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THE AIR FORCE RESEARCH LABORATORY
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High fidelity and multiscale algorithms for collisional-radiative and nonequilibrium plasmas

AFOSR Computational Math Review Meeting
July 2014

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TOC

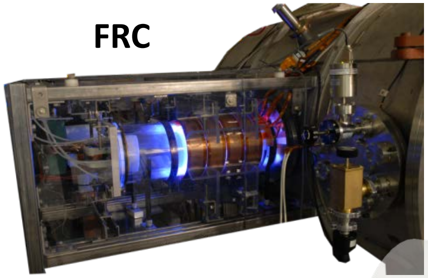
Spacecraft Plasma M&S

- Applications from Hall thrusters to plumes and gas discharges
- Complex physics: excitation/ionization, transport, radiative, material, etc.
- Multiple spatial-temporal and density scales.

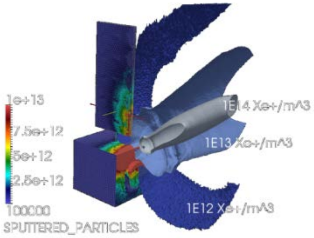
Current focus:

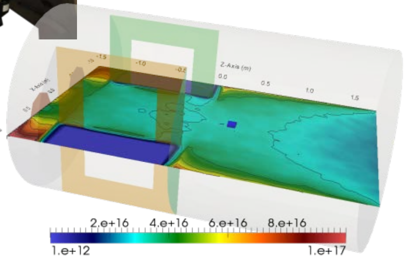
Develop advanced multiscale algorithms for plasma M&S with highly non-equilibrium condition and collisional-radiative kinetics

FRC

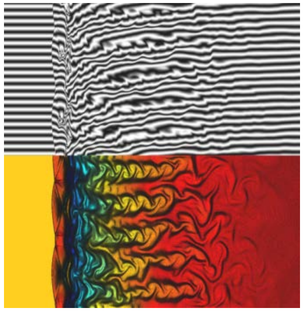


EP Plumes





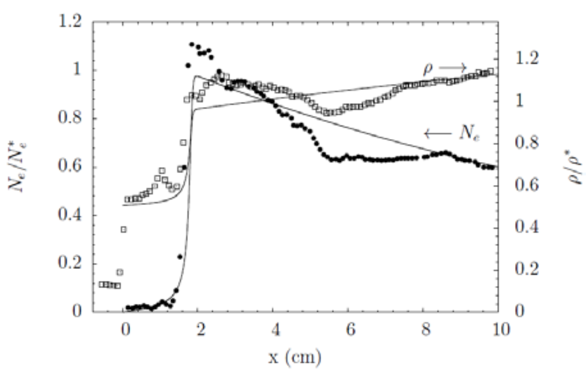
Chamber Environment



Ionizing shocks

Collisional-Radiative kinetics

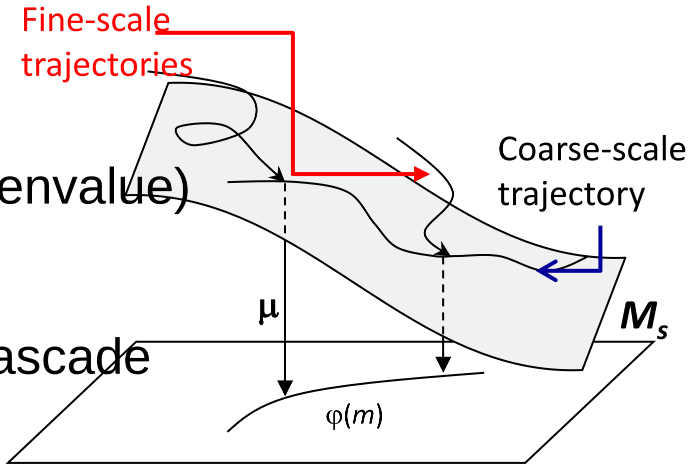
- **Non-equilibrium modeling of the atomic state distribution function (ASDF)**
  - Detailed state-to-state model of atomic transition, i.e., excitation and ionization
  - Rates derived based on ab initio cross section.
- **Examples: shocks**
- **Complications:**
  - Numerical stiffness



Atomic CR
Ar shock (31 levs)

Multiscale problem

- **Generic Multiscale problem:** $\dfrac{dy}{dx} = f_0(y,x) + \dfrac{1}{\varepsilon} f_1(y,x) \quad \varepsilon \to 0$
- **Various approaches possible: DNS, multi-grid/AMR, HMM, equation-free, etc.**
  – Some similarities between approaches
- **Traditional approach: scale separation** $y = y_s + y_f$
  – when ε→0, solve $\dfrac{dy_f}{dx} = \dfrac{1}{\varepsilon} f_1(y_s, y_f, x)$
  – Use "relaxed" solution for $\dfrac{dy_s}{dx} = f_0(y_s, y_f^*, x)$
  – Works slow manifold is attractive (neg. eigenvalue)
- **Complications:**
  – Pos. eigenvalues. Ex: instability, inverse cascade
  – Chaotic, stochastic fine scales, …
  – Non-separation of scales



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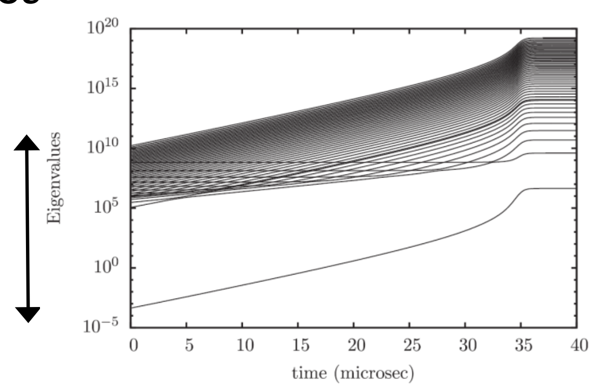
  - Works slow manifold is attractive (neg. eigenvalue)
- **Complications:**
  - Pos. eigenvalues. Ex: instability, inverse cascade
  - Chaotic, stochastic fine scales, …
  - Non-separation of scales: **CR kinetics**

