

Frank Pasemann

## Event-Based Simulations. Is there a Need for New Physical Theories?

2017

<https://doi.org/10.25969/mediarep/2240>

Veröffentlichungsversion / published version

Sammelbandbeitrag / collection article

### Empfohlene Zitierung / Suggested Citation:

Pasemann, Frank: Event-Based Simulations. Is there a Need for New Physical Theories?. In: Anne Dippel, Martin Warnke (Hg.): *Interferences and Events. On Epistemic Shifts in Physics through Computer Simulations*. Lüneburg: meson press 2017, S. 75–92. DOI: <https://doi.org/10.25969/mediarep/2240>.

### Nutzungsbedingungen:

Dieser Text wird unter einer Creative Commons - Namensnennung - Weitergabe unter gleichen Bedingungen 4.0 Lizenz zur Verfügung gestellt. Nähere Auskünfte zu dieser Lizenz finden Sie hier:

<https://creativecommons.org/licenses/by-sa/4.0>

### Terms of use:

This document is made available under a creative commons - Attribution - Share Alike 4.0 License. For more information see:

<https://creativecommons.org/licenses/by-sa/4.0>

# Event-Based Simulations: Is there a Need for New Physical Theories?

Frank Pasemann

Following the discussions concerning the role of computer simulations in the development of natural sciences, and especially for the physical sciences, at some point I was confronted with the statement that, as a result of these simulations, “there is a need for new theories in physics.” For me as a theoretical physicist this was a quite provoking appraisal, which showed up, almost naturally, in the debate on the interpretation of quantum mechanical predications. Based on the papers on event-based simulations (see Michielsen and De Raedt 2014) it was argued that for explaining quantum phenomena, like, for instance, the interference patterns in electron-scattering experiments, no quantum theoretical assumptions have to be made. The specific type of the described computer simulations will reproduce results of quantum theory showing that there exist macroscopic, mechanical models of classical physics that mimic the underlying physical phenomena. This is in contrast with statements like, for instance, that of Richard Feynman saying that the double-slit experiment “is impossible, *absolutely* impossible, to explain in any classical way, and which has in it the heart of quantum mechanics” (see Feynman 1989).

As a first reaction to this situation I had to reformulate the statement in terms of the question, which gave the title of my talk. Then I had to reassure myself about what I am willing to understand by a theory, by a physical theory, and, on the other hand, what kind of ingredients are necessary for setting up significant computer simulations of physical systems.

So, what I would like to present here are some general remarks about what I think are basic properties of physical theories; to make sure that we are talking about the same thing when demanding something new. And because the topic of this workshop is the context of computer simulations, and especially the simulation of physical experiments, I would like to add some general comments on simulations used for research in natural sciences. So I will not go into the specific simulations, which were presented in the first talk, and it is only at the end of my talk that I will try to imbed their event-based simulations into the scheme I will introduce.

Let me start with a description of a physical theory. I will do that in terms of a few simple but strong statements. This view is influenced mainly by the situation at the end of what may be called “the Old Science,” characterized by the state of theoretical physics around the 1970s when it was still able to predict, besides the outcome of quantum mechanical experiments, also the outcome of those in the high-energy domain. But I think with respect to quantum phenomena this view of an established theory is still valid.

Although this is trivial, if one wants to set up a new physical theory, or a new type of a theory, it should be clear in which domain of phenomena it should be placed. So the first statement will be: **Every physical theory describes a well-defined area of physical phenomena.**

There are of course different ways to identify such domains. For example, one may refer to the length scale, which is quite natural, and talk about subatomic or atomic phenomena, about the domain of everyday physics that is described by classical physics, or about phenomena on the cosmic scale.

One can also refer to the forces that dominate the physical processes in a certain domain, and one may distinguish between the physics of strong forces, of weak forces, of electromagnetic forces, and of gravitational forces. The scattering phenomena under consideration here are primarily related to the single particle phenomena in the atomic domain, that is, we are in the arena of quantum (field) theory.

At this point one should perhaps mention the observation that there is a large gap in existing theories concerning the number of particles involved in processes. We have very nice theories about single particles or single objects, and we can often handle systems with two objects quite nicely. For the other extreme (i.e., systems composed of very many particles) stochastic theories are very effective. Between these two extremes there is the interesting physics of “medium-sized” systems, which is difficult to describe

in detail. Even when dealing with just three objects the classical theories get into difficulties. We know that from the 1898 Poincaré paper (Gray 1997, 27–39), where he identified in the classical three-body problem a behavior that today is identified as chaos. I mention this because I believe that what computer simulations can do in the future, and are partially already doing now, is filling up this knowledge gap where reasonable theories do not (yet) exist. I will come to this again later.

