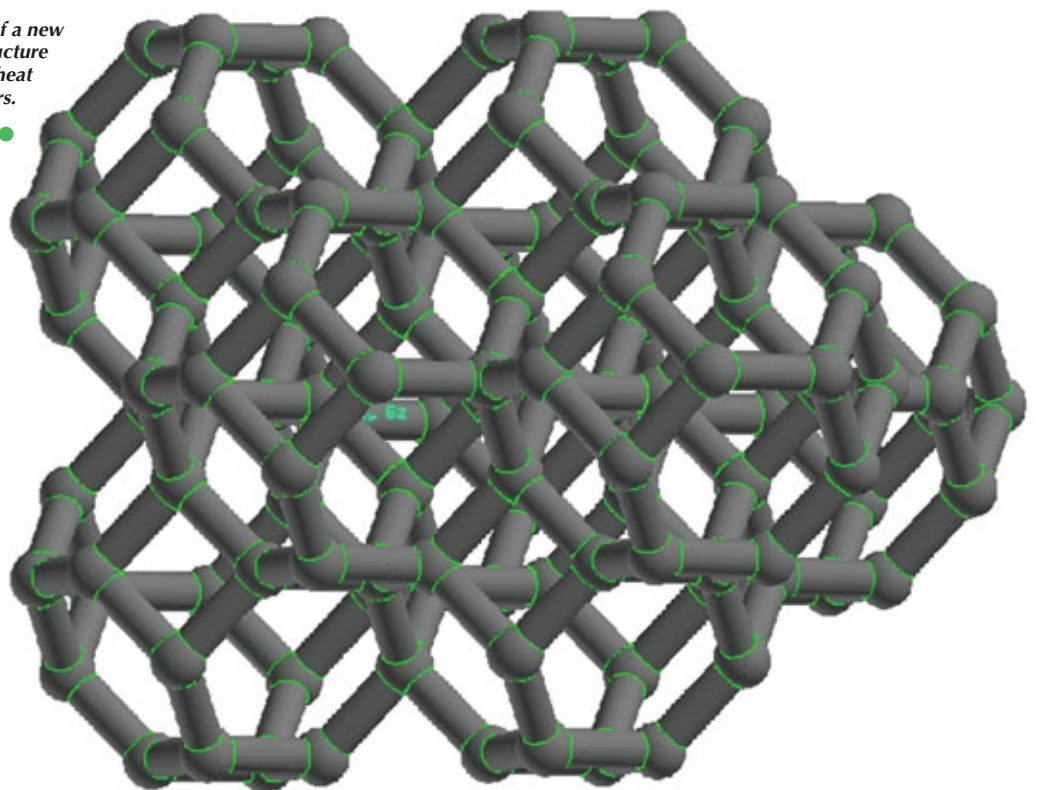


OPTIMIZATION OF COMPACT HEAT EXCHANGERS BY NUMERICAL SIMULATION

In the field of heat exchangers, researchers are pushing forward basic investigation of the mechanisms governing turbulent flows, of decisive importance but only partly understood, even as industrialists call for ever-higher-performing technological developments. At the center of these concerns, simulation tools play a major role.

Elementary model of a new metal-foam type structure designed to increase heat transfers.



CEA/GRETh

At the core of the problem, turbulence...

Making the flow turbulent is the best way of enhancing heat transfers between a fluid and a wall. This is why **turbulent** flows (see Box F, *Modeling and simulation of turbulent flows*) are present in the majority of industrial processes, and particularly in the field of heat exchangers, where the dominant disciplines are fluid mechanics and transfers. A good understanding of the mechanisms of single-phase turbulence is of major importance for the optimization of their performance. These flows inherently exhibit very marked characteristics: a fluctuating character, three-dimensional aspect and broad energy spectrum. These three aspects contribute to the difficulty of exper-

imental measurements and the widespread use of physical **models** (see Box A, *What is a numerical simulation?*).

Broadly speaking, there are two opposing standpoints: that of the fluid mechanics specialists, and that of the industrialists. The former rightly point out that the mechanisms governing turbulent flows are still not perfectly accounted for, and require basic investigation. The latter, more pragmatically, are led to make choices in the face of an ongoing process of technological development. These choices, such as that of new geometric shapes, are often made under pressing circumstances. Their relevance depends in part on the fluid mechanics software programs, which form one component, among others, of the decision-making process.



