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Current Trends in Heat Transfer Computations

A. F. Emery and R. J. Cochran
University of Washington, Seattle, Washington 98195
and
D. W. Pepper
Applied Research Projects, Inc., Moorpark, California 93021

Introduction

HEAT transfer is usually thought of as being composed of convection, conduction, and radiation with certain applications (e.g., structural heating and boiling), evidencing aspects of all three. Until recent years the computational aspects were usually anchored in the finite difference or finite volume methods and other esoteric methods were seen only in the context of solutions to very special problems, normally involving stiff equations or pertubation analyses. The physical models which underlay the computations ranged from simple to complex, but were most frequently based upon correlations of experimental data gathered slowly and with frequent inadequate resolution.

During the last decade heat transfer computations have undergone remarkable changes. Improved computer architecture, particularly work stations with graphical output, have led to significantly more complex codes and static or animated graphical displays for interpretation. Hardware implementation of formerly slow software processing has enabled the construction and visualization of two- and three-dimensional grids for problems that were up to now intractable, and the development of improved algorithms which relied upon finite Fourier (FFT) and other transforms. At the same time, high frequency, programmable data acquisition systems have led to the measurement of data of unusually high resolution and accuracy and have permitted the construction of sophisticated models to buttress the computations.

In this paper we wish to describe a variety of different problems which are being aggressively attacked computationally and the computational trends which they suggest. It is not our intent to describe the heat transfer modeling and computations in as much detail as the papers of the 50th anniversary of the *Journal of Heat Transfer*[1] which should be consulted for complete coverage and extensive bibliographies. Neither do we suggest that our descriptions constitute critical reviews of the works to be discussed nor that we possess any specific or unusual intellectual skills in these areas. Rather we hope to give a flavor of the different problems and ap-

A. F. Emery is Professor of Mechanical Engineering at the University of Washington. He specializes in heat transfer, fluid flow, finite element methodology, thermal stresses, sensitivity analysis, parameter estimation, inverse problems, and energy conservation.

R. J. Cochran has a B.S. in Mechanical Engineering from Washington State University and M.S. and Ph.D. in Mechanical Engineering from the University of Washington. He has worked for the Boeing Airplane Company since 1984 as an analyst specializing in thermal systems, radiation, active cooling, and the adaptation of finite element codes to non-linear thermal and solid mechanics. He is currently developing and applying finite element and finite volume CFD simulations for internal fluid flows in aircraft, some of which are main cabin airflow, electronic cooling, and air conditioning system performance.

Darrell W. Pepper, cofounder and CEO of Advanced Projects Research, Inc. (APRI), Moorpark, California, received his B.S. in Mechanical Engineering in 1968, his M.S. in Aerospace Engineering in 1970, and his Ph.D. in Mechanical Engineering in 1973, all from the University of Missouri—Rolla. He is also a faculty member at California State University—Northbridge, and is currently conducting a home study course on the fine element method for AIAA. Before starting APRI he was Chief Scientist of the Marquardt Company (1987-90) and he worked for 13 years for E. I. DuPont de Nemours at the Savannah River Laboratory in Aiken, South Carolina. His research interests include numerical heat transfer, finite element methods, and computational fluid mechanics. He is the author or coauthor of over 30 technical publications, including two books. He has also contributed two chapters to the *Handbook of Numerical Heat Transfer*.

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proaches being used for a wide variety of heat transfer problems.

We categorize, although imprecisely, the different topics as falling into: 1) algorithmic or computer improvements; 2) improvements of basic physical models; 3) coupled (conjugate) problems; 4) adaptive mesh and equation solvers; and 5) inverse and sensitivity approaches.

Although we have attempted to present the different cases according to a sequence which logically leads to comments on future trends, many of the cases display aspects of several categories and thus lead to some jumping and skipping through the topical sequence. Many of the examples are drawn from published reports but, by necessity, several have been obtained by personal correspondence and are not available in the open literature.

Radiation

Most radiation computations have concentrated on relatively simple problems in which the geometry and the surface radiative characteristics can be described analytically (planes, cylinders, etc.) or by very simple models (gray gases, bands, etc.). The computations have been restricted to solutions of the radiative transfer equation for gaseous absorption and emission or calculations of the radiosities. With increased computing power and imaging we find that very complex structures and radiative properties are being treated. Most of these computationally intensive studies tend to be associated with: 1) conventional view-factor calculations and associated thermal analyses using gray plane surfaces or Monte Carlo techniques; 2) modifications of 1) to consider angular dependence of emissivity, but isotropic reflectivity and absorptivity; 3) emission to distant observers (the signature problem); 4) bidirectional reflectivity; and 5) participating media.

Figure 1a is a schematic of the shuttle wing and the modeling of a single bay done by Ko and Gong.[2] Figure 1b shows how the temperature field varies with the model complexity and Fig. 1c illustrates the rapidity with which the number of view-factor calculations increases. Clearly, these computations are expensive and should be done using an optimal method. The different numerical methods currently used involve discretizing the surfaces into smaller subareas. These methods can be categorized in terms of the number of emitting and receiving subareas as indicated in Table 1.

Modern applications of the hemicube and projection methods depend upon computer graphics techniques to attain high-execution speed and accuracy. Emery et al.[3] surveyed the different methods and compared accuracy and speed for several realistic configurations. For isotropic surfaces the double area/contour integration and hemicube methods are recommended. Figure 2 compares the speed of these methods for a configuration with a variable number of obstructing surfaces. It is clear that the hemicube approach should be coupled with an adaptive search to minimize execution costs. The basic reason for the slow speed of the projection methods is their inability to utilize the principles of reciprocity. Angular dependence of emissivity can be easily included in these models, although reciprocity is lost, and rarely is the precise nature of the correct angular distribution known. If reflectivity and emissivity are angularly dependent (the bidirectional problem) the Monte Carlo method is generally used. Figure 3 illustrates the slow rates of convergence of this method—its major fault. The use of the Monte Carlo method is generally restricted to very complex geometries or to the validation of other methods. Improved geometric descriptions based upon solid modeling, adaptive ray launching, and accelerated searching by octree representations can provide significant increases in speed.

Normal thermal analyses are done using finite volume, finite difference, or finite elements which are defined in terms of nodal temperatures and the interpolating functions are rooted in these nodal temperatures. Because radiation absorption takes place over the entire surface it often tends to produce

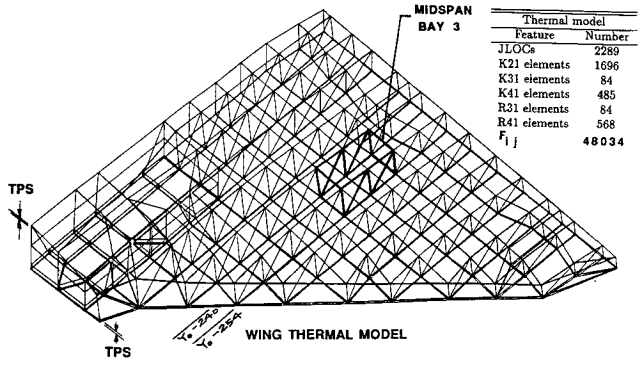


Fig. 1a Space Shuttle orbiter wing spar finite-element thermal model.

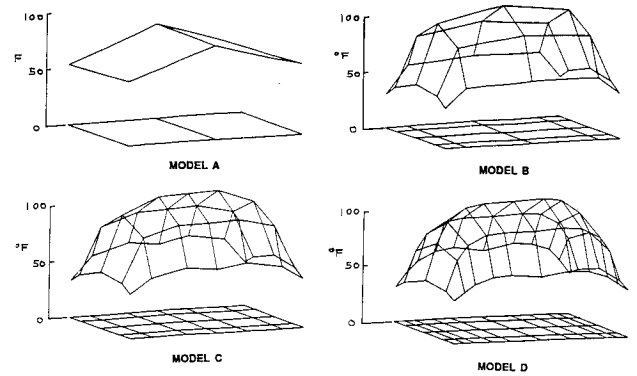


Fig. 1b Distribution of orbiter wing lower skin temperatures.

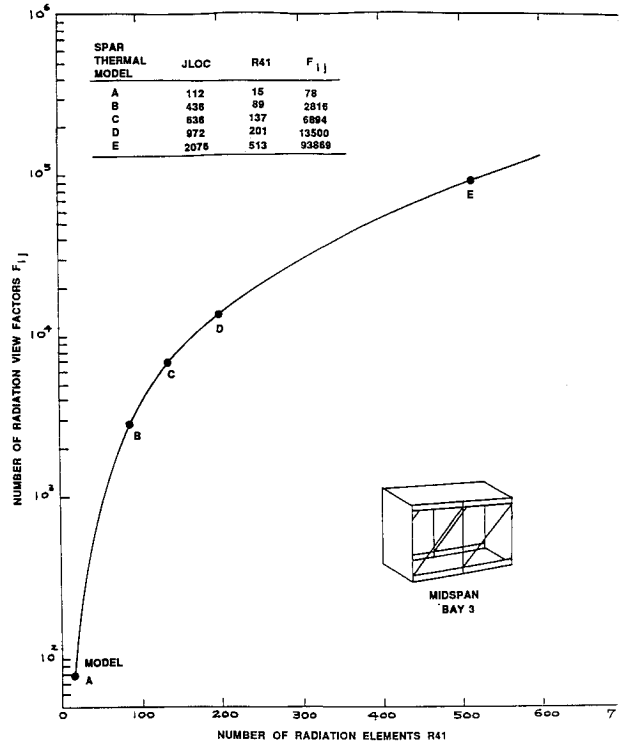


Fig. 1c Number of radiation view-factors as a function of number of radiation elements.

temperature fields with local maxima intermediate to the nodal positions. Consequently, very high densities of nodal points or elements are needed to accurately represent the resulting fields, particularly to avoid computed results in which the surface temperature exceeds the source temperature. Kumar[4] and Lobo[5] applied p-elements and spectral methods to these problems. Figure 4 displays the predicted temperature for a surface which is exposed to radiation and whose edges (x =

Table 1 Characterization of view-factor calculations

Method	Number of emitting areas	Number of receiving areas
Double area/contour integration	Finite and few	Finite and few
Hemicube	Finite and few	Finite and many
Nusselt projection	Finite and few	Infinite
Monte Carlo	Finite and many	Infinite
Exact integration	Infinite	Infinite

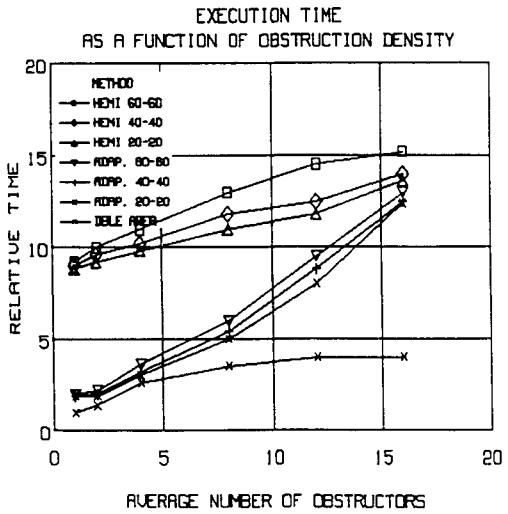


Fig. 2 Comparison of execution times for double area, ADAP, and hemi-cube methods for computing radiation view-factors.

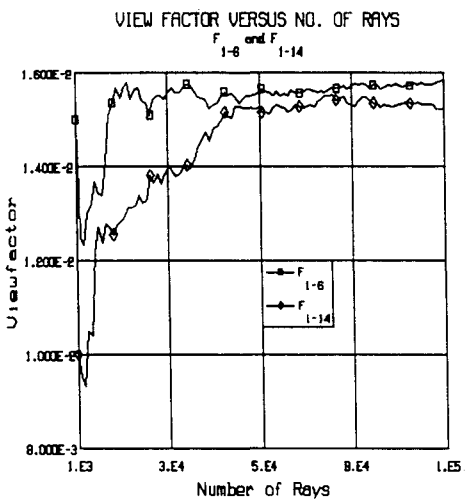


Fig. 3 Convergence patterns for the Monte Carlo method of computing radiation view-factors.

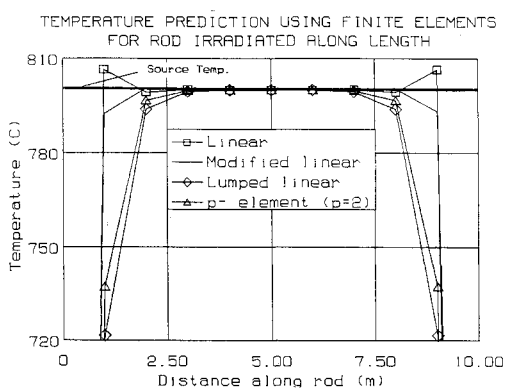


Fig. 4 Temperature predictions for an irradiated rod.

