Symmetry and Volume Compatibility in an r-z Staggered Scheme

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This work has been supported by the US DOE Advanced Simulation and Computing (ASC) Program, the DOE Office of Science ASCR Program, the Czech Science Foundation grant 14-21418S and RVO:68407700.

Motivation and Purpose

- **Develop a staggered Lagrangian scheme that preserves spherical symmetry while reducing the violation of the Geometric conservation law**

Outline of This Presentation

- **Introduction**
  - ◇ What do we do and why, staggered grid basics, notation
- **Existing staggered schemes: AW, GC and CV**
- **GCS: The symmetrized scheme**
  - ◇ Boundary conditions
  - ◇ Subcell pressures
- **Numerical results**
  - ◇ Sedov blast wave (sanity checks)
  - ◇ Coggeshall adiabatic compression (convergence study)
- **BONUS:**
  Wall heating removal by energy exchange à la Noh

Introduction: Spherically Symmetric Schemes

- **Why genuinely r-z, symmetry preserving staggered code?**
  - **AW** attractive because it **easily converts any Cartesian scheme** into an axi-symm. one
  - Drawback 1: adiabatic flows, no artificial viscosity:
    we would like to have an **accurate approximation to the thermodynamic relation**

    $$m_c \frac{d\varepsilon_c}{dt} + \mathcal{P}_c \frac{dV_c}{dt} = 0, \qquad \text{which would be true if} \qquad \sum_{p(c)} \mathbf{F}^{\text{p}}_{pc} \cdot \mathbf{U}_p = \mathcal{P}_c \frac{dV_c}{dt}$$

    This is not the case, in general, for area-weighted, where $\mathbf{F}^{\text{p}}_{pc} = r_p \mathbf{F}^{\text{p,Cart}}_{pc}$
  - Drawback 2: Area-weighted artificial viscosity may in general be **non-dissipative** and may **not conserve z-momentum**
  - In turn, typical existing genuinely r-z schemes **do not preserve spherical symmetry**

- **Relation to earlier work in staggered discretization:**
  - In **[Vachal, Wendroff, JCP 2014]** and **[Vachal, Wendroff, IJNMF 2014]** we **symmetrized artificial viscosity** by a correction of the r-component of the force
  - **Now** we are doing the same **also for pressure forces**

Staggered Grid Basics

- **Nodal dynamics are expressed in the system**

$$m_p\left(\mathbf{U}_p^{n+1}-\mathbf{U}_p^{n}\right)=\sum\nolimits_{c(p)}\mathcal{P}_c^{n+\frac{1}{2}}\mathbf{G}_{cp},\qquad\qquad \mathbf{G}_{cp}=\int_{t^n}^{t^{n+1}}\mathbf{g}_{cp}(t)\,dt$$

- **The nodal motion common to all our methods is**

$$\mathbf{X}_p(t)=\mathbf{X}_p^n+\mathbf{U}_p^{n+\frac{1}{2}}(t-t_n),\qquad \textbf{where}\qquad \mathbf{U}_p^{n+\frac{1}{2}}=\frac{1}{2}\left(\mathbf{U}_p^{n+1}+\mathbf{U}_p^{n}\right).$$

- **The energy dynamics are expressed as** $m_c\left(\varepsilon_c^{n+1}-\varepsilon_c^{n}\right)=-\mathcal{P}_c^{n+\frac{1}{2}}\sum\nolimits_{p(c)}W_{pc}$

- **Energy conservation requires that** $W_{pc}=\mathbf{U}_p^{n+\frac{1}{2}}\cdot\mathbf{G}_{cp},$

while entropy conservation requires that the energy equation be

$$m_c\,(\varepsilon_c^{n+1}-\varepsilon_c^{n})=-\mathcal{P}_c^{n+\frac{1}{2}}\,(V_c^{n+1}-V_c^{n}).$$

