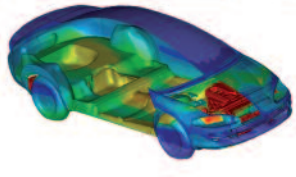
icons of CFD



Professor Suhas Patankar

Icons of CFD returns after a long absence, profiling the leading lights in the early days of CFD.

In the late 1980's, at the beginning of my PhD, I recall staring at several thousand lines of FORTRAN, which apparently coded the governing equations of fluid mechanics. This largely-uncommented 'spaghetti' appeared indigestible. Where to begin? I sought out my supervisor and he passed me an unassuming volume with the title: "Numerical heat transfer and fluid flow"[1]. I started to read, understood, and continued, until the last page was turned. The book explained with sublime ease and clarity how one could solve these equations, the pitfalls to be avoided, finishing touches to be applied, etc. I could even start to identify implementations of the numerical methods so clearly described, in the mess of code. It was no less than a revelation. The author of the book? Prof. Suhas Patankar.

Suhas Patankar was born in Pune, India, from where he received his Bachelor's degree in Mechanical Engineering in 1962, and a Master's in Technology two years later from the Indian Institute of Technology, Mumbai. He applied for, and won, an ICI Scholarship to Imperial College, London, where he was to make his mark, under the supervision of Prof. Brian Spalding - who we met in Benchmark - January 2010.

In the early-1960s, the group led by Spalding had just started out in CFD, focusing on the numerical solution of boundary layer flows. These are the thin regions which develop as flow passes over a solid surface. They can be approximated by partial differential equations which are classified as 'parabolic' in the main flow direction, i.e. they show a 'one-way' behaviour along the coordinate aligned with the main flow direction. What do we mean by this? Let Patankar be our guide[1]:

"A one-way coordinate is such that conditions at a given location in that coordinate are influenced by changes in conditions on *only one-side* of that location……Even a space coordinate can very nearly become one-way under the action of fluid flow. If there is a strong unidirectional flow in the coordinate direction, then significant influences travel only from upstream to downstream. The conditions at a point are then affected largely by the upstream conditions and very little by the downstream ones. The one-way nature of a space coordinate is an approximation. It is true that convection is a one-way process, but diffusion (which is always present) has two-way influences. However, when the flow rate is large, convection overpowers diffusion and thus makes the space coordinate nearly one-way."

Patankar's description allows us to easily understand the mathematical behaviour of the governing equations for boundary layer flows. This behaviour allows for significant simplifications in the numerical solution of such flows. The solution can simply proceed from known initial conditions at a given upstream location, being 'marched' downstream and, at any given time, the only flow conditions which need to be stored are those at the current and next downstream location. This minimises both computer storage and run time, which was of utmost importance with the precious, but limited, hardware available in the 1960s. Patankar successfully developed and applied such methods in his PhD on heat and mass transfer in boundary layers[2], later publishing the computational method and code – known as GENMIX - in a book[3] with Spalding.

GENMIX came to be widely used. But many flows of engineering interest are governed by equations which are 'elliptic', rather than parabolic, i.e. they show a two-way coordinate behaviour[1]:

"A two-way coordinate is such that the conditions at a given location in that coordinate are influenced by changes in conditions on *either side* of that location."

In an elliptic equation, information can propagate freely by convection and diffusion in each of the coordinate directions, i.e. both downstream and upstream. There are no limited regions of influence. In a flow which is modelled as elliptic, this means that the influence of a change in conditions – such as a local increase in pressure – is felt everywhere. The numerical 'marching' methods used in the solution of parabolic flows are no longer applicable, as the solution must instead be obtained for all points in the flow simultaneously.

After completing his PhD, Patankar worked as an assistant professor at the Indian Institute of Technology, Kanpur, from 1967 to 1970. In this period, Spalding's group became increasingly engaged in the numerical solution of elliptic flow problems. They had been successful in solving two-dimensional flows, but the methods* they were using could not obviously be extended to three-dimensional flows. To understand some of the difficulties in the solution of elliptic equations for fluid flow, we must now turn our attention to the governing equations.