In addition there are many special physical theories, like solid-state physics, quantum optics, hadron physics, plasma physics, and others. The point is, that for all of these theories there are of course still open scientific questions, and there are always limits of applicability. But despite this situation, there is still no cry for new theories. What is often done successfully is to take a well-established theory and develop an extension into a larger domain of applicability.

My next statement refers to the structure of a physical theory (Ludwig 2012): **A (well-established) physical theory is a kind of functor from the set of physical phenomena to a set of mathematical objects.**

Thus a theory corresponds to an unambiguous assignment of physical phenomena to certain mathematical objects, that is, it is a kind of mapping that preserves the relations between the corresponding objects. This functor is verified by physical experiments. Preferably it will be invertible, because one should be able to make verifiable (falsifiable) predictions from derived mathematical theorems.

Phenomena	Represented by
A stone	Point in phase space (six-dimensional Euclidean space for the space and momentum coordinates)
Moves on trajectory	Solution of a set of differential equations
The stone as a system	A vector field on phase space
Initial conditions	Initial position and momentum (or velocity)
Parameters	Mass, etc.
Boundary conditions	Restriction for applicable forces, friction, etc.

[Fig. 1] Phenomena and their Representations

To make clearer what this means let us look at a well-known example in classical mechanics. To describe what happens if we throw a stone in a certain direction what a physicist will do first is to abstract from the stone and reduce it to a description of a mass point (see Fig. 1). This mass point is then represented as (mapped to) a mathematical point (a zero-dimensional

object) in the so-called state space or phase space of the system. The observable trajectory of that stone will then be described as a solution of a set of corresponding differential equations.

The stone as a physical system (i.e., the stone together with all its possible trajectories resulting from all possible initial start points and initial velocities), is then described by a so-called vector field on state space. This will be a complete mathematical representation of all the motions this stone can realize. To obtain a specific trajectory, that is, a specific solution, one has to specify, besides the initial conditions, the relevant parameters of the system; for instance, the mass in this case. One also has to take relevant boundary conditions into account; for example, that the force one can apply is limited. Then one also has to specify those forces acting in addition to gravity on the system, such as friction. This is a satisfying classical characterization of a system like a stone. It is a heavily idealized mathematical description concerning measurable, physical quantities. It is not an attempt to describe the underlying real-world process that led to these measurements: this was stated by very many scientists, for instance by Feynman and Bohr.

If one accepts this definition of a physical theory then, of course, one must assert that quantum mechanics is a very well-established theory, and in fact it is—particularly as quantum field theory—the best verified physical theory we have so far. Why then should one ask for a new theory for this domain of atomic scale phenomena? There are at least two different arguments coming to my mind. One argument is based on the observation that quantum mechanics is a linear theory (linear in its state variables). Furthermore, following a more formal procedure to derive quantum mechanics from classical mechanics (Sniatycki 1980) one realizes that in principle one is able to quantize exactly only dynamically “trivial” systems like the harmonic oscillator (corresponding to a frictionless ideal pendulum). But the more interesting classical problems are of nonlinear and dissipative type, as I will discuss later. And one might question if there should be a more general “nonlinear quantum theory.”

Another string of arguments stems from the observation that somehow one runs into difficulties if one wants to extend the application of quantum mechanical principles, which work so convincingly on the atomic and nuclear levels, into other domains like that of strong forces or gravitation. From a theoretician’s point of view one would prefer to have a “theory of everything,” based on universal principles and unifying the description of all fundamental forces and their phenomena.

One may augment these statements about physical theories by saying that these theories—as idealizations clearly formulated in mathematical terms—are as good as the perturbation theories belonging to them. This is of course due to the fact that the real-world processes are always “noisy” and have to be tamed by experimentalists in laboratory settings.

A third simple statement I want to make is the following: **Every physical theory is only as good as its underlying abstractions.**

I think this is an essential aspect and I want to mention it here because it tells you that we should be very open when we are looking for new theories, and especially for those in the context discussed in this workshop. This is because we make some fundamental assumptions about observed phenomena like interference. Do we have to deal with particles or waves? Or do we need new concepts for whatever it is between the source and the detector of an experiment? And perhaps one should remember that all the abstractions we are using in non-classical physics are still coming from the macroscopic world. So they are deduced from what our sensors receive from phenomena in the macroscopic world. From that it seems clear that abstractions so derived may not be optimal for processes acting in a different domain of phenomena.

To be a little bit clearer about what I mean by that, let me give a few examples.

