An optimal, fully implicit, fully conservative, and equilibrium preserving Vlasov-Fokker-Planck code for spherical ICF capsule implosions

CSE 2017, Atlanta, GA

Metropolis Postdoctoral Fellowship, Thermonuclear Burn Initiative, LDRD

Got converted 2 days ago!!!

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Los Alamos NATIONAL LABORATORY EST. 1943

LA-UR 17-21529

Outline of talk

March 2, 2017

10:50AM-11:10AM

Grand Ballroom 2nd floor
MS222

- **Brief physics motivation**
- **Vlasov-Fokker-Planck**
  - Numerical challenges
    - Length and time scales
    - Discrete conservation and equilibrium preserving properties
  - Our solution
    - Adaptive grid and implicit solver
    - Discrete nonlinear constraints
- **Verification studies and preliminary simulation of imploding Omega capsule**
- **Conclusion**

Progress since last CSE (2015)

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- **At last CSE meeting:**
  - 0D2V grid adaptivity
  - Coarse grained asymptotics for disparate v_{th} ratio
  - Conservation (mass, momentum, energy) for collision operator and Vlasov pieces
- **Updates:**
  - Fluid electrons and electric fields
  - Spherical geometry and adaptivity in space
  - New equilibrium preserving discretization for the Rosenbluth-Fokker-Planck form
  - New null space preserving discretization for the geometrical inertial term
  - Suite of verification studies
  - Physics simulations

We have many updates. In fact so many that we cannot possibly cover all!

Main take away from this talk

- **Project began exactly 3 years ago (very high paced R&D)**
- **iFP is a first of a kind multi-scale simulation capability**
  - Fully implicit, scalable (both algorithmic and parallel)
  - Optimal grid adaptivity
  - Analytical equilibrium preserving property and other discrete null space preserving properties
  - Strict conservation enforced
  - Strict verification campaign against hydro limit and other codes

- **Began ICF physics campaign simulation**

  First capsule implosion simulation with hydro boundary conditions

How does ICF (indirect driver) work at NIF?

https://www.youtube.com/watch?v=Wg8R1IrAiM4

Recent ICF experiments have highlighted wide gaps in our understanding and predictive simulation capabilities

- **Contrary to radhydro simulation predictions, NIF's NIC and consecutive campaigns have failed to achieve ignition**

- **Recent OMEGA campaigns have highlighted serious deficiencies in our ability to**
  - Predict capsule **compression and yield** (both are over-predicted)
  - Predict time-dependent core mix (**especially when hydro instabilities** are not expected to play a role)

Hydrodynamics breaks down in certain regimes of ICF capsule implosion and a **kinetic model is required**

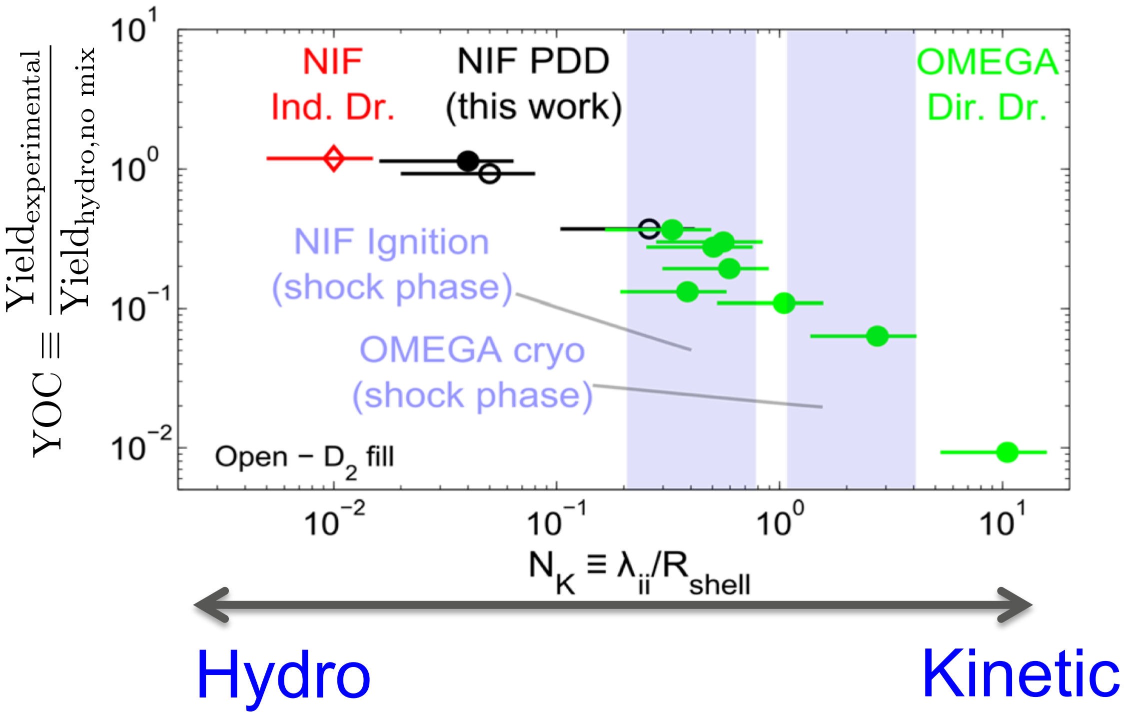


Figure from M.J. Rosenberg, PRL (2014)

Discrepancies btw experiment and simulations consistently increase with Knudsen number.

Radiation-hydrodynamics is not valid in many key stages in ICF implosion!

We need high fidelity Vlasov-Fokker-Planck code to understand impact of missing physics in hydro

- **Kinetic ions: Vlasov-Fokker-Planck is considered a first principles model for weakly coupled plasmas**

$$\frac{Df_i}{Dt} \equiv \frac{\partial f_i}{\partial t} + \vec{v} \cdot \nabla f_i + \vec{a}_i \cdot \nabla_v f_i = \sum_j C_{ij}\left(f_i, f_j\right)$$

- **Fluid model for electrons**

$$\frac{3}{2}\partial_t\left(n_e T_e\right) + \frac{5}{2}\nabla \cdot \left(\vec{u}_e n_e T_e\right) + \vec{u}_e \cdot \nabla P_e + \nabla \cdot \vec{Q}_e = \sum_{\alpha}^{N_s}\left[W_{e\alpha} + \vec{u}_e \cdot \vec{F}_{e\alpha}\right]$$

- **Quasi-neutrality and ambipolarity to close system**

$$n_e = -q_e^{-1}\sum_{\alpha}^{N_s} q_\alpha n_\alpha$$

$$\nabla \cdot \vec{J} = \nabla \cdot \left[q_e n_e \vec{u}_e + \sum_{\alpha}^{N_s} q_\alpha n_\alpha u_\alpha\right] = 0$$

$$\vec{a} = \frac{q_\alpha}{m_\alpha}\vec{E} = \frac{q_\alpha}{m_\alpha}\frac{\nabla P_e + \sum_{\alpha}^{N_s}\vec{F}_{e\alpha}}{q_e n_e}$$

Solving Vlasov-Fokker-Planck requires many algorithmic innovations

$$\frac{Df_i}{Dt} \equiv \frac{\partial f_i}{\partial t} + \vec{v}\cdot\nabla f_i + \vec{a}_i \cdot \nabla_v f_i = \sum_j C_{ij}\left(f_i, f_j\right)$$

$$C_{ij}\left(f_i, f_j\right) = \Gamma_{ij}\nabla_v \cdot \left[D_j \cdot \nabla_v f_i - \frac{m_i}{m_j} A_j f_i \right]$$

$$D_j = \nabla_v \nabla_v G_j \qquad A_j = \nabla_v H_j$$

$$\nabla_v^2 H_j(\vec{v}) = -8\pi f_j\left(\vec{v}\right)$$

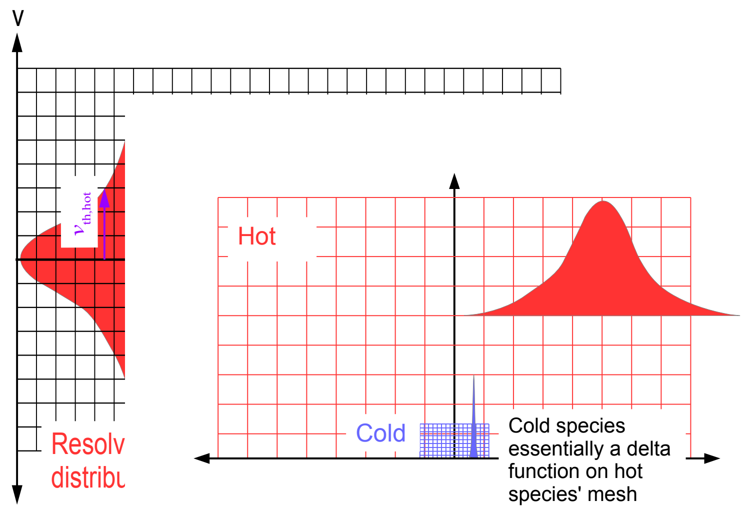
$$\nabla_v^2 G_j(\vec{v}) = H_j\left(\vec{v}\right)$$

