

ADVANCES IN VIRTUAL PROTOTYPING

Having a representation of an object and its behavior before a rough physical model is available is an option that is being taken up more and more widely in industry. Advances in virtual prototyping, which is becoming interactive thanks to real-time computations, are opening up new prospects for this type of simulation in many areas. CEA is an active participant in these developments.



Virtual image of the cockpit of the future Airbus A 380. The aviation industry is making increasing use of digital mockups to design its planes.

Airbus

From design to maintenance

Virtual prototyping used in industrial environments has already allowed reductions in development times, product industrialization costs, and associated training and maintenance costs. The computation capacities available are now making it possible to generate virtual environments representing manufactured systems with a behavior close to what it would be in the real world. They also allow visualization and handling in real time of these virtual objects, making interactivity possible.

Virtual prototyping is actually only the front end of a product life management (PLM) process taking on board all constraints related to manufacturing (robotics, ergonomics), and utilization and maintenance (training). All the computer-aided design (CAD) majors such as Catia (Dassault Systèmes) or PTC (Parametric Technology Corporation) now offer this approach. There is a demand from all buoyant industrial sectors, such as automotive, aerospace, transportation, energy,

but equally from architecture, and the cultural and medical sectors.

Presently, automotive and aerospace manufacturers still widely use physical mockups, for example to “prototype” assembly or maintenance operations. For use as visualization tools, however, such mockups do have a number of drawbacks. They are expensive and often obsolete before they can be used, since they do not always represent the latest version of the product. This is why these manufacturers are increasingly trying to substitute them by numerical (“digital”) mockups⁽¹⁾ and virtual-reality technologies. These should allow the realistic immersion of a human being in a virtual world, gaining substantial benefits in the process.

Development of haptic interfaces

As a first example, consider the design of the inside of a passenger vehicle. The designers wish to determine whether the driver can easily access the various fittings (car

radio, glove box, etc.). Current practice is to use physical mockups or stereoscopic visualization of a numerical model to prototype the inside of a passenger vehicle. It seems advisable to develop haptic⁽²⁾ interfaces allowing this virtual interior to be “touched.” By using such interfaces, ergonomics studies will cover a much broader area of expertise during vehicle design. This method is much faster, less expensive and more exhaustive than production of a physical prototype.

(1) The AIT (Advanced Information Technology) consortium defines the digital mockup as a “realistic computer simulation of a product with the capacity to perform all functions required for the design, manufacture and maintenance of the product and that is used as a platform for the development of the product and processes, for communication and decision-making, from initial design mockup to product maintenance and recycling.”

(2) Haptic: from the Greek *haptein*, meaning “to touch, manipulate” – related to the sense of touch. A haptic device reproduces the sensation of touch for the fingers or hand.

A second example in the automotive industry is assembly. Currently, assembly-line designers use parts made by stereo lithography to test part assembly and the associated tooling. Users consider that use of such current **simulation** software programs as Catia or Robcad is too complex for this type of operation. In the near future, designers will be able to use, on the one hand, stereoscopic visualization systems to prototype their lines, and, on the other hand, haptic interfaces coupled with real-time physical simulation software programs (calculation of collisions and contact forces) to prototype tasks. The goal? To make virtual prototyping tools usable by professionals in industry rather than by specialists, and with no need, for instance, to program a single line of code.

In the very short term, the other major applications of virtual prototyping and haptic feedback would thus seem to be virtual simulation of assembly and/or maintenance operations, and training for technical actions. However, all these technologies may also be used in the cultural sector. In the context of the European MUVII (Multi-User Virtual Interactive Interface) Project, CEA teams are developing the concept of the virtual museum visit with haptic rendering. The visitor will be able, for example, to view statues in stereoscopy and, most importantly, virtually touch them. The issue of whether virtual prototyping technologies have the ability to substitute entirely for the use of physical mockups is of immediate relevance. The computing power