Limitations of current tools

In the field of turbulent flows, **simulation** tools have relied essentially, so far, on a temporal-average approach requiring many **closure relations**, algebraic relations introduced to adjust the source terms of differential equations, of a more or less empirical character. Turbulence specialists take special care to tune models according to the particular cases – and these abound in the industrial domain. Such classical physical models are found wanting, for some conditions, particularly for zones close to walls, which limits their usefulness in the field of heat transfers. For example, recirculation in turbulent flows, or separation–reattachment processes, the mechanisms for which still lack a proper description.

Large eddy simulation

A new technique has recently appeared: *large eddy simulation* (LES). This consists in seeking to describe directly (in a non-stationary manner) the phenomena related to the largest vortices naturally present in a turbulent flow. The smaller vortices – those that dissipate the fluid's kinetic energy – will be described by a more general model. The principal original departure with such modeling is the way it opens up a whole field of investigation, by enabling numerical tools to yield not just a fixed image of the flow, but rather an animated film, allowing a reconstruction of its evolution over time. Simulation now has the ability to represent, in a particularly realistic manner, the motion of the largest vortices in the flow, which amounts to a major step towards a representation of the true nature of turbulence. Advances to be expected in the field of heat transfers in heat exchangers are thus numerous, and significant.

Commercial software policy

Requirements and expectations are great, in all industrial fields. The gamble is a huge one, since validation of LES is still left to the academic sector, and the advances to be made concern many specialties. As regards **numerical methods**, the accuracy and stability of the numerical schemas must be improved, and solving speed increased, and

in physics, model validation must be extended, starting with academic cases. At the halfway point between these two disciplines, compatibility must be ensured between the choices for the physical models and those for the numerical schemas. This is the approach that has been taken up by commercial **software**, with support from academic networks.

Just as, in the past, the inadequacy of the classical models was to be deplored, regarding fluid–wall heat transfers, it is apparent that the gulf remains great, between academic work and industrial reality, and that, in this respect, intensive validation on realistic problems is lacking.

GRETh's action

Faced with this situation, the activity developed by the Research Group on Heat Exchangers (GRETh: Groupement pour la recherche sur les échangeurs thermiques), at CEA's Grenoble Center, is twofold: carrying through the industrial validation of advanced thermal simulation models on the basis of heat-exchanger-related problems, and making available the models, and their domain of validity, to its industrialists' club, through the *software platform* concept.

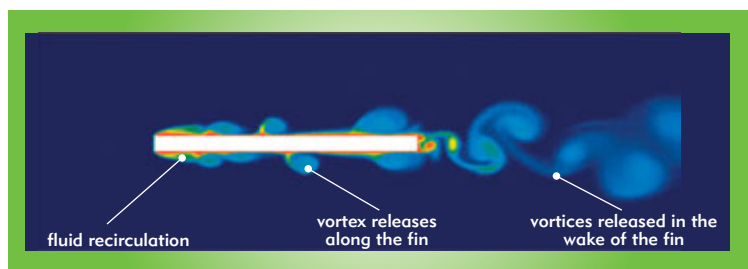
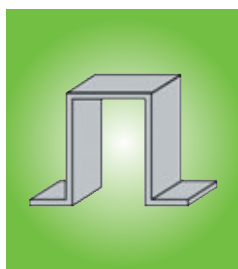
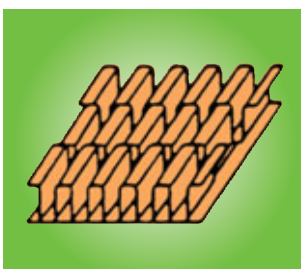
From industrial validation to industrialization

Compact heat exchangers occupy an increasingly important place in all areas of industry, particularly for the automotive, aviation, cryogenics, etc. sectors. They allow reductions in size, weight and costs for heat-transfer systems. One major scientific goal at stake is the prediction, by means of simulation, of flows and heat transfers in channels varying in size from 0.1 to 10 mm and featuring large geometric irregularities. One of the most representative geometries features offset strip fins (Figure 1).

With assistance from Ademe (Agence de l'environnement et de la maîtrise de l'énergie – the French Environment and Energy Control Agency), GRETh has undertaken work to increase the reliability of advanced numerical prediction tools, with a view to test numerical models and be in a position to select the highest-performing predictive



Figure 1. Snapshot of the air-temperature field at a given time around an isolated strip fin, with flow from left to right, obtained with CEA's Trio software. At left, diagram of such a fin and its offset layout, known as the offset strip fin (OSF) type.