- A nonlinear integral-differential equation
- Supports conservation of mass, momentum, and energy and positivity (numerically, these are constraints that must be ensured for long time accuracy and stability)
- Supports disparate length and time scales
- Supports a non-trivial null space (Maxwellian)

Challenges of the problem

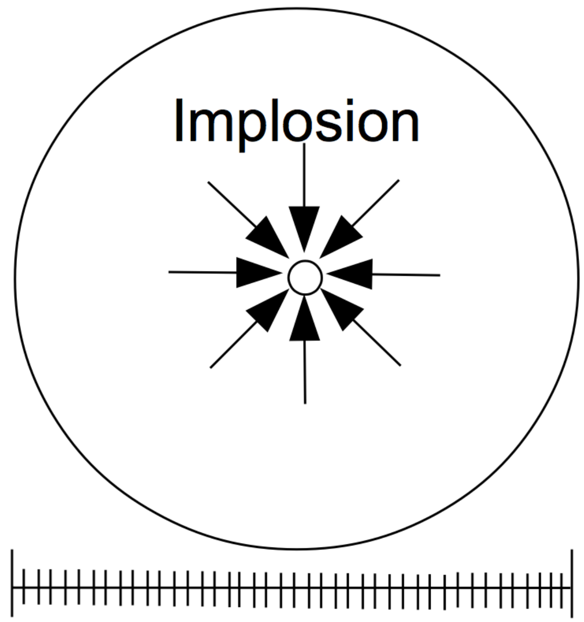
Mesh resolution challenges of VFP

- **Disparate temperatures during implosion dictate velocity resolution.**
  - $v_{th,max}$ determines L_v
  - $v_{th,min}$ determines Δv



Taitano et al., JCP, 318, 2016

- Shock width and capsule size dictate physical space resolution



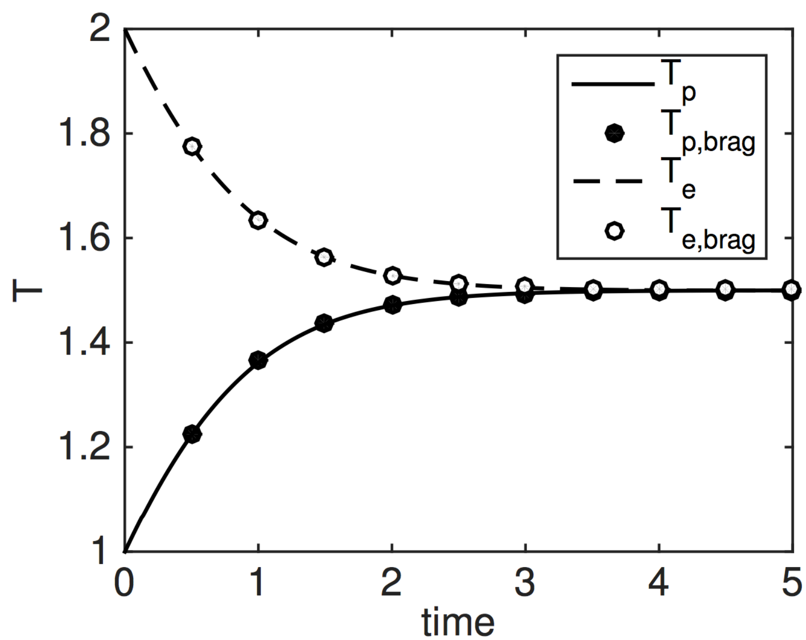
Static mesh with explicit methods, not practical

- Intra species $v_{th,max} / v_{th,min} \sim 100$
- Inter species $(v_{th,\alpha} / v_{th,\beta})_{max} \sim 30$
- $N_v \sim [10(v_{th,max}/v_{th,min}) x (v_{th,\alpha} / v_{th,\beta})]^2 \sim 10^9$
- $N_r \sim 10^3 - 10^4$
- **$N = N_r N_v \sim 10^{12} - 10^{13}$ unknowns in 1D2V!**

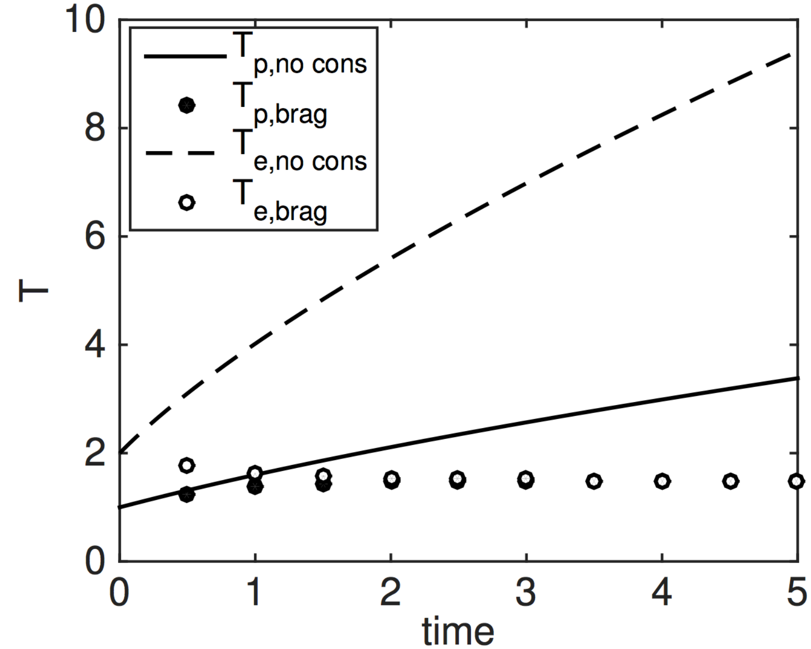
$$\Delta t_{exp}^{coll} \sim \frac{1}{10} \left(\frac{\Delta v}{v_{th}^{min}} \right)^2 \nu_{coll}^{-1} \sim 10^{-9} \, ns$$

