

Hydrodynamic Simulation of Counterstreaming Plasmas with a Multifluid Model

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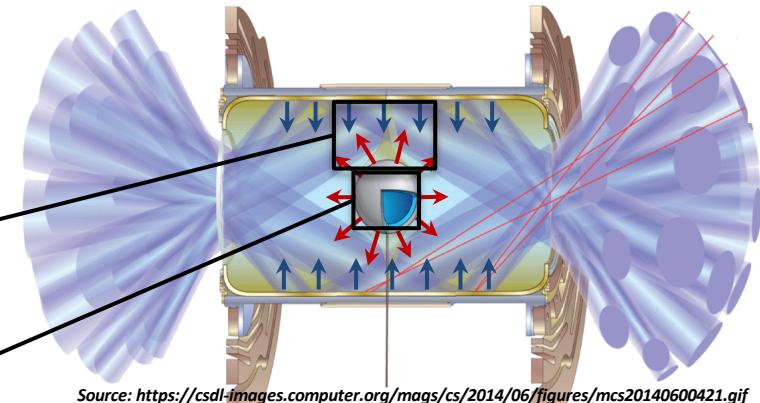
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Background and Motivation

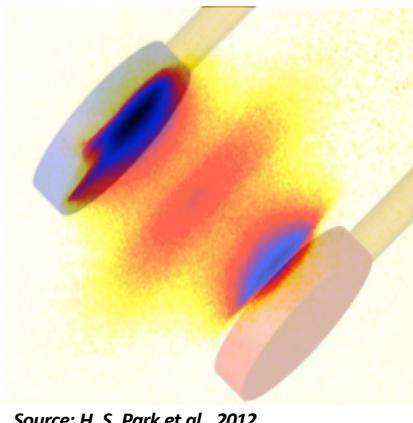
Inertial Confinement Fusion: Colliding plasmas from hohlraum wall and capsule

- 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

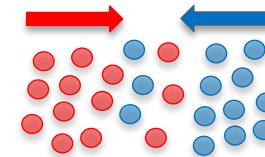


High Energy Density Physics (HEDP) Experiments

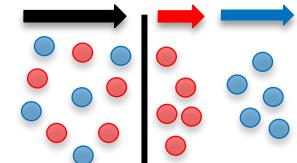


Carbon plasma streams ablating off paddles hit by laser beams and colliding with each other

Multifluid phenomena that we want to model



Interpenetrating plasmas



Plasma species separation

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

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

$$\alpha = 1, \dots, n_s$$

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

Interaction between species

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

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

$$Q_{\alpha,\beta} = Q_{\alpha,\beta}^{\text{fric}} + Q_{\alpha,\beta}^{\text{eq}}$$

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

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

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*

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

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

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

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

Electron pressure

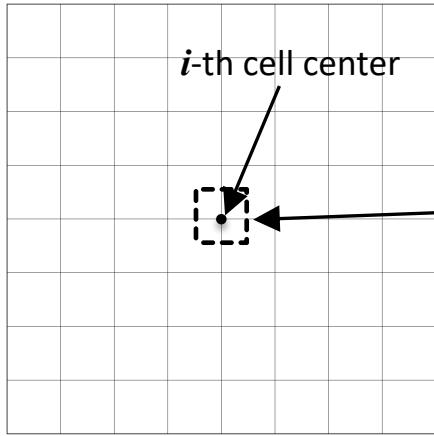
is the “augmented pressure” (hydro + e^-)

