Applied Mathematics for Industrial Flow Problems (AMIF)

An ESF scientific programme

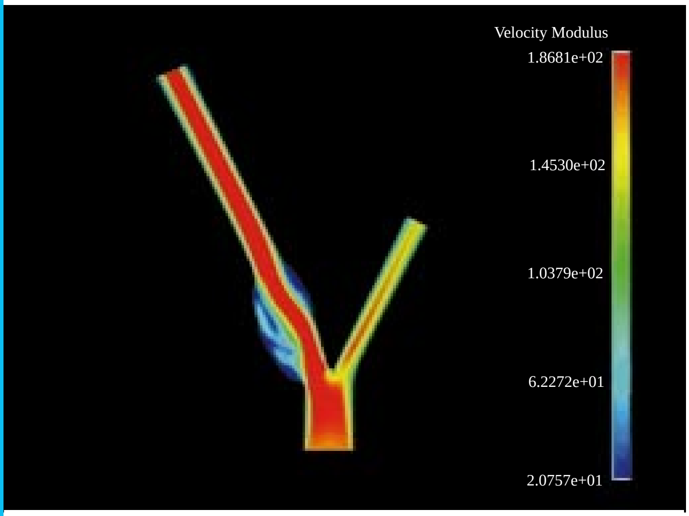
Fluid dynamics has extensive applications in a wide range of applied sciences, but at the same time constitutes the most difficult collection of problems in the whole of applied mathematics. However, with computers growing rapidly in power there is the potential to model increasingly complex mathematical models and fluid flows.

To exploit this potential fully, more advanced tools are needed for numerical simulations of complex realistic fluid flows.

This in turn demands a systematic investigation of fundamental mathematical models of fluid flows, and this is the objective of this ESF scientific programme.

The overall goal is to increase understanding of the mathematics underlying complex flow models, and then both improve existing numerical methods and develop new ones. These goals will be attained by combining expertise from different countries, as no single one has the resources to do it alone.

The research activity will embrace an unusually broad range of problems. This makes the best use of the programme's resources, because the problems are all inter-related, so that progress on any one will almost certainly lead to advances with the others.



Flow field in a human carotid bifurcation.

The European Science Foundation acts as a catalyst for the development of science by bringing together leading scientists and funding agencies to debate, plan and implement pan-European initiatives.

Introduction

Fluid mechanics has a long history dating back to the celebrated Euler equations in 1755, but many of the basic mathematical issues are still not fully understood. At the same time, the emphasis has switched from theoretical mathematical analysis to numerical approaches that exploit the power of modern computers. With the potential now for modelling realistic fluid flows to a much greater level of complexity on large computers, there is a pressing need for further progress with the fundamental mathematical models, leading to more advanced numerical simulation tools. Such fundamental models include not just the classical nonlinear partial differential equations, such as the Navier-Stokes equations that are widely used in numerical weather forecasting, but also modifications motivated by the need to reduce the complexity. For example, there are various turbulence models or coupled models that involve interaction between viscous and inviscid flows, fluids and structures.

Research on such challenging mathematical and computational issues will benefit from greater co-operation between different European research groups, helping the ESF achieve its overall goal of improving the mathematical understanding of the various models and existing numerical methods. This will lay the ground well for the programme's other goal, which is to propose new methods based upon the already known fundamental mathematical properties of the Fluid Mechanics equations.

The ESF programme

The programme is embracing an unusually broad range of research problems, including:

- compressible and incompressible flows and designs of models and algorithms capable of coping with both of these simultaneously;
- single and multi-phase fluid flows;
- reactive and turbulent fluid flows;
- flows in porous media;
- free-surface flows;
- viscoelastic and non-Newtonian fluid flows;
- modelling of turbulent flows (two-equation models, Reynolds stress models, and LES);
- multifields mathematical and numerical models, in particular for the coupling of fluids and solids, viscous and inviscid flows, rotational and irrotational flows, molecular and continuous regimes;

There are also some more specialised problems that may be addressed, including:

- electrochemistry and simplified models for electromagnetism;
- advanced models for semiconductor devices;
- shape design optimisation in aero-dynamics;

Although this is a wide range of problems, they are all closely interrelated, and will all benefit from new fundamental research covering the following:

1▪ development and analysis of mathematical modelling of fluid flows of practical relevance to some of the above problems;

2▪ simulation of these models by modern numerical methods;

3▪ development of effective numerical algorithms that exploit the latest parallel computers.