Atomic CR:
Hydrogen (40 levs)

15 orders of magnitude



Kinetic equation

- **Boltzmann equation:**
  - $\varepsilon \ll 1$: fluid regime
  - $\varepsilon \sim O(1)$: kinetic regime, need to resolve vfd

$$\partial_t f + \vec{v} \cdot \nabla_{\vec{x}} f = \frac{1}{\varepsilon} Q(f, f) + \ldots$$

$$Q(f, f) = \int_{R^3} \int_{S^2} \sigma(|v - v_*|, \omega)[f(v')f(v_*') - f(v)f(v_*)] d\omega dv'$$

$$Q(f, f) = 0 \rightarrow f(v) = \frac{\rho}{(2\pi T)^{3/2}} \exp\left(-\frac{|v-u|^2}{2T}\right)$$

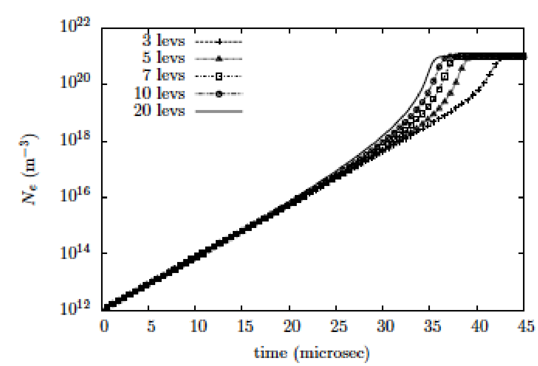
  - For collisional plasma (fully and partially ionized): need to include Coulomb collisions (FP), excitation/ionization, CX, etc.
- **Need efficient algorithms for collisional-radiative processes in both regimes and transitional regime.**

Translational Equilibrium

- **Moment method: derived by taking moment of the kinetic equations with fluid closure**
  - 5-moment model yields Euler/NS systems: multi-species, multi-temperature CR models.
  - Magnetized plasmas are often modeled with MHD with a hierarchy of descriptions: Ideal, resistive, Hall MHD.
  - Generalized model: multi-fluid (Braginskii, 1965)
- **CR kinetics = rate equations for each excited states**
  - Non-Boltzmann population of ASDF
  - Challenges: many states

$$
\begin{aligned}
\frac{dN_n}{dt} = & -\sum_{m>n} \alpha_{(m|n)} N_e N_n + \sum_{m>n} \beta_{(n|m)} N_e N_m + \sum_{m>n} A_{(n|m)} N_m \\
& + \sum_{m<n} \alpha_{(n|m)} N_e N_m - \sum_{m<n} \beta_{(m|n)} N_e N_n - \sum_{m<n} A_{(m|n)} N_n \\
& - \alpha_{(+|n)} N_e N_n + \beta_{(n|+)} N_+ N_e^2. \qquad (8)
\end{aligned}
$$

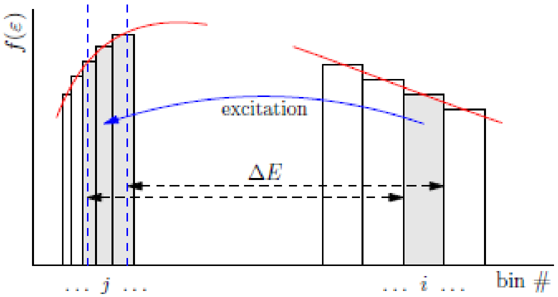
$$
\frac{dN_+}{dt} = \sum_n \alpha_{(+|n)} N_e N_n - \sum_n \beta_{(n|+)} N_+ N_e^2.
$$



Atomic hydrogen (20 levs)

Translational Non-equilibrium

- **Not-too-far from equilibrium**
  - Discretized EEDF yields rate equations for discrete elements (“bin”)
  - DB enforced at microscopic level
  - High-order, implicit and energy conserving
  - More efficient compared to MCC.
- **Far from equilibrium**
  - Particle methods with DSMC collisions
  - Can resolve anisotropic vdf
  - Drawback: slow convergence, reaction branching, singular rates, particles growth



$$\bar{n}_i = N_e \int_{\varepsilon_i}^{\varepsilon_i+\Delta\varepsilon} d\varepsilon\, f_e(\varepsilon)$$

$$\frac{d\bar{n}_i}{dt} = -N_l\, \bar{n}_i \sum_j \bar{k}^{\text{exc}}_{(j|i)} + N_u \sum_j \bar{n}_j \bar{k}^{\text{dex}}_{(i|j)}$$

$$\frac{d\bar{n}_j}{dt} = +N_l \sum_i \bar{n}_i \bar{k}^{\text{exc}}_{(j|i)} - N_u\, \bar{n}_j \sum_i \bar{k}^{\text{dex}}_{(i|j)}$$

Dynamical Regime

- **Examples: thruster plumes, gas discharges, LPI, etc.**
- **Require hybridization: fluid/kinetic**
- **Key challenges: smooth, efficient and consistent transition**
- **What we need:**
  - Multiscale statistics
  - Coarse-graining procedure for atomic state
  - Adaptive fluid-kinetic model
- **Current work:**
  - CR level grouping
  - Particle merging schemes
  - Multifluid model

Level grouping

- **CR modeling: level-grouping** ➡ $\mathcal{N}_n = N_{n_0}\sum_{i\in n}\frac{N_i}{N_{n_0}} \simeq \frac{N_{n_0}}{g_{n_0}}\underbrace{\sum_{i\in n} g_i e^{-\Delta E_i/T_n}}_{Z_n}$
  - Group effective rates of change

$$\frac{d\mathcal{N}_n}{dt} = -N_e\mathcal{N}_n\left[\sum_{m>n}\sum_{i\in n}\frac{g_i e^{-\Delta E_i/T_n}}{Z_n}\sum_{j\in m}\alpha_{(j|i)} + \sum_{m<n}\sum_{i\in n}\frac{g_i e^{-\Delta E_i/T_n}}{Z_n}\sum_{j\in m}\beta_{(j|i)}\right]$$

