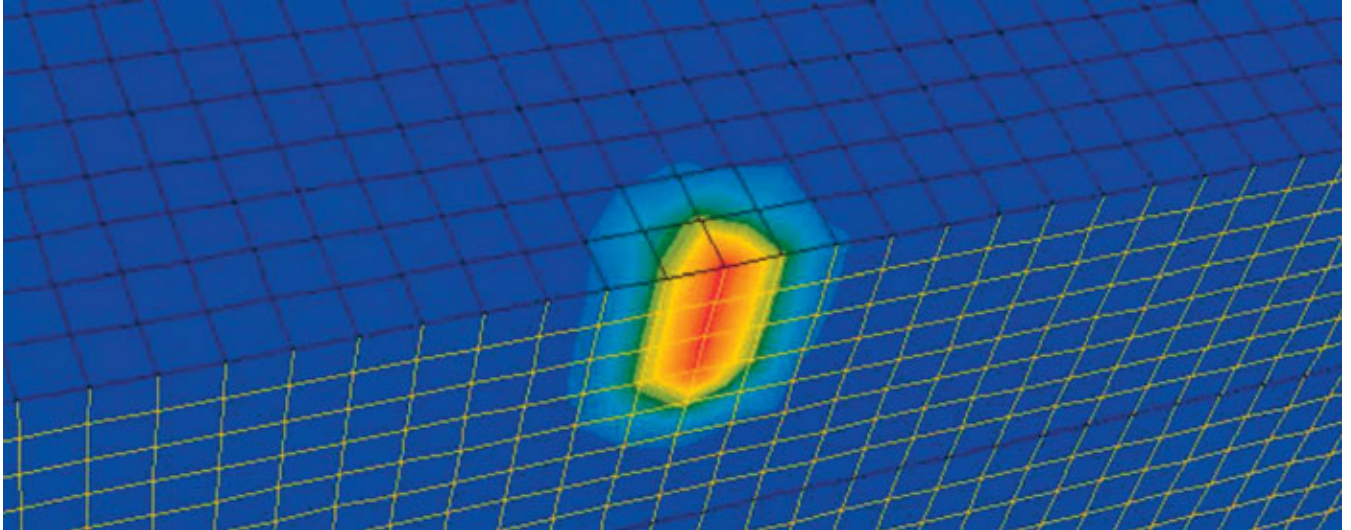


## VIRTUAL WELDING

*Numerical simulation is proving to be an effective means of controlling the main effects of welding and ensuring weld reliability. To be predictive, it must model, in a simplified but relevant manner, the interactions between the physics of the operation, weld pool behavior, thermics, metallurgy and the mechanics of the process.*



*Simulation, using the Fluent code, of the temperature distribution, modeled in 3D, following one pulse from the Nd:YAG pulsed laser during production of a fusion line at the center of an austenitic stainless-steel plate.*



### Indispensability of simple models

Welded joints are thought of, in more than one respect, as so many locations liable to constitute structural weaknesses throughout the life of a welded component. This is irrespective of the welding process, whether it consists in causing local, short-lived fusion of the joint (be it with the flame of a torch, an electric arc or the concentrated high-energy beam of a laser or electron gun), or forcing a transport of material to the interface by atomic diffusion (at high temperature and high pressure).

The singular character of welded joints is, first of all, physical-chemical: the very rapid heating to a high temperature, frequently to melting point, alters the arrangement of the material within the weld seam and across its immediate environment, over a width of only a few millimeters. The very existence of a melted zone is a source of radical alterations in the assembly's internal state. On the one hand, solidification of this zone results in a particular microstructure, distinct from the initial microstructure; and, on the other hand, welding dimensional shrinkage introduces residual stresses and distortions. This mechanical action is essentially due to differences in thermal expansion coefficients in the phases in contact, particularly between the liquid and solid phases. If these are not relaxed by heat, or mechanical, treatment, residual welding stresses will compound working stresses and can accelerate damage to

the component. Another consequence is that distortions, also concentrated around the joint, may induce displacements at the scale of the entire component and alter its dimensional characteristics. Finally, welding may induce defects in seam shape or, internally, cracks or cavities, all defects liable to impair the mechanical strength of the whole assembly.

In the great majority of cases, such difficulties do not amount to a genuine hindrance to the application of welding processes. In traditional sheet-metal work, they are overcome by the professional following standard practice. In cutting-edge industrial sectors, and particularly in the nuclear sector, risks related to welds are subject to specific treatment. From the design phase, dimensional specification codes consider a *joint coefficient* to be applied to the joints. Production development trials then form an unavoidable, protracted, and expensive phase. Particularly since optimization of the operating method may require revising the structure's design, by adjusting joint design and part size. Finally, non-destructive testing (NDT) is mandatory for welds deemed to be critical, after fabrication and possibly in service.

