Dundee Numerical Methods in MHD
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Arbitrary Lagrangian Euler codes for non-ideal MHD

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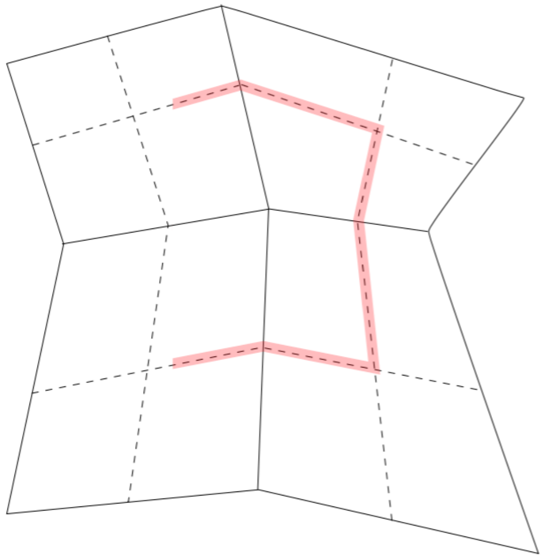

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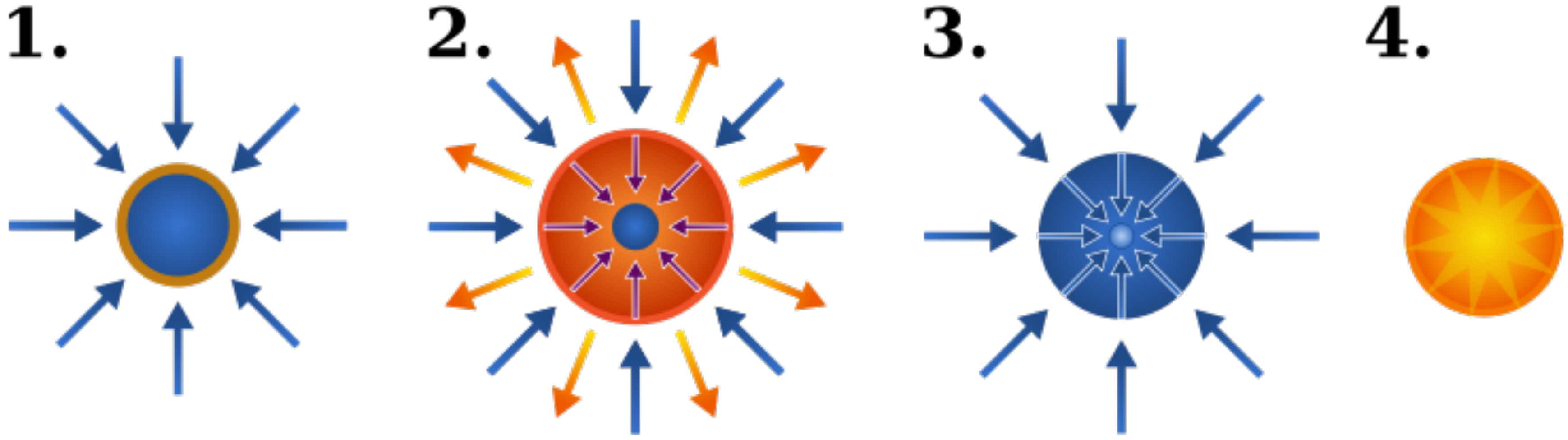
Overview

- What is the problem?
- Basics of laser-driven fusion
- Why this leads to ALE schemes
- Basic ALE algorithm
- Non-ideal MHD terms
- Some examples
- Status of the code development

Laser-fusion in a nutshell



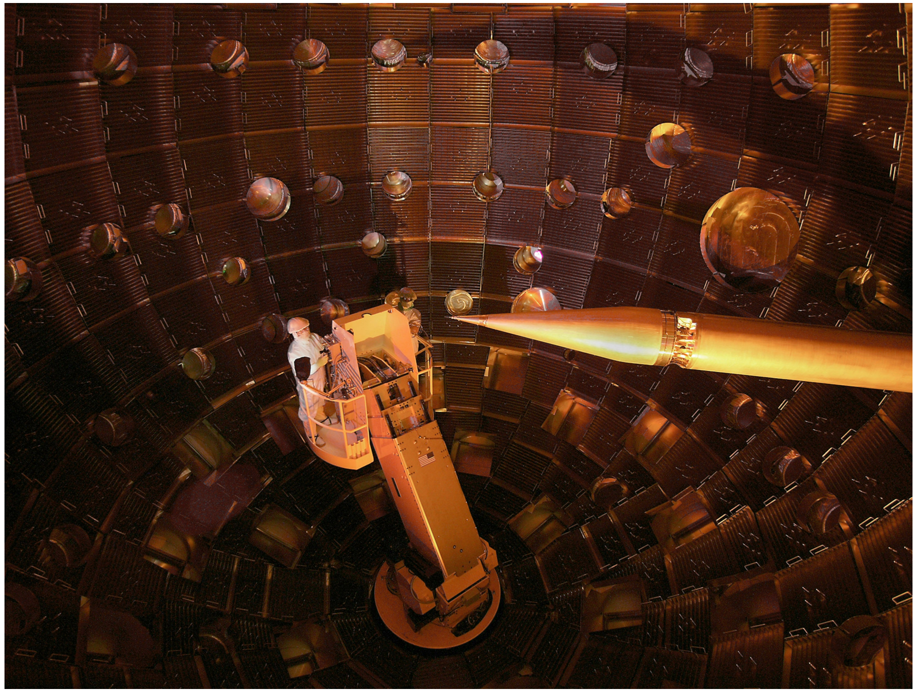
To achieve a gain of ~10 need…

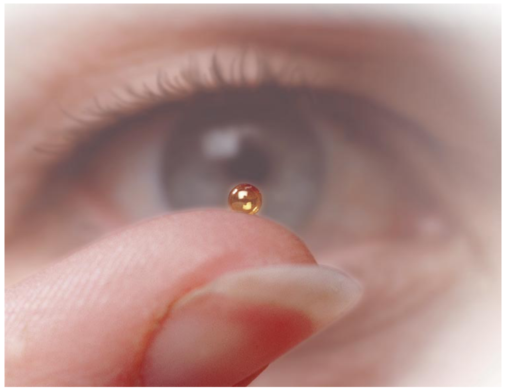
- Compress D-T fuel to ~1000 solid density
- Ignite fuel at $\sim 10^7$ K
- Requires implosion speed of ~ 350 km s^{-1} (about Mach 10)
- Drive time ~ 20 ns
- Laser energy ~ 1.8 MJ and peak power 500 TW ($\sim 5 \times 10^5$ Sizewell B)
- Peak ablation pressure ~130 Mbar
- Peak ignition pressure $\sim 10^5$ Mbar with burn, i.e. 10^{11} atmospheric
- Acceleration $\sim 10^{13}$ m s^{-2} about 10^{12} g

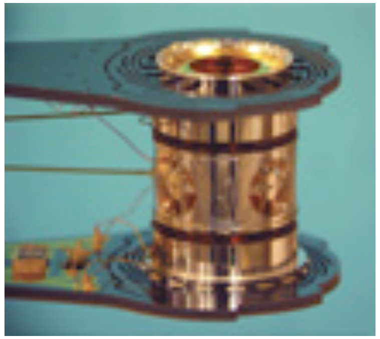
NIF was designed and built to create ignition conditions

- 192 Beams
- Frequency tripled Nd glass
- Energy 1.8 MJ
- Power 500 TW
- Wavelength 351 nm

National Ignition Facility (NIF)

