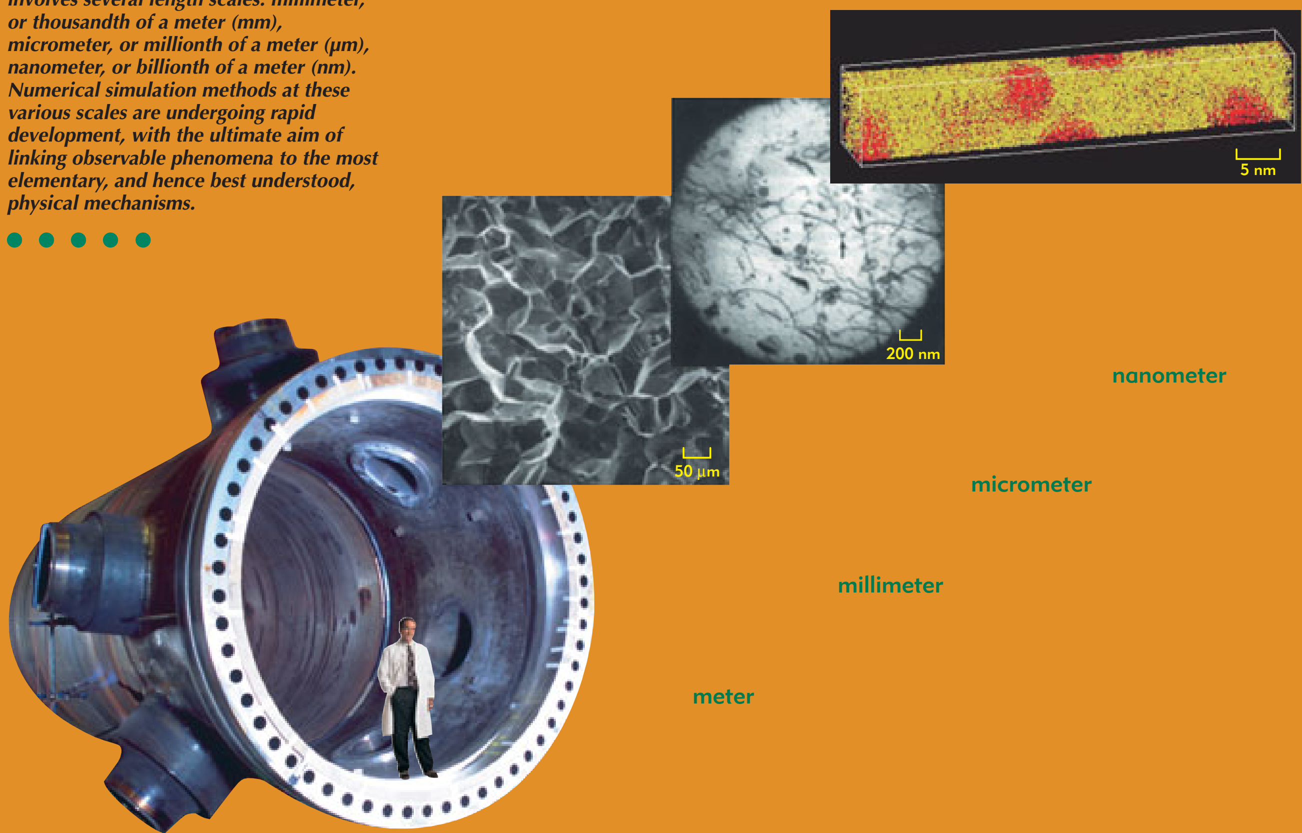
# SIMULATION OF MATERIALS

*In the nuclear industry, materials make a major contribution to enhancing the performance, reliability and safety of reactors and fuel-cycle facilities. Their behavior under irradiation is obviously of major concern for the metallurgist. Indeed, the action of ionizing radiation and neutron fluxes induces a structural change in the material, called aging, which can result in alteration of its properties. How to predict the behavior of materials over very long periods, extrapolate their evolution in new irradiation conditions, predict their properties in severe exposure conditions? Numerical simulation proves to be an essential tool, be it as a support to experimentation, to increase the "return on investment" or as sole recourse in cases where experimentation is unavailable.*




***The behavior of materials in service involves several length scales: millimeter, or thousandth of a meter (mm), micrometer, or millionth of a meter (µm), nanometer, or billionth of a meter (nm). Numerical simulation methods at these various scales are undergoing rapid development, with the ultimate aim of linking observable phenomena to the most elementary, and hence best understood, physical mechanisms.***

From left to right: R. Quatrain/Framatome – ANP – according to O. M. Yahya *et al.*, *Fatigue and Fracture of Engineering Materials and Structures* **21** (1998), pp. 1485–1502 – CEA – Rouen University (GPM)

## Materials exposed to extreme conditions

Materials performance is always the result of a compromise between their chemistry (bond types(1)), and their atomic structure and microstructure. Steel makers, in particular, know just how to optimize the properties of their material by working on these three components. In service, materials are subjected to various types of forcing which transform their characteristics. Exposure to irradiation (whether ionizing or otherwise) affects these three fundamental aspects. **Transmutations** cause changes in the chemical makeup of the materials, particularly of **fuels**. Electronic excitations modify chemical bonding in insulators. Nuclear collisions, by ejecting atoms from their equilibrium position, affect the atomic structure, resulting, e.g. in **amorphization**, in the creation of point defects such as vacancies (vacant crystal sites) and interstitials (atoms located between lattice planes). Ejected atoms can have sufficient kinetic energy to displace other atoms and thus cause cascades of atom displacements. Slow migration and clustering of the point defects thus generated induce changes in the microstructure: the formation or dissolution of **precipitates**, which affect mechanical strength (the ability to withstand significant stresses) and corrosion behavior, alteration of the network of **dislocations**, which governs the plasticity of materials, recrystallization, etc.
Another specific feature of the nuclear industry is the very high costs and the total lack, at times, of feedback. Thus, if we try to *predict* the behavior of materials over *time spans*

that are sometimes beyond any possible actual-size experiment – can aging of the materials be accelerated in a controlled manner? How to *extrapolate to new irradiation conditions*, presently unattainable (for **fusion** reactors or high-temperature reactors, for instance), the evolution of a material known only within a very narrow range of conditions (**neutron** energy spectrum, restricted range of temperatures, etc.)?
Materials are exposed to extreme conditions (nuclear collisions, highly powerful impacts, incursions into very high temperature and pressure conditions), conditions for which direct observation, at the relevant scale and **resolved** over time, is impossible: can the materials' properties be predicted for such extreme conditions, unattainable for elementary experiments?
Such questions have impelled a sustained effort to develop materials-modeling methods which, starting from the scale at which the physics of the processes is relatively well ascertained, attempt to reproduce the macroscopic behavior that is of practical interest. Four main types of tools are available for this.

## Tools for materials modeling

The modeling tools naturally fall into four categories, depending on whether the aim is:
• **modeling chemical bonding** (cohesion models). The aim here is to predict elementary defect properties, of use in coarser-scale modeling, and, hopefully, to monitor the evolution of chemical bonds under forcing. This involves calculations of *electronic structure* that are as predictive as possible;
• **modeling rapid events at atomic scale** (nuclear collisions, **shockwave** propagation, damage). These phenomena involve large numbers of atoms over numerous **atomic vibration periods**. ***Molecular dynamics*** is the appropriate tool;
• **modeling *slow* aging *kinetics***, i.e. slow kinetics of microstructure evolution or **relaxation**. A variety of methods are used, **deterministic** or **stochastic**, at the atomic, micron (1 µm = $10^{-6}$ m) or macroscopic scales;
• **going over from microstructure to properties of practical use**. For this step, the nuclear industry scarcely differs from other sectors, and the domain shows a rapid expansion.

### Modeling cohesion of solids

The tool is **simulation** "from first principles" (***ab initio***): matter is regarded as a crowd of nuclei and electrons; the latter, owing to their very small mass, adjust instantly to the motion of the nuclei. The image obtained is that of an electronic density adjusting to the actual positions of the nuclei. The determination of the electronic structure necessarily draws on **quantum mechanics**, and a remarkable theory, the so-called density functional theory (DFT), subject to various approximations, allows such calculations to be carried out for a large number of atoms in a reasonable amount of time. Ultimately, the modeler finds he has the total energy of a sample of matter expressed solely as a function of the nuclei's coordinates. From a numerical standpoint, the main problem consists in solving **Schroedinger's equation** for a large number of nuclei and electrons and covering the greater part of the periodic table of elements. The sizes of the systems under consideration range from a hundred to several thousands of atoms, depending on the compromise between accuracy and speed the numerical analyst is prepared to countenance.
What is to be done of the huge mass of data thus generated? First, the **model** used has to be qualified, since the starting point is an approximation of Schroedinger's equation. All structural properties can be evaluated: **equation of state**, **phase diagram**, atomic vibration spectrum (the set of the **crystal**'s vibration modes). The cohesion of solids, equilibrium volume, elasticity properties, the nuclei's vibrational properties are generally very accurately reproduced (to within a few per cent). The phase diagrams are modeled in more uncertain fashion (some tens of percentage points). **Actinides** are a remarkable exception, as illustrated in Figure 1, showing the observed and calculated equilibrium volume for those elements. The position, good as it is for the so-called light actinides, deteriorates once plutonium is reached. In the latter context, more sophisticated modeling approaches must be brought in, going beyond the mean-field approximation.(2)
The determination of a phase diagram, particularly the solid–liquid transition, constitutes a more complicated problem, as a simulation is carried out on a heterogeneous liquid–solid medium, too large to be simulated using an *ab-initio* approach. In order to effect calculations on such larger samples, the modeler adjusts the parameters of a **semi-empirical potential** to reproduce as accurately as possible the data from an ***ab-initio* calculation**. Such an approach was initially tested with the melting curve for iron, then extended to actinides (Figure 2).

(1) A **metallic bond** occurs between electrically positive elements (whose outer shell has few electrons): the electrons in the outer shells are delocalized. An **ionic bond** associates highly electro-positive elements and highly electro-negative elements (whose outer shell has many electrons): the electrons in the outer shells are trapped on the negative ions. The **bond** is **covalent** when an electron from the outer shell of one atom forms with an electron from the outer shell of a neighboring atom a pair shared by both atoms: for these electrons the density is a maximum between the atoms; an atom thus associates with several neighbors to saturate its outer shell.
(2) Such as the LDA+U method (see, for instance, J. Bouchet *et al., J. Phys. Cond. Mat.* **12** [2000], p. 1723) or the DMFT technique.