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, 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,⁽¹⁾ their prediction, in specific cases, remains tricky. Indeed, it must take into account the consi-

derable 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.

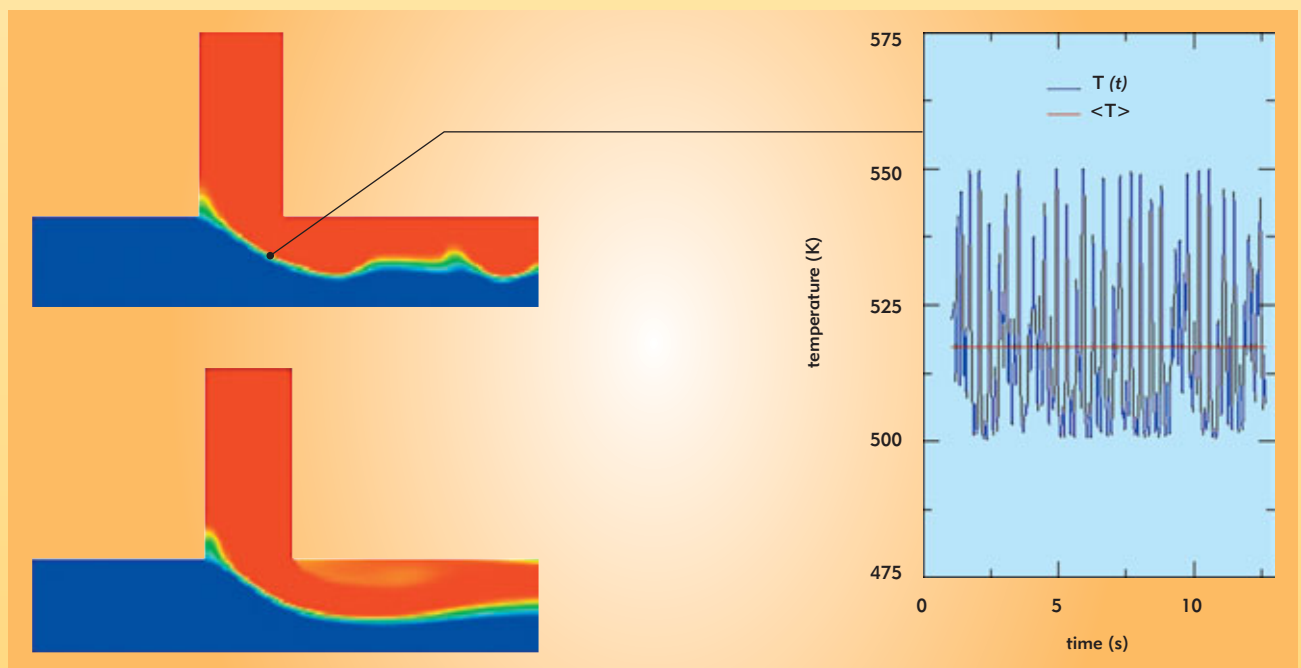


Figure. Instantaneous (top) and averaged (bottom) temperature field in a mixing situation. The curve shows the history of temperature at one point: fluctuating instantaneous value in blue and mean in red (according to Alexandre Chatelain, doctoral dissertation) (DEN/DTP/SMTH/LDTA).

model as regards a particular industrial problem. With the Trio software program developed at CEA, the best turbulence models are systematically tested on exchanger geometries comprising plates and fins whose characteristics are determined experimentally.

Two-dimensional and three-dimensional **thermalhydraulic** simulations of the flow around an isolated strip fin have been carried out, using two simulation tools. First, Trio enabled non-stationary simulations to be carried out, with various LES models. Then, the Fluent commercial computation tool was used to carry out stationary simulations with conventional turbulence models (of the Reynolds-averaged Navier–Stokes [RANS] equation type). These models yield the representative quantities for flow temporal averages.

The simulation results obtained are systematically compared with the literature or to laboratory experimental results: wall pressure-, friction- and heat-transfer-coefficient profiles, global pressure coefficient, and frequency of downstream vortex release.

The **meshes** used are of the order of 100,000 cells for 2D simulations, 1 million for 3D simulations. It is apparent that the numerical results are related to the turbulence models used, but also to their implementation. The results obtained in LES (Figure 1) allow identification of the mechanisms responsible for the increased heat transfer, by geometry-induced turbulence generation. The sequence of images enables visualization of the evolution over time of local mechanisms such as vortex growth, detachment and entrainment.

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.

