A Parallel 3D MHD code for core collapse supernova

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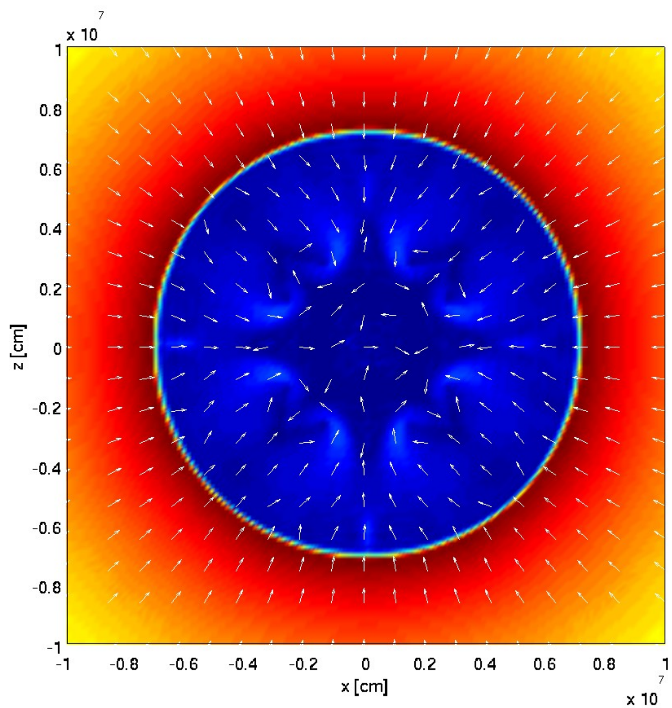

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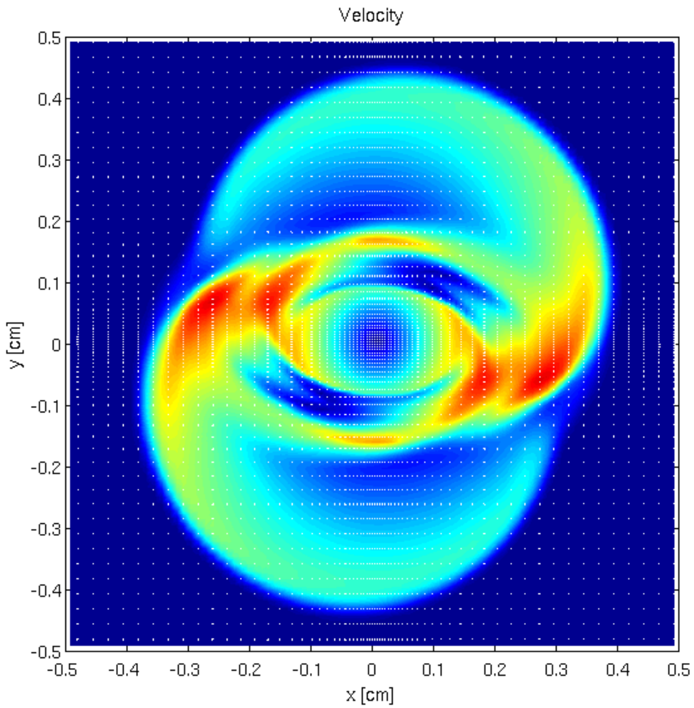

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Outline

Numerical Algorithms

i) Astrophysical motivation

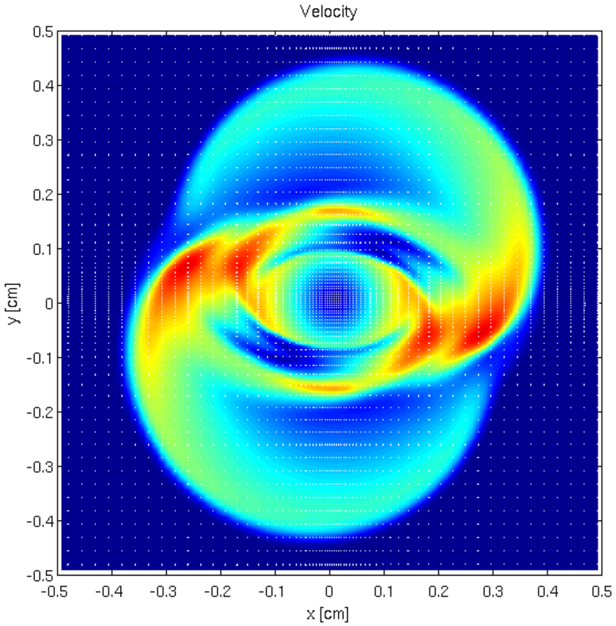
ii)Solving the MHD equations

iii)Keeping $\nabla \cdot \boldsymbol{b} = 0$

iv)Including gravity

v)Adapting the mesh

vi)Parallelization



Motivation

- Large class of astrophysical problems involve collisional systems where the mean free path is much smaller than all length scales of interest

$\Longrightarrow$ Can adopt a fluid description of matter

- Simplest case: single, ideal, non-magnetic fluid
- Next step: include magnetic fields

The MHD equations

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho v_i}{\partial x_i} = 0$$ Mass

$$\frac{\partial (\rho v_i)}{\partial t} + \frac{\partial}{\partial x_j}\left(\rho v_i v_j + P_* I_{ij} - b_i b_j\right) = \boxed{\rho \frac{\partial \phi}{\partial x_i}}$$ Momentum

$$\frac{\partial E}{\partial t} + \frac{\partial}{\partial x_j}\left[\left(E + P_*\right) v_j - v_i b_i b_j\right] = \boxed{\rho v_i \frac{\partial \phi}{\partial x_i}}$$ Energy

$$\left(\boldsymbol{b} = \frac{\boldsymbol{B}}{\sqrt{4\pi}} \right)$$

Magnetic flux $$\frac{\partial b_i}{\partial t} = \frac{\partial}{\partial x_j}\left(v_i b_j - v_j b_i\right)$$

No monopoles $$\boldsymbol{\nabla} \cdot \boldsymbol{b} = 0$$

$$E = \frac{1}{2}\rho v^2 + e + \frac{b^2}{2} \qquad P_* = p + \frac{b^2}{2}$$

EoS: $p = p(\rho, e, \ldots)$

The MHD equations (2)

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho v_i}{\partial x_i} = 0$$ Mass

$$\frac{\partial (\rho v_i)}{\partial t} + \frac{\partial}{\partial x_j} \left(\rho v_i v_j + P_* I_{ij} - b_i b_j \right) = \boxed{\rho \frac{\partial \phi}{\partial x_i}}$$ Momentum

$$\frac{\partial E}{\partial t} + \frac{\partial}{\partial x_j} \Big[\quad \cdots \quad \frac{\partial \phi}{\partial x_i}$$ Energy

$$\nabla^2 \phi = 4\pi G \rho$$

$$\left(\boldsymbol{b} = \frac{\boldsymbol{B}}{\sqrt{4\pi}} \right)$$

Magnetic flux $\quad \frac{\partial b_i}{\partial t} = \frac{\partial}{\partial x_j} (v_i b_j - v_j b_i)$

No monopoles $\quad \boldsymbol{\nabla} \cdot \boldsymbol{b} = 0$

$$E = \frac{1}{2} \rho v^2 + e + \frac{b^2}{2} \qquad P_* = p + \frac{b^2}{2}$$

EoS: $p = p(\rho, e, \ldots)$

Solution Algorithm: An Overview

- Algorithm from Pen et al. 2003, Liebendörfer et al. 2005
- Uses operator splitting:
  - Dimensional splitting: solves eqs in 1D
  - Split hydro and magnetic variables update
- Uses 2nd order TVD finite volume method for hydrodynamic and magnetic variables
- Uses constrained transport for $\nabla \cdot \boldsymbol{b} = 0$
- Correct operator ordering gives 2nd order accuracy in time

Notation

Conserved variables:

$$\boldsymbol{u} = \begin{bmatrix} \rho \\ \rho v_x \\ \rho v_y \\ \rho v_z \\ E \end{bmatrix}$$

Fluxes:

$$\boldsymbol{F} = \begin{bmatrix} \rho v_x \\ \rho v_x^2 + P_* - b_x^2 \\ \rho v_x v_y - b_x b_y \\ \rho v_x v_z - b_x b_z \\ (E + P_*) v_x - b_x \boldsymbol{b} \cdot \boldsymbol{v} \end{bmatrix}$$

$\boldsymbol{G}$ & $\boldsymbol{H}$ analog

Notation (2)

Conserved variables: $$\boldsymbol{u} = \begin{bmatrix} \rho \\ \rho v_x \\ \rho v_y \\ \rho v_z \\ E \end{bmatrix}$$

$$\frac{\partial \boldsymbol{u}}{\partial t} + \frac{\partial \boldsymbol{F}}{\partial x} + \frac{\partial \boldsymbol{G}}{\partial y} + \frac{\partial \boldsymbol{H}}{\partial z} = 0$$

