Supercomputing review

Numerical simulation for science and technology

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November 1988
Numerical simulations of meteorology and atmospheric pollution dispersion in an Alpine Valley

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A coupled system of three-dimensional numerical models of atmospheric processes has been applied to problems of pollutant dispersion carried within atmospheric flows in an Alpine Valley.

A regional scale meteorological model is used to reproduce conditions of flow and thermal stratification over complex terrain. The MESOCOV model contains the so-called primitive equations which describe, through conservation equations, the three-dimensional flow-field (Navier-Stokes), the temperature structure of the atmosphere (thermodynamic equation), and atmospheric moisture, cloud water, and rainwater. Additionally, physical parameterizations take into account atmospheric turbulence, cloud-induced thermodynamic perturbations, precipitation and radiative flux exchange. The model equations are solved by finite-difference methods, on a 32,000-point grid with a 20-second time step. A 24 hour simulation on the CRAY-2 requires approximately 1 hour of CPU time.

The problem of pollutant dispersion within atmospheric flows computed by the MESOCOV model is treated through a Lagrangean particle technique. The MICRO-L model makes use of the dynamic and thermodynamic data provided by the regional-scale model to transport and disperse a large number of individual particles which represent pollutant behaviour. The Lagrangean technique has the advantage of being independent of grid-size and can be applied to complex flow situations where strong wind-shear and flow reversals occur, and is certainly much more realistic than commonly used analytic Gaussian-type dispersion models.

As an example of the application of this method, the Chablais Valley has been chosen. Figure 1 gives a perspective view of the model domain, which covers a 20 km x 20 km area of the Alpine region; intervals between each point represent 500 m, and a 200-m interval is applied in the vertical. Figure 2 gives a plan view of the horizontal flow-field at 450 m above the valley floor, for a simulation of the case of February 14, 1988, on which real data are available for intercomparison purposes. Major height contours are superimposed for clarity. It is of interest to note that despite the strong flow above the main part of the Chablais valley, a significant contribution comes from drainage flow from Val d'Illiez to the SW. Flow separation also occurs above the town of Aigle, with some air being forced into a side valley to the east.

When releasing pollutants from some of the major industrial sources located in this region, through the Langrangean particle technique, the dispersion pattern for the flow field computed previously by MESOCOV, is given in Figure 3.

As the emission characteristics are different for each source, the behaviour of pollutant dispersion is extremely variable from one plume to another. This is especially visible for the two southermmost sources; the plume to the SW is injected high into the atmosphere and disperses laterally only slowly at the beginning; the plume to the SE remains at low levels and spreads over a very wide region, including some incursions into small side valleys. This figure gives only one mode of particle dispersion, corresponding to the cube root of total particles released.

Supercomputing review
November 1988
A cellular automaton model of diffusion and reaction in a porous medium: Concrete

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In this application, a cellular automaton model of diffusion and reaction in porous media is investigated. The specific case study is the carbonation of reinforced concrete.

Definition of the model

The model of diffusion provided by the random walk of a particle on a square lattice is driven by a simple rule: displace the particle with equal probability in any one of the four directions on the lattice. This rule is local and with it we update the position of the particle at each time step. The resulting dynamics simulate diffusive movement of the particle [1]. The same rule, adapted to constrain at most one particle per site and applied individually to each member in a population, governs the dynamics of the entire system, simulating diffusion in the population. This defines a model, discrete in space and time, in which local or microscopic rules imposed on the individuals drive the macroscopic behavior of the system. This is a cellular automaton [2]. With the stochastic rule, ours is a probabilistic automaton.

Because the rules of the automaton are locally applied, they can be locally modified, introducing local inhomogeneities. In this way we impose non-uniformity on local diffusion coefficients and simulate inhomogeneous and even non-linear diffusion. Further, the automaton rules can be augmented without changing the structure of the model. Thus by adding the local rule which describes the chemical reaction, we expand our model to simulate diffusion with reaction rather than just simple diffusion. In fact, by a rather simple expansion of the local rules, we introduce two diffusing species, two stationary species and the chemical reaction of the carbonation problem, increasing the model considerably in its scope.

Fourier's Law

In the asynchronous automaton only one particle at a time is randomly chosen and allowed to move, this random choice being equivalent to the use of a Poisson clock which orders the events [2]. In one dimension the corresponding master equations describe the evolution of the probability density as follows:

\[ \frac{\Delta P_j^n}{\Delta t} = \frac{1}{2} \frac{\Delta P_j^{n+1}}{\Delta x} + E_j^n \]

where \( P(x,t) \) is the probability that site \( x \) is occupied at moment \( t \) and \( \Delta t \) is the unit of time in the automaton, corresponding to one sweep of the configuration. Eq. (1) is just the discretized diffusion equation. Thus the asynchronous automaton, with its dynamics of non-interacting particles, reproduces the solution of this equation. The synchronous model, in which the entire population moves simultaneously, induces an interaction between particles due to the competition for free sites. It yields the following master equations in one dimension (2):

\[ \frac{\Delta P_j^n}{\Delta t} = \frac{1}{2} \frac{\Delta P_j^{n+1}}{\Delta x} + E_j^n \]

