Equivalences in Material Structures

by

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Abstract

Structure dictates every property and behavior of a material. Concepts of structure used within the field of materials science and engineering (MSE) are diverse, ranging from quantum level phenomena, to the practical development of macroscale components. The sheer volume of variables, scales, and models used to represent some aspect of material structure is immense. There is no current framework for bringing all of the concepts of material structure together, outside of a set of four relations, colloquially known as the materials paradigm. The paradigm relates process to structure to properties to performance, and serves as the ontological basis for the consolidated discipline of materials.

Given that general approach, this thesis offers a new framework for the interpretation, analysis, and validation of materials structures by incorporating concepts of general systems from outside of MSE. In this interdisciplinary work, concepts from various systems philosophies, quantum theory, information theory, category theory, and logic are described and selected as desirable components for a fuller notion of material structure. The idea of an enriched material structure leads to the construction of a functional framework for the analysis of aspects of materials systems on the basis of criteria of equivalence. If structure is more generally defined as that which is invariant across change, then equivalence is a natural determinate of shared structure. A multi-component structural equivalence framework is proposed, composed of five different senses of structure: definitional, empirical, informational, categorical, and theoretical.

The proposed structural equivalence framework organizes the different forms of structure which are drawn out of the multivariate analysis offered by each individual form. Through the rigorous definition of each form, models of materials structure in any arrangement can be equated with others, in order to parse out structure. Definitional equivalence can measure how much overlap the vocabularies and foundational concepts two models might share. Empirical equivalence can measure the overlap, or translatability, of the data sets produced by methods within each theory. Informational equivalence can measure the available communication pathways between data (and other) sets within models. Categorical equivalence can compare inherent, or associated, mathematical structures between models. Finally, theoretical equivalence can measure the overlap or translatability of two theories on the basis of the shared structure between the models of those theories (which take the other forms of equivalence into account). This thesis holds that these five senses of equivalence provide a richer version of abstract structural modeling and validation than is currently used.

Using this structural equivalence framework, different aspects of materials structure are investigated including: the general structural form of a conceptual multi-scale bridging technique between atomistic and continuum computational methods; a validation of informational structures produced by variances across X-ray diffraction results for copper samples processed in different manners; a survey of the general structures of creep models for copper; and an analysis of the variable used to represent average grain size in two different creep models for copper. The results of these investigations illustrate the utility—and current boundaries—of the structural equivalence framework when applied directly to concrete materials systems.

The work in this thesis is wide ranging, and offers contributions to multiple fields of study. For those in MSE, it offers new techniques of model validation, model construction, data analysis, and integration of methods from information science and logic. The novel approach of the structural equivalence framework also presents an opportunity for re-evaluation of historical data; a method to recontextualize experiments into the modern ‘vocabulary’ of the discipline. For those outside of MSE, it offers an insight into the approaches, techniques, and a touchpoint for integration of other fields with the vast created knowledge of MSE. Furthermore, this thesis offers an enriched materials ontology, inclusive of multiple structural concepts in an attempt to continue to build towards the goal of an all-encompassing science of materials.

Preface

Portions of the research presented in this thesis are being prepared for publication as K.P. Kucera, G.D. Hibbard, and J. A. Nychka "*Informational Equivalence in Materials Characterization*," [journal to be determined]. I, K.P. Kucera, was responsible for conceptualisation, methodology, investigation, data analysis, visualization, and manuscript composition. G.D. Hibbard and J. A. Nychka were supervisory authors and were involved in conceptualisation, methodology, visualization, and manuscript composition.

Portions of the research presented in this thesis were also manuscripts not currently published, or pending submission.

- K.P. Kucera, G.D. Hibbard, and J. A. Nychka, (2022). *Categories & Equivalence in Materials Science.* [Unpublished Manuscript]
- K.P. Kucera, M. Tiessen, C.J. Campbell, G.D. Hibbard, and J. A. Nychka. (2020). *Assemblage Dynamics and Comparative Complication*. [Unpublished Manuscript]

The remainder of this thesis is the unpublished, unfunded work of solely the author.

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Chapter 1

Introduction

> *The history of materials has been a long journey in search of knowledge in strange and difficult terrain, finally to return to the familiar scene with vastly better understanding.*
>
> – Cyril Stanley Smith, "Matter versus Materials: A Historical View"

1.1: Material Structure

The first time a person took a hammer to a piece of iron, there was no modern conception of atoms, of dislocations, or of strengthening mechanisms. There was simply the effect that—with each subsequent hammer blow—the material became more difficult to deform. Only through centuries of science and engineering advances were the cause and effect of structural changes to properties, like those of a hand-wrought piece of iron, discovered and cataloged. The reality that we inhabit involves a seemingly infinite number of systems from the macroscale to the atomic scale interacting with one another, structuring the world around us. Every conceivable object is definable as the set of interactions—both internal and external—of which it is a part, so a study of structure is inherently a study of sets of interactions and their behavior and evolution through various states.

To consider the concept of structure is to explore the one universal commonality between every material in existence, that their properties and behavior are dependent upon structure. As the world surrounds us in materials of every sort, structured objects and systems of structured objects are inescapable. In order to better understand the forces that structure these systems, and determine and predict the behavior of materials, models of these systems and mechanisms are designed and tested, providing quantitative analysis of their structure. This being the approach to the consensus understanding of the physical world, it would seem imperative that methods of designing, constructing, and combining the models of materials be rigorous and navigable from within, or across, any set of material theories.

Materials are not the only structured systems, nor the only objects that are modeled as systems. Mereological questions—those concerning the relationship between parts and wholes—abound throughout both the physical and social sciences, and have been studied by philosophers since antiquity. The physical sciences have used empirical and analytical techniques to great effect, in order to isolate new components of physical structure and study their properties and behaviors. Components only tell half of the story of the objects of our daily lives, though, and there have been many obstacles confronting efforts to fully explain systems of materials solely in terms of their constituent parts. Outside of the physical sciences, the past century has seen a variety of philosophers and social scientists who have worked to invigorate and expand the holistic philosophies of the early 19th century. If a goal of the physical sciences is to integrate holistic ideas into the existing frameworks of physical systems, it seems vital that the rigorously defined ontologies of various systems theories and philosophies be studied for conceptual landscapes which may bridge to the islands of scientific specialization.

In the field of Materials Science and Engineering (MSE), the keystone of the approach to model construction is a set of relations known as the materials paradigm. MSE has always been an interdisciplinary field [1], and the paradigm is the only heuristic that captures a general relationship shared between *any* materials system. A conception of the materials paradigm, and the relations between Process, Structure, Properties, and Performance (PSPP) is shown below in Figure 1.

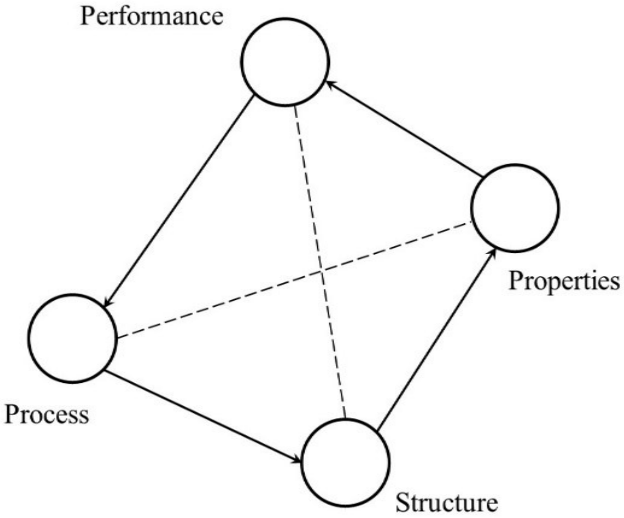


Figure 1: The common tetrahedral representation of the materials paradigm.

This paradigm illustrates the dependence of materials thinking on the concept of *structure*, a point discussed in more detail in section 2.1. The interdependence of the quantities of interest to MSE illustrates the degree to which models of material behavior are expected to incorporate variables representing the contributions of those structures. Every materials model relates structures, or some structural change, across landscapes of environmental energetic stimuli.

Given the importance of structure to materials modeling, it is important to be able to articulate what structure is, specifically in a materials context, and what the consequences of a structure-centric epistemology are with regards to the methods of model building within the discipline. The sheer number of materials, materials models, variables used across the materials modeling space, and contexts of interest to material behavior makes it difficult to knit together a rigorous, consolidated concept of structure across materials spaces. In order to elucidate a coherent theory of material structure, there should exist a framework against which the behavior of materials systems, variables, models, and states of systems can be compared and contrasted, and the relationships between these concepts can be mapped. Building this framework would require a coherent set of methods to determine when, where, and how there may exist equivalences between two concepts. These equivalence points will illuminate the various senses of materials structure, and how they are modeled.

Material objects are modeled as interacting systems of increasingly smaller objects. Models of lower scale phenomena serve to predict the behavior of macroscale objects. These models predict behavior on the basis of the manner in which collections and aggregates of objects interact with one another, and with the environment within which they are situated. There exist methods of this kind of process for physical systems containing levels of self-similar interaction objects. Cascading mereological (part-whole) relations have been treated with various techniques of bridging, the most successful of which is renormalization and the renormalization group. In physics, renormalization is a method of connecting small and large scale effects by accounting for the infinities in their respective models that arise due to self-interactions [2]. While this is an incredibly effective method, its specificity is such that direct application to various empirical models, or data analysis methods within MSE is not currently feasible, so this approach is not treated here.

The use of formulae, equations, and operations to predict variable evolution within materials systems presupposes that, within some range of values, there exist equivalent concepts and structures which may be tethered to one another in order to study complex, and connected, phenomena. What is the formal basis to determine whether or not one variable / state / model / theory is the same as another, as we chain these concepts together across the spectrum of materials science? Determining the answer to this question requires first determining what the epistemological methods of model building, and systems theories, have been to this point in MSE. The most generalized approach in the field is the aforementioned 'materials paradigm,' and every behavior or model can be tagged into one or more of the sets drawn between process, structure, property, and performance. What these concepts illustrate is that across scales and evolutions of state, material phenomena are interpretable as dispositions that physical systems, and components of physical systems, have in response to various stimuli. These stimuli govern how the cascading sets of relations through materials systems emerge, and show the boundaries of the physics and models used to predict phenomena.

Across this model space, experiments highlighting the behavior of materials systems point to different conceptual objects that can be used to determine the structure of those systems; structure both in the sense of the physical components, and of the invariants established within the model space that determine the bounds and efficacy of the models being used. Finding invariants across these interfaces means also determining where, and in what manner, various components of materials systems are equivalent to one another. If materials systems are compositions of assemblages of scaling and aggregating interactions, as all indications seem to be, then the question of when and how objects and relations are equivalent to one another becomes key to building a rigorous and precise network of structured models for materials systems.

To capture the full picture of phenomena, there must be a cascade of determinable equivalences. If we want to say that two objects are equal according to a theory, or between translatable theories—a theoretical equivalence—then we must first determine any conditional equivalences the theories may have. Specifically, we want to build models of theories which possess multiple equivalence determinates to capture the multiple conceptual forms of structure determined herein. Each form of equivalence allows for the construction of a robust and well-defined idea of material structure.

An idea of physical structure, built upon the structure of the experiments, models, and theories that give rise to the contents of that physical structure, is an approach which changes the epistemological priors and approaches of the discipline. The shift appears primarily in the migration from an object-based conceptualization of structure, to a relational one. Components of physical structure, in this sense, are rendered as collections of relations and meta-relations that are both more primed to highlight interactions with other objects, and well defined in terms of their local and global relational space.

With a method to illustrate the relational basis of materials science, we can then inform our definition of a general sense of 'system' and 'structure.' A meta-analysis of multi-scale materials structures can serve as a basis for analysis of systems and structure in general, with a framework of equivalences providing a means of testing connections between sets of interacting objects in any context. This approach forms a new basis for building, testing, and iterating upon models of materials systems, one centered on a local to global cascade of relationality, and based on the disposition of nodes of interaction.

Through the construction of this framework of equivalences, and application of it to multiple facets of materials research and modeling, we have developed a new approach to conceptualizing materials structure, and have created an apparatus for testing the cohesiveness and translatability of materials models in many different contexts. Through the use and refinement of this method, we believe that the modeling landscape of materials science and engineering can build a more rigorous web of connections between the theories and models which make up the modern science of materials. These connections can then be tested against a consensus framework of relational invariants representative of various material structures.

To summarize the above, this thesis hopes to provide detailed answers to the following research questions:

- What are the epistemological approaches to model construction and refinement within MSE, and in other systems theories?
- What criteria of equivalence can be formulated to capture the various senses in which variables, states, models, and theories are structured?
- Given a framework of the criteria of equivalence above, how would that affect the epistemological approaches to modeling within MSE?
- How does our interaction with materials systems inform our interpretation of the 'structure' of general systems?

1.2: Scope of This Work

This work is interdisciplinary, and aims to take a survey of approaches to the structure of systems from various social science perspectives and philosophies. This survey is then used to find general properties that a variety of systems of interacting objects may share. The synthesis of these properties can be used to inform the development of a novel interpretation of the concept of material structure. As stated, this idea of structure is based on finding a framework consisting of sets of relational equivalences between variables, models, states, or systems. Using these criteria serves as a method to analyze the interfaces between models, and can be used as a check on different types of models, including cross-functional and scale-bridging types.

Chapter 2 begins with a broad description of a materials ontology, the viewpoints and epistemological commitments of MSE. Section 2.1 takes this ontology and, through exploration of the manner in which the discipline approaches problems within the field, illuminates the key concepts needed to integrate the wide collection of materials problems into a universal framework. Section 2.2 goes into further depth on the concepts of system and structure within MSE. These sections serve as an overview of the current state of the field, and set a reference against which various ontologies and interpretations of systems theories may be compared and contrasted.

Following this background, section 2.3 presents a description of various approaches to systems from branches of philosophy. These include brief analyses of works by Alexander Bogdanov, Henri Bergson, Gilbert Simondon, Alfred North Whitehead, Bertrand Russell, and Gilles Deleuze. A relevant thread present through the analysis of these works is a concept of *process ontology*, the idea that systems may be defined as the emergence of behaviors of sets of relations that objects—including systems—may have as a whole.

This holistic approach helps to inform section 2.4, a summary of what is known as the relational interpretation of quantum mechanics, first proposed by Carlo Rovelli. This interpretation centers on the primacy of interaction between systems, and the resulting properties produced by these interactions. Although the theory deals with quantum systems, the applicability of the approach to larger systems is theorized by Rovelli [3] and is further expounded upon in this work. The concepts included set the groundwork to attempt a subtle shift in the proposed modeling approach from an object-oriented to a relational-oriented approach.

Changing the modeling interpretation also requires reinterpreting what kinds of data and information are produced by the general act of measurement. Section 2.5 discusses the downstream effect of an evolving view of systems building on the data meant to capture physical behavior and mechanisms of materials systems. The section includes discussion of how systems are measured, what types of data these measurements produce, and what commonalities sets of measurements can have. The characterization of the empirical content produced through measurement of materials systems allows for discussion of the structure of data sets, and the types of relations that appear specifically in empirical modeling.

Central to any analysis of data is the information theory pioneered by Claude Shannon in the mid-20th century. Section 2.6 explores how empirical, and other forms of data collected and produced within MSE, can be seen as a form of communication between systems, leading to a new set of relational functions between the data sets of MSE. These include those representative of engineering judgment, a crucial part of assessing performance criteria of materials systems. Through the steps of contextualization of data, different types of informational entropy are also explored, and their relevance to modeling within MSE are discussed.

Section 2.7 goes into more detail on the types and structures of models prevalent within MSE. These can include empirical models, analytical models, computational models, and other algorithmic / big-data models. The differences, and connections, between the modeling types are discussed, and then an analysis of what, if any, mathematical structures are used within each modeling category, and across the interfaces of combined models. Across this modeling space, MSE practitioners use a similar pathway of model construction and iteration proposed by M. F. Ashby [4], and that model building process is discussed in detail.

Collections of models are what constitute theories. Theories are built on models, variables, and data that can be grouped into a larger bin on the basis of some shared properties. Section 2.8 discusses the phenomenology of theory construction, and the interplay between models and the theories they construct. The structuring potential of theories and their models is discussed, as well as the establishment of criteria of equivalence between physical theories on the basis of the structure of their constituent models.

Judging relations between variables, models, systems, and theories requires an abstract set of tools in order to capture various forms of interactions. These tools should be mathematical in nature, and able to capture properties of like objects, sets of those objects, relations between the objects within the sets, and relations between sets of those objects. In light of those requirements, section 2.9 presents the field of category theory as a solution. A description of categories, morphisms, functors, and natural transformations—-among other mathematical objects—-is presented, along with their properties and potential applications. Categories are shown to fit the needs of criteria building, and as tools to capture the mathematical structure of objects of study. Discussion of applications to equivalence criteria and model building in the context of category theory is then presented.

Section 2.10 builds upon the concept of criteria of equivalence, proposing that the strength of the relation between two theories which share any sort of potentially equivalent objects—be they variables, states, systems, etc.—may be judged on the basis of a cascading framework of equivalence. This cascade of criteria includes discussion of five forms of equivalence, including definitional, empirical, informational, categorical, and theoretical. Each form builds upon the prior form, increasing the strength of equivalence between theories as greater connections are able to be identified between the two. These ideas of equivalence form the crux of the analysis performed in later sections.

In section 2.11, a through-line between all of the mentioned concepts is drawn, and the overall approach to building a comparative analytical framework is proposed. A synthesis of abstract theory and practical knowledge-building is illustrated, justifying the use of equivalence frameworks as a method of model and theory analysis. Contributions from each of the topics described are folded into the conceptual space of the materials paradigm and material structure. Armed with perspective from the far reaching survey presented in Chapter 2, a new materials ontology is proposed. This ontology incorporates the knowledge presented and provides a new foundation upon which the abstract comparative framework—the central contribution of this thesis—may be built. This section is intended to summarize the justification of the approach chosen, and to serve as a springboard for the discussion of the methods used within the thesis.

The methods of building the proposed framework are presented in Chapter 3. First, a general approach to the determination of equivalence is defined based on finding invariants within the object(s) being analyzed. This section defines the parameters of what to look for within the object(s) of interest. Following a general definition, each form of equivalence proposed is then explored in detail. The following forms of equivalence are formally defined in the indicated sections, and assigned postulates used to determine the basis of equivalence of that particular form:

1. Definitional Equivalence
2. Empirical Equivalence
3. Informational Equivalence
4. Categorical Equivalence
5. Theoretical Equivalence

After being defined, it is shown how these criteria fit together in order to form a cohesive and sensible progression, building the strength of structural equivalence as each set of criteria are met. Combined, the five forms of criteria define the structural equivalence framework.

Following this discussion, methods of rendering data and models in the context of the proposed framework are presented. This approach includes a proposal on methods to identify like objects within the landscape of materials, primarily on the basis of lists of applicable mathematical structures and potential mappings between them. Additionally, this section will provide an overview of a process of categorification, which takes data and information presented in a set-theoretic landscape and translates them into categorical terms. These discussions will lay out the manner in which each step of abstraction and generalization can be applied to various components of materials theories and models, creating the meta-analytic framework proposed.

With the methods in hand, Chapter 4 presents the results of the application of the proposed framework of equivalences, and model interpretative techniques, to a variety of applied materials modeling scenarios. The equivalence framework is specifically applied to different models in order to highlight its efficacy with regards to cross-model variables, cross-theory models, cross-system states, and cross-scale interfaces. Using these examples, the effectiveness of the equivalence framework is illustrated as a method of discovery for the structure, and structuring potential, of materials systems. Discussion around the examples elucidate the importance of translation (mapping) as a condition of equivalence. This section will go into detail on this point, showing that the ability to translate structures across the boundaries of modeled objects is the primary method of teasing out equivalences between the two (or more) objects of inquiry.

Following this discussion, Chapter 5 concludes the thesis and proposes future directions for the topics presented within. Using the preceding results, it is shown that this work presents a new conception of material structure. This novel concept is backed by the new methods of finding invariants, and conversely equivalences, within the mathematical structures of the objects of interest presented within this work. By finding and cataloging these equivalences for a variety of materials systems, a new method of checking combined models has been developed for any combination of like, abstract objects within materials systems. A description of potential uses within the discipline of MSE is presented for this framework.

In addition to the contributions to MSE, this interdisciplinary work also contributes new approaches to systems theories in other fields. These contributions are discussed in section 5.1, showing both that this work can lead to greater synthesis between MSE and various philosophies of science, and that the form of this analysis has the potential to open the whole body of materials research for analysis by non-engineering technical fields. Additionally, the limitations of this approach both directly to MSE, and for interdisciplinary applications are discussed, including the limits of using a meta-analytical framework on predictive and multiscale modeling, and the limits of data restructuring for use within the framework. Finally, in section 5.3 various proposals for future work are presented.

Chapter 2

Background and Literature Review

> *As humans, we belong to that component of nature given to organizing and structuring. We not only physically organize ourselves and our environment, but we also organize our perceptions of the physical world into abstract structures.*
>
> —L.L. Whyte, "Hierarchical Structures"

2.1: The Materials Paradigm

Currently within MSE practice, there is no single unified approach to the gamut of experiments and research projects conducted within the field. Overlapping with approaches from solid state physics, chemistry, and other engineering disciplines, experiments and research nominally contained within MSE are often set-up with different sets of assumptions and ontological priors. While research may involve metals, ceramics, polymers, etc., little is done to fit a given university's or department's research into a cohesive framework centered around a concept of what *all* materials have in common. This leaves a gap in creating definitions of unifying approaches to the way that materials *are*, and what they say about the ways in which materials systems *relate to one another*.

The most primitive, and closest analogous version of a materials ontology comes in the form of the oft invoked materials paradigm. As mentioned in Chapter 1, the materials paradigm is the general set of relationships between 'process,' 'structure,' 'property,' and 'performance,' (PSPP). Applied broadly, the paradigm states that, for *any* materials system, these sets of relations hold. Materials are generally differentiated from matter by their utility to human beings [5], and so the materials paradigm couches the performance aspects of materials systems—their appropriateness for use in various human contexts—in terms of the physical changes a structure undergoes, and the sets of properties instantiated by each structure produced for some human desire or need.

The modern form of the paradigm from Figure 1 came into existence over the course of several decades. First mentions of structure-process relations of materials begin as early as 1964 when Moffatt, et. al. discussed the centrality of them in their work *Structure and Properties of Materials* [6]. One of the first diagrams with all four elements of the modern paradigm appeared in the draft plan for the Materials Processing Center, opened in 1980 and pictured in Figure 2 below [1]:

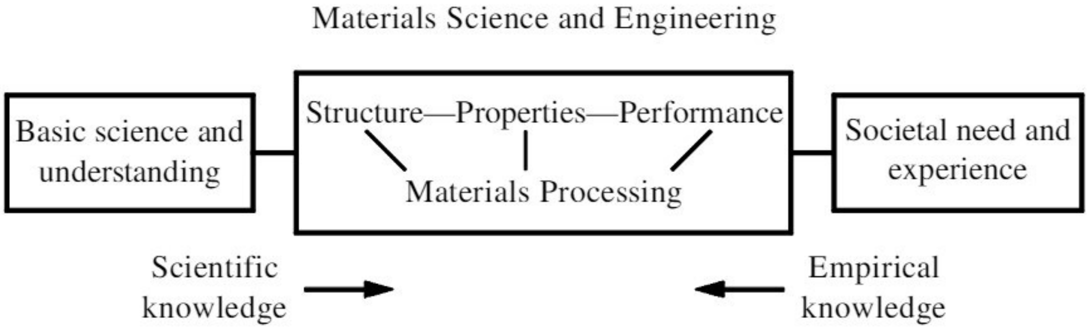


Figure 2: An early version of the materials paradigm, from [1].

Though not yet in the tetrahedral format, this draft is one of the first documented instances of all four of the PSPP elements being presented as interconnected, and central to an understanding of MSE as a unified discipline. Interestingly this also highlights the contributions of both empirical and analytical ("scientific") knowledge within the context of materials modeling.

Throughout the following decades, materials became an increasingly important focal point for research directions within the government of the United States. Reports such as *Materials and Man's Needs* [7] and *Materials Science and Engineering for the 1990s* [8] served as touchpoint reviews of the progress of MSE as a discipline, and were drivers of the unified approach of the sub-disciplines of the field. In the latter, the first recorded version of the materials tetrahedron appeared [8], relating the so-called "four elements of materials science and engineering" and shown below in Figure 3:

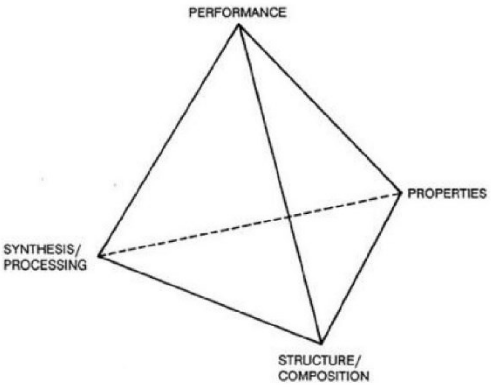


Figure 3*:* Materials tetrahedron relating the "four elements" from [8].

This iteration would eventually appear in most textbooks introducing students to MSE, and as a staple of introductory MSE courses. This conceptual framework began to fulfill the unspoken promise of the transition from separate fields of study to a centralized materials science by providing a conceptual node to which every materials system could connect. Though rarely presented as such, the set of PSPP relations forms the central concept around which any unity of materials may be built. It can, therefore, be classified as an *ontology*. The Oxford English Dictionary defines an ontology "a set of concepts and categories in a subject area or domain that shows their properties and the relations between them" [9], and it is clear to see that—in a qualitative manner—the materials paradigm qualifies as a materials ontology.

Generally, the paradigm was interpreted as giving equal importance to the process, structure, and properties in relation to how they affect the performance of a given materials system. Yet it becomes increasingly more clear that every aspect of materials systems relies on the physical structure that the system exhibits—the components and arrangement of those components at whatever scale is of interest to a particular observer. In this way, the idea of material structure and its downstream effects have become the most comprehensive definition of 'materiality.' As the modern sense of materials arose from practical encounters with the world throughout history, this conception of materials derives also from the way in which practitioners learn and are taught; from an epistemology of experience, like those described in the experiential learning theories of Kolb [10] or the constructivist theories of Piaget [11].

In this sense of materiality, the causal chain between sets of structural components and their relationships to the environment in which they are placed becomes clearer. Process is the reaction of material structure to energetic input; Properties are measures of the typical response of material structure to various stimuli; Performance is the response of material structure, and hence properties, to specific contexts of use. Each of the p-vertices of the tetrahedron involves some composition of structural changes, shorthand for specific arrangements, and evolutions of arrangements, of the components of physical structure that make up materials systems. These sets of relations can be summarized as:

$$\text{Performance} = \{\text{Structure - Property relations}\} \tag{1}$$

$$\text{Properties} = \{\text{Structure - Process relations}\} \tag{2}$$

$$\text{Process} = \{\text{Structure - Energy - Time relations}\} \tag{3}$$

This approach to the paradigm couches everything in terms of structure, and provides a structural lens to this ontology. Static structures have fixed properties, and dynamic structural evolutions—either natural or teleological—are disposed towards certain dependent pathways of change—known as mechanisms. This dispositional causation is the central method of interpreting the ways in which structural systems behave, with the {Structure-Energy} relations being synonymous with *thermodynamics* and the {Structure-Time} relations being synonymous with *kinetics.*

The paradigm serves as the most general guide for materials research and modeling, a compass pointing in cardinal directions. From even a cursory analysis, it is clear that structure is the most important, and indispensable, concept within this ontology. Structure is the causal engine that powers material properties and performance, the origin and terminus of processing, as well as the lens through which thermodynamics and kinetics are filtered into reality. Yet, often, cardinal directions are insufficient to find your way from one place to another, and what is needed is a detailed roadmap. How might the materials paradigm be enriched with even more detail? This work proposes that this enrichment can occur through the addition of conceptual density, specifically around alternative interpretations and forms of structure.

> *…when they are mingled with themselves and with one another there is an endless variety of them, which those who would arrive at the probable truth of nature ought duly to consider.*
>
> —Timaeus, "Plato's Timaeus"

2.2: Materials Systems and 'Structure'

Physical structure is the first and primary sense of structure present across the range of materials models. Materials systems are generally understood to be systems of various structural components occurring at length scales from the atomistic level (*nm* or *Å* scale) to the continuum level (*m* scale). At the lowest relevant scale, the arrangement of atoms—how they are structured—is mostly determined by interatomic bonding [6]. The strength of these bonds vary depending on the valence state of the atoms, and the number and type of elements within the system. In metals, bonding begets long range order and a crystalline structure, while in polymers or ceramics the types of bonds present produce a less ordered structure, with amorphous or semi-crystalline structures.

As atoms aggregate, new mesoscale structures are formed, such as molecules in polymers, or crystallite grains in metals. Materials systems with their various scales are considered hierarchical, where the lower scale components of a material necessarily comprise and (to some extent) inform the behavior of the scale immediately higher from it. While each subsequent scale does inform the next in an upward length scale cascade—and is causal *sine qua non*—there are also emergent phenomena at each new level [12].

One of the most important of these emergent phenomena with regards to the behavior of materials are often called defects. Within crystalline materials, such as most metals, there are a variety of defects which may often be categorized as interruptions within the long range order of the crystalline structure. These defects, which include vacancies, dislocations, and grain boundaries, have an outsized role on the arranging powers of points within these materials systems and an exaggerated effect on the properties of the macroscopic material objects. The same expression of non-idealized aspects of physical structure is true of all other classes of materials to some degree [13].

In the materials ontology derived from the materials paradigm, every small change in structure at any scale, has some effect on the properties of the material system, its processibility (how and through what mechanisms a processing change may be enacted), and on its performance in an application. What this entails is that, in order to fully characterize the ways in which materials systems behave, MSE practitioners want to be able to model all of these phenomena as simultaneously as possible. There exists an intense degree of difficulty to this aim, though, because of various challenges including the synthesis of various physical approaches, the many body problem, and the limits of computational power [14], [15].

As previously mentioned, materials are generally assumed to be interacting systems of various physical objects, arranged according to the laws governing those objects at different scales, e.g., bonding, or as C.S. Smith puts it "*a result of the interplay between the requirements of the physical forces operating between the individual parts and the mathematical requirements of space filling*" [5, p. 3]. Many of the organizing relations of a given physical component are relevant only in an intrascale manner, because the volume of affect of the interacting parts resides only on the length scale of those parts. Only in aggregation do the combined effects of individual interactions combine to feed the dispositional potential of the lower scale effects up the chain of length, and this is the emergent nature of multiscale materials systems.

Each of the relations of physical, material components is governed by the same physical forces found in physics, simply at different resolutions. For instance, atomic bonding is a result of the interaction space between nuclei of varying *Z*, their resultant electronic structures, and the electromagnetic (EM) bonding force between various assemblages of the nuclei and electrons. At the molecular scale, combinations of lower scale forces in the forms of ions combine using various configurations of their EM bonding force to create larger scale assemblages of nuclei and electrons. As bound atomic aggregates continue to grow in number, the types of new structures that are being formed diverge, and the classes of materials are roughly formed.

These senses of material, and of material structure, are historical, arising from the development of use and design of the various objects of ‘engineering’ or ‘design’ interest throughout time. While the structure of a metal or a ceramic can now be differentiated on the basis of some characterization techniques such as electron microscopy, processes of differentiation have existed as long as someone could judge whether one material was harder or softer than another, for instance. Indeed, with the exception of those macroscale objects which we judge primarily via direct sensory interactions, every individual measurement or interaction with the conceptual objects of substructure is mediated through a characterization device or technique. At every stage of the process, a model of varying complication is introduced and iterated upon in order to characterize the structure and process of structuring inherent in each material, and of each component in that material. In the engineering context, these models are designed specifically to be able to detect and predict the outcome of some mechanism of structural change that a material system will undergo within a specified environment.

The function of models within MSE at least implies that any method that would tie together different conceptions of various length scale phenomena would have to involve tying together the conceptual landscape, an abstracted version of the physical structures, or structures being measured, in the context of the technique being used for its measurement. If this implication is correct, then it is important for the conceptual landscape of models of multiscale materials systems to be well and rigorously defined. While the materials systems described by these models do follow various empirical and analytical formulas that inform our conception of the overall behavior of these systems, it is informative to look at other systems theories to see what they may be able to offer MSE on a conceptual basis.

And so each one, according as he has been accustomed to join and connect the images of things in this or that way, will pass from one thought to another.

—Spinoza, “Ethics*”*

2.3: Survey of Systems Philosophies

2.3.1: What are systems philosophies?

Systems philosophies, and approaches to systems theories, have been a part of the evolution of natural philosophy from the mereological theories of Plato and Aristotle [16]. Hypotheses about the physical structure of objects, comparisons between systems of objects, and their behaviors trace back to various Pre-Socratic philosophers, Plato, and Democritus. In the centuries that followed, debates about systems often centered around two concepts. One is sometimes called "corpuscular theory" [5]—the theory that every system is equal to a sum of its parts, and that the behavior of that system is describable wholly by accurate accounting of the behavior of its constituent parts. The other is sometimes known as "holism," a concept typically traced back to Aristotle that looks at a system as an emergent entity that cannot be reduced solely to the property of its parts [17]. These conceptual divisions are generally called *reductionism* and *antireductionism,* both of which include a variety of interpretations of reality based on the particular approach.

With the advent of characterization methods capable of perceiving smaller and smaller components of physical systems, along with the formalization of quantum electrodynamics, the 19th and 20th centuries saw an explosion of newly discovered components of physical structure. This boon of discovery had an effect of pushing research generally towards more reductionist subjects, trying to understand the individual properties and behaviors of newly discovered components of physical systems [18]. The resulting 'silofication' of many disciplines is still visible in overviews of the research of MSE, Physics, and other university departments.

Yet, concurrently with the trend towards further reductionism within the sciences, more holistic approaches to systems began to appear within various philosophies of science. One of the branches of this evolution arose from interpretations and iterations on the work of Ernst Mach, a "founder of the philosophy of science" who "more than anyone else bridged the divide" between philosophy and science [19]. While Mach himself was not a systems philosopher, he was massively influential on philosophers and scientists of the early 20th century who would lay the foundation for modern systems theories [20, p. 118]. One of Mach's biggest contributions was in recasting sensory events and measurements in relational terms, where instead of measuring objects directly, what human measurement entails is measuring the interaction between multiple objects. The manner in which systems interact is what produces properties of systems, i.e., it is the interaction itself which produces the properties. Phenomena are borne of relation, rather than manifesting from individual systems and their properties [20]. These ideas, along with his work in physics and other topics, directly influenced other philosophers and scientists of the early 20th century, and provided his contemporaries with topics worthy of debate.