As we have seen, objects like stones, cannon balls, bird feathers and things like that are in classical theories represented by mass points; that is, they are abstracted from all their properties like form, color, smell, roughness of the surface, and other properties that are thought to be irrelevant for the description of their movement in space.

Another essential concept is that of a free particle, meaning that there is no force acting on it. If one defines it, following in a way Aristotle in his *Physics*,<sup>1</sup> as an object that comes to rest at a finite time—which is what we will always observe—then the concept of a force like friction will not be developed. On the other hand, if, as with Newton (1999), a free particle is an object moving in a straight line with constant velocity then—by observing the orbit of the moon around Earth—one has to introduce a force, giving birth to the gravitational force. By the way: force is the most mystical concept in physics.

1 Compare for instance Rovelli, Carlo. 2015. “Aristotle’s Physics: A Physicist’s Look.” *Journal of the American Philosophical Association*, 1(1): 23–40.

Another powerful abstraction is that of a vacuum. If one states—following Galileo (1953)—that every object near the earth falls with a constant acceleration, this again is not what one observes in reality: if you throw a marble or bird feather from the tower of Pisa, you will observe that they fall to earth differently.

Formulating a rule like Galileo did is making a very strong abstraction, which makes a comprehension of the observed processes only then accessible; in fact there is no physical vacuum in the real world.

Deriving such powerful abstractions from observed processes has always been—and always will be—the cornerstone for the development of new physical theories. Is it possible to derive such abstractions from computer simulations of physical systems?

Another problem that might be of relevance in the context of this workshop is declaring what a fundamental physical object is. For example: What is an elementary particle like the electron for which we observe the described scattering phenomena, and how can we simulate it?

There was (and still is) a long debate going on about how to answer this question, and if it is really necessary to assume elementary objects into which the world can be dissected and from which it can be synthesized again. As far as I know, already Heisenberg's paper of 1955 claimed that there are no real physical criteria to discern between an elementary object and a compound system (Heisenberg 1957, 269), i.e., a system that is built of many convenient parts. This difficulty when dealing with a concept of fundamental or elementary objects is due to the situation in elementary particle physics (i.e., strong forces physics), during the 1950s and beginning of the 1960s, where one identified around 130 elementary particles according to the then actual definitions. Of course everyone then asked the question: What is elementary about 130 particles? Naturally, there then were some quite different approaches that tried to rethink what should be postulated as being elementary, or which tried to abandon the concept of something being fundamental at all. One may mention the S-matrix theory and bootstrapping (Chew 1966) or von Weizsäcker's Ur-Theory (von Weizsäcker 1985), among many others. Those were very inspiring days for theoretical physicists, which came to a sudden end with the postulation of quarks as fundamental objects. And this end of the "particle zoo" demonstrates the power of a theory, because the demanded existence of (initially three) quarks (Gell-Mann 1964, 214–215) comes from pure mathematical beauty, namely symmetry, and there is no other reason. Strangely enough, the theory claims that quarks are unobservable as free particles.

Based on the underlying group theoretical methods one was able to set up a theory not only for hadron physics, but also for the domain of electromagnetism and weak forces; a theory called the “standard model” today. This left us with the challenge of building up a unified theory of all forces (i.e., including gravitation)—a challenge that was not met until today.

Anyway, as was stated somewhere: “Without a guiding theory scientific explorations resemble endless forays in unknown territories. On the other hand, a theory allows us to identify fundamental characteristics, and avoid stumbling over fascinating idiosyncrasies and incidental features. It provides landmarks to orient ourselves in unknown grounds.”

But enough about physical theories! What to say about computer simulations of physical phenomena and their relation to physical theories? I think it is remarkable to observe that at the same time that there was great confusion about what the fundamental physical objects should be, there was a growing awareness that the most interesting phenomena in the physical world result from nonlinear effects; that is, nonlinear systems are ubiquitous—and as the mathematician Stanislaw Ulam observed, to speak of “nonlinear science” is like “referring to the bulk of zoology as the study of non-elephant animals” (Campbell 1985, 374).

