Plasma Simulations with Adaptive Cartesian Mesh

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DOE Plasma Science Center
Control of Plasma Kinetics

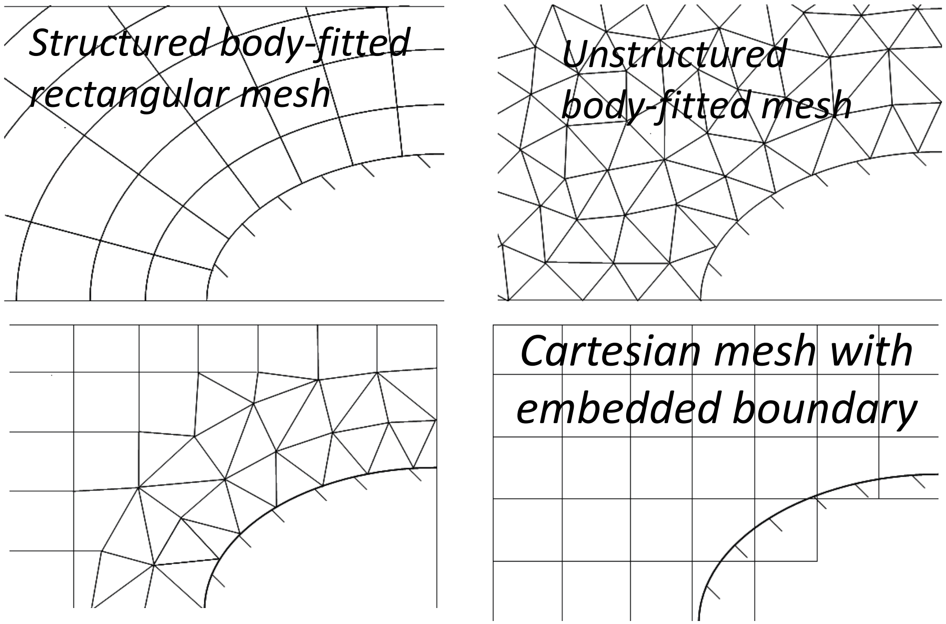
Center for Predictive Control of Plasma Kinetics: Multi-Phase and Bounded Systems

Agenda

- Adaptive Cartesian Mesh & 3rd wave of CFD
- What is Plasma ? Plasma technologies & computational challenges
- Commercial Software for Plasma Simulations
- Adaptive Mesh and Algorithm Refinement (AMAR)
- Unified Flow Solver
- Plasma Simulations with ACM
    - Minimal Plasma model: streamers
    - Extended Plasma model: Glow & Corona Discharges
    - AMPS, DSMC and PIC
- Exploring Basilisk: Gas Breakdown & Runaway Electrons
- Conclusions
- Key Publications

Adaptive Cartesian Mesh & 3rd Wave of CFD

- **Partial Differential Equations governing Plasma Dynamics are solved numerically using computational mesh**
- **The choice of mesh geometry and boundary treatment define accuracy and efficiency of simulations**



Combination of structured Cartesian mesh and hybrid unstructured body-fitted mesh near the wall

Adaptive Cartesian Mesh (ACM) with immersed boundaries has many attractive features:

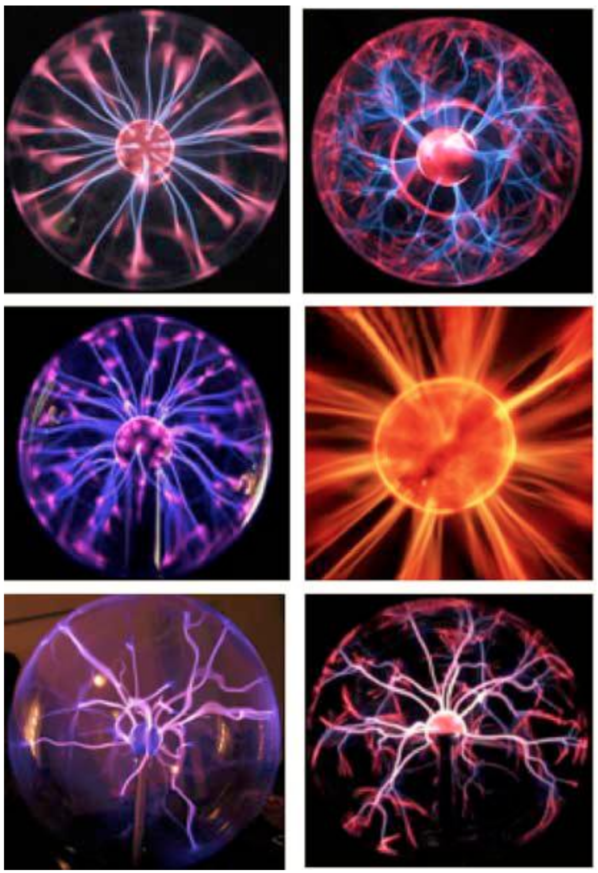
- **Geometry input from CAD tools**
- **Free surfaces and moving boundaries**
- **Parallelization: Space Filling Curves**

3rd Wave of CFD

- **Embedded CFD: FloEFD -> Mentor graphics-> Siemens**
- **Ansys Discovery (ACM+GPU)**

What is Plasma ?

The Greek word plasma means “formed or molded”. In 19th century, physiologist Jan Evangelista Purkinje introduced use of plasma to denote the clear fluid which remains after removal of all the corpuscular material in blood. In 1922, physicist Irving Langmuir proposed that the electrons, ions and neutrals in an ionized gas could similarly be considered as corpuscular material entrained in some kind of fluid medium and called this entraining medium plasma. However it turned out that there is no “fluid medium” entraining the electrons, ions, and neutrals in an ionized gas. Ever since, plasma scientists have to explain that they were not studying blood! – *after Paul M. Bellan, Fundamentals of Plasma Physics*

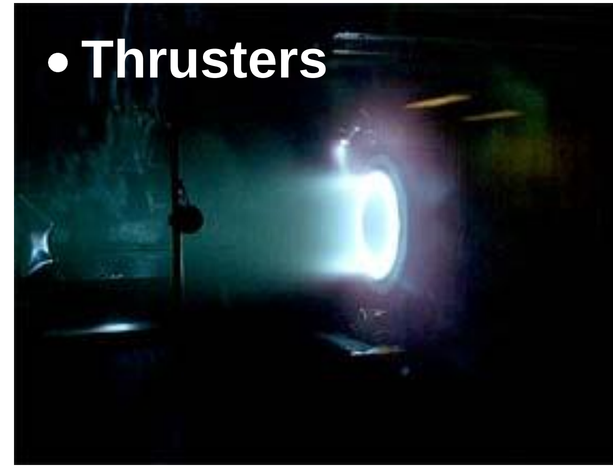


- **Plasma Is a quasi-neutral mixture of electrons, ions and neutrals**
- **Key properties of plasma are due to large difference of electron and ion mass**
- **The particle transport in plasma can be described by fluid or kinetic models**
- **Due to its non-equilibrium and nonlinear nature, plasma is prone to instabilities self-organization**

The motion of filaments in a plasma ball - Campanell et al, Phys Plasmas **17**, 053507 (2010)

Plasma Technologies

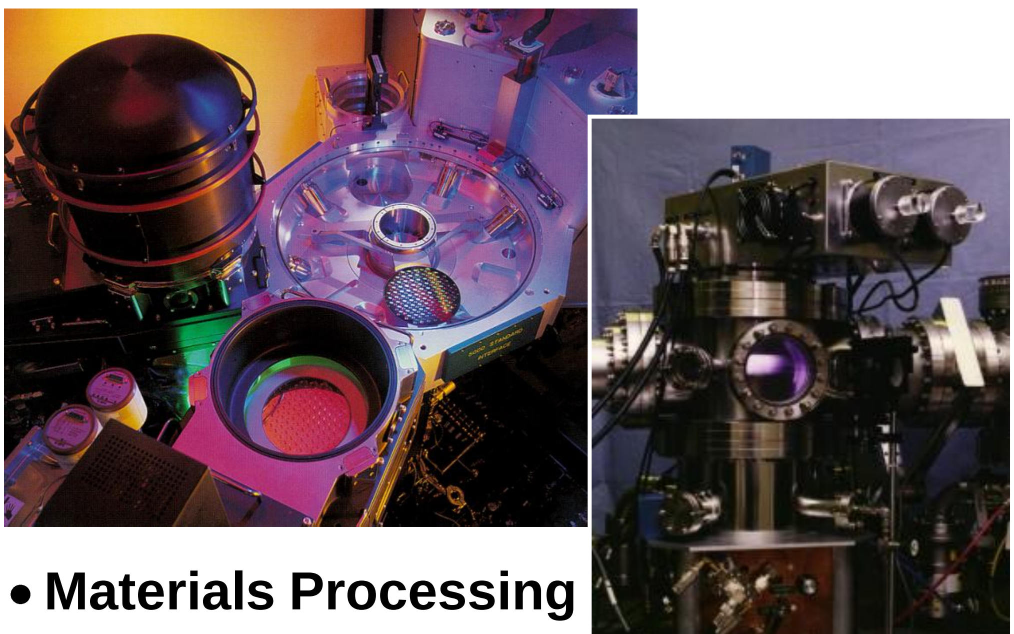
"The XXI century will be not only the century of informatics, biology and space exploration, but also the century of plasma technologies" A.I.Morozov 2006



- Thrusters

- Lighting

- Spray Coatings



- Materials Processing

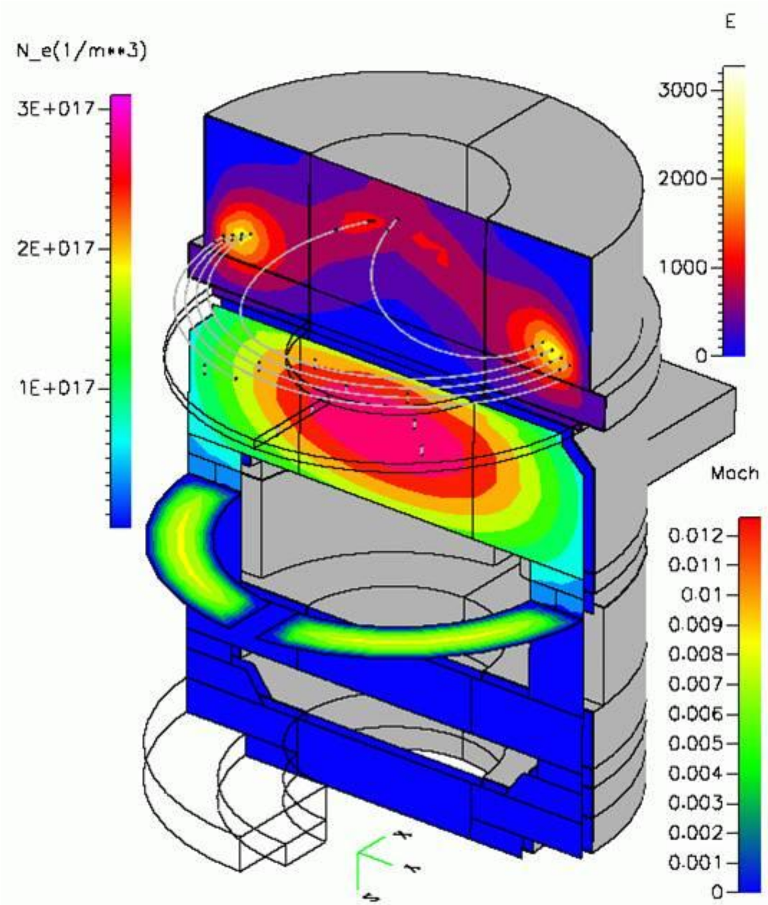
- Displays

Challenges of Plasma Simulations

Four major categories:

- **high spatial resolution is required in certain parts of the system (sheaths, shock layers, etc.) – using spatially uniform mesh results in a very large problem size**
- **kinetic solvers (both particle and grid based) are expensive computationally and require huge computer memory or large number of particles**
- **disparate time scales for electron and ions require long simulation time if both the electron and ion time scales need to be resolved**
- **coupling electromagnetics with charge transport results in highly non-linear problems (especially when ionization processes are important).**

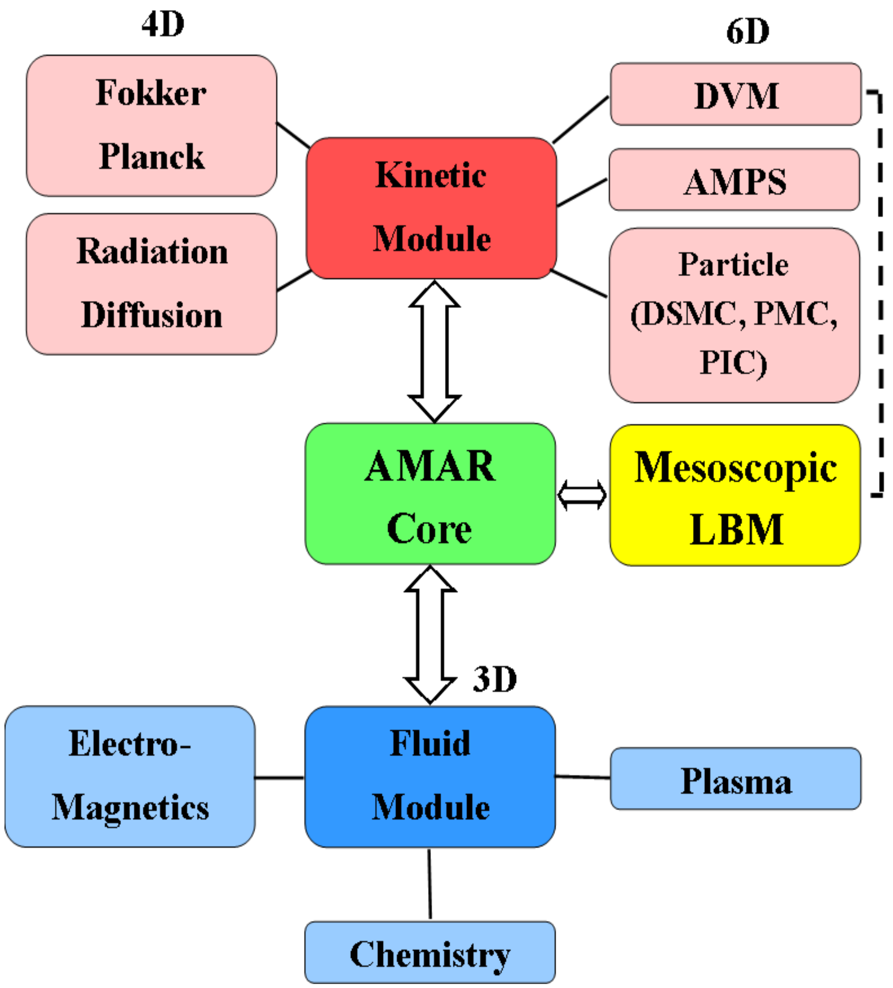
Commercial Software for Plasma Simulations



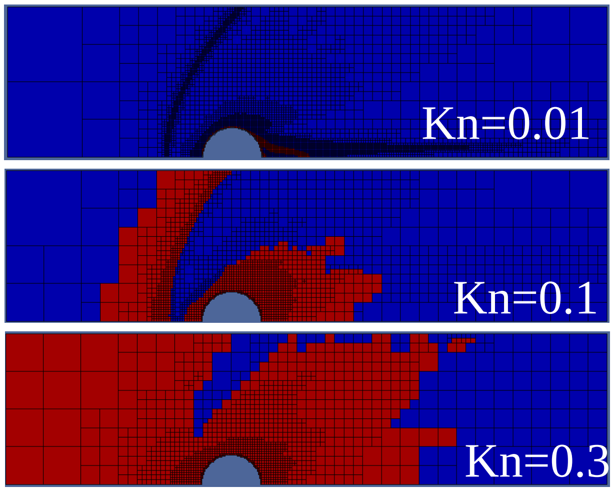
An example of 3D fluid simulations of an industrial ICP source performed with CFD-ACE+ software using body-fitted mesh techniques
J. Comput. Phys. 231 (2012) 839

- CFDRC developed commercial software, CFD-ACE+Plasma, to simulate plasma reactors and processes for material processing, semiconductor manufacturing, and lighting
- Gas mixtures and chemical reactions for:
  - rare gases (lighting, PDP)
  - O_2, N_2, Cl_2, H_2
  - Fluorocarbon plasmas (SF_6, C_2F_6, ..)
  - SiH_4 for deposition of SiO_2
  - Hydrocarbon plasmas (DLC films, CNT, etc)
- In 2004, CFD-ACE+ software was sold to ESI group.
- Around 2004, we selected Gerris as a framework for new multi-physics software with adaptive Cartesian mesh

Adaptive Mesh & Algorithm Refinement



Gas flow over a cylinder M=3



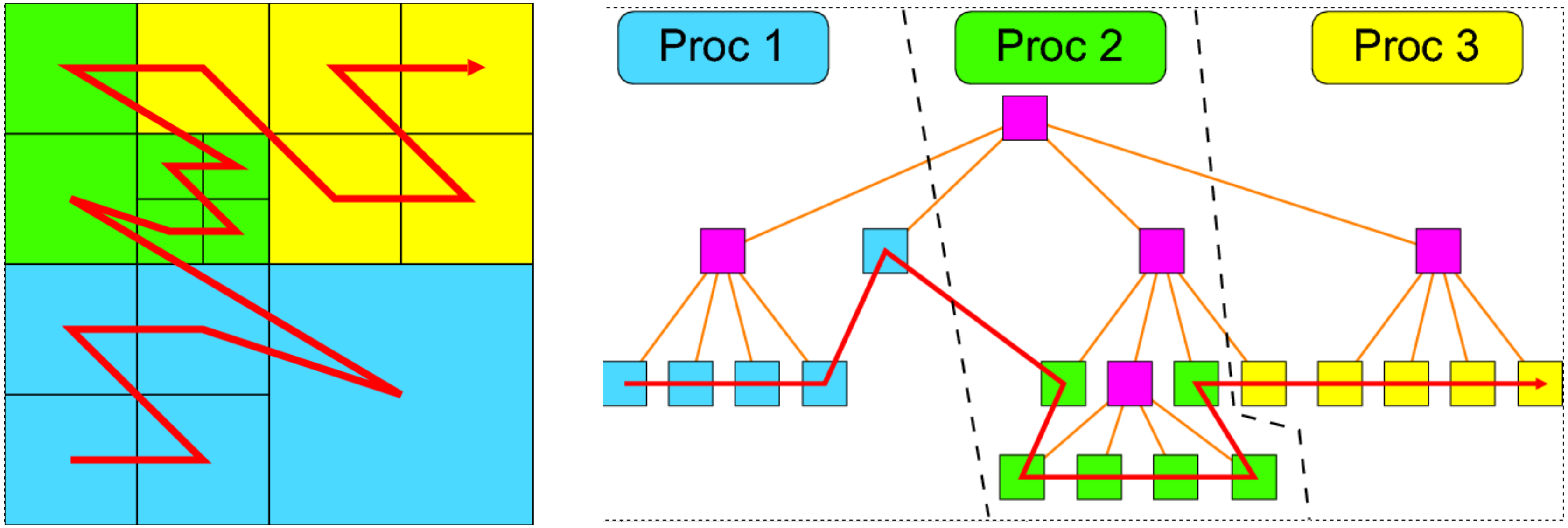
Computational grid with kinetic (brown) and continuum (blue) domains

- **Gas mixtures: different kinetic domains for heavy and light species**
- **Plasma simulations with AMAR require different criteria for electrons, ions and neutral species.**

V.I.Kolobov and R.R.Arslanbekov, Towards Adaptive Kinetic-Fluid Simulations of Weakly Ionized Plasmas, J. Comput. Phys. 231 (2012) 839

Space Filling Curves & Forest of Octrees

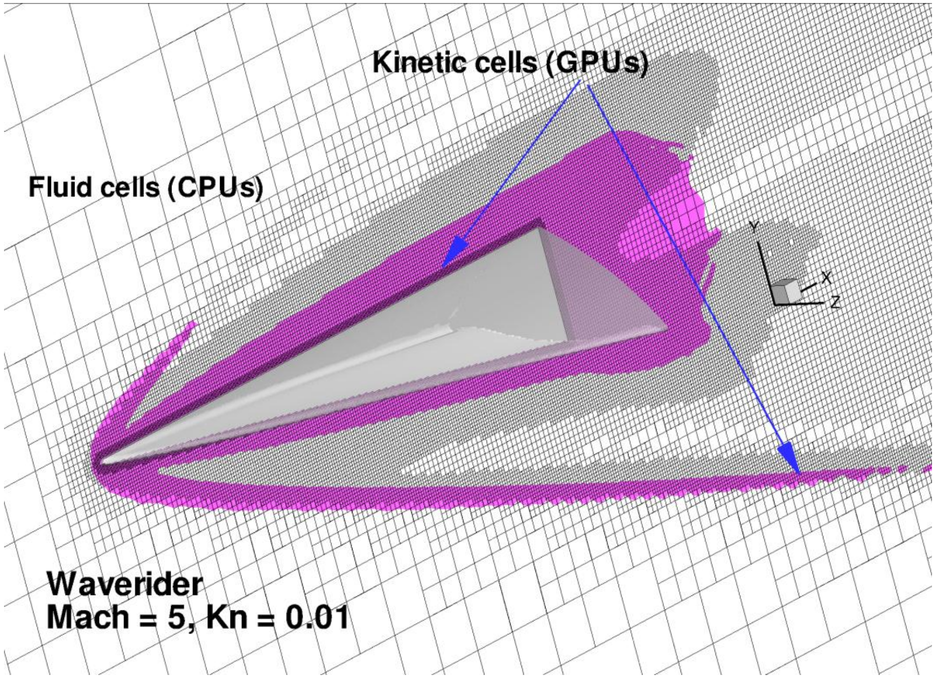
The procedure of domain decomposition is performed using SFC. Using SFC, 2D or 3D spatial data can be stored in a single dimensional array and domain decomposition is easily achieved by chopping this array into even pieces.