From Mach and others, philosophers of the era began to construct various schema of systems, both general and otherwise. Through their work, concepts about what systems were, how they were constructed, and why they behaved in the manner in which they do, evolved. These concepts were teased out in various ways, assessed, and iterated upon, creating many modern theories of systems. As has been established, materials are systems of physical objects, systems of structures, systems of properties, and behaviors, all which come together to form our conception of what it is to be a material. There are general relations that *every* material system shares, something that the first materials scientists and engineers had to have understood in order to undertake the consolidation of their various backgrounds under a single banner.

If it is a given that materials are systems, then a question becomes, "how might a science of materials be informed by various philosophies of systems?" Given the wealth of sources on the topic, and the desire to iterate upon our existing ontology of materials, a survey of systems theories is presented below. Through a brief and limited discussion of the ideas of six different philosophers—Alexander Bogdanov, Henri Bergson, Gilbert Simondon, Alfred North Whitehead, Bertrand Russell, and Gilles Deleuze—we will examine concepts and theories from each that will enrich the material ontology we seek to establish, and provide a roadmap towards a framework of structure to be applied to problems in MSE.

2.3.2: Bogdanov

Bogdanov was a Russian revolutionary, writer, physician, and philosopher who worked prodigiously across this broad range of fields until his death in 1928. He is generally considered to be the first to propose a theory of systems, what he called 'Universal Organizational Science,' or 'Tektology' after the Greek *τέκτον*, meaning 'builder' or 'mason' [21], [22]. Using this theory, Bogdanov cast matter, living organisms, and societal systems as dynamic entities, all governed by the same rules of what he called "positive selection" and "negative selection," the relations of systems undergoing changes in relation to their environment. The balance between selections he termed a sense of "structural stability" [23, p. 206].

Bogdanov also expanded upon some of Mach's ideas of perception, proposing that perceptions of physical objects were collective, a combination of both the sensations interpreted by an individual, but also the collected perceptions passed to an individual through learning. This idea made clear to Bogdanov that objects had both an internal and an external environment which affected their behaviors where, "*Each and every complex [his term for 'system'] is constantly tending toward its own internal equilibrium in a process of constant interaction with each other complex it is in contact with and, through them, with all other complexes*" [22, p. xlii]. These processes define the physical objects, and redefine for Bogdanov the central interest of systems. If systems are dynamic, with rich inner and outer flows of energy, then it is these processes of flow rather than centers of mass, or energy, which should be of primary interest. "*Thus the Tektological cosmos is constantly moving toward a myriad of local equilibria and, in this process, actively changing the conditions of those equilibria. Thus the cosmos does not exist as <u>state</u> but as <u>process</u>*" [22, p. xlii].

Characterized in this manner, it makes sense to say that Bogdanov was also one of the first to propose a *process philosophy*, an approach that characterized the inherent dynamism of systems. As Bogdanov saw it, the processes occurring in the growth and shrinking of a droplet of water, or in a collective of workers, must follow some of the same general laws, writing:

> "*My initial point of departure consists in the fact that structural relations can be generalized to the same degree of formal purity of schemes as the relations of magnitudes in mathematics, and on this basis organizational problems can be solved by methods which are analogous to the methods of mathematics*." [24, p. 209]

The structuring relations of Bogdanov's complexes were processes that could be generalized, and rendered as mathematical objects. Using this approach, the dynamics of organizing—structuring—powers of systems could be captured generally. These relations could be captured for any system, with differences being captured by the 'experience' or 'instrument' doing the organizing. "*All these unifying schemes are means of organizing experience; its instruments or 'forms.' The instrument of organization certainly depends on who organizes or develops the* *instrument and uses it, and on what is being organized; that is, on the material of experience"* [23, p. 30]. The idea that systems are collections of interacting objects, balancing an internal potential against an external potential, will sound familiar to those in MSE. Materials systems are modeled in this manner generically at many different length scales. What the 'Organization Science' of Bogdanov imparts upon an epistemology built for materials systems, characterized as a cascade of interconnected systems themselves, is the idea that a vital characteristic of those systems is the exchange of 'selective capabilities,' not only between the object and its environment, but between the various processes that comprise each individual level.

A tektological approach to materials systems would be one where the general forms of processes at the interfaces of the components of materials systems are captured mathematically, and integrated with the collective empirical knowledge of those components and their behaviors. Through this analysis, the structural sensitivities and stability of a system or component could be studied and organized. Even with these additions, questions remain of how to categorize these processes in terms of time, how they compare to the mechanistic ideas of atomic theories, and what a process-as-object sense of systems looks like. The nature of time is duration; processes endure; what does it mean for the processes of materials systems to persist in the manner in which they do?

2.3.3: Bergson

One enduring figure in philosophy was the influential French philosopher Henri Bergson, who was active around the turn of the 19th century, and into the first half of the 20th century. Through his works *Time and Free Will (1889), Matter and Memory (1896),* and *Creative Evolution (1907)*, Bergson built an enthusiastic following centered around his interpretations of creativity, memory, and conceptions of time and duration of experience. His work was influential across disciplines, ranging from a famous 1922 debate about the theory of relativity with Einstein, to winning the Nobel Prize for Literature in 1928 [25].

Bergson's philosophy was one of the first to regard the properties imbued upon objects as a relation between embedded concepts of the mind and the perception of the sensory inputs gained by interaction with the object. Properties of objects were contingent, relying upon "*modes of* *remembering [that] are further tempered through the degree of attention given in the perception of things, affecting not only the description of the object, but the features of the object itself*" [26, p. 33]. The objects being perceived are themselves collections of points in space, so-called "quantitative multiplicities." Bergson's version of multiplicities are static externalities whose rearrangements produce macro- changes in the collection. This concept of the object, though, belies the true nature of experience to Bergson, who says that:

> *"If these parts themselves suddenly dared to change, we would in turn divide them up into fragments. In this way, we will descend all the way down to the molecules that make up those fragments, to the atoms that constitute the molecules, to the generative corpuscles of the atoms, to the 'imponderable' at the center of which the corpuscle was formed by some simple swirling vortex [tourbillonnement]. In short, we will push the division or the analysis as far as is necessary. And we will not stop until we have reached something immutable*" [27, p. 14].

What is absent in this model, according to Bergson, is that this atomistic model produces too isolated and static a view of the world, and of life. The missing element is how these perception-images interact with time, a relation that defined Bergson's "qualitative multiplicity," which consists of a "temporal heterogeneity" [25] that organizes perception-states into a system, which gains emergent properties—"richer content" [28, p. 122]—as it assembles.

These multiplicities are the content of the world which are perceived, and they are always a mixture (hence the heterogeneity) of space-time perception-relations, or events of a particular duration which a person may perceive. In any given setting, there are numerous events of varying durations bombarding our senses, creating our view of reality. Bergson would say that these mixtures should be analyzed, and that the "pure" objects of one's perception should be studied, but that a mistake often made is that the objects of analysis are what he calls their "tendencies," or the relations between the events and their durations, rather than the elements making up the collections of events [29, p. 256]. The collections of relations that make up perception are open systems, dynamically evolving and not closed off to being affected by other systems.

Bergson speaks about his concepts of multiplicity and duration, *durée*, with regard to human perceptive capabilities, but goes on to surmise that the same approach to other systems would be valid, saying, "*Thus, nothing prevents us from attributing a durée—and thereby a form of existence analogous to our own—to the systems that science isolates, so long as those systems are reintegrated into the Whole*" [27, p. 17]. The reintegration of systems back into the "Whole" is another process of interactions, between systems external to us, between us and those systems, and between the interactions between systems and us, creating Bergson's sense of the world "*within the entanglement of the real and the individuality of the body [which] are reabsorbed back into the universal interaction that is surely reality itself*" [27, p. 17].

Through the construction of these ideas, Bergson thus concludes that the burgeoning separation of reality which the physics of his day was engaged in was in danger of losing a part of the sense of reality, if these notions were not used to feed the dynamics of whole systems. This conclusion led him to surmise that "*all division of matter into independent bodies with absolutely determined outlines is an artificial division*" [30, p. 259]. This deduction does not mean that Bergson was an idealist, which is to say he did not ascribe to the philosophy that reality exists only in the mind. The change in perception, the aggregation of durée, is descriptive of change in those systems and, "*the passage from one to another is also an absolutely real phenomenon*" [30, p. 258]. It is in the relation and reintegration between the individuated objects and the whole, through their interrelated and dynamically evolving durée that true images of reality are perceived.

Though organic systems, especially anthropological, were of primary interest to Bergson, his relational interpretation of systems provides conceptual clarity useful in our interpretations of inorganic systems as well. Within many physics and engineering practices, the division of nature into subordinate systems is a primary mode of analysis. What a Bergsonian interpretation of MSE systems adds to our ontology is the idea that, for all our studies of the individual components and levels of a materials system, the most important operation is the reintegration of these mereological perceptions into a model of the whole system. This reintegration requires a careful translation of the results of deterministic state changes of aggregations of 'closed' objects into the dynamic, ‘living,’ whole of the materials system. The relative kinetics of any two systems of these types is an interaction of durée of both systems, and an integration of both—rigorous mapping of the behaviors of the component systems to the whole system—is the best way to capture a consensus picture of the nearest reality-perception of the material object, a method that iterates upon itself constantly as new information of the system becomes available. In order to best utilize this idea, it is important to study the processes of individuation, and relation between those individuated objects, that produce the properties of interest to this relational framework. Study of things that stand out against the background—objects that take on properties so cacophonous that they break through the background noise of the æther—are key to understanding both mereological relations throughout systems, as well as how and why things individuate.

2.3.4: Simondon

Gilbert Simondon was another in a long line of practically *indistinguishable* French philosophers active in the mid-20th century who worked within the philosophy of technology. He is also known for integrating early ideas of information into his theories, as well as his theory of individuation. Many of these topics, and especially those relevant here, are detailed in *Individuation in Light of Notions of Form and Information* (1964) and *The Genesis of the Individual* (1964). These works present a systems ontology that centers upon the means by which objects and systems come into being, and one based on ideas of metastability and information exchange.

One of Simondon’s most well known concepts was that of individuation, a process of organizing by which systems come into being in the present moment. Simondon calls it “*...the singular manner in which the internal resonance of this matter about to take this form is established*” [31, p. 32]. Furthermore, per Simondon, this process is not one by which matter gains form, or by which form is instantiated in matter, but rather the relation between the two—the “operation” [31, p. 32]—*is* the object. In order to exemplify this, Simondon turns to the example of a brick.

In the hylomorphic sense, a brick is the combination of the matter of construction, the “clay,” and the form of a brick, generally a rectangular prism shape imparted onto the material by a mold of some sort, and each has their own haecceity or 'thisness.' The brick has 'brickness,' according to Simondon, not from some innate quality of the hylomorphic components, but rather only in the "*...operation through which the clay, at a given moment in an energetic system that consisted of the smallest details of the mold as well as the smallest pilings of this humid earth, has taken form under a certain pressure, distributed in a certain way, diffused in a certain way, and actualized in a certain way*" [31, p. 32]. This process, the molding of a brick, is the brick; systems are in a constant state of transformation, in one way or another, and each relation, or operation, which a system undergoes is in some manner actualizing that system. It is a process which involves the actualization of the relation between the internal and the external, where the system "*realizes an energetic exchange between the form and the matter up to the point that the ensemble ends in a state of equilibrium*" [31, p. 32].

Simondon's operation of individuation drives towards an equilibrium of actualization, which would sound like a familiar interpretation to any reader of thermodynamics. He is quick, though, to differentiate between a true equilibrium, or a null-energy state, and what systems actually undergo in what he terms their "becoming," as they evolve.

> *"Individuation has not been able to be adequately thought and described because only a single form of equilibrium was known, namely stable equilibrium; what was unknown was precisely metastable equilibrium; being was implicitly supposed in a state of stable equilibrium; however, stable equilibrium excludes becoming because it corresponds with the lowest level of potential energy possible…"* [32, p. 301-2]

His defining of metastability required the same kinds of variables as does thermodynamics, namely potential energies and entropy, but he believed that individuation, and its drive towards various metastable states, was inexhaustible. As an example, Simondon points toward crystallization, where a "*supersaturated solution… is capable of manifesting as wave or corpuscle, matter or energy, because every operation and every relation within an operation is an individuation that splits and phase-shifts pre-individual being, all while correlating the extreme values and orders of magnitude, which are initially without mediation*" [32, p. 302-3].

As crystals solidify, they are in a constant state of becoming. A crystal to Simondon *is* this operation of organizing and reorganizing in response to newly available metastable states as the results of the crystallization process become the antecedent to a new becoming [33, p. 10].

With a process of dynamic actualization as described above, how are different processes of individuation related to one another, since there are always multiple processes occurring as a system? Simondon says that they are communicating, in the form of information, and that "*the transmission of this information to the entire metastable environment is what [he] calls transduction, a process that is per se interminable*" [34, p. 481]. Processes communicate, they *inform* one another in asymmetric ways, and change the becoming of parts and wholes in a discordant eruption of life. This collection of information represents an "*ontology as a 'general theory of operations,' of the exchanges and modifications of being, of relation, whose importance lies in the fact that this action unites the means and principle discovering self-justification through the transductive practice at its interior*" [33, p. 18]. Through these processes—and relations between these processes—objects and systems, unities and their constituents, become the world around us, and information exchange is a way into our process of perceiving this interplay.

These concepts add even more tools to a materials ontology, and a process for further expanding our idea of structure and structuring. Many of Simondon's ideas reverberate with a tinge of familiarity, crystals and bricks, equilibrium and metastability, overlapping with the vocabulary of open materials systems. As with the organizational and multiplicities of durations, what Simondon proposes is again an idea of process as the object. In this sense, our ideas of materials ought to include (and to some degree do already) open metastabilities, and individuations as definitional for our structures. An atom, a molecule, a grain; these are not static entities kept in a vault, but rather *vital* entities that change, adapt, and reach plateaus of metastability as they relate within their own systems of influence.

Furthermore, each component of the structure of a system is in constant communication, both with its surroundings and with the wholeness of the object it partially comprises. This manner of communication implies that, in order to understand the processes of structure, we must be versed in the transductive manner in which structures communicate. It follows that a key quantity of structuring is information. Relation is communication, and communication infers that information-processes are an active part of the structure of systems. In a Simondonian sense, "*...philosophy is the authorizing of thinking all objective structural reality as a complex of relations; in short, the being of becoming*" [33, p. 18]. Communication is an abstract concept, a process with a nearly limitless application in the real spacetime that the world inhabits. The question becomes, how is it that from this primordial stew of signals and noise, physicality—our reality—takes hold?

2.3.5: Whitehead and Russell

In order better characterize processes, it is necessary to explore the related works of Alfred North Whitehead and Bertrand Russell, both English philosophers and mathematicians. Whitehead was likely best known as one of the primary architects of what is known as *process philosophy* [35], which indicated that—in a now common theme to this chapter—matter and the objects they make up are not independent, deterministic entities, but rather interdependent processes that organize the components of matter. Russell was a student of Whitehead's who, in his career, wrote extensively about mathematics, philosophy, history, and society, even winning the Nobel prize for literature in 1950.

Together, they wrote one of the seminal works on formal logic in the *Principia Mathematica* (1910). They also both wrote relevant philosophical works about the nature of systems and matter. Russell put forth his main theory in a work entitled *The Analysis of Matter* which concerned relations and their structuring potential. Whitehead composed *Process and Reality* (1929), which put forth a rigorous philosophy of science and mathematics that was concerned primarily with the processes of relation.

Whitehead wished to explore concepts of systems that would exist prior to their systemization, and found instead the *ursprung* of relation, which he determined to be the 'assemblage' [36]. While the systemization of things was fruitful for specialization—for drilling down to increasingly finer grained detail within a subject—assemblage looks for the primary relational capacities of things, tying the whole of the world together. Starting with assemblage, as

Whitehead saw it, informed systemization and, without it, rendered the results insensible. As an example, he conjured an image of steel, and described it saying, "*There are simplicities connected with the motion of a bar of steel which are obscured if we refuse to abstract from the individual molecules…*" [37, p. 16].

This sense of entities, which Whitehead takes to be processes between the whole (bar of steel) and its components (molecules), prompts one to ask not how these entities are in the world, but rather how they *become*. Becoming, then, is a process wherein parts become the whole of which they are a part, and the system becomes part of its environment. If we perceive it, the object then becomes part of our conception of the object. This phenomenon of perception is possible because "*being is located neither in the object itself nor in the subject that perceives it. This leaves becoming as primary*" [38, p. 63].

This conclusion prompts a further redefining of structure towards process, and towards a general theory by which we cognitively see the shape of how the universe shapes itself. Russell similarly wrote that:

> "*I say that I am acquainted with an object when I have a direct cognitive relation to that object, i.e. when I am directly aware of the object itself. When I speak of a cognitive relation here, I do not mean the sort of relation which constitutes judgment, but the sort which constitutes presentation*" [39, p. 108]

This object-relation as presentation is the same sort of mental becoming as described by Whitehead. The topic resurfaces in *The Analysis of Matter* as his differentiator between analytical and empirical knowledge, with "any degree necessarily dependent on perception" being termed as 'empirical' [40, p. 167-8].

All of these relations are preceded by Whitehead's concept of *prehensions*, which describes how objects and systems interact with their environment, and how that affects their becoming. Whitehead called prehension "*the general way in which the occasion of experience can include, as part of its own essence, any other entity*" [41, p. 177]. The prehensions of an object are a part of the structure of the object, and describe the potential inherent within objects to relate to other objects and systems, which is how "*materiality and physicality come to be*" [38, p. 63]. The manifold of relations which Whitehead proposes creates a framework by which the potential of a system can be understood in terms of the various perceived processes in response to some stimuli. Systems prehend their becomings, they contain within them the potential processes by which they can react and become something different, or new. These processes include our perceptions and interpretations of some system-object's becoming; prehensions existing within ourselves.

These concepts provide the tools by which one may delve further into the relational capacity of systems. Whitehead's prehensions, and Russell's perceptions, give us the vocabulary to differentiate between potential energies—at least qualitatively—as the potential to react to particular sets of relations. This idea corresponds nicely to the idea of material properties, a distillation of various reactions that materials systems have to different sets of environmental relations. Whitehead lends a fuller sense of process through the concept of prehension, one that can inform the materials ontology in its descriptions of processes—both in the philosophical and material sense. We have examined—very cursorily—how philosophies of systems, and systems-as-process construct a vital and vibrant ontology of reality. Yet, if only to avoid around the ire of Bergsonians, we should now take these concepts and assemble them into the whole of the account.

2.3.7: Deleuze

Gilles Deleuze was a French philosopher, and one of the foremost modern interpreters of the recent history of philosophy. His philosophical works were wide-ranging, and often revolved around other philosophers whose work Deleuze found to have been overlooked, or underappreciated. He wrote intentionally about Bergson and Simondon, and often played with ideas that can be traced back to Whitehead [42]. Through these interpretations, Deleuze constructed his own process ontology that built upon these influences, including varieties of many concepts such as assemblage, immanence, and becoming.

Deleuze’s interpretations consolidated much of the process thinking of the 20th century, and applied it far afield from whence it originated. Much of Deleuze’s oeuvre [including works with Felix Guattari] is often called ‘assemblage theory,’ and that is one of the concepts that he returns to often. The word ‘assemblage’ derives, in fact, from the English translation of the French word ‘agencement,’ which may also be translated as ‘arrangement’ [43, p. 18]. These assemblages are, as might be expected, more like the processes that result from a rearranging of some objects or systems, harkening back to Bergson’s multiplicities.

Assemblages are processes of things arranging, which Deleuze and Guattari termed a two-step process of becoming content and expressing that content. Deleuze also painted a vitalist picture of the world, wherein assemblages territorialize and deterritorialize, types of becoming as a relation between assemblages. These becomings differ slightly between Deleuze and his predecessors, with, for instance, Simondon “*heralding that singularity inaugurates the taking of form (the process of ‘in-formation’) within a potential field, while Deleuze sees in it what structures a potential field (and hence the process of differentiation)*” [34, p. 486]. For Deleuze, the structuring that is inherent in becoming, along with Bergson’s durée*,* serves as the basis for his differential ontology [44]. Structuring through the combined processes of ‘differentiation’ and ‘differenciation’—the former a part of Deleuze’s ‘virtual’ and reminiscent of ‘prehension,’ and the latter the process of actualizing from the ‘virtual;’ the content and the expression of that content—leads Deleuze to a vibrant process ontology that is widely applicable [45, p. 78]. Of particular interest is that Deleuze saw this vitalist framework as not only applicable to the mind, social systems, or organic life, but more than anyone else in the period, applicable to the vitality of inorganic systems.

In his work *A Thousand Plateaus* with Guattari, they write about metals in the context of Simondon’s brick, clay, and mold example, saying the vitality is found in metallurgy as it “*raise[s] to consciousness something that is only hidden or buried in the other matters and operations*” [46, p. 410]. It is not in exactly the same way that Simondon saw it, as metal *qua* metal in the act of becoming, but rather they see in metals and metallurgy a new form ascending on the operational boundaries, or “thresholds,” of the process of becoming. This interpretation is clarified as they write, “*the operations [in metallurgy] are always astride the thresholds, so that* *an energetic materiality overspills the matter, and a qualitative deformation or transformation overspills the form*" [46, p. 410].

Even though, for centuries, philosophers had been using metals and metallurgy as exemplars of the deadest, most inorganic systems that exist, in the meta-flow described above, Deleuze and Guattari see vitality. They write that, "*Matter and form have never seemed more rigid than in metallurgy; yet the succession of forms tends to be replaced by the form of a continuous development, and the variability of matters tends to be replaced by the matter of a continuous variation*" [46, p. 410]. The fact that metals (along with other materials) are 'processed' by their environments, either by design or ambiently, grants them the same sense of becoming afforded to organic matters. They confirm this "life" as a "material vitalism" which "*doubtless exists everywhere but is ordinarily hidden or covered, rendered unrecognizable, dissociated by the hylomorphic model. Metallurgy is the consciousness or thought of the matter-flow, and metal the correlate of this consciousness*" [46, p. 410]. Metals are, of course, not the same as organic materials, but in the exploration of their becomings Deleuze and Guattari find a qualitative structuring potential that shares similarities.

2.3.8: Contributions to a Materials Ontology

This all-too-short survey is not intended as comprehensive, and clearly there are many 'lines of flight,' (connections) that could be drawn from these systems theories to an ontology based around the materials paradigm. These philosophies also revolve around various conceptions of structure which differ from that of MSE, allowing for a melding of all notions to form a new materials ontology, further evolving our own idea of structure. Rather than collections of closed off objects, what this survey constructs is a picture of an organization of processes. These processes form physical objects, parts of those objects, and the environments that shape and form these objects. As scientists and engineers, we endeavor to understand how and why systems of physical objects behave in particular ways, and how we might predict those behaviors. These mechanisms constitute our models, which are representations of multiplicities of these organizations, various durations of interaction with the objects themselves, and representations of the objects through various means of characterization.

The objects-as-process are relations, individuated through their relation with their surroundings, process-clay in relation to process-mold. These systems are, by virtue of their potential energies, always in flux, clawing towards metastability. They become, and the various becomings relate to one another through information; the language that one system speaks to another within and without our perceptions. We sift through these becomings to prehend recognizable structuring potentials, and through these we hope to recognize various patterns of becoming. These processes, though derived from the organic and the social, feel equally as relevant to the world of inorganics—of metals, ceramics, polymers, and the like—and we have seen that the structuring potential of them can be couched in the same terminology, the same framework.

These objects are abstractions, and may not yet feel wholly applicable to the seemingly concrete systems that are the everyday experience of MSE practitioners. The idea of multivalent structure that they convey is one that has to be analyzed in several ways, and one that lends itself to a meta-analysis of the structures of the component processes. In MSE, materials, components of materials, properties, and behaviors are grouped in a variety of ways, so a framework which takes into account a multivalent structure, and does not throw out the vast knowledge of material practice, will need involve every concept of structure that has been used to this point.

We are left to conclude that the definitional structure of a set of materials processes, the measured empirical structure of materials experiments, the informational structure of materials data sets, and the mathematical structure of materials models must all be included in our theory of physical structure. In order to build this framework, we first look to each sense of structure, and the background needed to elucidate their concepts. Additionally, we look for any existing frameworks that may capture versions of the structuring similar to the conceptual structuring that has just been described, which leads us to the closest existing parallel, Relational Quantum Mechanics as described by Carlo Rovelli.

Nature is a theatre for the interrelations of activities.
All things change, the activities and their interrelations.
—Alfred North Whitehead, "Nature and Thought"

2.4: Relational Quantum Mechanics

Materials, as generally constituted, are not perceived as quantum systems. In the models used to study our original sense of physical structure, the components of materials systems are rather deterministic, and capable of being reconstructed through mostly Newtonian physics. This section does not represent an attempt to recast the macroscopic behaviors exhibited by materials systems in a quantum mechanical light, even though all systems *are* in fact quantum systems [3, p. 1658]. Rather, in the previous section we outlined a new sense of structure which can hopefully be applied to materials systems, and thought to look for any degree of analogous treatment in modern scientific applications. This treatment is the interpretation of quantum mechanics published by Carlo Rovelli in his ground-breaking paper *Relational Quantum Mechanics* (1996), and expounded upon in several of Rovelli's books including *Helgoland* (2021).

Rovelli opens his interpretation by proposing that the notion of the "absolute" or "observer-independent" states of systems are incompatible with the results of quantum research, due to the fact that two observers of one system can produce different accounts of the same event [3, p. 1637]. If this result is the case, then every result of a quantum mechanical experiment is relative to the observer. Therefore, as a system is measured, a consensus conceptual idea of the system is constructed, and these sets of measurements become "*a theory about the states of systems and values of physical quantities relative to other systems*." That every measurement of a system is relative to another system (or systems), leads to the conclusion that "*in quantum mechanics all physical variables are relational*" [3, p. 1648-9].

These conclusions already mirror some of those which were elucidated in the previous section. Measurements are always relative to the system performing the measurement (here the 'observer'), and the properties that are produced through sets of repeated measurements are averages of the set of relative measurements performed. Averaging these values does not produce some observer-independent concept of the system being measured, but rather gives the sense that the only independent factor within measurement systems is the form of the relation between the observer and the observed systems. One key to building a physics around this shift to a relational interpretation is to be able to in some way measure the relational capacity of systems, and for this Rovelli suggests *information*.

The form of information that Rovelli suggests is classic Shannon information, which he describes in this context as "*...a measure of the number of states in which a system can be—or in which several systems whose states are physically constrained (correlated) can be*" [3, p. 1641]. This basic, correlational sense of information does not take into account differences between observers or system types, so it is not exhaustive in its descriptive powers. Rather, as Rovelli notes, it is a necessary condition of relation for any other, more descriptive form of information. If two systems are correlated (and they all are), then there must exist some measure of the effect that this correlation has measured from the starting point of one correlative body, or the other.

Materials models are often created in an attempt to predict the behavior of some aspect of a materials system, and this predictive bent is also a part of Rovelli's treatment of information. While the information that one system has about another may vary, depending on the context of a measurement, there is a subset of that information which is "*useful for predicting future answers of possible future questions*" [3, p. 1656] which is called <u>relevant information</u>. Relevant information connects the measured, internal, informational qualities of a system, and relates them to how they may potentially affect some other system, in some other measurement. This type of information is important in a materials context, because it is the first connection towards building meaningful (here, important to human use) interpretations of materials systems behaviors. Relative relevant information:

> "*...is not the whole chain between physics and the full notion of meaning in the mental world, but it is the first link in this chain—the difficult one. It is the first step from the physical world, where there is nothing that corresponds to the notion of meaning, toward the world of the mind, whose grammar is based on meanings: signals that have meaning*." [20, p. 175]

This baseline of relation, and the types of information used to interpret it, are important to physics, and fields that deal with physics, because "*Physics is concerned with relations between physical systems. In particular, it is concerned with the description that physical systems give about physical systems*" [3, p. 1655]. Materials are physical systems, they contain physical systems, they interact with physical systems, and our teleological design of them consists of predicting how they will interact with particular physical systems. Much like Rovelli's interpretation of quantum mechanics, we are left to conclude that our own interpretation of the various 'mechanics' of materials should center around relations of the physical systems of materials. Materials systems are measured in different ways from smaller scale quantum systems, though, so the relational qualities of measurements must also be discussed.

> *The instrument presents an epistemic synthesis, seamlessly*
> *joining representation and action to render information.*
> *This synthesis does and must take place in a material medium.*
> —Davis Baird, "Thing Knowledge"

2.5: Measurement

Measurement within an MSE context can mean an enormous number of different things. Characterization techniques measuring properties in the field can range from acts as simple as swinging a hammer at a sample (Charpy impact testing), or probing atomic scale phenomena with electron beams (electron microscopy). In practicality, this diversity of approaches means that any theory of measurement within MSE would need to concentrate on the form that measurement takes, and the forms of data produced by the acts of measurement, rather than particular methods being employed, in order to study the relational capacities inherent in measuring materials systems.

In fact, across the various techniques used to measure, there are common relational qualities that are instantiated within the data sets produced by these measurement techniques. The type and form of data that a measurement produces are the important qualities for both ensuring that empirical data is contextualized properly within a set, and for translating that data for any possible analytical synthesis. In order to illustrate those qualities, measurement should be presented in the most general terms possible, which leads to three related concepts of measurement, all of which are relevant to our coalescing sense of structure. These are [47]:

- Mathematical measurement
- Informational measurement
- Measurement within models

Mathematical measurement is defined as "the mapping of qualitative empirical relations to relations among numbers (or other mathematical entities)" [47]. This approach takes the data produced by a measurement technique and assigns to it some sort of mathematical structure. This is a common practice, and perhaps the most widespread, as most physical experiments result in some form of mapping onto sets of mathematical relations—especially those of sets of numbers, e.g., $\mathbb{R}$, $\mathbb{Z}$, or $\mathbb{N}$. Additionally, this is the primary process of imbuing empirical models with an initial form of mathematical structure, something that will become important later in the thesis.

As might be expected, informational measurement is defined as "*the gathering and interpretation of information about a system*" [47]. Feeding forward from the previous section, we think of information measurements as exactly what was discussed, determining how much the measurement system (or observer system) knows about the system being measured. This process involves looking at the number of correlated states between the apparatus and the object being measured, and can set the boundaries for the mathematical measurements by qualifying how much information it is possible to transmit via measurement for a particular technique.

Finally, measurement within models takes the two prior forms, and uses them to create analytical models—combinations of empirical models that can then be used predictively on the basis of the combined phenomena they describe. Measurement within models is also defined as "*the coherent assignment of values to parameters in a theoretical and/or statistical model of a process*" [47]. This process is how, traditionally, various laws of physics come to be. Related experiments produce related empirical data sets, and these are assigned to variables in a model of some multivariate phenomenon. If measurement is the relation between components of a system mapped onto sets of numbers, then within these sorts of models this third sense is the measurement between a relation of those relations.

The combination of these three senses of measurement are adequate to the construction of materials models, and help to imbue the models that are a result of measurement with useful properties. For instance, S. S. Stevens assigned different types of measurements into different classifications in a classic 1946 paper entitled *On the Theory of Scales of Measurement*. In this paper, Stevens classifies measurements into one of four different scales [48, p. 678]:

1. Nominal – a "determination of equality"
2. Ordinal – a "determination of greater or less"
3. Interval – a "determination of equality of intervals or differences"
4. Ratio – a "determination of equality of ratios"

To each of these he assigned a 'group structure,' in order to classify types of measured data according to their inherent relational characteristics, and their most basic mathematical structure, respectively. This process allowed for direct comparison and contrast between the types of numbers and variables being produced by various forms of measurement. It is an example of the types of properties that the outlined senses of measurement can help imbue on sets of data, as well as helping to establish "*rules… under which numerals are assigned*" [48, p. 680].

The above example concerns primarily the mathematical structuring of measurement, so what of the other two types? Information and approaches to modeling both structure measurements in different ways to the inculcation of mathematical structure on data sets. The first sets rules and variables for what type of information measure can be seen once two systems are in relation. Beyond just the Shannon sense of information, other types arise to describe the relation of systems in different forms. Modeling also has unique approaches, ones that often change depending on the field, experiment, or context of the system being modeled. Both are explored in further detail in the following sections.

"...the elements useful for thinking the world are manifestations of physical systems to each other, not absolute properties belonging to each system."

—Carlo Rovelli, "Helgoland"

2.6: Information Theory

The technical concept of information was first proposed by Claude E. Shannon in *A Mathematical Theory of Communication* [49]. Since then, concepts of information have expanded to encompass a variety of different ways to measure signal, communication channels, variance, and the relational capacity of systems in a variety of different fields. Information has come to be synonymous with the concept of entropy as well, although it is not quite analogous with thermodynamic entropy. In many instances, the variety of entropy used becomes a measure of the information quantity that one system has about itself—as in the Shannon entropy of a system which is the probability of finding the system in a particular state—or about another system, or state of the original system [50].

This first sense of information, now called Shannon entropy, quantifies the uncertainty of a random variable. The equation given by Shannon is:

$$H(x) = -\sum_{x \in X} p(x)\, log_2\, p(x) \tag{4}$$

where *H(x)* is the entropy measured in *bits* for a base 2 logarithm, and *p(x)* is the probability of a particular variable, x, being selected [50, p. 13]. This measure corresponds to the information content, *I(x)*, of a distribution of variables by:

$$H(x) = \mathbb{E}[I(x)] \tag{5}$$

where $\mathbb{E}$ is the expectation value. These two equations serve as the basis—the minimal form of measurable information—for random variables and probability distributions. These expressions were initially formulated as a way of measuring the signal from a source to a destination as it is transmitted along a signal chain and encounters noise. The famous diagram showing this chain is shown below in Figure 4.