Fluxes: $$\boldsymbol{F} = \begin{bmatrix} \rho v_x \\ \rho v_x^2 + P_* - b_x^2 \\ \rho v_x v_y - b_x b_y \\ \rho v_x v_z - b_x b_z \\ (E + P_*) v_x - b_x \boldsymbol{b} \cdot \boldsymbol{v} \end{bmatrix}$$ $\boldsymbol{G}$ & $\boldsymbol{H}$ analog

Finite Volume Methods Basics

- Use integral form of eqs

$$\frac{\partial \boldsymbol{u}}{\partial t} + \frac{\partial \boldsymbol{F_i}}{\partial x_i} = 0$$

$$\int_{t^0}^{t^1} \mathrm{d}t \iiint_V \mathrm{d}x\, \mathrm{d}y\, \mathrm{d}z$$

$$\iiint_V \boldsymbol{u}(\boldsymbol{x}, t^1)\mathrm{d}V = \iiint_V \boldsymbol{u}(\boldsymbol{x}, t^0)\mathrm{d}V - \int_{t^0}^{t^1} \mathrm{d}t \iint_{\partial V} \boldsymbol{F_i}(\boldsymbol{x}, t) \cdot \mathrm{d}\boldsymbol{S}_i$$

Finite Volume Methods Basics (2)

- Use integral form of eqs

$$\frac{\partial \boldsymbol{u}}{\partial t} + \frac{\partial \boldsymbol{F_i}}{\partial x_i} = 0$$

$$\int_{t^0}^{t^1} \mathrm{d}t \iiint \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z$$

Quantity in volume V changes by fluxes through the boundary ∂V

$$\iiint\limits_V \qquad \iiint\limits_V$$

$$- \int_{t^0}^{t^1} \mathrm{d}t \iint\limits_{\partial V} \boldsymbol{F_i}(\boldsymbol{x}, t) \cdot \mathrm{d}\boldsymbol{S}_i$$

Finite Volume Methods Basics (3)

- Integral form suggests to discretize time into discrete steps Δt and space into finite volumes or cells

$$\begin{aligned}
\boldsymbol{u}_{i,j,k}^{n+1} = \boldsymbol{u}_{i,j,k}^{n} &- \frac{\Delta t}{\Delta x}\left(\boldsymbol{F}_{i+1/2,j,k}^{n} - \boldsymbol{F}_{i-1/2,j,k}^{n}\right) \\
&- \frac{\Delta t}{\Delta y}\left(\boldsymbol{G}_{i,j+1/2,k}^{n} - \boldsymbol{G}_{i,j-1/2,k}^{n}\right) \\
&- \frac{\Delta t}{\Delta z}\left(\boldsymbol{H}_{i,j,k+1/2}^{n} - \boldsymbol{H}_{i,j,k-1/2}^{n}\right)
\end{aligned}$$

Conservative!!!

Finite Volume Methods Basics (4)

- Integral form suggests to discretize time into

Cell indexing	$i,\ j,\ k$
Cell spacings	$\Delta x = x_{i+1/2} - x_{i-1/2} = \mathrm{const.}$ $\Delta y = y_{j+1/2} - y_{j-1/2} = \mathrm{const.}$ $\Delta z = z_{k+1/2} - z_{k-1/2} = \mathrm{const.}$
Cell volume	$V = \Delta x \Delta y \Delta z$
Numerical fluxes	$\boldsymbol{F}^n_{i+1/2,j,k} = \dfrac{1}{\Delta t}\displaystyle\int_{t^n}^{t^{n+1}} \boldsymbol{F}(\boldsymbol{u}(x_{i+1/2},t))\mathrm{dt}$

time average flux per unit area at boundary surface

Cell average of $\boldsymbol{u}$	$\boldsymbol{u}^n_{i,j,k} = \dfrac{1}{V}\displaystyle\int_V \boldsymbol{u}(\boldsymbol{x},t)\mathrm{dV}$

Finite Volume Methods Basics (5)

- Use operator splitting

Dimensional splitting:

$$\mathrm{L_x}: \quad \boldsymbol{u}^{n+1/3}_{i,j,k} = \boldsymbol{u}^{n}_{i,j,k} - \frac{\Delta t}{\Delta x}\left(\boldsymbol{F}^{n}_{i+1/2,j,k} - \boldsymbol{F}^{n}_{i-1/2,j,k}\right)$$

$$\mathrm{L_y}: \quad \boldsymbol{u}^{n+2/3}_{i,j,k} = \boldsymbol{u}^{n+1/3}_{i,j,k} - \frac{\Delta t}{\Delta y}\left(\boldsymbol{G}^{n+1/3}_{i,j+1/2,k} - \boldsymbol{G}^{n+1/3}_{i,j-1/2,k}\right)$$

$$\mathrm{L_z}: \quad \boldsymbol{u}^{n+1}_{i,j,k} = \boldsymbol{u}^{n+2/3}_{i,j,k} - \frac{\Delta t}{\Delta z}\left(\boldsymbol{H}^{n+2/3}_{i,j,k+1/2} - \boldsymbol{H}^{n+2/3}_{i,j,k-1/2}\right)$$

Magnetic field advection

- Operator splitting: solve alternatively for fluid and magnetic variables
- Magnetic field advected with constant velocity field from fluid update
- Additional numerical difficulty:

$$\boldsymbol{\nabla} \cdot \boldsymbol{b} = 0$$

Discuss only constrained transport... other methods projection method, 8-wave formulation
See Tòth 2000

- Magnetic field update also dimensionally split

Constrained transport

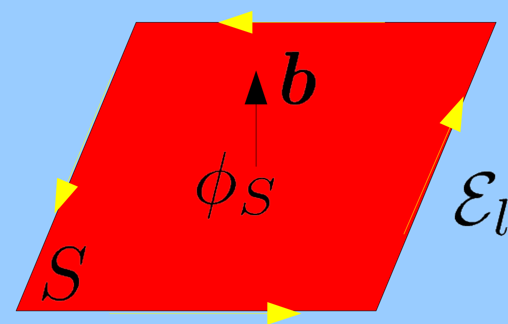
- Evans & Hawley 1988
- First discuss algorithm in general
- Idea: consider integral form of flux conservation equation

$$\frac{\partial}{\partial t}\phi(t) = \frac{\partial}{\partial t}\int_S b_i \mathrm{d}S_i = -\mathcal{E} = -\oint_{\partial S} \epsilon_{ijk} v_j b_k \mathrm{d}x_i$$

Temporal change in magnetic flux equals minus the total EMF around contour of the surface (fixed in space)

Constrained transport (2)

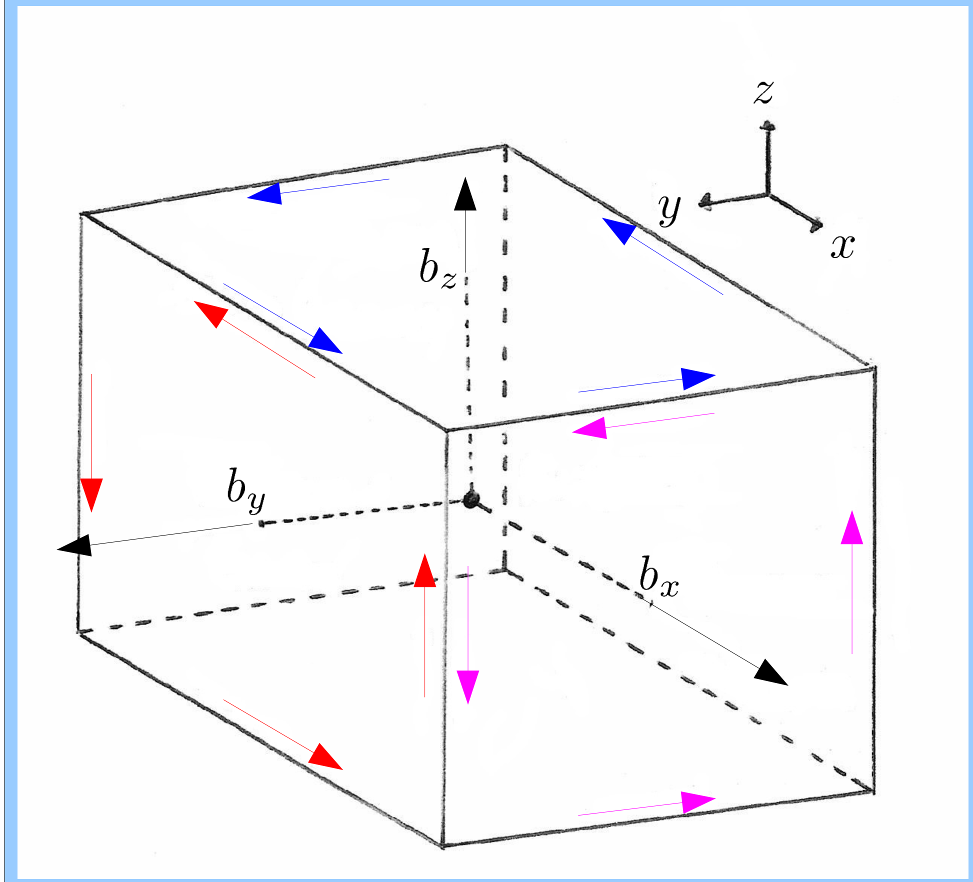
Suggests following discretization:



$$\frac{1}{\Delta t}\left[\phi_S^{n+1} - \phi_S^{n}\right] = -\sum_{l=1}^{4} \mathcal{E}_l$$

$$\boldsymbol{b}^{n+1} = S\phi_S^{n+1}\boldsymbol{n}$$

Constrained transport (3)



