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On the Narrative Form of Simulations

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Abstract. Understanding complex physical systems through the use of simulations often takes on a narrative character. That is, scientists using simulations seek an understanding of processes occurring in time by generating them from a dynamic model, thereby producing something like a historical narrative. This paper focuses on simulations of the Diels-Alder reaction, which is widely used in organic chemistry. It calls on several well-known works on historical narrative to draw out the ways in which use of these simulations mirrors aspects of narrative understanding: Gallie for "followability" and "contingency"; Mink for "synoptic judgment"; Ricoeur for "temporal dialectic"; and Hawthorn for a related dialectic of the "actual and the possible". Through these reflections on narrative, the paper aims for a better grasp of the role that temporal development sometimes plays in understanding physical processes and of how considerations of possibility enhance that understanding.

An Exemplary Simulation--Snowflakes

In a previous paper I have considered several simulations of physical processes and have argued that in important respects they exhibit properties of historical narratives, or more specifically natural-historical narratives. That is, they "explain" (as practitioners of simulation sometimes say) the processes they simulate by generating them as a development in time, an evolution or unfolding from a beginning scenario to an ending. A brief summary of one of those cases will establish some basics for continuing the discussion. The case concerns snowflakes.[1]

As part of his work on pattern formation in complex systems (here nonlinear, nonequilibrium, dynamical systems), the physicist Kenneth Libbrecht, began studying snowflakes. Contrary to the traditional expectation that they should exhibit highly symmetric geometrical forms, he already knew that they nearly always exhibit asymmetries and irregularities, conforming rigorously to no simple pattern. Using high resolution equipment Libbrecht obtained photomicrographs of both naturally occurring and artificially grown snowflakes, revealing their characteristics in unprecedented detail. In 2006 he published what he called a *Field Guide to Snowflakes*. Libbrecht's *Field Guide* and his extensive website contain an amazing diversity of natural forms.[2] The term "field guide" signals already that he takes the subject of pattern formation in snowflakes to be one of natural history. He writes further of snowflakes in terms of their "life history" and of constructing their "story." In brief, the growth of an individual snowflake is to be understood in the terms of a unique historical narrative.

This narrative quality in Libbrecht's remarks continues further in the work of two of his occasional collaborators. While he makes photomicrographs of real snowflakes, they do simulations, with comparable resolution (figure 1). In "Modeling Snow-Crystal Growth," the mathematicians Janko Gravner and David Griffeath have produced a computational model that replicates many of the basic forms or "habits" of snowflakes—dendrites, needles, prisms, etc.—along with their more intricate "traits"—sidebranches, sandwich plates, hollow columns, and a variety of surface effects—ridges, flumes, ribs, circular markings, and other more chaotic patterns.[3] Ironically, given this level of detail, their simulations produce only symmetric crystals. That is an artifact of the program. To reduce computer time, it generates only one-half of one arm, which is then reflected around a central axis in twelve identical half-arms.

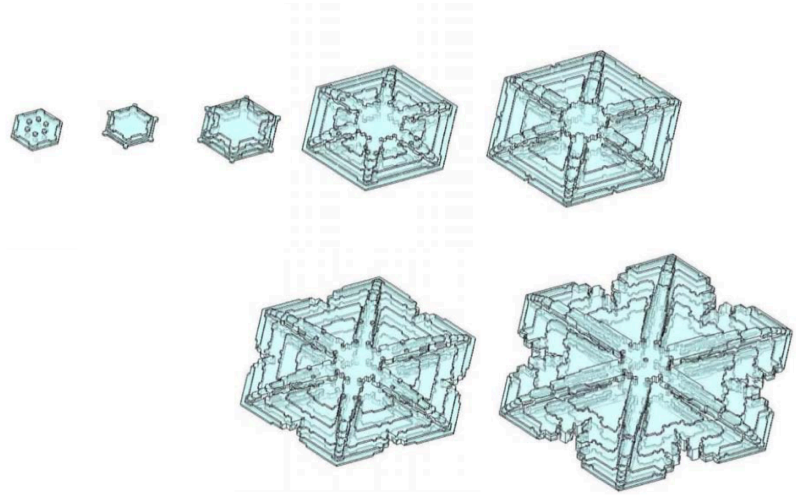
Figure 1. Simulated snowflakes. (Gravner and Griffeath, p. 13)

Gravner and Griffeath model snowflake growth at the mesoscopic level, that intermediate realm between microscopic molecules and macroscopic appearances, where neither quantum mechanics nor classical mechanics provides an approach directly from general principles. Instead, the model grows a virtual snowflake from a small "seed" crystal by successive addition of tiny hexagonal prisms. The crystal is imagined to be surrounded by water vapor and its growth is governed by only three phenomenological considerations: diffusion of water vapor from the crystal; freezing and melting in a narrow boundary layer; and attachment rates at the boundary favoring concavities. Despite this conceptual simplicity, however, implementation of the model in a continually updating cellular automaton requires many parameters and therefore large amounts of computing time. The evolution of a single snowflake takes about 24 hours on a modern desktop computer, even though restricted to full symmetry.

Gravner and Griffeath forthrightly acknowledge that it is not very clear just how their intuitively plausible parameters correlate with physical processes and that their simulations do not yet treat important issues of non-symmetry, randomness, singularities, and instabilities, that is, the full range of contingencies that affect growth. They nevertheless believe that their limited evolutionary simulations provide an understanding of many of the characteristics of natural snowflakes, both in general morphology and in the details of their traits.[4] Run many times over, with varying parameters, the simulations explore the space of possible snowflakes and their probable mechanisms of formation. These explorations also "discover" new properties, in the sense that they reveal features that might be found in real snowflakes. They thereby suggest new kinds of observations, which could probe the strengths and weaknesses of the model.

The known properties and new discoveries obtained in the snowflake simulations are natural historical in kind. Key terms are *trait*, *habit*, *morphology*, *seed, evolution*, *field guide*. The simulations generate a kind of taxonomy of snowflakes in which the traits of the different varieties are understood through the simulated history of their development in time, read as evolution (figure 2).

Figure 2. Evolution of a snowflake.
(Gravner and Griffeath, p. 6)



This evolution derives from a simple generative model operating under varying environmental conditions. That is, the simulations generate an evolutionary narrative that grows snowflakes as products of a development in which every individual emerges uniquely from its temporal path. If fully developed, this history would follow a tiny ice crystal falling for an hour or more through the contingencies of a turbulent atmosphere to acquire its final intricate form. Libbrecht draws the basic lesson: "Complex history; Complex crystal shape." Complexity and historicity are deeply entwined.

While more explicitly natural-historical than other examples, this snowflake generation nevertheless provides a fairly typical case of model-based simulations of complex physical processes, of their relation to historical narrative, and of their value for scientific understanding. Although I will limit my discussion here to complex systems, I do not think that limitation is essential. Rather, the narrative properties tend to be effaced when deductive mathematical systems are available. I take such deductive systems to be a subset of the more general form of narrative, obtained from it by idealization and abstraction. Although often obscured, the virtues of narrative knowing retain their potency.

One further aspect of the snowflake story requires immediate notice. It depends crucially on visualization to make it legible. That is not a matter simply of illustration. Rather visualization is the only effective means for following the growth process. To be understandable the simulation must incorporate visualization software for converting its calculations into an object accessible to the senses. Ideally, the software would show the evolution in a continuous movie. That goal will bring me to the simulation on which I will focus below, discussion of which will help to deepen the role of temporality in narrative understanding. But first a few general comments on the relation of model-based simulations to narrative.