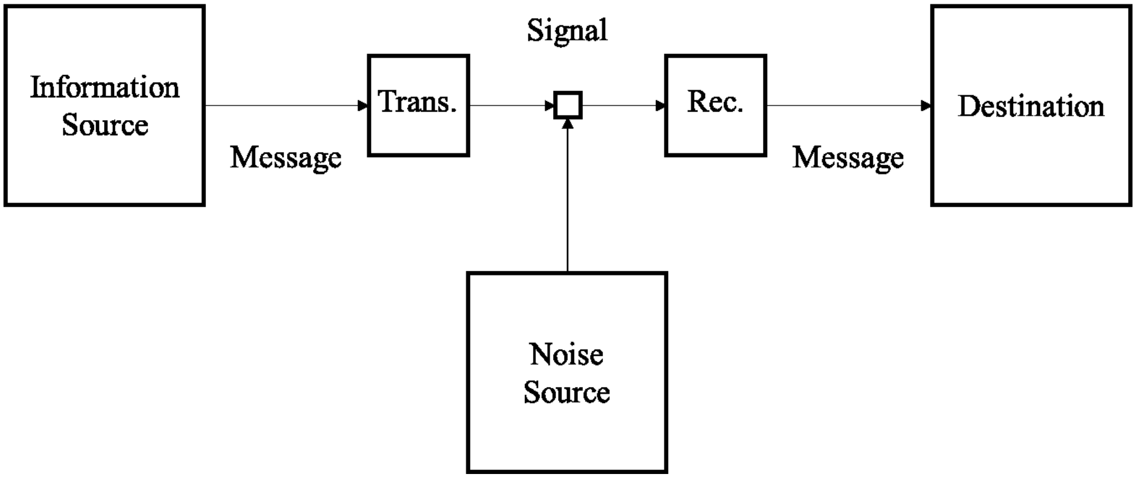


Figure 4: A signal chain which transmits signal (information) from the Source to the Destination, recreated from [49].

This diagram can also be interpreted as one side of a relation of signal transmitted, then received, between two systems. As discussed in previous sections, information is the "language" that systems use to communicate with one another, and each system can serve as both a 'source' and a 'destination.'

Information as a measure of the communication between systems can be interpreted in different ways. In the Shannon sense, information measures the 'entanglement' of two systems, and how much change one system may affect, or 'know,' about the other system. In the context of materials modeling, a type of information of interest is often in the contrast and comparison of experimental data to the results predicted by some empirical or analytical model. One of the best measures to directly analyze sets of modeled data, or data concerning state changes, is a quantity known as the relative entropy, or the Kullback-Leibler divergence. The relative entropy of two probability distributions is given by:

$$K(P\|Q) = -\sum P(x)\log\frac{P(x)}{Q(x)} \tag{6}$$

where *K(P‖Q)* is the relative entropy measured in bits for base 2 or nats for base *e* logarithms. *P(x)* and *Q(x)* are the discrete probability distributions based on sets produced by fluctuations of the independent variable in question, and that of the reference state, respectively [50]. The relative entropy is a statistical divergence, an asymmetric 'distance' between probability distributions that is always positive, and only zero if the distributions are completely equivalent to one another [51].

Related to both the Shannon entropy and relative entropy is the concept of *mutual information*. Given two random variables, *X* and *Y*, the mutual information, *I(X; Y)*, measures how much knowledge of one of the variables informs about the second, and is given by Equation 4 [50]:

$$I(X;Y) = \sum_{x\in X} \sum_{y\in Y} p(x,y) \log \frac{p(x,y)}{p(x)p(y)} \tag{7}$$

where *p(x, y)* is the distribution of both variables and *p(x)p(y)* is the distribution of the product of the variables. The mutual information is also equivalent to the difference between the Shannon entropy and the conditional entropy for two variables with:

$$I(X;Y) = H(X) - H(X|Y) \tag{8}$$

where *H(X|Y)* is the conditional entropy of *X* given *Y*. The mutual information of a variable with itself is equivalent to the entropy of that variable, which is why Shannon entropy is also called self-information [50].

With these three concepts of information, materials systems can be compared in terms of their relatedness, and relational potential, in the context of a measurement of structure, structural change, or structuring potential. Several of these types of information will also allow for a quantification of the relative relevant information discussed in section 2.5, which is the information between two systems that can be used to predict the effect one system has on another system. Every type of information presented here can be used for the creation of engineering judgment—the addition of informational structure from dedomena to data to information to judgment that contextualizes the use of materials in the application decision-making process, finding data that is distinctively distinct [52].

Finally, these various types of information provide a basis for establishing criteria of informational equivalence. Depending on the context of some experiment, model, or theory these measures of information can be judged across a comparative interface to see if there are compatible quantities, objects, and structures on the basis of their information and entropy form or content. Information is the key relational quantity when looking at the interaction and structure building across models or theories. The forms of those models and theories become important to the transmission of information, and before looking at the general structures of models and theories, we look first at the specifics of materials modeling.

> *So it is with all successful models: they unashamedly distort*
> *the inessentials in order to capture the features that really matter.*
> —M.F. Ashby, "Physical Modeling of Materials Problems"

2.7: Modeling within MSE

Modeling in MSE is typically centered around one of two broad goals: recording how natural and engineered materials are structured at all relevant scales, or measuring how these materials react to some energetic impetus in terms of some property of interest. Much existing research in the field covers one or both of these goals, for particular materials systems. In order to create the sum picture of any given materials system, various models from *ab initio* electronic structure calculations to molecular dynamics of atomic structures to finite element analysis of mesoscale structures are stitched together as a method towards creating a multiscale, continuum model of a material, which could serve as the ultimate predictive tool for material behavior, and a key element in the process of designing new materials [15].

Each of these modeling techniques (and others) uses a different set of physics or chemistry to predict how certain objects, e.g., atoms, molecules, will behave in some contextual energetic environment. The techniques of materials modeling will often use these different rules to represent the same object, at some interface of length or time scale. As stated in previous sections, material structure is commonly understood as the set of objects, at a particular scale, which may be manipulated to cause some change in material properties, but it may also be framed as the set of potential interactions of which a set of ‘objects’ is capable; for instance, the types of bonding made available by particular mixtures and quantities of atoms.

Materials models all revolve around the idea of structure, and often we wish to know in what ways the systems composed of these structures are able to contextualize the input of particular forms of energy—a process of structuring. Yet, for all of the models in use, and all of the empirical data collected to-date, there still exists a knowledge gap at the interfaces of different scales of phenomena. Various theories attempt to fill these gaps and, as these theories about material mechanisms and behavior are proposed, a variety of modeling techniques are used to determine the ‘structural’ or ‘behavioral’ basis of these phenomena. Additionally, techniques are extended to serve as predictors for potential behavior of materials in various environments.

The predictive capabilities of models also depend on the type of model being used. There are several approaches to modeling within MSE, beginning with empirical and physical, or theoretical, modeling [4], [53]. Empirical modeling consists of taking data resulting from any experiment and fitting some mathematical equation to it in order to get a sense of some specific material behavior, but is not predictive for those phenomena. Physical models are constructed from physical laws, and on the basis of their analytical power can be predictive of the behavior of various materials systems [4, p. 102].

As phenomena are better understood, and more causal elements within mechanisms are discovered, the physical models that encapsulate them have to change in order to enhance their predictive capabilities. This enhancement occurs through the iterative process of mathematical structuring, or adding the smallest set of new variables and relations to better capture the phenomena. This process is captured below in Figure 5:

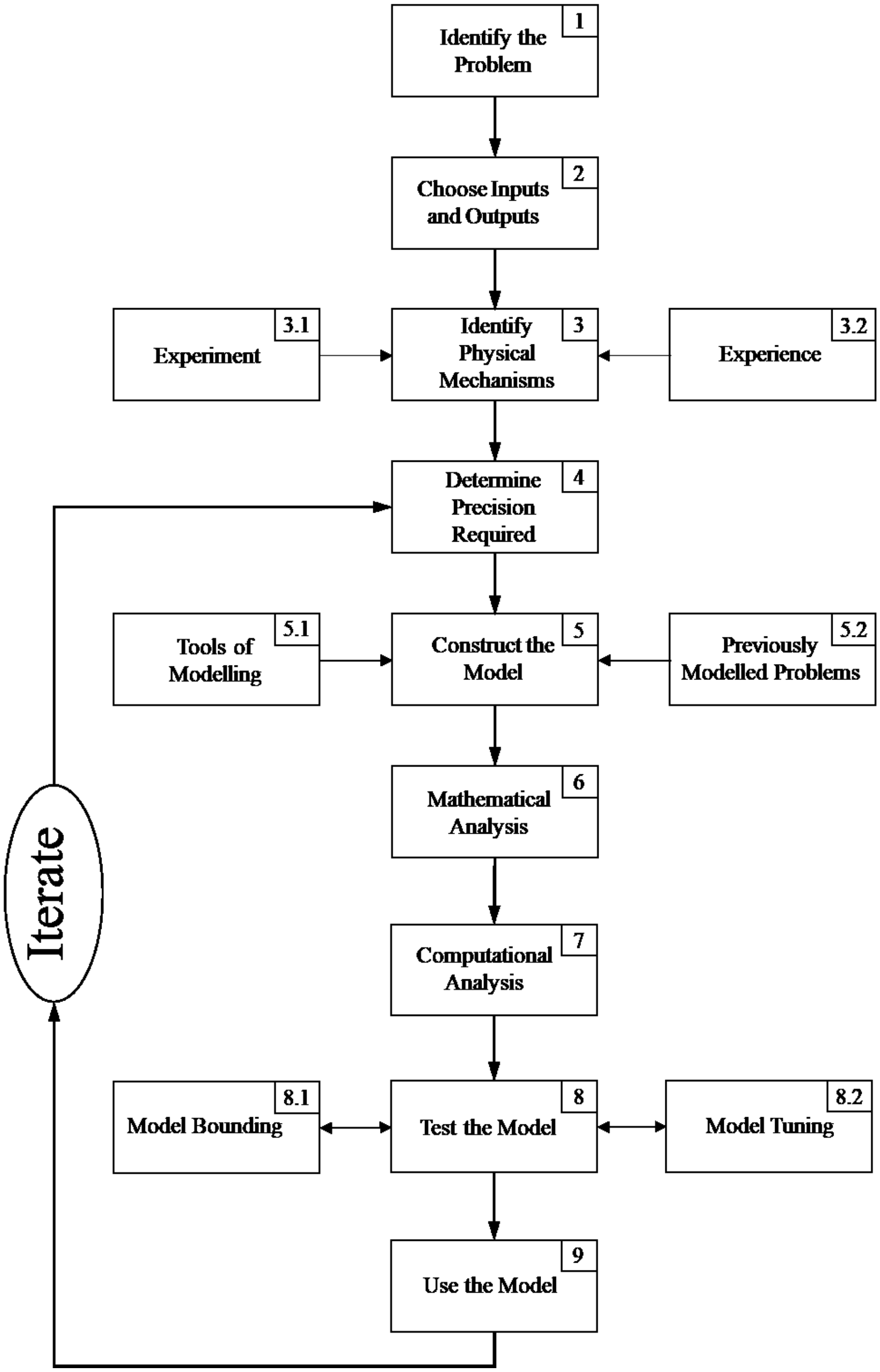
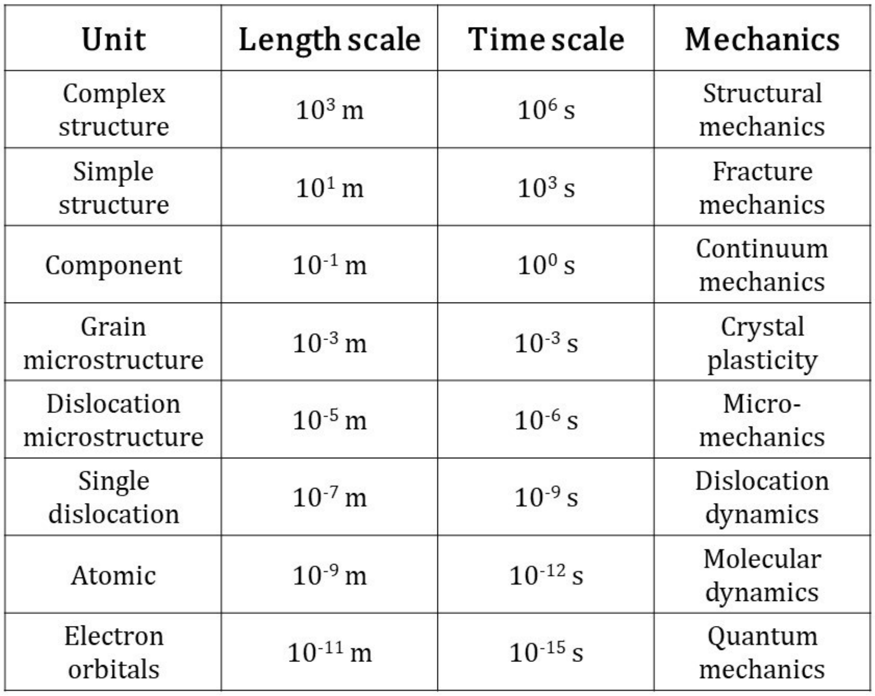


Figure 5: The process of constructing and iterating upon physical models, adapted from [4].

This flowchart shows various points within the process of constructing a physical model where various bits of structure may be added, tested, and then fully integrated. Structure can arise from direct experiment (Box 3.1), from analogous experiments (Box 3.2), from dimensional analysis

(Box 6), or from various calibration techniques (Box 8.2). These structures allow models to be checked, internally, and for two models to be compared and contrasted with one another. The structures of materials models become increasingly important as they are put in to use, not only because of their application as predictive of material behavior, but also because structures of various forms are key to testing and iterating upon models that bridge length scale effects in materials systems. Figure 6 below shows all of the scales currently deemed relevant in MSE:



Unit	Length scale	Time scale	Mechanics
Complex structure	10^{3} m	10^{6} s	Structural mechanics
Simple structure	10^{1} m	10^{3} s	Fracture mechanics
Component	10^{-1} m	10^{0} s	Continuum mechanics
Grain microstructure	10^{-3} m	10^{-3} s	Crystal plasticity
Dislocation microstructure	10^{-5} m	10^{-6} s	Micro-mechanics
Single dislocation	10^{-7} m	10^{-9} s	Dislocation dynamics
Atomic	10^{-9} m	10^{-12} s	Molecular dynamics
Electron orbitals	10^{-11} m	10^{-15} s	Quantum mechanics

Figure 6: The length / time scales relevant to material phenomena, and the physics that describe them, adapted from [14].

Within materials systems, at any given moment, there are changes of various mechanisms occurring at each of these scales simultaneously. In order to capture each sense described above, a variety of models, and model types, are required including empirical and physical modeling. While those two forms of modeling are the primary basis of our understanding of the physical structure and behavior, the advent of computers have introduced new forms of modeling: primarily computational and ‘big data’ (e.g., machine learning) modeling [53].

Each successive form of modeling, from empirical to physical to computational to ‘big data,’ incorporates the previous in their construction. The assumptions and structures that underlie each of these modeling types then feed forward into the assumptions and structures of the subsequent types. As is clear, iterations of models used within MSE integrate an enormous number of approaches, variables, and physics, and keeping the interfaces between these rigorously defined requires ideas about how theories and models interact and inform one another.

> *He looked across the sea and knew how alone he was now. But he could see the prisms in the deep dark water and the line stretching ahead and the strange undulation of the calm.*
>
> —Ernest Hemingway, “The Old Man and the Sea”

2.8: Theories and Models

Theories are ways of looking at the world, they are the collective, cognitive understanding of human experience, both internal and external. As we seek to understand the reality that we inhabit, we create theories about what things are, why they behave in particular ways, and how they are connected in the web of existence. Within these theories, patterns ebb and flow, coming in and out of focus. In order to illuminate these patterns, models are created which adhere to particular theories and map various phenomena in order to better understand them and, occasionally, predict them.

Materials models sit embedded in various material, physical, and chemical theories. In communicating structure across an interface of scale or phenomena, materials systems are often pragmatically stitched together. Yet, in studying the methods of these syntheses, it is also important to take into account how theories and models fit together and inform one another generally. Models are adherent to a particular theory, and theories can contain multiple models. It is, therefore, important to map out the ways in which theories inform the models of various aspects of that theory, and the ways in which models inform the structure of the theories of which they are a part.

As theories are primary to models, we first want to know what a theory is, how it is that we connect to theories, and how we use theories. In MSE, we use theory as a method of organization; for different material classes, for mechanisms of material behavior, or for collections of like properties. Theories guide our material design, and our design-of-use for the materials systems to be engineered; they are teleological blueprints. Theory is defined as "*the analysis of a set of facts in their relation to one another"* [54]. This definition fits with the idea of structure that has been outlined here so far. Theory is, then, a process of abstraction from some related set of things; it is information drawn from the data of the senses. The components of a theory share some relation, rules of interpretation, and ontological commitments that inform the manner in which that theory is used [55]. The cohesiveness of a theory is dependent on how the components of that theory, the models that represent the commitments of that theory, fit together. They are an assemblage, and the strength of a theory depends on where the boundaries of the theory are drawn.

Models are clearly integral components of a theory, acting as representations of the theory, or of components of the theory. These components are, naturally, relations and models are "*the representation of relationships between some formally defined quantities or qualities*" [56, p. 7]. Models describing qualitative relationships give a flavor of the ways in which systems behave, establishing a basic causal calculus that builds up the conceptual structure of the theories to which the models belong. Models describing quantitative relationships assign to the qualitative relations a mathematical formalism that allows for novel approaches of representation and, eventually, prediction. Both senses of a model can be constitutive of a theory, and a basis for comparison and contrast between theories of the same, or similar, phenomena.

Given how models constitute theory, they may be considered the structure of a theory [57]. Models relate to one another within the same theory, or may share structural similarities across theories. They inform the shape of theories, through iteration, and the shaping of the ontological commitments of the theory. Models serve as the invariants across transformations, echoing Max Born who said that complimentary theories should take the form of "...a set of invariants, characteristic of the entity" [58, p. 146]. Materials systems are qualitatively structured by various theories, and the models of these theories serve as the skeleton onto which the science of materials is grafted. Therefore, like other theories, once the structures of materials theories are invoked, it follows that the invocation "*will bring in its wake a <u>criterion of equivalence</u>; theories are equivalent if they agree on that structure*" [57, p. 3].

Thus, this discussion arrives at the conceptual crux of *structure*. Structure, across the various senses that have been discussed, is the sets of relations between the objects of a model or a theory that remain invariant across some change, or some comparison. Materials models contain so many, and such a variety, of structures that accounting for all of them makes a unified theory of materials difficult to parse. What is required are methods of abstraction for materials models in order to find structuring components, and a method of sorting and categorizing the components that are sussed out. Therefore, the approach needed for an analysis of structure is contained within an abstract mathematics capable of probing any structure that might arise in materials modeling, which is offered by category theory.

> *The first of these papers is a more striking case; it introduced the very abstract idea of a "category"—a subject then called 'general abstract nonsense'!*
>
> —Saunders Mac Lane, "The PNAS Way Back Then"

2.9: Category Theory

Category Theory is a mathematical field concerned with "structures and of systems of structures" [59]. As such, it centralizes the relations between collections of objects—and between the objects themselves—in the study of systems and how structures are preserved across different pathways of change in those systems. If structures can be thought of as models of context for objects and collections of objects, then the desire is for category theory to be used as a "universal modeling language" [60]. In addition to modeling structures, category theory also provides a connection to higher order structuring operations, and to algebras useful for comparison of even disparately structured systems. Using these conceptual tools, pre-existing in mathematics and accessible through category theory, an enormous variety of structures could be described within the same framework and compared on an axiomatic basis, centered around a conceptual object of category. To do so, the formal components of a category should be found or defined in any theory which we wish to connect to this network of transdisciplinary knowledge.

Categories are formally defined as mathematical objects, with a category, $\mathcal{C}$, consisting of several collections [61, p. 21]:

Definition 1: A Category, $\mathcal{C}$, is a mathematical object containing

- a set of objects of $\mathcal{C}$
- a set of mappings between the objects of $\mathcal{C}$, called morphisms
- a map from each object of $\mathcal{C}$ to itself, called an identity
- a set of morphisms that compose the other morphisms of $\mathcal{C}$, called composite morphisms

Each composition must also have two properties:

- composition must be *associative*, where given morphisms f, g, and h, then $f \circ (g \circ h) = (f \circ g) \circ h$
- composition must follow *identity rules*, where if f is a map from A to B, or $f: A \rightarrow B$, then $1_B \circ f = f$ and $f \circ 1_A = f$

There are two other concepts central to category theory that deepen the connective tissue that categories offer. The first is that of *functors*, which is a morphism, or operation, between two categories. The second is that of *natural transformations*, which is a morphism between two functors. All of the morphisms—those in the base category, as well functors and natural transformations—are 'structure preserving,' which in this context means they are required to translate the mathematical structure of the objects that they map. These three nested concepts allow for descriptions of complex structures, and an enormous number of different mathematical objects, an indication of the vast utility of these concepts.

Categories are moldable, and through processes of categorification any data renderable in set-theoretic terms can be converted into a category-theoretic version, which adds mathematical structure to the data. Each of the resulting objects should also share properties with their set-theoretic counterparts, rules they need to follow called coherence laws [62], that preserve the properties of the original sets, in the mathematical context. Once categorified, the adjusted models can be used to create cross-functionality, or to embed structure inherent in any sub-processes into a given model.

There are, potentially, many existing mathematical structures that can be grafted in various forms onto materials models. The first step is to find existing sets within materials models, determining how these sets are related to one another, determining what mathematical properties they may already possess, and determining which variables make up the domain and codomain for any identified set-theoretic relation. Ontology logs, or ologs [63], are also useful shorthand for representing the set- or categorical structures of models and their variables visually, an example of which is shown below in Figure 7:

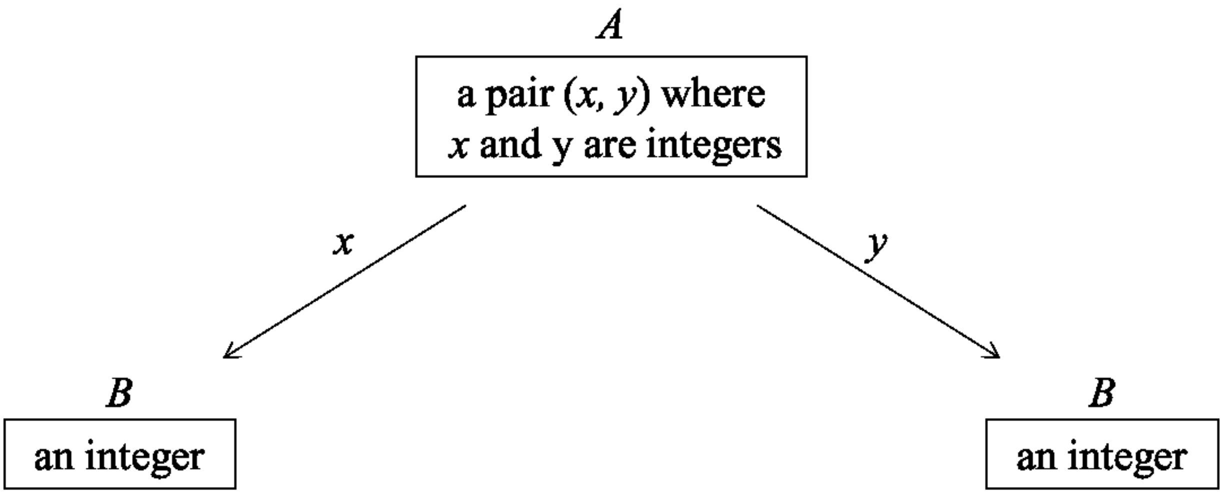


Figure 7: An example of an olog showing a mapping from a pair of integers to singleton sets of integers, preserving the structure of the set of all integers, ℤ. From [63].

Ologs are especially useful as knowledge representation tools because of the implicit mathematical structure embedded within them. If an olog can be created for a system, then the assumption is that each box is an object in a category, each arrow a morphism, and that the arrangement of the boxes and arrows follow the rules established in Definition 1. This feature of ologs is very useful in organizing the mathematical structures that are part of any system being represented. Ologs have been previously used in MSE research [64], [65], though the construction of the explicit categories based on the ologs drawn was not performed.

The tools of categorification and ologs both offer ways to analyze the structure of models, and also to determine the degree to which the structures that both tools illuminate are the same. The former, especially "*refines our concept of 'sameness' by allowing us to distinguish between isomorphism and equality. In a set, two elements are either the same or different. In a category, two objects can be 'the same in a way' while still being different*" [62, p. 7]. Isomorphism refers to a map that has a bijective inverse, such that if $f: A \rightarrow B$ and $g: B \rightarrow A$, then f is isomorphic if $g \circ f = 1_A$ and $f \circ g = 1_B$. Equality, in this sense, is where categories have a specific isomorphism out of the set of possible isomorphisms that can exist.

This property of categories is incredibly useful, because it offers a way to say that things are the same in one way, different in another, and gives the tools to differentiate. Materials by definition are the same *kinds* of things. Yet, clearly, they are different in an enormous variety of ways; metals are not plastics, iron is not copper, a single crystal is not a polycrystalline grain structure. Accounting for these differences while searching for similarities is the task set for MSE across a variety of contexts, and category theory offers the most diverse toolset to accomplish this task. Categories encapsulate a sense of structure that can inform models of materials, decipher embedded mathematical structures, find structure-preserving maps, and determine sets of invariants. It follows then that the use of categories, and the tools of category theory, is a process of finding equivalences between objects, systems, behaviors, and theories.

Whence things have their origin,
Thence also their destruction happens,
As is the order of things;
—Anaximander, "Fragment*"*

2.10: Criteria of Equivalence

Equivalence seems like a straightforward idea; if something is equal to something else, it is equivalent to it. Yet, that does not capture the full picture of what and how things—objects, systems, ideas, theories—may be the same, or similar. There are various senses of equivalence, and there are relations between senses of equivalence that may inform how two objects may share some degree of equivalence. As these objects are structured, their forms are drawn in comparison—in relation to—other systems and objects. A juxtaposition of equivalences in this comparison, either between objects or in states of the same object, illuminates these structures. Criteria of equivalence therefore become the key to recognizing novel forms of structure overall.

In building theories, and models of those theories, criteria of equivalence can serve as a blueprint for how each ought to be constructed. Theory being a set of like ideas or concepts, they gain conceptual heft as more senses of structure and equivalence are applied. Here we propose that there are at least five relevant senses of equivalence that can help to build a framework of structuring to serve as a new materials ontology. Theories of materials are designed to capture the required physical and behavioral aspects of a system in a way such that the system may be modeled, and predictions about the behavior of the system may be produced by that model. Iterations of materials theories aim to improve the accuracy and precision of the predictive capabilities of the models of a particular theory. The various forms of equivalence that exist within physical modeling help to build criteria of theoretical equivalence, and provide a rigorous framework to compare and contrast different theories to one another.

As the physical theories, and their representative models, are iterated upon each becomes more structured, and the criteria of equivalence serve as structuring frameworks. Many materials theories may be defined in terms of one of these types of equivalence, or some combination of them, to varying degrees. Through careful definitions of these sets, the relational structure of models at every step of materials system-building can be put into place in order to ensure that the behavior of variables and models is consistent in any context. For the physical structure of materials, complete equivalence of two material objects, or systems, requires that the objects should be equivalent in all five of the forms listed in section 1.2. These individual equivalence forms are generically defined as:

1. Definitional Equivalence

   Physical theories begin centered around groups of like, physical objects. We define sets of objects as equivalent on the basis of their definitional equivalence; we use the same set of descriptors to define the objects, relations between them, and similar properties they may share. This is a first criterion for definitional equivalence:

$$\{D\} = \{\forall d \mid d \in D_T\} \tag{9}$$

where *{D}* is the set of definitional equivalence criteria, D_T is the set of all descriptors of objects in theory *T*, and *d* is an individual descriptor. This set of descriptors is also an object that serves as the basis for a physical theory.

Across models, for some object *x*, some object *y* is definitionally equivalent to *x* to the extent that some set of descriptors of *x* composed of {nouns, verbs, adjectives, etc.} contains a subset that is also a set of descriptors of *y*:

$$\{D_x\} \Leftrightarrow_D \{D_y\} \leftrightarrow \exists\{d_y\} \in \{D_y\}, \{d_y\} \subset \{D_x\} \tag{10}$$

2. Empirical Equivalence

   A form of equivalence between two sets of experimental data which, at a minimum, share a data type. The data types also include the form of measurement taken [48]. It may include observational equivalence, if the form of empirical data comes in the form of a set of observations other than numerical data. Empirical equivalence, on the basis of shared techniques and theories, with a condition of definitional equivalence, is also assumed. For models of the same theory, empirical equivalence occurs when the models of the theory, *M(T)*, produce data that share a data type.

   For models of different theories, a condition for determining their empirical equivalence is that there exists a structured translation between the models. If *{e}* is any set of experimental data in the set of empirical results for a theory, $\{E_{T1}\}$, then for there to be empirical equivalence between theories T_1 and T_2, there must exist an injective map *f* from $\{E_{T1}\}$ to $\{E_{T2}\}$ [57].

$$f: \{E_{T1}\} \rightarrow \{E_{T2}\} \tag{11}$$

3. Informational Equivalence

There could exist a variety of senses of informational equivalence. One is the equivalence of entropy, the amount of information measured by Shannon entropy that a model or data set may contain. There are many existing physical quantities that are related to the amount of informational entropy of the system, and it can inform interpretations of both local parameters—for example, local order parameters such as extracopularity [66]—and defined properties of individual states of systems [67].

Another proposed form is the equivalence of relative entropy, which allows for a comparison of multiple states, $\{u_i\}$, of a system $\{U\}$, or of the form of a state change of two different systems, on the basis of its relative entropy, K, (the Kullback-Leibler divergence) measured against some reference state such as equilibrium, absolute zero, STP, etc. In order to determine informational equivalence, the proposed criteria are that the information measure of two states are equivalent.

$$|u_1(x)| = |u_2(y)| \Rightarrow K(x) = K(y) \tag{12}$$

This proposal does not necessitate that the states, u_{ij}, are exactly the same, but rather they have the same entropy relative to their respective reference states.

Using these forms of equivalence in tandem, a framework of comparison of materials systems, and the models of which these systems are comprised, can be constructed. This framework can serve as a basis of comparison and contrast for judging the equivalence, effectiveness, and predictive capabilities of models and scientific languages. Furthermore, building informational criteria can, in the vein of other treatments of empirical equivalence, build even stronger connections between the mathematical structure and empirical content of theories [68].

4. Categorical Equivalence

On its face, categorical equivalence is simply the criterion that the categories used to describe some set of data share some structure. If data within some model or set can be categorified, then some measure of categorical equivalence could be established. Categorical equivalence can be established between two categories if they are intertranslatable [57], up to an isomorphism.

This definition means, that for any two categories, A and B with functors *F* and *G,* share some categorical equivalence at an upper (isomorphism) and a lower (translation) bound, rendered as:

upper bound: $\exists F, G;\quad F: A \rightarrow B \;\; and \;\; G: B \rightarrow A \mid F \circ G = 1_B \;\; and \;\; G \circ F = 1_A$

lower bound: $\exists F \; or \; G;\quad F: A \rightarrow B \;\; and \;\; G: B \rightarrow A$

In between the isomorphism and the existence of functors are a variety of different degrees of equivalence depending on the amount of structure that is preserved. All of the gradients of equivalence can be used as the basis for judging what structures of materials models and systems are invariant, the core of the idea of structure.

5. Theoretical Equivalence

Theories are the most general objects through which science and engineering are performed. Each of the preceding senses of equivalence are potentially constitutive of theoretical equivalence. This assertion follows from the levels of structure that each other form of equivalence projects onto the theory of which they are a part, with a theory becoming stronger, or weaker, as it becomes more or less dense with structures, respectively. General theoretical equivalence is present, similar to the other senses, if the definitions, experiments, models, and categories of that theory are similar to those of another theory. This sort of structure preservation between two theories (*T*) and models of those theories (*M(T)*) is shown in Figure 8:

$$\begin{tikzcd}
T_1 \arrow[r, "f"] & T_2 \\
M(T_1) & M(T_2) \arrow[l, "f^{-1}"']
\end{tikzcd}$$

Figure 8: Theoretical equivalence shown on the basis of the structural preservations between models of those theories, adapted from Dewar 2022 [55].

The forms of equivalence criteria that have been outlined are definitional ($\Leftrightarrow_D$), empirical ($\Leftrightarrow_E$), informational ($\Leftrightarrow_I$), categorical ($\Leftrightarrow_C$), and theoretical ($\Leftrightarrow_T$). These kinds of equivalence criteria feed upwards and inform at every level the structure of the theory of which they are part. Figure 9 shows the nesting relation of the proposed equivalence criteria:

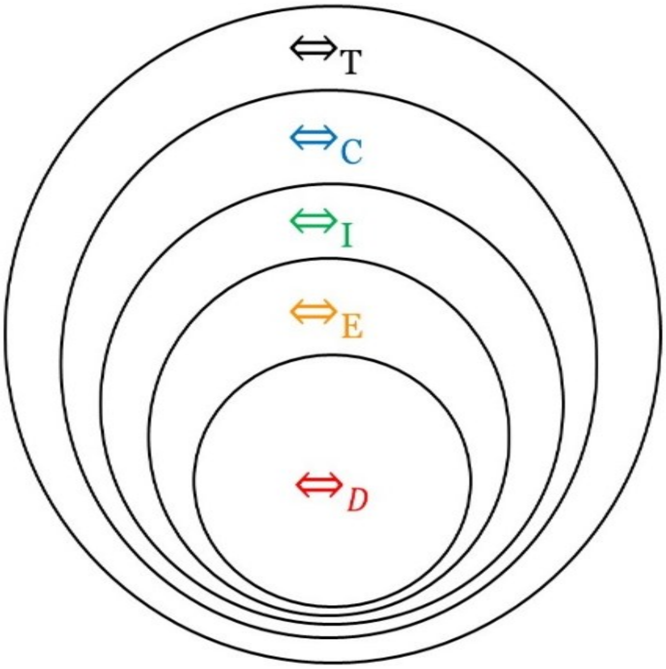


Figure 9: Nested equivalence criteria.

The criteria of equivalence introduced in this section are general, and capable of comparing and contrasting an enormous variety of structures. The structures can be presented in any of the five forms, or may be any system invariant that serves as the bases for these criteria. Through this framework, through these criteria, and with integration into the existing paradigm of materials, a new ontology of materials can be established.

History is process, knowledge is process.

—Carlo Rovelli, “Helgoland”

2.11: A New Materials Ontology

What is structure? Structure is sets of relations between “objects” (themselves sets of relations between other objects), including invariants, symmetries, and arrangements. From the outset, materials systems have been a composite of theory, experiment, data; all forms of structuring. Everything that informs how materials systems are instantiated in the world and how they behave revolves around structure. Previously, the idea has been that it is purely physical structure—objects like atoms, molecules, grains, or bars of a material—that is determinate of every property and behavior of a materials system. What is becoming clear is two-fold:

1. Physical objects can be thought of as a process of relations of systems being actualized.
2. This conception of objects requires new and multi-faceted ideas of structure in order to fully capture every sense of structure, and structuring, that presents itself within materials phenomena.

