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On the explanatory power of atomistic simulations

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Abstract

Given that explanation is at the heart of science and considering that computer simulations have become ubiquitous in a multitude of scientific fields, it is important to examine their role in the acquisition of scientific explanations. Even though philosophers of science are increasingly paying attention to the use of computer simulations in explanatory contexts, the concrete contributions that simulations can make to explanations deserve closer philosophical scrutiny. Zooming in on the case of atomistic simulations and starting from a counterfactual account of explanation, we here explore how such simulations can help scientists tackle three relevant challenges in the search for explanations. We argue that atomistic simulations can help access variables at explanatorily relevant levels of description, that they can help track the effects of changes in variables in a highly controlled and fine-tuned way, and that they can allow for a fine-grained account of the relative importance of various difference-makers. Considering a concrete example and illustrating how atomistic simulations are actually used in scientific practice to support explanations, our examination aims to contribute to a more comprehensive and nuanced view of their explanatory power.

Keywords Computer simulation · Scientific explanation · Difference-making · Molecular dynamics, explaining with models, atomistic simulation

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1 Introduction

Scientific explanation is a pertinent and controversial topic in the philosophy of science. Although the search for explanations is widely taken to be at the heart of science, it is often considered a challenging task – especially if the investigated phenomena are very complex and difficult or impossible to tackle by means of traditional scientific approaches. The nanosciences are a particularly illustrative example: At the nanoscale, the behavior of matter often deviates significantly from what would be expected on a macroscopic scale, leading to interesting scientific surprises and sparking a plethora of explanatory questions. Experiments to study such behavior are, however, often difficult to perform and phenomenological theories abstracting from molecular details often turn out to lead to inaccurate predictions.

Over the last decades, computer simulations have become increasingly important tools in science – in the nanosciences and elsewhere. Given their prevalence in scientific research, it is perhaps of little surprise that the role of computer simulations in scientific explanations is gaining more and more attention from philosophers of science (e.g. Durán, 2017; Boge, 2020).

However, there is no consensus on how explanations obtained with the help of computer simulations work, and philosophical contributions exploring in detail how computer simulations support explanatory reasoning in scientific practice are so far sparse.

In addition, discussions on the complexity and epistemic opacity of computer simulations have casted doubt on their potential to offer scientific explanations or understanding (Lenhard & Winsberg, 2010; Winsberg, 2010; Lenhard, 2019), highlighting the need for further exploration of their explanatory power. Being concerned with atomistic simulations, Lenhard, for example, suggests that the high degree of control provided by such simulations over the modeled system can come at the cost of increased epistemic opacity, potentially hindering explanation or understanding (Lenhard, 2006).

Given that atomistic simulations allow scientists to study how complex behavior emerges from atomic and molecular interactions – and given that they find applications across diverse scientific disciplines, including materials science, chemistry, and the life sciences, they make a particularly interesting case for exploring the explanatory power of computer simulations. While we acknowledge, in alignment with Lenhard's perspective, that atomistic simulations are sometimes used primarily for the purposes of prediction or control, we here argue that they can make highly important contributions to scientific explanations. And, as we will show, they do so not *despite* but partly *in virtue of* their capacity to grant scientists control over the respectively modeled system.

In a number of recent contributions it has been suggested that computer simulations provide explanations by allowing researchers to manipulate modeled systems in various ways, enabling them to draw what-if inferences about the explanandum (see e.g. Ylikoski, 2014; Kuorikoski & Ylikoski, 2015; Schweer & Elstner, 2023). This resonates with what is often referred to as the 'counterfactual account of explanation' in the tradition of Woodward (2003). In the counterfactual account, explanation is a matter of showing how the explanandum would have been different if the factors cited in the explanans had been different.

We here propose that the explanatory role of atomistic simulations can fruitfully be approached from within the counterfactual account of explanation. Schweer and Elstner (2023) recently highlighted that atomistic simulations can be powerful tools for assessing difference-making factors. Drawing on this, we here develop a more comprehensive account of the explanatory power of atomistic simulations.[1] By paying close attention to how these simulations are actually used in scientific practice, we explore their specific contributions to explanations. Also, in developing an account of the explanatory power of atomistic simulations, we make the case for greater philosophical recognition and appreciation of their relevance in scientific explanations– particularly in light of recent concerns raised about epistemic opacity.

Concretely, we proceed by examining how atomistic simulations can help scientists tackle three relevant challenges that may arise in the search for explanations.

First, there is what can be called the *challenge of accessing and selecting variables*, i.e., the challenge of depicting and accessing a suitable set of variables that potentially matter for explanation. Finding the relevant variables for explanations can be non-trivial, especially if the investigated target systems are complex and involve features on various levels of description. Second, there is the challenge that once a set of suitable variables has been depicted and accessed, obtaining an explanation involves assessing how the explanandum would have been different if the values of the respectively chosen variables had been different. It is, however, often not easy to actually *track* how the explanandum would be sensitive to changes of the chosen variables. Let us call this the *challenge of tracking variable changes*. Third, many explananda are sensitive to changes in not just one but a number of variables. Hence, there is the difficulty of having to evaluate the relative importance of each difference-making variable. Call this the *challenge of evaluating quantitative contributions*.

In what follows, we elucidate the explanatory power of atomistic simulations by showing how they can help scientists address these three challenges: Atomistic simulations can enable access to variables at relevant levels of description, they allow to perform manipulations in a controlled and often otherwise unfeasible way– and they can help with an assessment of the relative importance of various difference-makers. After providing some background about atomistic simulation (Sect. 2), we introduce a concrete illustrative explanatory problem where scientists used atomistic simulations to study the behavior of ions in atmospheric aerosols (Sect. 3). Having set the stage, we propose approaching the contributions of atomistic simulations to scientific explanations from within a counterfactual account in the tradition of Woodward (Sect. 4). Turning to computer simulations, we briefly discuss concerns about their explanatory power and outline how they can help scientists obtain real-world explanations in the first place (Sect. 5). Based on that, we introduce the three aforementioned challenges occurring when obtaining counterfactual explanations, and we discuss how atomistic simulations can help scientists tackle them (Sect. 6). In con-

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[1] This article is based on and substantially revised and expanded from Chapter 4 of the first author's doctoral dissertation (Schweer, 2025).

cluding, we summarize how our examination enhances a better understanding of the explanatory power of these simulations (Sect. 7).