- **The *Geometric Conservation Law (GCL)* $\equiv$ requirement that these expressions are same:**

$$\sum\nolimits_{p(c)}\mathbf{U}_p^{n+\frac{1}{2}}\cdot\mathbf{G}_{cp}=V_c^{n+1}-V_c^{n}$$

Existing schemes: AW and GC

- **Both assume that the force vector from cell c on edge e with endpoints p, q is**

$$\mathbf{f}_{ec} = \mathcal{P}_c \, \frac{r_p + r_q}{2} \, \mathbf{n}_{ec}.$$

- **Area-weighted (AW)** - see e.g. **[Caramana, Burton, Shashkov, Whalen, JCP 1998]**
  - **The contribution to the geometrical force factor is** $\frac{1}{2} \, r_p \, \mathbf{n}_{ec} \Rightarrow \mathbf{g}_{cp}^{\textbf{AW}} = \sum\limits_{e(c,p)} \frac{1}{2} \, r_p \, \mathbf{n}_{ec}.$
  - Is symmetric ($\equiv$ preserves spher. symm. on an equi-angular polar grid)
- **Non-symm. GCL Scheme (GC)** - **[Loubère, Shashkov, Wendroff, JCP 2008]**
  - **Contribution to geom. force factor** $(\frac{2}{6} r_p + \frac{1}{6} r_q) \mathbf{n}_{ec} \Rightarrow \mathbf{g}_{cp}^{\textbf{GC}} = \sum\limits_{e(c,p)} \left(\frac{2}{6} r_p + \frac{1}{6} r_q\right) \mathbf{n}_{ec}.$
  - Note the factors $\frac{2}{6}$, $\frac{1}{6}$, corresponding to Maire's cell-centered work
  - Edge normals $\mathbf{n}_{ec}$ linear $\Rightarrow$ integrand in the mom. eq. is a combination of rr and rz $\Rightarrow$
    * These terms quadratic in t $\Rightarrow$ $\mathbf{G}_{cp} = \int \mathbf{g}_{cp} \, dt$ can be done exactly with Simpson's rule
    * System $m_p \big(\mathbf{U}_p^{n+1} - \mathbf{U}_p^n\big) = \sum_{c(p)} \mathcal{P}_c^{n+1/2} \mathbf{G}_{cp}$ is nonlinear in $\mathbf{U}$ $\Rightarrow$ iteration required
    * **The use of Simpson's rule in this way is critical for GCL to be satisfied**
      $\Rightarrow$ **In all calculations below, we perform inner (velocity) and outer (energy) iterations**
  - It is well known, that GC is not symmetric.

Existing schemes: CV

- **“Control Volume” (CV)**
  - Suggested for cylindrical coordinates in **[Caramana, Burton, Shashkov, Whalen, JCP 1998]**
  - Half-edge normals multiplied by r-coord of their midpoints**:**

$$\frac{1}{2}\left(r_p + \frac{r_p + r_q}{2}\right) = \left(\frac{3}{4} r_p + \frac{1}{4} r_q\right)$$

$\Rightarrow$ **Contribution to geom. force factor is**

$$\mathbf{g}_{cp} = \sum_{e(c,p)} \left(\frac{3}{8} r_p + \frac{1}{8} r_q\right) \mathbf{n}_{ec}.$$

  - **Note that**

$$\mathbf{g}_{cp}^{\textsf{CV}} = \sum_{e(c,p)} \frac{3}{4}\left[\frac{1}{6} r_p + \left(\frac{2}{6} r_p + \frac{1}{6} r_q\right)\right] \mathbf{n}_{ec}$$

