A Multi-Species, Multi-Fluid Model for Simulating Plasma Interpenetration

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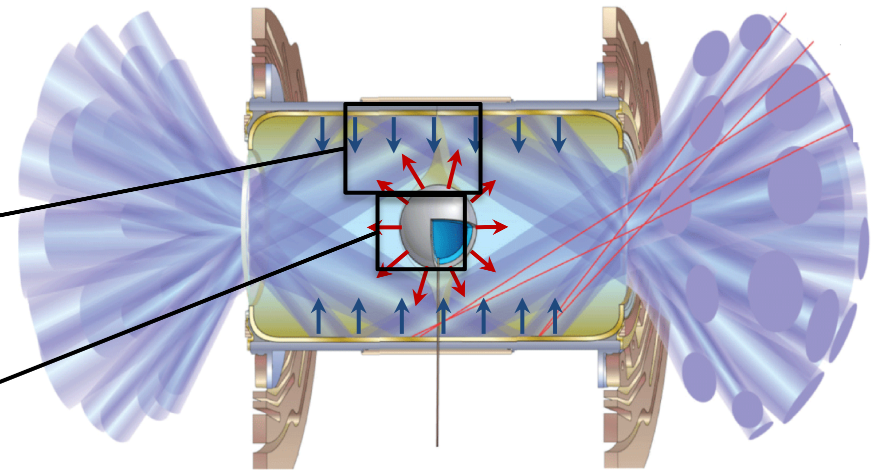
Background and Motivation

Inertial Confinement Fusion: **Colliding plasmas from hohlraum wall and capsule**

Interpenetration of plasma flows from capsule and hohlraum wall

- Large range of Z: $2 \leq Z \leq 60$
- Supersonic flows ($\Delta u \approx 10^8$ cm/s)

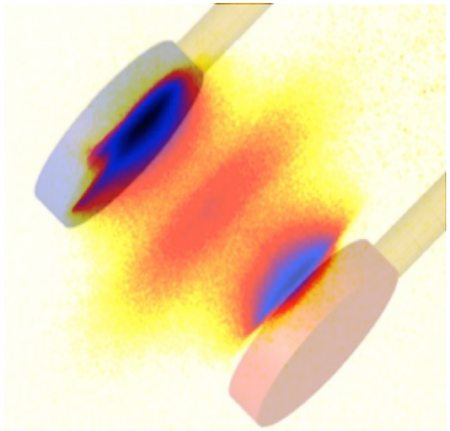
Species separation inside target capsule



Source: https://csdl-images.computer.org/mags/cs/2014/06/figures/mcs20140600421.gif

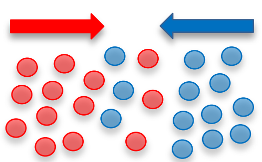
High Energy Density Physics (HEDP) Experiments

Carbon plasma streams ablating off paddles hit by laser beams and colliding with each other

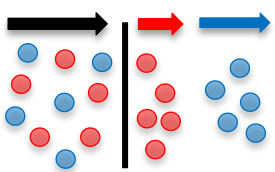


Source: H. S. Park et al., 2012

Multifluid phenomena that we want to model



Interpenetrating plasmas



Plasma species separation

Current simulation tools are *not sufficiently versatile*

Lack key physics

Single-Fluid Multi-species Hydrodynamic Solvers

- Example: *HYDRA, LASNEX*
- Single velocity field insufficient to model multiple inter-penetrating fluids
- Unphysical shocks

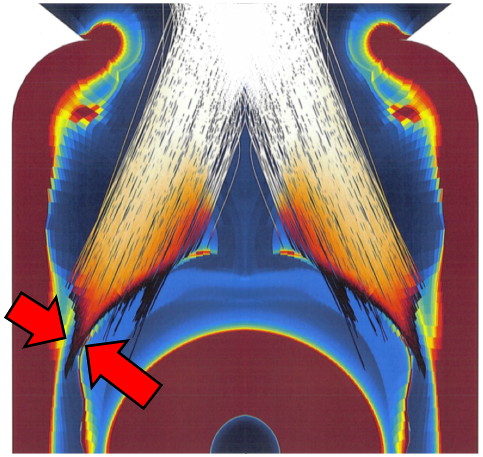
Collisional Kinetic Solvers

- Example: *LOKI, OSIRIS, PSC*
- High computational cost to simulate small volumes
- Impractical for experimental scales

Too Expensive

Simulation of **plasma dynamics in hohlraum** using *HYDRA*

Density pile—up predicted when plasma streams collide



Current workarounds: species diffusion models

Needs: physics beyond single-fluid theory – *multi-fluid*, multi-species, with local *kinetic effects*

Governing Equations: We solve the inviscid Euler equations for each ion species

$$\alpha = 1, \cdots, n_s$$

$$\frac{\partial \rho_\alpha}{\partial t} + \nabla \cdot (\rho_\alpha \mathbf{u}_\alpha) = 0$$

$$\frac{\partial \rho_\alpha \mathbf{u}_\alpha}{\partial t} + \nabla (P_\alpha + \rho_\alpha \mathbf{u}_\alpha \otimes \mathbf{u}_\alpha) = -Z_\alpha e n_\alpha \nabla \phi + \sum_{\beta \neq \alpha} \mathbf{R}_{\alpha,\beta}$$

$$\frac{\partial \mathcal{E}_\alpha}{\partial t} + \nabla \cdot [(\mathcal{E}_\alpha + P_\alpha) \mathbf{u}_\alpha] = -Z_\alpha e n_\alpha \mathbf{u}_\alpha \cdot \nabla \phi + \sum_{\beta \neq \alpha} (\mathbf{R}_{\alpha,\beta} \cdot \mathbf{u}_\alpha + Q_{\alpha,\beta})$$

