A Semi-Implicit Algorithm for the Simulation of High–Z Plasma Interpenetration

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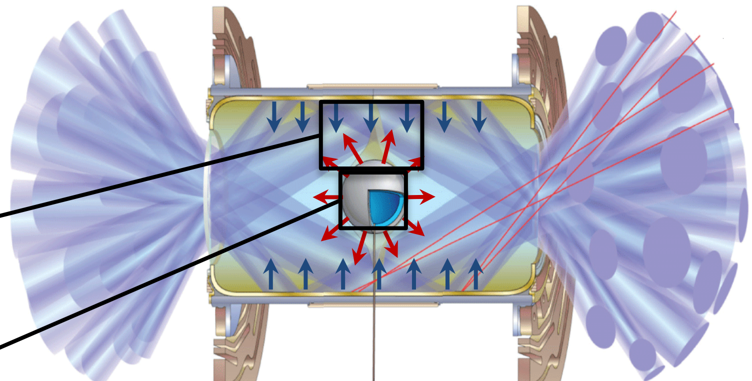
Background and Motivation

Inertial Confinement Fusion: Colliding plasmas from hohlraum wall and capsule

Interpenetration of plasma flows from capsule and hohlraum wall

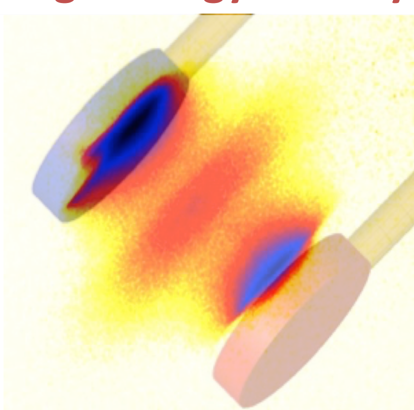
- Large range of Z: $2 \leq Z \leq 60$
- Supersonic flows ($\Delta u \approx 10^8$ cm/s)

Species separation inside target capsule



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

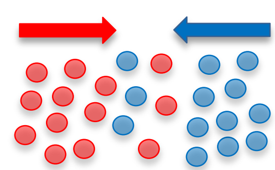
High Energy Density Physics (HEDP) Experiments



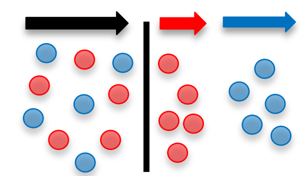
Source: H. S. Park et al., 2012

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

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

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

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

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

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

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

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

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

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*

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

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

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

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

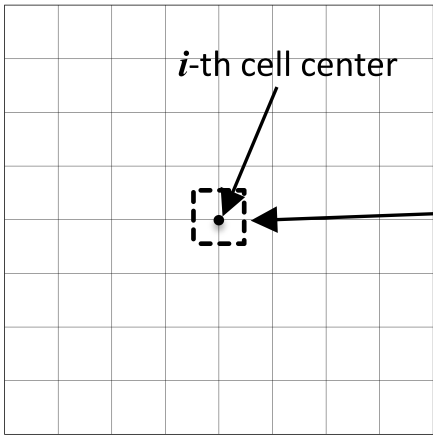
is the "**augmented pressure**" (hydro + *e*⁻)

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)



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

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

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

Cell-averaged / cell-centered solution

Face-averaged / face-centered fluxes

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

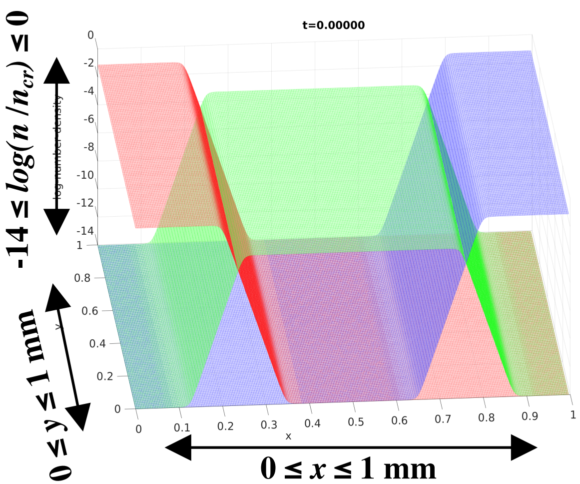
Strong shocks and gradients
O(1) to O(1e-14)