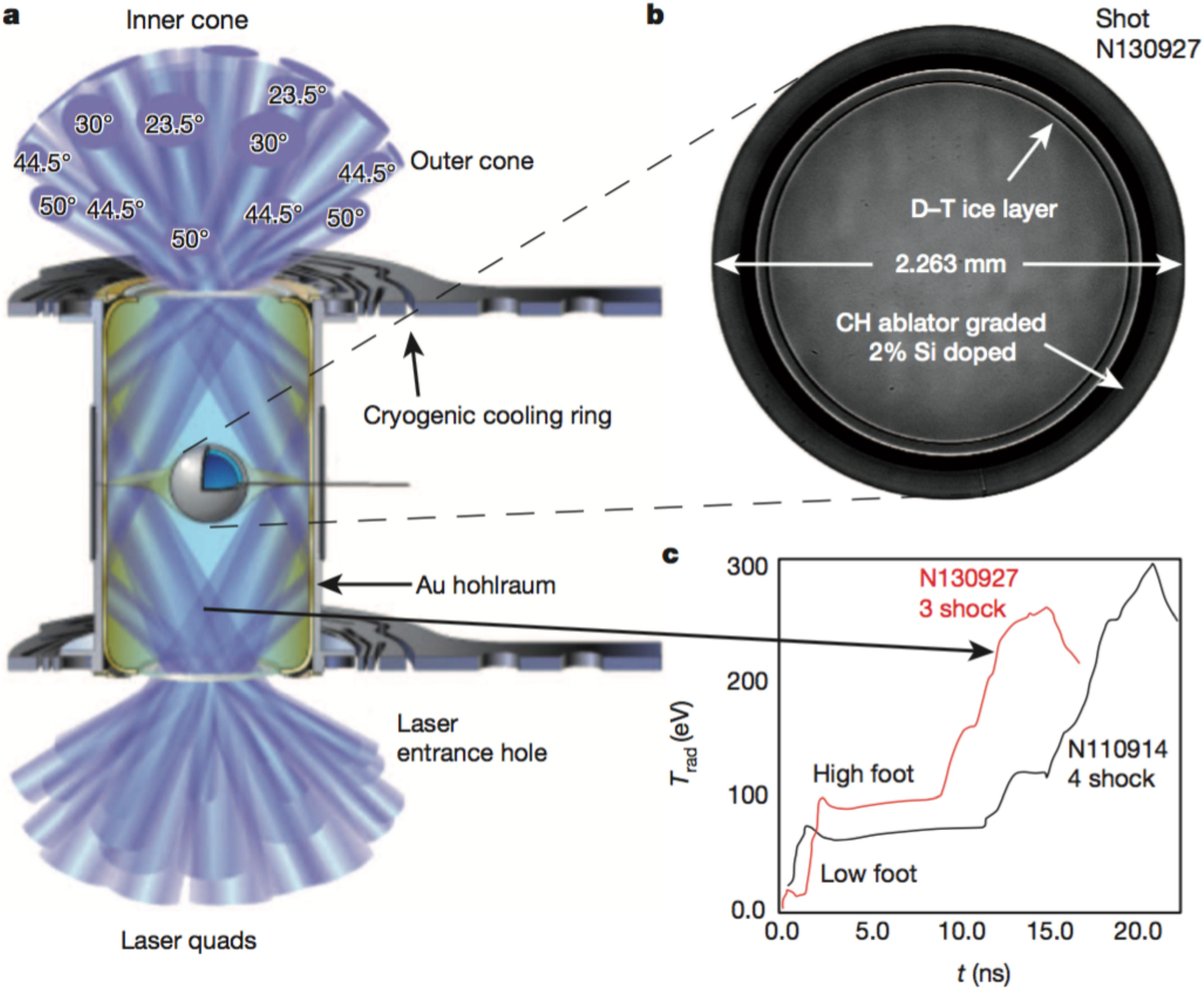






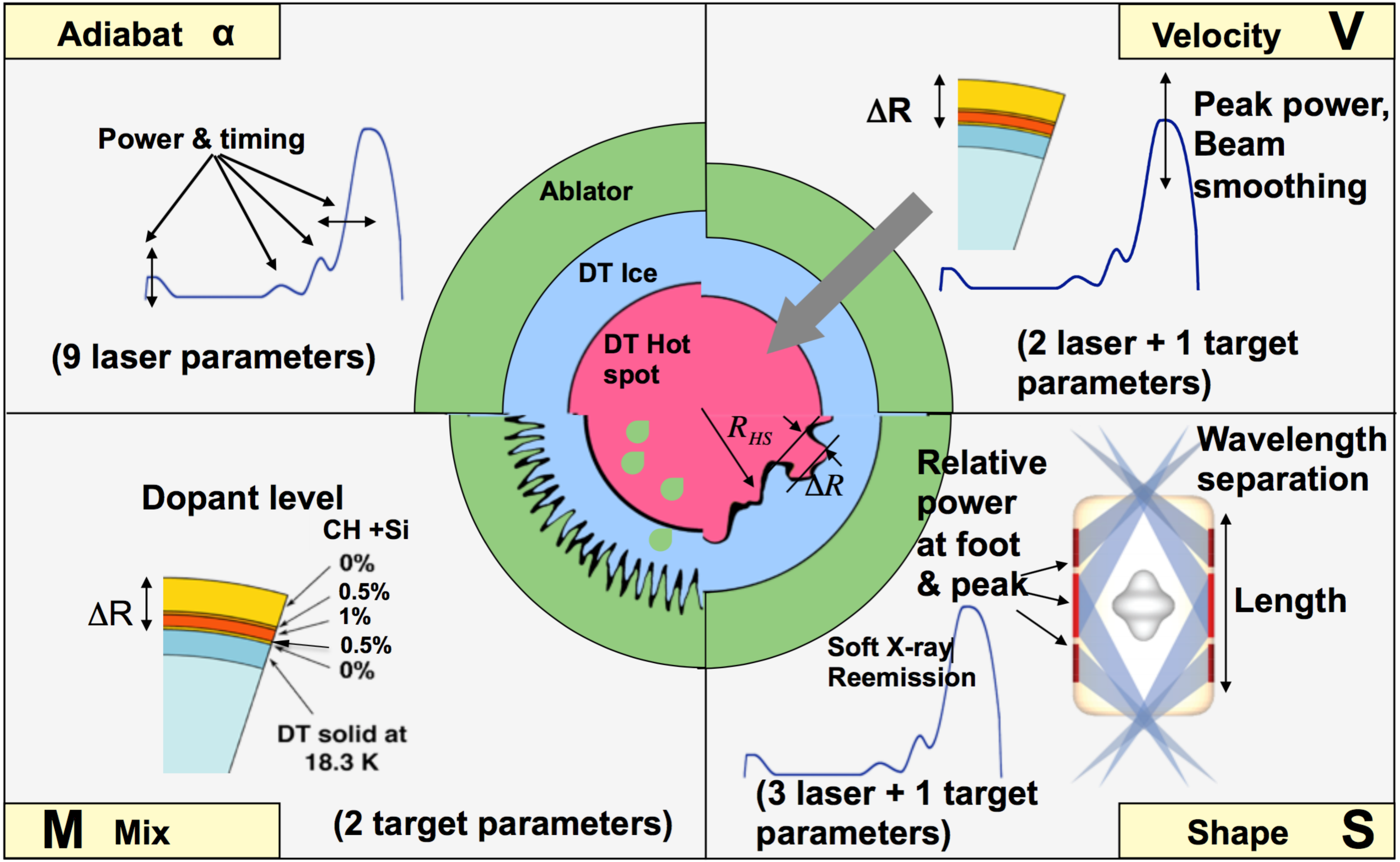
Lawrence Livermore National Laboratory (LLNL)

Few MJ laser energy to 100 MJ burn



O. Hurricane et al. Nature 2014

Fusion success = f(a,v,m,s)



Code specification

A target point design must…

- Handle converging and coalescing shocks at ~ Mach 10
- Handle tabulated EOS, NLTE and burn
- Preserve symmetry
- Prevent numerical mixing of materials
- Maintain accuracy for 30 x length contraction

Odin is an Arbitrary-Lagrangian-Eulerian code

- Lagrangian mesh - grid moves with fluid
- Second-order accurate with shock viscosity (Kurapetenko)
- Not in conservative form - compatible energy update (Caramana)
- Area-weighted r-z geometry for symmetry
- Include MHD as well as Euler solver
- Remap/rezone to relaxed grid if Lagrangian grid too distorted

Lagrangian Equations

$$\frac{D\rho}{Dt} = -\rho\nabla.\mathbf{v}$$

$$\frac{D\epsilon}{Dt} = -\frac{P}{\rho}\nabla.\mathbf{v}$$

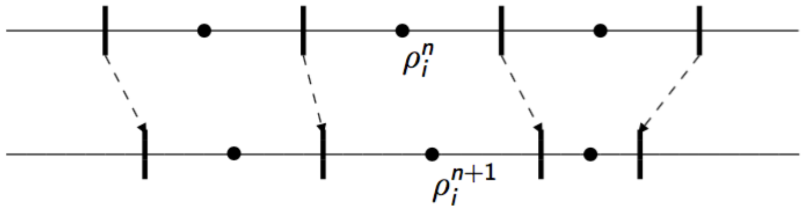
$$\frac{D\mathbf{v}}{Dt} = -\frac{1}{\rho}\nabla.P + \frac{1}{\rho}\mathbf{j}\times\mathbf{B}$$

$$\frac{D}{Dt}\left(\frac{\mathbf{B}}{\rho}\right) = \frac{\mathbf{B}}{\rho}.\nabla\mathbf{v}$$

$$\epsilon = \frac{P}{\rho(\gamma-1)}$$

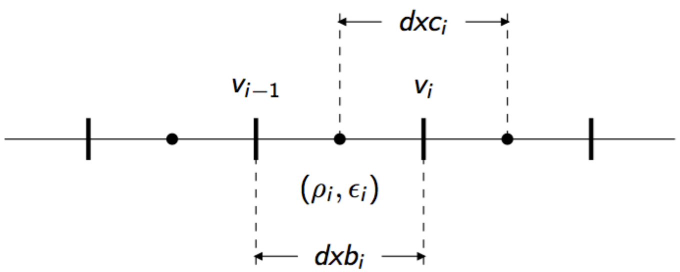
Lagrangian Grids

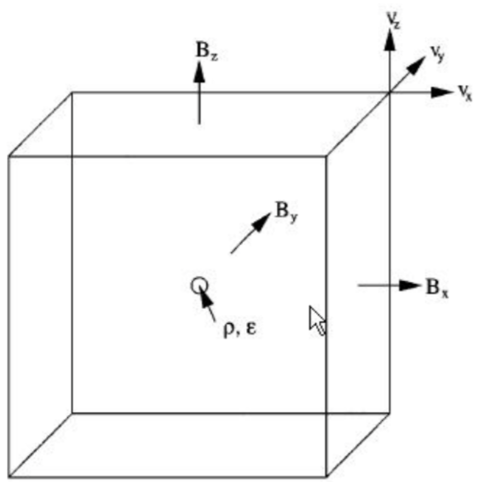
Lagrangian grid, i.e. $\frac{D}{Dt}$, updated variables move with the fluid.



Staggered Grid

- Variables $(\rho, \epsilon, \mathbf{v})$ not defined at the same grid location
- Define v as the velocity of cell boundaries
- ρ as cell averaged density defined at cell centre
- $\rho_i dxb_i$ is the mass in cell i





Momentum Equation

$$\int_{\Omega(t)} \rho \frac{D\vec{u}}{Dt} dV = - \int_{\Omega(t)} \nabla P dV.$$

$$M = \int_{\Omega(t)} \rho \, dV$$

$$\bar{f} = \frac{1}{V} \int_{\Omega(t)} f dV.$$

$$\tilde{f} = \frac{1}{M} \int_{\Omega(t)} f \rho dV,$$

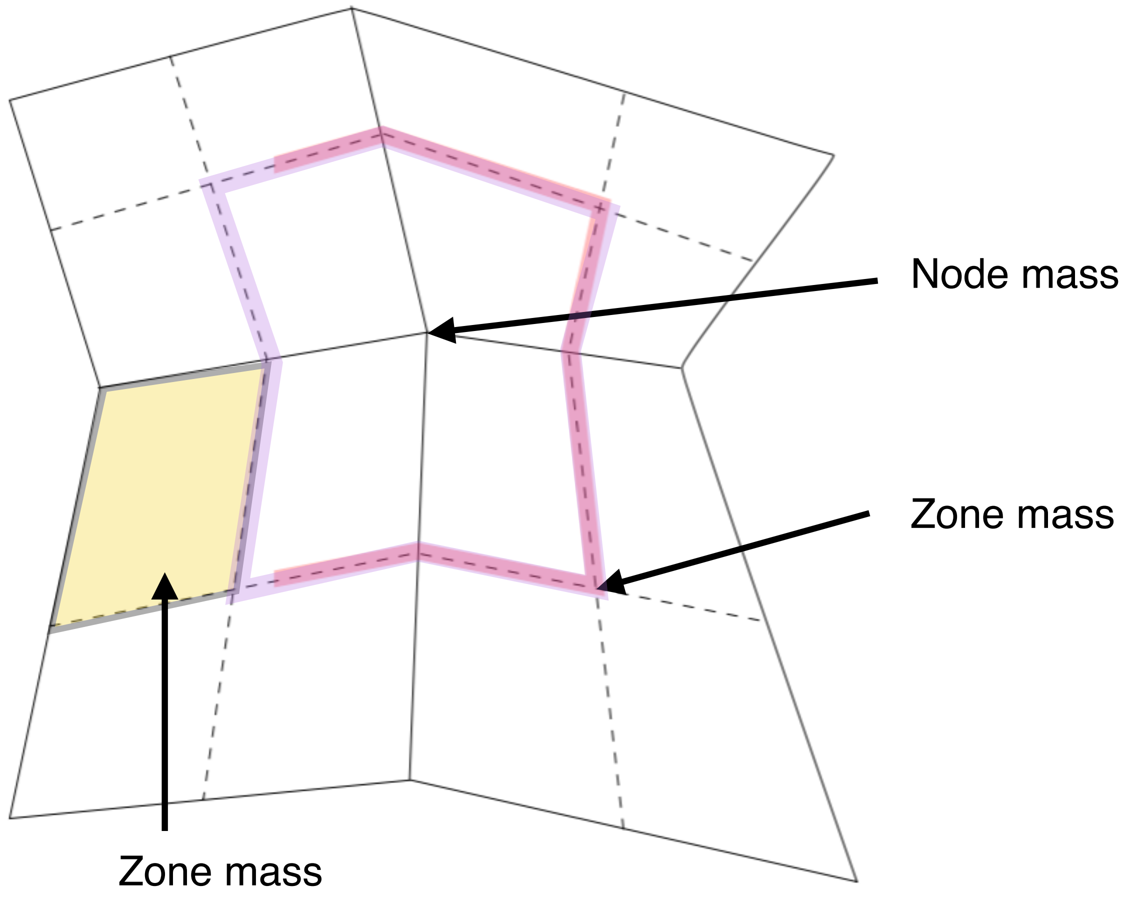
$$M \frac{D\tilde{\vec{u}}}{Dt} = - \int_{\partial\Omega(t)} P d\vec{S}.$$

$$\frac{D}{Dt} M = 0$$

Mass in cell/zone conserved

Momentum needs nodal mass

Assume corner masses are constant - the median mesh is Lagrangian



Compatible energy update

$$M^p \frac{Dv_x}{Dt} = \sum_{i=1}^{4} f_{x,i}.$$

$$M^z \frac{De_i}{Dt} = -\sum_{i=1}^{4} \vec{f_i} \cdot \vec{v_i},$$

M^z mass in cell/zone

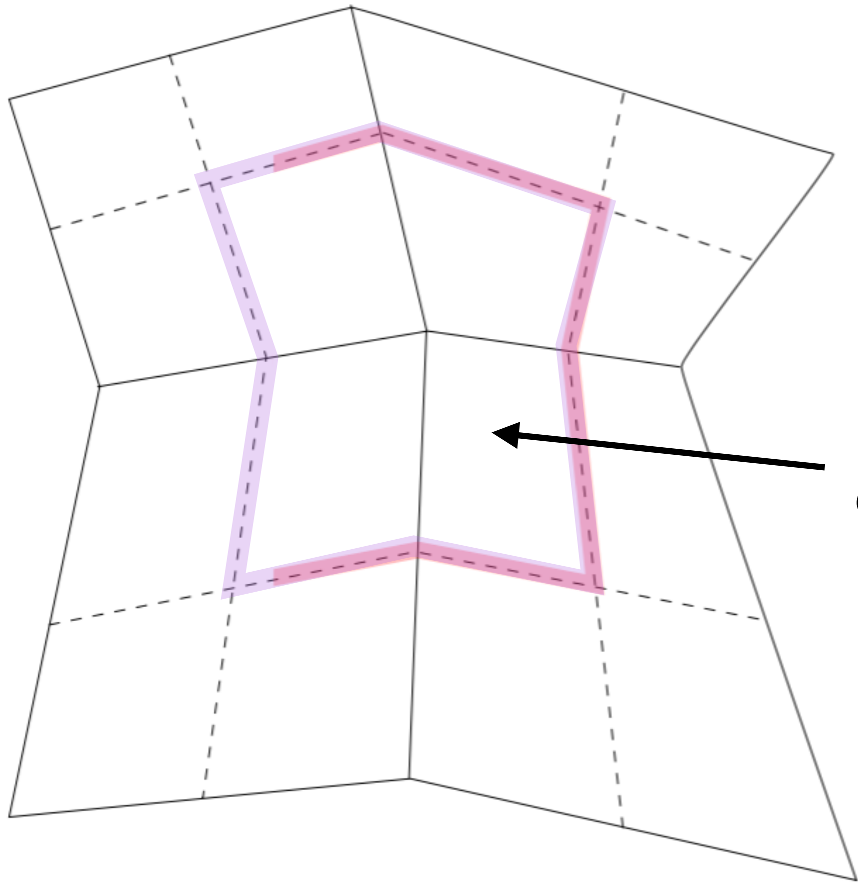
M^p mass in nodal volume about velocity

Provided same force is used in both updates energy is exactly conserved.

