General Presentation

> *"Attractive mathematics does not protect one from the rigors of digital computation."*
>
> J. H. Wilkinson, von Neumann Lecture
> Fall SIAM Meeting 1970, Boston.

The fast evolution of techniques and performance in Scientific Computing modifies how one approaches high-technology problems. The models are more complex and can take into account the complete phenomenon in its environment (nonlinear equations, unsteady behaviour, coupling between several physical and chemical aspects for example). Often, research and development give rise to documented software that is part of the deliverables. Engineering practice evolves as well. Parametric studies allow the integration of a large number of parameters, and this reduces significantly the number of prototypes.

Since Scientific Computing is at the heart of the development of high technologies in industry, the problem of assessing the robustness of numerical methods becomes increasingly important today.

Coupling

Taking into account more and more detailed phenomena closer to physical reality leads to an evolution of modelling techniques. This evolution is twofold: first, taking into account a much larger number of degrees of freedom at the lowest level of the description and second, an increase in the complexity of the description, that is, in the number of levels which have to be integrated. This evolution is made possible by the increasing availability of software which realizes the coupling of different physical phenomena, often on parallel platforms. However the overall behaviour of a complete system is sometimes hard to predict. It is in the interaction zone between two strongly coupled models that new phenomena can occur which require a qualitative study before any attempt at computation.

Chaotic computations

Until the seventies, the classical approach of proving the numerical convergence of approximation methods in exact arithmetic was sufficient in most cases to assess the validity of the computer simulations in finite precision. The global stability of the equations of computational physics at that time was, in general, strong enough to accept the perturbation induced by finite precision. However in the past two decades, and through extensive computer experiments, scientists and engineers became aware of the theoretical role of chaos (i.e. extreme sensitivity to initial conditions) in evolution phenomena ruled by certain nonlinear equations.

Nowadays, the new problems at the edge of instability that are encountered more often in physics and high technology challenge the classical approach. To assess the validity of chaotic computations, it is necessary to study the robustness with respect to machine precision of the stability conditions for numerical methods which have been proved convergent in exact arithmetic. This robustness can be derived from the stability properties of the physical phenomenon under study.

Computability in finite precision

A rigorous theory of computability in finite precision is presented. The key feature is the introduction of the quantity known as "machine precision", that is $1^+ - 1$, where 1^+ is the successor of 1 in the computer arithmetic, as a parameter ε which tends to zero. This corresponds to a mantissa of increasing length for the computer representation of numbers. Then the embedding of the floating point computations into the field of mathematical reals allows the use of the powerful tools of classical analysis to prove the convergence of the results of an *algorithm* (finite number of steps) towards the exact result computed in an arithmetic with precision ε, as $\varepsilon \to 0$. The Lax principle of equicontinuity in ε is the tool of choice. More generally, the convergence analysis of *numerical methods* in finite precision requires the coupling of the arithmetic with all the convergence parameters. Therefore, the numerical stability proved in exact arithmetic can become conditional to finite precision.

Numerical quality of computations

It is important to distinguish in a computer result the amount of error due to the arithmetic instability (curable) from the amount due to a possible mathematical or physical instability (unavoidable), but which can be studied by theoretical means. Wilkinson establishes the *optimal quality* of a reliable algorithm with respect to machine precision, or to the level of inaccuracy in the data, by means of a backward error analysis. We show how Wilkinson's principle can be extended to assess the optimal reliability of a numerical method with respect to the numerical and arithmetic parameters. This allows the user to choose the methods that are guaranteed to make the best use of the finite precision of the computer, and to match the quality of the algorithm with the level of uncertainty in the data.

Role of singularities

Singularities correspond to cases where the solution has no continuous derivatives in some parameter. The singularities of a general differentiable map can be very complex, but they are a set of measure zero. However their computational influence can be devastating, because it is when a computation takes place in the neighbourhood of a singularity, that results obtained in finite precision can vastly differ from their exact counterparts. Because singularities are rare, they are not preserved under general perturbations: a double root is computed as two close simple roots in finite precision. Therefore, there has been a tendency to underestimate their role in practice. But indeed, they play an essential role in the area of theoretical physics concerned with the reduction of theory (Berry (1991)). Often enough, a general theory based on elementary principles is reduced to a particular theory when some dimensionless parameter (say δ) tends to zero, for example. Then the key question is the nature of the limit as δ tends to zero, and very often it is highly singular. The type of singularity is important and the existence of singularities is directly connected to the emergence of new phenomena. For example, statistical mechanics reduces to thermodynamics when $\delta = \frac{1}{N}$ tends to zero, N being the number of particles. The pressure $P(v,t)$ as a function of volume v and temperature t can be derived from the principles of statistical mechanics by large N asymptotics. But the reduction runs into difficulty near a critical point $(v_c,\ t_c)$ where the compressibility $k = [-v(\partial P/\partial v)_t]^{-1}$ is infinite. The nature of the divergence of k as $t \to t_c$ is a power law, which determines the critical exponents. Thermodynamics is a continuous theory, except at critical points, which correspond to a new state of matter. Other areas in physics where singularities underlie some of the most difficult and intensively-studied problems today include the limit: wave optics $\to$ geometrical optics, or quantum mechanics $\to$ classical mechanics.