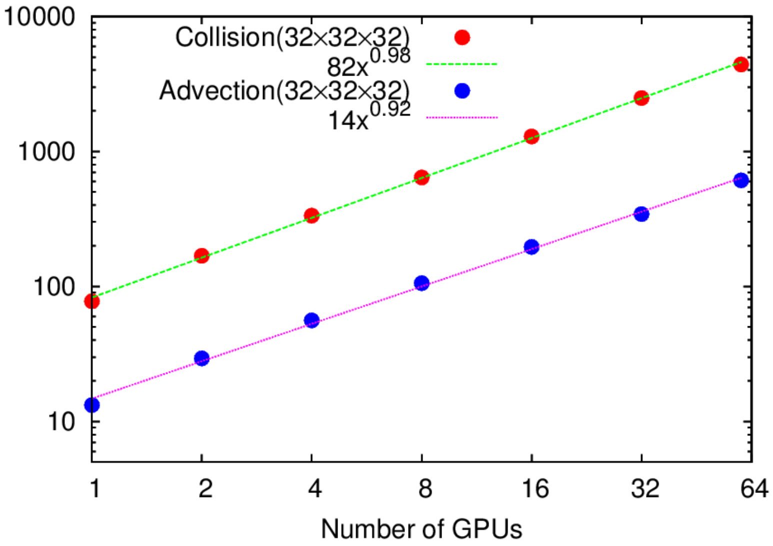


- During sequential traversing of cells by natural order, the physical space is filled with curves in N-order (Morton ordering). After this ordering of cells, all cells can be considered as a one-dimensional array.
- A weight is assigned to each cell, proportional to CPU time required for computations in this cell. The array modified with corresponding weights, is subdivided into sub-arrays equal to the number of processors.
- This method allows most efficient domain decomposition between different processors.

Unified Flow Solver

- **Hybrid kinetic-fluid simulations using CPU for the Navier-Stokes cells and GPU for the Boltzmann cells**
- **Cell-by-cell selection of the kinetic or fluid solvers based on a continuum breakdown criteria**

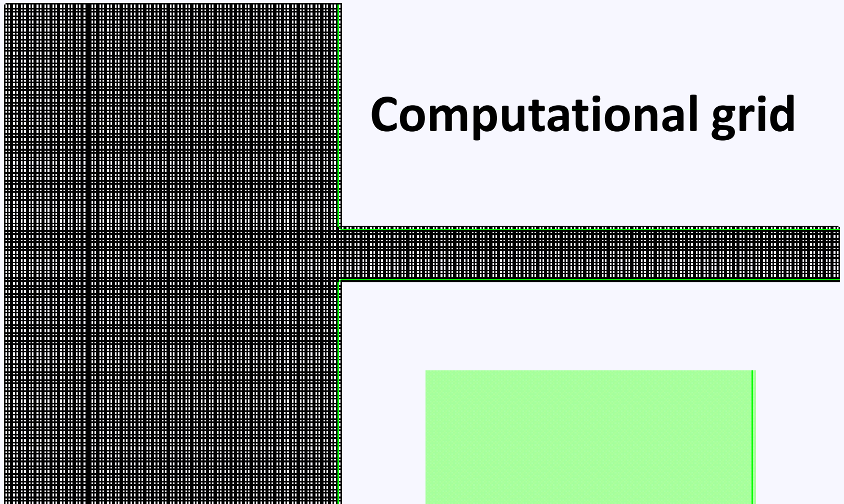




GPU acceleration of the Boltzmann solver

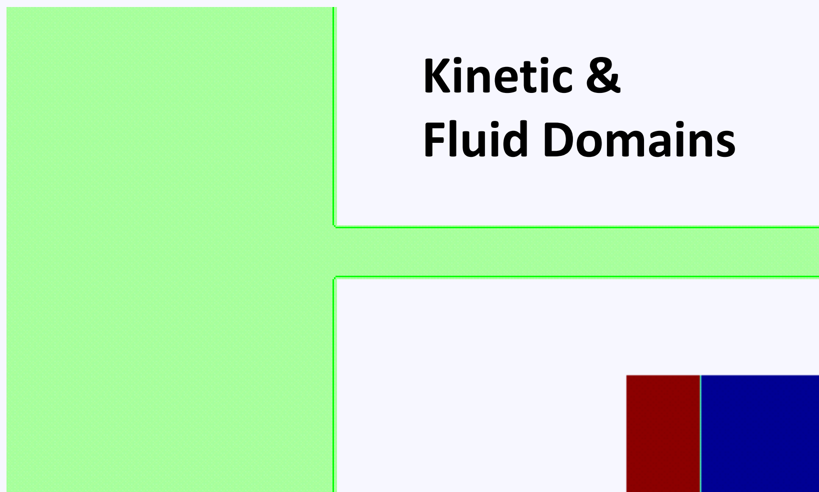
S Zabelok, R Arslanbekov, V Kolobov, Adaptive Kinetic-Fluid Solvers for Heterogeneous Computing Architectures , J Comp Phys 2015

UFS Simulations of Transient Problems



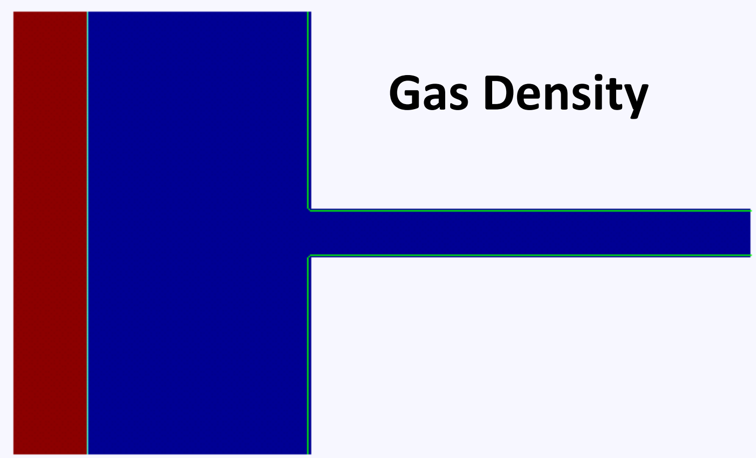
Computational grid

Shock Wave Penetration into Micro Channel



Kinetic & Fluid Domains

M=3
Kn=0.2



Gas Density

V.I. Kolobov, et al, Unified Flow Solver for Transient Rarefied-Continuum Flows, 28th Symposium on Rarefied Gas Dynamics, AIP Conf. Proc. 1501 (2012) 414

Minimal Plasma Model

A simplest set of equations for the electron and ion densities, and Poisson equation for electrostatic potential.

Electron diffusion and ion transport are neglected

$$\frac{\partial n_e}{\partial t} + div \ \ \vec{\Gamma}_e \ \ = \nu n_e \qquad \vec{\Gamma}_e = \mu \vec{E} n_e$$

$$\frac{\partial n_i}{\partial t} = \nu n_e$$

$$\nu = \nu_0 \exp\left[-\frac{E_0}{E} \right]$$

$$\Delta \varphi = 4\pi \ \ n_e - n_i$$

Mesh Adaptation criteria

$$\alpha = 20\left(\frac{n_e}{\max(n_e)} + \frac{n_e}{\max(n_e)} \right) + 3 \ \ \log_{10}(n_e) + \log_{10}(n_i) + \log_{10}(\nu_i) + \log_{10}(|E|)$$

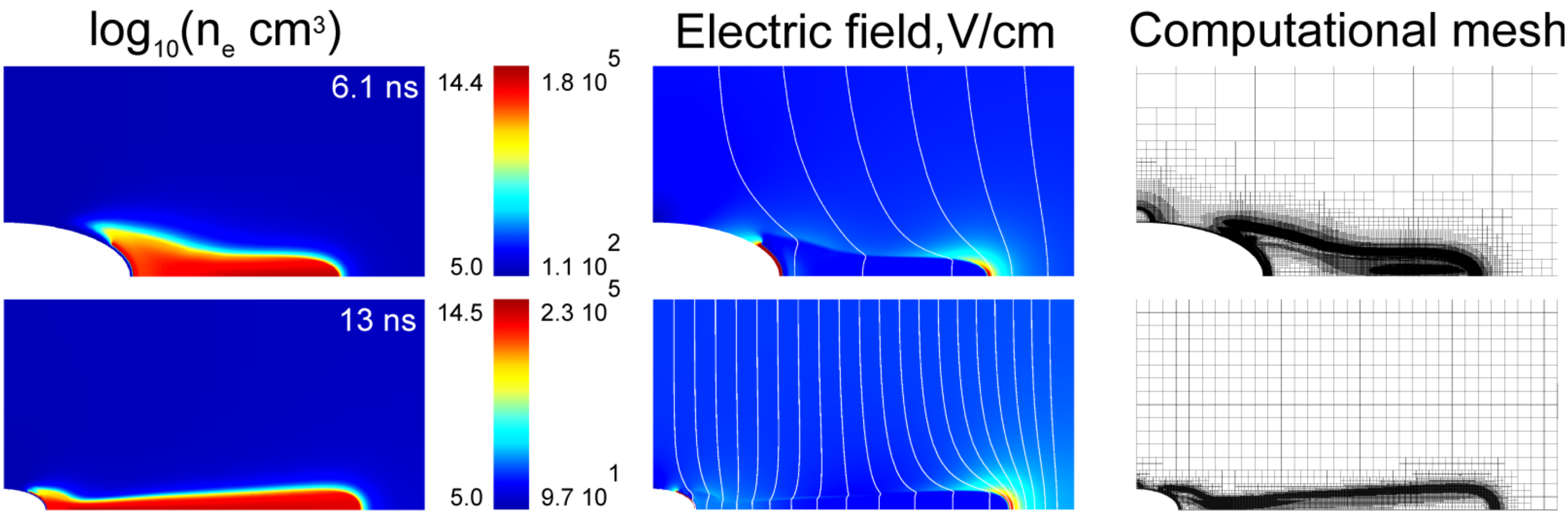
When gradient of α exceeded a fixed value $|\nabla \alpha| > 1$ in a cell, this particular cell was refined

When $|\nabla \alpha| < 1/4$ in a cell, this cell was coarsened

The procedure of mesh adaptation performed every 10 time steps

Streamer development in negative corona

2D axi-symmetric simulation of streamer development near a needle-like elliptic cathode and a flat anode: *p*=760 Torr



A constant electron density 10^5 cm^{-3} is assumed at the cathode surface. The streamer propagates with a velocity by an order of magnitude higher than the electron drift velocity .