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

Summary of Numerical Method

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

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



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

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

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

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

Cell-averaged / cell-centered solution

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

Face-averaged / face-centered fluxes

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

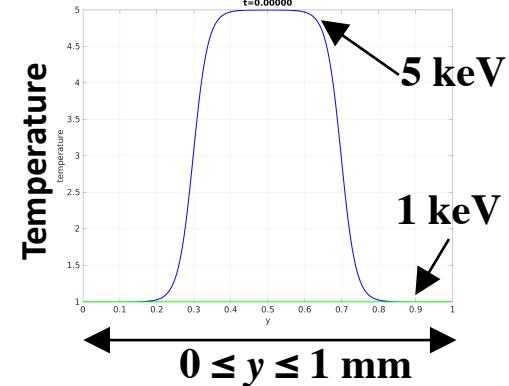
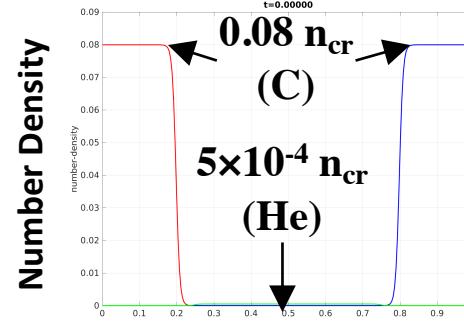
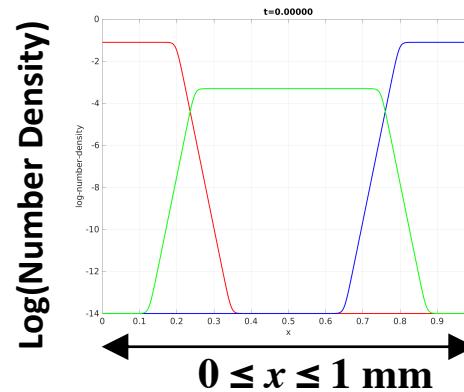
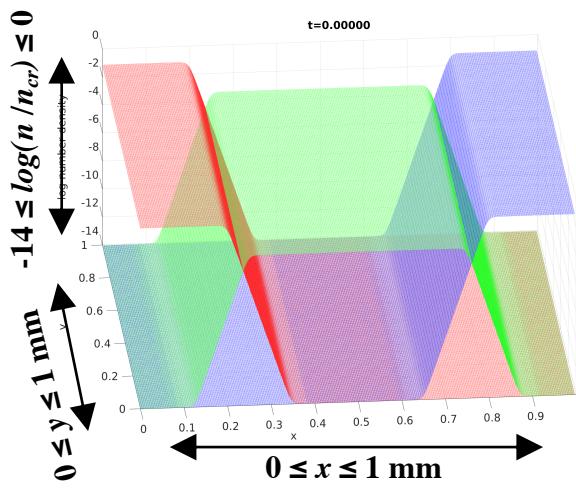


- Characteristic-based discretization
- 5th-order WENO scheme with Monotonicity-Preserving limiting

Example: Two Species Interpenetration with Gas Fill Problem Setup

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

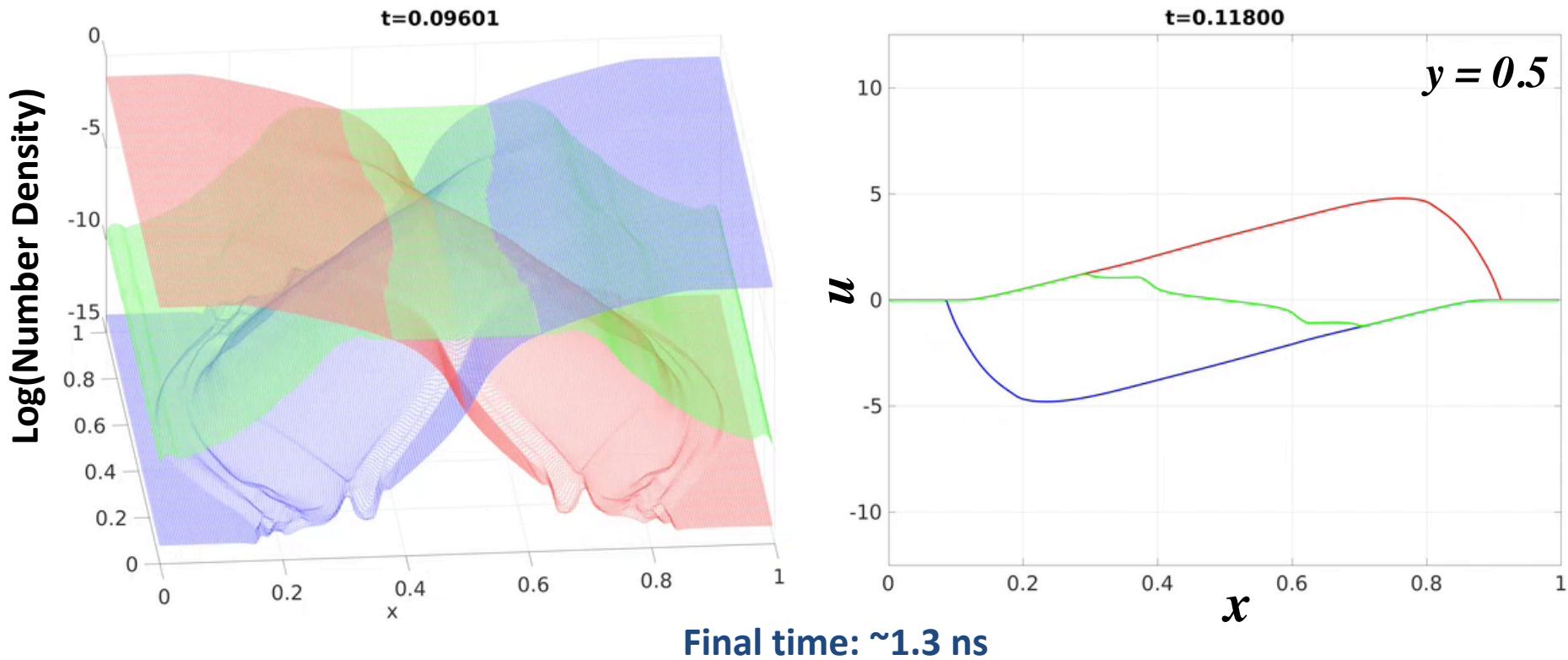
- Initial solution: two species piled up on either end (*smoothed slab density*); gas fill present in the space in between.
- Temperature variation along y – the plasmas are hotter in the center of the domain