The additional term in Eq. (2) results from the particle interactions in the model. Fig. 1 illustrates the effect of the synchronicity. The diffusion equation

\[ \frac{\partial u}{\partial t} = \frac{1}{2} \frac{\partial^2 u}{\partial x^2} \]

with \( u(0,t) = 0 \) and \( u(1,t) = 1 \)

has equilibrium solution \( u(x,t) = x \) (Fourier's law). The probability density of the asynchronous automaton at equilibrium simulates this solution, Eq. (1) with the above boundary conditions. In a study of the synchronous model at equilibrium, we have conducted 100 simultaneous one-dimensional simulations with these boundary conditions. The initial density of the particles, distributed so as to correspond to the equilibrium solution (the straight line) of the diffusion equation, Eq. (3), is shown in Fig. 1a. The steady state of the model appears in Figure 1b. The smooth curve is the result of the numerical iteration defined by Eq. (2) and the experimental curve is the particle dis-


Carbonation

Carbon dioxide from the atmosphere enters concrete pores as they are emptied by drying. Calcium hydroxide, Ca(OH)$_2$, present in the concrete as a hydration product, reacts with the incoming CO$_2$, in the presence of water, to form calcium carbonate, CaCO$_3$, and liberating more water in a series of reactions usually simplified as:

\[
\text{CO}_2 + \text{Ca(OH)}_2 \rightarrow \text{CaCO}_3 + \text{H}_2\text{O}.
\]

(5)

This transformation of Ca(OH)$_2$ once complete, lowers the pH of pore water below that which protects interior steel reinforcements from corrosion. The “carbonation zone”, in which all the Ca(OH)$_2$ has been transformed, progresses toward the interior reinforcements with the inward progress of the CO$_2$, threatening the integrity of the reinforcements once it reaches them. Of interest, then, is the progress of this reaction zone, under the influence of the state parameters: relative humidity, cement content, water-cement ratio, degree of hydration, etc... [4].

In a simple automaton simulation, CO$_2$ and H$_2$O are modelled as two populations of diffusing particles, Ca(OH)$_2$ and CaCO$_3$ as stationary populations of fixed particles and the carbonation reaction as described in (5). Fig. 3 shows the simulated behaviour of water in a specimen, in the presence of CO$_2$ and the carbonation reaction. The sample is initially saturated with water. The right border remains in equilibrium with an atmospheric relative humidity and the left border has a zero flux condition. Further examples are available on request.

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HREM Image Simulation on a Cray Computer

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Introduction

The interpretation of High Resolution Electron Microscopy (HREM) observed image intensities is almost irrelevant without simulation. One problem to solve in HREM is the interpretation of the contrast of the micrographs. For thin crystals, the contrast is due to first order wave interferences and then simple to compute; but when the crystal is thicker, the second order wave interferences do become significant and if they are neglected, a wrong contrast interpretation will be done. Including the second order in the calculation needed a more powerful computer to keep good accuracy and will increase the computing time as the square of the number of beams (Fourier components of the wavefield) that are included in the simulation (Saxton 1980). Therefore, for large simulation problems as dislocations, clusters with more than 300 atoms, voids, interfaces, the number of beams is so important that the simulations are prohibitive for small computers (computation time too high or memory too small).

Simulation and discussion

The method is called `multislice method in Fourier space` because a multislice theory is used (Cowley and Moodie 1957; Ishizuka and Uyeda 1977) and the transmission function of the crystal is calculated in the Fourier space with the electron scattering factors given by Doyle and Turner (1968) or Smith and Burge (1962). The image intensity is calculated using the theory of image formation under partially coherent illumination (Born and Wolf 1957). The simulation of large defects, voids, interfaces or dislocations needed the creation of files containing the atomic positions. Those files are called `supercells` by analogy with the crystal unit cell. The defect or the aperiodicity in the supercell introduces diffuse scattering in the reciprocal space between the Bragg reflections. This information is characterized by low frequencies in the reciprocal space, and thus requires a high sampling density.

In order to perform the simulation of faulted structures, part of the EMS software package (Stadelmann 1987) has been implemented to run on a Cray at EPFL. The software installed on the Cray allows to compute HREM images of crystals with sampling of the supercell of $2 \times 2 \times (n+m+c=20)$; the samples can be distributed to form a square supercell (1024x1024) or a rectangular supercell (4096x256, 64x16384, ...), in order to make the best match to the geometry of the supercell and to have a similar spacing along both directions in the supercell. The comparison of the computing time between a `small` system such as an IBM-AT plus DSI20 Board (Definicon System Inc.) and the Cray for the same simulation problem gives a factor of 50 to 100 faster for the Cray. Now, on the Cray-1, FFT are done by block for big images, because 1024x1024 complex samples don't fit into the memory, particularly small (1 Mwords). The calculations should be 10 times faster on a Cray 2 for example where they can all fit into the memory.

As example of application, the Figure 1. shows a gold cluster built up of 2869 atoms (Flueli et al 1988) and cut into 21 slices for the simulation. The edge dimension of the square slices amounts as much as 6.12 nm. The sampling is 1024x1024 in order to represent the atomic positions accurately. The calculation of the wave function at the exit side of the cluster takes 107 minutes of CPU time: 75% of the time for the calculation of the transmission function of all the slices, 19% for the FFT (Fast Fourier Transformation) and 6% for multiplications (instead of convolutions) and the Fresnel propagator. The full non-linear image calculation takes 250 seconds of CPU time with 1400 beams in the objective aperture of 12 nm.

Fig. 1. Gold icosahedral shaped cluster. Viewed along 5-fold symmetry axis. 2869 atoms.

The programs are easily portable on another computer system: they were developed on PDP11/34 (Stadelmann 1987), implemented on IBM-AT and other systems. They can also be installed on a Cray 2 with the idea to do all the calculations (including the FFT) in the main memory.