These conclusions shift interpretations of materials theories and models, but it remains that structure is also the center of the new materials ontology. Everything within materials research involves not only the common physical structure, but also definitional structure, informational structure, mathematical structure, and theoretical structure. Every form of structure is constitutive of material structure, with every different concept building towards an enriched materials structure.

Various philosophies of structure, of process, of relations lend conceptual heft to the approaches of modeling within MSE. These approaches result in comparisons of relational structuring; Process becoming comparisons of comparisons of relations between structures. Time introduces mechanism in the material sense, reframing an aspect of process as a Bergsonian durée*,* a duration between two states. Each system of process encapsulated by the philosophies reviewed in section 2.3 reorients the picture of systems as *relationally*, rather than object, oriented.

Perceptions of individual physical objects offer little information about the 'useful' potentials of an object (at least, in an engineering sense). What can be known of how a piece of iron will behave by looking at it, or by touching it with a bare hand? It is only through the iron object-system's interactions with some other system—say a hammer, or a heating element—that the perception of the iron system is further informed. That is to say, the concept of iron is not a direct sensory input of the iron system itself, but rather my concept of iron being a direct sensory input of a relation between the iron system and some third system.

This interpretation of how systems are constructed is akin to relational quantum mechanics in that it informs our interpretation of measurement, and of how the role of the observer changes in a relational context. Every measurable sense of materials that exists comes from the actualization of some property in response to the act of being measured. Quantifying the actualized, relational capacities of systems, and their structuring potential, involves characterizing the information of those systems. The information that arises from the relation of two systems is directly correlated to the amount of change that one system may affect in another, or a measure of change within a system that has already occurred.

Measures of information and informational relations become the basis by which various model types within MSE can be enriched. Through this enrichment material theories, and the models that comprise them, gain structure and can be analyzed in the abstract. The new materials ontology is an encapsulation of every way in which our conceptions of materials may be structured, and this structure becomes clear most broadly by illustrating the various equivalence criteria that can draw out the structures of each sense. Using all of the tools that have been described, a framework of structural equivalence, from the definitional to the empirical to the informational to the categorical to the theoretical, can be built.

Every criterion adds a novel type of structure to the idea of what a material is, and the process of establishing these criteria allows for a direct comparison of even the most disparate material systems. Every materials system is structured, so a method of creating the criteria of equivalence between two systems is the best way to find the rules of structuring, the true idea of universal materiality. As Bogdanov wrote:

> "*Practice and theory would benefit little if the entire matter came to the philosophical position that "everything is organization." Methods are necessary and important for practice and theory. In this regard, the inference is clear: "all methods are in essence organizational." The problem, therefore, is to understand and study every method as organizational*" [23, p. 6].

This sense of 'organizational' methods are exactly what is proposed herein. We understand the rules of organization as the essence of structure, and we search through various means to extract these rules. Using the tools embedded already within MSE, levels of abstraction, the tools of information and category theory, and a relational-process view of systems, a new paradigm of materials is crafted and we see how it is that this paradigm may be applied to different materials systems, experiments, behaviors, and applications.

Above all, a new materials ontology shows us that we are not isolated from materials any more than we are isolated from any other system. The only anthropological transcendence comes from our senses as nodes of relation that can recognize our own relational capacities. We are integrated into the world and the sensations relating to, and becoming, us are "natural phenomena in the world: the form in which the world presents itself to the world" [20, p. 126]. Though it is not often explored within the context of materials, the human process of conceptual becoming through relation to materials systems is central to our existence. As Morris Cohen, a luminary in the field of MSE phrased it, "Nature, in the form of the human mind, then starts to examine *itself*; to describe itself; to try to understand itself" [69, p. 516].

Chapter 3

Methods

> *...equivalence is a matter of positing the same structure,*
> *and structure is that which is invariant across equivalence.*
> —Neil Dewar, "Structure and Equivalence"

The meta-framework which results from the analysis presented in the previous chapter is designed to determine the structures of both models and theories of materials. The framework performs this task by establishing rules for determining equivalence between structures of various aspects of materials systems. The rules for determining equivalence provide a backdrop against which the invariants across some relational interface can be resolved. If some object, a theory, model, or state, meets these criteria for each form of equivalence, there is a basis for translating results from object to object knowing that key invariances will be maintained. Furthermore, we propose that this set of invariants *is* material structure, on the basis that they are key components which are measurable within the range of model efficacy, and across modeling and environmental interfaces.

As such, the method proposed herein for determining the structure of materials at various levels and interfaces involves five sets of equivalence criteria, and the structural equivalence framework that connects those criteria to one another. Instead of analyzing the data produced by materials models, simulations, or theories directly, this approach is to look at how the current analyses of materials systems are structured and analyze that structure. As presented in section 2.10, this analysis requires five different senses of equivalence. These forms of equivalence are tied together into a framework of equivalence, against which systems may be tested. Within this framework, invariances may be found and described for any objects of analysis, and thereby material structure may be defined. Any model, any system, within a set of materials objects can influence the way in which this framework can be constituted, so the abstracted rules by which structure is defined are vitally important.

Equivalence relations and classes are foundational within mathematics. The most basic equivalence relations are binary relations in some set, where $\{e\} \in E$ is the set of equivalence relations for a set $\{a\} \in A$. In order for a binary relation to be an equivalence relation within some set, it must be reflexive, symmetric, and transitive in that set.

Definition 2: Let E be an equivalence relation within R, where:

i. for all $a \in A$, aEa indicating *reflexivity.*
ii. for all $a, b \in A$, aEb implies bEa indicating *symmetry*.
iii. for all $a, b, c \in A$, aEb and bEc imply aEc indicating *transitivity*.
and (i), (ii), and (iii) are all true.

This basic sense of equivalence gives properties and structures to even the simplest of sets, and more structure can be built on the basis of this relation. If there exist within a set multiple equivalence relations, those that share properties are known as equivalence classes. Equivalence classes are sets of equivalence relations, and define the types of equivalence that sets of objects may have. Across mathematics there are equivalence relations and classes of many types that account for the varying degrees of equivalence that mathematical objects may possess [70].

The forms of equivalence built upon this type of relation are the backbone of the comparative technique that we propose. Every system, of physical objects, theories, models, etc., is interacting with, or defined in relation to, some other system. There is no system capable of manifesting properties, or of being measured, that exists in isolation. The relational nature of systems, therefore, make criteria of equivalence an incredibly suitable tool for divining structure. If no system is isolated, then the structure correlating to each proposed form of equivalence may be found in relief to some system in comparison. Therefore, the layers of juxtaposition proposed by this set of equivalences is—in our view—the most comprehensive method of proposing, identifying, and cataloging the structures present within any materials theory.

To this end, we wish to propose various interpretations of the five forms of equivalence so that they may be used in a materials modeling context. This framework is designed to be loose and abstract enough so that it allows connection with any model, of any material, at any scale. Portions of the framework borrow from the vocabulary and language of first-order logic, which is redefined to the particulars of materials theories as needed. Material structure, as has been discussed, is not simply the physical mass and bonding, but includes the meta-structural information of the models used to conceptualize material scale. The first equivalence of the simplest relational sort is that of *definitional equivalence.*

3.1: Definitional Equivalence

A degree of definitional equivalence generally means that given two theories and their constituent models, we may at least partially be able to define them in the terms of the other. To begin we will borrow a concept from logic and model theory, that of a *signature* which can be defined as a selected list of the non-logical symbols and algebraic operations from a vocabulary describing an object. The use of this terminology is intended to offer a more formalized treatment of material definitions, rather than to render them fully axiomatic. If this object is structured, then the signature is the union of constant, functional, and relational symbols and descriptors for that structure [71]. Using a signature is an efficient means of collecting all the definitional pieces of a theory into one place, and similar methods have been adopted elsewhere in materials research, even if not explicitly by name [72].

In materials modeling, our definitions are centered around the material type, dictated by the atomic or molecular structure of the material, classes of those materials, material properties and mechanisms of behavior. Sometimes these models consist of only one of these categories, or they may be coupled with other types of models incorporating aspects into either or both. For each we can follow section 2.10 and assign these materials definitional criteria as theories, and then establish sets of definitional descriptors for each, building a general definitional signature, Σ_{def}, for model sets.

> **Definition 3 (**olog Figure B.1**)**: Let Σ_{def} be the signature of definitions for a materials model. We define a set *M,* the elements of which are types of Σ_{def}. We then define three sets:

- Rel(Σ_{def}) - the set of all relational definitions for the vocabulary of a model, with descriptors the set $\{d_{Rel} \in M_{Rel}\}$, and maps <*unit*>: Rel(Σ_{def}) $\rightarrow M \times M$ for defining unit relations across the definition set;
- Func(Σ_{def}) - the set of functional definitions for the vocabulary of a model, divided by a relation *domc*, which divides the set into elements of various potential domains and codomains for pairs in M, <*domc*>: Func(Σ_{def}) $\rightarrow M \times M$, and with descriptors the set $\{d_{Func} \in M_{Func}\}$
- Const(Σ_{def}) - the set of constant definitions for the vocabulary of a model

Using this definition, we define the sets of descriptors for which there is a basis for establishing a theory. In qualitative terms, any set of descriptors that are determined to share some basis of similarity may be sufficient for the establishment of a shared theoretical vocabulary, which may then be used in the determination of definitional equivalence.

Then for any two signatures representing different materials theories, $\Sigma_{def}(T_1)$ and $\Sigma_{def}(T_2)$, there exists a definitional equivalence if there is a relation mapping at least some of the elements of one of the theories to the other, up to isomorphism. As with the generic equivalence relation, these sets should also have the properties of reflexivity, symmetry, and transitivity.

In other terms, given our two signatures of a materials theory $\Sigma_{def}(T_1)$ and $\Sigma_{def}(T_2)$, if a set X with elements $[x_1, \dots, x_n]$, where $X \subseteq \Sigma_{def}(T_2)$ is to be definable in terms of $\Sigma_{def}(T_1)$, then there must exist some formula φ such that:

Definition 4: There exists a definitional equivalence between theories T_1 and T_2

$$\exists\ \Sigma_{def}(T_1) \Leftrightarrow_D \Sigma_{def}(T_2) \text{ when for}$$

$$\{X\} \subseteq \Sigma_{def}(T_2) \quad and \quad x \in X, \text{ there is a function, } \varphi,$$

$$\exists \varphi \mid \Sigma_{def}(T_1) \ \vDash \ \varphi[x_1, \dots, x_n]\ when\ \varphi\langle x_1, \dots, x_n\rangle \in \Sigma_{def}(T_1)$$

meaning that the formula φ defines the terms of $\Sigma_{def}(T_2)$ in $\Sigma_{def}(T_1)$ [57]. There would necessarily also be a formula φ^{-1} mapping the terms in reverse, from $\Sigma_{def}(T_1)$ to $\Sigma_{def}(T_2)$.

Each form of equivalence can be measured for a degree of equivalence, calculated as the probability of there existing a map between an element, or elements, of the domain and codomain of the equivalence relation. The degree of definitional equivalence is then calculated as:

$$\overset{\circ}{\Leftrightarrow}_D = \frac{p(\ |x_i \times \varphi[x_i]|\ )}{|[x_i]|} \tag{13}$$

showing that as the density of maps increases from the definitional set $\Sigma_{def}(T_1)$ to $\Sigma_{def}(T_2)$, the degree of definitional equivalence between the two also increases.

This first criteria of equivalence exists mainly as a basis for the comparison and contrast of theories and models of them, provided a shared framework and vocabulary upon which other structures may rest. Some sense of definitional equivalence is a necessary component for the determination of empirical equivalence, primarily as a necessary prerequisite for the construction of comparable experiments.

3.2: Empirical Equivalence

The second form of equivalence in our conceptualization of structure is that of empirical equivalence. Empirical equivalence is, in general, a term used to describe when two theories start with different primary vocabularies, but are able to produce moderately equivalent experimental results or predictions. A classic example for this is Newtonian and Langrangian mechanics [73]. Here we take any result of experiment, hence any measurement, to be a basis for a comparison between the empirical contents of a theory. That is to say, the results of the experiment may be theoretical in nature—the measurement of yield strength, or of electric fields are contrived rather than *directly* empirical—but we assume them to be part of the empirical basis of materials theories on the basis of the dispensability thesis, like that proposed in [74], and do not differentiate the ontological determinative powers between direct observables and theoretical variables derived from experiment.

In a materials sense, our criteria of empirical equivalence will involve the juxtaposing of structured data sets resulting from various experiments either of different or the same materials theory, and determining the degree to which one data resulting from one theory is reproducible (and to what degree) in the other theory. This approach is supported by the scaffolding of definitional equivalence, a requirement for the establishment of empirical equivalence, as well as necessary unit assignment relations, from the powerset of all units notated as $\mathcal{P}\{u\}$ [75].

Therefore, for any two sets of empirical measurements pertaining to theories T_1 and T_2, rendered as $E_1\{T_1\}$ and $E_2\{T_2\}$, there is empirical equivalence when:

Definition 5: There exists an empirical equivalence between models E_1 and E_2

$$\exists\, E_1(T_1) \Leftrightarrow_E E_2(T_2) \quad \text{if} \quad \exists R\colon \{e_r\} \leftrightarrow 2^{\{u\}}$$

$$\text{and } (e_1 \in E_1) \overset{R}{\rightarrow} (e_2 \in E_2),\ (e_2 \in E_2) \overset{R}{\rightarrow} (e_1 \in E_1) \text{ up to isomorphism.}$$

This definition allows for the maps to combine operations which translate between experiment types, $\{e_r\}$, and a relation which maps the appropriate unit(s) onto the values. The overall set of units $\{u\}$, includes any conceivable base or derived unit, and the multirelation is a combination carrying both the numeric relation and unit conversion relation, as pictured in Figure 10, with $e_r u_c \in R$.

$$\begin{tikzcd}
\{E_1\} \arrow[r, "e_r"] & \{E_2\} & & & \\
& & \Longrightarrow & \{E_1\} \arrow[r, Rightarrow, "e_r u_c"] & \{E_2\} \\
\{U\} \arrow[uu, "u_1"] \arrow[r, "u_c"'] & \{U\} \arrow[uu, "u_2"'] & & &
\end{tikzcd}$$

Figure 10: An olog showing the expanded and collapsed versions of the multirelation of unit-preserving empirical equivalence, where $\{E_1\}$ and $\{E_2\}$ are different sets of empirical data, $\{u\}$ is the universal set of units with unit assigning functions u_1 and u_2, e_r is an empirical relation between the data sets, and u_c is a unit conversion relation.

As with the other forms of equivalence, there exists here a degree of probability that is determinate of the degree of equivalence between two sets of experimental values, measuring how much the ‘bits of evidence’ contained in both sets agree [76, p. 120]. If a multirelation exists, the degree of empirical equivalence is the probability that a value in the domain of the relation will map into the codomain. If that probability is 0, no empirical equivalence exists, and if that probability is 1, then it is a function, and an isomorphism.

$$\overset{\circ}{\Leftrightarrow}_E = \frac{\Sigma p(f\colon e_1 \rightarrow e_2\ )}{|\{e_1\}|} \tag{14}$$

Empirical equivalence, as constructed, is also associative, transitive, and symmetric. That is, for any elements of E_1, E_2, and E_3, which are, to any degree, empirically equivalent:

1. $E_1 \rightarrow (E_2 \rightarrow E_3) = (E_1 \rightarrow E_2) \rightarrow E_3$
2. *if* $E_1 \rightarrow E_2$ *and* $E_2 \rightarrow E_3$, *then* $E_1 \rightarrow E_3$
3. *if* $\exists f\colon E_1 \rightarrow E_2$, *then* $\exists h\colon E_2 \rightarrow E_1$

Empirical equivalence within a materials context entails the use of historical data, meaning that experiments deemed to measure equivalent properties at any point in time may be used a basis for determining the empirical equivalence of a similar system (e.g., the same material, or same class of material) within the bounds of the empirical model at hand. This assumption allows for the comparison of systems of material structures that may not have the same actualized properties, but may be considered empirically compatible in order for their equivalence to be ascertained [77, p. 265]. Depending on the problem being investigated, our form of empirical equivalence may be calculated for material structures (the physical elements and properties), variables, models, and theories; in whatever form the difference-making distinctions within the experimental framework may be found [77, p. 268].

3.3: Informational Equivalence

There could exist a variety of senses of informational equivalence, each based on the various measures of information that a system may have. The most basic is the equivalence of information entropy, or the amount of information measured by Shannon entropy that a model or data set may contain. As information entropy measures the amount of signal which is transmitted through some communication relation between two systems rendered as probability distributions, the equivalence of information can be used in various ways to determine the degree of affect that one system has in relation to another. There are many existing physical quantities that are related to the amount of informational entropy of the system, and it can inform interpretations of both local parameters and defined properties of individual states of systems [67].

First, for any version of information equivalence, empirical equivalence is a necessary prerequisite, meaning the distributions analyzed must either share empirical priors, or there must be an empirical translation between the two theories being analyzed. In its simplest form, the information equivalence measured via Shannon entropy would show that for two related objects that are rendered as probability distributions, how much dispositional power each has to affect change in the other; put in the context of related systems based on empirical data sets, it is the probability that the average element of the domain set is in relation to an average element of the codomain set. Recalling section 2.6, this entropy *H(x)* is given by equation (4).

This event can be as simple as a coin flip, or as complex as the measurement of some relation between material objects at the microscale. The equivalence criteria of this type of information is similar to the other forms in that empirical equivalence is a necessary precondition, and if a map between the data sets exists, then sets of information measures between those sets may be directly compared and contrasted on the basis of the probabilities of ‘event’ occurrence. If it is assumed that these sets are of discrete probability distributions, the criteria would then be given as:

Definition 6: For any two sets of information measures H_1 and H_2, if

$\{E_1, H_1\} \in T_1$ and $\{E_2, H_2\} \in T_2$ then

$\exists H_1 \Leftrightarrow_I H_2$ if $E_1 \Leftrightarrow_E E_2$ and $|H_1| = |H_2|$

This type of informational equivalence does not obtain degrees, but is rather true, or false; either two discrete distributions have the same Shannon entropy, or they do not. This property renders this type of informational equivalence in this form of minimal value to analysis of materials problems, as it pertains more to the properties of distributions which empirical methods may produce, rather than analysis of those distributions.

In order to obtain more relevant structure within materials science, we look instead to the equivalence of relative entropy, which allows for a comparison of multiple states, $\{s_i\}$, of a system $\{S\}$, or of the form of a state change of two different systems, on the basis of its relative entropy, K, (the Kullback-Leibler divergence, equation (6) in section 2.6) measured against some reference state such as equilibrium, absolute zero, STP, etc. The relative entropy for a set of empirical data of a given theory is shown by equation (15) as:

$$K(E_i \| E_{i0}) = -\Sigma E_i(x) \log \frac{E_i(x)}{E_{i0}(x)} \tag{15}$$

where, again, $K(E_i \| E_{i0})$ is the relative entropy measured in bits for base 2, or nats for base e logarithms. $E_i(x)$ and $E_{i0}(x)$ are the discrete probability distributions produced via analysis of an empirical data set at various points as the environmental variables are changed, and that of the chosen reference state, respectively. An olog of this process can be seen in Figure B.2.

Then, two systems undergoing the same change in environmental variables—e.g., two samples raised to the same temperature—can be contrasted in terms of the relative entropy shift produced by that change in variables. With a sufficient number of steps, a relation may be formed between the dynamic shift in the divergence of the domain distribution versus the measure of divergence of the codomain for a particular shift.

In order to determine this informational equivalence, there must then exist a map between the information sets defined by the relative entropy of the two empirical data sets, for the bounded range of appropriate environment values.

Definition 7: For some data set $\{e_i\}$, where $e_i \in E_i$, and probability distribution

$$P(e_i) = \frac{\Sigma(e_{i+\Delta i} - e_i)}{\Sigma(e_n - e_0)}$$

with bounds $[0, n]$ where (upper: $e_n \geq e_i$) and (lower: $e_0 \leq e_i$) then

$$K(E_i) = -\Sigma P(e_i) \log \frac{P(e_i)}{P(e_0)}$$

then, for E_1 and E_2, there exists an information equivalence

$$\exists K(E_1) \Leftrightarrow_I K(E_2) \text{ if } \exists f\colon [\, K(E_1) \vee K(E_2)] \rightarrow [K(E_1) \times K(E_2)] \text{ up to isomorphism.}$$

This proposal does not necessitate that the states, s_{ij}, are exactly the same, but rather compares the entropy produced by the same progression of environmental variables relative to their respective reference states. The definition includes the upper and lower bounds determined by the state variables of the system by capping the probability distributions at $[0, n]$.

Informational equivalence, at least of the two varieties presented here, are associative and transitive, but not necessarily $(\neg\Box)$ symmetric. That is, for various sets of information data $K(E_i)$:

1. $K(E_1) \rightarrow (K(E_2) \rightarrow K(E_3)) = (K(E_1) \rightarrow K(E_2)) \rightarrow K(E_3)$
2. if $K(E_1) \rightarrow K(E_2)$ and $K(E_2) \rightarrow K(E_3)$, then $K(E_1) \rightarrow K(E_3)$
3. $K(E_1) \rightarrow K(E_2) \neg\Box\, K(E_2) \rightarrow K(E_1)$

As previously stated, the form and properties of informational equivalence might change based on the form of information content being analyzed.

3.4: Categorical Equivalence

The forms of equivalence defined so far have dealt with comparing structures concerned with the relation of objects and the ways in which they are measured. A theory defines the objects of that theory, a kind of sameness relation, and then in scientific practices those objects are measured creating empirical data sets, and compared to one another in a relational capacity, producing information about the systems being measured. Across many systems within a given theory, there is room for additional, mathematical structure to be used to illuminate more general ways in which systems behave. Theories across different materials systems can adhere to behaviors defined by various similarities in the behaviors of their models. This structure, a comparison of the mathematical structure of the models used within MSE, is best analyzed using Categories, as covered in section 2.9.

Materials models describe various aspects of materials, and are generally bound in their range of efficacy; that is to say, some model of material behavior or structure might be valid at low temperatures, while another model is needed to describe the structure or its behavior at higher temperatures. Category theory provides a general, abstracted approach to classifying mathematical structures across a wide variety of objects, and states of those objects. This quality makes it an exceptional tool for tying together the varied forms of structure already outlined, and for serving as a final tier by which the criteria of theoretical equivalence may be enriched.

Categories of materials models may be based on any relevant similarity among a set of models. Categorical equivalence, then, becomes a method of determining the mathematical structure that sets of models may share. As with the other forms of equivalence outlined in this section, the previously described forms we take as necessary for the construction of the criteria of categorical equivalence. Building from the theory up, the mathematical structure of a theory is informed by the definitions of the objects of that theory, the results of experimental analysis of those objects, and the relational capacity of those sets of objects as interpreted through the informational structure of those sets.

Categorical equivalence is a common topic within the literature of philosophy of science, and thereby many criteria of categorical equivalence have been proposed. One such criterion proposed by JO Weatherall [78] holds that the categories made up of the models of a theory are equivalent if the "*functors realizing that equivalence preserve empirical content*" [79, p. 427]. Put another way, if the models of a theory are taken as the objects of a category, wherein the morphisms of that category are maps which preserve some sense of the structure of the models, then two categories of models are equivalent if both the mathematical and empirical structure of the categories are translatable up to isomorphism [79].

Coming from an abstract mathematics approach, there is no set prescription for what the empirical content, or its structure, may be. Yet, in many instances from materials models the content of experiments of a given theory are explicit, and the mathematical structure of the empirical data sets are rather loose, but bounded by the efficacy ranges of the models set upon those data sets. This bounded relationality informs how we model the physical arrangements, and behaviors of materials systems, both characteristics that produce information in the various forms of informational entropy. What these pre-existing approaches to materials modeling mean is that within the context of building a relational interpretation of materials structure, we may require that the criteria used to determine equivalence for categories of materials models are necessarily definitionally, empirically, *and* informationally equivalent.

While informational equivalence is a new formal requirement in the context of the literature of theoretical equivalence, it fits well within the framework, given that data sets and relations between data sets produce various measures of information which dictate how and how well the relations between these objects may be understood. Indeed, if we take it to be true that the objects of our interest at each step of criteria construction are simply nodes of relation, then we might say that "*the arrows carry all the information*" [79, p. 437]. If that is the case, the effect of variation of information on the mathematical structure of the models must surely follow.

Taking all of this into account, we propose that categories of materials models are constituted as follows:

Definition 8: A category of materials models, $\mathcal{C}_{\mathrm{Mat}}$, is composed of:

- A collection of objects, $\mathcal{O}_{\mathrm{Mod}}$, which are materials models of a given theory;
- A collection of morphisms, C_{con}, which are structure-preserving arrows (conversions) between the models;
- For every morphism f in C_{con}, a relevant domain set (source of morphism) $\{s(f)\}$ and codomain set (target of morphism) $\{t(f)\}$ of allowed transitions for the given models;
- A composition function for the morphisms of C_{con}, where, given morphisms f and g for a given domain and codomain, $g \circ f$ is their composite; and
- For every object $m \in \mathcal{O}_{Mod}$, an identity function id_m.

The elements of this category satisfy two axioms, those of 1) associativity, and 2) identity, stating that:

1. For models m_1, m_2, m_3, and m_4, and morphisms f, g, and h, if $f: m_1 \rightarrow m_2$, $g: m_2 \rightarrow m_3$, and $h: m_3 \rightarrow m_4$, then $f \circ (g \circ h) = (f \circ g) \circ h$.
2. For every object m, there is a function $id_m: m \rightarrow m$ called the identity function, where if a morphism $f: m_1 \rightarrow m_2$ exists then it follows that $id_{m1} \circ f = f = f \circ id_{m2}$.

The category $\mathcal{C}_{\text{Mat}}$ can contain models of similar physical objects, particular materials, or types of properties / behaviors which arise in the normal conduct of MSE practitioners. Using this form of the category, we may then propose criteria for determining the equivalence of these categories. We take the previously outline definitional, empirical, and informational equivalence criteria as necessary prerequisites for categorical equivalence, and propose that:

Definition 9 (olog Figure B.3**):** Given two categories of materials models, $\mathcal{C}_{\text{Mat-1}}$ and $\mathcal{C}_{\text{Mat-2}}$,
and $mod_{Mat-1} \in \mathcal{C}_{Mat-1}$ and $mod_{Mat-2} \in \mathcal{C}_{Mat-2}$
there exists a categorical equivalence
$\exists \mathcal{C}_{Mat-1} \Leftrightarrow_C \mathcal{C}_{Mat-2}$ if
$\exists f_{Mat}: mod_{Mat-1a} \rightarrow mod_{Mat-1b}$ and
$\exists g_{Mat}: mod_{Mat-2a} \rightarrow mod_{Mat-2b}$
such that $F \Leftrightarrow_{D,E,I} G$ up to isomorphism

This approach allows for the internal structure of the models as proposed to be preserved, via the excess structural requirements of the other forms of equivalence. This construction is also malleable enough that, as is the case with nearly every scientific theory, as new data and iterations upon existing models is input into the framework, the categories composed of them may be easily adapted to these changes without the necessity of completely replacing the proposed equivalence criteria. While those outlined above may be weak categories in a completed, mathematical sense, (weak being indicative of the category being more general, not lacking in some manner) they are sufficient to capture the variety of knowledge produced by the wide range of approaches to solving *materials problems*.

3.5: Theoretical Equivalence

The whole of the framework being constructed in this section is in the service of determining when, how, and to what extent, any proposed theory of materials may be equivalent. As stated, a framework of equivalence criteria is an effective method of structure determination because, as no 'real' object may gain properties or effect change in isolation, the structure of an object is only discernible in juxtaposition with another. Equivalence criteria illustrate how various senses of objects gain structure at every step of the construction of theories regarding those structures.

Theories exist prior to, and at each stage of this process. Therefore, theoretical equivalence is not measured in the same manner as the other forms of equivalence presented thus far, but is, rather, an assemblage of the other forms of structure, which is measured via the equivalence framework presented. A pair of theories may gain relatively weak equivalence on the sole basis of some definitional transition, whereas theories which produce all four forms of equivalence are relatively strongly equivalent to one another. None of the non-theoretical forms of equivalence are strictly necessary to declaring equivalence between two theories, but the structure added from adherence to each criteria strengthens the sense in which two theories may be equivalent. Table 1 illustrates this point for definitional ($\Leftrightarrow_D$), empirical ($\Leftrightarrow_E$), informational ($\Leftrightarrow_I$), categorical ($\Leftrightarrow_C$), and theoretical equivalence ($\Leftrightarrow_T$):

Table 1: A table, read L to R across each row, showing whether each defined form of equivalence is necessary (n) for another form of equivalence, or if it is merely informative (i) to that form.

	$\Leftrightarrow_D$	$\Leftrightarrow_E$	$\Leftrightarrow_I$	$\Leftrightarrow_C$	$\Leftrightarrow_T$
$\Leftrightarrow_D$	—	n	n	n	i
$\Leftrightarrow_E$	i	—	n	n	i
$\Leftrightarrow_I$	i	i	—	n	i
$\Leftrightarrow_C$	i	i	i	—	i
$\Leftrightarrow_T$	n	n	n	n	—

Theoretical equivalence is necessary for every other form, because each step in the structuring of a theory and its models necessitates a theory upon which to build. As each subsequent form of equivalence is expanded upon, the previous form becomes a necessary criterion of the next, while the new form is—through iteration—able to inform any changes in the criteria of the nested forms of equivalence. The ebb and flow of communication through the various forms of structuring shown here allow for the richest and most thorough analysis of models of materials theories.

In using four different forms of equivalence criteria, a "bestiary" of approaches to strengthening theoretical equivalence is formed and, in the process, the best approach to the new conception of material structure outlined in the background [79]. The sum of all equivalence criteria allows for comparison, contrast, and validation of materials theories at a variety of important levels, all of which build a framework capable of adaptation to a wide range of contexts within materials science, at whatever relative strength a theory, old or new, may possess. Theories, via their models, may also be analyzed for degrees of equivalence, illustrating where overlap between theories may occur, and adding to a burgeoning network of vetted materials knowledge.

The combination of all of these criteria of equivalences is, itself, a set of criteria; the structural equivalence framework. The ontology of MSE that has been outlined in this thesis offers new insight into how the senses of structure present throughout the practice and modeling of materials science are able to be synthesized, and the criteria of a holistic structural equivalence follows closely. Using this method allows for many aspects of materials to be analyzed in a way that permits faster, more direct comparison in future analyses as more aspects of more systems are expressed in terms of the central framework.

This approach is intended for use from any starting point within materials science. MSE is the study of structures and, through the construction of a means to test the equivalence of structures across multiple senses of materials modeling, this method of comparison via a framework of forms of equivalence is a rich tool for this study. In the next section, we explore the various use cases of such a framework in a materials context, looking at structuring processes of scales, states, models, and variables in a number of examples.

Chapter 4

Results and Discussion

You've never been out of college! You don't know what it's like out there!
I've WORKED in the private sector. They expect ***results****.*
—Dr. Raymond Stantz, “Ghostbusters”

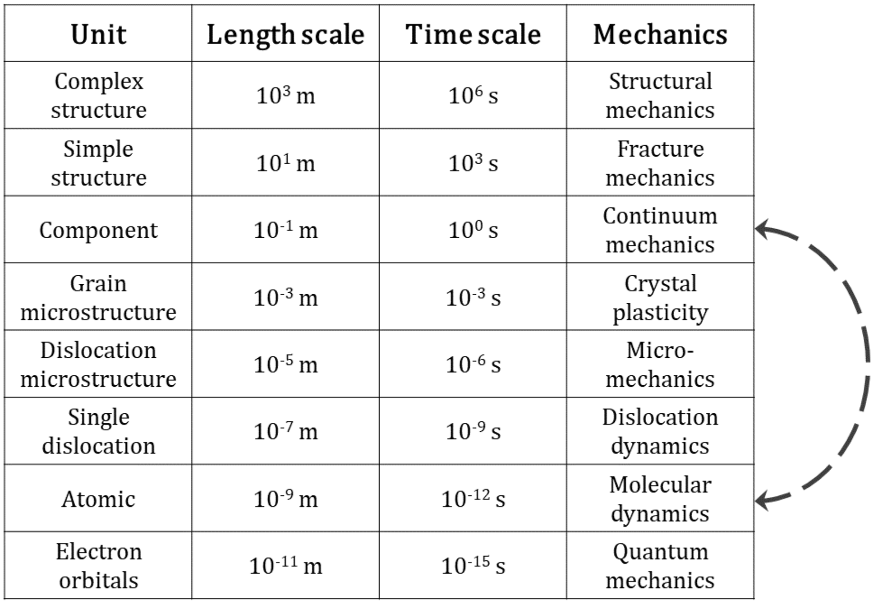
Equivalence criteria elucidate structure by providing the rules for determining when and how the relational quantities between objects in a system change as a system undergoes some evolution. Looking at the invariants of materials models through these evolutions invokes exactly the holistic sense of material structure that fits the variety of approaches with which an MSE practitioner explores material systems. Every entry point to the science of materials deals with some form of structure, be it a measurable variable, a mechanism, a state change of a system, or of some multiscalar phenomenon. For each approach, identifying and classifying structure and then adding to knowledge of particular materials systems, or classes of materials, is paramount.

In order to use this method on pre-existing bodies of research, or theories, two or more systems must first be chosen, isolating some object of overlap between them—for instance where some objects of two theories share qualitative definitional equivalence—and determining the extent of structural equivalence between the systems. The object for this method can be any thing of which there are defined properties within a materials theory. As the descriptions of materials systems within MSE consist of numerous overlapping theories, a framework of determining structural equivalence as defined here is wide-reaching and effective. At every point of a materials system, from the element(s) which comprise the atomistic structure, to the models of plasticity predicting the evolution of defect structures, to the macroscale behavior of material objects leading to the damage and / or failure of components, materials systems inhabit different physics, scales of energy, and interpretations of data and models. In order to illustrate the efficacy of the proposed program, four different problems within materials science are analyzed using the structural equivalence framework, and the results of each application are discussed.

