Procedia Computer Science
Volume 80, 2016, Pages 2433–2437
ICCS 2016. The International Conference on Computational Science

Second Order Upwind Lagrangian Particle Method for Euler Equations

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Abstract

A new second order upwind Lagrangian particle method for solving Euler equations for compressible inviscid fluid or gas flows is proposed. Similar to smoothed particle hydrodynamics (SPH), the method represents fluid cells with Lagrangian particles and is suitable for the simulation of complex free surface / multiphase flows. The main contributions of our method, which is different from SPH in all other aspects, are (a) significant improvement of approximation of differential operators based on a polynomial fit via weighted least squares approximation and the convergence of prescribed order, (b) an upwind second-order particle-based algorithm with limiter, providing accuracy and long term stability, and (c) accurate resolution of states at free interfaces. Numerical verification tests demonstrating the convergence order for fixed domain and free surface problems are presented.

Keywords: particle methods, generalized finite differences, meshless methods, smooth particle hydrodynamics

1 Introduction and Motivation

Smooth particle hydrodynamics (SPH) [2, 3] is a Lagrangian particle-based method that gain popularity due to its ability to handle complex free surface flows. Other important SPH properties are the conservation of mass and adaptivity to density changes. However, the major drawback of SPH is a very poor accuracy of discrete differential operators. It is widely accepted [4], including original SPH developers [3], that the traditional SPH discretization has zero-order convergence for widely used kernels. The limited success of SPH is based on the hidden Hamiltonian property: the discrete system effectively solves the Hamiltonian dynamics of particles interacting via special potentials, which is similar but not identical to the solution of the original fluid dynamics PDE's, thus leading to non-convergence. A number of "modern" or "corrected" SPH methods (see [3, 4] and references therein) improve certain features of SPH at the expense of other properties such as conservation or long-time stability, but still remain zero-order or at best 1st order convergent.

Selection and peer-review under responsibility of the Scientific Programme Committee of ICCS 2016

doi:10.1016/j.procs.2016.05.543

We have proposed a new Lagrangian particle method for solving compressible Euler equations that eliminates major deficiencies of SPH: accurate discretization of differential operators is achieved using weighted least-squares (WLS) approximations also known as generalized finite differences [6], and long term stability is achieved via upwind discretization methods. An algorithm for accurate resolution of states on free surfaces is also developed and tested. The method is also easily generalizable to coupled systems of hyperbolic and elliptic or parabolic PDE's.

2 Governing Equations

Following [1], we write the system of Euler equations in one spatial dimension in the Lagrangian form as

$$U_t + A(U)U_x = 0, \quad U = \begin{pmatrix} V \\ u \\ P \end{pmatrix}, \quad A(U) = V_0 \begin{pmatrix} 0 & -1 & 0 \\ 0 & 0 & 1 \\ 0 & K & 0 \end{pmatrix}, \quad K = \left(P + \frac{\partial e}{\partial V}\right) \Big/ \frac{\partial e}{\partial P}\,, \tag{1}$$

where V is the specific volume, u is the velocity, P is the pressure, and the equation of state (EOS) is in the form $e = f\,(P, V)$, where e is the specific internal energy. If the matrix A is diagonalized as $A = R\Lambda R^{-1}$, equations (1) become

$$U_t + R\Lambda R^{-1} U_x = 0 \quad \Longrightarrow \quad R^{-1}U_t + \Lambda R^{-1}U_x = 0, \tag{2}$$

where

$$R^{-1} = \begin{pmatrix} 1 & 0 & \frac{1}{K} \\ 0 & -\frac{1}{2\sqrt{K}} & -\frac{1}{2K} \\ 0 & \frac{1}{2\sqrt{K}} & -\frac{1}{2K} \end{pmatrix}, \quad R = \begin{pmatrix} 1 & 1 & 1 \\ 0 & -\sqrt{K} & \sqrt{K} \\ 0 & -K & -K \end{pmatrix}, \quad \Lambda = V \begin{pmatrix} 0 & & \\ & \sqrt{K} & \\ & & -\sqrt{K} \end{pmatrix}.$$

Based on the governing equations (2), we have developed stable, particle-based, upwind numerical schemes. Details are described in the next section.

3 Numerical Discretization and Main Algorithms

To solve numerically the hyperbolic system of PDE's (2), the medium (compressible fluid or gas) is discretized by a distribution of particles. Each particle represents a Lagrangian fluid cell of equal mass, and stores states of the continuum medium such as density (that is proportional to the number density of Lagrangian particles), pressure, internal energy, velocity, as well as material properties and pointers to data structures containing material models, such as the EOS.

