Numerical Experimentation: A Third Way to Study Nature

Marie Farge

Summary. We will outline the history of the numerical approach and trace back the origins of the use of computers to carry out simulations in mathematics and physics. We will then present the techniques used, by taking as example the finite-difference method to solve PDEs and discuss the nature and impact of numerical errors. Finally, we will argue that numerical simulation pertains more to experiment than to theory.

'Although this may seem a paradox,
all exact science is dominated
by the idea of approximation'

(Bertrand Russell, The Scientific Outlook, 1931)

1 Historical Sketch

The numerical approach goes back much further than the appearance of the first computers. In a paper submitted in 1822 [1], Charles Babbage already suggested using numerical machines to calculate astronomical tables. These machines were made up of an 'attic', where data were stored, and of a 'mill', where calculation took place. However, this consisted merely in numerically evaluating some solutions, already known analytically, and not, in fact, performing simulations in the modern sense. Numerical simulation is defined as solving the equations that describe the physical laws governing the system studied by using algorithms. One can trace its origin back to the year 1899, with the development of the finite difference method by Sheppard [2]. It was then developed by Richardson [3] who used it, from 1910 onwards to calculate the stress exerted upon a dam. Richardson later had the idea of numerically solving the equations of atmospheric dynamics in order to predict the weather. He designed for this a finite difference scheme, which now bears his name, and applied it to find out the atmospheric situation on May 20th 1910. After six

weeks of hard work he had only managed to compute the state of the atmosphere for two vertical columns, and the values he was obtaining then, for the wind and pressure fields, were already quite different from those observed. He then realized that to perform this calculation by hand, at the same speed as the current atmospheric evolution (which is the minimum required to have prediction rather than 'postdiction'), it would require 64,000 people to get a new state of the atmosphere every 3 h using a computational grid of $200 \times 200\,\mathrm{km}^2$ over the whole Earth. In a book published in 1922 [4] he went as far as to imagine a city with a huge theater at its center where 'a myriad computers are at work upon the weather of the part of the map where each sits, but each computer attends only the one equation or part of an equation'. Each one at a grid point, under the leadership of one person in charge of synchronizing the computation 'like the conductor of an orchestra in which the instruments are slide-rules and calculating machines!'. Such a project never came to pass, which is just as well since O'Brien et al. [5] showed in 1950 that Richardson's scheme is unconditionally unstable. The mathematical justification of the numerical approach was given by Courant, Friedrichs and Lewy in a paper published in 1928 [6]. They proved that discrete equations actually constitute an approximation of continuous partial differential equations (PDEs), as long as some stability conditions, known as 'CFL conditions', are satisfied.

Numerical simulation, in its modern sense, implies the use of computers to carry out calculations. Computers appeared at the beginning of the Forties. The first were the Z2 and the Z3, built in Germany by Konrad Zusse in 1939 and 1941, respectively, but they were destroyed during the war. Independently Turing at Cambridge, England, was developing calculators to decipher codes, but unfortunately most of the information about his work is still classified. The first computer built across the Atlantic was the Mark I, which was completed by Aiken in 1944 at Harvard University, with the help of IBM. Meanwhile, at the University of Pennsylvania, Mauchly and Eckert were designing the ENIAC, which was installed in 1946 at the Ballistic Research Laboratories of Aberdeen, Maryland. They then founded the company Univac, which in 1951 was the first to launch a computer on the market.

The first two people to have foreseen the impact that computers could have in mathematics and physics were von Neumann and Ulam. The latter recounts in his autobiography [7] that: 'Almost immediately after the war Johny and I also began to discuss the possibilities of using computers heuristically to try to obtain insights into questions of pure mathematics. By producing examples and by observing the properties of special mathematical objects one could hope to obtain clues as to the behavior of general statements which have been tested on examples'. He went on to show, for the sake of example, how numerical experiments could help study the regularity of some solutions to PDEs, and concludes by explaining that: 'In the following years in a number of published papers, I have suggested – and in some cases solved – a variety

of problems in pure mathematics by such experimenting or even merely observing'. Thus, right from the beginning, two of the essential contributions of computers to research in mathematics and physics were already foreseen, namely the possibility of experimenting with equations and of 'seeing' their solutions. These two points will be illustrated in the third part.