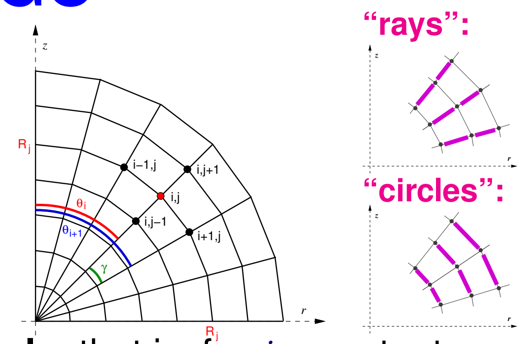
$$= \frac{1}{4}\mathbf{g}_{cp}^{\textsf{AW}} + \frac{3}{4}\mathbf{g}_{cp}^{\textsf{GC}}.$$

  - Even after Simpson’s integration we get

$$\mathbf{G}_{cp}^{\textsf{CV}} = \tfrac{1}{4}\mathbf{G}_{cp}^{\textsf{AW}} + \tfrac{3}{4}\mathbf{G}_{cp}^{\textsf{GC}},$$

$\Rightarrow$ **to symmetrize CV we only need to symmetrize GC.**

Symmetry analysis of GC



- **Assume fully symmetric data on an equiangular polar grid,**
  $\mathbf{X}_{i,j} = (r_{i,j}, z_{i,j}) = (R_j \sin\theta_i, R_j \cos\theta_i)$**,**
  $\theta_{i+1} - \theta_i = \gamma$ for all i**.**
- **Therefore assume also** $m_{i,j} = r_{i,j}\, A_j$**,**
  where A_j is indep. of the angle of ray with node (i, j)
- **The lack of symmetry in GC lies entirely with the radial component of** $\mathbf{g}$ **coming from the edges lying on the same circle,** that is, for j=constant
  - Symmetry ⇒ edges on the rays do not contribute to the force (normals opposite, press. equal)
  - Consider node $p = (i, j)$ with circle edges $(i + \frac{1}{2}, j)$ and $(i - \frac{1}{2}, j)$
  - In order for symmetry to occur, the total geom. factor from these two edges must have the form
    $$\mathbf{g}^{\text{circ}}_{i,j} = B_j\ \sin\theta_i\,(\sin\theta_i, \cos\theta_i), \tag{1}$$
    where B is independent of angle (= of i), because then the contribution to the acceleration is
    $$\frac{\mathbf{g}^{\text{circ}}_{i,j}}{m_{i,j}} = \frac{B_j}{R_j\ A_j}\,(\sin\theta_i, \cos\theta_i),$$
    which is spherically radial and has norm independent of angle.
  - Now insert for position $\mathbf{X}$ and normals $\mathbf{n}$ as in GC, drop const. index j, and consider the identity
    $$\underbrace{(r_{i-1} + 2r_i)(r_i - r_{i-1}) + (r_{i+1} + 2r_i)(r_{i+1} - r_i)}_{\text{6 times the z-component of } \mathbf{g} \text{ from GC}} = \underbrace{(r_{i-1} + r_i + r_{i+1})(r_{i+1} - r_{i-1})}_{= R_j^2\,[(2\cos\gamma + 1)\sin\gamma]\,2\sin\theta_i\ \cos\theta_i}$$
    RHS has the form of the z-comp. of (1) ⇒ **nonsymmetry of GC lies in the** r**-component of** $\mathbf{g}$
- **This points the way toward symmetrization of GC**

Symmetrization (GCS)

- GC will be **kept as is on the ray edges.**
- On circles, **the z-component** of the geometrical factor, being already symmetric, **will remain as is**
- **The r-component will be changed** as required for symmetry, namely

$$g_r = -\frac{1}{6}\left(r_{i-1} + r_i + r_{i+1}\right)\left(z_{i+1} - z_{i-1}\right), \quad \text{which is} \quad \frac{1}{6} R_j^2 \left[(2\cos\gamma + 1)\sin\gamma\right] 2\sin\theta_i \, \sin\theta_i$$

by adding a **correction to the r-comp.** and then accounting for that in the energy equation.