For 3D computational cell

- Place magnetic field on cell faces (So-called staggered mesh)
- Compute EMF on cell edges (requires velocity to be interpolated)
- For cell $\nabla \cdot \boldsymbol{b} = 0$ equivalent to

$$\sum_{\text{faces}} \phi_S = 0$$

Constrained transport (4)

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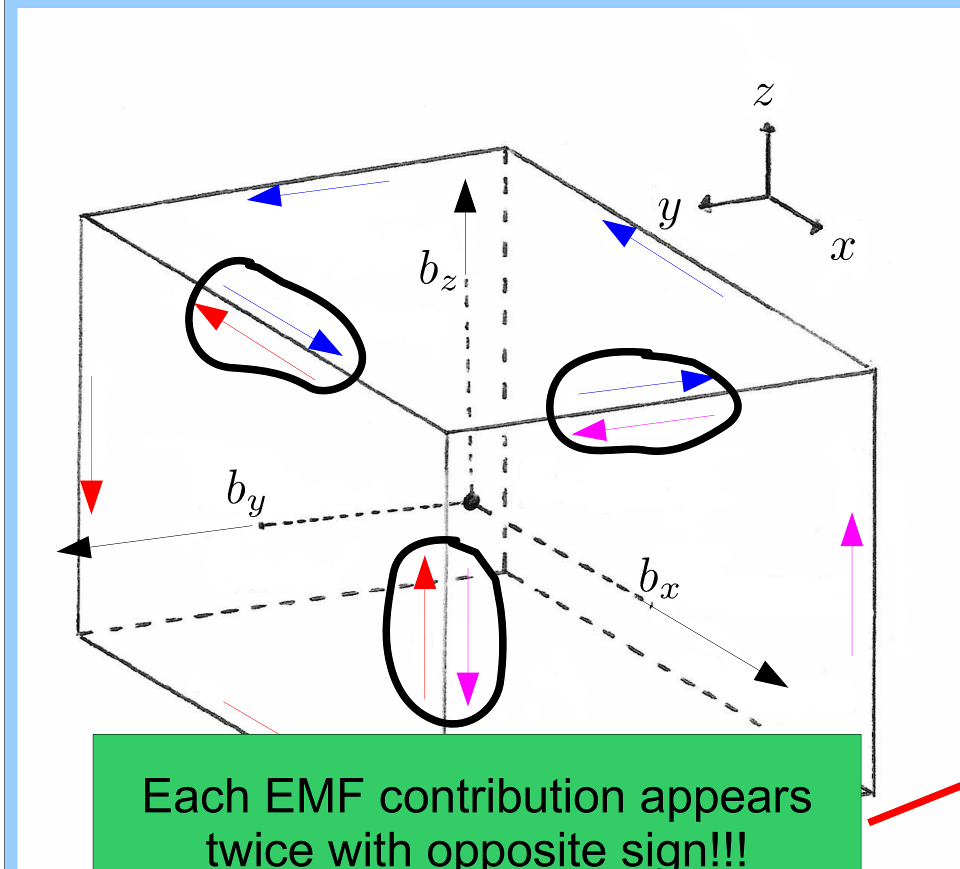


Each EMF contribution appears twice with opposite sign!!!

For 3D computational cell

•Place magnetic field on cell faces (So-called staggered mesh)

•Compute EMF on cell edges (requires velocity to be interpolated)

•For cell $\boldsymbol{\nabla} \cdot \boldsymbol{b} = 0$ equivalent to

$$\sum_{\text{faces}} \phi_S = 0$$

Constrained transport (5)

- Magnetic field equation dimensionally split
- Update by using 2D advection-constraint steps
- Example: b_y along x-direction

$$
\begin{aligned}
(b_x)^{n+1/3}_{i+1/2,j,k} = (b_x)^{n}_{i+1/2,j,k} + \frac{\Delta t}{\Delta y \Delta z} \Big\{ & +\Delta y \left[\overline{v_z}\overline{b_x} - \overline{v_x}\overline{b_z}\right]_{i+1/2,k+1/2} \\
- & \ \Delta y \left[\overline{v_z}\overline{b_x} - \overline{v_x}\overline{b_z}\right]_{i+1/2,k-1/2} \\
- & \ \Delta z \left[\overline{v_x}\overline{b_y} - \overline{v_y}\overline{b_x}\right]_{i+1/2,j+1/2} \\
+ & \ \Delta z \left[\overline{v_x}\overline{b_y} - \overline{v_y}\overline{b_x}\right]_{i+1/2,j-1/2} \Big\}
\end{aligned}
$$

$$
\begin{aligned}
(b_y)^{n+1/3}_{i,j+1/2,k} = (b_y)^{n}_{i,j+1/2,k} + \frac{\Delta t}{\Delta x \Delta z} \Big\{ & -\Delta x \left[\overline{v_y}\overline{b_z} - \overline{v_z}\overline{b_y}\right]_{j+1/2,k+1/2} \\
+ & \ \Delta x \left[\overline{v_y}\overline{b_z} - \overline{v_z}\overline{b_y}\right]_{j+1/2,k-1/2} \\
+ & \ \Delta z \left[\overline{v_x}\overline{b_y} - \overline{v_y}\overline{b_x}\right]_{i+1/2,j+1/2} \\
- & \ \Delta z \left[\overline{v_x}\overline{b_y} - \overline{v_y}\overline{b_x}\right]_{i-1/2,j+1/2} \Big\}
\end{aligned}
$$

Transport terms along x
Use TVD scheme

Constrained transport (6)

- Magnetic field equation dimensionally split
- Update by using 2D advection-constraint steps
- Example: b_y along x-direction

$$
\begin{aligned}
(b_x)^{n+1/3}_{i+1/2,j,k} = (b_x)^{n}_{i+1/2,j,k} + \frac{\Delta t}{\Delta y \Delta z} \Big\{ &+\Delta y \left[\overline{v_z}\,\overline{b_x} - \overline{v_x}\,\overline{b_z}\right]_{i+1/2,k+1/2} \\
&- \Delta y \left[\overline{v_z}\,\overline{b_x} - \overline{v_x}\,\overline{b_z}\right]_{i+1/2,k-1/2} \\
&- \Delta z \left[\overline{v_x}\,\overline{b_y} - \overline{v_y}\,\overline{b_x}\right]_{i+1/2,j+1/2} \\
&+ \Delta z \left[\overline{v_x}\,\overline{b_y} - \overline{v_y}\,\overline{b_x}\right]_{i+1/2,j-1/2} \Big\}
\end{aligned}
$$

Constraint terms along x
Use same flux as for b_y

$$
\begin{aligned}
(b_y)^{n+1/3}_{i,j+1/2,k} = (b_y)^{n}_{i,j+1/2,k} + \frac{\Delta t}{\Delta x \Delta z} \Big\{ &-\Delta x \left[\overline{v_y}\,\overline{b_z} - \overline{v_z}\,\overline{b_y}\right]_{j+1/2,k+1/2} \\
&+ \Delta x \left[\overline{v_y}\,\overline{b_z} - \overline{v_z}\,\overline{b_y}\right]_{j+1/2,k-1/2} \\
&+ \Delta z \left[\overline{v_x}\,\overline{b_y} - \overline{v_y}\,\overline{b_x}\right]_{i+1/2,j+1/2} \\
&- \Delta z \left[\overline{v_x}\,\overline{b_y} - \overline{v_y}\,\overline{b_x}\right]_{i-1/2,j+1/2} \Big\}
\end{aligned}
$$

Transport terms along x
Use TVD scheme

Constraint for $(b_x)_{i-1/2,j,k}$

Constrained transport (7)