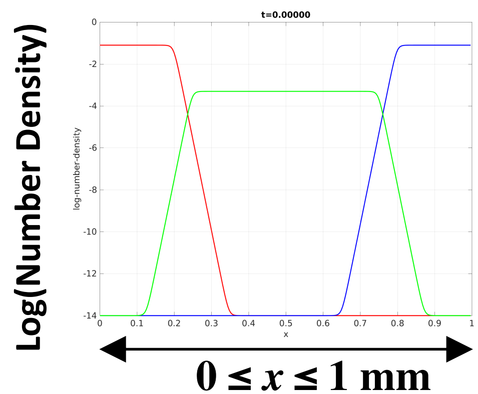
- **Characteristic-based discretization**
- **5th-order WENO scheme** with **Monotonicity-Preserving limiting**

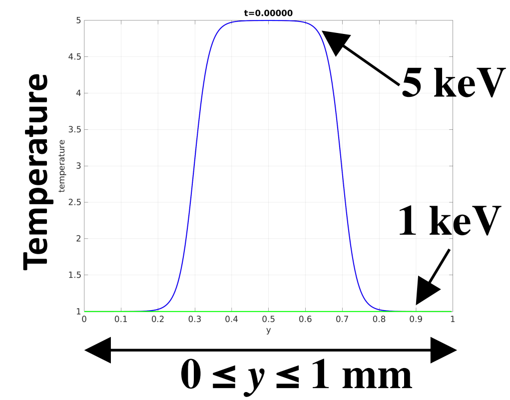
Example: Two Species Interpenetration with Gas Fill
Problem Setup

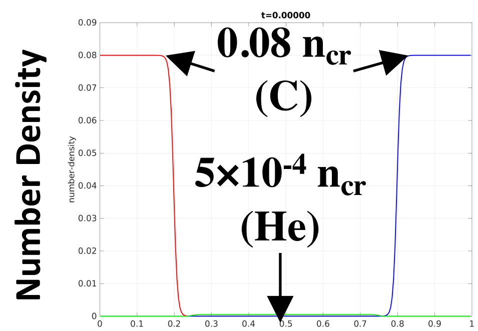
Interpenetration of *carbon* and *carbon* streams in the presence of *helium* gas fill (2D)

- **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









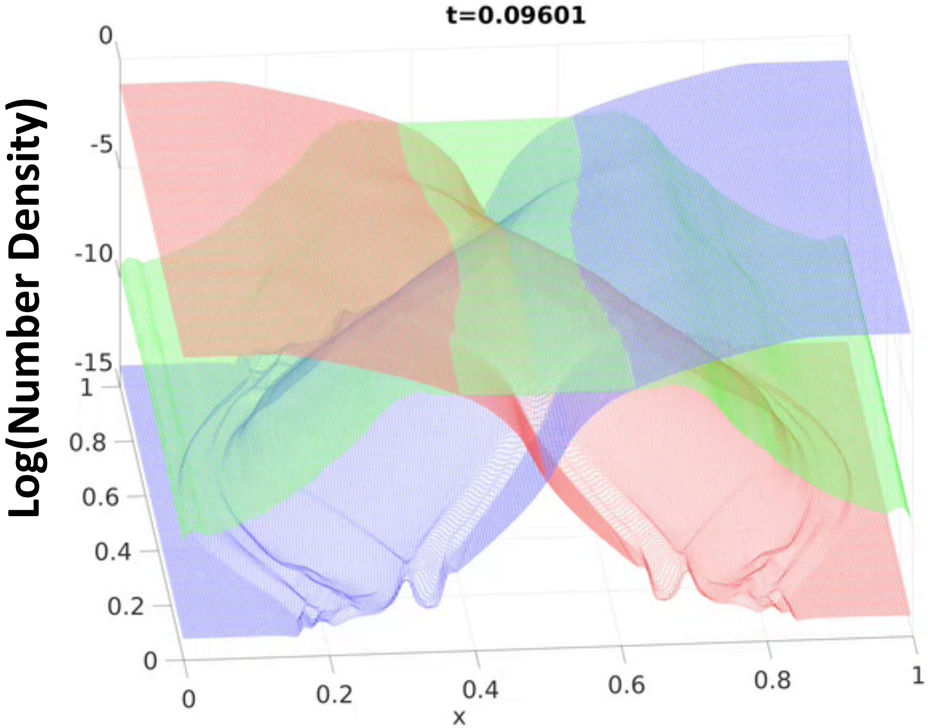
Boundary conditions:

