Journal of Computational Physics 266 (2014) 191–213

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

Hydrodynamic shock wave studies within a kinetic Monte Carlo approach

Irina Sagert [a,*], Wolfgang Bauer [b,c], Dirk Colbry [c], Jim Howell [c], Rodney Pickett [c], Alec Staber [c], Terrance Strother [d]

[a] Center for Exploration of Energy and Matter, Indiana University, Bloomington, IN 47308, USA
[b] Department of Physics and Astronomy, Michigan State University, East Lansing, MI 48824, USA
[c] Institute for Cyber-Enabled Research, Michigan State University, East Lansing, MI 48824, USA
[d] XTD-6, Los Alamos National Laboratory, Los Alamos, NM 87545, USA

ARTICLE INFO

Article history:
Received 14 October 2013
Received in revised form 23 January 2014
Accepted 15 February 2014
Available online 26 February 2014

Keywords:
Kinetic simulation
Monte Carlo
Shock waves
Fluid dynamics
Non-equilibrium

ABSTRACT

We introduce a massively parallelized test-particle based kinetic Monte Carlo code that is capable of modeling the phase space evolution of an arbitrarily sized system that is free to move in and out of the continuum limit. Our code combines advantages of the DSMC and the Point of Closest Approach techniques for solving the collision integral. With that, it achieves high spatial accuracy in simulations of large particle systems while maintaining computational feasibility. Using particle mean free paths which are small with respect to the characteristic length scale of the simulated system, we reproduce hydrodynamic behavior. To demonstrate that our code can retrieve continuum solutions, we perform a test-suite of classic hydrodynamic shock problems consisting of the Sod, the Noh, and the Sedov tests. We find that the results of our simulations which apply millions of test-particles match the analytic solutions well. In addition, we take advantage of the ability of kinetic codes to describe matter out of the continuum regime when applying large particle mean free paths. With that, we study and compare the evolution of shock waves in the hydrodynamic limit and in a regime which is not reachable by hydrodynamic codes.

1. Introduction

In fluid dynamics, when the characteristic length scale of a flow is smaller than the mean free path of its components, the continuum approximation which is assumed by the Navier–Stokes (NS) equations breaks down and the particle nature of matter must be taken into account [1]. Under these conditions, flows are said to be rarefied. The rarefaction of a flow is characterized by the Knudsen number K, which is defined as the ratio of the mean free path λ to a characteristic length scale of the system L:

$$K = \lambda / L. \tag{1}$$

While the continuum limit of hydrodynamics is applicable for $K \ll 1$, flows with $K > 0.01$ are not well described by the NS equations as these do not form a closed set in this regime [1]. Simulations of shock structures [1] and hypersonic flow [2], studies of space flight [3] and nano-scale devices [4], particle production in heavy-ion collisions [5–9], the dynamics of inertial confinement fusion (ICF) capsules [10–12], and neutrino–matter interactions in core-collapse supernovae (CCSN) [13]

* Corresponding author.

http://dx.doi.org/10.1016/j.jcp.2014.02.019
0021-9991/

are all examples of research areas which require the ability to model flows with $K > 0.01$. In our work we are especially interested in the modeling of ICF capsules and CCSN.

Despite the enormous efforts poured into achieving thermonuclear ignition of ICF capsules at the National Ignition Facility (NIF), satisfactory yield has not yet been obtained. The ICF capsule experiments at NIF are guided by complex numerical simulations. Codes which suggest that the employed techniques should have been successful in igniting the nuclear fuel, all use continuum hydrodynamics to describe the entire capsule system. However, the so-called *hot spot* of an ICF capsule where thermonuclear burn is expected to occur is approximately 25 μm across and has a density and temperature on the order of 100 g/cc and 10 keV, respectively [14]. In this environment, the mean free path of a thermal deuteron, a critical component of the nuclear fuel, is on the order of a few micrometers and the continuum approximation is not applicable. Further investigations found that non-maxwellian ion distributions resulting from shock front kinetic effects that deplete the ion distribution of fast particles [10–12,15–18] may alter the hydrodynamics and thermonuclear yield of ICF capsules. Other studies suggest that capsule yield can be diminished by kinetic effects associated with strong self-generated electric fields which can broaden the shock fronts [19,20]. With that, the physics of ICF capsules being possibly subject to strong non-equilibrium effects provides a strong motivation to develop a kinetic simulation code that is capable to fully resolve shock fronts in all regions of the capsules.