0 and 1) are maintained at 0. In order to conduct the heat to the fixed temperature edges, a very high gradient is needed. Linear elements can achieve such gradients only by predicting temperatures near the edge which exceed the source temperature. The figure illustrates how elements with enhanced basis functions can accommodate the very large temperature gradients and produce meaningful results.

IR signature analysis involves radiation from both the surfaces of the hot structure and from the exhaust plumes and thus requires the treatment of participating media and bidirectional surface properties. Billings[6] proposed extending the concept of Markov chains to treat bidirectional radiation. This is done using a two-parameter state definition of the chain—a method which is very similar to restricting the Monte Carlo approach to discrete ranges of parameters (sometimes called the "bin" method). Treatment of participating media requires the solution of the radiative transfer equation—generally done with discrete ordinates, zonal, or finite element methods, all of which are very time consuming and of varying accuracy. Tan[7] described an improvement to the Gaussian integration approach which reduces computational costs in a manner similar to the hereditary integral approach used to solve linear viscoelastic problems. Its drawback is a nonuniformity in spatial coordinates. A generic question for the bidirectional problem is the exact form of the reflectivity function. Billings[6] proposed the symmetric conditional probability density function which progresses smoothly from diffuse to specular reflectivity. Corlett[8] recently developed some relatively simple models which are rigorous and satisfy the necessary theoretical requirements (e.g., reciprocity, upper bounds, etc.)

The wavelength dependent radiation typically found in the IR signature problem is treated using either Monte Carlo or a banded spectral approach. The latter requires a separate solution for each band. Recognizing that hot engine cavities have a fixed geometry and that the wavelength dependence of most metals varies smoothly, Betchley[9] developed a technique in which the solutions for the second and higher numbered bands are treated as perturbations of the solution for the first band. With the use of the LINPACK solver package, Betchley obtained stable and robust solutions.

Mattick and McFall[10] proposed a high temperature gaseous radiation receiver for a space propulsion system (Fig. 5). Their analysis assumes that a gas absorbs the concentrated solar energy and subsequently radiates to the gray surfaces comprising the system. The candidate gas is treated as either a gray gas or one with three bands but it is still isotropic. The figure illustrates the effect of the nongray gas assumptions. Clearly, nonisotropic scattering and bidirectional properties should also be considered to give a more realistic and accurate assessment of this device.

Currently, even if radiative fluxes are efficiently computed, the subsequent calculation of surface fluxes and temperatures is still limited by the dense matrix associated with the radiosity method, its requirements of view-factor reciprocity and the sum of the view-factors to be unity, and its coupling with associated convective and conductive analyses. With the advent of computer graphics hardware implementation (particularly parallel systems) capable of handing solid modeling and imaging, we can expect much of the future radiation analyses to be based upon Monte Carlo simulation (or its descendents), interatively coupled to the finite element or spectral conductive and convective solvers.

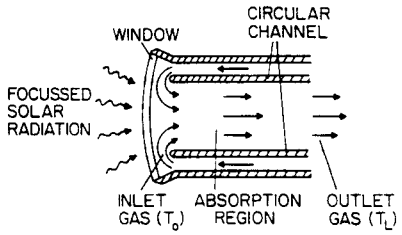


Fig. 5a Illustration of FGRH concept.

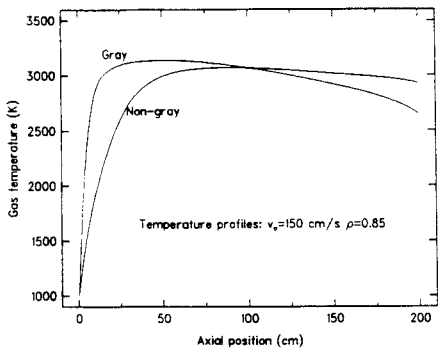


Fig. 5b Comparison of temperature profiles for gray and nongray gases.

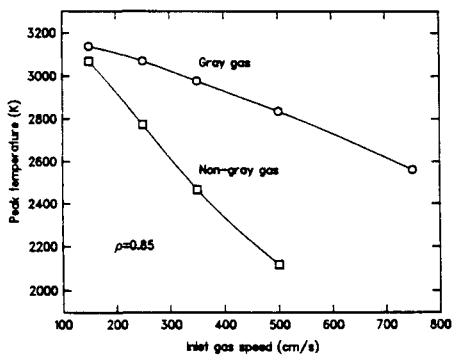


Fig. 5c Peak temperature vs inlet gas speed.

Finally, the understanding of these signature problems and other more general problems is significantly enhanced by computer graphics, especially ray tracing (Foley[11] and Glassner[12]) which permit the user to easily see if one surface can see another or to follow the progress of individual rays.

An area of importance is radiation to particles and particle-laden streams which are encountered in combustion systems and environmental pollution problems (droplets and aerosols). Such radiation is characterized by nonisotropic scattering and properties which are strong functions of temperature and wavelength.[13] In addition, the wide range of length scales in these problems (particularly those of the ash in contrast to the physical size of boiler components) poses severe computational problems unless the participating media is treated as a second fluid, rather than as single, interacting radiators.

Evaporation and Interfaces

A major concern in the design of propulsion systems is the change in liquid fuels which in the future are expected to contain more of the lower end of the distillation and will therefore be less volatile. These changes are likely to strongly affect the design of combustors which depend upon droplet evaporation. In contrast to the computationally intensive flow examples presented elsewhere in this paper, Bellan and Harstad[14] employed simpler numerical approaches to investigate binary fuels and to study the effects of turbulence and droplet drag models. The results suggest that the relative velocity between the droplet and the ambient fluid is a weak controlling parameter for both lean and rich mixtures. In further studies they have shown that the evaporation time does not depend upon the turbulence model used for dilute sprays (for charged or uncharged droplets) but does have a great effect on dense sprays.

Mattick and Hertzberg[15] proposed droplet and sheet sprays for cooling in space. Upon exposure, the droplets radiate energy (Fig. 6). Droplet vapor pressure must be low (10^{-7} Torr) to reduce the evaporative loss. Figure 6 illustrates how droplet rejection compares to that of a solid surface. Bruckner and Shariatmader[16] proposed a heat exchanger in which the droplets transfer heat to an inert gas (LDHX exchanger). The findings of Bellan[14] may be useful in choosing droplet size for the LDHX and some consideration of sheet flows when droplets are dense may be useful.

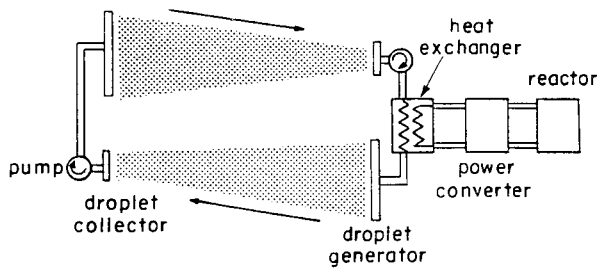


Fig. 6a Droplet radiator configuration.

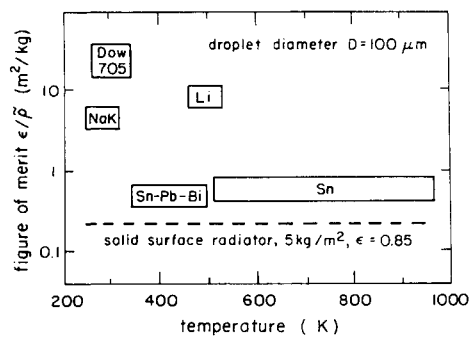


Fig. 6b Figure of merit for candidate radiator liquids.

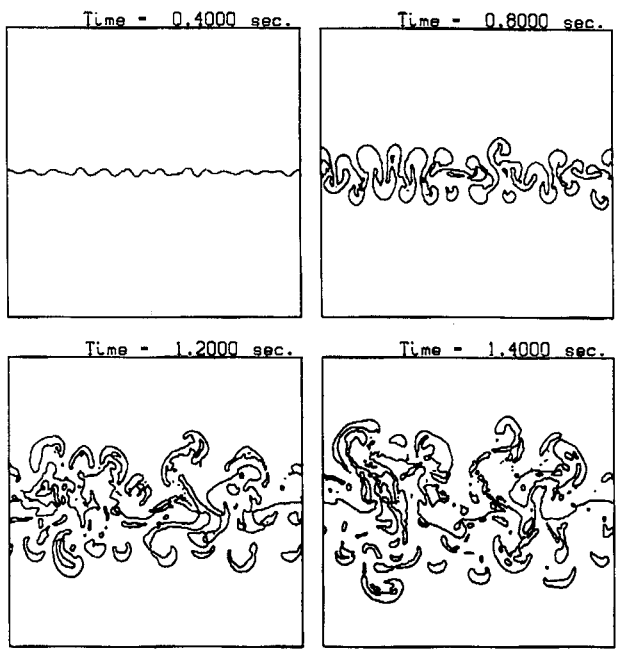


Fig. 7 Evolution of the inertially unstable interface in a 0.5-m domain with surface tension computed using fractals.

Webber et al.[17] studied inertially unstable fluid interfaces, a topic which may be pertinent to such sheet exchangers. Their results suggest that the interfaces have an effective fractal dimension and that this is lower in the presence of surface tension. Figure 7 illustrates one of their computed time histories of an interface. The idea of using fractals for heat transfer may be of interest in situations in which the process depends upon microscopic surface geometry (e.g., boiling) heat pipes, surface radiation, and contact resistance, or volume effects as found for dense droplets. Yao[18] recently shown that the conductivity of packed beds can be well-correlated using fractal dimensions between 1–2. Argoul[19] suggested that the energy cascading process of turbulence contains a multifractal nature.

An important interface is the free surface of a fluid flow as found in cavitating machinery systems, flow in heat pipes, and other general liquid-vapor flows. The numerical solution is difficult since the free-surface geometry changes along the path of the flow and usually cannot be fitted using a regular coordinate system. Rahman[20] utilized body-fitted coordinate systems to treat free thin films under reduced gravity, although the generality of the method remains to be proven.

Coupled/Integrated Problems

Traditionally, the only coupled problems which received significant computational attention were those of combined convection and conduction in fluids (thermal boundary layers) or in fluid-structure interactions (ablation, transpiration) or radiative-convective-conductive problems. Only recently have we seen significant strides made in fluid-structure interactions in which the structural deformations and stresses are an intrinsic part of the thermal process.

When convection, radiation, conduction, and chemistry are simultaneously present, the problems are frequently referred to as "coupled" and the solution techniques are called coupled or "integrated," although there is a subtle distinction between these two terms. For convective-conductive problems as found in heat transfer between fluids and solids, there are a number of different approaches. The simplest is when the fluid properties are independent of temperature and the velocity may be computed independently of the thermal field. The solution therefore only consists of solving for the temperature in the fluid and the solid. We call this the "zeroth" order coupling. The approach consists of establishing a grid in the fluid and the solid and requiring that the heat flux at the interface be continuous. For laminar flow this is not difficult, but some care must be taken in defining the grid if the conductivities of the solid and the fluid are significantly different. Kelkar et al.[21] developed a method for computing conjugate heat transfer in irregular geometries. The solution technique treats the entire temperature field in a unified manner by computing the equivalent conductances across control volume faces and is applicable to laminar as well as turbulent flows. An iterative solution proposed by Kelkar[22] can be utilized to handle a wide range of thermal conductivity ratios. Figure 8 illustrates the temperature fields for conductivity ratios ranging from 1 to 10,000 for laminar flow over cylinders. For turbulent flow there are two choices. First, we may assume that the fluid heat flux is molecular by establishing a sufficient number of points within the laminar sublayer. This causes computational problems (in the sense of a demand upon computational resources but not in a fundamental mathematical nature) because of the thinness of this layer which increases the grid density and number of nodes significantly. A further complication is that because of the need to retain reasonable aspect ratios within the computational grid, grid refinement must be done in both streamwise and normal directions, thus leading to block meshing with mesh interface problems. The second choice is to use empirical relationships for the heat transfer coefficient at the surface and to treat the fluid and solid as separate, but simultaneous, computational problems—a process we term "first"-order coupling.