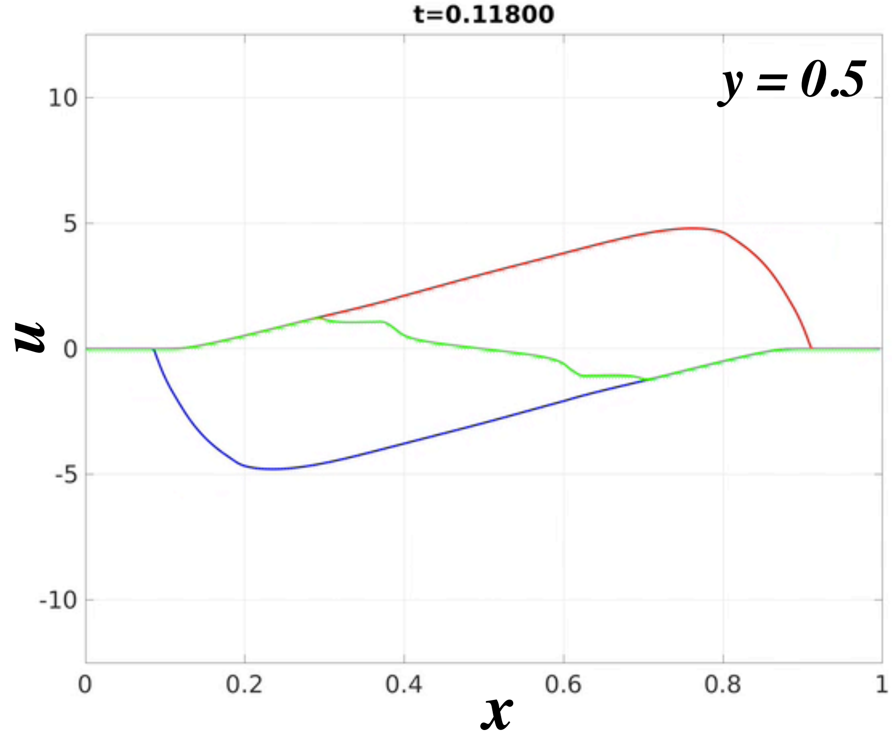
- Solid wall BCs along *x*
- Periodic along *y*

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: *ion species 1* due to *ion species 2*