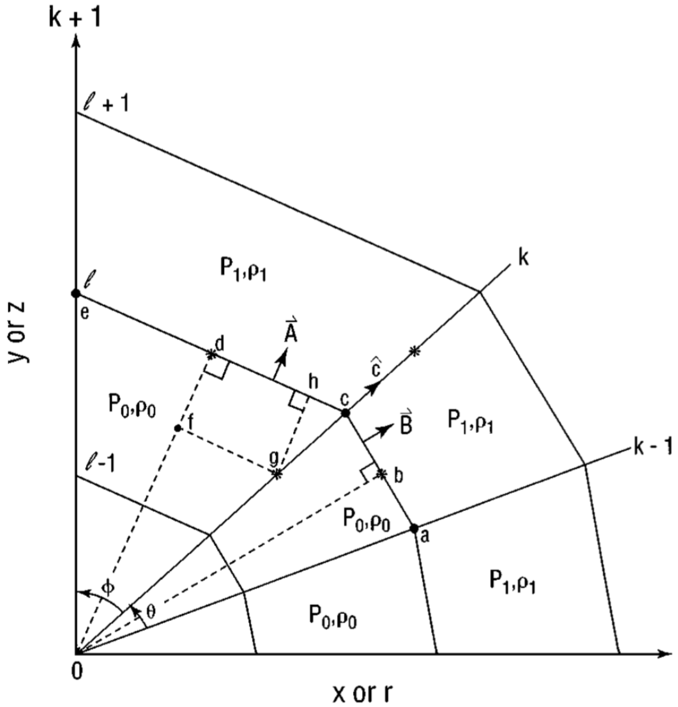
Requires a scheme to find nodal mass from zonal mass

In *x-y* simply use areas of sub-zonal mesh

Corner mass conserved in Lagrangian step



r-z Area Weighting



Control volume averaging in r-z

$$M^p \frac{Du_p}{Dt} = -\int P\mathbf{dS} + \hat{\mathbf{r}} \int \frac{P}{r} dV$$

Radial weighting in **dS** unlikely to be balanced by volume term in code.

Approach based on this method leads to loss of symmetry

Problem removed if $\int P\ r dr dz \simeq r_g \int P\ dr dz$

$$M^p \frac{D\mathbf{u}}{Dt} = -r_g \mathbf{F}_P$$

Re-factor calculations of nodal mass from volume mass using

$$M^p = r_g \sum_z \rho_z\ A_z$$

Edge Viscosity

Full scheme from Caramana et al. JCP (1998)

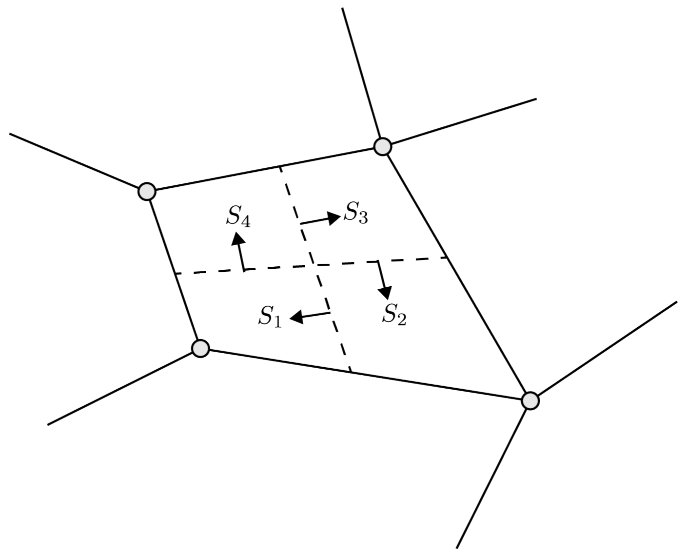
Limited away from shocks

Only apply on edge compression

$$\mathbf{f}_i = \rho_i \left\{ \frac{\gamma+1}{4}\Delta v_i + \left(\left(\frac{\gamma+1}{4}^2 \right) \Delta v_i^2 + c_s \right)^{1/2} \right\} (\Delta \hat{\mathbf{v}}_i . \mathbf{S}_i) \Delta \mathbf{v}_i (1 - \psi_i)$$

Shock jump from Lagrangian from Kuropatenko, 1967

For MHD usually replace sound speed with fast speed



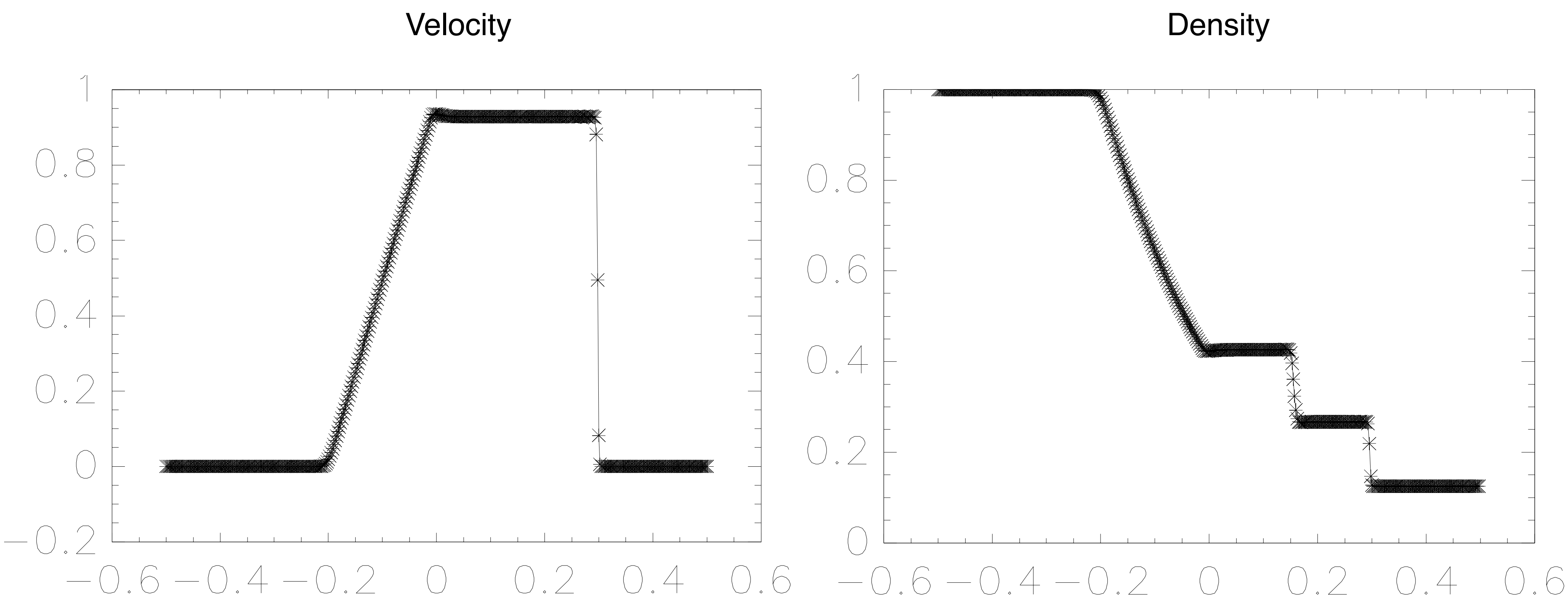
1D test - Sod's problem

Sod considered a one-dimensional tube of unit length $0 \leq x \leq 1$ and the following initial conditions at $t = 0$:

$$\rho(x,0) = \begin{cases} 1.0 & \text{for } x \leq \frac{1}{2} \\ 0.125 & \text{for } x > \frac{1}{2} \end{cases} ,$$

$$p(x,0) = \begin{cases} 1.0 & \text{for } x \leq \frac{1}{2} \\ 0.1 & \text{for } x > \frac{1}{2} \end{cases} ,$$

