Adaptive Kinetic-Fluid Models for Multi-Phase Plasmas

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Frontiers of Plasma Science
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Agenda

• Desirable features of future plasma codes:
  • Adaptive Mesh Refinement
  • Physics-based criteria for switching between fluid and kinetic models
  • Multi-material properties, phase transitions, interface tracking
  • Heterogeneous CPU-GPU computing
  • Semi-Implicit solvers to mitigate disparity of time scales

• State of the Art: Unified Flow Solver
  • Adaptive Mesh and Algorithm Refinement (AMAR)
  • Kinetic Solvers & Fluid Plasma Models
  • GPU-accelerated kinetic solvers

• Scientific problems calling for new computational methodologies
  • Streamers, sparks, arcs, …
  • Multiphase plasmas
  • Near-electrode phenomena, self-organization and pattern formation

• Physical Frontiers and Computational Challenges
An overview of existing hybrid plasma codes

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<th>Hybrid Kinetic-Fluid</th>
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<th>GPU</th>
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- There is currently no code that has all the desired capabilities.
- The Unified Flow Solver (UFS) developed by CFDRC has most of the desired capabilities.
- UFS combines Adaptive Mesh Refinement (AMR) technique with automatic cell-by-cell selection of kinetic or fluid solvers: an Adaptive Mesh and Algorithm Refinement (AMAR) procedure.
- Tree-based Cartesian mesh technique of UFS allows automatic generation of computational mesh for complex boundaries and dynamic mesh adaptation to solution and moving objects without human intervention.
Adaptive Cartesian Mesh

A 2:1 balanced grid is represented by octree. Additional constraints simplify the gradient and flux calculations:

(a) the levels of direct neighbors cannot differ by more than one;

(b) the levels of diagonal neighbors cannot differ by more than one;

Boundary Conditions

Cut-cell and IBM approaches. Cut cells are yellow, ghost cells are blue.

Fully threaded tree structure for efficient traversal, access to neighbor cells, cell level and spatial coordinates.

http://gfs.sourceforge.net
Adaptive Mesh & Algorithm Refinement (AMAR)


Gas flow over a cylinder $M=3$

• Gas mixtures: different kinetic domains for heavy and light species

• Plasma simulations with AMAR require different criteria for electrons, ions and neutral species.
Adaptive Mesh in Phase Space

Tree-of-trees data structure

- It is possible to use different topology ξ-grids for each r-space cells: velocity space of different sizes and (center) positions

- However, for efficient implementation of the advection operator, it is desirable to have similar topology ξ-grids so that each ξ-space cell in r-space cell can find a corresponding leaf, parent or children cell in neighboring r-cells

- Such implementation allows improved conservation when advecting VDF from one r-space cell to another

Tree-based ξ meshes “grown” in r cells, representing the concept of a tree-of-trees (ToT) data structure for a 2D2V case.

VDFs are stored in r- and ξ-cell centers. Advection in r-space requires calculating normal fluxes across cell faces of neighboring r-cells

R R Arslanbekov, V I Kolobov, and A A Frolova, Kinetic solvers with adaptive mesh in phase space, Phys. Rev. E 88 (2013) 063301
Hypersonic flow around a square

Gas temperature and r-grid for hypersonic flow over a square at $Ma = 30$, $Kn = 0.1$ (left); gas density, mean velocity and temperature along stagnation lines (right).

$r$-grid is adapted on gradients of density, mean velocity and temperature

$\xi$-grid adapted on gradients of VDF with a threshold value reduced near the wall to resolve reflected part of VDF.

2D2V, BGK model

Adapted velocity mesh and VDF contours for at different locations: free stream (left), inside shock wave (middle) and near the wall (right).

Direct Simulation Monte Carlo

Parallel simulations of rarefied supersonic flows over moving particles of different shapes

Adaptive Mesh Refinement for dynamic tracking of moving boundaries

Processor ID shown by different color

2D Simulations

Dynamic Mesh Adaptation

3D Simulations
UFS Simulations of Transient Problems

Computational grid

Shock Wave Penetration into Micro Channel

Kinetic & Fluid Domains

M=3
Kn=0.2

Gas Density

CPU-GPU Computing of Hypersonic Plasmas

Communication Blackout, Ablation, Thermal Protection Systems

- Developed CUDA kernels for three modules in UFS: DVM Boltzmann solver, DSMC module, and LBM solver
- Double digit speedups on single GPU and good scaling for multi-GPU have been demonstrated.

3D hybrid kinetic-fluid simulations of hypersonic flow over a X-51A waverider scramjet at M=5 and Kn=0.01 on a CPU-GPU NASA cluster with 58 GPU cards.

Total number of adapted computational cells is 3.5M, and total number of Boltzmann cells (brown color) is ~1.2M.