There was an upcoming feeling that new types of theories were needed to describe the diversity of these nonlinear phenomena. One may refer for instance to the work of Prigogine (Nicolis and Prigogine 1977) and Haken (1984). And new insights were driven in an accelerating sequence by the growing available computer power. There was the Lorenz equation (Lorenz 1963, 130–141), giving the first nonlinear model for weather dynamics. It was the first example of chaotic dynamics inherited by so many simple mathematical equations, as was shown in the famous book of Mandelbrot (1983). There was also a formulation of global nonlinear dynamics by Hirsch and Smale (1974), applied to physics (Abraham and Marsden 1978), which was progressively noticed in the 1960s and 1970s. Finally it became clear that a desirable nonlinear theory has to describe the behavior of something like “complex adaptive systems” (Gell-Mann 1994, 17–45), a concept that is still under development. This can be marked by the foundation of the Santa Fe Institute in 1984. Now, concepts like nonlinearity, chaos, fractals, emergence, and complexity gathered more and more attention, and at the same time physics as a leading science was superseded by biology.

Already in 1953 it was (probably) Fermi who invented something like the concept of numerical experiments by proposing that instead of simply performing the standard calculation doing pencil and paper work, one



could use a computer to test also physical hypotheses (Weissert 1997). At that time the Fermi–Pasta–Ulam group tried to understand the behavior of atoms in a crystal. To do simple things first, they reduced the problem to a one-dimensional problem considering a chain of mass points coupled by springs that obey Hooke’s law; that is, they introduced a linear interaction. This linear problem is then something one can handle with classical theories. Needing a chain of masses of infinite length one will end up naturally with statistical physics. In this situation it was asked, what happens if one puts into these linear equations a very small nonlinear term. The well-known answer from statistical physics was: the energy of the system will finally be equally distributed over all the possible modes of the mass chain.

So, a simulation of the system with the equations augmented by a nonlinear term was run, and what was observed was very surprising: the energy does not drift towards the equipartition predicted by statistical physics, but periodically returns to the original mode. This was very difficult to understand and it was not predicted by any theory. In fact, this result led to a new field in physics centered on soliton theory.

What I think should be mentioned here is something quite characteristic for simulations of nonlinear systems: almost unexpectedly there do appear to be phenomena adhering to the simulated system that are unexpected and unexplainable, and they become manifest only by chance. In the Fermi–Pasta–Ulam case “the quasi-periodic behavior wasn’t observed at first, because the computer was too slow to allow a simulation to run for long enough. But one day the computer wasn’t stopped as intended, and the calculation was left running. The researchers found to their great surprise that nearly all of the energy returned to the initial mode, and the original state was almost perfectly recovered” (Dauxois 2008, 55–57).

The situation at that time was nicely described by Norman Zabusky, who said, “Now with the advent of large computers, sophisticated graphical algorithms and interactive terminals, we can undertake large-scale numerical simulations of systems and probe those regions of parameter space that are not easily accessible to the theorist/analyst or experimentalist” (cited by Weissert 1997). The Fermi–Pasta–Ulam simulations showed for the first time that computer simulations as a scientific tool can lead to phenomena inherited by physical systems, which are neither predicted by, nor expected from, the theories then at hand.

Nowadays computer simulations find widespread application in many different domains. For instance, they are used for predicting the behavior of physical systems, for proving the existence of hypothesized effects, for testing alternative approaches to a problem, or to explore the behavior of a model in new or larger parameter domains. And sometimes computer simulations also reveal unexpected phenomena, hidden in well-established theories. The best example is perhaps the visualization of chaotic behavior in a simple quadratic map, like the logistic map  $f(x) = r \times x(1-x)$  (Feigenbaum 1978), where  $r$  is the parameter determining the general behavior. This first and well-known example already points to the decisive role of the chosen visualization of computer simulation results.

For more clarification, let me finally unfold what I mean by a computer simulation: **A computer simulation realizes the behavior of a model system under certain boundary conditions for a given set of parameters.**

I want to point out that to have a convincing simulation you have to make sure that all three ingredients—the model, its parameters and the boundary conditions—are well defined. Thus, computer simulations in general follow a standard setup: first, there is a model (or a set of models) of the physical system under study. The model is given by a set of mathematical equations, usually based on an appropriate physical theory. In general this set of equations will have a finite set of parameters for which the behavior of the system should be studied. The specification of the parameter domain is essential for conditioning the applicability of the results derived from the simulation. In addition, appropriate boundary conditions determining the “environment” and the initial conditions for starting a process have to be fixed.

It should be clear that every model picks up only certain aspects of a phenomenon and neglects others that are considered marginal with respect to the particular investigation. But the quality of the utilized models depends essentially on an appropriate mathematical formulation, eventually added by interesting terms, like in the Fermi–Pasta–Ulam case, or just by some interesting mathematically motivated equations. Models are of course always reasonable reductions, abstractions, approximations or analogs of the real physical systems they mimic. In addition, one often has to deal with a large set of parameters for which the behavior has to be tested, and that is what larger computer power is usually needed for.