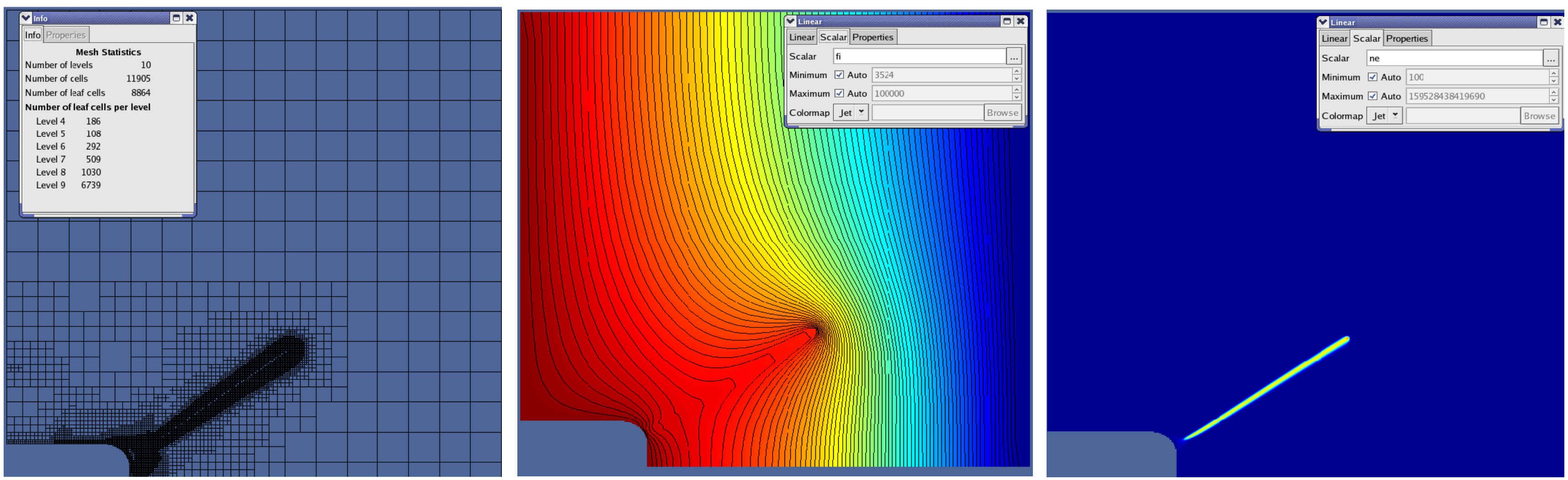
The calculated streamer velocity agrees with the classical estimate for the fast streamer velocity.

The plasma channel is formed on the axis of the discharge.

Streamer development in positive corona

2D axisymmetric simulations of positive corona discharge

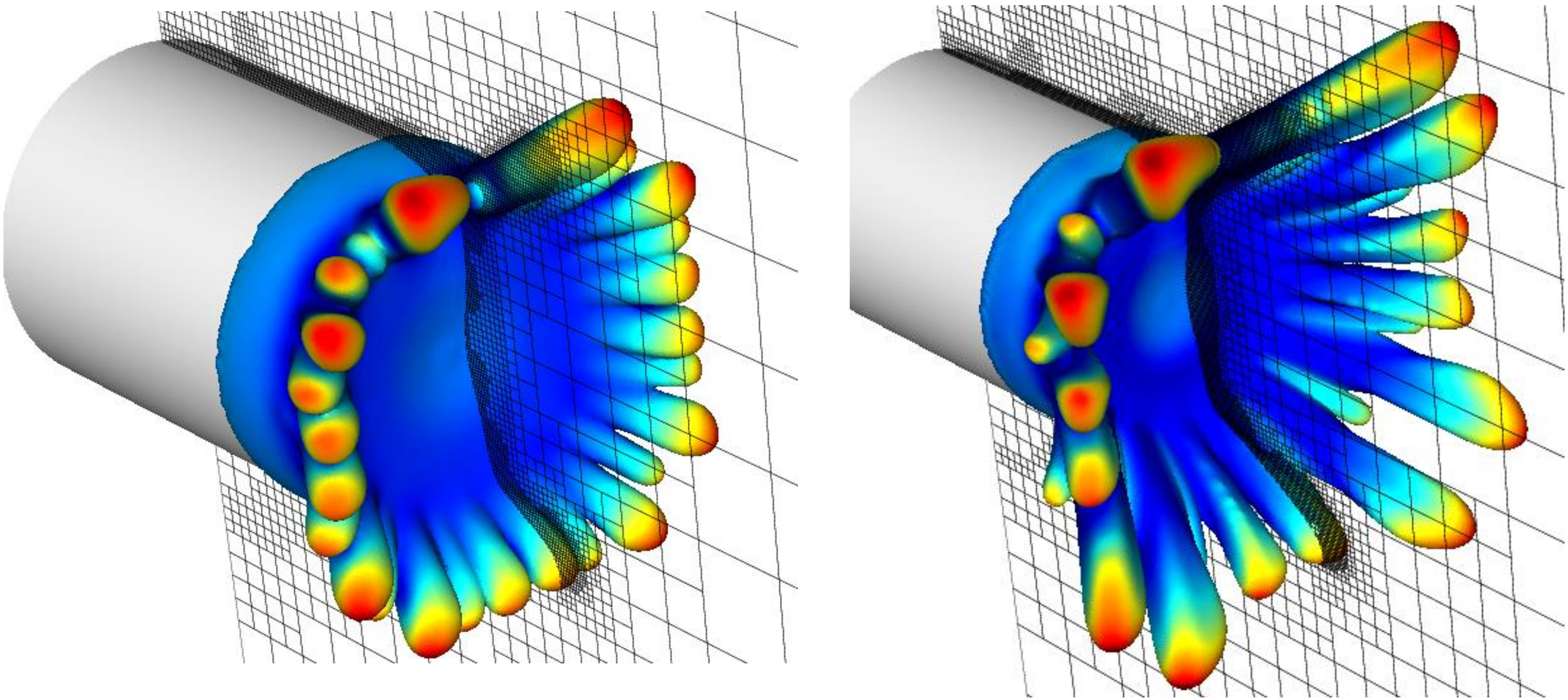
An off-axis toroidal channel was formed in our simulations.
This behavior was observed with different physical models for different electrode shapes.



The computational grid (left), electrostatic potential (center), and the electron density (right) for a streamer developing near a rod-shape anode.

Streamer development in positive corona

3D simulations revealed that the 2D axi-symmetric channels break into separate streamers. The streamers form near the anode with an almost periodic pattern and propagate in slightly different directions with different speeds. Only two streamers survived at a long distance from the anode. The code generates about 1.5 million cells during parallel simulations on 8 cores.



Computational grid, electron density contours at 10^7 cm $^{-3}$, and the electric field strength (color, maximum value 7 10^6 V/m) at 15 ns (left) and 20 ns (right)

Extended Plasma Model

• A set of equations for the electron and ion densities, and Poisson equation for electrostatic potential

$$\frac{\partial n_e}{\partial t} + div \;\; \vec{\Gamma}_e \;\; = \nu n_e$$

$$\vec{\Gamma}_e = -\mu_e \vec{E} n_e - D_e \nabla n_e$$

$$\Delta\varphi = 4\pi \;\; n_e - n_i$$

• Ion transport is included

• Multiple species ions are allowed by introducing species specific mass, diffusion coefficients, and ionization rates

$$\frac{\partial n_i}{\partial t} + div(\Gamma_i) = \nu n_e$$

$$\vec{\Gamma}_i = \mu_i \vec{E} n_i - D_i \nabla n_i$$

• Local field approximation for ionization rate

$$\nu = \nu_0 \exp\left[-\frac{E_0}{E} \right]$$

• Electron Energy Transport with account for electron thermal conductivity

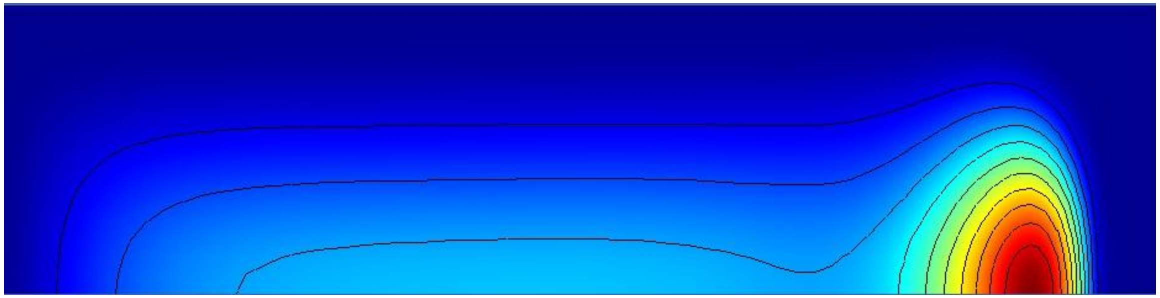
$$\frac{\partial n_\varepsilon}{\partial t} + \nabla \cdot \vec{\Gamma}_\varepsilon = S_\varepsilon \qquad n_\varepsilon = n_e \overline{\varepsilon}$$

$$\vec{\Gamma}_\varepsilon = -\frac{5}{3} \mu_e \vec{E} n_\varepsilon - \frac{5}{3} D_e \nabla n_\varepsilon$$

