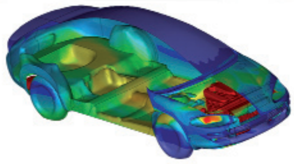
icons of CFD



Frank Harlow and Los Alamos National Laboratory

High in the mountains of New Mexico, the Los Alamos National Laboratory will forever be synonymous with 'Fat Man' and 'Little Boy'. Nuclear weapons research was indeed the genesis of Los Alamos, but its lasting contributions are far wider-ranging. In our previous Icons article we met Prof. Brian Spalding. In the late 1960's Spalding led a burgeoning CFD group at Imperial College, London. The luminaries in this Group made seminal contributions in the modelling of turbulence, the development of flow solvers and numerical discretisation techniques - all of which were essential in realising Spalding's vision of CFD as a widely-available engineering tool. However, much of the essential groundwork which Spalding and his Group built upon was undertaken at the Los Alamos National Laboratory. The creative force behind this early research was Frank Harlow.

In the 1950's, a key concern at Los Alamos was the fluid-like behaviour of materials under high compression, and in particular the interface between multiple materials. The standard modelling approach was to use a mesh which deformed with the material. This 'Lagrangian' treatment allowed the interface between materials to be accurately tracked. However, when the distortion was very large, not only was the method unstable, but the mesh became 'entangled' and the problem had to be re-meshed, by hand!

Frank Harlow joined Los Alamos in 1953 with a doctorate - not in fluid mechanics - but in quantum field theory. By 1957, Harlow had proposed and developed a radically different approach to the multiple material problem, based on a fixed mesh of cells. In this 'Eulerian' approach, particles are tracked across the fixed mesh. Harlow's 'Particle in Cell' (PIC) method allowed the modelling of transient compressible flow of multiple materials to be undertaken without any restrictions on the deformation of the interface.

The PIC method was a significant step forward. As a consequence, in 1958, the Fluid Dynamics Group (T-3) was created in the Theoretical Division at Los Alamos, with Frank Harlow as its first leader. The Group began with seven members, growing to 15 by 1970 and 25 by 1990. Weapons research was its first area of application, but throughout the 1950's and 1960's there was the freedom to explore many other aspects of CFD – including incompressible free-surface flows. It was the modelling of free-surface flows, such as breaking waves, that led Harlow to develop the so-called MAC method, 'Marker-And-Cell', with Eddie Welch, in 1965. In the MAC approach the free-surface is captured by tracking markers which locate the interface in the mesh.

Harlow and Welch's seminal 1965 paper on the MAC method influenced the development of engineering CFD for decades ahead. It was not so much the modelling of the free-surface that was influential – even though this was significant in its own right – but the numerical methods used to solve the fluid flow equations. There were at least three new developments introduced by Harlow:

- solution of equations for the primitive flow variables – velocity, pressure, etc. – rather than derived variables such as stream function and vorticity, the latter being the usual approach up to that time;
- solution of a Poisson equation* to obtain the pressure field;
- use of multiple, staggered, meshes for the pressure and velocity field.

In this short article we will focus on the third of these new developments; staggered meshes.

Why would one need or want to go to the trouble of using more than one mesh in a single flow computation? The problem is rooted in the numerical modelling of the pressure gradient term which appears in the momentum equations (the fluid-flow equivalent of Newton's second law of motion). If we use a single mesh at which all the flow variables – velocity, pressure, etc – are stored at the same node, then it turns out that there is the possibility for a pressure field to be computed which is completely non-physical, yet which appears to satisfy the momentum equations. This non-physical pressure field has the character of a checkerboard pattern, with the pressure oscillating between two distinct values from one node to the next – see Figure 1. Clearly, this is a highly undesirable feature of a numerical scheme.

Harlow and Welch's answer to this problem was to use multiple meshes; the mesh nodes at which pressure is solved are offset from those of the velocity field, as in Figure 2. For uniform meshes this leads to the velocity nodes being located midway between the pressure nodes, and vice-versa. The pressure gradient which drives the flow is then easily computed and, importantly, the pressure field becomes closely-connected to the velocity field, so avoiding non-physical checkerboard patterns in pressure.