**Numerical simulation** of the welding process may provide valuable assistance in controlling the main effects of the process and weld reliability (see Box A, *What is a numerical simulation?*). The scientific and technological stake? To provide predictive results, which entails considering, in a simplified manner, the interactions between the



physics of the process, fluid behavior in the weld pool, thermics, metallurgy and mechanics. Developments concern, in particular, models of interaction between part and process (input of heat and material), mechanical and metallurgical behavior laws for materials during welding, and instrumentation methods enabling validation of these models.

### Localization of residual stresses

Mechanical design codes for steel components in the nuclear sector are used from the design stage of a power station to prevent **fatigue**, fatigue creep<sup>(1)</sup> and (progressive or excessive) distortion problems. Based on elasticity analyses of the stresses generated by the various operating loads, these codes impose very conservative margins as regards risk of cracking. Despite this precaution, defects can occur close to welds, due to loading arising in an incident, or inadequate knowledge of materials behavior. To account for the defect's occurrence and predict its development between inspections, it becomes necessary to implement detailed damage models, and take into account the residual stresses introduced by the assembly operation. Indeed, in such a case, a weld can constitute a weak link, even if NDT finds it to be sound. Its weakness then is attributed to its state of residual stress and to the materials' work-hardening state,<sup>(2)</sup> generated during the post-welding cooling phase. Operating loads adding to this initial stress state, the cumulated total must be taken into account to predict fatigue, creep and stress-corrosion behavior. At the same time, work-hardening of steels can accelerate such damage, either by causing embrittlement of the material, or by accentuating the discrepancy in mechanical characteristics between base metal and weld. This latter phenomenon can lead to a concentration of distortions in either one.

Simulation of residual welding stresses and distortions requires a minimum amount of data: the material's thermal and mechanical behaviors must be characterized up to melting temperature, and there is a requirement for perfect knowledge of heat source evolution in space and time. Further, nothing must remain unknown as to the position of the various welding passes and deposit sequence, and the right thermal and mechanical boundary conditions must be stipulated. A correction, based on experimental data such as size of melted zones, and – as the case may require – temperature during welding remains an indispensable requisite.

Simulations thus enable comparison of different processes according to criteria such as maximum residual stress or work-hardening levels, and evaluation of the effect of modified operating conditions. Thus, for repairs to the Phénix reactor's steam generators, a preliminary numerical study allowed optimization of the welding process so as to minimize residual stresses and distortions suspected of markedly accelerating the damage process (Figure 1).

What is at stake, in the coming years, is the ongoing improvement of models, particularly for the requirements of future reactors, by looking into materials exhibiting phase transformations at high temperature.

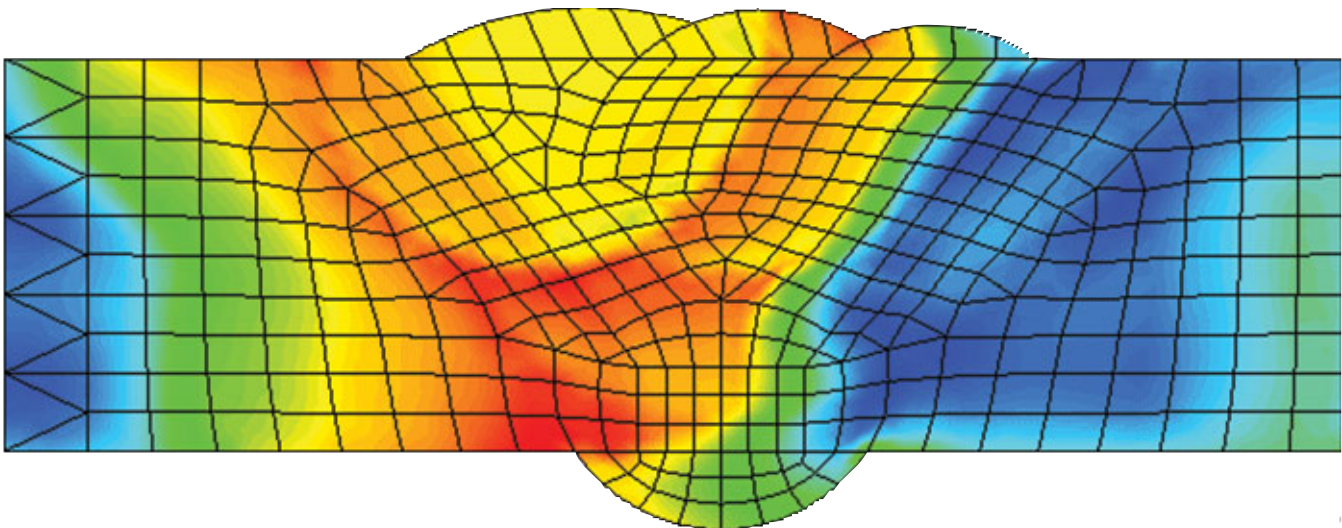
### Relevant thermics simulation: an unavoidable stage

The requirement for numerical simulation, in the case of Nd:YAG laser spot welding, originates in the wish to achieve better knowledge of assemblies fabricated by this method at CEA's Valduc Center. Indeed, these must

- (1) Irreversible deformation of a material subjected to mechanical stress.
- (2) Working a metal at a temperature below its annealing temperature.