Interaction between species

Assuming quasineutral, isothermal electrons*

$$\nabla \phi = \frac{T_e}{n_e} \nabla n_e + \frac{1}{n_e} \sum_\alpha R_{e,\alpha}$$

Electron momentum equation neglecting inertia terms and assuming

$$P_e = n_e T_e$$

Frictional drag

$$\mathbf{R}_{\alpha,\beta} = m_\alpha n_\alpha \nu_{\alpha,\beta} (\mathbf{u}_\beta - \mathbf{u}_\alpha)$$

Frictional heating and thermal equilibration

$$Q_{\alpha,\beta} = Q^{\mathrm{fric}}_{\alpha,\beta} + Q^{\mathrm{eq}}_{\alpha,\beta}$$

$$Q^{\mathrm{fric}}_{\alpha,\beta} = m_{\alpha,\beta} n_\alpha \nu_{\alpha,\beta} (\mathbf{u}_\beta - \mathbf{u}_\alpha)^2$$

$$Q^{\mathrm{eq}}_{\alpha,\beta} = -3 m_\alpha n_\alpha \frac{\nu_{\alpha,\beta}}{m_\alpha + m_\beta} (T_\alpha - T_\beta)$$

Reformulated Governing Equations

Ion Euler equations with isothermal, quasineutral e⁻

Advective nature of electrostatic force

- Included **electron pressure** on LHS with hydrodynamic pressure
- Derived the **eigenstructure** for **characteristic-based discretization**

Effect of discretization error in dense species on **dynamics of sparse species**

Reformulation of electrostatic source terms to *avoid sums/differences of terms of disparate scales*

$$\frac{\partial \rho_\alpha}{\partial t} + \nabla \cdot (\rho_\alpha \mathbf{u}_\alpha) = 0,$$

$$\frac{\partial \rho_\alpha \mathbf{u}_\alpha}{\partial t} + \nabla (\rho_\alpha \mathbf{u}_\alpha \otimes \mathbf{u}_\alpha + P^*_\alpha) = Z_\alpha T_e n_e \nabla \left(\frac{n_\alpha}{n_e}\right) + \frac{Z_\alpha n_\alpha}{n_e} \sum_\beta \mathbf{R}_{e,\beta} + \mathbf{R}_{\alpha,e} + \sum_{\beta \neq \alpha} \mathbf{R}_{\alpha,\beta},$$

$$\frac{\partial \mathcal{E}_\alpha}{\partial t} + \nabla \cdot \{(\mathcal{E}_\alpha + P^*_\alpha)\mathbf{u}_\alpha\} = Z_\alpha T_e n_e \nabla \left(\frac{\mathbf{u}_\alpha n_\alpha}{n_e}\right) + \frac{Z_\alpha n_\alpha}{n_e} \sum_\beta \mathbf{u}_\alpha \cdot \mathbf{R}_{e,\beta} + \sum_{\beta \neq \alpha} (\mathbf{R}_{\alpha,\beta} \cdot \mathbf{u}_\alpha + Q_{\alpha,\beta}) + \mathbf{R}_{\alpha,e} \cdot \mathbf{u}_\alpha + Q^{\text{eq}}_{\alpha,e},$$

Electron pressure

where $P^*_\alpha = P_\alpha + Z_\alpha T_e n_\alpha$

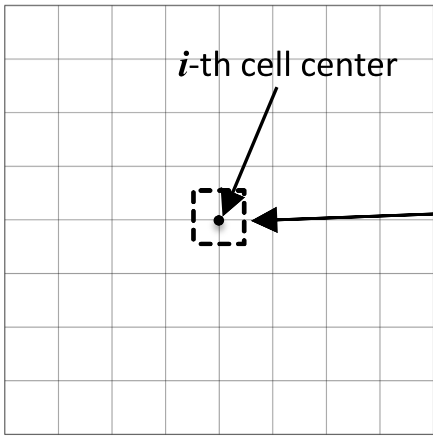
is the "**augmented pressure**" (hydro + *e*⁻)

Wavespeeds (eigenvalues) : $\mathbf{v}, \mathbf{v} \pm \sqrt{\frac{\gamma_\alpha P^*_\alpha}{\rho_\alpha}}$

Summary of Numerical Method

High-Order Conservative Finite-Difference/Finite-Volume Method

4th order finite-volume discretization (using the *CHOMBO* library) **with AMR**



3D Domain $\Omega \equiv \{\mathbf{x} : 0 \le \mathbf{x} \cdot \mathbf{e}_d \le L_d, 1 \le d \le 3\}$

discretized into computational cells

$$\omega_{\mathbf{i}} = \prod_{d=1}^{3} \left[\left(\mathbf{i} - \frac{1}{2}\mathbf{e}_d \right) h, \left(\mathbf{i} + \frac{1}{2}\mathbf{e}_d \right) h \right]$$