2 On atomistic simulation

Atomistic simulations are computer simulations used to study the structure and dynamics of systems described at the atomic and molecular level and to examine the processes underlying larger-scale phenomena. One particularly relevant class of atomistic simulations are molecular dynamics (MD) simulations. In their conventional[2] form, MD simulations start from an approximative description of various types of interactions that figure between the atoms of a given system. By numerically solving Newton’s equation of motion for the atoms of the system, MD simulations produce trajectories of the respectively modeled system in time.

2.1 From micro to macro

One important goal of MD simulations is to use a description of micro-level motion and interactions to obtain information about the energetic, structural or kinetic properties of a modeled system that undergoes a certain chemical reaction. The underlying theoretical framework for this purpose is statistical mechanics. More concretely, the idea of statistical mechanics is to bridge between a micro- and macrostate description of a system. Whereas the former is given in terms of the positions and velocities of the particles in it, the latter describes thermodynamic properties of a system such as its temperature. Many microstates can correspond to one and the same macrostate. When using statistical mechanics, the idea is to employ equations by means of which one can bridge from a description of particle velocities and positions to a thermodynamic description. Enabling a computation of atomic trajectories, MD simulations provide the resources for drawing inferences about larger scale, e.g. thermodynamic, quantities.

A particularly important thermodynamic quantity is the free energy.[3] Free energy changes along the course of a chemical reaction inform us when a given system is stable or whether a certain reaction runs spontaneously; and free energy differences are used to address a plethora of chemical problems, ranging from molecular conformational preferences over binding constants to absorption coefficients, just to name a few.

Having at hand trajectorial data obtained by MD simulation runs and using statistical mechanical methods, free energy differences can be computed. As an illustration, consider the change of a protein in solution from an unfolded to a folded state, as shown in Fig. 1.

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[2] There are also coarse-grained approaches that do not start from individual atoms but simplified ‘coarser’ representations of molecular systems. We here focus on conventional molecular dynamics, and we will later come back to certain limits of approaches that neglect atomic detail.

[3] In the following, we will focus on the Gibbs free energy G that applies to systems with constant pressure and temperature. For systems at constant volume and temperature, there is the Helmholtz free energy A.

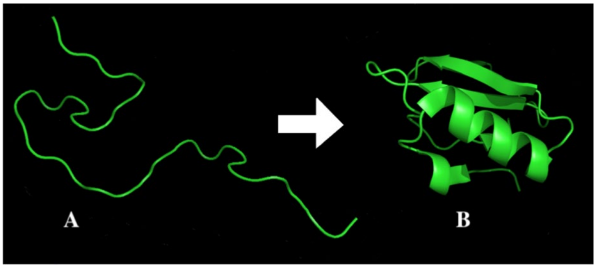

Fig. 1 Process of protein folding. A denotes the unfolded and B the folded state. Adapted from DrKjaergaard, public domain, via Wikimedia Commons

Using different snapshots of the trajectories, MD simulation data provide the resources to count how often the protein adopts a folded (B) or unfolded (A) conformation, respectively. Based on this, a probability $P(X)$ of finding the system in a certain state X can be assigned. The principles of statistical mechanics then make it possible to obtain free energy differences ΔG between two given states A and B of a system:[4]

$$\Delta G = G(B) - G(A) = -kT\ln\frac{P(B)}{P(A)} \tag{1}$$

Accordingly, by using statistical mechanics, MD simulations can be employed as bridging tools between a description of molecular configurations at the microscopic scale and a description of thermodynamic quantities.

2.2 Analysis of energetic contributors

When analyzing the occurrence of a certain molecular behavior or of a stable molecular arrangement, we are commonly interested in analyzing how the free energy of the system changes as such a behavior occurs or as such a structure forms– and the employment of statistical mechanical principles to derive free energy differences is what makes atomistic simulations such as MD simulations powerful tools for doing so.

Having obtained a free energy curve for a modeled system by means of simulation, we can ask for the energetic factors that determine the shape of the respective free energy curve. Concretely, a common question is as to how free energy curves are shaped by entropic and enthalpic contributions, respectively. (Gibbs) free energy changes ΔG relate to changes in enthalpy ΔH and changes in entropy ΔS as follows:

$$\Delta G = \Delta H - T\Delta S \tag{2}$$

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[4] In the case of proteins, it is important to note that one is dealing with a so-called rare event which requires appropriate sampling methods to make sure that the relevant parts of phase space are included (i.e., the relevant molecular conformations are ‘visited’) to accurately capture the transition path between the states.

Many biologically relevant chemical reactions are ‘entropy-driven’, meaning that their course is mainly determined by the increase of entropy. In molecular systems, an important interpretation of a system’s entropy is given in terms of conformational freedom: Roughly put, an increase in conformational entropy means that more ‘arrangements’ of the molecules in the system become possible. Consider the earlier-introduced case of proteins as an example: If a protein folds, the protein itself typically loses entropy because a folded state restricts the number of possible conformations.

Enthalpic changes, on the other hand, correspond to the effects that inter- and intramolecular interactions have on the energetics of the system. If, for example, a reaction leads to the formation of new non-covalent bonds, this will correspond to a release of heat and, thus, a negative enthalpy change. A common question when analyzing changes in the structure of a molecular system is how enthalpic changes are given rise to by certain features or parts of the system. In the example of protein folding, for instance, enthalpy changes could be due to the formation of hydrogen bonds or the presence of Van-der-Waals interactions. With the help of simulations, enthalpy changes can further be disassembled into contributions from different types of molecular interactions. This is, as we will show, an important feature when it comes to their explanatory power.

3 The difficult search for difference-making factors: an example

Having set the stage, let us make the scientific use of atomistic simulations more concrete by considering an illustrative example of how such simulations are practically employed by scientists to support explanatory reasoning.