For many interesting problems of today it is a quite difficult task to set up reliable models and to identify crucial parameter domains, because the intrinsic complexity of the investigated systems and their environments is still increasing due to the involved stochastic properties and nonlinearities. Furthermore, these systems are often composed of many subsystems, so questions like that of system-level organization, development, interdependence, and interactions of subsystems have to be considered carefully, as well as the interaction of the compound system with its often challenging environment. And the parameter sets then have to be thoughtfully adjusted to the posed problem. One therefore often has to go through a cyclic procedure: modeling, simulating, analyzing the results, adaptation of model and parameters, simulating again, and so on.

One way to categorize the many variants of practicing computer simulations is to follow John Holland (2012) by discerning data-driven models, existence-proof models, and exploratory models. These are outlined below.

The *data-driven models* are the common ones used to establish good predictions or a better understanding of processes of interest like climate, weather, traffic, car crashes, bomb explosions, and so on. For these simulations one usually has a given set of mathematical equations, which are derived from an established theory, and a well-defined set of parameters. A comparison of the simulation's results with observed data should then lead to a more precise simulation by adjusting relevant terms in the mathematical equations and tuning the respective parameters. These data-driven simulations mostly give answers of the causal if/then type: if the following initial conditions are satisfied then one will observe the following behavior.

*Existence-proof models* are used to prove the hypothetical existence of phenomena in certain not yet observed or explored parameter domains and initial conditions. A typical example for this category of computer simulations is von Neumann's hypothesis (von Neumann and Burks 1966, 3–14) that self-reproducing machines do exist. The positive answer to this question we nowadays enjoy as the game of life. Another of the many examples, which was also reported by newspapers, was that the existence of monster waves—which have long been around as a vivid fantasy of sailors—has now been proved by computer simulations. Physicists showed that a combination of linear and nonlinear terms in corresponding wave equations could lead to the spontaneous appearance of monster waves, which are not announced in advance by the slow buildup of a superposition of normal waves (Adcock, Taylor, and Draper 2015).

The goal of *exploratory models* is oriented towards answering questions concerning processes that correspond to rather abstract models of systems or to problems for which a theory or a reasonable mathematization is not (yet) available. They are often purely based on computer programs representing for instance something like *Gedanken* experiments. Often they are driven by the goal of realizing a certain fictional system or optimizing a desired procedure, but neither a mathematical method nor a reasonable theory is known for doing so. Exploratory computer-based models have much in common with the traditional thought experiments of physics. One selects some interesting mechanisms and then explores the consequences that occur when these mechanisms interact in some carefully contrived setting. These experimental settings are often not achievable in a laboratory; hence, the “laboratory” resides in the head.

To give again an example reported in the newspapers: artificial diamonds were realized in a microwave reactor. To achieve this result a group of scientists at the Diamond Foundry ([diamondfoundry.com](http://diamondfoundry.com)) company first simulated tens of thousands of different mixtures of ingredients in different reactor shapes to finally obtain in reality an extremely hot plasma under very high pressure at a certain localization. Other examples can be taken from synthetic biology. Here one of the goals is for instance to build regulatory circuits of proteins that are able to control cell behavior. With respect to basic research the aim is to construct—among others—a living artificial biological cell. In the first attempts computer simulations were used to identify a kind of minimal genome that allows for a living cell. Then this genome was chemically synthesized and injected into a bacterium (Hutchison et al. 2016) demonstrating that it is sufficient to realize a living cell. Without the tremendous computer power available it is impossible to find the necessary protein reactions.

For these exploratory simulations therefore (complete) knowledge about a system is not applied but generated. In fact, a theory-driven comprehension of observable real processes is replaced by an experience with possible structures and processes, which is based on specific simulations using large computer capacities. This kind of experience with the simulation of exploratory model systems, which may have no counterparts in the physical world, will not necessarily lead to new theories. But it leads to very many desired applications following the slogan, *I do not understand how it works, but I know how to do it*. With respect to the natural sciences, complex computer simulations often replace *tinkering in the lab* with *modeling in the computer*, and referring to scientific explorations without a theory one may state that *understanding is replaced by engineering techniques*.

After having described what I understand by a physical theory and having surveyed different types of computer simulations, I will shortly come back to event-based simulations.

The goal of these simulations was to demonstrate that for certain scattering experiments the results predicted by quantum theory are reproducible by assuming purely classical arguments. This is done by showing that the statistical distributions of quantum theory can be reproduced “by modeling physical phenomena as a chronological sequence of events whereby events can be actions of an experimenter, particle emissions by a source, signal generations by a detector, interactions of a particle with a material” (Michielsen and De Raedt 2014, 2).

