A multilevel adaptive particle-grid method for gas dynamics

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Abstract: We present a multilevel adaptive grid-based particle method, inspired by the adaptive mesh refinement (AMR) technique, applied to the compressible Euler equations. We show numerical results in two dimensions for the cylindrical Noh's infinite strength shock problem.

1 Introduction

Bergdorf, Cottet and Koumoutsakos, inspired by finite-difference Adaptive Mesh Refinement (AMR) methods first proposed by Berger and Oliger ([2]), introduced in [1] a class of techniques for particle methods that allow to refine dynamically the computational domain and adapt accordingly its particle discretization. These techniques use particle regridding as a key element. We have applied them to a grid-based point particle method for the Euler compressible equations.
In section 2, we first present the particle method, then recall the principles of the adaptive mesh refinement for particle methods. In section 3 we show numerical results obtained by computing the two-dimensional cylindrical Noh problem.

2 Presentation of the method

2.1 Grid-based particle method for the compressible Euler equations.

The method is in the spirit of the Particle-in-Cell (PIC) method pioneered by Harlow [4]: the general idea is to use particles to transport conservative quantities – so that the advection part of the equations is split apart in a Lagrangian fashion - and grid-based formulas to compute fields.

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We start from the compressible Euler equations written in a mixed Eulerian-Lagrangian formulation:

$$d(\rho J)/dt = 0$$

$$d(\rho Ju)/dt = -J \nabla p$$

$$d(\rho JE)/dt = -J \nabla . (pu)$$

$$dJ/dt = J \nabla . u$$

$$dx/dt = u$$

J is the Jacobian of the matrix $(\delta x_i / \delta \xi_j)_{i,j}$,where the x_i are the Eulerian coordinates and the ξ_j the Lagrangian coordinates.
d/dt is the Lagrangian derivative.
The operator ∇ represents spatial derivatives with respect to x.

Once the equations have been discretized on the particles, we obtain the following set of ODEs:

$$d(\rho_p V_p)/dt = 0$$

$$d(\rho_p V_p u_p)/dt = -V_p (\nabla p)_p$$
$$d(\rho_p V_p E_p)/dt = -V_p (\nabla .(pu))_p$$
$$dV_p/dt = V_p (\nabla .u)_p$$

$$dx_p/dt = u_p$$

where ρ_p is the density, u_p the fluid velocity, E_p the total energy, x_p the particle location and V_p the volume of the particle p.

The Lagrangian form of particle methods avoids the explicit discretization of the convective terms and the associated stability constraints.

Particle methods enable an automatic adaptivity, because particle positions are modified according to the local flow map. The local accumulation of particles near large velocity gradients results in a lack of particles in the rest of the domain. Then, it can damage the theoretical convergence rates. Thus, a critical issue for the accuracy of particle methods is the regularity of the particles distribution, and frequent regridding on regular locations is necessary to preserve it.
In this work, regridding is basically a way to define new particles with uniform volume, equal to the size of a grid cell. Thus, there is a strong relationship between the particles and the grid cells: at the beginning of each time step, one particle is located at the center of

each grid cell, and the values of the quantities carried by this particle are equal to those allocated to the cell. Consequently, regridding at every time step allows also to compute the spatial derivatives on a regular grid.

In order to perform regridding we use the interpolation formula M'_4 first suggested by Monaghan [5] . This formula preserves the first three momentums of the interpolated quantities, is continuously derivable, and requires the contributions of the 4 neighbouring particles. It represents a good compromise between smoothness and accuracy, at a reasonable computational cost. Let us recall the definition of M'_4 :

$$\begin{aligned} M'_4 &= 1 - 5/2\ |x|^2 + 3/2\ |x|^3 \quad \text{if } |x| \le 1 \\ &= 1/2\ (2 - |x|)^2\ (1 - |x|) \quad \text{if } 1 \le |x| \le 2 \\ &= 0 \qquad \text{if } 2 \le |x| \end{aligned}$$

This interpolation procedure needs the grid to be cartesian and uniform. Consequently, if the “physical” grid associated with the particles is not cartesian and uniform, as it is the case for the Noh problem, we use an explicit mapping that changes the “physical” grid into a uniform grid. Applying this mapping to the “physical” particles allows us to perform the interpolation on a uniform grid. We obtain the new “physical” particles by applying the inverse mapping to the particles resulting from this interpolation.