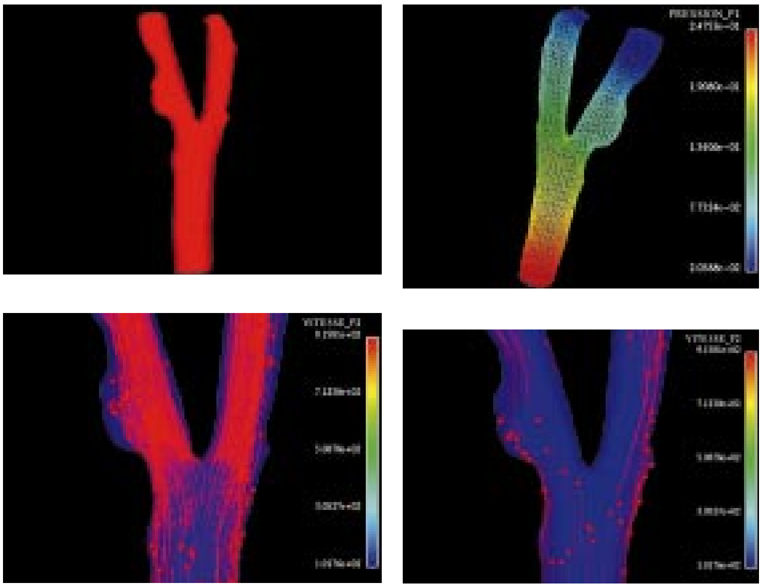
The programme runs for three years initially, with a further two years after revising the objectives in the light of earlier results and experience. It will include specialised workshops to discuss progress in particular aspects of the field, as well as tutorials and training sessions for researchers including some drawn from industry as well as universities. There will also be a conference of general interest spanning the whole field, and fellowships for young researchers.

Scientific background

The three themes of the programme, improving underlying mathematical theory, understanding existing numerical methods, and designing new numerical approaches, are strongly related. The programme is exploiting this, building on groundwork already laid by some recent work, such as research on compressible Navier-Stokes equations for rotating fluids like the earth's atmosphere. Much progress has also been made during the last 10 years on the one dimensional case of the Navier-Stokes equations. This work, combined with recent proofs and methods derived from the numerical analysis of incompressible Navier-Stokes equations, should lead to considerably improved understanding of numerical methods for the compressible Navier-Stokes equations.

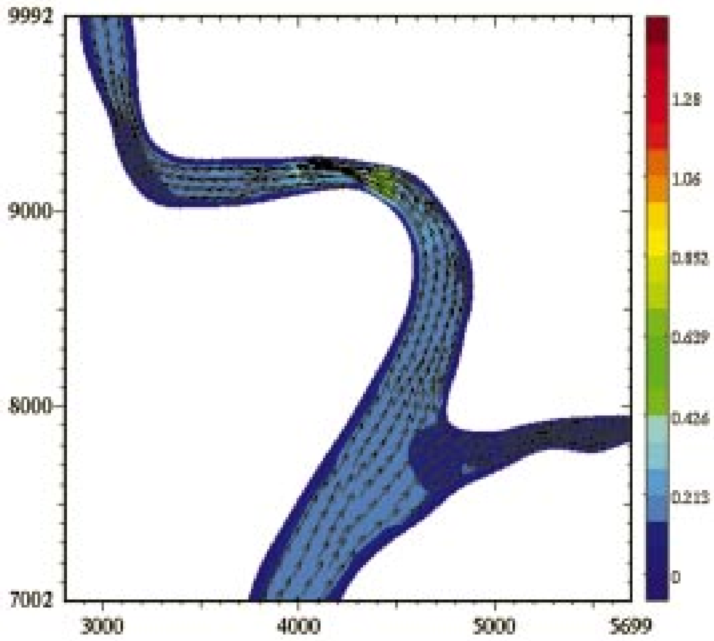
Such understanding is needed to develop new numerical approaches that exploit modern parallel computer hardware efficiently, but in this case at least the foundations have been laid. There are other applications where better mathematical understanding is needed, and here we describe briefly two important families of problem that, although not covering the complete field of interest, illustrate many of the scientific and mathematical issues that need to be tackled.