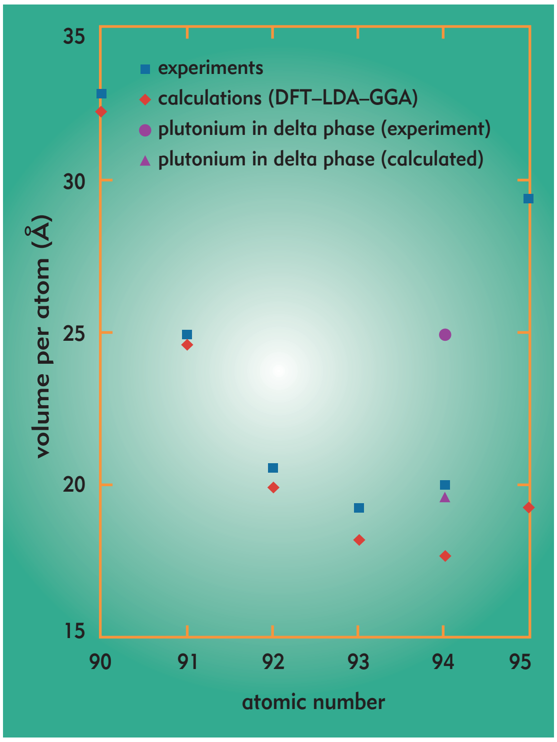



*Figure 1. For actinides, whose electronic structure is complicated by gradual filling of electronic sub-shell 5f, calculations performed with the density functional theory (DFT) in the local-density approximation–generalized-gradient approximation (LDA–GGA) are in good agreement with experiments, up to plutonium, of atomic number (number of **protons**) 94. The situation deteriorates considerably for plutonium in the delta phase (face-centered cubic) and even more so for americium (atomic number 95). (Calculations effected by N. Richard and M. Pénicaud.)*

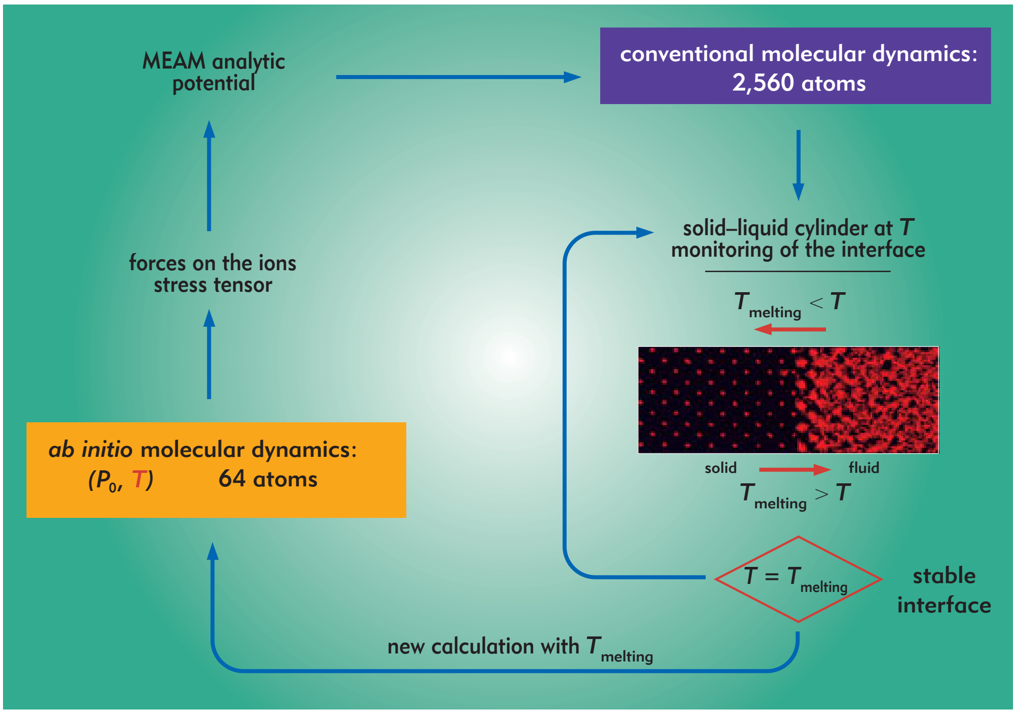
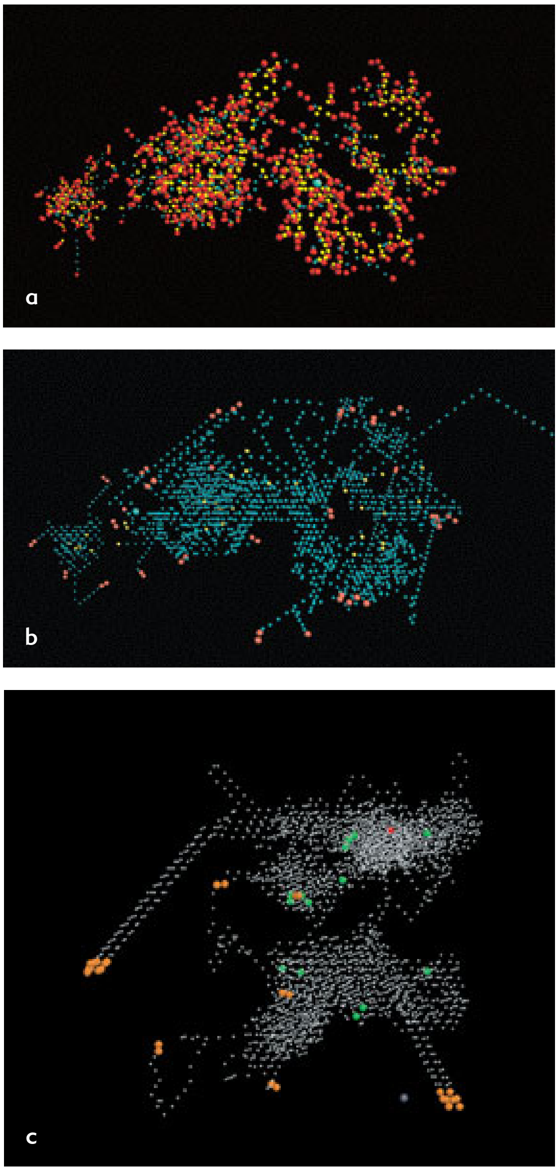



*Figure 2. Computation cycle aimed at the* ab-initio *determination of a melting curve. A semi-empirical MEAM (modified embedded atom potential) is adjusted to the results of* ab-initio *calculations carried out for a small system, compatible with the possibilities of computers (Box on left) for given temperature and pressure conditions. This potential is then used in a classical simulation (Box on right) for a much larger system, for the same thermodynamic conditions. Melting temperature $T_{melting}$ is reached when the solid-liquid interface has stabilized. An application of this process led to re-evaluation of the phase diagram of iron. (A. Laio, S. Bernard* et al.*, Science, Vol. 287, No. 5455, pp. 1027-1030, 11 February 2000).*

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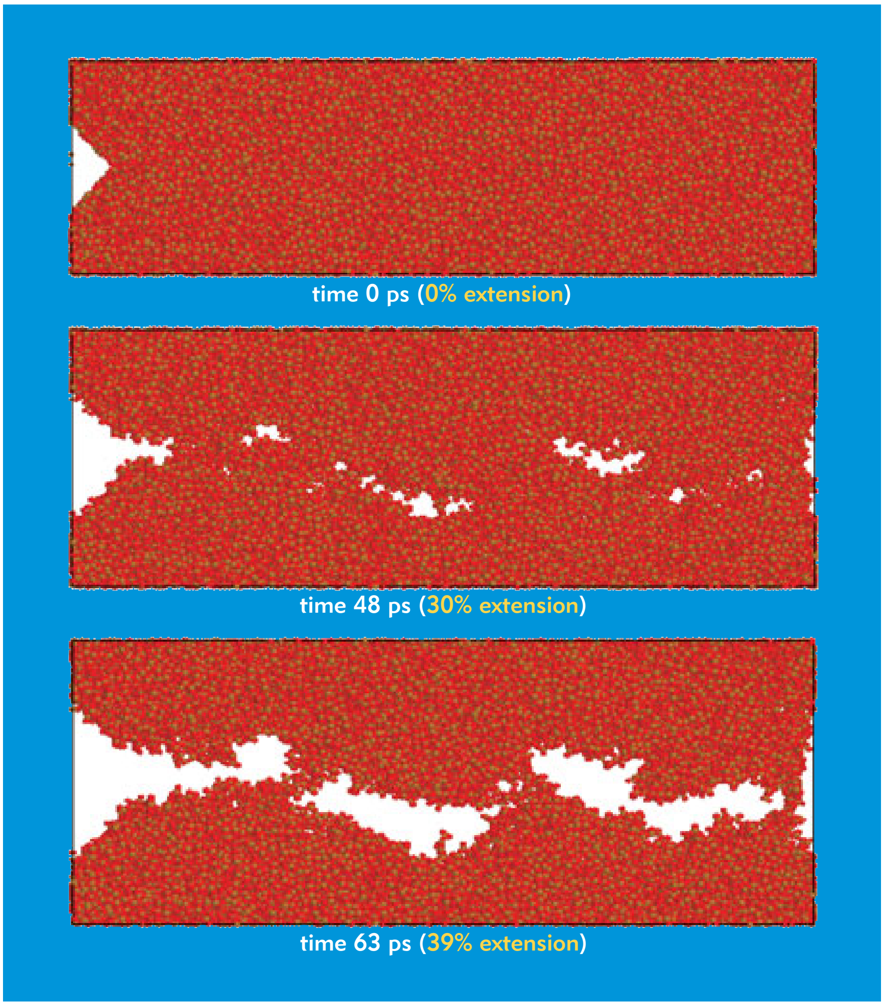
*Displacement cascades in a model of dilute solution of copper in iron, following a collision of 10 keV energy: (a) after 0.21 ps (about 2 atom vibrations), a large number of atoms (shown in red) are expelled from their lattice sites, left vacant (vacancies, shown in yellow); (b) after 15.27 ps (about 150 atom vibrations), most of the expelled atoms have found again a crystal site (in blue). A few point defects remain, isolated or in clusters; (c) at nanosecond scale, the clusters of interstitials are mobile and fill in vacancies as they go over them. After 3 ns, healing of the metal is quite advanced. Residual defects store only a few thousandths of the energy transferred by the collision.*

## Modeling rapid events at atomic scale

The tool here is molecular dynamics. Let us consider a set of atoms connected together by one of the energy models described above. Within the limits of classical mechanics, the atoms' trajectory is given by the integration of **Newton's equation**: an atom's acceleration is equal to the force it is subjected to, divided by its mass; the force is given by the variation in potential energy with position. This equation is integrated by means of a very fast, highly accurate **algorithm**. The modeler thus has the system's trajectory trough its phase space (position and momentum). Today's computers allow such calculations for ensembles comprising up to one billion atoms for physical timeframes of up to several hundreds of nanoseconds (1 ns = $10^{-9}$ s) for small systems, at least if the numerical analyst uses semi-empirical potentials. If potential energy is calculated from first principles, only a thousand atoms can be handled over a few picoseconds (1 ps = $10^{-12}$ s).

