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Review

Fluid dynamics in Group T-3 Los Alamos National Laboratory ☆ (LA-UR-03-3852)

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Abstract

The development of computer fluid dynamics has been closely associated with the evolution of large high-speed computers. At first the principal incentive was to produce numerical techniques for solving problems related to national defense. Soon, however, it was recognized that numerous additional scientific and engineering applications could be accomplished by means of modified techniques that extended considerably the capabilities of the early procedures. This paper describes some of this work at The Los Alamos National Laboratory, where many types of problems were solved for the first time with the newly emerging sequence of numerical capabilities. The discussions focus principally on those with which the author has been directly involved.

Keywords: Computational fluid dynamics; History of computing; Turbulence; Multi-field flow; Strong distortions; Incompressible flow; Relativistic fluids

1. Introduction

The year 1953 saw the arrival of the first big commercial computers at the Los Alamos Scientific Laboratory (now the Los Alamos National Laboratory). My employment in the Theoretical Division during that same year gave to a group of us the opportunity to become pioneers in the largely unexplored subject of numerical fluid dynamics. Several years before my arrival, the MANIAC computer had been developed in our Division, paving the way for the innovative creation of important new features of both hardware and software during the initial stages of the computer revolution, but I was not a part of that project.

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The first of the large computers to arrive here was the Model 701 from the International Business Machines (IBM) Corporation. This machine was great and marvelous for all of us and we were very excited to follow all sorts of exploratory pathways for the development of new techniques to solve hard problems. The 701 was a big monster; it occupied a huge room filled with cathode-ray tubes that contained the memory of 2048 36-bit words or 4096 16-bit halfwords. It was cumbersome, and it had troubles, but we loved it. We would come at any time in the night or day to run it ourselves. It was a hands-on operation. It was something that was very special to be involved with. We did not realize what a dawn of the computing era we were witnessing. At that time we programmed in machine language without the advantages of index registers. Both the address arithmetic and the problem-solving calculations were performed by fixed-point manipulations, although sometimes we used a subroutine called the Dual Interpretive Routine, which was very slow and cumbersome, but we could invoke it at selected places in our programs for doing floating-point arithmetic. By the time that Fortran arrived, we were so accustomed to the machine-language programming techniques that we felt suspicious of the new-fangled "black-box" approach and kept to the familiar tried-and-true procedures until well into the 1960s.

Soon after my arrival at Los Alamos it became apparent that fluid dynamics was the field for me. My main specialty at first was to look at what seemed very natural to me, namely supersonic flows, in which it is possible to imagine step-by-step the progress of sound waves across a computational mesh, and of the shocks that go through the fluid around various kinds of obstacles. I cut my teeth on supersonic flows with incompressible flows coming later.

There is much that could be told about the pioneering work in our Group, but I have limited the discussion to include only the topics with which I was directly involved, in collaboration with many creative and talented associates as described in the Acknowledgment section of this paper, and listed as co-authors in my publications in physics and mathematics [1–151].

One of the things about supersonic flows that I soon learned was that there were at that time two main ways to think about zoning space for resolving the behavior of a fluid. One of them we call the Lagrangian approach, which means having a mesh of computational cells that follow the motion of a fluid through its contortions and whatever processes that take place. The mesh could follow interfaces beautifully. The other, the Eulerian viewpoint, has a fixed mesh of cells that stay in one place in the laboratory frame and the fluid flows through it. This second approach is great for looking at large distortions; there is no movable computational mesh to get tangled. But on the other hand, it has problems if you want to follow a sharp interface between two fluids. Eulerian techniques tend to diffuse the interface and to smear out sharp shocks. (In those days we had only begun to experiment with very primitive interface reconstruction techniques.)

2. Particles in cells (1955)

These problems with each of the computational viewpoints led us early in our work to think about some way to combine the two. Martha Evans and I started spending part of our time exploring ideas for accomplishing this amalgamation, and we developed a technique that turned out, despite a lot of initial skepticism, to be very useful. This technique we call the Particle-in-Cell (PIC) method [3,4,9,16,19,26]. It is a computational technique in which there is an Eulerian set of cells together with Lagrangian marker particles that move through the cells. Each marker particle has a constant mass. At that stage of the development the particles did not carry velocity or energy; when a particle moved across a cell boundary its mass was subtracted from the donor cell and added to the receptor cell, and the event also signaled that momentum and energy should be transferred. For each of the transported quantities the amount was the mass weighted fraction of the totals in the donor cell.

This process can be viewed in two distinctly different ways. One of them is based on the idea of time splitting, in which a computational cycle is broken into two parts, the first being an update of the quantities

by all the processes except advection, while the second part moves the particles and accomplishes all of the advective fluxing. The second way, as recognized by Eleazer Bromberg (a visitor to our Group from the Courant Institute at New York University), is to consider that the mesh of cells is actually Lagrangian, so that the first part of the calculations in a cycle advances all the variables, including the mesh coordinates and the particle positions, and the second part maps the mesh back into its original configuration, leaving the particles at their new locations [4]. Some years later, Tony Hirt and Dan Butler of our Group discovered that instead of a complete mapping back to the original mesh each cycle, the mapping could be partial, leading to a technique that is called an Arbitrary–Lagrangian–Eulerian (ALE) method, which limits to either of the two viewpoints.