As previously mentioned, many simulations that focus on changes in the molecular arrangement of a system involve calculating free energy changes and assessing which factors of the modeled system contribute to these changes. The study introduced in the following aligns with this approach and offers insight into how atomistic simulations can be used in the search for explanations.[5]

3.1 The surprising presence of ions near the surface of aerosol droplets

Studying atmospheric chemistry, scientists have observed a host of climatically relevant chemical reactions occurring on sea-salt particles, ocean surfaces and on aerosols in laboratory contexts (Petersen & Saykally, 2006, 333–334). In an effort to explain these reactions, scientists suspected that certain ions might be present at water/air interfaces, influencing the reactivity of atmospheric aerosols (ibid.). Confirming such speculations, a number of recent experimental and computational studies have revealed that certain large polarizable[6] anions are indeed preferably located

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[5] Importantly, given that our focus is to offer an examination of how simulations help with scientific explanations, we do not aim to scientifically evaluate as to what eventually explains the phenomenon in question, but to offer an analysis of how simulations were used in the search for this explanation.

[6] Polarizability describes the likeliness of an ion to acquire an electric dipole moment when exposed to an external electric field.

near the surface rather than in the inside of aerosol droplets (Jungwirth & Tobias, 2002; Tobias et al., 2013).

The finding that certain ions can be found near the surface of aerosol droplets was rather surprising. According to a traditional scientific assumption, no atomic ions are present at interface regions between the air and aqueous solutions such as aerosol droplets (Jungwirth & Tobias, 2002). Originally, this assumption was backed up by considerations from within a classical continuum picture according to which water is treated as an idealized continuum medium with a certain dielectric constant and ions as ‘hard spheres’ with a uniform surface charge (Tobias et al., 2013, 344). From within a continuum perspective, it was assumed that when approaching the interface region between water and air, the ‘hard sphere ions’ are repelled from the surface by their image charge on the air side of the air/water interface (Tobias et al., 2013, 344).

Considering that ions at the air/water interface potentially interact with climatically-relevant reactive gases such as ozone in the troposphere (Jungwirth & Tobias, 2002, 6363), various research groups undertook efforts to explain this phenomenon–and computer simulations played a relevant role in the search for an explanation.

3.2 Simulation study by Caleman et al.

One of the simulation studies devoted to explaining the surprising presence of certain ions, known as large halide ions, at air/water interfaces is that by Caleman et al. (2011).[7] Tackling the question “of why the ions behave like they do” (Caleman et al., 2011, 6838), the researchers performed simulations for various ions, tracking their trajectories from the droplet center to the surface region. Building upon ideas from previous studies, Caleman et al. proceeded in various steps, examining first the role of various ion properties and then the role of energetic factors on the surface preference of large halide ions.

Polarizability. Before Caleman et al.’s study, various groups suggested that polarizability might be the main determining factor for the surface preference of large halide ions (see Petersen & Saykally, 2006). Specifically, one idea suggested was that the potential at the air/water surface induces a dipole in polarizable ions, which attracts them to the surface. In their simulation study, Caleman et al. examined how ion dipoles change as a function of the position of the respectively investigated ion in the droplet. If the polarizability of large halide ions mainly determined their surface preference, one would expect that those ions which show surface preference are most polarizable. Interestingly, the researchers found that while the dipole of the ions indeed increases slightly as they approach the surface, this increase is most pronounced for the small halide ion fluoride, which does not exhibit surface preference (Caleman et al., 2011). Therefore, they concluded that polarizability alone is insufficient to distinguish ions that exhibit surface preference from others.

Polarizability in combination with size. In a subsequent hypothesis tested by Caleman et al., the researchers explored whether an ion needs to be both polarizable and large to exert surface preference. Despite fluoride being the most polarizable ion, it is comparably smaller than the ions that exhibit surface preference. Conversely,

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[7] For an earlier (brief) philosophical discussion of this study see Schweer and Elstner (2023).

all ions showing surface preference have in common that they are both polarizable and large. If nothing but the combination of size and polarizability mattered, surface preference should also occur for fictitious ions that have same polarizability and size as the halide ions but an artificially inverted charge sign.

To investigate this, Caleman et al. conducted simulations for 'hypothetical cations' whose size and polarizability is identical to those of the halide ions which exhibit surface preference, but with artificially inverted charges. If polarizability in combination with ion size were sufficient for explaining surface preference, these hypothetical cations– given that they have exactly the same properties as the large halide ions but only differ in the sign of their charge– should also exhibit surface preference (Caleman et al., 2011, 6840).

However, the hypothetical cations did not show surface preference anymore. Hence, Caleman et al. concluded that the combination of polarizability and ion size alone cannot sufficiently explain surface preference. Vice versa, they inferred that the sign of the charge matters, too (ibid.).

Decomposition of free energy profiles. Since attempts to explain the surface preference of halide ions by referring solely to one or more of their properties remained unsatisfactory, Caleman et al. proceeded with an analysis of the thermodynamics of the modeled system. As has been sketched earlier, reactions are commonly analyzed in terms of how they are driven by enthalpy or entropy, respectively; and free energy profiles obtained by means of atomistic simulations can be used for such an analysis. Recall that the free energy of a system informs us about the point at which a system is at chemical equilibrium. Having computed free energy profiles of various ions as they migrate to the surface, Caleman et al. decomposed the obtained free energy profiles into contributions stemming from enthalpy on the one hand and entropy on the other hand (see Eq. 2).

It was found that for all halide ions, the entropy decreases as they move towards the surface, meaning that if nothing else were to play a role, the entropic contributions would make it energetically preferable for halide ions to stay in the bulk of aerosol droplets rather than migrate to the surface. In the case of the large halide ions, however, favorable enthalpic changes were found to make a dominant contribution to the location of the energetic minimum near the surface. This means that unfavorable entropic changes only partly counterweight the favorable free enthalpy near the surface. In other words, contributions stemming from molecular interactions in the system rather than entropic effects make the surface region energetically favorable for these ions (Caleman et al., 2011, 6839).

Even though entropic factors alone would make it favorable for the halide ions to remain in the bulk, the relative impact of enthalpic contributions outweighs these factors in the case of large halide ions (Caleman et al., 2011, 6840). In the case of the small halide ion fluoride, in contrast, the enthalpic changes are less pronounced so that they are overcompensated for by entropy reduction (ibid.).

