

Chapter 2

On the Success and Limitations of Reductionism in Physics

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2.1 Introduction

Natural sciences, and in particular physics, can look back over a track record of increasing predictive power with regard to the outcome of time evolutions, control, as well as the design of experiments of far-reaching technological and practical importance. But, their success has also brought deeper insights into the underlying laws that govern a wide variety of phenomena. Without doubt this success is based on methodological reductionism, i.e., the attempt to reduce explanations to smaller constituents (although not necessarily the smallest) and to explain phenomena completely in terms of interactions between fundamental entities. Included in the scope of methodological reductionism is theoretical reductionism, wherein one theory with limited predictive power can be obtained as a limiting case of another theory, just as Newtonian mechanics is included in general relativity. From the beginning we should emphasize that reductionism does not preclude emergent phenomena. It allows one to predict some types of emergent phenomena, as we shall see later, even if these phenomena are not in any sense the sum of the processes from which they emerge.

In the following, emergence is understood as involving new, sometimes novel properties of a whole that are not shared by its isolated parts. Emergent phenomena generated this way are therefore intrinsically nonlocal. Within the reductionistic approach we understand them as a result of local interactions, as characteristic of approaches in physics. Emergent phenomena definitely extend beyond simple formation of patterns, such as those in mass and pigment densities. Functionality may be an emergent property as well, as in cases where systems are built up of cells, the fundamental units of life. In our later examples, we shall not refer to “weak emergence”, where a phenomenon is predicted as a result of a model.

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Instead, we shall usually mean “strong emergence”, where nonlocal phenomena arise from local interactions.

Emergent features are not restricted to patterns in an otherwise homogeneous background. “Being alive” is also an emergent property, arising from the cell as the fundamental unit of life. The very notion of complexity is a challenging one. In our context, systems are considered genuinely complex if they show behavior that cannot be understood by considering small subsystems separately. Our claim is a modest one—it is not that complex systems can be understood in all their facets by analyzing them locally, but that complexity can often be reduced by identifying local interactions. Moreover, we do not adopt the extreme view which considers complex systems as inherently irreducible, thereby requiring a holistic approach. The art is to focus on just those complex features that can be reduced and broken up into parts. Why this is not a fruitless endeavor is the topic of the Sect. 2.2.

Section 2.2 deals with the “recipes” responsible for the success. They are abstract guiding principles as well as the use of symmetries, such as the principle of relativity and Lorentz covariance, leading to the theory of special relativity; the equivalence principle and covariance under general coordinate transformations, leading to the theory of general relativity, as well as the gauge principle and invariance under local gauge transformations (complemented by the Higgs mechanism for the electroweak part), leading to the standard model of elementary particle physics. These theories have extraordinary predictive power for phenomena that are governed by the four fundamental interactions; three of them involve the realm of subatomic and atomic physics at one end of the spatial scale, while gravity becomes the only relevant interaction on cosmic scales, where it determines the evolution of the universe.

Interactions on macro or intermediate mesoscopic scales, like the nano and microscales, are in principle produced by the fundamental interactions when composite objects are formed. In practice, they can be derived using a phenomenological approach that involves models valid on this particular scale. Beyond the very formulation of these models, reductionism becomes relevant as soon as one tries to bridge the scales, tracing phenomena on the macroscale back to those on the underlying scales. “Tracing back” means predicting changes on the macro and mesoscopic scales produced by changes on the microscale. A computational framework for performing these bridging steps is the renormalization group approach of Kogut and Wilson (1974), Wilson (1975) and Kadanoff (1977). The framework of the renormalization group goes far beyond critical phenomena, magnetism, and spin systems (see Sect. 2.2.2.1).¹ More generally, but very much in the spirit of the renormalization group, we now have what is called multiscale analysis, with applications in a variety of different realms. In general, it involves links between different subsystems, with each subsequent system having fewer degrees of freedom than its predecessor. The new system may still be

¹ For further applications, see also Meyer-Ortmanns and Reisz (2007).

complex, but the iterative nature of the procedure gradually reduces the complexity (see Sect. 2.2.2.4 below).

Sometimes one is in the fortunate situation where no intermediate steps are needed to bridge the scales from micro to macro behaviour. This can happen when static spatial patterns form on large scales according to rules obeyed by the constituents on the smaller scale, or when shock waves propagate over large distances and transport local changes. We shall illustrate pattern formation with applications as different as galaxy formation in the universe as well as spots and stripes on animals in the realm of living systems. We shall further use dynamical pattern formation in evolving strains of bacteria to illustrate increasing mathematical complexity, as more and more features are simultaneously taken into account. This leads us to conclude that any candidate for an equation of “everything” will be constrained to describe only “something”, but not the whole (see Sect. 2.2.4).

One may wonder why there is in general a need for bridging the scales in intermediate steps. Why not use a single step by exploiting modern computer facilities? After all, it is now possible to simulate a virus in terms of its atomic constituents (an example will be sketched in Sect. 2.2.5). The very same example we use to illustrate the power of up-to-date computer simulations could in principle also serve to demonstrate typical limitations of reductionism. Reductionism, pushed to its extreme, makes the description clumsy. It does not identify the main driving mechanisms on intermediate scales that underlie the results on larger scales. Reductionism then falls short of providing explanations in terms of simple mechanisms, which is what we are after. A more serious worry is that new aspects, properties, features, and interpretations may emerge on the new scale that a computer experiment may inevitably miss. In a fictive dialogue we debate the positions of an extreme reductionism with a more moderate version. As an example of the moderate version, we consider DNA from the perspective of physics and computer science. Even if there are no equations of theories that deserve the attribute “of everything”, or if a multitude of disciplines must be maintained in the future, one may still wonder whether some further steps towards a universal theory of complex systems are possible. Such steps will be sketched in Sect. 2.4.

2.2 On the Success of Reductionism

2.2.1 *Symmetries and Other Guiding Principles*

Physical theories are primarily grounded in experiment in that they are proposed to reproduce and predict experimental outcomes. What distinguishes them from optimized fits of data sets is their range of applicability and their predictive power. Some of these theories deserve to be classified as fundamental. To this class belongs the theories of special, general relativity and the standard model of particle physics.

In this section we would like to review some guiding principles that led to their construction, restricting what would otherwise be a multitude of models to a limited set.

2.2.1.1 The Special Relativity Principle

According to Albert Einstein the Special Relativity Principle postulates that all inertial frames are totally equivalent for the performance of all physical experiments, not only mechanical ones, but also electrodynamics. (In this way, Einstein was able to eliminate absolute space as the carrier of light waves and electromagnetic fields.) Insisting in particular on the constancy of the velocity of light propagation in all inertial frames, one is then led in a few steps to the conclusion that the coordinates of two inertial frames must be related by Lorentz transformations. (First one can show that the transformations must be linear, then one can reduce considerations to special transformations in one space direction, and finally one shows that the well-known γ -factor takes its familiar form $\gamma = 1/\sqrt{1 - v^2/c^2}$.)² If a physical law is invariant under these special Lorentz transformations, and also under spatial rotations and translations in space and time, it holds in any inertial system. The corresponding transformations between two arbitrary inertial systems are then Poincaré transformations. The reductionism arising from the special relativity principle (including the constancy of the velocity of light) leads to the restriction to formulate laws in inertial frames in flat space as equations between tensors under Poincaré transformations. In particular, it restricts the choice of Lagrangians, such as the Lagrangian of electrodynamics, to scalars under these transformations.