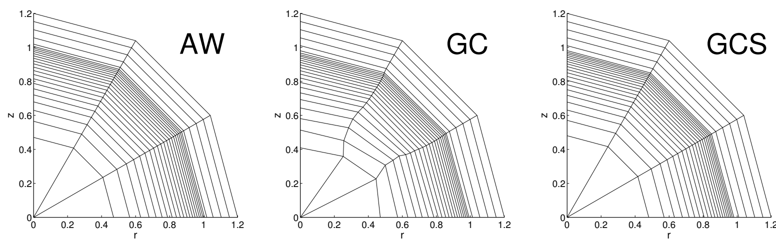
- **In fact, the correction is nothing more than g_r minus the GC geometric factor, namely,**
$\delta = -\frac{1}{6}(r_{i-1} + r_i + r_{i+1})(z_{i+1} - z_{i-1}) + \frac{1}{6}[(r_{i-1} + 2r_i)(z_i - z_{i-1}) + (r_{i+1} + 2r_i)(z_{i+1} - z_i)].$
- **Notice the identity for this correction δ:**

$$12\,\delta = (z_{i+1} - 2z_i + z_{i-1})(r_{i+1} - r_{i-1}) - (r_{i+1} - 2r_i + r_{i-1})(z_{i+1} - z_{i-1}).$$

- **In the symmetric case:**

$$\delta = \tfrac{1}{3}\, R^2 \sin\gamma\,(\cos\gamma - 1),$$

$\Rightarrow$ **δ is independent of angle**
$\Rightarrow$ **energy change is also symmetric.**

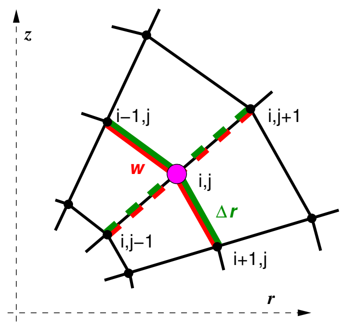


- Of course, **any deviation from GC will not exactly satisfy the GCL,** but (using Taylor expansion for $\sin\gamma$ and $\cos\gamma$) we see that **the correction δ is of 3rd order,** as is the error in entropy**.**

The z-axis Boundary Condition

- **Assume an equi-angular polar grid with symmetric data (pressure)**
  - **For an interior node (i,j), $i>0$, the z-component of acceleration in GC and GCS is**

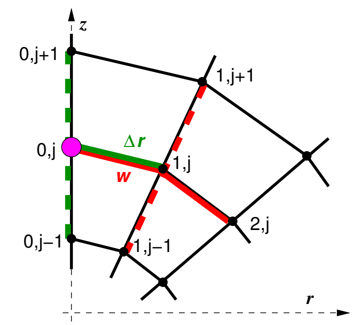
$$\frac{d\delta v_{i,j}}{dt} = \frac{1}{6} \underbrace{\frac{r_{i-1,j}+r_{i,j}+r_{i+1,j}}{m_{i,j}}}_{\text{denote } w, \quad \textbf{indep. on } i} \underbrace{\left(r_{i-1,j}-r_{i+1,j}\right)}_{\text{denote } \Delta r} \left(\mathcal{P}_{j+\frac{1}{2}} - \mathcal{P}_{j-\frac{1}{2}}\right).$$



Stencil of Δr and $w = \frac{\sum r}{m}$ for the acceleration

← of an interior point (i,j)

of a boundary ($z-$axis) point $(0,j)$ →



  - **On the z-axis ($i=0$ ray): We apply reflection $v_{-1,j}=v_{1,j}$ and use $\frac{\sum r}{m}$ from the first off-axis node $(1,j)$, because it is not defined on the axis (at $i=0$):**