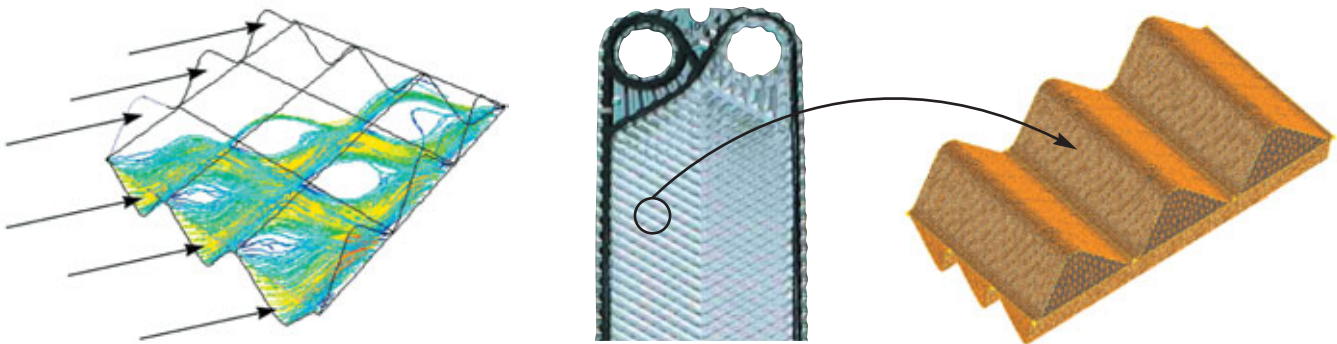
(1) One may mention the spectral distribution of turbulent kinetic energy known as the "Kolmogorov spectrum," which illustrates very simply the hierarchy of scales, from large, energy-carrying scales to ever smaller, less energetic scales.

(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.

Frédéric Ducros
Nuclear Energy Division
CEA Grenoble Center



Industrialization of these methods cannot occur without customer support of the consultancy type, the more so since such methods require ever-increasing specialization. For this purpose, GRETh has developed the software platform concept, which involves making the thermalhy-

draulic software programs and advanced models available to its industrialists' club, and working in close collaboration with the industrial partner, by giving access to its own resources and associating him as much as possible in tool use and implementation.⁽¹⁾ (Box).

Figure 2. Trajectories followed by the fluid inside a corrugated-plate heat exchanger with an angle of 60° to the flow direction. Obtained with the Fluent software, these results illustrate the work on local modeling of flows in exchangers of this type.



The example of developments in plate exchangers with Alfa-Laval-Vicarb

In the past, knowledge of the **thermohydraulic** performance of a heat exchanger resulted from a long list of trials, more or less consistent and complete. This is particularly true for compact heat exchangers, whose complex surfaces do not satisfy the correlations widely described in the literature. Improving a heat exchanger's performance thus involved many tests, but also some luck and a good part of feeling.

The arrival on the market of three-dimensional **numerical simulation software** programs has completely changed the position (see Box A, *What is a numerical simulation?*). Simulation, initially limited to one, then nine (Figure 2) and now thirty-six elementary cells, nowadays allows "numerization" of corrugated plates with very good consistency with standard formulas. With such a tool, it is possible to simulate geometric profiles that do not as yet exist, and would be expensive to manufacture prior to carrying out traditional trials – with findings subject to the possible mishaps of test loops.

Availability of this technology allows many more simulations to be achieved, to quantify the impact of the various parameters, and the visualization it makes possible is of great value for the understanding of local phenomena.

GRETh's lead in mastery of simulation software is a major asset when drawing up partnership contracts. Indeed, manufacturers do not always have in house the expertise and available resources to carry through increasingly complex projects, with ever-tighter deadlines.

The industrialists who call on GRETh for breakthrough technological developments have clearly understood the benefit of working in association with a laboratory that endeavors to go further than a mere demonstration of the potentials of the new methods, as illustrated by recently obtained results (Figures 2 and 3). GRETh also finds benefits in the good positioning of its work of systematic qualification, the increasing reputation

of its software platform – serving as meeting point for industrialists from widely diverse industries –, and the synergy between the various research programs carried out in non-competitive sectors, meeting the actual problems of industrialists.