The partners in the PERFRV project 1

The PERFRV platform project, as a center for experimentation in virtual reality on the theme of the design office of the future, brings together partners from the world of research and industrialists. The academic partners in this project are the Rennes and Rocquencourt Inria Centers, CEA/List, the Paris École des mines, the Chalon-sur-Saône Institut de l'image, Labri (Laboratoire bordelais de recherche en informatique – Bordeaux Information Technology Research Laboratory), LRP (Laboratoire de robotique de Paris – Paris Robotics Laboratory) and Limsi (Laboratoire d'informatique pour la mécanique et les sciences de l'ingénieur – Laboratory of Information Technology for Mechanical Engineering and Engineering Sciences). The industrial partners are: Adepa, EADS/CCR (centre commun de recherche Aérospatiale Matra – Aérospatiale Matra Joint Research Center), IFP (Institut français du pétrole – French Petroleum Institute), CLARTE (Centre lavallois de ressources technologiques – Laval Technological Resources Center), Dassault Aviation, GIAT Industries, PSA, Renault, Alstom Transport, EDF (Research and Development Division).

of PCs and associated graphics cards, due to the popularity of video games, has recently made it possible to consider massive deployment of these technologies in manufacturing industry.

The PERFRV project

At the end of 1999, two research workers – Raymond Fournier at CEA's List (Laboratoire d'intégration des systèmes et des technologies – Integration of Systems and Technologies Laboratory) and Bruno Arnaldi of Irisa (Institut de recherche en informatique et systèmes aléatoires – Information Technology and Random Systems Research Institute) at the Rennes Inria (Institut national de

recherche en informatique et automatique – French National Institute for Research in Computer Science and Control) – sought to set up an organizational framework for experimentation to enable development of innovative solutions in virtual simulation, based on concrete requirements formulated by manufacturers in the areas of design, training, maintenance, installation or assembly. The outcome of this initiative was the PERFRV (PlatE-foRme Française de Réalité Virtuelle – French Virtual-Reality Platform) project. This platform was recognized in June 2000 as meeting the RNTL (Réseau national des technologies logicielles – National Software Technologies Network) criteria, and funded by the French Ministry of Research. It is intended to work in support of a scientific program on a number of themes in real-time physical simulation of mechanical systems (which needs must rely on new **numerical modeling** methods): physical interaction – gesture and haptic feedback –, making it imperative to investigate innovative peripherals, collaborative work (multi-user interaction in virtual environments), and ergonomics of interfaces (Box 1). CEA/List is involved in several initiatives in the project, related to haptic rendering, ergonomics and physical simulation in real time. It is working, for instance, with EADS, Renault, PSA, Dassault Aviation and Inria on the assessment of the various possibilities for virtual-reality simulation of an operation of the assembly type. The typical operation consists in integrating an equipment into a complex environment, for example a hydraulic pipe into an Airbus engine pylon. What is at stake here is proposing an optimal solution for a problem of significance in the world of the aviation numerical workshop. This entails a detailed study of the operator's requirements for information and sensory feedback, and searching for a multimode solution, making use of peripherals, substitutions and sensory illusions.



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The immersive system and the two Virtuose arms in the Phare system allow highly realistic virtual work in 3D.

F. Vigouroux/CEA

The Phare platform

The Phare virtual reality platform developed by CEA/List comprises five main elements (Figure):

- a real-time physical simulator. Such a **graphical** simulator's principal purpose is to describe visually the virtual world and the objects contained in it. The various elements of the virtual scene have basic attributes (shape, location in space) and complementary attributes that enrich the realism (texture) or provide specific information on status (a color coding to indicate a heat level, for instance). This type of simulator also frequently provides further effects (lighting, camera movements, etc.) and sometimes animation and kinematic control functions.

In an actual scene, a number of physical processes are involved, which one may wish to simulate, be they thermal, wave, mechanical, dynamic, etc. Depending on the nature of these processes, the model equations used (diffusion, transport, etc.) and resolution methods will vary;

- a real-time optical motion-capture system supplied by ActiCM (CEA/List startup). Comprising 16 cameras distributed on four stands, this system uses optical 3D measurement sensors designed, made and marketed by ActiCM. Each of these sensors includes two digital video cameras, two pulsed infrared (IR) lighting systems and control electronics. Each has the capacity to give accurately, in three dimensions, the position of points as a rule materialized by adhesive reflective targets. These targets are passive, avoiding the need for cumbersome instrumentation on the moving object (quick positioning, no electrical leads). Lighting in the near IR is associated to each head to "activate" it. When positioned in sufficiently large numbers on an object, such targets make it possible to determine, at every instant, its position and orientation parameters in real time. Several sensors may be combined to monitor its movements;