The system 2 represents, in terms of transformed dependent variables, advection equations with the characteristic speeds 0, $\sqrt{K}$, and $-\sqrt{K}$. Writing it in a component-wise form and adding the subscripts l and r to the spatial derivatives to indicate that the corresponding terms, in the discrete form, will be computed using one-sided derivatives, we obtain the following system

$$
\begin{aligned}
V_t &= \frac{V_0}{2}\left(u_{xr}+u_{xl}\right)-\frac{V_0}{2\sqrt{K}}\left(P_{xr}-P_{xl}\right), && (3)\\
u_t &= \frac{V_0\sqrt{K}}{2}\left(u_{xr}-u_{xl}\right)-\frac{V_0}{2}\left(P_{xr}+P_{xl}\right), && (4)\\
P_t &= -\frac{V_0 K}{2}\left(u_{xr}+u_{xl}\right)+\frac{V_0\sqrt{K}}{2}\left(P_{xr}-P_{xl}\right). && (5)
\end{aligned}
$$

An important component of a particle-based numerical scheme is the calculation of differential operators based on states at the location of particles. Our method achieves accurate discretization of differential operators using the weighted least-squares (WLS) approximation also known as the generalized finite differences [6, 7].

The first-order ($O(\Delta t, \Delta x)$) upwind discretization of the system (3-5) is obtained using the 1st order WLS approximation of spatial derivatives , and the 1st order discretization of temporal derivatives of the state ($V,\ u,\ P$) at the location of particle j. After the updates of states of each Lagrangian particle, particles are advanced by a mixture of the forward and backward Euler schemes:

$$
\frac{x^{n+1}-x^n}{\Delta t} = \frac{1}{2}\left(u^n+u^{n+1}\right) \tag{6}
$$

The first order scheme is stable, provided that the standard CFL condition is satisfied: $dt <= l/max(c,u)$, where l is the smallest interparticle distance, but diffusive. To reduce the amount of numerical diffusion of the 1st order scheme and obtain higher order approximations in space and time, we propose a *modified Beam-Warming* scheme for the Lagrangian particle system. For the same reason as in the grid-based Beam-Warming method [8], an additional term is added to equation (1):

$$
U_t + A(U)U_x - \frac{\Delta t}{2}A^2(U)U_{xx} = 0 \Rightarrow R^{-1}U_t = -\Lambda R^{-1}U_x + \frac{\Delta t}{2}\Lambda^2 R^{-1}U_{xx}. \tag{7}
$$

Performing similar manipulations as in the case of the 1st order method, we obtain the system of equations in upwind form that involves 1st and 2nd order one-sided spatial derivatives. By discretizing spatial derivatives using the second order WLS, we obtain a numerical scheme that is second order in both time and space, $O(\Delta t^2, \Delta x^2, \Delta t\Delta x)$, and conditionally stable.

As is typical to a second order scheme, the modified Beam-Warming scheme is oscillatory in the location of strong solution gradients and discontinuities. This problem was resolved by developing a limiter method similar to the Van Leer limiter [8]. The multidimensional problems are solved using the Strang splitting method [5] that maintains second order accuracy.

In a simulation involving Lagrangian particles, it is critical that an efficient neighbor search algorithm is employed. If the matter is approximately uniformly distributed in the computational domain, a supercell search algorithm is used. For strongly non-uniform distribution, the search particle neighbors is based on the construction and search of quad (2D) and octrees (3D).

The fluid / vacuum interface is modeled in our method by using *ghost* particles in the vacuum region. A geometric algorithm places patches of ghost particles outside the fluid boundary, ensures their proper distance to the interface, and eliminates those particles that were placed too closely or inside the fluid. Then the ghost particles are assigned the physics states of vacuum pressure and fluid velocity, using WLS interpolation. The only functionality of ghost

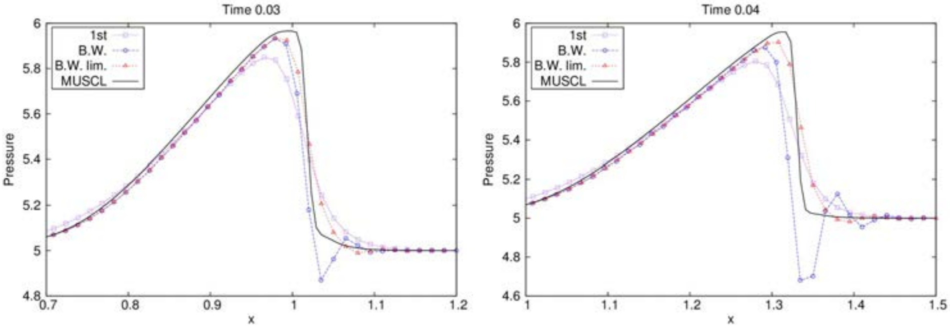

Figure 1: Gaussian pressure wave propagation with periodic boundaries at time 0.03 (left) and 0.04 (right). Coarse-resolution simulations results were used to illustrate the behavior qualitatively.

particles is to serve as neighbors of fluid particles when calculating spatial derivatives. This simple algorithm adequately handles the fluid / vacuum interface, but a Riemann solver-based algorithm will be used for interfaces in multiphase problems.