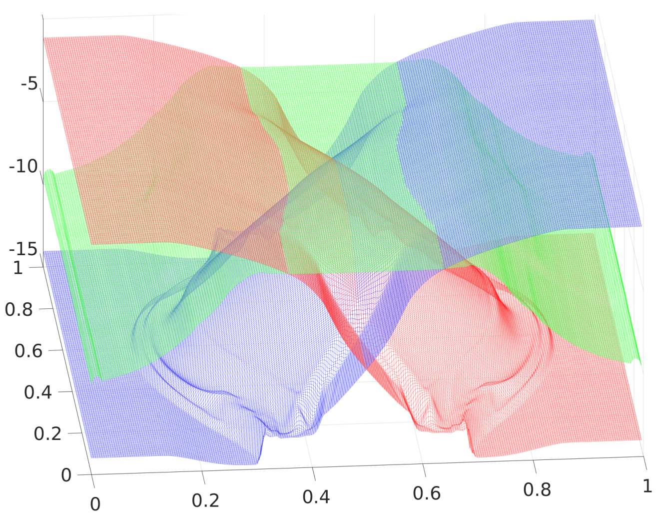
$$\begin{bmatrix} 0 \\ m_1 n_1 \nu_{12} \left(u_2 - u_1\right) \\ m_1 n_1 \nu_{12} \left(u_2 - u_1\right) u_1 + m_{12} n_1 \nu_{12} \left(u_2 - u_1\right)^2 + 3 \frac{m_1 n_1 \nu_{12}}{m_1 + m_2} \left(T_2 - T_1\right) \end{bmatrix}$$

where

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

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

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



Z = 1, m = 1

H → *H* ← *H*

CFL ~ *1*

Z = 40 *m = 197*	*Z = 2* *m = 4*	*Z = 6* *m = 12*

Au → *He* ← *C*

CFL ~ *0.001*

Z = 6 *m = 12*	*Z = 2* *m = 4*

C → *He* ← *C*

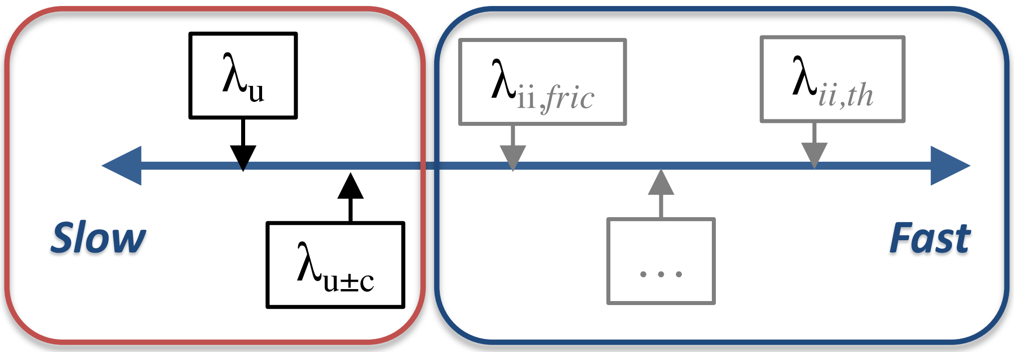
CFL ~ *0.05*

(CFL based on the hyperbolic term on the LHS)

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

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

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

Additive Runge-Kutta (ARK) Time Integrators

Multistage, high-order, conservative IMEX methods

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 $t_{n+1} = t_n + \Delta t$ $\qquad$ 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)~~

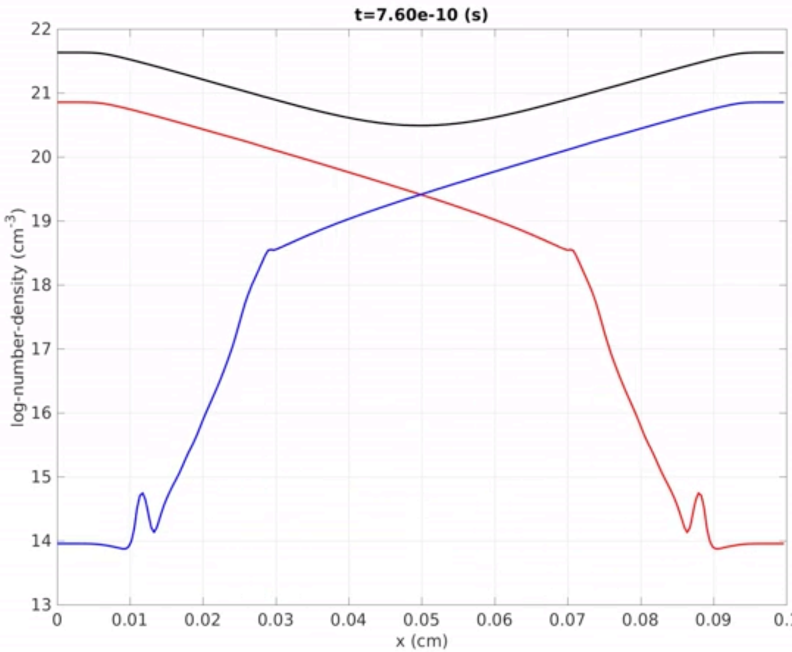
$$\mathcal{J}(y_k)\,\Delta y = \mathcal{F}(y_k)$$

