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Models in Scientific Inquiry

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Dedication

To the family, friends and community that made my research possible. I am especially grateful to my parents, Jody and Sandra Price, who fostered in me the resilience one needs to see a project like a dissertation through.

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Abstract

This dissertation studies how models become useful for scientific inquiry. Towards this study, I develop a theory on the cross-discipline transfer of mathematical models. The first part of this theory characterizes the way in which scientists must respond to the constraints in making a transferable model useable in their discipline. I invent the notion of a landing zone to identify the aspects of their domain that scientists prepare for the use of a transferrable model. The second part connects this response-to-constraints to cases of conceptual progress resulting from model transfer in biology and chemistry. The last part of this dissertation characterizes scientific inquiry as problem solving, where I invent a framework for identifying how scientists use models to frame problems so that they are easier to solve.

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Chapter 1: Introducing Model Transfer as a Doorway

This dissertation uses the scientific activity of model transfer as a doorway into a novel perspective on issues to do with modeling in science. Through characterizing how model transfer works, this dissertation provides an approach to understanding more generally what models do in science. Model transfer itself is an interesting puzzle; it seems peculiar that a concrete scientific representation like a model can target some scientific phenomena, can be used by scientists to study these phenomena, and then can represent something in a domain that studies completely different kinds of phenomena. One understanding would be that differences are only surface level and the phenomena of separate disciplines in fact share some essential connection. However, it does not seem to be the case that scientists understand this connection in this way, or at least their work indicates otherwise. In the cases I examine, scientists often fit these transferrable models, and the phenomena they target, into much different inquiries. Model transfer is also conceptually disruptive, producing tension and debate about foundational concepts similar to the tensions described by Thomas Kuhn taking place with scientific revolutions (Kuhn 1962). Whatever the connection between domains that allows for model transfer, there seem to be some interesting and messy details in the actual practice of transfer; details that provoke thoughtful

theorizing by scientists. I argue this interesting mess applies more generally to the use of models in science. We can learn about how scientific domains work conceptually, how models contribute to scientific aims, and how to understand the epistemic value of models through attending to model transfer.

Scientific domains are complicated. For a model to be transferable, scientists must disentangle it from its myriad connections to the phenomena and to the theory of its original domain, and then re-entangle it with the new domain. This process recalls the boggling complexity of attaching a transplanted organ, with numerous sorts of networks, blood vessels, nerve fibers and tissue, needing work for a functional re-attaching. In scientific domains, there exist various levels to which scientists need to reattach the model: the level in which scientists work towards solving problems with its phenomena, experiments and labs, as well as the theoretical and conceptual level where the meaning of scientific language gets determined, and where scientists imbue the characters in their story telling with meaning.

My dissertation explores the dimension of model transfer to do with grafting the transplantable model. Theorists have had less to say about this process of de-abstracting/de-idealizing — the scientific practice most analogous to grafting the organ back in the body. Accounts of model transfer so far focus on characterizing the process of abstracting a model (what, above, I call ‘disentangling’), i.e. making a model transferrable (Humphreys 2002 and 2004, Knuuttila and Loettgers 2014). Abstraction may be more straightforward to understand, especially for those trained in analytic philosophy. Abstraction is a

process of conceptual subtraction. For example, in formal logic we subtract the features of a proposition by replacing natural language words and grammar with symbols. Rendering a model generic through abstraction similarly involves removing or altering assumptions that are descriptive of domain-specific phenomena while keeping syntactic features intact. After the surgeon separates the organ, the surgeon must restore its capacity to function (or be useable by the body) when placed back in a context rendered similar-enough. The result of transfer is a model that scientists can use to represent phenomena that are similar yet different from the model's original use.

In developing a theory of model transfer what must we pay attention to? So far, the answer is: abstraction and the product of this abstraction — the transferrable core of models. The underlying assumption is that once we have understood what makes a model generic enough to transfer, we understand how it can apply across disciplinary lines. On what grounds is it scientifically reasonable to then use an abstractable-enough-to-transfer model to study different types of phenomena? The first part of my dissertation motivates the idea that these grounds cannot only be the process that renders the model generic, or the property of the model being generic. To provide an account of transfer we must pay attention to the interaction between generic (mostly mathematical) factors in constructing models and the world which scientists work within. Otherwise, an account of model transfer does not do justice to how scientists achieve transfer.

There is some history in approaching philosophy of science with an eye to formal structures first — mathematical and metamathematical. The largest such operations were the syntactic and semantic views of theories. My dissertation takes a lesson from the pragmatic turn in these understandings of scientific theory structure and applies it to understanding model transfer. One commonly cited problem with the semantic conception of models, for instance, is that it does not do justice to how scientists work with models. Seeing models as an entirely theory-derived, mathematical constructs does not account for how scientists achieve their aims in using models. In scientific practice, highly abstract 'theoretical' models rarely represent any observable system. Entirely theory-derived models end up representing highly idealized situations that do not obtain in the observable world. As the story goes, if we pay attention to how scientists construct models and how they use models, we realize that an account of modelling must pay attention to the interaction between different 'levels' in scientific domains — phenomena and theory for instance — to understand model construction and model use (Morgan and Morrison 1999). My dissertation takes this same general lesson about the turn in discussion about models from the semantic view to models as mediators, and applies it to discussion about model transfer. In my next chapter, I introduce the concept of the landing zone, to identify the interaction between the theoretical and practical levels in achieving model transfer.

Cartwright's (1983) description of theory entry highlights the part of modelling to which my investigations of model transfer draw further attention.

Theory entry here refers to the activity of scientists preparing descriptions of phenomena — facts — so that this description may be brought ‘under’ theory. Cartwright counts the preparing of these descriptions as preparing phenomena to meet the needs of theory. Meeting the needs of a theory includes preparing phenomena to meet the needs of the mathematics of a theory — i.e. its equations. The idea of preparing phenomena to meet the needs of mathematics is one that I draw upon to motivate analyzing what scientists do to make model transfer possible. For Cartwright, the fundamental mathematical laws of physics do not describe any objects in reality. Therefore, under her picture of scientific modeling, physicists must render fundamental laws into mathematical descriptions that ‘get the job done’. In order to decide on what form a mathematical law will take scientists must ‘...present the phenomenon in a way that will bring it into the theory’ (Cartwright 1983, p. 133). This “presentation”, as she calls it, is theory entry. Scientists prepare descriptions that allow them to know, for instance, what boundary conditions they can use, what approximation procedures are valid etc. An example she uses is of the Hamiltonian in quantum mechanics. The Schrödinger equation tells us how a quantum system evolves subject to a Hamiltonian; hence, to model a quantum system, one must know how to pick the Hamiltonian. Cartwright argues that when a physics student learns quantum mechanics, they are not just learning ‘the theory’; more importantly, they learn skills about how to make the theory useable, one of which is how to choose the correct model Hamiltonian. This choice depends on how one wants to set the stage for modelling, and other scientific activities. For

instance, the choice can depend on whether the ‘particle in a box’ Hamiltonian, linear harmonic oscillator, or coulomb potential offer more useful modes of theory entry. Deciding how to prepare the phenomena is an activity that has more to do with practical rules. Some of these rules are constraints on applicability imposed by theory — we need equations to be solvable and this constraint dictates which, for instance, Hamiltonian we use — some are rules of thumb learned through lab work or rules to do with norms of communication that make collaboration possible. Pragmatic considerations are necessary to make scientific work on phenomena using the theoretical laws of physics possible.

A similar sort of choice takes place in physical chemistry, where to use models from physics, pragmatic standards guide the fitting of abstract, theoretical mathematics to the phenomena, and preparing the phenomena to be the target of a transferable model. This modelling in physical chemistry is the focus of the next two chapters of my dissertation, where I use this history to build a case study to support my account of model transfer.

In my second chapter, I discuss how there exists a sort of scientific activity that seems to be the locus of theorizing with model transfer. This type of decision-making is analogous to what Cartwright means by theory-entry. It involves choices made in order to present the phenomena in a way that makes the phenomena modellable by a transferrable model. An example from Cartwright (and one applicable to quantum chemistry) would be the detailing of how a target system is ‘like’ a particle in a box when using a ‘particle-in-box’ Hamiltonian with a Schrödinger equation. I call this sort of a detailing a ‘landing

zone' in my first chapter. It is a thing to which transferrable model templates apply. I use two accounts of model transfer to set the stage for introducing landing zones: Knuutilla's (2011 and 2013) concept of a model template and Humphrey's (2002, 2004) concept of a computational template. These accounts are the foundation for my identification of the transferrable thing in model transfer. Although I agree with Knuutilla that conceptual features of model templates contribute significantly to scientific theorizing, just an account of model templates does not exhaust the scientific theorizing to do with model transfer.

My second chapter takes the concept I develop in the first chapter and uses it to characterize the impact that these practical considerations in preparing phenomena have on the theoretical level of scientific domains. I call this impact 'conceptual progress'. An upshot of attending to conceptual progress resulting from model transfer is that it offers a novel direction from which to approach puzzles in philosophy of science to do with interdisciplinarity and intertheoretical reduction.

A theory of model transfer promises to be an interesting analytic tool for approaching other puzzles in philosophy of science. My second chapter discusses one such puzzle about the connection between reduction and scientific concepts. The puzzle goes like this. Much of the modelling in chemistry uses mathematics transferred from physics. However, there exists tension between chemical and physical conceptions of phenomena for modelling. Roughly speaking, since the empirical concepts do not travel with the mathematics, there exists a puzzle about what determines the chemist's conceptualization of

phenomenon. In philosophy of chemistry, a classic question regarding the relationship between chemistry and physics at the theoretical level is about inter-theoretic reduction (Scerri 2007, Hendry 2010, Gonzalez, Fortin, Lombardi 2018). An idea in this discussion is that the meaning of chemical concepts could be 'traced back' to physics concepts if it were the case there was a strong inter-theory link like reduction. However, a chemist's conception of phenomena like bonding is not straightforwardly reducible according to dominant literature in philosophy of chemistry. Molecular orbitals, valence bonds, resonance, Pauli forces are just some examples of notions central to mathematical modelling in chemistry that confound inter-theoretic reduction. This leaves a question: where do these scientific concepts come from?

To answer this question, I examine the preparation that modelers make in order to transfer model templates. Modelers prepare phenomena by inventing new categories, or altering the meaning of current categories, in their domain as a response to the requirements of the model template's mathematics. Bader's topological atom is an example of an alteration to the category 'atom'. To characterize this preparation, I examine the assumptions these modelers make when using a model template, and debates about description of phenomena that take place surrounding these assumptions, to characterize how model transfer impacts conceptual progress. These impacts result in mini-paradigm shift like changes in the way that scientists view the world they work within. I argue this is because in order to make a model useful scientists must engage in a creative, intellectual pursuit, inventing new sorts of things. In the second chapter, I

compare the use of the virial theorem in chemistry brought about by the invention of the ‘topological atom’ and the use of the ideal gas law in ecology brought about by the invention of idealized populations. Both inventions resulted in debate over the conception of discipline-specific phenomena that I analyze as resulting from conceptual progress. Paying attention to these inventions to make model transfer possible locates a mechanism for the invention of scientific concepts, the mechanism that makes chemical concepts not straightforwardly reducible physical concepts.

My third chapter presents a positive framework accounting for the epistemic workings of transferable models, and modelling in general. This framework uses cognitive science theory on problem solving. Seeing model transfer through the lens of problem solving helps us to understand the activities that makes transfer possible, and how these models hold epistemic value for the investigations they see use within. Broadly, in the cognitive science literature, the activity of problem solving is split between two types of action, framing and searching. Mathematical models see use in scientific efforts to frame investigations and models hold value if this framing makes possible the use of heuristics in a search for the solution to problem.

Framing is the activity wherein problem solvers decide which aspects of the task environment are salient to solving the problem. Broadly, framing is the activity where scientists conceptualize the problem by determining what information is relevant to track and structuring the search around this information. Scientific models give scientists ways to organize and structure information

towards this end. Scientists may use model transfer to shake up (or reframe) an investigation that they see as spinning its wheels, or in need of a new perspective. In a scientific investigation, altering or reframing the problem will involve bringing in different sorts of mathematical tools for modelers to use from an outside source in the same way an everyday problem solver might bring new tools to bear on an intractable problem.

Chapter 2: The Landing Zone

1 — Discussion

Why are some scientific models especially transferable, seeing uses in domains much different from the one where they originate? There exists a short history of discussion concerning this question. In *Extending Ourselves,* Paul Humphreys draws up a unit of analysis for the invention and deployment of tractable mathematics - computational templates (Humphreys 2004). According to Humphreys, models are transferable if they have computational templates at their core. Tarja Knuuttila and Andrea Loettgers offer some modifications to Humphreys' analysis in two papers (Knuuttila and Loettgers 2011, 2014), arguing that there are also conceptual features of models that factor into the spread (transfer) of certain mathematical models. Both accounts of model transfer work towards a depiction of progress in the sciences as constituted by, in part, the redeployment of models in new domains. My contribution to this depiction is a new notion - the landing zone - a target system that makes possible the use of transferable mathematics in a new domain.

Two aspects of scientific modeling motivate Humphreys' analysis of model transfer. First, as Humphreys sees it, progress in the sciences largely involves a drive towards tractable application of mathematics: "Whenever you have a

sudden increase in usable mathematics, there will be a sudden, concomitant increase in scientific progress in the area affected" (Humphreys 2004, pp. 55). A drive towards tractability results in the spread of computational techniques across scientific domains. Therefore, an account of the dissemination of computational techniques that highlights the role of mathematical tractability ought to provide us with a new vector for depicting scientific progress. The story of model transfer is thus also a story about the advancement of the sciences. In analyzing model transfer, we may gain insight into the rationality of scientific progress.

Additionally, scientific models are, of course, insofar as they are mathematical, limited to the available mathematics. For instance, Newtonian models of the solar system employed calculus, and before them, the Ptolemaic models of the solar system employed the geometry of epicycles. Newton's invention of calculus drove development in modeling the solar system by providing usable methods for calculating planetary motion in celestial mechanics. Humphreys argues that in analyzing the invention and transfer of these mathematically tractable parts of models, we come to a novel perspective on how certain methodologies and modeling practices such as those found in Newton's celestial mechanics become available.

Analysis of the invention and deployment of tractable mathematics requires a unit of analysis, some *thing* that is the fundamental object of investigation. Accounts of scientific progress have typically invented such units of analysis - paradigms, research programs, theories. Humphreys invents the computational template. A computational template is a generalizable and

tractable equation, function, or computational method. Transferable models have computational templates at their core. Humphreys thinks, similar to the inventors of these other units of analysis, that we can make a cogent categorization of the sciences based on dominant computational templates. For instance, percolation theory, a way to describe the behavior of networks —clustering of nodes — sees use in a preponderance of models across domains. As a computational method, it makes possible the application of mathematics towards representing "phenomena as varied as the spread of fungal infections in orchards, the spread of forest fires, the synchronization of firefly flashing, and ferromagnetism" (Humphreys 2004, pp. 70). The invention and deployment of percolation theory as a computational template constitutes notable progress in the study of these phenomena.

Computational templates that see as wide of dissemination as percolation theory are rare yet influential. A computational template can be an equation, function or a computational method like percolation theory. According to Humphreys, computational templates are transferable because they are tractable and generalizable, features they owe to having a particular syntactic form. For instance, common to all uses of percolation theory is a function that describes the system state - the state of being 'magnetic' for the Ising model or the state of being 'infected' for fungal growth models. This state function's syntactic form, the relationship between variables, is invariant between applications, thus generalizable and transferable.

Knuuttila and Loettgers' 'model templates' constitute a second approach to

identifying the factors important to explaining model transfer, building on Humphrey's notion of a computational template. According to them, the analysis of syntactic form and the computational tractability that it affords does not exhaust the factors involved in model transfer. They write that model transfer "cannot be accounted for by tractability alone. In [the Ising model's] case, apart from mathematical forms and methods, a very general conceptual idea of the kind of mechanism of interaction involved was also transferred" (Knuuttila and Loettgers 2014, pp. 297). Model templates, they argue, facilitate the transference of models because they sensitize us to patterns shared by a variety of empirical systems. Their notion of a model template captures the "intertwinement of a mathematical structure and associated computational tools with theoretical concepts that, taken together, depict a general mechanism that is potentially applicable to any subject or field displaying particular patterns of interaction" (Knuuttila and Loettgers 2014, pp. 295). Thus, both computational and conceptual features of a particular mathematical tool contribute to its transfer. Futhermore, even though they characterize the Ising model template as being about a 'mechanism', the general conceptual idea at the heart of a model template does not need to be an idea about causal structure (Knuuttila and Loettgers 2016). They mention that ideas about, for instance, cooperative phenomena, have 'explanatory universality' just within physics due to mathematical explanation — instead of causal.

In this chapter, I will refer to the transferable mathematical core of a model as Knuuttila and Loettgers' 'model template' - an "abstract conceptual idea

embedded into a mathematical form or method". For the Ising model template that they discuss, these abstract conceptual ideas are "critical point phenomena", "phase transitions", and "equilibrium states" and they constitute a "conceptual framework that cannot be detached" from the model template (Knuuttila and Loettgers 2014, pp. 298). They are ideas concerning the existence of types of things. Since they constitute a "conceptual framework that cannot be detached from the model", for the Ising model template mathematics to be usable, critical point phenomena, phase transitions and equilibrium states must be assumed to exist.

Knuuttila and Loettgers' addition to this discussion highlights the conceptual features in model transfer. Since model templates are mathematics embedded with concepts about mechanisms and types of systems/objects, they carry with them ontological commitments. These conceptual features of templates factor in the construction of models to the extent that the target phenomena must be compatible with the model template's ontological commitments. To characterize this preparatory activity, I propose a complementary notion to that of a model template for discussion on model transfer, the 'landing zone'. As an addition to analyzing the *thing* transferred, this notion of a landing zone contributes towards analysis of the *things* to which templates may be applied. Model templates are not simply applied to a system, but a specifically prepared target. Broadly defined, a landing zone is a model's target system. It has two characteristic functional roles. First, it functions as the target for mathematical description for a model. Additionally, it functions to make

possible the use of transferable mathematics. Modelers design a landing zone to fulfil requirements for the use of a transferable model template. These two functional roles are definitive of a landing zone. Identifying features of scientific modelling that function as a landing zone complements discussion surrounding model transfer.

There are two motivations for further analysis of these features in modelling that I call landing zones. First, adding this notion to current accounts of model transfer identifies the ontological features of a target system that make possible the use of transferable templates. Second, it enables accounts of transfer to depict scientific decision making by providing a unit for analysis of salient features in the target system that are prerequisite for the use of transferable mathematics. A significant part of progress in model building is not only the invention of usable mathematics, but also the construction of a model (including, at least to some degree, its ontology) in a manner that makes model templates useable. This ontology, if the model transfer is successful, often becomes a prominent feature in a domain's modeling practice, as the case I introduce later in this chapter illustrates.

This appearance of a new sort of ontology also took place with the transfer of the Ising model template to neuroscience. The Ising model template's computational methods make modelling cooperative phenomena tractable. The model represents ferromagnetic materials as a lattice of nodes where each node has two states, spin up or spin down. The model thus contains a mathematical function that assigns a probability of realizing an ensemble of states. For

ferromagnetics, this is a function of temperature. Each node has an interaction with its neighbour; physicists specify this interaction as a constant in the state function which varies depending on the material modelled. In the typical two dimensional Ising model, each node interacts with four neighbors. The Ising model takes this mathematical description of the possible ensemble of microstates and uses a *partition function* along with a *state function* to describe the overall macro state of the system, its energy typically. For these mathematics to be useable —tractable —, scientists must prepare the phenomena.

The transfer of this Ising model template required neuro-scientists to prepare a similar description of neurons. One difficulty is that neurons are quite different from the ‘atoms’ in an Ising model system in many ways. For one, neurons in a biological network are not binary. Their interactions are chemical and electrical, and these chemical and electrical states vary continuously For instance, the neurons in a human brain interact by releasing neurotransmitters. The release of neurotransmitters depends on the action potential - a measure of the voltage of a neuron. There are a multitude of possible input and outputs for each neuron that affect the action potential, and action potentials can take on a continuous range of possible voltages. This myriad of possible values makes it so that neurons, unmodified, do not exhibit the sort of simple, cooperative interactions that make possible the application of the Ising model template. As described, this target system is thus not a suitable home.

So, in part, the notion of cooperative mechanisms embedded in the Ising model template makes neural networks a potentially relevant site for application.

However, there are important preparatory conditions for the use of this template in neuroscience as part of the Hopfield model — a model of memory in neuroscience that Knuuttila and Loettgers study in their article on model templates (2014). The conceptual and computational features of a model template by themselves do not completely depict the factors in this case of model transfer. For instance, in order to apply the template at the core of the Ising model as a representation of neural networks in the Hopfield model, there needs to be some feature invented as the target for description by the Hopfield model that makes possible the representation of neurons as binary- "[neurons] are rendered binary by introducing a threshold: if the summed up signals exceed a threshold, the neuron fires an action potential and goes over into a quiet state. The model neuron σ takes the value 1 in case it is active, and the value 0 if it is inactive" (Knuuttila and Loettgers 2014, pp. 293). This 'binary neuron' that exists in neither the domain of neurobiology nor the Ising model template is part of the landing zone, the lattice of neurons. It is a landing zone that Hopfield prepares by specifying the 'simple cooperating phenomena' as neurons with action potentials. The landing zone, along with the binary neuron, functions as a target for description by the Ising model template's state function by instantiating a necessary property - binaryness. This property makes possible the description of neurons as simple cooperating phenomena, thus functioning to make possible transfer of the Ising model template. The Hopfield model's target system is ontologically compatible with the Ising model template because it claims the same sorts of things exist. A similar mechanism, handshaking, is identified by

Bursten for the ontological compatibility of multiscale models (Bursten 2018). The ontological compatibility functioning of the landing zone is made possible by an ontological claim about the sort of thing that the model represents. In this case it is a claim that neurons are discreet. Much like how the Ising model template consists of mathematical methods embedded with concepts about what exists, target systems that function as landing zones provide an ontology built into a mathematical method. To be more specific, the landing zone provides an ontology in that the properties that the target system features instantiate are an answer to the question 'what exists?' In the Hopfield model's case, since Hopfield describes the binary neuron as having two values, this answer is "binary phenomena".