- $t_{sim} = 1$ ns
- **$N_t >= 10^9$ time steps**

Conservation is also critical



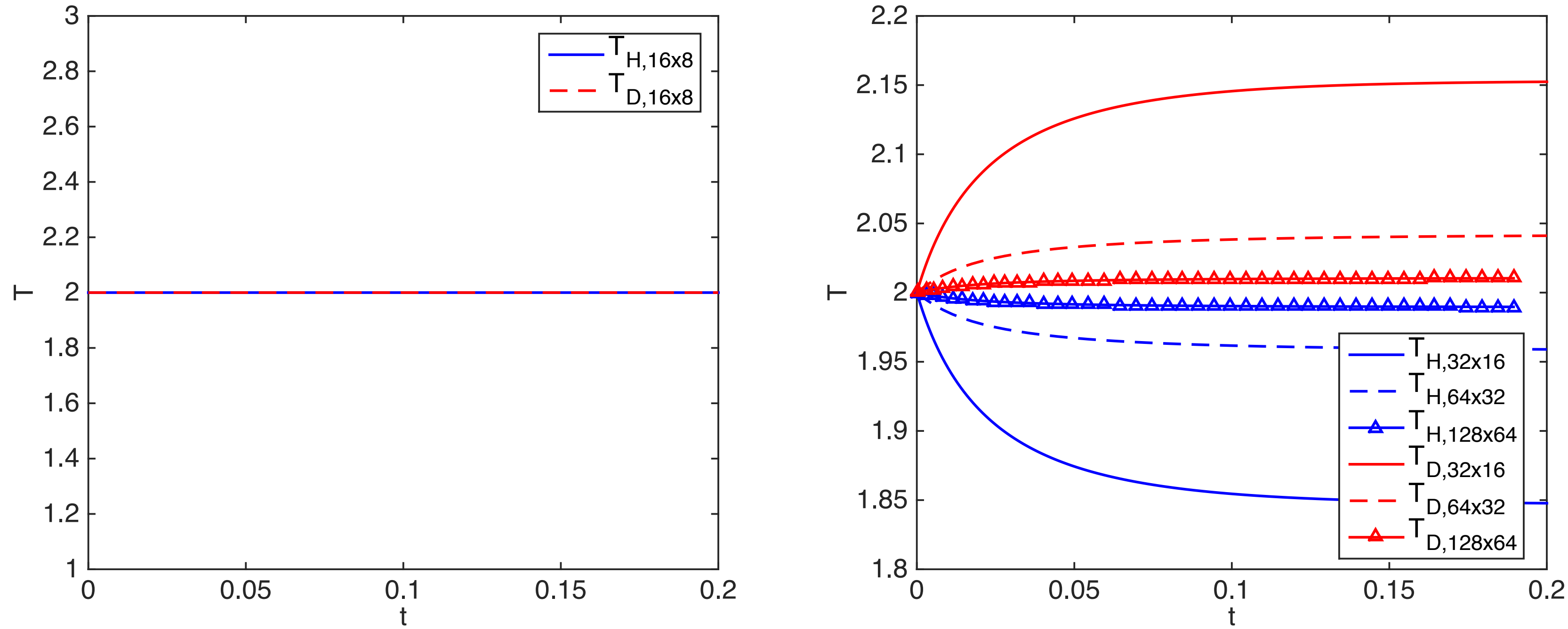
With conservation



No conservation

Taitano et al., JCP, 318, 2016

Equilibrium preservation is also critical



With equilibrium preservation

Without equilibrium preservation

Taitano et al., JCP, 2017, under review

Our solution:

Adaptive grid

Implicit solver

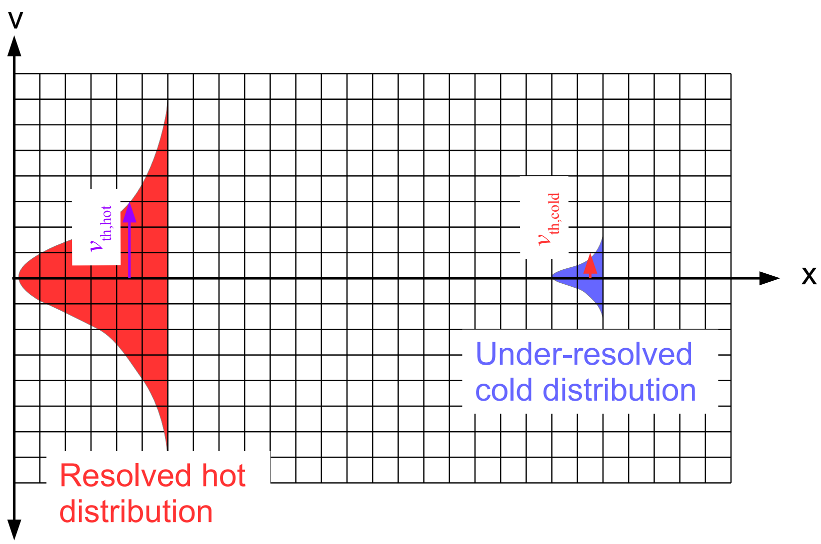
Exact discrete conservation

Adaptive mesh and implicit method makes problem tractable

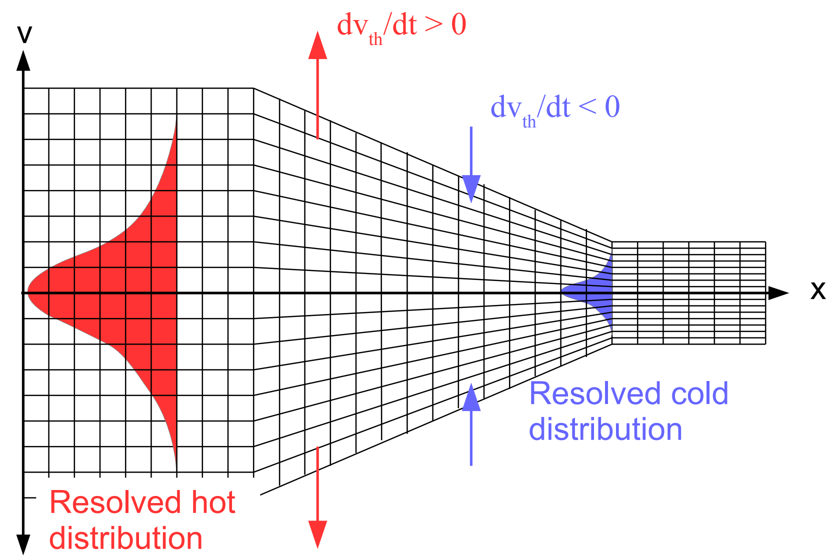
- v-space adaptivity with v_{th} normalization, $\widehat{v} = v/v_{th}$, $N_v \sim 10^4$-10^5
- Lagrangian mesh in physical space, $N_r \sim 10^2$
- $N = N_v N_r \sim 10^6 \sim 10^7$ (vs. 10^{12} with static mesh)

- Multigrid preconditioned optimal nonlinear implicit solver [*Chacon et al., JCP, 157 (2000)*], $\Delta t_{imp} = \Delta t_{str} \sim 10^{-3}$ ns
- $N_t \sim 10^3$-10^4 (vs. 10^{10} with explicit methods)

v_{th} adaptivity in velocity space allows optimal mesh resolution throughout domain