*Figure 1. Modeling, with the Castem 2000 finite-element code, of the distribution of Von Mises stresses after circumferential (TIG) arc welding of two austenitic stainless-steel pipes in a steam generator in the Phénix reactor, made in five passes. The highest stresses are observed at the foot of the first pass.*



meet certain specifications as regards defect (pore) size, allowable distortions and mechanical strength.

This welding principle is based on the local fusion of material at beam impact point. The duration of a laser pulse is about ten milliseconds, with a firing frequency of a few hertz. A partial overlap of spot welds ensures seam continuity, with an average width and depth of a few millimeters.

Feasibility of simulation for this type of welding has been demonstrated. The thermics approach under transient conditions required development of a subprogram for the Fluent v.6 software using the **finite-volume method**. It is thus possible to introduce into the simulation such process parameters as travel step, laser beam energy, pulse dura-

tion and frequency. Heat exchanges by natural **convection** and by radiation are taken on board. Energy input during welding is simulated empirically by stipulating an energy flux per unit volume over each pulse. Validation of this model is based on size prediction for the melted zone and experimental realization of a fusion line at the center of an austenitic stainless-steel plate<sup>(3)</sup> (see illustration at beginning of article). However, one should bear in mind the difficulty of achieving correct measurement of the temperature, owing to the steep thermal gradients generated and small size of the affected zone. A design of experiment was implemented to determine the relationship between melted pool shape and process parameters, and quantify the influence of the latter and their possible couplings (see *Behavioral modeling*). The findings constitute a validation base for the **modeling** effort.

The purpose of this purely thermics-oriented approach is to be able to consider thermalmechanical aspects in sequence. A future step will consist in further taking into account **thermalhydraulic** phenomena. More physical modeling will require a description of keyhole generation in the pool during the laser pulse, closure of which is the source of some defects (pores).

grades used and the amplitude of the distortions imposed by shrinkage during solidification. The occurrence of this defect being difficult to predict empirically, the industry seeks the ability to control this risk through numerical simulation of the process.

A local thermalmechanical criterion for crack initiation is being developed at CEA's Saclay Center. Conditions for cracking are investigated by means of a "weldability" test enabling forced occurrence of the defect in a material particularly subject to cracking, austenitic stainless steel. This Vareststraint (Variable Restraint) test consists in straining the material by bending it during production of a fusion line by the TIG (tungsten-inert gas) process. The defects obtained are then characterized in terms of quantity and length. Since there are limited possibilities as to local instrumentation, the experimental findings are complemented by a numerical simulation of the thermalmechanical conditions of the test. Now realistic mechanical simulation of the test requires use of an appropriate behavioral law for temperatures ranging from ambient temperature up to melting (about 1,400 °C). A campaign of mechanical characterization is thus carried out, selecting values and rates of distortion that are representative of what the material is subjected to during such tests. The findings, originating from tension and compression tests, allow a behavior law to be written, of the unified elasto-viscoplastic type, up to 1,200 °C, which is then extrapolated by way of viscoplastic behavior up to the melting domain (Figure 2).

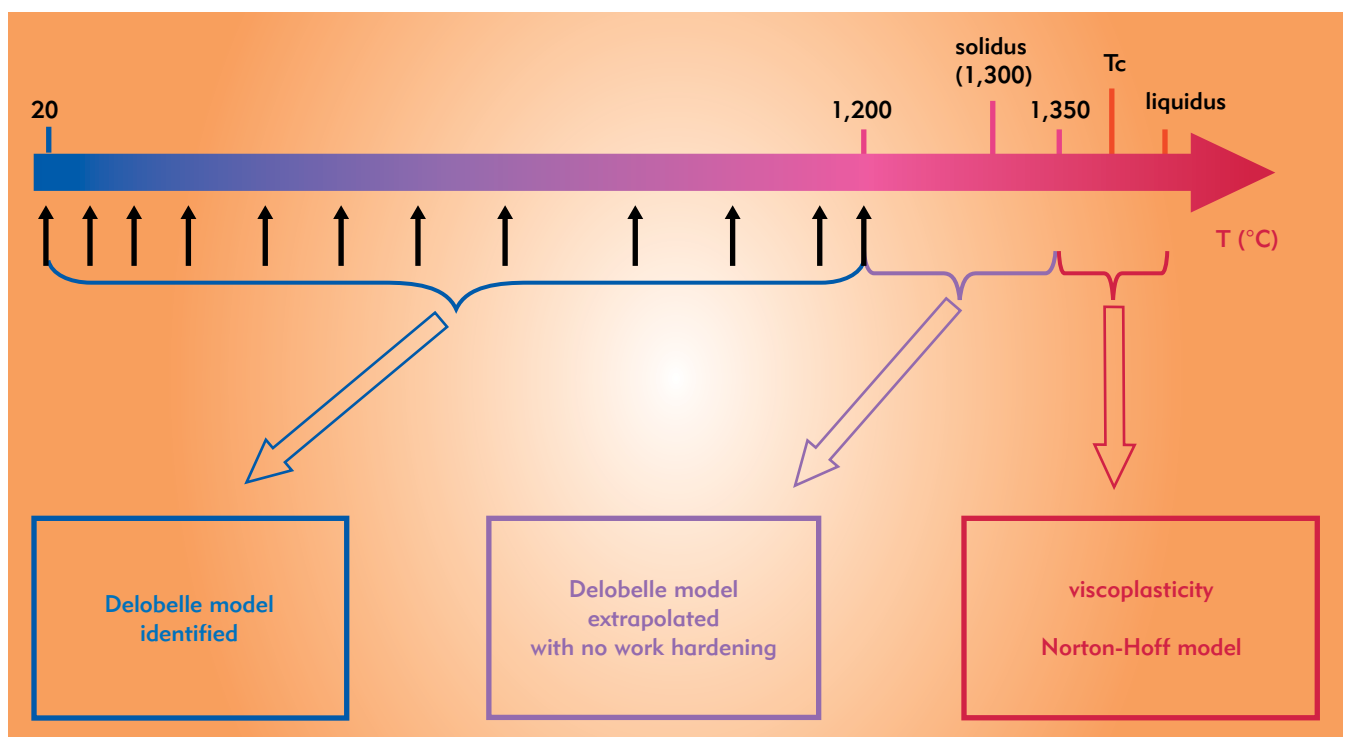
Thermalmechanical simulation by means of the Abaqus® **finite-element** code allows