Adding the notion of a landing zone to this discussion makes salient an important and potentially interesting factor in model transfer that neither previous account covers. To demonstrate that the notion of a landing zone is an important addition to the discussion on model transfer, I provide a case study on a model in chemistry constructed from two model templates. This model is the Quantum Theory of Atoms in Molecules (QTAIM) and the transferrable templates it uses are the virial theorem and density functional theory (DFT). First, I will be examining QTAIM's use of the virial theorem as a technique to make calculating kinetic energy tractable. The virial theorem is a model template and as such requires a target system to have an appropriate landing zone, an ontology that manifests features that make the template applicable. QTAIM uses the virial theorem as a computational method for making the calculation of kinetic energy

from electron density tractable. It has a well-known conceptual condition for its use as a technique that the landing zone of QTAIM satisfies, namely, that the system it describes be bounded and in equilibrium. QTAIM's landing zone, the topological atom, instantiates these properties, thus satisfying conditions for the use of the virial theorem. QTAIM also uses density functional theory as a computational method for rendering the quantum-mechanical description of atoms and molecules mathematically tractable. Again, there are ontological prerequisites for the application of DFT that the topological atom satisfies. Specifically, the topological atom provides a form to electron density that affords description of chemical properties in three dimensions.

2 — Using Physics in Chemistry

The problem with using mathematics from physics (for example, quantum mechanics) to describe chemical phenomena is that the mathematics is mostly intractable in this domain. Consider describing the state of a molecule - the 'position' of nuclei and electrons, and the potential and kinetic energies of these particles. There exists mathematics in physics used to describe the state of these same entities, the Schrödinger equation. It may seem that transfer of this mathematics to chemistry in describing the same features ought to be straightforward. However, molecules involve many more particles and a higher degree of complexity in their interactions than an individual atom. Even for the simple molecules, an oxygen-oxygen molecule for instance, a completely 'physics-based' computational approach is impossible. One could characterize

the history of modeling in 20th-century chemistry as progress towards inventing modifications of the Schrödinger equation that make its application possible.

Along with this computational challenge comes conceptual difficulties. How does a chemist make these mathematical modifications meaningful? It is not enough to draw up constraints and approximations. There exist different features in chemistry that these modified mathematics must describe while also avoiding unnecessary mathematical description of features that are not of interest to the chemist - the interactions within a nucleus for example. To make such modifications meaningful and rational, as in having good reasons for constraints and approximations, requires chemists to make some claim about what exists.

For example, a classical application of physics in chemistry is the description of ‘bond energy’. All bonding involves a lowering of the kinetic energy of a system. A modeler in chemistry will want to try to predict or describe the energetics of bonding - the reduction of kinetic energy for instance. To modify math from physics for this purpose requires a complete overhaul of the Schrödinger equation to solve chemical ‘wave functions’ - functions describing the states of bonding electrons. To specify these modifications requires some notion of what the new computational methods are about.

The chemical bond does not exist as an entity of concern for physics. So in transferring mathematics to describe bonding, a chemist will have to determine not only what modifications to make to the mathematics, but also how these modifications relate to the entities modelled. For instance, one of the first

methods invented to make quantum chemistry tractable, introduced by Linus Pauling, involved valence bond wave functions. Pauling eliminated spherical coordinates from quantum mechanical calculations, leaving only the angular component, making calculations derived from a Schrödinger equation tractable (Pauling 1960). Pauling's method required plugging in what chemists knew about bond angles for a molecule rather than leaving them as something to be calculated. These modifications required some *thing* to be hypostatized as that which the mathematics describes. Thus, Pauling invented the notion of a valence bond, providing cogency to his approximation of the Schrödinger equation. Drawing up the valence bond also involved making substantive claims about the nature of chemical bonds - that they were 'directional' or instance. So, the problem for chemists in transfering mathematics from physics is to not only invent tractable deployment, but also to prepare notions making this deployment meaningful.

Consider the seemingly uncontroversial notion that atoms exist in molecules. This ontology consists of two claims about the relation between molecules and atoms. These claims are that (a) atoms occur as separate entities, preserved in molecules, and (b) that interactions between these atoms contribute to the structure and properties of the molecule.

> "To retrieve [atoms in molecules] from accurate quantum mechanical wave functions presents a nontrivial challenge because, in fact, chemical binding results from electrons being shared between several atoms. To recover and identify atoms in an electronic wave function requires therefore a transformation of its representation in such a way that the wave function becomes constructed from subunits that exhibit atomic character" (Schmidt et al 2014, pp. 10).

This difficulty in choosing the most appropriate transformation of the wave function has shaped the transfer of physics to chemistry. Notions like resonance, valence bonds, and molecular orbitals guided these choices. An account of progress in quantum chemistry must inevitably connect these conceptual developments to transfer of mathematics. To follow is a brief history on these developments in modeling the chemical bond.

Since the development of the Heitler-London linear combination of atomic orbitals (LCAO) approach, applying quantum mechanics to chemistry has seen successive developments in making use of the Schrödinger equation less complex and more accurate. The twin developments of the valence bond (VB) approach by Pauling and Slater, and the molecular orbital (MO) approach by Mulliken and Hund, simplified mathematical description of chemical properties while making fundamentally different claims about the existence of bonds. They differ over what Weisberg and Hendry call the “structural conception of bonding” (Weisberg, Hendry 2008). The valence bond approach involved picking out one electron from each bonding atom and constructing a wave function that represents a localized, paired-electron bond. This LCAO method is based on the hypothesis that bonding is localized (Brush 1999) — by ‘localized’ I mean that there is an area positioned with respect to other features of the molecule that the method/model assumes the bonding electrons to likely be. Characteristic of valence bond models is the covalent bond, a directional, sub-molecular

relationship between individual atomic centers that is responsible for holding the atoms together (Weisberg 2008).

That the chemical bond is structurally defined and localized is a fundamental ontological claim in VB modelling methods. Concepts like resonance, and the structural conception of local, inter-atomic bonding, guide the interpretation of wave functions to make them a tractable description of chemical information. VB methods, informed by this ontology, approximate the molecular wave function using atomic wave functions in appropriate valence states. Values such as bond energy result from quantum mechanical resonance interaction between patterns of spin arrangements (Hiberty and Shaik 2014). Thus, the existence of a localized valence bond concept guides the transformation of the wave function from describing atoms to tractably describing chemical bonds between atoms.

Molecular orbital methods contrast with this approach by representing chemical bonds as delocalized. Contrary to VB approaches, these models distribute electrons throughout the entire molecule. Instead of considering electrons as either bonding or nonbonding, MO methods assign a continuously varying bonding power to all electrons in the molecule (Gavroglu and Simoes 2011). Chemists characterize molecular orbitals as bonding, nonbonding, or anti-bonding depending on their contribution to the overall bond order — number of bonds — in the molecule. This contrasts with VB's method of establishing a "symmetric" relationship in the position coordinates and an antisymmetric relation in the spin-coordinates between two electrons (Gavroglu and Simoes 2011). The

delocalized bond forms a basis whereby the MO approach develops approximate wave functions. MO theory is not constrained by representing bonds as directional and local because these sorts of bonds do not exist in the model systems of MO approaches. A delocalized bond ontology justifies different methods, for instance, developing a scheme to assign quantum numbers to electrons in molecules based on molecular spectroscopy data (Brush 1999). The delocalized perspective also allows for the mixing of ionic terms in the calculation of the molecular wave function (Weisberg 2008). These steps are given meaning by the implicit claim that molecular orbitals exist within the target systems of MO theory. Molecular orbital ontology provides a basis for interpretation of quantum mechanics in chemistry. For instance, it enables experimental data - molecular spectroscopy — to count as basis for inferring molecular orbitals from atomic orbitals. This is an important 'shortcut' for tractable use of quantum mechanics.

Finally, density functional theory (DFT) constitutes a notably different approach. In physics, DFT is a mathematical method that allows one to 'replace' the wave function with so-called 'density functionals' as carrier of basic information of a quantum system (Proft, Ayers, Geerlings 2014). This affords a 'quantum' definition of energy that does not use the Hamiltonian operator for instance - the part of a Schrödinger equation that makes describing molecular interactions difficult. However, for this DFT template to be useful in describing chemical properties, for it to be *transferable*, it needs specification. For instance, the exchange-correlation energy - a term in the Kohn-Sham energy functional - cannot be exactly expressed. Instead, modelers must approximate its value from

first principle considerations or parameterization (Proft, Ayers, Geerlings 2014). Thus, DFT requires other mathematical tools and more specific ontological claims in order to make it applicable in chemistry.

The general lesson from these different methods is that at some point chemists need to make weighty assumptions about phenomena in chemistry in order to make sense of methods for approximating a wave function. Some of these assumptions are incompatible, like the localized versus delocalized bonds of VB and MO. Either bonds exist in some location relative to other molecular features or they do not. This is what I have called so far an 'ontological' claim because making the assumption asserts that a sort of feature in chemistry either exists or does not — i.e. VB's assumption of localized bond asserts that bonds exist in a way that can be understood as localized,

The entwinement of ontological claims and model transfer in the history of using physics in chemistry prompts further analysis. Conceptual work in detailing what transferable mathematics describes is a substantial factor in the progress of chemistry modeling. Not only does it shape how mathematics eventually see use, but these ontological claims seem necessary for chemists to make sense of the use of certain computational methods. One particularly powerful and promising method, constituting a model template, is the virial theorem. The virial theorem provides a method for vastly reducing the complexity of descriptions of particle interactions in a molecule, and its transfer from physics to chemistry constitutes notable progress in chemical modeling. However, there exists well-known conditions for its use that a model's target must satisfy.

3 — The Virial Theorem as a Template

Bader's resituating of the virial theorem in physical chemistry afforded new methodology for modelling, extracting information about 'atoms' from electron density data. Central to the virial theorem is an equation relating time-averaged kinetic energy and potential energy ($T = -1/2V$). Using algebra and substituting domain specific equations for kinetic energy or potential energy allows a modeller to use this equation toward tractably describing these properties. Thus, the virial theorem, besides consisting of an equation, is also a model template. For instance, in its original use by Clausius, one can derive a function for modelling the kinetic energy of a set of particles. This derivation involves substituting in place of the potential energy part of the equation an expression to do with forces. The virial equation in classical mechanics affords the identification of kinetic energy with force. This relation between force and kinetic energy affords greater tractability in describing a system because it allows a modeller to essentially 'convert' a vector (force) description of a system into a scalar description, a conversion valuable for reducing the complexity in mathematically describing some systems. Scalars are typically less complex than vector quantities.

However, intermediate steps in this transformation of the virial equation into an equation relating forces and kinetic energy require characteristic assumptions about the target system. Very generally, the chosen special form of the virial theorem assumes that the target system is in bounded equilibrium; the target system is quasi-stationary and the individuals interact via an inverse square law type force. This assumption entails that a target system cannot be *too*

dynamic. For instance, it would be unwise to use the virial theorem-derived functions to model a group of particles part of an explosion — a supernova perhaps. A model so constructed would fail to accurately describe kinetic energy because an explosion is not a system in bounded equilibrium. Systems like our earth-moon planetary system, or the solar system are example of virial theorem applicable targets. The orbits are stable and periodic, meaning, for instance, the change in kinetic energy over time averages out to 0.

Like with the meaning of ‘clustering’ with the Ising model template, the meaning of ‘stable equilibrium’ depends on the domain where the virial theorem sees use. There are specific assumptions that are variously interpreted with this more general assumption. One such assumption is about the nature of interactions in the target system. In order to afford a simpler mathematical representation of forces, the virial equilibrium must hold true. Kinetic energy and potential energy must be in a stable ratio. If, for instance, outside potentials/forces influence the target system, then there is no guarantee that this ratio will remains stable for the entities of interest. Thus, one example assumption is that there are not ‘outside’ forces acting on the system. All interactions are only between entities being targeted by the model. Whether this is true or not depends less on the ‘real’ system and more on what the modeller stipulates as a target. Universal gravitation at the large scale makes any real star system an unsuitable target. However, the virial theorem still sees much successful use in stellar models. This is because modellers can delineate targets where the outside interactions cancel out, or become negligible - boundaries for

instance where gravitational potential are equal from all directions. The boundaries for these targets are spatial and temporal — stipulating where and for how long a given model applies. Besides the practical purpose of delineating a boundary as an area of application for a virial theorem model, the target system must be conceivable. To put it broadly, the target system must make sense; it must cohere with general conceptions about phenomena in a given domain.

Take for instance the first use of the virial theorem in quantum chemistry by Hellman and Slater (Hellman 1931 and Slater 1933). They separately proved that a chemist using the virial theorem could describe the kinetic and potential energy of a molecule when they knew the total energy. This version of the virial theorem came to be known as the “molecular virial theorem” (Gavroglu and Simões 2012). Using this form of the virial theorem, Slater built a model where kinetic energy was a function of the distance between nuclei in a molecule. This afforded a method to isolate the kinetic energy of the electron from that of the nucleus, approximating away nuclear motion, and making kinetic energy simpler to model for bonding. However, Slater’s use of the virial theorem required an idealizing assumption, “replace the coupling between electronic and nuclear motion with an [idealized] external force acting on the nuclei” (Slater 1933, p. 687). Thus, he assumed molecules were containers exerting a force on nuclei, keeping them in place. This conceptual strategy afforded the use of the virial theorem by providing the model with compatible assumptions, couching necessary virial theorem compatibility requirements in terms of chemistry’s domain-specific notions like molecule, nuclei, and inter-nuclear distance. This

conception of the molecule then put pressure on a chemist's understanding of bonding, whether bonding is caused by changes in potential or kinetic energy - the molecular 'box' expanding or shrinking. Despite first introduction of the virial theorem in this type of model almost a century ago, these debates about how to conceive of bonding are alive today (Backsey, Nordholm, Reudenberg 2018).

Thus, the virial theorem, as a model template, consists of a mathematical tool for modelling and also a corresponding conceptual requirement. I say conceptual because besides stipulating of mathematical 'boundaries - parameters or limits perhaps - for a model built using the virial theorem to be useful at all, its target must be something the discipline studies. So the target must both constitute requirements for the use of the virial theorem - boundedness- and also qualities characteristic of domain-specific phenomena.

Despite its usefulness in a wide range of applications, chemists regard the virial theorem as having the potential to be an unreliable mathematical tool. In chemistry, it is often the case the molecules are not good targets for application for the virial theorem. The aforementioned stability requirement limits modeling molecules using the virial theorem to ones that are in their 'ground state'. There is also controversy regarding whether models of bonding in chemistry target appropriately constrained systems for using the virial theorem (Burdett 1997). The stability requirement is open for interpretation. Some models, like Hellman's box model, formulate this stable target as a box shaped boundary limiting the positions of electrons. However, this results in controversial claims about the nature of bonding — that for instance bonding is the result of lowering in kinetic

energy of a molecule (Burdett 1997). Stable equilibrium is a widely known special condition of the application of the virial theorem in physics; similarly, in chemistry, the virial theorem's use as a computational method requires a target constituted of features that meet this condition. This is the aforementioned conceptual difficulty in transfering mathematics from physics — how to appropriately describe the ontology of such a target system.

The Quantum Theory of Atoms in Molecules (QTAIM) is a model constructed by Richard Bader in the early 1970s that holds an interesting place in the history of solving the difficulties in transferring math from physics to chemistry. QTAIM's attempt to make quantum mechanics useable involves several steps that take the wave function and make it into a mathematical description of 'topological atoms'. The last and most important step in this transformation is the use of the virial theorem as a computational method for calculating energy. With QTAIM, the goal is to make chemical quantities like bond energy calculable when given molecular formula. For instance, knowing that water has two hydrogen and one oxygen atom, QTAIM ought to describe the energy contribution of, for instance, oxygen to the molecule. Additionally, Bader constructed QTAIM to simulate the structure of the molecule, so we ought to be able to use the model to tell us the shape that bonded atoms form. These functions of the model depend on the usability of the virial theorem. It is the linchpin in making the math from physics useable - describing energy contribution and molecular shape. Moreover, the virial theorem has stringent ontological conditions for its use as discussed in the previous section. The virial

theorem requires that a target system instantiate characteristic assumptions about what types of things exists. Thus, the usability of the virial theorem is contingent on the ontological claims made in constructing QTAIM's target system.

The topological atom is the target system for QTAIM, constructed to fulfil the ontological requirement for application of the virial theorem. Topological atoms function in this way through a partitioning method. This method partitions a molecule into regions of electron density that are in equilibrium, affording the usability of the virial theorem by satisfying conditions for its transfer. To construct the topological atom, QTAIM partitions the molecule into fragments that additively contribute to properties of the molecule. These features of the topological atom are unique to quantum chemistry and indispensable to QTAIM's use of transferable math from physics. For the next parts of this paper, I will discuss this function where it concerns the usability of the virial theorem.

What follows here is a more technical description of how the topological atom makes possible the use of the virial theorem. The mathematical method behind its functioning begins with electron density information obtained through either experiment or using an electron density function (DFT). Electron density replaces the wave function as basic carrier of system information in this density functional template. This is the first aforementioned step in making math from physics useable. Partitioning electron density data then involves identifying the closed surfaces where the first derivative of the electron density is zero — thus, 'zero-flux boundary'. These surfaces become the stable boundaries separating

topological atoms in the molecule. A gradient field allows QTAIM to identify the vectors of steepest ascent through the electron density topology. Zero flux surfaces then partition atoms in the gradient vector field. These ‘stationary’ points in the electron density gradient, where there is no change in charge/electron density, are ‘saddle points’. Once these saddle points are identified, gradient paths (GP) that follow the line of steepest ascent to each of the stationary points, and a line of steepest descent, partition the surface.

The fragments partitioned by these GPs are virial fragments - topological atoms. The applicability of the virial theorem is a direct result of this spatial partitioning of a molecule. Each fragment is in virial equilibrium. With zero-flux boundaries dividing the molecule, one can derive a mathematical description of the total energy of the topological atoms using the virial theorem, allowing the modeler to differentiate between kinetic energy and potential energy using DFT functionals. As Bader puts it, “If the virial theorem exists for an atom - that is, for a region of space bounded by a zero-flux surface — one could use this theorem to define the energy of an atom in a molecule” (Bader 2011 p. 24). The way QTAIM defines the energy of the atom in a molecule using the virial theorem is through volume integration. In short, the virial theorem allows one to use computational methods from statistical mechanics. These computational methods make using quantum mechanics in chemistry tractable. In addition, the use of these methods is possible because of the topological atom’s zero-flux partitioning that then provides a spatially bounded atom in QTAIM’s model system. This partitioning method supplies the topological atom with properties

such as ‘in stable equilibrium’ and ‘transferable’. Since the topological atom instantiates these properties, it is ontologically compatible with the virial theorem.

4 — The Landing Zone

Before QTAIM, modeling approaches used chemical bond concepts as the characteristic features that guide the 1-electron wave function approximation (LCAO) towards calculating molecular energy and the energy of bond formation. For QTAIM, the fundamental consideration for tractable interpretation of the wave function is the topological atom - called ‘virial fragment’ in Bader’s early work.

> Rather than bonds, we choose as our fundamental parts mononuclear fragments of the system with boundaries defined in real space. We do so for two reasons: (a) all of the properties of such a fragment may be rigorously defined, and (b) theory and comparison with experiment indicate that such fragments are the fundamental building blocks for a total system (Bader 1975, pp. 36).

Bader frames the beginnings of QTAIM as a choice between two ontologies. Here we see justification of QTAIM’s ontological claims. Reason (a) results from Bader’s successes in using the virial theorem as a model template. Molecular fragments obey the virial theorem relation between potential and kinetic energy affording description of chemical properties using electron density. Reason (b) appears because Bader’s model successfully analyzes electron density data obtained from x-ray/neutron diffraction, assigning energies that cohere well with other observations of kinetic and potential energy.

Observations justify Bader’s construction of QTAIM’s target system. Some of Bader’s decisions in this construction connect to ontology of past chemistry,

“The atom played the central role in early chemical theories. The properties of a molecule were related to those of its constituent atoms” (Bader 1975, pp. 131). In later works, Bader cites Dalton’s early atomic theory as consisting of an ontology that chemistry could find itself rooted again with QTAIM (Bader 1990). Fundamentally, Bader’s intention is to build a target system with an ontology that diverges from the modelling practices of past quantum chemistry.

> “The quantum theory of atoms in molecules, QTAIM, demonstrates that every measurable property of a system, finite or periodic, can be equated to a sum of contributions from its composite atoms (Bader 1990). Indeed, without this possibility, the concept of the atom as the building block of matter loses its usefulness” (Bader and Matta 2012, pp. 254).

This possibility for mathematically describing chemical properties is the result of the topological atom’s functioning as a landing zone. For Bader, the topological atom’s successful functioning as a landing zone demonstrates the possibility of “a return to Dalton’s notion of an atom as a bounded space-filling object frees chemistry from the yoke of arbitrary models and definitions” (Bader and Matta 2012, pp. 256). This constitutes a sort of conceptual progress, a progress in transferring physics to chemistry by using a fundamentally different ontology in shaping this transfer. The successes of QTAIM then provides reason to take its ontology seriously. Indeed, since QTAIM’s development, topological modelling has seen a marked increase in use. Instead of depicting progress in the history of quantum chemistry as progress in theory or progress in mathematical description, we can also characterize a conceptual progress in the invention of target system features that make possible the transfer of mathematical tools.

Introducing the notion of a landing zone identifies the topological atom as a feature that functions by furnishing QTAIM with an ontology. It provides an ontology by being a vehicle for ontological claims. Presenting the topological atom as QTAIM's target system answers two ontological questions. These questions are 'what exists?' and 'what relations between things exist?'. The way a modeler answers these questions in building a model is to prepare features of a target system so that they instantiate a specific ontology. So, for instance, Bader designs the topological atom so that it is bounded and space filling. This answers the first question "what exists [in chemistry]?" with "spatially bounded and space filling atoms". Bader also designs the topological atom so that one can infer, additively, properties of the molecule from properties of the atoms. This answers the second question "what relations exist [specifically, between wholes and parts]?" with "additive relations exist [specifically, the properties of the whole are completely determined the properties of the parts]". These claims are substantially different from the ontology of VB or MO models.