Models and Narratives

I begin from two broad observations. The first is that natural scientists today are much more likely to appeal to models to ground their claims to understanding and explanation than they are to appeal to natural laws. The difference is rather fundamental in that the strength of the appeal to natural laws has often rested on the implicit assumption that the laws are “out there,” in nature, and not a product of human contrivance. An archetype is Laplace’s *System of the World* (1795), unified by the inverse-square law of gravitation, along with his conception of a being knowing all the laws, and therefore knowing simultaneously all past and future states of every atom in the universe. Models, on the other hand, typically carry the sense of things that we build and modify for our own purposes of understanding and action. Models are exploratory and provisional. They are limited in scope rather than universal and they typically work by analogy rather than necessity. And they are more likely to take up real-world contingencies. These properties lead to a second observation, that the practice of using models to explore the world tends to bring with it a more nearly narrative mode of understanding. The link between these two observations may be that narratives too are our constructions, designed to interrelate a limited range of materials within a coherent context to yield a meaningful interpretation. When coupled with models, the narratives tell us how the models work and how they relate to the world.[5]

If so, then the narrative aspects of model-based simulations may have much more in common with historical narratives than has usually been assumed. An exemplary expression from Paul Ricoeur's now-classic *Narrative and Time* (1984) will suggest how deeply the change in viewpoint cuts. In commenting on the role of contingency and complexity in history, Ricoeur sharply contrasted historians with his conception of physicists, relying on the view then current that physicists aim to eliminate contingencies by appeal to laws.

> [Historians] do not expect them [laws] to eliminate contingencies, but rather to provide a better understanding of their contribution to the march of history. This is why their problem is not to deduce or to predict but to understand better the complexity of intertwinings that have converged into the occurrence of this or that event. In this historians are different than physicists.[6]

But are they? If "complexity of intertwinings" is precisely what some physicists and other natural scientists want to understand through model-based analysis, then we ought to expect that they will behave more like historians. And they do.

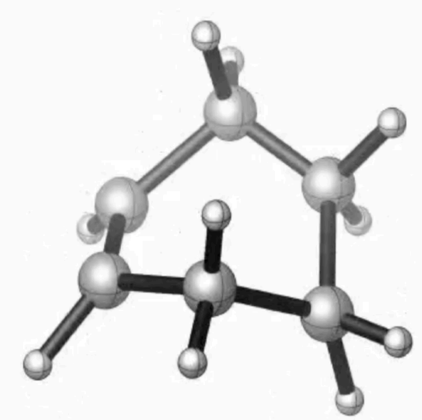
From this perspective, a broad field opens for fresh consideration of how narratives function in modeling, whether in the natural sciences or social sciences. I aim to show, in fact, that important aspects of what has been said about the properties of narrative by philosophers of history like Ricoeur – looking aside from their views on science – apply also to some model-based simulations. I will be arguing, for example, that contingencies often play a crucial role in the understanding of physical processes that some simulations provide. More generally, the use of models to explore the world and experiment on it often makes contingencies explicit and thereby deepens understanding.[7]

Finally, I will focus my discussion of the narrative form of simulations on the role of time. Not all simulations and not all narratives have a primarily temporal form, as will be evident from other papers in this special issue (Morgan, & others). Nevertheless, I want to show that the experience of temporal development or unfolding is critical for scientists' understanding of the simulated physical processes that I describe and that the way they make sense of these temporal simulations reflects key aspects of narrative. The question of temporality has long been at the center of productive debate among analysts of historical narrative. Does understanding come from following the story prospectively toward an ending or does it come from retrospective reflection on what has already happened? I consider first the virtues of the prospective view, then important aspects of retrospective judgment, and finally a dialectical perspective on their interrelation.

Following the Story

In 2012 the chemist Kendall Houk published his inaugural article for the National Academy of Sciences, in which he and his collaborators presented simulations of so-called Diels-Alder reactions, first described by Otto Diels and Kurt Alder in 1928, for which they were awarded the Nobel Prize in 1950. These are some of the most important reactions used in organic synthesis. They involve two reactants forming two carbon bonds to yield a six-membered ring. Figure 3 shows the product of butadiene reacting with ethylene, which is the example on which I will concentrate.

Figure 3. Bonding of butadiene plus ethylene.



Debate over the mechanism of the reactions has continued ever since their discovery, focusing especially on "the timing of bond formation,"[8] which is also my focus here. The basic question of whether the two C-C bonds form simultaneously or serially remained unresolved. As usual for such complex systems, a direct mathematical solution from quantum mechanical foundations was not possible. Attempted computational solutions remained ambiguous and experiments could not directly address bonding that occurred in femtoseconds (one millionth of one billionth of a second). Houk and his team sought to address the question by creating high resolution simulations of the process in time, which they presented as movies. These simple visual narratives form a key component of the published paper, for they present the findings in a compelling form. And like all good stories, they draw the viewer almost irresistibly into the experience of following the dynamic vibrations of the molecules as they approach one another, perhaps recede, and approach again. To appreciate the sense of expectancy that is produced requires watching the action. The published movies are available at this link: [9] http://www.pnas.org/content/suppl/2012/06/26/1209316109.DCSupplemental. Movies S1 to S3 are for the reaction of butadiene with ethylene.

A voiceover might give the plot summary as follows. In the beginning two molecules that feel an initial attraction begin to approach one another in a tantalizing dance, with all of their atoms in motion and seeming to explore a coupling that may or may not occur. They form a first bond between two of their carbon atoms and then continue the dance about one another, sometimes exceedingly briefly, sometimes much longer, before the final denouement when they form a second C-C bond. So ends the story of a Diels-Alder reaction in its usual form. At normal temperatures (298^0 K or 25^0 C) the succession of the two bonds for most reactions turns out to be so fast that they are essentially simultaneous (approximately 5 femtoseconds, or 5 millionths of one billionth of a second), while at high temperatures (about 1100^0 K) and for non-symmetric reactions, some trajectories involve an intermediate formation (a biradical) and the interval can be much longer (800 fs or more).

In an interview, Kendall Houk described the function of these apparently so simple movies within a professional scientific publication.

> ”This paper is *hard-core physical chemistry*, using molecular dynamics techniques to study the Diels-Alder reaction in detail to understand how it happens. We conducted a time-resolved study of how these reactions happen by creating simulations, *basically movies*, of molecules coming together and reacting. The idea is to understand how the reaction happens, not just that *a* goes to *b* and *b* goes to *c*, but to *actually follow* how the bonds are forming and how the atoms are moving as these things come together. Using the massive computer power we have now, we get a degree of resolution of the mechanism [in time] that was not really possible before. It takes a lot of computer time, but as a result we now have *unprecedented insight* into how this reaction occurs.”[10]

The movies are not just pretty pictures and not just fascinating to watch; they are integral to the understanding achieved in this piece of “hard-core physical chemistry.” Their great value lies in the temporal account they give of the process of bond formation, here literally to see it happening in a movie. According to Houk, it is this capacity to actually follow the motions in time that brings “unprecedented insight.”