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November 1988

Supercomputing review
The presented work describes the influence of pressure fluctuations on unsteady shock movements in transonic flows. It treats a model for the unsteady flow through blade passages in turbomachines operating in the transonic flow region, and has as particularity the sharp numerical capture of unsteady transonic shocks, the physical influence of the unsteady shock wave on the flow for different pressure oscillations and the resulting unsteady aerodynamic loads acting on a structure.

The solution of unsteady flows is of importance for the designer of several structures, such as bridges, airplanes, turbomachines and jet engines as the fluctuating flow might introduce large unsteady aerodynamic forces on the structure. These forces can often lead to failures and to the destruction of the element.

The prediction of unsteady forces is complex, especially in the transonic flow region, and makes unavoidable the use of complicated numerical schemes together with large computer capacities, first of all as regards to memory requirements and secondly computer time. In fact, in order to obtain unsteady solutions in the domain of computational fluid dynamics it is mostly necessary to first of all compute the steady-state results and thereafter introduce the unsteadiness into the flow by, for example, vibrating structures or time-fluctuating pressures. The computer time required for unsteady computations may thus be several times as large as the corresponding CPU times for steady-state flows. It is therefore important that the results from the numerical models used on complicated geometries are validated for relatively simple sample cases, where physical aspects of unsteady flows can be readily investigated and understood.

The study presents a numerical method, based on the flux vector splitting approach, to the problem of unsteady one-dimensional and two-dimensional inviscid transonic flows through nozzles with time-varying back pressure, with emphasis on the numerical determination of the unsteady shock position. With the method presented the steady-state and unsteady shock waves can be considered to be captured within two numerical cells. The model is first validated by comparison with exact (one dimension) and numerical (two dimensions) steady state solutions. It is thereafter applied to the problem of time-fluctuating back pressure in quasi one-dimensional and two-dimensional nozzles. The one-dimensional results are validated by comparison with a small perturbation analytical unsteady solution, whereas a few one-dimensional and two-dimensional sample cases are presented with the objective to understand fundamental aspects of unsteady transonic flows. These sample cases have been calculated on the CRAY 1S/2300 at the EPFL - Lausanne.

It is concluded that both the amplitude and frequency of the imposed fluctuating exit pressure are important parameters for the location of the unsteady shock. It is also shown that the average unsteady shock position is not necessarily identical with the steady state position, even for pressure fluctuations that normally would be considered to be a small perturbation around an otherwise undisturbed mean flow, and that the unsteady shock may, under certain circumstances, propagate upstream into the subsonic flow domain. The pressure jump over the shock, as well as the unsteady post-shock pressure, is different for identical shock-positions during the cycle of fluctuation which implies that an unsteady shock movement, imposed by an oscillating back pressure, may introduce significant unsteady lift and moment. This may be of importance for predictions of self-excited flow in diffusers and blade rows.

It is also noted that, although the sonic velocity is obtained in the throat of steady state quasi one-dimensional flow, this is not necessarily true for the unsteady solution. During part of the period with fluctuating back pressure the flow velocity may be subsonic at the throat and still reach a supersonic value later in the nozzle. In two-dimensional nozzles the flow may vary between completely subsonic, local supersonic or choked conditions. These phenomena depend on the frequency and amplitude of the imposed pressure fluctuation, as well as on the nozzle geometry.

The future work in the development of the program will be the computation of interblade channels (compressors and turbines) with the possibility to move the blades to compute unsteady flows in vibrating cascades.

The importance of large efficient computing capabilities for the numerical solution of unsteady transonic flows can best be judged by comparing the computational time for the sample case presented in Fig. 1. The computation mesh in this case was 14 x 60 cells, with one period corresponding to 1600 time-steps and a total of 6000 time-steps to first obtain a steady-state and then a fully periodic time dependent solution.

The CPU time for one period (1600 time steps) was 34 sec on Cray 15/2300. As this case takes too much memory on the Cyber 180-855, a test case of only 9 x 20 grid cells was run for the comparison. Table 1 compares the CPU time needed on different computers and shows that the present computation is about 330 times faster on the Cray 2 than on the Cyber.

Figure 1: Sinusoidal "bump"-flow. Unsteady solution for two dimensional sample case. Upstream Mach number = 0.675, mean exit pressure = 0.7369, amplitude of mean exit pressure = 0.12, reduced frequency = 0.369.
Pseudo 3-D Study using crooked line processing from the Swiss alpine western profile (Val d’Anniviers - Valais)

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The following text is the introduction and the conclusions of the paper submitted to TECTONOPHYSICS and it was presented at the international workshop and symposium on the probing of the continental crust: seismic probing of continents and their margins, Canberra, July 1988.

Abstract

First results are presented of the processing on one of the seismic lines of the Swiss National Program (FNRS) to study the deep geological structure of the Swiss Alps, located in the Anniviers valley (Val d’Anniviers-Valais) and called West Profile - Line 2. These results are produced by the group GRANSIR of the Geophysics Institute of the University of Lausanne.

The rough topography of the studied area gave rise to a crooked line geometry allowing the analysys of lateral dips across the Common Depth Point (CDP) swath which correponds to a Pseudo 3-D study. The coherence of the reflections of the seismic section has been improved by taking into account the lateral dips and correcting them before performing the CDP stack.

Preliminary geological interpretation of the reflections suggests the presence of large scale backfolds at depths between 10 and 20 km.

Introduction

The Swiss, French and Italian seismic reflection profiles through the Western Alps (Schweizerische Arbeitgruppe für Reflektionseismik, 1988; Bayer et al., 1987) exhibit high quality signatures which can be related to the surface geology and therefore present unique opportunities for the interpretation of seismic reflections.