- two Virtuose 6D-RV™ interfaces with six degrees of freedom and force and torque feedback, made by Haption (CEA/List startup) (Figure 3). Designed by CEA/List's Robotics and Interactive Systems Department and made by Haption, Virtuose 6D-RV™ is a haptic interface that enables its user to touch and handle objects located in the virtual environment, with high sensitivity. It offers many prospects for such sectors as manufacturing (virtual prototyping, training for technical actions), and medicine (remote surgery, assistance to the handicapped, rehabilitation), and for the general public;

- a **cluster** of PCs dedicated to graphics. The List site will be one of the first in France to use such a cluster for stereoscopic multi-screen visualization. The use of PC-type technologies for virtual prototyping is essential for deployment in an industrial environment;

- a stereoscopic visualization system made by Barco, comprising two 2.5 m × 5 m wall-and-floor work surfaces with stereoscopic retroprojections (active stereo).

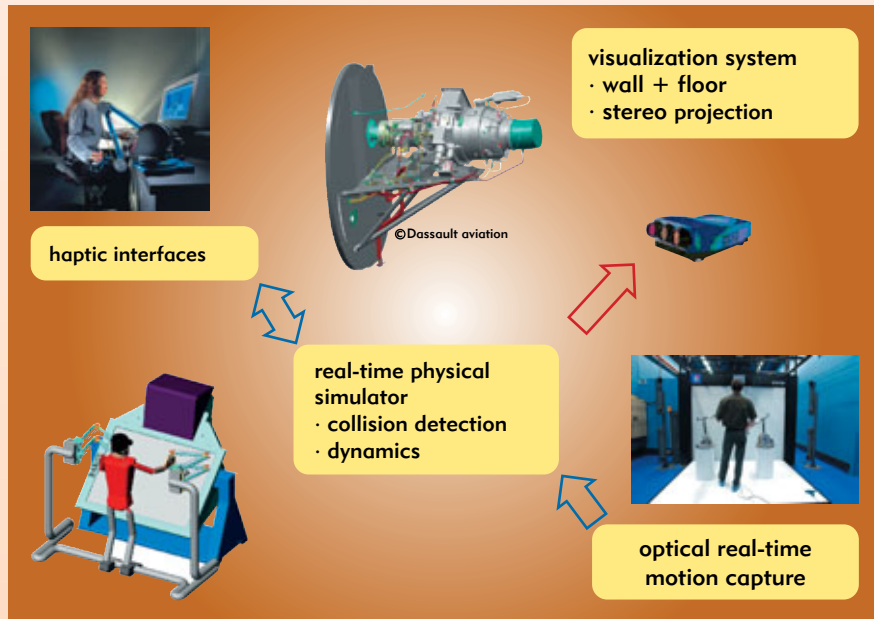
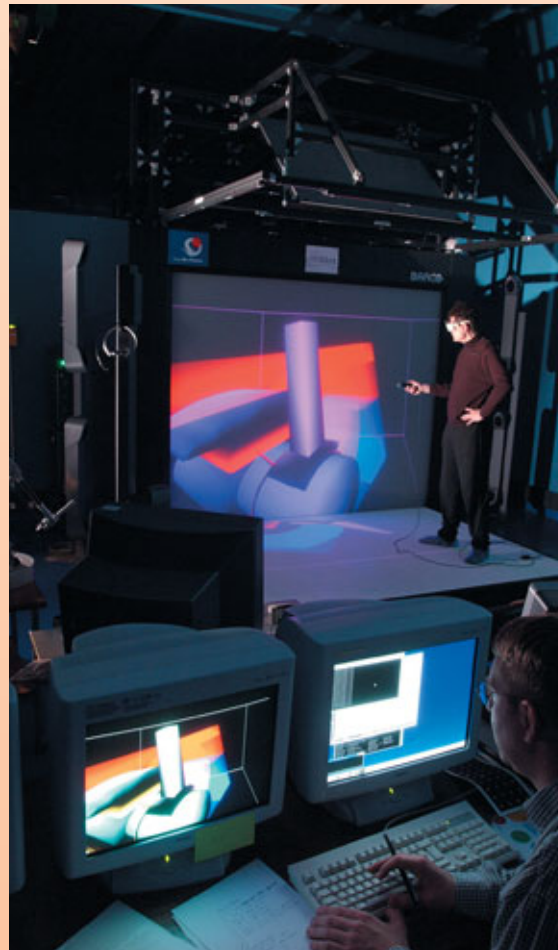