4.1: Multiscale Models

The full picture of any material is not captured by phenomena of a single length scale. Rather, a key component of materials is that interlinking, multiscale phenomena are integral to the understanding of macroscale material behavior. Linking the physical models at different length and time scales of a materials system is, therefore, paramount to improving the predictability of holistic materials models, which implies that models relating those tested within certain scales must be constructed. The interfaces at the bounds of scales are known as 'bridging' models, and are essential to creating linked, multiscale models [15]. The objects being bridged are different theories adhering to a specific scale of length. They are not only descriptions of different portions of the same system, but constitutive interfaces, wherein one theory fully describes the objects which make up the basic units of the other. Atomic theory begets molecular theory which begets microstructural theories, so on and so on. These theories have massive conceptual overlap, and are causally affective in relation to one another. This relationship means that, as is commonly assumed in practice, the terminal objects of each congruent theory are equivalent at the boundaries of their theories.

Because the separations of a material object into scales are subjective, any scale of length or time can be compared to another on the basis of their structure, and therefore their structural equivalences. Figure 11 below shows a version of Figure 6 illustrating the two scales of the materials hierarchy discussed in this section:



Unit	Length scale	Time scale	Mechanics
Complex structure	10^3 m	10^6 s	Structural mechanics
Simple structure	10^1 m	10^3 s	Fracture mechanics
Component	10^{-1} m	10^0 s	Continuum mechanics
Grain microstructure	10^{-3} m	10^{-3} s	Crystal plasticity
Dislocation microstructure	10^{-5} m	10^{-6} s	Micro-mechanics
Single dislocation	10^{-7} m	10^{-9} s	Dislocation dynamics
Atomic	10^{-9} m	10^{-12} s	Molecular dynamics
Electron orbitals	10^{-11} m	10^{-15} s	Quantum mechanics

Figure 11: The various scales and mechanics of materials science [14]. The arrow represents the connection between the two scales being discussed in this section.

As the figure illustrates, it may be theorized that the models at each scale are connected in some manner, and therefore capable of being analyzed using the structural framework proposed herein. A particularly rich vein of analysis occurs between atomistic models, represented generally by molecular dynamics (MD), and microscale mechanics, which can be modeled using various finite element (FE) models. Many existing bridging models have been created expressly to provide this specific connection [80], in order to solve materials problems as diverse as nanostructure mechanics, polymer-composite interfaces [81], crack propagation [82], [83] and damage mechanics in ceramics [84].

The MD method involves applying classical Newtonian forces to collections of individual atoms, and then using the resulting motion of the atoms to calculate various properties of the MD system [14]. When the atoms get close enough to interact in the simulation, the interaction force between the particles of an MD simulation is typically modeled through some selected pair potential, such as the Lennard-Jones potential, the Mie potential, of the embedded-atom model potential [14]. Measurement of the resultant arrangement of the particles at the desired time step,

δt, can then be used to analyze various formations within a simulated system—defects such as dislocations and grain boundaries—as well as properties of that system.

Larger scale phenomena often deal with continuous segments of materials, and are often analyzed using various FE techniques. FE analyses are numerical methods which involve breaking down some continuum into a finite number of smaller elements (usually of some known geometric shape), and then analyzing equilibrium criteria at the boundaries of each element relative to the nodes of adjacent elements, as the system is iterated through some process. The criteria for analysis can be across a variety of domains, including stiffness, heat conduction, fluid flow, and electrostatics [85].

These two simulation techniques are often used to represent various aspects of materials, and can be thought of as models *pertaining to* materials theories. Therefore, both models may be analyzed via means of ascertaining the structural equivalence, and the analysis would be applicable to any example of the two methods being bridged. In order to illustrate this point, the structural elements of both methods are drawn out in the subsequent sections. This approach demonstrates how models, or other objects, should be analyzed in a structural equivalence framework to look for the necessary elements that a valid translation between the two ought to possess. In order to determine the equivalence forms of both MD and FE methods, we begin by looking at the basic framework of both models.

4.1.1: Structuring Elements of Molecular Dynamics Models

The basic building blocks of MD are particles, or atoms, represented by a mass (m_i), a position (r_i), and a velocity (v_i). A simulation using MD will often involve a set volume (V) which is populated by a set number (N) of atoms. If a particular substance is being modeled, say a metal, then each atom within the volume will be set to occupy a lattice site within the given metal's crystal structure, and a mass assigned to each. Analyzing the system as it changes in time using Newton's equations of motion gives the basic form for the motion of an atom as:

$$\frac{d^2\boldsymbol{r}_i}{dt^2} = \frac{1}{m_i}\boldsymbol{F_i} = \frac{1}{m_i}\sum_{j\neq i}\boldsymbol{f_{ij}}(r_{ij}) \tag{16}$$

where $\boldsymbol{F_i}$ is the force on an atom, $\boldsymbol{f_{ij}}$ is the force of the i-th atom on j-th atom, and r_{ij} is the distance between the two. This model is the basic form of what is calculated for every time step of a run [12].

For an MD simulation of a given time step δt [s], the basic equations for the change in velocity and position for an atom is given by (17) and (18) respectively:

$$\boldsymbol{v_i}(t + \delta t) = \boldsymbol{v_i}(t) + \boldsymbol{a_i}(t)\delta t \tag{17}$$

$$\boldsymbol{r_i}(t + \delta t) = \boldsymbol{r_i}(t) + \boldsymbol{v_i}(t)\delta t + \frac{1}{2}\boldsymbol{a_i}(t)\delta t^2 \tag{18}$$

where $\boldsymbol{a_i}$ is the acceleration of the atom, assumed along with the force to be constant from time t to time $(t + \delta t)$ [14].

In addition to positions and mass, simulations will often use an interaction potential specifically conceived for the class of materials being simulated. This section is primarily focused on the general form of the molecular dynamics method, so we will use the classic Lennard-Jones potential to look at the structure of the model, but any potential model could be used in a future analysis. The Lennard-Jones potential (φ_{LJ}, [eV]) between two interacting atoms a_i and a_j, is generally rendered as:

$$\varphi(r_{ij}) = 4\epsilon\left[\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^{6}\right] \tag{19}$$

where r_{ij} [Å] is the distance between a_i and a_j, ϵ [eV] is the absolute value of the minimum of the potential, and σ [Å] is the distance at with the potential is zero. Often, this potential and resultant force equation will be normalized by ϵ and σ in order to simplify the calculation, and a standard cut-off value surrounding any atom is $r_c = 2.5\sigma$ [14].

Once these parameters are set, the MD simulation will apply a force of some variety to the constructed model and solve Newton's equations of motion for each atom within the volume for each time step *δt*. After each time step, the new positions and velocities for each atom, a_i, can then be used to calculate other properties [14].

Due to inaccuracies that arise in the numerical integration of Newton's equations after large numbers of time steps, various algorithms are used as correctives, including the Verlet algorithm [14]. Using this algorithm on a generic molecular dynamics model gives an updated estimate of velocity for each atom as a function of both the forward $\boldsymbol{r_i}(t + \delta t)$ and backward $\boldsymbol{r_i}(t - \delta t)$ position change, with:

$$\boldsymbol{v_i}(t) = \frac{\boldsymbol{r_i}(t+\delta t) - \boldsymbol{r_i}(t-\delta t)}{2\delta t} \tag{20}$$

Using this velocity, various thermodynamic properties of the system may be calculated including the potential energy *U* (21), the kinetic energy *K* (22), the Hamiltonian $\mathcal{H}$ (23) representing the total internal energy of the system, the instantaneous temperature *Θ(t)* (24), and the average temperature $\langle T \rangle$ (25) and pressure $\langle P \rangle$ (26).

$$U(r^N) = \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}\varphi_{ij}(r_{ij}) \tag{21}$$

$$K = \frac{1}{2}\sum_i m_i v_i^2 \tag{22}$$

$$\mathcal{H}(p^N, r^N) = K(p^N) + U(r^N) \tag{23}$$

$$\Theta(t) = \frac{2K(t)}{3Nk_b} \tag{24}$$

$$\langle T \rangle = \frac{\langle K \rangle}{3Nk_b} \tag{25}$$

$$\langle P \rangle = \frac{N}{V}k_b\langle T \rangle - \frac{1}{3V}\langle \sum_{i=1}^{N} r_i \cdot \nabla_i U \rangle \tag{26}$$

A general MD system is often presented as a microcanonical ensemble (NVE), and so it will also have a boundary condition wherein energy is conserved, and—for those with periodic boundary conditions—momentum is conserved [14]. Given these building blocks, we may now ask what the structures used to create an equivalence criterion for MD might look like.

In order to define a definitional structure of MD, a signature $\Sigma_{\text{def(MD)}}$ is chosen to represent the vocabulary of the method. MD typically operates in a three-dimensional Cartesian space, so much of the vocabulary of this method will be adaptations of physical parameters within that framework. While, again, we do not strictly adhere to the axiomatization rules of first-order logic, we take inspiration from work used to apply them to relativistic frameworks in [86], [87], [88].

As a reminder, the signature of a model consists of the relational Rel($\Sigma_{\text{def(MD)}}$), functional Func($\Sigma_{\text{def(MD)}}$), and constant Const($\Sigma_{\text{def(MD)}}$) definitions for the vocabulary of a model. For MD, we define these sets for some set of arbitrary (in this context) variables $\{x, y, z \in X\}$ as follows:

- Rel($\Sigma_{\text{def(MD)}}$) has as elements:
    - Bodies, B(x), of which atoms, At(x), are a subset, both unary relations.
    - Quantities, Q(x) a unary relation
    - <, a binary ordering relation
    - Ca(x, y), a binary Cartesian relation
- Func($\Sigma_{\text{def(MD)}}$) has as elements:
    - $+ / \circ$, binary function symbols for operations
    - T(x, y), a binary time function
    - M(x), a unary mass function
- Const($\Sigma_{\text{def(MD)}}$) has as elements:
    - Or^d, the origin of the simulated volume with *d* number of coordinates
    - δt, a time step

Using this signature $\Sigma_{\text{def(MD)}}$, as the basic definitional structure of the model, all of the other objects of MD can be constructed within definitional models $S_{def(MD)}$, defined as:

$$\langle S; B, At, Q, +, \circ, <, Ca, T, M \rangle \tag{27}$$

The atoms of a simulation, $At(x) \subset B(x)$, define the primary bodies of the simulation. The space in which those relations are defined is a quantity Q^d, where d is the dimension of our space, and elements such as $p \in Q^d$ may also be defined as d-tuples where $p = \langle p_1, p_2, \ldots, p_d \rangle$. For MD, $d=3$ and the coordinate system is defined as a volume in only positive regions, $Q^{3+}(Or^3)$. Given a linearly ordered field, the field operations for this space are the set {0, 1, -, /, √}, and a vector-space can be constructed using Q^n (for any n-tuples of quantities) and, for any $p, q \in Q^n$ and $\lambda \in Q$ (where λ is a scalar), the set $\{p+q, -p, \lambda p\} \in Q^n$ [86].

This vector-space can then be used to construct the velocity vector definitions for the Cartesian simulation space, for the atoms of the simulation $At(x)$. For each $At(x)$, there is a relation $Ca(p_i, Or^3)$ that defines where a spatial component of an element $x \in Q^3$, p_x, is relative to the constant representing the origin. This property of the signature allows for the length of the vector to be defined for any set of $\{p_i, q_i\} \in Q^3$ as:

$$|p_i q_i| := \sqrt{\sum_{i=1}^{n} (q_i^2 - p_i^2)} \tag{28}$$

and the direction of the vector to be defined by the ordering relation, <, relating any two of the time function for p and q where $T(p, \delta t) < T(q, \delta t)$.

The velocity of an element $At(x)$ is also defined by quantities p and q, where for those quantities relative to element x, the velocity $\boldsymbol{v_x}$, is defined as:

$$\boldsymbol{v_x} := \frac{|Ca(q_x, Or^3) - Ca(p_x, Or^3)|}{|T(q_x, \delta t) - T(p_x, \delta t)|} \tag{29}$$

The position and velocity of any atom within an MD simulation are the bedrock definitional variables through which any of the thermodynamic variables, and other properties, may be derived. The definitional structure, as captured in the signature $\Sigma_{\text{def(MD)}}$ should then contain all of the necessary components for that derivation, although further work should be done to express the full breadth of the theory in the same near-first-order logic used here.

With definitions in hand, the next set of criteria is based around the empirical structure of the MD theory. As illustrated in section 3.2, the empirical structure is constructed by obtaining a set of empirical data, unitized through a multirelation on the empirical relations of a model and the powerset of units, standard and derived. The empirical relations of MD models are not directly experimental in this context—though it is not uncommon for empirical models of pair potentials to be used [89] within an MD simulation—but rather we assume the results produced by a simulation as representational of the empirical data sets of the model.

Then, it follows that the raw empirical results of an MD simulation are, as has been shown, sets of time-evolved position ($\boldsymbol{r_i}$) and velocity ($\boldsymbol{v_i}$) measurements, $e_{MD} = \{\boldsymbol{r_i}, \boldsymbol{v_i}\}$. These results themselves are structured by the models used in their calculation, mainly in equations (18) and (20) describing the evolution of the position and velocity of an atom within an MD simulation. The time-step relations are the first maps included in the set of empirical relations, $\{Em_{MD}\}$. The thermodynamic relations, along with those which derive other properties from e_{MD}, are also included within $\{Em_{MD}\}$, so that any structuring process of the basis of the initial empirical data sets can also be used for building empirical equivalence criteria for these parameters.

Another relation within the empirical set, which is key to the creation of equivalence criteria, is that of assigning units. As stated in section 3.2, these relations rel_u are taken to be multirelations where any given empirical relation em_i carries with it the units from the powerset of units both measured and derived from the set of base SI units [90], shown in Definition 5. In an MD simulation, the basic relations are time-step calculations of position and velocity evolutions, so we could take the isolated unit relation $rel_u(em_{MD(i)})$ as:

$$r_{i(u)}\left(em_{MD(i)}\right) \colon [L] \rightarrow [L] \tag{30}$$

$$v_{i(u)}\left(em_{MD(i)}\right) \colon [LT^{-1}] \rightarrow [LT^{-1}] \tag{31}$$

where L and T are some unit of length and time, respectively. The structure of the empirical data set of an MD experiment is then, simply, the relations which hold for a particular model being simulated, in terms of the evolution of the state (r) and vector (v) spaces of the system, along with the requirement for carrying units.

The elements of the empirical structures of an MD experiment may then serve as the basis for an informational structuring. Recall from section 3.3 that information derived from sets of empirical data carry the structure for ascertaining the interaction capabilities, and structuring potential, of a system. The criteria informed by Shannon entropy structures any potential data channel between two interacting systems, carrying forward the boundedness of the "source" set of random variables, while the criteria informed by relational entropy structures any potential state space evolution of a system with data related to different states of that system.

The information of each reviewed information model is a probability measure, meaning that the sets of MD data measuring the probability of some outcome of interaction will be a set of probabilities, bound to specific sets of values on the basis of the validity bounds of the empirical models used to produce the probability distributions analyzed. For a simple MD model, this approach could measure the information produced by some finite number of time steps by way of the average velocity v of the atoms within the system, and no other bounds, as:

$$H(\boldsymbol{v}) = -\Sigma p(\boldsymbol{v})\ log_2(\boldsymbol{v}) \tag{32}$$

This information criterion could, on the other hand, account for some restriction on the simulation, such as 'the system being modeled must be in the solid state,' necessitating a potential restriction of the MD model to ensure that the temperature of the simulation always falls within (0 K to T_M) for the system being modeled. This approach would ensure that the only valid information content related to the measured system corresponds to the random velocities able to be produced within the given temperature range for the system. All this to say that the structure of the information criteria is wholly dependent on the 'design of experiment' that produces the data sets being analyzed.

This characteristic is also true for the relative entropy within a system. When using the relative entropy as a measure for the potential state evolutions of a system, it is also paramount to check the 'experimental' boundary conditions $\{B_i\}$ that produced the data correlating to the related states. If, in a particular MD simulation, the evolution of defect structures as a function of temperature is being measured, then perhaps the max. / min. temperature and the max. / min. dislocation density (ρ) might serve as the bounds for the data set to be analyzed. Then, the set of relative entropy values for this experiment from some temperature range (T_0, T_i) might be modeled as:

$$K(\rho(T_i)\|\rho(T_0)) = -\Sigma\rho(T_i)\log\frac{\rho(T_i)}{\rho(T_0)} \tag{33}$$

with as many temperature increments in that range as desired, and the random dislocation density measured at each. The experimental data upon which the probability distributions are based, structure the sets of information-bearing probabilities.

All of the forms of structure heretofore then further inform the mathematical structure of the models of a given theory. Having elucidated the forms of the models produced within an MD approach, we can now create a category of MD models, $\mathcal{C}_{\mathrm{MD}}$. Following section 3.4, we define $\mathcal{C}_{\mathrm{MD}}$ as the collection of models (objects) of MD, meaning $\{\{\Sigma_{\mathrm{def(MD)}}\}, \{E_{MD}\}, \{I_{MD}\}\}$, and the morphisms $C_{con(MD)}$ between elements of those sets—the relations established in the preceding text. The set of models are then further structured with composition and identity requirements, and the basic categorical structure of the theory of MD is thus set.

While further specifications based on the particular parameters of an MD simulation could be set, we take the elements described as the basic structure of the theory. These elements are summarized in Table 2 below:

Table 2: A summary of the structuring elements to be used as equivalence criteria, derived for the theory of Molecular Dynamics (MD).

Theory of Molecular Dynamics (MD)

Form of Criterion	Objects	Relations	Boundaries
Definitional	$\Sigma_{def(MD)}$; $S_{def(MD)}$	$Rel(\Sigma_{def(MD)})$; $Func(\Sigma_{def(MD)})$; $Const(\Sigma_{def(MD)})$	N/A
Empirical	$\{e_{MD}\} \in E_{MD}$	$Em_{MD}: \{em_{MD(i)}\} \leftrightarrow 2^{\{U\}}$	State variable boundaries; Units
Informational	$H(e_{MD(i)})$; $K(e_{MD(i)} \Vert e_{MD(0)})$	$H(e_{MD})_{[B1 \text{ to } B2]}$ $K(e_{MD})_{[B1 \text{ to } B2]}$	Empirical model boundaries
Categorical	$\mathcal{C}_{MD}$	$C_{con(MD)}$	Empirical model boundaries

This table provides all the structure necessary for the construction of translations from MD to another theory, and thereby the criteria for determination of the equivalence of another theory to MD.

4.1.2: Structuring Elements of Finite Element Models

The basic building blocks of FE methods are elements of some geometric variety, discretized from some object with a continuous surface or volume. The object of analysis could be almost any variety of object, across variations in geometry, material type, or use. The method is commonly used to solve so-called “field problems,” or problems where the values of some dependent variables are known at the boundary of an element, and must be solved for in the remainder of the physical domain of the element [91].

Finite element approaches solve—for every element—a problem where some type of externally applied forces, $\boldsymbol{f_i}$, are transmitted through a matrix, $\boldsymbol{K_{ij}}$, of relational variables dependent on the type of problem, to solve for some general manner of displacement, $\boldsymbol{u}_j$, at the nodes of the elements, as shown below:

$$\boldsymbol{K_{ij}} \cdot \boldsymbol{u_j} = \boldsymbol{f_i} \tag{34}$$

Note, the displacement $\boldsymbol{u}_j$ is not related to the length displacement of deformation, though that is a problem common to FE analysis, but here is meant only as a general displacement relative to the field of interest. This calculation can also be done in reverse, where the displacement is known and the goal is to solve for the applied external forces, or stiffness matrix [92].

At the boundaries between elements, the equations describing the field of a particular variable must be equal, so at the heart of FE is a process of solving partial differential equations (PDEs) for these boundaries. This process is accomplished by creating equations that pair various 'shape,' or 'interpolation' functions, $\{N_i\}$, with an approximated function representing the field variables being modeled, $\tilde{\boldsymbol{u}}(x, y)$ [92]. As FE is also a numerical solution to a set of analytical equations, $\tilde{\boldsymbol{u}}(x, y)$ is an approximation because the exact solutions to the PDEs are not easily solved.

Interpolation functions are generally polynomial functions of some degree, intended to relate the unknown quantities within the body of the element to the known quantities of the associated nodes of that element [93]. These functions are similarly bound depending on which node is being analyzed, where for some index j, N_j approaches unity at node j and approaches 0 at the other nodes of the same element [92], and two common types of functions used for this application are Lagrange and linear polynomials [93].

When the set of displacements $\{\boldsymbol{u}\}$ are unknown, the form of the solution is a functional $\chi(u)$, given by equation (35) as:

$$\chi(u) = \int\limits_{v} f\left(\{u\}, \frac{\partial\{u\}}{\partial \boldsymbol{r}}, \dots\right) dv + \int\limits_{s} g\left(\{u\}, \frac{\partial\{u\}}{\partial \boldsymbol{r}}, \dots\right) ds \tag{35}$$

where *v* and *s*, are the volume and surface of an element, *f* and *g* are functions of them, respectively, and ***r*** are coordinatized position vectors [93]. As previously stated, FE problems are solved by assumptions of boundary conditions, one of which is the minimization of $\chi(u)$, also known as the "principle of minimum potential energy" [85, p. 113], where:

$$\frac{\partial\chi(u)}{\partial\{u\}} = \begin{Bmatrix} \frac{\partial\chi}{\partial u_1} \\ \frac{\partial\chi}{\partial u_2} \\ \vdots \end{Bmatrix} = 0 \tag{36}$$

Solving this equation illustrates the equilibrium state of the system based on the field being studied, and the type, number, and distribution of the elements chosen [93].

The sets of displacements are, again, often known at the nodes (*n*) and unknown in the continuum (*c*) of the element itself, so $\{u\}$ can be broken down into two subsets, $\{u\}^c$ and $\{u\}^n$. Equation (34) above, with a matrix of various shape functions (N_i), can then be reformulated as (37), with conditions (38) and (39):

$$\{u\}^c = [N]\{u\}^n \tag{37}$$

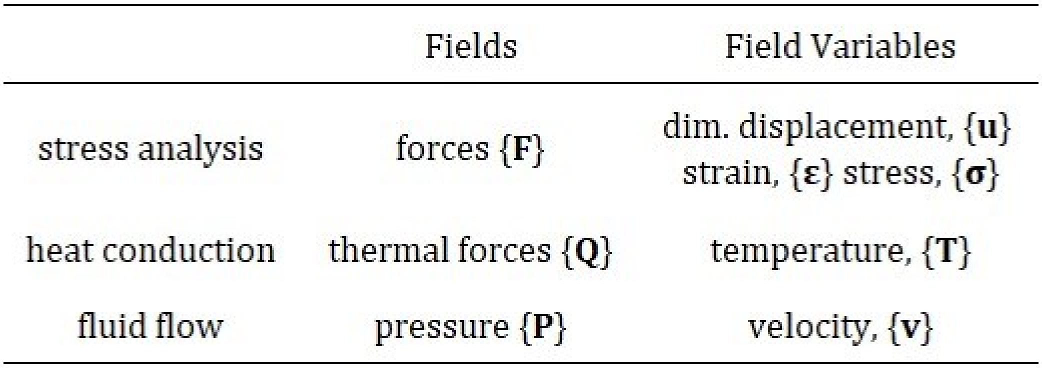
$$\chi(u) = \Sigma\chi^e(u) \tag{38}$$

$$\frac{\partial\chi(u)}{\partial\{u\}} = \Sigma\frac{\partial\chi^e(u)}{\partial\{u\}^e} = 0 \tag{39}$$

where the superscript *e* represents a single element of the analysis [93].

Once the set of element equations has been derived for the set of elements to be analyzed, they are all assembled in order to create the subsequent set of field equations for the problem. This analysis can be performed for a variety of scientific and engineering contexts, a survey of which is provided below in Table 3.

Table 3: A short survey of areas in which FE analysis can be performed, characterized by their representative fields and field variables, adapted from [93].



	Fields	Field Variables
stress analysis	forces $\{\mathbf{F}\}$	dim. displacement, $\{\mathbf{u}\}$ strain, $\{\boldsymbol{\varepsilon}\}$ stress, $\{\boldsymbol{\sigma}\}$
heat conduction	thermal forces $\{\mathbf{Q}\}$	temperature, $\{\mathbf{T}\}$
fluid flow	pressure $\{\mathbf{P}\}$	velocity, $\{\mathbf{v}\}$

Each element is situated within the wider coordinate system of the object that has been discretized, so equations at nodes, boundaries, and within the body of an element may be constructed. For the entire structure of the object, the sets of equations have the general form:

$$[K]\{\boldsymbol{q}\} = \{\boldsymbol{R}\} \tag{40}$$

where $[K]$ is known as the global “stiffness” matrix, and is a function of the interpolation functions, $\{q\}$ represents the vectors of the unknown quantities at the nodes, and $\{R\}$ is the set of vectors representing known parameters resulting from the applied field, a function of a given field’s dispersion to the nodes of an element [93]. The global stiffness matrix $[K]$ is the sum of the individual stiffness matrices of the elements, or:

$$[K] = \sum_{1}^{N} [K_e] \tag{41}$$

where N is the total number of elements in a given analysis. Solving this global set of equations for $\{\boldsymbol{q}\}$ is often accomplished through various algorithms used for solving systems of linear equations [93]. Once these equations have been solved, any further derived quantity that is related to, or a function of the elements of $\{\boldsymbol{q}\}$, can also be found on the basis of these results; for example, the strain $\{\boldsymbol{\varepsilon}\}$ or stress $\{\boldsymbol{\sigma}\}$ values resulting from some dimensional displacement (as shown in Table 3). Once all the equations of the discretized elements of an object have been solved, the analysis is complete and the results of it may be interpreted and used for various purposes [93].

The structural analysis of a theory of FE proceeds in much the same manner as that of MD. As with the definitional structure of MD, we choose a signature to represent the definitions of the theory in order to build out a definitional equivalence criterion for FE. The objects of FE, especially those that might be of use in an engineering context, are often three dimensional and made of various materials. An FE simulation, therefore, will also utilize three dimensional Cartesian space. The basic material quantities of FE are variable, because its analysis can—as has been shown—account for various physical properties of an object. FE, as foundationally constituted, is also static; an object and its elements could be cycled through a kinematic event and snapshots of steps within the event taken, but that capacity is not directly embedded within the method.

Setting out the definitional structure, for some set of arbitrary variables $\{x, y, z \in X\}$, the signature of an FE simulation, $\Sigma_{\text{def(FE)}}$, is as follows:

- Rel($\Sigma_{\text{def(FE)}}$) has as elements:
    - Bodies, B(x), of which elements, El(x), are a subset, both unary relations.
    - Quantities, Q(x) a unary relation
    - <, a binary ordering relation
    - G(x), a scaled unary geometry relation
    - Ca(x, y), a binary cartesian relation
- Func($\Sigma_{\text{def(FE)}}$) has as elements:
    - $+ / \circ$, binary function symbols for operations
    - D(x, y, z), an n-ary discretization function
    - N(x, y), a binary interpolation function
    - Am(x, y), a binary counting function
- Const($\Sigma_{\text{def(FE)}}$) has as elements:
    - Or^{d}, the origin of the simulated volume with *d* number of coordinates
    - {G}, a set of known geometries

Echoing the analysis for MD, using this signature $\Sigma_{\mathrm{def(FE)}}$, as the basic definitional structure of the model, all of the other objects of FE can be constructed within the set of definitional models $S_{def(FE)}$, defined as:

$$\langle S; B, El, Q, G, +, \circ, <, Ca, D, N, Am \rangle \tag{42}$$

The primary definitional objects of FE are elements, which are a subset of bodies, $El(x) \subset B(x)$. The elements of an FE simulation are discretized in a particular space, and we construct the definitions in the same manner as an MD simulation, as they both occur in three-dimensional Cartesian space. The objects of space are, therefore, also a quantity Q^d with elements $p \in Q^d$, the coordinate system is defined as a volume in only positive regions, $Q^{3+}(Or^3)$, and with the field operations for this space—the set {0, 1, -, /, √}—a vector-space can be constructed using Q^n where for any $p, q \in Q^n$ and $\lambda \in Q$ (where λ is a scalar), the set $\{p+q, -p, \lambda p\} \in Q^n$ [86].

Defining the object as an initial body, $B(x_0)$, elements may be defined through the discretization function with:

$$El(x_i) := D\big(B(x_0), Ca(p_i, Or^3), G(p_i)\big) \tag{43}$$

Here, the element is defined as being discretized relative to the original body, mapped with respect to the origin in a three-dimensional space, and given a set geometry. Through this operation the nodes and boundaries, along with the surface and volume, of each element may be defined.

Next, with the nodes and boundaries defined, the interpolation functions are defined at any point within the volume of the defined element. Any potential geometric object defined within or across some element, $El(x_i)$, must be definable in terms of a quantity relative to any other part of the element. This interpolation function is defined as:

$$N_{ij} := El(x_i) - El(x_j) \tag{44}$$

where N_{ij} interpolations the element space from some ith to some jth portion of the element.

These interpolation functions provide a pathway between points within the field of interest in the element, but as defined do not carry values for the fields of interest with them. As noted in the name of the theory, the discretization of a continuous body provides *finite* elements and a numerical method of analysis, which is ideal for this treatment as we can define a function which counts values rather than integrating them. This counting function can be defined as:

$$Am(x_{ij}) := N_{ij}\left(Q(x_i) - Q(x_j)\right) \tag{45}$$

which is defined to 'count' the amount of some quantity Q at some variable (here a coordinate) relative to another variable, scaled by the interpolation function connecting the two variables.

These three definitions define the foundational definitional structure of the theory of FE analysis. Using these definitions, every other part of an FE simulation can be derived and used for various applications of the FE method. It is assumed once more that the as-captured signature $\Sigma_{\text{def(FE)}}$ contains all of the necessary components for those and other derivations, but for use in outlining the set of definitional equivalence criteria, these definitions are, again, deemed sufficient.

With the definitional structure of FE theory in place, the empirical data sets of the FE method must be constructed. The data sets of FE include the geometric data on the body being discretized, as well as that of the chosen element geometry. The set also includes any field which may be applied to the elements of a simulation, along with the field variables resulting from that application. Each applied field will have a different multirelation on the set of elements, to account for the difference in units assigned to various points in the element.

The set of empirical relations of FE, $\{em_{FE} \in Em_{FE}\}$, will include those discretizing the volume and surface of the object, as well as spatial relations between points within the coordinate space of the element. Additionally, the set includes all of the interpolation functions selected for a given analysis, and the relations applying a field onto the discretized geometry. The units in each multifunction will rely on the field being used. For example, an analysis of stress states on a body under external loading could have a multirelation of:

$$em_{FE(i)}: \{u_i\} \leftrightarrow \{[L]\} \tag{46}$$

where some empirical relation, for some element point i, carries with it both a set of displacements and some length units, $[L]$.

The empirical structure of FE is, therefore, the set of empirical relations used to discretize the coordinate space of the object, apply a field of interest, and linearize the set of relations formed by the first two steps. These relations must be bound by the same conditions presented in equations (38) and (39) above, and must carry the appropriate set of units through any translation. Any boundary condition of the specific field selected for an FE simulation must also be instituted, e.g., the melting temperature, T_M, for a material being subjected to thermal forces.

The informational structure of FE is similar in construction to that of MD, namely an analysis of the types of information describing the state of the FE system. First, a relation structuring the probabilities of achieving some state of the fields being analyzed across element geometry using $H_{FE}(x_i)$. Then, another relation structuring the relation between established states of a system, $K_{FE}(x_i \parallel x_0)$, that analyzes the probability of some state x_i coming into existence from a starting state of x_0. These information relations are also bound by whatever conditions bind the empirical data sets, in whatever realm of physics is being studied in a given FE simulation.

Naturally, these all feed in to the mathematical structure indicated by the category of FE models, $\mathcal{C}_{\mathrm{FE}}$. The category has, as objects, the set of all FE models defined as $\{\{\Sigma_{\mathrm{def(FE)}}\}, \{E_{FE}\}, \{I_{FE}\}\}$. The category has, rather predictably, as morphisms, the set of conversion relations $C_{con(FE)}$, which consists of those described in each section above. $\mathcal{C}_{\mathrm{FE}}$ is structured with both a composition function, and an identity function, and its models obey their respective boundary conditions. There are, of course, many variations on an FE simulation that could be instituted, but the above is a quick description of the basic structures of the theory. As with the theory of MD, the Table 4 below summarizes these structures for a theory of FE:

Table 4: A summary of the structuring elements to be used as equivalence criteria, derived for the theory of Finite Element (FE) analysis.

Theory of Finite Element (FE) Methods			
Form of Criterion	Objects	Relations	Boundaries
Definitional	$\Sigma_{def(FE)}$; $S_{def(FE)}$	$Rel(\Sigma_{def(FE)})$; $Func(\Sigma_{def(FE)})$; $Const(\Sigma_{def(FE)})$	N/A
Empirical	$\{e_{FE}\} \in E_{FE}$	Em_{FE}: $\{em_{FE(i)}\} \leftrightarrow 2^{\{U\}}$	State variable boundaries; Units
Informational	$H(e_{FE(i)})$; $K(e_{EF(i)} \mid\mid e_{FE(0)})$	$H(e_{FE})_{[B1 \text{ to } B2]}$ $K(e_{FE})_{[B1 \text{ to } B2]}$	Empirical model boundaries
Categorical	$\mathcal{C}_{FE}$	$C_{con(FE)}$	Empirical model boundaries

4.1.3: Translations

Table 2 and Table 4 summarize, abstractly, the structures that have been proposed for models of the theories of MD and FE, respectively. Each criterion of equivalence proposed for both theories is proposed in shape, nimble enough to capture the variety in models of both theories, and strengthening the equitability of each theory as criteria are added. If one were to set out to prove the sense in which a model of MD was equivalent to a model of FE—a not uncommon proposition within MSE—then this work proposes that the equivalence of the models ought to be validated on the basis of the forms of equivalence proposed above.

There are numerous methods that have been proposed for bridging these two specific theories [80] - [83], [94]. This work does not set out to find, or create, a perfect bridging model for multiscale materials methods, but rather to provide a framework through which bridging models could be analyzed and validated. As any particular bridging method is applied to a model linking MD theory with FE theory, it ought to translate from one to the other while maintaining as much of the structure of the theory of the domain of the translation, up to isomorphism.

Figure 12 illustrates this concept via an olog between a representation of MD and one of FE. Table 5 below the figure postulates the form of the translations that would be necessary to establish how, and to what degree, some bridging model would establish equivalence between the theories.