Reference quantities:

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

Example: Two Species Interpenetration with Gas Fill



- **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} ($9.0320e+21 \text{ cm}^{-3}$);
Length: 1 mm; Time: $3.2314e-09$ s;
Velocity: $3.0946e+07 \text{ cm/s}$

Stiffness of Collisional Terms for High-Z Species

Ion–ion collisional interaction term: *ion species 1* due to *ion species 2*

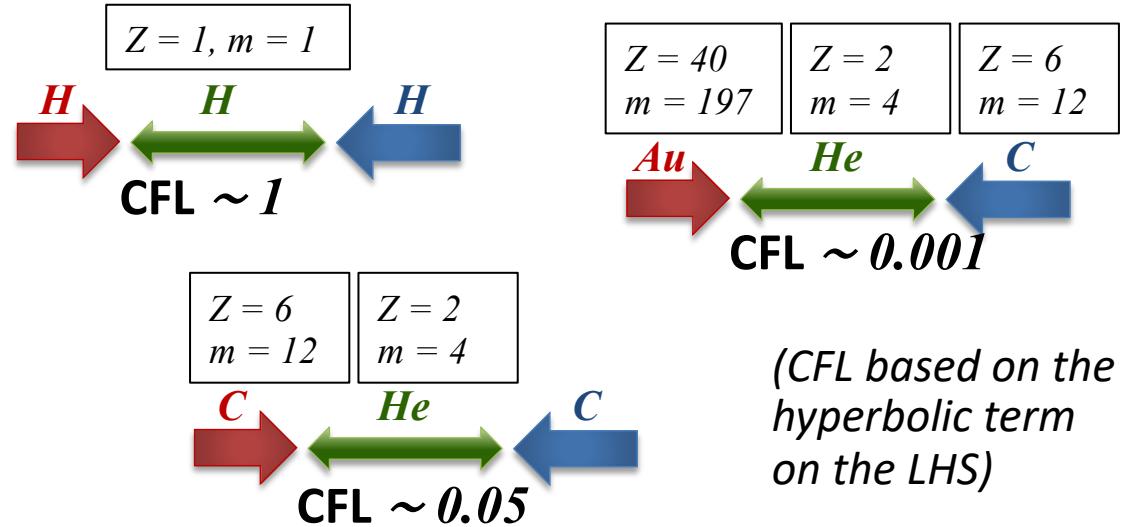
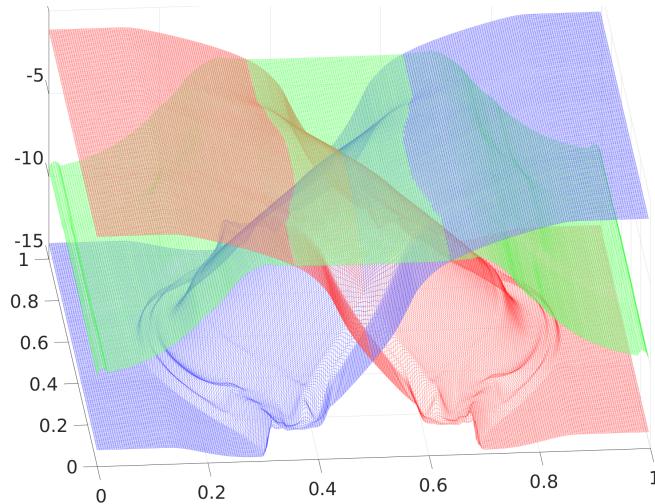
$$\left[\begin{array}{c} 0 \\ m_1 n_1 \nu_{12} (u_2 - u_1) \\ m_1 n_1 \nu_{12} (u_2 - u_1) u_1 + m_{12} n_1 \nu_{12} (u_2 - u_1)^2 + 3 \frac{m_1 n_1 \nu_{12}}{m_1 + m_2} (T_2 - T_1) \end{array} \right]$$