During the Second World War, part of von Neumann's research in Los Alamos was about the development of numerical schemes and the definition of a stability criterion, which bears his name, allowing one to choose optimal space and time steps when discretising parabolic equations with a finite difference scheme. Von Neumann never published this work (which can, nevertheless, be consulted in his complete works [8]); indeed, he deemed it too approximate, since it did not take into account, either the nonlinear terms, or the boundary conditions. Nonetheless, such a method is still widely used and is being developed, yielding very general extensions where the discretization of the boundary conditions plays a role. In 1949 von Neumann and Richtmyer conceived a numerical technique to calculate the shocks which appear in compressible flows [9]; at the time, the problem was still out of reach analytically due to the presence of singularities. The method which they adopted consisted in introducing some dissipative terms in the equations to spread the shocks and creates boundary layers that were at least of the size of the computation in order to smooth out any singularities. The technique is still very much in use today. Von Neumann then set out, along with Charney and Fjörtoft, to integrate numerically an atmospheric barotropic circulation model, i.e. which neglects the temperature variations along the isobar surfaces. This model used the vorticity equation instead of the primitive equations with pressure–velocity form, and suppressed the flow to be quasi-geostrophic – i.e. with a stable horizontal stratification – and nondivergent, i.e. supposing the fluid to be incompressible. The computational grid was of 15 times 18 grid points and only covered the US, which corresponded to a space resolution of 736 km. The numerical resolution, carried out in 1950 on the ENIAC of Aberdeen, made it possible to calculate a 24 h meteorological evolution on the 5th, the 30th and the 31st of January, and of the 13th of February 1949. In their article [10], the authors made the following remark: 'It may be of interest to remark that the computation time for a 24-h forecast was about 24 h, that is, we were just able to keep pace with the weather. However, much of this time was consumed by manual and I.B.M. operations, namely by reading, printing, reproducing, sorting, and interfiling of punch cards. In the course of the four 24-h forecasts about 100,000 standard I.B.M. punch cards were produced and 1,000,000 multiplications and divisions were performed'. The authors then compared the predicted fields with those obtained and endeavoured to account for the prevision errors that were observed. According to them, they were due to too coarse a computational grid and to the fact that the baroclinic effects (i.e. the pressure variations) had been disregarded. This first numerical simulation, performed in collaboration with Smagorinsky from

the US Weather Bureau and Mrs. von Neumann who was programming the ENIAC, is at the origin of the present dynamical models used to study meteorology and climatology, e.g. general circulation model (GCM) which take into account the whole planet.

In the beginning of the 1950s John von Neumann completed his computer, called EDVAC, at the Institute for Advanced Studies in Princeton and then built a second one, which was installed by Metropolis in Los Alamos where it remained in use until 1971. On this latter machine, von Neumann and Fermi undertook the simulations of the first hydrogen bomb, and particularly the study of hydrodynamic instabilities such as the Rayleigh–Taylor instability [11], as well as the calculation of neutron cross-sections. On this occasion Ulam proposed the Monte-Carlo method, for which, in order to solve problems involving a large number of particles, one chooses a subset of statistical samples instead of studying all possible configurations. This technique, which is widely used nowadays, does not give an exact solution, but merely an estimation for a given error, and it allows the resolution of problems that would otherwise remain unsolved.

From very early on, Fermi has foreseen the use of computers and he undertook, along with Pasta and Ulam, to study numerically the evolution of a system of interacting particles that was marginally nonlinear. To their great surprise, they discovered that, instead of leading to energy equipartition, on the contrary, the system presented quasi-periodical solutions, which contradicted the ergodic hypothesis of statistic mechanics [12]. At the beginning of the 1960s, Kruskal and Zabusky took over the same research program but considered a quadratic rather than a cubic nonlinear interaction; they showed that the system was described by the Korteveg-de Vries equation. They integrated it numerically and found wavelike solutions, whose behaviour recalled that of the particles (since they preserve their shape and their velocity after interaction). They called them 'solitons' [13–15]. These numerical experiments paved the way for a whole row of new problems concerning nonergodic dynamical systems where are still at the frontier of statistical physics.