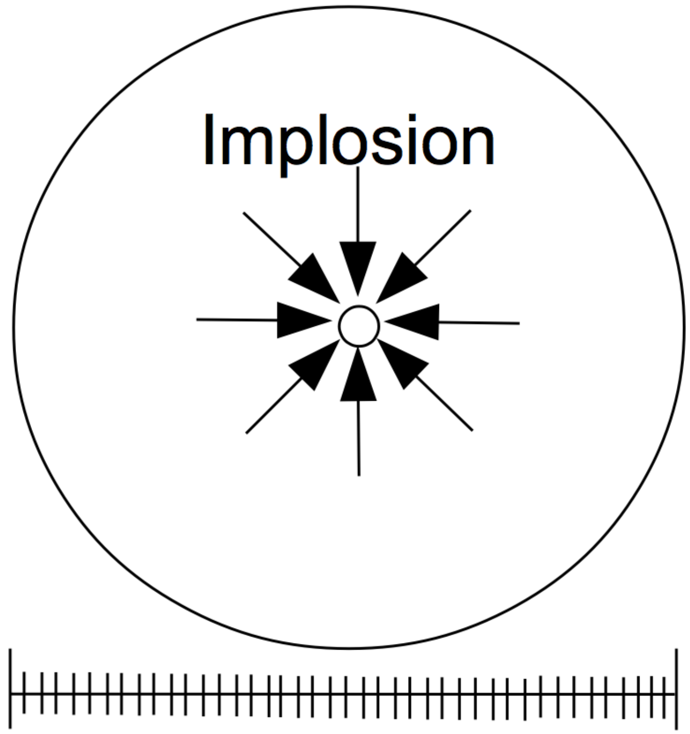


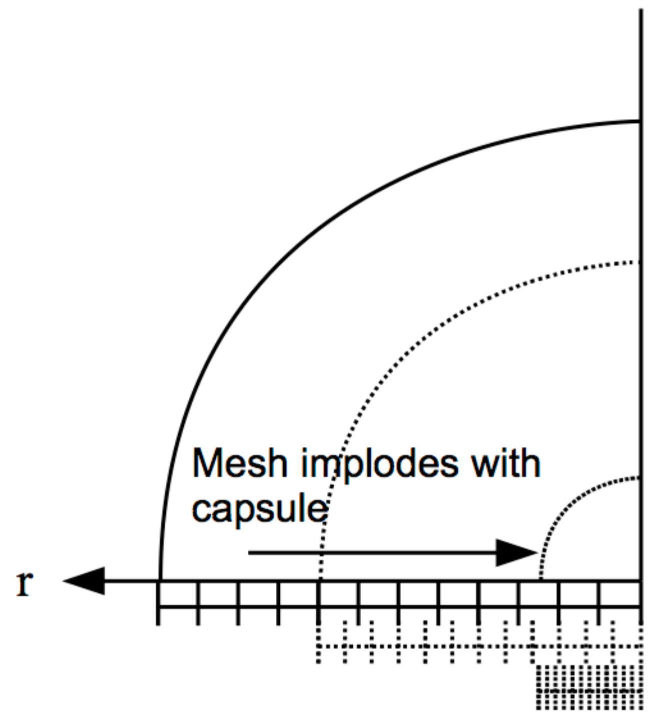
Static Mesh



v_{th} adaptive Mesh

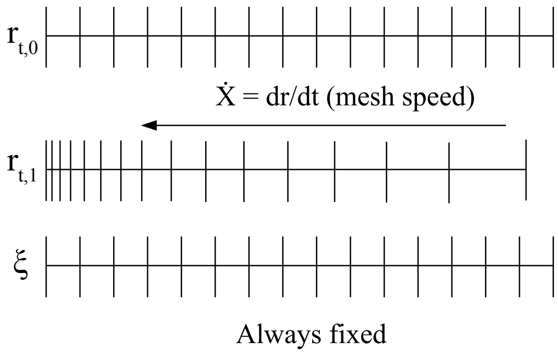
Moving mesh in physical space:
Implode mesh with capsule to track shock

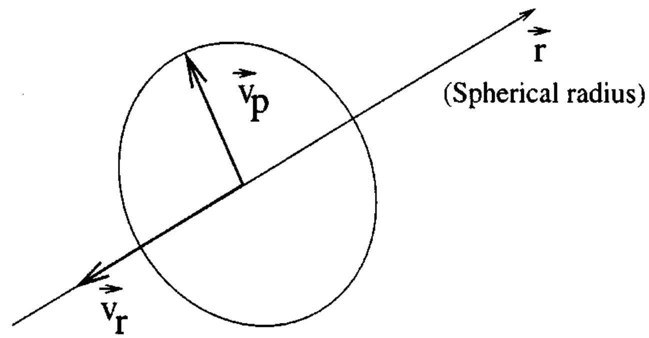




To have grid adaptivity, we transform the equation

1D spherical (with logical mesh); 2D cylindrical geometry in velocity space





Coordinate transformation:

$$\widehat{v}_{||} \equiv \frac{\vec{v}\cdot\widehat{\vec{r}}}{v_{th,\alpha}}, \quad \widehat{v}_{\perp} \equiv \frac{\sqrt{v^2 - v_{||}^2}}{v_{th,\alpha}}$$

Jacobian of transformation:

$$\sqrt{g_v}\left(t, r, \widehat{v}_\perp\right) \equiv v_{th,\alpha}^3\left(t, r\right) r^2 \widehat{v}_\perp$$

$$J_{r\xi} = \partial_\xi r$$

Adaptivity introduces inertial terms in the conservation equation

- **VRFP equation in transformed coordinates**

$$\partial_t \left(\sqrt{g_v} J_{r\xi} f_\alpha\right) + \partial_\xi \left(\sqrt{g_v} v_{th,\alpha} \left[\widehat{v}_{||} - \widehat{\dot{r}}_\alpha\right] f_\alpha\right) +$$

$$\partial_{\widehat{v}_{||}} \left(J_{r\xi}\sqrt{g_v}\widehat{\dot{v}}_{||} f_\alpha\right) + \partial_{\widehat{v}_\perp} \left(J_{r\xi}\sqrt{g_v}\widehat{\dot{v}}_\perp f_\alpha\right) = J_{r\xi}\sqrt{g_v}\sum_\beta^{N_s} C_{\alpha\beta}\left(f_\alpha, f_\beta\right)$$

$$\widehat{\dot{v}}_{||} = -\frac{\widehat{v}_{||}}{2}\left(v_{th,\alpha}^{-2}\partial_t v_{th,\alpha}^2 + J_{r\xi}^{-1}\left(\widehat{v}_{||} - \widehat{\dot{x}}\right) v_{th,\alpha}^{-1}\partial_\xi v_{th,\alpha}^2\right) + \frac{\widehat{v}_\perp^2 v_{th,\alpha}}{r} + \frac{q_\alpha E_{||}}{J_{r\xi} m_\alpha v_{th,\alpha}}$$

$$\widehat{\dot{v}}_\perp = -\frac{\widehat{v}_\perp}{2}\left(v_{th,\alpha}^{-2}\partial_t v_{th,\alpha}^2 + J_{r\xi}^{-1}\left(\widehat{v}_{||} - \widehat{\dot{x}}\right) v_{th,\alpha}^{-1}\partial_\xi v_{th,\alpha}^2\right) - \frac{\widehat{v}_{||}\widehat{v}_\perp v_{th,\alpha}}{r}$$

Inertial terms due to v_{th} adaptivity and Lagrangian mesh

Taitano et al., JCP, 318, 2016
Taitano et al., JCP, 2017, in preparation
Taitano et al., JCP, 2018, in preparation

v_{th} adaptivity provides an enabling capability to simulate ICF plasmas

- **D-e-α, 3 species thermalization problem**
- **Resolution with static grid:**

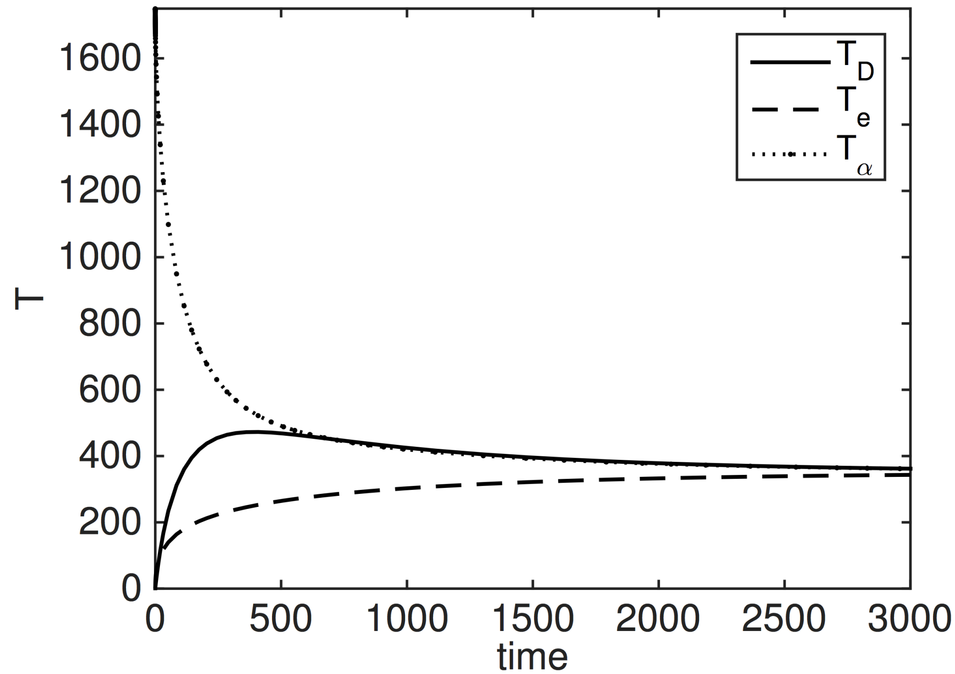
$$N_v \sim 2\left(\frac{v_{th,e,\infty}}{v_{th,D,0}}\right)^2 = 140000 \times 70000$$

- **Resolution with adaptivity and asymptotics:**

$$N_v = 128 \times 64$$

- **Mesh savings of**

$$\sim 10^6$$



Taitano et al., JCP, 318, 2016

Our solution:

Adaptive grid

Implicit solver

Exact discrete conservation

Implicit solver strategy: Preconditioned Anderson Acceleration

- **We drive the nonlinear residual to zero**

$$R = \partial_t f + VE(f) - \left[\underline{\underline{D}} \cdot \nabla_v f - \underline{A} f\right] = 0$$