An interesting consequence of the transport of momentum and energy in mass-weighted proportions of the amounts in the donor cell is that the process introduces an effective artificial viscosity that serves to remove some of the numerical instabilities that otherwise would have to be removed by means of an explicit artificial viscosity. The strength of the effective viscosity was calculated by means of a truncation-error analysis. The double-mesh zoning, the time splitting ideas, the donor-cell concept, and the use of truncation-error analysis all subsequently developed into procedures that have received wide usage in the world of computer fluid dynamics.

The early versions of the PIC method had various restrictions and difficulties in its application to the problems that we wanted to solve. Principal among these was the necessity to use a fairly large number of particles in each cell in order to reduce the fluctuations that occur as a result of particle passage across a boundary. Cells that have completely emptied create troubles for their neighbors, so that it was important to avoid that circumstance if possible, or else invent some type of remediation by which to avoid the interpretation that an empty cell represents a region of vacuum. Bart Daly, Dan Butler, and Tony Amsden made major contributions towards the remediation of these difficulties. In 1966 Tony Amsden wrote a report that is still a major resource for the early PIC techniques [4].

We did not have the computer memory and speed that are available today, so that at first we solved only relatively simple problems in two space dimensions. We also discovered that with the earliest formulation, it was necessary to restrict the time increment per cycle to half of what is allowed by the velocity-limiting part of the advective stability constraint, in order to prevent particles from crossing over each other. Because the formulation was completely explicit, we also were limited to consider only the problems that had no regions with low Mach number other than those that had been initialized to uniform pressure and zero velocity. Cells having more than one material were difficult to treat correctly if each material had a complicated equation of state, so that all of our early test calculations were performed using polytropic-gas descriptions allowing us to simply sum the partial pressures. Conservation of linear momentum was ensured by the way in which the equations were formulated, but conservation of energy was an issue that revolved around whether the equations should transport internal energy or total energy. Many of these issues have subsequently been resolved.

To demonstrate the validity of the PIC method for solving complex problems we investigated a variety of circumstances involving the strongly distorting dynamics of several materials driven by the passage of a shock over the configuration [9]. Examples include: passage of a shock over a bubble, the compression of rectangular slabs of one material imbedded in another material, the refraction of a shock over an oblique interface (for which there is good experimental data with which to compare), and the instability of a perturbed interface between two materials. Additional examples are described in [5,7,8,15,26].

3. Low-speed flows

The PIC method was developed for application to fluid flows that are subjected to large distortions involving significant compression during the course of the problem. Designed for flows that have Mach

number greater than about 0.1, the finite-difference equations could be solved explicitly. For calculations of flow at lower Mach numbers, it was at first speculated that good results could be obtained from the compressible-fluid codes by simply decreasing the time step per cycle. This procedure is not only more expensive in computer time, but also has significant difficulties in obtaining accuracy as the flow approaches complete incompressibility. For this type of problem we developed two very different methodologies.

One of these techniques is based on the properties of the vorticity and stream function. Jacob Fromm in our Group investigated the idea that the evolution of these quantities could be calculated numerically, and he soon worked out a procedure that was highly successful. The approach works especially well for confined flows in two space dimensions, where the vorticity vector always points in the third direction, and the boundary conditions can be expressed as constraints on the velocity. The transport for vorticity is solved explicitly for each time cycle of the calculation, and the negative of the updated value is used as the source term in the Poisson equation for the stream function. In the early days of this technique we used a Jacobi or Gauss–Seidel relaxation procedure to solve the equation. Each cycle ended with the extraction of the new velocities from the stream function. The most interesting of the output for a calculation was the pattern of time varying streamlines, obtained from contours of the stream function. Our most famous application of this technique was to the investigation of the von Karman vortex street generated by the flow of an incompressible fluid by an obstacle, which in those days was constrained to be rectangular. For low Reynolds numbers we obtained a steady flow pattern with two downstream vortices, but at higher flow speeds the street emerged and had the correct shedding frequency. We were ecstatic, and published these first-in-the-world calculated results, which were subsequently reprinted in a Japanese reprint series [18,22,23].

The other of the two techniques that we developed for incompressible flow works directly with the primitive variables of velocity and pressure. The principal incentive for this alternative development was to have a procedure that allows for the use of pressure boundary conditions, for applicability to free-surface flows in both two and three dimensions. We called the resulting method the Marker-and-Cell (MAC) technique [27]. It uses marker particles to show the fluid contortions and to follow the changing position of the free surface, at which we could apply pressure boundary conditions (later generalized to include the full stress conditions).

Eddie Welch and I realized that the principal challenge for developing a numerical technique to solve incompressible fluid flows using the primitive variables is to find a way to ensure that the divergence of the velocity field vanishes. For the first version of the MAC method we attempted to describe the fields of velocity and pressure with co-located (cell-centered) values in a mesh of rectangular cells. The procedure was to be completely Eulerian, with the fluid flowing through the stationary mesh. We knew that a crucial requirement was to achieve the incompressibility constraint through the determination of pressures in each computational cycle consistent with the desired objective. In effect the achievement of that goal also will remove the sound-speed restrictions on the time step per cycle; sound signals could propagate to all parts of the mesh instantaneously. The only problem with the idea soon turned out to be the difficulty in expressing the divergence constraint with cell-centered placement of velocities.