where

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

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

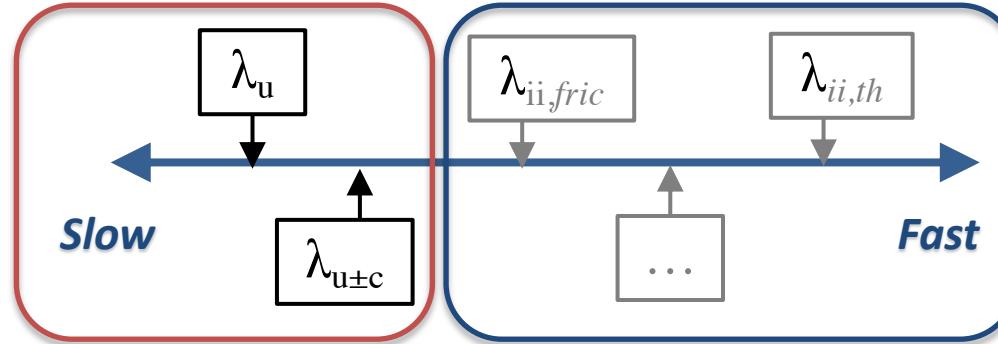
$$\propto Z_1 Z_2 \sqrt{\frac{m_1 m_2}{m_1 + m_2}}$$



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)

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

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

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

Additive Runge-Kutta (ARK) Time Integrators

Multistage, high-order, conservative IMEX methods

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

Stage solutions

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

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

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

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

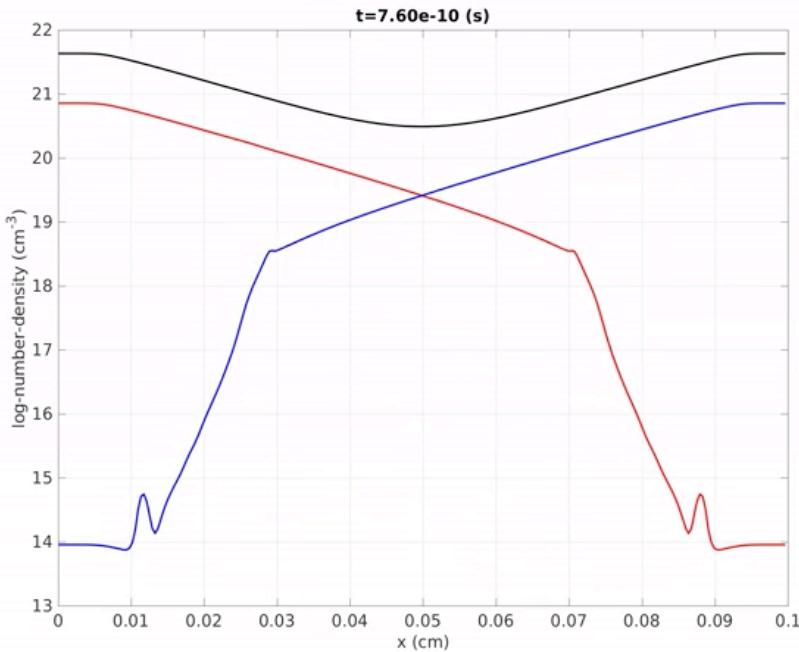
$$\mathcal{J}(y_k) \Delta y = \mathcal{F}(y_k)$$