Since models like QTAIM introduce ontology that may be divergent from that common to a scientific domain, answers to these questions need to demonstrate that the claims are reasonable. More than just describing the ontology of the target system, the topological atom demonstrates that this ontology has epistemological value. It does so by showing that its design affords key chemical information - molecular structure and bond energies. It does so by making possible the use of tractable mathematics. In order to make use of, for instance, the virial theorem as a transferable template, these aforementioned

ontological questions require specific answers.

In other words, scientists construct landing zones in part by imposing ontological claims about their domain that are justified in part because they enable the transfer of useful models. Landing zone claims also give meaning to transferable mathematics, allowing a modeler to take certain calculations as information about domain-specific properties, like with the virial theorem. The quantities it describes are only information about atoms when these quantities are specified. Returning briefly to the discussion on model templates, both Knuuttila and Humphreys acknowledge the need for a template to be specified by the scientists using them.

This account of landing zones helps us understand in a bit more detail what is going on with specification. Humphreys' (2004) mentions briefly about ontology's place in model construction as a part of specification. Claims about ontology are necessary for the use of transferable mathematics not only in that they make possible the use of a specific template, but also in providing meaning. Computational templates as a generalizable syntactic form need their unspecified form mapped to domain-specific concepts in order to be meaningful for a domain. This mapping involves what Humphreys calls construction assumptions. For Humphreys these assumptions comprise a quintuple — (Ontology, Abstraction, Idealization, Constraints, Approximations). They guide correction of a template to a specific phenomenon, and these assumptions are mathematical except for ontology. Ontology is necessary to turn a general model into a model about a specific type of system, guiding specification of the other elements of the

quintuple. “Although a multinomial model in statistics may be a model of many different phenomena, it is a model of dice-tossing only when the objects are deliberately specified as dice” (Humphreys 2004, pp. 78). Ontology guides specification of mathematics assumptions like constraints. For example, the multinomial distribution for a six sided dice-tossing model requires that the value of $k = 6$. The ontology of this model - six-sided dice - guides how the math is specified. It does so by answering ‘what exists?’ for the model system. Thus, it gives meaning to the mathematics by giving reason for the transformation of a general multinomial function into a function with specific constraints. Since the notion of a landing zone identifies what instantiates these claims for a model, it identifies what Humphreys refers to here as ontology. In this way, the landing zone is an extension to Humphreys work, identifying the features of models that instantiate necessary assumptions for the specification of transferable mathematics.

5 — Functional Groups

This section goes into greater detail on how the topological atom’s ontology prepares for the *meaningful* transfer of mathematics, and how this ontology connects to the conception and study of other phenomena in the domain. Since the topological atom’s partitioning method provides a form to electron density that makes depicting molecular structure with the density functional theory (DFT) model template possible, it affords identification of what chemists call ‘functional groups’. A functional group is a collection of atoms in a molecule that generally have the same structure across molecules, and that, in

biology, share a function because of this similarity in structure. The functioning, roughly, has to do with shape. By affording direct identification of the shape of 'sub-units' like functional groups, the topological connects QTAIM to other phenomena in chemistry that valence bonds and molecular orbitals cannot — in as direct a way, using one model. QTAIM represents atoms as a three dimensional objects using the topological atom as a sort of cookie cutter for electron density. "A display of [partitioned charge density] for a molecule will make visible to the eye, without further mathematical analysis, the definitions of its atoms and of a particular set of lines linking certain pairs of nuclei within the molecule-its molecular graph" (Bader 1990, pp. 14). With QTAIM's target system, molecules have a clear, identifiable structure. This is part of what Bader calls "recovering the concept of a functional group".

In some domains of chemistry, functional groups are phenomena of interest. Valence bond and molecular orbital theory models do no prioritize the representation of these phenomena because the atom is not a bounded, spatial *thing* for these models. Particular "functional" groupings of atoms exhibit characteristic properties that enable one to detect their presence in any molecule and to predict the properties resulting from their shape (Bader 2007). QTAIM's topological treatment of the molecule provides easily partitioned subunits. A result of this approach is that structures like functional groups become more immediately accessible in its representation. This is in contrast to the MO approach, where the delocalized bonding ontology results in target systems that cannot provide information about functional groups.

QTAIM's identification of functional groups depends on two aspects of the topological atom. First, a topological atom's shape affords inference about chemical properties. "The atoms of QTAIM that look the same (that is, have the same form in real space) exhibit the same properties" (Bader 2013, pp. 262). This is a result of mathematical methods for integrating over volume from QTAIM's use of the virial theorem. In addition, the topological atom is transferable on the basis that its shape determines its identity. A chemist using QTAIM can identify functional groups within different molecules by their shape in the topology of electron density. Thus, the topological atom prepares the DFT template, and the virial theorem, as a source of information about functional groups and molecular structure, providing meaningful transfer of these templates.

Features of the topological atom make possible the mapping of general and transferable mathematics to domain specific concepts like functional groups. Specification of a model template requires ontology, that the target system instantiate claims about the existence of things and relations. This specification provides general mathematics with meaning. A modeler can then use this mathematics as a source of information about domain-specific phenomenon. For instance, the use of density functional theory for identifying functional groups. Without the unique ontology of the topological atom, mapping chemical properties to three-dimensional shape, this information about functional groups is not available using density functional theory. The charge density it provides only has meaning because Bader specifies, in constructing QTAIM, that certain regions are topological atoms.

6 — Conclusion

Chemistry faces a generic problem. Quantum mechanics is relevant and important for describing chemical phenomena, but the fundamental kinematical and dynamical equation, the Schrödinger equation, is intractable for molecules. The history of modeling in chemistry is a history of inventing or transferring tractable forms of this equation. Concomitant with the invention and deployment of tractable quantum chemistry is conceptual work towards making this invention or transfer meaningful. In the history of addressing this problem, bonds were the dominant ontological notion for constructing target systems. The Quantum Theory of Atoms in Molecules is a model that diverges notably from this ontology. By transferring the virial theorem it makes possible the replacement of a Schrödinger equation with density functionals, thus rendering description of chemical phenomena using mathematics from physics tractable. This model fits in this history of solving the generic problem not only by transferring a new tool, but also by constructing a new thing to which transferable mathematics applies - the topological atom. It is this additional factor in model transfer that motivates complimenting current analysis with a new notion — the landing zone.

QTAIM consists of a landing zone — the topological atom — for the use of transferable model templates from physics — the virial theorem and density functional theory. A landing zone is a target system that functions to make use of transferable model templates possible. There are two aspects to this functioning. First, a landing zone satisfies conditions for the interpretation of transferable templates with respect to approximations, constraints and parameterization. This

allows a modeler to answer questions about the ontology of the target system that are necessary in deciding how a scientific domain is to use a model template. For instance, the topological atom provides QTAIM with a target where atoms have spatial definition and sharp boundaries. This then allows Bader to construct QTAIM as a model that combines density functional theory and the virial theorem as model templates.

Second, a landing zone functions by providing an ontologically compatible target system. Bader designs the topological atom to be ontologically compatible with the virial theorem, providing a target system that the virial theorem can describe.

The target systems hypostatized by past chemical modeling practices differ significantly from each other. What accounts for these ontologically different target systems in the history of transferring physics to chemistry? Bader, in more recent work, makes it clear that what accounts for these different ontologies is the preparatory activity in applying physics to chemistry. “It is readily demonstrated in a few lines beginning with Schrödinger’s equation that to apply physics to an atom in a molecule, the atom must be a bounded space-filling object” (Bader 2004, pp. 8387). These differences result from landing zone type preparation for model transfer. QTAIM’s ontological claims are opposed to a perspective on atoms in molecules that predominantly guides molecular orbital (MO) and valence bond (VB) approaches. “Most chemists would probably describe a molecule as consisting of approximately spherical, overlapping atoms or ions” (Haaland et al. 2000, pp. 1079). Contrary to this description of atoms

found in VB and MO methods, the landing zone for Bader's QTAIM functions by instantiating a bounded space-filling target for application of the Schrödinger equation. With this topological atom as QTAIM's target system, the model enables one to "apply the full predictive power of quantum mechanics to the analysis of chemical problems" (Bader 2009, pp.273). Thus, the topological atom provides a basis for the extraction of chemical information from mathematics transferred from physics, "the predictive power of quantum mechanics". Additionally, the ontological claims that make this use of mathematics possible are important conceptual features for QTAIM. Introducing the notion of a landing zone identifies the role of ontological claims in model transfer.

Since the topological atom has well-defined boundaries, the virial theorem becomes a usable computational method. Just like how it would not be possible to use site-seeing helicopter in a dense forest without preparation, clearing trees and leveling the ground, the use of the virial theorem in QTAIM requires preparation, the designing of an area for its application. The notion of a landing zone allows us to identify this constitutive and preparatory aspect of model transfer.

Chapter 3: Model Transfer and Conceptual Progress

1 — Introduction

In the previous chapter, I examine how Richard Bader invented the phenomena of a topological atom as a landing zone for the transfer of the virial theorem. To perform this examination, I define the notion of a landing zone. A landing zone is a target system which scientists prepare for the use of a model template. This target system can encompass a phenomenon, or more abstractly, encompass multiple phenomena. Part of this preparation includes stipulating the sort of things that exist in a domain. Often it is the case that scientists redefine these phenomena partially (or even totally in QTAIM's case), stipulating new categories of things to exist in a scientific domain. I call this an 'ontology', referring to the implicit claims made by scientists in stipulating new types of phenomena, like topological atoms. Preparing a landing zone requires scientists to plan how to organize information in a domain, often in new ways. Bader created a new plan for organizing electron density information by analogy to topographic maps of mountains in order to make the virial theorem applicable.

As was the case with QTAIM's introduction to chemistry, the preparation of landing zones introduces what I will call 'conceptual progress'. Conceptual progress is the introduction of new concepts, or significant redefining of existing

concepts, in a scientific domain for the use of a new model template. I use the term ‘progress’ because I wish to connect conceptual change that brings about the application of novel model templates through model transfer as constituting scientific progress. If scientists transfer a model template it means that they have successfully made use of it towards solving some problem, or a the very least successfully prepared a space for the model template’s use that is meaningful enough to be the subject of debate by other community members. Thus, analysis of model transfer provides a new vector in characterizing puzzles to do with the conceptual differences between scientific domains — intertheoretic reduction and interdisciplinarity. Scientists reconceive domain-specific phenomena to make possible the use of transferable templates. These new conceptions of phenomena introduce conceptual pressure and drive theorizing. To motivate this perspective on model transfer, I detail two stories of transfer from chemistry and biology that have telling parallels.

To follow is a brief sketch to reiterate philosophical discussion on model transfer that I cover in Chapter 2. Paul Humphreys invents his notion of a computational template in *Extending Ourselves (2004).* A computational template is an equation, function, or other computational method that is both generalizable and tractable. They are genuinely cross-disciplinary in that they draw together computational methods across scientific domains, domains that often have very little in common. Additionally, computational templates have a particular syntactic form that is invariant through the domains where they find use. Models constructed from the same computational template will, for instance, bear similar

relationships between variables. However, it is their tractability that ultimately accounts for their dissemination. Computational templates promote the useability of mathematics in modeling. Thus their transfer to a new domain constitutes progress in the mathematical modeling of phenomena of that domain.

Knuuttila and Loettgers respond that tractability alone is not sufficient to account for model transfer. In addition to features like tractability and generalizability, they think there are conceptual features belonging to templates that explain their dissemination. Depicting these conceptual features prompts augmenting Humphreys' notion of a computational template with that of a model template. To put it simply, a model template is mathematics embedded with general concepts. For instance, with the Ising model's transfer to the Hopfield model, besides mathematical or syntactic form, a very general conceptual idea of the kind of mechanism of interaction was also transferred (Knuuttila and Loettgers 2014).

To depict this dynamic between the thing that is transferred and the thing to which it applies, I introduce the notion of a landing zone in the previous chapter. The features that are characteristic of landing zones are their function in model transfer and their function as a target for mathematical models. This type of feature in model transfer functions by providing a scientific domain with a target system that is ontologically compatible with concepts embedded in model template mathematics. For instance, the binary neuron introduces into neuroscience 'simple cooperating phenomena'. Both the Ising model template and this domain then have matching ontology in that they answer the question

‘what exists?’ with ‘simple cooperative phenomena’. This matching of ontology is a necessary condition for transferable model templates to be useable in a new domain. Not only do scientists need the neurons to be binary but they need to understand what physical quantities — temperature, energy, and entropy — mean in this new context.

Besides accounting for what makes transfer possible, introducing analysis of landing zone target systems provides discussion about model transfer with a new vector for approaching questions about conceptual innovation and modelling. One of these questions is — where do scientific concepts come from (Nersessian 2008)? This is an especially relevant question for a domain like physical chemistry, where modelling predominantly uses transferable mathematics from physics; however, chemists use these models to study phenomena not present in physics — like chemical bonding. These models do not target the phenomena of physics. Instead, these models — molecular orbital models for instance — represent phenomena that is in some way similar yet different from the phenomena of physics. A chemist's conception of this phenomena is at the very least not straightforwardly reducible according to dominant literature in philosophy of chemistry. There are arguments from the ‘bottom-up’, that the theoretical peculiarities of quantum mechanics preempt representation of molecular structure (Gonzalez, Fortin, Lombardi 2018), from the ‘top-down’, that there are dimensions to molecular structure that present day quantum mechanics cannot explain (Hendry 2010), or that the relationship between the use of mathematics in chemistry and physics is too loose to apply

classical notions of reduction (Scerri 2007). Molecular orbitals, valence bonds, resonance, Pauli forces are just some examples of notions central to mathematical modelling in chemistry that confound inter-theoretic reduction. Taking for granted this loose connection, where do these concepts, featured center-piece in chemical models that use quantum mechanics, come from?

My suggestion is that literature on model transfer can aid in answering this question by providing a mechanism for the generation of new concepts through conceptual pressure. Two features of model transfer indicate this affordance. First, model transfer introduces conceptual pressure to a domain. When scientists use novel mathematical tools, debates about highly theoretical matters follow, including ontological matters. Dissemination of mathematical techniques across cultural and domain-specific barriers seems to prompt scientific theorizing on the nature of the phenomena these disseminating tools model (Lalli 2015). This theorizing, for instance, the drawing up of landing zone target systems, is part of the conceptual strategy for resituation of abstract things like model templates. Abstract and transferable, model templates require de-abstraction for use as a concrete model in a domain. Strategies towards this end may require conceiving of phenomena in tension with entrenched modelling practices, thus introducing conceptual pressure — tension between notions about the essential characteristics of phenomena. Additionally, some model templates have well-known conditions for their use. The virial theorem is one example, where a model using it must include characteristic assumptions. These assumptions require, as with the binary neuron, a preparing of phenomena in *a particular way*. Domains

where the virial theorem travels see the introduction of similar modelling assumptions, and conceptions of phenomena. Thus, paying attention to model transfer provides a way to trace the origin of new scientific concepts to a domain.

Both cases I present in this paper exemplify the reconceiving of phenomena and resulting conceptual pressure that follow from model transfer. These new conceptions spark scientific debates that cleave deeply into philosophical matters, matters like ontology, and the epistemology and methodology of modeling. The first case involves the transfer of the ideal gas law to biology by R.A. Fisher. Fisher's model revolutionized modeling in biology by introducing a method to treat population level selection mathematically, in a similar way to ideal gases. Fisher makes possible the use of novel statistical methods by introducing a novel model target system — populations consisting of velocities instead of individual animals. This reconceiving of a population as a landing zone plays a vital role in Fisher's transfer of the ideal gas law as a model template, and sparked debates about the constitution of populations that persist today.

The second case of model transfer is Richard Bader's construction of the Quantum Theory of Atoms in Molecules (QTAIM) model. This model allows chemists to mathematically describe the state of a molecule and depict its structure. Bader uses a model template to construct this model, the virial theorem. The virial theorem has well-known conditions for its use in a model. For instance, the virial theorem only applies to systems that are in stable equilibrium. Bader introduces a new target system — the topological atom — to satisfy this

requirement of the virial theorem, making possible its transferability as a tool to analyze charge density. The success of the topological atom as a target for transferable templates results in debate over the appropriate way to conceive of phenomena, like the ‘atom in a molecule’, for the use of mathematics from physics in chemistry. By analyzing this landing zone feature, the topological atom, we depict the conceptual development to do with modeling in chemistry.

2 — The Fisher Model of Genetic Fitness

Starting in 1918, the statistician R.A. Fisher began working on problems in genetics. Fisher developed a statistical model of evolution from this work that used the ideal gas law to investigate the role of selection in producing variation. Before his work, biologists believed that natural selection was incompatible with mendelian inheritance. In other words, it was not clear how there can both statistical variation in inherited traits and traits that persist because they are advantageous; the *persistence* of advantageous traits and statistical *variation* seemed in tension for mathematical description. Fisher used equations at the core of the ideal gas model in physics to make tractable the description of natural selection in mendelian populations, thus creating a method for describing both natural selection and mendelianism (Fisher 1958). In short, Fisher invented a way to statically describe the survival of a mutant gene so that ‘persistence of the fittest’ could connect to ‘statistical variation of genes’. Morrison, in her paper, “Physical Models and Biological Contexts”, goes into detail on Fisher’s use of the ideal gas law (Morrison 1997). As her argument goes, analyzing Fisher’s model solely as a representation does not accurately depict its functioning. Instead, we

should pay attention to its use as an instrument. Fisher used his model as an "instrument for mapping biological concepts into a mathematical framework that could enable one to make specific concrete claims about evolutionary dynamics" (Morrison 1997, pp. 324). Morrison's description of the functioning of Fisher's model highlights the aspect of model transfer that I think is particularly relevant to analyzing conceptual progress. This is the relation between the domain specific concepts and the mathematical structure of transferable templates that Morrison characterizes as a mapping.

As a model template, the gas law sees use in a preponderance of models across various domains. The core equation expresses a simple relation between pressure (P), temperature (T) and volume (V) ($PV = nRT$) — where *n* is the number of moles in the gas and R is a constant. The ideal gas law takes different forms depending, but the 'pure' form there are classic assumptions that physicists make. These assumptions are that molecules are infinitesimal compared to the gas itself and that the intermolecular forces are negligible. As Morrison puts it, physicists must "specify a model of the molecular system" that meets these requirements in order for the ideal gas law to be useable (Morrison 2002). Evolutionary biology, however, does not deal in molecules or gases. How was the preparation for the use of this model even conceivable by Fisher? According to Morrison, Fisher invents a new 'model' that treats populations as gases. For Morrison in this context, a model is "a particular way of conceiving of how a population should be structured and theorized, conceptions that are presupposed in both Fisher and Pearson's application of statistical techniques"

(Morrison 2002, pp.60). This model is a particular conception of a biological population that functions to make possible the application of a further model, the model that includes statistical techniques. One such statistical technique had Fisher using the velocity distribution law (maxwell-boltzman) for calculating the distribution of the frequency ratio for different Mendelian factors (genes). What Morrison calls ‘model’, a particular way of conceiving of a population, is also what I call a landing zone. It functions as the target of the Fisher’s statistical techniques, his use of the ideal gas law, by providing the appropriate description of phenomena (populations and genes).

Morrison’s first sense of model, as an ontological conception and presupposition for mathematical description, is a landing zone. It is these target models that are of particular interest in analyzing model transfer. Attending to these features in accounts of scientific modelling allow us to explain idealizations as a something useful (for transfer) even though they misrepresent real phenomena (because they do not function as representations). Fisher’s “model provided the instrument for investigating the role of selection in human populations by replacing actual populations with idealized ones” (Morrison 1996, pp. 320). These idealized populations made possible the application of a statistical model by mapping biological concepts (i.e. population) to ontology that would satisfy requirements for the use of the Ideal Gas model template. What I call the ideal gas law model template could also be called the ‘kinetic theory of gasses’ template since the mathematical core of what Fisher uses is the velocity distribution law. In short, Fishers used a maxwell boltzman-like function to assign

fitness to genes in a population undergoing natural selection by replacing velocity with a variable expressing ‘fitness’ in this equation. An important factor was the separation of gene fitness from mendelian allele variation. This was accomplished by assuming ideal-gas-like conditions (that roughly PV = T) Fisher’s model uses a different equilibrium condition, specifying that there are no external forces acting on fitness — i.e., predation, enough animals for statistical analysis to be meaningful etc. Morrison calls the reasoning Fisher uses to make this connection a ‘mapping’ because it ‘maps’, defines a connection, from conditions for the use of mathematics (ideal gas criteria) to descriptions of phenomena. Such reasoning makes the interpretation of a distribution ratio as being about a mutant gene’s propagation through a population meaningful. As Fisher’s justification for this transfer of the ideal gas law goes, the “distribution of the frequency ratio for different factors may be calculated from the condition that this distribution is stable, as is that of velocities in the Theory of Gases” (Fisher 1918). By ‘factors’, Fisher means genes. Inventing a target that is analogous to both the velocities in the theory of gases and evolutionary populations satisfies the condition for stable distribution, while at the same time making the model congruent conceptually with evolutionary biology.