Decomposition of enthalpic contributions. In a subsequent step, Caleman et al. proceeded with a more detailed analysis of how enthalpic changes affect ion movement in droplets. Note that in the examined case, changes in enthalpy can be interpreted as being composed of two kinds of molecular interactions, namely those between water molecules and the ion on the one hand, and those between water molecules and other water molecules on the other hand. Even though Caleman et al. suspected that effects on the local arrangement of water molecules are not the key factor for the surface preference of large halide ions[8], it could still be the case that their presence more subtly affects how the different kinds of molecules in the systems interact. Caleman et al. thus further decomposed the enthalpic profiles of all ions into the contributions stemming from the water-water interactions and water-ion interactions, respectively. This was facilitated by interpreting enthalpy changes $\varDelta H$ along the reaction coordinate r describing the distance between droplet center and surface as the sum of time-averaged[9] water-water and water-ion interaction potentials V (Caleman et al., 2011, 6839):

$$\Delta H\left(r\right)=\left\langle \Delta V_{water-water}\left(r\right)\right\rangle +\left\langle \Delta V_{ion-water}\left(r\right)\right\rangle \tag{3}$$

The obtained profiles show that water-water interaction energies decrease as the ions approach the surface. At the same time, water-ion interaction energies increase. As Caleman et al. (2011, 6840) argued, the obtained profiles suggest that the partial desolvation of large halide ions enables more favorable water-water interactions. Only when arriving at the proximity of the droplet surface, losses in ion-water interactions start to become energetically more dominant over gains in favorable water-water interactions, preventing the ions from ‘leaving’ the droplet entirely (Caleman et al., 2011, 6839). Conversely, their results suggest that alkali cations are energetically favored in the bulk because their desolvation hardly affects water-water interactions (ibid.).

In other words, according to Caleman et al., large halide ions migrate towards the surface of droplets because a particular factor becomes more pronounced than for other ions, namely how their presence negatively affects how water molecules exert interactions with other water molecules. As the researchers argue, this is different in the case of other ions whose presence hardly affects interactions between water molecules and makes them prone to stay in the bulk. Hence, large halide ions differ from other ions in that enthalpic effects are specifically pronounced for these ions, more precisely the effects by water-water interactions. A disturbance of the latter is what, according to the simulation study by Caleman et al., eventually makes a difference for them be energetically preferred near the surface.

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[8] Testing this, Caleman et al. examined if the presence of large halide ions in bulk water ‘disturbs’ the preferred local structure of surrounding water molecules. However, having employed a certain method to quantitatively describe how the local structure of fluids is affected by the presence of a given particle, Caleman et al. found in their simulation study that even though the orientation of water molecules to a respective ion seems to be somewhat sensitive to whether the ion is near the surface or in the bulk of a given droplet, the effects on the local structure are similar for all ions– i.e. they are not specific for those ions that show surface preference. Hence, they inferred that changes in the local structure of water molecules do not seem to be the main factor for why large halide ions show surface preference.

[9] The square brackets denote the averages over the MD trajectories.

4 Explanation and difference-making

Before analyzing the explanatory contributions of atomistic simulations, let us characterize the explanation sought in contexts such as the ion example. The case of ions in aerosols concerns the stability or expectedness of a particular molecular arrangement. When explaining why large halide ions differ from other ions in their tendency to move to the surface of small aerosol droplets, we seem to be interested in depicting a number of factors upon which the expected surface preference of these ions depends (cf. Schweer & Elstner, 2023). And since we are interested in the expectedness of a stable molecular arrangement, it seems natural to ask specifically for those dependence relations that hold under a range of variations. In this regard, the explanatory setting in the ion example arguably resembles many other problems in molecular science and beyond.

Many contemporary accounts of scientific explanation agree that scientific explanations are concerned with dependence relations. More specifically, it has been suggested that obtaining scientific explanations involves depicting a number of factors that make a difference for the explanandum (Woodward, 2003; Woodward & Hitchcock, 2003; Ylikoski & Kuorikoski, 2010; Bokulich, 2011; Rice, 2021).

According to what can be called the counterfactual account of explanation, explanations are exhibitions of systematic patterns of counterfactual dependence (Woodward, 2003, 191). As Woodward puts it, “[an] explanation must enable us to see what sort of difference it would have made for the explanandum if the factors cited in the explanans had been different in various possible ways” (ibid., 11). In his famous wording, explanations are answers to what-if-things-had-been-different questions (Woodward, 2003, 11). To Woodward, the dependence relations that figure in explanations can be addressed as relations between variables. When asking for an explanation, we are interested in how changing the value of various explanans-variables would change the explanandum.

In what follows, we suggest that the explanation sought by scientists in contexts such as that of the ions can best be captured and rationalized from within a counterfactual, or difference-making, account of explanation. That is, when searching for an explanation, we are looking for a number of factors that make a difference for the explanandum.

5 Explaining with (computational) models

The aim of this paper is to enhance a philosophical understanding of the explanatory power of atomistic simulations. Therefore, before dealing with the concrete contributions that such simulations can make to explanations, it is worthwhile to briefly address the preliminary question of how it is *possible* for them to support the assessment of dependence relations in real-world targets in the first place.

Rather than directly intervening on or interacting with the target system, drawing inferences from computer simulations requires working with a computationally-implemented model of the target system. In the case of halide ions, we need a model containing information about the molecules of the system (i.e., the respective ion and surrounding water molecules) and their interactions, as well as a starting geometry and appropriate boundary conditions.

A comprehensive account of how scientific models can contribute to the assessment of difference-making factors is offered by Bokulich (2011, 2014, 2017). For the context of our paper, we suggest that Bokulich's account offers a fruitful starting point for understanding how explanations given with the help of computer simulations draw on scientific models.

Bokulich formulates three key features of 'model explanations'. The first feature of model explanations is that the explanans makes reference to a scientific model (Bokulich, 2011, 39). As Bokulich puts it:

> "Model-based explanations (or model explanations, for short) are explanations in which the explanans appeal to certain properties or behaviors observed in an idealized model or computer simulation as part of an explanation for why the (typically real-world) explanandum phenomenon exhibits the features that it does" (Bokulich, 2017, 104).

The second feature of model explanations is that the model should 'reproduce' the relevant properties of the target system and offer information about how the target system would have been different if certain aspects of the model had been different (Bokulich, 2011, 39). Bokulich draws on Woodward's counterfactual framework[10] and suggests that the counterfactual structure of the model should in relevant ways be isomorphic to the counterfactual structure of the target system (Bokulich, 2011, 39).