- Magnetic field equation dimensionally split
- Update by using 2D advect
- Example: b_y along x-di

$$(b_x)^{n+1/3}_{i+1/2,j,k} = (b_x)^{n}_{i+1/2,j,k}$$

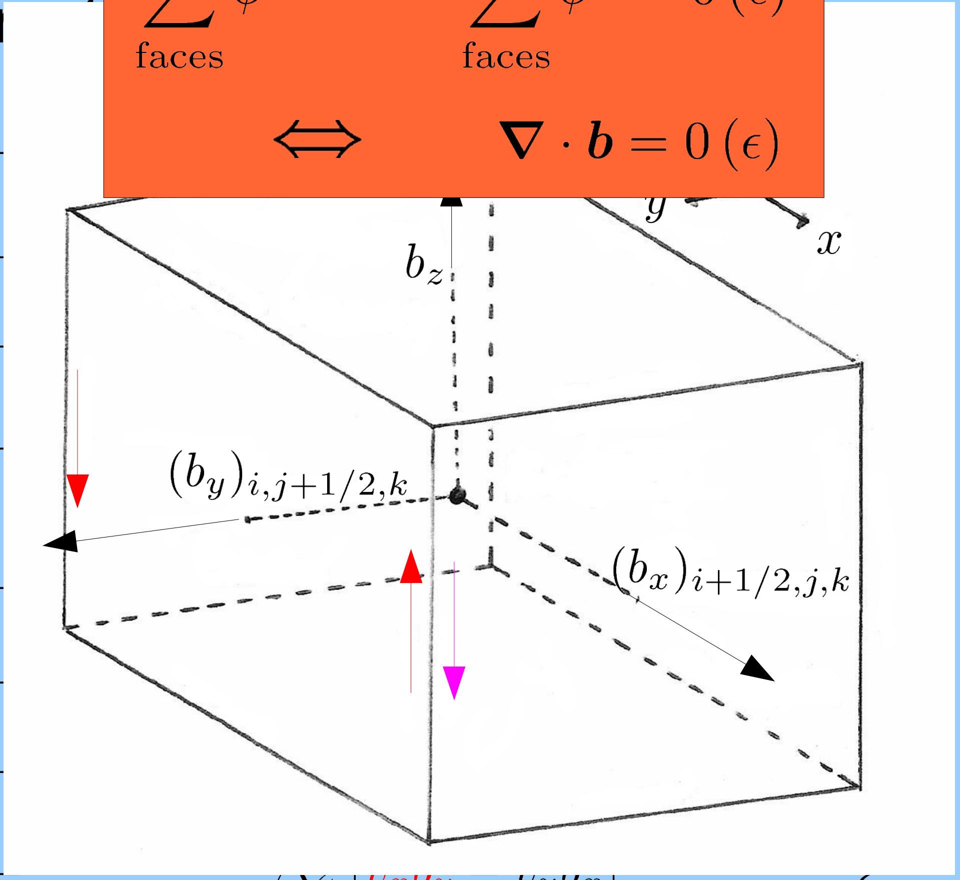
Constraint terms along x
Use same flux as for b_y

$$(b_y)^{n+1/3}_{i,j+1/2,k} = (b_y)^{n}_{i,j+1/2,k}$$

Transport terms along x
Use TVD scheme

$$\sum_{\text{faces}} \phi^{n+1/3} = \sum_{\text{faces}} \phi^{n} = 0\,(\epsilon)$$

$$\Leftrightarrow \quad \nabla \cdot \boldsymbol{b} = 0\,(\epsilon)$$



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Connecting fluid and magnetic update

- Operator splitting used
- Ordering of operators gives 2nd order accuracy in time

Forward sweep

$$L_x^{HD} L_x^b L_y^{HD} L_y^b L_z^{HD} L_z^b \boldsymbol{u}^n = \boldsymbol{u}^{n+1}$$

Backward sweep

$$L_z^{HD} L_z^b L_y^{HD} L_y^b L_x^{HD} L_x^b \boldsymbol{u}^{n+1} = \boldsymbol{u}^{n+2} + O(\Delta t^2)$$

Incorporating gravity

- Fundamental ingredient for astrophysical simulations
- Use operator splitting

$$L^{HD}: \quad \frac{\partial \boldsymbol{u}}{\partial t} + \frac{\partial \boldsymbol{F}}{\partial x} + \frac{\partial \boldsymbol{G}}{\partial y} + \frac{\partial \boldsymbol{H}}{\partial z} = 0$$

$$L^{b}: \quad \frac{\partial b_i}{\partial t} = \frac{\partial}{\partial x_j}\left(v_i b_j - v_j b_i\right)$$

$$G: \quad \frac{\mathrm{d}\boldsymbol{u}}{\mathrm{d}t} = \boldsymbol{S}$$

$$\boldsymbol{S} = \begin{bmatrix} 0 \\ -\rho\partial\phi/\partial x \\ -\rho\partial\phi/\partial y \\ -\rho\partial\phi/\partial z \\ -\rho\boldsymbol{v}\cdot\nabla\phi \end{bmatrix}$$

Simple $\boldsymbol{u}^{n+2} = \boldsymbol{L}GG\boldsymbol{L}\boldsymbol{u}^n$

Incorporating gravity (2)

- Difficulties:

  1) EoS is called with as input the internal energy

$$p = p(\rho, e, ...)$$

The internal energy is computed by subtracting the kinetic and magnetic energies from total energy

$$E = \frac{1}{2}\rho v^2 + e + \frac{b^2}{2}$$

This may lead to negative internal energies and make the code crash!

Weak coupling of gravity to MHD

-

$$\left[\; -\rho \boldsymbol{v} \cdot \nabla \phi \; \right]$$

Incorporating gravity (3)

- Difficulties:

2) Consider a steady flow: $$\frac{\partial \boldsymbol{F}}{\partial x} + \frac{\partial \boldsymbol{G}}{\partial y} + \frac{\partial \boldsymbol{H}}{\partial z} \approx \boldsymbol{S}$$

Both fluxes and source term may be large expression

Very unlikely that potentially large changes in $\boldsymbol{u}$ cancel by the splitting: $\boldsymbol{u}^{n+2} = \boldsymbol{L}\boldsymbol{G}\boldsymbol{G}\boldsymbol{L}\boldsymbol{u}^{n}$

Even if cancellation exact, what about small perturbations in steady flow?

Weak coupling of gravity to MHD

$$-\rho \boldsymbol{v} \cdot \nabla \phi$$

Incorporating gravity (4)

- Improve coupling by
  - Directionally splitting
  - Include half of the gravity before and after a fluid update

$$
\begin{aligned}
G_x/2: &\quad \frac{\mathrm{d}\boldsymbol{u}}{\mathrm{d}t} = \frac{\boldsymbol{S}_x}{2} \\
L_x^{HD}: &\quad \frac{\partial \boldsymbol{u}}{\partial t} + \frac{\partial \boldsymbol{F}}{\partial x} = 0 \\
G_x/2: &\quad \frac{\mathrm{d}\boldsymbol{u}}{\mathrm{d}t} = \frac{\boldsymbol{S}_x}{2}
\end{aligned}
\qquad
\boldsymbol{S}_x = \begin{bmatrix} 0 \\ -\rho\partial\phi/\partial x \\ 0 \\ 0 \\ -\rho v_x \partial\phi/\partial x \end{bmatrix}
$$

Incorporating gravity (5)

- Further problem:
  - The gradients induced in $\boldsymbol{u}$ by gravitation may be wrongly interpreted as part of a propagating wave during the fluid update (flux limiters!)