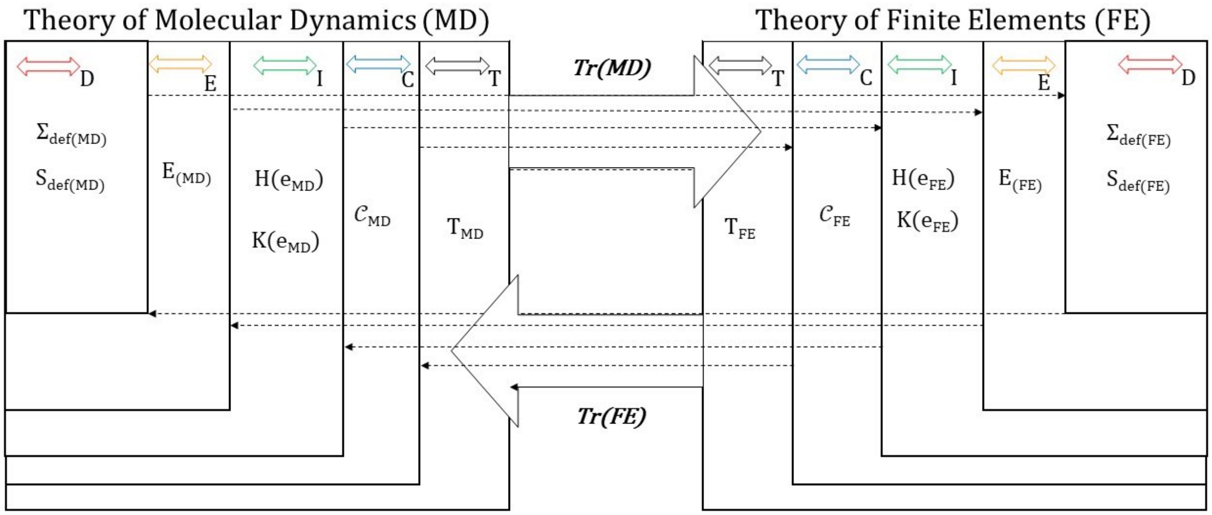


Figure 12: An olog of the translations between MD and FE, and between FE and MD on the basis of their respective equivalence structures.

Table 5: A summary of the abstract translations necessary to validate equivalence between MD and FE models.

Translations Between MD and FE Theories			
Form of Criterion	MD → FE	FE → MD	Boundaries
Definitional	$\Sigma_{def(MD)} \rightarrow \Sigma_{def(FE)}$	$\Sigma_{def(FE)} \rightarrow \Sigma_{def(MD)}$	N/A
Empirical	$E_{MD} \rightarrow E_{FE}$	$E_{FE} \rightarrow E_{MD}$	State variable boundaries; Units
Informational	$H(e_{MD}) \rightarrow H(e_{FE})$; $K(e_{MD}) \rightarrow K(e_{FE})$	$H(e_{FE}) \rightarrow H(e_{MD})$; $K(e_{FE}) \rightarrow K(e_{MD})$	Empirical model boundaries
Categorical	$F: \mathcal{C}_{MD} \rightarrow \mathcal{C}_{FE}$	$G: \mathcal{C}_{FE} \rightarrow \mathcal{C}_{MD}$	Empirical model boundaries

The translations pictured above are the form, and function, of a method of validating equivalence between two theories. In the abstract, any two material theories—any theories—are able to be compared and contrasted in this manner. The specifics of a particular model of a theory may change, the boundary conditions might change, etc., but the approach of structural juxtaposition based on illustration of various forms of structure outlined in the preceding section, will remain consistent.

Now that the most abstract portions of this method of analysis have been demonstrated, other flavors of the application of this framework may also be illustrated. The next section will provide detail on informational structure and equivalences. Specifically, what sort of structures are found in an informational analysis of state change measured by a particular method of characterization of a material, using the X-ray diffraction method.

4.2: State Change Models

Even the most straight-forward techniques of characterization within MSE involve the interaction of phenomena at two length scales, often a micro- or mesoscale being tied to macroscale phenomena. As the body of materials knowledge grows, the effects of various physical components within materials systems on their behavior becomes more complex, occasionally necessitating the re-evaluation of models concerning related materials phenomena. Much like the problem of bridging within multiscale modeling, the calibration of models intended to faithfully recreate empirical results across scales can be difficult and time consuming. The question presented by this intersection of research offers an opportunity for an analysis of the ways in which the structure of models interacts with the empirical data produced by characterization, which is best analyzed through characterization of *information*.

With sets of relations between components of systems, and between systems interacting, information is a natural language for materials systems and materials models are full of informational relationships. As has been shown, an analysis involving various forms of information content deriving from the probabilistic nature of many empirical relations adds necessary structure to theories. The stochastic nature of measured variables, juxtaposed to the deterministic nature of the equations designed to describe the phenomena, provides ample room to investigate signal and noise across various empirical / analytical boundaries. Exactly how quantities of information can be used in analysis of materials systems is a question with, likely, many useful answers, one of which is the determination of when *states* of a system are informationally equivalent, and what that tells us about pertinent structural forms in materials models. This type of analysis is best performed by calculating and assessing values of relative entropy for different states of a material system.

Structural modeling, and studying the behavior of those physical structures, is at the heart of MSE. One of the classic characterization methods used to determine various aspects of physical structure in materials is X-ray Diffraction (XRD). XRD has been used to study an enormous swath of materials, and can measure the degree of crystallinity of a sample, the lattice parameter of crystals, and the phases present within the sample, among other things. By bombarding the sample being measured with x-rays of a known wavelength, at specific angles of incidence, these measurements can be calculated based on the resultant intensities of x-rays diffracted by the material. Diffraction is described by well-known empirical relations, including Bragg's Law and the Laue equations. XRD also produces patterns with well-known analytical methods, representative of the structure of the material [95].

One common method of representing XRD data is by plottingthe intensity of the diffracted beam, I [a.u.], versus the diffraction angle 2θ [°]. Various structures will have different possible sets of reflection planes, based on satisfying Bragg’s Law, that can help to identify specific materials via the intensity peaks being measured at specific diffraction angles [13]. These peaks, given a completely static environment, would be straight lines indicating the precise angle where diffraction may occur, but in practice there are a number of deviatory factors including grain size, strain, temperature, and instrumental effects which lead to the broadening of the peaks in measured XRD patterns. Other factors such as absorption, texture, polarization, and temperature can affect the intensity and location of the peaks of a diffraction pattern [95].

Using the equivalence criteria framework, the variety of results obtained via XRD characterization can be analyzed for elements of the forms of structure outlined herein.

Specifically, we wish to look at the variations produced in XRD patterns in copper metal samples to show the information content in the form of the relative entropy shift produced by varying independent variables which cause peak shifting, namely changes in temperature [*T*] and percent reduction [*%red*], due to cold-working—deformation of a metal at low (~ < 0.4T_M) temperatures. The data produced by this method must first be turned into probability distributions of the resultant intensity data, then the shift in the discrete probability distributions produced by the peak shifting experiments may be quantified. This analysis is applicable to any set of data, of any characterization technique, with some random variable able to be rendered in probability distributions.

The relative entropy, as shown in equation (15), is in this context a quantification of the variance of an empirical model, or the increase in the number of informational states available, relative to some reference state of that model. An increase in the relative entropy correlates to a larger number of accessible configurations of information at some value of an independent variable of the model. Using this analysis, we can design criteria for the determination of the equivalence of states of a system, measured via XRD, on the basis of their information content.

For a single characterization technique, the analysis of states via information assumes both definitional and empirical equivalence on the basis that a technique and its resultant data share both a set of definitions and empirical relations, those assigned to a theory of XRD. Therefore, in order to quantify the type of information that is needed for this analysis, we begin by defining our set of measured variables. XRD patterns, as stated, are typically illustrated on an 2D Cartesian plot, with diffraction angle [2θ] on the x-axis and intensity [*I*] on the y-axis. Measured peaks of intensity will occur at specific angles where the incident X-ray beam diffracts, giving a characteristic pattern.

The set of data used to calculate the probability distribution of an experiment includes the intensity, *I*, and angle 2θ, which we define as $\{X\}$, with every element $x \in \{X\}$ equal to some combination of $[I, 2\theta]$. Given these sets, we then select a bin size in order to convert the experimental data into probability distributions. Here, a half degree of 2θ was chosen because it is roughly a quarter the size of the base of the largest peak analyzed, deemed sufficient to capture different sections of each peak. Then every element *x* from {*X*} was mapped into a bin, *n*, of 2θ from 0° to 180° degrees.

Once the measured data is binned, the probability that some element of intensity, *x,* might be found in each *n-2θ* bin is calculated where:

$$p(x) = \frac{\Sigma x_n(2\theta = i, i + 0.5)}{\Sigma x_n(2\theta = 0, 180)} \tag{47}$$

An example calculation using the above equation may be found in Appendix A.1.

The probabilities are calculated for every half degree *2θ* from 1° to 120° [*2θ*] for temperature variable patterns. The sum of all *Σp(x)* for the collected data should be equal to 1, which it is for each set analyzed herein. Calculating a probability *p(x)* for every *2θ* bin *n* produces a probability distribution, *P(x),* for any diffraction pattern. In order to perform the relative entropy analysis, one of the diffraction patterns, and its resultant distribution must be chosen as a reference. Here, we choose a reference state of copper at 0 K, based on a lattice parameter calculated by Giri and Mitra [96], which was then used to produce a representative powder diffraction pattern for copper using the Match! Powder Diffraction software [97]. The probability distribution produced by this powder diffraction data set is set as our model distribution, *Q(x)*. Figure 13 displays the calculated reference pattern for copper at 0K.

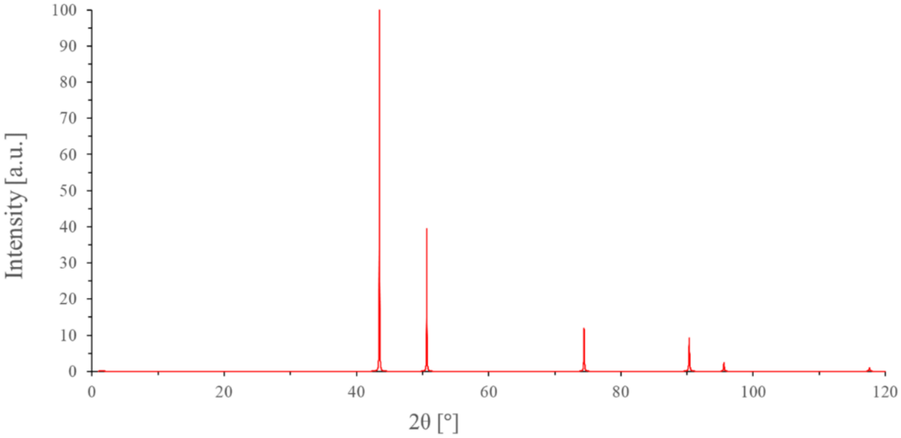


Figure 13: The 0 K XRD pattern for Cu, which serves as *Q*(x), or the reference pattern, for the temperature evolution analysis. Pattern produced using Match! [96]

Similarly, the diffraction patterns for copper at temperatures of 303K, 403K, 503K, 603K, 703K, and 803K were produced with lattice parameter data from [98] and the Match! Powder diffraction software [97]. In all cases it was assumed that the lattice parameter for copper used to calculate all higher temperature diffraction patterns expanded isotropically, and that $a = b = c$. The evolution of temperature produces a noticeable shift in the peaks, as shown below for the Cu(200) peaks in Figure 14.

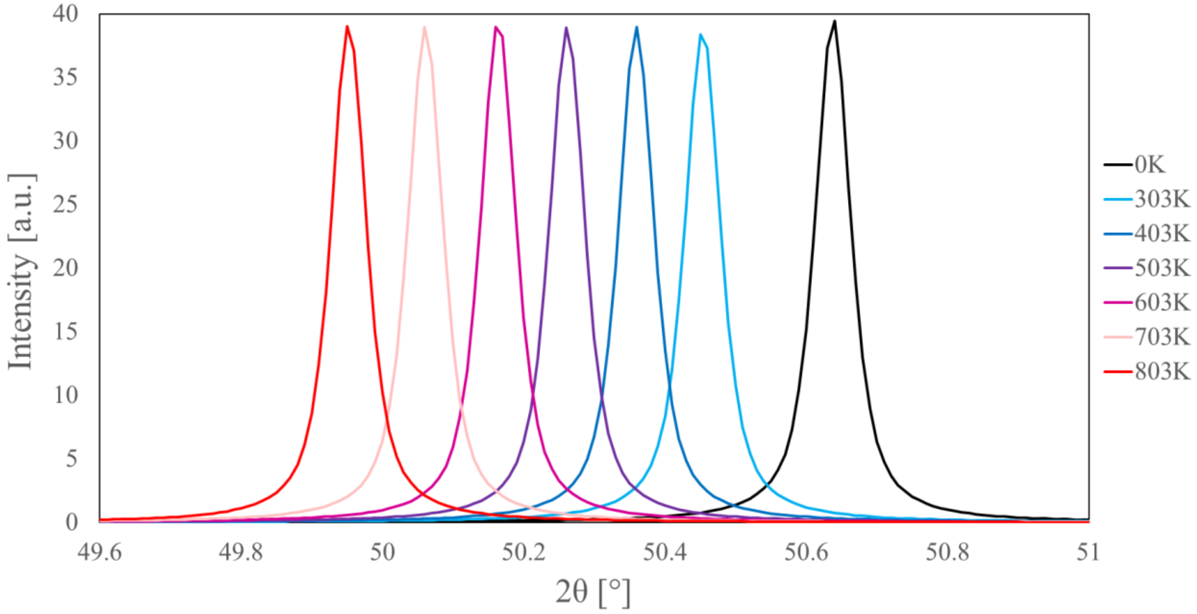


Figure 14: The shifts of the (200) XRD peaks to lower values of 2θ for Cu due to increasing temperature, which correspond to a shift in the intensity probability distributions, $P(x)$.

The peaks produced in Figure 14 should theoretically be straight lines as the calculations involved differ only by a change in the lattice parameter, a [Å]. The minute peak broadening of approximately 0.08° [2θ] (as measured by full-width of the peak at half of the maximum intensity) that each calculated peak exhibits is due to the datasets which form the standard in Match!, and the instrumental broadening of those referenced experiments, which is much lower than the typical broadening seen due to instrumentation [95]. The software allows, and encourages, the creation of XRD pattern standards for known materials as a comparative baseline and, if none are uploaded prior to an analysis, defaults to records of the Crystallography Open Database (COD) [99]. The records contained in the COD are open source data, uploaded and published by authors and institutions for use in research, the results of which are then used in the calculation of the XRD patterns produced by Match! The broadening apparent in Figure 14 is then likely due to the instrumentation used in the studies which produced the pure copper reference patterns for the COD. While the data produced in this method may be inappropriate for use in other experiments due to these factors, it is still in a form which is acceptable for use within this framework as an evaluation of the method of informational analysis because the method measures only deviation from the reference, and this section is intended only as proof that this form of measurement is feasible. If this were an analysis of straight line intensities with broadened peaks, the trend of the relative entropy would remain unchanged, though the values of entropy produced would be higher as the distribution of the intensity data would change more, in contrast to to the analysis above.

Diffraction patterns representing copper undergoing a series of cold working steps were mapped into Microsoft Excel from [100, p. 4] and used to produce intensity vs. 2θ data sets using the WebPlotDigitizer [101]. Figure 15 contains these patterns plotted next to one another, where the effect of processing the material can be seen via the contrast in the position and shape of the peaks. In contrast to the calculated temperature patterns, these patterns display more variance and peak broadening, with the shift especially prominent for the Cu(220) peak, a result of changes in crystallographic texture, and microstrain from the increase in the dislocation density due to cold-rolling [95].

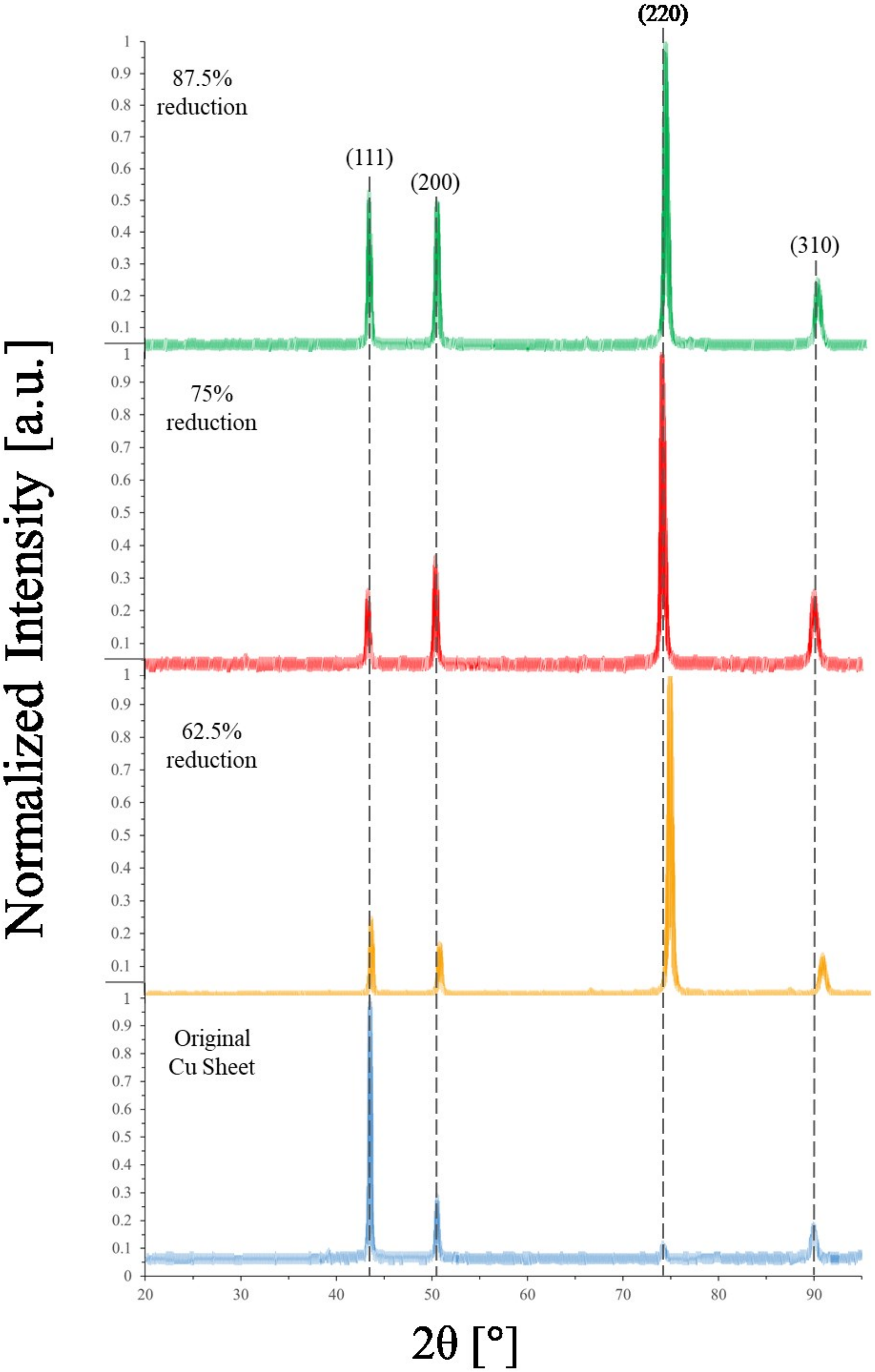


Figure 15: Normalized XRD intensities of cold-rolled Cu sheet, shown with the %reduction of the original thickness, indicative of rightward peak shifting and broadening that can occur due to cold-work reduction, adapted from [100].

With the data in this format, the probability distributions of the sets of intensity data can now be calculated. As the probability distribution of each pattern is calculated, the relative entropy of any two distributions can be obtained. In this instance, we are interested in the ‘distance’ of an experimental distribution from a reference distribution that represents the current ‘ideal’ of some combination of material and characterization technique—here the pattern of the polycrystalline copper calculated at 0 K for the temperature evolution, and the undeformed copper sheet pattern for the cold-working reduction. A slightly different version of equation (6) using the natural logarithm was also calculated, based on the assumption that the natural log renders the results as a more direct proportional difference [102]:

$$K(x) = -P(x) \ln \frac{P(x)}{Q(x)} \tag{48}$$

Once the distributions have been entered into this formula, the content of the XRD patterns—the distribution of intensity measurements across the span of incident angles—can be analyzed. The shifts and changes in the shape of the XRD peaks represent the relationship between physical states of the system, which are being measured by the relative entropy. Higher temperatures produced the highest values of relative entropy compared to the reference state for temperature evolution, and a reduction of 62.5% produced the most relative entropy for the cold-worked set. The relative entropy shifts due to increasing temperature are summarized below in Table 6.

Table 6: The relative entropy produced for the copper XRD patterns as the temperature is increased. For both $K(x)$ [bit] and $K(x)$ [nat], there is a positive correlation with temperature.

Temp. [K]	***K(x) [bit]***	***K(x) [nat]***
0	0	0
303	0.384	0.885
403	0.594	1.367
503	0.713	1.641
603	0.795	1.832
703	1.214	2.795
803	1.877	4.322

Similarly, Table 7 shows the change in the relative entropy due to cold-working T1 copper sheet [100]. The analysis method, and form of the results, should be replicable for any XRD pattern in copper, and in other crystalline materials systems. In fact, assuming that any given characterization technique has a set of material standards which may be utilized to formulate a desired reference state, this type of analysis should be equally valid across a range of techniques. The choice of reference data is subjective, depending on the analytical design-of-experiment, or available data.

Table 7: The relative entropy produced for copper XRD patterns after cold-working. The amount of information gained spikes at the lowest reduction % of the set, then steadily decreases.

% Reduction	***K(x) [bit]***	***K(x) [nat]***
62.5	1.477	3.401
75.0	1.035	2.384
87.5	0.831	1.913

The meta-analysis of a system through relative entropy, based on the distribution of experimental data, measures how much additional information is necessary to describe a state of a system relative to a reference state. The amount of information the state of a system contains relative to a reference state is indicative both of a change in the contribution potential of conceptual parts of physical material structure (atoms, grains, defects, and the like), as well as the effect of environmental variables on those parts and their arrangements. In this analysis, the physical structure of the reference state of copper is comparatively idealized. As each of these variables is altered, the XRD data reflects the change in the structure, and in the symmetries inherent to the reference state, an interruption in the relatively ideal nature of the crystalline lattice which necessitates a larger number of variables be determined to fully describe the system. The relative entropy is a measure of the change of that data, for a specific characterization technique, in the context of the variables of that state.

This sense of information is where a rigorous idea of informational equivalence within materials models can begin to form. These measurements show how the overall information of the system increases against a reference, as Figure 16 illustrates the increase in the relative entropy as the temperature increases for copper.

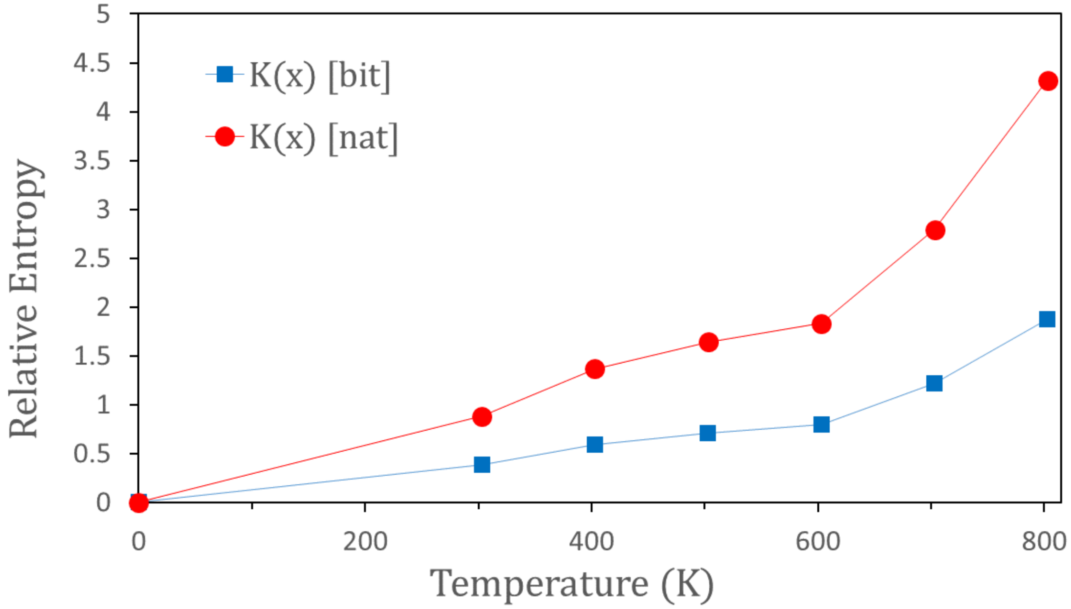


Figure 16: The increase in relative entropy as temperature increases for copper, as measured via XRD.

The amount of relative entropy *K(x)* increases at each step of temperature increase. The diffraction patterns analyzed for this figure show only the effect of temperature on the lattice parameter, making the results of this analysis—in effect—the isolated dispositional power of temperature on the lattice parameter, as mediated through the probability distributions of XRD. We previously noted that, if two systems (or two states of a system) are empirically equivalent, which we take as a necessary condition to the determination of informational equivalence, then determining the informational equivalence becomes a matter of determining the relevant informational criteria. Quantifying the isolated temperature effect on the expansion of the lattice parameter is one method of highlighting where the criteria for information equivalence might arise.

The shift due to multiple steps of cold-working, against its own undeformed reference state, exhibits a different pattern. Figure 17 shows the relative entropy shift for the cold-working of T1 copper sheet, reduced from a thickness of 8 mm to 3 mm, 2 mm, and 1 mm, respectively [100].

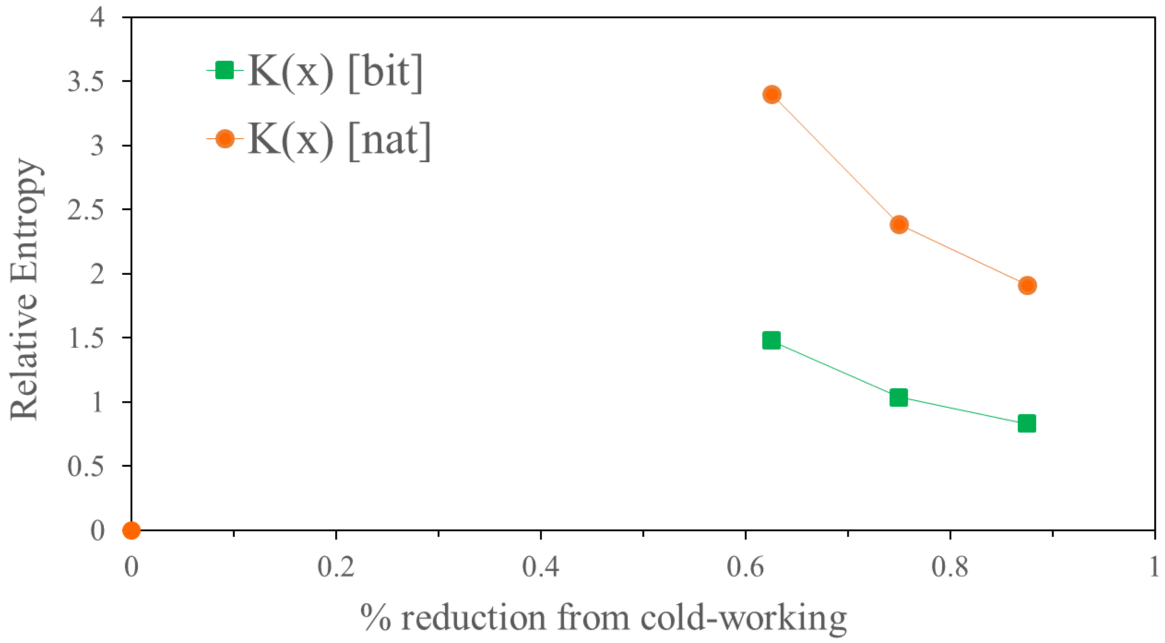


Figure 17: The relative entropy increase in copper as the % reduction due to cold-working, as measured by XRD.

Here, the relative entropy increases dramatically upon the first rolling step, then decreases gradually with further steps. The shape of the shift in the relative entropy presented here reflects the sizable shift of the (200) peak to larger values of 2θ that can be seen in Figure 15. The authors of that study suggest that these shifts in the XRD pattern are due to texture effects in the rolling deformation of the sheet [100]. The apparent inflection in the relative entropy shift also seemingly corresponds to the plateauing of the dislocation density increase during cold-working due to saturation [103]. Regardless, the divergence data shows that the initial rolling steps have a greater effect on the shape and distribution of intensity data than subsequent steps.

Both of these experiments involve a copper system, both having the effect of their processing steps measured by XRD. This overlap in material and experimental technique indicate that the ‘problem’ involving a comparison of these two sets of data can already claim both definitional and empirical equivalence. With those equivalences assumed, it is now possible to see in what sense, if any, the state change evolution of the heating of a copper sample is informationally equivalent to the state change evolution of a copper sample due to cold-working. The first step of this analysis is to see how the empirical relations central to each processing model overlap; are they able to occur under the same set of circumstances? Figure 18 illustrates the meaning of this step:

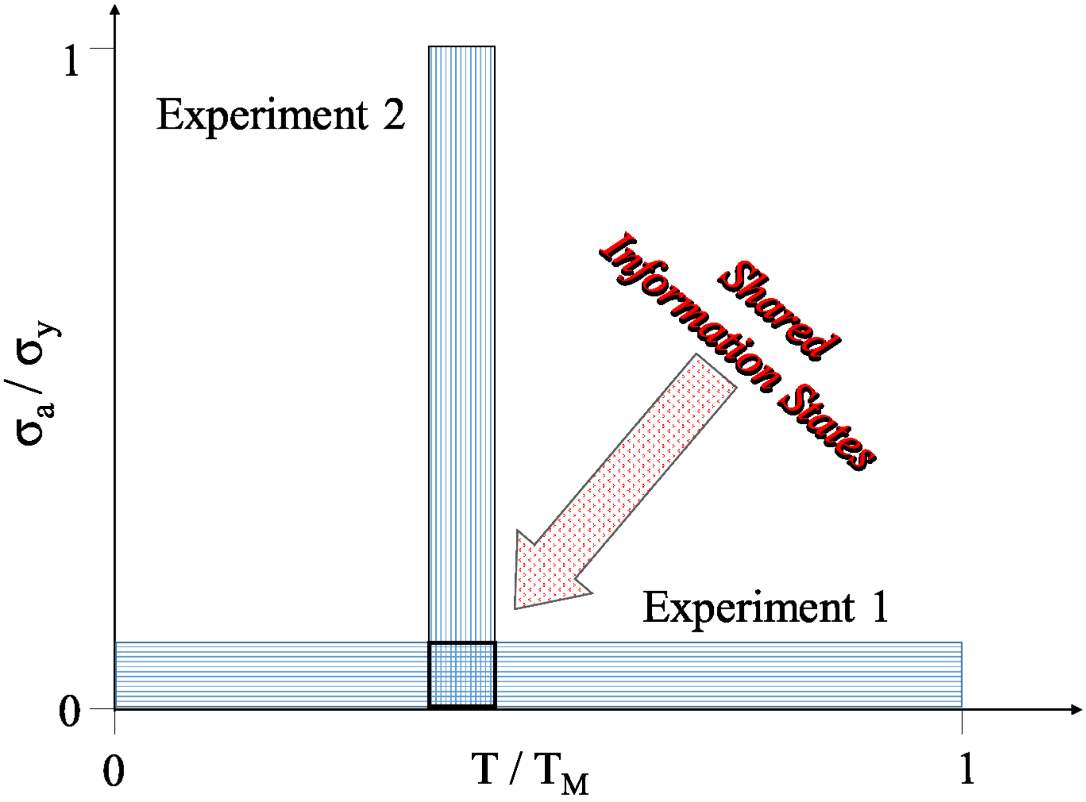


Figure 18: Representative empirical bounds for two experiments involving applied stress (σ_a) normalized by the yield stress (σ_y), and the temperature (T) normalized by the melting temperature (T_M). The overlap of the two are the boundary conditions for shared information states of the two experiments.

In the hypothetical system shown, two experiments are valid in different ranges of normalized stress (σ_a / σ_y) and normalized temperature (T/T_M). Whatever the relationship in general between these two variables, the hypothetical empirical relation—and therefore the measures of information—are valid only in the overlapping range of state variables.

The first set of experiments in this section describe the evolution of the lattice parameter of copper (*in silico*) as a result of the steady increase in the temperature of the system. The lattice parameter is a property of the crystalline solid state of copper, and is a valid measure of the system in all states where copper is in the state of a crystalline solid. If it is assumed that the sample is pure, the crystal structure of copper will stay the same throughout its solid temperature range so the only bound on that experimental model is the melting temperature, giving an effective empirical boundary of T from [0, 1358] K.

Turning to the cold-work experiment, the definition of cold-work for metals holds that it is deformation performed under the recrystallization temperature of the material. For copper, this temperature is given as a range with an upper bound of around 500 K, though this number may vary based on other parameters [13]. This definition, plus the availability of data only from room temperature experiments gives cold-work an effective empirical boundary of T from [0, 500] K. Cold-work also introduces defects into a metallic system, nucleating new dislocations as the deformation adds energy to the system. The dislocation density of a system has been empirically measured in relation to temperature, so rough ranges of empirical overlap in terms of [T, ρ] can be drawn for these two experiments [104]. As the temperature is raised, the dislocation density, ρ, will decrease in a copper system, where in a non-cold-worked specimen the range would be roughly [120×10^8, 8.5×10^8] cm^{-2} for a temperature range of [298, 973] K [104]. In a cold-worked sample, the dislocation density increases as the amount of deformation is increased, and the range for that process would vary roughly from [10^8, 10^{12}] cm^{-2} for a reduction range of [0%, 70%] [103]. Given these ranges, we can construct a chart, Figure 19, illustrating the empirical overlap for the shown ranges of (T/T_M) and ($\rho/\rho_{\max}$), where we $\rho_{\max}$ to be the measured saturation dislocation density of roughly 10^{12} cm^{-2} [103].