Figure 2. Prediction of the mechanical effects of welding involves a relevant description of material behavior over a very wide temperature range. In this case, for an austenitic stainless steel, an elasto-viscoplastic behavior law, identified up to 1,200 °C, is extrapolated up to the solid-liquid transformation region.

### Predicting the occurrence of defects during welding

The risk of seam cracking during welding is mainly linked to the composition of the

(3) Steel characterized by a cubic face-centered structure (assembly of atoms).



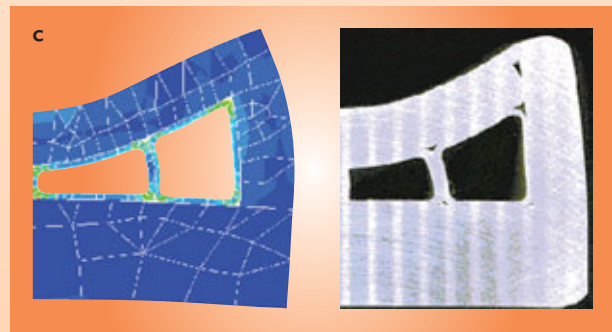
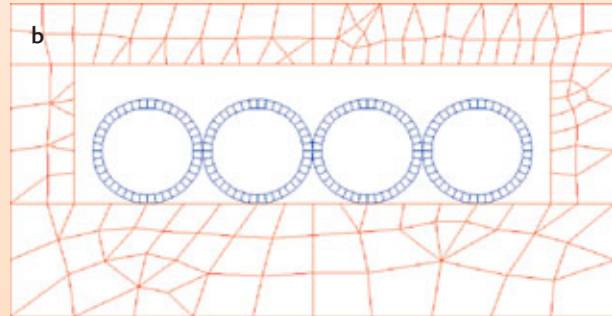
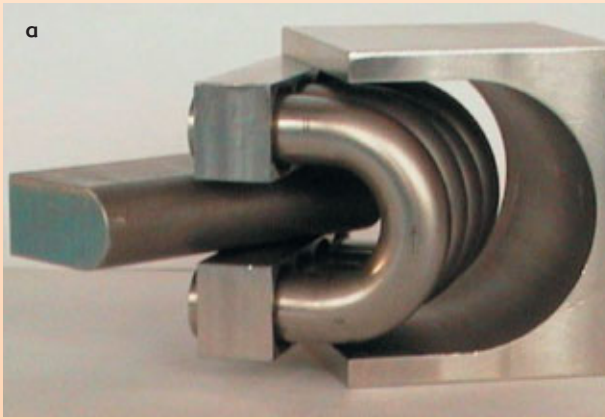


## What a hot isostatic pressing simulation can predict

Numerical simulation of a diffusion-welding operation by hot isostatic pressing (HIP) enables, in particular, prediction of dimensional evolutions in a component assembly fabricated by this technique, during the temperature- and pressure-loading cycle.

One of the specific features of this technique bears on the difficulty of predicting squeeze for the various components, i.e. the way the parts to be assembled (example: Figure A) will move with respect to one another and deform to fill the unavoidable gaps. The **mesh** of a section of a complex part (Figure B) takes such gaps and clearances into account. Two flows may occur in this part. The first one, which is desirable, is the expansion of the tubes related to gas circulation inside of them until they come into contact with each other, and with the top and side plates, thus welding. The second, unwanted, one is sagging of the top plate.