Let us briefly clarify as to what this means in the case of complex molecular models. For problems such as the surface preference of halide ions, the computational model that underlies a simulation takes the form of a so-called 'force field', together with a starting configuration of the atoms in the system, and appropriate boundary conditions. Force fields are parametrized potential energy functions that provide an estimate mathematical description of the relevant types of interactions between the atoms of a systems. Each type of interaction that is considered relevant for a given problem (think, for example, of Van-der-Waals interactions or bond stretching energies) should be reflected in a term of a given force field.

That is, in order for the counterfactual structure of the computational model to be 'isomorphic' to the target system in relevant regards, the parameterized energy terms should adequately reflect the relevant types of interactions between the atoms in the

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[10] At the same time, Bokulich departs from Woodward by dropping the interventionist underpinnings of his account. In Woodward's causal-interventionist framework, the antecedents of counterfactuals are made true by so-called interventions, heuristically to be understood as manipulations that could potentially be performed in an idealized experimental setting (Woodward, 1997, 29). Interventionism restricts Woodward' account to causal explanations. Bokulich suggests letting go of interventionism and proposes that the counterfactual dependence relations which figure in model explanations can have different origins, allowing for a distinction between different types of model-based explanation– causal explanation being just one of them (Bokulich, 2011, 40). While exceeding the scope of this paper, it would be an interesting topic for future work to scrutinize in more detail how computer simulations support such different types of counterfactual explanations.

target; such that in a simulation context, the model can be worked with as a ‘stand in’ for the target.[11]

This also brings us to Bokulich’s third feature of model explanations, namely that they require a justificatory step in which the domain of applicability of the model, as well as its representational scope are assessed (ibid.). In other words, there needs to be a justification that the model indeed reflects the relevant features of the target system to be explained (Bokulich, 2008, 226). According to Bokulich, the required justification is typically based either on theory that ‘backs up’ the model’s domain of applicability, or on empirical considerations, or a combination of both (Bokulich, 2011, 39).

In the simulation of molecular systems– such as ions in aerosols– the required justification indeed typically involves both theoretical and empirical reasoning. The computational modeling of molecular systems looks back to a decades-long history of development of numerical methods, as well as the careful calibration and stepwise improvement of computational models in light of theoretical predictions and experimental data. The parametrization of force fields, for example, can be based on calculations from quantum mechanical theory, but it can also be a matter of fitting of the model with experimentally-accessible properties, often in a ‘hand’-tuned and incremental way. Certainly, activities such as the choice of the functional form of a molecular model or its parametrization can potentially introduce errors and hence cause distortions or unintended computational artefacts (see also Ylikoski, 2014, 329). The credibility of the conceptual models upon which computer simulations requires careful evaluation (see e.g. Gelfert, 2019) and the potential of computer simulations to contribute to explanations owes much to their respective conceptual models (Krohs, 2008).

6 Disentangling the explanatory power of simulations

Starting from a counterfactual account of explanation and zooming in on the case of atomistic simulations, the remainder of the paper explores how these simulations can help with the search for explanations. It has been argued that atomistic simulations, such as that used by Caleman et al., can be powerful tools for the assessment of difference-makers (Schweer & Elstner, 2023). While the perspective offered in the following aligns with this idea, better understanding the explanatory power of atomistic simulations and their role in the search for explanations necessitates a finer-grained account of the contributions that they make to explanations.

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[11] Yet is is important to note that in the case of force-field models (other than may be the case in certain highly idealized models), those elements of the model which are supposed to capture the counterfactual structure of the system are not necessarily identical to the candidate difference-making factors to be cited in explanations given with the help of such models. Even if the structure of the target is ‘preserved’ in relevant regards by a computational model by means of appropriate parametrized energy terms, the relevant difference-making factors will need to be extracted from such models by drawing systematic inferences with simulations. In a sense, this ‘extraction’ is precisely what our paper aims to give a more detailed picture of.

In the case of large halide ions, atomistic simulations could help with the search for an explanation both by ruling out potential candidate explanations– such as one that draws on the size and polarizability of these ions alone– and by enabling a fine-grained analysis of the variables that actually do make a difference for the explanandum. By discussing the simulation study by Caleman et al. as well as further examples, we will in the following outline three contributions that atomistic simulations can make to counterfactual explanations: they can (i) help access variables at the relevant levels of description, they can (ii) help track the effects of changes in such variables in a highly controlled and fine-tuned way, and they (iii) allow for an assessment of the relative importance of various difference-making factors.

6.1 Selecting and accessing relevant variables

In the counterfactual account, obtaining an explanation of a given phenomenon starts with depicting a number of variables that potentially matter for the explanandum. The selection of appropriate variables can be a challenging task and is a scientific rather than a philosophical problem (Woodward, 2016).

Arguably, the challenge of identifying explanatorily relevant variables is especially acute when dealing with complex systems consisting of a multitude of components that exert intricate interactions, often spanning multiple levels of description. In such situations, numerous variables could potentially impact the explanandum and it may not be immediately obvious at which level of description they are located.

One possible problem in explanatory practice is that the chosen model for studying a system may be too ‘coarse’ to account for explanatorily relevant variables. This was the case in the ion example before simulations had entered the stage. Remember that the properties of solution surfaces were traditionally studied using continuum models that treat the solvent as a polarizable continuum rather than a set of individual molecules that exert particular kinds of interactions. Whereas such models come with the advantage of being applicable to large molecular systems that would otherwise be difficult to examine, they neglect many molecular details, such as the asymmetric solvation of positive and negative charges in water (Petersen & Saykally, 2006, 344). Although relying on theoretical continuum models can certainly be useful if the aim is to investigate electrostatic interactions over larger molecular distances, these models reach their limits in situations in which molecular structure or the effects of short-range interactions matter (ibid.).