The quality of the alpine outcrops and the presence of axial plunges allows reconstructions of the morphology of different geological units by using the hypothesis of cylindrical structures (Escher et al., 1987). Such reconstructions show the importance of the 3-D approach in alpine studies.

Through 3-D seismic studies are routine in oil exploration, this is not the case in orogenic areas where the rough topography prevents them technically and/or financially. Nevertheless, 3-D numerical ray tracing programs applied to areas of large lateral dips, point out that it is really important to take into account the 3-D aspect of the problem for the geological interpretation. In fact, it may turn out that the projection of the CDP line to the surface is well off the seismic line, because of the lateral dipping of the reflectors (Brown et al., 1988).

In the case of a crooked line survey of the Western Profile Line 2, the GEOMIVECTEUR™ software of CGG (Compagnie Générale de Géophysique) running on the supercomputer CRAY 1S/2300 of the Federal Institute of Technology in Lausanne (Ecole Polytechnique Fédérale de Lausanne, EPFL) (Levato et al., in press) provides tools to perform pseudo 3-D studies. The technique has two main advantages: on one hand it provides valuable information concerning the lateral dipping of the reflectors and on the other hand it improves the final stack by correcting the lateral dipping of the reflectors which otherwise may give rise to destructive effects when the seismic traces are added together. As part of the Swiss seismic reflection project (NFP20), three profiles have been designed trough the Alps: to the East, the West and the South (Figure 1). The Western profile is composed of four lines. In this work we present the results obtained on Line 2 (Val d’Anniviers).

West Profile Line 2 runs NS parallel to the Rhône valley along the Anniviers valley for 21 km. It has been vibrated by CGG. The NFP20 project has charged W. Frei with the coordination of the field work. The crooked line processing gave rise to 490 CDP (from 6 to 495) spaced at 40 m from each other. The elevation increases from 540 m to the North to 1750 m to the South.

The West Profile Line 2 runs from Sierraz to Zinal and cuts across the following units (from N to S): the Helvetic Wildhorn nappe and Aar basement, the Penninic Monte Leone, Pontis and Siviez-Mischabel nappes and their meta sedimentary cover rocks. The general structure shows the ductile superposition of the Southern units upon the Northern ones and a younger large-scale backfolding.

Conclusions

The results of the pseudo-3D processing on West Profile Line 2 are very satisfactory. The quality of the stack (Figure 1) has been improved by using the CGG pseudo-3D technique which corrects the lateral dips occuring along the profile and gives the order of magnitude of the lateral dip. The improvements have been quite important even if the lateral dip is relatively weak, of the order of 10 degrees. Therefore, this technique seems to be valuable in regions of complex tectonics like the Alps where important lateral dips are likely to occur. It is interesting to notice how the complex tectonics cause disadvantages as well as advantages for reflection seismic surveys.

On one hand, the rough topography may cause problems during the acquisition and the processing. In fact, very often the geographic environment limits the choice of the location of the profile and therefore, the recording conditions may not be optimum. Moreover, large variations in elevation mean a careful examination of the statics during the processing.

On the other hand, the Alps are rich in outcrops which can be correlated to deep seismic features, allowing a correspondence between reflections and geologic interfaces. The Line 2 seismic profile has made it thus possible to discover large fold structures of Lepontine style underneath the Valais Alps.
Figure 1: Dynamic stack of West Profile Line 2 after lateral dip corrections.
Pseudo3-D Study using crooked line processing from the Swiss alpine western profile - line 2.

Acknowledgement

The Swiss National Foundation of Scientific Research has financed the NFP/PNR20 project to study the geological basement of the Swiss Alps. We thank J.L. Epard, M. Marthaler, H. Masson and Ph. Virendaz for discussions and preliminary geological field work and B. Dumont for working on the first arrivals of the seismic data, to compute the velocities and thicknesses of the weathered zone. Our thanks are due to F. Perret for setting up all the figures.

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The numerical simulation of hypersonic flow is discussed in the context of the European space shuttle HERMES. Results are described of numerical simulations of the heat load on the shuttle surface upon re-entry into the atmosphere.

Introduction

During the last five years, research on hypersonic gas flows has experienced a rapid increase in interest. Stimulated by ambitious plans such as the European space shuttle HERMES, the National Aero-Space Plane (NASP) and the space based Aero-assisted Orbiter Transfer Vehicle (AOTV) of the United States, the reusable satellite launcher HOTOL of the United Kingdom and the German Sänger project many research groups in Europe and the United States have initiated or re-initiated research on hypersonic flow.

Numerical Simulation of Hypersonic Flow

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figure 1 — An artist's impression of the HERMES space shuttle.
research has a 30-40 year old history. In the 1950's and 1960's hypersonic flow research was stimulated by ballistic missiles and the first manned space flight programmes. Since no large computer facilities were available, theoretical research was focused on making suitable simplifications to the mathematical equations describing hypersonic flow and solving a greatly reduced set of equations. For simple geometries, aerodynamical properties such as drag could be predicted in agreement with experiment. Although experimental hypersonic flow research received much more attention than theoretical research during this period, its limitations should be recognized. For example, the HERMES space shuttle on re-entry into the atmosphere will fly at Mach 25 (corresponding to a speed of 7500 m/s). While a Mach 25 flow can be simulated in an experimental facility, it is not possible to simulate at the same time the corresponding dissociated air with a stagnation temperature of around 7000 K.