2.2.1.2 The Equivalence Principle and General Relativity

Einstein wanted to eliminate “absolute space” in its role in distinguishing inertial frames as those in which the laws take a particularly simple form. He put the equivalence principle at the center of his considerations. According to the (so-called) weak equivalence principle, inertial and gravitational mass are proportional for *all* particles, so that all particles experience the same acceleration in a given gravitational field. This suggests absorbing gravity into geometry, the geometry of space-time, to which all matter is exposed. The equivalence principle led Einstein to formulate his general relativity theory. From Newton’s theory, it was already known that mechanics will obey the same laws in a freely falling elevator as in a laboratory that is not accelerated and far away from all attracting masses. Einstein extrapolated this fact to hold, not only for the laws of mechanics, but so that all local, freely falling, nonrotating labs are fully equivalent for the performance of *all* experiments.

² For the derivation see, for example, Rindler (1969).

(Therefore the simple laws from inertial systems now hold everywhere in space, but only locally, so that special relativity also becomes a theory that is supposed to hold only locally.) This extrapolation amounts to the postulate that the equations in curved space-time should be formulated as tensor equations under general coordinate transformations, where curved space-time absorbs the effect of gravity. Due to the homogeneous transformation behavior of tensors, the validity of tensor equations in one frame ensures their validity in another frame, related by general coordinate transformations. This postulate finally led Einstein to the theory of general relativity that has been confirmed experimentally to a high degree of accuracy.

2.2.1.3 Gauge Theories of the Fundamental Interactions

In the previous sections on the relativity principle, the postulated symmetries referred to transformations of the space-time coordinates and restricted the form of physical laws. In the theories of strong, weak, and electromagnetic interactions, we have to deal with internal symmetries. Here it is not only the right choice of the symmetry group which is suggested by conserved matter currents, but also the prescription of how to implement the dynamics of matter and gauge fields that lead to the construction of gauge theories and finally to the standard model of particle physics.

Hermann Weyl was the first to consider electromagnetism as a local gauge theory of the $U(1)$ symmetry group (Weyl 1922). Let us first summarize the steps in common to the construction of electromagnetic, strong, and weak interactions as a kind of “recipe”. As result of Noether’s theorem, one can assign a global (space-independent) continuous symmetry to a conserved matter current. The postulate of local gauge invariance then states that the combined theory of matter and gauge fields should be invariant under local (that is space-dependent) gauge transformations. Obviously, a mass term, which is bilinear in the matter fields $\psi, \bar{\psi}$ and contains a partial derivative, violates this invariance. To compensate for the term that is generated from the derivative of the space dependent phase factors in the gauge transformations, one introduces a so-called minimal coupling between the matter fields and the gauge fields, replacing the partial derivative by the covariant derivative in such a way that the current is covariantly conserved. It remains to equip the gauge fields with their own dynamics and construct the gauge field strengths in such a way that the resulting Lagrangian is invariant under local gauge transformations.

Let us demonstrate these steps in some more detail. Under local gauge transformations, matter fields $\psi_c(x)$ transform according to

$$\psi_c(x) \rightarrow (\exp(-i\Theta^a(x)T_a))_{cc'}\psi_{c'}(x) \equiv (g(x)\psi)_c(x). \quad (2.1)$$

Here T_a are the infinitesimal generators of the symmetry group $SU(n)$ in the fundamental representation, $\Theta^a(x)$ are the space dependent group parameters,

$a = 1, \dots, N$, with N the dimension of the group, and $c, c' = 1, \dots, n$, where n characterizes the symmetry group $SU(n)$. Gauge fields $\mathcal{A}_{\mu, cc'}(x) = \bar{g}A_{\mu}^a(x)(T_a)_{cc'}$, which are linear combinations of the generators T_a , with \bar{g} a coupling constant, transform inhomogeneously according to

$$\mathcal{A}'_{\mu}(x) = g(x)(\mathcal{A}_{\mu} - i\partial_{\mu})g^{-1}(x). \quad (2.2)$$

In general, this equation should be read as a matrix equation. In the language of differential geometry, the gauge field corresponds to a connection, it allows one to define a parallel transport of charged vector fields $\psi_c(x)$ from one space-time point x , along a path \mathcal{C} to another point y . This parallel transport can then be used to compare vector fields from different space-time points in one and the same local coordinate system. It thus leads to the definition of the covariant derivative D_{μ} :

$$[(\partial_{\mu} + i\mathcal{A}_{\mu})\psi(x)]_c dx^{\mu} =: (D_{\mu}\psi)_c(x) dx^{\mu}. \quad (2.3)$$

The path dependence of the parallel transport is described infinitesimally by the field strength tensor $\mathcal{F}_{\mu\nu}(x)$ with $\mathcal{F}_{\mu\nu}(x) = \bar{g}F_{\mu\nu}^a(x)T_a$. In terms of gauge fields, $F_{\mu\nu}^a(x)$ is given by

$$F_{\mu\nu}^a(x) = \partial_{\mu}A_{\nu}^a(x) - \partial_{\nu}A_{\mu}^a(x) - \bar{g}f^{abc}A_{\mu}^b(x)A_{\nu}^c(x), \quad (2.4)$$

with structure constants f^{abc} specific to the gauge group. For $U(1)$, the last term vanishes, whence it is characteristic of the nonabelian gauge groups. In geometric terms, the field strength tensor is given by the commutator of the covariant derivatives

$$D_{\mu}D_{\nu} - D_{\nu}D_{\mu} = i\mathcal{F}_{\mu\nu}(x). \quad (2.5)$$

The last equation reflects the fact that the parallel transport is path dependent if there is a non-vanishing field strength, in very much the same way as the parallel transport of a vector in Riemannian space depends on the path if the space is curved. The field strength of the gauge fields then transforms under local gauge transformations $g(x)$ according to the adjoint representation of the symmetry group:

$$\mathcal{F}_{\mu\nu}(x) \rightarrow g(x)\mathcal{F}_{\mu\nu}(x)g^{-1}(x). \quad (2.6)$$

This construction principle leads for (quantum) electrodynamics to the familiar Lagrange density

$$\mathcal{L} = -\frac{1}{4}F_{\mu\nu}F^{\mu\nu} + \bar{\psi}^{(l)}(x)(i\gamma^{\mu}D_{\mu} - M_l)\psi^{(l)}(x), \quad (2.7)$$

with $D_\mu = \partial_\mu - ieA_\mu$. By construction it is invariant under the local $U(1)$ transformations given by

$$\begin{aligned} A_\mu &\rightarrow A_\mu(x) + \partial_\mu \Theta(x), \\ \psi^{(l)}(x) &\rightarrow e^{ie\Theta(x)} \psi^{(l)}(x), \\ \bar{\psi}^{(l)}(x) &\rightarrow \bar{\psi}^{(l)}(x) e^{-ie\Theta(x)}, \end{aligned} \quad (2.8)$$

where $\Theta(x)$ is a space-dependent phase, l labels the electron or muon, ψ is a Dirac spinor representing the matter fields, and A_μ represents the photons. For quantum chromodynamics, the resulting Lagrange density takes the same form as in (2.7):

$$\mathcal{L} = -\frac{1}{4} F_{\mu\nu}^a F^{a,\mu\nu} + \bar{\psi}(x)(i\gamma^\mu D_\mu - M)\psi(x), \quad (2.9)$$

where we have suppressed the indices of the mass matrix M and the quark fields ψ . Note that ψ here carries a multi-index α, f, c , where α is a Dirac index, f a flavor index, and c a color index, and all indices are summed over in \mathcal{L} . The gauge transformations (2.1) can be specialized to $T_a = \frac{1}{2}\lambda_a$, with $a = 1 \dots, 8$ and λ_a the eight Gell-Mann matrices, and $c, c' = 1, 2, 3$, for the three colors of the $SU(3)$ color symmetry. The covariant derivative takes the form $D_\mu = \partial_\mu - ig\frac{\lambda_a}{2}A_\mu^a(x)$, where the gauge fields A_μ^a now represent the gluon fields mediating the strong interaction, and the field strength tensor $F_{\mu\nu}^a$ is given by (2.4) with structure constants f^{abc} from $SU(3)$. Note that the quadratic term in (2.4) represents the physical fact that gluons are also self-interacting, in contrast to photons. So in spite of the same form of (2.7) and (2.9), the physics thereby represented is as different as are quantum electrodynamics and quantum chromodynamics.