• CANTERA link implementation is underway for complex reaction mechanisms

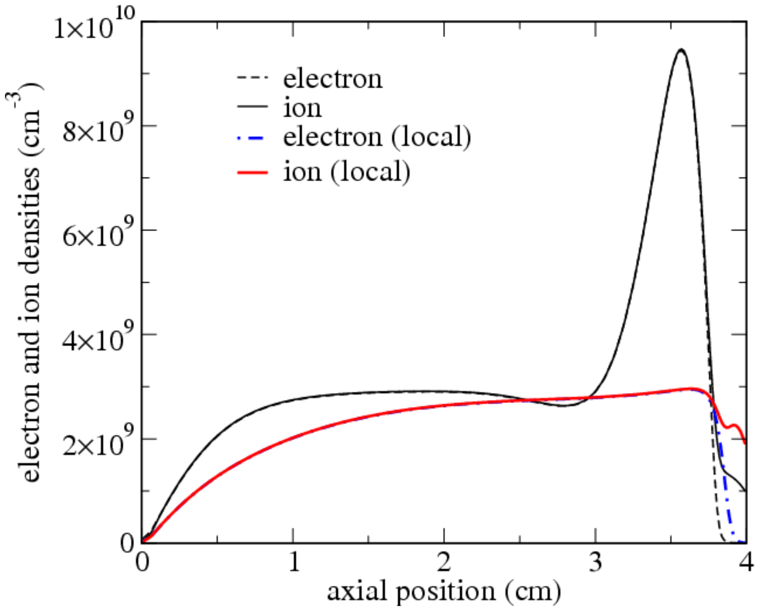
Effect of Electron Energy Transport

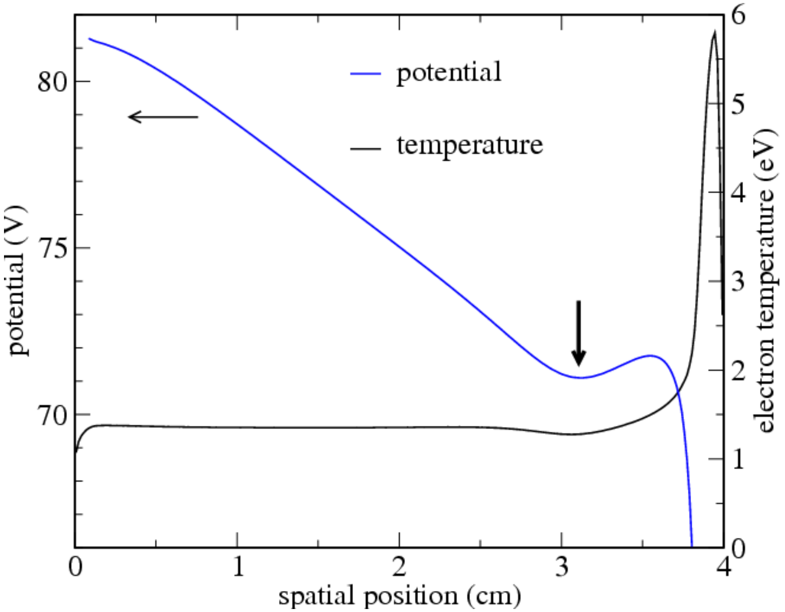
2D axi-symmetric simulations



The model reproduces basic structure of classical DC glow discharges

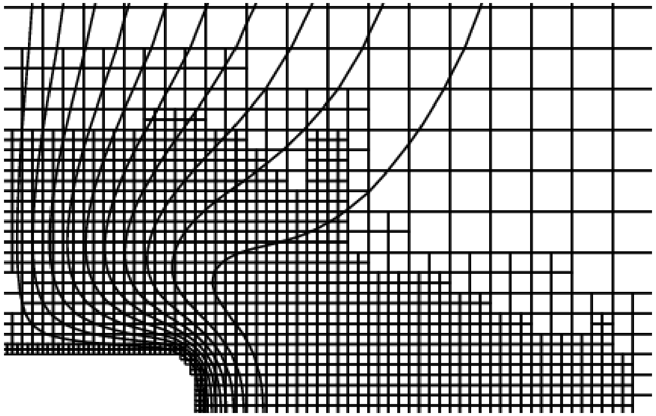
Spatial distribution of electron density

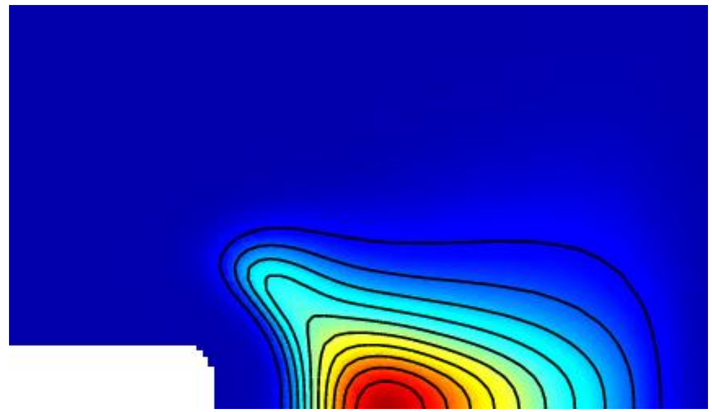




Axial distributions of electron and ion densities (left), electrostatic potential and electron temperature (right) with account of electron thermal conductivity

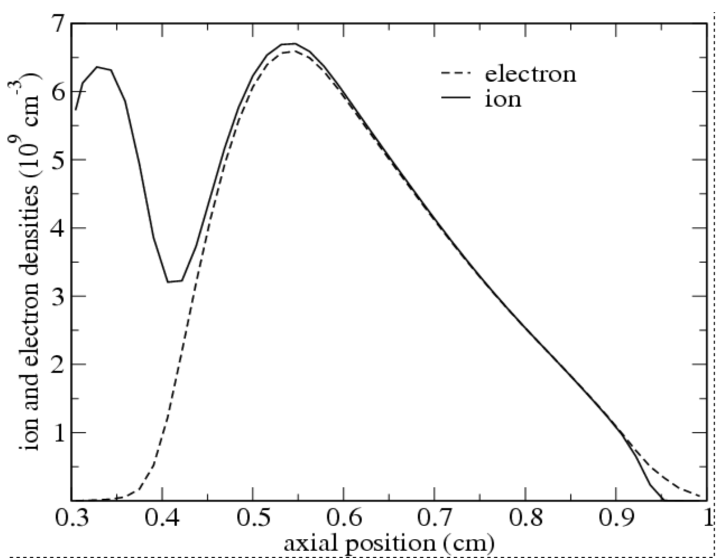
Discharges with Rod Shape Cathode

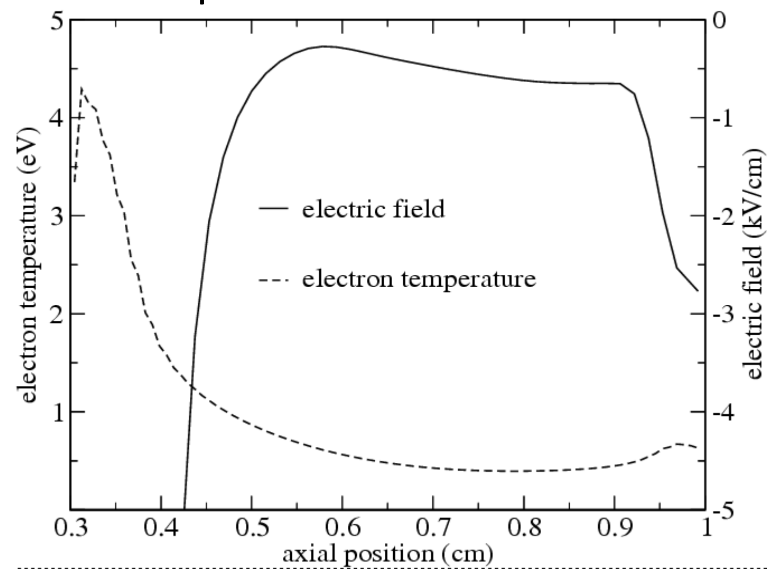




15 Torr
32 µA

Computational grid and the electrostatic potential (left), and electron density contours (right) for a glow discharge between a rod cathode and a planar anode.

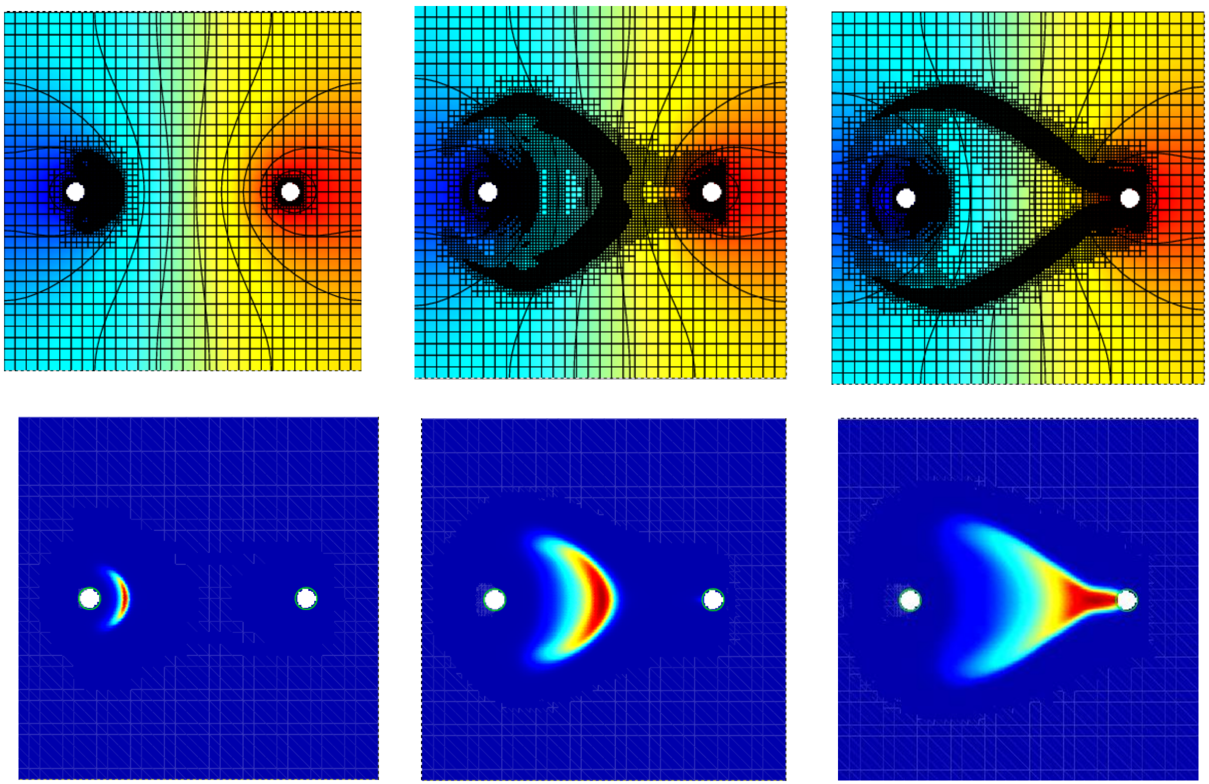




Axial profiles of the electron and ion density (left), the electron temperature and the x-component of the electric field (zoom on the plasma region)