To conclude this first part, in which we have tried to cast light upon some of the works grounding the numerical approach, we would like to quote Ulam once more. His vision of mathematics is after all couched in a language that does somehow recall that of Thom [7]: 'The recent study of the mathematics of morphogenesis and the possibility of studying experimentally on the computer the dynamics of competitions and conflicts between different geometrical configurations, on the model of life's struggle, could lead to new mathematical concepts. [...] The use of the computer seems, not only practical, but absolutely essential for such experiments which require to follow those games and fights over a large number of stages and steps. I believe that the experience gained by following the evolution of such processes will have a fundamental influence that may, one day, finally generalise, or even replace, in mathematics the exclusive immersion in formal axiomatics we presently have'.

2 Simulation or Simulacrum?

In a footnote from his book 'Stabilité Structurelle et Morphogénèse', René Thom remarks: 'classical Euclidian geometry can be considered as magic. At the price of a minimal distortion of appearances (the point with no extension, the straight line without any thickness), the formal language of geometry adequately describes spatial reality. In this sense one could say that geometry is successful magic'. We believe that numerical simulation can also be considered as 'successful magic', at the cost, this time, of a minute distortion of the equations, this distortion being exerted the other way around. Indeed, this method consists in replacing the differential equations by discretized algebraic equations; and one notices – here comes the magic – that their numerical processing allows to reach solutions which adequately describe the physical reality. However, such an astonishment is not so much the lot of the sole numerical approach as that of the entire physics: 'The most incomprehensible thing of the world is that it is comprehensible'(Einstein).

A numerical simulation unfolds in five stages:

1. *Defining the problem.* The phenomenon (e.g. physical, biological, economical) to be studied is defined and the questions the numerical simulation aims to answer are stipulated.
2. *Choosing the mathematical model.* The problem is typically, but not always, described using a system of integro-differential equations defined in space and time, with suitable initial and/or boundary conditions chosen to ensure that the problem is well posed, i.e. such that solution depends continuously on them. In practice, many problems are actually ill-posed, e.g. inverse problems such as deconvolution or tomography using Radon transform, and require adhoc procedure to deal with.
3. *Discretizing of the continuous equations.* The continuous variables are replaced by a set of discrete and finite values, given only for a subset of points, evenly distributed in space and time, which defines the computational grid. Moreover, each integro-differential equation is replaced by a finite set of algebraic equations which are verified at each point of the computational grid. This procedure corresponds to the finite-difference method, although there exist other methods based on a similar principle. For instance, spectral methods decompose each continuous variables into an infinite series of orthogonal functions, chosen according to the problem and its geometry; the series is then truncated to a finite number of terms, and the norm of the discarded terms evaluates the truncation error.
4. *Choosing of the numerical algorithm.* The algebraic equations are solved using a numerical algorithm chosen according to its computational efficiency, memory requirement and numerical precision on the computer one uses, which could be of different types (scalar, vectorial, parallel, or a combination of these).

5. *Programming the computational code*. One selects the programming language, according to his preference and practice, and then the most efficient compiler available on his computer. These choices should be made in order to maximize computational performances, but also to guarantee readability and portability of the code, keeping in mind that several people will have to use it, modify it and implement it on different computers having different compilers, which both evolve on very short time scales.
6. *Testing the code*. After having written down the computer program, one checks the convergence of the numerical scheme by reducing the space and time steps until the solution does not change anymore. The code is then used to solve a known case or, should such 'test case' be missing, at least verify that the structural consistency (the conservation of symmetries and invariants) of the numerical scheme is correct. These tests are also important to estimate the observed numerical errors and compare them to their theoretical values predicted by numerical analysis theorems.
7. *Analysing and visualizing the results*. Present computers perform number crunching at a tremendous rate (up to several teraflops, i.e. trillions floating point operations per second) and therefore generate huge datasets which have then to be analyzed and represented. A numerical simulation then requires signal processing (e.g. statistical analysis, filtering, denoising) and visualization as a laboratory experiment does.