  - Internal structure of group is assumed Boltzmann (T_n)
    - Piecewise exponential
  - This does NOT mean the entire ASDF is Boltzmann!!
  - Group temperature must be determined ➡ additional conservation equation, e.g.: $\frac{d\mathcal{E}_n}{dt} = -N_e\mathcal{N}_n\left[\sum_{m>n}\sum_{i\in n}\frac{g_i e^{-\Delta E_i/T_n}}{Z_n}\sum_{j\in m}E_i\alpha_{(j|i)} + \sum_{m<n}\sum_{i\in n}\frac{g_i e^{-\Delta E_i/T_n}}{Z_n}\sum_{j\in m}E_i\beta_{(j|i)}\right]$
  - Procedure?
    - Solve: $(\Delta E)_n(\boxed{T_n^*}) + C_v(\boxed{T_n^*})\delta T_n^* = \boxed{\frac{\Delta\mathcal{E}_n^{(k)}}{\mathcal{N}_n^{(k)}}}$ with: $\Delta\mathcal{E}_n = \sum_{i\in n}(E_i - E_{n_0})N_i = \mathcal{N}_n\boxed{(\Delta E)_n}$, $\boxed{C_v(T_n)} = \frac{d}{dT_n}(\Delta E)_n$

iterated

computed

tabulated

    - **However…** $(\Delta E)_n \simeq o(\epsilon)$, $C_v(T_n) \simeq o(\epsilon)$ where $\epsilon = e^{-\Delta E_1/T_n}$ ➡ $\delta T_n^* = o(\epsilon)/o(\epsilon)$

Level grouping

- **CR modeling: level-grouping**
  - Other approaches?
    - Sub-partitioning: lowest level n_0 and total $\mathcal{N}_n$ (no need for $\mathcal{E}_n$)

$$\delta T_n^* \simeq \frac{T_n^{*2}}{\mathcal{Z}_n(T_n^*)(\Delta E)_n(T_n^*)}\left[\frac{\mathcal{N}_n^{(k)}}{N_{n_0}^{(k)}} g_{n_0} - \mathcal{Z}_n(T_n^*)\right] \quad = o(\epsilon)/o(\epsilon) \text{ ...fails}$$

    - Sub-partitioning: lowest level n_0 and upper distribution $\mathcal{N}_{n'}$

$$\delta T_n^* \simeq \frac{T_n^{*2}}{\mathcal{Z}_n'(T_n^*)(\Delta E)_n(T_n^*)}\left[\frac{\mathcal{N}_n'^{(k)}}{N_{n_0}^{(k)}} g_{n_0} - \mathcal{Z}_n'(T_n^*)\right] \quad = o(\epsilon)/o(\epsilon) \text{ ...fails}$$

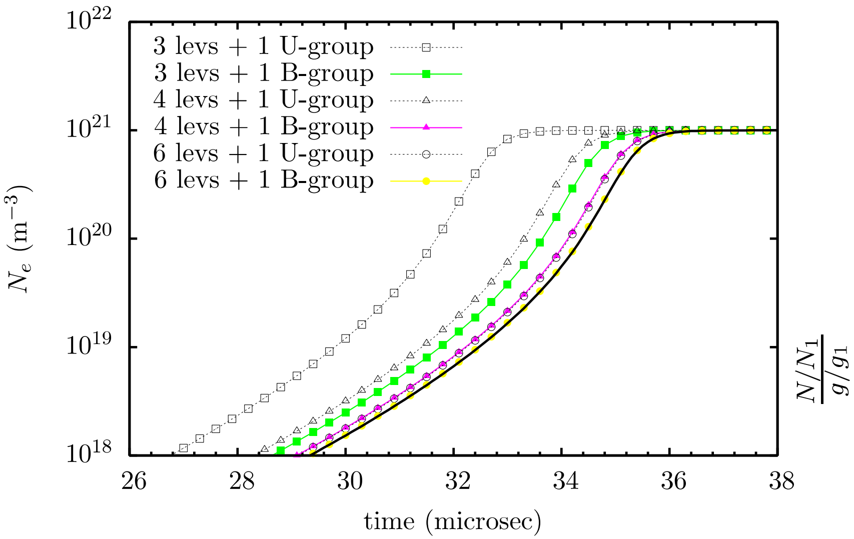
    - Approximate $\mathcal{Z}_n$ by expanding around mean energy: $\overline{\Delta E}_n = \frac{1}{g_n}\sum_{i\in n} g_i \Delta E_i$.

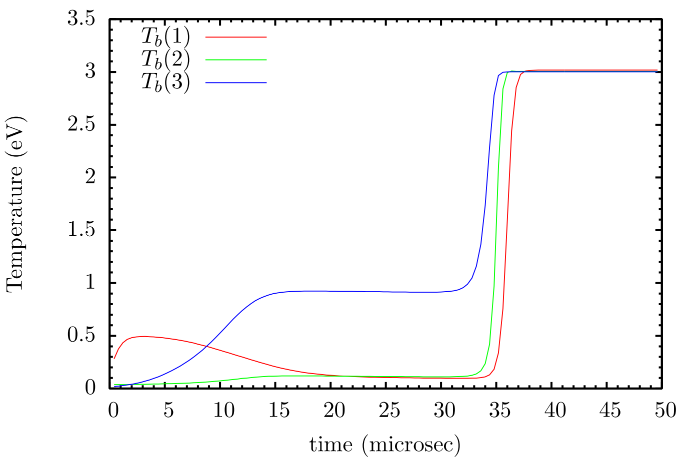
$$\mathcal{Z}_n(T_n) = e^{-\overline{\Delta E}_n/T_n}\sum_{i\in n} g_i\left[1 - \cancel{\frac{\delta_i}{T_n}} + \frac{1}{2}\frac{\delta_i^2}{T_n^2} + \ldots\right] \qquad \text{where} \quad \delta_i \equiv \Delta E_i - \overline{\Delta E}_n$$