Figure. Principle schematics for the Phare virtual reality platform.

photos F. Vigouroux/CEA



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An operator moves in three-dimensional space rendered in the Phare platform by a stereoscopic visualization system comprising two wall-and-floor work surfaces, and stereoscopic projectors.



F. Vigouroux/CEA

Designed by CEA/List and made by its Haption startup, the Virtuose 6D-RV arm is a haptic interface allowing objects to be touched and handled in a virtual environment with high sensitivity.



Phare, List's response

List's Robotics and Interactive Systems Department (SRSI: Service robotique et systèmes interactifs) has been developing for over thirty years remotely operated systems with force feedback for the monitoring and control of robots for a variety of applications: nuclear, offshore and medical, for assistance to the handicapped and remote surgery. Its activity calls for strong expertise in mechanics, electronics, automation and control, computers, man-machine interface (MMI) and systems ergonomics. This

multidisciplinary character, together with the technological R&D brief imparted to it, enable SRSI to offer a global approach that is unique in France, for the integration and implementation of virtual-reality systems.

To meet the requirements of the PERFRV project, and more generally its own specific virtual-reality requirements, CEA/List has set up the Phare platform, combining a real-time physical simulator, real-time motion-capture system, interfaces with six degrees of freedom and force feedback, a "cluster" of PCs dedicated to graphics processing, and a stereoscopic visualization system (Box 2).

Real-time physical-rendering simulators, which basically simulate mechanical and dynamic processes, appeared a few years ago. In virtual, interactive prototyping, indeed, mechanical interactions between the various subsystems must be computed in real time. There are two main reasons behind this development: the rising demand from the video games sector for more realistic simulation of dynamics and interactions, and the power of IT systems, which now make it possible to use model equations appropriate for this type of physics. One of List's major R&D aims in this area will consist in developing or adapting computation codes to take on board the constraints of real time and interactivity. The real-time motion-capture system makes it possible, for example, to control in natu-

ralistic fashion an *avatar* ("numerical dummy") representing an assembly operator and thus to investigate the ergonomics of an assembly station. List is also developing algorithms that allow tracking of the movements (posture, arms, fingers) of the individual piloting the avatar.

In the area of haptic interfaces, one of the List team's major R&D goals is to develop algorithms enabling improved haptic rendering and new generations of interfaces, for instance portable interfaces.

All in all, the PERFRV project and the Phare platform are an opportunity for List research workers and engineers to take a major part in the field of virtual interactive prototyping in Europe. They will also give them the opportunity to use these interactive simulation developments in areas as broadly varied as culture, medicine or video games. ●

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What is a numerical simulation?