This invention of a velocity-like population was in tension with existing notions about the constitution of populations, resulting in conceptual pressure and scientific debate. Morrison covers this controversy in her 2002 paper, “Modeling Populations: Pearson and Fisher on Mendelism and Biometry”. As Morrison points out, Pearson disagreed not only with Fisher’s statistical

methodology, but more importantly, his conception of a population. “Pearson had a very specific notion of how populations could be described or constituted, one that was presupposed in his application of statistical techniques and one that Fisher did not subscribe” (Morrison 2002, pp. 61). One example of how these notions diverged is that Fisher’s idea of a population included indefinite mendelian factors (genes). There are a limited number of genes that determine a phenotype. Similarly, any real population of animals is going to include a number of animals, animals that mate to pass on their genes and animals that die. Fisher’s model idealizes these details, assuming that numbers of individuals are indefinite and assuming that genes get passed on by chance. Fisher’s adoption of the ideal gas law model template assumptions, that the number of *things* modeled (molecules or animals) was assumed to be ‘large enough’ for biologists to treat the group statistically; like with molecules in ideal gasses, Fisher’s model treats *things* (animals) as indistinguishable. “We may imagine, in respect of any pair of alternative genes, the population divided into two portions, each comprising one homozygous type together with half the heterozygotes, which must be divided equally between the two proportions. The difference in average statures between these two groups may then be termed the average excess (in stature) associated with the gene substitution in question” (Fisher, 1930a, p. 30). Fisher’s model categorized populations of animals by their genes in order to describe fitness (stature) as a statical property (‘average excess’ in the case of this quote) of a particular gene.

Pearson thought this too abstract and unrealistic. Generally, the disagreement “centered on how populations should be characterized with respect to the individuals they comprise” (Morrison 2002, pp. 62). For Pearson, populations ought to be characterized as non-homogenous classes where each individual of a population is distinguishable. This came from a perspective on ontology wherein no two physical entities are exactly alike; instead they form a class with variation about a mean (Pearson 1930). However, knowledge of individuals was simply not important for Fisher. His model made it so one could describe successful genes statistically, glossing over details like actual inheritance — which, because of mendelian variation, was not a tractable way to describe the persistence of traits in a population. Fisher’s model made it possible to avoid variation between individuals in a population, like how the treatment of the properties of individual molecules in the modelling of ideal gases allows for tractable description of microstates like kinetic energy. Thus, the introduction of Fisher’s new landing zone, and its successful use in transfer of the ideal gas for statistical description of the distribution of traits, challenged the use of conceptions of a population as a target for mathematical modeling in biology. This debate over the target of statistical techniques cleaved deeply into ideas about general ontology. As Morrison ultimately argues, Pearson’s objections were not just methodological, but philosophical.

Morrison concludes this paper remarking that viewing the construction of Fisher’s model outside of the lens of typical questions to do with representation affords a rich and interesting story about conceptual development in evolutionary

biology. I draw a complementary lesson from Morrison's story. There is a feature discussed in this story that plays a fundamental role in affording use of the ideal gas law and one that becomes the subject of debate; thus it is taken as introducing serious challenges to conceptions about ontology of biology. According to Morrison, it is the construction of a certain sort of model that affords Fisher's use of the ideal gas law, one that underlies the conceiving and structuring of his evolutionary notion population as a population of vectors. This sort of conceiving of a population is an idealization, but this was not just a debate over the presence of idealizations. The debate between Fisher and Pearson was over what kinds of idealizations to use in preparation for mathematical modeling (Morrison 2002).

Model templates like the ideal gas law are simply not possible to use unless the phenomena are conceived a certain way. Thus a model template's transfer to a new domain requires reconception of phenomena. Idealizations like a vector populations for instance make possible mathematical representation by a model built from the ideal gas equation and associated mathematical tools — i.e. the variety of equations of state derivable from the ideal gas law. The ideal gas law requires phenomena conceived as ideal gases for its use. Populations of animals in biology require some stretch of imagination to render them applicable for this model template, resulting in a notion of a population in deep tension with existing conceptions — thus also in tension with biological theory to do with populations. Conceptual pressure results. This development is mirrored in chemistry with the case of Bader's transfer of the virial theorem.

Morrison's description of a target-model, some *thing* that maps domain-specific concepts to a piece of transferable mathematics is an apt characterization of the sort of landing zones I looked at in Chapter 2 for the virial theorem. The transferability of the virial theorem necessitates the reconceiving of phenomena in a domain that wishes to use it, and this target must instantiate certain qualities for the virial theorem to be applicable. This means that whatever the new target system is, it is likely going to conflict with previous conceptions of the same phenomena, like the conflict between Fisher's conception of a population and Pearson's conception. In order to make the ideal gas law useable, populations needed to be reconceived, a *certain way*, *like* gasses. This reconception for Fisher's model meant that a population now was a homogenous class of things. Model templates, the transferable units in model transfer, are not simply applicable. The activity of model transfer come concomitant with conceptual pressure as the reconception of existing phenomena meets the needs of mathematical application and result in tension with other notions of phenomena.

3 — The Topological Atom as a Landing Zone

The quantum theory of atoms in molecule (QTAIM) is a model built using the virial theorem template that chemists can use towards several different ends. An established method for making quantum chemistry less complicated is the replacing of the Schrödinger equation with density functionals. Roughly, this involves the assumption that a three dimensional electron cloud approximates the state of electrons in a molecule. One of QTAIM's uses is to give chemical

meaning to this electron cloud. The virial theorem is a fundamental part of this use. It constitutes the basis for identifying atoms in molecules, and then distributing properties to these atoms. However, the virial theorem's resituation depends on a specific conceptual strategy at the heart of QTAIM. QTAIM represents atoms as closed, hard-shelled things that additively contribute to the total energy of the electron cloud. This general notion about mereology, how parts relate to wholes, along with the associated topological method for carving up electron density makes possible the use of the virial theorem in this context. QTAIM is not unique either as a model that represents atoms as bounded, hard-shelled things or a model that uses the virial theorem in chemistry. However, the relationship between this representation of atoms and QTAIM's resituation of the virial theorem bears novelty and significance.

Richard Bader used the virial theorem as a model template in constructing QTAIM. In order to meet the requirements discussed in Chapter 2 for the use of the virial theorem, instead of the 'molecular virial system' of Slater and Hellman, Bader prepares a reconception of the atom to act as a target. One key difference between these uses of the virial theorem is the data that the models analyze. Bader developed his model to use empirical data from electron density. Slater and Hellman's use of the virial theorem corroborated with empirical data but did have as direct of a connection; one had to plug in known bond lengths and angles for isntance. Bader designed QTAIM to not only simulate molecular structure but to overlay this structure in the form of topology onto observations about electron density.

Bader discovered that he could partition charge density — electron density — into spatial regions that are in virial equilibrium, regions where the virial theorem equation is true of the relation between potential and kinetic energy (Bader and Beddall 1972). This partitioning of charge density allowed him to invent a new method for using the virial theorem in chemistry as a tool for analyzing charge density data. This new method is attached to a reconception of the atom — called virial fragments in Bader's earlier work (Bader 1975). Later, he refers to these partitioned units of charge density as the topological atom; it is a similar thing to atoms of other chemistry modelling practices in that they are the parts of molecules. However, Bader's conception of the atom conflicts sharply with other notions of an atom that underlie, for instance, molecular orbital models. Bader's topological atom has spatial boundaries consistent with a notion of the atom that goes back to Dalton — the idea of bonding atoms being touching spheres that do not overlap — and they relate additively to the whole molecule, consistent with other methods that relate sum properties. Because of these features, the topological atom affords the use of the virial theorem, and at the same time constitutes the source of conceptual pressure within the QTAIM model.

The general affordance of the virial theorem at the methodological level is a more tractable mathematical representation of the forces within a molecule. Steps towards this simpler representation of the forces relevant to chemists require assumptions about the interactions in a molecule. With QTAIM, this involves the interpretation of the assumption about interactions: boundedness;

the target is bounded so that the only interactions are between entities in the target system — no ‘outside’ interactions. These conditions are difficult to meet in chemistry where modelling practices conceive of intra-molecule parts — electrons — essentially ‘roaming’ the entire molecule. From the perspective of modelling practices where the molecule is conceived of as consisting of overlapping orbitals, these conditions are problematic to define.

For Bader’s QTAIM, the ‘outside’ forces condition is met by the zero-flux boundary of the topological atom. The surface of this region of charge density is bounded such that the interactions being targeted by QTAIMs mathematical tools are internal to the subsystem. Of course, ‘realistically’, all nuclei in a molecule exert force on each region of charge density. It just so happens that Bader’s partitioning allows one to ignore this because the nuclear potentials all equal out within nuclear basins partitioned by QTAIM’s zero-flux boundaries. A property of the surfaces partitioning charge density in QTAIM is the neutralization of nuclear potentials. Thus, topological atoms come built in with a feature that licenses the assumption that there are no outside forces, outside with respect to the target, and the virial theorem becomes useable. Among the affordances of this assumption and the resulting applicability of the virial theorem, it unlocks the ability to bundle description of multiple potentials (nuclear-electron, electron-electron, nuclear-nuclear) into one expression, increasing tractability in describing the state of an atom in a molecule.

This tractable feature in the mathematical methods of QTAIM requires the meeting of virial theorem conditions. Bader had to reconceive the atom to meet

the boundedness condition. Entwined with this reconception is the meeting of conditions for new methods in mathematical modelling. The applicability of the virial theorem allows Bader to construct QTAIM as a tool for representing regions in charge/electron density as atoms in a molecule. Because one can use functions derivable from the virial theorem to integrate over a three-dimensional region of charge density, QTAIM affords a relation between the three-dimensional shape of an atom and some quantity — kinetic energy. Each atom has quantities that depend on its shape. Bader calls this dependance on shape 'transferability' because the model identifies functional groups (Chapter 2) and atoms with their shape in electron density meaning that the same atom is transferred when a molecular change happens rather than destroyed by having some essential part stripped away (electrons). The ideal of QTAIM is such that, for instance, a hydrogen (topological) atom in water would have the same properties, shape and kinetic energy, in another molecule. The possibility of approaching this ideal depends on both the conception of the topological atom and the transferable mathematics it makes possible.

> The identification [between kinetic and potential energy in the virial theorem] satisfies in a single stroke the two essential requirements of the atoms of 'conceptual chemistry' — additivity and transferability of properties. It is common sense that two identical pieces of matter must possess identical properties and consequently, two atoms possessing identical charge distributions, that is, atoms indistinguishable in real space, must exhibit identical properties." (Bader 2009, p.10)

As Bader's argument goes, the successful functioning of the topological atom as a target for the virial theorem prompts some chemists to treat this conception of

this atom seriously. One can use this notion of an atom as foundation for interesting and successful models of chemical phenomena.

The topological atom became a vehicle for model transfer. Thus, properties of this target system became a point of contention in Bader's following discourse. As he argues, the success the topological atom as a new sort idealized target system motivated taking the conception of this target system seriously - that atoms ought to be thought of as spatially bounded subunits of a molecule.

> "Not only do the theorems of physics such as the virial theorem not apply to the model of overlapping atoms, such a model does not recover the essential chemical observation regarding the characteristic properties exhibited by functional groups. Overlapping atoms have no individual identities but are merged with the densities of all of the atoms in the system. A chemical atom on the other hand can exhibit near transferable behaviour even when the neighbouring atoms are radically different" (Bader and Matta 2013, p. 263)

Fundamental to Bader's position are concerns about what makes possible an ideal suite of mathematical tools from physics. Certain tools only apply to certain conceptions of phenomena that meet the general requirements of a model template — bounded equilibrium for the virial theorem. Bader's modelling strategy is to meet these requirements by reconceiving them in domain-specific terms. For chemistry, the interactions in bounded equilibrium are nuclear-electron potentials. The topological atom's zero-flux surface makes ignoring the effects of other nuclei on a region of charge density possible. Concomitant with this domain-specific reconception is a conceptual framework — the topological atom as space-filling, bounded by a non-penetrating hard shell, mereologically distinct

parts of a whole molecule. Since this framework conflicts with conceptions of the atom underlying other chemistry modelling practices and also makes possible the application of the virial theorem, the topological atom presents conceptual pressure in chemistry modelling.

4 — Conceptual Pressure and Model Transfer

The lesson of this chapter is that the source of conceptual progress ought to be what theorists pay attention to in characterizing intertheoretic connections between domains — i.e. the connection between physics and chemistry. This is the sort of characterization that is in the background of attempts to reduce chemistry to physics, for isntance. As chapter 2 highlights, model templates require scientists prepare phenomena in a way that results in new concepts or the alteration of old concepts. Accounts of reduction will miss the connection that these concepts in chemistry have to the pragmatic dimension to landing zone type conceptualization — at least as theorists classically model reduction, on a deductive, or some other truth preserving relationship, between theoretical terms across domains. As I highlighted in this chapter, scientific preparation for model transfer has connections to the theoretical-level of a domain — remaining agnostic to a domain having *a theory* — the level of scientific activity where scientists determine the meaning of the categories in which they use to discuss and frame their investigation of phenomena. This section motivates that the pragmatic dimension to the introduction of these concepts also impacts this theoretical-level by examining the source of disagreement between Bader and his interlocutors in chemistry. This debate takes a form that indicates the impact

that introduction of concepts like the topological atom or Fisher's population has is not just due to theoretic ideals — like simplicity — but due to the sort of landing zone type activity looked at last chapter. Thus, I argue, there exists in model transfer and important mechanism for understanding where scientific domain-specific concepts 'come from' in the sense of giving reason for why scientists think of phenomena the way that they do.

Fisher's transfer of the Ideal gas resulted in impactful debates that lasted for decades. Bader's transfer of the virial theorem also resulted in subsequent debates that lasted for decades, but were less impactful in his domain. Instead of only being about the methodology of scientific modelling, both debates covered philosophical topics like mereology, how to conceive of the constituent parts of molecules. For instance, the methodology side of the debates had to do with the sort of topics that a philosopher of science would discuss, like what sort epistemic achievements modeling ought to accomplish. Bader's opinion was that mathematical modelling in chemistry ought to be centered on a concept of the atom that was 'reducible' to physics instead of the tricky to reduce chemical bond. At the same time, Bader desired what he thought of as intuitive mathematical representations in three dimensions instead of Hilbert space. Part of his epistemic strategy was to explain the structure of functional groups, a major link between theoretical chemistry and other branches of chemistry. These methodological and epistemic strategies required a concomitant conceptual strategy for the use of the model templates he transferred, identifying parcels of electron density as the phenomena that the virial theorem was to be used to

model — topological atoms. It is this conceptual strategy that plays a key role in the debates introduced with QTAIM. More than, for instance, just QTAIM's use of the virial theorem to analyze electron density, or just the notion of reducibility or intuitive representations, it is the conceptual framework that includes ideas of how whole relate to parts for the use of the virial theorem that is the source of conflict. In short, the source of disagreement is the dynamic between the theoretic level and the methodological level in this case of model transfer.

In the following paragraphs I describe the pragmatic dimension to molecular orbital theory's conceptual strategy. The essence of molecular orbital theory modelling is an understanding of electrons as delocalized over the whole molecule instead of localized between atoms. This understanding of electrons licenses the way MO models make the use of wave functions tractable for describing bonds. However, as discussed by Harré and Llored in "Mereologies as the grammars of chemical discourses", this understanding of electronic structure comes with a particular mereology of the molecule. "Constituent atoms of molecules are not parts of those molecules when we look at the total entity in the light of molecular orbitals" (Harré and Llored, 2011, pp. 73). This is because, if the criterion for the identity of atoms is the composition of the electron shell, then the criterion cannot be met by the constituents of molecules within MO theory (Harré and Llored, 2011). MO theory approaches modelling the properties of molecular orbitals and bond orders, abstract bonding relations, properties that cannot be instantiated by any one atom. Thus, the concept of an 'atom' plays a particularly 'background' role in MO theory's strategy.

As Llored highlights in his later 2014 paper, this feature of MO-modelling results from its “whole-part methodology”. For instance, early MO-modelling uses the linear combination of atomic orbitals approach, where a molecular wave function is made by adding together the wave functions for atomic orbitals. However, atomic orbitals do not contribute ‘additively’ to the molecular wave function because they come associated with a coefficient in the LCAO expression of a molecular wave function. Llored points out these coefficients are determined by two integrals:

> (1) the Coulomb integral which is related to the electron energy in a unique atomic orbital φ1 or φ2 , and (2) the exchange integral which deals with the energetic coupling between the two atoms inside the molecule. As this type of coupling exists once the molecule is created, we can conclude that each coefficient depends upon the whole molecule, and not solely upon its corresponding atom or nucleus! (Llored 2014, 146)

The representation of repulsion and coupling interactions between, for instance, two electron orbitals depend first on the whole molecule, not any property of individual atoms. Bader complains of the arbitrariness of overlapping atom models like molecular orbital models for the following reason. It does not really matter what nuclei either of the orbitals belong to, they are essentially interchangeable depending on the aims of the MO-modeler. Whereas, with QTAIM, the conceptual strategy constrains the methods for distributing molecular properties to parts, narrowing the possible mathematical tools for analysis. Either modelling method for assigning properties to parts has its virtues, but their attached notions about mereology conflict, thus these notions serve as props for debate in chemistry.

As Llored depicts Bader's debates in his 2014 paper, Bader's conflict with MO modelling methodology is due to differences in an approach to mereology that is about how this mereology makes possible a method for using the virial theorem. Bader's approach to modelling molecules fundamentally represents molecules as constituted by additive parts. Each topological atom, because of the applicability of the virial theorem, additively contributes to the properties of a molecule. For instance, knowing the potential and kinetic energies of each atom in a QTAIM molecule, a chemist knows the energy of the whole. This is not true of MO-theory models, where no property of any individual atom maps, additively, to properties of a molecule. The transferability of the virial theorem towards this sort of mathematical representation depends on QTAIM's partitioning scheme. Since QTAIM partitions charge density into regions of space that meet the requirements for virial equilibrium, conceiving of molecules as constituted by additive parts is possible. The applicability of the virial theorem depends wholly on this conception of a molecule as consisting of spatially well-defined subunits. This also happens to constitute the core of Bader's conflict with MO modelling.

> The notion that atoms overlap one another stems from the use of atomic-like functions (improperly termed atomic orbitals) in the expansion of a molecular orbital or in expressing a valence bond wave function. The overlap integral for example, forms the core of Coulson's book on valence (Coulson 1961). The point of the present paper is simple: to demonstrate that a return to Dalton's notion of an atom as a bounded space-filling object frees chemistry from the yoke of arbitrary models and definitions and places it in realm of physics (Bader and Matta 2012, p. 256).

Bader emphasizes that his disagreement is not only with MO methods (the use of atomic orbital functions) but also the sort of idealizations that make the use of these functions possible. The introduction of Fisher's model featured similar

debates that are telling of the reasoning behind introducing new concepts. Debates were not that these conceptions are simply ‘right’, — i.e. atoms simply are ‘bounded and space filling’ thus other descriptions are false — but that there was an epistemic value tied to their use in strategizing the use of transferrable models.

> The orbital model has been extended beyond its intended use of predicting and providing electronic structure of a system, by associating the forms of individual orbitals with the assumed spatially localized pairs of bonded or non-bonded electrons, and by attempting to define atomic properties in terms of coefficients of atomic-centered basis functions appearing in the expansion of molecular orbitals. (Bader 1990, pp. 131)

The orbital model Bader refers to here, the target of molecular orbital mathematics, does not license definite assignment of properties to atoms in molecules. There exists no one-to-one mapping between features of a molecular orbital model and the parts of the molecule as there is with QTAIM. Llored calls this molecular orbital’s whole-part strategy. It is a strategy insofar as it involves a particular conception of the mereology of molecules that then guides approximating quantum mechanics (physics) to make it possible to use in chemistry. Ignoring some particularities of electron interactions and three-dimensional position in the linear combination of atomic orbitals using coefficients is one example. MO-theory’s conception of the molecule works as a strategy because it limits what sort of mathematical methods are possible to use, while affording others.

Strategies like the one that MO’s conception of the molecule makes available for ignoring some particularities of electron interaction while focusing on

others particularities impact the meaning of domain specific concepts. Scientists take seriously a new conception even if it is ‘just’ useful for making calculations easier, or transferring a model. Thus, we ought to understand the meaning of these conceptions — the molecular orbital molecule, the topological atom — by their connection to transferable mathematics like model templates and the strategies that the combination of computational methods and embedded concepts license — MO models are widely used because the strategy looked at in this section is incredibly useful and easy to apply for describing bond energies. A new concept that plays such a role constitutes conceptual progress. The lesson here is that an understanding of supposedly emergent concepts — molecular orbitals, topological atoms — that pays attention to conceptual progress better captures scientific reasoning in these domains than an analysis of whether these concepts can be ‘reduced’ to physics.

Bader spent decades debating chemists on the proper use of physics in chemistry for modelling. These debates centered on how certain sorts of target systems were not conducive to an ideal use of mathematics from physics. This includes the existence of bond related phenomena like resonance and molecular orbitals (Bader 1985, 1990, 2009). Bader’s debates reach topics besides mereology. For instance, a common criticism of QTAIM is that it promotes a conception of molecular structure that dismisses ‘the chemically relevant differences between ‘ionic, polar, covalent, H-bonding and van der Waals nonbonding and other interactions’’ (Wang et al. 2010). Bader argues that these interactions only “differ one from another in the manner in which the electron

density is distributed" (Bader 2011). Bader argues that chemists ought to not think of ionic, polar and covalent bonds as chemical kinds because QTAIM's conception of electronic structure makes an alternative tractable use of description of molecule energy. Another recent debate is whether chemists ought to consider Pauli repulsion a force. From the lens of QTAIM's conception of the atom, 'Pauli forces' do not exist (Bader 2006). This makes bond methods for modeling the structure of molecules using physics incoherent (Poater, Solà, and Bickelhaupt, 2006). Whether to conceive of the structure of molecules as due to Pauli forces or not depends on notions about the constitution of molecules. Conceptions about what sort of thing transferable mathematics should target is a sticking point in these debates about ontology and the methodology of model transfer.

Paying attention to what I have called conceptual progress offers a perspective where we can better understand Bader's debates. These debates are not simply about the meaning of concepts and/or what concepts more closely align with epistemic standards like 'truth'. For instance, the debate surrounding molecular orbital models was not simply conceptual, having to do only with how a chemist ought to think of mereology, or purely methodological, what sort of mathematical methods a chemist ought to use in modelling, but an entwinement of the two. The entwinement I think is captured by the idea that transference of mathematics — model templates — requires conceptualizing to make its application possible. It is not any conceptualization but a conceptualization that makes a particular model template possible to use. This activity introduces

complexity into model transfer. Bader's QTAIM consists in not just a use of new mathematical methods for modelling the state of molecules but a novel 'whole-part strategy' in chemistry. QTAIM's whole-part strategy depends on a certain mereology of molecules. The target for its use of transferable mathematics — the topological atom — must be conceived of as having an additive relation between parts of the molecule and the whole molecule. Understanding the dynamic between certain targets, and the associated conceptualization of phenomena, and model template transfer extends to an understanding of conceptual innovation.