In his emphasis on following the process, the practicing chemist here highlights what a well-known philosopher of history identified long ago as an essential feature of narrative: followability. In *Philosophy and the Historical Understanding* (1964), William B. Gallie analyzed the concept at length. That he supposed he was showing “why historical understanding [of human action] must differ in kind from the understanding that is the goal of the sciences"[11] now appears rather ironic, since much of his discussion of followability would seem to apply to model-based simulations in the physical sciences. And in fact, Gallie himself in his 2nd edition disavowed his former insistence that historical narrative depended essentially on its appeal to individual human action and human interest, recognizing "the clear fact that in a good deal of cultural history—histories of the arts and the sciences and of technologies and all 'pre-history'—the required story-worthy individuals are not to be found."[12] Replacing them with story-worthy molecules does little to vitiate several aspects of followability that Gallie highlighted.

One such aspect is the reader's sense that the story is proceeding toward an end and of being drawn along by it. A similar sense of expectation becomes remarkably strong when watching the Diels-Alder movies. As is said of narratives, they connect together a chain of events not simply as a sequence but as a natural unfolding guided by an implicit telos, a development within which the viewer is looking toward an ending, typically the double C-C bond, but then perhaps not! Thus the narrative has a purposive quality that is built into its structure. But the results it yields (or reveals) regarding the bonding process and bonding time are not ones that could be deduced or predicted on the basis of the starting point and any general conditions governing change.

This unpredictability, according to Gallie, is another key aspect of narratives, which gain much of their power from the way in which they incorporate contingencies that appear along the way. Such contingencies inhere in every historical situation and every historian encounters them in doing the research that ultimately enters the narrative they write. The challenge for the historian is to give full recognition to these contingencies and to the surprises they yield, while nevertheless including them coherently in the development that leads to the ending. This effort will be successful, in Gallie's terms, just in case the reader finds the contingencies "acceptable" within the narrative and with respect to the ending. They cannot derail the narrative nor can they appear from nowhere. They must be acceptable for the followability of the story.

> Almost every incident in a story requires, as a necessary condition of its intelligibility, its acceptability, some indication of the kind of event or context which occasioned or evoked it, or, at the very least, made it possible. This relation, rather than the predictability of certain events given the occurrence of others, is the main bond of logical continuity in any story.[13]

For the Diels-Alder movies as well as the evolution of snowflakes I have called this relation a natural "unfolding." The term is one that Gallie sometimes used and that several of the authors in this volume have also adopted. It leaves open the question of causal analyzability under laws while preserving the requirement that earlier developments establish the conditions of possibility for later ones. In philosophy of science there is a burgeoning literature that treats such unfolding under the name of "mechanism." Although I will not pursue it here, it seems promising for evolutionary simulations. (See Crasnow's discussion in this issue.)

The issue of causality emerged for Gallie not because he thought causes do not exist in history but because there are too many of them and they are irretrievably entangled, as in "the convergence of the different kinds of causal lines that met at Sarajevo in 1914," such that they do not constitute "a single comprehensive causal system." He called such systems "complex,“ without yet knowing that the same term was already coming to characterize a wide range of physical systems in the "sciences of complexity" and their exploration in "dynamical systems theory" (Libbrecht's field of physics).[14] Although the two meanings of complexity differ in technical terms, the results of interest here are much the same: complex systems are sensitive to many sorts of contingencies that affect their unfolding and make it unpredictable in detail. They require for their followability, therefore, an approach that is less reductive and less deterministic than deduction from causes governed by laws. Historians typically find this versatility in narratives while physical scientists often use simulations based on models that mirror observed complexity and capture relevant contingencies. The parallels, I am arguing, are extensive.

Enriching the Narrative

In attempting to explicate what it is about narrative history that yields trustworthy knowledge, Gallie distinguished *understanding*, obtained directly by following the narrative, from *explanation*, which for him came into play when the narrative seemed to lose its followability and required supplementary support or clarification.

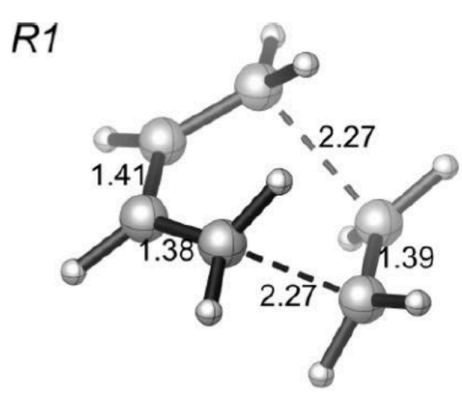
> Historical *understanding* is the exercise of the capacity to follow a story, where the story is known to be based on evidence …. But to follow an historical narrative always requires the acceptance, from time to time, of *explanations* which have the effect of enabling one to follow further …. [15]

Gallie was here attempting to distinguish narrative from deductions and from other explanatory material, which he regarded as scientific in form and as "ancillary" with respect to the priority of the narrative itself. Since this dichotomous mode of distinguishing narrative from science is not viable, neither is Gallie's formulation of the distinction of understanding from explanation. Nevertheless, his discussion raises an important point. The basic story in a historical narrative does not stand on its own. It relies on a great deal of supporting information and analysis that both explicates the narrative and deepens its meaning. For works of history, the enrichment appears partly in the introduction, partly in expository sections of the main text, and partly in the footnotes.

A similar enrichment accompanies the Diels-Alder movies as visual narratives of chemical bond formation. They require a detailed description of the model and of how the simulation works, including its development in time, so much so that these technical discussions constitute the main body of the text. They provide an elaborated verbal and graphical account of aspects of what the movies show in a consolidated fashion. In contrast to Gallie, I will simply treat this "explanatory" material as an integral part of the full narrative, which I now summarize.

Houk's presentation begins with a literature review, which positions the new analysis in relation to previous work, followed by a summary of what will be shown

Figure 4. Saddle point for butadiene plus ethylene
(bond lengths shown in angstroms)



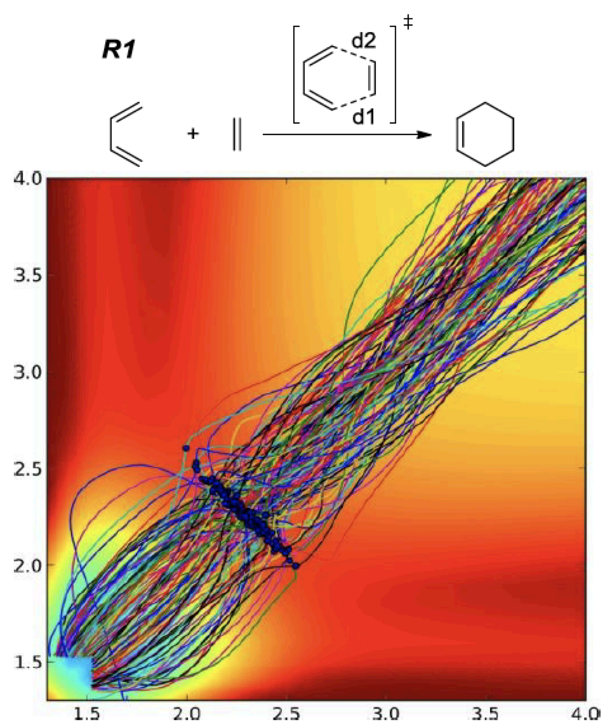
through the movies. An extended discussion follows of the starting point for the simulations, the so-called transition state through which the system must pass in order to reach stable bonding. Figure 4 shows the configuration at the middle of this transition state, where the distance between C-C bonds is 2.27 Angstroms.