Dynamics of pulsed breakdown

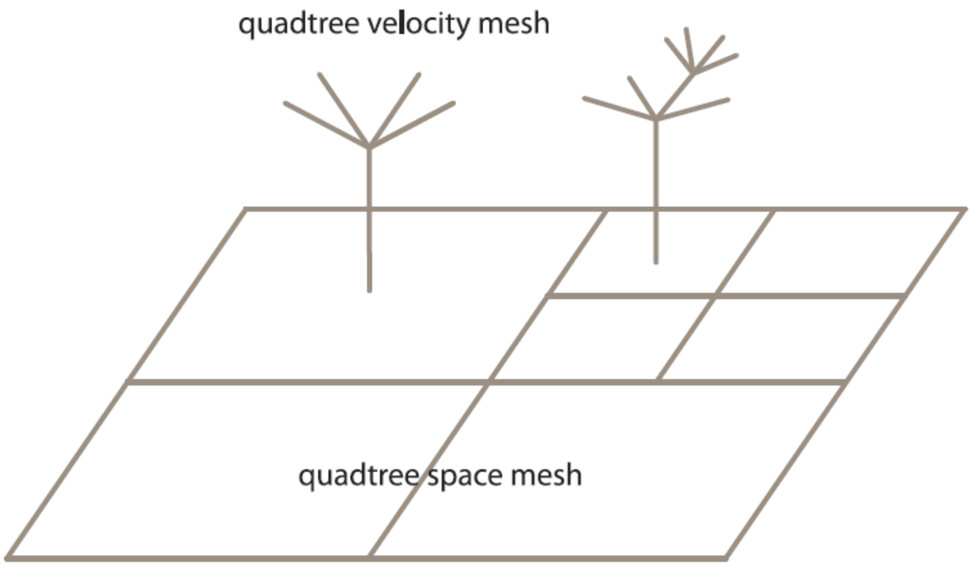
Gas breakdown between two wires of radius 100 nm separated by a 1 μm distance. A voltage of amplitude 0.2-4 kV applied between the wires to initiate the gas breakdown induced by field emission. Gas pressure 1-100 atm.



Micro Plasma is formed at a sup-picosecond time scale

Computational mesh and electrostatic potential (top), and electron density (bottow) at three time moments during gas breakdown between two wires.

Adaptive Mesh in Phase Space



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

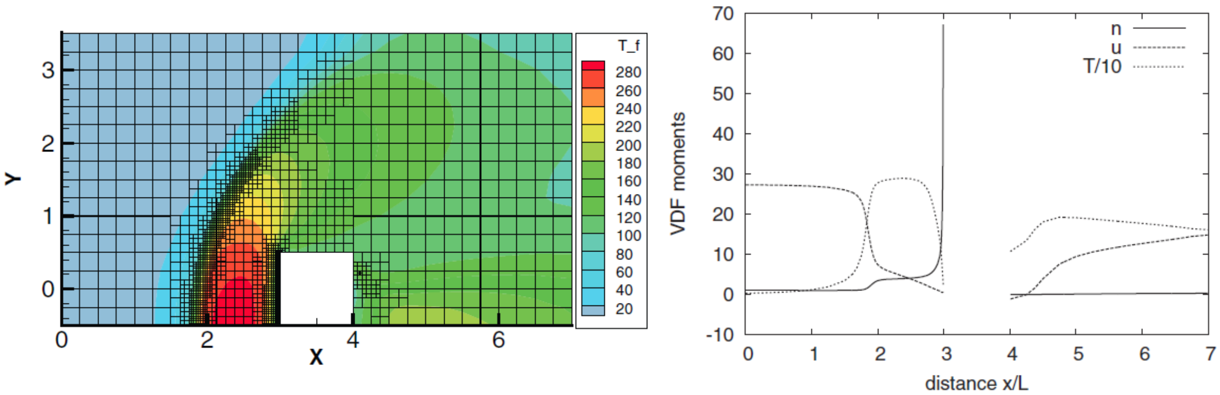
Tree-of-trees data structure

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

- 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 child cell in neighboring r-cells

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

Hypersonic flow around a square

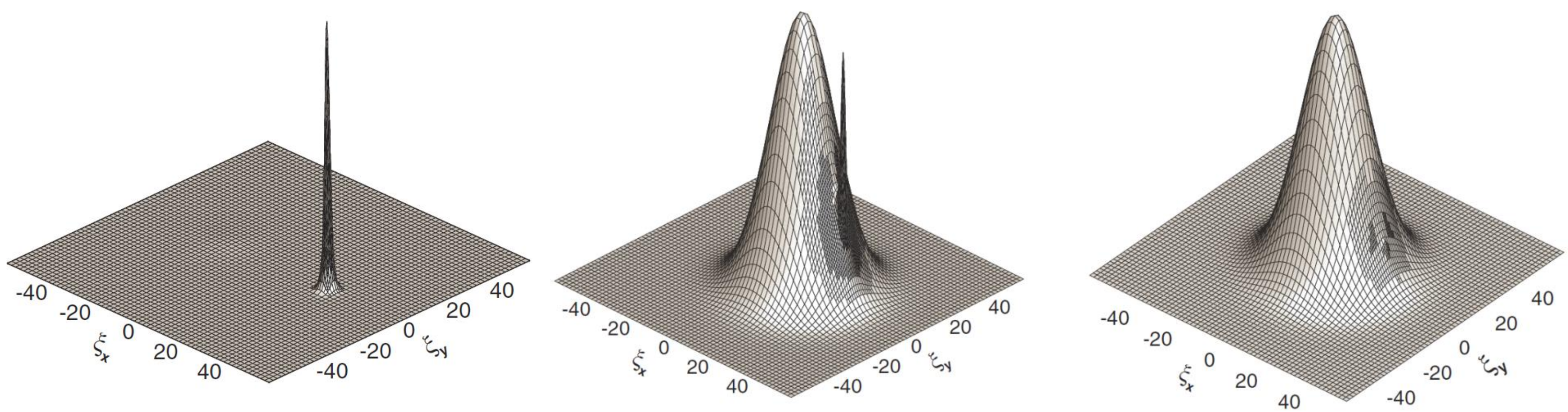


Gas temperature and r-grid for hypersonic flow over a square at Ma = 30 , Kn = 0.1 (left) ; gas density, mean velocity and temperature along stagnation lines (right).

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

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

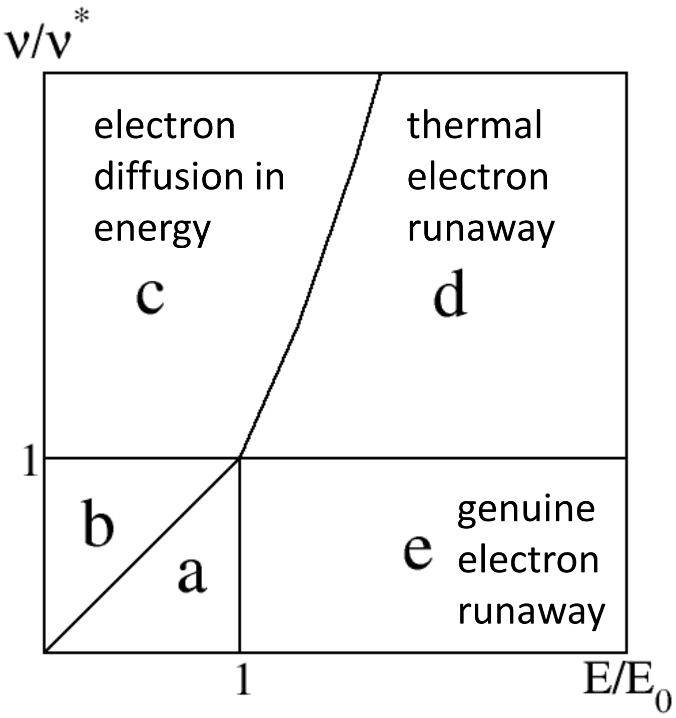
2D2V, BGK model



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

Phys. Rev. E 88 (2013) 063301

Electron Kinetics in Low Temperature Plasmas



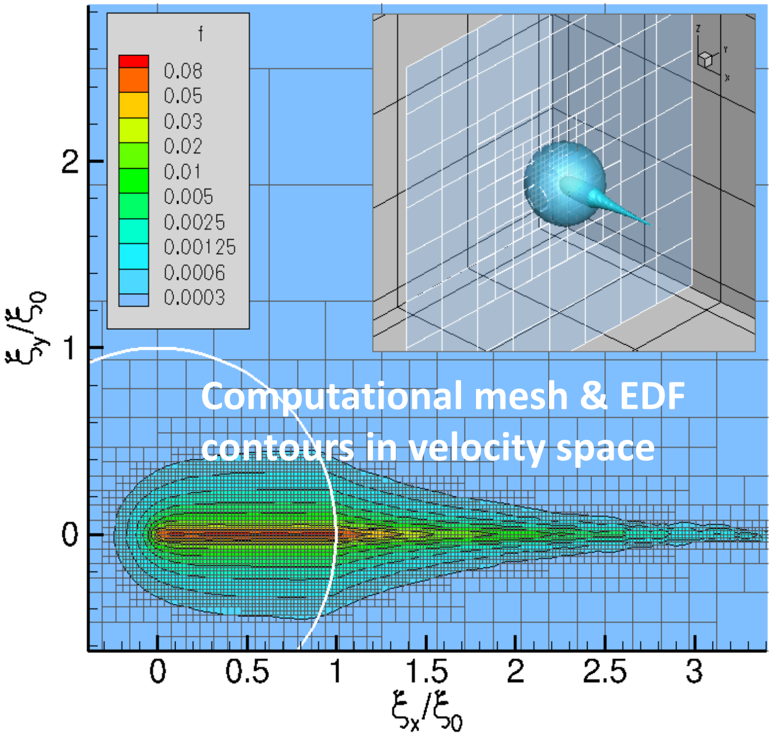
Different regimes of EDF formation:

a : electron streaming;
b : isotropic "body", anisotropic "tail"

V Kolobov, Advances in electron kinetics and theory of gas discharges, Phys. Plasmas 20, 101610 (2013)