The American Space Shuttle was designed mainly using the data from wind tunnel experiments, with empirical methods being used to account for incomplete simulations. The shuttle flight results showed that although some aerodynamical coefficients were predicted correctly, others were under-estimated by up to 80%, especially for high Mach numbers. The experience with the American Space Shuttle illustrates the lack of basic understanding of hypersonic flow; this needs to be resolved when designing the next generation of re-entry vehicles.

With the arrival of supercomputers, having high computational speed and large memory, the possibility now exists to undertake detailed numerical simulation of hypersonic flow. This has led to a revival in this field of research. The situation now exists where experimental and numerical simulation of hypersonic flow have become equally important; this is exemplified in the development program of the HERMES space shuttle.

The HERMES space shuttle (see Fig. 1), which will be a third the size of the American Space Shuttle, will carry a crew of three and a payload of up to three tons to low earth orbit. The HERMES shuttle will be launched by an Ariane 5 rocket, the first flight being forseen for 1996. On re-entry into the upper atmosphere, a large heat load will be experienced on the leading surfaces of the shuttle, and the dissociating air will affect its aerodynamical stability. Detailed numerical simulations are therefore necessary to determine the optimal geometry and thermal protection for the shuttle.

Modelling of Hypersonic Flows

The mathematical formulation of the physical laws governing flow around a body takes the form of a coupled set of nonlinear partial differential equations, the Navier-Stokes equations. Often, the viscosity of the fluid plays a role only in a thin layer surrounding the body. It is then possible to solve a reduced set of equations for this thin boundary layer, and solve the Euler equations describing inviscid flow in the external region.

Hypersonic flow is distinguished from supersonic flow by the occurrence of chemical and radiative processes. These processes are initiated by the strong shock waves occurring in a hypersonic flow. The temperature behind the shock waves is sufficiently elevated so that the air is dissociated and chemical reactions take place, and also radiative heat transfer becomes important. These chemical and radiative processes must be incorporated in the model describing hypersonic flow.

Solving the complete set of equations governing hypersonic flow is a formidable task, even for the present generation of supercomputers such as the Cray 2. It is therefore imperative that numerical codes be developed that utilize efficiently the computer's resources.
Hypersonic flow research at the EPF-Lausanne

Within the framework of the HERMES project, the Institut de Machines Hydrauliques et de Mécanique des Fluides (IMHEF), the Department of Mathematics and the ASTRID-project group are carrying out a research programme on hypersonic flows. The objectives of this programme are:

— Modelling of high speed flows taking into account both chemical and radiative processes
— Developing numerical tools to simulate re-entry flows, adapted to supercomputers (in particular, the Cray 2)
— Developing software to visualize large scale calculations.

With these objectives in mind, several computer codes have been developed or are currently under development.

To gain experience in the physical and numerical phenomena associated with the simulation of hypersonic flows, a relatively simple computer code was developed to simulate the flow conditions in the boundary layer. This code uses a finite-difference method to discretize the mathematical equations in two-dimensional geometry. Since the boundary layer equations alone are solved, only the region behind the shock wave is treated, the shock wave itself not being considered.

Figure 2 shows temperature contours for the flow over an adiabatic flat plate calculated both without and with the effects of chemical and radiative processes. For the conditions considered, it is seen that these processes cause a strong reduction in the temperature of the boundary layer.

Chemical and radiative processes are currently being incorporated into an Euler code to simulate realistically the external flow region. This code, which uses a finite-volume discretization, employs a shock-fitting technique to locate the position of the shock wave.

The two-dimensional external flow over the nose section of the HERMES shuttle has been studied using the Euler code. Figure 3 shows an example of calculated temperature contours. Across the bow shock, located close to the upper edge of the coloured region, a sharp change in temperature is observed. Also evident in Fig. 3 is the canopy shock, which originates at the discontinuity of the shuttle surface caused by the cabin.

A computer code that solves the Navier-Stokes equations in three-dimensional geometry is currently under development at the EPF-Lausanne. The aim is that this code will be fully optimized for use on the Cray 2 computer, much attention being given both to vectorization and multi-tasking in order to diminish the computational time. Since the Cray 2 has a large central memory, minimizing the memory requirements takes a secondary role. The maximum number of grid points to be used in the calculations will be of the order of a million. It is estimated that the CPU time required for a hypersonic flow simulation will be between 5 and 100 hours, depending on the complexity of the physical model considered.

Conclusions

Although recently much progress has been made in the understanding of hypersonic flows, there remain many unresolved problems. Only with the incorporation of realistic chemical and radiative models into three-dimensional codes can numerical simulations address these problems. In this article we have shown that for full-scale numerical simulation of hypersonic flow, the use of supercomputers such as the Cray 2 is indispensable.
Using advanced semiconductor technology for basic semiconductor physics, and vice versa

M. Posternak, DP-IPA and ASTRID & A. Baldereschi, DP-IPA and IRRMA

In the computer industry, scientists have realized that the performance of silicon circuits has just about been maximized, and they are turning to other semiconductor materials, like gallium arsenide for the next-generation supercomputers. For instance, the Cray-3, which will be commercialized in 1989, will be based on the GaAs technology. Indeed, GaAs integrated circuits can operate at speeds up to five times that of silicon-based equivalents. The key parameters for understanding the special properties of this semiconductor material are bandgap, electron mobility, and excess-carrier decay time. Gallium arsenide’s bandgap is direct (while silicon’s one is narrower and indirect), enabling electron decay without access to modern supercomputers, whose technology is precisely based on theoretical results. Considering the above relationship between computer and basic research, it is amazing to note this feedback process governing computer simulations of new semiconductor materials and their use as ingredients in computer technology.