Now, what is the setup of these simulations? To begin with we have three different models: one for the source, one for the detector, and one for what is in *between*. All these models are claimed to be derived from properties ascribed to objects of classical physics. All of these models have several parameters that can be tuned in such a way as to reproduce the interference pattern observed in laboratory experiments (*ibid.*).

According to the classifications given above, to which categories can we assign event-based simulations? Of course they do not use data-driven models. But they have aspects of existence-proof simulations in so far as they try models of classical systems able to reproduce the observed interference patterns. Although they are exploring the effects of different models and parameters concerning the involved subsystems (source, detectors, and the “between”), they are not exploratory computer simulations because the behavior of the compound system to be reproduced is given beforehand by the laboratory experiments.

What hampers event-based simulations—as they stand now—to give guidance for the development of a new physical theory is then obvious. It is of course the role of the models and parameters in this context. Replacing an electron with a “messenger” in a scattering is for the moment only an exchange of the naming for what is “between” the source and the detector. But the quantum mechanical electron has many additional properties, like quantum numbers identifying it as a lepton, and therefore makes possible the prediction of the outcomes of many other experimental settings. For every new type of experimental setup the “messenger” has to be modeled anew, together with different models for the source and especially for the detectors. Furthermore, all these models have many tunable parameters, which allow adapting simulation results to those obtained from the physical experiments performed in a laboratory. Another question is if event-based

simulations can make observable predictions of new phenomena—as any convincing theory is expected to provide.

To summarize: my impression is that at the moment the event-based simulation approach merely replaces for a certain set of physical experiments the “mysterious” quantum theoretical interpretations with a no less “mysterious” signal messenger or “mailman.” If in the future there will be an accumulated experience with event-based simulations giving a more consistent view of how to describe microscopic, atomic, or even subatomic phenomena, my view may be changed. Knowing about the impact of computer simulations on generating new concepts and “world views” one may still hope to excavate certain properties of the physical world, or powerful abstractions of those, which then can inspire or trigger a new type of physical theory having a formal mathematical description.

## References

- Abraham, Ralph, and Jerrold E. Marsden. 1978. *Foundations of Mechanics*. Reading, MA: Benjamin/Cummings Publishing Company.
- Adcock, Thomas AA, Paul H. Taylor, and Scott Draper. 2015. “Nonlinear dynamics of wavegroups in random seas: unexpected walls of water in the open ocean.” *Proceedings of the Royal Society A*, 471 (2184).
- Campbell, David K. Jim Crutchfield, Doyné Farmer, and Erica Jen. 1985. “Experimental Mathematics: The Role of Computation in Nonlinear Science”, *Communications of the ACM* 28 (4): 374–384.
- Chew, Geoffrey F. 1966. *The Analytic S Matrix: a Basis for Nuclear Democracy*. New York: WA Benjamin.
- Dauxois, Thierry. 2008. “Fermi, Pasta, Ulam, and a mysterious lady.” *Physics Today* 61 (1): 55–57.
- Feigenbaum, Mitchell J. 1978. “Quantitative Universality for a Class of Nonlinear Transformation.” *J. Stat. Phys.* 19 (1): 25–52.
- Feynman, Richard. 1989. *The Feynman Lectures on Physics: Commemorative Issue, Vol. 3 Quantum Mechanics 1-1*. Boston: Addison Wesley.
- Galilei, Galileo. 1953. *Dialogue Concerning the Two Chief World Systems*. Translated by Stillman Drake. Los Angeles: University of California Press.
- Gray, Jeremy. 1997. “Poincaré in the archives—two examples.” *Philosophia Scientiae* 2 (3): 27–39.
- Gell-Mann, Murray. 1964. “A Schematic Model of Baryons and Mesons.” *Physics Letters* 8: 214–215.
- Gell-Mann, Murray. 1994. *Complex Adaptive Systems*. Boston: Addison-Wesley.
- Haken, Hermann. 1984. *The Science of Structure: Synergetics*. New York: Van Nostrand Reinhold Company.
- Heisenberg, Werner. 1957. “Quantum theory of fields and elementary particles.” *Reviews of Modern Physics* 29 (3).
- Hirsch, Morris, and Stephen Smale. 1974. *Differential Equations, Dynamical Systems, and Linear Algebra*. New York: Academic Press.
- Holland, John H. 2012. *Signals and Boundaries: Building Blocks for Complex Adaptive Aystems*. Cambridge, MA: MIT Press.