- **Consider a fixed point map of form:**

$$G(f_k) = f_k - P_k^{-1} R_k = f_{k+1}$$

- **If** $P_k = J_k$ **, Newton's method**
- **Anderson updates the solution by using history (nonlinear) of solutions to accelerate convergence via:**

$$f_{k+1} = \sum_{i=0}^{m_k} \alpha_i^{(k)} G\left(f_{k-m_k+i}\right)$$

Two stage operator splitting in PC operator

$$P^{-1}R = P_x^{-1}P_v^{-1}R$$

Step 1: Velocity space operators (including collisions)

$$P_v = \partial_t \circ + VE_v \circ - \left[\underline{\underline{D}} \cdot \nabla_v \circ - \vec{A} \circ\right]$$

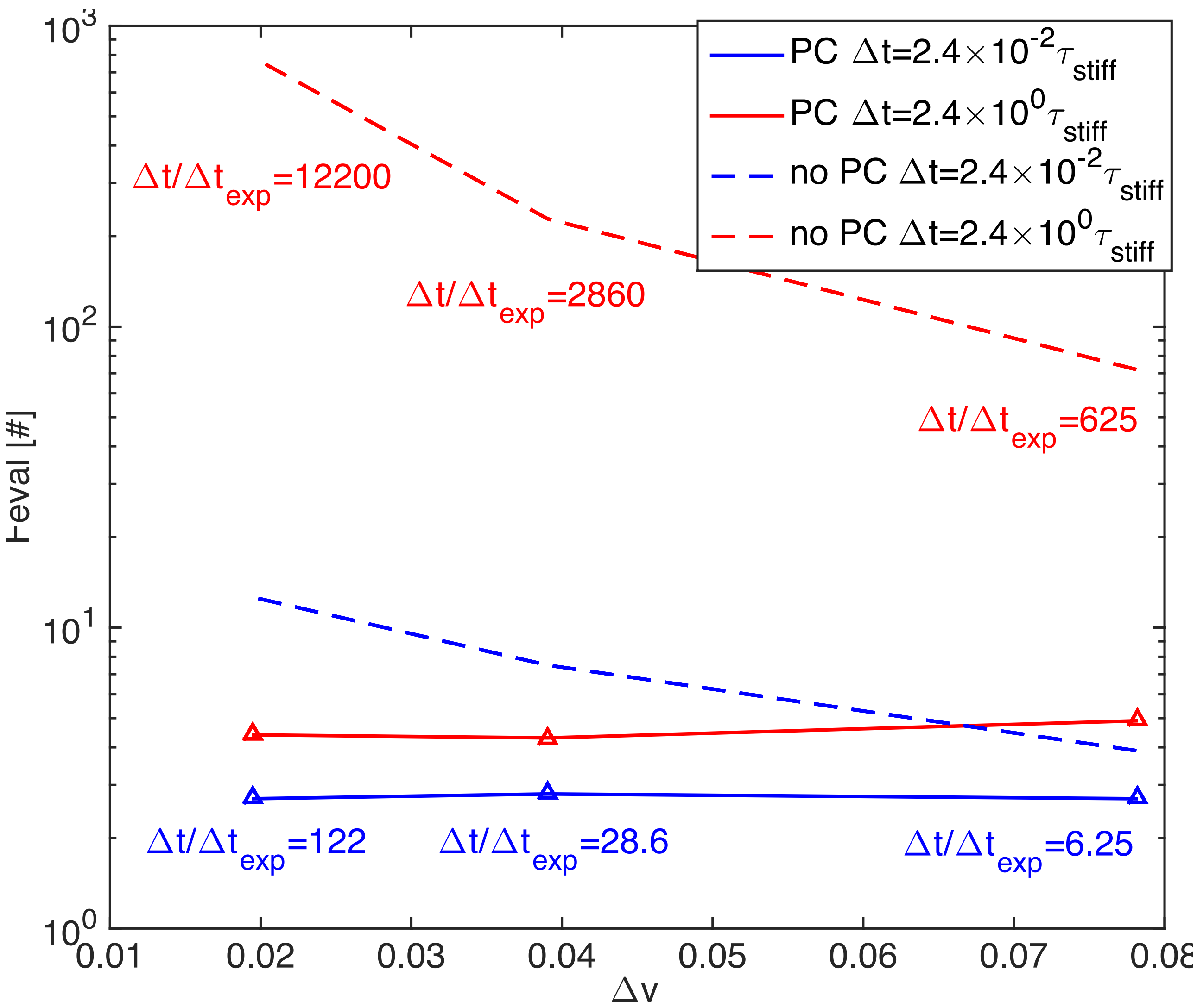
Step 2: Streaming operator

$$P_x = \partial_t + v\partial_x \circ$$

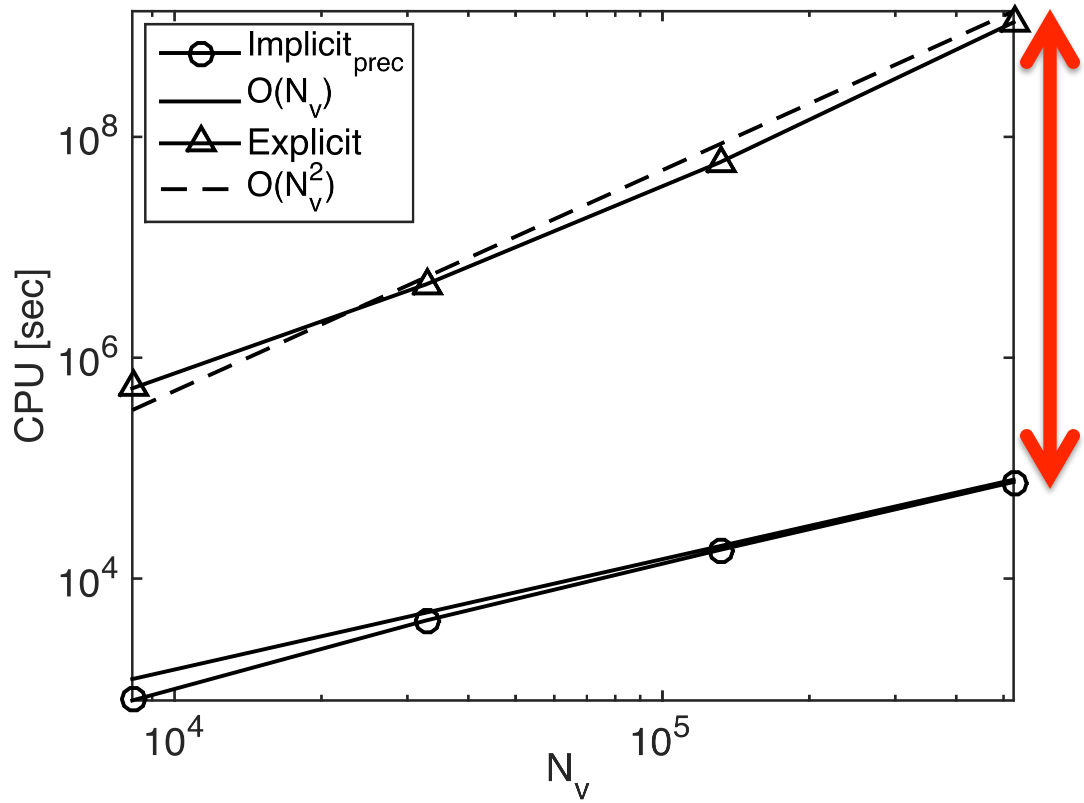
Preconditioner is a convergence *accelerator!*

No splitting error will be present in the actual solution (driven by the nonlinear residual)