A

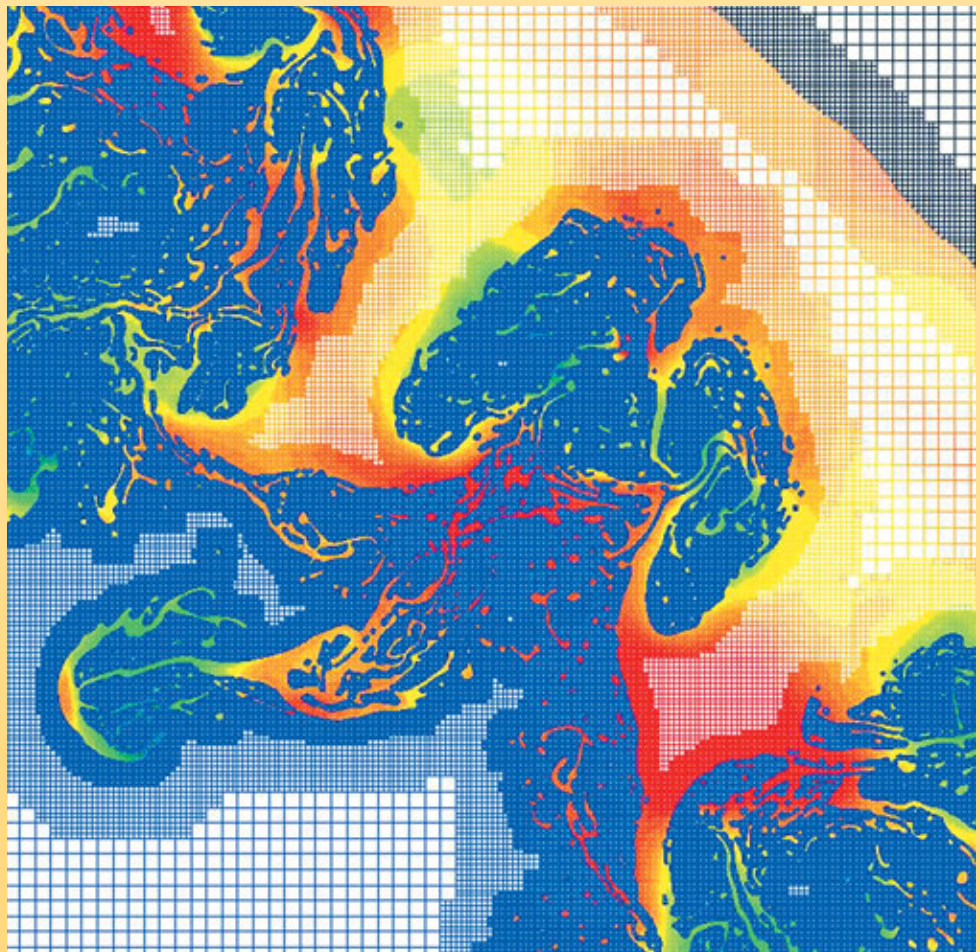
Numerical simulation consists in reproducing, through computation, a system's operation, described at a prior stage by an ensemble of **models**. It relies on specific mathematical and computational methods. The main stages involved in carrying out an investigation by means of numerical simulation are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

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.

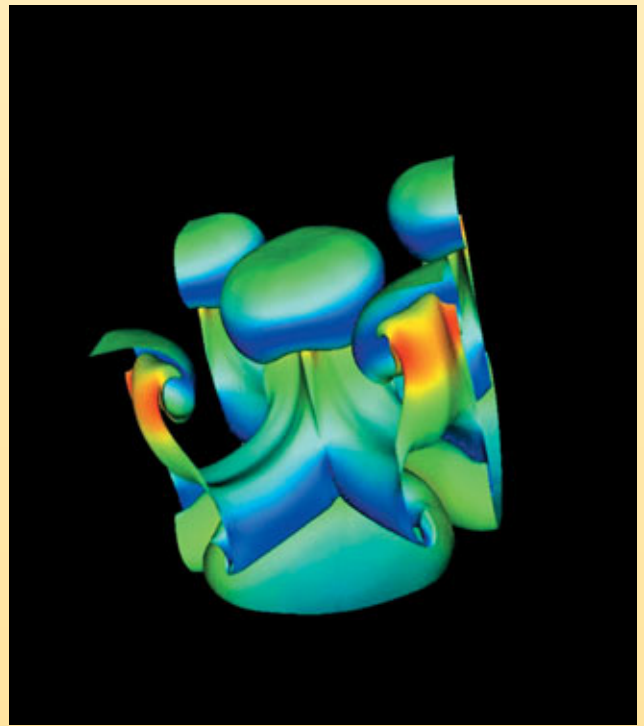
How does a numerical simulation proceed?