$\mathbf{i}$: 3-dimensional integer index (i, j, k)
h: grid spacing

$$\frac{\partial \bar{\mathbf{u}}_{\mathbf{i}}}{\partial t} = \frac{1}{h} \sum_{d=1}^{3} \left(\left\langle \hat{\mathbf{F}}_{\mathbf{i}+\frac{1}{2}\mathbf{e}_d} \right\rangle - \left\langle \hat{\mathbf{F}}_{\mathbf{i}-\frac{1}{2}\mathbf{e}_d} \right\rangle \right)$$

Cell-averaged solution

Face-averaged fluxes

$$\mathbf{u} = \begin{bmatrix} \vdots \\ \rho_\alpha \\ \rho_\alpha \mathbf{v}_\alpha \\ \mathcal{E}_\alpha \\ \vdots \end{bmatrix}$$

Spatially-discretized ODE in time (integrated in time using **4th order Runge-Kutta method**)

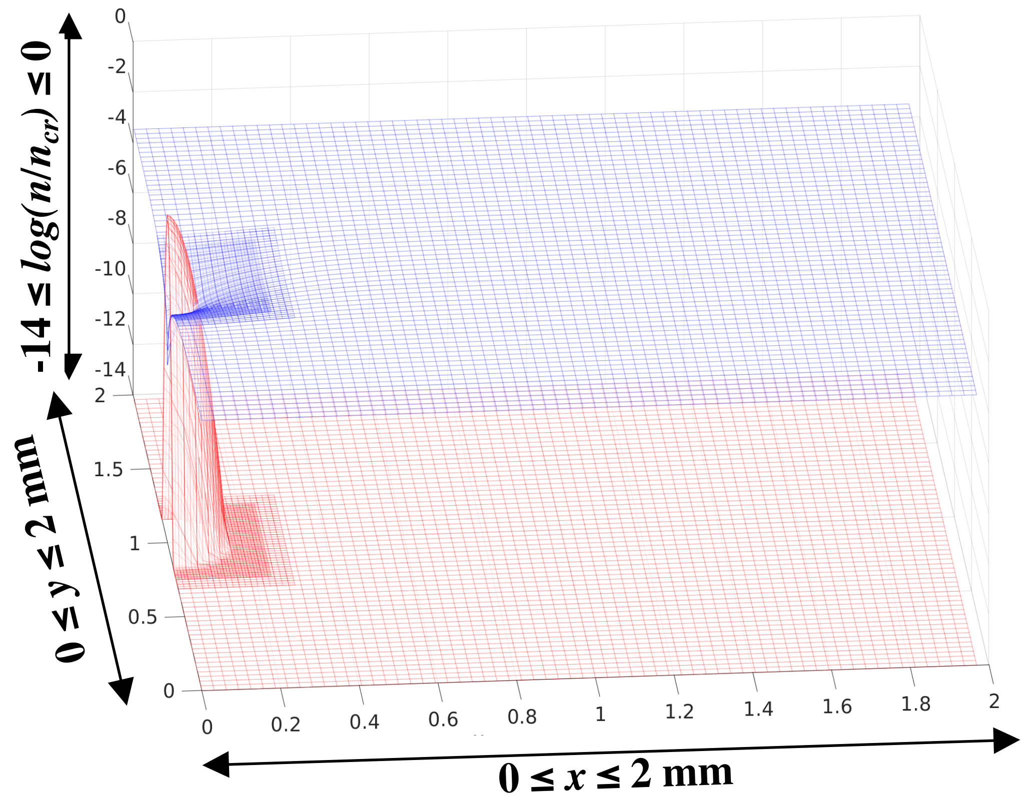
Strong shocks and gradients
O(1) to O(1e-14)

- **Characteristic-based discretization**
- **5th-order WENO scheme** with **Monotonicity-Preserving limiting**

Example: Single Species Expansion into Gas Fill with AMR – *Initial Setup*

Expansion of a *carbon* blob in the presence of *helium* gas fill (2D)

- **Initial solution:** a carbon species piled up on one end (*Gaussian blob* density); gas fill present in the space everywhere else.
- **Boundary conditions:** Solid wall BCs along *x* and *y*



Reference quantities:
Mass: *proton mass* (1.6730e-24 g);
Number density: n_{crit} (9.0320e+21 cm^{-3});
Length: 1 mm; Time: 3.2314e-09 s;
Temperature: 1 keV (1.6022e-09 ergs)

