Improving Particle-in-Cell advection modeling using deforming particle kernels

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The particle-in-cell (PIC) method [1] is a flexible hybrid approach well suited for the modeling of multi-phase/multi-component flows. It uses a network of Lagrangian particles superimposed on a Eulerian grid (see Fig. 1). The grid represents the discretization of the physical domain and is used to determine the velocity field and the quantities affected by motionless processes (diffusion, radiation, source, reactions...). The particles carry information about several quantities (composition, temperature, momentum...). Their position is determined individually, usually by advecting them along their characteristics, via the interpolation of the Eulerian velocity field. The physical quantities are continuously transferred back and forth between the particles and the grid, through averaging. The latter involve particles kernels and grid shape functions. The method heavily relies on the choice of the particle kernels and on their meaning, which varies depending on the applications. The original PIC method [1] has been adapted to a variety of research domains. Despite a spatial accuracy often confined to first-order in practice it remains popular for many applications (dispersion of atmospheric and oceanic pollutants, geodynamics, computer graphics, MHD, astrophysics...) because the advection of Lagrangian particles significantly reduces numerical dissipation compared to purely Eulerian methods.

Unfortunately, PIC methods suffer from the clustering and the rarefaction of the number of particles in regions characterized by intense deformation. This phenomenon also concerns incompressible flows for which several grid cells can become completely empty of particles while others are over-represented (Fig. 1). Typical remedies involve: (1) the use of a large number of particles, often generating a prohibitive extra computational cost; (2) the redistribution of the particles in order to maintain a homogeneous sampling of the domain, which induces numerical dissipation that progressively degrades the accuracy of the solution.

I will present an evolution of the PIC method based on a new formulation of the particle kernels that takes into account the strain history in the vicinity of the particles. This new method, named DPIC, allows for a considerably more uniform spatial sampling by the particles with a reasonable computational extra cost (~ 50% relative to the PIC approach using the same number of particles). The DPIC method with only 4 particles per cell (in 2D) generates a solution whose accuracy is comparable to the standard PIC approach with more than 64 particles per cell. Therefore, at comparable precision this new approach allows reducing the computational cost by more than one order of magnitude. This gain is even more important for cases requiring the knowledge of the Lagrangian deformation (as common for applications in geodynamics [2], and more generally to characterize mixing and dispersion in a given flow). The DPIC approach could also be adapted to purely Lagrangian methods (SPH, vortex method), which are also prone to spatial sampling problems.

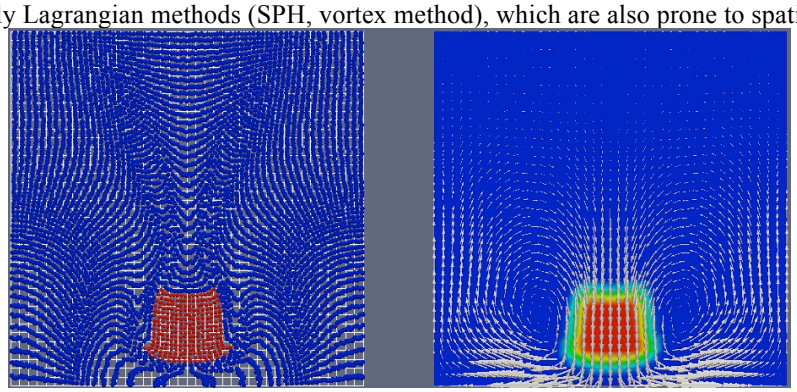

Figure 1. Example of the application of the PIC method, as proposed in [2]. Gravitational flow resulting from the presence of a more viscous and denser, initially square, body (red) relative to the surrounding fluid (blue). Left: Position of Lagrangian particles superimposed on the Eulerian grid. Right: Eulerian velocity field (calculated on the grid) and compositional field (obtained by averaging over the particles' population).

References

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