What does the modeler do with such trajectories? Two quite separate things. When statistical mechanics allows it, he *calculates* macroscopic quantities by integration along the trajectory, effecting this in various thermodynamic ensembles (for instance, by setting constant values for total energy, volume and number of particles, or for temperature, or pressure, etc.). If this should not be feasible, using visualization tools, he *observes* those few atoms whose configuration is causing the alterations in the properties of the material being modeled. This is truly "computer microscopy", the researcher having the

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*Silica glass is reputedly fragile, however the crack-propagation mechanism was revealed only recently, by molecular dynamics. Pores open and grow until they join in the neighborhood of "non-bridging" oxygen atoms – i.e., atoms not shared by two neighboring $SiO_2$ tetrahedrons. The same simulation carried out for a crystalline form of $SiO_2$ results in cleavage (breaking due to splitting along a crystallographic plane), as observed experimentally.*

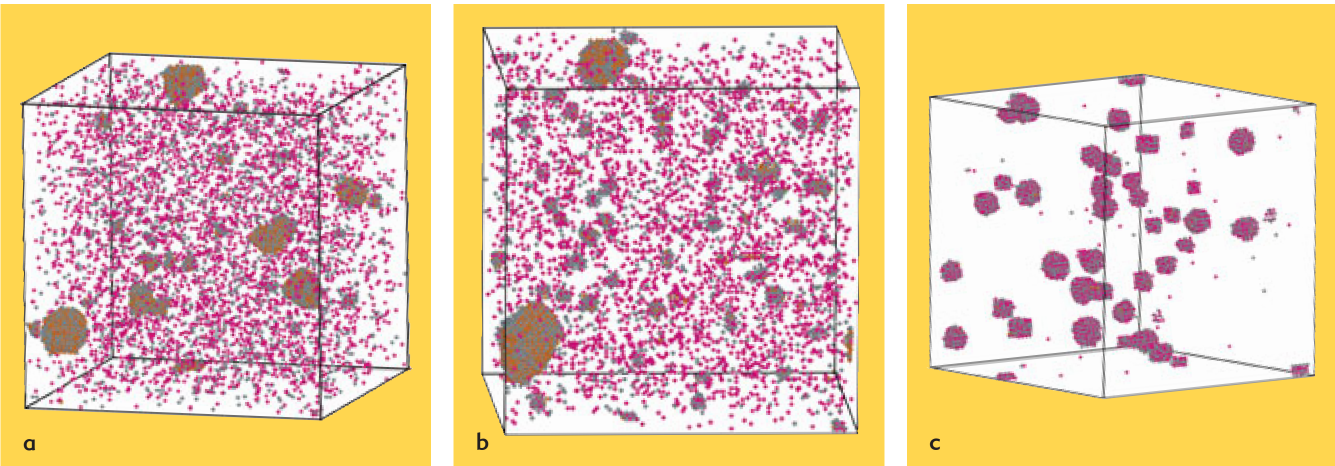
ability, through a variety of techniques, to observe, characterize and see in operation the atomic configuration he has identified. This approach is, for instance, the principal source for the notions generally entertained by physicists today as to atom-displacement cascades, an essential stage in irradiation damage in materials.

These techniques are beginning to bear fruit for problems of plasticity or of fracturing, where the atomic scale is relevant.

## Modeling the slow evolution of microstructure

Very often, microstructure evolution is controlled by the diffusion of point defects, or of clusters of such defects. In this case, various techniques enable realistic modeling, i.e. with a correct time scale, of the "kinetic path" followed by the microstructure. The *kinetic Monte Carlo method at atomic scale* is the most accurate, since it simulates the

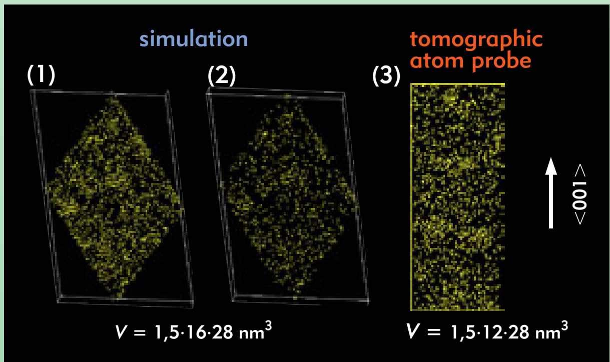
*Precipitation of niobium carbide in a steel, simulated by kinetic Monte Carlo method at atomic scale: (a) after 2 seconds, the initial solid solution (niobium atoms are shown in red, carbon atoms in gray) has given rise to transient iron carbides (gray and yellow clusters); (b) after 30 seconds, stable precipitates of niobium carbide appear which, as they grow, cause the iron carbides to dissolve; (c) after half an hour, only the niobium carbides remain. The algorithm has the capacity to handle two separate elementary time scales, that of interstitial carbon jumps (rapid time scale) and that of the vacancy jumps enabling iron and niobium diffusion (slow time scale).*




Usinor–CEA collaboration

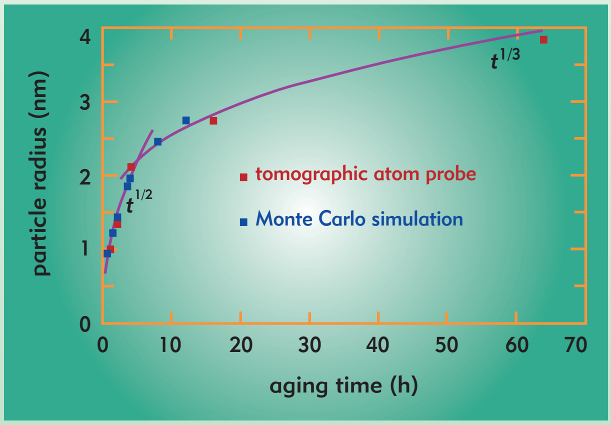
## Comparing simulation and experiment: the tomographic atom probe

Transformation paths in alloys can be observed directly *at atomic scale*, thanks to the tomographic atom probe. By individually stripping ions from a metal point cut from the alloy, accelerating them in an electrical field and measuring their flight time to a localization detector, it is possible to work back to the spatial distribution of the various types of atoms making up the alloy. The volumes that may be analyzed by this technique are of the same order of magnitude as those that may be simulated with the kinetic Monte Carlo method at atomic scale. Direct comparison of simulation and experiment is then feasible, and has successfully been carried out in collaboration with Rouen University (France) in the relatively complex case of precipitation in ternary nickel–chromium-aluminum (Ni-Cr-Al) alloys.
A Ni – 14.8 at% Cr – 5.2 at% Al alloy was aged at 600 °C for increasing periods of time and examined with the tomographic atom probe at various stages of its decomposition. A kinetic path of the "nucleation growth coarsening" type is observed.




CEA-Rouen University collaboration (Pr. D. Blavette and Dr. C. Pareige)

***Figure a.** Three-dimensional distribution of aluminum along the <001> direction of alloy Ni – 14.8 at% Cr – 5.2 at% Al aged at 600 °C for 1 hour. In (1), configuration obtained by simulation with 100% of aluminum atoms represented. In (2), configuration obtained by simulation with 50% of aluminum atoms represented (this factor of 1/2 corresponds to the detection efficiency achieved by the tomographic atom probe). In (3), experimental distribution obtained with the tomographic atom probe for the same alloy.*




CEA--Rouen University collaboration (Pr. D. Blavette and Dr. C. Pareige)

***Figure b.** Size of precipitates as a function of aging time, observed by the tomographic atom probe and simulated with the Monte Carlo method.*

For **numerical simulations**, the **model** is **parameterized** on the experimental data available in the literature [solubility limits in binary and ternary alloys, some diffusion coefficients, crystallographic structure of the $Ni_3(Al,Cr)$ compound arising through precipitation]. Comparison of the simulated results to the tomography results (Figure a) showed that Monte Carlo simulation correctly describes, both qualitatively and quantitatively, the kinetic path of the transformation. After early formation of ordered aluminum-rich zones (approximately 1 nm in diameter), these zones grow and become enriched in Al, then, in a later stage, Cr depletion occurs. The simulation perfectly accounts for this process as well as, quantitatively, for the evolution over time of particle density, phase composition and particle size (Figure b).

sequence of successive jumps by the defects, taking into account all the known physics of these jumps. Very long time scales can be simulated. Up to one billion defect jumps in iron have been simulated, which, at the temperature of a **pressurized-water reactor** vessel, is equivalent to 87 years. Volumes remain small, since the modeler is working at atomic scale (see Box).
Using recently developed theoretical tools (*self-consistent kinetic mean-field method*), the modeler knows how to carry over from this very precise description (each given atom at each given site at each instant) to a probabilistic description. Concentrations at every point as a function of time are the solutions of coupled **partial-derivatives equations**. This leads back to the so-called "phase-field" methods, but this time on an atomistic foundation, providing them with a realistic definition of physical time, while not remaining restricted to the atomic scale (Figure 3).

One technique currently being developed at CEA's Saclay Center is the ***event kinetic Monte Carlo method*** (EKMC). This is a promising method, as it is not restricted to the atomic scale and adjusts automatically to changes in time scale. The microstructure is schematically reduced to dislocation lines, **grain boundaries** and defect clusters; mobile entities (point defects, minor impurities, helium generated by nuclear reaction, etc.) are identified by their position. Simple models describe the probability that a given mobile entity be captured, within a certain time span, by each of the constituent elements of the microstructure. A **Monte Carlo** algorithm determines the sequencing of the various events and the time intervals separating them. This algorithm opens the way to modeling complex phenomena (size effects of atom displacement cascades, precipitation **catalyzed** by impurities, competition between various morphologies of defect clusters) in relatively complex materials.