Finally, the combined action of electromagnetic and weak interactions is constructed along the same lines, with an additional term in the action that implements the Higgs mechanism, to realize the spontaneous symmetry breaking of $SU(2)_w \times U(1)$ to $U(1)_e$ (where the subscript w stands for “weak” and e for “electromagnetic”) and give masses to the vector bosons W^+ , W^- and Z mediating the weak interactions.

The similarities between the local gauge theories and general relativity become manifest in the language of differential geometry and point to the deeper reasoning behind what we called initially a “recipe” for how to proceed. In summary, the pendants in local gauge theories and general relativity are the following:

- The local space $\mathcal{H}(x)$ of charged fields $\psi(x)$ with unitary structure corresponds to the tangential space with local metric $g_{\mu\nu}(x)$ and Lorentz frames.
- The local gauge transformations correspond to general coordinate transformations.
- The gauge fields $\mathcal{A}_{\mu,cc'}(x)$, defining the connection in the parallel transport, correspond to the Christoffel symbols, which describe the parallel transport of tangential vectors on a Riemannian manifold.

- The covariant derivatives correspond to each other; from an abstract point of view, the idea behind their construction and their transformation behavior is the same.
- The field strength tensor $\mathcal{F}_{\mu\nu,cc'}(x)$ corresponds to the Riemann curvature tensor R^i_{kmn} .

The overarching mathematical structure between gauge theories and general relativity is formulated in the theory of fiber bundles.

The standard model of particle physics has been confirmed experimentally to a very high level of accuracy. It brings order into the otherwise confusing zoo of elementary particles. Before its formulation in terms of local gauge theories, there were a variety of effective, phenomenological models, based merely upon symmetry requirements, with a rather limited range of predictions as compared to the standard model. It was the recognition of electrodynamics as a local gauge theory of $U(1)$, and the extension of the postulate of local gauge invariance to the strong and weak interactions, together with an implementation along the lines of differential geometry and general relativity, that led to its construction and eventual success. Seminal contributions along the way were made by Weyl (1922), Yang and Mills (1954), Glashow (1961), Weinberg (1967), Salam (1968), to name but a few,³ and Kibble (1961), Sciama (1962), Hehl et al. (1976), and others in relation to the formulation of gravitational theory as a local gauge theory.

2.2.2 Bridging the Scales from Micro to Macro

2.2.2.1 The Renormalization Group Approach

The renormalization group is neither a group nor a universal procedure for calculating a set of renormalized parameters from a set of starting values. It is a generic framework with very different realizations. Common to them is the idea of deriving a set of new (renormalized) parameters, characteristic of a larger scale, from a first set of parameters, characteristic of the underlying smaller scale, while keeping some long-distance physics unchanged. The degrees of freedom are partitioned into disjoint subsets. Specific to the renormalization group is a partitioning according to length scale, or equivalently, according to high and low momentum modes. These successive integrations of modes according to their momentum or length scales are the result of an application of the renormalization group equations. Since the change in scale goes along with a reduction in the number of degrees of freedom, the iterated procedure should lead to a simpler description of the system of interest, which is

³ For a reference on “The Dawning of Gauge Theory”, see also the book (O’Raifeartaigh 1997) with the same title.

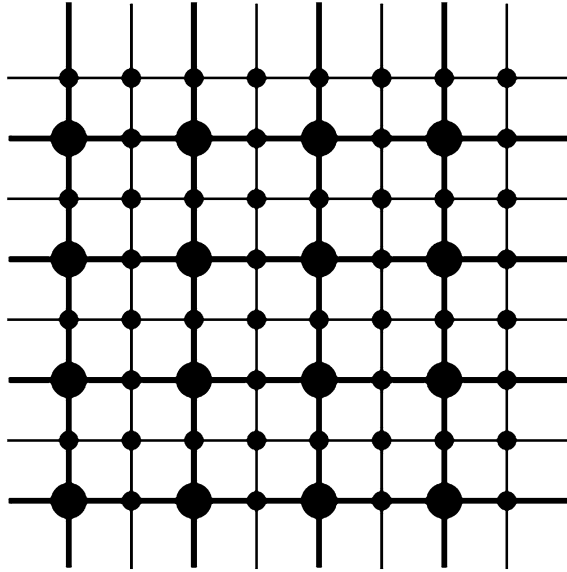


Fig. 2.1 Square lattice of size 8×8 in $D = 2$, with an assigned block lattice of scale factor $l = 2$

often the long-distance physics. The renormalization group provides a computational tool. There are different ways to implement the change of scale but for simplicity, we choose the framework of block spin transformations as an example.

2.2.2.2 Renormalization Group for a Scalar Field Theory

Let us consider the theory of a single (spin-zero bosonic) scalar field on a D -dimensional hypercubic lattice $\Lambda = (a\mathbb{Z})^D$ with lattice spacing a . In order to describe the block spin transformations, we have to introduce some definitions. The scalar fields make up a vector space \mathcal{F}_Λ of real-valued fields $\Phi : \Lambda \rightarrow \mathbb{R}$. The action S_Λ is a functional on these fields, and the partition function is given by $Z_\Lambda(J)$ with

$$Z_\Lambda(J) = \int \mathcal{D}\mu_\Lambda(\Phi) \exp(-S_\Lambda(\Phi) + (J, \Phi)_\Lambda), \quad (2.10)$$

where $J \in \mathcal{F}_\Lambda$ stands for an external current and $\mathcal{D}\mu_\Lambda(\Phi) = \prod_{x \in \Lambda} d\Phi(x)$, while $(J, \Phi)_\Lambda = a^D \sum_{x \in \Lambda} J(x)\Phi(x)$. Let us now define a block lattice Λ_l for $l \in \mathbb{N}$ by decomposing Λ into disjoint blocks. Each block consists of l^D sites of Λ (see Fig. 2.1 for $D = 2$ and $l = 2$).