To overcome this impediment we changed to placement of velocity components at the edges of each computational cell. In our first two-dimensional version, the four sides of each cell received the normal component of velocity, placed in the center of the edge. This arrangement has subsequently come to be known as a staggered mesh. To derive the equation for pressure we used the well-established trick of taking the divergence of the moment equation, and thus obtained a Poisson equation for the pressure, which in those days we solved by using the Jacobi method to relax the field. We also tried a Gauss–Seidel relaxation procedure, finding faster convergence, but at the price of altering the vorticity, which, during the iteration, is conserved to within round-off with the slightly slower Jacobi technique. Later, Tony Hirt discovered that a simple Newton–Raphson technique works much better and faster, at the same time improving considerably the process of inserting the desired boundary conditions on pressure and velocity.

In effect the MAC-method calculations take place in a time splitting process, with one part consisting of updating the velocities in response to all of the terms (body forces, advection, viscosity, etc.) except the pressure gradients, and the second part accomplishing the calculation of pressures that return the velocity to a state with vanishing divergence but without changing the vorticity that was updated in the first part.

After some initial struggling, we found that the MAC method worked very well, and we tried solving a wide variety of problems with results that exceeded our most optimistic expectations. One example that we calculated was the same von Karman vortex street that we had studied with the vorticity-and-stream-function method. An interesting discovery was that the advection of velocity should not be accomplished with the donor-cell method that we often used in order to give greater numerical stability to the calculations; that procedure simply produced too much effective artificial viscosity so that the desired instability would never occur. To overcome this difficulty, we used instead the second-order centered advection, knowing that one of the adverse effects is to allow for the growth of a slowly developing numerical instability. It turned out that the instability was not overly detrimental to the calculation except in the region upstream of the obstacle. It was discovered only later by Tony Hirt that the presence of velocity gradients has a significant effect on the nature of the second-order advective scheme that we used, reducing the instability in regions of deceleration and enhancing it where the flow is increasing in speed.

With this new MAC technique we explored a large variety of flow problems: the broken-dam configuration in which the instantaneous removal of the dam frees the water to rush forward and interact with an obstacle with such force as to splash over the top; the opening of a sluice gate so that water could rush out with such power as to create a backward-breaking wave; the interaction of a jet of water impinging into a pool of water on a flat plate; the formation of a hydraulic jump, or bore; the generation of a waterfall; the rise of a bubble in a fluid; Rayleigh–Taylor instability carried to large amplitudes with the development of the classical "mushroom" configurations at the tip of the downward moving spike; the splash of a liquid drop into a pool of fluid. These results were being obtained for the first time in the world, and we were pretty excited to see them and to publish them in both Laboratory reports and refereed journals [28–30,33,35,37,49,50].

4. All-speed flows (1971)

The next challenge that we faced was to combine the explicitness of the high-flow-speed techniques with the implicitness of the low-flow-speed techniques, so as to obtain a general procedure that could work well for flows with both magnitudes of speed. Tony Amsden and I realized that the key to the development lay in specifying the quantity that we wanted to bring to zero in a generalized Newton–Raphson iteration scheme. As it turned out there were two appropriate quantities that satisfied our needs. At first we used the equation for conservation of mass, including any possible sources and sinks. Later, Tony Hirt used the difference between the pressure and the equation-of-state expression for pressure as a function of density and specific internal energy. The essence of a computational cycle using the first convergence criterion consisted of a purely explicit update of velocities and internal energies and an iterative solution for determining the modified new densities and velocities that satisfied the equation for conservation of mass. The first criterion was incorporated by Tony Amsden into a code called SIERRA and tested on some problems in which the overall flow was far subsonic but the effects of sound-signal propagation was essential to represent. We published the method and results, but soon realized that there were significant improvements that could be made and accordingly wrote a second paper to describe these modifications [40,48,53]. (If anyone thinks that all of our developments took place in a direct fashion with no glitches along the way, I have to assure you that lots of false starts and turns occurred in virtually every project that we undertook.) Use of the second criterion for convergence worked well also, as long as the flow was not too far subsonic.

This new method for combining all flow speeds into one technique is called the ICE method. It has been exciting to see the numerous extensions that these ideas have fomented. Applications have been accomplished with a variety of new codes developed in our Group and elsewhere in the world for problems involving internal combustion engines, multiphase flows, national defense issues, nuclear reactor behavior, climate, etc. Both Eulerian and Lagrangian versions have been successfully used, and other exotic numerical techniques have also incorporated these ideas.

5. Publications

Many of these results were published in reports and journal articles (see Bibliography), but not without some opposition. There was, for example, a conversation that was reported to me, which took place around 1955 between two of the upper-level managers of the Theoretical Division, one of whom said, "Look, what is this stuff? This PIC method that they're trying to publish a paper on will never work! There will never be computers big enough and fast enough to solve problems with all of the particles that you need in order to resolve what's going on. I don't think we should publish this." And the other person said, "Hey look, maybe it's not useful or won't work all that well. But on the other hand, it's something that was tried, something that people will learn from. We probably should mark it down and it'll go into the annals of things that were tried and didn't work very well but at least it will have been recorded." I'm happy that the second point of view prevailed and that the ideas found their way into print.

Another type of opposition occurred in our interactions with editors of professional journals, and with scientists and engineers at various universities and industrial laboratories. One of the things we discovered in the 1950s and early 1960s was that there was a lot of suspicion about numerical techniques. Computers and the solutions you could calculate were said to be the playthings of rich laboratories. You couldn't learn very much unless you did studies analytically. The truth, of course, has turned out to lie in the complementary interaction between calculations and analysis, and in the validation of both through comparisons with experiments. I think some of these early suspicions were partially justified, although we found as time went by that many universities, industries, and governmental agencies began to solve problems of interest using numerical techniques.