**Numerical simulation** of temperature and pressure rise for this part shows that sag is significant and that the chosen cycle does not ensure closure of the final porosity. The plastic deformation field is compared with a photograph of the assembly sectioned after HIP (Figure C). The comparison shows the model correctly predicts the relative motions of the actual components. Once validated, it enabled the specification of the plate thicknesses and HIP cycle required to weld this assembly satisfactorily.



interpretation of the observations and measurements. Comparison of the experimental and numerical findings leads to the suggestion of a thermalmechanical criterion for initiation of solidification cracking, for which predictions are in good agreement with test observations (Varestraint and others).

### Welding without fusion at 1,000 °C at 1,000 bars

Numerical simulation also concerns diffusion welding under hot isostatic pressing (HIP), which allows assembly of parts with highly complex geometries. In this technique, the various elements are positioned in a container which is put under a vacuum, welded shut and then placed in the HIP vessel. Solid-state welding of the various surfaces is achieved by simultaneous application of high temperature (80–85% of melting temperature) and high pressure (1,000–1,500 bars). As it is highly reproducible, insofar as the heat source is controlled, this process lends itself naturally to numerical simulation. Prediction of residual stresses developing during cooling of

the welded part relies on equations classically used for welding involving local fusion, with catering for the liquid phase and solidification being omitted in this case. Stresses are due to the presence of a thermal gradient in the parts and/or differences in the expansion coefficients for the various materials in the assembly. Simulation involves multimaterial thermalmechanical models, taking into account, if required, phase change in the solid state and alterations of local properties (see Box). Thus, as in the previous examples, simulation ultimately serves to optimize the welding operation.

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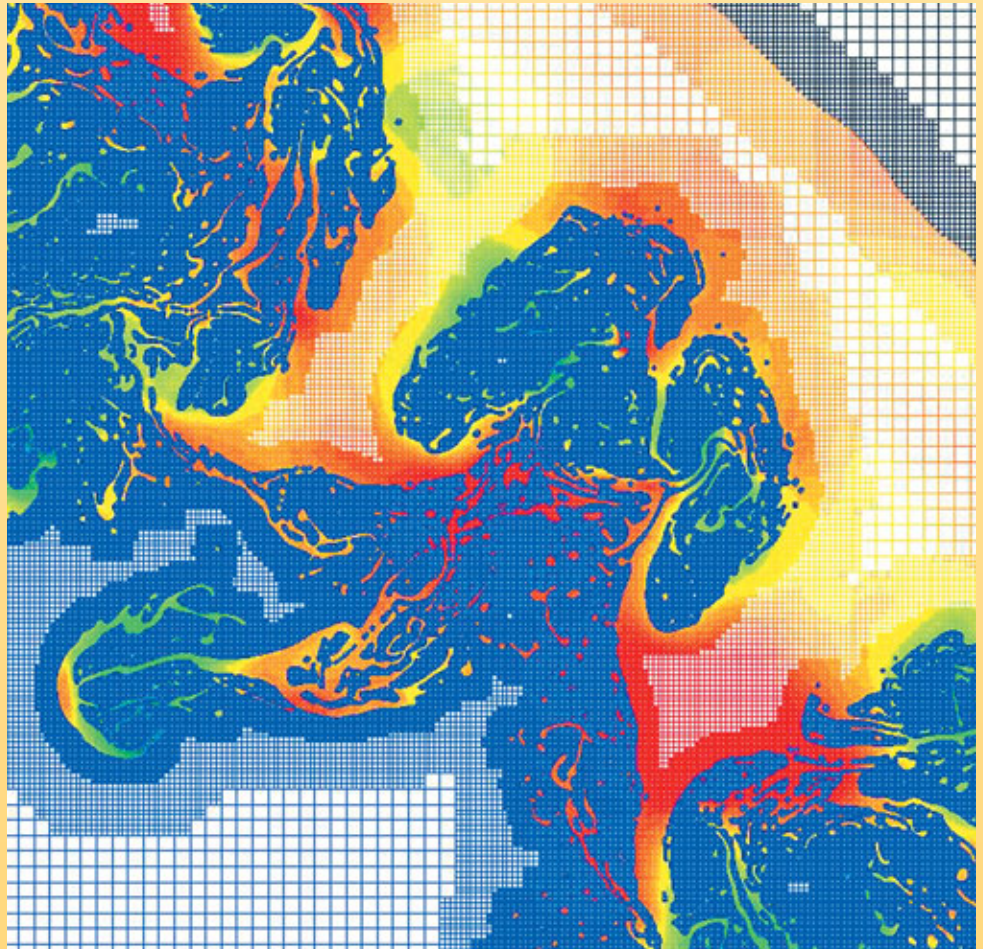
**Numerical simulation** consists in reproducing, through computation, a system's operation, described at a prior stage by an ensemble of **models**. It relies on specific mathematical and computational methods. The main stages involved in carrying out an investigation by means of numerical simulation 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.