Though fairly narrow in energy, the transition state is relatively broad in terms of bonding distances for the two C-C bonds and thus includes a spectrum of starting geometries for the two reactants. For each run of the simulation – and each corresponding movie that could be made – a specific starting point within the transition state is selected by random sampling from a distribution of possible positions and velocities. The distribution itself is obtained by quasi-classical techniques to yield an approximation to a quantum-mechanical probability distribution. It is just here, within the random selection of starting points, that the variability of the process enters along with its unpredictability.

From the beginning scenario of starting points, the narrative of the process of bonding proceeds. I give it in a simplified form but with enough detail to indicate how the full narrative is constructed. Four images (figures 5-8 below), all referring to the particular reaction of butadiene with ethylene, will suffice.[16]

For each of the selected starting points, the simulation generates a unique bonding history, which could be depicted in its own movie. To follow the histories more deeply, however (and in the manner of Gallie's explanatory material), the Houk team explores specific aspects of them as "trajectories" of the C-C bonds, focusing on bonding distance. The bundle of threads in Figure 5 shows these bond trajectories for the butadiene-ethylene example, for which the two bonds are symmetric.

Figure 5



Each sinuous thread, running from top right to bottom left, plots on the horizontal and vertical axes the distances between carbon atoms for the two forming bonds. The complicated vibrations of all of the other atoms of the reactants, which would appear in the full movie for any one of these threads, are taking place in the background, so to speak.

Each trajectory actually consists of two parts, computed in forward and backward directions from the transition state (the dark region, consisting of dots at the starting points). Thus "forward and reverse trajectory simulations from the same initial geometry give the complete trajectory that connects reactants, transition state, and product."[17] As the trajectories pass through the transition state they proceed toward the small square area at bottom left, where both bond distances are less than 1.5 Angstroms (10^{-8} cm) and the bonds have formed, ending the histories. Taken together, the full bundle of these complete trajectories (numbering either 128 or 256) gives a fairly comprehensive view of the full range of possible bonding histories for the reaction, including occasional outliers.

Figure 6

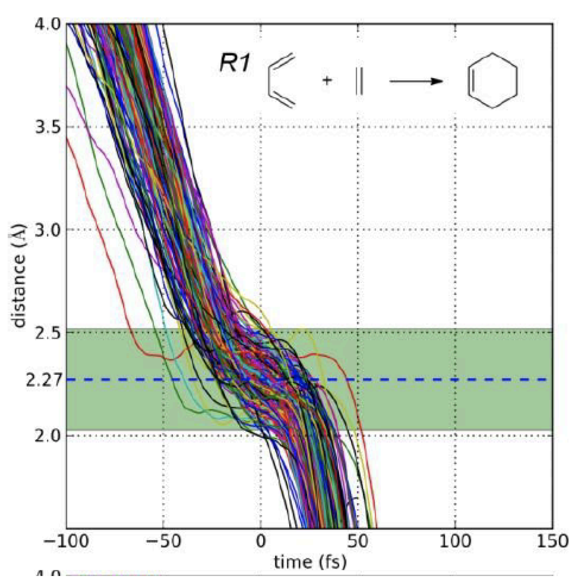
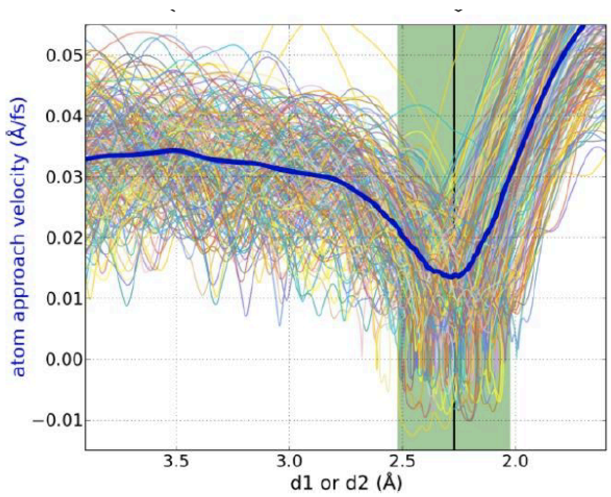


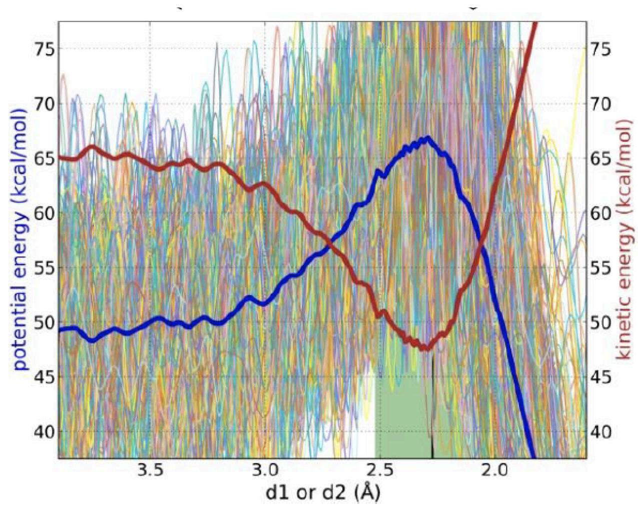
Figure 6 gives a set of complementary plots in the time dimension, showing how the distance for either one of the two symmetric C-C bonds decreases with time as the reactants pass through an appropriately defined "transition zone" (shaded). Since the slope of the curve gives the velocity of approach, the trajectories show how the velocity decreases and then increases again while passing through the transition zone.

Figure 7



Even more dramatically, Figure 7 plots the relative approach velocity of the two bonds as a function of the bond distance for one of them. The individual curves display wide oscillation, while the median velocity (solid dark curve) highlights an expected sharp dip through the transition zone followed by rapid acceleration as the bond forms. The trajectories also reveal the interesting fact that the relative velocity sometimes turns negative within the transition zone.

Figure 8



Finally, figure 8 plots potential energy as a function of bond length. From the wildly oscillating individual trajectories, curves for median values extract a marked hump in potential energy across the transition zone, while the curve for kinetic energy shows a corresponding dip. The median curves for the bundles of trajectories thus depict the energy barrier that the reactants must surmount in order to complete their bonding.

It will be apparent that the four graphic depictions of reaction trajectories, figures 5-8, along with their verbal descriptions, give technical specificity to key aspects of the temporal process of bond formation and its variability. They thereby enhance the followability of the narrative as it would be presented in the movie of any one of the specific trajectories, in the sense that they allow an interrogation of the movie that would not be possible by simply watching it directly. What they do not supply, and the movie does, is the capacity "to *actually follow* how the bonds are forming and how the atoms are moving as these things come together," which is what Kendall Houk identified as the source of "*unprecedented insight* into how this reaction occurs." This relationship between the experience in time that the movie affords and the analytic specification of key features of its technical content is what gives the full narrative its power for understanding.[18]

Synoptic Judgment

Another important perspective on the power of narrative is that of Louis Mink whose probing essays from the 1960s and 70s are collected in his *Historical Understanding* (1987). Like Gallie, Mink was concerned to show how historical understanding differed from natural science as conceived in the deductive theoretical mode (n.2) and he hit on an attractive idea. Unlike historians, he thought, scientists could detach their results from the evidentiary arguments that supported them, so that these results could be used by others in subsequent analysis and in different contexts in a cumulative fashion. (This property he took to be "possible in science because – and only because – of its [deductive] theoretical structure," which already suggests a severe limitation of the argument when a deductive theory is not available, as in most complex systems.) In contrast, Mink argued that historians' conclusions were "ingredient" to the narrative that contained them, meaning that they could not be detached from it while maintaining their meaning, because "their meaning refers backward to the ordering of evidence in the total argument."[19] Again, "The narrative is not a story supported by evidence, but the statement of the evidence itself, organized in narrative form so that it jointly constitutes the unique answer to specific questions."[20]