In the writing of reports and papers for publication we felt that it was important for readers who might wish to try our techniques that the writing be as complete as possible, even to the inclusion of the lengthy finite-difference equations. We were eager to have confirmation from other investigators that the techniques could be used on the various computers that were rapidly becoming available to the world, and give meaningful results for solving actual problems that could arise in both engineering and scientific investigations.

The part of the presentations that we found to be especially important was, and continues to be, the graphics. To absorb the meaning of vast amounts of computed data requires for all of us the pictorial depiction of results in ways that display the essence of what is going on. At first our visual displays were obtained by the tried and true method of plotting by hand. Hundreds of PIC particles have been plotted by that tedious procedure. A tremendous improvement came with the availability of the Cal-Comp machines, which mechanically plotted the position of each particle with much greater speed and accuracy than we could accomplish by hand. But the greatest achievement of convenience and accuracy came with the capability of the computer itself to produce the desired graphics. Microfisch films became our tool for this purpose, and many hours were spent with a Microfisch reader examining the graphs and pictures and trying to determine the best way to interpret the results of our calculations. The next improvement came with the capability for the computer to record the configurations of our flow calculations on 35-mm film. The result was our first opportunity to make movies of the changing structure of the flow! When I was told that COLOR depictions were soon to be possible, my first reaction was to think that we already had all of the

capability that we needed, and color would be an excessive luxury. How very wrong this old-fashioned viewpoint has turned out to be. One challenge that gave us some grief was how to develop good hidden-line routines. With all the current superb graphics packages available now it's amusing to remember how primitive our activities were in those days.

6. Early difficulties (1960, 1970)

We had some exciting successes in the early days of the PIC, MAC, and ICE developments and applications, but not every numerical method that we tried worked out well. One example that we tried for compressible flow was our experimentation with some ideas for eliminating the underlying mesh of computational cells, and putting all of the calculations onto the particles themselves. Each particle had its own mass, velocity, and internal energy, and the density associated with its location was to be obtained by examining the positions of the nearest neighbors [12,17,25]. We called the technique a Particle-and-Force (PAF) method because the dynamics of the system were determined on the basis of inter-particle forces derived in such a way as to represent the effects of an appropriate equation of state for the material. A rather elaborate statistical theory was developed for the formulation of the forces. The idea is the forerunner of various techniques referred to, collectively, as Free Lagrangian. At our stage of the development, the PAF technique worked fairly well for a single material in two dimensions. Its main difficulties were seen in application to problems with two or more interacting materials. We also were hampered by the inability, at that time, for determining nearest-neighbor particles in a consistent way that was not excessive in computer resources. Bill Meixner, Bart Daly, and Eddie Welch joined with me in writing several reports on our findings, but we have not pursued this line of investigation any further, especially because of the brilliant accomplishments for this type of computations developed elsewhere.

A second line of investigation resulted in what we call the Dynamics-of-Contours (DOC) method [51]. The main feature of this approach is the automatic creation of a computational mesh of cells that is neither Lagrangian nor Eulerian, but is composed instead of cell boundaries that follow contours of constant density. This approach works fine for one-dimensional problems but has significant difficulty when applied to two-dimensional configurations subjected to strong distortions. Some of this difficulty was later removed by Norman Zabusky and other investigators, but the technique has not received much acceptance by potential users.

7. Multi-field flows (1971)

Having worked with marker particles in computational cells it seemed like a natural extension for us to consider the transport of real, physical particles carried by a surrounding fluid. The process is called multi-field flow. Multi-field flow refers, for example, to the motion of bubbles in oil, to raindrops in the air, to particles of sand in water, and to dust in the atmosphere. Much previous work had been done to develop the governing equations for this type of dynamics, based on straight-forward extensions of the Navier–Stokes equations for the dynamics of a purely homogeneous fluid. The particles or bubbles and the fluid are both represented by continuous fields that can interpenetrate. Local pressure equilibrium is assumed between the fields. As a result, the formulation contains one especially disturbing feature: it is mathematically ill-posed, which means that as you get to smaller and smaller scales of flow, the solutions start wandering off in directions of their own, ultimately becoming arbitrarily far from each other, even for very small differences in the initial conditions.

Another related difficulty arose in trying to represent the processes that take place on the scale of each individual particle, in particular the detailed exchanges of mass, momentum and energy. The concept of

continuous fields for both components of the materials means that these exchanges can only be described in a bulk constitutive fashion. As a result, there was no way that the dynamics could be expected to follow the formulation for scales smaller than the inter-particle spacing. Thus Tony Amsden and I built our solution technique for multi-field flow on the assumption that the only results that could be meaningful are those that occur at scales significantly larger than the average value of that spacing, so that the problem of ill-posed behavior did not trouble us very much [62]. We soon realized that any corrective procedure to remove the ill-posed nature of the equations would be fine to incorporate as long as it did not interfere with the solutions at those scales for which the equations are physically meaningful. In particular, the existence of physical instability, which is related to the transition of the flow to turbulent, needs to be preserved at all the scales that are relevant to the problem of interest. A little experimentation showed that the addition of a small amount of artificial viscosity to each field works very well in curing the problem.