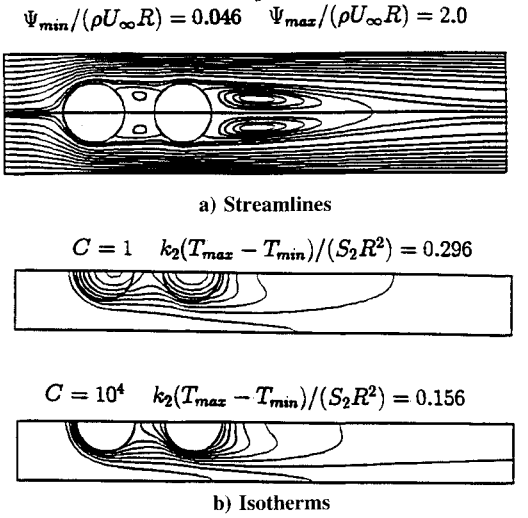


Fig. 8 Streamlines and isotherms for different conductivity ratios for flow around an array of heated cylinders.

The design requirements of hypersonic aircraft has introduced unique challenges for heat transfer analysis because, due to weight constraints, the airplane requires active cooling systems. This is in contrast to the passive insulation systems developed for the Space Shuttle. The airplane structure will have areas of very intense localized aerodynamic heating at stagnation points, leading edges, and in the neighborhood of shock-shock interaction. The active cooling systems include convection cooled panels, transpiration, and heat pipes. Due to the interaction of those cooling systems with the structure of the airplane, coupled thermal-fluid structural analysis is required. Accurate prediction of convection cooling in regions of intense heat flux for the cooled panels is necessary. The predictions have to include variable fluid property effects because of the wide range of operating temperatures of the coolants. Transpiration cooling has also proven to be very effective.[23] An example of such an analysis is the two-dimensional porous flow calculations combined with a real-gas boundary program for designing a nose tip reported by Young.[24] Coupling in this case was provided by convective heat transfer correlations which matched the heat flux at the fluid/structure interface. Faghri[25,26] analyzed heat pipe performance to estimate the effects of multiple, intense, heat sources, start-up transients, and initially frozen conditions which are relevant to the National Aerospace Plane (NASP) and to aircraft subject to laser weapon fire. The analyses have been based on standard finite difference two-dimensional modeling of the wall and the wick coupled with a one-dimensional analysis of the vapor flow.

A better approach, particularly for temperature-dependent fluid properties, is to simultaneously compute the velocity and thermal fields. Although computationally expensive, the process is conceptually simple, requiring only that the Navier-Stokes equations be solved in the fluid domain using one of the methods described above for matching of the heat flux at the interface. A better coupling, the "second"-order coupling, is achieved in some finite element[27] and finite-volume[22] codes by assuming that the entire region is filled with a fluid and that a solid is simply a fluid of infinite viscosity.

For external flows, the coupling is usually done using an integrated approach. The inviscid flowfield is computed by first ignoring the boundary layer. It is then considered as the freestream condition for the boundary-layer flow which is then solved for and the boundary-layer flow is then taken as the boundary condition for another calculation of the inviscid flow. This iterative process is continued until convergence. Similar approaches are used for transpiration, ablation, and blowing. In addition, when structures are involved and their deformations influence the velocity and thermal fields, such

integrated approaches with sequentially iterative solutions of each aspect are employed[28] (Fig. 9). Temperature and stresses in cooled struts have been determined by linking a PATRAN generated geometrical mesh with an aerothermal load program, SINDA, a structural deformation program, MARC, and a coolant fluid heat transfer code.[29] Some integrated programs, such as McDonnell Douglas' FATSO,[30] include optimization/optimal control codes to permit modification of shape or operational parameters during the sequential/iterative solution process.

In contrast to the sequential integrated approach, true coupling poses its own special problems, the most obvious of which is the differing time and spatial scales of several processes; it is handled by simultaneously solving for all field values. Grids for velocity and temperature must be concentrated near the interfaces, whereas those for structural deformation frequently need densification at other portions of the mesh, such as at structural discontinuities (cracks), and zones of plastic deformation. Time scales are usually different, particularly for dynamic structural behavior when characteristic times are often long in comparison to characteristic advection or combustion times. The common solution has been to employ a mixture of explicit and implicit codes, leading to time interpolation between the output of the two codes. With the advent of very high-speed computing, there is a movement to all explicit codes, even for the structural calculations. Grigoropoulos[31] treated laser melting of crystals using an explicit simultaneous evaluation of the temperature, the radiative properties, and the fraction of melting throughout the solid.

Probably the truest coupled codes are those used in welding where fluid flowfields, electric and magnetic fields, temperature fields, and solid mechanic variables are simultaneously computed. Each node then represents a multitude of field variables and the time-steps and grid spacing are controlled by the most critical aspect. Although computing can be done on single processor machines, this approach really awaits the massively parallel machines which are now projected for the near future.

A major application of numerical heat transfer has been the estimation of stresses and deformations associated with welding. The simulations range from complex coupled codes to simple empirical modeling. Typical of the complex coupled simulations are those reported by Callebresi[32] in which stresses are predicted in the immediate vicinity of the fusion zone. Such calculations take into account material properties, process variables, and fracture sensitivities. Validation of the results depends very strongly upon experiments which are difficult to make and analyze. In general, these codes are unique in that they predict the molten weld behavior and weld size along with metallurgical changes as the material passes through the austenitic/martensitic transformations. Considerable work has been done in predicting the free convection motion within the weld pool, but accurate descriptions of the subsequent solidification and metallurgical changes are still in development. An interesting application is the determination of the shape of a ball formed by arc-heating of a wire tip.[33] The shape was numerically determined by solving equations based upon minimum energy principles and a perturbation scheme. Temperature fields in the molten mass were determined by using a body-fitted coordinate system. A simpler model has been used by Emery and Jones[34] to determine the sensitivity of welding thin plates to process parameters. This model relies upon measured weld bead widths and uses material properties defined in terms of temperature. Although the details of the molten weld bead convection are ignored, all other aspects (conduction, convection, radiation, and plasticity) are treated. Figure 10 shows the agreement of measured and predicted deformations. Sensitivities of the residual stresses to surface radiation, convection, weld bead radius, heat sinking, and welding speed have also been reported.

Finally, welding simulations are often used not to study the weld itself, but to study the overall stresses in the body; usually at such distances from the weld that the details of the weld bead are not critical. Knorovsky and Burchett[35] used three-dimensional thermal stress analyses to study the effect of heat-sinking on glass-metal seals. Heat-sinking reduces the maximum temperatures experienced by the seals, but introduces significant and reversed thermal gradients, therefore, its effect is not easy to predict. Coupled stress calculations are currently being made.

In contrast to welding—which provides a thermally continuous junction between materials—the common methods of riveting or bolting lead to significant contact resistances

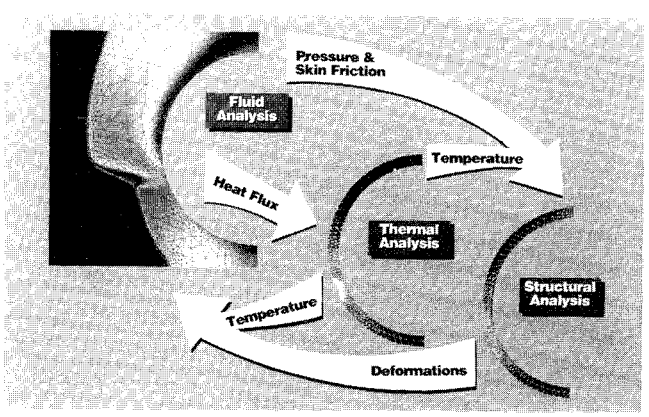
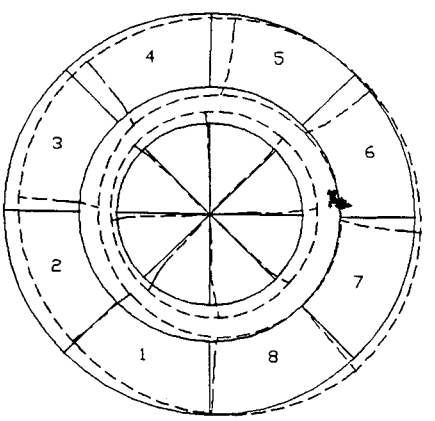
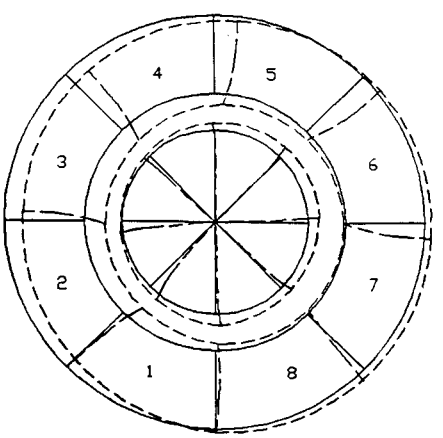


Fig. 9 Integrated fluid-thermal-structural analysis with adaptive unstructured meshes.



a) Magnified experimental deformations



b) Magnified analytical deformations

Fig. 10 Axisymmetric welding test coupon.

which are functions of flatness, roughness, hardness, material properties, and gap convection and radiation. Similar effects are found in assembling electronic packages. Surprising results are found where the joint conductances appear to depend upon the direction of heat flow. Figure 11 is a schematic of a typical surface and the gross heat flux lines.[36] The effect of heat flow direction may well be due to the local surface shape which can cause local reverse convection cells. While two- and three-dimensional Navier-Stokes-based flow calculations (including buoyancy and radiation) are likely to help us understand what is transpiring, such calculations will probably be unusually difficult and expensive to make and hard to interpret. The effects of pressure, which modifies the surface shape, and therefore, the convection and radiation, require the use of coupled codes. It will be interesting to see if fractal effects can be superimposed on gross motions to enhance our understanding.

Finite Difference, Volume, Element, and Spectral Elements

Finite-difference methods constitute the backbone of most computational fluid dynamics (CFD) codes and almost all early thermal analyzers. By using different stencils, user specified accuracy could be achieved to fit almost any problem as long as a regular grid system was used (rectilinear, polar, spherical, etc). Most grids were orthogonal and numerous methods have been developed to handle boundaries which do not fit the grid.[37] For problems which do not fit the simple regular grid systems, it is common to map the field onto a regular grid by a grid transformation. Such transformations require care and raise the question of accuracy since the numerical approximations can be expressed in two different ways. Consider a nonuniform grid in the x direction which is mapped onto a regular grid in ξ. The differencing can be represented as $\partial/\partial x$ where the differencing on the unequal grid reduces the accuracy unless care is taken or as $(\partial/\partial\xi)(\partial\xi/\partial x)$ where the accuracy depends upon the transformation, and large values of $\partial\xi/\partial x$ may multiply the error in $\partial/\partial\xi$ to unacceptable values. However, because of their simplicity, finite-difference techniques are still in use and under development (see the following section on internal flows). Kelkar[21] recently described improved methods of handling nonorthogonal grids. One must be careful describing the finite-difference approach since in some forms it reduces to the finite-volume method. Many FV codes use staggered grids to ensure conservation of physical quantities. Shih and Tan[38] give a good discussion of the effects of grid staggering.

Unfortunately, the general shape of practical parts is not easily accommodated by such regular grids and temperature-dependent properties reduce the accuracy of the high-order stencils. Thus, most practical and commercial programs are based on finite-volume concepts—a natural outgrowth of the RC network analog. Although most finite-volume solvers employ structured grids, they can be used with unstructured grids with only a minimal modification, but their accuracy is rarely more than first-order.

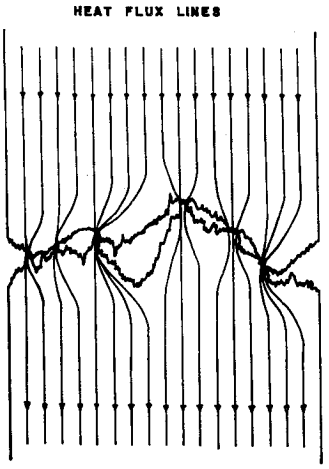


Fig. 11 Heat flux lines across an interface.

Over the last three decades, structural engineers have developed the finite-element technique and provided innumerable examples of the ease with which it can treat the most general problems. Not only is the method probably the easiest to apply, but its theoretical foundation is unusually well-developed and understood.[39,40] It should be noted that its ease-of-use has also led to it being one of the most misapplied tools. Routinely applied to structures and conduction, it is just beginning to make headway in radiation[41] and fluids.[42] Several commercial programs exist, such as FIDAP and FLOTRAN, which are capable of solving both laminar and turbulent fluid flows with heat transfer. The laminar flow solution capabilities are very robust and yield accurate solutions for complex domains. Turbulent flow simulation has been demonstrated with finite elements, but the stability of the solution algorithms is still questionable for two-equation models. Current trends include the refinement of equation coupling and linearization methods. In addition to fully coupled solution algorithms, successful solutions have been obtained with projection methods (SIMPLE type of algorithm).[43,44] These methods make use of a Poisson equation for pressure, which leads to a reduction on the incompressibility constraint that allows equal-order interpolation of pressure and velocity.[45] Several excellent articles dealing with the use of finite elements in solving the Navier-Stokes equations,[46] the least-squares finite-element method,[47,48] creeping flow,[49] advection,[50] body-fitted coordinates,[51] and mapping to regular domains,[52] should be consulted. Eliasson[53] has used finite elements for the easy display of streamlines.