This distinction, however, seems to be overdrawn for practitioners in either domain, whether in history of natural science, and to be more a matter of degree and of purpose than of detachment altogether. For example, the conclusion from the

Diels-Alder simulations that the time between C-C bonds is on the order of 5 fs is surely a detachable finding. Equally detachable are the median values for energy barriers and for the percentage of reactions that proceed through an intermediate formation (below). But those numbers are bare abstractions from a narrative whose broader aim is to convey an understanding of how the reaction proceeds. And chemists concerned with that understanding of the temporal process, including those who want to understand how the reaction will function in their own attempts at synthesis, will have to watch the movies repeatedly while also studying the bundles of highly variable trajectory plots that follow specific aspects over the whole course of the reaction. In this sense, there is no understanding of the simulated process that is detachable from the simulations. So, to the degree that the conclusions of historical narratives are non-detachable, so too are those of the simulations, for they provide effectively a historical narrative of the reactions.

However one judges the non-detachability claim, Mink associated with it another holistic conception of historical narrative of great importance. In crafting his narrative the historian aims to organize a complex interplay of events, actions, and contexts in such a way that they hang together in a coherent interpretive synthesis. This capacity Mink originally labeled "synoptic judgment." "The suggestion is that the distinctive characteristic of historical understanding consists of comprehending a complex event by 'seeing things together' in a total and synoptic judgment which cannot be replaced by any analytic technique."[21] He soon realized that this narrative mode of comprehension needed to be distinguished more carefully from other modes of comprehension, which also consisted of grasping things together in a single mental act. Most pertinent here is Mink's distinction of the *theoretical* mode, characteristic of natural science in his conception, from what he now called the *configurational* mode, characteristic of (but not limited to) historical narrative. In the theoretical mode one grasps together a set of objects under a general law. Thus “iron rusts” and “paper burns” become instances of a type of chemical reaction understood theoretically as oxidation. By contrast, in the configurational mode, a letter burning would be comprehended within a single complex of relationships – a friendship, a misunderstanding, a change of plans – perhaps constituting a narrative.[22]

With respect to the Diels-Alder simulations, it would certainly be possible to conceive them in the theoretical mode as instances of a generalization (though not of the deductive law form) about the dynamics of a certain class of reactions (concerted cycloaddition reactions), and in fact that is part of Houk’s mode of reporting them.[23] But it is by no means the most important part. Much more prominent, as I have stressed above, is his emphasis on understanding the process as a whole, described more nearly in the configurational mode. He apparently seeks to “grasp together,” in Mink’s terms, the entire bonding process in a single thought. Thus the movie, supplemented by the graphical plots (figures 5-8) elaborating aspects of it, depicts a complete history, with a definite narrative structure of beginning (reactants attracting), middle (movement through the transition state), and end (stable bond). As thus visualized, the single thought – bonding – includes within it the entire history. (Indeed, as developed further below, it includes the whole set of possible histories for each reaction.) This conception of configurational comprehension I take to be a critically important feature of simulations conceived as narratives.

What now becomes important to consider is that the Diels-Alder simulations as Houk presents them are preeminently about the temporal dynamics of the bonding. So the grasping together in a single thought is the grasping together of a development in time as a single thought. The question is whether time in this act of "seeing-things-together" is actually important to understanding. To this question, Mink answered with an unequivocal no; and yet time seems to be crucial to Houk. I will come down on the side of Houk, but first a bit on Mink's argument, which he presented most forcefully as a dismissive critique of Gallie, whose stress on the followability of a narrative he thought wrongheaded, and just wrong.

Understanding a historical narrative, according to Mink, has little to do with following the story and its contingencies. That would be the position only of a naïve reader who did not already know the ending. No historian could have the experience of contingent events being made acceptable by the story directing them toward an expected but open conclusion. "It is not following but *having followed* which carries the force of understanding."[24] By this Mink meant that one understands a narrative retrospectively, not prospectively, for it is only in retrospect that one can understand the significance of what has happened at any point. Furthermore, it is only in retrospect that one can grasp the narrative together in a single thought, which he took to imply that the temporal order of the events that it incorporates is not an essential feature of understanding. The "actions and events, although represented as occurring in the order of time, can be surveyed as it were in a single glance as bound together in an order of significance."[25]

This conception, with qualifications, has much to recommend it for the Diels-Alder simulations. With respect to figures 5-8, for example, the plots of the trajectories of bond formation can literally be surveyed at a glance and contemplated in their entirety. One sees the whole course of the velocity decreasing through the transition zone and the full shape of the potential energy barrier that must be overcome. But does this capacity for retrospective inspection and analysis legitimate Mink's more radical claim that the overview essentially eradicates temporality, that "in the understanding of a narrative the thought of temporal succession as such vanishes" so that "time is not of the essence of narratives"?[26]

Mink's most extreme formulation of this claim rested on the idea that "the human project is to take God's place," where God's knowledge is referred to Boethius's concept of the *totum simul*, "in which the successive moments of all time are copresent in a single perception, as of a landscape of events."[27] It is telling that Mink's references for this notion, with respect to theoretical comprehension, were Laplace and the ideal of all-embracing laws of nature in the deductive vision of scientific knowledge. That is of course the vision that fails for complex systems and for which simulations from models now offer a potent alternative. Even with respect to configurational comprehension Mink took the timeless *totum simul* to be the highest degree of comprehension.[28] I find it quite difficult to reconcile this view with the practices of those simulators who model the evolution or unfolding of systems in time as their source of understanding. The expression of this unfolding in Houk's movies provides an epitome.

Temporal Dialectic

I do not, however, want in any way to undercut the retrospective comprehension that Mink so effectively highlights as synoptic judgment and configurational comprehension, quite the opposite, but rather to interrelate it with the prospective sense of progression toward an ending that Gallie articulated as followability. In this I will draw on Paul Ricoeur, who in *Time and Narrative*, gave extensive reflections on "Defenses of Narrative," including those of Gallie and Mink. As one would expect from his title, Ricoeur took Mink's claim "that time is not of the essence of narratives" to be a self-defeating denial of the narrative form itself as a mode of understanding. He found this denial actually expressed in Mink's *totum simul* as an ideal, for it would have no place for the sequential form of narrative, or emplotment, to connect together the complex interrelations of the world.[29]

Ricoeur proposed instead that narrative always involves a constant interaction between two dimensions of time, which correspond to the emphases of Gallie and Mink. It involves a "temporal dialectic" between an "episodic" dimension (basically a temporal sequence of events, a la Gallie) and Mink's configurational dimension. The plot interrelates these two dimensions as the narrative moves along, making it possible to follow the story while continually grasping it together in a kind of feedback loop. In configurational terms, the plot "construes significant wholes out of scattered events," thereby "eliciting a pattern from a succession" as a single thought.[30] But episodic time is not thereby abolished, for the "single thought" encompasses the development as a development in time. Ricoeur's episodic/configurational dialectic can be captured by modifying Mink's own memorable metaphor of two views of a river. In reflective configurational comprehension, Mink remarked, "time is no longer the river which bears us along but the river in aerial view, upstream and downstream seen in a single survey."[31] But like anyone who has descended a turbulent river in a canoe, Ricoeur would surely have said that these are two very different experiences of temporality, and that their interplay is necessary to understanding river-time. I would now say the same for Kendall Houk's trajectories of bonding, as well as for snowflakes.