Preconditioner is effective in reducing iteration



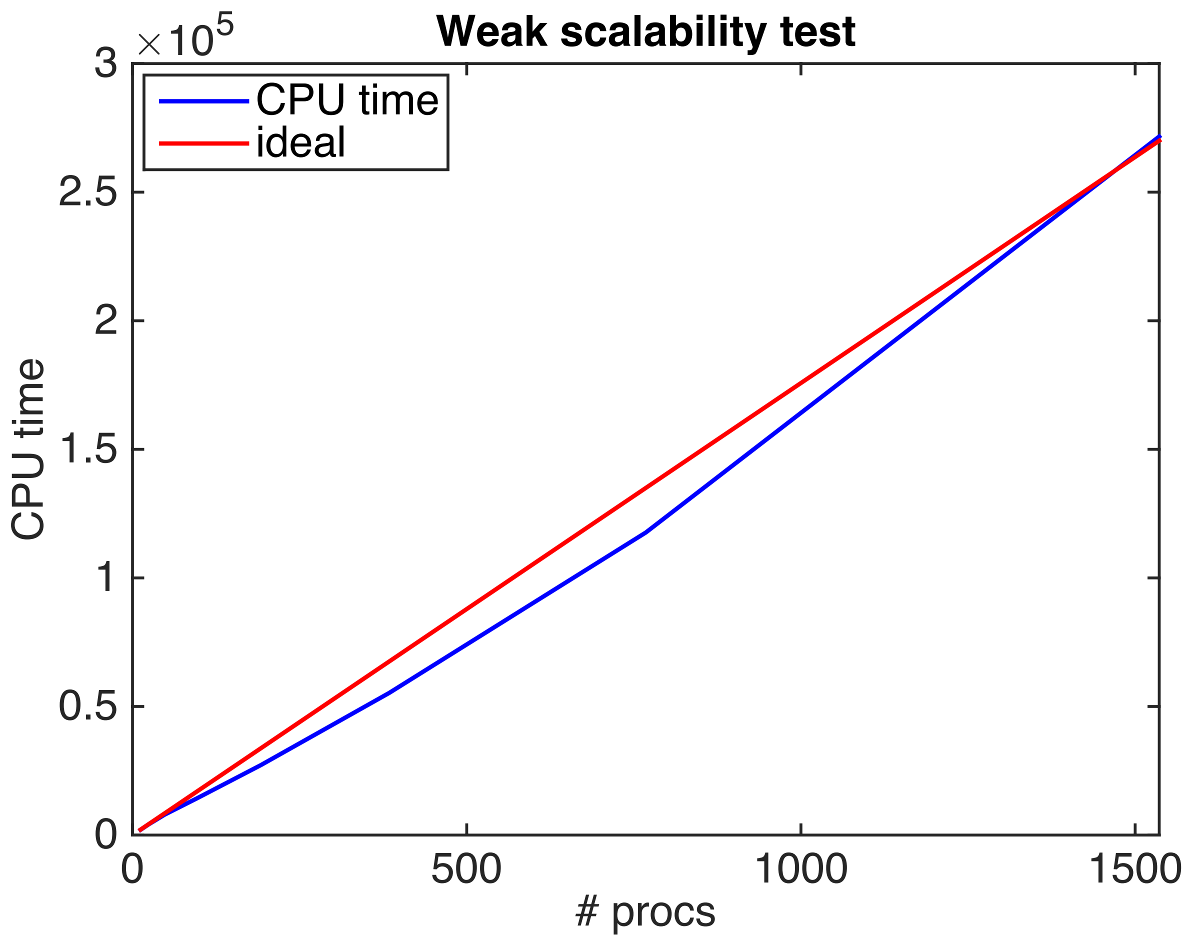
Implicit solver performance is optimal



4 orders of magnitude more efficient than explicit methods

Solver CPU time versus size of unknown

The code is scalable



Our solution:

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Rosenbluth-FP collision operator: conservation properties results from symmetries

$$C_{\alpha\beta} = \Gamma_{\alpha\beta} \nabla_v \cdot \left[\vec{J}_{\alpha\beta,G} - \frac{m_\alpha}{m_\beta} \vec{J}_{\alpha\beta,H} \right]$$

Mass

$$\langle 1, C_{\alpha\beta} \rangle_{\vec{v}} = 0 \quad \Rightarrow \quad \left. \vec{J}_{\alpha\beta,G} - \vec{J}_{\alpha\beta,H} \right|_{\partial \vec{v}} = 0$$

Momentum

$$m_\alpha \langle \vec{v}, C_{\alpha\beta} \rangle_{\vec{v}} = -m_\beta \langle \vec{v}, C_{\beta\alpha} \rangle_{\vec{v}} \quad \Rightarrow \quad \left\langle 1, J^{\|}_{\alpha\beta,G} - J^{\|}_{\beta\alpha,H} \right\rangle_{\vec{v}} = 0$$

Energy

$$m_\alpha \left\{ \left\langle v^2, C_{\alpha\beta} \right\rangle_{\vec{v}} \right\} = -m_\beta \left\{ \left\langle v^2, C_{\beta\alpha} \right\rangle_{\vec{v}} \right\} \Rightarrow \left\langle \vec{v}, \vec{J}_{\beta\alpha,G} - \vec{J}_{\alpha\beta,H} \right\rangle_{\vec{v}} = 0$$

2V Rosenbluth-FP collision operator: numerical conservation of energy

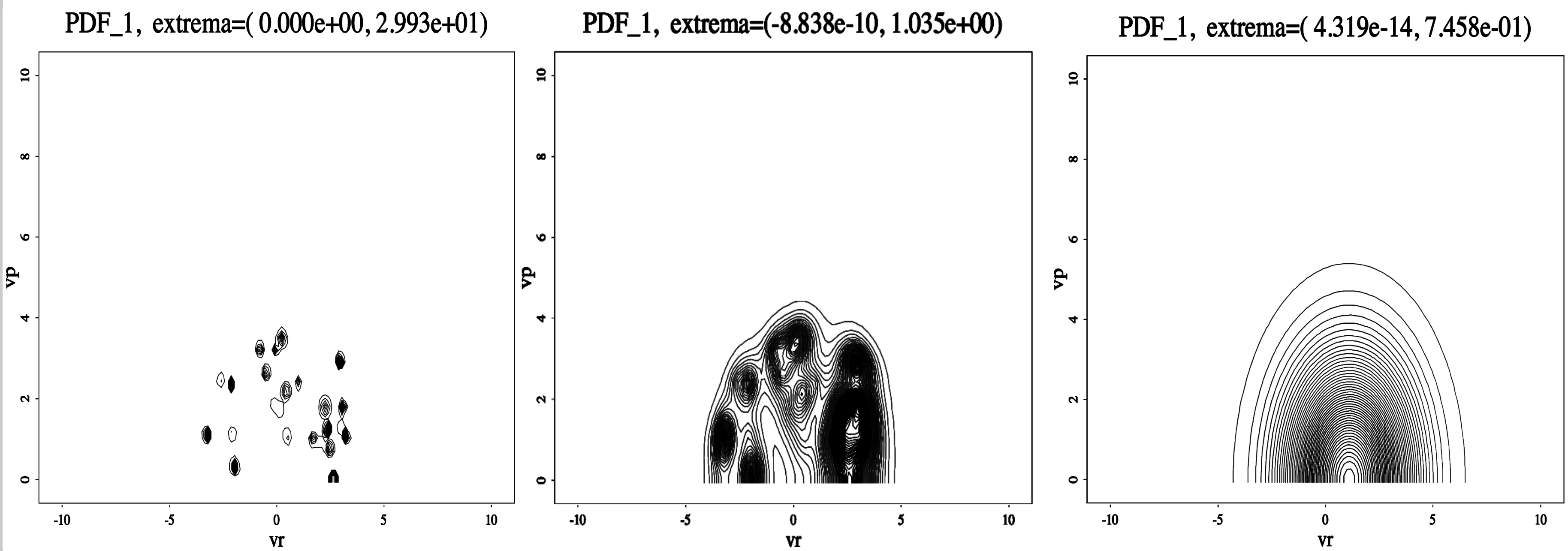
- **The symmetry to enforce is:** $\left\langle \vec{v}, \vec{J}_{\beta\alpha,G} - \vec{J}_{\alpha\beta,H} \right\rangle_{\vec{v}} = 0$
- **Due to discretization error:** $\left\langle \vec{v}, \vec{J}_{\beta\alpha,G} - \vec{J}_{\alpha\beta,H} \right\rangle_{\vec{v}} = \mathcal{O}\left(\Delta_v\right)$
- **Introduce a constraint coefficient:**

$$\left\langle \vec{v}, \gamma_{\beta\alpha} \vec{J}_{\beta\alpha,G} - \vec{J}_{\alpha\beta,H} \right\rangle_{\vec{v}} = 0 \qquad \gamma_{\beta\alpha} = \frac{\left\langle \vec{v}, \vec{J}_{\alpha\beta,H} \right\rangle_{\vec{v}}}{\left\langle \vec{v}, \vec{J}_{\beta\alpha,G} \right\rangle_{\vec{v}}} = 1 + \mathcal{O}\left(\Delta_v\right)$$

$$C_{\alpha\beta} = \Gamma_{\alpha\beta} \nabla_v \cdot \left[\gamma_{\alpha\beta} \vec{J}_{\alpha\beta,G} - \frac{m_\alpha}{m_\beta} \vec{J}_{\alpha\beta,H} \right]$$