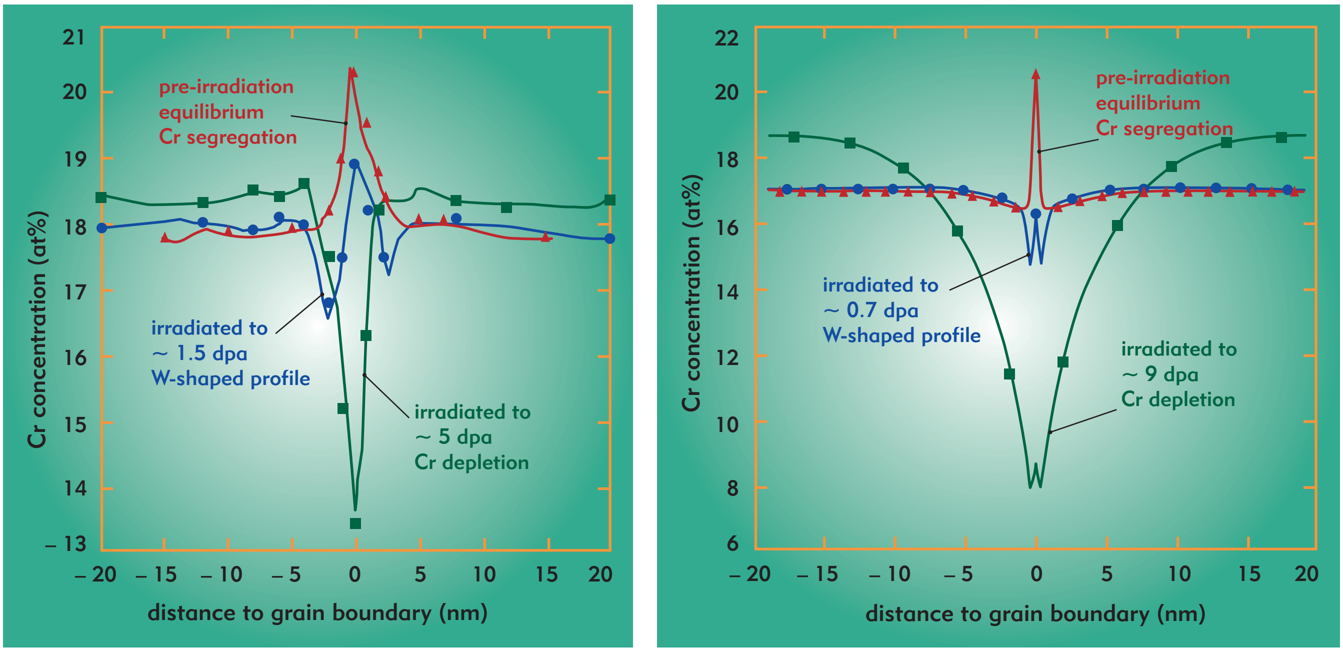


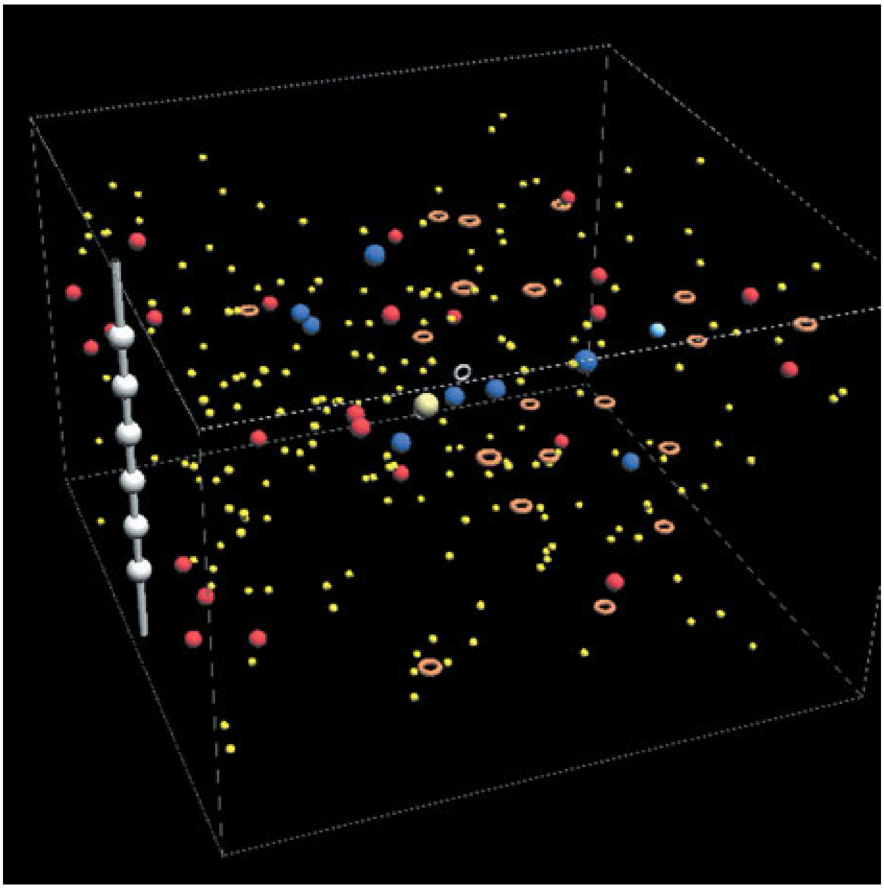

*Figure 3. Irradiation-induced segregation at the grain boundaries of an austenitic steel (made of iron, chromium, nickel and a little carbon). On the left, concentration profile for chromium (Cr) as a function of the distance to the grain boundary for increasing irradiation doses, expressed in dpa (displacements per atom), observed using analytical electron microscopy. On the right, concentration profile for Cr predicted by the chemical-kinetic model over network developed at CEA (M. Nastar* et *al.*, *MRS, Vol. 481 [1998], p. 383).*

Volumes of several µm$^3$ are routinely simulated for long periods (one hour or more). These time and space scales adjust automatically to microstructure evolution.

Finally, the modeler often uses homogeneous chemical-kinetic models to describe the competition between irradiation defect generation and their elimination by recombination, agglomeration or diffusion towards the discontinuities in the crystal lattice. These techniques are very powerful in yielding trends for microstructure evolution as a function of irradiation conditions.

## From microstructure to engineering properties

This step is not specific to the nuclear industry and benefits from the current developments in modeling methods. This is the preferred domain for multi-scale modeling, which can take the most diverse forms. The



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*Event Monte Carlo method (Jerk). Simulation of the microstructure as it develops in nickel containing a few ppm of helium and another impurity, during irradiation, resulting from the combination of a large displacement cascade and numerous subsequent small cascades. The microstructural elements taken into account include a dislocation, loops, cavities (vacancy cluster) containing varying amounts of helium, clusters with or without trapped impurities (simulated volume of 1 µm³ over one half-hour).*

most usual is the inclusion of quantities evaluated by means of fine-scale modeling (such as the anchoring force of dislocations by clusters of defects) in simple models of classical physical metallurgy (for instance flow-stress models) (see Figure 4).
Fine-scale models are also capable of yielding ingredients for sophisticated theories (for instance on phase stability in alloys undergoing irradiation). It should be noted that certain couplings between models or between a model (of microstructure evolution, for instance) and a macroscopic theory (such as a constitutional law in solid mechanics) are not always feasible in the current state of the art. Further theoretical developments are still required.

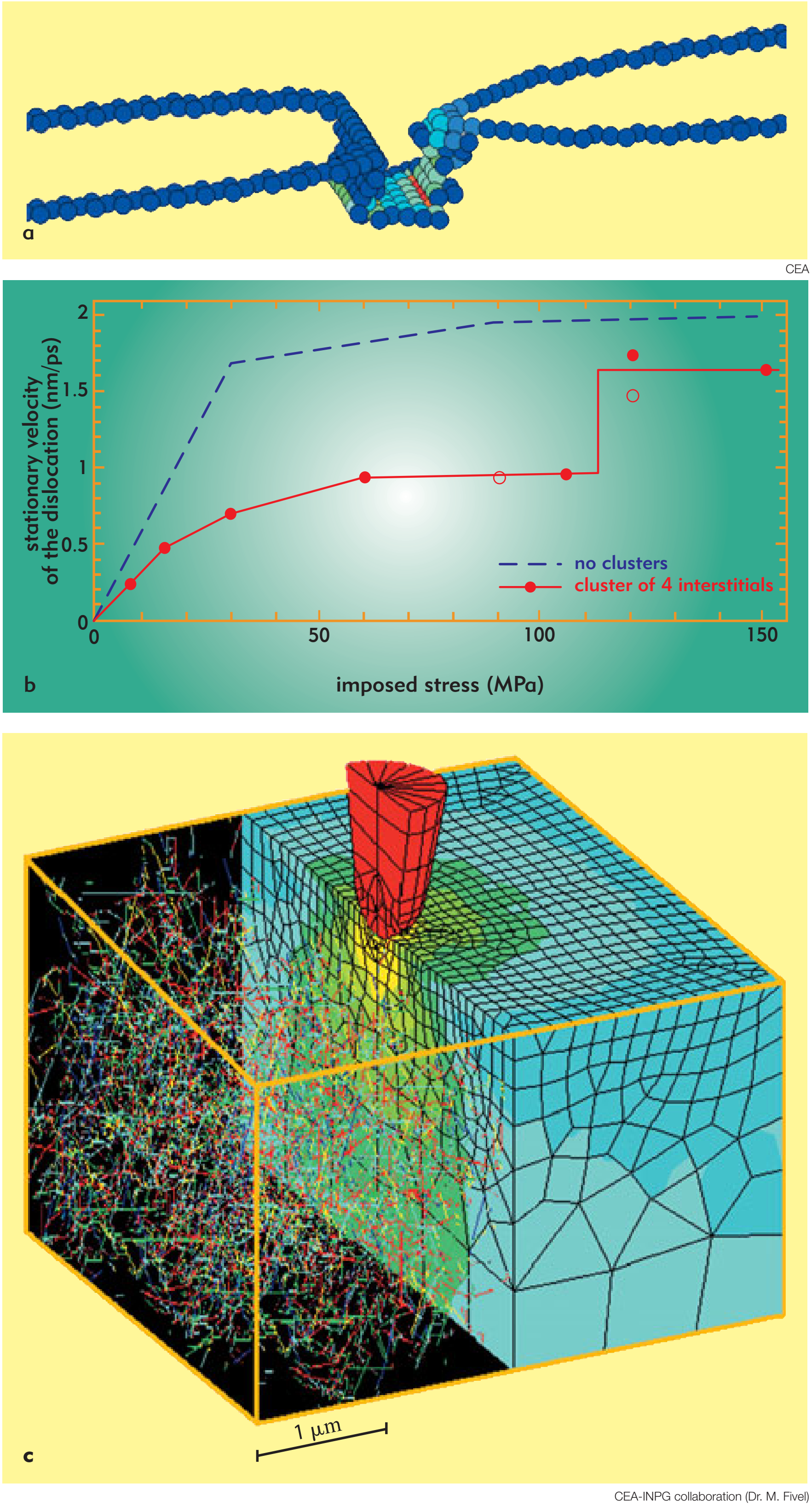
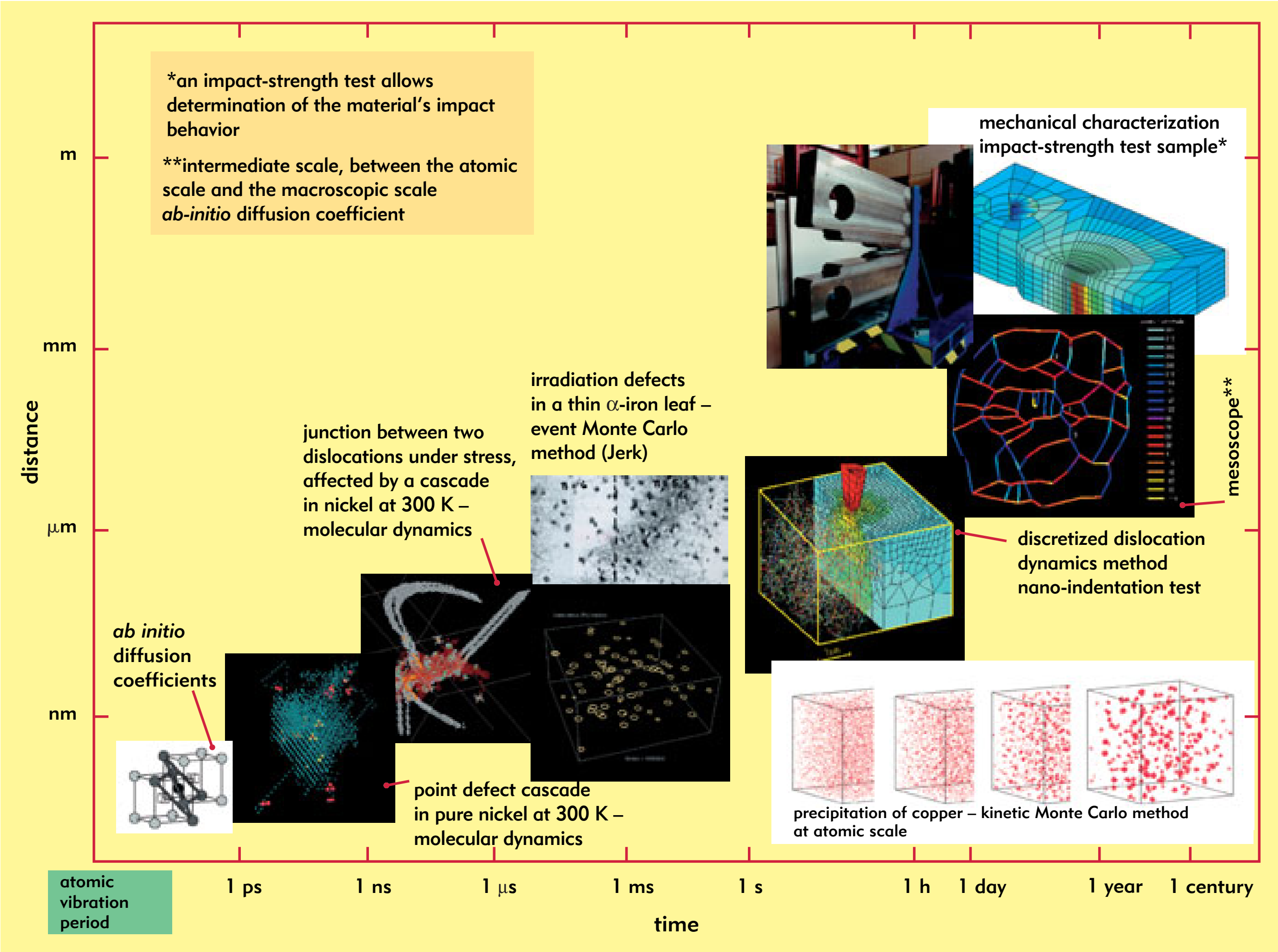