Example: Single Species Expansion into Gas Fill with AMR – Solution Evolution

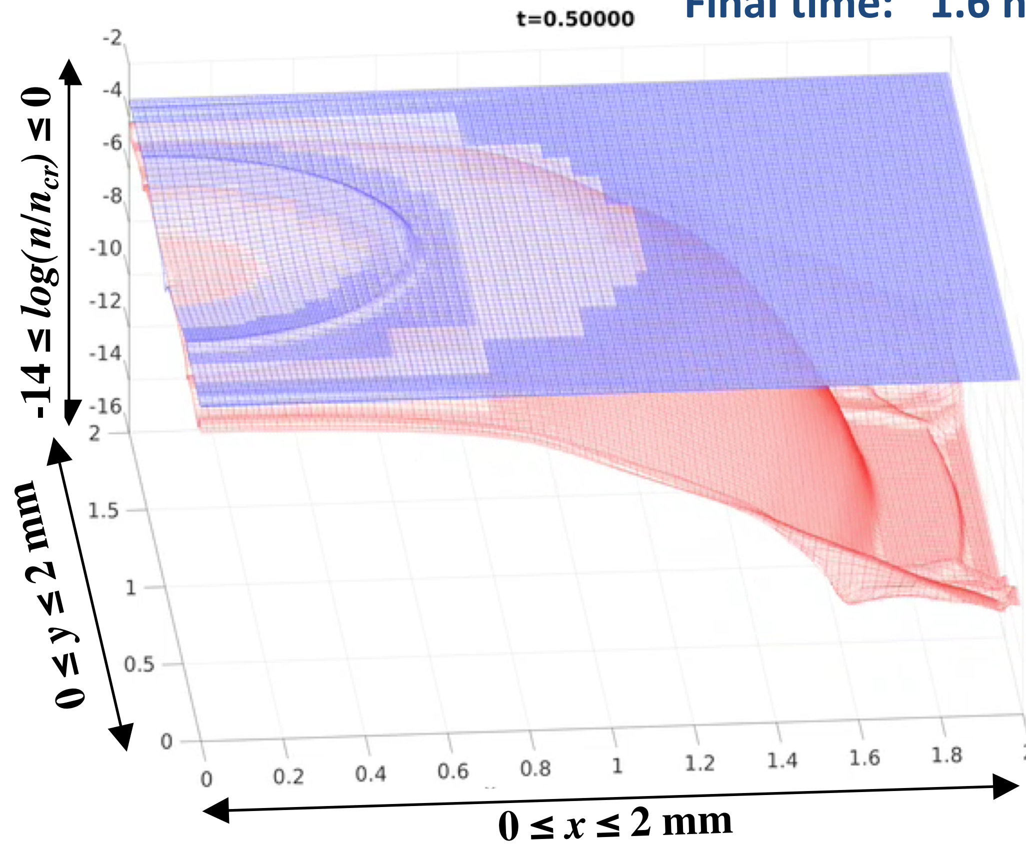
Expansion of a *carbon* blob in the presence of *helium* gas fill (2D)

- **Initial solution:** a carbon species piled up on one end (*Gaussian blob* density); gas fill present in the space everywhere else.
- **Boundary conditions:** Solid wall BCs along *x* and *y*

AMR: Refined mesh adaptively generated in regions of high gradients

Reference quantities:
Mass: *proton mass* (1.6730e-24 g);
Number density: n_{crit} (9.0320e+21 cm^{-3});
Length: 1 mm; Time: 3.2314e-09 s;
Temperature: 1 keV (1.6022e-09 ergs)

Final time: ~1.6 ns

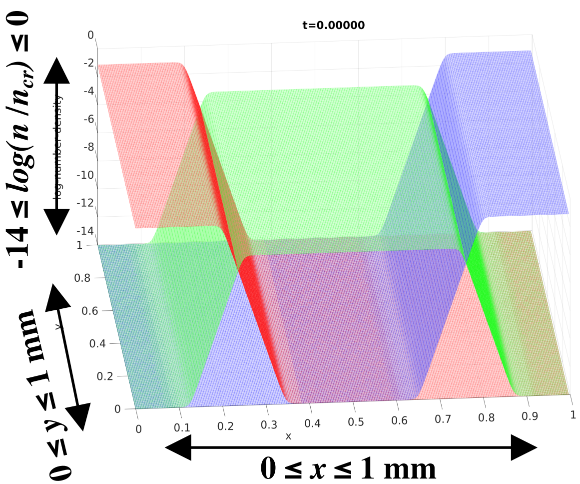


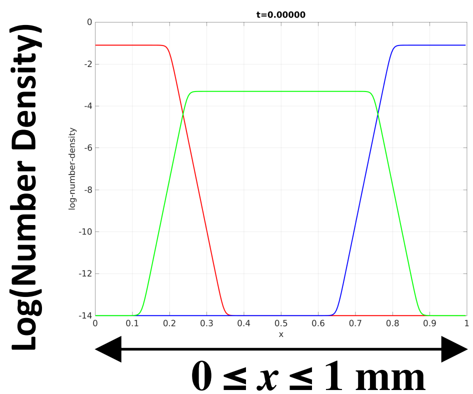
Example: Two Species Interpenetration with Gas Fill

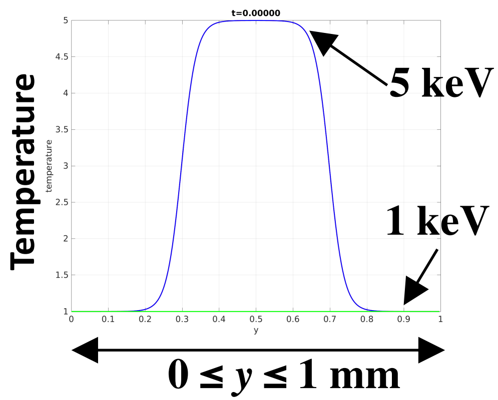
Problem Setup

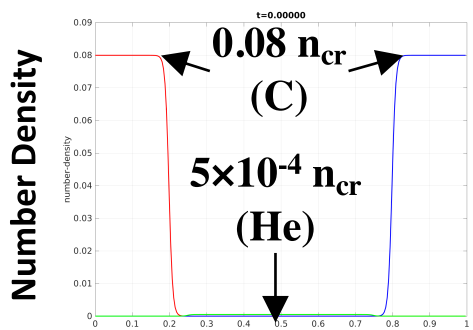
Interpenetration of *carbon* and *carbon* streams in the presence of *helium* gas fill (2D)