For fully coupled solution algorithms, the higher order accuracy of quadratic, mixed-method elements may still prove to be useful. This is especially true when attempting to resolve the heat transfer between a turbulent fluid flow and the surface by way of a two-equation turbulence model. The choice of stable, higher order elements for both continuous and discontinuous pressure interpolation is another area of importance. Figure 12 illustrates the variety of quadrilateral elements currently in use. The discontinuous pressure elements provide a better constraint ratio for maintaining incompressibility than do the continuous pressure elements. They also provide an additional level of local element mass conservation.[54] To date, turbulent flow simulations have made use of only continuous pressure elements. These turbulent simulations include equal-order projection methods,[55] and upwinding.[56] Benim[57] used discontinuous pressure elements for internal flows—with the intention of treating flames—and found good agreement in accuracy and computational speed with finite-difference calculations.

Increased accuracy in the finite elements is achieved by employing higher order basis (trial or interpolating) functions. These formulations often introduce off-diagonal terms in the element matrices which raise questions about their physical significance. For example, consistent quadratic elements have negative off-diagonal capacitance terms. As a result, a number of empirically-based lumping (diagonalization) techniques have been developed for different applications. Such modifications, which have their genesis in finite-volume methodology, detract from the solid mathematical basis of the finite-element method.

During the last several years a number of articles have appeared dealing with the spectral finite-element methods, partly because of the ease with which such methods can easily be adapted to parallel processing, but more so because of their inherent accuracy.[58–61] These spectral methods are based upon infinitely differentiable basis functions which converge "spectrally fast." In general, they have utilized orthogonal, structured grids. The semidiscrete form of the Navier-Stokes equations is achieved through a three-step, time-splitting scheme. The first step explicitly accounts for the nonlinear

Continuous Pressure

Nodal Layout	Name	Interpolation Functions
	Q2(8)-Q1	• velocity - serendipity biquadratic □ pressure - bilinear
	Q2-Q1	• velocity - biquadratic □ pressure - bilinear
	Q2-Q1+	• velocity - biquadratic □ pressure - bilinear augmented by a constant
	4XQ1-Q1	• velocity - bilinear on 4 quadrilaterals □ pressure - bilinear

Discontinuous Pressure

Nodal Layout	Name	Interpolation Functions
	Q2-P1	• velocity - biquadratic □ pressure - linear
	Q2-P1(3)	• velocity - biquadratic □ pressure - linear
	R2-P0	• velocity - restricted biquadratic □ pressure - constant ○ normal velocity - restricted biquadratic
	AQL	• velocity - enriched bilinear □ pressure - constant

Fig. 12 Stable continuous and discontinuous pressure quadrilateral elements.

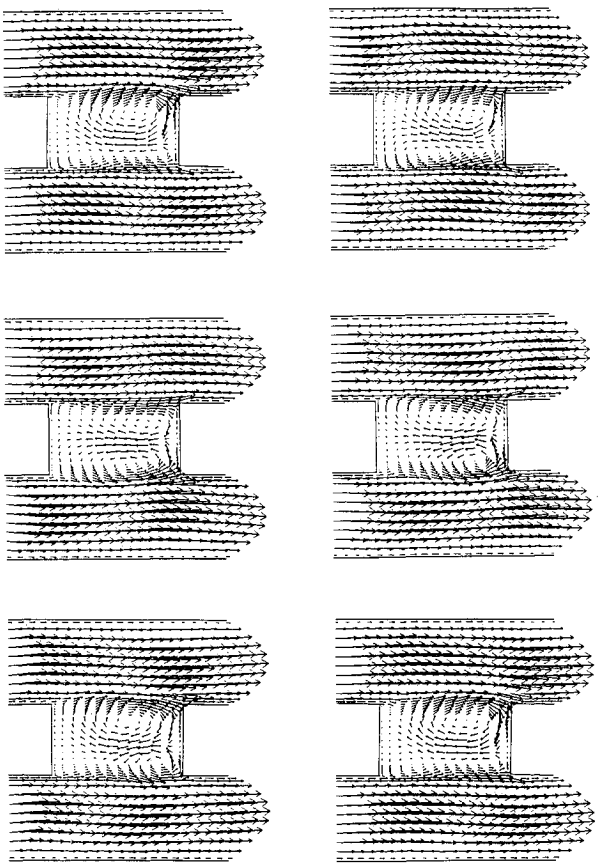


Fig. 13 Periodic vortex history.

convection contributions and introduces the only stability requirement of the scheme. After this first step the problem has been reduced to a Stokes problem which is decomposed into an elliptic Poisson and Helmholtz equation for the pressure and viscous terms, respectively. The pressure and velocities are solved with the same basis function and on the same mesh. The occurrence of spurious modes in the pressure (a problem common to some finite element techniques) is circumvented through a weak imposition of both the incompressibility conditions and the boundary conditions on the velocity. Numerical efficiency is achieved through the use of collocation for the nonlinear convective step and static condensation with the variationally formulated Stokes problem. The static condensation decouples the boundary nodes and their associated DOF from those in the interior, making this procedure ideally suited for parallel implementation. The enrichment of the basis function provides exceptional accuracy with a reasonable increase in computing costs; this is much better than can be obtained by refinement of the mesh as is usually employed in finite-difference and finite-element solutions.

Amon[62] used spectral methods to study internal flows. Figure 13 illustrates the steady periodic growth and decay of a vortex in a passageway connecting 2 two-dimensional channels. Similar calculations have shown how flow destabilization in a slot markedly affects the mixing and convective transport. Lombard and Riley[63] used spectral techniques to study finite amplitude internal gravity waves in stratified media; waves whose amplitudes are large enough to produce density inversions.

Internal Forced Flows/Turbulence

Full Navier-Stokes solutions have been presented for a number of interesting internal flows. Evans and Greif[64] employed a full Navier-Stokes solution to study chemical vapor deposition (CVD) reactions for laminar flow in rotating systems and channels. Their aim was to observe the effects of wall thermal boundary conditions and spin rates. Both effects caused fundamental changes in the flow patterns. In addition, the simulations have shown the existence of instabilities in CVD channel reactors. Chang et al.[65] studied the flow between corotating disks representative of computer disks to observe the existence of horizontal roll vortices and the effects of turbulence. Considerable effort was spent in addressing the turbulence modeling—a common feature of almost all studies which utilize the k-ε turbulence models. The calculations were done with a turbulence model which included wall shear and curvature corrections. Although their calculations considered only steady, nonperiodic states, the results were in good agreement with experiments. It was found that axial blowing protected the flow from the gradient steepening effects of rotation at the shroud.

In order to provide a bench mark solution for the study of outflow boundary conditions and mesh sizing, Gartling[66] used the finite element method with a structured regular grid to study isothermal flow over a backward-facing step. Due to the three separate recirculation zones found in this flow at a Reynolds number of 800, it is also a good test problem for the study of upwinding errors. Vradis[67] used regular grids and a strongly implicit algorithm in which the continuity and momentum equations are solved simultaneously to consider the effect of variable viscosity for the same problem. Figure 14 illustrates the effect of different viscosities on the reattachment point.

Complex flows are sometimes computed by using structured grids in which the grid lines have been transformed so that at least one set defines the streamlines and the boundaries. These transformations are generally derived by an algebraic transformation from the x-y system to the ξ-η system. Over the last decade significant efforts have been invested in defining robust transformations and the results have been reported in numerous symposia.[68] Although most transformations involve both ξ and η, some studies have successfully transformed only one coordinate. Faghri[69] used this idea to

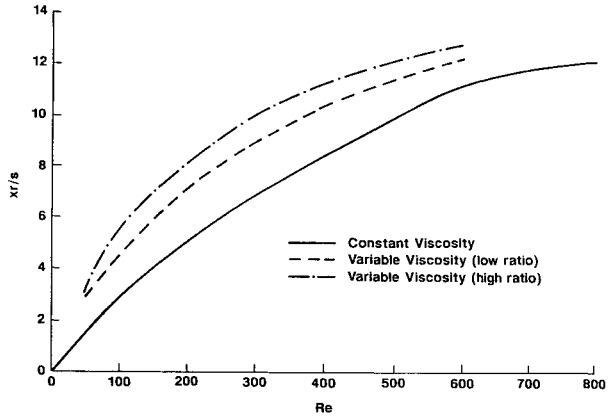


Fig. 14 Reattachment length vs Reynolds number.

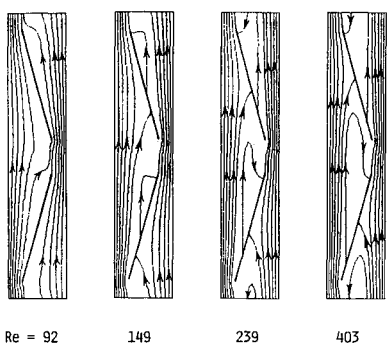


Fig. 15 Streamline diagrams for flow using boundary fitted coordinates.

treat a number of duct problems and flow through honeycombs. Figure 15 shows the streamlines for flow through a series of interrupted plates with each plate being at an alternate angle to the flow. Similar results have been obtained for flow through nonparallel plates and honeycombs with good agreement with measured results. Kelkar and Patankar[70] used this method to study the effect of offset fins in compact heat exchangers. It should be noted that these efforts have led to a revitalization of the finite-difference approach and have provided an alternative to the finite-element method.

An area of continuing work is the prediction of convective heat transfer in bends and curved ducts.[71] As recently pointed out by Iacovides and Launder[72] and Launder,[73] the numerical prediction of the turbulent flow in three-dimensional square-sectioned bends requires the use of near-wall wall sublayer models and algebraic second-moment closure. This level of turbulence modeling is required in order to predict the effects of the secondary velocity field induced by this flow on the local Nusselt number within the duct. They note that the flow in circular-sectioned bends creates similar difficulties. The effects on the heat transfer in the downstream pipe or duct are also significant as pointed out by Humphrey et al.[74]

Free Convection

Mason[75] applied a laminar Navier-Stokes solver to study the effects of geometry and heating rates in closed containers. The properties were considered to be independent of temperature and the volumetric heating rates were linear proportional to pressure. At low heating rates (P = 1 atm) for a container wall held at a constant temperature, the maximum temperature was higher and its location higher for a hemispherical/cylinder container than for a sphere. Increasing the heating rate raised the temperature (not linearly), raised the location of the maximum temperature point, and produced a significant temperature inversion.

Chenoweth and Paolucci,[76,77] have studied flows in cavities and slots to examine the effects of large temperature differences and destabilization using a staggered interlaced grid and a variant of Patankar's SIMPLE algorithm.[78] Using over 200 simulations they determined the different flow regimes as a function of Rayleigh number, aspect ratio, and temperature difference (Fig. 16). The Boussinesq assumption is used in almost all free convection simulations although there are questions about the consequences of its use. Figure 17 displays results for different aspect ratios and values of $\varepsilon = \delta T/T_0$ for a Rayleigh number of 10^5. The flow on the right side of the figure is for a negligibly small value of ε = 0.005, while its neighbor to the left is for ε = 0.6. When the Boussinesq

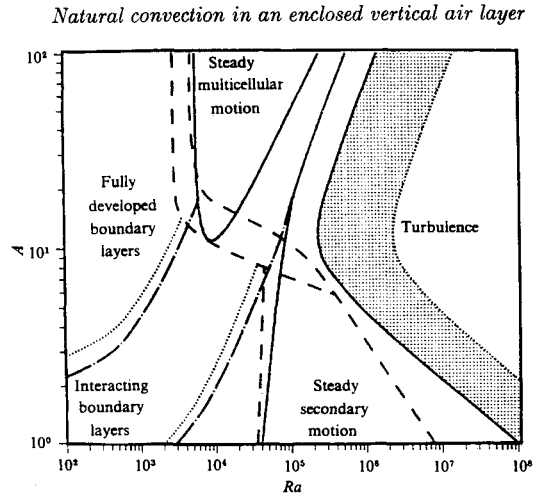


Fig. 16 Natural convection flow regions dependence upon A, Ra, and ε (A = aspect ratio, Ra = Rayleigh number, and $\varepsilon = T_{hot} - T_{cold}/T_{mean}$).