A major leap in predictive capability

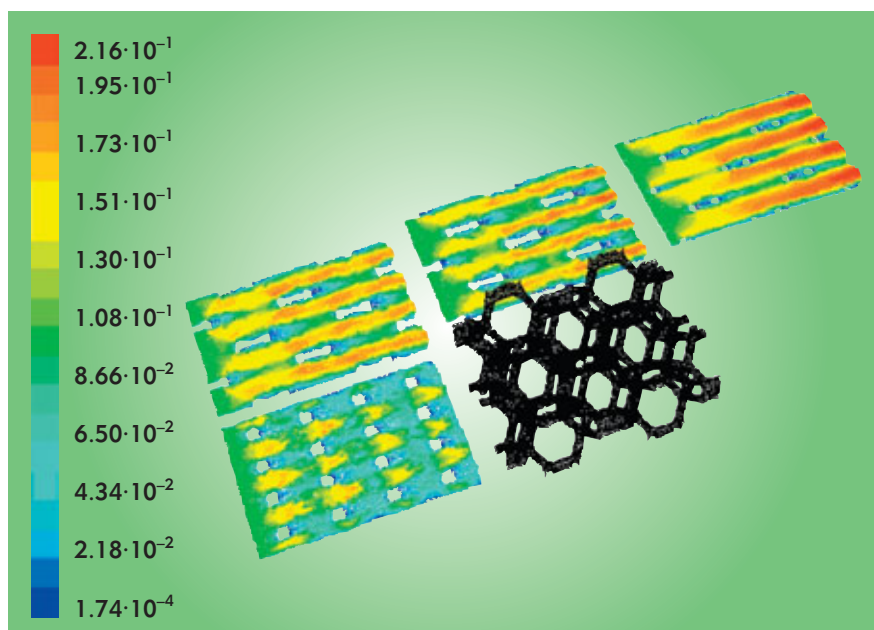
Manufacturers are increasingly turning to simulation for the specification of better geometries at millimeter scale, where the economic stakes are, currently, and where it is hard to get fast, reliable experimental characterization. In its endeavor to meet this challenge, GRETh is providing elements for the qualification of the new numerical simulation methods, such as LES, in the field of compact heat exchangers.

These methods are opening up a new field of investigation by numerical means, bringing forward a major leap in the ability of engineers to predict heat transfers. Consequently, they are steering experimental investigations towards finer measurement. With validation based on mean temperature or pressure values no longer being adequate, it is also important to measure the fluctuations for these quantities.

Pierre Mercier and Patrice Tochon
Research Group on
Heat Exchangers (GRETh)
Technological Research Division
CEA Grenoble Center

Figure 3. Flow inside a metal foam (see illustration at the beginning of the article), computed by the Fluent software. These are the first results of a project aiming to characterize a new structure of this type, intended to increase heat transfers.

(1) This concept allows good tuning to meet demand, from day-to-day service to jointly funded doctoral thesis.



What is a numerical simulation?

A

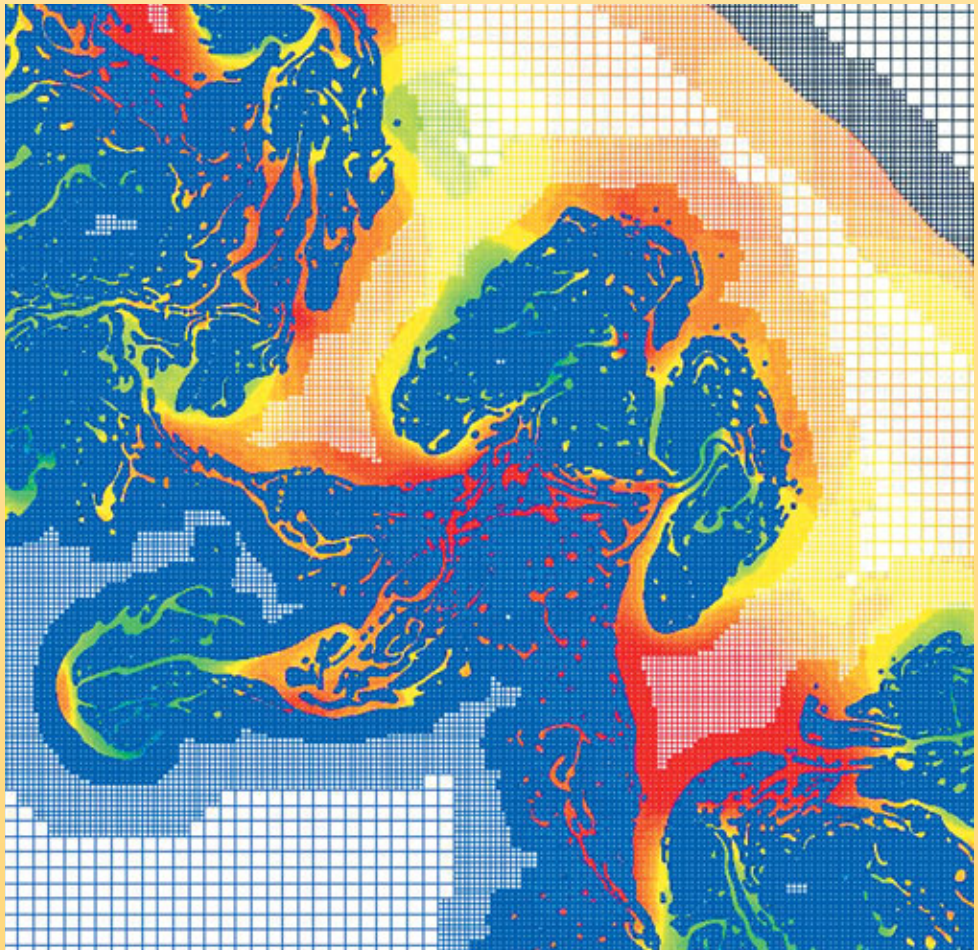
Numerical simulation consists in reproducing, through computation, a system's operation, described at a prior stage by an ensemble of **models**. It relies on specific mathematical and computational methods. The main stages involved in carrying out an investigation by means of numerical simulation are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