- **Initial solution:** two species piled up on either end (*smoothed slab* density); gas fill present in the space in between.
- **Temperature variation along *y*** – the plasmas are hotter in the center of the domain









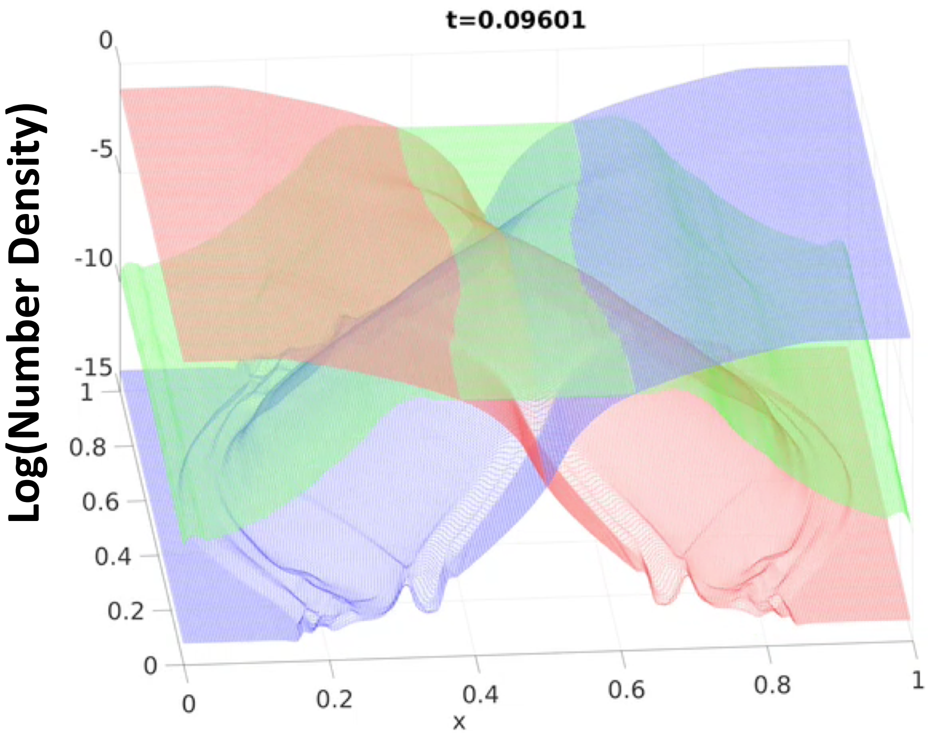
Boundary conditions:

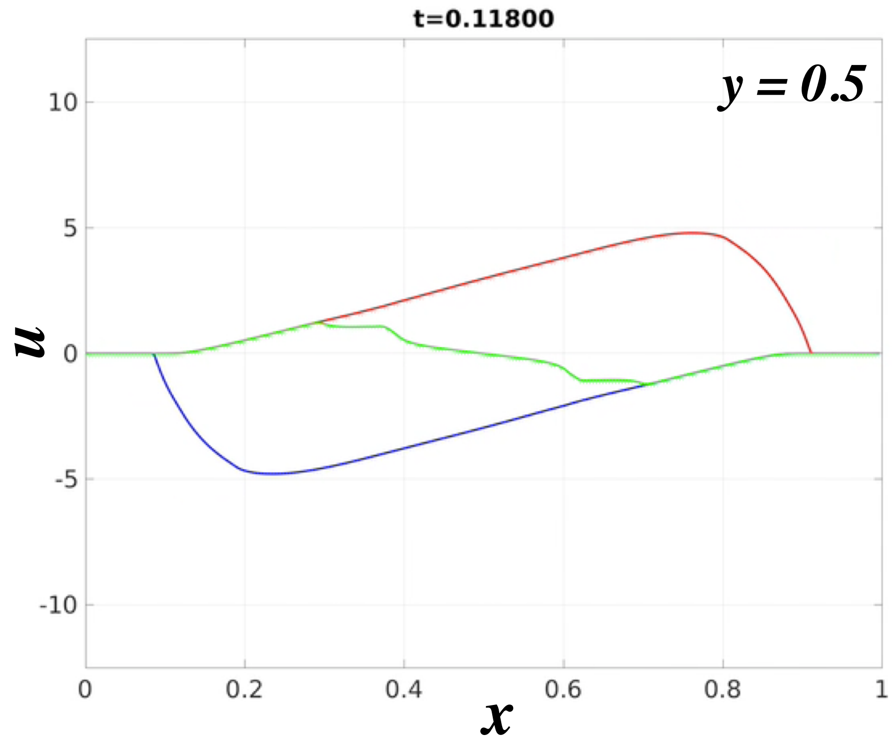
- Solid wall BCs along *x*
- Periodic along *y*

Reference quantities:

Mass: *proton mass* (1.6730e-24 g)
Number density: n_{crit} (9.0320e+21 cm^{-3})
Length: 1 mm
Temperature: 1 keV (1.6022e-09 ergs)

Example: Two Species Interpenetration with Gas Fill





Final time: ~1.3 ns

- **Species interaction** prevents one species from reaching the other end of the domain along *x*
- The fill gas is pushed towards the center of the domain by the carbon streams.