Subtract hydrostatic equilibrium gradients in flux construction

Zingale et al. 2002, similar but only PPM

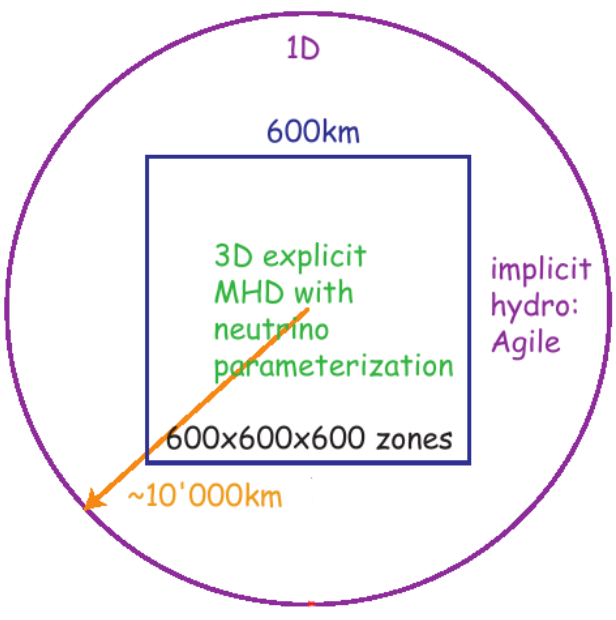
Assuming

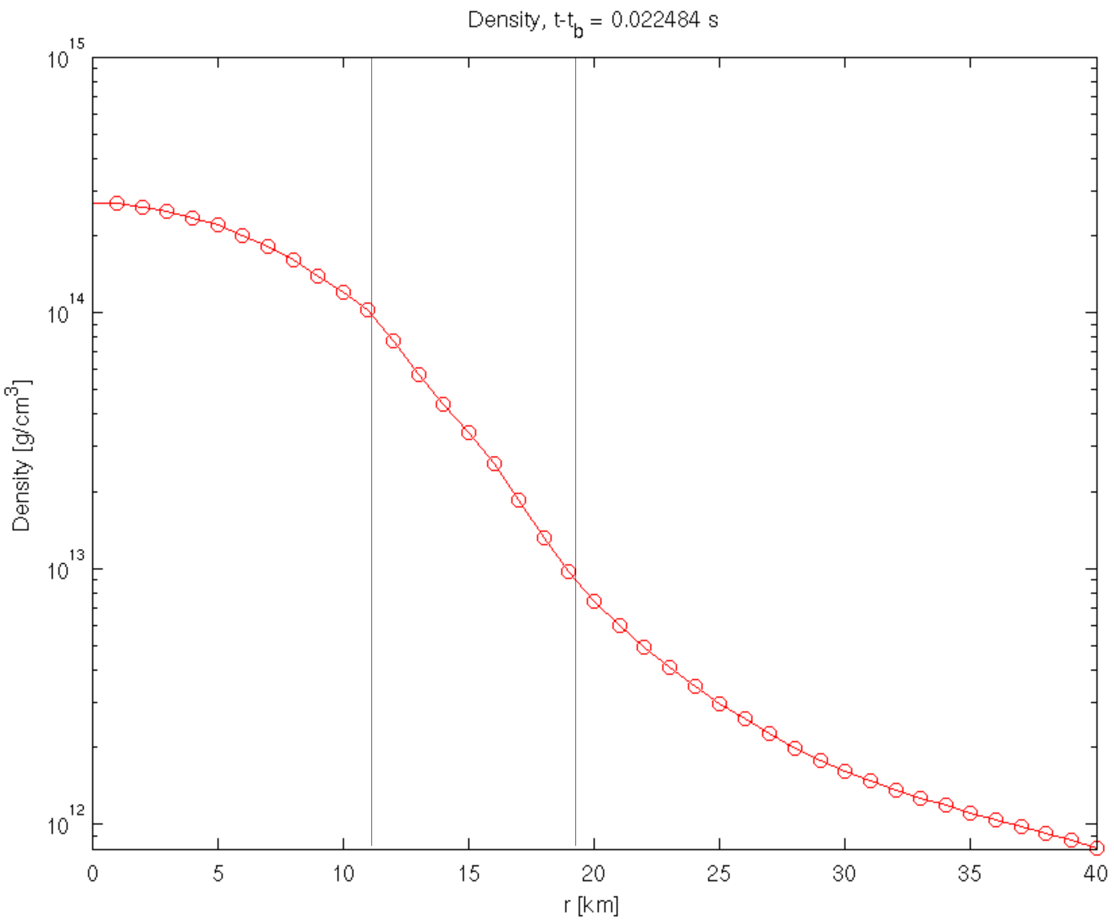
$$\frac{\partial Y_e}{\partial x} = 0, \ \frac{\partial s}{\partial x} = 0 \ \Rightarrow \ \frac{\partial}{\partial x}\begin{pmatrix}\rho \\ \rho v_x \\ E\end{pmatrix} = -\frac{1}{c^2}\begin{pmatrix}\rho \\ \rho v_x \\ E+p\end{pmatrix}\frac{\partial \phi}{\partial x}$$

Sound speed

Adapting the mesh

- Motivation





Adapting the mesh (2)

- Simplest approach
  - Use non-equidistant Cartesian mesh

$$\Delta x_i = x_{i+1/2} - x_{i-1/2} = f(i)$$
$$\Delta y_j = y_{j+1/2} - y_{j-1/2} = f(j)$$
$$\Delta z_k = z_{k+1/2} - z_{k-1/2} = f(k)$$

- Better:
  - Adaptive Mesh Refinement (AMR)

Adapting the mesh (3)

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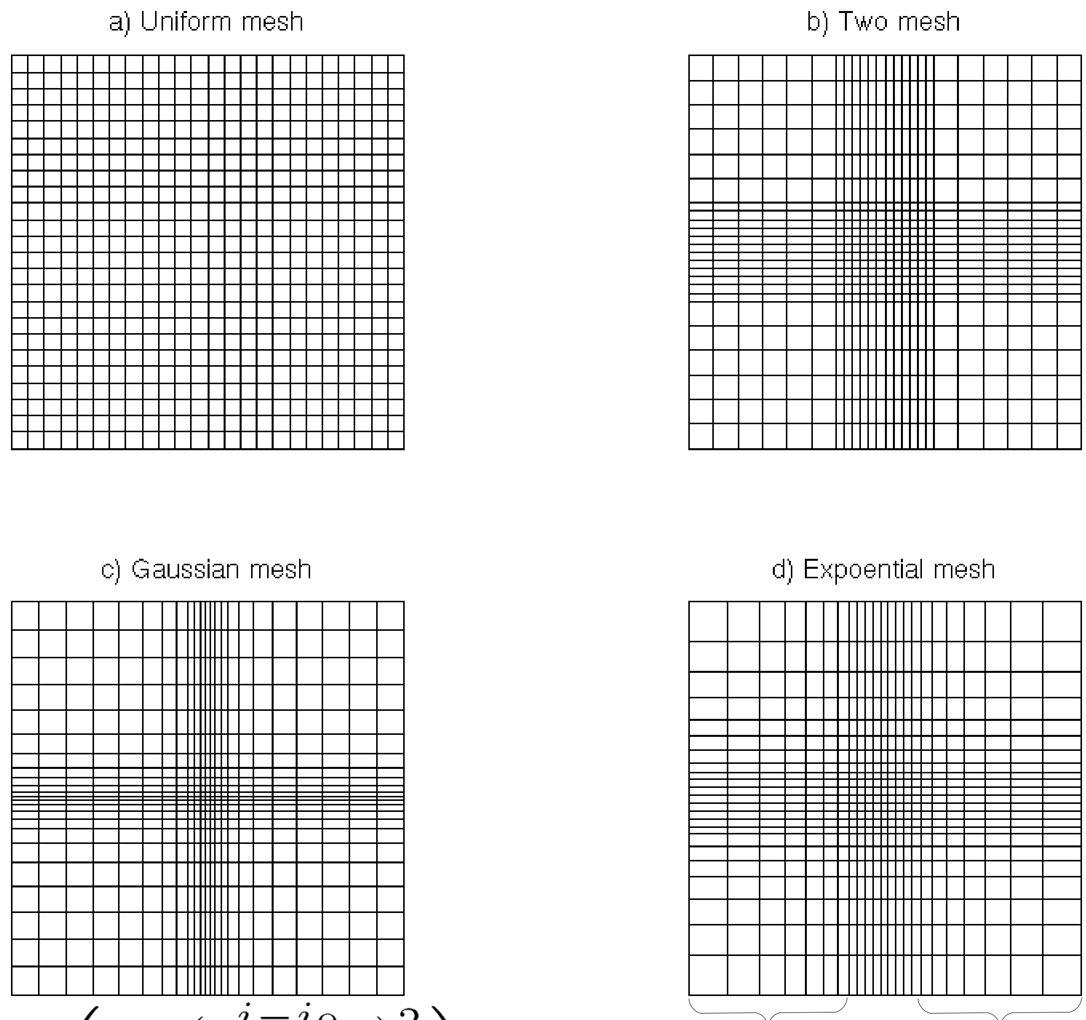