4 Numerical Results

In this section, we present simulation results obtained with the Lagrangian particle method, including the free surface algorithm.

In the 1st test, we study the propagation of pressure waves in gas with constant initial density $\rho = 0.01$ and the initial Gaussian pressure distribution $P = 5 + 2\exp -100x^2$ in the domain $-1.5 \leq x \leq 1.5$ with periodic boundaries. The polytropic gas EOS is used with $\gamma = 5/3$. The goal of the simulation is to demonstrate the accuracy of the proposed algorithm in resolving nonlinear waves with the formation of shocks. The benchmark data is obtained using a highly refined, grid-based 1D MUSCL scheme. The results, shown in Figure 1, are labeled as *1st* for the first order WLS approximation, *B.W.* for the Beam-Warming scheme with the second order WLS approximation, and *B.W. lim.* for the Beam-Warming scheme with the second order WLS approximation and limiter, respectively. As expected, first order scheme is diffusive, while the Beam-Warming scheme is dispersive near discontinuities. However, results demonstrate that the proposed limiter method effectively reduces oscillations near sharp edges, resulting in the second order of convergence. We have also verified that the Lagrangian particle method accurately resolves waves in stiff materials with large values of parameters defining the stiffness and the sound speed. In both cases, the second order convergence was obtained.

The second problem is a verification test for the motion of free boundary. A liquid disk, modeled using the stiffened polytropic EOS model with $\gamma = 6$, $P_\infty = 7000$, and initial $\rho = 1$, has initially a Gaussian distribution of pressure. The resulting pressure wave interacts with the free boundary and causes oscillation of the disk radius. A well-resolved 1D problem was used as a benchmark solution, and second convergence order was achieved. The verification test and the fact that the pressure wave maintains good symmetry after many reflections from the free surface demonstrate that the proposed method for modeling vacuum with ghost particles works well with the overall algorithm. We have also obtained simulations of gas expansion into vacuum (see Figure 2, right) and confirmed their accuracy by comparing to theory.

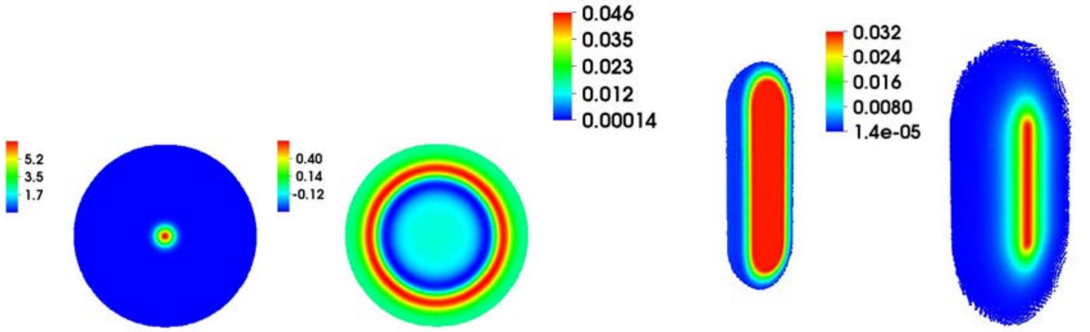

Figure 2: 2D simulation of liquid disk with free surface (two left images). 3D simulation of gas expansion into vacuum (two right images show pressure distribution).

5 Conclusions and Future Work

A Lagrangian particle method has been proposed for the simulation of Euler equations describing compressible inviscid fluids or gases. The method greatly improves the accuracy and convergence order of SPH. The main contributions of our method are (a) significant improvement of approximation of differential operators based on weighted least squares approximations and convergence of prescribed order, (b) an upwind second-order particle-based algorithm with limiter, providing accuracy and long term stability, and (c) accurate resolution of states at free interfaces. Numerical verification tests demonstrate the second convergence order of the method, including problems with free surfaces. Future developments will include new high resolution particle-based WENO-type solvers and coupled multiphysics problems.

Acknowledgement. This research has been partially supported by the DOE Muon Accelerator Program. This manuscript has been authored in part by Brookhaven Science Associates, LLC, under Contract No. DE-SC0012704 with the US Department of Energy.

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