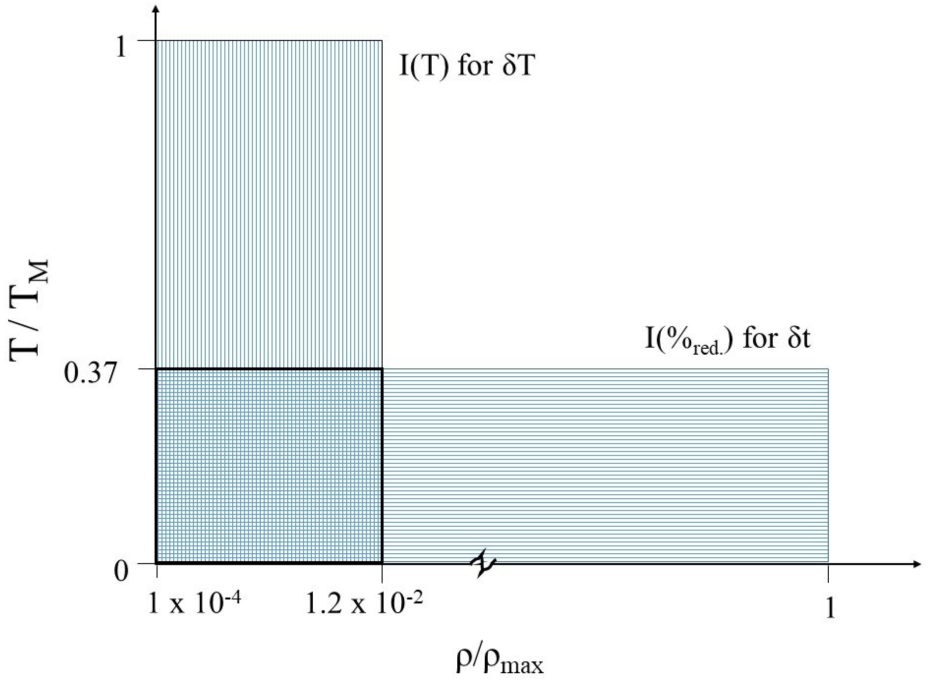


Figure 19: The empirical overlap of both XRD experiments on the basis of temperature (T) and dislocation density (ρ).

The upper bound of (ρ/ρ_{max}) for the temperature experiment is roughly equivalent to 10% reduction [103], and the upper bound of (T/T_M) for the cold-work experiment corresponds to a recrystallization temperature of 500 K [13]. Looking back at the equivalence criteria in section 3.3, a region of state variable overlap has been established, providing a validated region wherein some measure of informational equivalence may be found for the XRD probability distributions related to these variables.

At the most basic level, within the ranges of empirical overlap for the selected state variables [T, ρ], and given the translatability of the empirical sets, we hold that that any state that has equivalent relative entropy to another has the same structuring potential, and is therefore informationally equivalent. The accumulated empirical data in this region is, unfortunately, rather sparse. Without running further experiments within the desired ranges, the analysis is forced to center on rudimentary methods of line-fitting within the regions of validity.

Looking at Figure 16 and Figure 17, it can be seen that while the ranges of temperature and percent reduction for the relative entropy shift are present on each graph, there are no values for either. Within these regions the values can be calculated based on trendlines fit to the existing data, if only to give a rough idea of where overlap might occur. Fitting both *K(x)* [nat] data sets with a 2nd order polynomial allows for two equations to estimate where the relative entropy produced by each experiment might overlap. Solving for the relative entropy measure in the regions where there is overlap, an estimate of ~0.11375 [nat] is produced, signaling a tacit informational equivalence of these two models, based on the proposed criteria, albeit a value corresponding more or less to the lower bounds of the systems.

Clearly, this analysis could benefit from a richer supply of experimental data, or the opportunity to run specific XRD tests in order to compile larger and more tailored data sets. If this approach was to be used in order to conduct an analysis of unknown systems, or mechanisms, relative to known systems, the data would also need to be of higher quality than those calculated for Figure 14 as well. In building an analytical technique with this method, care will need to be given that the data used meets the rigor of the standards for whatever characterization technique is being used to conduct the informational analysis, in order to minimize the sources of error. What the current level of analysis *does* indicate is that, given a set of experiments, the relation between two models on the basis of the information required to describe the evolution of states is present and quantifiable. Relative entropy is a form of relative information, it is representative of a physical correlation between two states of a system, and the number of possible pathways between those states constrained by the empirical bounds of the model [105].

If a network of state change models for a material system can be synthesized, then the relative entropy produced is a useful parameter for measuring the relative potential of a system given a specific mechanism of change, or in particular environments. As informational equivalence matures as a concept, a variety of interactions within a material system may be better understood in terms of their affect, here meaning the measure of the ability of some object (say a material subsystem) to create change in another with which it is interacting. Mechanisms are often differentiated in this manner, and so we turn to look at comparable mechanisms of creep as our next subject of interest.

4.3: Mechanistic Models

An enormous variety of materials phenomena are captured in models, and stitched into various theories of materials. The set of the phenomena includes not only multiscale hierarchies, or the evolution of experimental behavior, but also the various modes of change that a material may undergo, what are known as mechanisms. Take, for example, a phenomenon called creep. Creep is defined as the high temperature (>0.4 T_M) plastic deformation of a material over time, while under constant loading [13]. There are numerous analytical models which describe creep at various loading and thermal conditions, each separated by specific pathways by which the creep is believed to occur. Often, the models describing the creep mechanisms are shown in terms of their strain rate $\dot{\gamma}$, or the rate at which the permanent deformation occurs within a given environment.

The mechanisms of creep do not occur independently of one another. For a given material, in some environment, a single mechanism may contribute more than another to the total strain rate of the system, but that does not prevent the other mechanisms from occurring simultaneously. If these mechanisms work in concert, and are all understood to contribute to the overall strain rate of the system, then these mechanisms should have equivalent structures in the context of that variable. The partial additivity of the strain rates produced by different mechanisms of creep are exemplified best by Equation 3.2 of [72], showing that the overall strain rate of a polycrystalline system is a combination of the strain rates of individual competing mechanisms. Specifically, because we assume that the mechanisms already share definitional (all mechanisms of creep), and empirical equivalence (data all translatable given their shared rate equations), then the search is narrowed to overlapping informational and categorical equivalences.

A manner of presenting these particular mechanisms are charts known as 'deformation-mechanism maps,' where the dominant mechanism (greater than 50% of the total strain rate) for a given environment of stress and temperature is mapped [72]. Figure 20 shows a deformation-mechanism map for copper with a grain size of 100 μm and axes of normalized shear stress [σ_s / μ] (where μ is the shear modulus), and normalized temperature [T/T_M]:

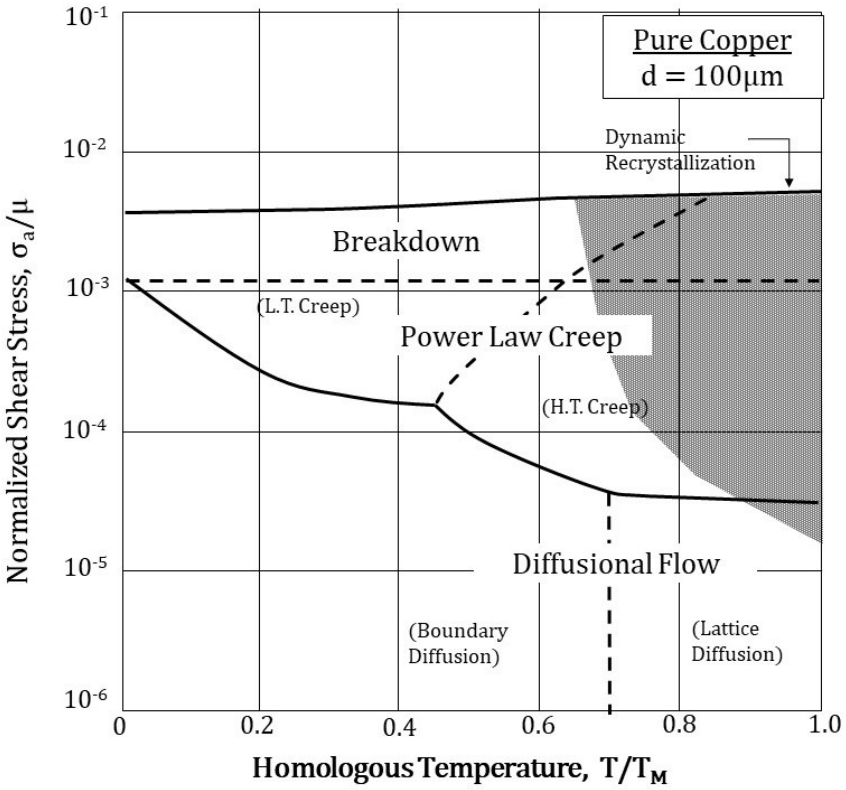


Figure 20: The deformation-mechanism map for pure copper at a 100 μm grain size, recreated from [72].

As can be seen, there are three different mechanisms of creep over this range of normalized temperature and stress. The mechanisms from right to left are: 1) diffusional flow, 2) power-law creep, and 3) power-law breakdown. Each of these mechanisms has a range of [σ_S, T] values for which it is the dominant mechanism, and the bold lines indicate boundaries where the mechanistic contribution to the strain rate is numerically equivalent for adjacent mechanisms. Given this framing, the structures of the informational and categorical equivalence criteria for these creep models can be illustrated but, first, the specific definitions, variables and empirical models corresponding to each mechanism are listed below.

One of the mechanisms is 'diffusional flow' creep, which is where grains (collections of atoms in an ordered crystal, all with the same crystallographic orientation) are deformed due to the diffusion of vacancies (point interruptions in an ordered lattice structure) through the volume of the grains, or along the grain boundaries (the interface between grains of different crystallographic orientations). There are, in fact, slight variations on the equations of diffusional flow creep depending on whether the diffusion is occurring along the grain boundaries (Coble creep), or through the lattice of the material (Nabarro-Herring creep). Figure 21 below illustrates the basics of creep: how a sample is tested, the three stages of creep, and a microscopic depiction of the diffusional flow mechanisms [72].

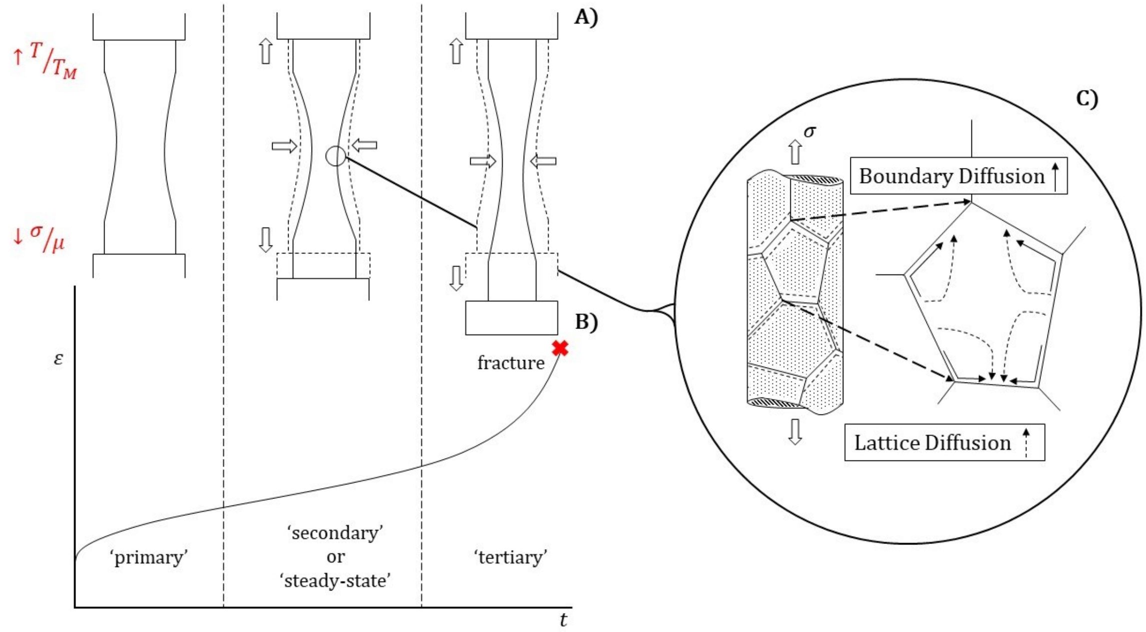


Figure 21: (A) a representation of a creep test, with a sample deforming slowly at elevated temperatures and a constant, low applied force. (B) a typical creep curve with the three stages of creep labeled, (C) a representation of the physical mechanism of diffusional flow creep. (C) recreated from [72].

Assuming that both lattice and boundary diffusion contribute, the combined strain rate equation for both Coble and Nabarro-Herring mechanisms is given by:

$$\dot{\gamma}_{DF} = \frac{42\sigma\Omega}{kTd^2} \cdot \left(D_v + \frac{\pi\delta D_b}{d}\right) \tag{49}$$

where 42 is a constant related to the periodic shape of grain boundaries [106], σ is the applied stress, Ω is the atomic volume of the material, k is Boltzmann's constant, T is temperature, d is average grain size, D_v is the volumetric diffusivity, δ is the average grain boundary width, and D_b is the grain boundary diffusivity [72]. As seen in Figure 20, both flavors of diffusional flow are dominant at low levels of applied stress (roughly 10^{-4} to 10^{-6} [σ_s / μ]) and high temperatures (roughly 0.6 to 1.0 [T/T_M]).

Another mechanism is ‘power-law’ creep, where the plasticity of the material is governed by the movement of dislocations (a plane of missing atoms within the crystal lattice). Dislocations moving through a lattice have two different methods of movement, glide and climb. The former is where a dislocation moves along the direction of the slip plane, “gliding” along the lowest energy pathway available to it through the lattice. The latter is where a dislocation “climbs” in the lattice normal to its slip plane via the aid of the diffusion of nearby vacancies. Both mechanisms can occur within this regime of creep, often in tandem, with lattice diffusion favored at high temperatures and low stresses, and core diffusion favored at low temperatures and high stresses [72]. Figure 22 illustrates this mechanism pictorially:

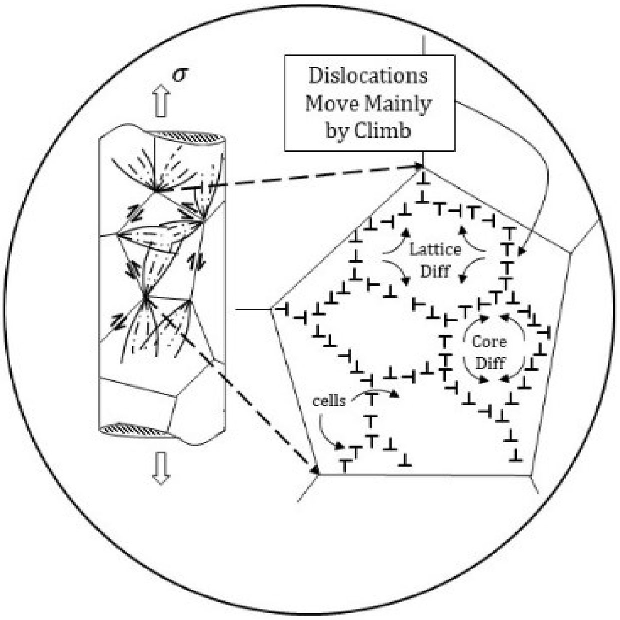


Figure 22: The central concept of power-law creep, where at high temperatures dislocation climb is a major contributor to plasticity, recreated from [72].

The strain rate contributions of power-law creep are empirically modeled following equation (50):

$$\dot{\gamma}_{PL} = \frac{A_2 D_{eff} \mu b}{kT} \cdot \left(\frac{\sigma_s}{\mu}\right)^n \tag{50}$$

where A_2 is a dimensionless fitting constant, D_{eff} is the effective diffusion coefficient, b is the Burger's vector, μ is the shear modulus, and n is the power-law exponent, which is given as $n = 4.8$ for Cu. For low temperature creep, the exponent becomes $(n+2)$ [72].

At values of $[\sigma_s / \mu]$ above ~10^{-3}, the power-law behavior of equation (50) no longer fits the experimental data, so another model must be used. This model is known as 'power-law breakdown,' and is a mechanism of creep similar to power-law, but in a regime of higher applied stresses the mechanism is increasingly governed (in the sense of contribution to the overall strain rate) by dislocation glide [72], as shown in Figure 23:

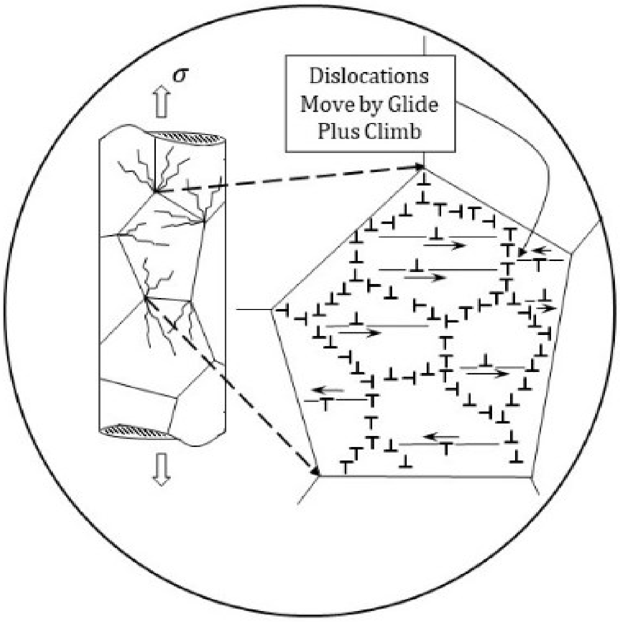


Figure 23: As the applied stresses are increased, the dislocations in a crystal increasingly move by 'climb,' aided by more diffusion of vacancies through the system. Recreated from [72].

The model for how power-law breakdown contributes to the strain rate is slightly different from equation (51) above, and at stresses, σ_s, below a certain threshold will reduce to that power law equation. Above that level, the strain rate is given as:

$$\dot{\gamma}_{PLB} = A'_2 \frac{D_{eff}\mu b}{kT} \cdot \left[sinh\left(\alpha' \frac{\sigma_s}{\mu} \right) \right]^n \qquad (51)$$

where A'_2 is the adjusted fitting constant, and α' is an adjusted unity constant, both fit to empirical data of creep above the power-law breakdown boundary.

These three mechanisms describe the majority of the pathways available to a pure copper metal of 100 μm grain size to creep at the microstructural level. All the physical mechanisms—the migration of dislocations and vacancies, along with grain boundary sliding—are all occurring concomitantly, but each dominates the contribution to the overall strain rate in specific environmental ([σ, T]) circumstances. Equation (51) for the power-law breakdown regime is a more general version of the power-law model, and reduces to the power-law equation (50) at low enough levels of stress [72]. Therefore, because power-law breakdown creep occurs by the same set of defect mechanisms, but is outside the boundaries of the simpler model, the two rates can be consolidated and presented together, which we will show as "power-law general" (PLG).

The combined strain rate $\dot{\gamma}_{comb}$ is a sum of all the contributions, so would be given in this case by:

$$\dot{\gamma}_{comb} = \dot{\gamma}_{DF} + \dot{\gamma}_{PLG} \tag{52}$$

Within the complete set of the constituent models, there are three independent variables (σ_s, T, and d) which are compressed into bound sets, meaning there are fixed ranges of values, beyond which the particular model breaks down, as the power-law equation does above ~10^{-3} [σ_s / μ]. It is assumed for the purposes of this study that all other variables in the equations above are constants. While the bounds of each model will feed forward as part of the equivalence analysis, they do not change the manner in which the criteria are determined. Starting with the information equivalence, the sets of strain rates determined by each set of [σ, T, and d] is a 3-tuple of the form:

$$[\dot{\gamma}_{comb} \quad \dot{\gamma}_{DF} \quad \dot{\gamma}_{PLG}] \tag{53}$$

These models, as currently constituted whenever an analysis like this one is performed, represent the reference state of each creep mechanism. When calculated, they fully define the strain rate behavior for each mechanism across the environments of creep. During creep experiments like those run to produce the models above, the sets of instantaneously measured strain rate data, which can vary from the models, can be treated as a stochastic variable and therefore amenable to a probability analysis.

It is assumed that, given the differences in environment necessary to isolate each mechanism, that experiments are designed to test one mechanism or the other, and not multiple simultaneously. Accounting for potential variations in experimental design and testing apparatus, the probability of a particular strain rate [s^{-1}] being measured for these mechanisms can be given as $p(\gamma_{\mathrm{PLG}})$ and $p(\gamma_{\mathrm{DF}})$ respectively. Given a set of data, each of these is the probability of selecting a particular value for the strain rate among the set of measured rates. The combined strain rate above combines the probability of the two rates, probabilities that are taken to be independent as they reflect different experiments and different data sets. The probability of the combined strain rate data set can then be given as:

$$p(\dot{\gamma}_{comb}) = p(\dot{\gamma}_{DF}) \cdot p(\dot{\gamma}_{PLG}) \tag{54}$$

Through the summative quality of the strain rates produced by various mechanisms of creep, there is an empirical relation between the quantities of the random variable of the experiment and so we may compare the informational equivalence of each individual mechanism on that basis. The distributions would be informationally equivalent with respect to the average amount of information of the experiment (the Shannon entropy $H(x)$) if:

$$H(\dot{\gamma}_{DF}) = -\sum_{\gamma \in \dot{\gamma}_{DF}} p(\gamma) \log p(\gamma) = -\sum_{\varepsilon \in \dot{\gamma}_{PLG}} p(\varepsilon) \log p(\varepsilon) = H(\dot{\gamma}_{PLG}) \tag{55}$$

These amounts would measure how much uncertainty exists in the sets of probabilities for each measured strain rate for each mechanism, and their evaluation illustrates the stochasticity of one measurement relative to the other.

The probability distributions produced by measurement of each mechanism may then, also, be compared to the predicted results given by each constitutive equation, via the relative entropy. A relative entropy measure of 0 would indicate that the model is perfectly predictive, with any other value indicating a shift away from that model. This is a common use for this measure and different forms of relative entropy minimization are used in a number of fields [107], [108]. Here, that measure would be given as:

$$K(\dot{\gamma}) = -\Sigma p(\dot{\gamma}_i) \log \frac{p(\dot{\gamma}_i)}{p(\dot{\gamma}_m)} \tag{56}$$

This equation states that the relative entropy for any mechanism of creep on the basis of its strain rate is the sum of the probability of measuring a particular strain rate via experiment $(\dot{\gamma}_i)$, relative to the value predicted by some model of creep, $(\dot{\gamma}_m)$. The form of this equation is also the same for the overall strain rate.

Returning to the equivalence criteria, we hold that an equivalent shift in the probability distribution of two mechanisms is saying that both systems require the same amount of excess (relative to the model) information in order to describe them. Formally, this means that the models of each mechanism are held to be informationally equivalent in this sense if they produce the same amount of relative entropy, or:

$$K(\dot{\gamma}_i) \Leftrightarrow_I K(\dot{\gamma}_j) \quad iff \quad K(\dot{\gamma}_i \parallel \dot{\gamma}_m) = K(\dot{\gamma}_j \parallel \dot{\gamma}_m) \tag{57}$$

In order to determine the categorical equivalence of the mechanisms of creep, we must first determine how a category of creep would be constructed. For creep as a mode of failure, we can contextualize any model of plasticity that fits within the creep regime as a constitutive mechanism of creep. The models of these mechanisms, as we have seen, are related to one another in a variety of senses, but specifically in their contributions to the overall strain rate of the system during a creep test. In this context, we take the morphisms between the sets of objects for each model to be these additive contributions to the total strain rate. Each mechanism is taken to have an identity function, and the morphisms follow the composition rule, producing a rudimentary category of creep models, $\mathcal{C}_{\text{creep}}$, illustrated in a Lawvere diagram.

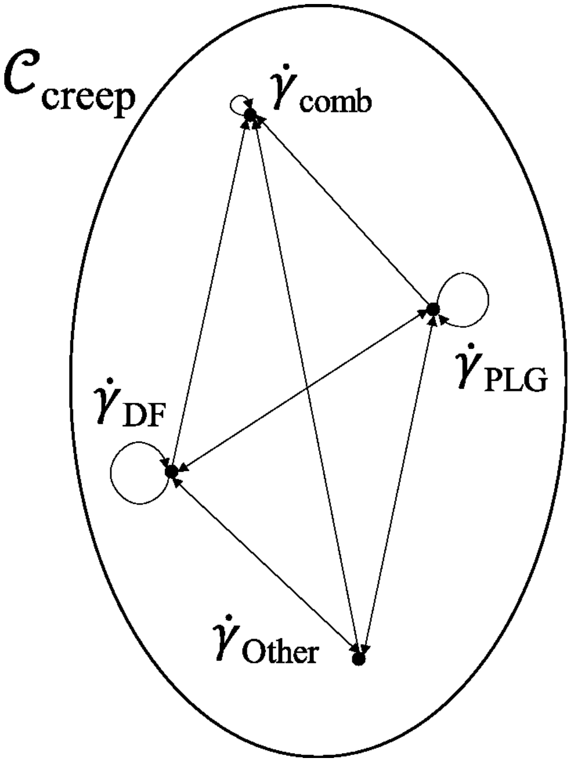


Figure 24: A Lawvere diagram of the proposed category of creep models, where γ_{Other} represents all other mechanisms of creep which may contribute to the overall strain rate.

The elements of each model of creep, assumed here to be subcategories of creep, are functions of the state variables of any experiment run to test a given mechanism. Across the two dominant models for copper, general power-law creep and diffusional flow creep, there are three variables which are thought to govern their behavior: applied stress [σ], temperature [T], and average grain size [d]. Given sets of variables $\{\sigma, T, d\}$ with elements in the domain set of a model, it is clear that the remaining variables, which we will call f and assume they are correctly formatted, can operate as a morphism mapping these sets to the codomain set $\{\gamma\}$, where:

$$f \colon \{\sigma, T, d\} \to \{\dot{\gamma}\} \tag{58}$$

As each of the domain sets is bound—for each material there will be min / max values of σ, T, and d—then this mapping shows the entire space of potentiality for any given model with regards to its creep behavior. Each model follows roughly the same selection process, illustrated by the olog in Figure 25 for diffusional flow creep of copper below:

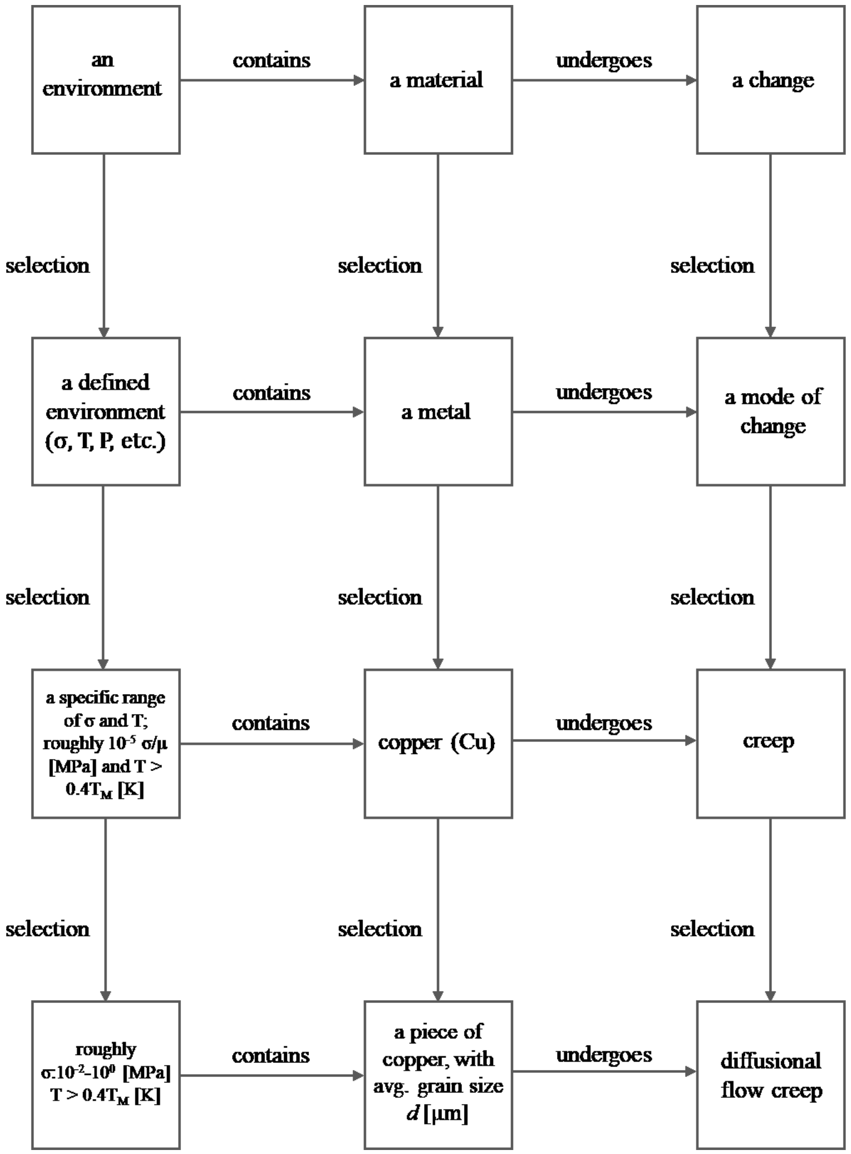


Figure 25: An proposed olog created to illustrate the conceptual flow building to a particular mechanism of creep, here diffusional flow creep of copper. Values derived from [72].

Each of the mechanisms of creep is relatable within the same conceptual framework, and they each include elements and morphisms within their individual subcategories that produce a strain rate. This result indicates that, for their differences, there is a mathematical structure in the categories of general power-law creep and diffusional flow creep that is equivalent. The equivalence adds another morphism to the category of creep, a comparative relation wherein the structure of the model for each constitutive equation of a mechanism is equivalent to that of a different mechanism.

$$\forall \dot{\gamma}_{ij} \in \mathcal{C}_{creep}, \qquad \exists F(\dot{\gamma}): \dot{\gamma}_i \to \dot{\gamma}_j \tag{59}$$

meaning for any mechanism of creep, γ_{ij}, within the category of creep there is a functor between the subcategories, *F*, that relates the mathematical structure of *i* to *j* on the basis of whether or not a value for strain rate is recoverable from that subcategory. If *F* exists, there must also be a functor *G* such that:

$$\forall \dot{\gamma}_{ji} \in \mathcal{C}_{creep}, \qquad \exists G(\dot{\gamma}): \dot{\gamma}_j \to \dot{\gamma}_i \tag{60}$$

because if one model shares that sense of mathematical structure with another, it follows that the inverse relation would also be true. On this basis, we can declare that the mechanisms of creep are categorically equivalent. The analysis of equivalences presented here are based on specific empirical models, derived from specific experimental data sets, meaning that calculating data from them to do a numerical version of this analysis would be invalid. In order to complete a quantitative equivalence analysis, new tests measuring strain rates for some system should be performed and then compared to these models.

4.4: Variable Models

Mechanisms of creep, like the ones illustrated in Figure 21, Figure 22 and Figure 23, have been shown to be equivalent in several ways. The models of these mechanisms are built around the reaction of a materials system to the sets of independent variables that drive the specific pathways of the evolution of the state of that system. Clearly, in addition to the other structures pertinent to modeling changes within systems, the structures inherent to each variable also structures the model of which it is a part. If a particular variable is being used across different models, are the instances of that variable structurally equivalent to one another across the models?

In order to work towards an answer, some overlap of variables between two of the models of creep mechanisms should be considered. Creep is prevalent within polycrystalline metals, structures where atoms at the nano- to micrometer length scales are arranged in an ordered, repeating pattern. There are several patterns which occur frequently in polycrystalline metals, including crystal structures such as fcc, or face-centered cubic, bcc, or body-centered cubic, and hcp, or hexagonal close-packed. These crystal structures, and specifically the unit cell, are a convenient shorthand for a specific atomic stacking pattern, and all of the symmetry operations that go along with a given crystal type.

Inherent to all crystalline structures are interruptions of the repeating lattice patterns, termed defects. There are a variety of defects, but the three most important for describing metallic structures and their behavior are vacancies, dislocations, and grain boundaries, corresponding to point, line, and planar defects, respectively. Grain boundaries are numerous within polycrystalline metals, and physically arise from the fact that—as a metal is cooled from a liquid to a solid state—it will generally nucleate crystal lattices (grains) from many independent points, each with a different orientation relative to one another.

The behavior of polycrystalline metals are heavily influenced by their defect structures. Collections of vacancies, dislocations, and grain boundaries exercise a significantly disproportionate amount of influence on material properties from strength to electrical conductivity. Defects also affect how material change occurs at the microstructural scale, especially for the mechanisms of creep. In many nominally pure metals, at low levels of constant stress and high temperatures, the dominant mechanism is diffusional flow creep, which is illustrated in section 4.3 in Figure 21. This mechanism is caused by a potential energy gradient within the grain boundaries, which promotes the diffusion of vacancies through their volume and/or along the grain boundaries, as the grains slide and elongate in the direction of loading [72].

The rate of deformation caused by this mechanism is captured by the combined Coble/Nabarro-Herring equation (49), where the average grain size is represented as *d* [72]. The combination of the two equations somewhat obscures the fact that the two mechanisms of diffusional flow have different relations to the average grain size of the material. Separated, the Coble relation (61) and Nabarro-Herring relation (62) can be shown as:

$$\dot{\gamma}_{NH} = A\frac{\sigma\Omega}{kT}\cdot\frac{D_v}{d^2} \tag{61}$$

$$\dot{\gamma}_{Coble} = 42\frac{\sigma\Omega}{kT}\cdot\frac{\pi\delta D_b}{d^3} \tag{62}$$

where the only addition from the combined equation is *A* in (61) which is a geometric fitting constant for the Nabarro-Herring relation [72].

As these formulas indicate, the contribution of the average grain size to the strain rate produced is different depending on if the vacancies within the lattice are diffusing along the grain boundaries (Coble creep), or through the volume of the lattice (Nabarro-Herring creep), where the former scales as d^{-2}, and the latter as d^{-3} [72]. The form of the grain size scaling factors is directly related to the geometric considerations of each mechanism. Diffusion along a grain boundary is a form of travel across a plane created by two adjacent grains (often modeled as cells), so the geometry that the vacancy traverses is best described by an area, described by d^2. Diffusion through a volume, as one might guess, is a journey for a vacancy in a three-dimensional space, described by d^3. The geometry of diffusion, and therefore the geometry of a grain, is an important consideration for the structuring of these processes.