Many theories have been suggested to explain the explosion mechanism of CCSNe [21–27]. The most commonly accepted model is based on energy deposition by neutrinos that are produced in the central high temperature and high density region of the collapsed stellar core into cooler less dense regions of infalling nuclear matter [21,22,28]. Simulations suggest that this so-called neutrino heating can power fluid instabilities that grow to large amplitudes and eventually power an explosion [29,30]. To study such a scenario, an accurate description of the supernova hydrodynamics and neutrino transport in three dimensions (3D) seems to be inevitable [31–34]. While for 1D simulations, it is possible to solve the full Boltzmann equations for neutrino propagation [35–37], in two or three dimensions this approach becomes computationally too expensive and approximations have to be made [38–41,96]. Monte Carlo neutrino transport has the potential to scale better for multi-dimensional calculations and has been suggested as an alternative approach for CCSNe studies (see [42] and references therein). Most simulations have been operating with nuclear equations of state which evolve only one representative heavy nucleus. More modern approaches apply equations of state that describe low density and low temperature nuclear matter as a full statistical ensemble of present nuclei (see e.g. [43,44]). The inclusion and evolution of the latter could alter weak interaction processes and thereby the efficiency of neutrino heating as well as impact supernova nucleosynthesis [28,45–47]. It has been demonstrated in previous works that a kinetic approach has the capability to treat baryon and neutrino dynamics identically and thereby evolve an ensemble of nuclei as well as model out-of-equilibrium neutrino–matter interactions [13,48]. Preliminary studies conducted with such an approach found that out-of-equilibrium neutrino–matter interactions with nuclei close to the neutron drip line could significantly impact the dynamics of CCSN explosions [13,48]. However, more detailed calculations are necessary to confirm the observed effects.

It is the long-term goal of this work to contribute to the modeling of systems which are influenced by out-of-equilibrium phenomena, such as ICF capsules and CCSN. For this, we develop a kinetic code that is capable to resolve macroscopic 3D hydrodynamic flows and describe non-continuum behavior. Our approach is based on a combination of two kinetic methods for solving the Boltzmann equation – the Direct Simulation Monte Carlo technique (DSMC) and the Point of Closest Approach (PoCA) method. Together, these two methods can provide the computational feasibility to model large scale systems while maintaining spatial accuracy of the simulations. The latter is crucial for the study of shock fronts which play an important role for ICF capsules and CCSN dynamics.

This work serves as an introduction to our kinetic Monte Carlo code as well as a demonstration of its ability to evolve shock fronts in 2D and 3D setups. After a brief introduction to kinetic methods in Section 2, we describe our simulation setup in Section 3. In Section 4, we present our results for shock wave modeling for matter in the hydrodynamic regime while Section 5 is devoted to shock fronts in matter with large particle mean free paths. Finally, we close with a summary and outlook in Section 6.

2. Kinetic methods

2.1. The Boltzmann equation

The governing equation for non-continuum flows is the Boltzmann equation of kinetic theory. It is a nonlinear integro-differential equation that describes the time evolution of a statistical distributions of particles in a fluid that undergo binary collisions. The Boltzmann equation is valid for all Knudsen numbers and leads to the continuum description in the limit of small mean free paths [49]. For a fluid comprised of N different particle species, the Boltzmann equation for the probability distribution function (PDF) of the ith particle species is [50]:

$$\frac{\partial f_i(\vec{r},\vec{p},t)}{\partial t} + \frac{\vec{p}}{m_i}\cdot\nabla f_i(\vec{r},\vec{p},t) + \vec{F}\cdot\frac{\partial f_i(\vec{r},\vec{p},t)}{\partial \vec{p}} = I_{i,\mathrm{coll}}. \tag{2}$$

Hereby, $\vec{r}$, $\vec{p}$, and m_i are the position, momentum, and mass of particle i respectively. $\vec{F}$ is the external force field, and $f_i(\vec{r},\vec{p},t)$ is the number of particles of species i that are found in a differential phase space neighborhood of $\vec{r}$ and $\vec{p}$ at time t. The term $I_{i,\mathrm{coll}}$ on the right hand side of Eq. (2) takes into account the changes in f_i that are induced by two-body collisions. $I_{i,\mathrm{coll}}$ is generally a sum of integrals involving the pre- and post-collision PDFs of all species present [50]. It is this