As concerns large halide ions, the simulation study by Caleman et al. demonstrated that the charge sign of large halide ions matters for whether these ions move to the surface, and that a (computational) atomistic model accounting for the asymmetrical distribution of charges in water molecules is required to explain their behavior. To the extent to which continuum models fail to incorporate the asymmetric charges in water, they principally seem unsuited for providing an explanation of the observed surface preference of large halides, as they do not offer sufficient access to molecular detail (Caleman et al., 2011, 6840). Rather than using a variable that captures the solvent charge distribution as whole, it turned out that the distribution of charges in the molecules of the solvent matters; and hence, that finer-grained variables are needed to explain the surface preference of certain ions in these solvents. [12]

Atomistic simulations allow for this level of detail, and part of their explanatory power stems for their capacity to grant access to details that are beyond the reach of coarser continuum models.

However, this is only one part of the story of their significance in accessing explanatorily relevant variables. While access to small-scale details can be decisive in explanatory contexts, explanations that cite nothing but features on the level of individual atoms or molecules and their interactions are often unsatisfactory. Consider again the case of halide ions. Even if *some* molecular-level details matter for why large halide ions are preferably located near the surface of droplets, an as detailed as possible story about the exact chain of molecular interactions leading to an ion's movement to the surface of aerosol droplets would be misguided because it would contain an enormous amount of irrelevant details, and because it would fail to give an idea of why the behavior of large halide ions was to be expected. Just as many other explanatory problems in the sciences, the problem of halide ions in aerosols is a problem that concerns the occurrence of a *stable* (molecular) arrangement: it describes a tendency of such ions, when being present in small droplets, to reliably migrate to the surface of these droplets. An explanation that is solely given in the language of individual molecules and their movement could not render intelligible why the behavior of these ions is expectable, and why it occurs invariantly against a range of changes in the micro-setup of the system.

In some sense, explaining halide surface preference is interesting in the first place because the phenomenon remains stable under a range of possible variations in the microdetails of the system and because it occurs frequently enough to potentially matter for chemical reactions in atmospheric aerosols.

In recent philosophical discussions, it is recognized that explanatorily relevant variables are often located at *intermediary* levels of description between small and large. On such levels, variables can be found that code for the stability, robustness or expectedness of larger-scale explananda (Green & Batterman, 2016; Batterman & Green, 2020; Batterman, 2021).

Atomistic simulations can help with accessing variables at such intermediary levels of description. To fully understand their explanatory power, it is important to see that besides offering access to small-scale details, atomistic simulations make it possible to access and select variables that code for the stability, robustness or expectedness of the explanandum. In particular, atomistic simulations allow to draw systematic *connections* between small-scale details and intermediary variables in the aforementioned sense.

Let us elaborate. Remember that the surface preference of large halides was explained by showing how the presence of these ions near the surface subtly affects a particular *type* of interactions present in the droplet, namely water-water interactions,

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[12] This is, however, certainly not to say that continuum models cannot be explanatory. Whether or not these models are suited for providing an explanation depends on the level at which the relevant variables are located. Determining this level in a specific case is, to some extent, an empirical rather than a philosophical task.

which– as Caleman et al. pointed out– turned out to be mainly responsible for why large halides would move to the surface of droplets.

Although water-water interactions occur at the molecular level, understanding their impact on the surface preference of large halides necessitated an analysis of how the presence of these interactions leads to the expected ions' positioning near the surface. The variables which code for the expectedness of molecular arrangements are thermodynamic ones, perhaps most importantly the free energy– as it provides information about the point at which a system is in chemical equilibrium. Free energy differences can be obtained from micro-state descriptions of a system by means of statistical-mechanical methods. By employing such methods, atomistic simulations can function as bridges between 'small-scale' trajectory information and thermodynamic variables.

In their simulation study, Caleman et al. derived free energy profiles and then dissected them into their corresponding enthalpic and entropic components. This approach allowed them to engage in a detailed evaluation of how various energetic factors influence the phenomenon under investigation. After identifying that enthalpic contributions predominantly influence the energetic minimum near the droplet surface, Caleman et al. further analyzed these contributions. Concretely, they separated the enthalpic contributions into the average contributions arising from water-water interactions and water-ion interactions. This led to the result that the energetic minimum near the surface primarily stems from water-water interactions.

Even though the obtained explanation partly relied on including detail about the properties of molecules, their approach required more than a purely molecular-level perspective: What was at stake is how different types of molecular interactions contribute to a chemical reaction leading to a stable larger-scale molecular arrangement. Instead of focusing on the detailed path of molecular interactions that leads to ion movement towards the surface, Caleman et al.'s simulation allowed them to evaluate how specific *types* of these interactions contribute to forming a stable molecular arrangement. The thermodynamic variable of free energy is what codes for the stability of this arrangement– and hence, for the expectedness of halide surface preference. Being based on the application of statistical mechanical principles, their simulation enabled Caleman et al. to decompose the free energy and select several intermediary-level variables whose impact on the explanandum could then be analyzed in detail (see Fig. 2). In other words, by step-wise decomposing the free energy and analyzing how different types of molecular interactions contribute to an arrangement where large halide ions are near the droplet surface, atomistic simulations were tools for selecting a set of aggregated or reduced variables, and for analyzing in detail their significance to the explanandum.

On the one hand, some molecular details *did* play an important role in the explanatory story provided by Caleman et al.– such as the asymmetric distribution of charge in water. On the other hand, explaining why the surface preference of large halides was to be expected - or why these ions would reliably go to the surface– required referencing larger-scale features of the modeled system. To fully grasp the explanatory significance of water-water interactions, it was important to understand how these interactions influence the energetic properties of the modeled system at higher scales. In other words, accessing and selecting variables that code for the expectedness– or

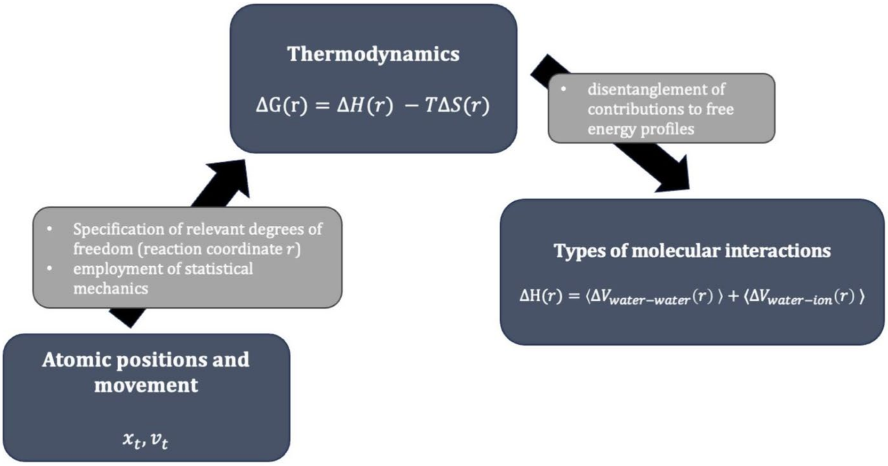

Fig. 2 Atomistic molecular dynamics simulations as tools for accessing variables on different levels of description

stability– of the explanandum was necessary. For these tasks, the relevant resources were provided by atomistic simulations.