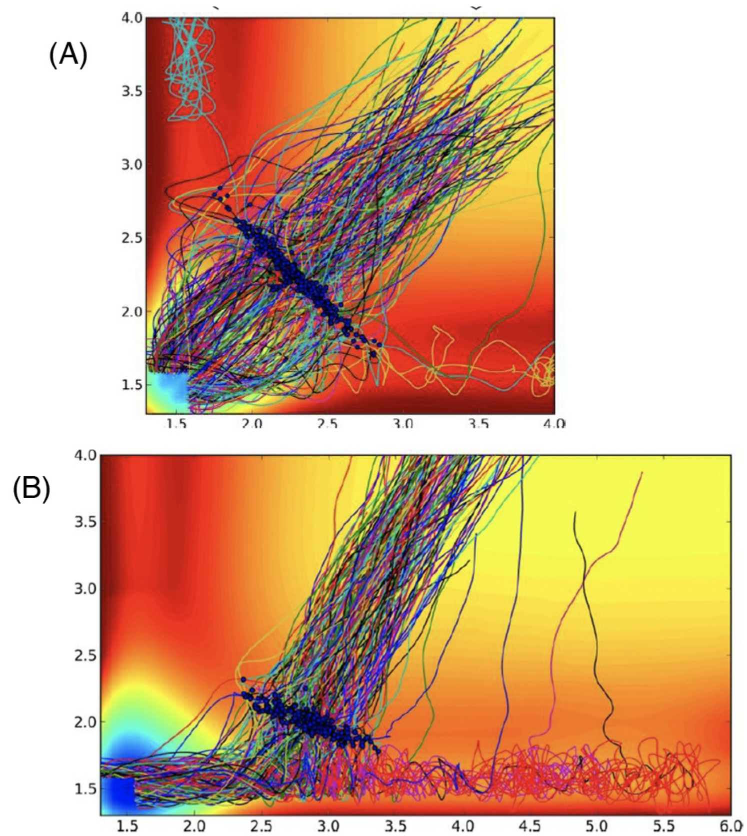
The Gallie-Mink discordance raises a further major issue requiring comment, namely the role of contingency. While Gallie's forward-looking perspective welcomed contingency as a motor of historical narrative, Mink viewed the historian as striving to eliminate contingency. With respect to Gallie's remarks on the complexity of causal lines leading to Sarajevo and the inherent contingency of what happens, Mink responded: "*tracing lines backwards* is exactly what an historian does, and *there are no contingencies going backwards* (if there were there would be no lines)."[32] Ricoeur objected to this reasoning on the ground that historians are continually rethinking the narratives they either write or read and in this are much more like the naïve reader than Mink allowed. Thus "the process of tracing forward again what we have already covered going backward may well reopen … the space of contingency that belonged to the past when it was present."[33] I would argue in fact that it is precisely the job of a good historian to keep the "space of contingency" open, rather than to close it down, and to explore the possibilities of that space.

It seems unlikely that to "run the film backward," as Mink suggested, will succeed in eliminating the importance of contingencies in understanding complex systems. The Diels-Alder trajectories and movies suggest a different conception. Granted, running any one of the movies backward will take the viewer through precisely the same movements in reverse. But every rerunning of the simulation from a randomly selected starting point, mimicking the effect of contingencies, produces a somewhat different history, and a different movie, sometimes quite different. This rerunning, which I take to be somewhat analogous to the rewriting and rereading so characteristic of historians, is one of the important ways in which simulations deepen understanding of the processes they model.

Possibility and Exploration

The significance of this rerunning of simulations emerges more clearly for the Diels-Alder reactions if we think of each of them in terms of the whole bundle of bonding trajectories that represents it (here standing in for the full histories that could be shown in movies). The single thought of bonding then encompasses not only one trajectory but all of the trajectories that the reactants could have followed through the many different randomly sampled starting points. The effect of this broader comprehension becomes quite striking for the symmetric reaction of butadiene with ethylene depicted in figure 5 when the temperature is elevated from 298^0 K. to 1180^0 K as in figure 9A. The bundle of trajectories is now much more tangled and irregular, more like a swarm. A significant percentage (such as those stretching out to the right along the bottom of the plot) go through a different mechanism, an intermediate formation (biradical), which leads to quite long time gaps between the two C-C bonds, increasing from about 6 to 800 fs. Movie S3, corresponding to one of these trajectories, gives an excellent sense of why they are so tangled, as it displays a dance between the C-C bonds that is tantalizingly long. This latter mechanism is even more in evidence in figure 9B and Movie S5 for a different, asymmetric, reaction simulated at the lower temperature, with time gaps over 1400 fs (Movie S5 at http://www.pnas.org/content/suppl/2012/06/26/1209316109.DCSupplemental).

Figure 9. Trajectory plots at high temperature (A) and for an assymmetric reaction (B), with some passing through intermediate formations (biradical).



This suggests too how rerunnings of the simulations, as represented in the bundles of trajectories, quite literally explore Ricoeur's "contingency space" for the various ways in which the reaction could proceed. They map out the space of possibilities as real developmental possibilities and facilitate the grasping together in a single thought of the whole process of bond formation.[34] To put the point a bit differently, in following any one *actual* bonding history, we are immediately aware of its place among other *possible* histories. And this knowledge of the possible deepens our understanding of the actual.

An analogous relation of the actual to the possible has been made the basis for a penetrating account of how historical explanation is related to understanding by the philosopher of social and political theory, Geoffrey Hawthorn, in his *Plausible Worlds: Possibility and Understanding in History and the Social Sciences* (1991).[35] It turns on counterfactuals and on what he calls initially a paradox. A successful historical *explanation*, on Hawthorn's account, connects the conditions and actions of actual developments with other actualities, but the force of the explanation depends on its implication of other possible developments that might have been realized but were not.

> "Its success as an answer to the question 'why?' will turn on the plausibility of the reasoning – the model, mechanism, or what J. L. Mackie called the inductively arrived-at 'running on' – that we invoke to make the connection. The plausibility of this reasoning will turn on the counterfactual it suggests.[36]

The seeming paradox is that, in connecting actualities, the successful explanation opens unrealized but realistic possibilities, and it is just in this opening of possibilities that *understanding* is located. Houk's simulations have something like this character. The credibility of any one actual movie or trajectory depends on its place within the entire spectrum of possible trajectories. As Hawthorn said of history, "It promises that kind of understanding . . . which comes from locating an actual in a space of possibles." He took his cue here from Robert Nozick in *Philosophical Explanations* (1981), who suggested that "explanation locates something in actuality . . . while *understanding* locates it in a network of possibility." He cited also an astute passage from Robert Musil's *Man without Qualities*, "If there is such a thing as a sense of reality … then there must be something that one can call a sense of possibility." Things might really have been different. [37]

The paradoxical relation of explanation to understanding, as Hawthorn presented it, began from the view that historians have understood explanations as providing a causal account of a sequence of particular events, an account that aims to be so tightly constructed rationally and evidentially that it is irresistible, explaining away contingencies and making it difficult to believe that any alternative development was possible. He summarized this view: "however the world may appear to be or really is, to understand it is to make it coherent. The coherence is ours and in it, the loose ends of mere possibles have no place." He offered a paraphrase of Kierkegaard that recalls Mink's view: "Life may have to be lived forwards, but the historian is privileged to understand it backwards."[38]

Retrospective explanations, on this view, exclude the counterfactuals that they actually imply or suggest, for to every cause adduced as important to an outcome, if that cause had not been operative the outcome would have been different. And yet, the more one examines the particularity of the apparent causes in play for specific situations and agents, the more contingent they seem. And here is the crucial point: "if the counterfactual is itself not plausible, we should not give the explanation the credence we otherwise might."[39] So even as the pursuit of ever more detailed explanation hones in on what actually happened, the nearby possibilities of what might plausibly have happened, but did not, increase. This increase is where understanding lies, it "comes from locating an actual in a space of possibles."