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

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

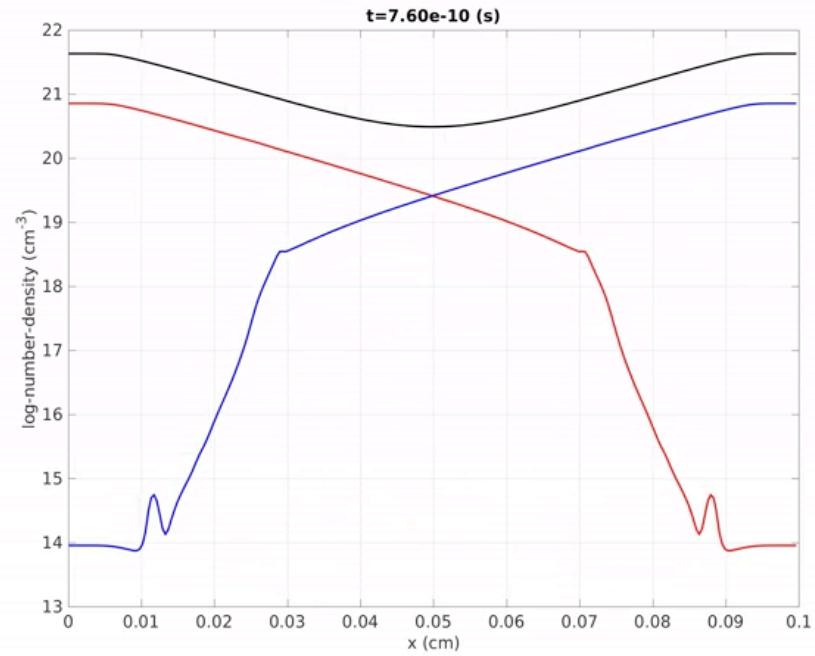
Low-Z Example: 1D Carbon–Carbon Interpenetration

Interaction of two counterstreaming carbon fluids



ARK4 (6-stage, 4th order, 5 implicit stages)
CFL = 0.5

~ 1200 time steps, 1 hr 40 mins



RK4 (4-stage, 4th order)
CFL = 0.05

$\sim 12,000$ 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

High-Z Plasma Simulations: Difficulties with Implicit Solve

Nonlinearity and Stiffness:

- Collisional terms are highly nonlinear
- Time step is 100-1000 times larger than collisional scales

Near-Vacuum Conditions and Strong Shocks:

- In parts of the domain, density corresponds to "numerical vacuum"
- Newton iterations result in nonphysical intermediate states

Nonconvergence of Newton iterations with the usual initial guess (*GMRES converges okay!*)!

Step Limiting: Reduce the step size obtained from GMRES by a factor till next guess is physical

Positivity Preservation: “Post-process” Newton guess to replace negative densities/pressures by some positive value

Operator-Splitting-based Initial Guess

instead of previous step/stage



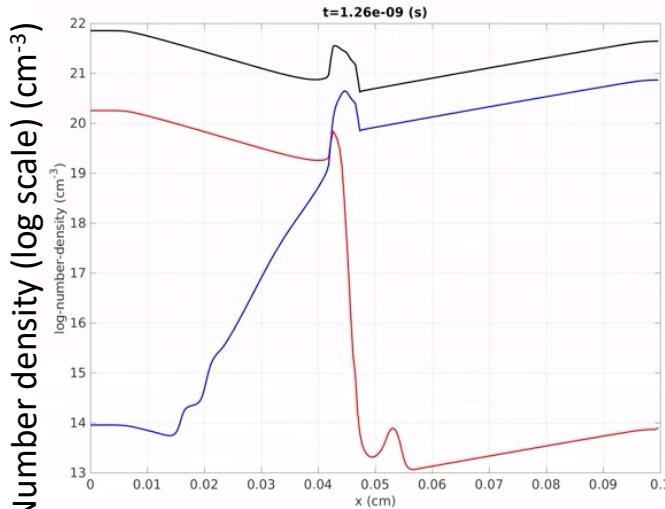
Evolve stiff RHS terms at collisional Δt (**cheap**)