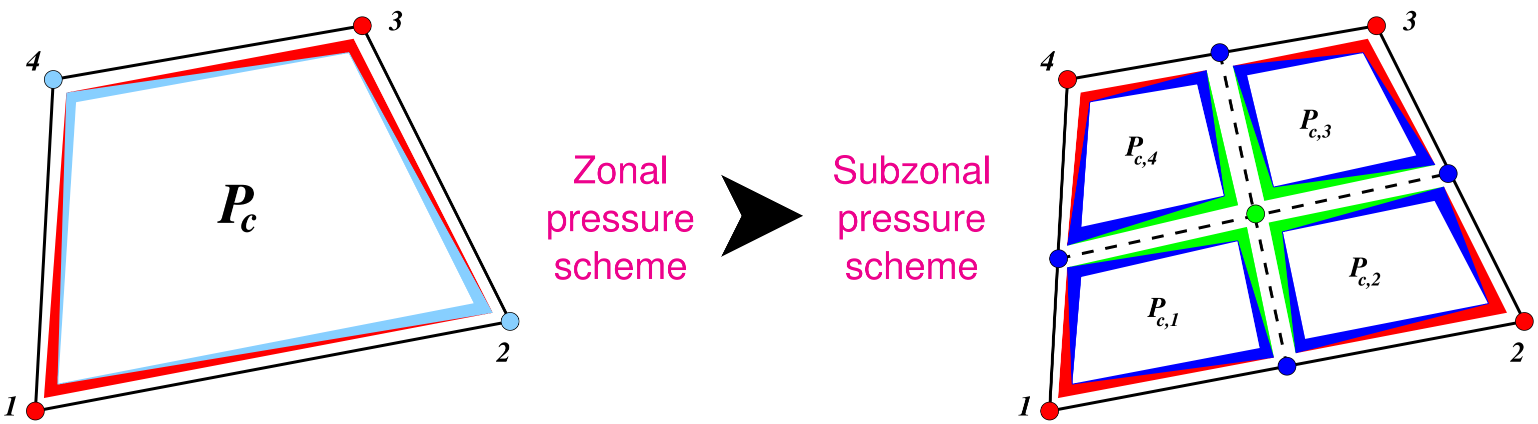
$$\frac{d\delta v_{0,j}}{dt} = \frac{1}{6}\frac{0+r_{1,j}+r_{2,j}}{m_{1,j}}\, 2\left(-r_{1,j}\right)\left(\mathcal{P}_{j+\frac{1}{2}} - \mathcal{P}_{j-\frac{1}{2}}\right) = -\frac{1}{3}\frac{r_{1,j}+r_{2,j}}{m_{1,j}}\, r_{1,j}\left(\mathcal{P}_{j+\frac{1}{2}} - \mathcal{P}_{j-\frac{1}{2}}\right)$$

- **Such choice of acceleration of nodes on z-axis also makes sense for a general grid.**
- **Similarly for the AW approach we get**

$$\frac{d\delta v_{0,j}}{dt} = -\frac{1}{2}\frac{r_{1,j}}{m_{1,j}}\, 2\, r_{1,j}\left(\mathcal{P}_{j+\frac{1}{2}} - \mathcal{P}_{j-\frac{1}{2}}\right) = -\frac{r_{1,j}^2}{m_{1,j}}\left(\mathcal{P}_{j+\frac{1}{2}} - \mathcal{P}_{j-\frac{1}{2}}\right)$$