All of this seems quite pertinent for both cases of simulation that I have discussed, in each of which actualities and possibilities are produced within the same generative model. Whether for the whole taxonomy of snowflakes or the bundles of trajectories for a Diels-Alder reaction, the simulations quite explicitly explore the counterfactual world of realistic possibilities in order to gain a more thorough understanding of what actually happens for any particular snowflake or trajectory. Whether in history or physical science, then, explanation (of actualities) and understanding (of possibilities) are inherently linked. A better explanation is one that makes the nearby alternatives more immediately present to what actually happens in a given case.

Interestingly, if unsurprisingly, Hawthorn's analysis of explanation in relation to understanding ultimately vitiated the conception of explanation that originally stood behind his discussion as a foil, namely, the view that it is causal laws and general theories that explain.[40] Drawing on a number of philosophical critiques of the idea of laws said to be laws of *nature*, or laws *in* the world, he proposed to "forget laws altogether" and to focus on a different conception of explanation. It is a pragmatic conception emphasizing relativity to our interests and purposes, and it provides an answer to the question "why?" as a narrative: "it tells a story which is guided by contrasts with what we want to explain. It succeeds, where it does, by giving descriptions which in the conventions of telling that story to that kind of audience, are relevant *as* explanations."[41] In Hawthorn's plausible worlds, context, contingency, and indeterminacy are the features that have to be assimilated in our understanding of the story. For this purpose, it is not the distinction of science from non-science that counts (or indeed I would add, of explanation from understanding), but of the actual from the possible, since "each turns on the other."[42] He could offer no new name for this dialectical mode of understanding but it will be apparent that it bears a close relation to Ricoeur's episodic/configurational dialectic, for which it provides a grounding in the logic of counterfactuals.

Conclusion

I have been pursuing an understanding of the role of temporality in simulations of physical processes in complex systems by taking the Diels-Alder simulations as an epitome and placing some of their specific features in parallel with what have been seen as definitive characteristics of narrative knowing. 1.) Most immediately, Kendall Houk's stress on being able to directly follow the process of the reaction in a movie correlates quite closely with Gallie's emphasis on the followability of a narrative through its contingencies. 2.) Repurposing Gallie's account of how explanatory material ancillary to a narrative enhances followability, I find that graphical plots of specific aspects of the reaction, extending over its full course (bonding distances, bonding distance vs. time, velocities, and potential energies) greatly enrich understanding of what the movies contain in consolidated form. 3.) These same graphical plots appear to give a clear picture of what Mink meant by the synoptic judgment and configurational comprehension that narratives afford. The plots provide at a glance overviews of the entire course of the reaction, ready for retrospective analysis. 4.) And yet Mink went too far in eradicating temporal order from the configurational mode. Ricoeur reasserts the significance of time in an episodic/configurational dialectic that reopens the "space of contingency" that Mink wanted to close. The relation of episodic movies to configurational trajectory plots in the Diels-Alder simulations captures the point rather well. 5.) Hawthorn similarly reopens the key role of contingency in his analysis of the relation of the actual to the possible in the understanding that historical narratives provide. Analogues for this relationship can be seen for the Diels-Alder simulations in the relation of any single actual trajectory to the entire bundle of possible trajectories and in the relation of the more direct bonding trajectories to those through intermediate formations.

I conclude that understanding how simulations produce knowledge about real processes in complex systems benefits greatly from recalling basic features of narrative knowing. I conclude also that thinking in terms of a dialectic between following and configuring illuminates the role of temporality in simulations of these processes.

A final observation from Hawthorn may be helpful. As an illuminating analogue to the contingency that figures so prominently in historical narrative, he offered the unrealized possibilities of biological evolution and the improbability of the species we know to exist today. This was a topic much-discussed by Stephen J. Gould at the time. Whether or not one wants to go so far as Gould in promoting the improbability of evolutionary history, the contingency of particular developments is apparent.[43] The evolutionary corollary has seemed quite appropriate also for the simulated natural histories of snowflakes, and I would extend it as well to the Diels-Alder reactions. In both cases it is the capacity to follow a process through its developmental history, or to follow its growth, while simultaneously learning to recognize diverse alternative possibilities, that yields understanding.

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[1] M. Norton Wise, "Science as Historical Narrative," *Erkenntnis*, *75* (2011), 349-376, special issue on *What Good is Historical Epistemology*, ed. Uljana Feest and Thomas Sturm. I have relaxed here my earlier stress on how simulations often "explain" by

growing their product not because I think it mistaken but in order to avoid confusion with the senses of explanation used by the authors I cite below and in order to join it with a broader conception of understanding. See n. 7 below.

[2] K. Libbrecht, *Field Guide to Snowflakes* (St. Paul: Voyageur Pr., 2006). Many images online at http://www.its.caltech.edu/~atomic/snowcrystals/

[3] Janko Gravner and David Griffeath, "Modeling Snow-Crystal Growth: A Three-Dimensional Mesoscopic Approach," *Physical Review E*, *79* (2009), 1-18 (color images online): traits, p. 1; habits, p. 17.

[4] A complaint could arise here that the model of growth of a snowflake from hexagonal prisms does not represent a "true" or correct quantum mechanical theory of the interaction of water molecules, thus obscuring truth even while aiding understanding. A possible response could be that the prism model with its parameters operates at the mesoscopic level and that at that level it aims to give a true theoretical account. Such a response need not invoke the idea of a merely approximately correct model; it could insist instead on the irreducibility of the mesoscopic description to a microscopic molecular one. An interesting possibility for such a claim could be the existence of quantum "protectorates," or mesoscopic domains in which characteristic features are not sensitive to changes at the quantum mechanical level, so that the higher level description is as "fundamental" as it gets. That is, there may be nothing about snowflakes considered macroscopically that depends on a microscopic description. On protectorates and their possible relevance to "complex adaptive matter" and even evolutionary diversity see Robert B. Laughlin and David Pines, et al., "The Middle Way," [Electronic Version], *Proceedings of the National Academy of Sciences*, *97* (2000), 32-37.