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.

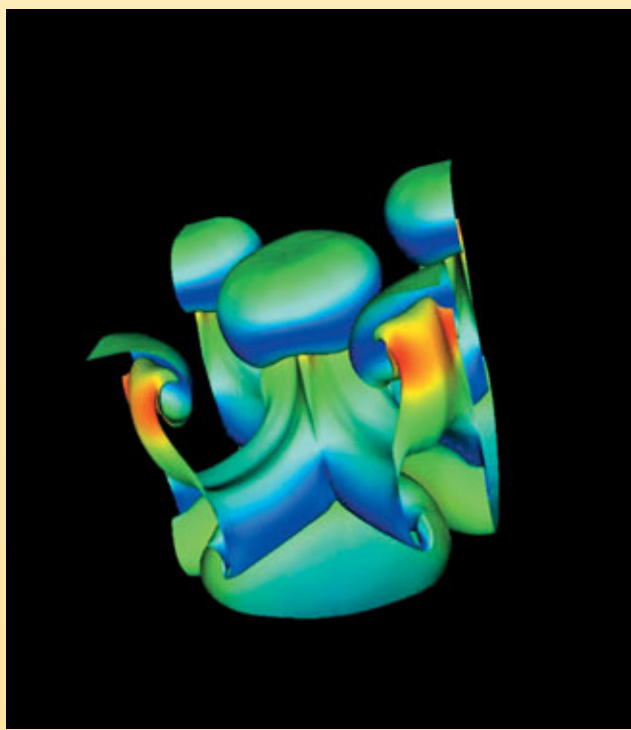
How does a numerical simulation proceed?

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-



CEA

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,⁽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.

Bruno Scheurer

Military Applications Division
CEA DAM-Ile de France Center

Frederic Ducros and Ulrich Bieder

Nuclear Energy Division
CEA Grenoble Center

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 tube-plate (section of the velocity field, at left on Figure E), and instantaneous temperature in the water box (at right).

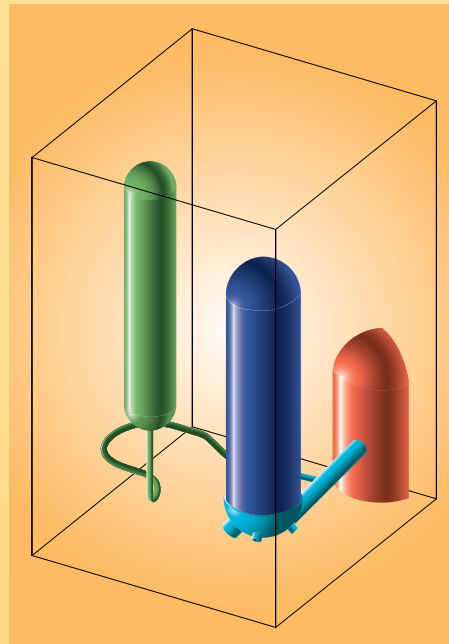


Figure A. Overall computation domain, including part of the reactor vessel (shown in red), the outlet pipe (hot leg, in light blue), steam generator (dark blue), and pressurizer (green).