By describing the nature of the numerical errors, we would like to evaluate the risk of simulation being a *simulacrum*, i.e. the risk that one might be misled by a fake representation of the *phenomena*. For the sake of example, we will confine ourselves to studying numerical errors encountered in the finite-difference method, and will briefly tackle the case of the Monte-Carlo method. This discussion boils down to the following problems: existence and uniqueness of the solution (are the equations well-posed?), consistency (is the phenomenon under study akin to that predicted by the simulation), stability (does the numerical code amplify errors and diverge?) and convergence (does the approximate solution remain sufficiently close to the exact solution?).

2.1 Existence and Uniqueness

Regarding the mathematical formulation of the phenomenon one wishes to simulate, the first question to arise deals with the existence and, for evolution problems, the uniqueness of the solutions of the equations, for the chosen boundary conditions. Typically, the problems solved by using numerical methods are two-fold:

– *Initial value problems* (Cauchy problems), where the computation is performed from an initial state, considering appropriate boundary conditions, by solving PDEs, which could be, either elliptic (e.g. diffusion equation), parabolic (e.g. transport equations), or hyperbolic (e.g. wave equation),

– *Boundary value problems*, where there is no time evolution and the values inside the computational domain should only satisfy the boundary conditions; they are also called, figuratively, 'jury problems', since the values inside the computational domain should 'agree' with those at the boundary. Elliptic equations (e.g. Poisson's or Laplace's equations) in general belong to this category.

If the equations are linear, one can generally rest assured that one solution does exist, insofar as one has a sufficient number of boundary conditions to close the system and that one only studies the evolution forward in time. Nonetheless, one of the most useful applications of the numerical approach is the treatment of nonlinear problems, which are described by nonlinear equations for which there seldom exist theorems proving existence and uniqueness of their solutions, neither analytical methods to solve them. Let us take, for the sake of the example, the case of fluid dynamics, whose fundamental equation are the so-called 'Navier–Stokes equations'. One can guarantee the existence and uniqueness of their solutions, but only for Reynolds numbers (defined as the ratio between the nonlinear and the linear terms of Navier–Stokes equations) below order one [17]. Conversely, for large Reynolds numbers, if existence of the solutions (in the weak sense) is well established [18, 19], it is not the case for their uniqueness, except in dimension two [20, 21]. Indeed, beyond a critical value, which corresponds to the transition laminar and turbulent regimes, uniqueness has not yet been proven in dimension three, since one then does not know any longer how to control the nonlinear terms [22] without increasing dissipativity (e.g. the power of the Laplacian which takes care of viscous damping) [23, 24]. As for Euler equation (which corresponds to zero viscosity), the problem of existence and uniqueness for all times has been solved in dimension two, but not yet in dimension three [25].

When there is no uniqueness of the solutions, then, the problem is ill posed (in Hadamard's sense), i.e. there is no continuity between the solution and the data. In most cases uniqueness is intimately linked to the regularity for all times. Nowadays, computers play an important heuristic role to study such properties, either by studying Taylor expansions of the solution, or, thanks to direct numerical simulations (DNS), by estimating when a singularity may intersect the real axis [26] which would result in finite-time blow-up of the solution.

2.2 Consistency and Precision

When one discretizes a differential equation one must wonder whether the algebraic approximation is indeed consistent, i.e. is the discretized equation equivalent to the differential equation which one is trying to integrate? The idea of consistency spans the two following properties:

– The discretized equation must tend towards the continuous equation when the space and time steps tend towards zero.

– The discretized equation must preserve the structure (e.g. Hamiltonian, sympletic) structure and the symmetries of the differential equations, or, more precisely, its invariance group must be a subgroup (as large as possible) of that of the original differential equation.