The first is the modelling of turbulent and reactive flows, where direct numerical simulation (DNS) has been used to compute all scales of motion of a turbulent flow. The problem is that highly turbulent flows with a large Reynolds number cannot be modelled effectively by



Numerical simulations of blood flow in a real vascular geometry. At the top: on the left: real geometry of a carotid artery reconstructed by a set of Computed Aided Tomography; on the right: corresponding mesh for Finite Elements simulations. On the bottom: Numerical results: visualisation of blood flow in two different instants of the heart beat (systole on the left, diastole on the right) (simulations with N3S by EDF).

Detail of the scalar and vector velocity field on a meander of the Po river, during a simulation of the influence of mareal tides on the water circulation in the last portion of the river.



DNS. This is because at this level of complexity, the time scales needed to represent the turbulence are much smaller than those that can be allowed for the step and mesh spacings of the DNS. Therefore conventional DNS cannot capture the turbulent diffusion.

There are several difficult problems that need to be solved to model such turbulent diffusion correctly. The first is to reduce the scale of the model without losing sight of the big picture. Multiscale methods have been adopted, such as large eddy simulation (LES), which provides a direct numerical simulation of large vortical structures, but at the same time models the exchange mechanism that transfers energy from high to low frequencies (and therefore from small rapidly changing local eddies to larger more slowly changing motions). LES therefore models large scales of motion explicitly, while treating smaller scales by some approximate parameterisation. However LES has a problem with boundary conditions, since experiments have found that coherent local structures exist there that require a major modelling effort to represent accurately.

Further complexity can be added to the flow structure by chemical reactions or combustion. For turbulent combustion, as opposed to diffusion controlled combustion, Montecarlo techniques are usually adopted for the transport of the probability density function, rather than using DNS.

The second family of problem of particularly great interest concerns computation of supersonic flows and shock waves. This field really started during the Second World War, leading to the invention in 1950 by von Neumann and Richtmyer of a numerical technique for capturing shocks as rapid internal transitions.

The original numerical schemes that stemmed from this were all linear, where equations converge if they are stable, which was the case if the “frozen” difference schemes with constant coefficients were also stable, as in turn can be checked by Fourier transform and matrix analysis.

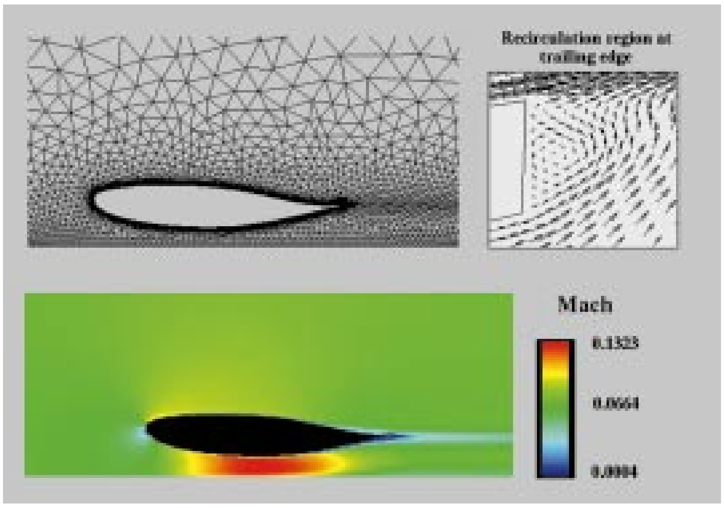
Nowadays the most efficient numerical schemes are nonlinear, but proof of convergence is much harder. However, an important design principle is that conservation laws should be approximated by difference equations, employing a numerical flux that approximates the physical flux. Then if an entropy function can be defined for a given system of conservation laws, it is important that the numerical method employed to construct approximate solutions should avoid increasing entropy. This can be done through numerical dissipation, which provides stability and damps unwanted oscillations generated by higher order schemes around discontinuities and stiff layers. This can be done in various ways, for example by uncentered, upwind like schemes, which are discussed further under *Aims and objectives.*

Of particular relevance to the ESF programme is the fact that extension of such techniques to multidimensional vector problems is still an active area of investigation, involving cross fertilisation between different groups. In particular, there is a fertile exchange of ideas between those involved with the finite element approach using nonlinear stabilisation, and researchers into the finite volume method using node-centred unknowns and dual cells.