Each step of the algorithm consists of the following sequence:

- compute spatial derivatives on the grid by standart centered finite differences,
- update particles quantities $\rho_p\ J_p$, $\rho_p J_p u_p$, $\rho_p J_p E_p$ and J_p on the grid (generally with a 2 or 4 order Runge Kutta time stepping),
- update particle locations x_p thanks to the new velocities obtained from the ratio of the updated quantities $\rho_p J_p$ and $\rho_p J_p u_p$,
- remesh particles on the fixed grid,
- possibly apply an artificial viscosity to treat shocks.

2.2 Adaptive mesh refinement for particle methods

Due to the regridding, the volume of the particles and thus the accuracy of the computation are strongly related to the size of the grid cells. To improve the adaptivity of the method to the physics of the flow, and consequently obtain a better accuracy of the numerical

solution, a new class of techniques with variable grid-sizes has been introduced by Bergdorf, Cottet and Koumoutsakos in [1]. Following the pioneering work of Berger and Oliger on AMR, the idea was to define blocks of piecewise constant grid-sizes that can ajust dynamically, based for instance on a posteriori error estimates. As in [3], the method is heavily based on overlappings of the subdomains, that allow particles around the block-interfaces to exchange informations during the interpolation in order to maintain a consistent approximation at the desired resolution everywhere.

To understand how blocks communicate, we consider two blocks with different grid sizes: a coarse one and a finer one. We assume that at the beginning of the algorithm step all particles provide a consistent approximation of the solution. In each block we distinguish two parts:

- the zone 1, where we are sure this assumption is still valid after one algorithm step (with possible motion of the grid),
- and the zone 2 : the rest of the block.

In zone 1 we distinguish again two domains: the first one, where the interpolation process only needs particles from zone 1, and the second one, where this process needs particles from zone 2 too, that are not “reliable”. In the first domain, the interpolation is done in the usual manner, with contributions of the particles from the block that we are considering, for instance the fine one. In the second domain, as in zone 2, the new particles are created with an interpolation performed on particles from the other block, that is, the coarse one. This leads to overlapping conditions between the blocks to ensure that these coarse particles are located in zone 1 of the coarse block.

3 Numerical illustration: the 2D cylindrical Noh Problem

The Noh problem is an implosion problem, difficult to solve numerically, and thus, a challenging test for hydrodynamics codes.
The initial density is uniform, the specific internal energy negligible, and the velocity uniform and directed toward the origin. The gas is supposed to be polytropic, with adiabatic index $\gamma = 5/3$. This configuration leads to an infinite strength shock instantly reflecting from the origin and propagating outwards (see [6],[7]).

3.1 Initial conditions

Physical properties	***Values***
Density	1.
Pressure	0,001
Radial velocity	1.
Tangential velocity	0.

The computational domain is: $(r, \theta) \in [0, 1] \times [0, 360]$.
We used a fine grid ($\Delta r = 1/400$, $\Delta \theta = 6°$) near the origin, to solve the shock with a good accuracy, and a coarse one ($\Delta r = 1/50$, $\Delta \theta = 6°$) everywhere else, with $\Delta t = 0.0005$ for the fine grid, and $\Delta t = 0.004$ for the coarse grid.

3.2 Results

Figure 1 shows the results obtained with the multilevel particle method compared to the analytical solution, at t = 0,6 s.
The results are in good agreement with the analytical solution. Concerning the multilevel aspect of the simulation, we remark that the transition between the fine and the coarse grids, located at this time around 0.2, is unnoticeable, which means that the communication procedures between the grids work well. On the other hand, we recognize a wall-heating effect, typical of Lagrangian methods for this problem, near the origin: the density is under-evaluated, while the specific internal energy is too high. We hope to reduce this phenomenon in the future by giving a special care to the treatment of the artificial viscosity for the particles in contact with the origin.