If we consider as example finite-difference schemes, it is of much importance that the first property should be verified, and it is, indeed, the case of the most known discretization schemes. As for the second property, on the other hand, it is only verified for centred finite differences, there, unknown values at grid points are expressed in terms of an even number of values at neighbouring points.

In practice, of course, one uses time and space steps that are not equal to zero. Therefore, even if a discretization scheme is consistent, it will nonetheless introduce errors, which are called truncation errors. The precision of the numerical results depends on both:

– The *round-off error*, which stems from the limited size of the memory words (usually 32 or 64 bits) of the computer which is used
– The *truncation error*, which is directly linked to the order of the discretization scheme (i.e. to the order of the neglected terms in the Taylor's series expansion of the differential operators).

Typically, for first-order schemes the truncation error has a diffusive effect on the solutions, which thus smooth the gradients. For second-order schemes the truncation error does have, conversely, a dispersive effect that is characterized by the appearance and spreading of spurious oscillations in high gradient regions (e.g. shocks, fronts) [27]. The behaviour of the truncation error varies according to the order of the discretization scheme, but its amplitude, on the other hand, does only depend on the space step. Therefore, it is always possible to limit the truncation error by reducing the size of the computational grid. As for the round-off error, however, it does not depend on the discretization scheme but on the precision of the computer one uses. In practice, this error is always negligible in comparison to the truncation error.

2.3 Stability and Convergence

Once it is verified that the chosen discretization scheme really is an approximation of the PDEs problem, one should raise two questions:

– Is the calculation process stable, that is to say, does not it amplify the round-off errors at the risk of diverging?
– If it is stable, does the numerical solution converges towards that of the PDEs problem when space and time steps are tending towards zero?

Lax's [28] equivalence theorem does state that: 'Given a properly posed initial-value problem and a finite-difference approximation to it that satisfies the consistency condition, stability is the necessary and sufficient condition

for convergence'. Thus, insofar as one has already answered affirmatively to the questions of paragraphs II.1. and II.2., the problem of stability and of convergence does come to one sole and only question: is the numerical scheme converges?

Generally one studies the stability of a scheme by carrying out the harmonic analysis of a perturbed solution. One checks that the frequencies' amplitudes in the power spectrum remain bounded when the number of time steps increases, so as to prevent the round-off errors from increasing and the computation from diverging. This is the principle of von Neumann's analysis. It shows that the explicit schemes (i.e. those for which the unknowns are explicitly expressed in terms of the values computed at the previous time step) are unstable or conditionally stable, whereas the implicit schemes (i.e. those for which the unknowns are implicitly expressed in terms of both previous values and unknown values at the neighbouring points) are unconditionally stable [27]. Von Neumann's analysis thus allows us to estimate, depending on each case, the maximal time step able to preserve the stability of the solutions, i.e. a time step that is sufficiently small for the computation to follow the flow evolution [27]. (To draw an analogy, one can think of the focusing of the obturation time of a camera lense in function of the speed at which the photographed object moves). If one adopts the viewpoint of stability, the analogy between the numerical experience and the laboratory experience allows us, for a given price, to reach a certain spatial and temporal resolution, just as the resolution and the dynamical behaviour of a numerical simulation depend on the chosen grid size and consequently on the available computation resources.

Nevertheless, von Neumann's criterion does merely apply to the simplest linear problems, since it does take into account neither nonlinear effects, nor incidence on stability of the discretized boundary conditions. In view of the impossibility in which the numerical analysts are to establish stability criteria that are adapted to the numerical treatment of nonlinear equations, we are suggesting to resort to a more physical analysis, that some may condemn as a rather too intuitive one. This approach draws upon the analogy there is between the mechanisms which govern the physical problem (e.g. physical instability) and those which ensure numerical stability. It proceeds from the following principle: 'To obtain numerical stability there must be hydrodynamic stability at the scale of the computational mesh' [27]. The hydrodynamic stability is conditioned by the balance which exists, at a certain scale, called the dissipation scale (Kolmogorov's scale built upon the molecular viscosity), between the advective forces governed by the nonlinear terms and the diffusive forces described by the linear terms of the Navier–Stokes equation. One incurs the risk that instabilities may develop if the nonlinear terms take over the linear terms, i.e. when, the advective forces dominate the diffusive forces. Similarly, numerical instabilities appear in a simulation when, on the scale of the computational mesh, the nonlinear advective terms take over the linear diffusive terms; in this case the smallest perturbation, introduced for instance