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

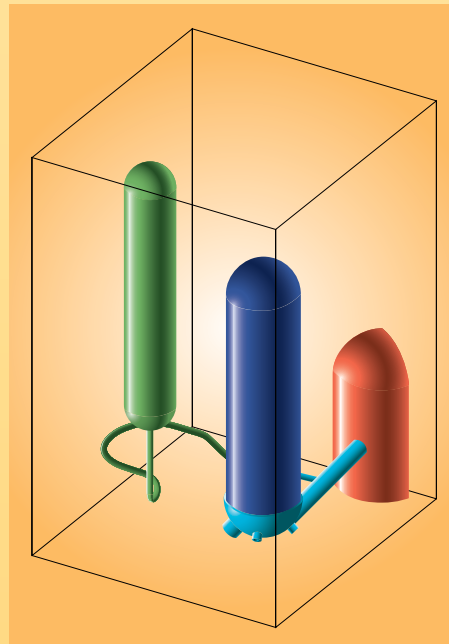


Figure A. Overall computation domain, including part of the reactor vessel (shown in red), the outlet pipe (hot leg, in light blue), steam generator (dark blue), and pressurizer (green).

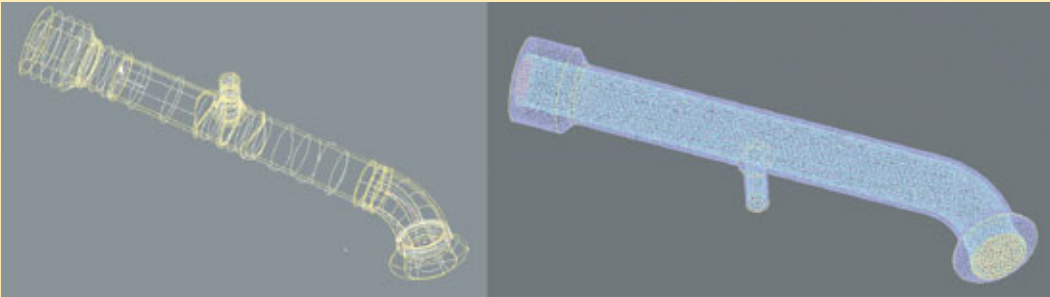
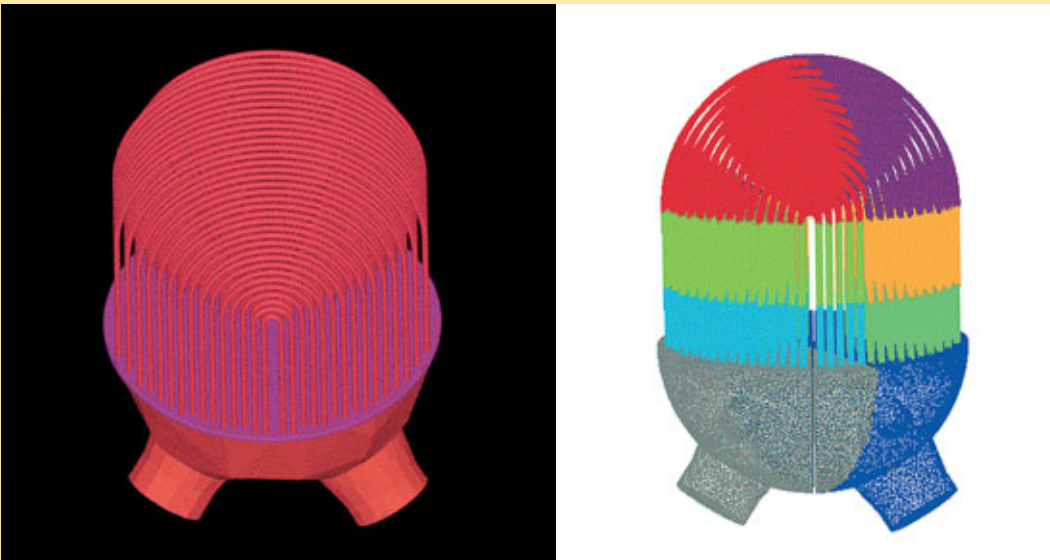


Figure B. CAD model of the hot leg of the reactor vessel outlet (left) and unstructured mesh for it (right).



Figures C et D.