5 — Conclusion

Characteristic of both cases of model transfer examined in this paper is the preparation of domain specific phenomena. Scientists invent a new kind of thing for application of a model template. Epistemological and methodological debates result from the conceptualizing of this thing. These debates involve discussion about what sort of things mathematical modeling ought to target — for instance, whether it is the spatially overlapping molecular orbitals or the spatially bounded topological atom. Each choice entails a suite of idealizations and assumptions. Are the phenomena of chemistry mereologically additive or not? Are atoms transferrable subunits of a molecule? These questions are implicit in the preparation done to make transferrable mathematics useable because of the aligning done by scientists between phenomena and model template concepts. Model transfer instigates conceptual pressure. The concept of conceptual pressure has a slightly metaphorical use; I wish to characterize through using it

that the increase in tension amongst scientific concepts in a domain with the addition of new conceptualizations of phenomena is similar to the changes that take place in an enclosed gaseous system when one adds new molecules. At least in the cases I have covered so far, and I suggest this can cover much of modeling in chemistry, the reconception of domain-specific phenomena in order to make possible the application of a transferable model template is the driving force behind conceptual pressure. The reconception in order to make sense of the new sort of target (model/system/phenomena) comes entangled in a rich web of assumptions. This motivates analysis of conceptual developments in chemistry through the lens of model transfer.

In QTAIM's case of model transfer, Bader introduces an alternative conception of the constitution of molecules embedded in the topological atom as a target for transferable mathematics. This new conception becomes the centerpiece of debate about ontology and methodology like the case of Fisher's model

Philosophical discussion on model transfer identifies these features as landing zones. They are a feature in modeling that functions to make possible the transfer of a model template. They also function as a target for a model constructed from a transferable template. These two functions are related. A model template's use in a new domain requires a target that is ontologically compatible. A landing zone is the result of reconceiving domain specific phenomena in a way that makes phenomena ontologically compatible with the conceptual framework embedded in a particular model template. For instance,

embedded in the virial theorem model template is a conceptual framework that makes the mathematics meaningful only for things in stable equilibrium. As a tool for analyzing charge density in chemistry, these conditions are met by Bader's atoms. Both the topological atom and the virial theorem answer 'what sorts of things exist?' with 'things that are in stable equilibrium'. Thus, they are ontologically compatible. In the case of QTAIM, the topological atom is the feature that functions to make possible the application of the virial theorem in a density functional theory framework.

Analysis of landing zone features like the topological atom tells a story of conceptual progress by model transfer in the Fisher model and QTAIM cases. A significant source of mathematical modelling in chemistry is the transfer of mathematics from physics. Existing theory on model transfer provides a framework for analyzing the thing that is transferred — model templates — and the thing to which transferrable templates apply — landing zones. The latter becomes a source of new scientific concepts. This is an account that still needs refinement, but, as I have argued in this chapter, there exists promise in applying the framework in characterizing conceptual pressure in chemistry. For instance, how do contrasting mereologies of the molecule arise? They are the result of model transfer, the reconceiving of domain-specific phenomena in making transferable mathematical tools applicable.

The sort of analysis performed in this chapter provides an avenue for understanding conceptual innovation that does not rely on an account of 'scientific theory' or models of reduction. In the case I look at in this chapter,

model transfer imparts conceptual change at a smaller scale. Models of intertheoretic-reduction like Nagel's are now widely rejected as overly simplistic by philosophers. My chapter 3 suggests a source of difficulty for reduction is that, at least with chemistry, the intertheoretic connection is complicated by the sort of conceptualization required for model transfer. To elaborate, consider Nagel's model of reduction. It requires postulating scientific theories as syntactic objects. Such models of reduction also require postulating that domains then have logical relation between laws (Nagel 1949, 1961, 1970). This is a problematic conception for sciences like chemistry that do not have general scientific laws in the way that physics does — by general, I mean full coverage in the sense of Hendry (2012). Chemistry laws are of limited scope. Hence, Nagelian type models of reduction need a notion of bridge laws to justify 'a reduction'. Derivability of laws and connectability through bridge laws are the two necessary conditions for reduction. However, as I show in Chapter 2 and 3, the concepts that a reductionist would like to explain through a reductionist model — the chemical bond is such and such phenomena from physics — have an inexorably pragmatic dimension. The meaning of concepts like the chemical bond are complicated by the reason for which the concept is invented, to make model transfer possible.

The connection between scientific domains examined in this chapter consists of a transfer of a model template and the introduction of new notions that make the model template useable. Scientists react to the concepts

embedded in model templates, preparing phenomena so it makes sense to use the template to model in their domain. Fisher did this with the introduction of the ideal gas law. Using the ideal gas law's distribution of velocities method to model the inheritance of traits within a species required Fisher to prepare the domain of evolutionary biology for seeing species as homogenous kinds and not composed of individuals. Thus, through model transfer, the spread of computational methods like that seen from statistical mechanics to biology in the ideal gas law case influence biologists' conception of species.

In Chapter 3, I also mention how methodological advantages further motivate scientists to accept the new concepts introduced through model transfer as legitimate. With QTAIM, the methodological strategy afforded through transferring the virial theorem was the 'whole-part' relationship between atoms and molecules. Scientists using QTAIM could identify molecular properties from information about electron density (or 'simply' from the volume a topological atom takes up within a molecule). Molecular orbital and valence bond models promote different strategies; these strategies allow organization of 'electronic' information based around bonds. In the next chapter, I examine in more detail how scientists use things like model templates, or models, to organize information, or how a model could bring about a 'strategy'. Bringing about a new strategy or way of organizing information is a major epistemic achievement.

In the next chapter, I create an account to characterize more specifically the epistemic achievement to do with model transfer. This account uses problem solving in order to explain the epistemic value of model transfer. Scientists use models to frame investigations. And, in Fisher's case, scientists also use models to reframe an investigation that was spinning its wheels — biologists at the time were considering getting rid of the notion of natural selection because of the difficulty in characterizing it statistically. Scientific investigations are a sort of problem-solving, and framing is a type of activity necessary for problem solving. How scientists frame an investigation makes possible the use of different problem-solving strategies. Problem solving literature refers to these problem-solving strategies as heuristics. Thus, my account ties a models' epistemic value to its affordance of heuristics when used by a scientist to frame an investigation. For example, suppose a chemist wanted to investigate into why certain molecular geometries were prolific. Bader's QTAIM model would allow a rather efficient strategy for predicting bond angles and bond lengths from electron density. Thus, scientists could frame, using QTAIM, the investigation around electron density information whereas this is not such an efficient strategy coming from a valence bond or molecular orbital model. My next chapter elaborates in more detail what I mean by framing and its relationship to information.

Chapter 4: Problem Solving and Epistemic Value

1 — Introduction

There has been some history of focusing on problem-solving in the sciences in attempts to understand scientific progress. I wish to take the strategy of shifting focus onto problem-solving from the accounts of progress to use in accounting for the epistemic value of modelling. Among the well-known attempts regarding progress are Kuhn and Laudan (Kuhn 1962, Laudan 1977). Both used the solved problem instead of the established truth as the unit of scientific achievement for their accounts of scientific progress. For Kuhn, the scientific community spends most its time pursuing a sort of puzzle solving (Kuhn 1962, pp. 35). Roughly, scientists take in the exemplar puzzles in their field, develop a know-how for solving similar puzzles to these exemplars, and go about adding to their discipline's stock of solved puzzles — an intra-discipline measure of success. Kuhn’s conception of scientific activity was in opposition to the depiction of science at the time of the empiricist tradition. Again, roughly, this tradition depicts science as operating by making predictions (in the form of hypotheses), designing experiments based on those predictions, and inferring from the veracity of predictions the truth of theories (Hempel and Oppenheim 1948, Hempel 1965). Within this image of science, the community of scientists were

either chipping away at the discipline's previously thought to be true theoretical generalizations or adding to them on the basis of confirmed hypotheses. However, this special epistemic authority to access and modify what the discipline held to be core 'truths' was unrealistic according to Kuhn, who compared this image of science to learning about national culture from a tourist brochure (Kuhn 1962). This access is only available in times of unprecedented epistemic turmoil. Most scientists work to solve problems, puzzles deemed pursuitworthy by their similarity to paradigmatic cases instead of determined to be pursuitworthy in virtue of explicable rules.

Laudan's account of scientific inquiry similarly prioritizes problem-solving in analyzing the reasoning for the pursuitworthiness of theories (Laudan 1977). Laudan thinks this reasoning is about the capacity of a research tradition to solve empirical problems rather than about justification from empirically verifiable truths. By shifting focus from justification of discoveries to promise of problem-solving, his proposed epistemology of science offers an account of scientific rationality that prioritizes the aspect of scientific reasoning that is ‘forward-looking’ in the sense that it is reasoning about how to proceed forward with an investigation despite great uncertainty. The upshot of accounts like Laudan’s and Kuhn’s is that they afford the characterizing of scientific reasoning in cases where there is not enough evidence to justify a theory’s choice but perhaps there is good reason as far as promise for problem-solving or heuristics.

The virtue of Kuhn’s and Laudan’s accounts is that they bring into perspective everyday scientific inquiry. I wish to use a similar reprioritization of problem-solving for describing what models do. Seeing scientific inquiry from the perspective of

prioritizing problem-solving is accounting for the epistemic goodness of scientific activities — experimenting, modelling, hypothesizing, theorizing — by their contribution towards either solving problems or framing problems so that they are easier to solve. By pursuing reprioritization of the value of problem-solving in accounting for the goodness of modelling, I do not wish to deny that scientists 'seek the truth' in inquiry. Instead, developing such an account shifts the focus of philosophical analysis from justification and verification to the reasoning that scientists often use to work, the use of heuristics to decide on pursuitworthy activities in spite of uncertainties. Taking this shift in perspective from general rationality of science to the epistemology of modelling can be helpful in illuminating what models do in science. Broadly, models make problem-solving easier. They simplify computational tasks, help the setup of experiments, provide reason to pursue a path through a problem space and make the oceans of data navigable.

First and foremost, scientists use models to solve problems. The lens of truth-first epistemology offers cognitive achievements as the scientific reason for modelling — learning about the world, understanding, explanation. However, it is a fairly uncontroversial view on models themselves that they are essentially distorting of the world. Models distort by consisting of assumptions about the world that simplify complex systems, postulate entities and mechanisms for the sake of computational ease, or otherwise constrain the representation of phenomena. To represent usefully, a model must be dissimilar to its target — a fullscale map of Britain would be useless for navigation — and this way in which a model becomes useful is the real trick to a model's value to scientific inquiry. Truth-first epistemology

sees model distortion as either an obstacle to epistemic value — a Galilean Idealization waiting for computational power to catch up to demand (Weisberg 2007) — or a side-effect of value — i.e. irrelevant features to the explanatory task (Strevens 2008, McMullin 1968). I use a problem-solving lens on the epistemic value of modeling to offer an alternative account, placing the distorting features of modeling closer to the positive practical goals of scientific inquirers.

In this Chapter, I use an information processing framework for characterizing problem-solving borrowed from cognitive science and develop this framework to analyze a major achievement in science, the discovery of Neptune. The upshot is a truth agnostic depiction of modelling that captures the creative, intellectual activities of scientists. Scientists are inventors, of worlds, mechanisms, models, where realism or realistic-ness is left for debate after scientific action has been taken, for the purpose of solving the problems at hand. Science is mostly a forward-looking intellectual endeavor. An approach that paints such a picture of scientific modeling gets at the epistemic standards of scientists.

The epistemic achievements resulting in the discovery of Neptune were borne out by the use of rather inaccurate models. Therefore, the achievements are poorly characterized if one looks mostly at the model-world relationship — how scientists learned, understood or explained something about Neptune through these models. Instead, what models of Neptune allowed scientists to do is understand with greater certainty how to frame the problem of Uranus' anomalous orbit. There exists a connection between epistemically successful problem solving and having a well-

framed problem in the sciences. Well-framed problems allow for the use of heuristics and community-borne wisdom.

To characterize having a well-framed problem as an epistemic achievement to which models contribute, I will be borrowing some conceptual tools from cognitive science accounts of problem-solving. These accounts formalize the cognitive process of problem-solving towards characterizing the activity as a *search* of a *problem space*. I will be using their terms to elaborate on scientific problem-solving. This elaboration involves first a brief detailing of Simon and Newell's information processing account of everyday problem-solving (Simon and Newell 1972), a philosophical retooling of their concepts towards the purpose of analyzing scientific decision-making to do with modelling, and then an application of these concepts to the historical case of the discovery of Neptune.

2 — Problem-solving as Information Processing

In this section I will introduce the information processing (IPS) account of problem-solving and indicate its affordance in accounting for the problem-solving value of scientific modelling. In their seminal work *Human Problem-solving*, Allen Newell and Herbert Simon (1972) introduce an information processing account of what they call "human problem-solving". Their account provides a mathematical and computational depiction of problem-solving. They define a problem as any instance when "someone wants something and does not know immediately which series of actions they can perform to get it" (Newell and Simon 1972). To solve a problem, a problem solver engages in a mental search of a problem space for the state changes to the task environment they can bring about leading to the desired result.

The task environment is the problem-solving situation. It consists of the object(s) of interest to the problem solver and their properties, properties including the capacities of these objects to change with a manipulation of the enviroment. Problem solvers represent the task environment using a representation similar to network graphs, a *problem space*, where nodes represent possible states of the task environment and edges represent possible state changes (i.e. transition between possible states). Therefore, the problem space represents possibilities as well as the thing in itself and since the problem space is a representation there is a possibility of failure. Problem spaces reflect what the problem solver believes about the possible changes to the task enviroment. The problem space consists of an initial state, states that the problem solver could practically bring about by manipulating the task enviroment and a (or several) goal state(s). The problem space is a representation in that it contains information encoded in states that is about something — for example, the information encoded in a state in the problem of navigating a mall could be given by a series of questions with yes or no answers about the position of the navigator in the mall.

A problem-solving state is a complete description of the features of the task environment the problem solver can manipulate. It is complete in that it encodes all the information relevant to the problem-solving. Relevance is determined by the problem-solving agent's framing (in the sense of interpretation) of the constraints that define the problem; more on constraints later. The state is a description in that the information consists of answers to yes/no questions about the thing(s) being manipulated by the problem solver. The state encodes the properties of the thing(s)

that the problem solver is manipulating to solve the problem — e.g., in navigating the mall the state is the position of the navigator with respect to the mall described by the set of questions, for example, "Am I at gamestop? Yes/no, Am I at the flower shop? Yes/no, etc." The goal state is the state of the problem-solving enviroment that meets the constraints on the solution to the problem. The problem solver does not have the solution to the problem if they just comprehend the goal state. A solution to a problem is a path through the states in a problem space that begins at the initial state and ends at a goal state.

The assumption for this branch of cognitive science is that when problem-solving, humans search this problem space for solutions similar to a Turing machine. To make such search possible, the information processing theorists argue, problem solvers must find ways to limit their search to a computable amount of detail. This literature calls such limiting *framing*. I will go into greater detail on framing later in this paper. But, in short, framing is the grappling with ‘conceptual’ issues with the problem. An example is changing what information the problem space states encode so that a particular sort of heuristic is useable.

Simon later uses IPS accounts to understand the psychology of scientific discoveries (Simon 1999). I wish to borrow upon this line of thinking for depicting the non-truth-related epistemic affordance of modelling in science. Heuristics are strategies for searching a problem space. A classic example is ‘backup avoidance’, where a problem solver chooses the next node of a problem space (next state to bring about) based on whether their path has led them through this node before. As a heuristic, backup avoidance is a rule of thumb; like all heuristics, the rule directs

the agent's preference in searching but does not act as a hard constraint. With back-up avoidance, the agent is to prefer state changes that do not bring about nodes already visited in the problem space, but such choice is always *possible* while still following the heuristic. To make backup avoidance useful, the problem space ought to encode information that makes the preference conceivable to the agent. Whether or not a strategy is useful depends on framing as much as it depends on the problem at hand. A poorly framed problem can make an otherwise useful strategy, useless. With backup avoidance one can imagine an agent who is just not paying attention to enough detail in framing the problem space states to distinguish between already visited states and novel states — this may an unrealistic example since it would require an agent to have a single node problem space, more detailed examples explored later.

Beyond psychology, heurists play a key positive epistemic role in making scientific epistemic achievement through problem-solving possible. In order to be useful though, a problem needs to be framed well enough that for the solver to deploy these strategies. In a way, having a well-framed problem is an epistemic achievement because it affords the use of strategies and community born wisdom for handling problems. Much of community born wisdom is in the form of tacit rules on how to approach problems that parents (for instance) teach children by doing. Most people were never were taught explicitly to use something like backup avoidance.

The person who knows more precisely what they need to know (but do not yet know) is able to use framing more successfully. The mall navigator in the

previous paragraph knew that they needed to know the stores they were passing instead of the smell of the air or a trillion other details our senses can discern in an enviroment, turning a time-consuming impractical meandering into a decisive hunt. After all, if one spends their time clothes shopping spending three hours meticulously wandering the parking lot looking for their store, they may as well not even go. Similarly, if their problem space encodes the details of every tile and every footstep they take in the mall, they would find themselves quickly overwhelmed. One way to think of good framing is that it is finding the successful compromise between too much information and not enough information to make the strategies we have inherited through generations of learning to be human useable.

There is a scientific equivalent to this imperative that is epistemic. We do not have eternity to inquire. In this sense, formulating a well framed scientific problem is a major epistemic achievement, one that is often borne out by a new application of a model through model transfer. This chapter will form a basis for explicating what is especially epistemically valuable about activities like model transfer. To have a well framed problem implies one knows to a significant extent what one needs to know. A difficulty in this framework borrowing is that scientific problem-solving involves complexities usually not found in the everyday variety studied by cognitive scientists. Scientific problems are often ill-defined; e.g. there may exist no algorithm for determining whether something is a solution (Reitman, 1964, Simon, 1973.) Goal states are uncertain until a solution has been found. For example, that Uranus' peculiar orbit was due to another planet was not known until well into the scientific investigation.

With this complexity in mind, at its most general, a scientific problem is a demand for something and constraints on what counts as fulfilling the demand (Nickels 1988). The solution is a path through problem space states that begins at an initial state and ends at a goal state. The goal state encodes information about the constraints on the problem. One can understand the constraints as formulable in terms as a set of questions that have yes or no answers. — Is the store a clothing store? Is it named Belks? Does it have great deals? Is the Belks in the mall I am in? This set of questions are the *constraints* on the solution. These constraints are part of what a problem-solver uses to define the problem space that they search — ie. restricting the nodes of the space to ones that encode information about location relative to stores instead of floor tiles or smells. A problem space typically consists of nodes that encode the states of affairs that the agent can practically bring about in the task enviroment — e.g. navigating a mall. A human problem-solving agent cannot teleport to the store, so the problem space would likely not have node where the agent is at the entrance directly connected to the node encoding the state of the mall where the agent is at the store.

For everyday problem-solving, there is usually more certainty about the goal state. For scientific problem-solving, the goal state is usually less ‘fully’ characterized, and the agent’s problem space often is more often shared by a community of inquirers. Some everyday problem-solving involves community inquiry. Science just happens to be a complex enough of an activity with a great deal of uncertainty about the goal state of problem-solving. This results in heuristics being trickier to use. Understanding the way in which scientific problems make possible

community inquiry is one of the side goals my proposed account can shed light on. The focus in this paper is on how scientific problem solvers frame problems so that heuristics are useable.

3 — Problem-Solving With a Derivation

To help illustrate the relation between framing and heuristic use, consider an example of problem-solving most philosophy students are quite familiar with, doing derivations in formal logic. A student will be given an argument in a formal language and asked to use a proof system, rules of inference, to derive the conclusion from the premises. With a derivation the goal state is more certain for the solver than I suggest a scientific problem would be. They know what the last line needs to be and that it has to be licensed by a rule of inference. There is some uncertainty about what rule but not the syntax of the line. A typical derivation problem will tell the student exactly what the final line must look like. However, just writing the conclusion down does not count as a solved problem. This is because a derivation only counts as a solved derivation if the operation follows the constraints given by the rules for symbol manipulation by the proof system and the particular problem at hand. A solved derivation must include a path from the premises to the conclusion consisting of a series of formal sentences where each sentence is licensed according to a rule of inference applied to some sentence in the series before it.

At first glance it would seem there is not much similarity to navigating a mall. A derivation is done typically on paper. Navigating a mall takes place in physical space. The constraints on a derivation are a set of rules for symbol manipulation. The constraints on finding a store are physical. However, typically, people do not

perform the task of navigation by physically trying out all options until one works. We think through the problem.

Cognitive scientists would rightly point out that there is a similarity between these two seemingly different activities when viewed as searches of a problem space. In navigating a mall, one is mentally trying out different paths through the various places one can find oneself in the mall. If in this particular mall a hallway contains, in sequence, a gamestop (G) between the flower shop (F) and the Nike store (N), and we are at the flower shop then a valid path would be F -> G -> N. G -> F -> N is not a valid path from any navigation state of this mall hallway. If the navigator thinks it is a valid path then they need to update their conception of what stores are where or face likely future difficulties in solving navigation problems. This is an issue of a problem solver struggling to map constraints onto their problem space. Even though this is a problem about navigating a physical space, the activity of the good problem solver is mostly occurring in a 'mentally' searchable space. A good problem solver is setting up this space with the right constraints or discovering the paths leading to a solution efficiently.

Still, only having the right idea of valid paths is not going to make one a successful navigator. Consider the situation where a mall is a figure eight with two loops. In this case we could navigate all day long around valid paths through the bottom loop while our store remains unfound in the top loop. This seems easily solvable from the perspective of our experience navigating but from a perspective of nowhere there is no in principle reason to navigate away from places that we have already been.