by the discretization of the boundary conditions or by truncation errors, is amplified by the nonlinear terms before having had time to be damped by diffusion, and the calculation diverges. Thus, to guarantee numerical stability, one must choose a computational mesh which is sufficiently fine for diffusion to dominate at the smallest scale. This is further expressed by saying that the grid Reynolds number (ratio of the advective terms upon the diffusive terms at the scale of the grid) must always remain inferior to 1. In practice, the destabilizing effect of the nonlinear terms cannot really be felt below a Reynolds of 4 [29].

Until now, we had only been dealing with models built according to the equations that govern the physics of the *phenomena* which we are studying: the computer is used to integrate these equations and, given the numerical errors, the link between the underlying theory and reality solely hinges upon the adequation of underlying theory and reality. There is a second category of numerical models for which this link is much more questionable, namely Monte-Carlo methods, that we have already mentioned in the first part. Indeed, these models are based on stochastic processes, which seem to have no relation a priori to the phenomenon under study but whose statistical behaviour proves to be similar as long as one chooses adequate statistical samples. In this case, the computer is used as a random number generator and, among all realizations thus obtained, one only keeps those having enough physical 'realizability', e.g. which verify the conservation and symmetry properties of the phenomenon one wishes to simulate. The relevance of such models to reality rests upon the partial isomorphism which exists between stochastic processes and differential equations. This approach turns out to be highly heuristic, and in practice there are only two ways in which to test these models: either by comparing them to laboratory experiences, or by performing a large number of simulations and check that the variance of the set of solutions is sufficiently small value; unfortunately this is usually is too costly in terms of computation time to be done thoroughly.

To conclude, we think that the question 'simulation or simulacrum of the phenomena?' is not specific to the numerical approach, but to the entire field of physics. The study of the phenomena with the help of numerical simulation does not seem to us to be more 'artificial' than this very study carried out thanks to experiments as complex as those used in physics nowadays: the risk of *simulacrum* is not greater when one studies the behaviour of dynamical systems thanks to computers than when one observes that of the particles thanks to accelerators or that of galaxies thanks to telescopes. Indeed, the distance between the phenomena and their observation is such that one always needs theoretical principles to discern what one holds as true from the rest of the artifacts.

The terms '*simulacrum*' and 'simulation' have a pejorative connotation and mean, for the first, 'image, idol, representation of false gods' but also 'action faked to mislead', and for the latter, 'disguise, fiction' [30]. Such a terminology may well hide some symbolic meaning, where one finds again

the opposition between ideas and idols [31], laws and observables, where one encounters both the risk of an illusory fascination exerted by the computer and the original dependency which links that same computer to the military-industrial *nomenclature*. But, to answer the question, we had rather avoid using both terms, 'simulation' or 'simulacrum', and use instead the word 'experimentation', which corresponds a lot better to what simulation is used for in mathematics and physics, that is to say, the possibility to experiment with the equations or with the principles governing the phenomena under study.