To solve problems we used a straight-forward extension of the MAC-method ideas, employing the Newton–Raphson technique in each computational cycle to find the pressure that brings the velocities to values that ensure overall conservation of mass.

A more challenging problem was that of determining meaningful descriptions of the exchange processes. The drag of the interpenetrating fields upon each other was especially important to represent accurately. We postulated that the momentum exchange takes place by means of combined viscous drag and form drag, but were soon concerned that the formulation was based on the identification of which was the dispersed field, and which was the surrounding continuous field [66]. For widely separated spherical particles in water the identification was not ambiguous, and the drag formula was reasonably good as long as there were no appreciable particle-to-particle interactions. For bubbles in water, however, the flow circumstances could easily reverse the identification to that of droplets in air. We developed a procedure that covers the behavior through the transition from one circumstance to the other, and it has worked reasonably well for many problems of interest to us. We have even applied the momentum-exchange equations to circumstances in which the entities (bubbles or droplets) are expected to deform appreciably during the dynamics, and we still got reasonably good results.

The other exchange processes (of mass and energy) were especially important for problems in which there are phase transitions, as for example in steam-water flows. Here was a crucial area for our developments, because of an assignment to consider the behavior of pressurized water reactors during a hypothetical blow-down in which you might have very hot pressurized water suddenly released to atmospheric pressure, forming bubbles and droplets and sending a potentially disastrous pressure pulse through the entire piping system of the reactor [77].

Applications by Bart Daly and others in our Group to reactor safety analysis under the auspices of the US Nuclear Regulatory Agency were remarkably successful, and the initial studies proved so meaningful that a whole new Division of the Laboratory was created to extend our multi-field technique to the calculation of the entire hot-water piping system of the reactor. Many other types of problems were also solved in our Group, including the transport of pollutants in the atmosphere around buildings in an urban setting [60], and the dynamics of fuel droplets in the cylinder of an internal combustion engine. These activities received substantial funding from agencies and industries outside the Laboratory. Many other examples are given in [64–67,81,99,100].

8. Relativistic fluid dynamics (1975)

A completely different type of application of our numerical techniques arose with problems of relativistic fluid dynamics. Large accelerators at several Laboratories in the world were obtaining data on the effects of atomic-nucleus collisions at very high energies for which the effects of Einstein's relativity are very important. To address the problem of interpreting these experimental results, Ray Nix from our nuclear

physics Group and Fred Goldhaber from the State University of New York were discussing the possible applicability of a liquid-drop model. With their specification of the appropriate relativistic fluid dynamics equations, Tony Amsden and I set to work to modify the PIC method for applicability to such problems as the impact of a neon nucleus on the nucleus of a uranium atom. We put the uranium atom into the laboratory frame of the computational mesh, so that in the initial conditions the neon nucleus was appreciable shortened in the direction of its trajectory. One of the goals of the study was to obtain the distribution of fragments that propagated away from the point of collision, and the results of the calculations were remarkably successful in duplicating the experimental results. Six papers were published on our part of the project [68,69,71,72,74,76], and other investigators then took the ideas and have been continuing the studies with PIC-method calculations even to the present time.

9. The spread of numerical fluid dynamics

The development of numerical methods for solving material dynamics problems of a wide variety of kinds occupied my attention for many years. Up to about 1968, I felt confident in knowing about the dissemination and extensions of our techniques to most parts of the world, but at the same time began to realize the genius of other method developers in creating new techniques. Numerical fluid dynamics had become an important and respectable science, and my directions of investigation began to change.

10. Turbulence (1967)

We had long realized that turbulence occurs in many of the fluid-flow circumstances of interest to both scientific studies and engineering applications. Turbulence is like any of the fine-scale processes that we have to represent in the behavior of a fluid, whether it be a gas, a liquid, a plastic flowing metal, or any other deformable material. It is like heat, which represents the effects of molecular fluctuations. Thermal energy describes part of the collective behavior of the molecules, but its transport does not require the determination of every molecular trajectory. The thermal energy per unit mass of the material is transported as though the molecular assemblage were continuous. Could turbulence behavior likewise be described by the evolution of some appropriately-chosen field variables? The answer, of course, had been partially known for many years. Turbulence energy transport equations had been proposed by Rota in Germany and by P.Y. Chow in China, and had subsequently been generalized to transport the full Reynolds stress, but there was a big unresolved problem: Can we find a transport equation for the determination of an appropriate length scale from which to calculate several required rate functions? These rates in the transport equation include the rates of return to isotropy and of decay. To describe the evolution of an appropriate length scale, Paul Nakayama and I introduced a transport equation for the rate of energy dissipation, epsilon [38,45]. Thus was born the K–epsilon model that has been used in our calculations and in computations performed by many other investigators throughout the world. A notable example is the work of B.E. Launder and D.B. Spalding. The model turned out to be very useful, and we tried solving many problems with it. The results often worked out nicely, but sometimes they were not as good as we wished, especially when the mean flow of the fluid was rapidly changing. Only somewhat later did we discover a spectral approach to the analysis that helped to extend the range of applicability. It was, however, a new and exciting sort of adventure and we enjoyed the challenge of testing the model by applying it to a wide variety of fluid-flow circumstances.