- Hutchison, Clyde A. III, Ray-Yuan Chuang, Vladimir N. Noskov, Nacyra Assad-Garcia, Thomas J. Deerinck, Mark H. Ellisman, John Gill, Krishna Kannan, Bogumil J. Karas, Li Ma, James F. Pelletier, Zi-Qing Qi, R. Alexander Richter, Elizabeth A. Strychalski, Lijie Sun, Yo Suzuki, Billyana Tsvetanova, Kim S. Wise, Hamilton O. Smith, John I. Glass, Chuck Merryman, Daniel G. Gibson, and J. Craig Venter. 2016. "Design and synthesis of a minimal bacterial genome." *Science* 351 (6280): aad6253.
- Lorenz, Edward N. 1963. "Deterministic nonperiodic flow." *Journal of the Atmospheric Sciences* 20 (2): 130–141.
- Ludwig, Günther. 2012. *Foundations of Quantum Mechanics I*. Berlin: Springer Science & Business Media.
- Mandelbrot, Benoît B. 1983. *The Fractal Geometry of Nature*. San Francisco: W.H. Freeman.
- Michielsen, Kristel, and Hans De Raedt. 2014. "Event-based simulation of quantum physics experiments." *International Journal of Modern Physics C* 25 (08): 1430003.
- Newton, Isaac. 1999. *The Principia: Mathematical Principles of Natural Philosophy*. Berkeley, CA: University of California Press.
- Nicolis, G., and I. Prigogine. 1977. *Self-Organization in Nonequilibrium Systems: From Dissipative Structures to Order Through Fluctuations*. New York: Wiley
- Sniatycki, Jędrzej. 1980. *Geometric Quantization and Quantum Mechanics*. New York, Berlin: Springer Verlag.
- von Neumann, John, and Arthur W. Burks. 1966. "Theory of self-reproducing automata." *IEEE Transactions on Neural Networks* 5 (1): 3–14.
- von Weizsäcker, Carl Friedrich. 1985. *Der Aufbau der Physik*. Munich: Hanser.
- Weissert, Thomas P. 1997. *The Genesis of Simulation in Dynamics*. Berlin: Springer Verlag.

## Discussion with Frank Pasemann

Stefan Zieme: I'd like to go back to the very beginning, to the first statement you made. You said every physical theory describes a well-defined area of phenomena. My question would be what to your belief is a phenomenon, and even further can there be a phenomenon without a theory?

Frank Pasemann: I used it here in the naïve sense, referring to objects, processes or facts observed in the physical world by our senses. Talking about physics I naturally understand our measuring apparatuses to be an extension of our human senses. What was called an "event" by Kristel [Michielsen] and Hans [De Raedt] is related to that. Can there be a phenomenon without a theory? To a certain extent this question refers to a kind of chicken-and-egg problem. I would say in general you do not need a theory to observe something I called a phenomenon. On the other hand a theory sometimes claims that something—an effect, a process—should be observable and it gives a name for it. For what we were discussing here I would call the observable "interference pattern" predicted by quantum theory a phenomenon, but not the electrons, quantum probability waves, or any kind of descriptive "messenger." These are wordings used in the specific context of theories or simulations.

Hans-Jörg Rheinberger: If you are coming from biology and not from physics, this is I would say an everyday situation, that you can have and even stabilize and reproduce phenomena without having a theory in the background. You can do genetics – classical genetics – in a quantitative manner without having to know anything about the material constitution of the hereditary units. I think that's very common in the life sciences.

FP: I believe that the development of the biological sciences had a great influence on the way we are reflecting natural processes today because, compared to the standard physical systems, biology has to deal with much more complex and differentiated structures. Perhaps biologists are much closer to thinking in terms of dynamics, of "noisiness," of networks and coherent subsystems. That is perhaps the point where the "New Science" is developing.

Eric Winsberg: I think that's also the case in physics. I think the expressions you used, stable and reproducible, those are I think what are characteristic of phenomena. It's not just something that you see happen in the world, but it's something that can be reproduced consistently and



you get the same kind of data pattern from a variety of different apparatus and such. Which may or may not fall under a theory—it's when you have stable and reproducible phenomena that don't fall under a theory that you think well, gee, maybe I need new theory.

SZ: Let me give an example: I thought about what is the phenomenon, what stage to understand it. Looking at the sky every night, you can produce data about where the planets go. You can look at the data, you can have a pattern of recognition, you can say they move in an ellipsis. It's the phenomenon, the data or the ellipsis. Because ellipsis is not a phenomenon. Firstly it's wrong, they don't move in an ellipsis. They can only do so if you choose a theory. My question was where would you put the phenomena? At which stage? I think you are at the second stage.