3 Numerical Experiment

We would like to illustrate the role played by the computer in physics by choosing, for the sake of the example, the study of turbulence, that is to say, the study of dynamical systems having a chaotic behaviour. The turbulence is a rather beautiful source of 'formless forms', which is the first type of unstable morphologies according to Thom's classification, who gives the following description: 'Certain forms are shapeless because they present an extremely complicated structure; being chaotic, they offer to analysis only little or no element to identify' [16]. It is precisely that type of morphologies which is encountered in the two-dimensional turbulent flows (see the figure earlier). The study of turbulent flows has a distinctive status from the epistemological viewpoint, insofar as the Navier–Stokes equations governing the fluid dynamics have always been unanimously admitted and only their integration poses problem. In an unpublished (but available in his complete works) article from 1946, written in collaboration with Goldstine [32], von Neumann emphasized the originality of this field in comparison with the rest of physics: 'The phenomenon of turbulence was discovered physically and is still largely unexplored by mathematical techniques. At the same time, it is noteworthy that physical experimentation which leads to these and similar discoveries is a quite peculiar form of experimentation; it is very different from what is characteristic in other parts of physics. Indeed, to a great extent, experimentation in fluid dynamics id carried out under conditions where the underlying physical principles are not in doubt, where the quantities to be observed are completely determined by known equations. The purpose of the experiment is not to verify a proposed theory but to replace a computation from an unquestioned theory by direct measurements. Thus wind tunnels are, for example, used at present, at least in large part, as computing devices of the so-called analogy type to integrate the nonlinear partial differential equations of fluid dynamics. Thus it was to a considerable extent a somewhat recondite form of computation which provided, and is still providing, the decisive mathematical ideas in the field of fluid dynamics. It is an analogy method, to be sure. It seems clear, however, that digital devices have more flexibility and more accuracy, and could be made much faster under present conditions. We believe, therefore, that it is

now time to concentrate on effecting the transition to such devices, and that this will increaser the power of the approach in question to an unprecedented extent'. Thus, with a stunning intuition given the possibilities of computers in 1946, von Neumann was suggesting to replace laboratory experiments by numerical experiments in order to study fluid mechanics problems, and especially turbulence. Such foreknowledge/insight was even rather optimistic when one thinks that the idea to replace wind tunnel experiments by numerical experiments was revived by NASA in 1978 ('Numerical Wind Tunnel' project of NASF) but had to be postponed sine die since the performances of the most powerful computers are still insufficient to numerically compute, without any adhoc turbulence model, flows with large Reynolds around complex three-dimensional geometries [33]. However, the progresses that have been made over the last thirty years, regarding as much the computers as the algorithms, are hardly imaginable. One example will be sufficient to illustrate this: to compute the flow past an airplane wing using Reynolds equations (averaged Navier–Stokes equations with first-order closure), one needs less than half an hour nowadays, whereas the same simulation tried forty years ago with the algorithms and computers then available would have been 10,000 times more expensive and the calculation of only one realization of the flow would have taken about 30 years [34]. But the advantage of numerical experimentation is not to replace laboratory experimentation, which would be, really, a dangerously illusory program insofar as simulation, just as theory, needs laboratory experiment to confirm or infirm its predictions, at least on a few test cases. No, the advantage of numerical approach is to open up new fields of experimentation that are out of reach in a laboratory: numerical experimentation should not replace laboratory experimentation but complement it.

The study of the two-dimensional turbulence is a particularly interesting case to illustrate the originality of the numerical approach in physics (see Fig. 1). Indeed, two-dimensional turbulence is practically out of reach in laboratory since it is encountered in large scale atmospheric and oceanic flows (and even then, this is a mere approximation). To study it, one needs to consider planetary scale, which is why simulation is the only method left in this case to actually experiment rather than observe. The numerical approach represents a break from the traditional scheme Thom had in mind when he wrote: 'From the epistemologist's point of view two types of morphological disciplines can be distinguished. Some disciplines are experimental: man can create the morphology under study (in physics, chemistry), or intervene, more or less brutally to say the least, in its development (as in biology). Other disciplines on the other hand are solely observational: no experimentation is possible either because of spatial distance (astronomy) or temporal distance (geology, paleontology, ethnography, history) or finally for ethical reasons (psychological and social phenomena)' [35]. This classification may indeed be widened since, some purely observational sciences could now be considered as numerically experimental sciences; for instance it is the case of paleoclimatology, the study

Fig. 1. Vorticity field computed by direct numerical simulation of a two-dimensional turbulent flow using a pseudo-spectral method [39]

of planetary atmospheres or that of galaxies' evolution. Numerical simulation thus allows us to turn purely observational sciences into experimental ones.