Reference quantities:
Number density: n_{crit} (9.0320e+21 cm^{-3});
Length: 1 mm; Time: 3.2314e-09 s;
Velocity: 3.0946e+07 cm/s

Stiffness of Collisional Terms for High-Z Species

Ion–ion collisional interaction term: Frictional force & heating, and thermal equilibration of *ion species 1* due to *ion species 2*

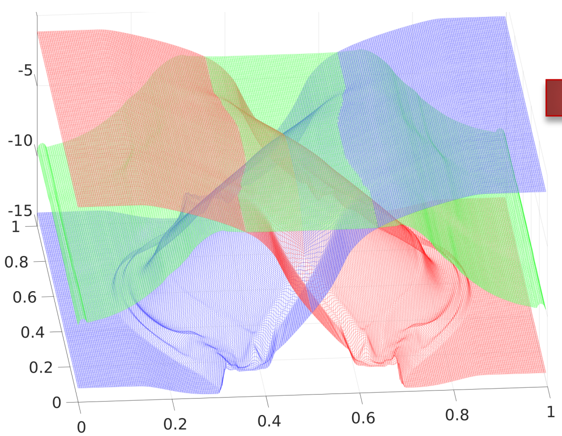
$$\begin{bmatrix} 0 \\ m_1 n_1 \nu_{12} (u_2 - u_1) \\ m_1 n_1 \nu_{12} (u_2 - u_1) u_1 + m_{12} n_1 \nu_{12} (u_2 - u_1)^2 + 3 \frac{m_1 n_1 \nu_{12}}{m_1 + m_2} (T_2 - T_1) \end{bmatrix}$$

Typically, $n \propto (1/Z)$

where

$$\nu_{12} = \left(\frac{4\sqrt{2\pi}}{3} \right) \frac{Z_1^2 Z_2^2 n_2 \Lambda}{m_1 m_{12}} \left[r (u_1 - u_2)^2 + \frac{T_1}{m_1} + \frac{T_2}{m_2} \right]^{-\frac{3}{2}} \left(\frac{e^4 n_0 x_0}{T_0^2} \right)$$

$$\boxed{\propto Z_1 Z_2 \sqrt{\frac{m_1 m_2}{m_1 + m_2}}}$$



$Z = 1$, $m = 1$

H → ***H*** ← ***H***

CFL $\sim$ ***1***

(CFL based on the hyperbolic term on the LHS)

$Z = 6$, $m = 12$ | $Z = 2$, $m = 4$

C → ***He*** ← ***C***

CFL $\sim$ ***0.05***

$Z = 40$, $m = 197$ | $Z = 2$, $m = 4$ | $Z = 6$, $m = 12$

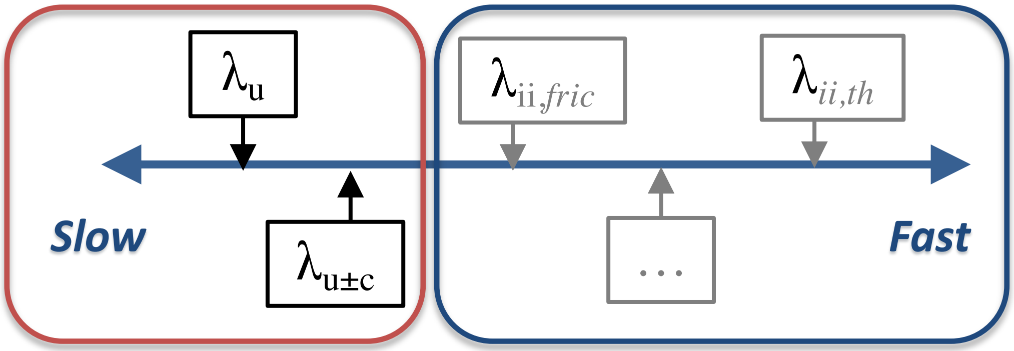
Au → ***He*** ← ***C***

CFL $\sim$ ***0.001***

Implicit-Explicit (IMEX) Time Integration

Resolve scales of interest; Treat implicitly faster scales

Advective and acoustic time scales (nonstiff terms)



Collisional time scales – ion-ion and e^--ion friction & thermal equilibration **(stiff terms)**

Explicit time integration *Implicit time integration*

ODE in time

Resulting from spatial discretization of PDE

$$\frac{d\mathbf{y}}{dt} = \mathcal{R}(\mathbf{y})$$

IMEX time integration: *partition RHS*

$$\mathcal{R}(\mathbf{y}) = \mathcal{R}_{\text{stiff}}(\mathbf{y}) + \mathcal{R}_{\text{nonstiff}}(\mathbf{y})$$

Linear stability constraint on time step

$$\Delta t \left(\lambda \left[\frac{d\mathcal{R}_{\text{nonstiff}}(\mathbf{y})}{d\mathbf{y}} \right] \right) \in \{ z : |R(z)| \le 1 \}$$