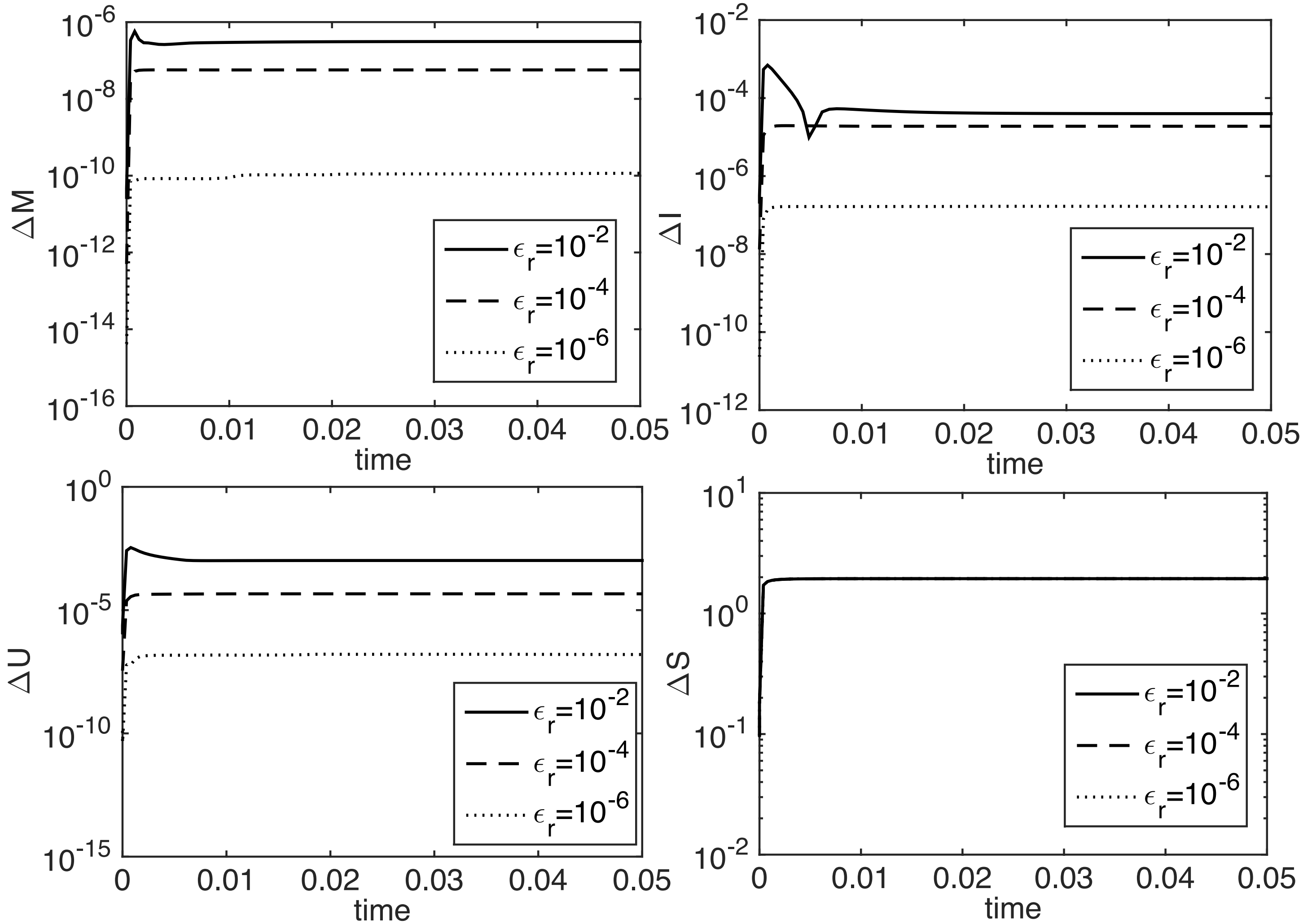
Taitano et al., JCP, 297, 2015

Single-species initial random distribution thermalizes to a Maxwellian and HOLDS IT



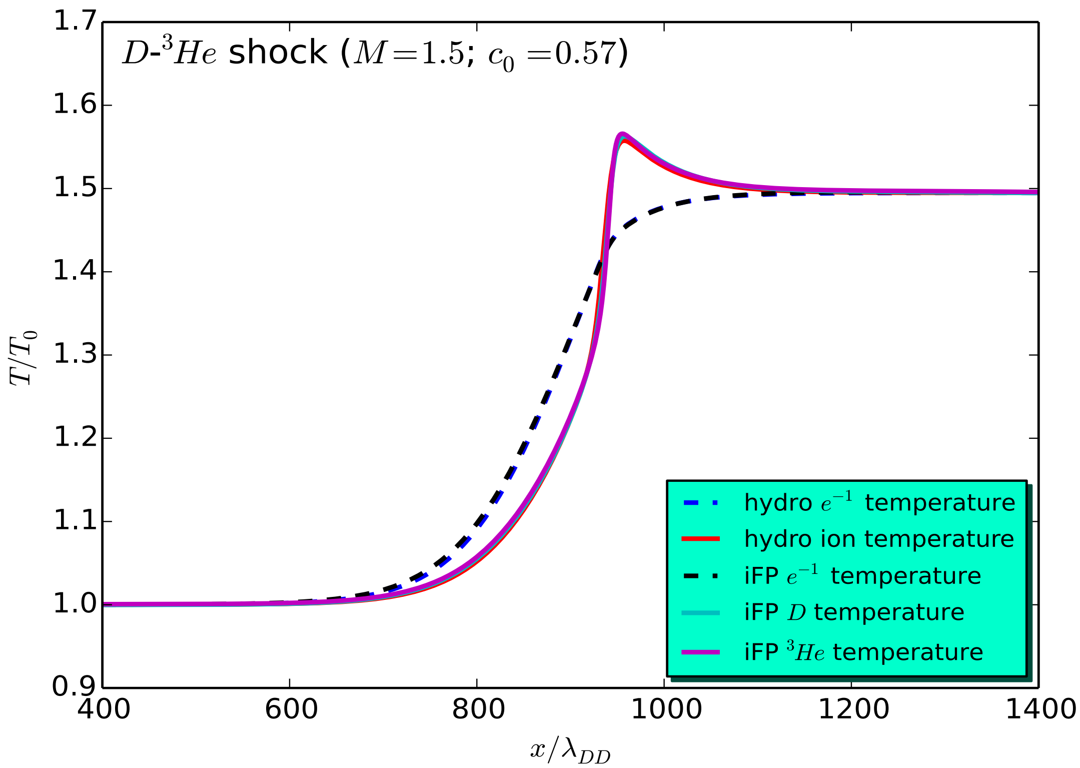
Taitano et al., JCP, 297, 2015

Conservation properties enforced down to nonlinear convergence tolerance



Taitano et al., JCP, 297, 2015

The end product is a reliable code



- **Comparison between a reference iFP and fluid simulation for a two ion species M=1.5 (weak) shock problem**

First capsule implosion simulation

First implosion calculation

- D-He^3 fill Omega capsule simulation with hydro boundary for fuel [O. Larroche, PoP, 2012, collaborator]
- **Studied to investigate Rygg effect** [J. R. Rygg et al. PoP, 2006]
- FPion was first used to investigate fuel stratification to explain reactivity drop by Rygg et al.