Numerical simulation is half-way between theory and experiment without replacing either, since theory, simulation and experiment are all interrelated. Just as an experiment requires a theory to be interpreted, and a theory requires an experiment to be refuted (or, as some would say, 'falsified'), a numerical simulation equally requires a theoretical model for its formulation, and also experimental results for its validation. In return, it can enrich the intuition of theoreticians and allow them to solve problems out of reach analytically, to imagine a larger number of cases, and to present the results in a graphical form which represents information in a more concise way. A numerical simulation allows the experimentalist to study the behaviour of a system by varying one parameter independently of the others, to know the value of the fields at all points in a given domain and to visualize phenomena which are too fine, too fast or too remote to be observed through conventional means. We think that numerical simulation reintroduces in physics the traditional notion of 'thought experiment' ('Gedankenexperiment'), now on a new scale, just as the thought experiments of Lucretius, Bruno, Galileo, Einstein or Bohr once did: by reasoning on the basis of an 'imaginary' experiment, one tries to predict a behaviour that might challenge theory at its very foundations. For

instance, the numerical experiment of Fermi-Pasta-Ulam has questioned the ergodic hypothesis on which all statistical mechanics is based. The numerical approach could also reveal the phenomenology hidden in fundamental equations, and hence improve the validation of simplified models: for example the numerical solution of Newton's equation to go beyond the three-body problem and study the formation of galaxies, the solar system's stability or any other n-body problems (for n larger than 3). Likewise, numerical experiments allow us to solve the Navier–Stokes equation for a large number of degrees of freedom in order to better understand turbulence in fluids and plasmas.

Numerical experiment is thus a third way whose specificity is the heuristic use of computers. This new approach is quite distinct, by its methods and its requirements (in particular in terms of academic curriculum), from both theory and experiment. Kenneth Wilson [36] recounts that: 'In the Sixties most scientists believed that a good theorist seated in front of a computer could instantly produce good science. It was overlooked that before gaining any decent results a long and difficult training period was necessary to overcome the very strict constraints dictated by computers (whatever their power). A large scale numerical experiment is as difficult to succeed as a proper experiment or an analytical calculation leading to good results [...] For three centuries students have been trained to perform experiment and theory; the best are selected and only those can continue; a similar system should now be implemented for numerical simulation. This would not be easy, students and teachers alike will have to carry out many unsuccessful simulations before the training effort bears fruit'. The numerical approach has its own practice, one which is indeed difficult to transmit. Zabusky [37] alludes to 'synergetic computational style' and he goes on to write: 'I have found it difficult to relate this mode of working via lectures. Perhaps this mode is still an art form understood by committed practitioners in benign computer environments and learned only by apprenticeship'. This impression is confirmed by Roache who, in the introduction to his classic book on numerical simulation, 'Computational Fluid Dynamics' [29], stipulates that: 'the newcomer to computational fluid dynamics is forecast in this field there is at least as much artistiry as science'. Similarly, Turkel, in his review published in 1983 in 'Progresses in Numerical Physics' [38], states that: 'the coding of large scale problems is as much art as it is science with a large reliance on intuition and folklore'.

Should we regard this as an indiscretion of youth or is it intrinsic to the numerical approach? Is the fact that numerical simulation is still perceived as 'amateur practice' due to its youth or is intrinsic to its methodology? Is this not always the case for any research domain too young to have become ossified? We believe that theoreticians, experimentalists and numericians will better contribute to their common enterpriser, namely the evolution of concepts and the explanation of phenomena, by keeping and affirming their singular identity, while yet engaging in vigorous core interaction on the foundations. As a matter of fact, this 'differentiation of the species' should not surprise us, since the distinction between theoreticians and experimentalists, just as that

drawn between mathematicians and physicists, is quite recent in our history. Should the choice of the numerical approach not ultimately be, as elsewhere, a matter of taste, of personal sensitivity, and, indeed, why not, of vocation?

> *'One cannot escape the feeling that these mathematical formulae have an independent existence and an intelligence of their own, that they are wiser even than their discoverers, that we get more out of them than was originally put into them'.*
>
> (Heinrich Hertz)

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