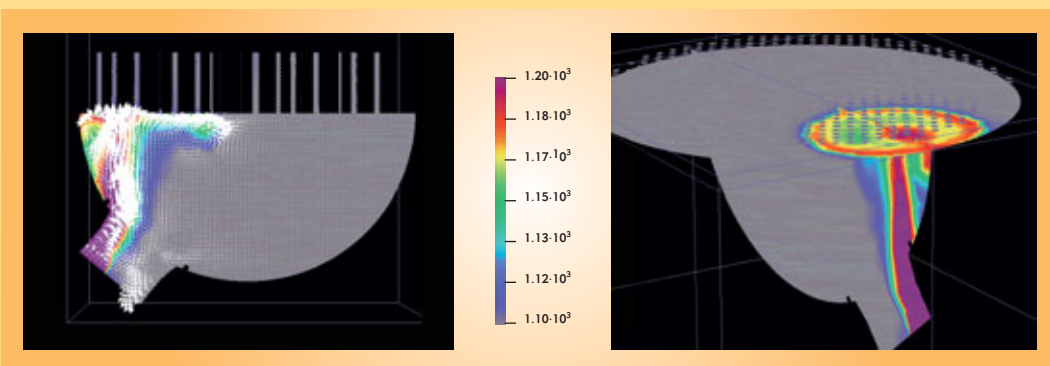


Figure E.

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).

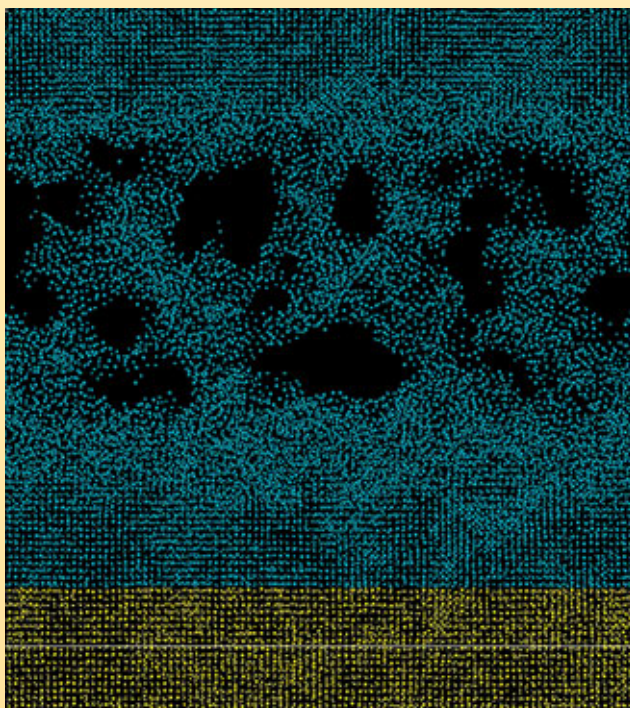
Currently, there are three main types of supercomputers: vector supercomputers, clusters of mini-computers with shared memory, and clusters of PCs (standard home computers). The choice between these architectures largely depends on the intended applications and uses. Vector supercomputers have very-high-performance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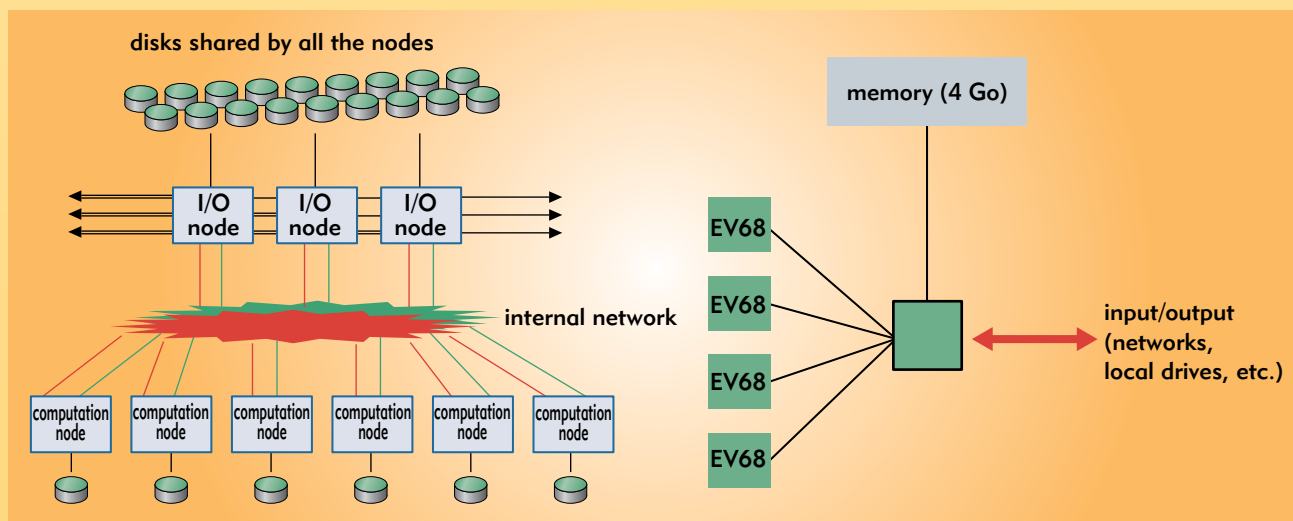