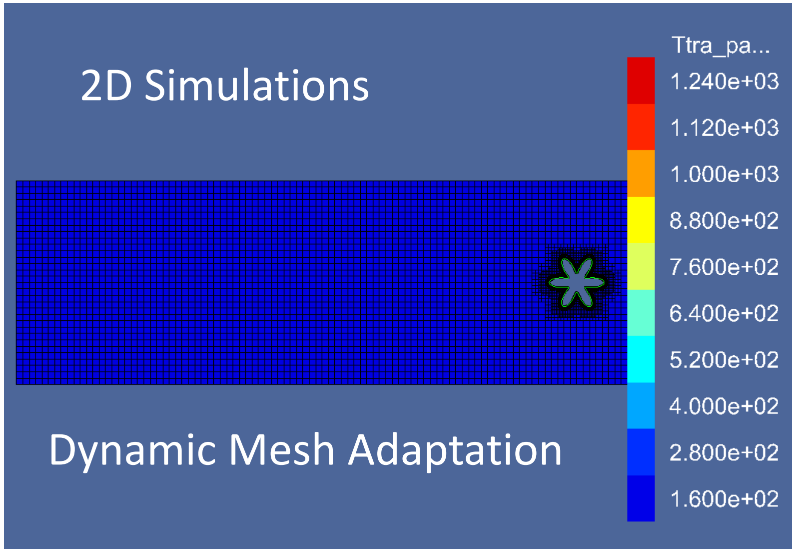
Kinetic solvers for electrons **in different regimes of EDF formation:**

- **Fokker Planck (collisional, slow)**
- **Vlasov (nearly collisionless regimes)**
- **Boltzmann (fast runaway, anisotropic)**

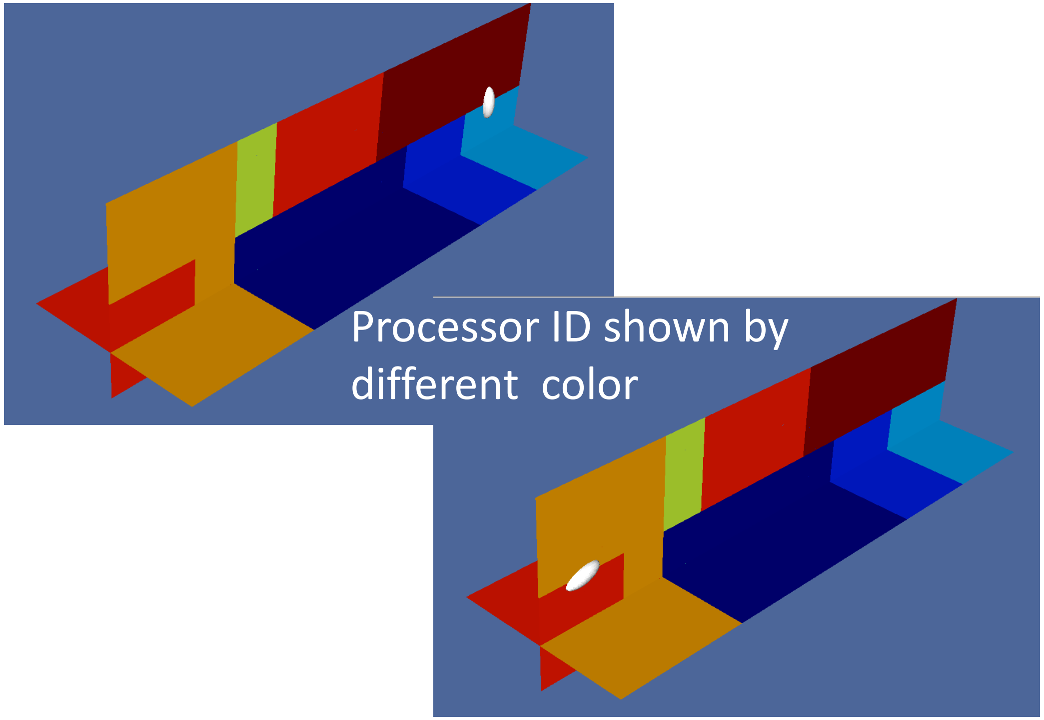


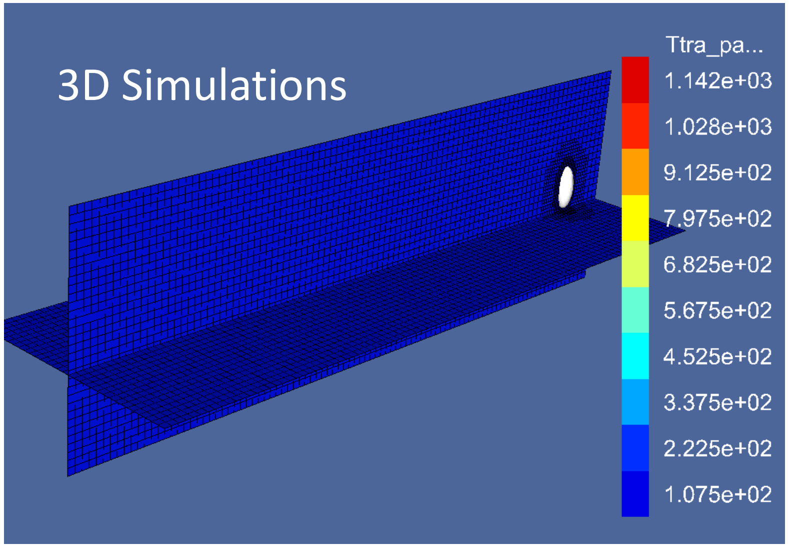
Adapted mesh in velocity space

Particle Models: Direct Simulation Monte Carlo



Adaptive Mesh Refinement for dynamic tracking of moving boundaries

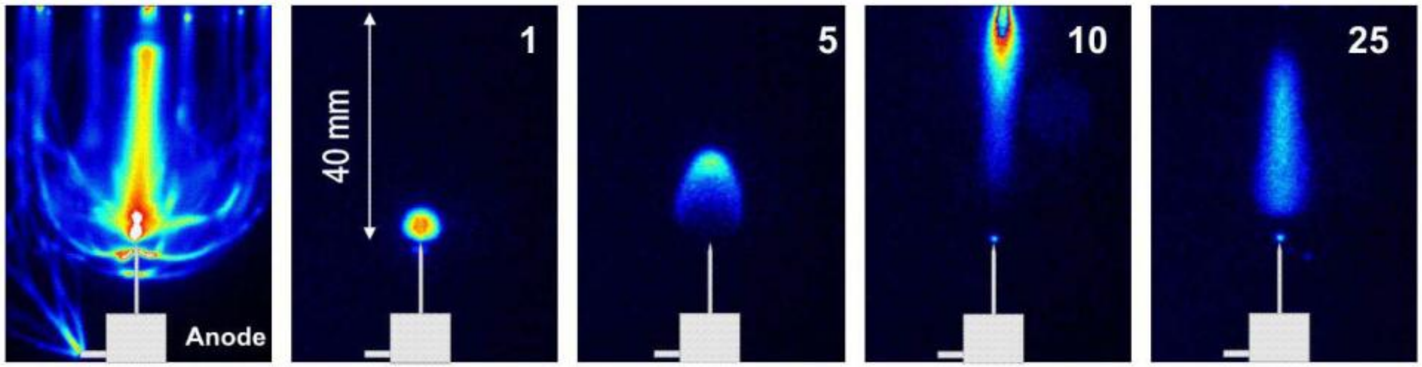




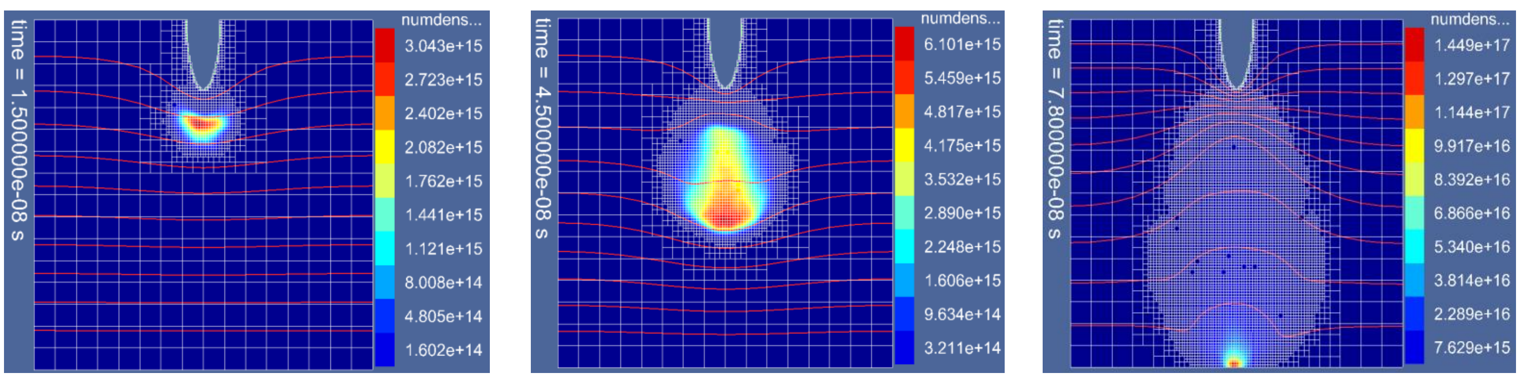
Parallel simulations of rarefied supersonic flows over moving particles of different shapes

Gas Breakdown: Experiment & Simulations

Integral and subsequent ICCD images of nanosecond discharge in air initiated by HV pulse with short (11 ns) rise time: Air, 680 torr (IEEE TPS 2008)



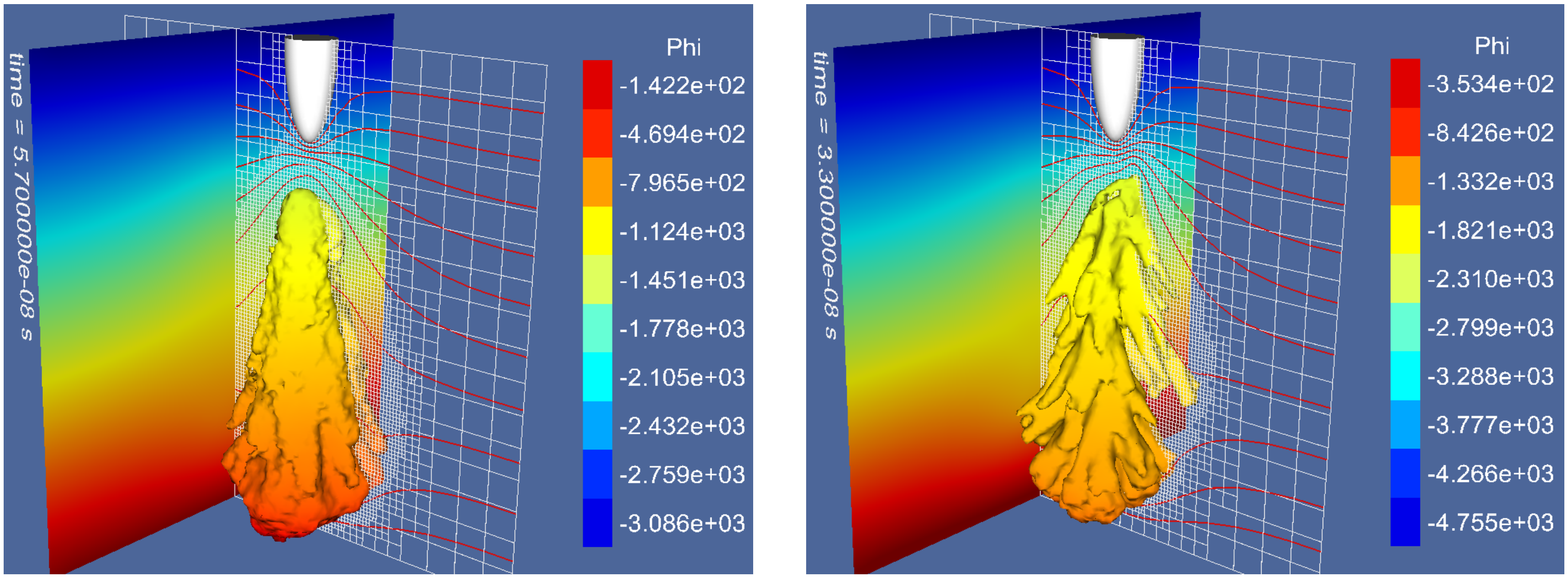
2D fluid simulations: Ar, 100 Torr, needle-to-plane geometry, 40 mm gap, 2.5 kV