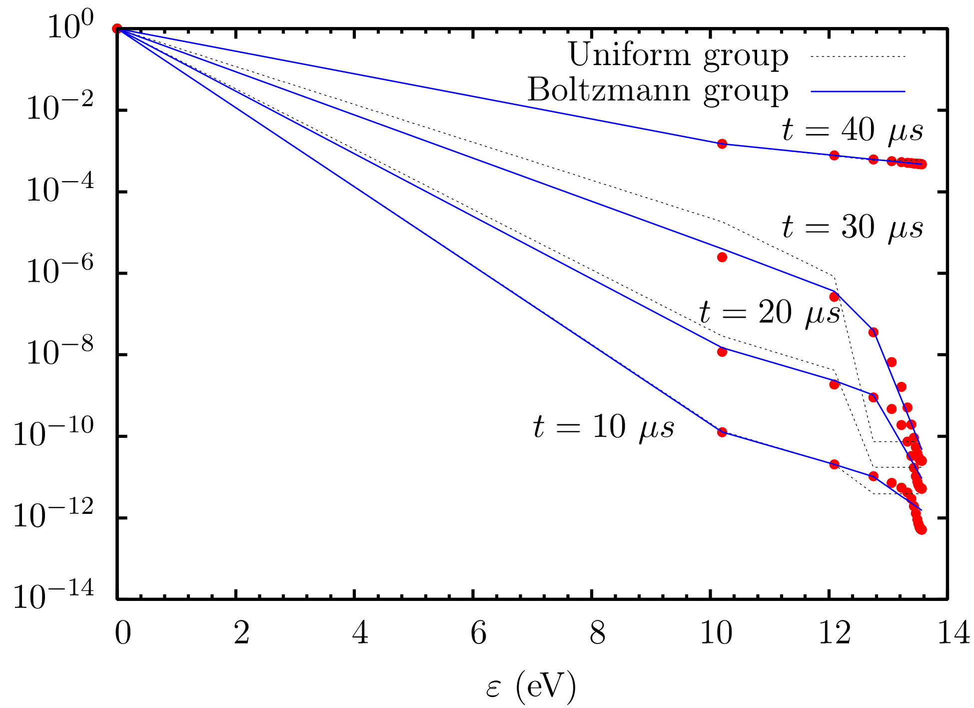
      - With n_0, $\mathcal{N}_n$ partitioning: $1/\ln(1+\varepsilon)$ ...fails
      - With n_0, $\mathcal{N}_{n'}$ partitioning: $1/\ln(\varepsilon)$ ...succeeds!
        - Improve with successive iterations… $\mathcal{Z}_n'(T_n) = \bar{g}_n'(T_n)e^{-\overline{\Delta E'}/T_n}$

Level grouping: 0D test

- **Isothermal heat bath**







Works very well (also tested in cooling regime).
Much better than uniform (standard) grouping.

Level grouping: Energy conservation

- **CR modeling: level-grouping**
  - Look at uniform bins – 2 formulations:

$$\cancel{\bar{\alpha}^E_{(m|n)} = \sum_{j\in m}\sum_{i\in n}\frac{g_i}{g_n}(E_j - E_i)\alpha_{(j|i)}}$$
$$\cancel{\bar{\beta}^E_{(m|n)} = \sum_{j\in m}\sum_{i\in n}\frac{g_j}{g_m}(E_j - E_i)\beta_{(i|j)}}$$

$$\bar{\alpha}^E_{(m|n)} = (\bar{E}_m - \bar{E}_n)\sum_{j\in m}\sum_{i\in n}\frac{g_i}{g_n}\alpha_{(j|i)}$$

Energy conserving!

$$\bar{\beta}^E_{(m|n)} = (\bar{E}_m - \bar{E}_n)\sum_{j\in m}\sum_{i\in n}\frac{g_j}{g_m}\beta_{(i|j)}$$

  - Right-form is product of Energy x d$\mathcal{N}_n$/dt…
    - Conservation follows from definition $\mathcal{E}_n = \bar{E}_n \mathcal{N}_n$
  - Same principle can be applied to Boltzmann groups:
    - Start with:

Δ(overall group population) : $\mathcal{N}_n$

$$\frac{d\Delta\mathcal{E}_n}{dt} \equiv \sum_{i\in n}\Delta E_i \frac{dN_i}{dt} = \frac{d}{dt}\left(\mathcal{N}'_n\langle\Delta E\rangle_{n'}\right) = \langle\Delta E\rangle_{n'}\boxed{\frac{d\mathcal{N}'_n}{dt}} + \mathcal{N}'_n\boxed{\frac{d\langle\Delta E\rangle_{n'}}{dt}}$$

Δ(internal structure) := $C_{v,n'}\frac{dT_n}{dt}$

    - Express in terms of conserved variables:

$$\frac{d\mathcal{E}_n}{dt} = [E_{n_0} - \omega_{n'}]\frac{dN_{n_0}}{dt} + [E_{n_0} + \langle\Delta E\rangle_{n'} + \xi_{n'}]\frac{d\mathcal{N}'_n}{dt}$$

with $\xi_{n'} = \dfrac{C_{v,n'}T_n^2}{\left(\overline{\Delta E'}_n + T_n^2\frac{d\ln\bar{g}_n}{dT_n}\right)}$ and $\omega_{n'} = \xi_{n'}\dfrac{N_{n'}}{N_{n_0}}$

Level grouping: Energy conservation

- **CR modeling: level-grouping**
  - Finally…Procedure shown to be equivalent to replacing energies by “effective” (condition-dependent) values (≈ EOS)

Excitation:

$$\bar{\alpha}^{E}_{(m_o|n_o)} = \left(\bar{E}_{m_o} - \bar{E}_{n_o}\right) \cdot \bar{\alpha}_{(m_o|n_o)}$$
$$\bar{\alpha}^{E}_{(m'|n_o)} = \left(\bar{E}_{m'} - \bar{E}_{n_o}\right) \cdot \bar{\alpha}_{(m'|n_o)}$$
$$\bar{\alpha}^{E}_{(m_o|n')} = \left(\bar{E}_{m_o} - \bar{E}_{n'}\right) \cdot \bar{\alpha}_{(m_o|n')}$$
$$\bar{\alpha}^{E}_{(m'|n')} = \left(\bar{E}_{m'} - \bar{E}_{n'}\right) \cdot \bar{\alpha}_{(m'|n')}$$