At IPA and IRRMA, we use state-of-the-art methods for computing structural and electronic properties of GaAs and other semiconductors, on the basis of the Density-Functional Theory. Briefly, two approaches are available for solving on a first-principles basis the electronic part of the problem. In all-electron methods, the Coulomb singularities of the nuclei appear explicitly in the potential, and the wave functions have strong oscillations in the core region, while they are only slightly modulated in the interstitial region. In pseudo-potential methods, the effective potential is smooth; there are no core electrons, and the wave function oscillations in the core region are strongly reduced, but the price to be paid is non-locality, due to orthogonalization to inner states of distinct character. Computer codes based on these approaches, and designed for parallel processors of the next generation, are planned at ASTRID.

As an example of the selective information which can be extracted from computer simulations, we show here the valence-charge density of a 3x3 GaAs/AlAs superlattice, calculated in a plane exhibiting bond formation, using the FLAPW method. In the top panel displaying the total valence charge of the crystal, the density is high, and it is hard to see the bonds and to discriminate between the two materials. By subtracting from the crystal density the quantity obtained by superposing the corresponding spherical atomic densities, we obtain a much lower charge density, which is displayed in the second panel. The contours spacing is five times smaller, and the broken (dotted) lines indicate the zero (negative) contours. It shows now clearly the covalent bonds resulting from the formation of the crystal, but the differences between the two materials remain weak. In the bottom panel, we display finally the antisymmetric part of the latter quantity, relatively to GaAs/AlAs interface. The order of magnitude of the density has still decreased by about a factor of 5. The weak changes in the differential charge density between the two materials appear now. Clearly, the calculation of the electronic structure is in general only one step in the derivation of physical quantities, and the use of the supercomputer doesn’t stop here.
Numerical Flow Simulation

by Alain Drotz, IMHEF-DME — EPFL Lausanne

Figure 1 — Axial view of a Francis Runner

Flows around airplanes, cars, trains, boats or inside turbines, compressors or pumps involve very complex physical phenomena such as three dimensional turbulent boundary layers, vortex sheets, wakes and solid wall influences. The study of these phenomena is called Fluid Dynamics. The base of this study is the principle of conservation of physical properties, for example, mass or energy. Fluid Dynamical problems are difficult to solve due to the non-linearity of the equations (the Navier-Stokes equations) describing the flow processes. Only for simple geometries and by using simplifying assumptions is it possible to obtain an analytical solution.

With the arrival of supercomputers having a great central memory capacity and a vast computing power, numerical simulation of three dimensional flow problems has become possible.

The explicit pseudo unsteady centered method for the Euler equations.

The base of the numerical simulation is a discretized form of the partial differential equations describing the flow. The approach followed here is based on the assumption that the physical properties do not vary strongly between neighbouring grid points in space. This assumption implies that the solution of the discretized equations converges to the solution of the original system of partial differential equations if the grid spacing tends to zero. The discretized equations are constructed by integration of the partial differential equations over a volume surrounding each grid point. This discretization method, called the finite volume method, is applied to the Euler equations. The Euler equations are based on the assumption that the Reynolds number of the flow is large, so that the viscous terms in the Navier-Stokes equations can be neglected.

The Euler equations have a hyperbolic character and can be solved using a pseudo unsteady integration method in time.

Flow simulation in a hydraulic turbine using the CRAY Supercomputer.

To illustrate the numerical simulation procedure, the complex problem of the flow simulation in a hydraulic turbine will be presented. The aim of this project, presently under development at IMHEF, is, in the medium term, the simulation of a complete hydraulic installation (Fig. 1), consisting of a spiral duct, the stay vanes, the wicket gate, the runner and a draft tube. Such a calculation requires the decomposition of the calculation domain into several subdomains, each subdomain corresponding to an element. Flows around airplanes, cars, trains, boats or inside turbines, compressors or pumps involve very complex physical phenomena such as three dimensional turbulent boundary layers, vortex sheets, wakes and solid wall influences. The study of these phenomena is called Fluid Dynamics. The base of this study is the principle of conservation of physical properties, for example, mass or energy. Fluid Dynamical problems are difficult to solve due to the non-linearity of the equations (the Navier-Stokes equations) describing the flow processes. Only for simple geometries and by using simplifying assumptions is it possible to obtain an analytical solution.

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Graphical software has been developed for Hewlett Packard workstations. This software allows for the visualization of the three-dimensional geometries used in the calculations on the CRAY, as well as the visualization of the calculation results, i.e.,
- grid surfaces
- isoline surfaces
- stream lines
- and so on.

This software runs interactively and allows for manipulation of the created pictures. Examples of the graphical representation are shown in Figs. 3 and 4. These figures show the pressure distribution on the runner; the colours ranging from red to blue represent the pressure evolution from high pressure to low pressure.

An application of the numerical method is the calculation of the interblade domain of a turbine. Figure 2 presents the grid for the calculation domain, with the pressure field on the lateral surfaces. The interblade volume constitutes for the turbine under study 1/13 of the complete turbine. The grid generator used to discretize the calculation domain is based on transfinite interpolation. Presently, work is being undertaken to develop an adaptive grid generator, which allows for the adaptation of the grid during the solution process.

The Euler code, which can be used for internal as well as external flows and for arbitrary geometries, has been completely vectorized for use on the CRAY-15 and CRAY 2. The use of parallel processing on the CRAY 2 is presently under study.
The ASTRID group\(^1\) presented by Silvio Merazzi, GASOV-EPFL Lausanne

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The computational mesh must be discretized into regular subdomains. Fig. 1 displays a typical mesh of 3 regular subdomains.