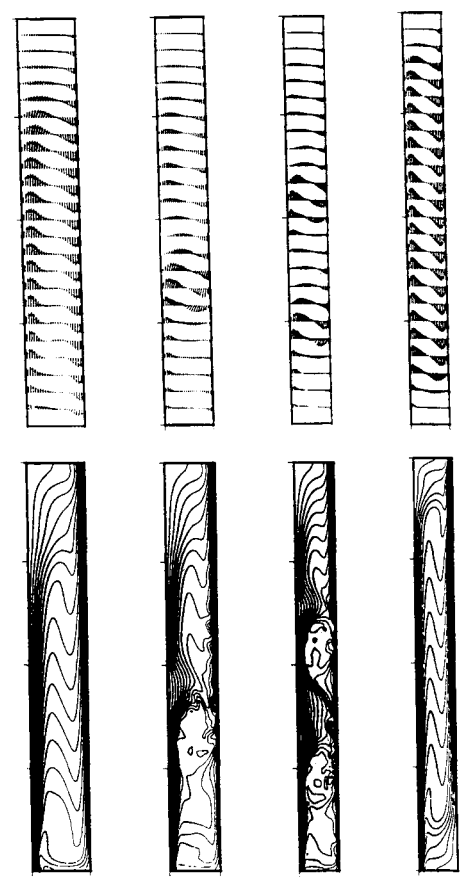


Fig. 17 Velocity and isotherm fields for $Ra = 10^6$ showing effects of ε and A: a) ε = 0.6 and A = 7; b) ε = 0.6 and A = 8; c) ε = 0.6 and A = 10; and d) ε = 0.005 and A = 10.

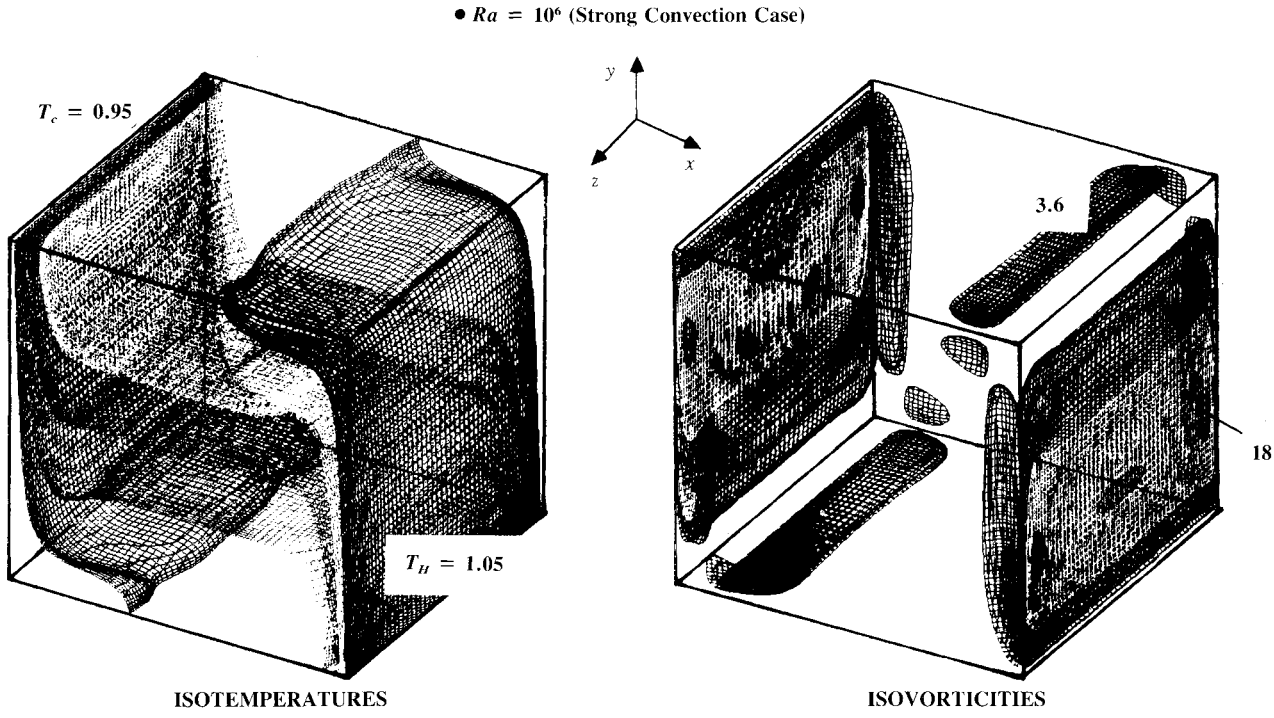


Fig. 18 Three-dimensional natural convection in a cavity.

assumption is used the calculated flow is well-behaved and is single-celled. However, when the assumption is not utilized the flow displays multiple cells with rather intense vortical motion. Their work suggests that an accurate representation of the fluid properties is critical to producing realistic flow simulations and that the Boussinesq assumption must be used with great care. They have also studied the origin of the chaotic motion within the cell. At low Rayleigh numbers and for small aspect ratios, the instability arises from the internal waves generated near the corners where the vertical flows turn to become horizontal. For other aspect ratios, the instabilities are generated within the boundary layers.

Gardner[79] and Douglass[80] investigated the linear stability of axisymmetric natural convection and the effect of Prandtl number for flows between closely-sized concentric spheres, with the inner sphere being warmer than the outer sphere. The flow regimes are characterized by a bifurcation in which flows are steady for low Grashof numbers and quasiperiodic for higher values, but both are always axisymmetric. The effect of the Prandtl number is reversed, with small *Pr* yielding periodic flows and large *Pr* producing a steady flow. The computations clarify the experimental observations of Bishop[81] and Yin[82] in which the different flow patterns were thought to be associated with artifacts of the experimental approach.

Although almost all published free convection in enclosure studies have been two-dimensional, Humphrey[83] has suggested that three-dimensional results are likely to be fundamentally different and predictions of turbulence may be much different between two- and three-dimensional flows. Fusegi et al.[84] concentrated their studies on the three-dimensional aspects of internal free convection. Figure 18 illustrates how the horizontal vortices bend down at the side walls to influence the temperature field.

The preceding examples have concerned flows in enclosures of reasonable aspect ratios in which only a few cells of motion exist. Liakopoulos et al.[85] studied the convective flows in tall cavities using the spectral approach (by way of the NEKTON program). Their interest is in examining the multiplicity of cells which result from the unstable flow in tall cavities and in simulating the flow over heat sources which represent electronic components.

To and Humphrey[86,87] studied mixed free- and forced-turbulent convection in heated cavities to simulate solar receivers and heated rooms. Their analyses were based upon a variable physical property code to couple the momentum and the energy equations, and both k-ε and algebraic turbulence models. Abrous and Emery[88] and Silva[89] used a similar k-ε model to simulate the combined effects of local heating and infiltration into a closed cavity. Figure 19 shows how the local shelf separating a cold window and heater affects the vortex located adjacent to the surface heater.

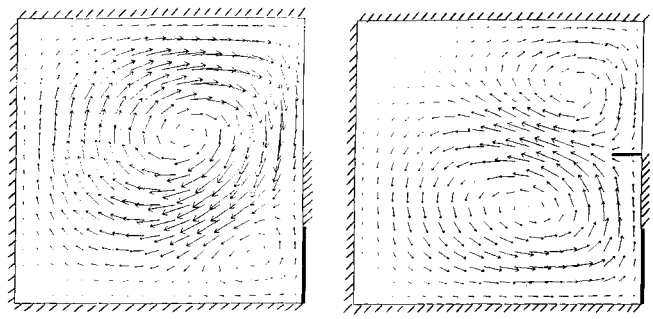


Fig. 19 Effect of a horizontal partition placed directly above a simulated wall heater.

Bench mark calculations of laminar-free convection have been summarized in the workshop results presented by deVahl Davis[90] and we feel that algorithms for such laminar flow are mature. By contrast, little is known about the correspondence between the different methods of computing turbulent-free convection, particularly with the added complexity of the need for low Reynolds number turbulent models. A workshop on turbulent natural convection in a square cavity is to be held at Delft University in 1992.[91] This should go far in defining optimal algorithms and providing a turbulent flow bench mark solution.

Mesh Generation, Adaptive Grids, and Solvers

Finite-difference, volume, and element methods all require the discretization of the domain into a finite number of nodal points. The different algorithms essentially make use of a Jacobian transformation from the physical coordinate system to a local computational coordinate system. Finite-difference and volume methods normally employ orthogonal grids, as the transformation is carried out in the global domain by

making use of grid metrics. The isoparametric finite-element method performs a local transformation at the element level. This relaxes the conditions on orthogonality, but restrictions on maximum element aspect ratio and distortion still exist. Although the finite-element method can utilize unstructured grids, most analyses use blocks of structured grids with special interface elements or connectivity. Such grids are usually based upon an I–J logic sequence which requires that no I or J line disappear or be created within the block. Multiblock, orthogonal, structured mesh generation in three dimensions is currently available in a variety of programs (e.g., the EAGLE code, Thompson,[68] and GRIDGEN of Steinbrenner[92]).

A structured grid implies that a fixed number of nodal points along each mesh line is maintained. This provides an implied neighbor nodal point location that is useful in finite-difference and volume algorithms when forming difference formulae. An unstructured grid implies no constraint on the location and numbering of the mesh points (Fig. 20). Because of this, a mesh connectivity must be provided for each element or volume of the grid. For unstructured mesh generation, triangularization algorithms are currently capable of generating two- and three-dimensional meshes in multiply connected domains. Unstructured quadrilateral meshes have recently become available in the IDEAS SUPERTAB program and the QUADMESH algorithm of Talbert and Parkinson.[93] Refinement of these meshes often requires lofting and smoothing algorithms for parts with sharp curvature. Such meshes usually interface to CAD programs for extraction of geometric and material data.

Most FD, FV, and FE programs guarantee at most C_0 continuity between elements or volumes and depend upon mesh refinement to produce C_1 and higher continuity (this is true even of p and spectral finite elements which possess very high internal accuracy and continuity). Some finite-element programs have attempted to provide C_1 continuity, but the execution costs and resulting accuracy are not much different than those obtained by mesh refinement. Such mesh refinement—usually termed h-adaptive meshing—has become an important trend as an automatic feature of integrated solvers. These adaptive mesh algorithms attempt to minimize the error in a numerical solution by refining the mesh in areas that require a fine mesh and making it courser where such refinement is not needed. Wieting[94] describes an adaptive method which measures the need for adaptation by estimating second derivatives throughout the model. The refinement is done by solving an elliptic equation with the second derivatives as a forcing function. Figure 21 illustrates how the refined mesh produces better results. Note that the structured grid away from the wall has been replaced by an unstructured grid, but near the wall the structured grid has been retained, even though it is significantly densified. Interestingly, the number of nodes is only slightly reduced. Figure 22a shows the adaptive grid used for shock reflection calculations, and Figure 22b displays the resulting shock profile.[95]

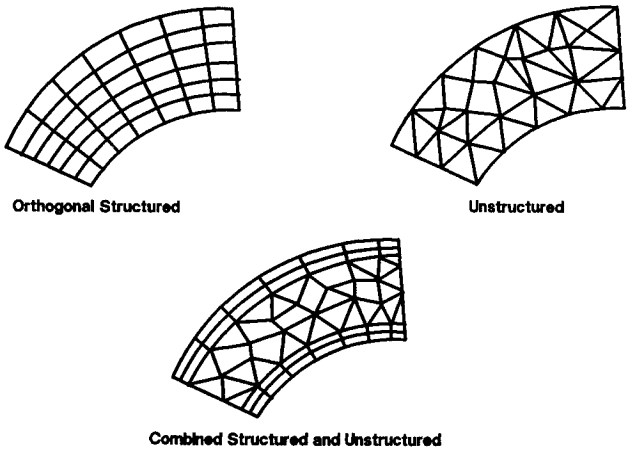


Fig. 20 Methods for discretization of a domain.

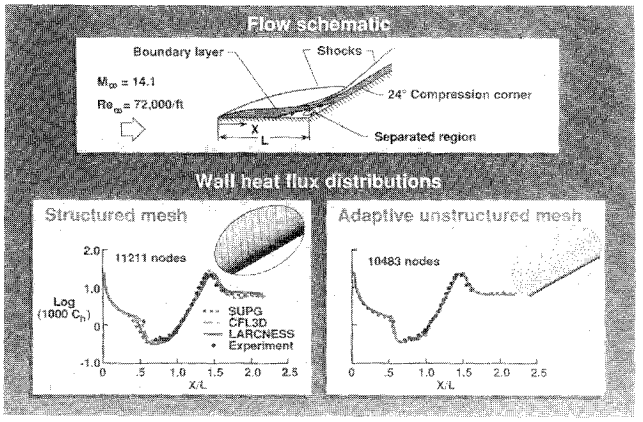


Fig. 21 Two-dimensional unstructured mesh solvers calibrated on compression corner flow.