Ionization:

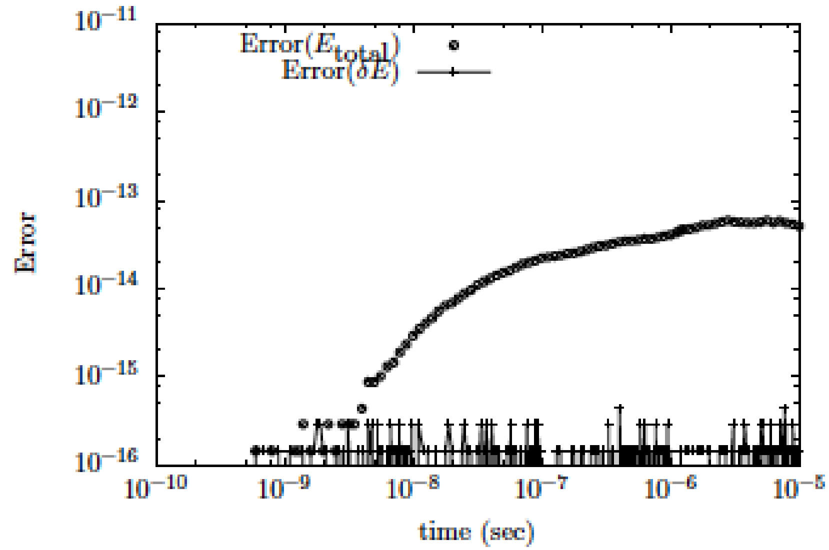
$$\bar{\alpha}^{E}_{(+|n_o)} = \left(I_H - \bar{E}_{n_o}\right) \cdot \bar{\alpha}_{(+|n_o)}$$
$$\bar{\alpha}^{E}_{(+|n')} = \left(I_H - \bar{E}_{n'}\right) \cdot \bar{\alpha}_{(+|n')}$$

with

$$\bar{E}_{n_o} = E_{n_o} - \omega_{n'}$$
$$\bar{E}_{n'} = E_{n_o} + \langle \Delta E \rangle_{n'} + \xi_{n'}$$

- **NOW**, energy is conserved

(down to round-off)



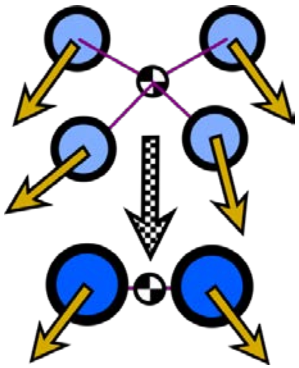
Particle Merging Schemes

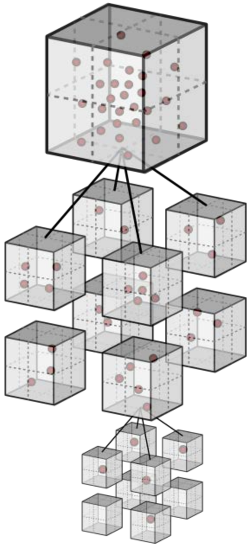
- The schemes consists of merging 3 or more particles to 2. Mass, momentum and kinetic energy are exactly conserved; Electrostatic energy also conserved in physical space.

- Split analogously defined by merging only fractions of original particles.

- To inhibit thermalization, an octree in velocity space is used so that only near neighbor particles are merged.

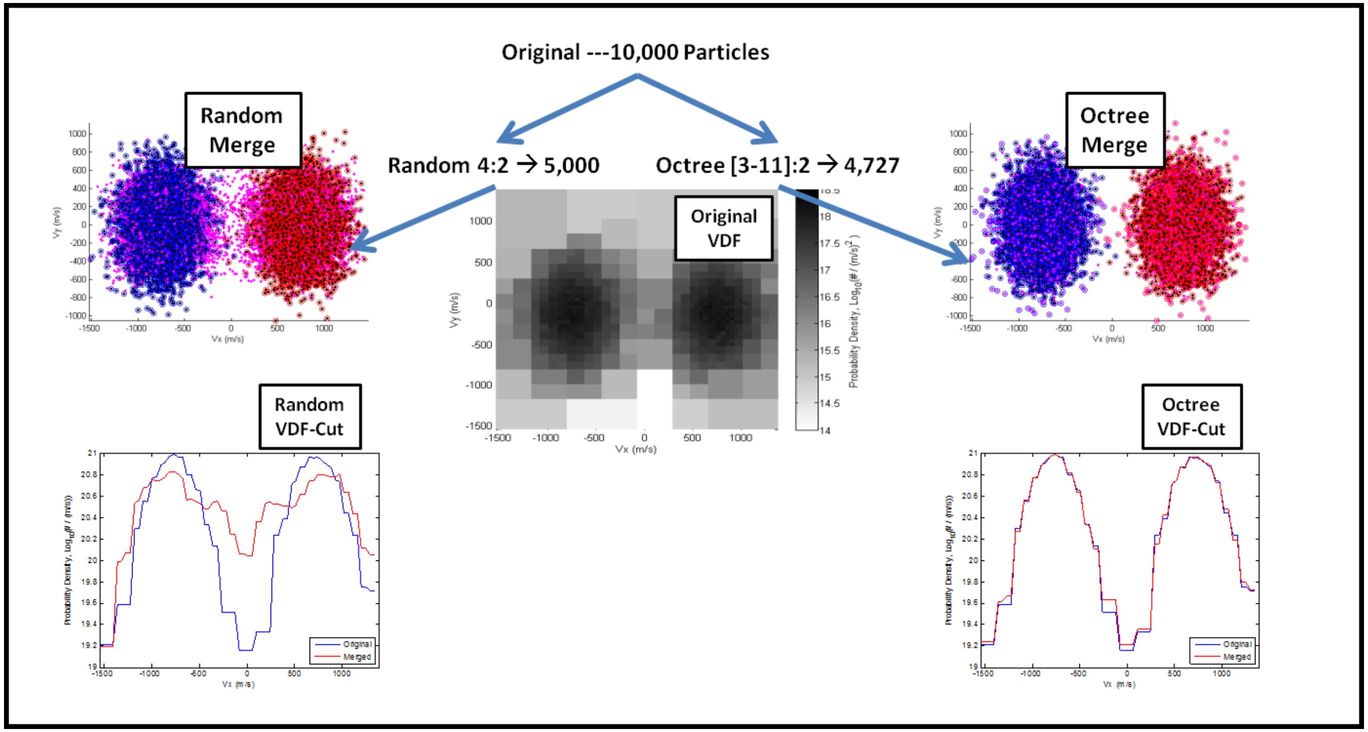
- Higher-moment conserving schemes obtained with increased number of merge result particles generated.