[5] The best recent account of this relation is Mary S. Morgan, *The World in the Model: How Economists Work and Think* (Cambridge: Cambridge University Press, 2012). On simulation modeling of complex systems (but without narrative) see Johannes Lenhard, "The Great Deluge: Simulation Modeling and Scientific Understanding," in Henk de Regt, Sabina Leonelli, and Kai Eigner (eds.), *Scientific Understanding: Philosophical Perspectives* (Pittsburgh: University of Pittsburg Press, 2009), 169-186, and his general analysis and survey, "Computer Simulation," in Paul Humphreys (ed.), *The Oxford Handbook of Philosophy of Science* (Oxford: Oxford University Press, 2015), accessible from Oxford Handbooks Online (www.oxfordhandbooks.com). The relation of models and narratives is a theme of Angela N. H. Creager, Elizabeth Lunbeck, and M. Norton Wise (eds.), *Science without Laws: Model Systems, Cases, Exemplary Narratives* (Durham, NC: Duke University Press, 2007).

[6] Paul Ricoeur, *Time and Narrative*, trans. Kathleen McLaughlin and David Pellauer, 3 vols. (Chicago: University of Chicago Press, 1984-1988), I, 154. Ricoeur was expressing the widespread "Hempelian" or "Deductive-Nomological" conception of scientific explanation as requiring deduction from general laws, identified for historians with the oft-reprinted paper by Carl G. Hempel, "The Function of General Laws in History" [1942], in C. G. Hempel (ed.), *Aspects of Scientific Explanation, and Other essays in the Philosophy of Science* (London: Macmillan, 1965), 232-243. Most

of the philosophers of history discussed below also understood "science" in this way. Despite its drawbacks, it may have sharpened their reflections on narrative.

[7] A vexed debate lurks here over the meaning of understanding versus explanation. I will be attempting to lead discussion away from this question and toward a more liberal view of understanding, which does not depend on the dichotomy (this in spite of the fact that for several of the authors I cite the dichotomy – typically in Hempelian form – was immediately present to their thinking about narrative). The philosophical literature on understanding in science (rather than explanation) is growing, but so far it is thin on what narrative has to offer. De Regt, et. al., *Scientific Understanding*, contains many useful articles on the meaning of understanding in a wide variety of sciences.

[8] Kersey Black, Peng Liu, Lai Xu, Charles Doubleday, and Kendall N. Houk, "Dynamics, Transition States, and Timing of Bond Formation in Diels-Alder Reactions," *Proceedings of the National Academy of Sciences*, *109*, no. 32 (2012), 12860-12865, on 12860. http://www.pnas.org/content/109/32/12860.full

[9] It may be best to use the Chrome, Safari, or older Explorer browsers, or download to, e.g., Windows Media Player. If unsuccessful contact nortonw@history.ucla.edu.

[10] Interview with Beth Azar, "QnAs with Kendall N. Houk," *Proceedings of the National Academy of Sciences*, *109*, no. 32 (2012), 12839. My emphasis.

[11] W. B. Gallie, *Philosophy and the Historical Understanding* [1964], 2nd ed. (New York: Schocken Books, 1968), 3. Gallie, like Ricoeur after him, followed Hempel's characterization of natural science (n. 6).

[12] Gallie, *Philosophy*, 4.

[13] Gallie, *Philosophy*, 26.

[14] Gallie, *Philosophy*, 92-93, 118. See also the Ricoeur quotation of n. 6.

[15] Gallie, *Philosophy*, 105. My emphasis.

[16] All of the figures are from Black, et. al., "Dynamics" and its Supplementary Material. http://www.pnas.org/lookup/suppl/doi:10.1073/pnas.1209316109/-/DCSupplemental

[17] Black, et. al., "Dynamics," 12862.

[18] This understanding could of course be wrong, if the simulation does not in fact correspond to the actual dynamics of the reaction, but that is difficult to judge in the absence of direct experimental confirmation. The question of validity then becomes one of consistency, whether with respect to other experimentally confirmed results, to the successful extension of the results in a chain of synthesis, or to theoretical considerations.

[19] Louis Mink, "Autonomy and the Historical Understanding," *History and Theory*, *5* (1966), 24-47, reprinted in Louis Mink, *Historical Understanding*, ed. Brian Fay, I. O. Golob, and R. T. Vann (Ithaca and London: Cornell U. Pr., 1987), 61-88, esp. 79.

[20] Louis Mink, *Mind, History, and Dialectic: The Philosophy of R. G. Collingwood* (Bloomington: Harper & Row, 1969), 193. See Paul Roth's article in this issue for the significance of this claim and his development of it.

[21] Mink, "Autonomy," 82.

[22] Louis Mink, "History and Fiction as Modes of Comprehension," *New Literary History*, *1* (1970), 541-548, in Mink, *Historical Understanding*, 42-60, on 51-53.

[23] Mink considered the different modes of comprehension to be incompatible, in the sense that they could not be combined in a single act. He offered only anecdotal evidence. He did acknowledge that one could select different modes as appropriate to a particular inquiry. Mink, "History and Fiction," 551f, in Mink, *Historical Understanding*, 53.

[24] Mink, "History and Fiction," 545, n.9, and 546, in Mink, *Historical Understanding*, 47, n. 9, and 48.

[25] Mink, "History and Fiction," 554, in Mink, *Historical Understanding*, 56.

[26] Mink, "History and Fiction," 554-555, in Mink, *Historical Understanding*, 56-57.

[27] Mink, "History and Fiction," 549, in Mink, *Historical Understanding*, 51.

[28] Mink, "History and Fiction," 549-551, 554, in Mink, *Historical Understanding*, 51-53, 56.

[29] Ricoeur, *Time and Narrative*, I, 160.

[30] Paul Ricoeur, "Narrative Time," *Critical Inquiry*, *7* (1980), 169-190, on 178.

[31] Mink, "History and Fiction," 554f, in Mink, *Historical Understanding*, 57.

[32] Louis Mink, "Philosophical Analysis and Historical Understanding," in Mink, *Historical Understanding*, 118-146, on 136.

[33] Ricoeur, *Time and Narrative*, I, 158.

[34] The function of these rerunnings is reminiscent of work by Adam Toon, "Playing with Molecules," *Studies in History and Philosophy of Science, Part A*, *42* (2011), 580-589, on the way in which chemists "play" with models of molecules in much the same way as children play with dolls and trucks in games of make-believe. They learn the possibilities and constraints for the bonding of particular sorts of molecules, Toon argues, through their visual and tactile manipulation of the models and their imaginative participation with them, as though they were actually manipulating the molecules themselves. On the importance of manipulation of models in time, see also, Lenhard, "Great Deluge," 170, 178.

[35] Geoffrey Hawthorn, *Plausible Worlds: Possibility and Understanding in history and the Scocial Sciences* (Cambridge: Cambridge University Press, 1991). I will omit from my discussion one of Hawthorn's primary concerns, with practical reasoning, which he often contrasts with causal reasoning. My selection, while somewhat distorting, focuses an aspects more relevant to the relation of history to natural science.

[36] Hawthorn, *Plausible Worlds* 16.

[37] Hawthorn, *Plausible Worlds*, 17, 10, 4. Nozick (1981), 12; Musil (1979), 12. I thank John Beatty for pointing me to Hawthorn. See his careful analysis (this issue) of the significance of alternative possibilities for understanding and explanation.

[38] Hawthorn, *Plausible Worlds*, 9.

[39] Hawthorn, *Plausible Worlds*, 16.

[40] Hawthorn, *Plausible Worlds*, 168, 185.

[41] Hawthorn, *Plausible Worlds*, 25.

[42] Hawthorn, *Plausible Worlds*, 169-177, 187.

[43] Hawthorn, *Plausible Worlds*, 17f, n. 19.