$$u(x,0) = 0 \; .$$



Eulerian grid

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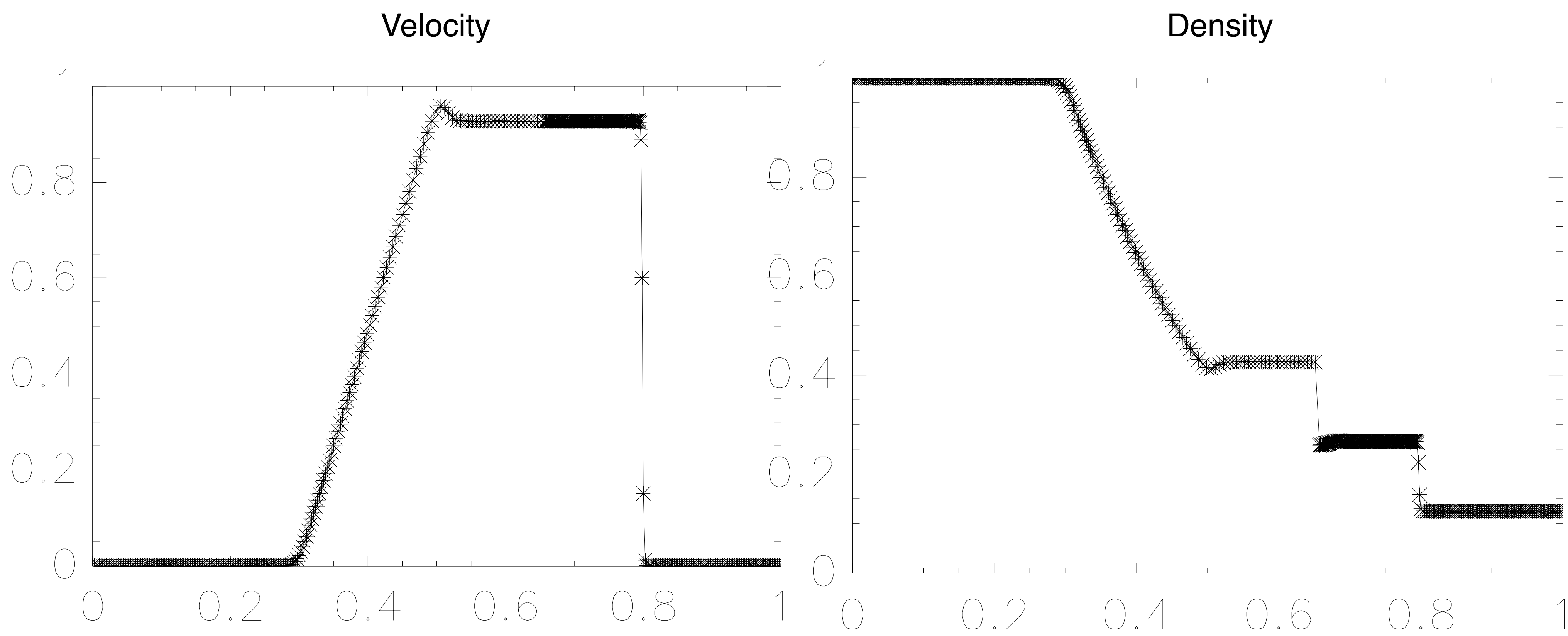
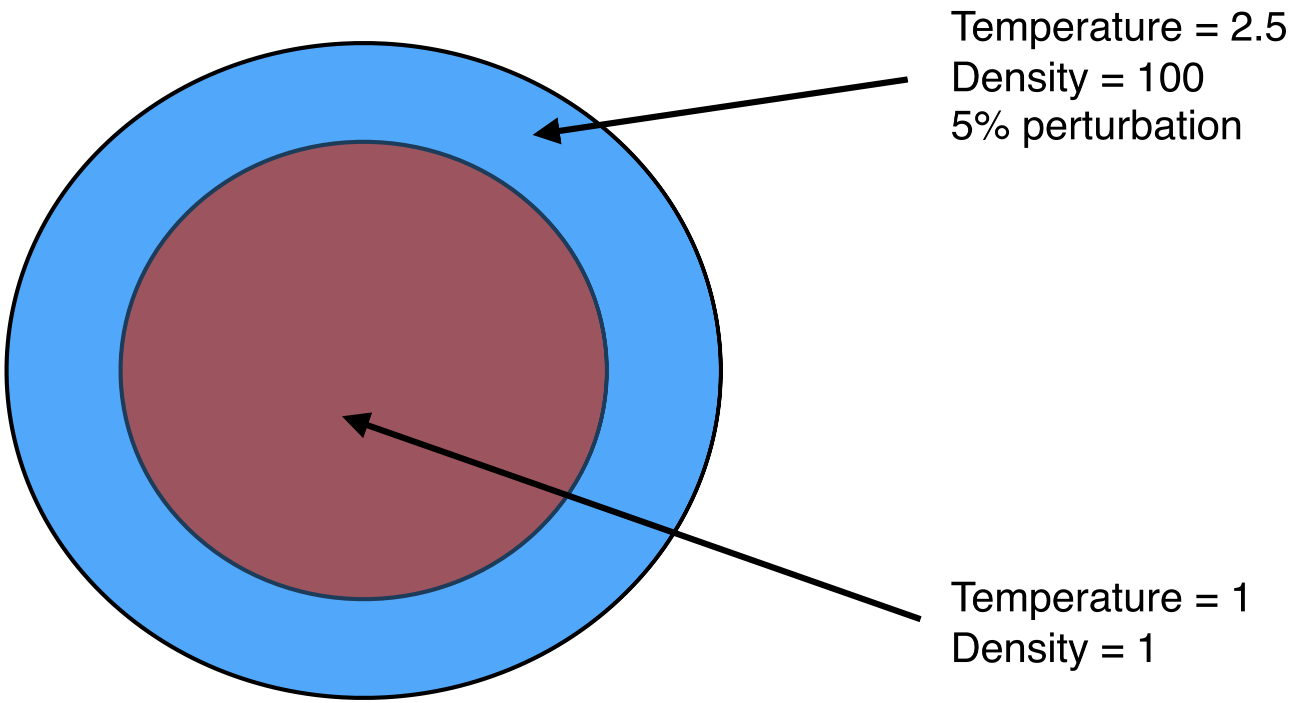


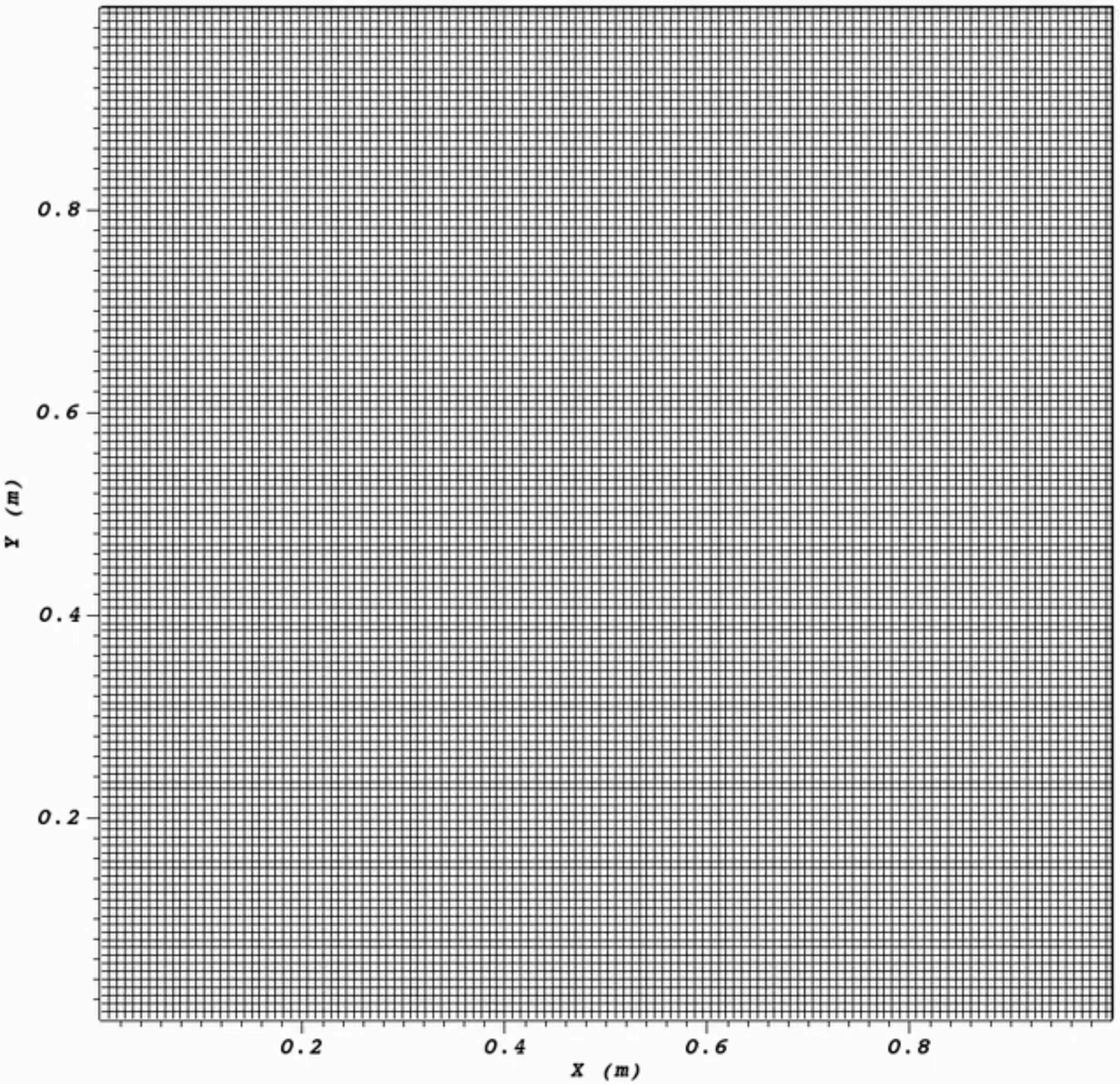
Lagrangian grid

Spherical shell test

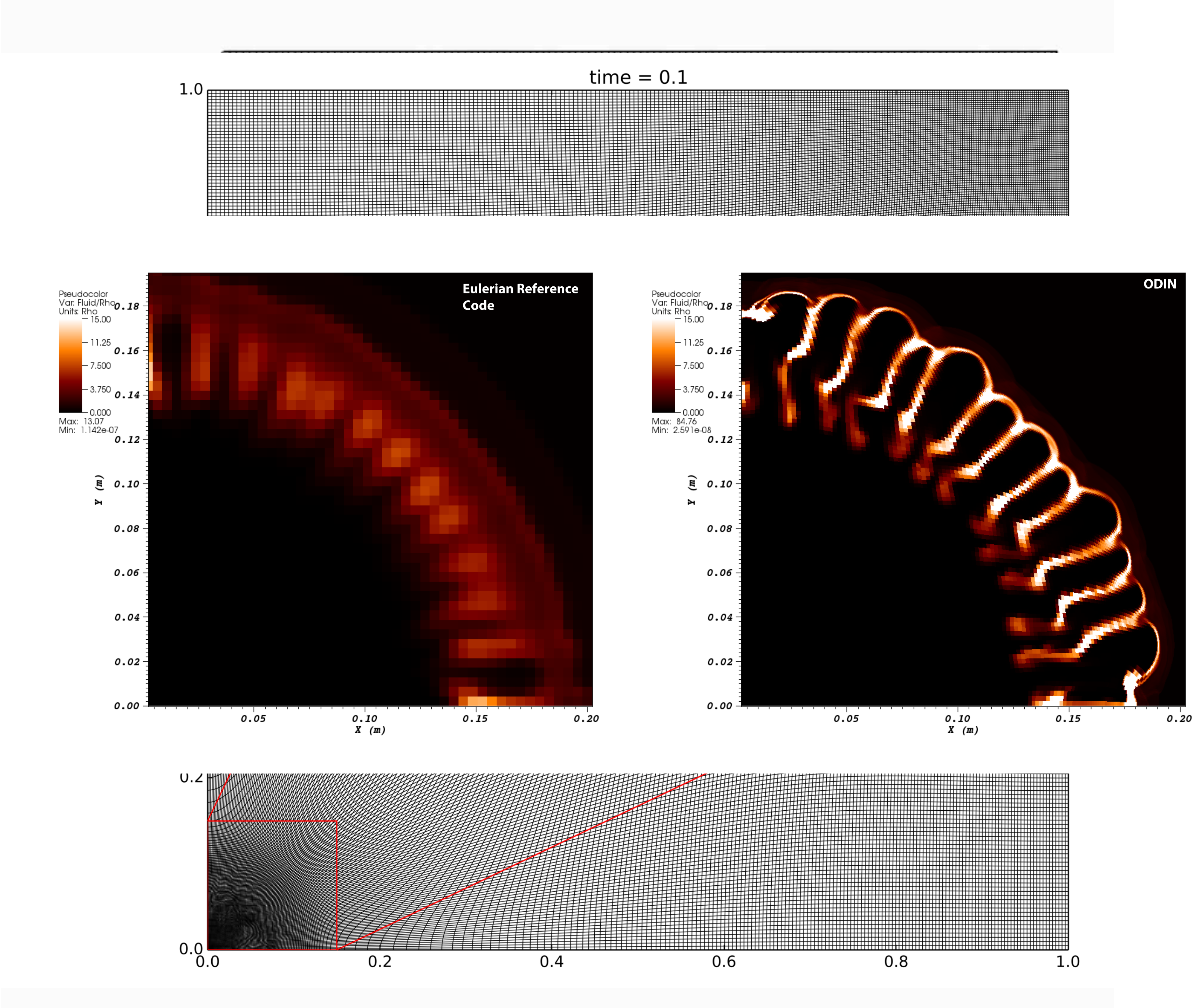


Includes remapping to relaxed grid (Winslow) until core collapse then locked grid