$$\Delta x_i \left(e^{-\left(\frac{i-i_0}{n/2+1}\right)^2}\right)$$

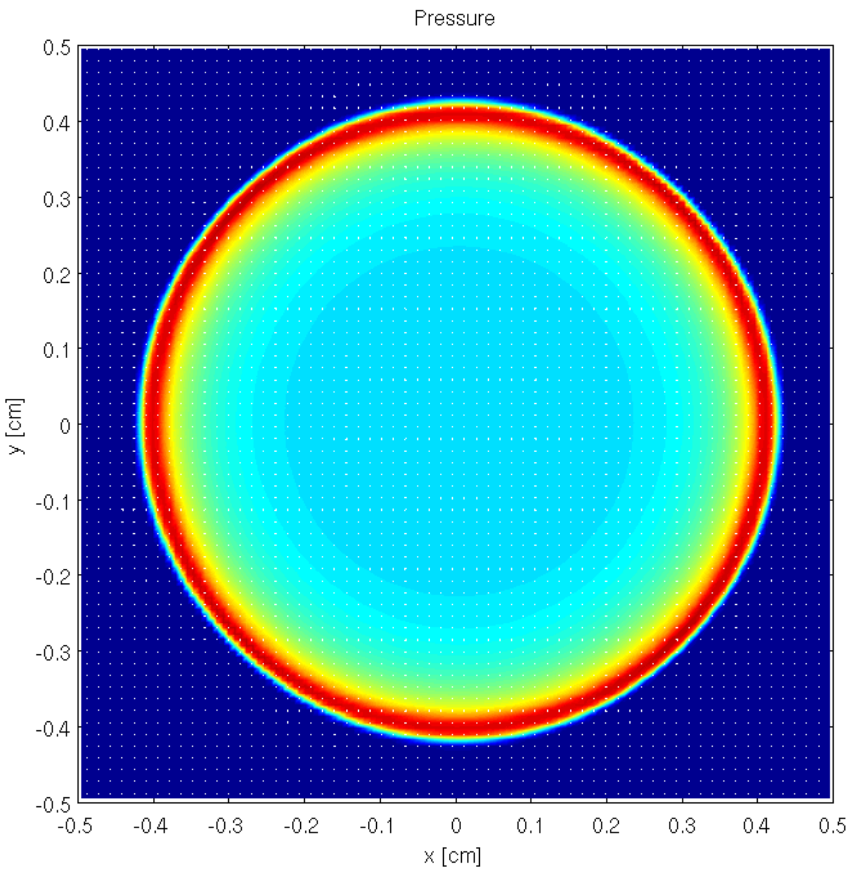
$$\Delta x_i \propto e^{ai}$$

Adapting the mesh (4)

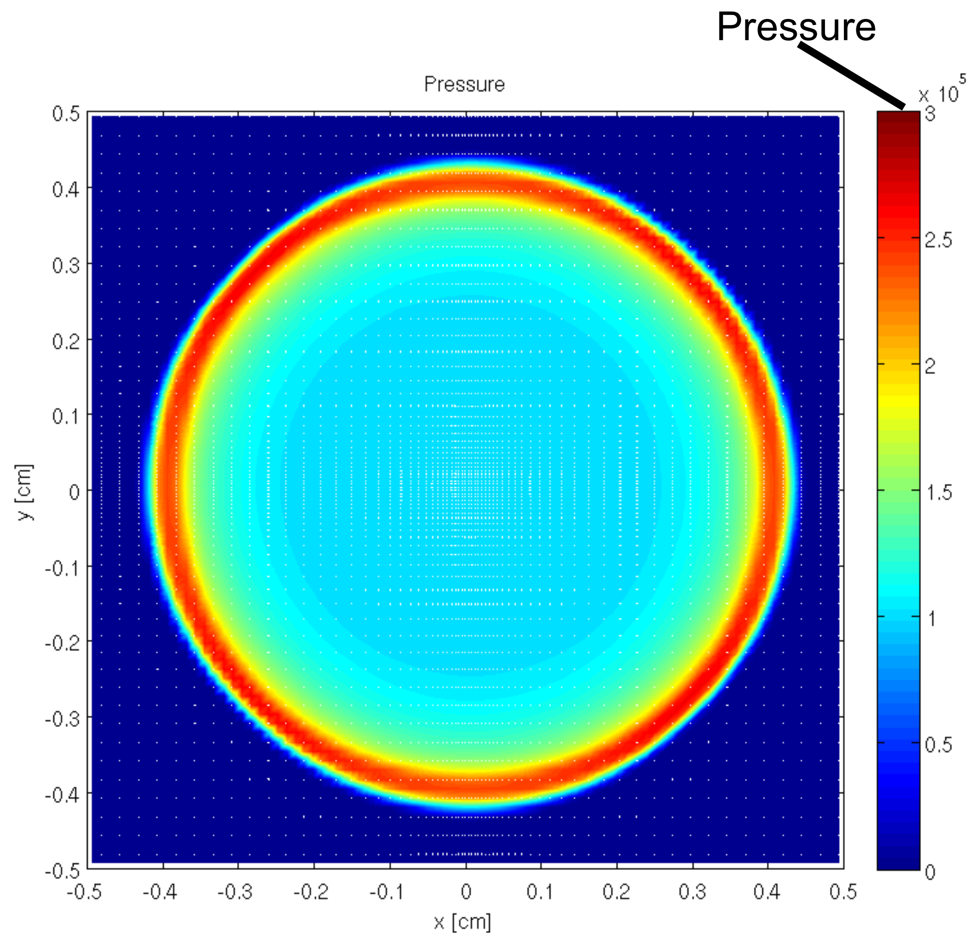
- Testing
  - Sedov-Taylor blast wave (point explosion)
  - Magnetic explosion
  - Braking of a magnetic rotor
- Comparison between uniform and non-uniform meshes

Adapting the mesh (5)

- Sedov-Taylor blast wave (point explosion)