The renormalization transformation R_l of the action S_Λ , leading to the effective action S'_Λ , defined on the original lattice Λ , is defined via the Boltzmann factor

$$\exp(-S'_\Lambda(\Psi)) \equiv \exp(-(R_l S_\Lambda)(\Psi)) = \int \mathcal{D}\mu_\Lambda(\Phi) P(\Phi, s_l \Psi) \exp(-S_\Lambda(\Phi)), \quad (2.11)$$

where a commonly used choice for the block spin transformation is given by

$$P(\Phi, s_l \Psi) = \prod_{x \in \Lambda_l} \delta[(s_l \Psi)(x) - \frac{1}{b}(C\Phi)(x)], \quad (2.12)$$

with block averaging operator C defined by

$$(C\Phi)(x) := \frac{1}{l^D} \sum_{y \in \text{block}(x)} \Phi(y). \quad (2.13)$$

So the effective action $S'_\Lambda(\Psi)$ in terms of the block variables Ψ results from a path integral over all Φ of the Boltzmann factor $e^{-S_\Lambda(\Phi)}$ under the constraint that the average value of $\Phi(y)$ over all sites of a block (normalized over the number of these sites, viz., l^D , and multiplied by a scale factor $1/b$) takes a prescribed value $\Psi(x)$ for each block, where the block is labeled by $x \in \Lambda_l$. The rescaling operation $(s_l \Psi)(x) : = \Psi(x/l)$ with $x \in \Lambda_l$ accounts for the fact that lengths and distances on the block lattice reduce by a factor of $1/l$ when measured in units of the block lattice distance as compared to units on the original lattice. Note that the way the constrained integration is realized here amounts to an integration over short wavelength fluctuations with a wavelength λ satisfying $a < \lambda < la$. The effective action S'_Λ then describes the fluctuations of the scalar field with wavelength $\lambda > la$. The choice of the block variable as some rescaled average (by a factor of b) over the variables of the block is plausible as long as the average values are good representatives for the whole ensemble of variables. If the variables are elements of a certain group like $SU(3)$, the sum is no longer an $SU(3)$ element, so it is obvious that the naive averaging procedure will not always work. For block variables that are spins with two possible values, one may use the majority rule instead. If the majority of spins points “up” within a block, the representative is chosen to point up, etc.

2.2.2.3 Renormalization Group for the Ising Model

An alternative option for selecting a block variable is decimation. In the simplest case of the Ising model in one dimension, decimation amounts to the choice of block spins as spins of a subset of the original chain, for example, choosing as block spin the spins of every second site. In the partition function, this amounts to taking the partial trace. When the resulting partition function in terms of a trace over the

reduced set of variables is cast in the same form as the original one with the Ising action in the Boltzmann factor, one can read off what the renormalized parameters (of the effective Ising action on the coarse scale) are in terms of the original parameters (of the Ising action on the underlying scale). Writing for the Ising action

$$S = -k \sum_{\langle ij \rangle} s_i s_j - h \sum_i s_i - \sum_i c, \quad (2.14)$$

with coupling k , external field h , and constant c ,⁴ $s_i \in \{\pm 1\}$ and $\langle ij \rangle$ denoting nearest neighbors, one obtains the following relations for the renormalized parameters k' , h' , c' in terms of those of the original action:

$$\begin{aligned} \exp(2h') &= \exp(2h) \cosh(2k+h) / \cosh(2k-h), \\ \exp(4k') &= \cosh(2k+h) \cosh(2k-h) / \cosh^2 h, \\ \exp(4c') &= \exp(8c) \cosh(2k+h) \cosh(2k-h) \cosh^2 h. \end{aligned} \quad (2.15)$$

For the derivation of these relations, see for instance (Yeomans 1992). Here it should be emphasized that the result is exact, since the effective action on twice the scale, resulting from the decimation, can be exactly cast into the form of an Ising model without truncation of other terms. Usually, further terms are generated in the effective action under a renormalization group transformation. Exact self-similarity with respect to the action is the exception rather than the rule.

The successes of the renormalization group in relation to critical phenomena are as follows:

- One can explain why second-order phase transitions fall into so-called universality classes.
- One can predict an upper critical dimension for a given universality class.
- One can derive scaling relations as equalities between different critical exponents.
- Once can explain why critical exponents take the same values if calculated from above or below the critical point.

Our examples of a scalar field theory and an Ising model are simple dynamical systems. In the vicinity of critical points, the conjecture of self-similar actions over the spatial scales could be suggested, for example, by visualizing the blocks of aligned spins: at the critical point the linear block size varies overall length scales, so it is natural to define the block spin in such a way as to represent a whole block by another spin. In general, block variables should be representative of the whole block, in the sense that they project onto the appropriate degrees of freedom. They should also guarantee that the dynamics becomes simple again on the coarse scale in terms of these variables. A choice of block variables for which the effective

⁴ Keeping the constant c from the beginning, although it appears to be redundant in (2.14), one can claim that the new action has the same form as the old one.

action contained many more terms than the original one, of which all remained relevant under iteration of the procedure, would fail. Therefore there is a certain skill involved in making an appropriate choice, and this is an act of “cognition” that cannot be automated in a computer simulation.

Although from a rigorous point of view it may be quite hard to control the truncations of terms in the effective actions, a closer look at the mesoscopic or macroscopic scales reveals that there do exist new sets of variables that afford a relatively simple phenomenological description, even if it is not feasible to derive them within the renormalization group approach. In a similar spirit to the renormalization group is multi-scale modeling, which we consider next.

2.2.2.4 Multi-scale Modeling

Multi-scale modeling is an approach that is now also used outside physics, in engineering, meteorology and computer science, and in particular in materials science. There it can be used to describe hierarchically organized materials like wood, bones, or membranes (Fratzl and Weinkammer 2007). Typically, one has a few levels with non-self-similar dynamics and different variables for each level. The output of one level serves as input for the next. The number of variables for each level should be limited and tractable. As an example, let us indicate typical levels in bones. Starting with a cube of the order of a few mm^3 of trabecular structure of a human vertebra, we zoom to the microscale of a single vertebra, then further to the sub-microscale of a single lamella, then to the nanoscale of collagen fibers, and finally to the genetic level (see, for example, Wang and Gupta 2011). Conversely (and different research groups may proceed either top-down or bottom-up), once we succeed in understanding the regulation of bones on the genetic level and its impact on intracellular processes, identifying its impact on cell–cell communication, then on ensembles of cells, and finally on the whole organism, we will be able to treat bone diseases on the genetic level. Moreover, by understanding self-healing and restructuring processes of bones, we may be able to imitate nature’s sophisticated design of bone material. Here reductionism leads to the “industry” of bionics and biomimetics, which is already booming for many applications.

2.2.3 When a Single Step Is Sufficient: Pattern Formation in Mass and Pigment Densities

Sometimes one is in the lucky situation that the scales from micro to macro distances can be bridged in a “single step”, that is in a single set of equations, as the inherent local rules lead to patterns on a coarse, macroscopic scale. We would like to give two examples from very different areas, cosmology and biology.

2.2.3.1 Pattern Formation in the Universe

Let us first illustrate the great success of reductionism for the example of galaxy formation in the universe. For a detailed description we refer to (Bartelmann 2011) and references therein. Based on two symmetry assumptions (that of homogeneity and isotropy of space) and the theory of general relativity, one first derives the Friedmann equations. Together with the first law of thermodynamics and an equation of state for matter, one arrives at the standard model for the structure and evolution of the universe. In particular, assuming that dark matter gives the main contribution to the total mass and that it can be approximated as pressureless, the equations governing the evolution of the dark matter density are the continuity equation for mass conservation, the Euler equation for momentum conservation, and the gravitational field equation of Newtonian physics (here the Einstein equations of general relativity are not even needed in view of the final accuracy). The three equations can be combined into one, viz.,

$$\ddot{\delta} + 2H\dot{\delta} - 4\pi G\bar{\rho}\delta = 4\pi G\bar{\rho}\delta^2 + \frac{1}{a^2}\nabla\delta\nabla\Phi + \frac{1}{a^2}\partial_i\partial_j[(1+\delta)u_iu_j]. \quad (2.16)$$