*Figure 4. Irradiation-induced hardening, an instance of multi-scale modeling (the hardening stems from the elimination of point defects, in clusters, on dislocations): (a) molecular-dynamics simulation of the pinning down of a dislocation (which can no longer move) by a cluster of interstitials generated by irradiation; (b) measurement, on that same simulation, of the anchoring force for the dislocation exerted by the interstitial cluster; (c) simulation, by the so-called discretized dislocation dynamics (DDD) method, of a nano-indentation test making it possible to evidence hardening due to irradiation. This test consists in forcing a diamond point into the material and monitoring the penetration depth as a function of applied force, at nanometric scale.*

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***The gamut of materials-modeling methods available or under development, at various space and time scales.***

## Simulation and experiment: an indispensable comparison

One of the major industrial challenges at stake for materials modeling is to develop predictive modeling of materials performance. This can only be achieved by the incorporation, by way of the phenomenological theories, of data gained at smaller scales. The ensemble of knowledge attaching to such approaches is gradually taking form, allowing each specialist in his own field (mechanics, corrosion, etc.) to turn to such tools as if in a vast numerical laboratory, dedicated to the multi-scale modeling of materials.

Given the complexity of materials and their evolution in service, particularly under irradiation, it is unthinkable to develop models without constantly comparing them to experimental findings. "Elementary" experiments are infinitely tougher judges of the realism and robustness of a model than measurements of the macroscopic, composite properties of materials. Such elementary experiments are all too rare; they must be encouraged concurrently with the development of modeling methods.

This approach will flourish under the combined effect of the considerable growth in computation (and visualization) resources and the miniaturization of the experimental setups.

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# What is a numerical simulation? A

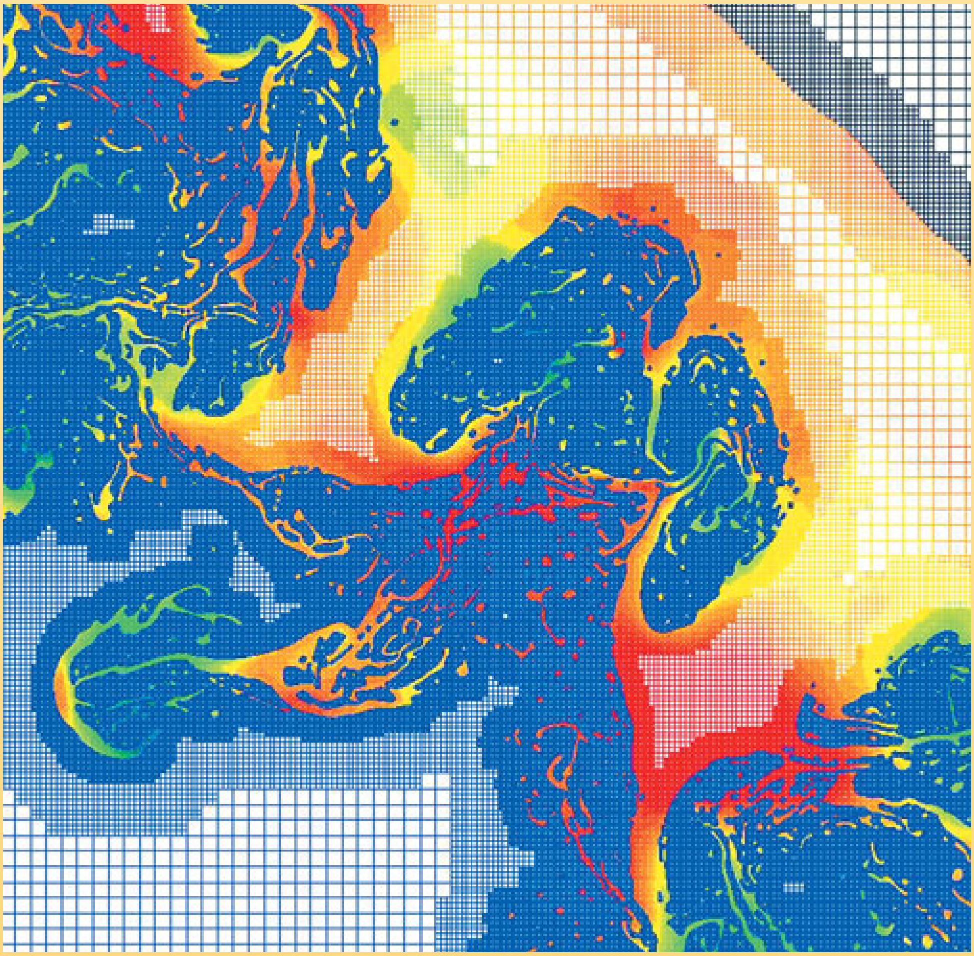
**Numerical simulation** consists in reproducing, through computation, a system's operation, described at a prior stage by an ensemble of **models**. It relies on specific mathematical and computational methods. The main stages involved in carrying out an investigation by means of numerical simulation are practices common to many sectors of research and industry, in particular nuclear engineering, aerospace or automotive.

At every point of the "object" considered, a number of physical quantities (velocity, temperature…) describe the state and evolution of the system being investigated. These are not independent, being linked and governed by **equations**, generally **partial differential** equations. These equations are the expression in mathematical terms of the physical laws modeling the object's behavior. Simulating the latter's state is to determine – at every point, ideally – the numerical values for its parameters. As there is an infinite number of points, and thus an infinite number of values to be calculated, this goal is unattainable (except in some very special cases, where the initial equations may be solved by analytical formulae). A natural approximation hence consists in considering only a finite number of points. The parameter values to be computed are thus finite in number, and the operations required become manageable, thanks to the computer. The actual number of points processed will depend, of course, on computational power: the greater the number, the better the object's description will ultimately be. The basis of parameter computation, as of numerical simulation, is thus the reduction of the infinite to the finite: **discretization**.

How exactly does one operate, starting from the model's mathematical equations? Two methods are very commonly used, being representative, respectively, of **deterministic computation** methods, resolving the equations governing the processes investigated after discretization of the variables, and methods of **statistical** or **probabilistic calculus**.

The principle of the former, known as the **finite-volume method**, dates from before the time of computer utilization. Each of the object's points is simply assimilated to a small elementary volume (a cube, for instance), hence the *finite-volume* tag. Plasma is thus considered as a set or lattice of contiguous volumes, which, by analogy to the makeup of netting, will be referred to as a **mesh**. The parameters for the object's state are now defined in each mesh cell. For each one of these, by reformulating the model's mathematical equations in terms of volume averages, it will then be possible to build up *algebraic relations* between the parameters for one cell and those of its neighbors. In total, there will be as many relations as there are unknown parameters, and it will be up to the computer to resolve the *system* of relations obtained. For that purpose, it will be necessary to turn to the techniques of **numerical analysis**, and to program specific **algorithms**.

The rising power of computers has allowed an increasing fineness of discretization, making it possible to go from a few tens of cells in the 1960s to several tens of thousands in the 1980s, through to millions in the 1990s, and up to some ten billion cells nowadays (Tera machine at CEA's Military Applications Division), a figure that should increase tenfold by the end of the decade.