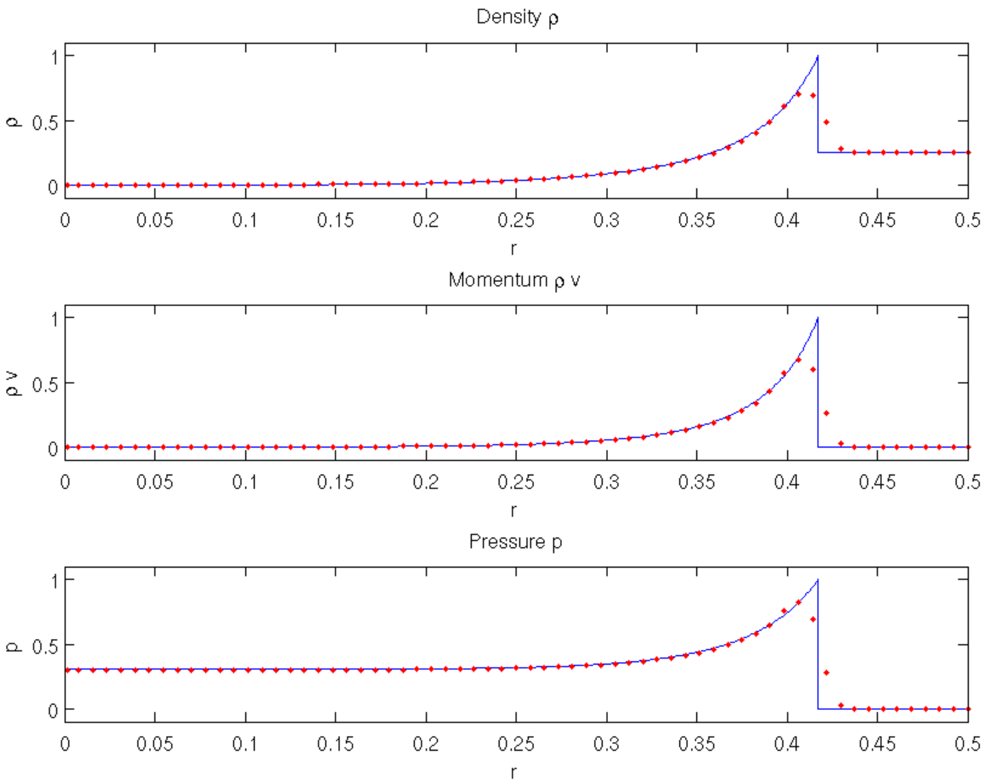
Uniform mesh



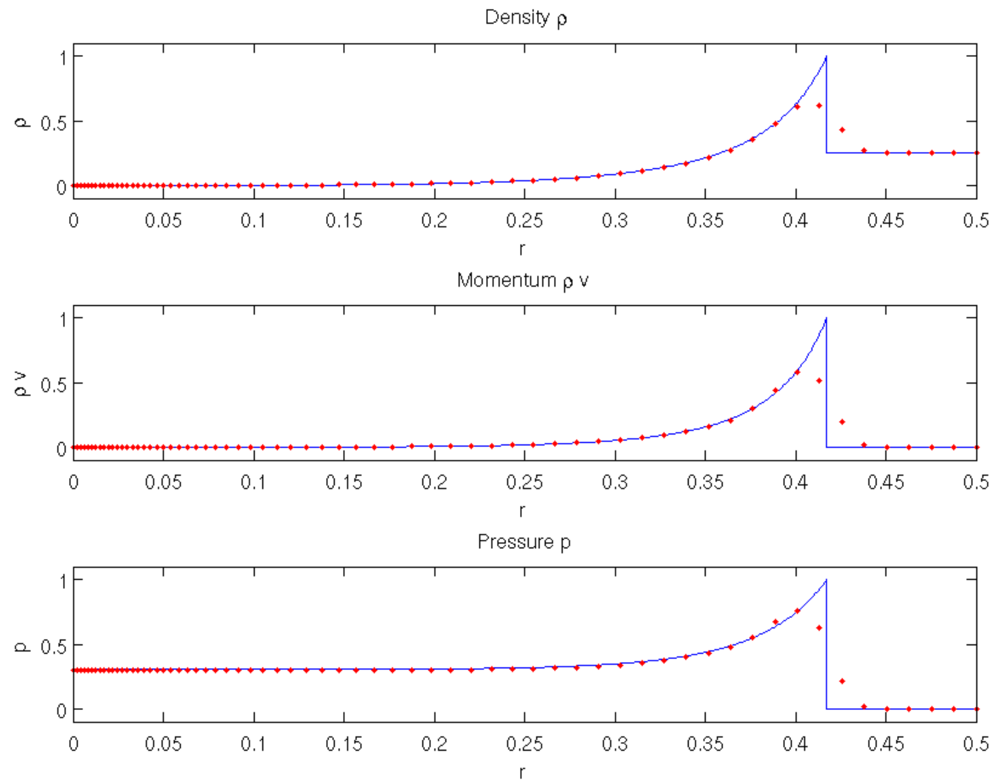
Gaussian mesh

Adapting the mesh (6)

- Sedov-Taylor blast wave (point explosion)
  - Comparison to analytic solution



Uniform mesh



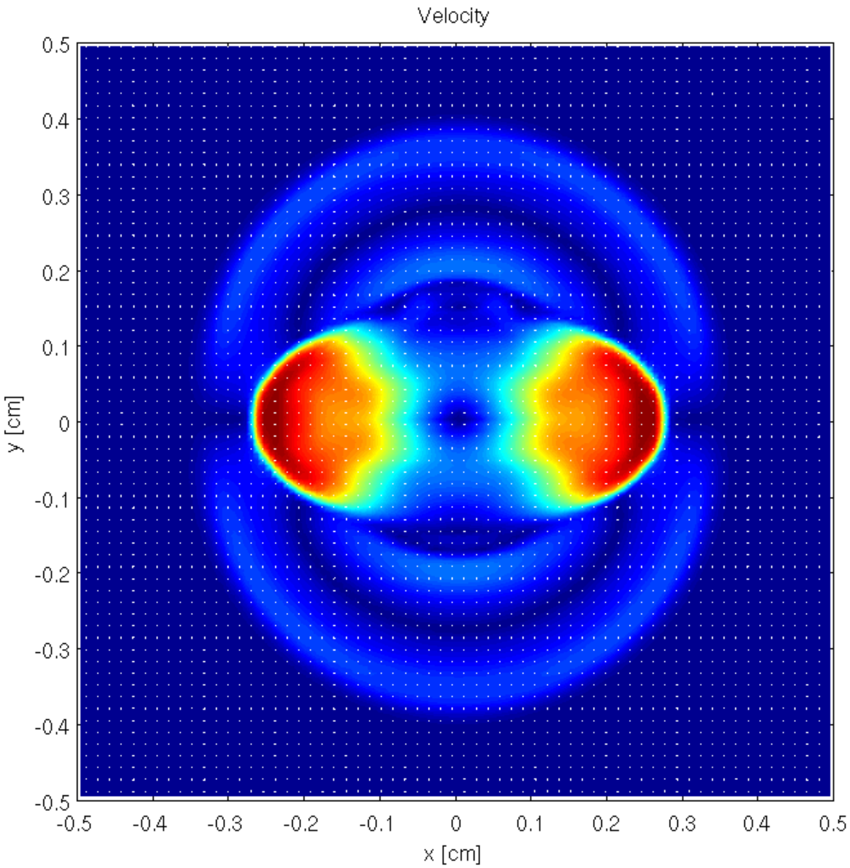
Gaussian mesh

Adapting the mesh (7)

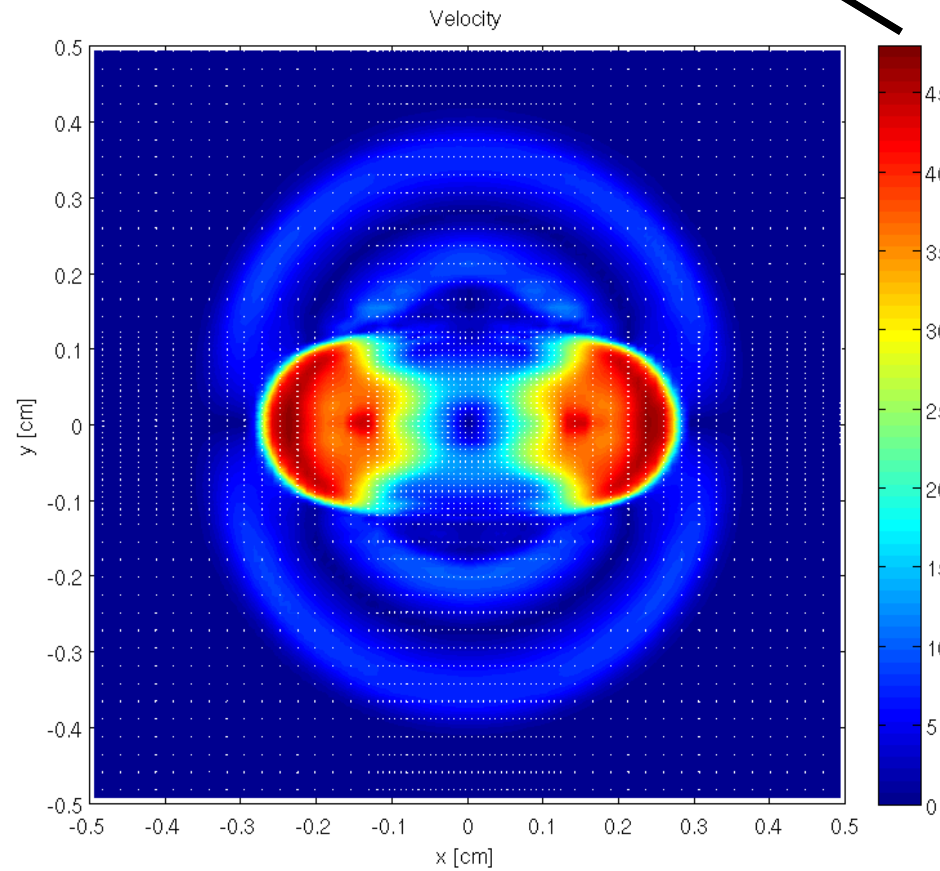
- Magnetic explosion (Sedov-Taylor + Magnetic field)