Cognitive problem-solving accounts suggest that what makes a good problem solver then is the ability to use heuristics to narrow down the set of valid paths when searching a problem space — a valid path through the problem space is simply a path that uses the space's existing nodes and edges. To experienced mall navigators, if we found ourselves coming across the same stores again and again, we would probably try a different path. This would be to apply a more sensitive version of backup avoidance where we avoid states like the ones we have already been through — similarity avoidance. A heuristic is a suggestive as opposed to demonstrative rule on how to search a problem space — a 'rule of thumb'. It is suggestive in that, unlike a demonstrative rule, like a logical rule, heuristics point more ambiguously to a conclusion. Heuristics are also suggestive in that they do not guarantee something about the problem state change (that for instance the path is going to be a solution path); this is unlike how a rule of inference guarantees that the next line is entailed by the ones that the rule is used on. Using similarity avoidance requires one to frame the problem in a way that encodes information that would enable one to assess the similarity of each location visit in the problem space. Backing up is not prohibited by this heuristic. So, one can think of heuristics as applying desirability weights to the edges of the problem space graph. To have the similarity avoidance weighting be useful there needs to be the right framing, one that allows the recognition of the similarity of states with the right amount of detail. There are two ways of seeing this framing. The first is a setting up of the agent problem-solving space to include only paths that take one through each store once. Or, more realistically to our typical non-optimal mall navigation, finding ones' navigation is

taking one past the same stores and reframing the problem space to encode information that would allow for a strategy like similarity avoidance.

Likewise, a derivation solver is also searching for paths through the possible sentences one can create by manipulating symbols through application of rules of inference. Each new sentence must be licensed by a rule. For any derivation problem, the paths are constrained by sentences one starts with and the rules of inference for the language one uses. Take for example a relatively simple derivation where a beginner logic student will be asked to demonstrate through the use of a proof system that it is a valid argument. If one is given the argument: [premise 1] Fa -> Gb, [premise 2] Fa & Gb, [conclusion] Gb, then the premises and the rules of inference combined define the complete problem space for this derivation problem.

One can write down an infinite series of sentences (and still solve the problem eventually) exploring all possible valid conclusions from these two sentences. No one has the time for that. A slightly practiced derivation solver is going to rightly constrain their search of paths to ones that involve using rules that have to do with the (->) and (&) symbol. A competent derivation solver will have a problem space that prioritizes rules that eliminate connective symbols. In the case of a derivation, each node of the problem space represents a unique series of formal sentences and each edge connecting a node represents an additional line brought about by a rule of inference usage.

Derivation 1

> Nodes: derivations in which the first two lines are premises 1 and 2 (justified by the rule ‘P’), following by N many lines (for any N—this space is infinite) each of which is a wff with a correct justification.

Goal states: any node in the space whose last line is Gb

Edges: for each node in the space with N lines, there is an edge to every node in the space with N+1 lines such that the two nodes match on their first N lines.

In this problem space
Node 1a:

1. Fa → Gb P
2. Fa & Gb P
3. Fa 2, &E
…
#. Gb ??,??, →E

would have an edge to the Node 1b (part of a suboptimal path):

1. Fa → Gb P
2. Fa & Gb P
3. Fa 2, &E
4. Gb & Fa 3, &I
…
#. Gb ??,??, →E

For navigating the mall, a state could be a position that the navigator is in with respect to the mall. Typically, a navigator represents this state as proximity to stores, or other landmarks, so this information is typically encoded as questions about which landmarks are nearby. For both these instances of problem-solving, a solution is a path through these states that end in a goal state. Hence there is a distinction between ‘the goal state’ and ‘the solution’. A derivation is not counted as solved by writing down the conclusion just the same as navigating a mall is not solved by finding oneself at the store one is looking for — it would be more accurate to say that the problem has gone away. The goodness of the solution is connected to the efficiency of the path. A fifty-line proof for the derivation mentioned above counts but it is not a 'good' derivation even though it counts as solved.

What makes the difference between a good derivation solver and a bad one is determined by their ability to use heuristics. One heuristic mentioned is the one that prescribes preferring one type of rule when navigating the problem space possibilities — preferring elimination rules if the conclusion has fewer connectives than the premises. So, this heuristic would suggest to the competent problem solver of Derivation 1: ‘do not follow the edge from 1a to 1b’. This heuristic does not count as a constraint though. Rule preference does not determine what counts as a goal state and does not otherwise determine which paths count as valid. One would not be a good deriver if one followed this rule without thinking carefully. Some problems can only be solved by introducing negations or more connectives as part of the path to the goal state for isntance.

To use the rule preference heuristic, however, does require certain framing. The deriver has to encode information about not just what rule is useable on a sentence but also what type of rule (elimination or introduction). This is a relatively easy distinction to make once one knows a little bit about the proof system. Framing a scientific problem so that the problem solver encodes the right information for heuristic use is a much more complex task because the problem spaces are usually much more complex and the problems themselves are not as well defined as a derivation. There is not a formal language with its own rule system for scientific investigations (yet!), and I would suggest such a language would be undesirable.

4 — Framing and Constraints

Framing is an activity where an agent characterizes a problem space using constraints. There are two ways constraints characterize a problem space. First, a

bit about the verb characterize. In the sense I use it here, characterize means to describe the important features of a thing. So, constraints characterize in the sense they are descriptions of the information encoded by the problem space states. For instance, the states of a logic derivation are about sentences in a formal language. There are explicit rules to doing derivations; some are symbolic such as the rules of inference for a proof system, some are expressed in a natural language — e.g. “a line must be licensed by a rule of inference". These rules determine the edges of the problem space. No valid path can consist of edges that are not a rule of inference. There is also an implicit dimension to such constraints, and this is the dimension where framing is an intellectual and creative activity is required. Such explicable rules or constraints provide guidelines for human problem solvers on what information is more or less relevant to solving the problem. In the derivation example, the problem solver most likely will interpret the “a line must be licensed by a rule of inference" rule that the states to attend to have to do with line information and rule information. This agent’s problem space nodes are about 'lines' of symbols and 'rules of inference'. So, constraints are explicable descriptions on valid solutions to a problem. But constraints also have an implicit dimension in that they tell a problem solver what information to represent — i.e. locations in a mall, rules of inference used etc. They tell a problem solver this but this implicit dimension to constraints also underdetermine the information encoded by the agent’s problem space.

There are two senses of framing corresponding to these two dimensions to constraints. To reframe a problem an agent can change (drop, add, or amend) the

nodes of their problem space by changing the description of the problem. This sort of reframing is a change in the description of the problem — i.e. "I am searching for the store in the top half of the Mall instead of the whole Mall". The other sort of framing involves changing the sort of information that nodes encode. With this type of framing, an agent changes the interpretation of the constraints to a problem. So, for instance, with the rule "All lines must be licensed by a rule of inference" one might keep track of just individual rules or if one is having a hard time deploying certain heuristics, one can include a rougher grained categorization of the sort of rule used (elimination or introduction rules). Even though it is somewhat obvious to a human derivation solver that these two classes of inference rule exist, for a machine search there would have to be two classes explicitly defined as containing the five elimination rules and five introduction rules — or perhaps the derivation solver is using a proof system where the rules go by their latin names and thus there exists the extra conceptual work of recognizing some rules as eliminating connective and some rules as introducing connectives. Another way to put this implicit dimension to constraints is that it consists of the entities and properties implied to exist in the task enviroment by the explicit description.

Finally, another important action from work on problem solving to translate to this philosophical framework is *registration*. Registration in this literature is a sort of framing. It is a sort of framing that falls under the second sense I discuss in the previous paragraph, when a problem solver changes the information that a problem space’s nodes encode. Registration is the making of a connection between some node in the problem space to an empirical fact in the task enviroment. This

connection then counts as framing because it requires the problem solver to refresh the problem space, either adding the empirical fact as a sort of information encoded by nodes, or if this sort of information was already encoded, updating the information encoded in nodes. The classic example of this activity in cognitive science literature is the use of the “you are here arrow” in a mall map to connect the problem solver’s problem space to their actual location; often registration involves the use of representations like maps in order to accomplish this sort of connection. In this instance, registration encodes a node in the problem space with information about the location of the problem solver — “Is the problem solver here? Yes” — and all other nodes with ““Is the problem solver here? No”. A general way to look at registration is that it is a framing that problem solvers often use to ‘refresh’ the problem space information with respect to new empirical facts made available to the problem solver or changes made by the agent to the task enviroment. To contrast registration with framing in general, problem solvers will change the information encoded by the problem space by interpreting rules for a game or instructions. This is not a registration because there is no problem-space node to empirical fact within the task enviroment connection. As a sort of framing, problem solvers also use registration to give structure to a problem space so that heuristics are useable. This paper will explicate such an instance of registration in the next section.

5 — How Framing Matters

For some detail on how framing matter for heuristic use, consider a comparison between two games well studied by cognitive science literature, tic-tac-toe and number scrabble. An agent’s framing is impactful of the agent’s ability to

problem solve. Tic Tac Toe is a simple to understand game; for the majority of game players, agents are usually searching through the same problem spaces. For instance, the goal state is commonly grasped amongst game players, three of the player's symbols exist in a row in the game play area.

Testing whether the constraint of three-in-a-row is satisfied involves answering the following set of questions {"Are my (Xs or Os) in a row across the top three cells?", "Are my (Xs or Os) in a row across the middle three cells?", … etc.}. A problem space according to this win condition constraint would be the game tree of tic tac toe, a directed graph that 'begins' with the more limited number of initial game moves and branches off to include all end states. Thus, the nodes encode answers to yes/no questions about the state: "Is there an X on the top left cell and an O on the middle cell?" along with answers to yes/no questions about potential states "If agent 1 put an X on the top left cell will the game state consist of an X on the top left cell and an O on the middle cell?". Nodes of this problem space represent the state of the game and edges represent the moves to potential states; a player is not allowed to erase their moves so edges leading back to the initial states do not exist.

Framing matters for even simple games like tic tac toe. This becomes apparent in the attempt of cognitive scientists to understand how problem solvers transfer problem-solving methods to new problems. One such case is the transfer of a strategy known as the 'corner move' from tic tac toe to a similar game, number scrabble. The game play area of number scrabble consists of a list of 9 numbers and the game play consists of each player taking a turn picking a number. Once a number is picked it is crossed from the list. The game ends when a player has

chosen three numbers that add up to 15. To most players who are familiar only with tic tac toe, there will appear to be not much similarity between the two games. However, their game trees are isomorphic, thus there exists a ‘complete’ problem space that is shared by both games. It is complete in that it comprises all possible game states and moves.

Corner move strategies require the player to recognize that a particular state counts as a ‘corner’. One way number scrabbles players come to this recognition is the ‘magic square’ setup number scrabble. One can think of this setup as the use of a simple model to interpret information about the task enviroment. (Figure 4.1)

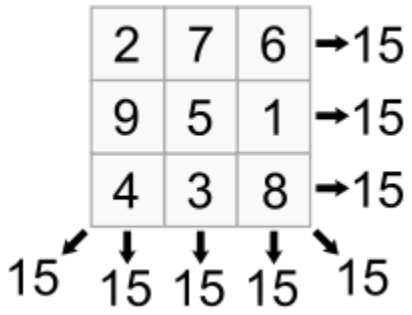

Figure 4.1 A magic square is a grid where each cell is filled with a different positive integer and the sum of integers in the rows, columns and diagonals of the square are equal.

A game player using this magic square model can register certain branches of the tic tac toe game tree (problem space) to the task enviroment of number scrabble. This registration encodes the empirical facts of ‘2’, ‘6’, ‘4’, and ‘8’ written as symbols in a game play area as ‘corner states’ in a problem space — in the problem space these states would have the information “Is this a corner? Yes” encoded. This makes it so the player can frame the problem space for use of the corner move heuristic in the same way our derivation solver must recognize certain states as involving a type of

rule in order to use more advanced derivation solving heuristic. However, in this case, the categorizing of states is a mentally difficult task that would require not insignificant mental math while simultaneously doing the problem-solving task. The magic square offloads this cognition allowing for simpler identification of corner states so that the problem solver can correctly encode this information and then use the corner move heuristic. Framing matters and models like the magic square can aide by giving reasons for encoding information into problem spaces. Scientists use models similarly to frame their inquiries.

6 — How Framing Matters in Science and How Models Help

For an illustration of how scientists use models to solve problems, I will be using the example of the problem with Uranus' perturbed orbit. This problem resulted in the discovery of Neptune in the 1800s, a significant scientific achievement at the time, brought about by the use of mathematical models of the planet developed by John Adams and Urbain Le Verrier. These models were quite inaccurate. None of the predicted values would result in a scientist learning about the planet. They were significantly far from predicting the real mass and orbital characteristics of the actual planet. One might therefore wonder how such models could have enabled the discovery of Neptune, or indeed whether they should be credited with providing such help. But, when their use is understood within the framework of problem-solving, we can see that these models provided a tool scientists used to reframe an intractable problem into one to which they could apply heuristics to make a successful search feasible.

Uranus was discovered in 1781. A slow-moving planet, it orbits the sun every 83 years. Because of this slow orbit, it was not until several decades after Uranus' discovery that astronomers noticed that Uranus did not follow an orbit predicted by laws of planetary motion (Bamford 1996). Uranus' strange orbit posed a problem for scientists studying the motion of planets. Either the scientific laws that they used to model Uranus' orbit needed revising, or there needed to be special rules or assumptions made for Uranus. There were a number of conflicting candidate solutions. Some proposed that a comet had hit Uranus before its discovery, some hypothesized that there was a physical medium that affected the movement of Uranus, some correctly thought that there was an undiscovered body interacting gravitationally (Smart 1947). It seemed an intractable problem to astronomers since they had fairly well catalogued the visible objects in the sky by this point. In fact, the solution to this problem—the undiscovered influencing body, Neptune—was observed several times and recorded as a star (Bamford 1996)

Scientists' understanding of the problem of Uranus' perturbed orbit changed significantly over the course of the problem's existence. At first the problem was not well understood, prompting divergent investigations that did not have much in common. Questions like "Did a comet hit Uranus?", "Is there an intra-solar system ether?" guided investigation. In the language of my framework so far, the scientific community were investigating a not well framed problem. The goal states encoded different information, and so did the states of the problem space — for example, information about possible comet locations as well as information about the distance of an ether from the sun. In short, they did not know well what they did not know yet

resulting in an agent problem space characterized by questions like “Did the comet hit Uranus in 1788?... 1789… etc.)”, “Does the ether extend past 9 AU? … 10 au? Etc.” This results in a richer problem space, with many more nodes and where each edge taken constitutes less progress in the search for a solution.

Similar to the case of what I call the ‘magic square’ model of number scrabble, modeling here gave the scientific community reasons for reframing the problem and changing how they characterized the problem space, dropping nodes about ether and comets. The development of models of a perturbing planet provided the scientific community not with knowledge of Uranus, Neptune, or any object, or property, in the solar system, but knowledge of what they did not know. Having well framed, and interpreted, constraints involve knowing for instance that the solution to the problem would include an answer to “is my instrument pointing at Neptune?”, and encoding the right information to make a search of the sky by reference to a star chart efficient.

7 — Case of the Discovery of Neptune

The discovery of Neptune is taken as an exemplar achievement of the scientific method. There was the established theory of Newtonian gravity, a discrepancy with Uranus’ orbit, an attempt to ‘refine’ the theory by adding laws or entities — in Uranus’ case, models - , a prediction using the refined theory, and then verification. However, it is commonly known that the prediction leading to the discovery of Neptune was a failure. The problem has its origins in 1821 when French astronomer Alexis Bouvard published tables describing Uranus’ orbit, forty years after the planet’s approximate orbit had been calculated. By 1837, British Royal

Astronomer George Airy, declared Uranus' half a degree difference in longitude with respect to predictions of its orbit the most puzzling problem in contemporary astronomy (Smart 1947). Airy suggested that the laws of gravity might not be exactly according to the inverse square of distance, comprising one of the competing ways in which the problem was framed. John Adams and Urbain Le Verrier began work contemporaneously in 1843, having the idea that Uranus' anomalous orbit was due to gravitational interaction with an unseen planet, on seeking to refine the ideal orbit model of Uranus. To do this, they based a model of Uranus orbit on corrections to Bouvard's tables of Uranus' orbital data; it was a model of what Uranus' orbit ought to be according to the laws of gravitation. By comparing this ideal model of Uranus to Uranus' actual orbit both Le Verrier and Adams were able to estimate the mass and distance of the 'perturbing body', which of course turned out to be Neptune. Using these estimates as parameters, they created a model of the planet that they were supposing caused Uranus' anomalous behavior. However, these models produced by Le Verrier and Adams were inaccurate regarding predictions of the actual planet's orbit. The main orbital parameters their models predicted — distance from the sun, period of orbit and eccentricity — were in some cases several factors removed from the true values. See figure 4.2 for a two-dimensional plot of these orbits.

Despite these inaccuracies, it was these mathematical models that guided Galle and d'Arrest towards an observation confirming the existence of Neptune in 1847. John Adam's model did not result directly in discovery, but the timing of his

model's construction and documentation about the models' use for the unsuccessful, British search justified awarding the discovery to Adams as well as Le Verrier.

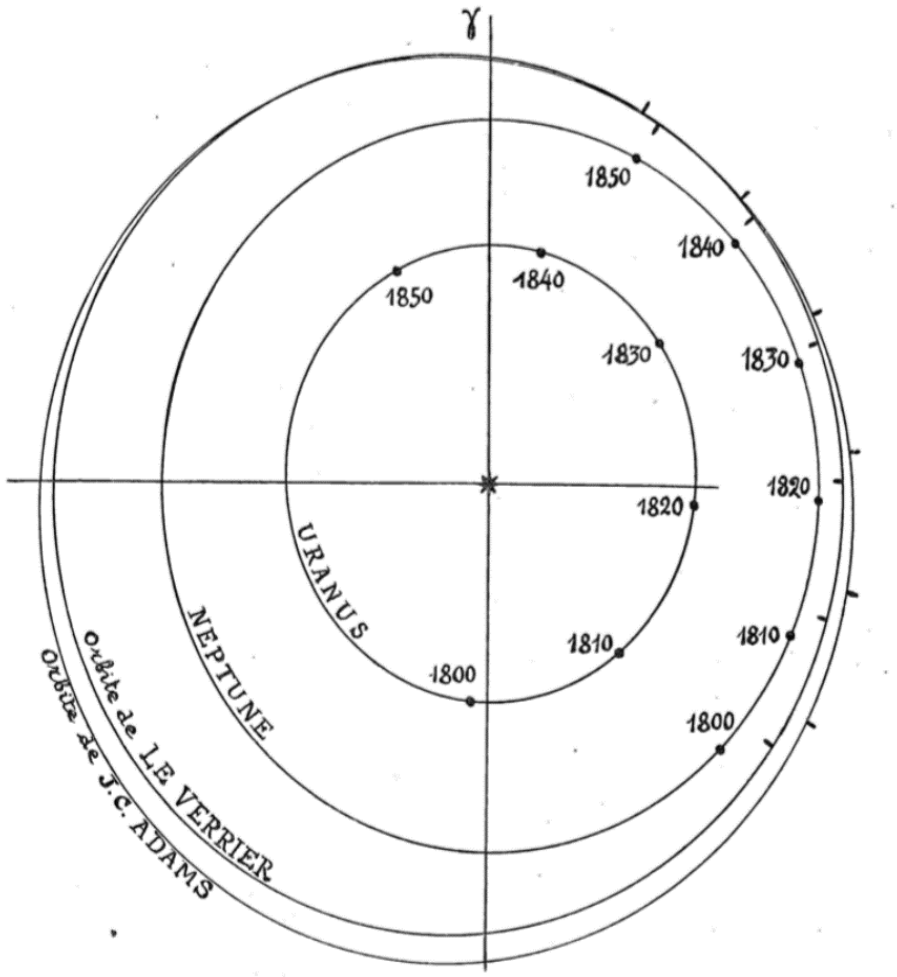

Figure 4.2 Two dimensional plot of Le Verrier's and Adams' models orbits. Neptune was observed 1846. At that time, the model orbit predictions lined up with Neptune's position well enough to guide a search from astronomers.

Some controversy resulted soon after the discovery of Neptune, as post-discovery observations revealed these inaccuracies. American astronomer, Sean Walker, investigated into Neptune's true orbit soon after the discovery by Galle, finding that Le Verrier and Adams' models predicted a planetary orbit with much different properties than Neptune's actual orbit. (See table 4.1). Benjamin Pierce, a

Harvard astronomer at the time, claimed: "the planet Neptune is not the planet to which geometrical analysis had directed the telescope; and that its discovery by Galle must be regarded as a happy accident" (Smith and Hubbel 1992) The criticism by the scientific community that Peirce exemplifies called into question the extent to which Le Verrier and Adams deserved credit for the observation of Neptune because of the models that they constructed.

Table 4.1 — Table of Values Predicted by Modeling Compared to Actual Orbit

orbit	**Le Verrier**	**Adams**	**Walker**	**Neptune**
Semi-major axis (AU)	36.15	37.25	30.25	30.11
Discovery distance	33	32		
eccentricity	0.10761	0.12062	0.00884	0.009456
Orbital period (yr)	217.4	227.3	166.4	164.8
Mass (mSun)	0.00011	0.00015	0.000067	0.000515

A perspective of modelling using the problem-solving framework I presented earlier in this chapter provides a defense of giving epistemic credit to Adams and La Verrier for the discovery of Neptune. Le Verrier's model gave astronomers a way to frame the search for a hidden body such that heuristics were useful. The use of Adam's model provides a contrast case for the successful framing of a problem for the use of heuristics since it led to an unsuccessful search. The model was the same as Le Verrier's as far as predictions about Neptune. It was the use of Adam's model specifically for problem solving that was different, and different in a way that emphasizes the epistemic value of model use towards problem solving. The goal of

this section is to show that what accounts for the epistemic value of these models is their contribution to problem-solving instead of the aspects in which they are ‘true’ of the world.