Here $\delta \equiv (\rho - \bar{\rho})/\bar{\rho}$ are the density fluctuations around the mean density $\bar{\rho}$, H denotes the Hubble function, G the gravitational constant, Φ the gravitational potential in Newtonian gravity, $-\nabla\Phi$ the gravitational force, \vec{u} the velocity of matter with respect to the mean Hubble expansion of the universe, and $a(t)$ the scale factor entering the Friedmann model. By deriving the initial density fluctuations in the early universe from the observed CMB (cosmic microwave background) data under the assumption of cold dark matter and evolving the resulting Gaussian fluctuations with respect to (2.16) in time, one can reproduce the formation first of filamentary or sheet-like structures as they are experimentally observed in large-scale galaxy surveys, then of galaxy clusters and galaxies. The quantities to be compared between experiment and theory are the power spectra of the variance of fluctuation amplitudes, and these are measurable over a vast range of scales. This is clearly a striking success of the reductionistic approach, starting from symmetries and basic laws of physics, to arrive at an equation for the mass density fluctuations that is able to reproduce structure formation from the scale of about 1 Mpc (1 megaparsec $\approx 3 \times 10^{22}$ m)⁵ to cosmic scales.

On the other hand one has to admit that the considered observable, the mass density fluctuations, is a universal but simple characteristic that keeps its meaning over a vast range of scales, and the only relevant force on large scales is gravity. The formation of functional structures of the kind occurring within biological units is incomparably more difficult to trace back to a few “ingredients” as input, as the

⁵ This estimate depends on the applicability of (2.16). One megaparsec is supposed to be an estimate for a lower bound if the mass density fluctuations refer to dark matter. Density fluctuations of gas in cosmic structures may be described as a fluid down to even smaller scales.

struggle to construct precursors of biological cells so clearly demonstrates in the study of artificial life.

2.2.3.2 Pattern Formation in Animal Coats

We would like to add another example of pattern formation, based on different mechanisms and in a very different range of applications. This is pattern formation in animal coats. The mechanism goes back to Turing (1952) who suggested that, under certain conditions, chemicals can react and diffuse in such a way as to produce steady state spatial patterns of chemical or morphogen concentrations. For two chemicals $A(\vec{r}, t)$, $B(\vec{r}, t)$, the reaction–diffusion equations take the form

$$\begin{aligned}\frac{\partial A}{\partial t} &= F(A, B) + D_A \nabla^2 A, \\ \frac{\partial B}{\partial t} &= G(A, B) + D_B \nabla^2 B,\end{aligned}\tag{2.17}$$

where F and G are nonlinear functions of A and B that determine the reaction kinetics and D_A , D_B are the diffusion constants. According to Turing's idea, spatially inhomogeneous patterns can evolve by diffusion driven instability if $D_A \neq D_B$. (Special cases of $F(A, B)$ and $G(A, B)$ include the activator–inhibitor mechanism, suggested by Gierer and Meinhardt (1972).) In particular, one can derive the necessary conditions on the reaction kinetics and the diffusion coefficients for a process of reacting and diffusing morphogens, once the set of differential equations (2.17) is complemented by an appropriate set of initial and boundary conditions. Murray suggested (Murray 1980, 1981) that a single (reaction–diffusion) mechanism could be responsible for the versatile patterns in animal coats. It should be noticed that pattern formation does not directly refer to the pigment density. What matters are the conditions on the embryo's surface at the time of pattern activation. Pattern formation first refers to morphogen prepatterns for the animal coat markings, and it requires a further assumption that subsequent differentiation of the cells to produce melanin simply reflects the spatial pattern of morphogen concentration. Solving the differential equations for parameters and geometries which are adapted to those of animals (like the surface of a tapering cylinder to simulate patterns forming on tails) leads to remarkable agreement between general and specific features of mammalian coat patterns.

The important role that the size and shape of the domain have on the final pattern (spots and stripes and the like) can be tested through a very different realization of the related spatial eigenvalue problem

$$\nabla^2 \vec{W} + K^2 \vec{W} = 0.\tag{2.18}$$

In relation to animal coats, \vec{W} represents the fluctuations about the steady state concentration in dimensionless units, and solutions reflect the initial stages of pattern formation. In a different realization of (2.18), \vec{W} represents the amplitude of vibrations of a membrane, a thin plate, or a drum surface, since their vibrational modes also solve (2.18). Time-average holographic interferograms on a plate, excited by sound waves, nicely visualize patterns and their dependence on the size and form of the plate. Varying the size (for a plate, this is equivalent to varying the forcing frequency) generates a sequence of patterns in the interferograms that bear a striking resemblance to a sequence of simulated animal coats of varying sizes (Murray 1993 and references therein).

The reductionism here amounts to explaining the variety of patterns in animal coats in terms of a single set of equations (2.17) with specified parameters and functions F and G , assuming that the morphogen prepatterns get transferred to the finally observed pigment patterns. Moreover, analysis of this set of equations also allows one to study the sensitivity to initial conditions. In the biological implementation, it is the initial conditions in the embryonic stage that matter for the final pattern. It should be noticed that beyond the universal characteristics of these patterns (spots, stripes), the precise initial conditions at the time of activation of the reaction–diffusion mechanism determine the individuality of the patterns. Such individuality is important for kin and group recognition among animals. The role the pattern plays in survival differs between different species. If it does play a role, the time of activation in the embryonic phase should be well controlled. These remarks may give some hints regarding the fact that, although the basic mechanism behind pattern formation sounds rather simple, its robust implementation in a biological context raises a number of challenging questions for future research.

2.2.4 From Ordinary Differential Equations to the Formalism of Quantum Field Theory: On Increasing Complexity in the Description of Dynamic Strains of Bacteria

Dynamic strains of bacteria provide another example of pattern formation. In this section we use these systems to demonstrate a generic feature that is observed whenever one increases the number of basic processes that should be included in one and the same description at the same time. It is not only, and not necessarily, the number of variables or the number of equations that increases along with the different processes, but also the mathematical complexity of the required mathematical framework. Including different processes in one and the same framework should be contrasted with treating them separately, in certain limiting cases. These processes may be their self-reproduction and destruction, or birth and death events, caused by their mutual interactions, all this leading to a finite lifetime of individuals

and therefore to demographic noise, and also their movement via diffusion or active motion, and their assignment to a spatial grid, restricting the range of individual interactions.

As an example of such a system that can be treated in various limiting cases, we consider strains of bacteria in microbial experiments in a Petri dish, reproducing, diffusing, going extinct, and repressing or supporting each other according to certain rules. All these features can be observed in the spatially extended May–Leonard model (May and Leonard 1975). This model is intended to describe generic features of ecosystems such as contest competition, realized via selection, and scramble competition, realized via reproduction. The selection events follow the cyclic rock–paper–scissors game according to the following rules:



This means that the N individuals occur in three species A, B, C , where A consumes B at rate σ if they are assigned to neighboring sites on a two-dimensional grid of linear size L , and similarly B consumes C and C consumes A at rates that here are chosen to be the same for simplicity. The reproduction rules are:



Hence, A reproduces at rate μ if the neighboring site of A is empty, and B and C accordingly. It is assumed that the lattice sites have a finite carrying capacity, viz., zero or one. In addition, the individuals are allowed to move. One option is to let the individuals exchange their position with a nearest neighbor at rate ϵ , leading to effective diffusion. Here we use a realization of the model as described in (Frey 2010). The overall goal is to predict the space-time evolution at large times as a function of the inherent parameters, and in particular to predict and characterize the kind of pattern formation that happens on the spatial grid (The conditions that ensure the coexistence of different species on the grid are of primary interest, in view of one of the core questions of ecology: the maintenance of biodiversity.).