Spherical compression test



Spherical compression test



Ideal MHD in Odin

Lagrangian B-field update

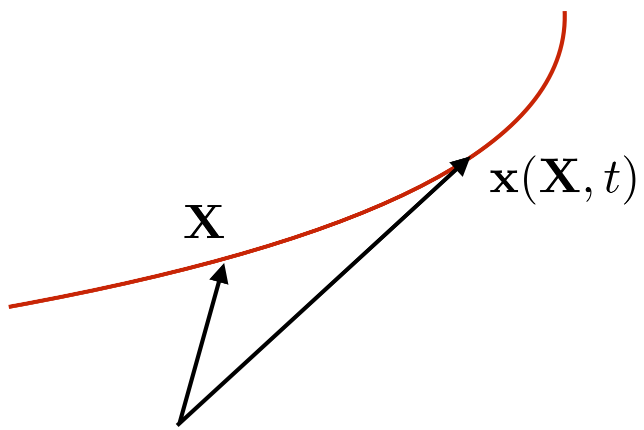
- Adapted from Craig & Sneyd, Astrophysical J., **311,** 1986
- B-field staggered to cell faces to preserve div.B=0 by constrained transport (Evans & Hawley) so really only know fluxes through surfaces, not vector B-field on surface

$$\mathbf{x}(\mathbf{X},0) = \mathbf{X}$$

$$\frac{B_i}{\rho} = \frac{\partial x_i}{\partial X_\alpha}\frac{B_i^0}{\rho_0}$$

$$\frac{\rho_0}{\rho} = \frac{\partial(x_1,x_2,x_3)}{\partial(X_1,X_2,X_3)} = \Delta_0$$

$$B_i = \frac{\partial x_i}{\partial X_\alpha}\frac{B_\alpha^0}{\Delta_0}$$



Use Cauchy solution to update cell-centred B-field using but initial X-grid may not be uniform

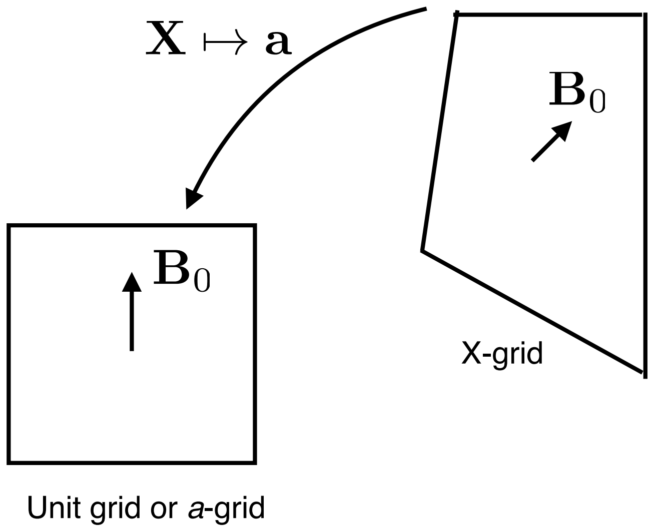
Ideal MHD in Odin

The pre-initial B-field

- If initial grid not coordinate aligned above scheme inconvenient
- Transform initial conditions back on to unit grid, the *a-grid*

$$B_i = \frac{\partial x_i}{\partial a_\alpha} \frac{\bar{B}^0_\alpha}{\Delta}$$

$$\bar{B}_i = B^0_\alpha \frac{\partial a_i}{\partial X_\alpha} \frac{\partial(X_1, X_2, X_3)}{\partial(a_1, a_2, a_3)}$$



Orszag-Tang Vortex

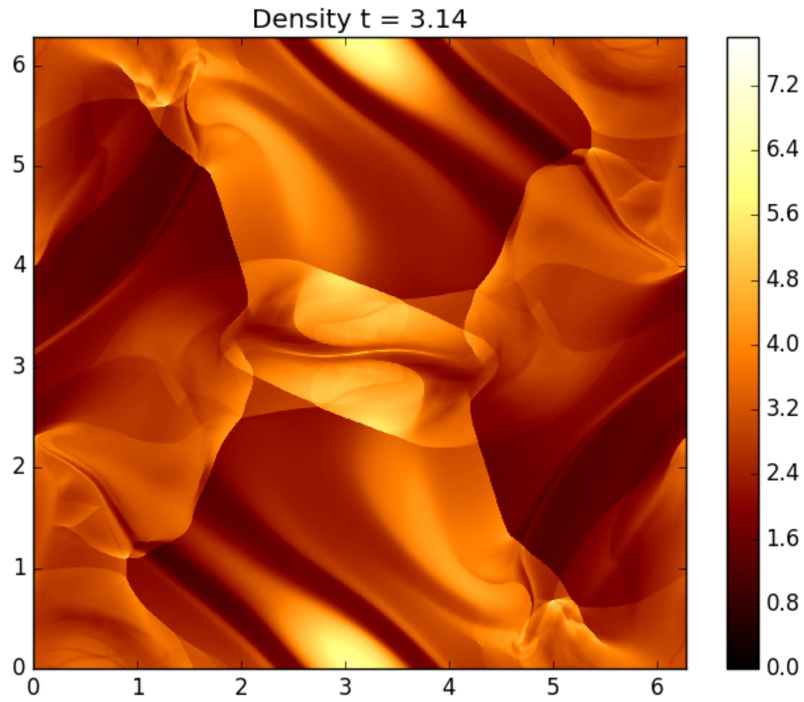
Problem Definition

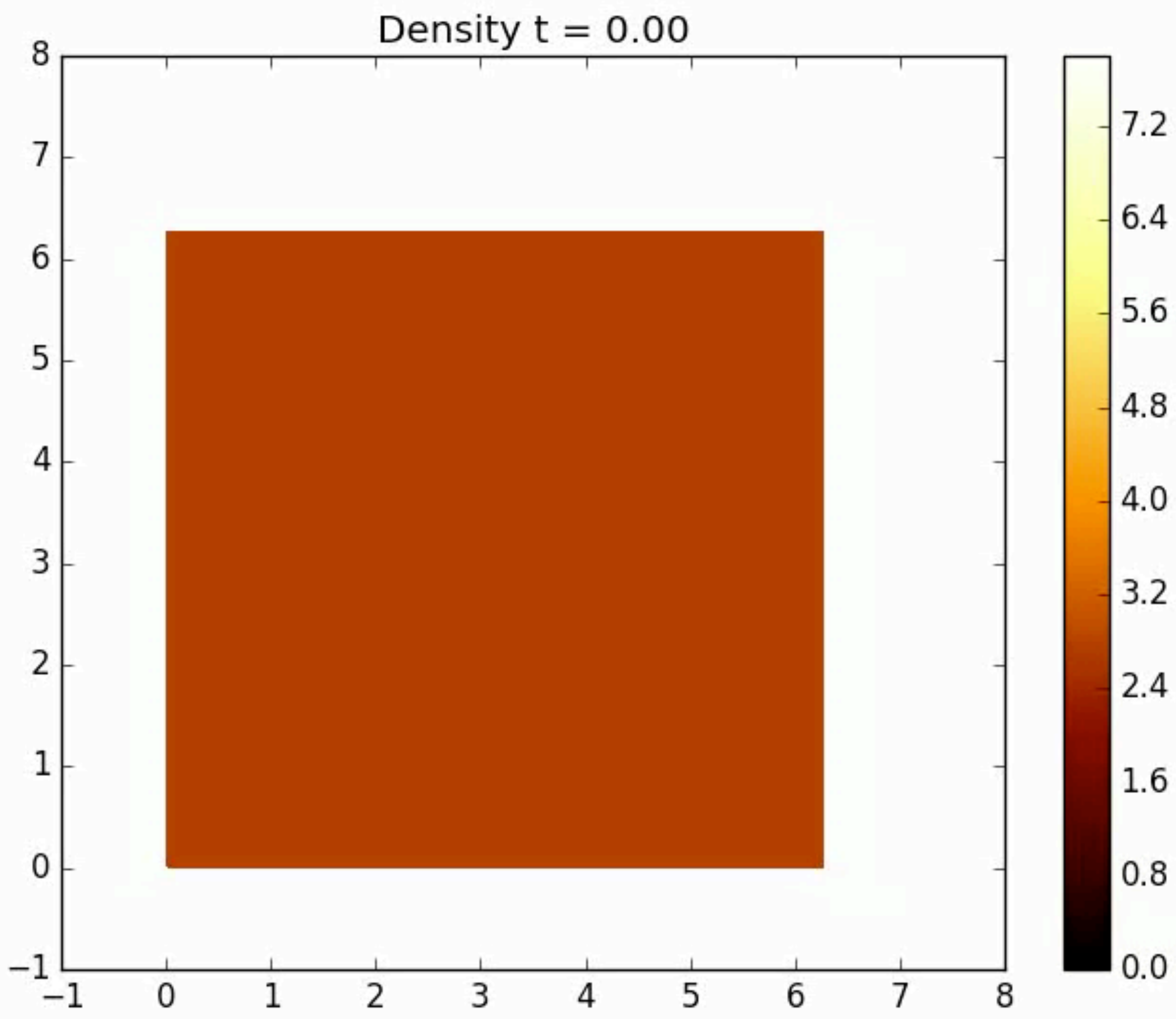
$$\rho = 1.0 \; p = \frac{5}{3}$$

$$v_x = -\sin y \qquad v_y = \sin x$$

$$B_x = -\sin y \qquad B_y = \sin 2x$$

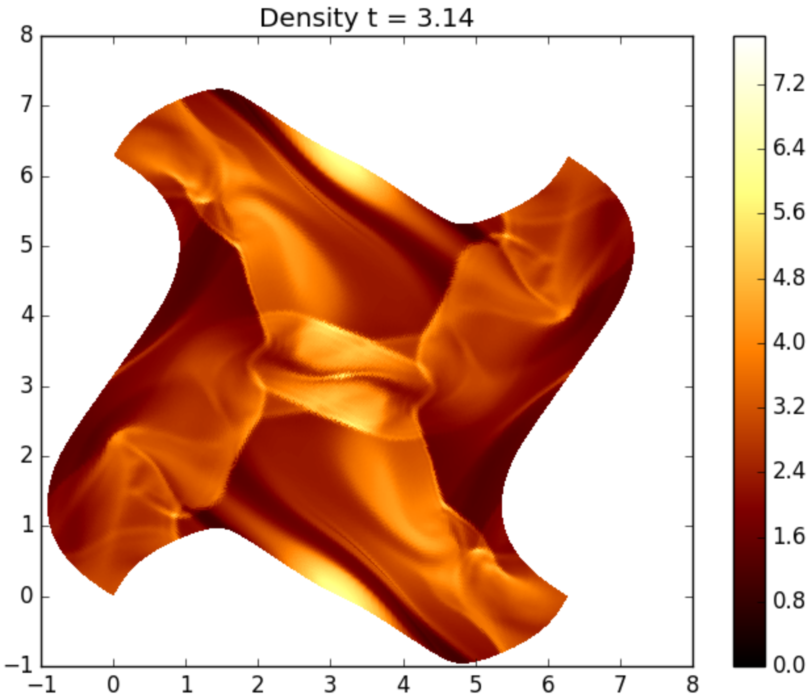
Run Lagrangian Mode until t=1.0. Then lock grid, and run Eulerian until t=3.14

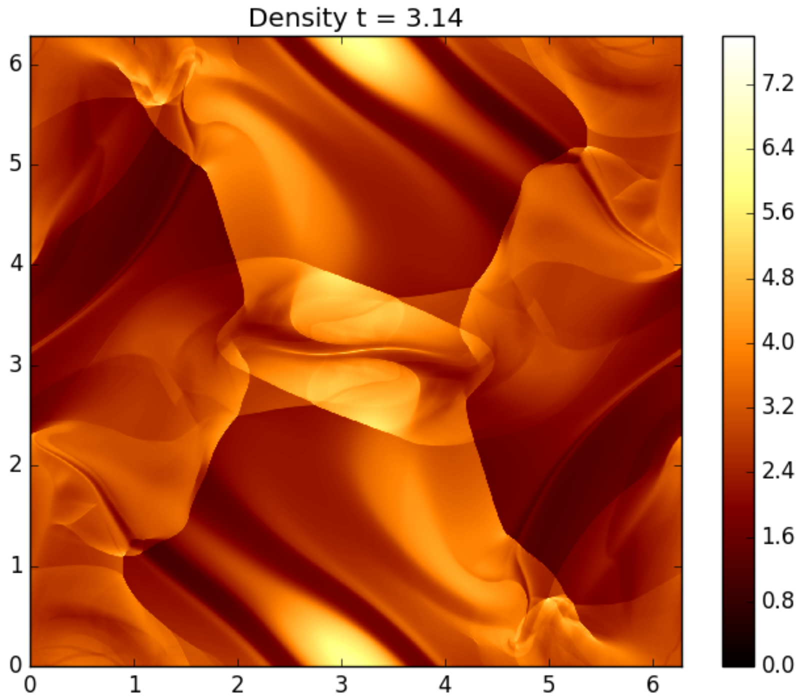




Density t = 0.00
8
7
6
5
4
3
2
1
0
−1
−1
0
1
2
3
4
5
6
7
8
7.2
6.4
5.6
4.8
4.0
3.2
2.4
1.6
0.8
0.0

Orszag-Tang





Density at t=3.14 for ALE Orszag-Tang vortex.