One class of problems that we could not address with the first version of these turbulence transport equations involved circumstances in which there are two or more fluids with different densities or a single fluid with continuous variations of density. At the same time we were interested in the application of our

model to fluids that are compressible, sometimes with strong shocks or rarefactions. To describe the effects of variable density required the introduction of two new descriptive variables together with transport equations to describe their evolution. The two new descriptive quantities are the variance of the density fluctuations and the mass flux relative to a coordinate system in which the volume flux is zero. The basic Navier–Stokes equations for the derivations are the same as we used for obtaining the constant-density K–epsilon model. By means of suitable manipulations, Rick Rauenzahn and Didier Besnard (visiting from France) joined with me in adding two more equations to describe the transport of the two new quantities [112,129]. Using the initials of the developers, the new technique came to be known as the BHR method. The first application was to Rayleigh–Taylor instability, in which the mixing interpenetration of the materials across an interface is driven by a normal pressure gradient. Comparisons with abundant experimental data that had been obtained in British and Russian Laboratories showed good agreement for the growth of mixing-layer thickness even into the far non-linear regime. The results for the mean density profile across the layer, however, were not satisfactory. The root of the problem lay in troubles associated with the calculation of the length scale, which was too small at the edges of the mixing layer. The missing element of the theory was demonstrated to lie in the rapid pressure-wave propagation to the edges of the layer. Using as guidance the linearized equations for low-amplitude Rayleigh–Taylor instability analysis, Michael Steinkamp and I saw that the missing element of the model was associated with the ''non-local'' spreading of the long-wave-length disturbances, which transport important acceleration to the fluid beyond the edges of the mixing layer. With an integral spreading function for the Reynolds-stress source term the results were excellent. Many other unstable mixing processes have been investigated with considerable success. It should be noted that a turbulence transport model for variable-density fluids, developed independently by scientists in the Soviet Union, is very similar to the BHR model.

One of the interesting things that we realized at that time was that there are two major differences between turbulence and heat. With heat there is usually a rapid return to some kind of equilibrium after the fluid is subjected to a disturbance. In addition, the length scale associated with molecular fluctuations is essentially the same as the mean free path, for which the variations are easily calculated. With turbulence, the behavior is quite different; there is a distribution of length scales that can vary significantly with position and time, and the return to equilibrium or to any kind of self-similarity is very sluggish, taking place in times that are comparable to the overall elapsed time of interest. If you disturb a material with a rapid transient of drive, it will respond with the development of a strong departure from equilibrium, which persists for considerable time. To be more specific, we mean by non-equilibrium the distortion of the distribution of Reynolds-stress components from a ''universal'' self-similar form. The distribution of energy among all the wavelengths can look very strange, with humps and gaps in its structure.

The idea of strong problem dependence on the distribution of energy across the size scales leads to the speculation that a spectral theory for the turbulence might be appropriate. It was felt that a close relation to the behavior of gas molecules could be found. For a gas with a mean free path that is comparable to the size of the macroscopic scales of the configuration, the idea of a nearly universal distribution of molecular velocities (the Maxwell–Boltzmann distribution) was well known to be incorrect in circumstances with rapid changes in the dynamical drive of the system, or with large differences in the temperature and/or velocity of adjacent walls. For such circumstances it was necessary to transport a probability distribution function for the velocities. Could a similar analysis procedure be found for turbulence? We learned that exploration of this idea had taken place in France some years earlier, with results that seemed promising as a basis for developing the type of transport equations that are needed for this type of circumstances.

To proceed with the derivation, Chuck Zemach joined with us in writing the Navier–Stokes equations for two different points in space, so as to derive a way to examine the correlation of fluctuations that could occur in the dynamics at those two positions [124]. As the distance becomes large the correlations vanish. Thus a Fourier decomposition of the two-point equations with respect to the separation variable could be expected to describe the dynamics of the distribution function for such two-point correlations as those of

velocity fluctuations (the spectral form of the Reynolds stress). In many respects the result resembles the Boltzmann equation. In particular, appropriate moments of the equation over all of spectral space reduce to the K–epsilon equations if the assumption of a "universal" form for the spectral distribution is made. When that assumption is not valid, the spectral equations themselves can be solved to follow the evolution of the non-equilibrium behavior.

To test the spectral equations Tim Clark and Patrick Spitz (visiting from France) extended them to include the presence of density variations, and we applied them to both pressure-driven and shear-driven interface instabilities. The buoyancy calculations, including the important non-locality of pressure-wave effects in physical space, gave excellent results. The technique, described in several publications by Mike Steinkamp, Tim Clark and myself, has been called the SCH method [134,135]. For shear-driven instability, there was, however, a missing feature in the equations associated with a well-known process that continuously creates vortices of larger and larger sizes (called vortex pairing in a free shear layer). To represent this process, Peter Wilson and I found that a modified version of the Kraichnan-Spiegel non-locality formula in spectral space could be made to work very well.

With our spectral–transport model, Peter Wilson and I decided to test the equations with one of the classic non-equilibrium (non-self-similar) problems, namely that of the combined pressure-driven AND shear-driven instabilities at an interface between two fluids. The calculations for each separately had given excellent results for the development of the self-similar spectral structures. With our new modifications, the calculations showed that the presence of both shear and buoyancy produces a continuing non-equilibrium in which the spectral structure has ever-changing features that continue until the occurrence of ultimate late-time dominance of the buoyancy effects.

Perhaps the most useful of the results of the spectral derivations is that they furnish a procedure for solving problems numerically for which the K–epsilon model and its variants are not capable of capturing important effects of spectral non-equilibrium. They have also furnished for the first time a procedure by which the evolution equation for epsilon could be derived, instead of simply postulated on the basis of dimensional and geometric arguments.