Grains are geometric spaces. By definition, they maintain certain geometric properties even as grains change shape. These properties can be drawn out of any treatment of a grain structure by stereometric grain size calculation methods, like those presented in ASTM Standard E 112 [109]. This methodology, dependent on a meticulous random sampling of measurement sections with points, lines and planes, produces the following invariants for three-dimensional grains:

$$\frac{\bar{N}}{\bar{L}} = \frac{2\bar{l}}{\pi\bar{A}} = \frac{S}{2V} \tag{63}$$

$$\frac{\bar{l}}{\bar{A}} = \frac{\pi S}{4V} \tag{64}$$

$$\frac{\bar{n}}{\bar{A}} = \lambda 2V \tag{65}$$

$$\frac{\bar{n}}{\bar{l}} = \frac{2\lambda}{\pi S} \tag{66}$$

$$\frac{\bar{n}\bar{L}}{\bar{A}\bar{N}} = \frac{\lambda}{S} \tag{67}$$

where (when drawing the intercept lines used in the measurement methodology) *S* is the total area of an isolated volume, *V*; λ is an intersecting line of average length L, N is the average number of intercepts the line makes, A is the average area of an intersecting plane, l is the average total length of a plane's intercepts with the surfaces, and n is the average number of points where the λ lines intersect a plane [5]. These relations hold as long as all of the random sections selected for the analysis are averaged over a sufficient number of geometric objects applied to the grain structure. These relations geometrically structure the approach to the measure of average grain size, and it turns out that L/N is the measure of average three-dimensional grain diameter encapsulated in the variable *d* [5].

This measurement provides the last pieces in the puzzle for assembling a structural equivalence for the average grain size variable. Looking again to the framework of equivalences, it may be assumed that all grains within pure metals are definitionally equivalent. Grains across the class of all metals and alloys are measured using similar methods, including the method described above using stereometric methods to calculate the average grain size, and are mapped to the set of length units. Any measurement that meets those criteria for measuring the average grain size is empirically equivalent to another.

The information structure of grains would depend on the context of the interaction between a 'grain-object' described by a distribution of grain size measurements, and the 'object-system' with which the grain is interacting. In the context of a grain structure, the Shannon entropy could be used to indicate how close the average grain size measurement is to an expected mean, indicating the uniformity of the average grain size. In the context of creep, the relative entropy could be employed to try and correlate how much a shift away from some reference (*d* at STP, say) in grain size affects the shift away from a reference strain rate produced. As with the other analyses in this work, the informational structure is always dependent on the type of relation between objects being studied.

Most pertinent to this discussion, though, is the relation of the grain and its mathematical structure to the mathematical structure of the creep mechanisms. In order to discuss that relation, the categorical structure of grains must first be constructed. The invariant relations described above in equations (63) - (67) provide a hook into categorizing grain structures (or, general structures involving grains). Given a set of objects, $\{gs\}$, a category of *grain structures* can now be constructed. This category, $\mathcal{C}_{\mathrm{gs}}$, could be defined as:

Definition 10. A discrete category of grain structures, $\mathcal{C}_{\mathrm{gs}}$, consists of…

- a collection of three-dimensional volumes corresponding to the measurement of a collection of geometric objects (grains) at some mesoscale of a material system, called *grain structures*, $\{gs\}$, as well as a set of variable geometric objects of 0, 1, 2, and 3 dimensions, $\{x\}$, $\{\lambda\}$, $\{A\}$, $\{V\}$, the combined set of which will be called $\{go\}$.
- a collection of morphisms, including a set $\{f\}$ mapping the geometric objects to the grain structures where f_i: $\{x_i, \lambda_i, A_i, V_i\} \rightarrow \{gs_i\}$, a set $\{i\}$ mapping the geometric quantities to one another, and a set $\{h\}$ mapping grain structures to one another.
- an identity morphism for any object in $\mathcal{C}_{\mathrm{gs}}$, e.g., id_{gs}: $gs_i \rightarrow gs_i$
    - a composition function for any elements of $\mathcal{C}_{\mathrm{gs}}$, where, for morphisms s_a and s_b, there exists a morphism s_c, called the composite, where if s_a: $[gs]_1 \rightarrow [gs]_2$ and s_b: $[gs]_2 \rightarrow [gs]_3$, then s_c: $[gs]_1 \rightarrow [gs]_2$ and $s_c = s_b \circ s_a$.

Given this definition, grain structures, the invariant relations, and the average grain size can be constructed using the maps from the collection of geometric objects to a particular grain structure.

Due to the notion that grains as physical objects are a casual element within materials models, the structure of a grain structure as a variable should carry with it every sense of equivalence that allows grain structures to have the same dispositional, causal power across models. The same average grain size corresponding to a map g_i: $[\lambda_i]_n \rightarrow [gs_i]$, has the capacity for diffusion of vacancies via both established pathways. This proposition means that the categorical equivalence of a grain across these two models is a function of whether or not the specific geometry conducive to the specific mechanism is a map within the set of maps of $\mathcal{C}_{gs}$. Put more formally:

There exists a categorical equivalence, $d_{Coble} \Leftrightarrow_C d_{NH}$

iff $[j \in HomSet(f, h)]$ such that

$j_{Coble}: [f(V), h(gs_i)] \rightarrow [gs_j]$, and

$j_{NH}: [f(A), h(gs_i)] \rightarrow [gs_j]$, and

for $i_1: f(V) \rightarrow f(A)$ *and* $i_2: f(A) \rightarrow f(V),\ i_2 \circ i_1 = i_1 \circ i_2$

For the same measured grain structure, $[gs_i]$, the two measures of average grain size are equivalent if, and only if, there exists a mapping of a volume (cell) mapped on the structure and an area (grain boundary) mapped on the structure that are able to create an equivalent, subsequent grain structure. This definition shows that, as long as the geometric invariants of equations (63) - (67) hold, and a grain structure can project both a volume and an area corresponding to diffusion pathways forward, then the characteristic grains represented in both models by the average grain size are mathematically equivalent to one another, and are therefore categorically equivalent. This category is specific to a particular pure metal, able to undergo particular mechanisms of creep, so is not universal. Rather, with enough categories of this form, there is opportunity for similar mathematical structures to be found across material classes and mechanisms.

Chapter 5

Conclusions

> *Science needs a soul which would show respect*
> *and love for its subjects of study and would stress harmony*
> *and communication with the rest of the universe.*
> —Rita Arditti, "Science and Liberation"

MSE has always been interdisciplinary in spirit. The drive to consider materials as a consolidated field of study finds roots in the interdisciplinary work between metallurgists, physicists, and chemists working on the Manhattan Project [110], a drive that speaks to the search for some general concept of what it is that all materials have in common. The first versions of the materials paradigm gave equal measure to the four components of process, structure, properties, and performance. Yet, as decades worth of empirical research and analysis show, structure is the sole cornerstone of a science of materials; everything else within MSE is set in reference to structure.

That is it. *Structure* is the answer to what unites all sciences of all materials. Structure governs behavior, structure selects for applications, changes in structure determine every material property, and structure is the foundation of every aspect of a material that delights, awes, or adds comfort to the lives of the people that use them. Cyril Stanley Smith wrote that structure was a "universal metaphor" [5, p. 389], that within any system, of any medium, the mind seeks the pattern of interactions between things. If structure is a universal metaphor, then the human mind is effectively Joe Brody in *The Big Sleep*, shaking two patterns together for a month, trying to get them to mate.

Hard-boiled metaphors aside, it is clear that the key to creating, designing, and contextualizing materials is to be able to structure our concepts of them. Structure is the process of relating, and our richest picture of what materials are comes into focus when every manner of relating to material objects is taken into account. The thrust of pre-MSE materials research, and science in general, in the 20th century was one of isolation and reduction. Enormous advances came about due to work isolating components of physical systems and probing at them to see how they responded, but the work of recontextualizing this science into the greater fabric of life remains incomplete [111, p. 210].

In some small way, new techniques for relational and holistic analysis of systems is what we hope to have contributed to in this thesis. Human beings do not interact with materials systems, or with any system, solely on the basis of experiment and quantification. There is a far richer landscape of interactions, one in which each of us is our own small node. Recognizing patterns, human beings define things; we see, hear, and feel them with varying intensities; we strive to predict how and why the systems outside of ourselves behave in the manner in which they do; and, of course, we *do* test and probe them, measuring their capacities in numerous ways. No single, isolated measure of a material system is complete.

Furthermore, this analysis of systems in general is amenable to, at a minimum, the philosophical concepts outlined in section 2.3. The SEF is designed to capture the various senses of structuring which, historically, the process philosophies of the 20th century honed in upon. Various senses of mereological relationality; processes of individuation and organization; the duration of relationality between systems; assemblages and boundary drawing; flows of information and perception; each of these is realized by one of more parts of the SEF. If this framework is amenable to these theoretical concepts—some of the most important systems ideas of recent history—then there is no reason to think that it would not be amenable to analysis and treatment by contemporary philosophers of science and systems, such as structural realists, or pluralists. Further iteration of the SEF with contemporary philosophical ideas of relationality and systems can serve to make the framework more robust and, thus, strengthen the ontology of materials.

The process of building theories of materials, their models, and their various relational capacities expressed through the proposed structural equivalence framework also follows the roadmap of MSE model building, shown in Figure 5. The structural equivalence framework is an attempt to capture every entry point to the analysis of materials systems, and combine them into an abstract model of what it is to *be* a material. The rest of the thesis builds upon the definitions presented for these entry points, and adds detail through analysis of materials models. The path to the fullest concept of materials, through iteration of the proposed framework of structuring relationality, and—through a scaffolding of multiple forms of structure—is what we have attempted to construct.

5.1: Summary of Results

In this thesis, it was posited that an expansion of the concept of structure could add new tools to the modeling, design, and discovery of materials. A wide-ranging literature review was performed in order to illustrate what the current state of the field is, and to explore what various other disciplines offer in terms of structure and structuring concepts. Using these concepts, the materials paradigm and the concept of material structure was redefined in a manner allowing it to encompass more aspects of material structure than ever before. This framework of structural equivalence, consisting of five different forms of structure used in MSE, was then evaluated in different material contexts in order to test the efficacy of its framing and validation applications.

In answer to the research questions, this thesis presented the following answers:

- The epistemological approach to models within MSE was determined to be centred around the materials paradigm, the set of PSPP relations that govern material behavior. Furthermore, the process of building models within MSE was illustrated by Figure 5, then expanded upon in the text. The centrality of structure, mainly physical structure, was determined to be the guiding principle of the current approach. Systems according to other theories were covered in detail in section 2.3.
- Equivalence criteria of five different types were proposed to fully capture the swatch of ideas that are represented by ‘structure’ in materials modeling. Each of these five equivalence types were explored in detail, and specific criteria for each in the context of materials were proposed. These included definitional, empirical, informational, categorical, and theoretical equivalence. These types of equivalence were then used to analyse a selection of materials problems in chapter 4.
- Through the construction of an enriched materials ontology, the structural equivalence framework, and exploration of different types of materials problems, it was shown that

new types of structure could be successfully added to the epistemological approaches of MSE. By taking abstract structure into account, fuller accounts of materials concepts—and therefore a fuller network of representative models—can be built into the existing knowledge base of MSE.

- This treatment also illustrated the accessibility of materials research for the general study of systems, across disciplines. By molding such abstract approaches into a framework that can be applied to materials systems, new avenues of research and analysis into mereological and general systems have been opened.

The specific conclusions of the chapters of this thesis were as follows. In Chapter 2, the materials paradigm was presented and discussed as it is currently constituted. Physical structure being a central component of the paradigm, a brief glance at current conceptions of physical structures was presented at multiple length scales of interest to the field. The current iteration of structure in-hand, a survey of various philosophical approaches to systems theories was presented. Through this survey, a through line of systems thinking related to objects, relations, and perception was drawn through the portions of the works of Bogdanov, Bergson, Simondon, Whitehead, Russell, and Deleuze. The survey was intended to look for grounded philosophical ideas to enhance the concept of structure within MSE, so the selections presented build upon the idea of what systems are, how they are constructed, and how we relate to them. This conceptual approach is the first treatment of systems theories with a philosophical bent that has been applied to materials science and engineering, and is novel in both its approach and in its potential utility to both fields as a nucleation point for future research.

Using this survey of systems philosophies, a new ontological framework for materials was proposed, one centered on the relations and relational capabilities of interacting systems. This ontology casts the concept of structure not as groups of physical objects—cannonballs stacked on increasingly, infinitesimally smaller battlements—but rather as a network of relational processes. Structure in all its forms is a duration of perception—as interaction, as measure, as experiment—where objects experience ‘becoming’ solely in relation to other objects, and this becoming permeates every scale, every facet of reality. This interpretation of structure opens new ways for material systems to be studied, and is another contribution to potential philosophical treatment of materials, either by MSE practitioners or others.

Taking this new conception of structure, the remainder of Chapter 2 introduces the theoretical tools necessary for realizing the proposed ontological framework for materials. First, a brief survey of the relational interpretation of quantum mechanics (RQM) of Carlo Rovelli was presented as an example of other scientific fields where a similarly relational interpretation of physical systems has already been taking hold, but in a much less applied fashion. Looking for the keys to its success, it was surmised that processes of measurement, and the information relations between systems, were two key components of building relational structure. A quick overview of measurement theory and information theory set the background for what kinds of tools could be used from each, and how they might relate to theories of material structure.

These tools, being applied to materials systems, would be used to construct and iterate upon models of those systems, leading to a brief overview of the general approaches to modeling in MSE. The length and time scales of import were briefly discussed, as well as how different levels of structures are treated with different methods, methods which ideally are to be connected at the interfaces. The MSE approach to modeling is similar to the approaches of other scientific modeling, so the general topic of how models relate to theories was discussed and used as a springboard to present the proposed mathematical solution to model building, category theory.

After a general introduction to category theory, the concept of equivalence was presented as a potential solution to ferreting out forms of structure within modeling. Though the idea of using equivalence criteria as a method of finding structure within relations and processing comes from a treatment of categories—looking for mathematical structure—it was then shown that equivalence criteria appear in all manner of forms. The utility of equivalence criteria as a framework building concept was discussed and, in order to capture the fullest sense of materials structure, five forms of equivalence criteria were proposed. The last section summarized the equivalence framework and its embodiment of the new materials ontology, and the new conception of structure.

Chapter 3 presented the proposed framework of equivalence criteria for materials models, encompassing five forms of equivalence that include definitional, empirical, informational, categorical, and theoretical structures. The components of each sense of structure were defined, and formal equivalence criteria were proposed. Fitting within a framework which is being called ‘Structural Equivalence,’ it was shown how each of the five forms of equivalence fit together and inform one another. The utility and potential applications of this framework were briefly discussed before examples in the following chapter.

The framework of structural equivalences is the main contribution of this work. The framework incorporates every sense of structuring that arose from the literature review, and provides a nuanced, flexible tool for analyzing the structures of models. The meta-analysis that this equivalence determination method provides can inform the derivation, construction, or iteration of models within MSE and, most likely, in other fields as well. Presented thusly, the method is a tool for exploring the structure of theories in general, as well as a method of validation for existing models. The framework captures the essentials of structure in various senses, but is also robust enough to itself be iterated upon as new concepts of structure arise, or new criteria of equivalences proposed. The idea of informational equivalence, specifically, is a novel approach to data analysis within MSE, building on treatments of the concept within computer science [112], [113].

Chapter 4 took this structural equivalence framework and applied it to four different scenarios within MSE. First, the framework was applied to two theories of modeling—molecular dynamics and finite element methods—that are often presented together in terms of how one might bridge multiscale problems within the field. A brief background on the approaches and mathematics of each theory led to an analysis of the structures of both theories. If two theories are to be linked, it is important that the link between the two be arranged in such a way that the structure of both theories is either intact, or translated across the bridge formed by that link. This section illustrated that, if a bridge between MD and FE is to be constructed, the form of the structures of each would need to feed through. The basic shape of the structural equivalence criteria for both MD and FE were derived and presented formally, including the potential structure of any translation between the two. The purpose of this analysis was to show how the framework is used for problematizing questions within MSE, and to provide a meta-model for structural comparisons with existing bridging models for multiscale problems that use MD and FE theories.

In section 4.2, the framework was then applied to characterization methods within MSE, specifically looking at two different materials processes for the same material system (copper) in terms of their effects on X-ray diffraction measurements. Assuming definitional and empirical equivalence, the informational and categorical structures of the models based on published XRD data were sussed out and illustrated. For both data sets, a computational set looking at temperature effects and an empirical set looking at cold-working effects, an information analysis was performed calculating the divergence of the probability distribution of XRD data from that of a chosen reference distribution.

This analysis showed the informational effect of processing, and proposed a method for measurement of information structuring potentials on the basis of experimental data. The two sets were confirmed via calculation of the relative entropy to have at least a trivial information equivalence, and the work needed to further confirm that equivalence was outlined. This example illustrated how various notions of state change within materials models could be treated, and specifically how the informational equivalence criteria could be used to analyze the data produced by specific characterization methods as long as the results could be rendered as probabilities. Methods of finding information equivalence and proposing various informational equivalence criteria should, then, be valid for any characterization or computational technique. While this text presents only two forms of information as criteria, it is acknowledged that any measure of information could serve as the basis for constructing new criteria, all dependent upon the context of use.

Section 4.3, showed a method of using the structural equivalence criteria to compare multiple mechanisms of a single failure mode, creep. This analysis looked at the dominant mechanisms of creep for a single material, again copper, and compared the models on the basis of the structure that would be produced by an informational data analysis, and at the categorical structure that follows from the mathematical form of each strain rate equation describing the particular mechanism. Concerning the former, only the shape of the analysis was presented as the only data in hand at the time of this thesis were the data used to construct the models, and therefore inappropriate for measuring relative entropy as the model data is used as a reference in that method. If a full information analysis was to be performed, new measurements of strain rates across the gamut of applied stress and temperature fields would need to be taken, and that data (taking the measured strain rate as the stochastic variable) then turned into probability distributions to measure against the model. As stated in the text, this form of model iteration is used with some frequency in other contexts, known as relative entropy minimization [106].

The categorical structure of the models of two mechanisms of creep, a general power law mechanism and a general diffusional flow mechanism, were both analyzed and shown to be equivalent. This equivalence was determined on the basis of their shared relation to a strain rate variable, one that was additive across all mechanisms of creep. Because both models could be structured to produce the same form of a variable, and that each of the forms of that variable produced by the individual models could then be added together, it was shown that both mechanisms show at least a tacit mathematical structure on that basis. This is a new form of analysis and validation for materials models—one based on the mathematical structure itself—and it points towards a novel method of enriching the physical and analytical models of MSE. Integration of existing mathematical structures into the models of MSE on the basis of combined categorical features could add many analytical tools to the modeling of materials.

Finally, section 4.4 presented a more detailed analysis of an overlapping variable of the two diffusional flow creep models that were analyzed, specifically the average grain size of a polycrystalline metal. The use of average grain size as a variable was discussed in terms of the physical geometry of each of the mechanisms, and the proportional relationship between them was explored. In order to compare geometric properties, a method of the determination of grain size on the basis of geometric relations was reviewed, and the pertinent details for a categorical analysis extracted. A brief discussion of the form of information analysis that could be done was outlined, followed by a definition of a category of grain structures.

This category was defined in order to capture the mathematical structure that variables of grain size—and specifically the measure of average grain size used in the two dissected models—all share in common. The category illustrated an example of how to construct structural (in the sense of the framework presented in this thesis) requirements of variables across models, a novel method of analysis for MSE contexts. The two instances of average grain size were then determined to be mathematically equivalent on the basis of their categorical structure.

This thesis proposes a new ontology of materials, outlines what specific elements that ontology adds to the concept of material structure, then proposes a framework for validating structures across materials theories on the basis of that new ontology. The framework of equivalences that is presented here is a first attempt to combine multiple senses of structure in a method of material model analysis. The method provides new connective pathways between MSE and multiple other disciplines, including philosophy, physics, logic, computer science, and mathematics, that can be explored within the context of structure and structuring processes. The method also creates novel ways to analyze materials systems, approaches that take structural aspects of each of those disciplines into account.

5.2: Limitations

The meta-analytical techniques proposed by this thesis are potentially abstract in nature. A limitation to their uses within MSE might be that it is difficult to construct a research question for specific systems, or specific contexts, where the various forms of structure within the equivalence framework are easily identified. Formal definitions, or data in the form of probabilities, or some mathematical structures for a materials model may be difficult to conceptualize, or obtain, potentially stripping this method of some of its potency. Access to data sets, in particular, remains a challenge for using this type of analysis on existing or historical materials models. The methods proposed herein are also agnostic to the quality of models and data with which they are used. If the models are inaccurate, or the data is corrupted in some manner, the techniques of determining structural equivalences will not inherently flag poor results, or correct for them. Outliers resulting from bad models will only become apparent in relation to analysis of larger data sets, or known models.

Finally, the framework presented here can require potentially time-consuming preparation, meaning that its application to engineering problems which require quick answers and turnaround might not be practical. If, however, analysis of a system using the structural equivalence framework has already been prepared for the context of some test, then the results of that test and the analysis of those results should be readily amenable to the method presented here.

5.3: Future Work

The nature of this project lends itself well to the speculation on future applications of the proposed framework. Due to the framework being constructed from theories spanning multiple disciplines, it follows that there are various approaches from many different starting points on analyzing the results of this thesis, both initializing from MSE and from other fields.

5.3.1: Future Work in MSE

Within MSE most future projects would most likely be application of the framework to materials problems, and iteration upon the equivalence criteria and the framework itself. Specifically:

- A database of historical models like those analyzed in sections 4.3 and 4.4 could be constructed. The database would be an incredibly useful tool for the study of the evolution of models within MSE, and a repository of the various approaches and assumptions that have classically been used. The entries would allow modellers to search for specific structural contributions when studying the evolution of particular models of materials phenomena over time.
- Further definitions of information could be used to create new informational equivalence criteria for different types of data. There are many formulations of information, and each measures a different aspect of data sets. An expansion of the criteria used for analyzing information in materials contexts could create new analytical tools for use within materials modeling.
- Using specific information models to create metrics, rather than measuring divergence, could open the door to creating mathematical manifolds of the various senses of materials space. If manifolds representing materials space could be formulated, a vast array of mathematical tools become available for use in analyzing materials, branching the field even further out into abstract topological studies.

- In addition to manifolds, the analysis of materials systems might benefit from the application of other mathematical structures, e.g., rings, loops, groups, etc. Category theory is a natural door into the application of those structures as categories are already used for the comparison of structure across abstract mathematical objects. If materials models are categorized, then new mathematical structures can be tested for their efficacy within materials research.
- More work to validate the proposed studies in Chapter 4 could be done, specifically: using the proposed form of a bridging model from section 4.1 to study the structures of existing bridging models; a full test suite of XRD patterns to map the information across the full range of temperatures and cold-working conditions, rather than the limited amount obtained here; and a full test suite for strain rates produced by various creep mechanisms, in order to compare the models used historically to new creep data on a structural equivalence basis.
- Integration of renormalization techniques into the methodology of the SEF could provide another powerful tool to analyze scale bridging techniques specifically. Therefore, an analysis of renormalization and renormalization group methods should be undertaken using the SEF to determine the structural processes of both, and the promising potential of using both as the basis for criteria of equivalences.
- The methods embedded within the SEF can serve as a springboard for the refinement of existing theories, or construction of new theories, within the field.

5.3.2: Future Work in Other Fields

Materials are the bridge between quantum physics and human beings. The scales of interest for materials are the connective tissue between what is commonly considered to be the fundament of nature and ourselves, making materials essentially the medium of communication between us and whatever it is that comprises us and everything surrounding us. The study of material structure is a study of that connective tissue, and a means for relating to it. That sentiment encapsulates the opinion that materials and the models arising from MSE ought to be studied more often by those outside of our field. Specifically:

- A first-order logic treatment of materials models could standardize and simplify the types of relations standard to the field, but could also provide logicians with new frameworks to access well-studied phenomena in a systematic method.
- Materials provide a variety of entry points for the study of aggregates, and therefore also for the study of the behavior of aggregated mathematical structures assigned to small scale phenomena. The mathematics of quantum theories mediated through the collective experience of MSE could help to build a more holistic modeling language.
- The study of communication of materials systems, either by measurement, by convention, or through modeling, could add new approaches and measures to the field of information theory. Materials communicate in an enormous variety of ways, and an informational analysis of materials systems could enrich the understanding of noise and signal in the communication pathways of aggregates.
- Structural and realist philosophers might also find connection points from this work, as the philosophical priors outlined in section 2.3 touch on many well established topics. Specifically, a metaphysical study of material relations could add experiential heft to the topic and make concepts within systems philosophies more accessible to every day experience.

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Appendices

Appendix A: Sample Calculations

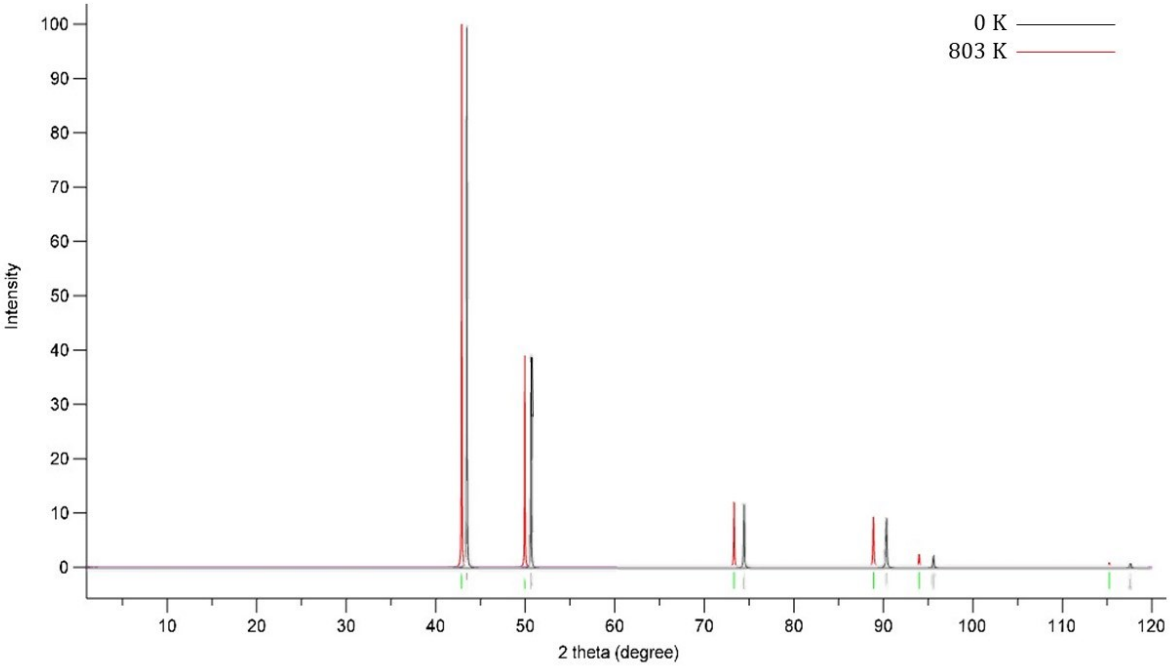

Figure A.1: The shift in the XRD pattern shown from 0 K(black) to 803 K (red). Produced using Match! [92].

Table A.1: Intensity data for the XRD pattern of Cu at 0 K between 43° and 43.5° 2θ

Angle [2θ]	Intensity [a.u.]
43.00	0.24502
43.01	0.25545
43.02	0.26657
43.03	0.27843
43.04	0.29112
43.05	0.30470
⋮	⋮
43.50	57.28875

$$p(x) = \frac{\Sigma x_n(2\theta = i, i + 0.5)}{\Sigma x_n(2\theta = 0, 180)} \tag{47}$$

$$p(x)_{0\,K} = \frac{\Sigma(0.24502, 0.25545, \dots, 57.28875)}{1557.48921} = 0.397395$$

Table A.2: Intensity data for the XRD pattern of Cu at 803 K between 43° and 43.5° 2θ

Angle [2θ]	Intensity [a.u.]
43.00	4.65621
43.01	3.90223
43.02	3.31532
43.03	2.84984
43.04	2.47477
43.05	2.16837
⋮	⋮
43.50	0.13995

$$p(x)_{803\,K} = \frac{\Sigma(4.65621, 3.90223, \dots, 0.13995)}{1557.48921} = 0.028399$$

Appendix B: Selected Ologs

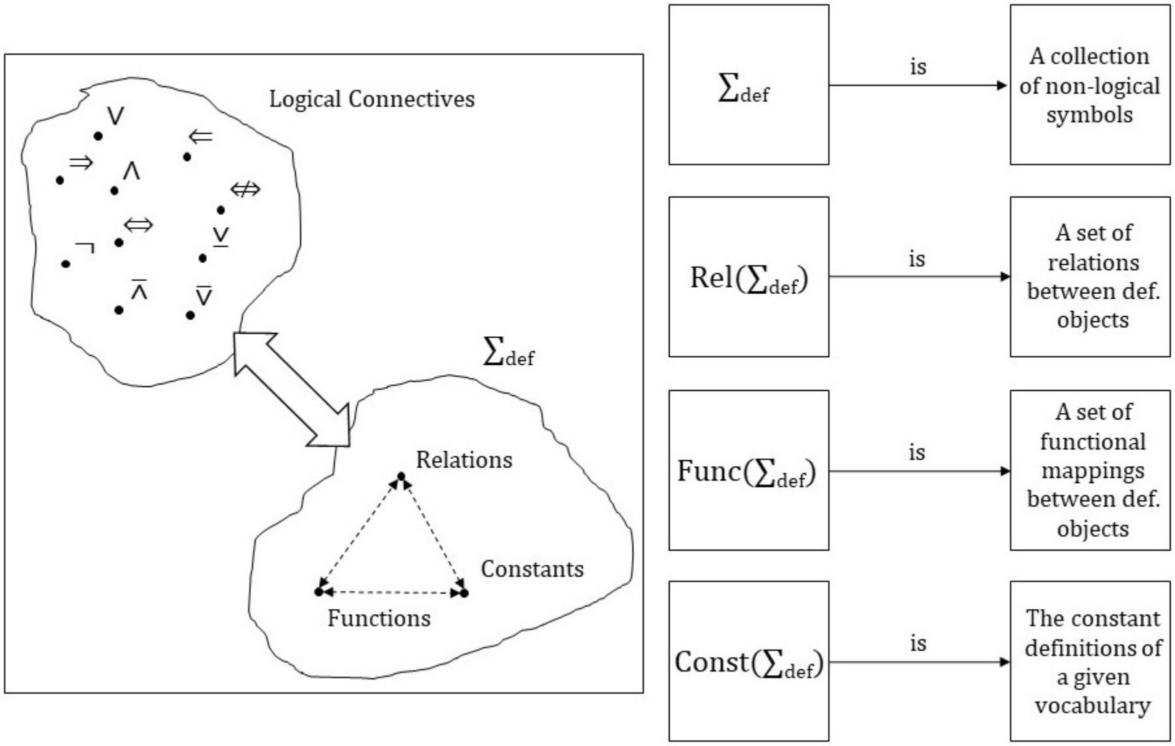

Figure B.1: Ologs illustrating Definition 3.

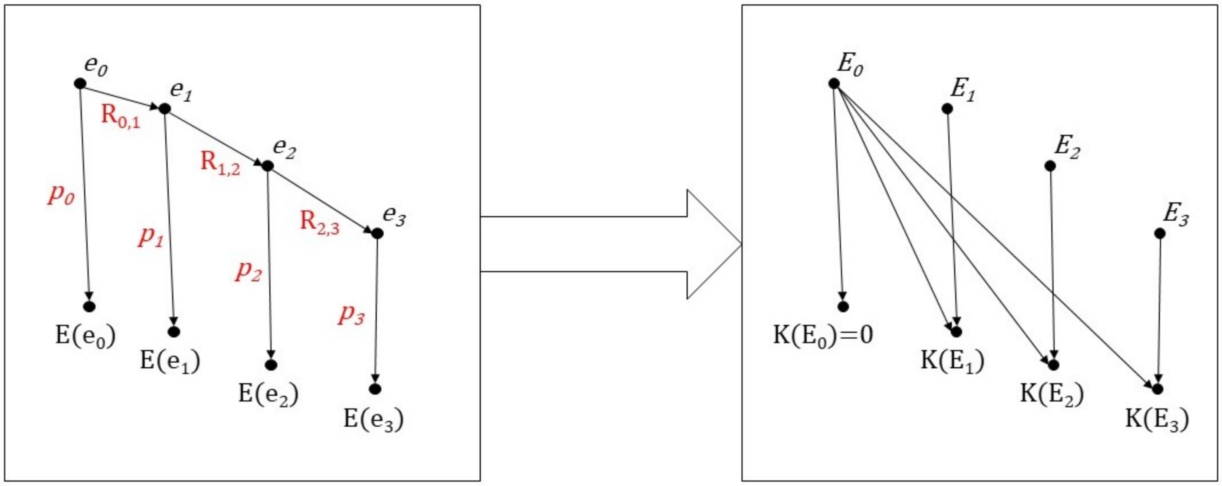

Figure B.2: An olog illustrating the creation of probability distributions for some random variables, $\{e\}$, and how the relative entropy of those distributions is found.

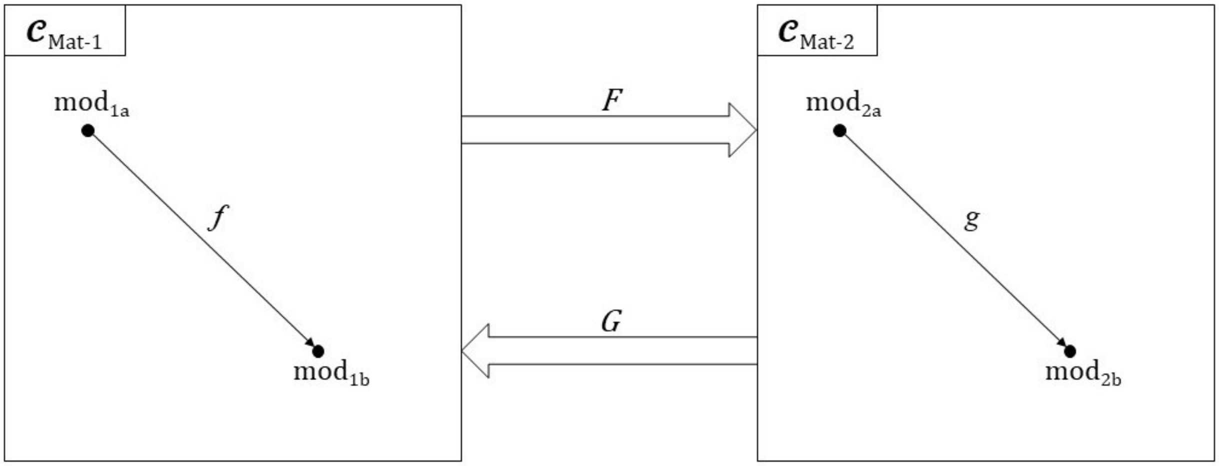

Figure B.3: Olog illustrating Definition 9.