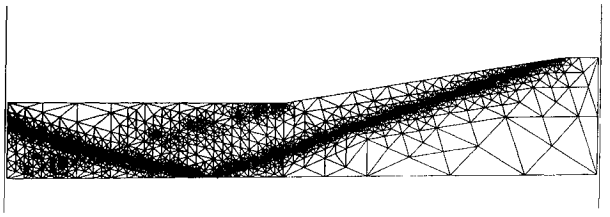


Fig. 22a Adapted mesh plot.

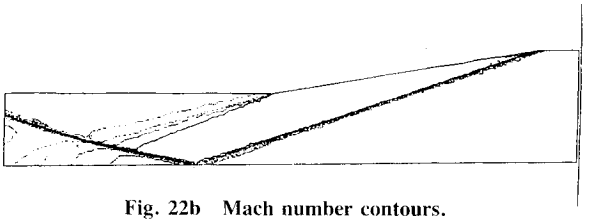


Fig. 22b Mach number contours.

Mesh refinement in structured grids is, in general, not as efficient as in unstructured grids. This is due to the fact that the mesh refinement must be carried out throughout the block in order to maintain the I-J logic structure. This leads to an unnecessary increase in the number of nodal points unless hand-tailoring of the blocks is done. The solution to global refinement is to use local grid refinement in order to resolve the local flow scales more efficiently. Figure 23 illustrates a mesh that is refined locally at the regions of shock waves and shear layer. In this approach, special consideration must be paid to the interfaces between the different blocks. Structural computations frequently make use of interface continuity enforced by "slide lines," which, while appropriate to Lagrangian grids,[96] are frequently inexact and not fully developed for fluid flow.

The generality of unstructured grids has led to methods to convert such grids to resistance capacitance values for use with finite volume thermal analyzers. Hartvigsen and Cochran[97] used the mathematical equivalence of finite-element and finite-volume conductivities to generate three-dimensional models. This hybrid approach allows the use of unstructured meshes for detailed component analysis coupled with the flexibility of general thermal analyzers (such as SINDA) to treat the coupled fluid/solid thermal problems.

Adaptive modeling can be used effectively with adaptive mesh refinement. Figure 24a illustrates the different flow regimes postulated to exist about a solid rocket motor drag skirt and Fig. 24b illustrates the adaptively generated grid.[98] In this case, the choice of equations was made by the user, not by the program. Ideally, while the program is refining the mesh, it should be able to decide what type of modeling should be

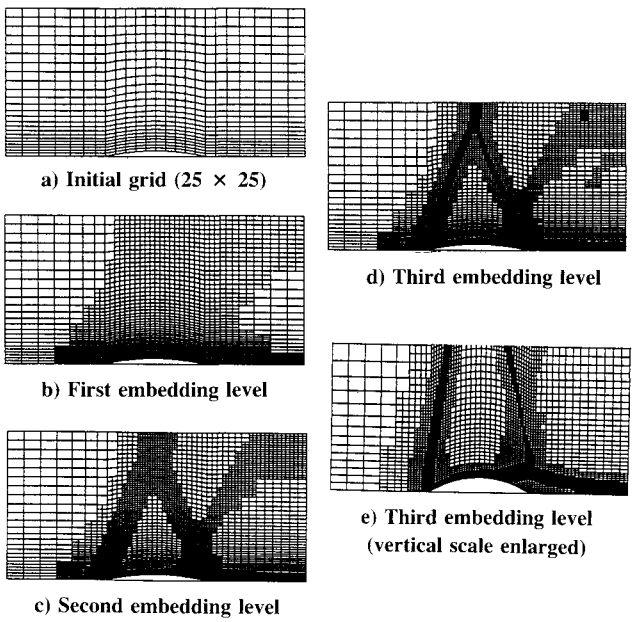


Fig. 23 Adaptive grid evolution for circular arc cascade.

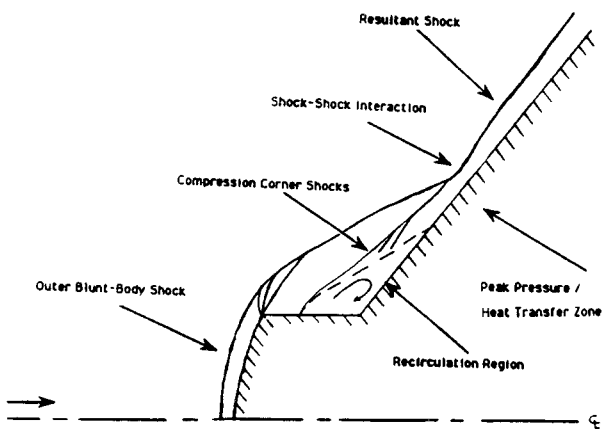


Fig. 24a Schematic of the flow around the solid rocket motor + flare.

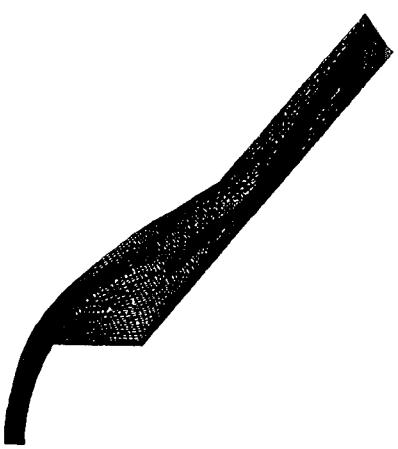


Fig. 24b Adaptively generated grid.

done within each region since the two decisions can be expected to interact. Such adaptive modeling has been done by Sindir[99] for NASP in which the program automatically chooses between Euler, Navier-Stokes, finite rate chemistry, and frozen chemistry equations. Excellent examples of the use of adaptive grids can be found in the modeling of gaseous turbulent reacting flows in combustors of complex shapes.[100]

Turbulence Modeling

Considerable effort originally began during the 1960s and 1970's to develop higher order turbulence closure models, in lieu of mixing-length models in use since the early 1900s. Some improvement has been seen in the use of higher order turbulence closure for a few problem classes, but the complexity and trouble involved in using such schemes raises questions about their usefulness for general problems.

Algebraic relations or "zero-order" models, have seen widespread use and are still in use today. The basis of these models is rather straightforward: the local rate of production of turbulence and the rate of dissipation are approximately equal. Although such models do not account for the advection of turbulence, i.e, the spatial distribution of the flow velocities, they are mathematically simple and can be easily incorporated into numerical codes. One of the most widely used models today is that of Baldwin and Lomax.[101] Based on previous works by van Driest,[102] Klebanoff,[103] and Cebeci and Smith,[104] an inner and outer set of relations are used to define a mixing length and a turbulent viscosity. Many of the NASA-based finite-volume codes currently being used for NASP use this model.

The next level of closure deals with the solution of the turbulent kinetic energy equation along with an empirical relation for the dissipation of turbulent kinetic energy. Such models saw some popularity in the late 1960s and early 1970s; some meteorological and geophysical simulations employ these "one-equation" models for transport calculations.

By far, the most prevalent type of turbulent closure is the "two-equation" model advocated in the early 1970s, frequently referred to as the k-ε model. Many industrially oriented problems have been successfully simulated by using the two-equation approach. In this form of closure, the turbulent kinetic energy and the dissipation term are modeled in their primitive form, i.e, the partial differential equations are solved numerically. This higher form of closure allows one to account for the past history of the flow and has been shown to yield more accurate solutions to a wide class of problems. However, as one proceeds to resolve higher forms of correlation terms, it turns out that more empiricism must also be used (e.g., to account for triple correlation terms and dissipation). The literature is full of articles reporting the slight alteration of empirical constants used with two-equation models. One of the best studies of this approach is that of To and Humphrey[85,86] who compared the k-ε and the algebraic stress models and investigated the effects of variable density. They concluded that the algebraic stress model did not provide enough increase in accuracy to justify its additional complexity.

An excellent discussion of the use of the k-ε for turbulent reacting flows is given by Correa.[100] The discussion includes comments about curvature, swirl, nonisotropic eddy viscosity, algebraic stress models, countergradient diffusion which has been observed in flames, pressure gradients, and the time-scale problem of scalar turbulence.

Moving up the closure chain, one then addresses the task of resolving the double correlation terms—or Reynolds stresses—themselves from governing partial-differential equations. Such efforts now require the solution of multiple equations; e.g., to resolve recirculating flow, one needs to solve for three shear stresses, three normal stresses, and ten triple correlation terms, in addition to the momentum and energy equations (and species concentration, if needed). Application of this form of closure is somewhat rare and requires considerable computer resources to model even the simplest of problem configurations. However, results are usually dramatic and clearly show improved accuracy in resolving regions of intense shear and recirculation. Some effort is now underway to incorporate second-order closure in modeling atmospheric motion over irregular terrain,[105] and three-dimensional flow around submarines.[106] On the other hand, both the second-order and the two equation models obtain length scale information from the dissipation rate equation. This limits the

accuracy of the models and may detract from more sophisticated and more difficult computational models.

Finally, some effort is underway to employ direct numerical simulation of all the important scales of turbulence including the time-dependent large-scale eddy motion. Such simulations of this wide spectrum of fluid motion require extensive supercomputer resources and generally utilize spectral/pseudospectral methods to solve the full form of the Navier-Stokes equations. Although examples of direct simulations in the literature are rather idealistic, the insight and corroboration with stochastic turbulence theory are rather good. Much of this work is discussed by Gottlieb and Orszag[107] and Canuto et al.[61]

One of the most important points to consider when numerically simulating turbulent flow is grid resolution. In order to accurately resolve turbulent flow near a surface, a grid point must lie within the laminar sublayer (i.e., within $y^+ \leq 5$). Much effort is generally spent in developing a good mesh, therefore, considerable patience and a good mesh generator are required.

Incorporation of chemistry with turbulence into the overall solution scheme—and the subsequent interaction with the flow process—is the ultimate challenge. In high-speed flows, the assumption of a perfect gas is no longer valid due to the high temperatures associated with the flow. As a result, the air molecules dissociate and ionize. Therefore, chemistry becomes particularly important if one is to obtain a reasonably accurate flow solution. The problems associated with chemistry and hypersonic flow have become particularly apparent in the NASP effort. For supersonic flows several approaches have been used with success and are currently being advanced to hypersonic flows.

One approach is based on simple equilibrium and finite-rate chemistry models with finite-volume (Lagrangian-based SALE) techniques as described by Pratt[108] and Kashiwa.[109] Although limited to inviscid two-dimensional problems, results agree with experiments for limited species reactions. Figure 25 shows the predicted results for a strongly overdriven (superdetonative) case. The agreement between the experiment and the predictions is taken as proof that the chemistry and shock modeling are correct. When the velocity almost matches the Chapman-Jouget speed, high-frequency oscillations exist behind the combustion front. Figure 25b does not show these oscillations. Pratt has speculated that these instabilities arise at the stagnation point and the mesh refinement at this point was inadequate to accurately represent them. If so, this is an ideal opportunity for adaptive grid refinement. Wilson[110] has used a second-order spatial discretization and an adaptive grid procedure developed by Gokcen[111] which assigns different weights to the temperature, chemistry, and pressure to obtain excellent agreement with Lehr's[112] seminal experiments. When adaptive grids are used, the flow solutions are fairly accurate in resolving shocks as demonstrated by Shuen and Yoon[113] in modeling shock-induced combustion using implicit flow solvers; the computer codes are based on the RPLUS family of flow solvers, and have been optimized for solution on Cray class machines.

A second approach utilizes the finite-element method with a two-equation turbulence model and finite-rate chemistry. Eighteen species equations based on hydrogen-oxygen reactions have been successfully calculated by Chung and Kim.[41] Incorporation of adaptive unstructured grids are under development utilizing linear triangular elements. Parallelization of this code should greatly improve its performance.

Turbulence is extremely complex. Available approaches presently use various types of closure models ranging from simple mixing length schemes to sophisticated Reynolds stress equations. Direct simulation for general configurations are not yet achievable; also, a universally accepted turbulence closure model is not yet available. Considerable effort is still needed to resolve turbulence in a tractable manner for a wide range of problems; many existing models work well on some specific flow configuration but work poorly on others. For the present, close collaboration of turbulent flow modeling with experimental verification on various classes of problems appears to be necessary.