Density at t=3.14 for 1600^2 LARE2D calculation.

Odin with 256^2 grid

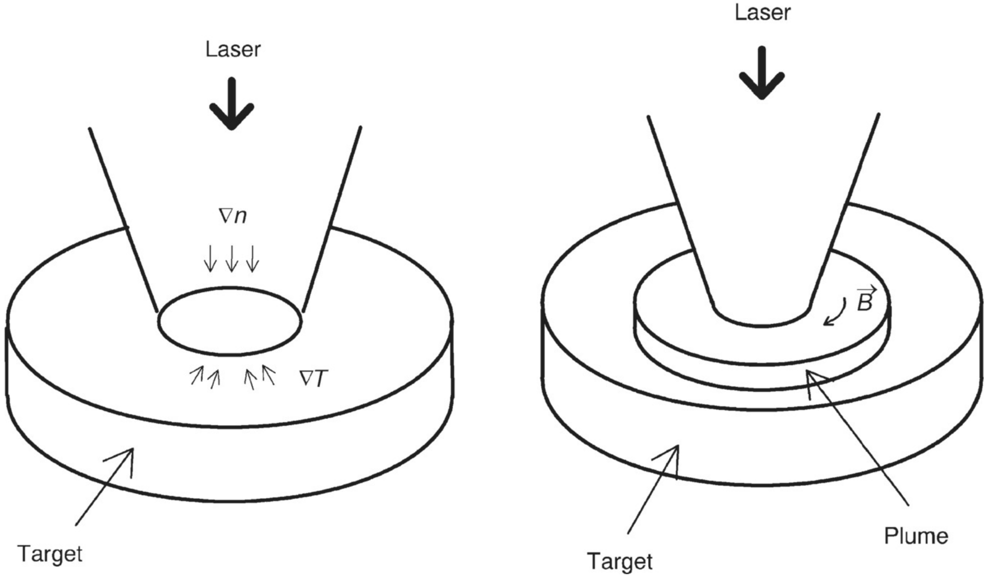
Biermann battery field generation

Pressure term in generalised Ohm's Law

$$\mathbf{E} + \mathbf{v} \times \mathbf{B} = \eta \mathbf{j} - \frac{1}{en_e} \nabla P_e$$

Combines with Faraday's law to give

$$\frac{\partial \mathbf{B}}{\partial t} = \nabla \times \left(\frac{1}{en_e} \nabla P_e \right) = - \frac{\nabla n_e \times \nabla k_B T_e}{en_e}$$



$$\boxed{\frac{\partial \mathbf{B}}{\partial t} = \nabla \times \left(\frac{k_b T_e}{e} \nabla \ln n_e \right)}$$

[1] C.K. Li *et al.*, Phys. Rev. Lett **102** (2009)
[2] G. Gregori *et al.*, Nature **481** (2012)
[3] L. Biermann, Z. Naturforsch **5** (1950)

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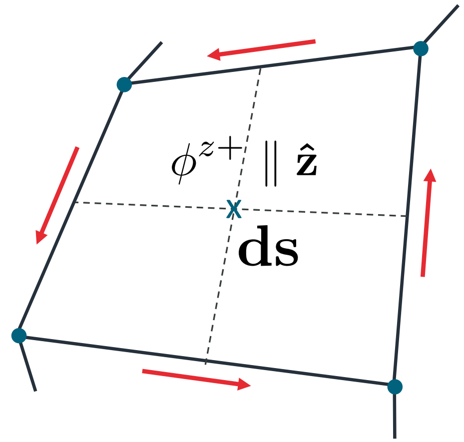
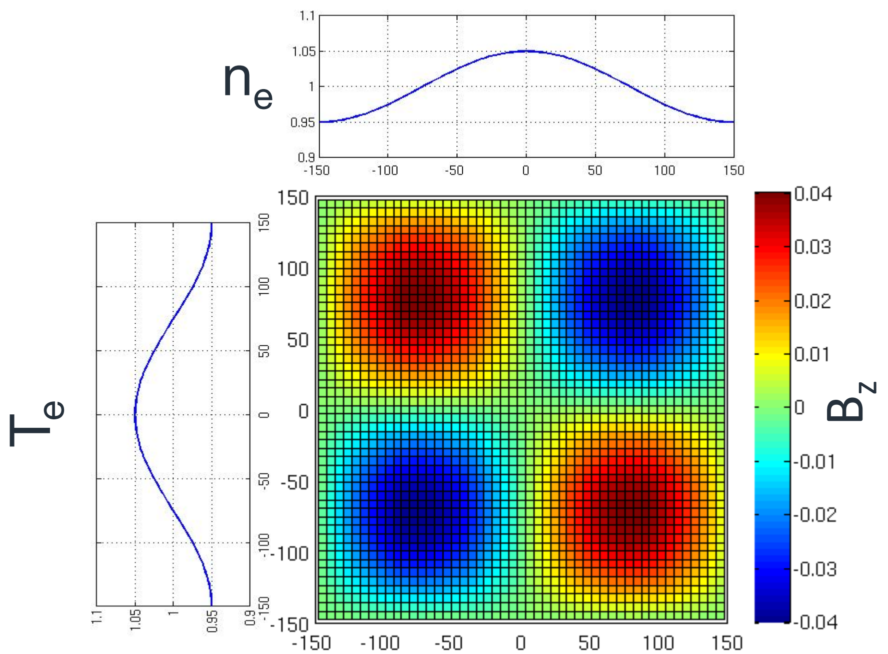
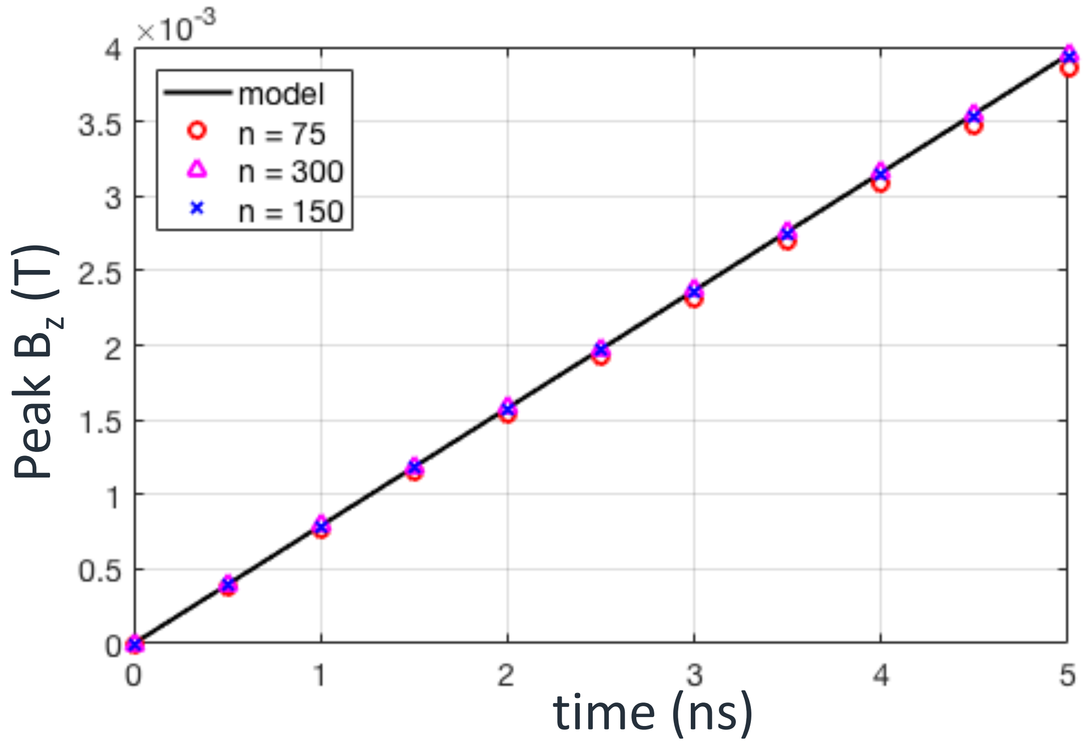
Biermann battery - implementation

- B-fields in Odin defined as fluxes ⊥ to cell faces
- Field generation in z-direction only
- Update total cell fluxes via line integrals



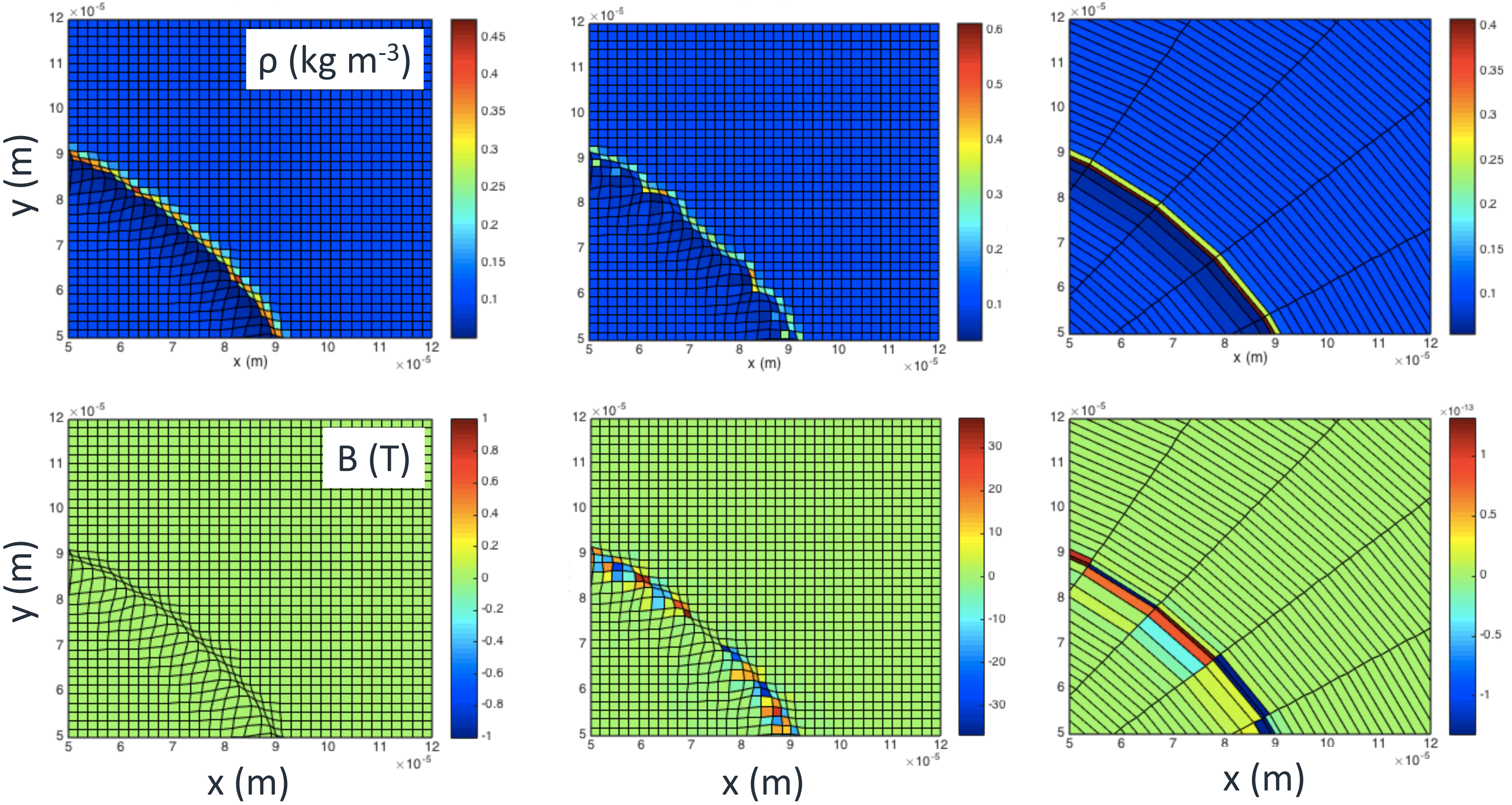
$$\frac{\partial}{\partial t}\int_S \mathbf{B}\cdot\mathbf{ds} = \oint_C \left(\frac{k_B T_e}{e}\nabla \ln n_e\right)\cdot\mathbf{dl}$$