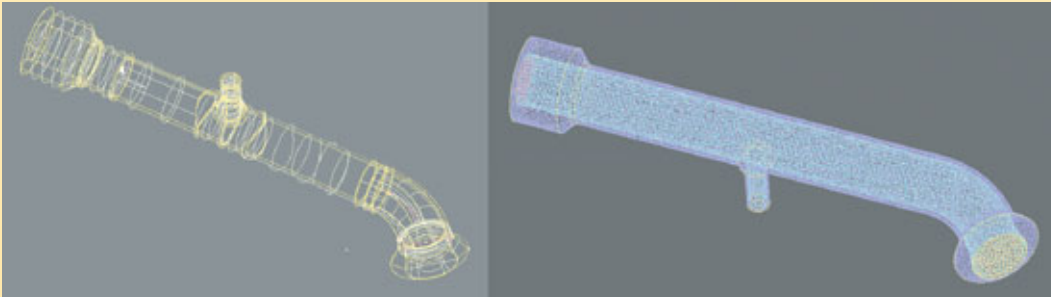
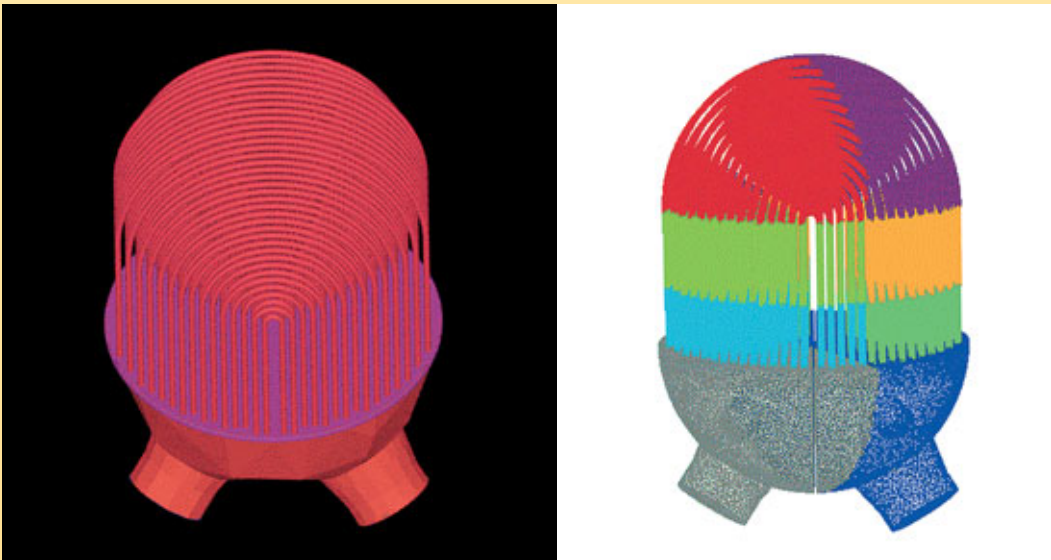


Figure B. CAD model of the hot leg of the reactor vessel outlet (left) and unstructured mesh for it (right).



Figures C et D.

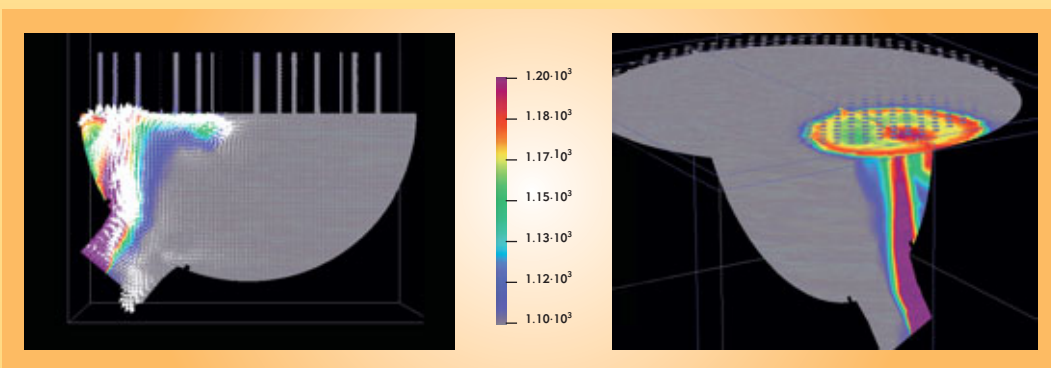


Figure E.