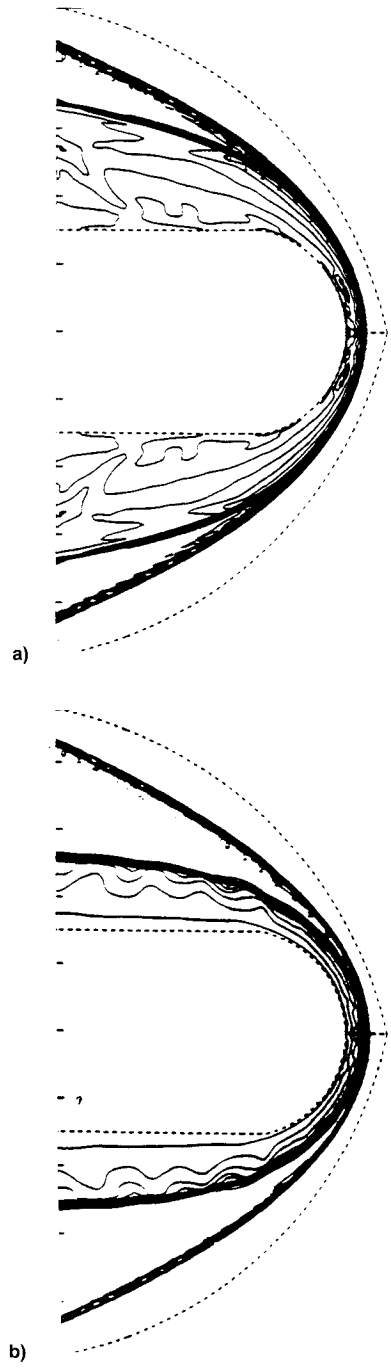


Fig. 25 Combustion behind a bow shock: a) overdriven ($W > D$), and b) nearly matching ($W \approx D$).

If one wished to model a three-dimensional turbulent compressible flow with chemistry using second-order closure, a total of 40 governing equations would have to be solved numerically. Assume the problem domain requires approximately 3×106 nodes (to insure a very fine grid in the boundary layer), and a time-step of at least 10^{-6} s. Likewise, assume at least 18,000 time-steps are needed to converge to a steady state. Using a supercomputer with a 200 Mflop capability, the calculation would require nearly a year to reach steady state. On the other hand, using a 2000 node parallel computer with 200 Gflop performance, the solution could be achieved within 7 hours.

Sparse Matrix Solvers

Sparse matrices occur when solving engineering problems involving heat transfer, fluid flow, acoustics, some structural analysis, and related nonlinear problems. The equilibrium solution of these boundary-value problems generally requires the solution of large systems of simultaneous equations and the overall solution speed of many programs often depends on the efficiency of the matrix solvers used to solve elliptic equations. A number of good banded symmetric matrix solvers for a wide class of machines exists in the literature. However, in cases where the matrix is nonsymmetric such solvers are relatively rare and not easily available.

In many instances involving finite-difference/finite-volume simulations, tridiagonal (ADI/time-split) or pentadiagonal (strongly implicit) algorithms can be efficiently utilized. However, when the mesh is unstructured, particularly in finite-element techniques, such simplifications are not amenable. These sets become very large and require large amounts of core memory. In addition, the matrix is nonsymmetric and ill-conditioned. In general, the matrices become quite sparse and require efficient sparse matrix solvers to yield timely solutions. In most finite-element models currently in use today some form of Cholesky-skyline decomposition technique is employed. Careful attention is generally paid to optimizing this solver for the computer being used since it is easy to fill memory even when the matrix is less than 1% dense (Ortega and Voigt[114]). Hasbani and Engelman[115] demonstrated the use of block-out of core solvers for column storage methods. Using asynchronous *I/O*, the problem can run as fast as if all of the matrix is in memory.

Frontal solvers have been very successful in overcoming these restrictions.[116] Duff[117] claims performance values near 80 Mflop using this technique. The frontal solver concept has also been extended to coarse grain parallel methods by Benner et al.[118] The use of substructuring (creating diagonal block matrices) and block/frontal techniques also gives good performance and can be parallelized. With the recent introduction of new interative algorithms for nonsymmetric matrices the possibility of using sparse storage is being examined.[119] The drawback to this method for the fully coupled solution algorithms is the need for preconditioning. The projection methods provide better conditioned matrices in that the Poisson equation is symmetric and positive definite and the momentum equation (although nonsymmetric) does not have zeros on the diagonal. Mixed implicit-explicit techniques which treat some elements implicitly yield reduced global matrices.[120] In contrast, purely explicit methods dispense entirely with the need for sparse matrix solvers[45] since they require only the manipulation of the dense element level matrices. The structural counterparts of these are the dynamic codes such as HONDO[121] and DYNA[122] which use finite elements to form the element matrices but solve for the dynamic structural response using a time-centered (i.e., explicit) approach.

An interesting commercial matrix solver has recently appeared which yields fast solutions on a variety of low-end workstations, as well as Alliant and Convex parallel machines. The solver, called fast matrix solver (FMS)[123] is partially written in machine language and is structured to automatically vectorize and/or parallelize, depending on the computer. Also, overlays and reduced matrix operation are employed to shrink storage requirements. By utilizing FMS one can greatly reduce the number of FORTRAN statements required to assemble and store matrices.

Preconditioned conjugate gradient methods have recently reappeared as viable alternatives to Gaussian elimination methods. First developed by Hestenes and Stiefel,[124] the method has been shown to yield impressive solution speedup for certain problems. Although iterative in nature, they are actually direct methods which converge to the exact solution in no more than N steps for systems of size N (assuming no rounding error). However, with rounding error this no longer occurs and the method lost favor until recently. For a certain class of sparse problems (elliptic equations), conjugate gradient methods converge in less than N iterations. The tricky part of using conjugate gradient methods is in establishing the condition number (or preconditioner); the smaller the condition number the faster the convergence. Use of the incomplete Choleski conjugate gradient methods are fairly successful.

Commercial Software

Numerous commercial codes are available for structural analysis and conduction heat transfer; many of these companies have been in existence for over 20 yr, and provide reasonably priced, user-friendly software for a variety of machines. Commercial software packages for CFD and related nonlinear problems are not so prevalent. However, a few of the existing codes appear to have wide appeal and a good share of the marketplace. Likewise, several NASA-based CFD codes are well documented, work well (for the intended problem class), and can be obtained either directly from NASA or commercially (at low-to-moderate fees) through COSMIC. Nearly all the commercially available codes have been bench marked on various problems and evaluated on various classes of computers.

All CFD codes use one of several methods for solving the equations of motion and energy. Certainly each software package has its own merits and limitations; however, no one package appears to be superior. All the computer codes utilize either finite-difference/finite-volume or finite-element methods to discretize the problem domain into a set of grid points; these meshes are either structured or nonstructured, depending on the solution strategy. Once the mesh is constructed (which in itself can be a formidable task) the partial-differential equations are reduced to a set of algebraic equivalent equations which are solved either iteratively or by direct techniques.

A few of the well-established CFD codes presently available utilize the finite-volume method. The reasons for using the finite-volume method lie in its ease of use, integral based conservation properties, and the requirement of low levels of smoothness for the flow variables. Such methods have been around for many years and continue to be used in both incompressible and compressible flows with shocks. Two of the more popular codes today are PHOENICS and FLUENT. Both models now utilize boundary-fitted coordinates (BFC) to model irregular domains, and offer several time-step algorithms for solution of the resulting equations. In addition, both models employ mixing length, two-equation, and algebraic stress models for turbulent closure. PHOENICS can be used to solve either incompressible or compressible flows with heat transfer and combustion. A new compressible code known as RAMPANT is being prepared by the developers of FLUENT; FLUENT is an incompressible code much like PHOENICS—in fact, both codes stem originally from work done by Gosman, Launder, and Spalding (see Patanker[78]), and their colleagues at Imperial College in the 1960s and 1970s to develop fluid simulation programs which included turbulence. RAMPANT uses an unstructured triangular-based grid (analagous to a three-node triangular finite-element) with adaptive features; however, the solution proceeds as though it were a finite-volume method. The code will be available for workstation, mini-supers, and Cray class machines by mid 1991.

FLOW3D is a finite-volume-based code originally developed at Los Alamos National Laboratory by Hirt et al.[125] This code solves two- and three-dimensional incompressible flow problems and includes the ability to handle free surfaces. The code cannot account for irregular domains other than by employing staggered orthogonal blocks in a structured grid. If the grid is fine enough, solution accuracy is not overly compromised. The source code is available for purchase.

Computer Hardware Trends

An increasing interest in the use of computers which utilize pipeline or parallel architecture has occurred since 1970. Early efforts were spent on development of parallel algorithms in the mid 1960s, but the machines did not materialize until the 1980s. As a result of this lag, vector and high-speed sequential logic developed as an alternative means for solving very large scientific problems. The first Cray-1 was delivered to Los Alamos National Laboratory in 1976.

Advances in integrated circuits and materials since the Cray-1 have led to a plethora of "supercomputer" class machines. We now have the Cray-2 and Cray-YMP machines with nearly gigaflop computing power and huge storage capabilities, along with rather expensive price tags; the upcoming Cray-3 is proposed to be significantly faster than the present class of machines. Likewise, smaller computer companies, e.g., Alliant and Convex, have developed "mini-supercomputers" which take advantage of smaller footprints, air cooling, and parallel/vector architecture to achieve nearly comparable performance to the Cray machines (Fig. 26). In a similar vein, parallel oriented companies such as Ncube, Masspar, Intel, and Thinking Machines, have declared that massive parallelization is the way to higher performance while maintaining lower cost. The merging of these two approaches appears questionable for now, but will likely occur as new designs and technological advances develop in the future. From an engineer's point of view, the most significant change has been the development of desktop workstations with color graphic output for visualization. Figure 27 gives an idea of current capabilities and prices.[126]

By the year 2000, it is anticipated that there will be an increase from today's 10 million transistors on a chip to a billion on a chip—with the cost essentially unchanged. Likewise, a gigabit chip with a nanosecond access time is forecast which will consume less than a watt of power. Both Japan and the United States are actively pursuing research in these new technologies.

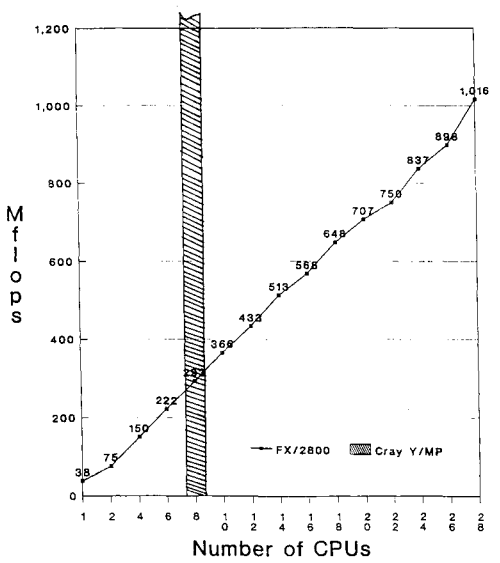


Fig. 26 Comparison of Alliant FX/2800 and Cray Y/MP performance.

Price Range	Representative Computer Systems	LINPACK Benchmark (n = 100) (mflops)
$5-10,000	33 MHz 486 PC Clone	1.4
	Sun IPC	1.7
$10-20,000	Sun SPARCstation 2	4.2
	IBM RISC System/6000-320	9.0
$100,000	Stardent 3020 (2 proc.)	11.0
$1,000,000	Convex C-220 (2 proc.)	21.0
	Alliant FX/2800 (8 proc.)	22.0
$10,000,000	Cray Y-MP/832 (8 proc.)	275.0

Fig. 27 Price performance of current computer systems (n is the number of equations and mflops is millions of floating point operations completed per second).

In the early days of computing, software advances were constantly demanding more and more powerful computers. Today, computer architecture is changing so rapidly that once a system is purchased it is largely obsolete. For software which advances more slowly it is not uncommon that a software package must be rewritten to take "advantage" of a specific hardware platform. Even a simple piece of software written for the PC must undergo modifications as it migrates upwards in machine class to the Cray. If one wishes to optimize the performance of the code on a parallel computer the code will likely have to be rewritten from scratch.

Many feel that the bigger the computer, the more powerful the computer. A sequential computer consists of a memory unit, a processor, and some sort of communications system. The processor fetches a sequence of instructions from memory and each instruction is decoded and carried out in specified operations in registers or memory locations with addresses contained in the instruction. This results in a step-by-step algorithm common to most programming languages and logic in algorithm development. The simplicity and universality of the method make it very appealing; such methods are employed in PCs and workstations.

The concept of building larger machines involves several arguments. First, the cost of such a computer is roughly proportional to the square root of its speed.[127] Therefore, a computer four times faster would cost only twice as much. Secondly, assume that a total of N jobs are in various stages of execution in a pipeline of processors. An N-stage pipeline has the same throughput as the single processor, but N times longer response time. Although the pipeline achieves parallelism it is less responsive than an equivalent single processor. Alternately, there is a limit to the amount of computing power which can be squeezed into a box. The speed-of-light is 3×10^8 m/s in a vacuum; signal transmission speed in silicon is about 3×10^7 m/s. A chip about 3 cm diam can propagate a signal in about 10^{-9} s. Since a nonparallel floating-point chip can perform at most one operation during one-signal propagation, the chip can support about 10^9 floating point operations/s. Therefore, single-processor machines are not likely to exceed 1 gigaflop.