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.

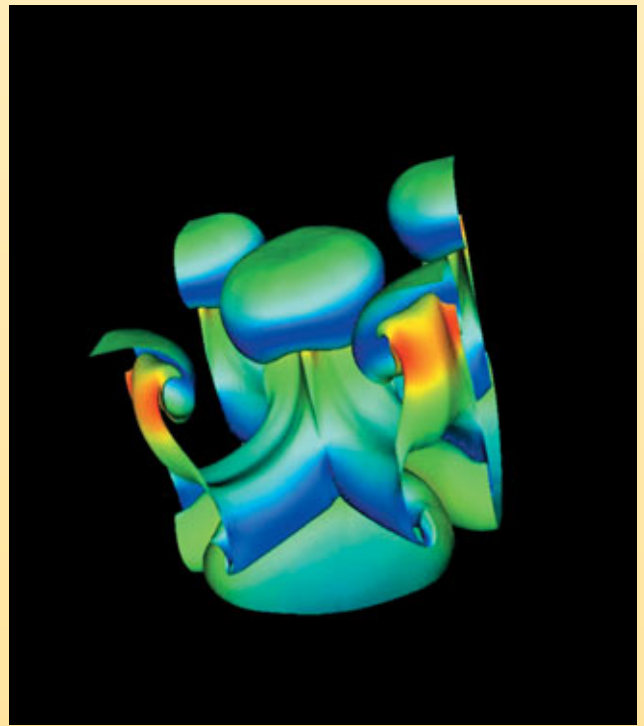
## How does a numerical simulation proceed?

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) –, fol-



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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.

lowed 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,<sup>(1)</sup> mesher,<sup>(2)</sup> 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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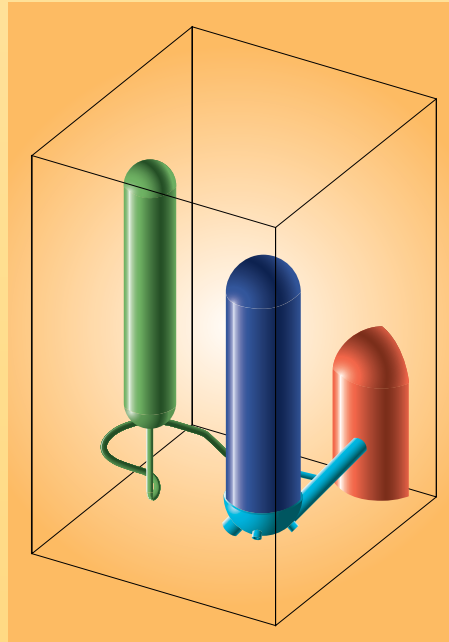
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## The example of a thermalhydraulics computation

Implementation of a numerical simulation protocol may be illustrated by the work carried out by the team developing the **thermallydraulics** 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 tube-plate (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).*

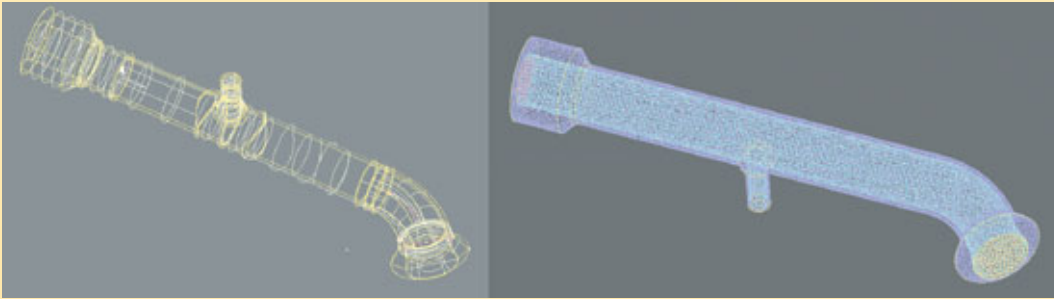
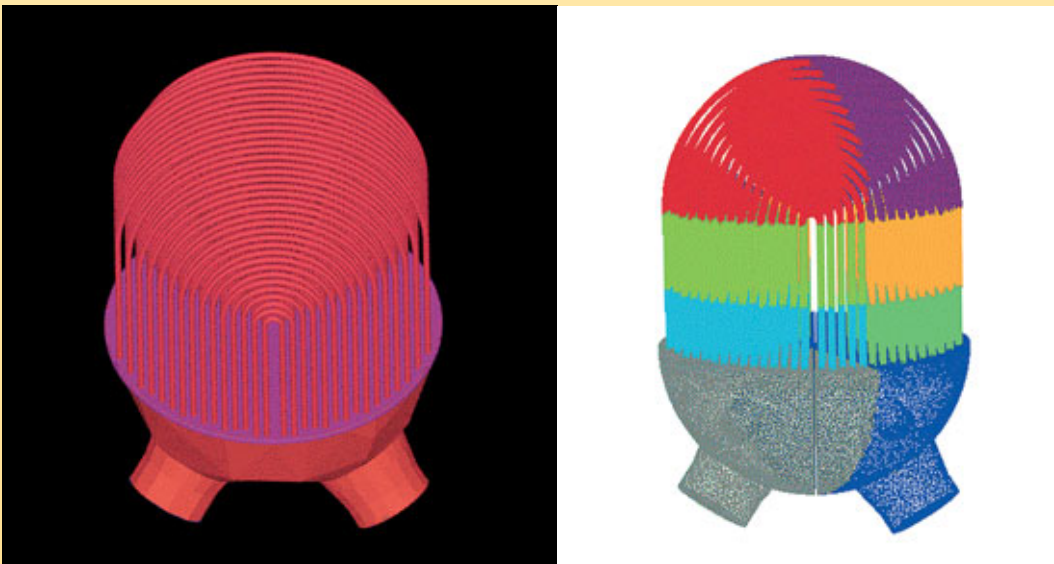