*Example of an image from a 2D simulation of instabilities, carried out with CEA's Tera supercomputer. Computation involved adaptive meshing, featuring finer resolution in the areas where processes are at their most complex.*

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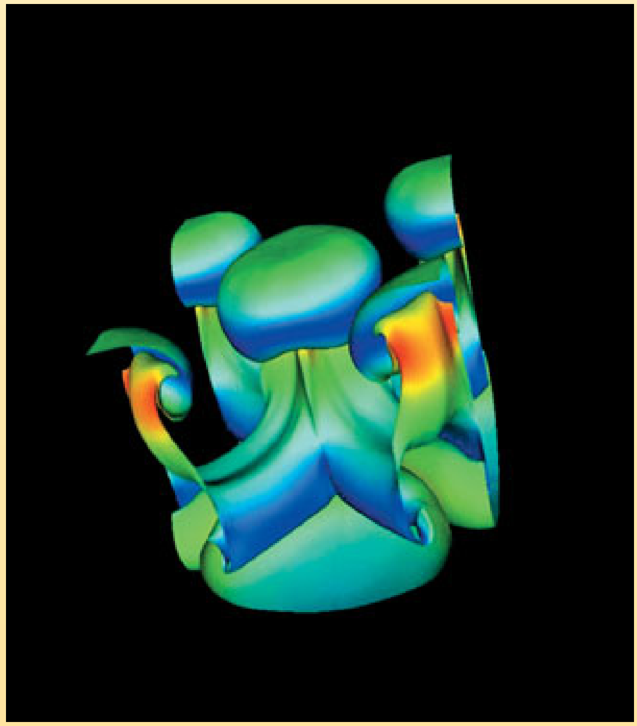
A refinement of meshing, **adaptive remeshing**, consists in adjusting cell size according to conditions, for example by making them smaller and more densely packed at the interfaces between two environments, where physical processes are most complex, or where variations are greatest.
The finite-volume method can be applied to highly diverse physical and mathematical situations. It allows any shape of mesh cell (cube, hexahedron, tetrahedron…), and the mesh may be altered in the course of computation, according to geometric or physical criteria. Finally, it is easy to implement in the context of **parallel computers** (see Box B, ***Computational resources for high-performance numerical computation***), as the mesh may be subjected to partitioning for the purposes of computation on this type of machine (example: Figure B).
Also included in this same group are the **finite-difference method**, a special case of the finite-volume method where cell walls are orthogonal, and the **finite-element method**, where a variety of cell types may be juxtaposed.
The second major method, the so-called **Monte Carlo** method, is particularly suited to the simulation of *particle transport*, for example of neutrons or photons in a **plasma** (see *Simulations in particle physics*). This kind of transport is in fact characterized by a succession of stages, where each particle may be subject to a variety of events (diffusion, absorption, emission…) that are possible *a priori*. Elementary probabilities for each of these events are known individually, for each particle.
It is then a natural move to assimilate a point in the plasma to a particle. A set of particles, finite in number, will form a representative sample of the infinity of particles in the plasma, as for a statistical survey. From one stage to the next, the sample's evolution will be determined by random draws (hence the method's name). The effectiveness of the method, implemented in Los Alamos as early as the 1940s, is of course dependent on the statistical quality of the random draws. There are, for just this purpose, *random-number* methods available, well suited to computer processing.



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***3D simulation carried out with the Tera supercomputer, set up at the end of 2001 at CEA's DAM-Île de France Center, at Bruyères-le-Châtel (Essonne* département*).***

Finite-volume and Monte Carlo methods have been, and still are, the occasion for many mathematical investigations. These studies are devoted, in particular, to narrowing down these methods' convergence, i.e. the manner in which approximation precision varies with cell or particle number. This issue arises naturally, when confronting results from numerical simulation to experimental findings.

# How does a numerical simulation proceed?

Reference is often made to *numerical experiments*, to emphasize the analogy between performing a numerical simulation and carrying out a physical experiment.
In short, the latter makes use of an experimental setup, configured in accordance with initial conditions (for temperature, pressure…) and control parameters (duration of the experiment, of measurements…). In the course of the experiment, the setup yields measurement points, which are recorded. These records are then analyzed and interpreted.
In a numerical simulation, the experimental setup consists in an ensemble of computational programs, run on computers. The **computation codes**, or **software** programs, are the expression, via numerical algorithms, of the mathematical formulations of the physical models being investigated. Prior to computation, and subsequent to it, *environment software* programs manage a number of complex operations for the preparation of computations and analysis of the results.
The initial data for the simulation will comprise, first of all, the delineation of the computation domain – on the basis of an approximate representation of the geometric shapes (produced by means of drafting and CAD [computer-assisted design] software) –, followed by discretization of this computation domain over a mesh, as well as the values for the physical parameters over that mesh, and the control parameters to ensure proper running of the programs… All these data (produced and managed by the environment software programs) will be taken up and verified by the codes. The actual results from the computations, i.e. the numerical values for the physical parameters, will be saved on the fly. In fact, a specific protocol will structure the computer-generated information, to form it into a numerical database.
A complete protocol organizes the electronic exchange of required information (dimensions, in particular) in accordance with predefined formats: modeler,[1] mesher,[2] mesh partitioner, com-

(1) The modeler is a tool enabling the generation and manipulation of points, curves and surfaces, for the purposes, for example, of mesh generation.
(2) The geometric shapes of a mesh are described by sets of points connected by curves and surfaces (Bézier curves and surfaces, for instance), representing its boundaries.

putation codes, visualization and analysis software programs. *Sensitivity* studies regarding the results (sensitivity to meshes and models) form part of the numerical "experiments."
On completion of computation (numerical resolution of the equations describing the physical processes occurring in each cell), analysis of the results by specialists will rely on use of the numerical database. This will involve a number of stages: selective extraction of data (according to the physical parameter of interest) and visualization, and data extraction and transfer for the purposes of computing and visualizing diagnostics.
This parallel between performing a computation case for a numerical experiment and carrying out a physical experiment does not end there: the numerical results will be compared to the experimental findings. This comparative analysis, carried out on the basis of standardized quantitative criteria, will make demands on both the experience and skill of engineers, physicists, and mathematicians. Its will result in further improvements to physical models and simulation software programs.

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## The example of a thermalhydraulics computation

Implementation of a numerical simulation protocol may be illustrated by the work carried out by the team developing the **thermalhydraulics** computation software Trio U. This work was carried out in the context of a study conducted in collaboration with the French Radiological Protection and Nuclear Safety Institute (IRSN: Institut de radioprotection et de sûreté nucléaire). The aim was to obtain very accurate data to provide engineers with wall heat-stress values for the components of a pressurized-water reactor in case of a major accident involving turbulent natural circulation of hot gases. This investigation requires simultaneous modeling of large-scale "system" effects and of small-scale **turbulent** processes (see Box F, ***Modeling and simulation of turbulent flows***).
This begins with specification of the overall computation model (Figure A), followed by production of the CAD model and corresponding mesh with commercial software programs (Figure B). Meshes of over five million cells require use of powerful graphics stations. In this example, the mesh for a steam generator (Figures C and D) has been partitioned to parcel out computation over eight processors on one of CEA's parallel computers: each color stands for a zone assigned to a specific processor. The computations, whose boundary conditions are provided by way of a "system" computation (Icare–Cathare), yield results which it is up to the specialists to interpret. In this case, visualization on graphics stations of the instantaneous values of the velocity field show the impact of a hot plume on the steam generator's tubeplate (section of the velocity field, at left on Figure E), and instantaneous temperature in the water box (at right).

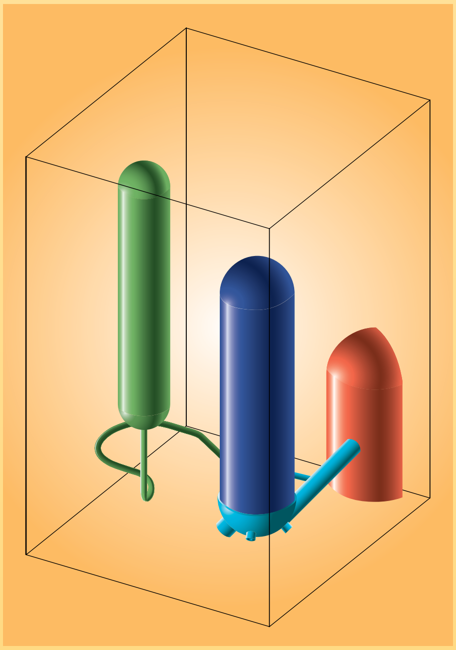


***Figure A. Overall computation domain, including part of the reactor vessel (shown in red), the outlet pipe (hot leg, in light blue), steam generator (dark blue), and pressurizer (green).***

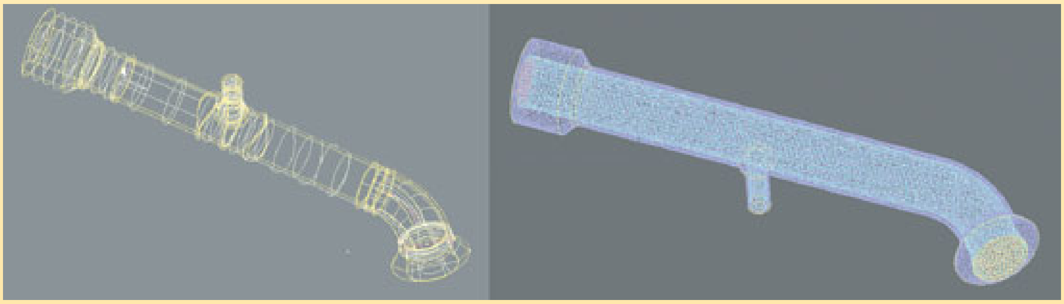
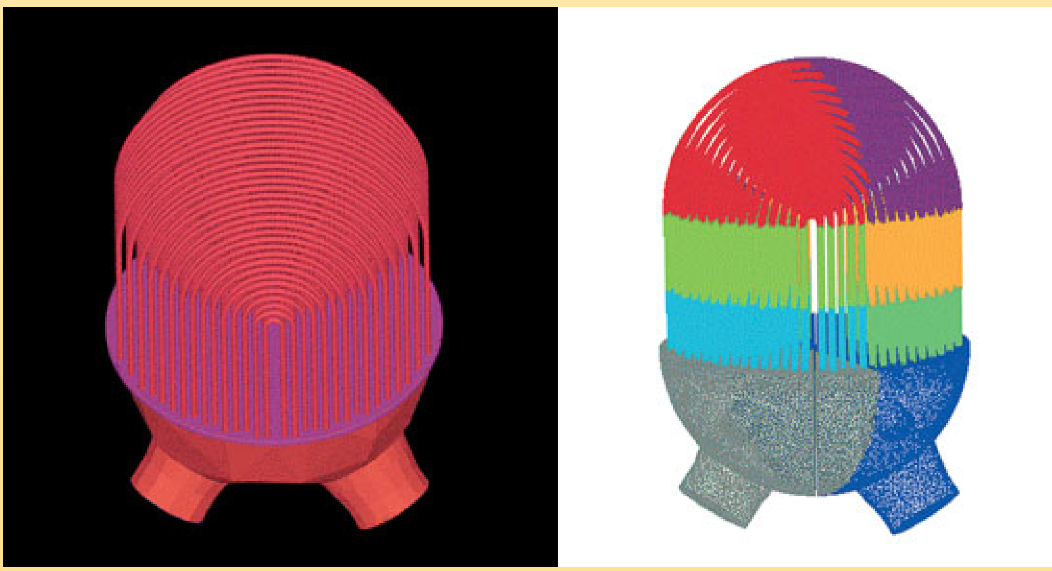