The main physical principles which apply are conservation of mass, Newton's 2nd law of motion applied to fluid flows (i.e. rate of change of momentum depends on the net force applied), and conservation of energy.

The conservation of mass leads to an equation which contains the three velocity components, u, v, w and density ρ. The application of Newton's second law of motion leads to momentum conservation equations for each of the three coordinate directions, and in each of these equations all of the velocity components appear, together with the pressure, p. Finally, the energy equation relates the changes in local internal energy with the prevailing temperature field.

In the case of a compressible flow, with heat transfer, the five conservation equations typically contain seven unknowns: the three components of velocity, u, v, w; pressure, p; density ; internal energy per unit mass, e; and temperature, T. In order to form a closed set, we need two further equations. For compressible flows, thermodynamics provides the necessary link. The internal energy is related to temperature by the relationship $e = C_vT$, where C_v is the specific heat at constant volume. An equation of state can be used to close the conservation equations through the missing link: density ρ, which varies as a result of changes in pressure and temperature. Usually, a simplifying assumption is made that the gas is a calorifically perfect gas behaving according to the ideal gas law, i.e. $p = \rho RT$, where R is the gas constant.

The solution of these governing equations, usually referred to as the Navier-Stokes equations in honour of their 19th Century French and English founders, is problematic. The equations are non-linear and highly coupled. For instance, every velocity component appears in the mass conservation equation and in each of the three momentum equations. Furthermore, whilst the pressure appears in each momentum equation, it has no separate transport equation which would readily allow its determination throughout the entire flow field. We now begin to see why numerical solution of the fluid flow equations is far from trivial.

For compressible flows, it is possible to solve for the density field by using the mass conservation equation, and for the temperature field by using the energy equation. The pressure field can then be obtained from its equation of state, as above.

But what about incompressible flows, in which density is essentially constant, i.e. most liquid flows and those of gases at low Mach number? Here the difficulties become, if anything, even more profound. The problem is how to solve for the pressure field, if density is constant. In the absence of heat transfer, we have only the mass conservation and momentum equations. Pressure appears in the latter equations, but not the former. If we can somehow obtain the correct pressure field, the resulting velocity field will then satisfy the mass conservation equation. That is the key difficulty: obtaining the correct pressure field. It is compounded by the elliptic nature of the incompressible fluid flow equations, which demands that the pressure and velocity fields must simultaneously satisfy these equations throughout the entire three-dimensional flow domain.

Such was the nature of the difficulties being tackled by Spalding's group in the late 1960s. Although some headway was being made on the pressure-velocity problem in three-dimensional elliptic flows, with an algorithm known as SIVA[4] (Simultaneous Variable Adjustment), it was proving very complex. It was obvious at the time that a superior alternative was needed to SIVA, and which would provide a way to calculate three-dimensional elliptic flows as easily as those in two-dimensions.

At this point, in 1970, Patankar returned from India to take up a research post in the Imperial College group. He immediately set to work on the problem. Within the space of just a few weeks he had formulated a far better approach. He presented his algorithm to the research group at its weekly progress meeting. It was immediately clear that it had significant advantages over the SIVA method. Soon, almost the entire research group was using Patankar's algorithm, whose acronym, SIMPLE, was almost as brilliant as its formulation.

This is not the place to describe the SIMPLE algorithm in detail. Patankar does so with great clarity in his book[1], as well as in his classic paper with Spalding[5]. In addition, almost every book published on general CFD methods makes at least a passing reference to his algorithm, such has been its lasting impact.