The role their models of Neptune played in its discovery was not one of providing a prediction that was later verified by observation, or learning about the world. Instead, the role of their models in the discovery of Neptune is best understood as framing the problem of Uranus’ perturbed orbit in a way that reduced the complexity of searching a problem space in two ways. The first is that the framing allows for the dropping of many nodes associated with the comet hypothesis or altering the inverse square law. The second way is by encoding information into the problem space about model predictions for Neptune allowing for astronomers to use heuristics — like the role of the magic square in number scrabble which allowed for the encoding of certain nodes with ‘corner’ making the ‘prefer taking a corner’ heuristic useable.

An adept player of tic tac toe most likely would know of corner moves since the strategy’s availability is more obvious given the game’s task enviroment. But when confronted with the list from 1 to 9 of number scrabble, the availability of the corner move strategy is not going to be obvious simply from the rules and task enviroment. The typical player would require the magic square model to help them frame the game in a way that makes this game play strategy accessible. One way to understand the availability of this heuristic to the game player is through registration. Suppose a master tic tac toe player was to play number scrabble for the first time. No doubt this player is familiar with the corner move. Most likely this familiarity is not

with a path through the game's directed graph game tree — as experiments showing the different performance profiles between number scrabble and tic tac toe suggest (Kirsh 2009). The familiarity is with the 3 by 3 grid with corner squares. It is the familiarity of the corner as seen by the game player with the magic squares framing that attunes the player to availability of a search heuristic. In order to understand the accomplishment of this task, like with the person navigating a mall, the crucial step is to map the problem space onto the task environment, thereby encoding the problem space with new information. This is the action of registration.

Similarly, the astronomers searching for Neptune needed a 'magic number' to aide in framing the problem for a successful search. Consider the hypothesis that a comet hit Uranus. If astronomers were trying to find a planet OR (inclusive) a comet, and the problem space nodes represent states of ‘searching the night sky’ (pointing a telescope at a bright object), then the disjunctive framing of a planet and comet adds extra information to each node. Such framing expands the area of the night sky — task enviroment — the astronomers would need to search since comets do not orbit on the same plane as planets. Additionally, Le Verrier and Adam’s models encoded, with greater precision, information about which nodes would provide a likely observation, allowing for the use of heuristics. The model orbits of Neptune failed to trace the true orbit, but when the model orbits were used to register Neptune’s position for a search of a problem space representing the two-dimensional star chart/night sky, these models afforded the use of heuristics like backup avoidance and hill climbing to achieve discovery. To illustrate how astronomers used these heuristics, this chapter will later contrast a competing

search for Neptune that did not make use of these models for framing or heuristics (nor of other potentially useful heuristics), resulting in failure.

What ended up aiding the astronomer Johanne Galle was that the orbital model of Le Verrier provided structure to his search using star charts. Just as magic square registration encodes the number scrabble player's problem space with information about corners, registration using the inaccurate Neptune models encoded information about Neptune likelihood-of-observation to the scientific problem space, connecting nodes in this problem space to certain bright objects in the sky. Astronomers use maps called 'star charts' to catalogue these bright objects. Le Verrier and Adams' models provided an invaluable tool for guiding an observation of Neptune because the method that astronomers use to discover new things includes a mapping of observations to these two-dimensional star charts; such representations are close in structure to the problem space scientists were operating within. In the case of Neptune, astronomers accomplished the registration of the problem space onto the task environment using star charts along with the models predicting Neptune's location — see Figure 4.5 for the star chart that Galle used. First, these models afforded the framing of the problem of a search for a planet by limiting the nodes that astronomers searched (see figure 4.4 for an illustration of this reasoning). They were inaccurate models but accurate enough to allow for the dropping of nodes associated with celestial objects recorded in other star charts.

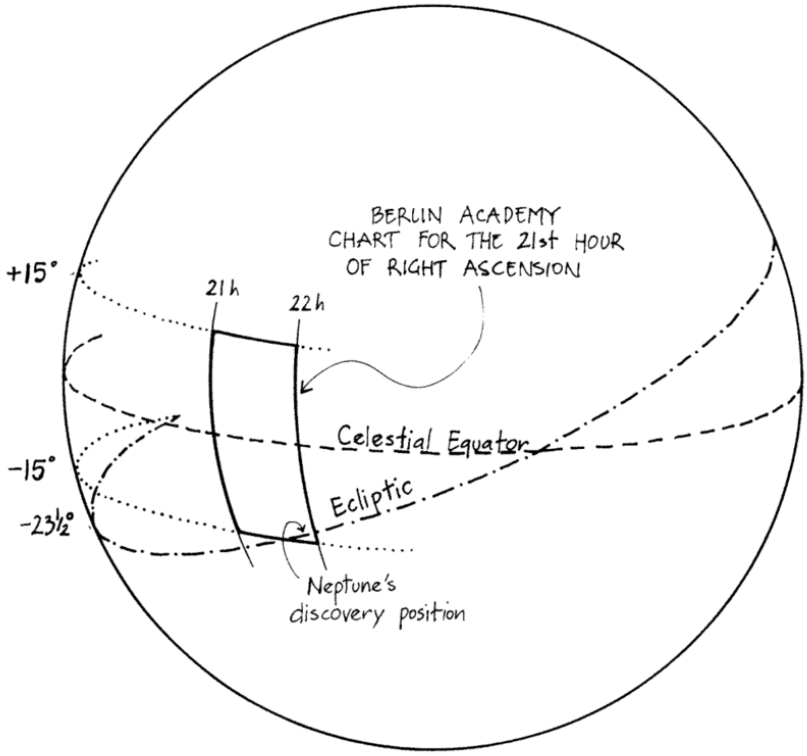

Figure 4.4 shows the Berlin star chart used to discover Neptune superimposed over the region of the globe that Astronomer's were searching for Neptune in. This superimposing is analogous to the registration used to make the problem space searchable: astronomers connected the Berlin chart (a representation) to the searched enviroment to guide their actions.

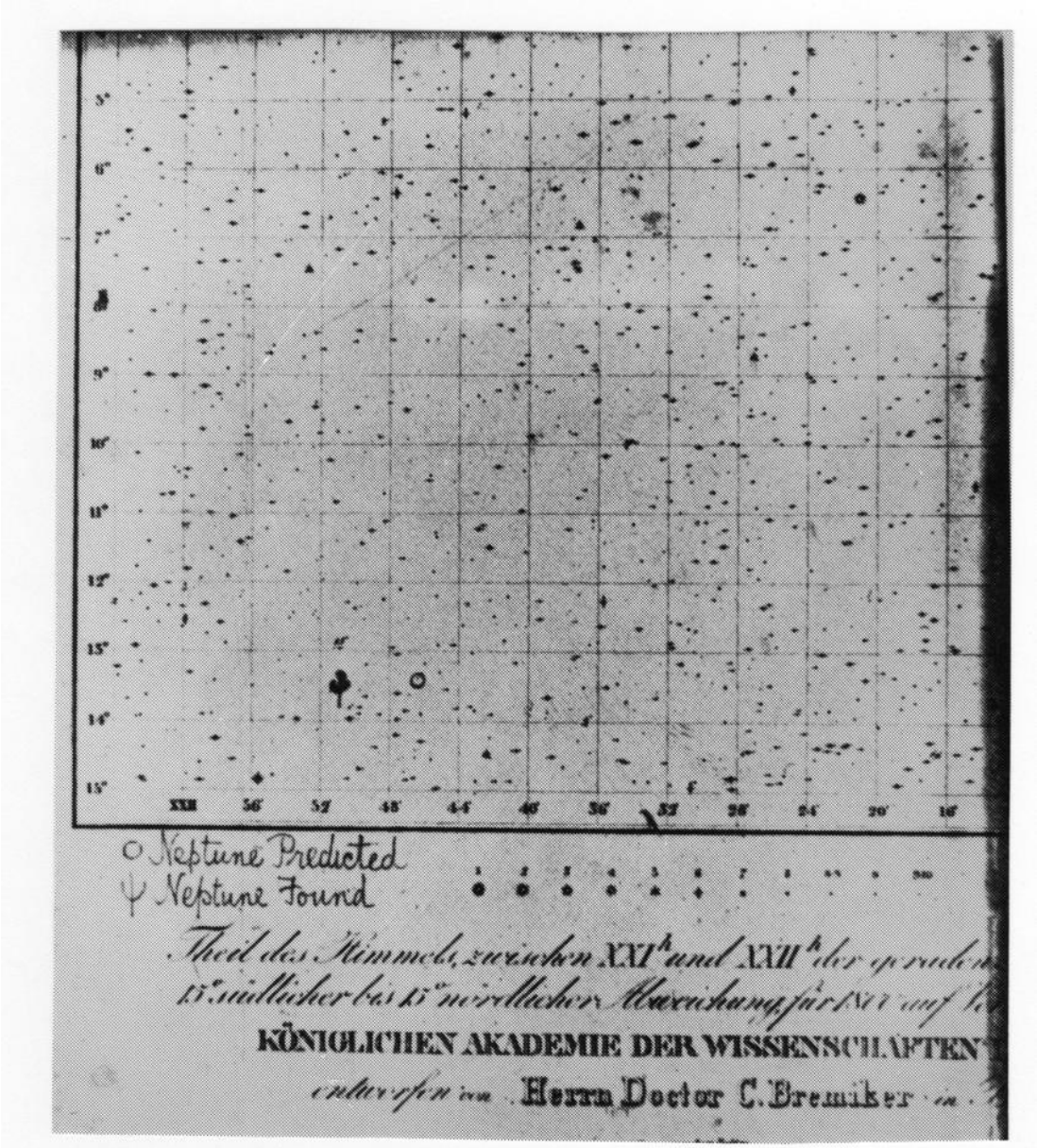

Figure 4.5 is the Berlin star chart that Galle used to guide his search for Neptune. The problem space he framed his search had nodes in a one to one correspondence to the stars on this chart, with information about the closeness to the model prediction encoded in each node.

Dissimilarly from the number scrabble example, problem spaces in scientific problem-solving are typically less defined than the game tree of games like number scrabble, consisting of constraints more open to interpretation in framing the problem; the allowable moves in tic-tac-toe are very much not open to interpretation. And often there is more uncertainty regarding the goal state. It is these characteristics of scientific problems that requires great and increasing division of labor, specialization and interdisciplinary activities (like modeling) in order to solve. The problem space in operation for Neptune's discovery was the space of possible locations an astronomer could observe. There were practical limits on these observations. Astronomers could not, and still cannot, travel about freely in space to find a planet like one may navigate a mall. One can think of the limit son observation of the sky similar to how physical walls limit one's navigation however. There are certain lengths of time needed for a trained eye to observe through a telescope in order to distinguish a planet like Neptune from background stars. The limits on observation imposed by instruments at the time meant that a practically successful search required a well framed problem. Astronomers needed a problem space that included fewer nodes, but also more information that could direct a search only to a much smaller region.

Both Adams and La Verrier were considered co-discoverers of Neptune because of the similarity of their models. However, Adam's orbit model did not see use in successful observation. The astronomer tasked with using Adam's model, James Challis used a strategy that provides an example of a failure to appropriately

frame a search resulting in suboptimal heuristic selection. Challis' plan was to: "Sweep over, three times at least, the zodiac belt 30 degrees long and 10 degrees broad, having the theoretical place of the planet at its center" (Grosser 1962 p.108). This plan however explicitly avoided information provided by modeling. Additionally, this search area was much larger than it needed to be, containing many celestial objects far from the modeled locations of Neptune — it was a problem space that encompassed many more nodes than Galle's.

Challis' sweeping was enormously labor intensive, each sweep estimated to take 300 observatory hours. One historian describes this strategy as "searching for a particular bright pebble on a beach by removing one by one thousands of other pebbles from a large area where one had been told the desired object was lying" (Grosser 1962 p.108). This description of Challis' strategy describes a strategy that was undirected. While this framing uses the model prediction of Neptune to frame the problem space — in the first sense of determine which nodes and edges exist — it does not do so in the second sense — encoding. Challis did not encode closeness-to-modeled-Neptune into the nodes of his problem space. In the words of my problem-solving framework, he framed the problem space (but not very precisely) in the first sense by using Adam's Neptune model to limit the nodes searched, but did not use the second sense of framing, the sense in which registration applies, to encode the information needed to direct the use of heuristics. Galle's strategy, in contrast, used closeness-to-model-Neptune information to direct the search operation inwards towards the predicted location — whether that edge lead more 'inwardly' to the modelled location influenced Galle's choice of edges for

each observation. When pressed on his choice of strategy, Challis asserted that organizing the search for a new planet with a mathematical (theoretical) model to "undertake observations in reliance upon merely theoretic deductions" was unusual, and that he "thought the probability of discovery was small until a much larger portion of the heavens was scrutinized" (Grosser 1962 p. 135). One way to understand Challis' failure is that it resulted from not using the mathematical model to encode information into his problem space. There was no connection made from problem space node to bright objects in the task enviroment as far as "Is this near the predicted location of Neptune? Yes/no". This failure manifested in a bad search strategy, one that took into consideration too many possibilities, many of which would likely have been avoided with better framing. Adams' model of Neptune did not have any 'pull' or weighting on Challis' use of a star chart.

One way to describe the missing ingredient in Challis' search is in terms of heuristics. One such heuristic would involve something like "hill-climbing" — call it 'model-directed searching' — where the search operation involves moves with respect to a rule of thumb about making the current observation state closer to an ideal state — ideal state in this case is the model-predicted location of Neptune on the star charts. Instead of orienting the sweep vaguely around the predicted area, Challis' search likely would have been more successful had he used a heuristic like model-directed searching. His actual sweeping strategy included many changes of states in the problem space that went along edges away from the predicted location leading to a search too inefficient to achieve discovery.

Galle, instead, encoded in his problem space what the model's predicted location of Neptune. As a result, his search could use heuristics like 'model directed searching'. I suggest this is analogous to how a mall navigator uses a 'you are here arrow', to encode the problem space with information about the navigator's current position. This sort of encoding is what I call registration. Galle used registration to encode problem space nodes and edges with information about whether a node was 'nearer' or 'farther' from the Le Verrier's model prediction. Starting from stars closer to the predicted location, he prioritized the next observation in a vaguely orbit like pattern around where Le Verrier's model projected Neptune onto his chart. The actual prediction (O on Figure 4.2) was not where Neptune was found. Nevertheless, this tighter focus allowed Galle to spend an appropriate amount of search time comparing the relative movements of the objects to then make an observation and verify that observation. This search was one we can understand as done in a problem space encoded with different information from the one in which Challis worked. Galle's problem space had nodes that not only encoded the information about a stars' previous observation but also how close it was La Verrier's model prediction.

Galle registered the Neptune model in a way that gave his problem space structure that made the use of a heuristics like hill climbing possible. Galle observed closely around the projected spot of Neptune and as he moved closer, he made the discovery. Challis on the other hand swept a very large area, ignoring the shadow cast by Adam's Neptune model on his charts, directing his search as a line-by-line sweep. Successful framing looks like Galle's use of Le Verrier's model. The 'truth' in

this situation was that Neptune was observable in both astronomer's problem spaces. The epistemic standard that makes the important difference here, however, is not truth but effective framing for problem solving.

Galle framed the problem effectively in two senses. First, he successfully framed the constraints on the problem to limit nodes representing the stars found on "21st hour" star chart (Figure 4.5). This framing dropped a significant number of nodes from the search. Secondly, Galle interpreted the constraints on the problem so that his problem space encoded information about closeness to model prediction. This second aspect of framing involves registration. There existed some prediction of Neptune's position based on La Verrier's model. This prediction by itself, like one's location in the mall, is useless without it being contextualizing done through registration. In the mall case, registration connects your current location to the overall navigation by recognizing 'you are here' on the map and connecting your problem space to the empirical fact of your location. In this scientific analogy of the mall navigation, Galle marked the star chart with Neptune's location as predicted by La Verrier's model, and connected his problem space to an empirical fact about the location of an object in the sky marked by the chart (one located at x, y degrees at z time). This registration gave weight to directions in Galle's search pattern. He valued moves that would bring him closer to Neptune's projected position on the star chart. Thus, returning to Benjamin Pierce's 'happy accident' claim, the mathematical model of Neptune's orbit may have been inaccurate but was indispensable in directing a successful search.

8 — Conclusion

Registration in the discovery of Neptune case of problem-solving identifies how a model may successfully contribute to the growth of scientific knowledge, and it also fits in a more general scientific activity (one not necessarily involved in problem-solving). This is the previously mentioned activity of de-idealizing or concretizing. The actual space containing Neptune is quite vast and far removed from the experiences of astronomers. The two-dimensional star chart is a more concrete representation. It saw use by astronomers to keep track of observations they already made to utilize backup avoidance heuristics, and included detail depicting observations made by astronomers, detail that is similar to the experience of one observing a region of the sky. Adams and La Verrier's models ‘live’ in the three-dimensional problem space with terms describing Neptune's change in position with respect to time. The activity of registration takes the path traced in the actual world by model Neptune’s orbit and connects this path to an empirical fact about observable objects in the astronomer’s world (the world of night skys and star charts). Another way to put this is that registration is an activity performed between two representations, one typically more abstract to one that is typically more concrete. For instance, a clear way to understand the transfer of corner moves from tic tac toe to number scrabble is that the game player is registering a branch of the game tree (problem space) shared by both games to the play area of number scrabble. Play areas, like charts, are closer to our lived-in world of work and human problem-solving, but in order to use more generic things to help us solve problems

like heuristics, and community borne wisdom, we must make a successful connection from the abstract to the concrete.

Thus, looking into registration provides insight into how models become useful, and thus epistemically valuable. Models become useful when scientists use them to register a problem space to empirical facts in a task enviroment. An astronomer mapping observations with a star chart makes ‘backup avoidance’ applicable just like a number scrabble player using the magic square frame makes ‘corner moves’ applicable, by connecting the problem space to the world through the intermediary of a model (star chart or ‘magic square’). Broadly speaking, using learning about the world as an epistemic standard is not sufficient as a standard to capture this reasoning because it is reasoning about using rules of thumb to navigate uncertainty instead of deducing true conclusions from assumptions. Galle’s search could have failed; maybe the telescope got bumped at the crucial observation. However, in comparison to Challis’ strategy, Galle was better geared for success given the information his problem space encoded, information that had almost nothing to do with ‘truth’ given the Neptune model’s inaccuracies.

Models help us think more efficiently through possibilities. Since problem solving is a search through *possible* transformations in an environment that will bring about the desired state, problem solving provides an apt framework to understand the value of models in science. I have argued for the usefulness of this framework through a case study on the discovery of Neptune. This discovery was one of the crowning achievements of the use of models in science. The achievement in using models however was not the result of scientific reasoning following the epistemic

standard of ‘truth’. Models of Neptune were inaccurate. The reasoning leading up to discovery had to do with efficiency, time needed to make observations and how best to manage limited resources and uncertainties. Considering these factors in Neptune’s discovery, I make the case that using a problem-solving framework for understanding the value of models in science provides the advantage of accounting for the role models play in scientific inquiry.

The framework developed in this chapter helps to account for the epistemic value of model transfer to the sciences. The search for dark matter is an investigation in science that provides fertile ground for analysis of the connection between model transfer and scientific inquiry. Before the 1930s, the virial theorem saw use in modelling thermodynamic systems. Following its introduction to astrophysics, the virial theorem comprised a key method for scientists to frame the search for dark matter by giving scientists an idea of the amount of missing matter that could be ‘dark’. In the language of my framework, astrophysicists used the virial theorem to encode problem space nodes with the masses that scientists used to search for beginning dark matter candidates. To follow is a short history on this use of the virial theorem.

I would suggest the search for dark matter has much more to do with the use of models for framing than even the Neptune case. It was the transfer of the virial theorem that allowed astrophysicist to identify a discrepancy with the mass estimates of phenomena in their domain. The first type of models that were used to estimate mass were luminosity models. Luminosity models provide estimates of mass from the total observed flux of radiation. The other sort of models are

dynamical models. The ability for a scientist to construct these models was brought about by several changes to physics in the 1920 and 30s at the practical level: the availability of spectroscopy data from nearby systems and our sun, the availability of more powerful telescopes, and long exposure photographing techniques (Vanderburgh 2001). With these factors it was possible for scientists to observe the apparent motions of distant galaxies by comparing red-shift or blue-shift to spectrograms. Having access to the relative velocities of distant galaxies and clusters of galaxies allowed scientists to construct dynamical models. Scientists soon noticed a discrepancy from already empirically established luminosity models (Oort 1933, Babcock 1939, Smith1936, Zwicky 1937). Oort and Babcock invented dynamical models targeting our own Milky Way galaxy and the nearby Andromeda galaxy. Smith and Zwicky instead modeled nearby clusters of galaxies using the virial theorem (Vandeburgh 2001, Trimble 2013).

In 1933, Zwicky first published on the possibility of using the virial theorem to model the dynamics of galactic clusters (Zwicky 1933). This paper compared various methods for measuring of the distance of extra-galactic nebulae from earth, comparing the new methods of measuring distance using red shift to methods using luminosity. He found that redshift data allowed for more precise estimates of distance. Greater precision in distance measurements allowed for more precise measurement of galaxy velocity since part of what astrophysicists' used to estimate velocity was the galaxy's distance from earth.

With greater precision in velocity data, Zwicky noticed the beginnings of a promising area of scientific inquiry. Red shift data showed curious measurements for

velocity distributions in dense galaxy clusters. As Zwicky puts it, “the great dispersion of velocities in the Coma system (and in other dense nebular clusters) harbors a problem that is not yet understood" (Zwicky 1933, pp. 223). Found at the end of this paper is his use of the virial theorem as a first step towards *framing* this problem. Zwicky makes use of the virial theorem similar to how the Le Verrier’s and Adams’ models framed the anomalous Uranus orbit problem as a search for Neptune. By using the virial theorem to model the distribution of velocities in the Coma cluster, Zwicky was able to describe an estimate of *missing* mass in the Coma cluster. This use of the virial theorem turns a puzzling observation— “the velocities of these things are unusual!”— into a problem, “there is significant a missing factor in the mechanics of this system”. For models of the orbit of Uranus, this missing factor turned out to be a new planet. Zwicky’s use of the virial theorem *frames* a problem “not yet understood” into one that is a scientific investigation into a missing factor in the mechanics of a sort of astrophysical system.