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).

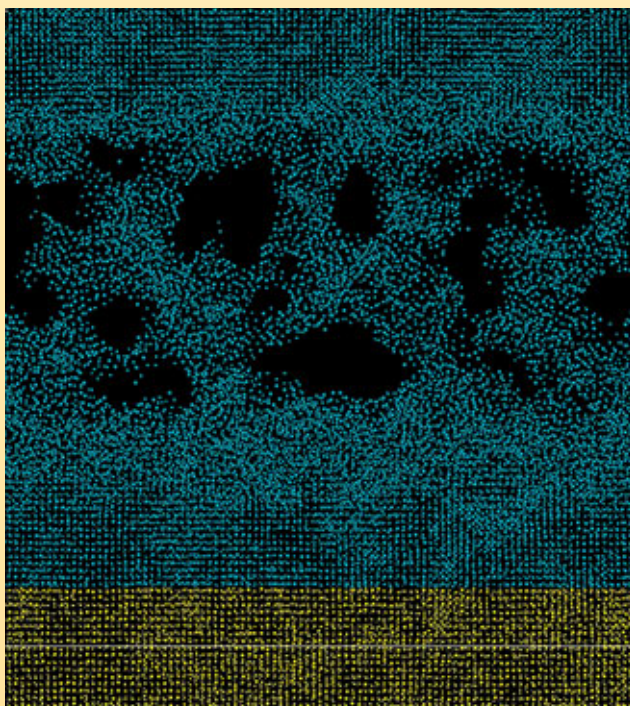
Currently, there are three main types of supercomputers: vector supercomputers, clusters of mini-computers with shared memory, and clusters of PCs (standard home computers). The choice between these architectures largely depends on the intended applications and uses. Vector supercomputers have very-high-performance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



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 ($0.02 \mu\text{m}$ 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.

François Robin

Military Applications Division
CEA, DAM-Ile de France Center

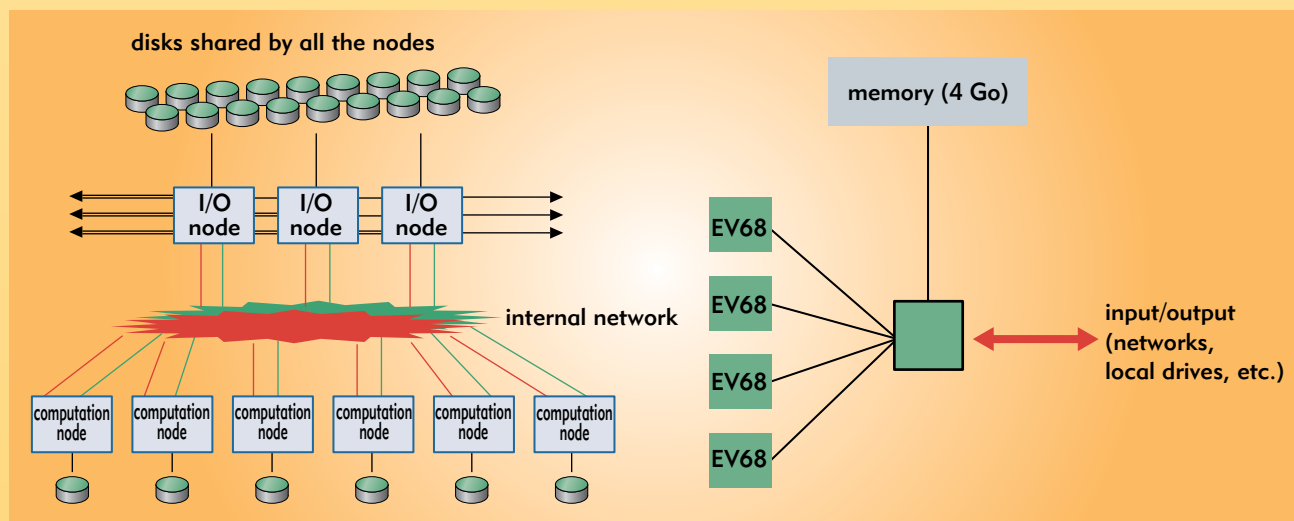


Figure. Architecture of an “SMP-cluster” type machine. At left, the general architecture (I/O = input/output), on the right, that of a node with four Alpha EV68 processors, clocked at 1 GHz.