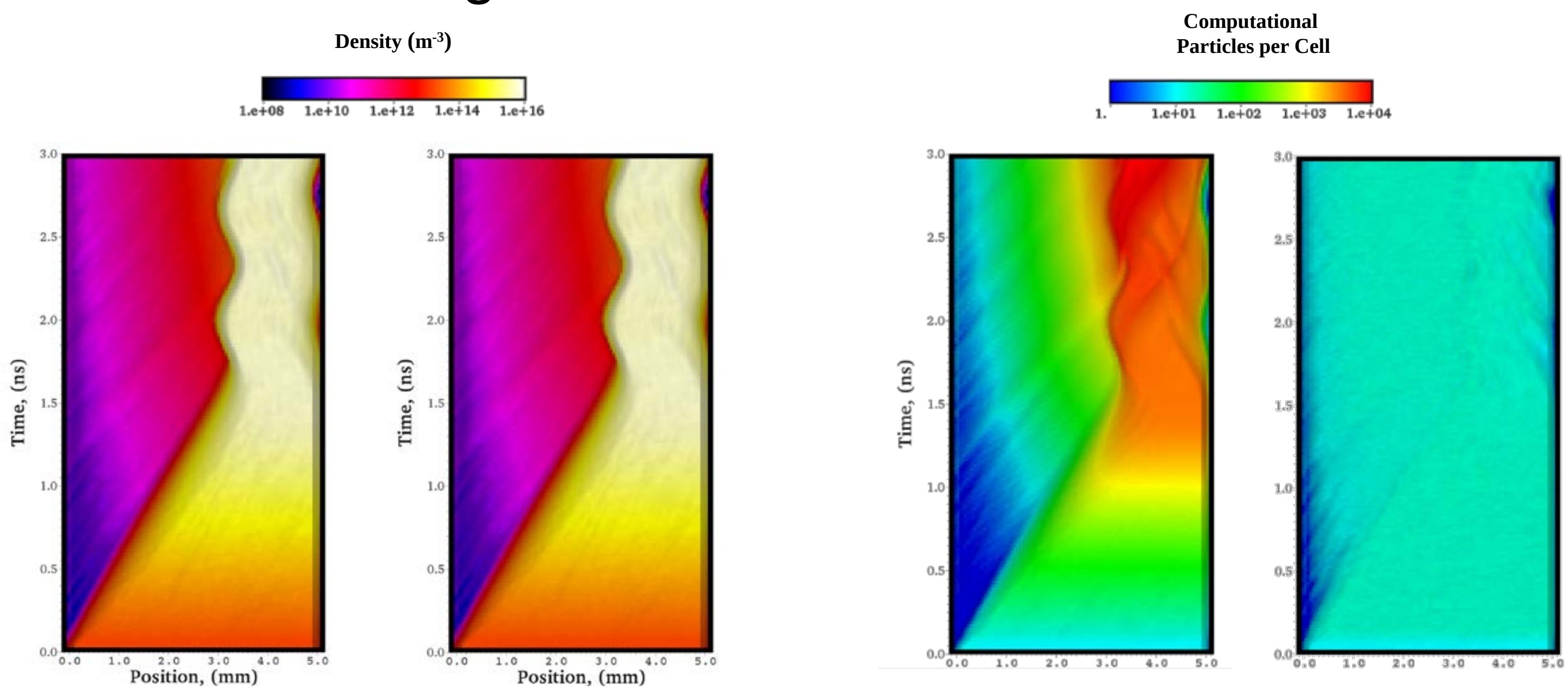
Examples

- **from 0D …**



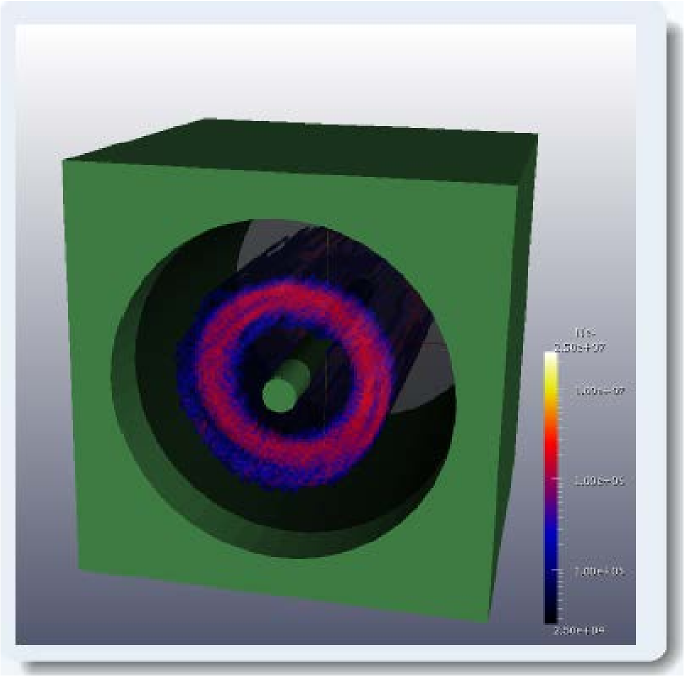
Examples

- **from 0D to 1D3V…**
  - Gas discharge with ionization.



