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PIC AND ITS PROGENY

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ABSTRACT

The Particle-in-Cell (PIC) method was developed to solve numerically for the strongly contorting dynamics of several materials in two or three space dimensions. Related numerical techniques with Lagrangian marker particles are also discussed in this brief survey. An extensive bibliography lists many of the earlier publications describing these techniques.

A generic challenge for numerical fluid dynamics is to solve for the time-varying behavior of several materials undergoing large distortions and significant slippage in two or three space dimensions. Despite forty years of intense effort and considerable progress, much of the basic challenge remains. No sooner has one difficulty been overcome than another arises. In addition we demand more: higher accuracy, faster algorithms, greater generality, and a variety of embellishments, including the presence of turbulence, multiphase interpenetration, phase transitions, relativistic effects, chemical or nuclear energy release, interactions with electromagnetic fields, and material strength including elastic-plastic and fracture effects.

Most traditional numerical techniques can be classified as Lagrangian or Eulerian. In their purest forms, each has significant advantages and disadvantages. Lagrangian techniques, with a coordinate system that follows the fluid motion,

permit sharp resolution of material interfaces but suffer from mesh tangling when distortions become severe. Eulerian techniques, with a fixed coordinate system, are robust in the face of strong distortions, but suffer from the diffusion of any discontinuity traveling with the fluid.

Numerous variants and hybrids have been devised to mitigate the disadvantages of the traditional techniques. One of these is the Particle-in-Cell (PIC) method, which combines an Eulerian mesh of computational cells with a Lagrangian mesh of marker particles.

In its initial form, the PIC method is characterized by

- Lagrangian marker particles; mass at points
- Eulerian cells; momentum and energy at cell centers
- Velocity weighting for particle motion
- Donor-cell (upwind) advection, carried by particles
- Calculation cycle split into phases
- Explicit formulation, valid for Mach Number $\gtrsim 0.3$

Numerous calculations with the original PIC formulation explored shock interactions with material interfaces and the deformations that could occur during hypervelocity impact or explosive-driven contortions. Many of these are described and illustrated in the references listed below.

Variants of the original formulation were explored by a number of investigators. Some of these added new elements of physics: radiation flow, multiphase interpenetration, relativistic effects, and high-explosive energy release. Others explored variations in the numerical procedure: smearing out the particles to reduce the jarring effects of discrete point-particle transport, removal of the mesh of Eulerian cells with one or another procedure for calculating particle interactions, or demotion of the particles to the role of markers only.

This last direction is especially characteristic of the Marker-and-Cell (MAC) method for incompressible flow calculations. Developed shortly after Fromm's very successful stream-function-and-vorticity technique for confined incompressible flows, the MAC method was devised for calculating flows with free surfaces. In its original and extended forms, the technique is characterized as follows.

Original MAC

- Eulerian mesh
- Primitive variables (pressure and velocity)
- Staggered variable placement
- Marker particles to show free surface
- Implicit formulation

Some Extensions

- Two materials
- Surface tension
- Creep flow
- Multiphase interpenetration

Splashing drops, sloshing waves, interface instabilities, creeping flows, and three-dimensional pollution transport are among the early studies utilizing the MAC approach.

Whereas the MAC method used particles only as markers, the Particle-and-Force (PAF) technique departed from PIC in the opposite direction. The particles became paramount and the cells were eliminated entirely. Fluid-like behavior was accomplished by means of interparticle forces, chosen so as to correspond to a desired equation of state. This early "free-Lagrangian" technique was moderately successful in application to some two-dimensional test problems, but suffered from fluctuations that especially manifested themselves in ragged behavior of material interfaces. There has been essentially no further work on the interparticle-force approach

beyond the original explorations; modern "free-Lagrangian" and related techniques have followed somewhat different approaches to the treatment of interactions among particles.

It may stretch the definition of "particle" methods to include the Dynamics-of-Contours (DOC) technique in this summary. The "particles" no longer follow elements of fluid; instead they trace the motion of points (or surfaces in multiple space dimensions) at which the densities of mass, momentum, and energy have specified values. The incentive for this approach is that it automatically ensures fine spatial resolution in regions of steep gradients. The technique is especially appropriate in one space dimension, where tests exhibit an excellent degree of accuracy. In two space dimensions, usefulness is limited by some difficult topological constraints, which subsequent investigators have partially overcome (Zabusky and associates).

The original PIC method found considerable use in the two decades after its invention, and variants of it have been used well after that time. The Soviets apparently have made extensive use of the technique, which they call the Large-Particle method. The originators of the PIC method, however, slacked off from its usage in the late 1970's, partly because of difficulties with the method itself, partly in response to needs for other types of methodology (e.g. for far-subsonic multiphase flow problems), and partly in response to other interests (e.g., the transport theory of turbulence).

Difficulties with the method perceived at that time (but greatly alleviated by innovative developments in recent years) include

- Ringing (or bunching) of particles
- Fluctuations from discrete-particle transport effects
- Difficulty in the accurate resolution of thin shells of material
- Lack of rotational and translational invariance

While PIC-method usage was declining, there was considerable emphasis on techniques with staggered meshes, resulting in the development of Arbitrary-Lagrangian-Eulerian (ALE) techniques, principally with velocities at vertices. Implicit techniques extended the calculational capability to all flow speeds and the ideas of mesh adaptability became popular.

In recent years, descendants and cousins of PIC have re-emerged. The advantages of cell-centered velocities for calculations of distorting material interfaces with slip have been exploited by means of extended Godunov techniques to couple pressure and velocity fields. Many new ideas are being explored for particle representations without the underlying Eulerian grid. Clothed with a variety of improvements, PIC itself is demonstrating new muscle for robust problem solving. Many of these recent directions are discussed in detail in other parts of this volume.

Acknowledgment

Developments and application of PIC, MAC, and related techniques have been accomplished only with the dedicated and inspired collaboration of many people, to whom I am extremely grateful. Many of their names appear in the following bibliography.

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