Adapted computational mesh and kinetic domain (brown cells, top) and Mach number (bottom) around a Waverider scramjet.
Multi – Fluid Plasma Models

- Fluid plasma models with “traditional” body-fitted mesh techniques have reached predictive capabilities (semiconductor manufacturing, lighting and other applications)
- Fluid models with AMR have been introduced for simulations of shock waves, ionization fronts, streamers, etc. where “traditional” methods lack efficiency

An example of 3D fluid simulations of an industrial ICP source for semiconductor manufacturing performed with CFD-ACE+ software using body-fitted mesh techniques

Plasma simulations with AMR: Computational grid, electron density contours at $10^7$ cm$^{-3}$, and the electric field strength (color, maximum value $7 \times 10^6$ V/m)
Electron Kinetics in Low Temperature Plasmas

Kinetic solvers for electrons in different regimes of EDF formation:
- Fokker Planck (collisional, slow)
- Vlasov (nearly collisionless regimes)
- Boltzmann (fast runaway, anisotropic)

Different regimes of EDF formation:
- a: electron streaming;
- b: isotropic “body”, anisotropic “tail”

Formation of Electron Groups in Gas Discharges

Three groups of electrons in the cathode region in DC glow discharges

High Frequency Plasmas: Need for Hybrid Codes

Experimental EEDF and simulated electron density (a) and temperatures (b) in CCP as a function of the number of super-particles in a cell [J. Phys. D: Appl. Phys. 38 (2005) R283]

Electron heating regimes

“Numerical noise level in PIC codes can be as much as $10^4$ times higher than Vlasov simulations. The noise can therefore be viewed as playing a somewhat similar role to that of particle collisions, and consequently introduces an artificial phase randomization and stochastization even if particle collisions are removed” [Plasma Sources Sci. Technol. 24 (2015) 044002]
Plasma in Contact with Liquids

- When liquid acts as one of the electrodes, its surface is deforming and evaporating.
- Specific patterns are formed at the liquid surface depending on gas pressure, discharge power, and liquid resistance (pH factor).
- The pH values of the solution decrease with time (from 7.67 to 3.65 within 5 min), indicating increase of H+ concentration.
- A double layer is formed beneath electrolyte surface.

The sign of anode fall and the nature of anode spots (both metal and liquid electrodes) remain poorly understood.

Anode fall vs gas pressure, $p$, in mercury for different currents, $i = 10$ (1), 3 (2), 0.3 (3), 1 (4), 0.1 (5), and 0.05 A (6). Tube radius 1.5 cm
Electric Breakdown & Plasma Formation in Liquids

There is still no comprehensive theory of electrical breakdown in liquids. Two major mechanisms are discussed:

- An extension of gaseous breakdown, based on avalanche ionization of atoms caused by seed electron impact.
- The formation of gaseous bubbles, which have lower dielectric strength and trigger the breakdown of the liquid.

The prevalent opinion today is vapor formation followed by plasma generation in the vapor phase. Discharge development in liquids on the picosecond time scale is similar to the ionization wave propagation in gases.

Adaptive Cartesian mesh and the Volume of Fluid (VoF) solver provide adequate methodology for solving multi-phase flows with bubbles and droplets.
Explosive Electron Emission in Cathodic Arcs

- Explosion center (ecton) emits a portion of electrons and liquid metal jet from micro-craters (radius ~1 μm)
- The explosion lasts for ~10 ns
- Metal vapor pressure for a Cu cathode at ecton current of 3 A is $10^8$ Pa - non-ideal plasma
- The physics of such explosions is partially known from studies of exploding wires and crater formation by meteorites (WDM?).

- Positive ions move in the “wrong” direction (against electric field): gas-dynamic mechanism of ion acceleration (up to 50-100 eV) by plasma expansion
- Arc currents ~kA are produced by multi-ecton phenomenon
- Oscillations of arc voltage confirm multi-ecton mechanism

Scientific Frontiers & Computational Challenges

- **Coupling particle kinetics and electromagnetics** for multi-component mixtures of reacting charged and neutral particles

- **Identification of switching criteria** for cell-by-cell dynamic selection of kinetic and fluid models for different plasma components

- **Closure relations for fluid models** in collisional and collisionless plasmas

- **Electrons**: special sensors in phase space are needed to select different kinetic and fluid models depending on
  - electron energy
  - space variations (trapped or free electrons)

- **Multi-Phase Capabilities**:
  - Phase transitions, interfaces phenomena
AMAR extensions to Multi-Phase Plasmas

- Advance kinetic solvers (both grid and particle based)
- Electron Kinetics (domain decomposition in phase space)
- Adaptive Hybrid Plasma Models
- Hybrid Model of Radiation transport
- Multi-phase capabilities

Grid Generation and Domain Decomposition

Define geometry of the system & generate octree mesh.

Domain decomposition:
- define sub-domains containing different phases (flags) to apply different sets of equations in different subdomains.
- assign computational cells with different weights to processors using SFC

Interface Tracking:
- calculate dynamic positions of material interfaces, mass transport through interfaces, surface charge accumulation, surface tension, evaporation, melting and other interface phenomena

Adapt mesh and computational load