Examples

- **from 0D to 1D3V and 3D3V …**
  - Annular test case
  - More test cases underway

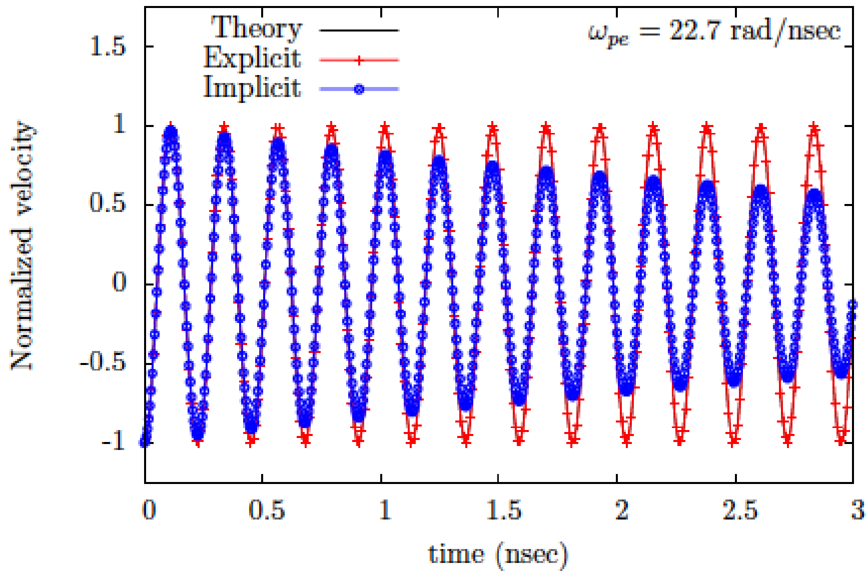


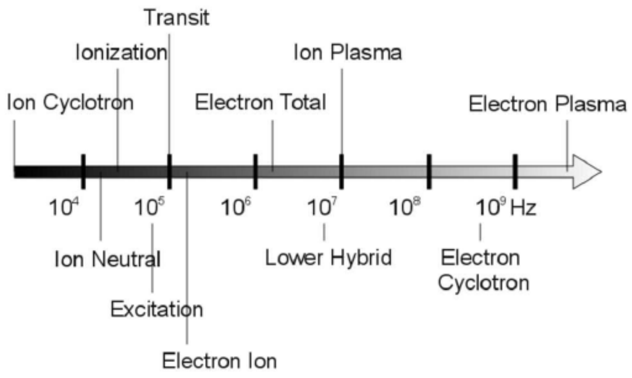
Multi-fluid equations

- **Multi-fluid model:**
  – Develop series of models for variable conditions:

Electrostatic → + Magnetostatic → Electro-magnetic → 3-fluid

  – Use implicit models to eliminate constraint of sequence of fast time scales: c, v_e, $\omega_{ps} = \sqrt{\frac{n_s q_s^2}{\epsilon_0 m_s}}$ $\omega_{cs} = \frac{q_s B}{m_s}$
  – Price to pay: lack of resolution misses physics…





Multi-fluid equations

- **Multi-fluid model:**
  - 5-moment:

$$\partial_t \rho_s + \nabla \cdot (\rho_s \mathbf{u}_s) = \omega_s^\rho$$

$$\partial_t(\rho_s \mathbf{u}_s) + \nabla \cdot (\rho_s \mathbf{u}_s \mathbf{u}_s + \mathbb{P}_s) = Z_s e n_s (\mathbf{E} + \mathbf{u}_s \times \mathbf{B}) + \mathbf{f}_s^m$$

$$\partial_t \varepsilon_s + \nabla \cdot (\mathbf{u}_s \varepsilon_s + \mathbb{P}_s \cdot \mathbf{u}_s) + \nabla \cdot \mathbf{q}_s = \mathbf{j}_s \cdot \mathbf{E} + \omega_s^\varepsilon$$

  - Add Maxwell's equations:

$$\nabla \times \mathbf{E} = -\partial_t \mathbf{B} \qquad \nabla \cdot \mathbf{E} = \frac{e}{\varepsilon_0}(Z_i n_i - n_e)$$

$$\nabla \times \mathbf{B} = \mu_0 \mathbf{j} - \frac{1}{c^2}\partial_t \mathbf{E} \qquad \nabla \cdot \mathbf{B} = 0$$

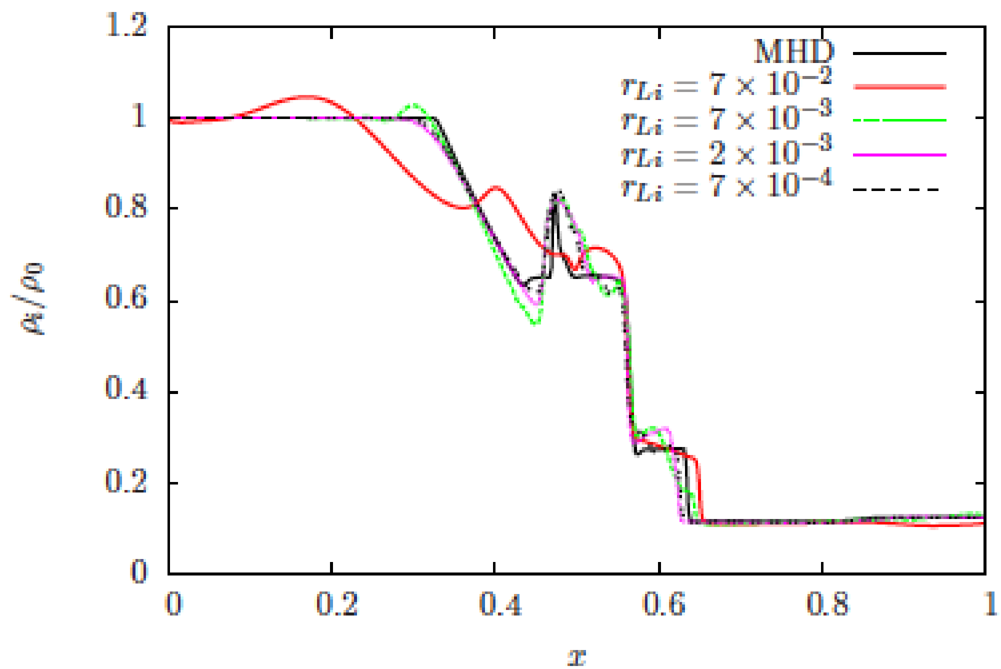
  - Add collisions:
    - Elastic – Bragiinski terms
    - Inelastic – warning! Rates depend on both T and relative velocity

$$k_i = n_n n_e \int\int f_n f_e g \sigma_i''(g; \Omega_1, \Omega_2) d\Omega_1 d\Omega_2 d^3 v_n d^3 v_e \;\Rightarrow\; k_i = k_i(T_e, |\mathbf{u}_n - \mathbf{u}_e|)$$