FP: And let me make a remark also about stability. The nice thing about our everyday world is that it is almost stable; there is no stability in an absolute sense. Of course we would not exist if atoms and the things composed of them were not stable on a certain time scale. But stability is still a concept to think about, due to the fact that often only a configuration of elements is relatively stable, not their parts. Think about a dynamic equilibrium. Due to the relative stability of the macroscopic physical world we were able to develop first of all classical mechanics, giving a deeper understanding of our everyday world. But as we see nowadays that is not the whole story.

For me the phenomena are the moving planets in the sky. Measuring their advancing positions will result in a set of data. Now, an ellipsis for me is primarily a mathematical object. It may be used to fit the data of the planets' positions. But the ellipsis may also be a solution curve of some differential equations, provided by a physical theory, representing the idealized movements of celestial bodies.

SZ: Do you think it is necessary to have a theory as you have described it for the development of physical science?

FP: No, not at all. I therefore referred to a "well-established" theory like classical mechanics or quantum mechanics. If you are active in a new field or stumble over some new phenomena it may be better to forget about such a definite theory. In these situations usually one will talk about things in terms of working definitions; for instance, one uses terms like roughness, fractality, chaos, nonlinearity or complexity to point to repeating patterns of observations and properties. Most of

the time a mathematical theory comes after certain relations between phenomena are aggregated and consolidated. So a mathematical theory can refer to a deeper understanding of what determines these relations.

MW: What if you would introduce the media of science into your world view? It all looks so ideal once again. It has no materiality, theory building is coming and going. I do not understand yet how theories could come and go? What do you think about introducing the concept of media on which sciences rely? That would change this ideal situation.

FP: Yes, theories are coming and going, that is a "natural process." How did Newton come up with his theory, and where is his theory going? It simply was absorbed in another, more comprehensive theory. Other theories have to go because new ones generate better data, produce more interesting, verifiable predictions, and the like.

As I said, as mathematical theories they are idealizations. Take classical electrodynamics: you can write it down in two equations with only a few symbols. It is a "medium" to understand all the electromagnetic phenomena of the everyday world. It has an epistemological function, and as such it depends on the actual "world view"—that's what I referred to as abstractions. I suppose that theories, as media of science, are forms of organizing our scientific experience of the physical world. Perhaps mathematical theories are a sort of "hot media" in the sense of McLuhan, and what one is using a theory for depends very much on the community that is trying to apply it. With the widespread use of computer simulations, as a kind of "cool" medium perhaps even the "hotness" of theories will change.

Moreover, if we call the mathematical theories "hot" theories, it's the "cool" theories that have a substantial impact on the developing sciences. Think about "chaos theory," which is still based on different "working definitions" but has influenced many, and not only scientific, fields of interest.

On the other hand, take a beautiful mathematical theory like string theory: because the community is able or willing to think about operations in 11 or 13 dimensions, its influence on our "world view," our technological or social development (at the moment), is quite negligible. It seemingly does not have the aura of a popular medium.

But to answer your question: I do not know if using the notion of media of sciences for physical theories will change the way we will try to

understand physical phenomena. Anyway, to say it in today's parlance: it is cool to have a theory.

Arianna Borrelli: You mentioned that computer simulation could contribute, for example in this case of complex systems, where you don't really have any mathematical tools, but before, earlier in your talk you mentioned the interesting questions open at the theoretical level. For example unification—you spoke about unification of forces. I was wondering, don't you think, for example, simulations could contribute to that? Of course unification between say electromagnetism and gravity is what everybody is working on—I mean not everybody, but many. Of course there could be possibility of trying to unify quantum mechanics and quantum field theory, which are not unified. I don't know if anyone is working on that. I was wondering, I ask you because this is something I often wonder about because there's a lot of talk about unification at this high level and there is so little unification at the level where one could also work. So I was just wondering, since we have talked before about this problem of one particle and of many particles. Could that be a possibly interesting or promising direction?

FP: Yes, of course. The point is that in the "old" days you could sit down, have some nice idea, write some equations on paper, and then calculate the possible effects. Nowadays we are confronted with more sophisticated problems. To get some reasonable results from your possibly good ideas it will take substantial computer power, a group to work on them, and not least, quite a bit of money. With respect to unification I can for instance imagine using simulations to study physics in higher dimensions, without relying on mathematical devices like group theory. If in these simulations your apple still falls down to earth and, in addition, all the other observed (and possibly not yet observed) processes are presented, then perhaps you have understood something essential—without having (yet) a theory.