Evolve nonstiff RHS terms at convective Δt



Example: 1D Gold – Carbon Interpenetration

Interpenetration of **carbon** and **gold** streams in vacuum

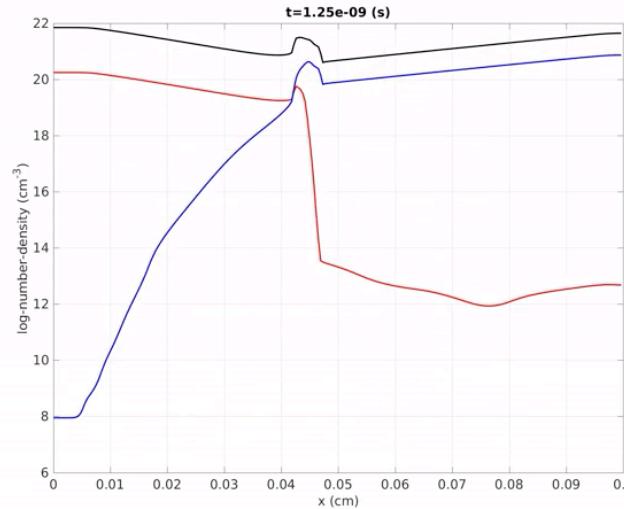


ARK 2e

- 2nd order, 3-stage (2 implicit stages)
- Simulation time: **~7.5 hours** (~2000 time steps)
- Time step: $\Delta t \approx 2e-4$



Sim. time integrated with actual TI: 0.300 (75.%)
Sim. time integrated with backup TI: 0.0998 (25.%)

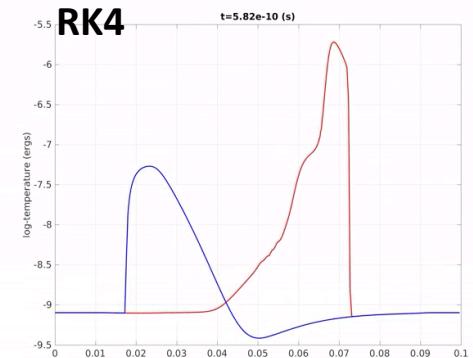


RK4

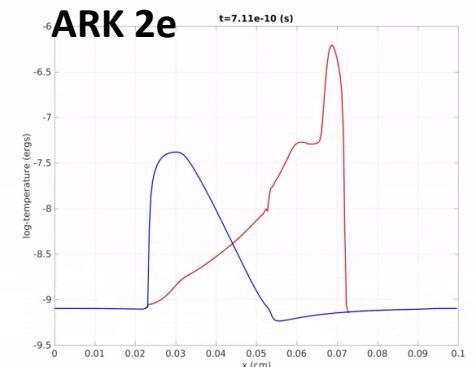
- Simulation time: **~12 hours** (~ 126,600)
- Time step: $\Delta t \approx 3e-6$

But, **ugly oscillations** in temperature (and pressure)

RK4



ARK 2e



Essentially no gain from using IMEX method!

Conclusions and Future Work

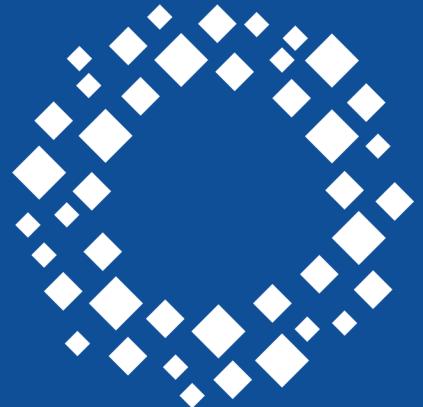
Summary

EUCLID: EUlerian Code for pLasma Interpenetration Dynamics

- Developed a **3D, parallel 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

- Improve implementation of **IMEX time integrators**
 - Implement an efficient preconditioner
 - Currently investigating using artificial viscosity to smooth out spurious oscillations
- 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.



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