An $N \times N$ matrix multiplication takes about N^3 operations. A problem twice as large requires a processor eight times faster to complete the calculation in the same time. By comparison, a processor twice as fast can multiple two matrices of size $2^{1/3}N$ in the same time, i.e., about 25% larger. Hence, linear growth in problem requirements results in superlinear increases in computing power to execute in the same time. For example, a 100,000 × 100,000 element matrix requires 160 gigabytes to solve the matrix. Similarly, one must also consider the role of job partitioning whereby jobs are partitioned into sequences of components (pipelines). It is now well known that parallel decomposition can lead to a machine of the same throughput and response time at a fraction of the cost of a single processor—assuming that the job can be partitioned into independent (equal) pieces.

All parallel computers use multiple processors. The major differences in parallel computers lie in their classification according to the relationship of memory to processors and number of instruction streams.[128] The relationships between memory and processors are known as distributed memory and shared memory. Likewise, multiple instruction, multiple data (MIMD) and single instruction, multiple data (SIMD) define the type of instruction technology. In a MIMD system, the processors work on separate instruction streams (tasks) at the same time. In SIMD, the processors all operate on a single instruction stream simultaneously. Synchronous behavior is automatic in SIMD machines; in an MIMD machine the syn-

chronization must be programmed in. Likewise, MIMD machines make use of either shared or distributed memory while a SIMD machine utilizes only distributed memory. The iPSC/2 and iPSC/860 computers built by Intel are examples of MIMD machines; the Alliant FX/Series of computers are SIMD-based. Farhat[129] provides an overview of how these different architectures affect the implementation of the finite-element methods.

One of the current barriers to more widespread use of parallel computing lies in the software requirements. Much of the older computer languages, such as FORTRAN and C, execute one statement at a time. Thus, one needs to direct and coordinate the use of the parallel processors within the program. Considerable efforts must generally be exerted in rearranging a computer code to maximize the use of all the processors. Alliant, for their "coarse-grained" parallel machines (i.e., a machine consisting of anywhere from 4 to 28 processors) uses a clever compiler which allows the use of existing sequential code by embedding "directives" within the code to parallelize various parts. This permits the user to "break-over" into parallel computing without undue software hurdles. Unfortunately, such software doesn't as yet exist for the "fine-grained" (massively parallel) machines.

Much of the current research into parallel-programming languages is aimed at helping the programmer to code problems without having to delve into concurrency processes (concurrent executions) and how parallel processes communicate interactively. New languages have been developed such as Occam and Parlog which assist in parallel programming; unfortunately, such languages vary widely in style. On the other hand, one notices the advent of commonality among scalar machines in the operating language Unix; Unix allows one to run a code on a variety of computers with commonality of statements.

While the race for increasingly faster machines still exists between vector and parallel machines, it is the parallel machine that will ultimately win out. Vector machines now function at 10^9 floating point operations/s, and will reach 10^{10} before the year 2000. Massively parallel machines already close to 10^{10} in performance will reach 10^{13} flops by the year 2000. To illustrate, suppose that a computer were built consisting of 4000 interconnected 25-megaflop processors. The machine would have a peak computing power of 100 gigaflops. Compared to a 100 megaflop machine, a 10-h job would take only 30 s; a 100-h job would take only 6 min. Likewise, vector machines are 10–15 times more expensive than parallel processors. Cray is currently working on a new machine which will incorporate massively parallel processors with a vector approach but will utilize reduced instruction sets.

Parameter Estimation and Sensitivity Analyses

The usual research paradigm is as follows: A complex experiment is designed and run. A simulation model is created, the simulation performed, and the results compared. The basic premise is that if the model agrees with a large number of measured results (presumed to be independent variables, under a number of different experimental protocols), then the basic model and its parameters are taken to be correct. If agreement is not found, then either the model parameters or the model itself are changed until agreement is achieved, which may not happen. Unfortunately, the measured quantities or the imposed boundary conditions may not be those that can be easily manipulated in the model. For example, heat fluxes may be prescribed in the neighborhood of a poorly defined and highly conductive material, leading to significant and ill-defined losses from the system. The simulation will be done by imposing a well-defined flux and trying different loss mechanisms until agreement is found. Because these loss mechanisms may be poorly understood, there is a natural reluctance to quantify them in a way that the model can utilize their characteristics. If agreement is found, whether it is fortuitous or not is generally unknown.

What must be done is to design the experiment in conjunction with the simulation. This requires that we move away from deterministically defined experiments and modeling to procedures that account for uncertainties in properties and experimental conditions. The inverse heat conduction method of Beck and Arnold[130] is one such approach which handles the uncertainties while estimating system parameters.

Another technique is to characterize the uncertainties as stochastic phenomena. The analysis is performed by using either a statistical or a nonstatistical approach. The statistical method deals with Monte Carlo simulations using different sampling techniques. Repetitive tests are conducted in which one or more parameters are varied and the resulting response of interest is statistically analyzed. The nonstatistical method, unlike sampling, is based upon an analytical treatment of uncertainty. For nonlinear systems, perturbation methods are the most commonly used. One such perturbation method is the first- and second-order–second-moment analysis which can be used for uncertainty modeling. This method determines the first- and second-order derivative of the responses with respect to the system parameters. These derivatives are in effect the sensitivities, thus this method is often referred to as sensitivity analysis. This approach can be conveniently incorporated into finite-element programs. One of the special features of this method is the ability to introduce correlations between physical parameters. For example, one does not impose independent heat transfer coefficients over the surface of the structure, but recognizes that a change in a value at one spatial location often implies a change at another location.

As an example, a preliminary study was conducted to estimate the temperature sensitivities of a thermal protection system experiment.[131] A typical TPS panel is shown in Fig. 28. The question is whether the temperatures measured at the points A, B, and C were sensitive to the experiment. If not, then agreement between simulated and measured temperatures is of little value. A transient analysis was carried out to determine the sensitivity to material conductivities and surface emissivities. Figure 29 illustrates a typical estimate of temperature sensitivity to the emissivity. We see that the temperature is very sensitive when the emissivity is small, and negligibly sensitive when it is large. From the figure, a match

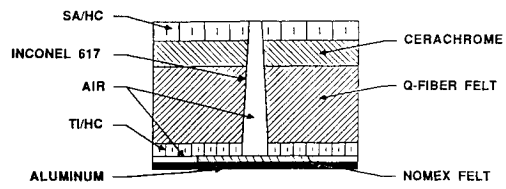


Fig. 28 Cross section of a thermal protection system (TPS) panel.

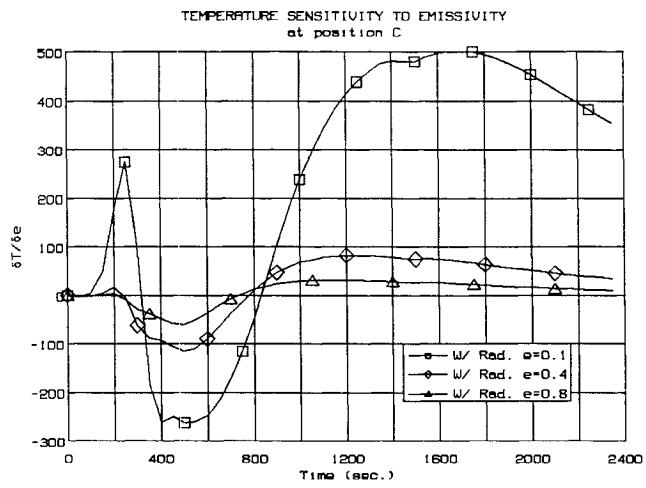


Fig. 29 Time history of temperature sensitivity to emissivity.

between measured and predicted temperatures at 800 s implies little about the accuracy of the stimulation model.

Conclusions

We see four trends from the topics described herein and in other published papers: 1) detailed computations of complex problems utilizing detailed models; 2) the use of commercial software by industry and academia; 3) graphical display for visualization and detailed analysis; and 4) a change in the philosophy of attacking coupled problems. Each of these trends depends upon increased computing power and each has a positive and negative side.

Detailed Computations of Complex Problems Utilizing Detailed Models

We expect to see many more complicated problems—in terms of geometry, coupled effects, and models of the physical processes—treated to a degree of detail unheard of just a few years ago. On the negative side, many of the simulations will be poorly constructed and carried out. Often the computations will be made perfunctorily, and the results will be presented as sets of data points with little attention paid to extracting useful information which can explain the physics of the problem. This is a particular danger in the highly nonlinear problems that are likely to be treated. Frequently, we already see solutions in which the computations are the aim, not the solution to the physical problem posed. With increased computing power, the need to exploit the mathematical modeling found in pertubation theory, linearization, and asymptotic expansion will decline and the physical insight that these approaches gave will be absent from much of the reported analyses.

On the positive side, this power when used intelligently will reveal insights obtainable in no other way. The work of Chenoweth and Paloucci[76] in using highly accurate solutions to develop maps of free convection flow behavior and of Humphrey and To[86,87] in studying turbulence models is representative of the best use of computations. Both of these relied heavily upon a deep understanding of the problem examined.

Use of Commercial Software by Industry and Academia

With carefully crafted programs which are well-supported by technical staffs, we can expect to see more analyses done by industry and by academic researchers with commercial software. The desire to treat larger and more difficult problems, with the associated attention needed to be paid to vectorization, parallelization, *I/O*, and graphical output for interpretation, will make these programs very attractive. With the exception of unique problems which require unusual approaches, we anticipate that writing individual programs will not be efficient. Debugging and validating such individual codes consumes a major fraction of code development effort, which can be better used in studying the problem, not the code. Commercial codes will become computing platforms onto which specialized models and techniques can be crafted. User-defined models of turbulence and radiative properties, e.g., will be inserted as object modules into these platforms. Such commercial code will eliminate the need for input and output processing and will provide robust nonlinear solvers.

Of course there will be a flip side to this. Unlike the ubiquitous calculator, whose every step is well-documented and verifiable, such large commercial codes will contain hard coded numerical and physical approximations. Users will have to be intimately familiar with these limitations and how they may affect the solution or interact with user-defined object modules. Documentation of the codes, both of the theory and of the processing, will have to be complete and exact. Users will need to spend significant amounts of time becoming familiar with the capabilities and peculiarities of the codes. The tendency of a small number of people to become "gurus" while the majority become "code jockeys" will increase.

Graphical Display for Visualization and Detailed Analysis

One of the greatest and most welcome advances in numerical computation has been the emergence of high-quality graphical display of the output. Such output ranges from displaying countors or vectors to the complete animation of flow and temperature fields. Modern graphic terminals have outstanding resolution and a wide range of color renditions. Software libraries are available for users who wish to develop their own graphical displays and commercial codes almost always come with graphical output. Almost every technical trade magazine contains numerous ads for finite-element and finite-difference programs which are highlighted by reproductions of their graphical output. However, it is interesting to note the implications of the differences: *Mechanical Engineering*, the monthly ASME publication, contains many full-page ads for commercial programs; on the other hand, *Aerospace America*, the monthly AIAA publication, contains almost no such ads. Why the difference? We suspect that most CFD analyses are still done with home-grown codes, with only a few commercial codes in current use, whereas, the more general thermal/fluid problems are treatable by commercial finite-element codes which are more friendly to the general user. Aerospace problems usually involve high-speed flows which are advection dominated, while the lower-speed flows associated with internal flows are a more balanced mix of advection and diffusion, particularly for turbulent flows. Presently, the finite-element methods are of limited accuracy and computational speed for advection dominated flows. There is considerable effort currently devoted to developing finite-element methods for very high Reynolds numbers and high speeds and we can expect to see more commercial codes with visualization available soon.

Change in the Philosophy of Attacking Coupled Problems

This area may represent the most fundamental change in computing practices since it applies in the most direct way to the analysis of experiments and the design of actual systems. Its use will require significant changes in codes and in the information needed for input. So much current computation takes place under the assumption of a precise knowledge of properties and boundary conditions, that a change to a statistical prescription of these will require entirely new data banks of information. This will be particularly true if spatial and temporal correlations are to be used.

Overall, we believe that the increased hardware and algorithmic computing capabilities show much promise and that we will be able to use computing for engineering design and not just to further study numerical solutions. Meaningful commercial and pedagogical decisions will be made on the basis of these numerical solutions.

Acknowledgments

We thank the individuals who shared their computing experiences with us and with whom, over the last several years, we have had many enjoyable and insightful conversations about the value and the future of engineering computations.

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