$$\boldsymbol{b} = b_0 \boldsymbol{e}_x,\; b_0 > 0$$

Abs. Magnitude of velocity



Uniform mesh



Two mesh

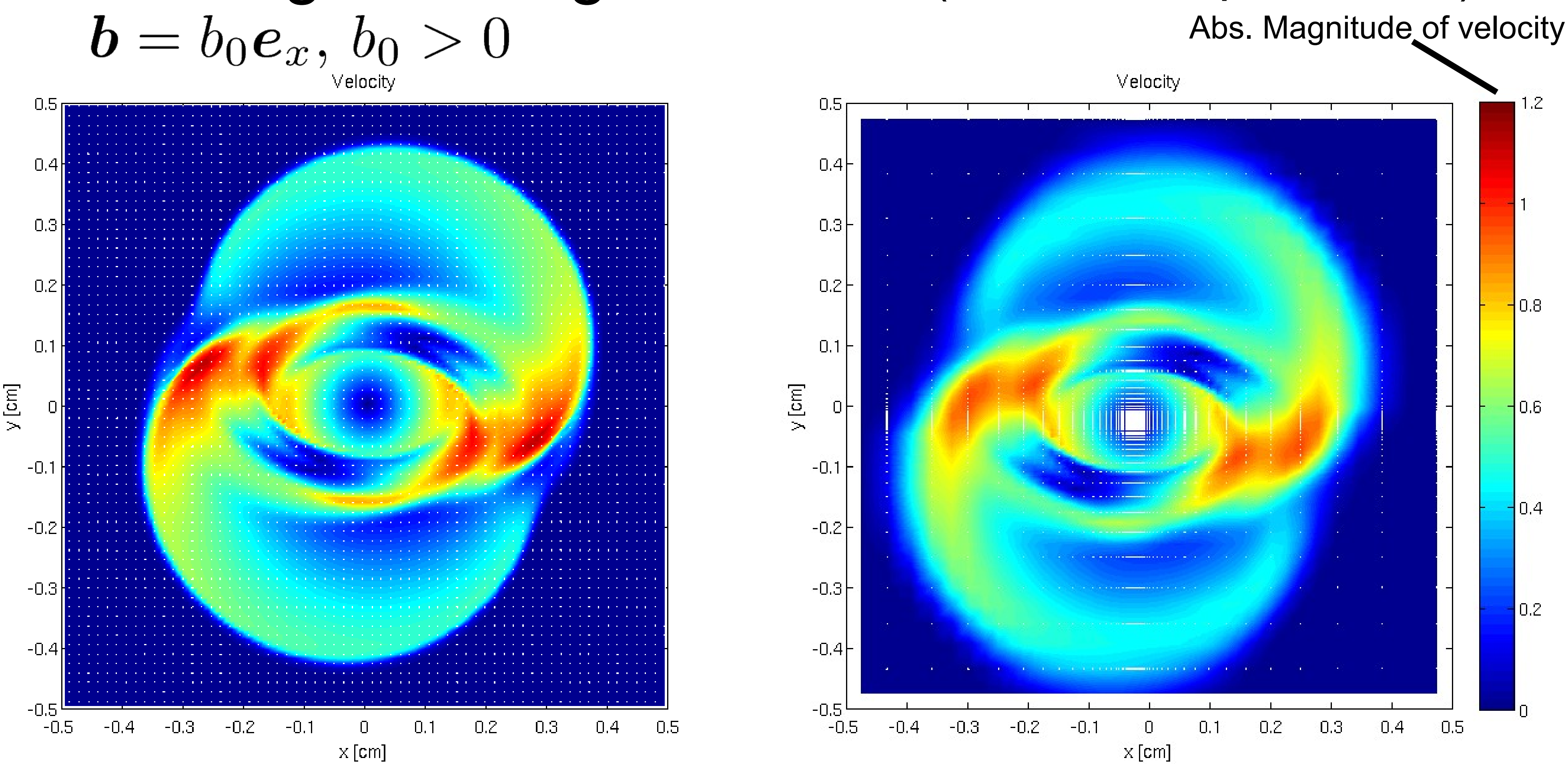
Adapting the mesh (8)

- Braking of a magnetic rotor (Balsara & Spicer 1999)
  - Dense, rapidly spinning cylinder (the rotor) in a light ambient fluid
  - Domain threaded by an initially uniform magnetic field
  - Rapidly spinning rotor causes torsional Alfvén waves to be launched (angular momentum lost)
  - Model for angular momentum loss of collapsing gas clouds in star formation (Mouschovias & Paleologou 1980)

Adapting the mesh (9)

- Braking of a magnetic rotor (Balsara & Spicer 1999)

$$\boldsymbol{b} = b_0 \boldsymbol{e}_x,\ b_0 > 0$$

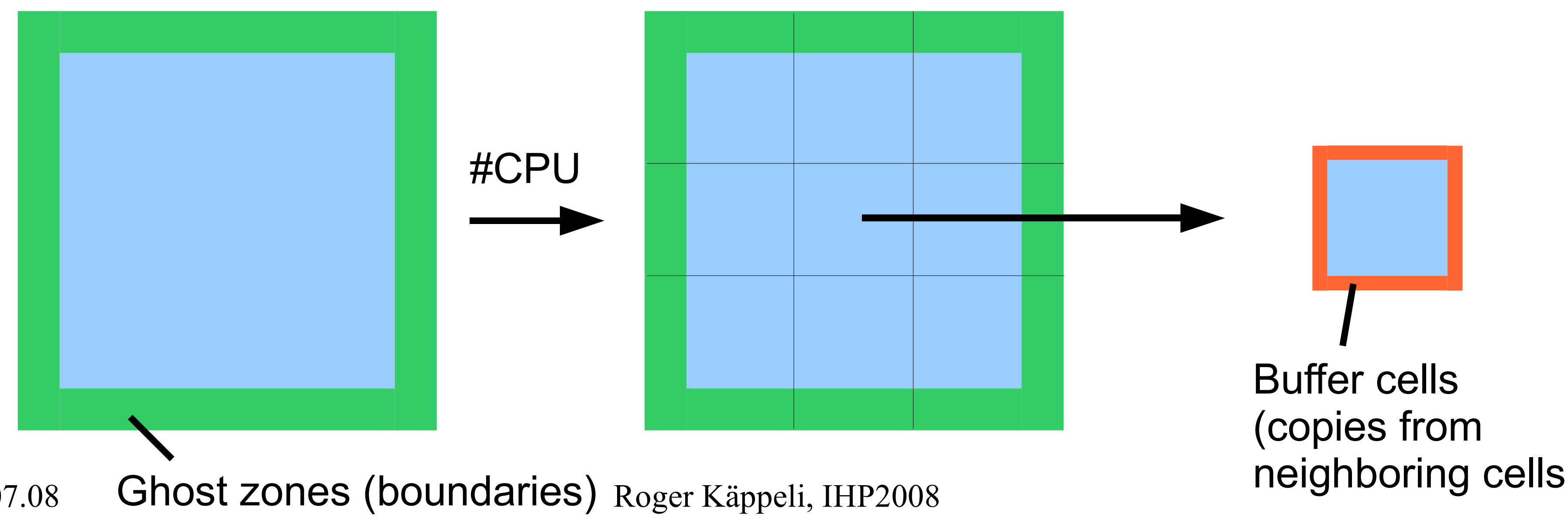


Uniform mesh

Exponential mesh

Parallelization

- Using Message Passing Interface (MPI)
- Cubic domain decomposition (chosen to min comm.)
- Use of non-blocking communication to overlap communication with computation

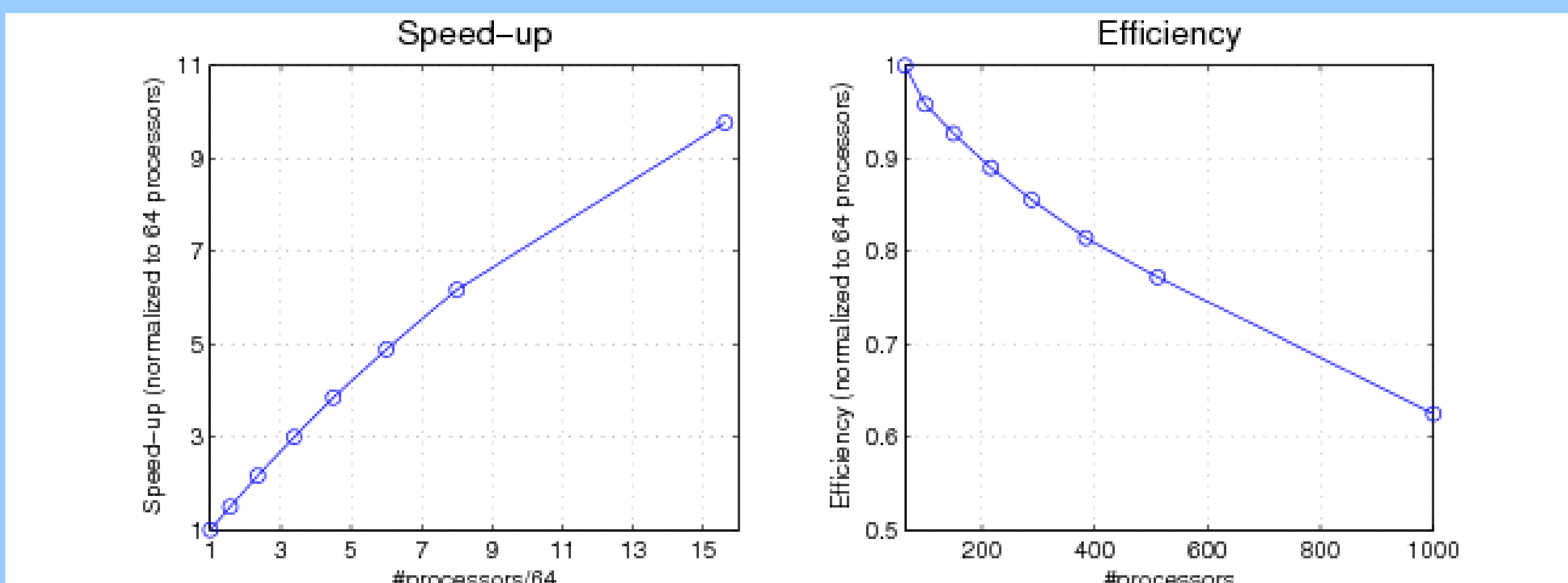


Parallelization (2)

Parallel Performance

Test case: 600x600x600 zones for 40 time steps

Test performed @ Swiss Super Computing Center CSCS



From S. Scheidegger

Summary

- Presented (partly) the MHD algorithm of our code
- Gravity incorporation into MHD code
- Improving the resolution by “adapting” the mesh
- Parallelization