11. Some applications of numerical methods

In the development of new solution techniques for fluid dynamics we needed to perform many types of test problems in order to validate the relevance and accuracy of the procedures. A few of these test problems are described above. At the same time, however, we undertook a variety of large-scale applications, first because they were interesting and relevant ways to increase our confidence in these new techniques, and second for the pragmatic purpose of developing sources of funding for our work. The Laboratory, along with many other scientific institutions in this country, found that the federal support for research was dwindling in the late 1960s, so that we needed to make contacts with various other government agencies that were still able to support projects of interest to their specific needs. We had computational tools that were new and powerful, and soon found that there was great interest in other agencies for us to apply our capabilities to problems of relevance to their requirements. A small number of examples are mentioned here to indicate the scope of our activities.

The reactor-safety analysis program is one of these projects, which is described above. Another, undertaken under the auspices of the US Environmental Protection Agency, was the analysis of pollution transport by winds through urban areas with streets and tall buildings. Bob Hotchkiss, Tony Hirt, Larry Cook and I used an extension of the MAC method with the inclusion of heat transport for representing buoyancy effects, and a particulate transport equation to describe the combined effects of gravity-driven settling, drag with the air, and turbulent diffusion. Sources of the pollution included the emission from automobiles and the effluence of material from rooftop vents. The calculations were applied to various

configurations of buildings and circumstances of wind direction and speed [60]. More particularly, we examined the pollution transport in the Broadway Street Canyon in downtown St. Louis, Missouri. The calculations worked so well that many research institutions built on our methodology to include complex terrain and many other factors contributing to the reality of specific pollution-transport circumstances.

Geothermal energy extraction was another challenge that we addressed, using our multi-field solution techniques. The particular circumstances of interest to one of the experimental Divisions of our Laboratory involved the hot dry rocks that lie buried in the heart of the mountains just to the west of Los Alamos. The technique employed in the field requires two deep holes to be drilled into the rocks. Cold water is pumped down into one of the holes, is heated by the rocks, and extracted through the other hole. Success requires a connection between the holes, and especially that the cold water fracture the rocks in order that the flow region would continuously enlarge for many years of energy extraction. Bill Pracht and I used a multi-field approach to study the problem, and the results we obtained continued to influence the program for many years [56].

Another thing that was of considerable interest in the early 1970s was the behavior of tornadoes. At that time there had been a major tornado in the city of Lubbock, Texas. This was an incredibly devastating storm, which did not behave like an ordinary tornado; there was something strange and different about it. To investigate what had happened, the US National Science Foundation gave us a grant to apply our numerical techniques to the analysis. Lee Stein and I calculated the dynamics of converging flow with various magnitudes of preexisting vorticity, and found that we could distinguish between a single-cell tornado and a double-cell tornado. In the first type the potential for damage is strong; while in the second type the potential for damage is enormously greater. Within the single-cell structure the central updraft extends upward into the spawning clouds, whereas within the double-cell tornado the centrifugal acceleration is so great that the air is thrown outward, and above a vertical stagnation point the velocity reverses and air travels downward from the clouds. The violence of the rotation can lead to the formation of a set of smaller tornadoes traveling around the central one, whose paths had been observed in damage patterns after the storm was over, and also has been observed in dry tornadoes, often called dust devils. For the milder type of tornado we were able to compare our results with those that had been obtained in a laboratory vortex chamber at another institution, with results that lent significant confidence to the validity of our calculations [61,63].

A very different type of study that we did was to investigate the dynamics of a biological cell, in which the internal circulation can give the cell the ability to crawl along a surface or to send out fingers that are called pseudopods. The work required the collaboration of Micah Dembo, a biologist in our Laboratory, because many of the relevant aspects of the internal structure of the cell were completely unknown to Mat Maltrud and me. We were very excited about the calculations, and enjoyed the publicity that came from publication of the results in several journal articles [106,108].

A fascinating project that I especially enjoyed was the development of a large computer code to describe the behavior of a wildfire propagating through a forest. The configuration that Rod Linn and I wanted to represent is fully three-dimensional; the forest is situated on rugged terrain consisting of deep canyons, riverbeds, flat-topped mesas, and various other relevant geological formations that might be present. The challenge is to incorporate into the code complex physical processes over a large range of scales, along with the chemistry of hydrocarbon release and combustion, and with boundary conditions representing realistic weather conditions such as the time-varying wind speed, intensity and scale of turbulence, and humidity. Self-determination of propagation rates, transition to crowning, automatic choice of the most likely burn path, and the effects of spotting are among the answers that we wanted to extract from the calculations. It was clear from the start of this project that no calculation is ever going to be able to predict the exact outcome of a particular wildfire; the best that can be expected is a meaningful description of the relative probabilities for the different possible scenarios to develop. The practical value of these calculations is to complement the excellent rapid-scoping techniques that have been developed by the US Forest Service, and

by other fire-mitigation agencies for estimating the behavior of wildfires. Some of the goals include the development of urban-planning strategies to minimize potential threats to new housing developments, the training of fire fighters, and the planning of controlled burns in forest regions that are considered to be especially susceptible to disastrous wildfire activity. Combining our developments with the atmospheric code of Jon Reisner, we tested the calculations by comparison with well-documented actual fires in California, Colorado, New Mexico, and Florida, with excellent results [136,141].