If we want to approach the problem in full generality, as it has just been posed, we would need either numerical simulations or the quantum field theoretic framework⁶ from the outset (for an example, Ramond (1989).) Instead, let us start with the various limiting cases and assume three species with a total of N individuals, interacting according to the rules of (2.19), (2.20) in all the following cases:

⁶ The formalism of quantum field theory can be applied to systems which are fully classical. See (Mobilia et al. 2007)

1. N infinite, no spatial assignment, no explicit mobility.

When the population size of the three species A, B, C goes to infinity, and the individuals are well mixed in the sense that they are neither assigned to the space continuum nor to a spatial grid, we obtain the following set of ordinary (nonlinear) differential equations (ODEs) for the corresponding concentrations of the three species a, b, c :

$$\begin{aligned}\partial_t a &= a[\mu(1 - \rho) - \sigma c], \\ \partial_t b &= b[\mu(1 - \rho) - \sigma a], \\ \partial_t c &= c[\mu(1 - \rho) - \sigma b].\end{aligned}\tag{2.21}$$

Here ρ denotes the overall density, and μ and σ are as defined below (2.19) and (2.20), respectively. These equations deterministically predict the time evolution of species concentrations.

2. N finite fluctuating, no spatial assignment, no explicit mobility.

Let us keep the species well mixed, not assigned to a grid, but keeping N finite and fluctuating. Now the appropriate description is in terms of a master equation for the probability P to find N_i individuals of species i ($i \in \{A, B, C\}$) at time t (under the assumption of a Markov process):

$$\partial_t P(N_i, t) = f(P(N_i, t), P(N_i \pm 1, t); \mu, \sigma),\tag{2.22}$$

where the right-hand side is a function f , depending on the probabilities for finding states with N_i or $N_i \pm 1$ individuals at time t , the latter being states from which a decay or creation of one individual contributes to a change in $P(N_i, t)$. Note that we now obtain a deterministic description of the probabilities of finding a certain configuration of species rather than of the concentrations themselves.

3. N infinite, concentrations spatially assigned as $\vec{a}(\vec{r})$, with diffusion.

Now we obtain a deterministic reaction–diffusion equation, that is, a set of coupled partial differential equations (PDEs) of the form

$$\partial_t \vec{a}(\vec{r}, t) = D \Delta \vec{a} + \vec{F}(\vec{a}),\tag{2.23}$$

where $\vec{a}(\vec{r}, t)$ denotes the vector of three space-time dependent concentrations of species, and \vec{F} the appropriate function of \vec{a} , given by the right-hand side of (2.21), while D is the diffusion constant with $D = \epsilon/2N$ finite for $N \rightarrow \infty$, so that ϵ has to increase accordingly.

4. N finite fluctuating, species spatially assigned to a grid, but high mobility.

Becoming more realistic and keeping N finite and fluctuating while moving in space, it is in the low-noise approximation that the spatiotemporal evolution of the system can be described by concentrations of the species, evolving in the

space-time continuum, and the result can be cast in a set of stochastic partial differential equations (SPDEs):

$$\partial_t \vec{a}(\vec{r}, t) = D \Delta \vec{a}(\vec{r}, t) + \vec{F}(\vec{a}) + C(\vec{a}) \vec{\xi}. \quad (2.24)$$

Here $\xi_i(\vec{r}, t)$, $i = A, B, C$ denotes Gaussian white noise, Δ is the Laplacian, and $\vec{F}(\vec{a})$ is the former reaction term. In principle, a noise term in these equations could have three origins: the stochasticity of chemical reactions according to (2.19) and (2.20), a finite fluctuating number N when it is not forced to be conserved, and the motion of individuals. The noise term $C(\vec{a}) \vec{\xi}$ in (2.24) represents only the noise in the reactions (2.19) and (2.20) (along with non-conserved N), where the noise amplitudes $C(\vec{a})$ are sensitive to the system's configurations $\vec{a}(\vec{r}, t)$. As argued in (Frey 2010), noise due to mobility can be neglected as compared to the other sources in this limit (4). Note that it is only in the low-noise approximation that one obtains equations for the concentrations \vec{a} rather than for the species numbers N_i , and assigned to a space continuum rather than to a grid. The effect of finite N is indirectly represented by the noise term. Equivalent to (2.24) would be the corresponding Fokker–Planck equations for the respective concentration probabilities.

5. N finite fluctuating, species spatially assigned to a grid, and low mobility.

This no longer corresponds to a limiting case. When in contrast to case (4) the exchange rate of species is no longer high compared with the reaction events, the former continuum description in terms of SPDEs breaks down, the low-noise approximation fails, and the field theoretic formalism is required as an analytical complement to numerical simulations. One should express the transition amplitude of an initial to a final occupation number distribution as a path integral over all occupation number configurations, where the path is weighted by an appropriate action that should be derived from the corresponding master equation. It depends on the specific interaction rules and the model parameters. The essential assumption is that each configuration is uniquely characterized by the occupation numbers N_i of the lattice site \vec{r} with species $i = A, B, C$.

In summary, the subsequent inclusion of demographic fluctuations (due to annihilation, creation, local interactions), spatial organization, and diffusion leads to increasing complexity in the required mathematical description. The actual solutions to the equations of our example can be found in Frey (2010) and references therein. In the detailed version of Frey (2010), it is interesting to focus on the qualitative changes in the predictions that are missed by projecting on certain limits like high mobility or infinite population size. For example, in the limit discussed under (1), transitions in which certain species go extinct would be completely missed.

In this example, our agents were bacteria, but it is obvious that the bacteria may be replaced by more or less complex agents like humans or chemical substances, while adapting the wording accordingly. The principal need for simultaneously including all these aspects into a single framework comes from the requirement of

not missing those phenomena that only occur in the simultaneous presence of all the available options when the system evolves. In general, it is not only that predictions obtained in certain limiting cases may be modified outside the validity range of the limit, but, more importantly, additional phenomena may also show up.

These results also shed some light on the meaning of any “Equation of Everything”. As soon as “everything” is cast into the form of a (differential) equation, it corresponds to a projection. A theory, cast into the form of a path integral, itself corresponds to a selection of cases in which the system can be described by the time evolution of functionals, depending on configurations in terms of discrete occupation numbers. This framework is indeed quite generic, though apparently not the most abstract one that is achievable (see Sect. 2.4).

2.2.5 Large-Scale Computer Simulations: A Virus in Terms of Its Atomic Constituents

As we have seen in the previous sections, bridging the scales requires a number of iterations between the micro and macro levels, unless the mechanism of pattern formation is the main focus of interest. In the iterative procedure, on each level one has to deal with a number of degrees of freedom that is considerably reduced as compared to the original full set on the smallest scale. Most important is therefore a suitable choice of variables on the intermediate scales, in terms of which the dynamics becomes tractable. On the other hand, in view of today’s high level of computer power one may wonder about using a brute force method instead, and numerically simulating the laws from the micro- to the macroscale in a single step. This means following the many paths (worldlines) of all individual constituents over a certain amount of time from the subatomic or atomic scale to the scale of macromolecules, deriving biophysics in terms of particle physics via large-scale computer simulations. Indeed, simulating a nano-machine like a virus in terms of its atomic constituents is feasible, as the following example of the mosaic tobacco virus will show.