Figure. Architecture of an “SMP-cluster” type machine. At left, the general architecture (I/O = input/output), on the right, that of a node with four Alpha EV68 processors, clocked at 1 GHz.

Modeling and simulation of turbulent flows

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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,⁽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.

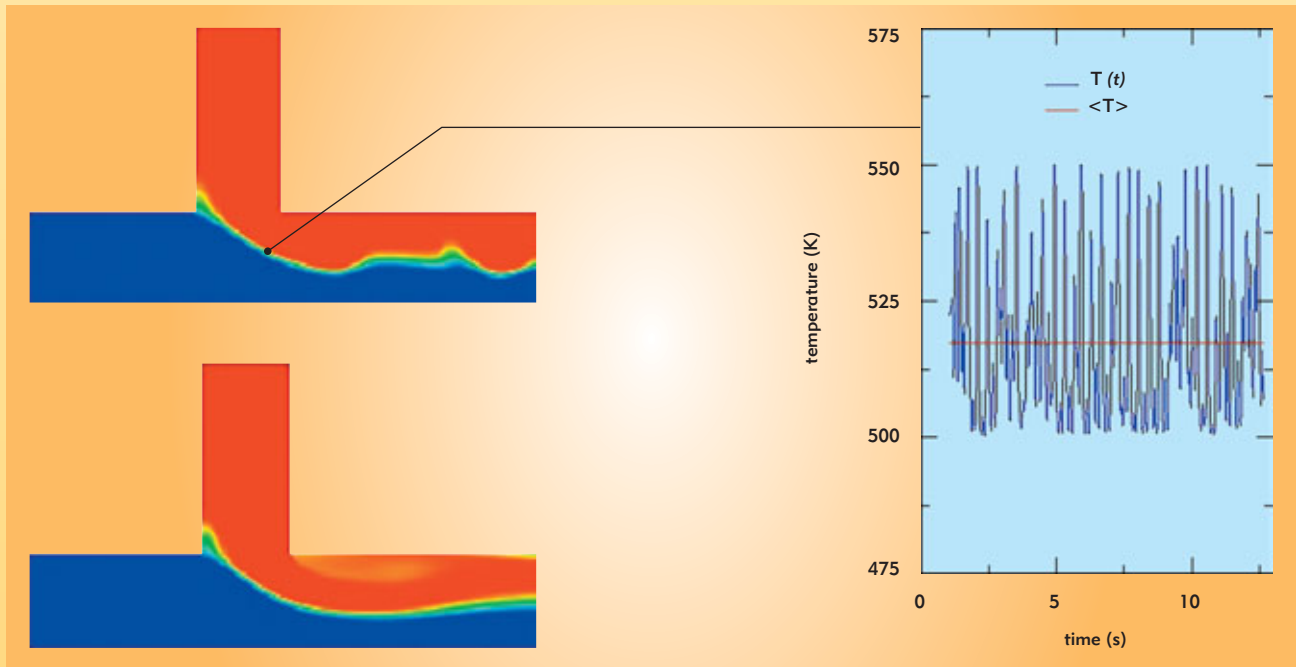


Figure. Instantaneous (top) and averaged (bottom) temperature field in a mixing situation. The curve shows the history of temperature at one point: fluctuating instantaneous value in blue and mean in red (according to Alexandre Chatelain, doctoral dissertation) (DEN/DTP/SMTH/LDTA).

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.

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