*Figure B. CAD model of the hot leg of the reactor vessel outlet (left) and unstructured mesh for it (right).*



*Figures C and D.*

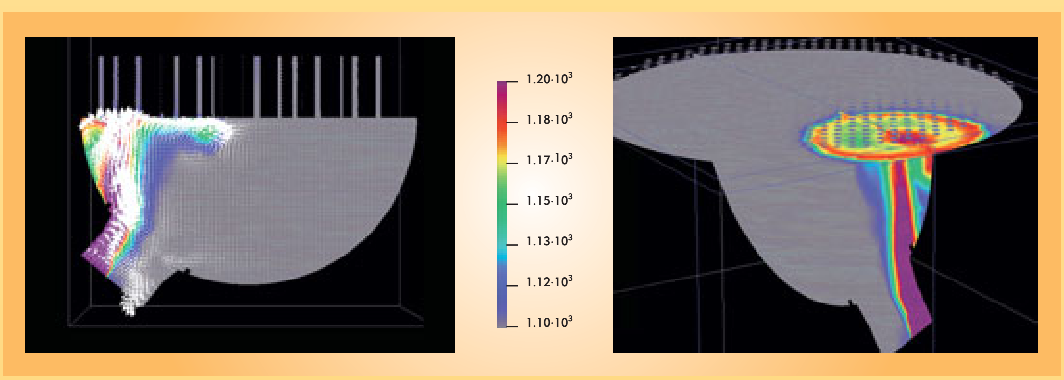



*Figure E.*

# Computational resources for high-performance numerical simulation

B

Carrying out more accurate **numerical simulations** requires the use of more complex physical and numerical **models** applied to more detailed descriptions of the simulated objects (see Box A, ***What is a numerical simulation?***). All this requires advances in the area of simulation software but also a considerable increase in the capacity of the computer systems on which the software runs.

## Scalar and vector processors

The key element of the computer is the processor, which is the basic unit that executes a program to carry out a computation. There are two main types of processors, **scalar processors** and **vector processors**. The former type carries out operations on elementary (scalar) numbers, for instance the addition of two numbers. The second type carries out operations on arrays of numbers (vectors), for example adding elementwise the numbers belonging to two sets of 500 elements. For this reason, they are particularly well suited to numerical simulation: when executing an operation of this type, a vector processor can operate at a rate close to its maximum (peak) performance. The same operation with a scalar processor requires many independent operations (operating one vector element at a time) executed at a rate well below its peak rate. The main advantage of scalar processors is their price: these are general-purpose microprocessors whose design and production costs can be written-down across broad markets.

## Strengths and constraints of parallelism

Recent computers allow high performances partly by using a higher operating frequency, partly by trying to carry out several operations simultaneously: this is a first level of **parallelism**. The speeding up in frequency is bounded by developments in microelectronics technology, whereas interdependency between the instructions to be carried out by the processor limits the amount of parallelism that is possible. Simultaneous use of several processors is a second level of parallelism allowing better performance, provided programs able to take advantage of this are available. Whereas parallelism at processor level is automatic, parallelism *between processors* in a parallel computer must be taken into account by the programmer, who has to split his program into independent parts and make provisions for the necessary communication between them. Often, this is done by partitioning the domain on which the computation is done. Each processor simulates the behavior of one domain and regular communications between processors ensure consistency for the overall computation. To achieve an efficient parallel program, a balanced share of the workload must be ensured among the individual processors and efforts must be made to limit communications costs.

## The various architectures

A variety of equipment types are used for numerical simulation. From their desktop computer where they prepare computations and analyze the results, users access shared computation, storage and visualization resources far more powerful than their own. All of these machines are connected by networks, enabling information to circulate between them at rates compatible with the volume of data produced, which can be as much as 1 **terabyte** (1 TB = $10^{12}$ bytes) of data for one single simulation.

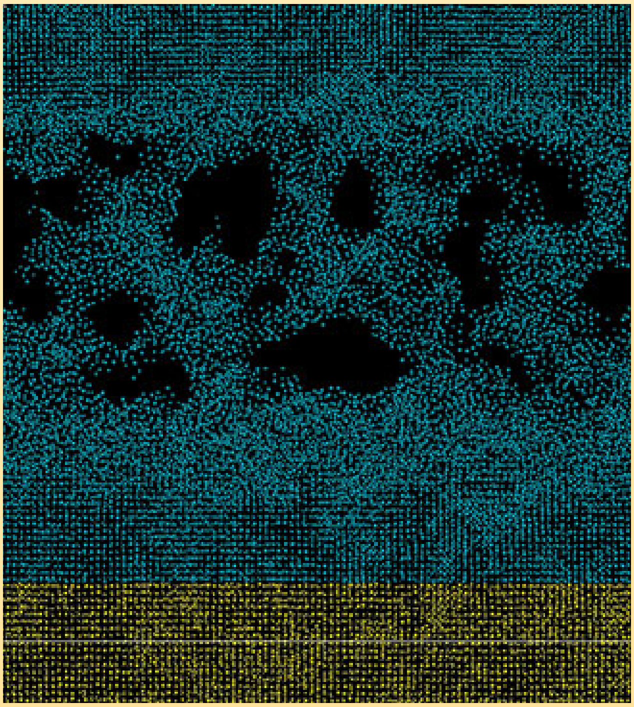
The most powerful computers are generally referred to as **supercomputers**. They currently attain capabilities counted in **teraflops** (1 Tflops = $10^{12}$ floating-point operations per second).

Currently, there are three main types of supercomputers: vector supercomputers, clusters of mini-computers with shared memory, and clusters of PCs (standard home computers). The choice between these architectures largely depends on the intended applications and uses. Vector supercomputers have very-high-performance processors but it is difficult to increase their computing performance by adding processors. PC clusters are inexpensive but poorly suited to environments where many users perform numerous large-scale computations (in terms of memory and input/output).

It is mainly for these reasons that CEA's Military Applications Division (DAM) has choosen for its Simulation Program (see *The Simulation Program: weapons assurance without nuclear testing*) architectures of the shared-memory mini-computer cluster type, also known as **clusters of SMPs** (symmetric multiprocessing). Such a system uses as a basic building block a mini-computer featuring several microprocessors sharing a common memory (see Figure). As these mini-computers are in widespread use in a variety of fields, ranging from banks to web servers through design offices, they offer an excellent performance/price ratio. These basic "blocks" (also known as *nodes*) are connected by a high-per-

***Installed at CEA (DAM-Ile de France Center) in December 2001, the TERA machine designed by Compaq (now HP) has for its basic element a mini-computer with 4 x 1-GHz processors sharing 4 GB of memory and giving a total performance of 8 Gflops. These basic elements are interconnected through a fast network designed by Quadrics Ltd. A synchronization operation across all 2,560 processors is completed in under 25 microseconds. The overall file system offers 50 terabytes of storage space for input/output with an aggregate bandwidth of 7.5 GB/s.***

# Computational resources for high-performance numerical simulation (cont'd)



CEA

*Parallel computers are well suited to numerical methods based on meshing (see Box A, What is a numerical simulation?) but equally to processing ab-initio calculations such as this molecular-dynamics simulation of impact damage to two copper plates moving at 1 km/s (see Simulation of materials). The system under consideration includes 100,000 atoms of copper representing a square-section (0.02 µm square) parallelogram of normal density. The atoms interact in accordance with an embedded atom potential over approximately 4–6 picoseconds. The calculation, performed on 18 processors of the Tera supercomputer at Bruyères-le-Châtel using the CEA-developed Stamp software, accounted for some ten minutes of "user" time (calculation carried out by B. Magne). Tests involving up to 64 million atoms have been carried out, requiring 256 processors over some one hundred hours.*

formance network: the cumulated power of several hundreds of these "blocks" can reach several Tflops. One then speaks of a **massively parallel computer**.

Such power can be made available for one single parallel application using all the supercomputer's resources, but also for many independent applications, whether parallel or not, each using part of the resources.

While the characteristic emphasized to describe a supercomputer is usually its computational power, the input/output aspect should not be ignored. These machines, capable of running large-scale simulations, must have storage systems with suitable capacities and performance. In clusters of SMPs, each mini-computer has a local disk space. However, it is not advisable to use this space for the user files because it would require the user to move explicitly his data between each distinct stage of his calculation. For this reason, it is important to have disk space accessible by all of the mini-computers making up the supercomputer. This space generally consists in sets of disk drives connected to nodes whose main function is to manage them. Just as for computation, parallelism of input/output allows high performance to be obtained. For such purposes, parallel overall file systems must be implemented, enabling rapid and unrestricted access to the shared disk space.

While they offer considerable computational power, clusters of SMPs nevertheless pose a number of challenges. Among the most important, in addition to programming simulation software capable of using efficiently a large number of processors, is the development of operating systems and associated software tools compatible with such configurations, and fault-tolerant.