    - Multi-fluid CR model from fundamental principles being developed (incl. detailed balance)

Multifluid equations

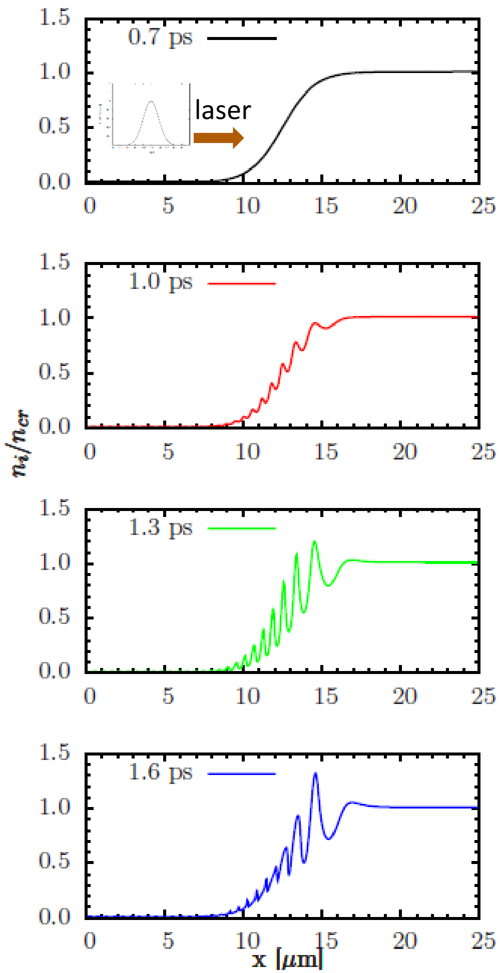
- **Electromagnetic shock: generalized Brio-Wu[1]**
  - FV with WENO reconstruction and RK3

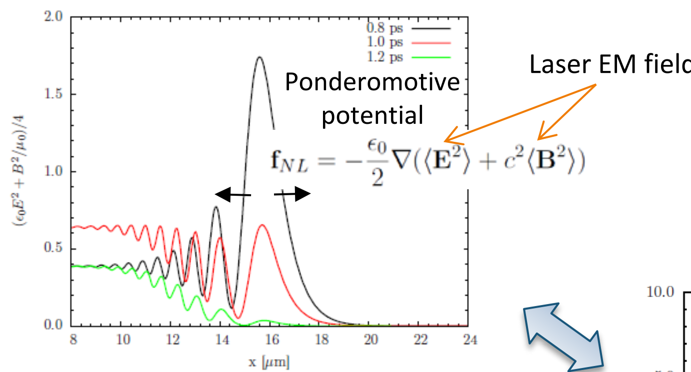


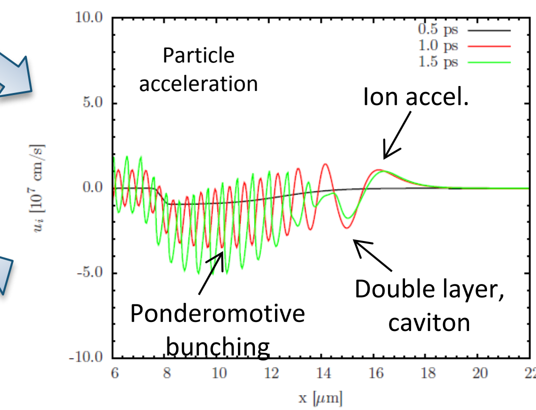
[1]Shumlak & Loverich, JCP 2003

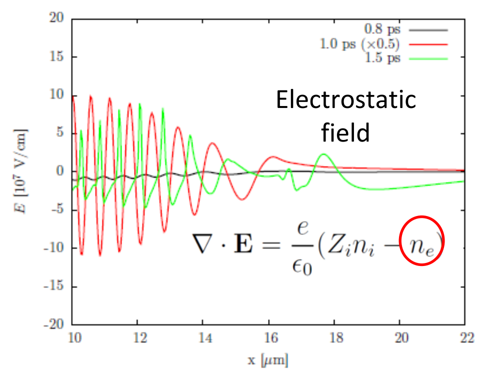
Laser-Plasma Interaction

- **Ion acceleration due to ponderomotive force**









$$\partial_t(\rho_e \mathbf{u}_e) + \nabla \cdot (\rho_e \mathbf{u}_e \mathbf{u}_e + p_e \mathbb{I}) = -e n_e \mathbf{E} + \rho_e \nu_{ei} \mathbf{w}_{ei} + \mathbf{f}_{NL}$$

$$\partial_t(\rho_i \mathbf{u}_i) + \nabla \cdot (\rho_i \mathbf{u}_i \mathbf{u}_i + p_i \mathbb{I}) = Z_i e n_i \mathbf{E} - \rho_e \nu_{ei} \mathbf{w}_{ei}$$

Conclusion

- **Multiscale algorithms for nonequilibrium flows with CR kinetics**
  - Particle merge/split for particle management, efficient sampling, inelastic collisions …
  - Level grouping schemes of electronic states, for dynamical coarse-graining of ASDF.
  - Multifluid equations to efficiently capture electron "hydrodynamics"
- **Ongoing works:**
  - High-order particle merging schemes
  - Multi-D simulation with level grouping
  - Modeling of inelastic collisions in multifluid