This virus is rod-shaped. Its ribonucleic acid (RNA) is surrounded by a coat of proteins. Its name comes from the fact that it causes mosaic-like symptoms in plants. The virus causes abnormal cellular function that does not kill the plant but stunts growth. Its deleterious effect is not restricted to the tobacco plant, since it can infect other plants as well. In order to combat the virus and control its spreading, one should understand its key regulators and survival mechanisms. A step in this direction was taken by the molecular dynamics simulations described in Freddolino et al. (2006) with up to one million atoms over a time interval of 50 ns. The simulated virus consists of a capsid, composed of 60 identical copies of a single protein, and a 1,058 kb RNA genome. It is modeled by 949 nucleotides out of the complete genome, arranged into 30 double-stranded helical segments of 9 base pairs each. Only the RNA backbone in the 30 stems was resolved at atomic resolution. These numbers should give some hints on the structure of the virus, but

they are not sufficient for a complete description, which cannot be provided in this context. One of the results states that the capsid becomes unstable without RNA. This has implications for assembly and infection mechanisms.

The reductionism here amounts to the fact that one “only” has to know Newton’s equations of motion (as an approximation of the original quantum mechanical system) with the appropriate forces and the appropriate interaction topology on the atomic level to let the system evolve. The success of this approach lies in the important insights it provides on how to control this virus. A further advantage of such *in silico* experiments is the ease of manipulating the virus. One may rarefy certain constituents more easily than *in vitro*, to check their effect on the evolution of the remainder. In this way the simulation can explore strategies to combat the virus that can be used later *in vivo*. However, it should not be thought that this kind of realization of reductionism, down to the atomic level, comes cheaply. There is no such thing as a free lunch, and this is a case in point. Rather advanced computer algorithms are needed along with parallel computing and a sophisticated network between the parallel processors to obtain the results in a reasonable time (see Freddolino et al. (2006) for further details). On today’s laptops, these simulations would take decades. In general, the CPU time of molecular dynamics simulations is easily of the order of millions of CPU-hours.

Still we may be tempted to extrapolate the computer power of today and ask when we shall be able to simulate *humans*. If we were able to do so, would that mean that biophysics explains life? Apart from numerous medical and technical applications, let us list some typical topics addressed in biophysics, such as the efficiency of nano-machines, the control of cell logistics,⁷ the communication of nerve cells, the emergence of macroscopic features from local forces acting at junctions of the cytoskeleton, and the intermediate energy states of cellular fusion and fission events. Addressing these topics using tools from biophysics will lead to deeper insights into the fascinating nano and micro worlds, leaving open, however, the core mystery of how life emerges from non-living ingredients, the topical goal of artificial life studies.

We would like to add a remark on the demands and feasibility of computer simulations today. In the example of the tobacco virus, the computer simulations bridge the scales from atoms to macromolecules. Therefore to outsiders of particle physics, it may come as a surprise how demanding first-principle calculations are when they merely bridge the subnuclear scale of quarks and gluons to the nuclear scale of mesons and baryons. Let us consider typical first-principle calculations in (lattice) quantum chromodynamics, implemented on a space-time grid of size $128^3 \times 256$. In order to calculate decay constants or excited states of the mass spectrum of mesons or baryons to an accuracy of the order of a few percent (for the experts, using the framework of staggered fermions), the number of required floating point operations is estimated to take of the order of 200 years if 10^{12} floating

⁷ It is instructive to consider cells as factories with a production output that has to be delivered at a certain time.

point operations are executed per second (in short, 200 Tflops/s-years). This means that about 50,000 processing units (cores) would be required to run for 1 year (Khaleel 2009). This should indicate the effort required for numerical first-principle calculations, even if one stays within the realm of particle physics. The compact notation for the Lagrangian in (2.9), the one that enters the path integral formulation of quantum chromodynamics, may obscure the extent of this effort to the outsider. The fundamental interactions between elementary particles are anything but elementary to handle.

Whatever an appropriate formulation of this kind of suggested “conservation law” might be, we may say that, whenever reductionism is pushed to its extreme, it will exact a price from us. It is as if hidden subtleties pop up and take revenge for the decomposition into simple constituents, so that the effort required of us is kept constant.

2.3 Limitations of Reductionism

2.3.1 *A Fictive Dialogue For and Against Extreme Reductionism*

To present the different mind-sets with respect to an extreme version of reductionism, we start with a fictive dialogue between two representatives, one, called PRO, extrapolating the power of reductionism to the extent that particle physics ultimately explains everything, and CON, pointing out the limitations of reductionism.

PRO: Knowing the laws on the fundamental scales, that is, on the scale of elementary particle physics, we can explain the whole world, at least in principle.

CON: Certainly some aspects, such as the reason why atoms stay together unless the temperature gets sufficiently high, and things like that, but not all. You are confusing the fundamental scale with fundamental phenomena. What is special about the scale of particle physics, or, more precisely, about the Planck scale (as the smallest scale we can talk about using classical notions of space), is its extreme value, but fundamental phenomena and fundamentally new phenomena occur also on larger scales.

PRO: I disagree, for the following reason. Let me be overly optimistic and extrapolate the present computer power by orders of magnitude as compared to today. We do know the laws of the four fundamental interactions in their ultimate form of local gauge theories (including gravity). Let us postulate initial conditions, which are extrapolated backwards in time from the CMB data observed today, to represent the soup of elementary particles at the end of the Planck epoch and the beginning of a universe in which we may use classical notions of space and time. Now let us rerun the tape of evolution in silico, at least in some sequences, with a supercomputer of a future generation. My claim is that the supercomputer would reproduce the formation of protons and neutrons out of the quarks and gluons,

nuclei, atoms, molecules, macromolecules, proteins, nanomachines, and to cut a long sequence short, life. Or, to quote M.L. Goldberger and W. Panofsky from Anderson (2011): “Other branches of physics [than particle physics]...are interesting, challenging, and of great importance. The objectives are not a search for fundamental laws as such, these having been known...since the 1920s. Rather, they are the application of these laws.”

CON: To directly reply with another quote from Anderson (2011): “If broken symmetries, localization, fractals and strange attractors are not “fundamental”, what are they?” Even if computer simulations were to predict the emergence of molecular machines in the same way as they predict the emergence of spontaneous symmetry breaking in a magnet, they would fail to explain emergent features on each scale in simple terms, they would fail to provide a coarse-grained description on the coarse scale, to generate acts of cognition like interpreting DNA as a carrier of information.

PRO: On each scale there are new emergent features due to the act of cognition, I agree, but cognition is subjective. It is only ourselves who interpret DNA as a carrier of information, and even the selection of objects that are declared to be elementary on the coarse scale is down to us; it is our choice. This cannot and need not be reproduced by the supercomputer when it starts from the initial set of elementary particles and evolves them towards the nanoworld.

CON: Cognition of the kind declaring that composed objects are new elementary ones on a larger scale may sound subjective, but it has an objective pendant. Consider the fact that physical processes on the coarse scale may not be able to resolve the composition of composite objects. In processes with a typical momentum transfer that is much smaller than the mass scale, characteristic of the structure of the bound state, the structure cannot be resolved and the bound state will appear to be an ordinary particle. Fundamental fields and composite fields should then be treated on a completely equal footing (Ellwanger et al. 1994). As an example, consider mesons. On energy scales typical for mesons, which are quark–antiquark bound states, the particles are much more simply described in terms of mesonic degrees of freedom than in terms of their constitutive quark and gluonic degrees of freedom. Beyond the phenomenological level, here the mathematical derivation itself suggests to introduce new degrees of freedom on the lower energy scale. Last, but not least, changing the scale gives rise not only to new objects that should be considered as elementary, but also new interactions between them.