12. Scale bridging

In recent years, I have become strongly interested in the potential for analytical–computational studies of systems with many degrees of freedom (like our turbulence studies using Reynolds-decomposition techniques), in which a probability distribution function (PDF) can be evolved by means of equations based on the Liouville principles of conservation in a generalized phase space. We have applied these ideas to a variety of problems. One of them, with Mike Steinzig, is to the development of grains in the solidification of a binary alloy, for which the mean grain size and distribution of sizes need to be calculated as functions of cooling rate and relative proportions of the two metals in the alloy [147]. Another, with Eric Harstad, is to the behavior of a polymer molecule during the non-equilibrium dynamics taking place at high strain rates, for which the Liouville approach resembles that of the techniques used to study Brownian motion [149]. The response of a polymeric foam to mechanical deformations has also been studied by Mark Schraad and me [151]. We follow the evolution of a probability distribution function for the variations of strain and stress in a random distribution of cell sizes. To describe the effects of strain-rate variations in the foam we include a version of the two-field equations to represent the movement of air through the matrix of cells.

13. Social problems

An interesting question arose from our investigations of scale-bridging techniques using PDF transport: If we can represent the combined behavior of individual molecules, and if we can represent the bulk effects of turbulence eddies, can we go one step further and model the collective behavior of groups of people? To answer this question we worked on the development of model equations that we thought could be relevant. I had two summer students who worked with me, Don Sandoval and Kent Genin, and we developed essentially the same technique that works well for molecular dynamics and for turbulence dynamics, but involves one important new factor, and that is the presence of what we call soft variables [121]. By soft variables, we mean properties in addition to such deterministic quantities as the position and the velocity of the individual person, namely the thoughts associated with excitement and fear.

A major challenge, of course, is to quantify the intensity of these emotional responses and to relate them to the behavior of the individual. In a rampaging mob, for example, the descriptions can be expressed in terms of either running towards something if the person's excitement is great enough or running away from something if his fear is great enough. We developed a relatively simple model and published a report about our application to the behavior of two platoons of soldiers in battle with one another under a variety of different circumstances. Now, almost 15 years later, I am finding that these types of models are starting to be of increasing interest to people, both in questions of international politics and economics, as well as the behavior of mobs of people, and most recently in issues of Homeland Defense. I predict that social dynamics (both slow and fast) with soft variables will become a major field of computational activity in the coming decades.

14. Additional interests

When I first came here it seemed important to do things besides science. My family was and continues to be a major source of delight. To my wife, Patricia, I am especially grateful for more than 50 years of loving friendship and support. In my spare time, paleontology became a significant activity for quite a while and Professor Patrick Sutherland from the University of Oklahoma and I wrote a major treatise on the fossil brachiopods of the upper Carboniferous of north-central New Mexico. I have also developed a lot of interest in the Indian pottery of the southwestern part of the United States. The Native Americans of this area are famous for manufacturing pottery using the same techniques developed many centuries ago. I have written six books on the subject and am working on three more, two of them already at the publisher; these are described in Section II of the Bibliography [152–174]. Also, since 1968, it has been both a challenge and a continuing source of recreation to paint well over a thousand pictures of the Indian pottery and of many other scenes that are typical of the activities of southwestern Indians, cowboys, and motorcycle riders.

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I have lived a lucky life, being in the right place at the time when something new and exciting was happening. The activities have succeeded only through a combination of pure luck and pure joy, and especially as a result of having wonderful people to work with. Indeed each of the projects described in this paper could only have succeeded with the collaboration of many remarkable associates.

The people with whom I published reports and papers during the pioneering years for each project are listed in the Bibliography. To each of my co-authors I shall always be more grateful than words can ever express. There have been many other people in our Group who have made marvelous progress in the field of numerical fluid dynamics and also of continuum dynamics in general, with whom I have interacted through many inspiring technical discussions. I am especially grateful to Frank Addessio, Tony Amsden, Didier Besnard, Jerry Brackbill, Dan Butler, Tim Clark, Tom Cook, Bart Daly, Ruth Demuth, Martha Evans, Jake Fromm, Dick Gentry, Rob Gore, Eric Harstad, Tony Hirt, John Hopson, Marty Horn, Bob Hotchkiss, Norm Johnson, Bucky Kashiwa, Dana Knoll, Rod Linn, Mat Maltrud, Len Margolin, Ron Moses, Paul Nakayama, Peter O'Rourke, Bill Pracht, Rick Rauenzahn, Murray Rudman, Hans Ruppel, Manjit Sahota, Don Sandoval, Mark Schraad, Mike Steinkamp, Mike Steinzig, Brian VanderHeyden, Eddie Welch, Peter Wilson, Chuck Zemach and Duan Zhang for many years of friendship, support, and numerous stimulating discussions. The publications listed below show only a part of the work accomplished by our Group. Virtually every new development saw many years of applications to problems, accomplished by later Group members and by researchers at many other places around the world. To all of them I wish to express my gratitude for their interest and for the wonderful feedback that they have expressed.

In addition, there have been literally hundreds of university students who have taken advantage of this Laboratory's student programs, and have come to Los Alamos for summer activities in our Group. Fifteen of them have stayed here for two or three years to work with me on the research and writing of their Ph.D. dissertations for nearly as many universities. All of them have brought their youthful enthusiasm to add immensely to the excitement of our work, and to the accomplishment of our missions.

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Extensive listings of publications resulting from some of our early activities are contained in the papers:

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