Figure B. CAD model of the hot leg of the reactor vessel outlet (left) and unstructured mesh for it (right).



Figures C and D.

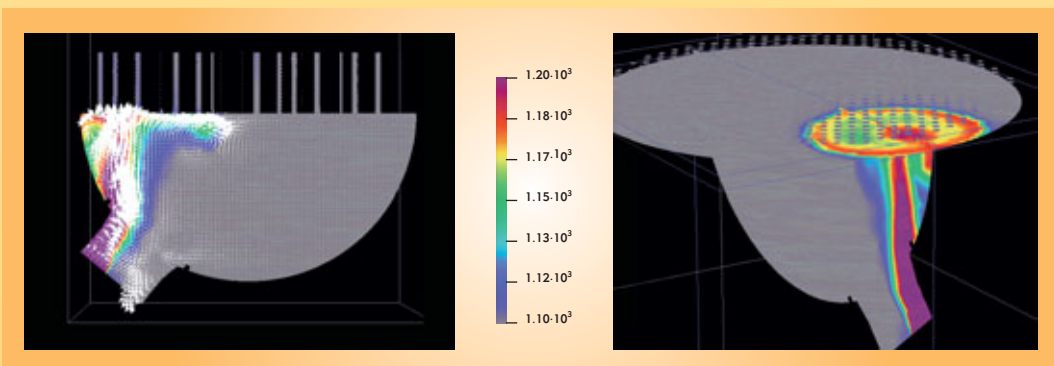


Figure E.



# 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 develop-

ments 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).

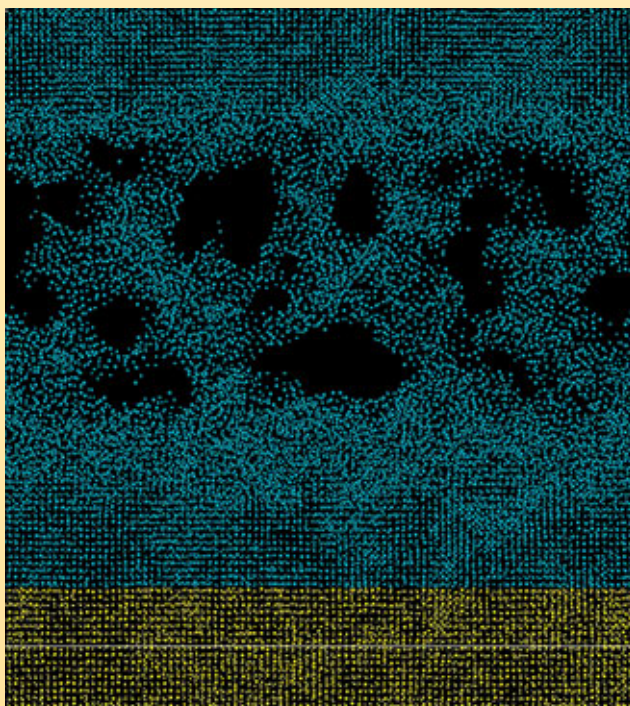
Currently, there are three main types of supercomputers: vector supercomputers, clusters of mini-computers with shared memory, and clusters of PCs (standard home computers). The choice between these architectures largely depends on the intended applications and uses. Vector supercomputers have very-high-performance 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 chosen 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)