The computational drift in the neighbourhood of a singularity depends on its type but also, for singularities of the same mathematical nature, it depends on their individual strength for diffusion into the regularity domain.

Spectral instability and nonnormality

Nonnormal matrices ($AA^* \neq A^*A$) are prone to spectral instability. If the conditions for numerical stability are not robust enough to spectral perturbations, the numerical stability in exact arithmetic is at risk. The spectral instability is often inherited from Physics. High nonnormality can occur in Physics and Technology whenever there exists a strong coupling between different phenomena, giving rise to physical instabilities.

Such extreme situations can be encountered when the spectrum of a family of operators depending on a parameter exhibits a *severe discontinuity* as the parameter varies. However it is possible that the pseudospectra remain continuous. The continuity of pseudospectra allows the use of Trefethen's principle to guarantee the convergence of numerical methods in exact arithmetic under conditions on the pseudospectra, which are robust with respect to nonnormality.

Influence on Numerical Software

In finite precision, the computation necessarily creates perturbations. Therefore, the numerical stability may guaranteed only under restrictive conditions coupling machine precision to discretization parameters such as time and space mesh sizes. Reliable software reflects the instability which is in the equations; it does not create it. Under the influence of certain parameters of the problem, such as the departure from normality for a matrix, the Reynolds number in CFD, or the resistivity in MHD, singularities which are isolated in exact arithmetic can be *coupled by the computation.* This coupling, which is at first local, can gradually become global as the relevant parameters evolve. This results in the emergence of new collective phenomena which mimic physical reality at the edge of chaos.
However, there exists another potential danger for Numerical Software which cannot happen in exact computation: the quality of the convergence may be seriously reduced by nonnormality. The danger is present for iterative solvers as well as finite algorithms. This should be a matter of serious concern for software developers.

Qualitative Computing

In ill-posed situations, the mathematical or numerical instability is so high that we cannot hope for a conventional control of the computational error, as was possible in less ill-conditioned situations. Classical computation seems meaningless at first because none of the digits in the results are correct. However, there may exist a broad spectrum of intermediate situations between right and wrong on the computer. In Qualitative Computing, the aim is not anymore to control the computing error (it does not tend to zero) but rather to extract meaning from wrong results. When the computation cannot deliver full information on the exact solution, because the problem is singular, then the computation –by means of a reliable method– can still deliver relevant *partial information* about the singularity.

Experimental mathematics

The presentation of the theory of computability in finite precision is complemented by a software toolbox PRECISE (**PR**ecision **E**stimation and **C**ontrol **I**n **S**cientific and **E**ngineering computing) to help the user set up computer experiments to explore the impact of finite precision on the computation at regular points and in the neighbourhood of singularities. This tool has a good explicative power, and can often be used predictively as well. It provides an estimate of the distance to the nearest singularity viewed by the computer, together with the order of this singularity. It is available electronically.

Sense of errors: for a rehabilitation of finite precision computations

Roundoff errors are often considered negatively, as a severe limitation on the purity of exact mathematics. However we wish to argue, by means of two examples, that computation in exact arithmetic is not always the choice which is the most appropriate to describe the mathematical or physical reality. The first example deals with Lanczos or Arnoldi method which could not compute multiple eigenvalues if they were run in exact arithmetic. The second example concerns the logistic. The gradual divergence of (1.27) to solve the logistic equation (1.25) presented in Chapter 1 disappears if the computation is exact (one gets essentially the various fixed points of $x = f^k(x)$). However, the experimental diagram for CO_2 lasers (Glorieux (1988)) reproduces the computed logistic and not the family of fixed point solutions. Finite precision has the property to make visible the zone of gradual divergence which has physical meaning.

Exact computation in simulations is a sensible aim, but only if it is exact with respect to the appropriate reference, the reference which makes sense for the simulation. It may not be useful to compute exactly a transient solution with no physical existence because its instability is too high.

As every physicist knows, no equation is exact; therefore we believe that finite precision computation can be closer to physical reality than exact computation.

So, it appears possible to *transform the limitations of the computer arithmetic into an asset.* Finite precision computation in the neighbourhood of a singularity can be put into remarkable correspondence with physical phenomena at critical points. Because finite precision necessarily introduces perturbations into the computation, the computer results follow *laws of computation* which might shed some light on certain critical phenomena. To close this introduction on a poetic note, one can cite rainbows in the sky, or the glittering of the sea under the sun, which can be explained by perturbations of the caustics that appear in the limit of wave optics, when the wavelength tends to zero (Berry (1978)).