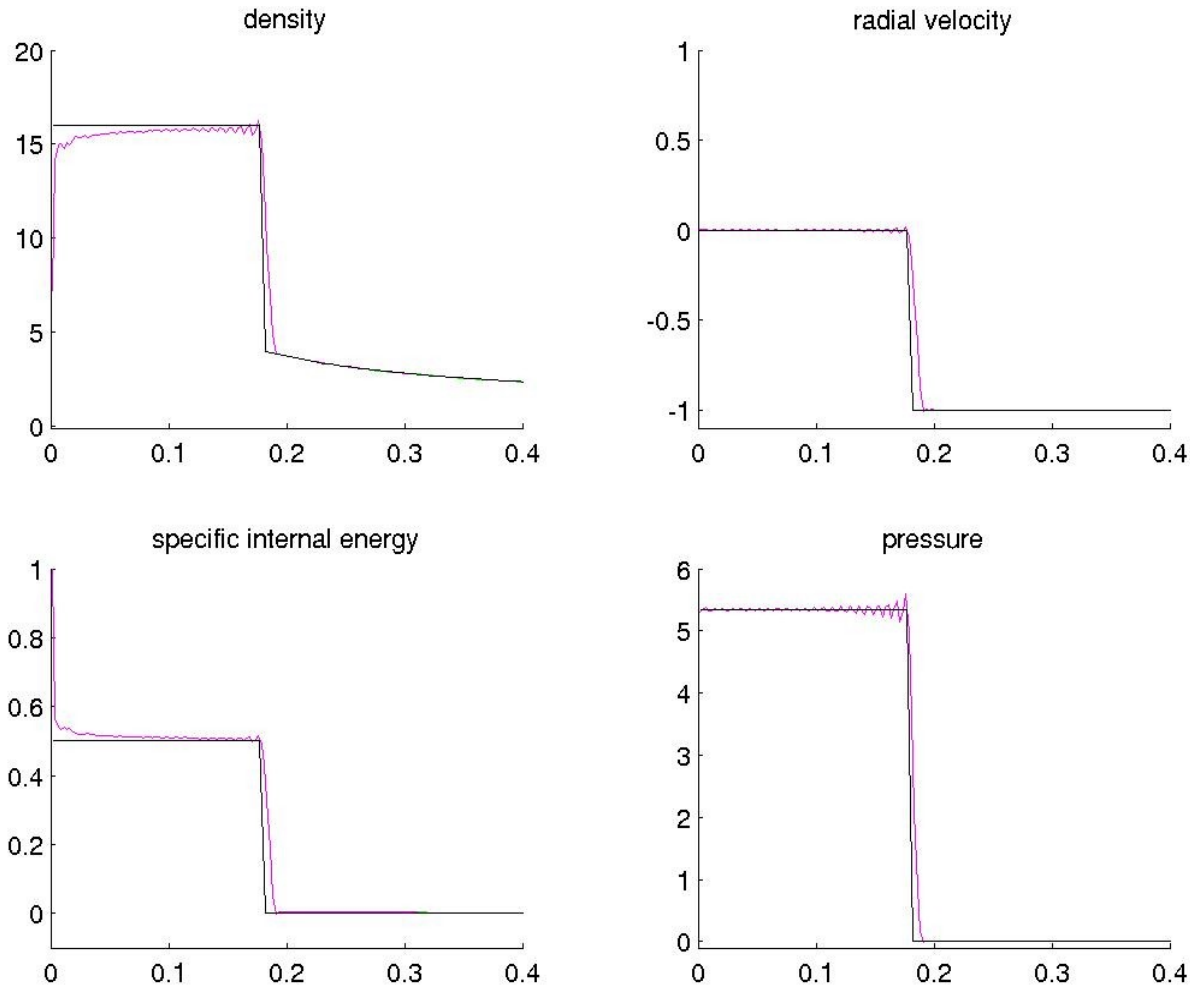

Figure 1: the Noh Problem

4 Conclusion

We have presented a two-dimensional application of an adaptive mesh refinement technique for grid-based particle methods. Numerical results performed on the Noh problem on one hand validate the communication procedure between the grids, which is heavily based on the existence of overlapping zones and on the regridding technique, and on the other hand show that the grid-based particle method itself is well-suited for the simulation of compressible gas dynamics.

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