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

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

Low-Z Example: *1D Carbon–Carbon Interpenetration*

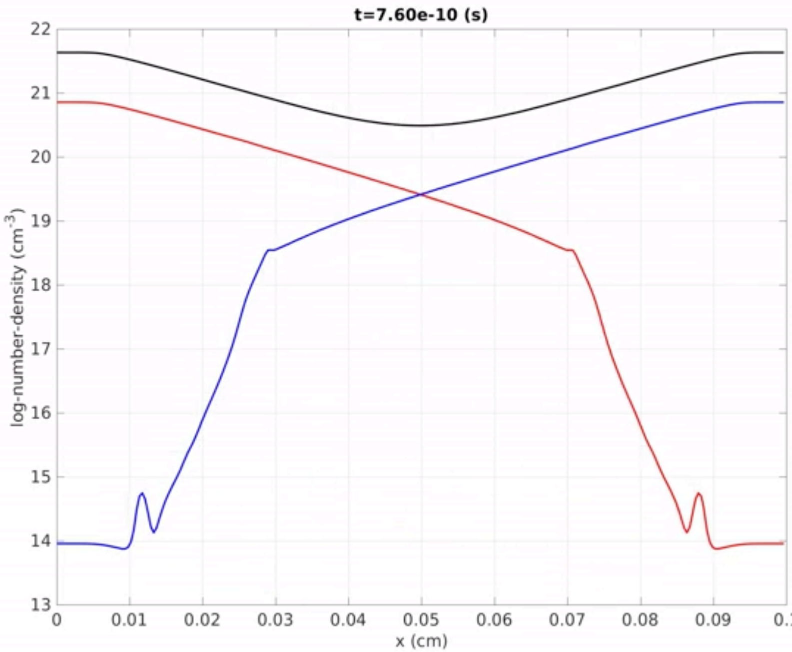
Interaction of two counterstreaming carbon fluids