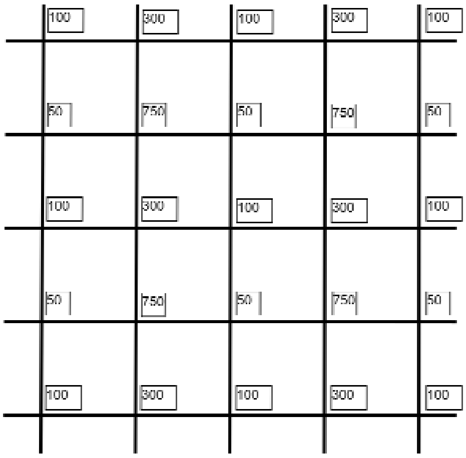


Figure 1: Checkerboard pressure field.

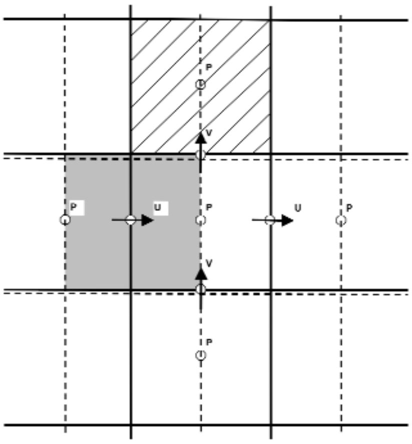


Figure 2: A staggered mesh, for primitive flow variables. **

Spalding's CFD group at Imperial College were aware of the MAC method, but initially were not using staggered meshes. However, they soon encountered the problem of checkerboard pressure fields when solving for the primitive flow variables. As a consequence they took on board the staggered mesh approach. In conjunction with the 'SIMPLE' solution algorithm developed by Patankar and Spalding (1972) this approach became the default numerical method (in one form or another) in most engineering CFD software for several decades. The use of staggered meshes has been gradually superceded by a method which allows the use of a single mesh (Rhie and Chow, 1983), but in its time it was a very significant breakthrough with a long-lasting impact.

It would be wrong to give the impression that Harlow's early contributions to CFD were all in the field of numerical methods. In the 1960's he was also working on turbulence models. Together with Paul Nakayama he set out the basis of the now-ubiquitous $\mathbf{k}-\varepsilon$ turbulence model (Harlow and Nakayama, 1968). Essentially, this work on turbulence models appears to have been proceeding roughly in parallel on both sides of the Atlantic; at Los Alamos, and Imperial College London – with both groups reaching broadly similar conclusions (Runchal, 2008).

The Los Alamos T-3 Group benefited widely from the creative leadership of Frank Harlow throughout the 1960's and beyond. The Group refined the original 'PIC' method under Harlow's direction, it becoming 'FLIC' – FLuid-In-Cell. The MAC method was also further developed in collaboration with Tony Amsden (1970), becoming 'SMAC' – Simplified MAC.

Harlow continued as leader of the T-3 Group at Los Alamos until 1973. He has said that 1968 was the last year that he could keep up with all of the CFD developments around the world (Johnson, 1996). Perhaps this is a measure of the very rapid growth in CFD research and development which has continued since the late 1960's. Of course this was a time when there was wide interest in science and technology; Harlow and Fromm (1965) even wrote a popular science paper on CFD, published in Scientific American.

The Los Alamos T-3 Group has continuously expanded the breadth and depth of their CFD development and applications since their inception. The interested reader can find further information in Johnson (1996) and on the T-3 web-site (http://t3.lanl.gov/). Frank Harlow was an instrumental part of this early growth but also contributed massively until his retirement in 2003, after 50 years continuous service.

Harlow published over 150 research papers during his time at Los Alamos. This was all the more impressive an achievement as Harlow worked outside of academia. Remarkably, he has also published widely in the field of anthropology and palaeontology, writes on Indian pottery, and is an accomplished painter. During a special symposium in his honour, in 2003, colleagues remarked that: "Harlow was our mentor and brought out the best in people, and whether he was the Group Leader or not he was always the group leader". He is truly an 'Icon of CFD'.

Icons of CFD continues in the next issue of Benchmark, focusing on Prof. Suhas Patankar and his 'SIMPLE' solution algorithm.

*Footnote: A Poisson equation for pressure takes the form: $\nabla^2 P(x,y,z) = f(x,y,z)$
It is a 2nd-order partial differential equation.

** The mesh cells surrounding pressure nodes (P) are shown as solid lines and a single mesh cell is indicated by the cross-hatching.

The mesh cells surrounding U-velocity component nodes are shown as dashed lines and a U-velocity component mesh cell is indicated by the shaded region.

The V-velocity component nodes are shown, but the staggered V-component mesh is not drawn for reasons of clarity.

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