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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  $\mu\text{m}$  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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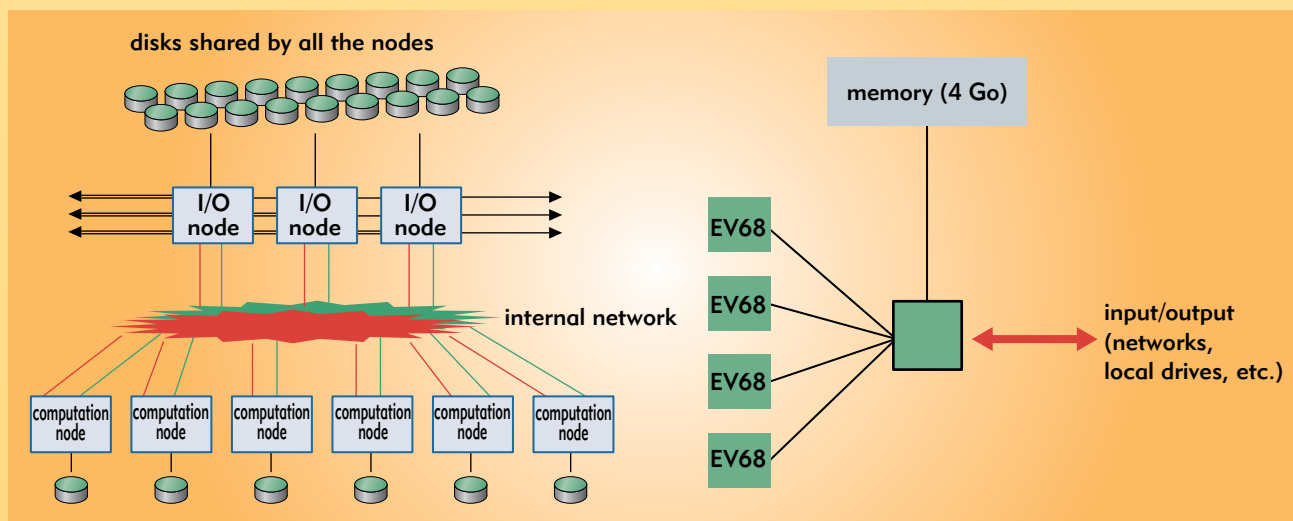


Figure. Architecture of an “SMP-cluster” type machine. At left, the general architecture (I/O = input/output), on the right, that of a node with four Alpha EV68 processors, clocked at 1 GHz.

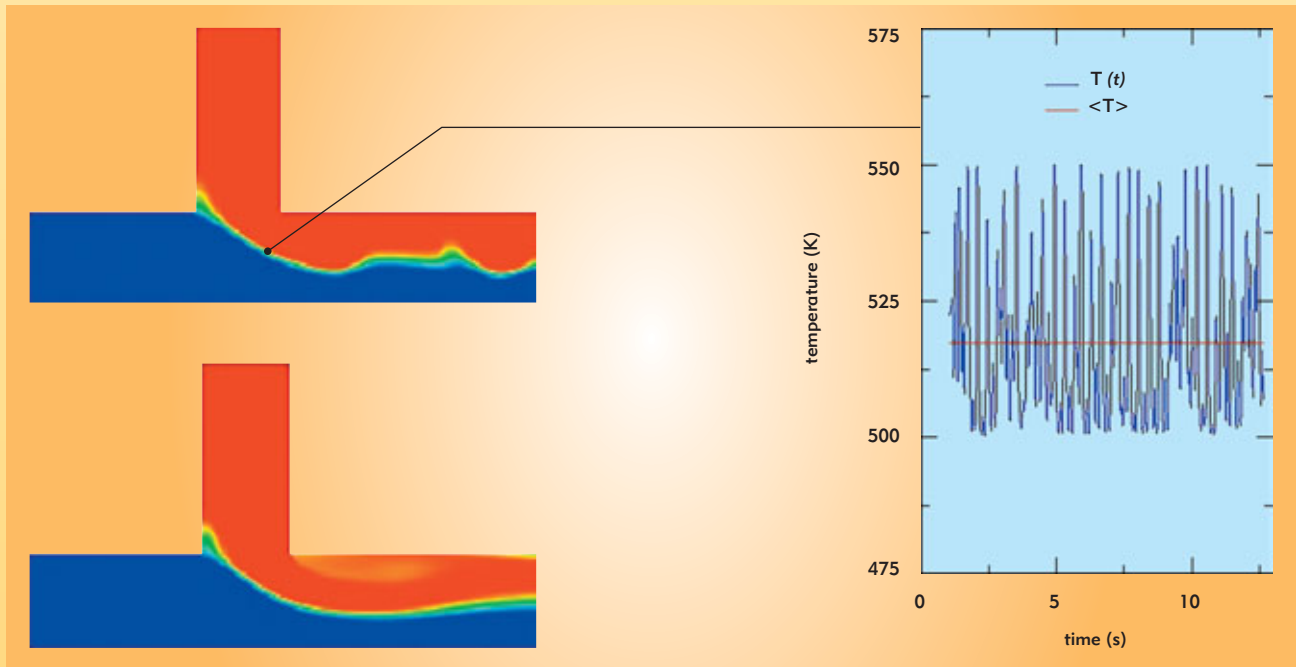
# Modeling and simulation of turbulent flows

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**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, paradoxically, 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,<sup>(1)</sup> their prediction, in specific cases, remains tricky. Indeed, it must take into account the consi-

derable range of space and time scales<sup>(2)</sup> 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<sup>(3)</sup>) 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,<sup>(4)</sup> 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.<sup>(1)</sup>

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.

(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.

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