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***

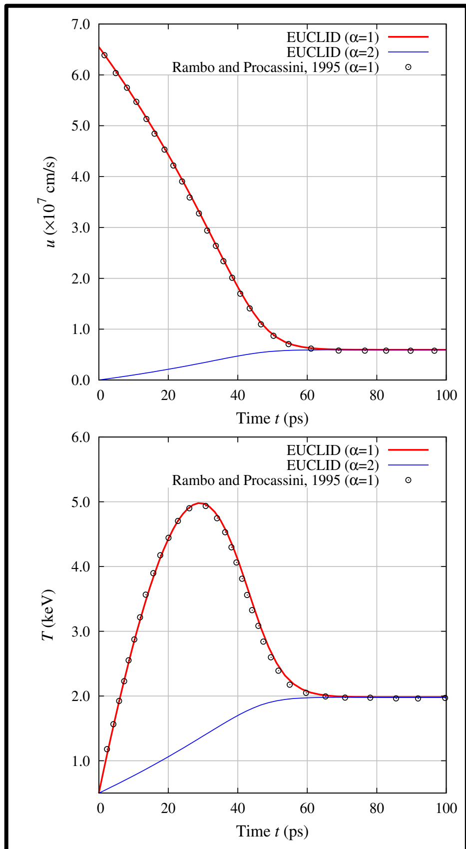
~ 12,000 time steps, 7 hrs 15 mins

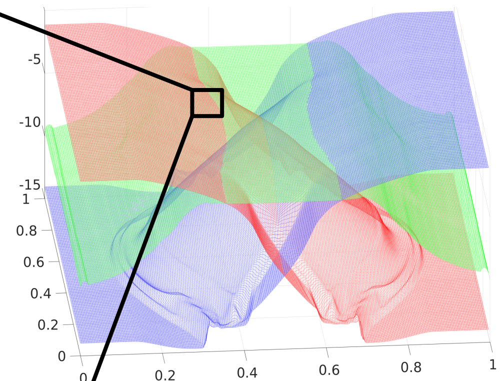
No preconditioner implemented yet; however, note *implicit term is block diagonal (no spatial derivatives)*

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

High-Z Plasma Simulations: Difficulties with Implicit Solve

Time step $\Delta t \gg$ collisional scales





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*)!

Current Attempts to Improve Convergence (1)

Near-Vacuum Conditions & Strong Shocks

If next Newton guess is nonphysical (negative density/pressure)

Higher value of "numerical vacuum", $n_{vac} = 10^{-6}$ or 10^{-8}, *instead of* 10^{-14}

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

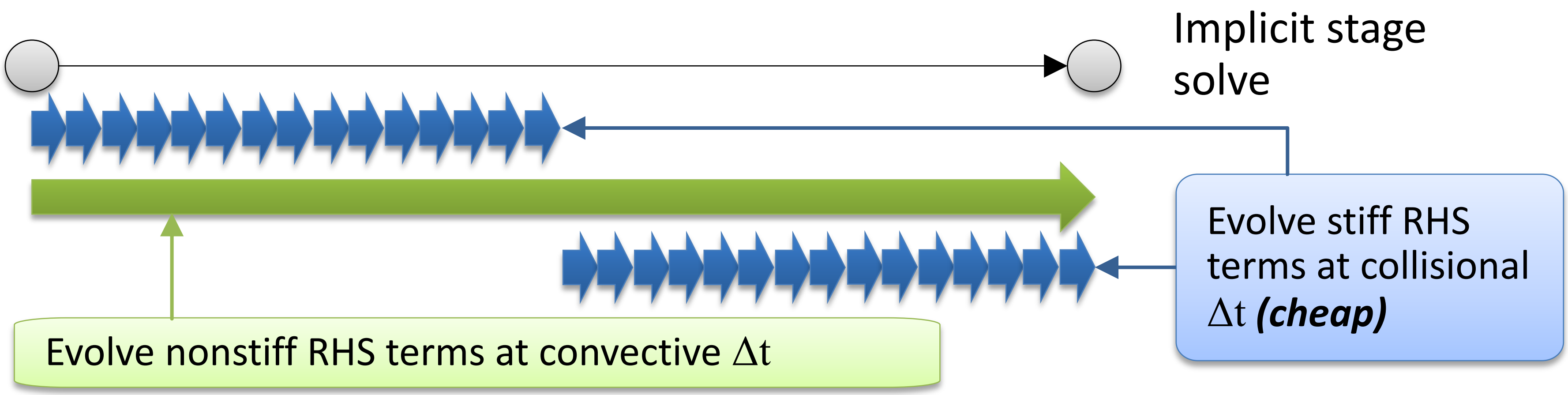
Positivity Preservation: *"Post-process" Newton guess to replace negative densities/pressures by some positive value*

Both approaches lead to ***stalling*** (residual does not converge) for difficult solves

Current Attempts to Improve Convergence (2)