Time step constrained by eigenvalues (time scales) of ***nonstiff component of RHS***

Additive Runge-Kutta (ARK) Time Integrators

Multistage, high-order, conservative IMEX methods

Butcher tableaux representation

Explicit RK

$$\begin{array}{c|ccccc} 0 & 0 & & & \\ c_2 & a_{21} & 0 & & \\ \vdots & \vdots & \ddots & 0 & \\ c_s & a_{s1} & \cdots & a_{s,s-1} & 0 \\ \hline & b_1 & \cdots & \cdots & b_s \end{array} \quad + \quad \begin{array}{c|ccccc} 0 & 0 & & & \\ \tilde{c}_2 & \tilde{a}_{21} & \gamma & & \\ \vdots & \vdots & \ddots & \gamma & \\ \tilde{c}_s & \tilde{a}_{s1} & \cdots & \tilde{a}_{s,s-1} & \gamma \\ \hline & b_1 & \cdots & \cdots & b_s \end{array}$$

DIRK

Time step: From t_n to $t_{n+1} = t_n + \Delta t$ $\quad$ s → number of stages

Stage solutions

$$\mathbf{y}^{(i)} = \mathbf{y}_n + \Delta t \sum_{j=1}^{i-1} a_{ij} \mathcal{R}_{\text{nonstiff}} \left(\mathbf{y}^{(j)} \right) + \Delta t \sum_{j=1}^{i} \tilde{a}_{ij} \mathcal{R}_{\text{stiff}} \left(\mathbf{y}^{(j)} \right), \quad i = 1, \cdots, s$$

$$\mathbf{y}_{n+1} = \mathbf{y}_n + \Delta t \sum_{i=1}^{s} b_i \mathcal{R} \left(\mathbf{y}^{(i)} \right)$$ *Step completion*

Kennedy & Carpenter, J. Comput. Phys., 2003

Implicit Stage Solution

Requires solving nonlinear system of equations

Rearranging the stage solution expression:

$$\underbrace{\frac{1}{\Delta t \tilde{a}_{ii}} \mathbf{y}^{(i)} - \mathcal{R}_{\text{stiff}}\left(\mathbf{y}^{(i)}\right) - \left[\mathbf{y}_n + \Delta t \sum_{j=1}^{i-1} \left\{ a_{ij} \mathcal{R}_{\text{nonstiff}}\left(\mathbf{y}^{(j)}\right) + \tilde{a}_{ij} \mathcal{R}_{\text{stiff}}\left(\mathbf{y}^{(j)}\right) \right\} \right] = 0}$$

$$\mathcal{F}(y) = 0$$

Jacobian-free Newton-Krylov method (*Knoll & Keyes, J. Comput. Phys., 2004*):

Initial guess: $y_0 \equiv \mathbf{y}_0^{(i)} = \mathbf{y}^{(i-1)}$

Newton update: $y_{k+1} = y_k - \mathcal{J}(y_k)^{-1} \mathcal{F}(y_k)$

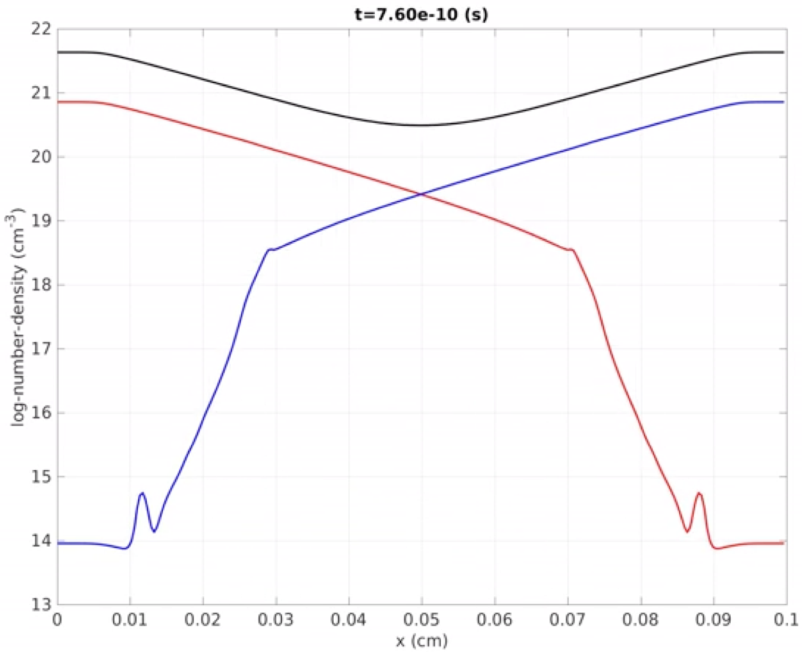
GMRES solver (preconditioned)

$\mathcal{J}(y_k)\,\Delta y = \mathcal{F}(y_k)$

Action of the Jacobian on a vector approximated by *directional derivative*

$$\mathcal{J}(y_k)\,x = \left.\frac{d\mathcal{F}(y)}{dy}\right|_{y_k} x \approx \frac{1}{\epsilon}\left[\mathcal{F}(y_k + \epsilon x) - \mathcal{F}(y_k)\right]$$