PRO: Why do you need your coarse-grained description, which is supposed to hold only on a single scale, the scale under consideration, if the supercomputer evolves the formation of larger and larger composed objects out of the fundamental ones? Let it go on and simulate humans.

CON: I need it precisely for my understanding in terms of simple mechanisms. I need this kind of understanding to abstract universal features from different realizations, to be inspired to new ideas, and in particular to design the new computer generations you are looking forward to.

2.3.2 DNA from the Standpoint of Physics and Computer Science

Let us illustrate the CON perspective from the previous dialogue using the example of DNA. From the physics standpoint, DNA is a flexible macromolecule with a certain charge density and electrophoretic mobility, and a helix–coil transition. It stretches, melts, and changes twist under tension (Gross et al. 2011). It consists of two entangled polymers of helicoidal structure and its configuration depends on the degree of hydration and the ionic strength of the solution. The structure and state of DNA is also triggered and determined by its interaction with many other biomolecules, especially DNA-binding proteins or enzymes, which can compact, align, or bend DNA. Essentially two type of forces stabilize the double helix structure: hydrogen bonding between complementary bases and stacking interactions of the base pair plateaux. DNA is certainly a challenging object from the perspective of physics. During transcription and replication, it undergoes large conformational changes, like other polyelectrolytes. Due to large amplitude motions, nonlinear dynamics must be taken into account (Yakusheich 1998) and thermal fluctuations play an important role in its functioning. Earlier, physical experiments on DNA were performed by methods from condensed matter physics, while more recently, new powerful techniques have been developed. In particular, single-molecule experiments nowadays allow one to measure forces in the pN range (10^{-12} N), so that the elastic properties and interaction forces of single DNA molecules can be investigated directly (Bustamente et al. 2003). Together with experiments, theoretical models were developed which require tools from statistical physics and nonlinear dynamics. So it is definitely the laws of physics that both enable and constrain the basic functions and modes of performance of DNA.

However, no computer simulation in terms of its atomic constituents could create the insight that DNA acts as a carrier of genetic information, nor would it be able to establish a possible bridge to computer science that we want to sketch in the following. In an “act of cognition”, one may wonder why DNA makes use of four characters (ACTG) in its alphabet and 20 amino acids plus one stopper. A look at searching problems in computer science may shed some light on this very choice of numbers (Patel 2001), although it is currently too early to claim that computer science will eventually explain this choice. A particular class of search problems there refers to search in an unsorted database with N distinct randomly arranged objects. The task is to locate a certain object by asking a set of Q questions. The set should be minimal. If the search is performed as a quantum search procedure, it has been shown by Grover (1997) that, for given N , the number of queries Q is determined by

$$(2Q + 1) \sin^{-1} \left(\frac{1}{\sqrt{N}} \right) = \frac{\pi}{2}, \quad (2.25)$$

so that asymptotically $Q = \pi\sqrt{N}/4$. Note that for given N , Q may not be an integer, so that a small error remains if it is chosen as such, but the search is accelerated by a

factor of \sqrt{N} as compared to classical search procedures. For small N , we obtain $Q = 1$ for $N = 4$ and $Q = 3$ for $N = 20.2$. As pointed out by Patel (2001) in this connection, base pairing during DNA replication corresponds to one yes/no query, to distinguish between the $N = 4$ possibilities of characters ACTG. The triplet code of DNA has $Q = 3$ consecutive nucleotide bases carrying $N = 21$ signals. Three base pairings between the t-RNA and m-RNA transfer this code to the amino acid chain. This may suggest that DNA provides the hardware that is best suited for the implementation of a kind of quantum search algorithm. A quantum search may be realized in classical hardware (Bhattacharya et al. 2002). Therefore the fact that DNA behaves as a whole as an object from classical physics is not an immediate objection.

This example shows that more and more phenomena emerge on the scales of biophysics, along with new phenomena, new properties of composites, and new rules governing their interactions. The qualitative variety proliferates so greatly that other disciplines than physics are needed to understand them, i.e., approaches from a range of different perspectives are needed.

2.4 Outlook: A Step Towards a Universal Theory of Complex Systems

In the previous sections we have pointed out that it is not meaningful to talk about a “World Formula” or a “Theory of Everything”, although such extrapolations occur repeatedly in the literature. Still there are striking universal features across the scales and between dynamical systems. Does the mathematical framework developed so far capture them in a satisfactory way or can we go a step beyond stochastic partial differential equations and the field theoretic formalism, to a more abstract and more generic level of description?

Let us first summarize some striking facts, using the terminology of Mack (2001) in terms of “death”, “growth”, “motion”, and “cognition”. So far we have seen similar fundamental processes on very different scales such as annihilation in particle physics, deletion in chemical processes, extinction of species, which may be summarized under “death”; creation in particle physics, replication in biology, composition, fragmentation (as the reverse process), and recombination, summarized under “growth”; diffusion, drift, migration, summarized under “motion”; and, last but not least, the emergence of new degrees of freedom from scale to scale, the creation of new links between objects with matching internal structure, summarized under “cognition”. Moreover, what induces death and growth in the former sense shares common features. We distinguish interactions as attractive or repulsive, activating or repressive, excitatory or inhibitory, short- or long-ranged, leading to binding and unbinding events, fusion or fission, selection or coexistence, competition or frustration (The very notion of frustration, familiar from the context of spin physics, is already a more generic concept than is usually assumed (see Mack (1981)).).

One may suspect that, although these analogies are evident, they hold at best on a superficial level. However, there is a formal manifestation in a framework that captures these analogies. It is the framework of (quantum) field theory, which can be applied whenever the state of the system can be described by a distribution of occupation numbers assigned to sites of a grid, and in which the time evolution refers to functionals of these occupation number distributions, as we mentioned earlier. However, when field theory is successfully applied to ecological systems⁸, for example, this does not imply that biology is “physics” after all. It is merely the mathematical complexity of the description that is shared between the different areas of application. Still, although the language used in the field theoretic formalism is very generic, it may not be the most abstract one that is accessible for applications in physics.

A further step may be the framework of local category theory, as proposed by Mack (2001). Laws then correspond to regularities of relations, graphically represented as links, that is, relations between objects and agents, the latter being represented as nodes of a network. *Systems* are defined as such networks equipped with a minimal set of axioms. The axioms are from category theory, the mathematical theory of relations, extended by a notion of locality that is not restricted to locality in space-time. The dynamics of these defined systems is described in terms of certain *mechanisms*: motion, growth, death, and cognition, examples of which we gave above. Formally, mechanisms are conditional actions of basic local structural transformations. Motion, for example, is then characterized by the fact that indirect links become direct. The dynamics can be stochastic or deterministic. The only information put into the systems is *structure*. Systems differ by their structure, which is characterized by constitutive constraints and conservation laws. Nonlocal phenomena emerge from local interactions leading to new functionality via cooperation.

Remarkably, the framework uses a mathematical language that is abstract enough to include the gauge theories of fundamental interactions, the dynamics of space-time, basic life processes, and—going beyond the material properties of the world—even propositional logic. With this brief outline of Mack’s proposal, we refer the interested reader to the original reference and references therein.

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⁸ For an example in which the field theoretic formalism was used in connection with ecology, see again (Mobilia et al. 2007).

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