Electron density, adapted grids, and isolines of electrostatic potential at 15, 45 and 78 ns

3D PIC-ACM Simulations of Gas Breakdown

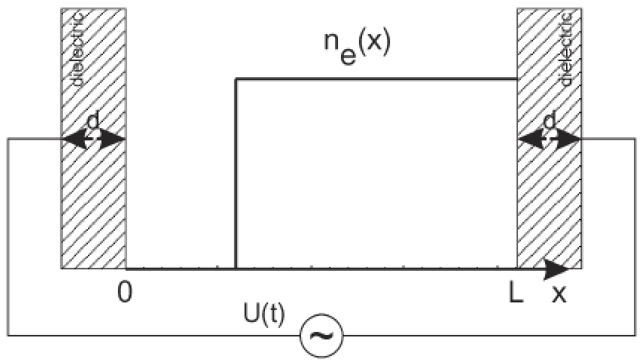
Argon, 100 Torr , applied voltage 3 kV (left) and 5 kV (right)



Isosurfaces of electron density (at 10^{16} m^{-3} and $5{\times}10^{16}$ m^{-3} levels), adapted grids, and isolines of electrostatic potential at 57 (left) and 33 (right) ns.

AMR capabilities are crucial; Computational cost of PIC is prohibitive at higher pressures, hybrid models are needed

Understanding Gas Breakdown Dynamics

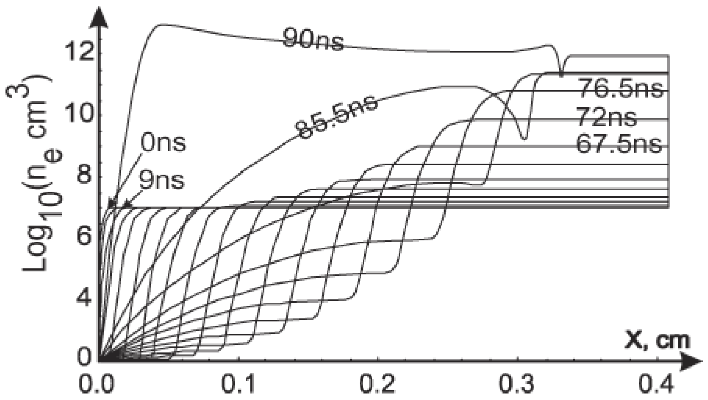


$$\frac{\partial n_e}{\partial t} + \nabla \cdot \mathbf{\Gamma} = S \quad (1)$$

$$\mathbf{\Gamma} = -\mu n_e \mathbf{E} \quad (2)$$

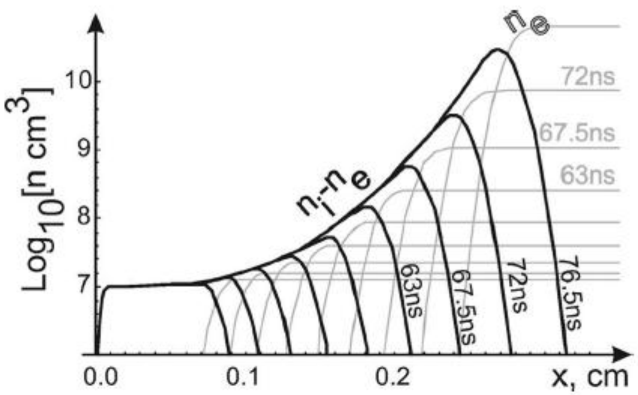
$$\frac{\partial n_i}{\partial t} = S \quad (3)$$

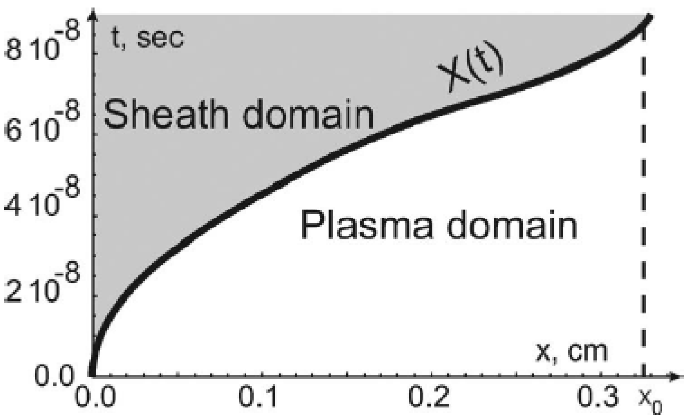
$$\nabla \cdot \mathbf{E} = 4\pi(n_i - n_e). \quad (4)$$



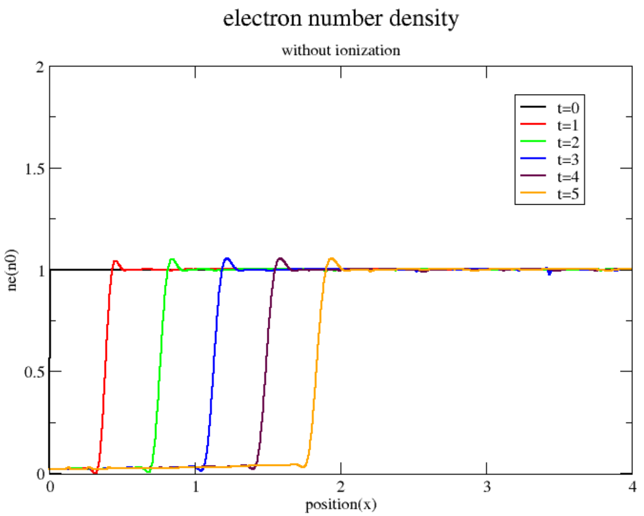
Theory of Pulsed Breakdown of Dense Gases and Optimization of the Voltage Waveform

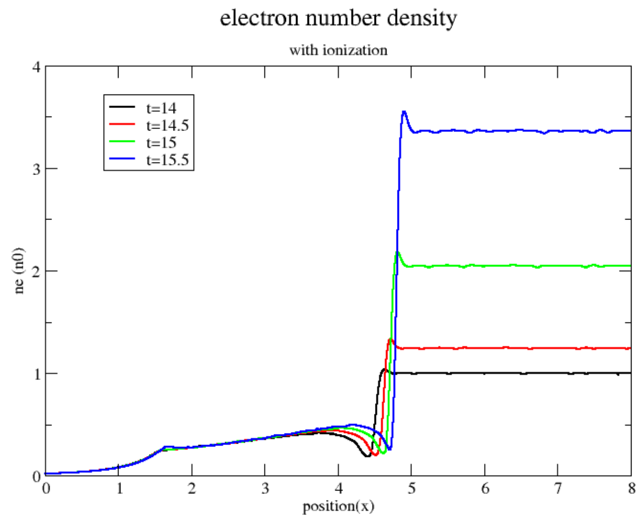
IEEE Trans. Plasma Sci. 36 (2008) 131





Minimal plasma model and kinetic solver for fast runaway electrons in Basilisk





Comparison of fluid model results with analytical solutions is in progress

Kinetic equation for velocity distribution function of runaway electrons

$$\frac{\partial f}{\partial t} + \nabla\cdot(\mathbf{v}f) + \frac{1}{m}\frac{\partial}{\partial \mathbf{v}}\left[\left(F(\mathrm{v})\frac{\mathbf{v}}{\mathrm{v}} - e\mathbf{E}\right) f\right] + \frac{\partial}{\partial \mathrm{v}_i}\left[D_{ij}\frac{\partial f}{\partial \mathrm{v}_i}\right] = I$$

Using spherical coordinates in velocity space

$$U = \mu \mathrm{v}; \qquad V = eE\mu - \nu p; \qquad W = eE\frac{(1-\mu^2)}{p}; \qquad D_\mu = \nu p^2(1-\mu^2)$$

$$Y = \mathrm{v}^2 f$$

$$\frac{\partial Y}{\partial t} + \frac{\partial}{\partial x}\, UY + \frac{\partial}{\partial \mathrm{v}}\, \mathrm{V}Y + \frac{\partial}{\partial \mu}\left[WY + D_\mu \frac{\partial Y}{\partial \mu}\right] = \mathrm{v}^2 I$$

This equation was coded in Basilisk

Coupling Fluid and Kinetic Solvers

- How to couple kinetic and fluid solvers in Basilisk ?

- In Gerris, for each spatial cell we create a GfsSimulation object (sim pointer).

- Each sim object has grid, events, boundary & initial conditions, etc.

- Each sim object (velocity space) is controlled by a separate parameter (.gfs) file

- Q1: Is it possible to do the same in Basilisk? This way we can couple 3D physical space with, 3D3V kinetic solvers.

- Q2: Maybe Basilisk can offer better ways ?

Desirable Features of Future Basilisk

- **Bring treatment of solid objects (e.g., from STL files) to the Gerris level using the cut cell (+ cell merging) approach.**

- **Make solids with cut cell work with MPI**

- **Proper and robust VOF treatment in cut cells (cut cells can have both fluid 1 and fluid 2)**

- **Multi-Domain capabilities with non-grid aligned boundaries (e.g., cut-cell) defined using static or moving VOF. Capability to set boundary conditions at solid-fluid interfaces and MPI support.**

- **More than 2 fluid capabilities (?), e.g., 3-fluid VOF.**

- **GPU acceleration support**

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DOE Plasma Science Center
Control of Plasma Kinetics

Key Publications

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