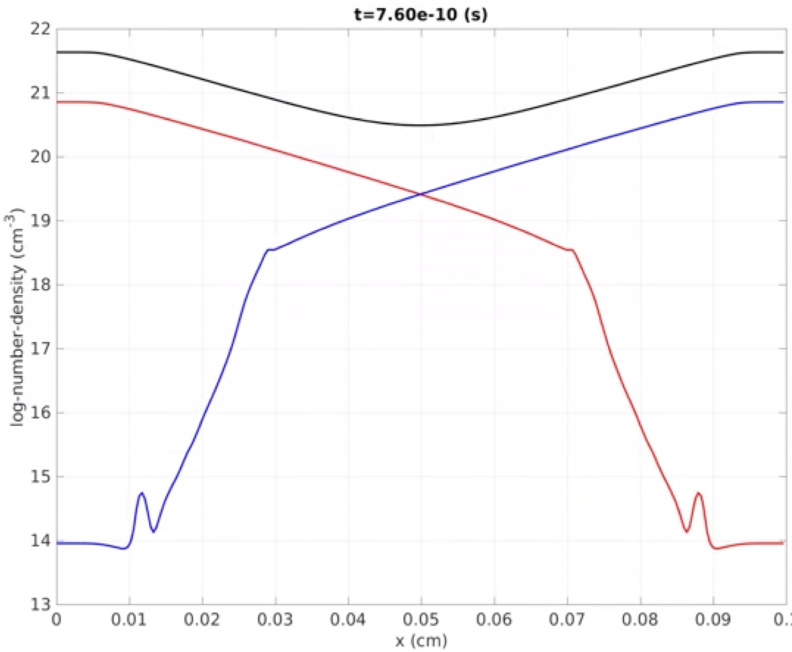
Work-in-Progress: Preliminary Example
1D Carbon–Carbon Interpenetration



ARK4 *(6-stage, 4th order, 5 implicit stages)*

CFL = $\mathbf{0.5}$

~ 1200 time steps, 1 hr 40 mins



RK4 *(4-stage, 4th order)*

CFL = $\mathbf{0.05}$

~ 12,000 time steps, 7 hrs 15 mins

No preconditioner implemented yet; however, note *implicit term is block diagonal (no spatial derivatives)*

Good agreement between IMEX and explicit solutions; need to verify convergence

Conclusions and Future Work

Summary — **EUCLID: EUlerian Code for pLasma Interpenetration Dynamics**

- Developed a **3D, parallel, AMR-capable multifluid flow solver**
- Implemented the *quasineutral, isothermal electron model* as a computationally tractable electron model for our target applications.
- *Verified EUCLID for accuracy and convergence* (benchmark cases, manufactured solutions)
- *Simulated flows motivated by laboratory astrophysics experiments and ICF hohlraums.*

Current and Future Work

- Implementation of **IMEX time integrators**
  - Newton's method convergence difficulties for large time steps
  - Implement an efficient preconditioner
- Conduct **simulations of plasma interpenetration experiments** (e.g. *Ross et al., 2013, Le Pape et al., ongoing*)
- Investigate *higher-fidelity electron models*, for example, adding an electron energy equation.
- Add *source terms to energy equations to simulate heating*

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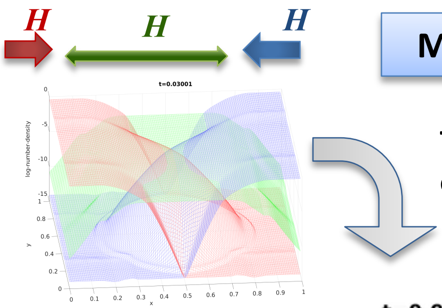
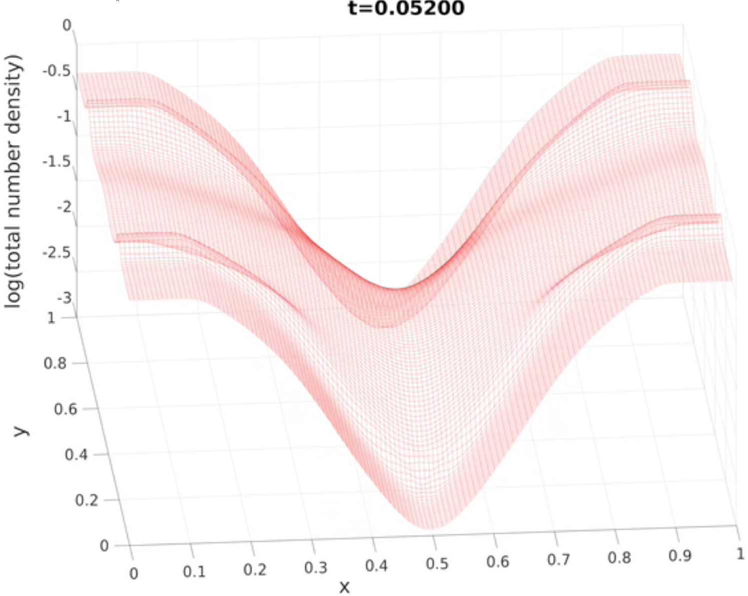
Multifluid vs. Single Fluid Simulations - *How do the solutions differ?*

Interpenetration of two *hydrogen* streams in the presence of *hydrogen* gas fill (2D)

Multifluid Simulation



Total density (sum of the 3 densities)



Single-fluid Simulation