Nonlinearity and Stiffness

→ ***Operator-Splitting-based Initial Guess*** instead of previous step/stage



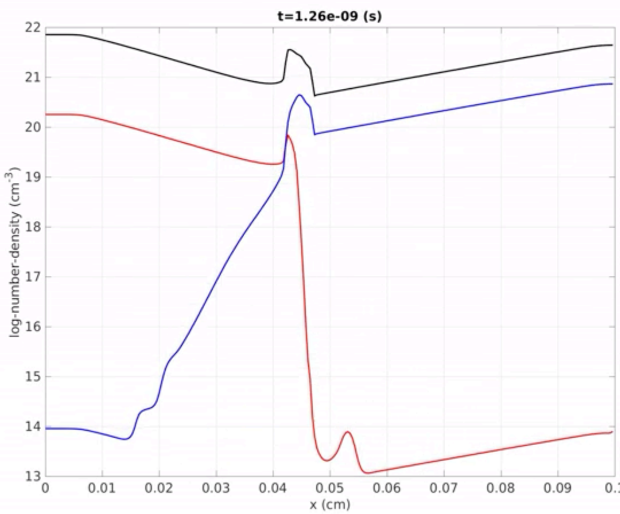
"Backup" Explicit Integration

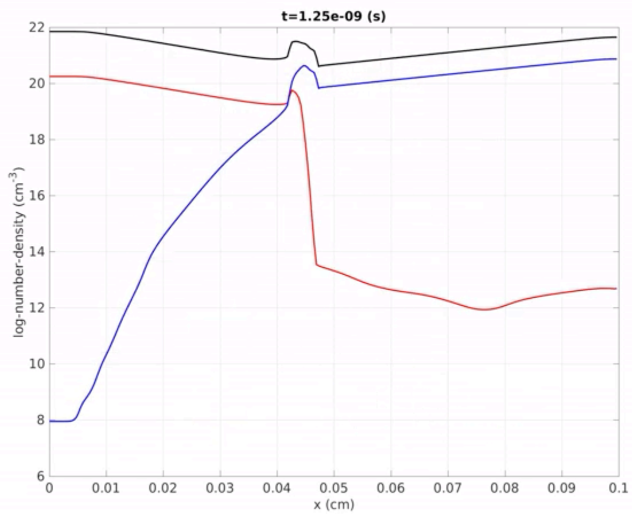
- There are *still situations during the simulation when implicit stage solve fails*
- Use RK4 to integrate 1/10th of ARK time step, then hand it back to ARK

Example: *1D Gold – Carbon Interpenetration*

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

Number density (log scale) (cm^{-3})





ARK 2e

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

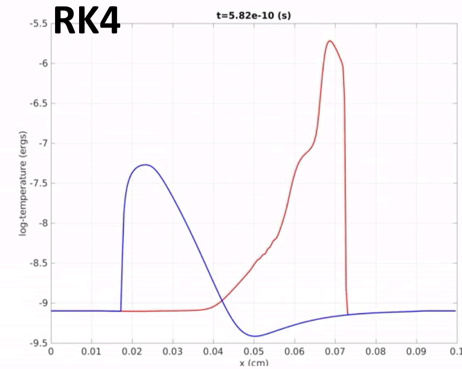
RK4

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

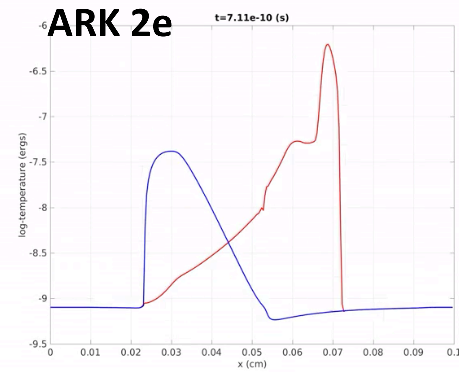
```
Sim. time integrated with
actual TI: 0.300 (75.%)
Sim. time integrated with
backup TI: 0.0998 (25.%)
```

*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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