Aims and objectives

The ESF programme has identified a number of specific fields that need to be tackled urgently, and concurrently, to allow more complex flows to be resolved. Among specific fields to be addressed is computation of low speed flows on structured grids. Although there are currently more computing methods being developed using unstructured grids, structured grids remain more attractive for highly compute time and storage intensive applications. Examples include direct and large-eddy simulation of turbulence. Until now this has only been feasible on very simple grids, mostly with Cartesian coordinates. The whole area needs to be developed further in order to transfer such simulations to more general geometries, and to bridge the gap between the domains of incompressible and compressible flows in a better way than is possible at present. The latter is required for some applications in technology fields where there are large variations in density, examples being combustion or study of catalytic action in chemistry. It is also needed for flows that incorporate both low and high speed flows. Improvements are also needed here on the algorithmic efficiency of domain decomposition, together with application of parallel computing methods both over and within subdomains.

Work is also needed on multidimensional upwinding techniques, which allow the impact of multiple time-variant parameters to be incorporated into models. Multidimensional schemes are needed for the solution of the scalar advection equation. Multidimensional upwind methods comprise two processes: the



Flow field around a Formula 1 car aileron.

decomposition step, in which an appropriate discrete form of the equation system is split into simple components, and the distribution step, in which each of these components is then allowed to evolve in time via a technique in which a cell-based quantity, called the fluctuation, is distributed to the nodes of the grid. These genuinely multidimensional upwind schemes are therefore based on the concept of fluctuation distribution where the underlying representation of the solution is a continuous piecewise linear function with the unknowns stored at the grid nodes. This approach looks on the surface more like a finite element method rather than a finite volume one from which it differs radically.

The focus of most current research on multidimensional upwinding is on the decomposition state. Now the decomposed form of the Euler equations can be divided roughly into two groups, simple wave models and approximate diagonalisations. The latter applied to a preconditioned form of the equation has at last provided a sound basis for schemes which yield reliably accurate steady state solutions to the two dimensional Euler problem.

The quality of solutions obtained using multidimensional upwinding or indeed any numerical scheme depends intimately upon the grid upon which the discretisation is defined. Often it will not be desirable to have nodes evenly distributed throughout the whole zone. In practice, there will be some regions where a more accurate solution is required, or where the solution varies more rapidly, in which case a concentration of nodes greater than the average is required. A two dimensional example is the modelling of air flow around an isolated aerofoil section, where it is desirable to concentrate nodes around the shocks, with fewer elsewhere. To do this it is necessary to know where the shocks are, and in general this is tackled using an algorithm that moves grid points towards regions where the error in the solution is likely to be high, for example where the flow gradient is high. The ultimate objective is to produce a grid on which the global error of the discrete solution is minimised for the given number of nodes.

Equally important, given that it means more detailed models with greater numbers of dimensions can be run, is to improve the computational efficiency of the adopted numerical methods. The programme will address some interesting instances of multifield approaches, which simplify the mathematical description of the problem at hand by a combination of various differential models and numerical schemes.

The final area worthy of special mention is the field of stabilised methods, which constitute a systematic methodology for improving stability without compromising on accuracy. But one of the difficulties of stabilised methods such as SUPG is their dependence on certain parameters whose value is not completely determined by the theory. As the numerical solution is quite sensitive to the fine tuning of these parameters, the robustness of the algorithm can be poor. The programme will apply various techniques that resolve this parameter issue. One such approach employs finite element spaces enriched with bubble functions which result in completely parameter free schemes, because the stabilisation constants can be explicitly computed.

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