In essence though, the algorithm consists of an iterative procedure, in which the pressure and velocity fields are solved sequentially. The algorithm starts from a guessed pressure field, with the pressure and velocity components being updated via simplified formulae relying on 'pressure corrections'. Although these correction formulae are simplified, the algorithm nevertheless ensures that at the end of every iteration the velocity field exactly satisfies the mass conservation equation. When the solution has converged, meaning that sufficient iterations have been made to ensure that both the mass conservation and the momentum equations are solved to tolerably small residuals, the magnitude of the pressure corrections becomes vanishingly small. This means that the simplifications made in the correction formulae become irrelevant to the final converged solution.

**During the period 1965 to 1970, Spalding's group were successfully solving two-dimensional elliptic flow problems using the stream function – vorticity method. When applied to two-dimensional flows, this approach results in two scalar quantities (stream function and vorticity) being derived from the primitive flow variables, i.e. velocity. Solution for two scalar quantities was straightforward, but the extension of the method to three-dimensions posed many problems.*

Patankar had realised that as long as the pressure and velocity fields were being progressed towards a converged solution of the discretised equations, the correction formulae need only be approximate. As well as ensuring computational simplicity, this allowed a significant degree of flexibility to be introduced into the algorithm. For instance, differing degrees of under-relaxation can be introduced for the different flow variables, suited to particular applications, i.e. some flow variables can be allowed to change rapidly from one iteration to the next, whilst others are damped if rapid changes are causing the solution to diverge.

SIMPLE means: Semi-Implicit Method for Pressure-Linked Equations. The wording 'semi-implicit' essentially refers to the fact that, at each grid node, the algorithm corrects the velocity field by using pressure corrections at just the immediate neighbouring grid nodes – even though the velocity field is, of course, affected by pressure variations throughout the flow domain. The basic SIMPLE algorithm has been successfully enhanced by several authors, including Patankar himself – with SIMPLER (SIMPLE Revised)[1], and variations such as SIMPLEC[6], and can be extended to unsteady or compressible flows.

It is hard to over-state the importance of Patankar's SIMPLE algorithm and its variants. For the three decades after its invention it was the default solution algorithm for almost every vendor of finite volume-based CFD software for industrial applications. Since the turn of the century, other solution algorithms have come more to the fore, based on strongly coupled flow solvers. Even so, there are still many CFD codes in industrial and academic circles which use the SIMPLE algorithm, or offer it as an option.

Patankar's algorithm, and indeed the wider research group led by Spalding, benefited significantly from the pioneering work on numerical methods for fluid flow undertaken by Frank Harlow and colleagues at Los Alamos, as outlined in Benchmark – April 2010. However, it was Patankar's insight in developing the SIMPLE algorithm that allowed the full potential of the early Los Alamos work to be realised - in the form of a practical solution method applicable to a very wide range of flows.

In 1973, Patankar joined the University of Waterloo in Canada for two years, and then in 1975 became a faculty member of the University of Minnesota in the Department of Mechanical Engineering, where he continues his research and teaching, as Professor Emeritus. He is President and founder, in 1987, of Innovative Research, Inc., a company providing application-specific software products and consulting services for fluid flow, heat transfer and related processes. He has won numerous awards for teaching and research, including, in 2008, the prestigious Max Jacob Memorial Award from the ASME.

Prof. Suhas Patankar has had a lasting influence on generations of fluid dynamicists. I would urge all those using CFD software to read his 1980 book. Even though some of its methods have been superseded, it nevertheless provides easily understood insights into many of the fundamentals of the numerical modelling of fluid flows - and which are equally applicable to the present day. Patankar is truly an 'Icon of CFD'.

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The author has, in part, drawn substantially from David Tatchell's insightful blog which reflects on the commercial CFD industry, and would like to acknowledge this source of material. See http://blogs.mentor.com/davidtatchell/

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Icons of CFD continues in the next issue of Benchmark, stepping back in time to the days of CFD before computers, profiling Lewis Fry Richardson, whose research in the early part of the 20th Century has had a lasting impact.