White Paper for Frontiers of Plasma Science Panel

Date of Submission: 11 June 2015

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<td>• Statistical mechanics of plasmas</td>
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Type of presentation desired at Town Hall Meeting: Oral

Title: Adaptive Kinetic-Fluid Models for Multi-Phase Plasmas

Corr. Author: Vladimir Kolobov

• Institution: CFD Research Corporation and University of Alabama in Huntsville

• email: vik@cfdr.com

Co-Authors: Robert Arslanbekov, CFD Research Corporation

Uri Shumlak, University of Washington

Gary Zank, University of Alabama in Huntsville

The research frontier and the scientific challenge

Plasma dynamics are characterized by a wide range of spatial and temporal scales covering particle transport and electromagnetics. Depending on conditions, transport of neutral and charged particles in partially ionized plasmas is best described by either atomistic (kinetic) or continuum (fluid) models. Kinetic description is much more detailed and much more expensive computationally compared to the continuum description and should be used only when necessary. Depending on conditions, the continuum multi-fluid description may be adequate for some plasma components whereas other component(s) should be treated by kinetic models.

Adaptive kinetic-fluid simulations apply kinetic solvers in selected regions of phase space for efficient description of different scales. Appropriate models are selected using sensors locally detecting phase space regions where a kinetic approach is required. For gas dynamics in mixed rarefied-continuum regimes, this methodology has been successfully implemented using an Adaptive Mesh and Algorithm Refinement (AMAR) methodology first introduced for DSMC-fluid coupling.\(^1\) A Unified Flow Solver (UFS) has been developed to combine Adaptive Mesh Refinement (AMR) with automatic selection of kinetic (Boltzmann) and fluid (NS) solvers based on continuum breakdown criteria.\(^2\)

The extension of the AMAR technique to plasma simulations poses scientific challenges due to the disparity of temporal and spatial scales typical to plasmas.\(^3\) Continuum breakdown criteria for electrons, ions and neutrals are quite different and strongly depend on plasma conditions. Furthermore, different kinetic models could be used for electrons depending on electron energy and the plasma type (collisional vs collisionless, magnetized vs non-magnetized).\(^4\) Nevertheless, first steps towards adaptive physics algorithms that dynamically create and remove localized kinetic patches within global fluid plasma models have been made. In particular, two-way coupling of a global Hall magnetohydrodynamics with a local implicit PIC model (MHD with Embedded PIC regions (MHD-EPIC)) has been demonstrated for space plasmas.\(^5\)

Multi-fluid plasma models can capture essential physics of multi-component reacting mixtures of ions, electrons, and neutrals. Such models have been successfully implemented using finite volume\(^6\) and high-order discontinuous Galerkin methods\(^7\) with the treatment of atomic and molecular physics.\(^8\) High-order finite volume methods have been applied to solve the kinetic Vlasov equation.\(^9\) The two-fluid plasma model has been used to study drift turbulence instabilities,\(^10\) which may be related to the experimentally observed anomalous resistivity.
Today’s simulations could benefit from using a combination of massively parallel GPUs and fast multicore CPUs. However, the existing computational algorithms must be redesigned for heterogeneous CPU-GPU architectures. Kinetic solvers are well suited for parallel computing. Impressive acceleration and excellent multi-GPU scaling have been demonstrated by several groups using particle and mesh-based methods. Coupled Vlasov and two-fluid codes have recently been demonstrated using GPU for Vlasov solvers in locally selected kinetic domains.