The virial theorem let him proceed on uncertainty of the 'actual' characteristics of the Coma cluster to some measurement of mass — knowing only the velocities of these galaxies relative to the Milky way. The mass estimates using the virial theorem have a large margin of error, so astrophysicists often rule out its use as a predictive tool (Trimble 1987). However, the mass estimate error is significantly smaller than the factor of 200-400 predicted by Zwicky’s mass discrepancy. Thus, Zwicky’s use of this model template constitutes another instance in science where the value of modelling is not sufficiently characterized by epistemic standards of accuracy, but by looking at how these models are useful for problem solving. Like the original model

of Uranus' ideal orbit, Zwicky's virial theorem mass model provides a way to set up a problem space to search for solutions. For the Neptune problem, this framing led to the dropping of various nodes associated with the hypotheses about ether, comets and laws of gravity changes, vast simplifying the problem space.

As the investigation into dark matter continues, scientists propose candidate types of dark matter particles (e.g. WIMPs) or alterations to the laws of gravity at large scales (e.g. modified Newtonian dynamics) that end up being considered or eliminated ultimately based on whether they close the gap in compared to newer models of mass discrepancy. Thus there exists much room for understanding the scientific use of models to frame problems, and how this framing promotes the use of heuristics, in the search for dark matter. I suggest that using the framework I develop in this dissertation would reveal a connection between scientific reasoning in the current investigation into dark matter and instances of model transfer. This connection is not just as far as conceptual innovation goes, but towards the practical level at which models see use — justifying the construction of a new detector for instance. The investigation of dark matter is especially hard to conceptualize because it seems like the search is not just for a type of thing we already know about but for possibly a new type of fundamental particle. Such great uncertainty requires an enormous effort in coordination between scientists, and the use of mathematical models to organize information so that this search can use generations of community borne-wisdom.

Chapter 5: Conclusion

In Chapter 1, I raise an issue with accounts of model transfer, that they do not sufficiently account for what makes a transferrable model useable in a new domain. I argue that by paying attention to what scientists do to make such models useable offers insight into how modeling in general connects to a scientific domain's theoretical level — the level where scientists determine the meaning of their concepts and categories — and the practical level — the level at which scientists experiment, discover and observe. In Chapter 2, I propose a concept to identify the thing to which scientists apply transferrable models — the landing zone. I argue scientists create landing zones in order to meet the requirements of a transferrable model template by preparing phenomena so that it is modellable. In Chapter 3, I argue that paying attention to this landing zone type preparation gives us a new direction for understanding conceptual innovation in the sciences, and a depiction of the conceptual machinery that confounds analysis of the intertheoretical connection between domains like physics and chemistry. In Chapter 4, I illustrated the affordance of a problem-solving account of the epistemic value of modelling using the Neptune case. Such an account allows us to understand the epistemic value of inaccurate, or

otherwise ‘untruthful’, models in scientific inquiry. These models allow scientists to frame investigations to make problem solving easier. However, the discovery of Neptune is not a case of model transfer, so it does not fit the motif for the cases I examined in the first three chapters of this dissertation; Adams and Le Verrier developed their models using methods from within the domain of physics for describing orbital characteristics.

The connection that the case of Neptune’s discovery, examined in Chapter 4, has to the rest of the dissertation is that it is a particularly striking example of the use of models for inquiry. The discovery of Neptune is an exemplar scientific achievement in the use of (inaccurate) models at the practical level to frame a problem. Thus, a case study of it reveals what successful model use, in general, looks like — successful framing for the use of heuristics. This standard then provides us with a way to characterize when scientists render a transferrable model useful to the practical level of their domain — towards successful problem solving. Generally, models are ‘useful’ to a domain if scientist can use them to frame an investigation for the deployment of heuristics. Framing either involves a dropping or altering of information in problem space nodes. One way scientists frame, or reframe, problems is through registration, an activity where models are an invaluable tool. Since registration involves processing empirical facts in the task enviroment as information to be encoded in the problem space, the connection between problem space and task enviroment must be conceivable to the scientists — there is a congruence between the categories the scientists recognize in the task enviroment and the categories

scientist use to conceptualize their overall investigation. In the Neptune case, it would be difficult to imagine a successful use of Le Verrier's model for framing if astronomers did not recognize bright objects in the sky as potential planets.

The landing zone type activity — conceptual progress — I examine in Chapter 3 is what establishes a model's connection with the level of scientific theorizing and the level of scientific practice that makes models useful for problem solving. Fisher reconceived the biological category of a population in order to make his use of a model template from statistical physics meaningful in connection to other methods in biology. His debates with biologists at the time are evidence of the impact this conceptualization had at the level of theorizing in this domain. The problem that Fisher sought to solve was a more 'theoretical' one than the Neptune case. His problem had to do with making mathematical description of mendelianism compatible with description of natural selection. I suggest that taking the framework I develop in Chapter 4 back to this case would characterize the work Fisher does as problem solving — this however would require quite a bit more work as Fisher's use of modeling did was not as focused on community inquiry as with the Neptune case, nor was it as straightforwardly a 'search' for something missing.

Conceptual innovation like the invention of a new notion of atom — topological atom — or a new conception of biological populations — what I call velocity populations — is a response to the requirements of making a transferrable model template useable in a new domain, what I identify as the 'landing zone' in Chapter 2. The virial theorem, for instance, has well-known

conditions for its use that partially determined Bader's conception of the atom in preparation for modeling phenomena such as functional groups. An area of future application of the research in this dissertation is characterizing precisely the way in which Bader's (and other chemist's) transfer of models became useful for framing various problems. Generally, I suggest Bader saw that the transfer of the virial theorem would accomplish framing within chemical problems of reduction, where the problem space is set up to search for paths to 'bring back' phenomena like functional groups to physical chemistry. It is more apt to see Bader's reductive goal with QTAIM as sort of Kuhnian puzzle solving than the hard-line reduction Bader himself suggests, that attempts to justify the elimination of chemical concepts because of epistemic standards associated with truth.

Chapter 4 depicts the epistemic upshot of conceptual innovation brought about by preparation for model transfer. Landing zones are what make a model useful for framing scientific investigations. A useful model is one which may be used to frame a problem by encoding information from the task enviroment into a problem space. I suggest that for such encoding to be feasible, there must be some congruence between conceptualization of phenomena in the task enviroment and the model. My proposal for future research is analyzing the epistemic value of model transfer along this dimension — how conceptual innovation affords landing zone congruence, and further, how this innovation then results in successful framing and reframing scientific investigations for the use of heuristics. There is opportunity to use this research in understanding the use of models in the search for dark matter.

Bibliography

Bacskay, G., Nordholme, S., Reudenberg, K. 2018. “The Virial Theorem and Covalent Bonding.” Journal of Phys. Chem A. *122* (39), pp 7880—7893 10.1021/acs.jpca.8b08234

Bader, R., Beddall, P. 1972: “Virial field relationship for molecular charge distributions and the spatial partitioning of molecular properties.” J. Chem. Phys. 56, 3320—3328

Bader, R. 1975. “Molecular Fragments or Chemical Bonds.” *Accounts of Chemical Research* 8 (1): 34—40.

Bader, R. 1985. “Atoms in Molecules.” *Accounts of Chemical Research* 18 (1): 9—15.

Bader, R. 1990. *Atoms in Molecules: A Quantum Theory.* Clarendon Press, Oxford.

Bader, R. 2006. “Pauli Repulsions Exist Only in the Eye of the Beholder.” *Chemistry — A European Journal* 12 (10): 2896—2901.

Bader, R. 2007. “Everyman's Derivation of the Theory of Atoms in Molecules.” *The Journal of Physical Chemistry A*, *111*(32), 7966-7972

Bader, R. 2009. “Bond paths are not chemical bonds.” *The Journal of Physical Chemistry A*, *113*(38), 10391-10396.

Bader, R. 2011. “On the Non-Existence of Parallel Universes in Chemistry.” *Foundations of Chemistry: Philosophical, Historical and Interdisciplinary Studies of Chemistry* 13 (1): 11—37.

Bader, R., and Matta, C. 2013. “Atoms in Molecules as Non-Overlapping, Bounded, Space-Filling Open Quantum Systems.” *Foundations of Chemistry: Philosophical, Historical and Interdisciplinary Studies of Chemistry* 15 (3): 253—76.

Ballesteros-Paredes, J. 2006. “Six Myths on the Virial Theorem for Interstellar Clouds.” Monthly Notices of the Royal Astronomical Society 372 (1): 443—49. https://doi.org/10.1111/j.1365-2966.2006.10880.x.

Bamford, G 1996. “Popper and his commentators on the discovery of Neptune: A close shave for the law of gravitation?” *Studies in History and Philosophy of Science Part A* 27 (2):207-232.

Burdett, J. 1997. *Chemical Bonds — A Dialogue.* Wiley: New York.

Bursten, Julia. 2018. “Conceptual Strategies and Inter-Theory Relations: The Case of Nanoscale Cracks.” *Studies in the History and Philosophy of Modern Physics* 62: 158–65.

Boeyens, J. 2015. “Wave-Mechanical Model for Chemistry.” *Foundations of Chemistry: Philosophical, Historical and Interdisciplinary Studies of Chemistry* 17 (3): 247—62.

Brush, S. 1999. “Dynamics of Theory Change in Chemistry: Part 1. The Benzene Problem.” *Stud. Hist. Phil. Sci., Vol. 30, No. 1, pp. 21—79, 1999*

Burdett, J. 1997. *Chemical Bonds — A Dialogue.* Wiley: New York.

Cartwright, N. 1983. *How the laws of physics lie.* Oxford University Press

Eberhart, M., and Jones, T. 2013. “The Two Faces of Chemistry: Can They Be Reconciled?” *Foundations of Chemistry: Philosophical, Historical and Interdisciplinary Studies of Chemistry* 15 (3): 277—85.

Elliott-Graves, A., Weisberg, M. 2014. “Idealization.” Philosophy Compass 9:176—85.

Fisher, R. 1918. "The Correlation Between Relatives on the Supposition of Mendelian Inheritance". Transactions of the Royal Society of Edinburgh. 52 (2): 399—433. doi:10.1017/s0080456800012163

Fisher, R.A., 1930. The evolution of dominance in certain polymorphic species. *The American Naturalist*, *64*(694), pp.385-406.

Gavroglu,K., Simoes, A. 2011. *Neither Physics nor Chemistry: A History of Quantum Chemistry*. MIT Press.

Galison, P. 1997. *Image & logic: A material culture of microphysics*. Chicago: The University of Chicago Press.

Gelfort, G. 2010. “Mathematical formalism in scientific practice.” *Studies in History and Philosophy of Science*

González, Juan Camilo Martínez, Sebastian Fortin, and Olimpia Lombardi. 2018. “Why Molecular Structure Cannot Be Strictly Reduced to Quantum Mechanics.” *Foundations of Chemistry*, March. https://doi.org/10.1007/s10698-018-9310-2.

Grosser, M. 1962. The discovery of Neptune . Harvard University Press.

Hempel, Carl G. and Paul Oppenheim, 1948, “Studies in the Logic of Explanation”, *Philosophy of Science*, 15(2): 135—175. doi:10.1086/286983

Haaland, A., Helgaker, T., Ruud, K., Shorokhov, D. 2000: “Should gaseous BF3 and SiF4 be described as ionic compounds?” J. Chem. Edu. 77, 1076

Harré, R., LLored, J. 2011. Mereologies as the Grammars of Chemical Discourses. Foundations of Chemistry. 13. 10.1007/s10698-011-9103-3.

Hellmann, H. 1931. “On crystal interferences of the spin-electron.” Z. Phys. 69 (1931) 495-506.

Hempel, C.G. and Oppenheim, P., 1948. Studies in the Logic of Explanation. *Philosophy of science*, *15*(2), pp.135-175.

Hempel, C. 1965b, “Empiricist Criteria of Cognitive Significance: Problems and Changes”, in Hempel 1965d: 101—119.

Hendry, R. 2008. “Two Conceptions of the Chemical Bond.” *Philosophy of Science* 75 (5): 909—20.

Hendry, R. 2010. “Ontological Reduction and Molecular Structure.” *Studies in History and Philosophy of Science Part B: Studies in History and Philosophy of Modern Physics* 41 (2): 183—91. https://doi.org/10.1016/j.shpsb.2010.03.005.

Hettema, H. 2013. “Austere Quantum Mechanics as a Reductive Basis for Chemistry.” *Foundations of Chemistry: Philosophical, Historical and Interdisciplinary Studies of Chemistry* 15 (3): 311—26.

Hiberty, P., Shaik, S. 2014. “Bridging Cultures.” *The Chemical Bond: Fundamental Aspect of Chemical Bonding* edited by Gernot Frenking and Sason Shaik. Wiley-VCH.

Hiberty, P., Shaik, S. 2014. “Bridging Cultures.” *The Chemical Bond: Fundamental Aspect of Chemical Bonding* edited by Gernot Frenking and Sason Shaik. Wiley-VCH.

Hohenberg, P., Kohn, W. 1964. “Inhomogeneous Electron Gas.” *Physical Review* 136: 864-871

Humphreys, P. 2002. “Computational Methods.” Philosophy of Science, 69 (3): 1-11

Humphreys, P. 2004. *Extending Ourselves: Computational Science, Empiricism, and Scientific Method*. Oxford University Press.

Hubbell, J. G., & Smith, R. W. 1992. Neptune in America: Negotiating a discovery. *Journal for the History of Astronomy*, *23*(4), 261-291.

Jones, M. 2005. “Idealization and Abstraction: A Framework.” In Idealization XII: Correcting the Model, ed. Martin R. Jones and Nancy Cartwright, 173—217. Amsterdam: Rodopi.

Kirsh, D. 2009. “Problem Solving and Situated Cognition”. *The Cambridge Handbook of Situated Cognition*:264-306.

Klahr, D. Simon, H. 1999 “Studies of Scientific Discovery: Complementary Approaches and Convergent Findings”

Knuuttila, T., and Loettgers, A. 2011. “The Productive Tension : Mechanisms vs. Templates in Modeling the Phenomena.” In *Models, Simulations, and Representations*, edited by Paul Humphreys and Cyrille Imbert. Routledge.

Knuuttila, T., and Loettgers, A. 2014. “Model Templates Within and Between Disciplines: From Magnets to Gases — and Socio-Economic Systems.” *European Journal for Philosophy of Science*, 1—24.

Knuuttila, T., and Loettgers, A. 2016. “Model Templates within and between Disciplines: From Magnets to Gases—and Socio-Economic Systems.” European Journal for Philosophy of Science 6:377—400.

Krajnović, D. (2016). The contrivance of Neptune. *Astronomy & Geophysics*, *57*(5), 5-28.

Kohn, W., Sham, J. 1965. “Self-Consistent Equations Including Exchange and Correlation Effects.” *Physical Review* 140 (4a): 1133-1138

Kuhn, Thomas(1962). *The Structure of Scientific Revolutions*, Chicago, Unoversoty of Chicago Press. 2nd edition.

Labarca, M, and Lombardi, O. 2010. “Why Orbitals Do Not Exist?” *Foundations of Chemistry* 12 (2): 149—57.

Lalli, R. 2015. "'The Renaissance of Physics' Karl K. Darrow (1891-1982) and the dissemination of quantum theory at the Bell Telephone Laboratories" Pisano R (ed) *A Bridge between Conceptual Frameworks*. Sciences, Society and Technology Studies. Springer

Laudan, Larry (1977). *Progress and Its Problems*, Berkeley, University of California.

Lenhard, J. 2014. "Disciplines, Models, and Computers: The Path to Computational Quantum Chemistry." *Studies in History and Philosophy of Science Part A* 48 (December): 89—96.

Lode, P., Popelier, A. 2014 "The QTAIM perspective of Chemical Bonding." *The Chemical Bond: Fundamental Aspects of Chemical Bonding* edited by Gernot Frenking and Sason Shaik. Wiley-VCH

Llored, Jean-Pierre. 2014. "Whole-Part Strategies in Quantum Chemistry: Some Philosophical and Mereological Lessons". HYLE--International Journal for Philosophy of Chemistry, Vol. 20, No. 1 (2014), pp. 141-163

Joypazadeh, H., and Shahbazian, S. 2014. "What does shape a topological atom?". *Foundations of Chemistry*, *16*(1), 63-75.

McMullin, Ernan, 1968, "What Do Physical Models Tell Us?", in B. Van Rootselaar and J.
Frits Staal (eds.), *Logic, Methodology and Philosophy of Science III* (Studies in Logic and the Foundations of Mathematics 52), Amsterdam: North Holland, pp. 385—396. doi:10.1016/S0049-237X(08)71206-0

Meyer, M. 1988. *Questions and questioning*. W. de Gruyter.

Morgan, Mary S., 1999, "Learning from Models", in Morgan and Morrison 1999: 347—388. doi:10.1017/CBO9780511660108.013

Morgan, M. 2014. "Re-situating Knowledge: Generic Strategies and Case Studies." Philosophy of Science 80:1012—24.
Morgan, M. 2018. "Exemplification and the Use Values of Cases and Case Studies." *Studies in the History and Philosophy of Science*

Morrison, Margaret. 1997. "Physical Models and Biological Contexts." *Philosophy of Science* 64: S315–24.

Morrison, M. 2002. Modelling populations: Pearson and Fisher on mendelism and biometry. British Journal for the Philosophy of Science 53 (1):39-68.

Morrison, Margaret, and Mary S. Morgan. 1999. “Models as Mediating Instruments.” In Models as Mediators: Perspectives on Natural and Social Science, ed. Mary S. Morgan and Margaret

Mulliken, R. 1932. “Electronic structures of polyatomic molecules and valence III. Quantum theory of the double bond.” *Phys. Rev. **41**, 754*

Mukhopadhyay, S. and Bhattacharyya, K. 2005. Confined systems and the modified virial theorem from semiclassical considerations. Int. J. Quantum Chem., 101: 27-32. doi:10.1002/qua.20220

Narsessian, N. 2005. “Abstraction via generic modeling in concept formation in science” Martin R. Jones and Nancy Cartwright (eds.), Idealization XII: Correcting the Model. Idealization and Abstraction in the Sciences.

Nersessian, Nancy J. 2008. Creating Scientific Concepts. Cambridge, MA: MIT Press.

Newell, A., & Simon, H. 1972. *Human problem-solving* . Prentice-Hall, Inc

Nickles, Thomas. 1978. "Scintific Problems and Constraints" PSA 1978, Vol. 1, 134-148

Nickles, Thomas. 1981. " What is a problem that we may solve it?", Synthese 47, 85 — 115

Parr, R., Ayers, P., and Nalewajski, R. 2005. “What Is an Atom in a Molecule?” *The Journal of Physical Chemistry A* 109 (17): 3957—59.

Pauling, Linus. 1960. *The Nature of the Chemical Bond...* Vol. 260. Cornell university press Ithaca, NY.

Proft, F., Ayers, P., Geerlings, P. 2014. “The Conceptual Density Functional Theory Perspective of Bonding.” *The Chemical Bond: Fundamental Aspects of Chemical Bonding* edited by Gernot Frenking and Sason Shaik. Wiley-VCH.

Poater, J., Solà, M. and Bickelhaupt, M. 2006. “Hydrogen—Hydrogen Bonding in Planar Biphenyl, Predicted by Atoms-In-Molecules Theory, Does Not Exist.” *Chemistry — A European Journal* 12 (10): 2889—95.

Portides, D. 2010. “Seeking representations of phenomena.” *Studies in History and Philosophy of Science*

Reitman, W. R. (1964). Information-processing models in psychology. *Science*, *144*(3623), 1192-1198.

Scerri, Eric R. 2007. “Reduction and Emergence in Chemistry -- Two Recent Approaches.” *Philosophy of Science*, Part I: Contributed Papers, 74 (5): 920—31. https://login.pallas2.tcl.sc.edu/login?url=http://search.ebscohost.com/login.aspx?direct=true&db=phl&AN=PHL2121633&site=ehost-live.

Schmidt, M., Ivanic, J., Reudenberg, K. 2014. “The Physical Origin of Covalent Bonding.” *The Chemical Bond: Fundamental Aspects of Chemical Bonding* edited by Gernot Frenking and Sason Shaik. Wiley-VCH.

Sukumar, N. 2013. “The Atom in a Molecule as a Mereological Construct in Chemistry.” *Foundations of Chemistry: Philosophical, Historical and Interdisciplinary Studies of Chemistry* 15 (3): 303—9.

Slater, J. 1933. "The Virial and Molecular Structure," Journal of Chemical Physics, 1(10), pp. 687-69

Simon, Herbert A. 1973. "The structure of ill structured problems." *Artificial intelligence* 4.3-4 : 181-201.

Smart, W. M. 1947. John Couch Adams and the discovery of Neptune. *Popular Astronomy*, *55*, 301

Strevens, M., 2008, *Depth: An Account of Scientific Explanation*, Cambridge, MA, and London: Harvard University Press.

Strevens, M. 2016. “How Idealizations Provide Understanding.” In Explaining Understanding: New Perspectives from Epistemology and the Philosophy of Science, ed. Stephen Robert Grimm, Christoph Baumberger, and Sabine Ammon, 37—49. New York: Routledge.

Vorms, Marion. 2011. “Representing with Imaginary Models: Formats Matter.” Studies in History and Philosophy of Science A 42:287—95.

Vorms, M. 2014. “The birth of classical genetic as the birth of two disciplines.” *Studies in History and Philosophy of Science*

Wang, S.-G., Qui, Y.-X., Schwarz, W.H.E. 2010. “Antibond breaking-the formation and decomposition of He@adamantane”. *Chem. Eur. J. 16, 9107—9116* (2010)

Weisberg, Michael. 2007. “Three Kinds of Idealization.” Journal of Philosophy 104:639—59.

von Oertzen, W., Freer, M. and Kanada-En’yo, Y. 2006. “Nuclear Clusters and Nuclear Molecules.” *Physics Reports* 432 (2): 43—113.

Weisberg, M. 2008. “Challenges to the Structural Conception of Bonding”. Philosophy of Science, 75 (December 2008) pp. 932—946.