Biermann battery – catastrophe

Biermann : OFF	Biermann : ON	Biermann : ON
(x, y) grid	(x, y) grid	(r, θ) grid



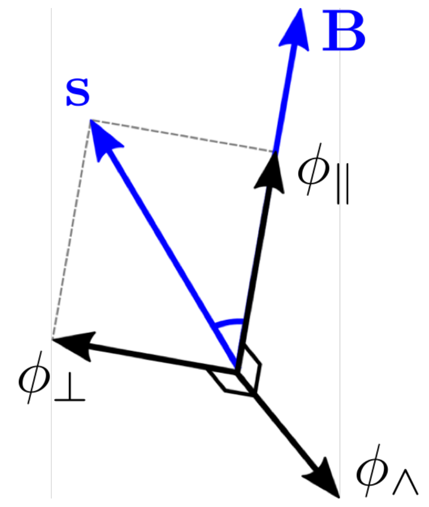
Maximum B ≈ 40 T

Maximum B ≈ 10^{-13} T

Thermal conduction with B-fields

- Temperature governed by diffusion equation

$$\rho \frac{\partial U}{\partial t} = -\nabla \cdot \mathbf{q}$$



- Anisotropic heat-flow (in presence of B-field)

$$\kappa = f(\omega\tau)$$

$$\mathbf{q} = -\underline{\underline{\kappa}} \cdot \nabla T$$

$$\mathbf{q} = \underbrace{-\kappa_{||}\mathbf{b}\left(\mathbf{b} \cdot \nabla T\right)}_{\mathbf{q}_{||}} \underbrace{- \kappa_{\perp}\left(\mathbf{b} \times \left[\nabla T \times \mathbf{b}\right]\right)}_{\mathbf{q}_{\perp}} \underbrace{- \kappa_{\wedge}\mathbf{b} \times \nabla T}_{\mathbf{q}_{\wedge}}$$

Parallel — Perpendicular — Righi-Leduc

[1] E.M. Epperlein & M.G. Haines, Phys. Fluids **29** (1986)

[2] S.I. Braginskii, Rev. Plas. Phys. **1** (1965)

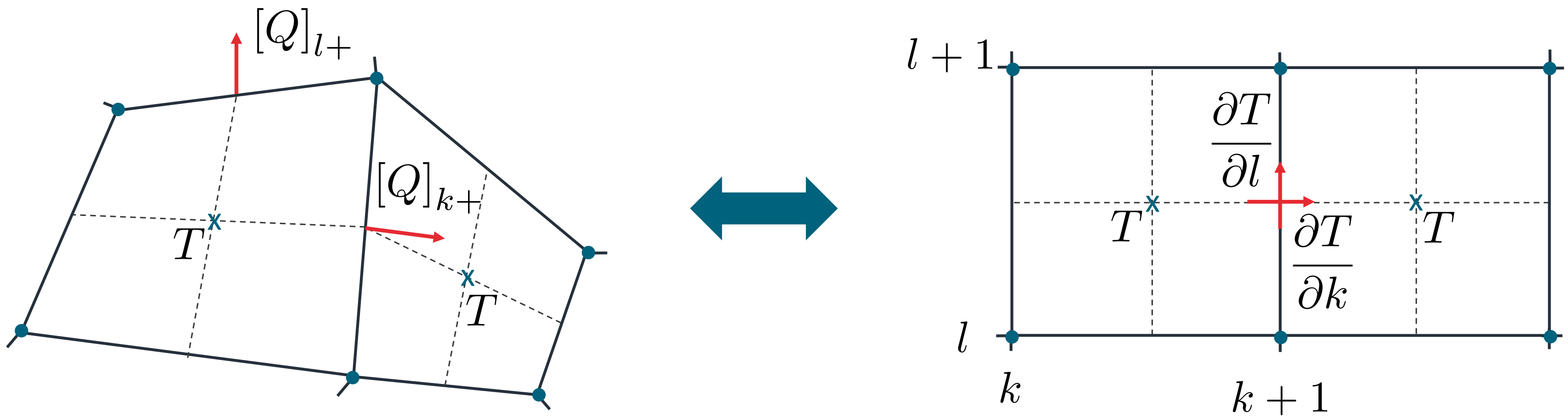
[3] C.A. Walsh *et al.*, Phys. Rev. Lett. **118** (2017)

Isotropic thermal conduction in Odin

- Take control volume integral + divergence theorem

$$\frac{\partial}{\partial t}\int_V \rho U \, dV = -\oint_S \mathbf{q}\cdot\mathbf{dS}$$

- Implement gradients on index grid due to distorted mesh



Total heat-fluxes

$$\begin{cases} [Q]_{k+} = -\frac{\kappa_\perp}{J}\left\{\left(\frac{\partial T}{\partial k}\right)|\mathbf{r}_l|^2 - \left(\frac{\partial T}{\partial l}\right)\mathbf{r}_k\cdot\mathbf{r}_l\right\} \\ [Q]_{l+} = -\frac{\kappa_\perp}{J}\left\{\left(\frac{\partial T}{\partial l}\right)|\mathbf{r}_k|^2 - \left(\frac{\partial T}{\partial k}\right)\mathbf{r}_k\cdot\mathbf{r}_l\right\} \end{cases}$$

[1] G.J. Pert, J. Comp. Phys. **42** (1981)

Anisotropic TC on the ALE grid

- Anisotropic heat-flow derivation based on coordinate transformation approach used by Pert [1]

- Recall $\mathbf{q} = -\kappa \nabla T$ for isotropic heat-flow:

$$[Q]_{k+} = -\frac{\kappa_\perp}{J}\left\{\left(\frac{\partial T}{\partial k}\right)|\mathbf{r}_l|^2 - \left(\frac{\partial T}{\partial l}\right)\mathbf{r}_k \cdot \mathbf{r}_l\right\}$$

- Anisotropic TC yields $\mathbf{q}_{\|}, \mathbf{q}_\perp, \mathbf{q}_\wedge$ components

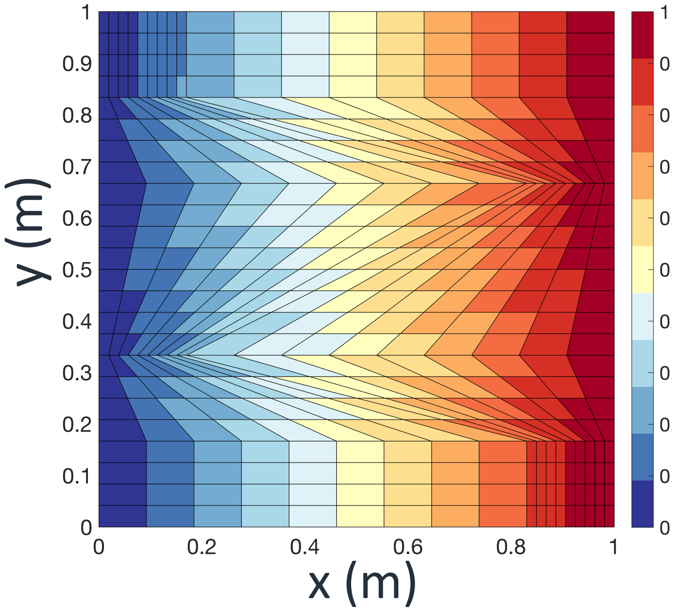
$$\begin{cases} [Q_{\|}]_{k+} = -\frac{\kappa_{\|}}{J}\left\{\left(\frac{\partial T}{\partial k}\right)|\mathbf{b}\times\mathbf{r}_l|^2 - \left(\frac{\partial T}{\partial l}\right)[(\mathbf{b}\times\mathbf{r}_l)\cdot(\mathbf{b}\times\mathbf{r}_k)]\right\} \\ [Q_\perp]_{k+} = -\frac{\kappa_\perp}{J}\left\{\left(\frac{\partial T}{\partial k}\right)\left[|\mathbf{r}_l|^2 - |\mathbf{b}\times\mathbf{r}_l|^2\right] - \left(\frac{\partial T}{\partial l}\right)[\mathbf{r}_k\cdot\mathbf{r}_l - (\mathbf{b}\times\mathbf{r}_l)\cdot(\mathbf{b}\times\mathbf{r}_k)]\right\} \\ [Q_\wedge]_{k+} = +\frac{\kappa_\wedge}{J} b_z J\left(\frac{\partial T}{\partial l}\right) \end{cases}$$

[1] G.J. Pert, J. Comp. Phys. **42** (1981)

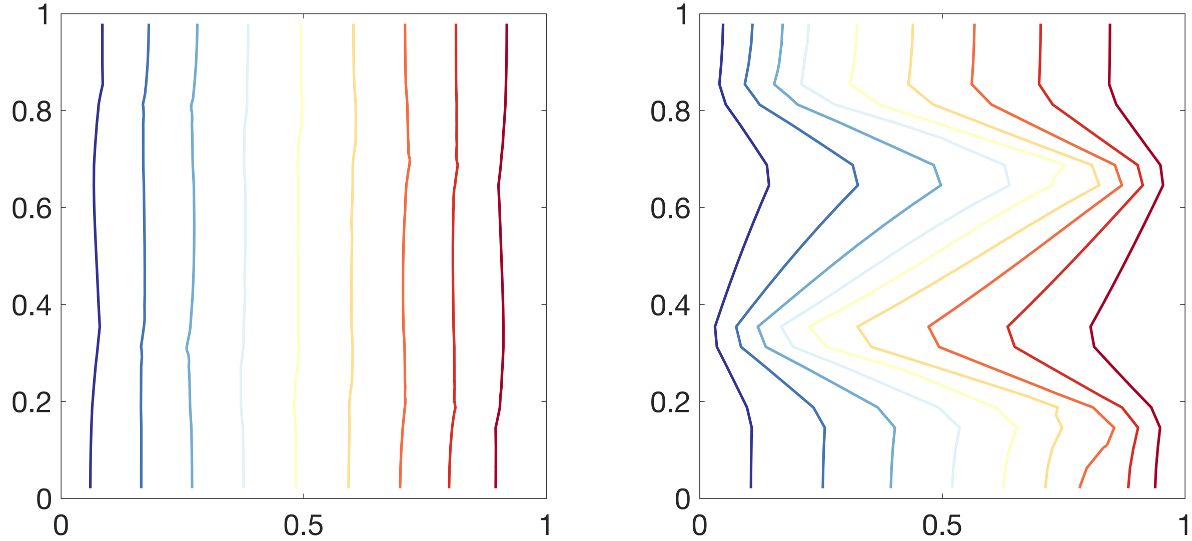
Conduction testing – Kershaw grid

- Test heat-flow on the Kershaw [1] grid - strongly distorted
- Expect linear T_e gradient in x-direction

Temperature (eV)



T_e isotherms



9-point stencil　　5-point stencil

- Standard '5-point' spatial stencil leaves strong grid imprint
- Full ('9-point') stencil required to produce correct isotherms