The connectivity between subdomains must be regular.

A single discretization operator must hold within a subdomain.

One of the main tasks of the ASTRID team consists of the development of the basic command modules and utilities. Numerical models and algorithms may then easily be embedded in the system by application programmers, thus providing for test bed. In other words, the designers of the ASTRID system currently concentrate their efforts on the following kernels:

- Data structure design and data base design \([1,2]\) in a network of workstations and computational servers.
- Adaptive mesh generation \([3]\) and post-processing \([4]\). Fig. 2 displays an initially equally spaced grid that has been adapted to the solution.
- User-interface design and command languages.
- Design of utilities, such as specialized graphics \([4]\) and process monitoring packages.
- Integrated documentation \([5]\).

ASTRID problems are always modeled on a graphics workstation, where the initial MEMCOM input data base resides. The input data

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1 E. Bonomi, M. Flueck, R. Herbin, S. Merazzi, T. Richner, V. Schmid, T. C. Tran
2 French acronym for Scientific Applications in Research and Development

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Figure 3 — Viscous flows (step test case)

base (or the instructions to create one) are then submitted by the ASTRID Network Monitor to the computational server (CRAY2). Once ready, selected results are automatically transmitted back to the workstation for post-processing.

The following examples give a short account of the basic modes of operation of a typical ASTRID application [6]. The mathematical model consists of $Q_1-P_0$ finite element approximation of the stationary incompressible Navier-Stokes equations. The corresponding set of nonlinear equations is solved by LU factorization (true Newton method). The viscosity is chosen as the continuation parameter.

The first example demonstrates the fluid flow in the well-known 2-dimensional step problem. The domain is decomposed into 3 regular subdomains, each 50 by 50 cells in size. The stationary solution is determined on the CRAY2. Once available, the velocity field is returned from the server to the workstation, where the stream function is computed. Fig. 3 displays the particle trajectories visualized by means of a color-shading technique.

The second example shows a two-phase non-mixing fluid flow in an electrolytic aluminum melting pot (Alusuisse SA, Chippis). The 3-dimensional Navier-Stokes equations are solved by means of the technique outlined above. Fig. 4 displays the model and the flow component perpendicular to the vertical slices cut through the model.

References


Figure 4 — Flow in aluminium melting pot (free interface and vertical slices)
Stability of Magnetic Fusion Experiments

by U. Schwenn *, EPF Lausanne
* on leave from Max Planck Institut für Plasmaphysik — Garching

Introduction

The major aim in magnetic fusion research is to build in the next 50 years or so a commercially exploitable thermonuclear reactor based upon the nuclear fusion reaction
\[ \text{D} + \text{T} = \text{n} + ^{4}\text{He} + 17.6 \text{MeV} \]

To get this reaction working the two components D (Deuterium) and T (Tritium) have to be heated up to temperatures of the order of 100 millions of °K. In order to reach such temperatures the fully ionized gas has to be kept away from material walls by confining it by means of strong magnetic fields.

The two main experimental configurations are the Tokamak and the Stellarator. In the Tokamak concept the magnetic field necessary for confinement is produced by an external toroidal field and by a poloidal field induced by a very strong longitudinal electric current in the plasma. The Stellarator has almost no net longitudinal current, equivalent to a magnetic field generated by external coils such as those shown in Fig. 1.

The Model of Ideal Magnetohydrodynamics (MHD)

A plasma in a magnetic bottle behaves like a mixture of fluids which can be described by the fluid equations coupled to the Maxwell equations. If one neglects the relative motion between ions and electrons and considers the plasma as only one averaged fluid, one uses the magnetohydrodynamic (MHD) equations. In the special case of an infinitely good conducting gas (with resistivity = 0), one uses what are called the ideal MHD equations. This most simple model describes surprisingly well the equilibrium state of a magnetically confined plasma, and the rapid unstable global motions which can destroy the confinement on a microsecond timescale.

The equilibrium equation
\[ \nabla p = (V \times B) \times B \]
describes the balance between thermal and magnetic pressure. Experimental physicists use this equation to reconstitute relevant physical quantities such as mass density, currents and temperatures. The computation of such equilibria is routinely done for Tokamaks and Stellarators.

Three Dimensional MHD Stability Code TERPSICHORE

If we perturb such an equilibrium with a sufficiently small displacement we can follow in a linearized model. The time dependence can be separated by
\[ \xi(r, t) = \xi(r) e^{i\omega t} \]

This leads to a symmetric eigenvalue problem
\[ -\alpha^2 P'' = \tilde{R}(\xi(r)) \]

where \( P \) is the equilibrium mass density and \( R \) is the linearized plasma response operator.

After appropriate discretization (finite elements and/or Fourier techniques) the above equation becomes a discrete matrix eigenvalue problem of the form
\[ A x = \omega^2 B x \]

A negative value of \( \omega^2 \) implies an unstable equilibrium.

Since one decade codes like ERATO/1/ based on this concept have been applied to two dimensional configurations successfully. Thus it was possible to derive a scaling law for the stability limit of \( \beta \) in Tokamaks. This reactor relevant quantity measures the ratio of the average plasma pressure to the applied magnetic pressure. This \( \text{Troyon limit} \) writes
\[ \beta < \beta_c = 2.5 \text{ I/A} [\%] \]

where \( \beta \) is a normalized total current and \( \beta_c \) is the ratio between major and minor radius of the plasma torus. This scaling law was verified by many experiments and has been used for the design of new ones.