6.2 Tracking variable changes

Once appropriate variables are depicted and accessed, another important step in obtaining explanations following the counterfactual account is to examine how the explanandum is– or would be– sensitive to changes in the value of these variables.

In many real-world scientific contexts, potentially explanatorily-relevant manipulations are difficult or even impossible to conduct, and it can thus be difficult to say what their effect on the explanandum would be. In other words, since the behavior of many scientifically-interesting systems depends on the intricate interplay and interdependency of a large number of components, tracking the effect of (hypothetical) changes on particular variables is often hardly feasible– especially when dealing with scales that are difficult to access using traditional experimental approaches.

It is recognized in the philosophical literature that computer simulations can be powerful tools for exploring how the behavior of the modeled system changes under varying conditions. According to Ylikoski, computer simulations can contribute to explanations by increasing the number of possible what-if inferences (Ylikoski, 2014). Discussing the case of agent-based simulations in the social sciences, Ylikoski (2014, 331) states that with such simulations, "[…] we can systematically study how the changes in the assumptions change the outcomes." Similarly, dealing with dynamic mechanistic explanations in cognitive science, Bechtel and Abrahamsen (2010) name the expansion of parameter value spaces as one important regard in which the explanatory power of simulations can be rendered intelligible. As they put it: "A model provides a means of exploring a much larger space of parameter values than would be feasible experimentally, and thereby of projecting how the actual mechanism would behave under a variety of conditions" (Bechtel & Abrahamsen, 2010, 325).

While we agree with these statements, we propose that the manner in which computer simulations facilitate variations in input variables deserves further attention. Beyond allowing scientists to explore a broader range of possible parameter values, computer simulations provide a particularly high degree of control over changes in such values. In this way, they enable scientists to perform manipulations whose effects would otherwise be difficult to track. This matters for explanation because according to the counterfactual account, the interest lies not only in observing how the modeled system would behave under various input conditions, but also in systematically tracking patterns of dependence between input variations and output. When it comes to the explanatory power of simulations, it is important to see how they allow researchers to track in a controlled way how changes in the factors mentioned in the explanans correspond to changes in the explanandum.

Considering studies on nanoparticles, computational physicist Amanda Barnard puts it as follows:

> "Unlike our experimental colleagues, we have the luxury of being able to systematically test the relationship between our results and a particular parameter (such as temperature, pressure, charge, etc) *independently*, and we can see precisely how each parameter affects a system, while keeping all others constant. In a conventional experiment, if one physical parameter is changed, there are consequences and other experimental parameters change in response to it." (Barnard, 2010, 2, emphasis in original).

As Barnard's words suggest, it can be notoriously difficult in experimental practice to associate alterations in the input with changes in the output. One aspect of what makes computer simulations valuable in real-world explanatory contexts is their role as 'tracking tools' for changes in the value of the explanans variables.

To give another example, consider research on the biological function of proteins. Here, typical questions are, for example, why a certain enzyme functions in a specific way or how a given transport protein facilitates its transport function. It is widely assumed that the function of proteins depends significantly on their structure– specifically, the three-dimensional arrangement of amino acids from which they are assembled. In protein structures, various characteristic regions may be present. When investigating a protein's function, a common question is how the presence of particular regions impacts the overall protein function to be explained. Experimentally tracking how changes in these specific regions affect the protein's function can be difficult. However, computer simulations allow us to isolate and even remove specific regions of the protein, enabling us to evaluate how the model would respond to these manipulations.[13]

This is similar in the case of large halide ions in aerosol droplets. Recall that the ions that are found near the surface of droplets share two common features: high

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[13] As a concrete example, consider the case of aquaporins mentioned in (Sect. 6.3, as discussed e.g. in Yarnell (2004).

polarizability and large size. To find out whether the specific combination of these two properties is what gives rise to their peculiar tendency to migrate to the droplet surface, Caleman et al. ran simulations for ‘hypothetical cations’ whose size and polarizability were identical to those of the investigated large halide ions but whose charge was artificially inverted. The researchers reasoned that if nothing but the combination of these two properties were responsible for the surface preference of large halide ions, the explanandum should occur invariantly against changes in *other* properties of the ions.[14] Given that the artificial cations did, however, not show surface preference, Caleman et al. inferred that the combination of size and polarizability alone cannot explain the surface preference of large halides and that, vice versa, the sign of the charge matters, too.

This explanatory maneuver is remarkable: Not only did computer simulations easily make it possible to set the charge sign of the ions to a counterfactual value[15], but they ensured that other features of the modeled system could be kept constant. In this way, the dependence of the explanandum on alterations in certain candidate explanans variables could be examined in a controlled and fine-tuned way.

6.3 Evaluating quantitative contributions

In many scientifically interesting explanatory situations, hypothetical changes in the values of more than just one variable are considered relevant to the explanandum. When faced with such situations, we seek to understand the extent to which each of the selected variables is responsible for a given outcome. Just as depicting variables and tracking changes in their values can be challenging, assessing the relative significance of each selected variable is often no easy task. Even when there is agreement on the relevant variables for a given explanatory problem, disagreements may persist regarding the relative importance of each variable to the explanandum. Given that idea of ‘relative importance’ may be somewhat vague, Woodward proposes to conceptualize disagreements about the relative importance of various factors as (empirical) disagreements about the relative sensitivity of various explanatory relationships (Woodward, 2006, 44). Relatively insensitive relationships are relationships that would continue to hold under a range of potential changes in the actual circumstances (Woodward, 2006, 2). If the explanandum is relatively insensitive to

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[14] That is, if only polarizability and size mattered, changing the sign of the charge of the ions while keeping everything else constant should, for example, not have an effect on the occurrence of surface preference.