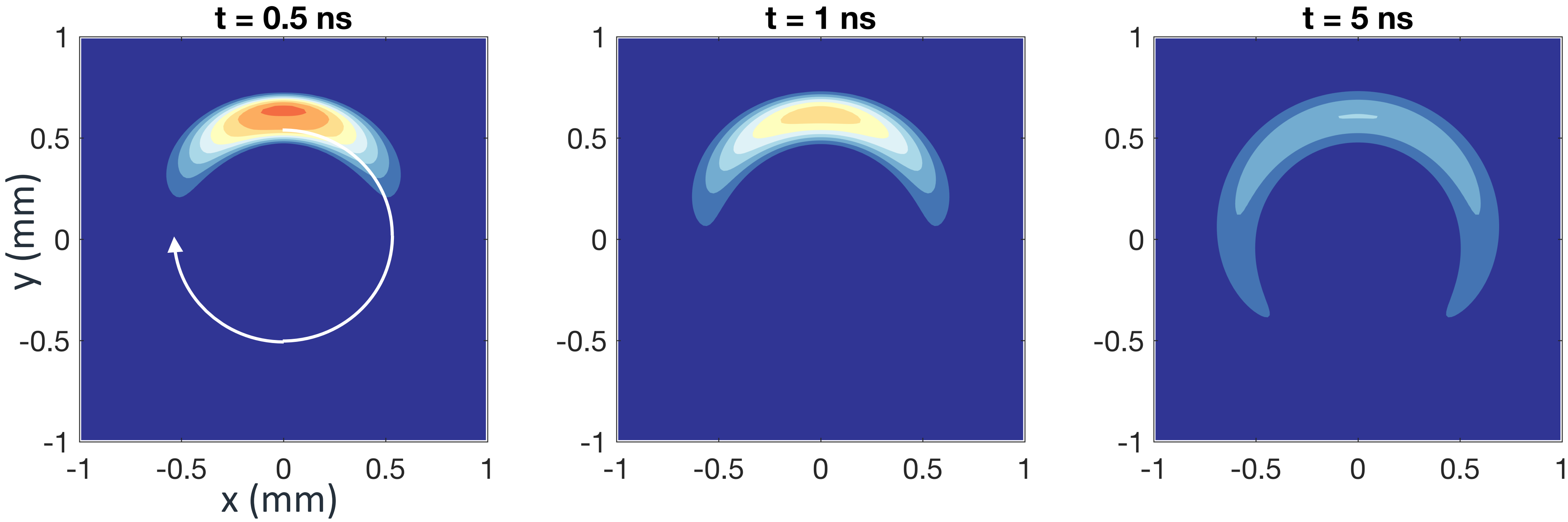
[1] D. Kershaw, J. Comp. Phys. **39** (1981)

Conduction testing – Parrish & Stone test

- Heat-pulse annulus in circular B-field profile

$$T(r,\theta)\begin{cases} T^* \text{ when } (0.5 \le r \le 0.7), \left(\frac{11\pi}{12} \le \theta \le \frac{13\pi}{12}\right) \\ \text{else } T_0 \end{cases}$$

$$B_0 = 100\,T$$
$$T_0 = 100\,eV$$
$$T^* = 120\,eV$$



- Super time-stepping [2] stages limited to ~ 25

[1] I. Parrish & J. Stone, Astro. J. **633** (2005)

[2] C.D. Meyer, Mon. Not. R. Astro. Soc. 422 (2012)

Extended MHD effects

- Odin core code uses ideal MHD
- Generalised Ohm's law

$$en_e\left(\mathbf{E}+\mathbf{C}\times\mathbf{B}\right)=-\nabla P_e+\mathbf{j}\times\mathbf{B}+\frac{m_e}{e\tau}\underline{\underline{\alpha}}^c\cdot\mathbf{j}-n_e\underline{\underline{\beta}}^c\cdot\nabla T_e$$

frozen-in flow resistivity thermoelectric

- Scalar resistive diffusion

$$\frac{\partial\mathbf{B}}{\partial t}=\nabla\times[\eta\mathbf{j}]$$

- Nernst advection – B-fields advect with electron heat-flow

$$\frac{\partial\mathbf{B}}{\partial t}=-\nabla\times\left(\frac{\beta_\wedge}{e|B|}\nabla T_e\times\mathbf{B}\right)=\nabla\times\left(\mathbf{v}_{\mathrm{N}}\times\mathbf{B}\right)$$

[6] E.M. Epperlein & M.G. Haines, J. Phys. D **17** (1984)

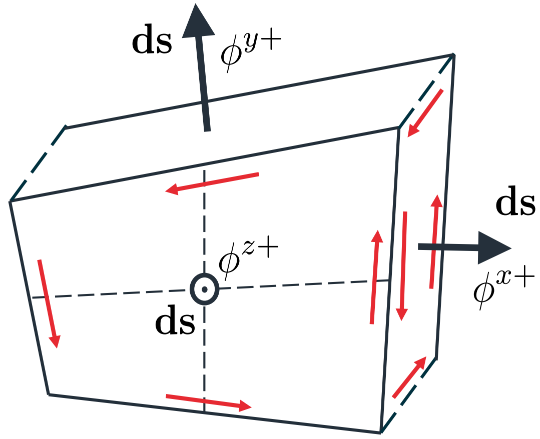
[7] S.I. Braginskii., Rev. Plas. Phys. **1** (1965)

Scalar resistive diffusion testing

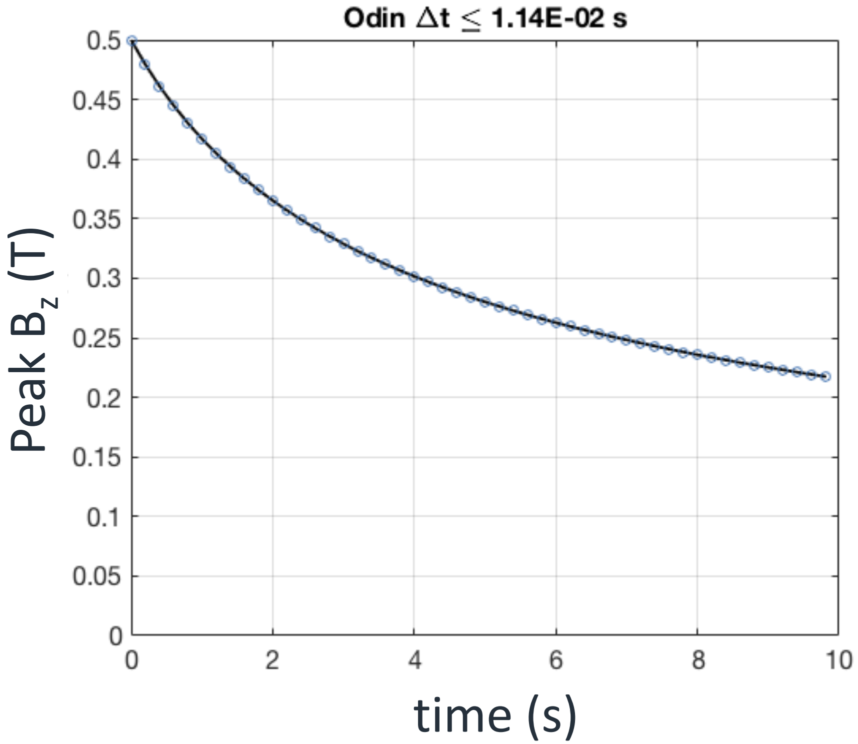
- Calculate B-field fluxes

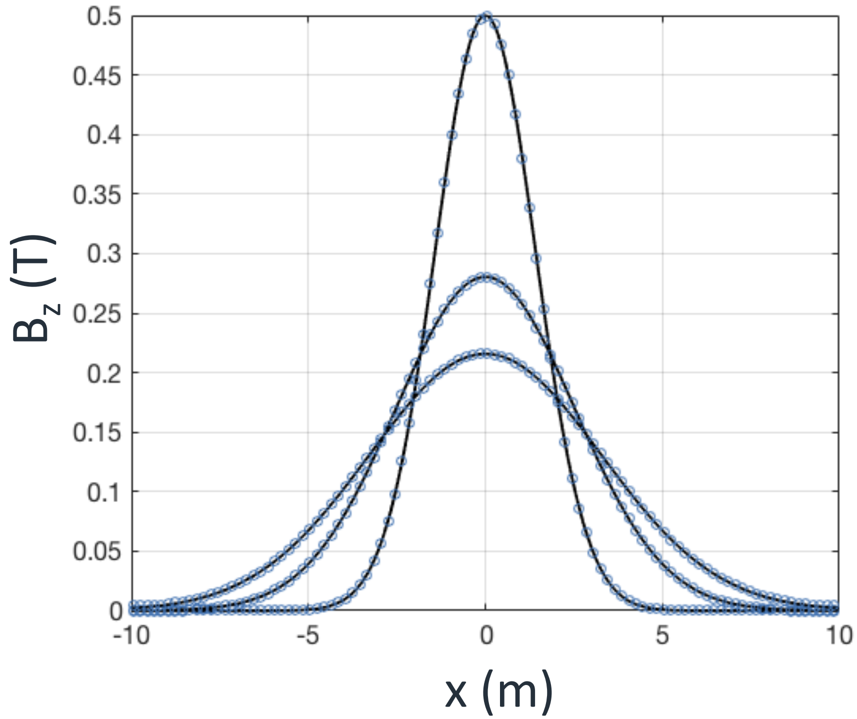
$$\frac{\partial}{\partial t}\int_S \mathbf{B}\cdot\mathbf{ds} = -\frac{m_e}{e^2}\oint_C\left(\frac{\alpha_\perp^c}{\tau n_e}\mathbf{j}\right)\cdot\mathbf{dl}$$

$$\mathbf{j} = \frac{\nabla\times\mathbf{B}}{\mu_0}$$



- Test: decay of a Gaussian B-field perturbation





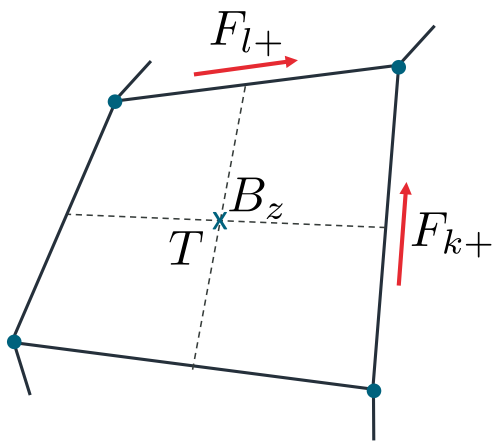
Nernst advection implementation

- B-field fluxes by surface integral

$$\frac{\partial}{\partial t}\int \mathbf{B}\cdot\mathbf{dS} = -\frac{1}{e}\oint\left(\beta_\wedge \nabla T\times\hat{\mathbf{b}}\right)\cdot\mathbf{dl}$$

$$\frac{\partial}{\partial t}\phi_z = -\frac{1}{e}\left\{F_{K+} - F_{L+} - F_{K-} + F_{L-}\right\}$$

$$\begin{cases} F_{K+} = \int_{K_+\,\mathrm{edge}} \beta_\wedge \nabla T\times\hat{\mathbf{b}}\cdot\mathbf{dl} \\ F_{L+} = \int_{L_+\,\mathrm{edge}} \beta_\wedge \nabla T\times\hat{\mathbf{b}}\cdot\mathbf{dl} \end{cases}$$



- Use 9-point stencil as with heat-flow calculation

$$F_{K+} = \frac{\beta_\wedge b_z}{J}\left(\mathbf{r}_K\cdot\mathbf{r}_L\frac{\partial T}{\partial L} - \mathbf{r}_L\cdot\mathbf{r}_L\frac{\partial T}{\partial K}\right)$$

$$F_{L+} = \frac{\beta_\wedge b_z}{J}\left(\mathbf{r}_K\cdot\mathbf{r}_K\frac{\partial T}{\partial L} - \mathbf{r}_K\cdot\mathbf{r}_L\frac{\partial T}{\partial K}\right)$$

Current status of Odin

- Ideal MHD Lagrangian step with arbitrary remap to smoothed grid (ALE-MHD)
- x-y or r-z 2D geometry
- Laser-ray tracing package
- Anisotropic thermal conduction for long mean-free-path
- Multi-group radiation transport
- Multi-material interface reconstruction on remapping
- Arbitrary EOS currently SESEME or FEOS
- Non-ideal MHD includes
  - Biermann battery term
  - Resistivity
  - Nernst field advection

Aim is for full simulations of laser-driven fusion experiments by the end of 2018 and then released as a ‘service’ from mid-2019

THE UNIVERSITY OF WARWICK

Thank you for listening