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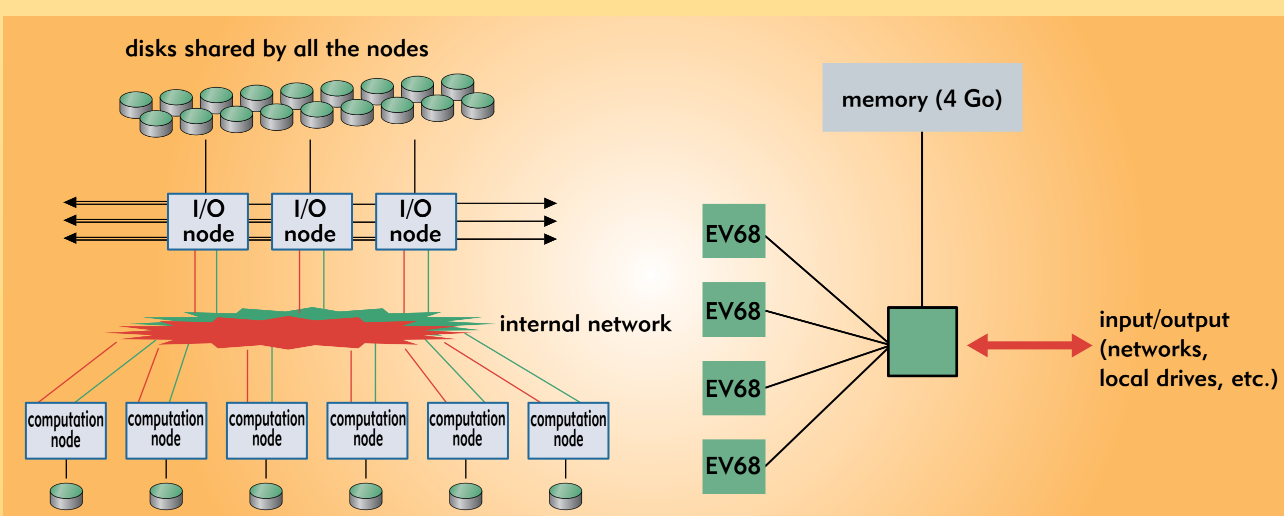


*Figure. Architecture of an "SMP-cluster" type machine. At left, the general architecture (I/O = input/output), on the right, that of a node with four Alpha EV68 processors, clocked at 1 GHz.*

# Modeling and simulation of turbulent flows F

**Turbulence**, or disturbance in so-called turbulent flow, develops in most of the flows that condition our immediate environment (rivers, ocean, atmosphere). It also turns out to be one, if not the, dimensioning parameter in a large number of industrial flows (related to energy generation or conversion, aerodynamics, etc.). Thus, it is not surprising that a drive is being launched to achieve prediction for the process – albeit in approximate fashion as yet – especially when it combines with complicating processes (stratification, combustion, presence of several phases, etc.). This is because, paraxodically, even though it is possible to predict the turbulent nature of a flow and even, from a theoretical standpoint, to highlight certain common – and apparently universal – characteristics of turbulent flows,(1) their prediction, in specific cases, remains tricky. Indeed, it must take into account the considerable range of space and time scales(2) involved in any flow of this type.

Researchers, however, are not without resources, nowadays, when approaching this problem. First, the equations governing the evolution of turbulent flows over space and time (Navier–Stokes equations(3)) are known. Their complete solution, in highly favorable cases, has led to predictive descriptions. However, systematic use of this method of resolution comes up against two major difficulties: on the one hand, it would require complete, simultaneous knowledge of all variables attached to the flow, and of the forced-flow conditions imposed on it,(4) and, on the other hand, it would mobilize computational resources that will remain unrealistic for decades yet.

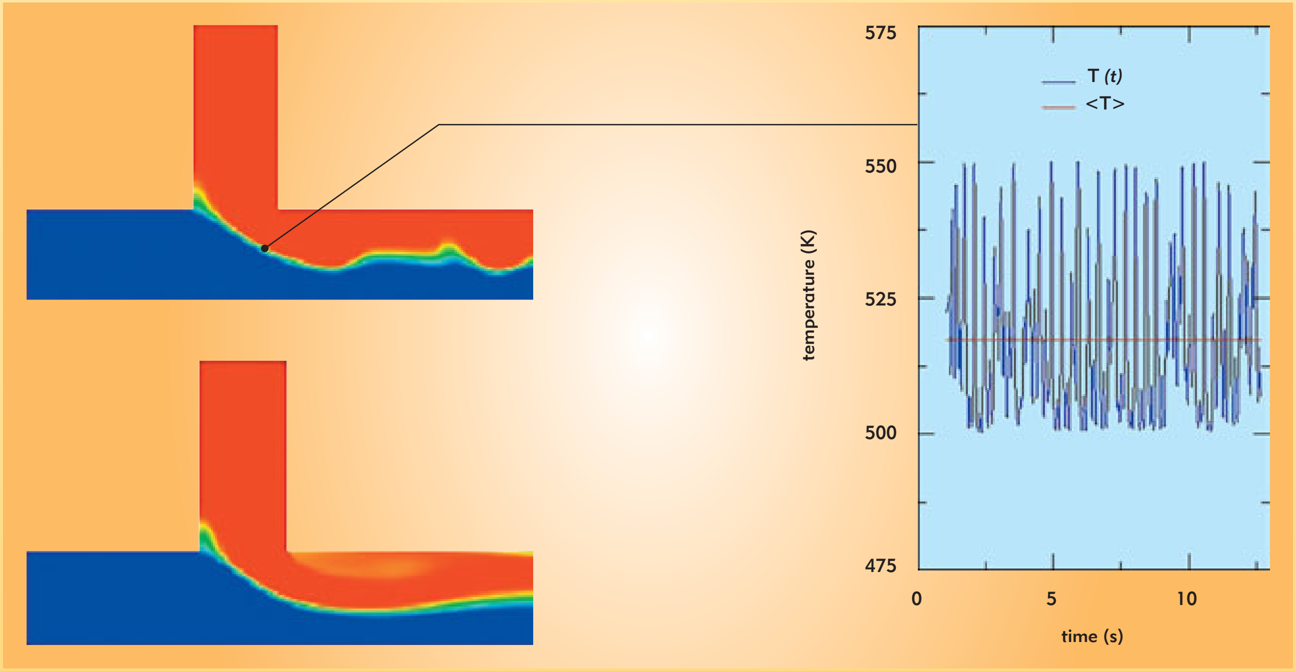


*Figure. Instantaneous (top) and averaged (bottom) temperature field in a mixing situation. The curve shows the history of temperature at one point: fluctuating instantaneous value in blue and mean in red (according to Alexandre Chatelain, doctoral dissertation) (DEN/DTP/SMTH/LDTA).*

The sole option, based on the fluctuating character of the flow due to turbulent agitation, must thus be to define and use average values. One of the most widely adopted approaches consists in looking at the problem from a statistical angle. The mean overall values for velocity, pressure, temperature… whose distribution characterizes the turbulent flow, are defined as the principal variables of the flow one then seeks to qualify relative to those mean values. This leads to a decomposition of the motion (the so-called Reynolds decomposition) into mean and fluctuating fields, the latter being the measure of the instantaneous local difference between each actual quantity and its mean (Figure). These fluctuations represent the turbulence and cover a major part of the Kolmogorov spectrum.(1)

This operation considerably lowers the number of degrees of liberty of the problem, making it amenable to computational treatment. It does also involve many difficulties: first, it should be noted that, precisely due to the non-linearity of the equations of motion, any average process leads to new, unknown terms that must be estimated. By closing the door on complete, deterministic description of the phenomenon, we open one to modeling, i.e. to the representation of the effects of turbulence on mean variables.

Many advances have been made since the early models (Prandtl, 1925). Modeling schemas have moved unabated towards greater complexity, grounded on the generally verified fact that any new extension allows the previously gained properties to be preserved. It should also be noted that, even if many new developments are emphasizing anew the need to treat flows by respecting their *non-stationary* character, the most popular modeling techniques were developed in the context of *stationary* flows, for which, consequently, only a representation of the flow's temporal mean can be achieved: in the final mathematical model, the effects of turbulence thus stem wholly from the modeling process.

It is equally remarkable that, despite extensive work, no modeling has yet been capable of accounting for all of the processes influencing turbulence or influenced by it (transition, non-stationarity, stratification, compression, etc.). Which, for the time being, would seem to preclude statistical modeling from entertaining any ambitions of universality.

Despite these limitations, most of the common statistical modeling techniques are now available in commercial codes and industrial tools. One cannot claim that they enable predictive computations in every situation. They are of varying accuracy, yielding useful results for the engineer in controlled, favorable situations (prediction of drag to an accuracy of 5–10%, sometimes better, for some profiles), but sometimes inaccurate in situations that subsequently turn out to lie outside the model's domain of validity. Any controlled use of modeling is based, therefore, on a qualification specific to the type of flow to be processed. Alternative modeling techniques, meeting the requirement for greater accuracy across broader ranges of space and time scales, and therefore based on a "mean" operator of a different nature, are currently being developed and represent new ways forward.

The landscape of turbulence modeling today is highly complex, and the unification of viewpoints and of the various modeling concepts remains a challenge. The tempting goal of modeling with universal validity thus remains out of order. Actual implementation proceeds, in most cases, from compromises, guided as a rule by the engineer's know-how.

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(1) One may mention the spectral distribution of turbulent kinetic energy known as the "Kolmogorov spectrum," which illustrates very simply the hierarchy of scales, from large, energy-carrying scales to ever smaller, less energetic scales.

(2) This range results from the non-linearities of the equations of motion, giving rise to a broad range of spatial and temporal scales. This range is an increasing function of the Reynolds number, Re, which is a measure of the inertial force to viscous force ratio.

(3) The hypothesis that complete resolution of the Navier–Stokes equations allows simulation of turbulence is generally accepted to be true, at any rate for the range of shock-free flows.

(4) This is a problem governed by initial and boundary conditions.

# Molecular modeling

C

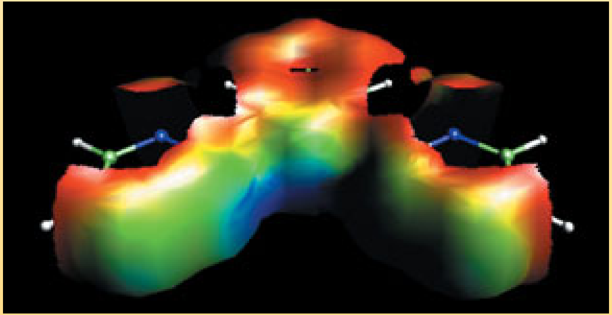
Researchers in biology, chemistry and the physics of materials increasingly use computational tools that enable them to model the behavior of molecules as a function of their structure. The accuracy of these approaches is now such that they are employed for the design of molecules and materials with specific properties.

A broad range of **theoretical** tools is available, including those based on the methods of quantum chemistry, grounded molecular mechanics and molecular dynamics.

**Quantum chemistry** is grounded on the laws of quantum mechanics and serves, above all, to describe the electronic structure of molecules. This is important for the understanding of processes such as chemical reactions.

*Classical* **molecular dynamics** simulates the motions of atoms in molecular systems, and the evolution of their spatial configuration, using the equations of classical mechanics. It gives access to structural, dynamic and thermodynamic properties.

Like quantum chemistry, **molecular mechanics** is a method that enables the investigation of the structure and behavior of molecules but it is less costly, faster and can be used to describe systems consisting of thousands of atoms, such as **biological macromolecules**.



CEA/DEN/J.-P. Dognon

***Representation of the electrostatic potential around the molecule, bis-triazinyl-pyridine (BTP) calculated by a quantum-chemical method. This molecule was developed for the Sanex process that separates actinides and lanthanides.***