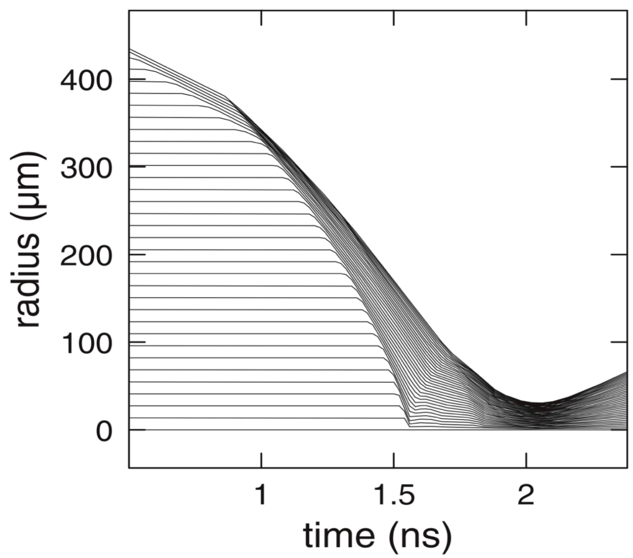
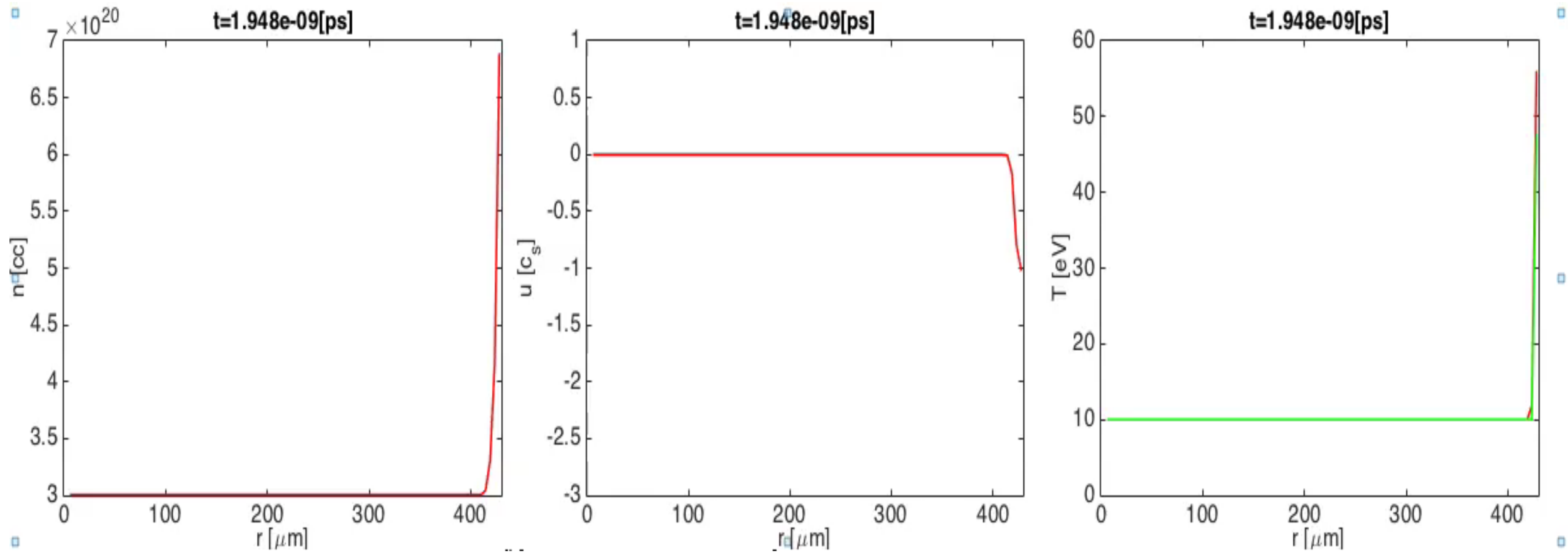
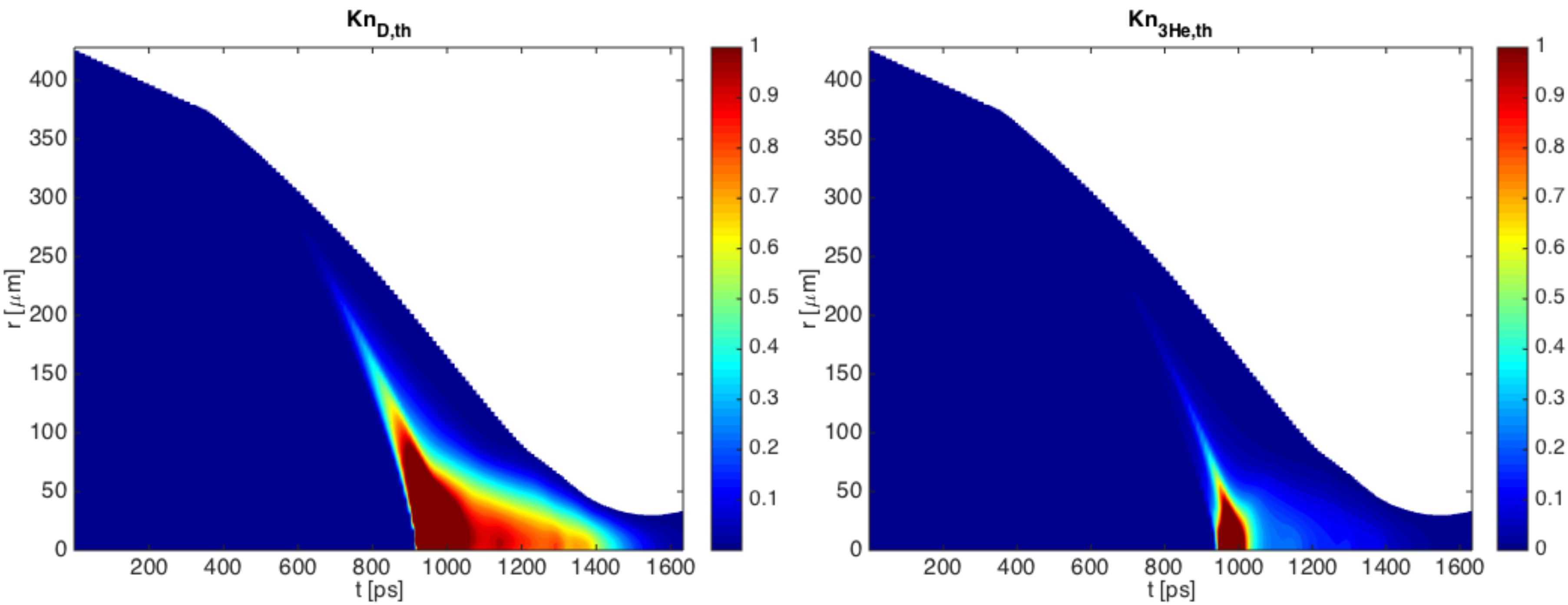


FIG. 3. Lagrangian (r, t) diagram of the fuel in the hydrodynamical simulation, from which initial and boundary conditions are extracted for the kinetic calculation.

Simulation observes fuel stratification. We might be able to explain experiment (current effort)



Kn reveals that D mean free path is on order capsule size for an appreciable time post shock convergence



$$Kn = \frac{\lambda_{mfp}}{R_{capsule}}$$

Main take away from this talk

- **Project began exactly 3 years ago (very high paced R&D)**

- **iFP is a first of a kind multi-scale simulation capability**
  - Fully implicit, scalable (both algorithmic and parallel)
  - Optimal grid adaptivity
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  - Strict conservation enforced
  - Strict verification campaign against hydro limit and other codes

- **Began ICF physics campaign simulation**

  First capsule implosion simulation with hydro boundary conditions

Future Work

- **Capsule implosion with self consistent pusher species included**

- **Investigate more ICF relevant physics**
  - Rygg (inverse) effect
  - Kinetically enhanced pusher mix into fuel
  - Kinetic effects on fuel convergence reduction

- **Implementation of neutron and thermal radiation transport packages to investigate multi-physics aspects of ICF implosion**

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- Collaborators : CEA, MIT, LLNL , Kinetic Effects Group at LANL

Q & A

is the logo pretty?