The approach to advancing the frontier and the development of new research tools and capabilities

To advance this frontier, we propose to develop a multi-phase plasma simulation tool using adaptive kinetic-fluid models for heterogeneous computing architectures. The new tool will have a) ability to dynamically switch between fluid and kinetic solvers for different plasma species, b) robust auto-mesh generation and adaptive mesh refinement algorithms, c) implicit solvers adapted for massively parallel CPU-GPU systems, and d) multi-phase capabilities for treatment of phase transitions and inter-phase phenomena. Our technical approach consists of advancing the previously developed AMAR methodology shown in Figure 1 (left part). AMAR provides the highest level of adaptation and allows using different physical models in different parts of the computational domain. The UFS framework enables coupling of continuum (fluid) solvers with the kinetic solvers on a cell-by-cell basis. The computational domain is decomposed into kinetic and fluid cells using continuum breakdown criteria for mixed rarefied-continuum flows (see Figure 1, right part). This methodology is also used in our hybrid radiation transport model coupling a Photon Monte Carlo (PMC) solver with a diffusion model of radiation transport, with the solver selected based on the local photon mean free path.

The Kinetic Module in the AMAR framework can solve Boltzmann, Vlasov, and Fokker-Planck kinetic equations for different species using different methods. Eulerian kinetic solvers use the Discrete Velocity Method (DVM) for solving kinetic equations. The statistical particle methods (such as DSMC and PMC) are based on Lagrangian transport models. In addition to the original DVM Boltzmann solver in UFS, we have recently developed a particle-based DSMC solver, an Adaptive Mesh in Phase Space (AMPS) methodology, and a mesoscopic LBM solver. Some of the kinetic solvers have been adapted for heterogeneous CPU-GPU computing on multi-GPU systems. The Plasma Module has multi-fluid solvers linking to database for atomic physics and the chemistry Module for chemical reactions.

We will advance the AMAR framework in several directions:
- Develop a new PIC Module and Maxwell solvers for heterogeneous CPU-GPU computing exposing the inherent parallelism of the kinetic and electromagnetic solvers.
- Develop implicit solvers and new regularization algorithms for dynamic AMAR execution on heterogeneous CPU-GPU architectures.
- Develop physics-based switching criteria to dynamically select kinetic and fluid models for different plasma species (electrons, ions, neutrals) on a cell-by-cell basis.
- Develop new capabilities for multi-phase plasma simulations for treatment of phase transitions and interphase phenomena, and heterogeneous chemical reactions.

Impact of proposed research on plasma science and related disciplines and societal benefits

The proposed research leverages ongoing work at CFD Research Corporation and the DoE Plasma Science Center (PSC) on plasma kinetics in multi-phase systems. A combination of several methodologies will offer revolutionary advances to outperform existing tools in a very significant way:
- Combining AMR capabilities with abilities to solve different sets of equations in different parts of computational domain (phases), simulate phase transitions, track moving interfaces, and use adaptive kinetic-fluid solvers for charge transport, atomic physics and chemistry.
- Designing computational algorithms to fully utilize capabilities of modern heterogeneous computers using multi-core CPU-GPU hardware.

2
• Open collaborative framework enabling implementation of additional models from relevant fields
to be developed by academia and user community.

A very broad range of applications from space sciences to biology and medicine will benefit from the proposed advances. Technologies using low temperature plasmas in gas, liquid, and solid media are now increasingly being used for biomedical, environmental, space, and energy applications, often at interfaces of physical and life sciences. The proposed tool will help advance plasma science and industrial applications of LTP by offering high-fidelity, user-friendly software with self-aware physics to academic and industrial researchers developing plasma technologies. The project will help clarify many essential problems of LTP science including space sciences, pulsed power sources driven by runaway electrons, streamer and spark dynamics in laboratory and atmosphere, plasma-induced phase transitions, and plasma particle interactions with liquids and bio tissues. Many relevant phenomena, which are poorly understood now, will be investigated using the new capabilities.

Figure 1. AMAR architecture (left) and UFS demonstration (right) for gas flow around a cylinder at $Ma = 3$, $Kn = 0.01, 0.1,$ and $0.3$ (from top to bottom): adapted computational grid with kinetic (red) and continuum (blue) domains.
Figure 2. Residual charge distribution measured for a surface streamer discharge using pockels crystals \(^13\) (left); CFDRC simulations of streamer formation in corona discharge (center); Electric breakdown in liquid (right).

References