[15] There are many other interesting counterfactual interventions that can be performed by means of (atomistic) simulation. One can use atomistic simulations to artificially alter the strength of molecular bonds or the magnitude of electrostatic interactions, among others things. Another interesting example from scientific practice where computer simulations make it possible to perform counterfactual interventions is computational alchemy. With the help of alchemical simulations, protein wild types can, for instance, be ‘morphed’ into mutants, allowing researchers to examine how hydrogen bond networks change. Additionally, these simulations can be used to artificially transform potential drug molecules into other compounds. Through such transformations, scientists can study the effects of these changes on bonding strengths and stability. Besides performing interventions that would be difficult to do experimentally, computer simulations can be used to study scenarios that violate or by design manipulate the laws of nature (cf. Humphreys, 2004, 116).

a particular factor, various changes could occur under which this factor still brings about the explanandum.

Let us revisit the case of research on structure-function relationships in proteins. As we have previously discussed, the biological function of proteins is believed to depend, to a signficant extent, on their structure. Even if there is agreement on which structural regions within a protein might potentially impact its overall function, there can still be disagreement on the *extent* to which each of these regions is responsible for the protein function. An illustrative example of this is the case of aquaporins[16]. These channel proteins are located in cell membranes, where they play a crucial role in regulating the selective flow of molecules between the inside and outside of cells. A number of studies have examined as to why aquaporins are highly permeable for water molecules but not for protons (e.g. Burykin & Warshel, 2003, 2004; de Groot et al., 2003; de Groot & Grubmüller, 2005). Whereas researchers largely agreed on which potential candidate structural regions of the channel protein could potentially prevent protons from travelling through the membrane channel, disagreement persisted about the relative weight of these structural regions (see Yarnell, 2004). By allowing researchers to trace free energy changes along the channel and by comparing the magnitude of the energetic barriers erected by various structural regions, computer simulations could help scientists tackle this problem (cf. Schweer & Elstner, 2023). Rather than just showing that various energetic barriers were present, simulations enabled scientists to reason how changing the energetic contributions of a certain region would affect the explanandum.

Similarly, in the case of halide ions in aerosols, MD simulations could enable a more detailed account of the structural peculiarities at the interface region, and of the complex interplay of various energetic factors that give rise to the observed ion behavior. Even before simulations had entered the stage, it was of course to be expected that the behavior of ions– just as in the case of other complex systems– is determined not just by one or two major factors but by the fine-tuned interplay of various contributors: as in many other cases, explanatory interests therefore concern the precise *extent* to which each factor matters. As Caleman et al. (2011, 6838) state, progress in force fields that underlie molecular dynamics simulations “finally allows establishment of the surface preference for all halide and alkali ions quantitatively.”

A major part of what made molecular dynamics simulations explanatorily valuable was that they could enable a quantitative comparison of how different types of interaction contribute and underlying molecular interactions for surface preference. Large halide ions prefer to be near the surface of droplets because their properties are such that the gain in water-water interactions *quantitatively* dominates over the energetic effects of a loss in water-ion interactions.

While it is clear *that* the free energy minimum of the ions’ path towards the surface is changed by the effect of various energetic contributions, insight into how sensitive the explanandum is to these contributions is to be acquired by means of quantitative comparison. Such a detailed comparison is hardly possible by means other than simulation and, thus, underscores their explanatory power. Besides granting access to explanatory-relevant variables, and besides making it feasible to track how changing

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[16] For a detailed discussion of the example, see Schweer and Elstner (2023).

them changes the explanandum, atomistic simulations could contribute to explanation by helping analyze the size of the contributions of different types of molecular interactions to the free energy profiles.

To sum up, atomistic simulations can provide the resources for a quantitative comparison of the effect of various changes to the respectively investigated model. This matters for explanation because in the case of complex systems, it is often expected that the delicate interplay of various factors rather than a single factor gives rise to the phenomenon or behavior to be explained. Hence, a third way in which atomistic simulations contribute to scientific explanations is by helping scientists to more precisely estimate and compare the degree to which various factors affect the occurrence of the explanandum.

7 Conclusion

In this paper, we have examined the explanatory power of atomistic simulations by shedding light on various ways in which they can support explanatory reasoning in scientific practice. Drawing on a counterfactual account of scientific explanation in the tradition of Woodward (2003), and as it has been further developed for explanations with the help of models by Bokulich (2011), we have outlined three ways in which atomistic simulations contribute to scientific explanations, namely by (1) offering epistemic access to variables at relevant levels of description; by (2) enabling scientists to effectively track how changes in the values of various variables affect the explanandum; and by (3) offering a framework for quantitative analysis.

Even though we have mainly focused on atomistic simulations, much of what we have shown applies to other cases where computer simulations are used to study complex systems: Computer simulations can be tools for accessing variables that code for the stability or robustness of the behavior of systems, they can allow us to track how the explanandum is sensitive to a range of variations in the investigated model– often in ways that would otherwise remain unfeasible; and they can help determine in a fine-grained manner the relative importance of various variables. In this sense, computer simulations can play an important role for both ruling out potential candidate explanations as well as analyzing in detail the factors that make a difference for the explanandum.

In offering a practice-oriented perspective on how computer simulations are concretely used by scientists in the context of scientific explanation, our analysis has aimed to advance a finer-grained understanding of their importance in explanatory reasoning and promote greater philosophical appreciation of their explanatory power.

Not least, our approach also inspires a critical and nuanced view on the issue of epistemic opacity and the complexity of simulations. At least in the discussed context, the use of simulations turned out to be conducive– rather than a hindrance– to obtaining explanations or understanding complex phenomena. For example, while previous contributions have suggested that the complexity of computational models can impede analytic understanding by prohibiting a detailed understanding of how particular components of computational models contribute to the simulation result (Winsberg and Lenhard, 2010), our analysis points in quite a different direction: As we have argued, atomistic simulations can help access and isolate specific features of complex modeled systems and, relatedly, track in detail the effect of these features on the explanandum. This, as we have suggested, is part of what makes them powerful tools in contexts of scientific explanation.

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