So far no systematic stability analysis could be done for genuine three dimensional equilibria, like modern Stellarators or realistic Tokamaks. Because of the now existant reliable 3D

Figure 1: Field coils for new Stellarator design.

Figure 2: Boundary shape of a modern Stellarator plasma.
Stability of Magnetic Fusion Experiments

equilibrium codes (see figure 2) a new 3D stability code, TERPSICHORE, was developed. This code has been designed to run optimally on multiprocessor CRAY-computers. The two most costly modules, namely the matrix construction and the eigenvalue solver, run at very high speed. For the eigenvalue solver 380 Megalopps have been measured on a single CRAY 2 processor.

TERPSICHORE has been applied to a straight I = 2 Stellarator configuration (see figure 3). Good agreement was obtained with the HERA code described in /1/. A typical unstable eigen-solution is shown in figure 4.

Acknowledgements

The author is indebted to the co-workers of this project, namely D.V. Anderson, A. Cooper, R. Gruber and J. Nührenberg. Thanks go as well to P. Merkel for figures 1 and 2, to S. Meruzzi, the ASTRID group, and the computer center staffs at IPP Garching and EPFL.

References


The use of supercomputers in image rendering and computer animation

by D. Thalmann, Computer Graphics Lab - EPFL, Swiss Federal Institute of Technology, Lausanne, Switzerland

It is commonly believed that supercomputers should be mainly used for numerical computations and image rendering may be performed by super graphics workstations. Unfortunately, this is not the case; new super graphics workstations have the capabilities of a very fast rendering of images, but they always assume geometric models based on polygonal meshes and bicubic patches. Hidden-surface removal is based on the z-buffer approach, light model is the classical Phong model and surface shading is based on the Gouraud intensity interpolation model. With such an approach, images which were rendered in several minutes using a traditional computer like a VAX, may be rendered in a few seconds on new super workstations. Unfortunately, these methods are relatively old and do not allow to render a large class of images. In particular, the following aspects were not taken into account in the workstation hardware: shadows, solid textures, refraction, complex shading models like the Cook-Torrance model, which is the only shading model with a physical reality. Images with these features may be rendered on workstations, but they don’t take advantage of the hardware and the CPU time is still very important. For these specific rendering algorithms, CPU time is still critical and supercomputers have also an important role to play in the rendering process.

Scientific visualization needs more complex rendering methods; polygonal meshes and bicubic patches are generally insufficient for representing most natural phenomena which require fuzzy object modelling. Fuzzy objects, as defined by Reeves [1] are objects that do not have smooth, well-defined and shiny surfaces. Their shapes are irregular and ill-defined and may change with time. In computer animation, fuzzy objects like clouds, smoke, fire and water and fluids in general are frequently required but difficult to represent. A few new methods have been developed in software, but not incorporated in the workstation hardware. Among these new methods, the best well-known methods are particle systems and fractals. The potential of these methods for scientific visualization has probably no limits.

Particle systems

A particle system, as defined by Reeves, is a collection of particles that together represent a fuzzy object. Over a period of time, particles in the system are born, move, change and die. For each new particle generated, values are determined for the following attributes: initial position, velocity, size, color, transparency, shape and lifetime. Global dynamic attributes like <<rates of change>> are also defined in the particle system to control motion and transformations. Particle rendering can be complex because particles can hide each other and transparency and shadows are also often required. However, for explosions and fires, Reeves describes a very simple algorithm based on the assumption that each particle is
The use of supercomputers in image rendering and computer animation

displayed as a point light source. A pixel gains light when it is covered by a particle; the amount depends on attributes like the particle’s transparency and color. A particle’s size and shape determine the covered pixels. A hierarchy of particle systems can also be defined to control complicated fuzzy objects. Unlike Reeves’ work, our particle systems may intersect with other surface-based modeling primitives. Our rendering method is based on a scan-line A-buffer algorithm [2], which is an extension of the processing of translucent polygons. Moreover, we have introduced a way of defining any evolution law to the numerous particle attributes: color, velocity, acceleration, transparency, size. The almost unlimited number of possibilities of the technique should allow to represent phenomena like fluid motion. However, good results are only possible with a very large number of particles, which is very CPU time consuming.

Fractals

Mandelbrot [3] has studied the structure of complex natural objects and succeeded in describing them well introducing a new kind of geometry: fractal geometry. He shows that objects constructed in his geometry, called fractal objects, can represent the shape of mountains, the pattern of stars in the sky and fluid networks in the organism. Fractal geometry has become a new field of mathematics and it seems to provide a clearer look at our universe. In our implementation, fractal polygons are created using subdivisions of meshes of triangles. But the midpoint is randomly generated inside a revolution volume where the axis is the edge itself. Based on this implementation, we have studied [4] the impact of three geometric parameters for controlling this algorithm: the edge threshold, the eccentricity of the smallest cylinder surrounding the revolution volume and the displacement of the revolution volume towards the segment center. The generation of very large number of triangles is unfortunately expensive and requires the power of a supercomputer. The rendering itself may be performed using the workstation hardware.

Applications of new techniques

These new techniques may be applied to numerous applications of scientific visualization. For example, they may be applied to the visualization of microclimate conditions. As we know, in Switzerland, we have a lot of microclimates, and we have the problem to visualize a lot of meteorological situations and their dynamic changes. In particular, specific rendering methods should be developed for representing humidity, clouds, fog and atmospheric pollution. New rendering techniques are also required for visualization of rivers including characteristics such as pressure, temperature, pollution and even evolution of living organisms.

An experience of representing fluid flow results from the ASTRID group [5] using particle systems is under way.

References