GCS: Subcell pressure forces

- A technique to **reduce grid distortion,** see **[Caramana, Shashkov, JCP 142, 1998]**
- **We extend the** p-c **notation:** $s(c)$ are the subcells, $a(s)$ the nodes of s, and $\sum_{s(c)} V_s = V_c$
- These nodes are **averages of the cell nodes,** that is, there is a matrix α_{ap} such that
$$\mathbf{X}_a = \sum_{p(c)} \alpha_{ap} \mathbf{X}_p \qquad \text{with } \alpha_{ap} \geq 0, \quad \sum_{p(c)} \alpha_{ap} = 1.$$
For example: for quad cells take quad subcells with $\mathbf{X}_c = \frac{1}{4} \sum_{p(c)} \mathbf{X}_p$ and $\mathbf{X}_e = \frac{1}{2}(\mathbf{X}_p + \mathbf{X}_{p'})$.
- It follows that $\mathbf{U}_a = \sum_{p(c)} \alpha_{ap} \mathbf{U}_p$.
- **Each subcell will be treated exactly as the cells are.** That is, we set
$$\mathbf{G}_{sa} = \frac{\Delta t}{6} \sum_{e(s,a)} \left(\left(2\, r_p^{n+1} + r_{p'}^{n+1}\right) \left(\tfrac{2}{6}\mathbf{n}_{es}^{n+1} + \tfrac{1}{6}\mathbf{n}_{es}^{n}\right) + \left(2\, r_p^{n} + r_{p'}^{n}\right) \left(\tfrac{2}{6}\mathbf{n}_{es}^{n} + \tfrac{1}{6}\mathbf{n}_{es}^{n+1}\right) \right)$$



- With subcell pressures $\mathcal{P}_s$, **the subcell nodal forces are now** $\mathcal{P}_s\, \mathbf{G}_{sa}$.

GCS: Subcell pressure forces

- **The cell nodal forces taken to be as in (16)-(17) of [Caramana, Shashkov, JCP 142, 1998],**

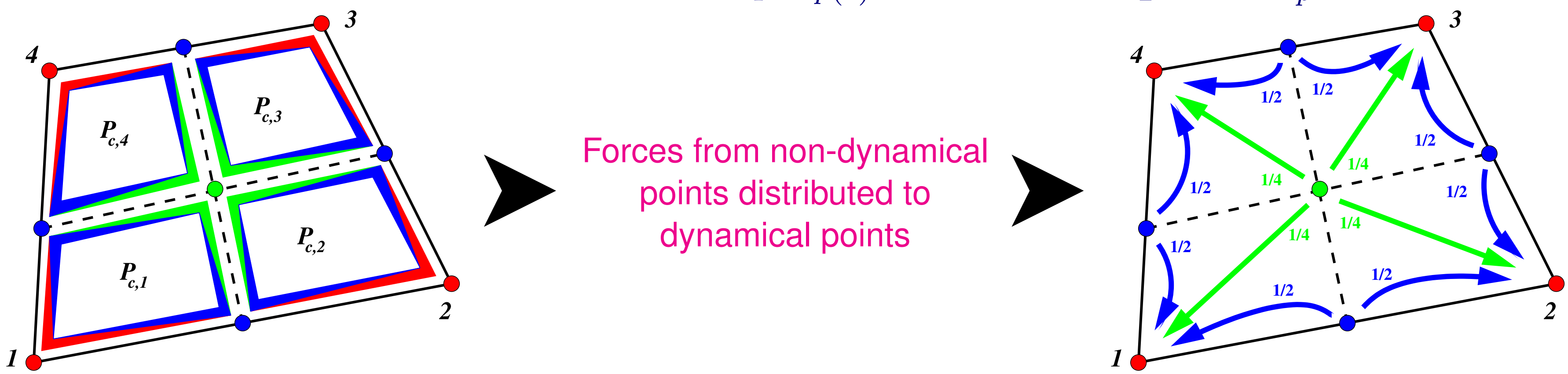
$$\mathbf{F}_{cp} = \sum_a \alpha_{ap} \sum_{s(a)} \mathcal{P}_s \mathbf{G}_{sa}, \qquad \textbf{(1)}$$

so that $\quad m_c\,(\varepsilon_c^{n+1} - \varepsilon_c^n) = -\sum_{p(c)} \mathbf{U}_p \cdot \sum_a \alpha_{ap} \sum_{s(a)} \mathcal{P}_s \mathbf{G}_{sa} = -\sum_s \mathcal{P}_s (V_s^{n+1} - V_s^n)$,

which reduces to $m_c\,(\varepsilon_c^{n+1} - \varepsilon_c^n) - \mathcal{P}_c (V_c^{n+1} - V_c^n)$ if the subcell pressures are equal

$\Rightarrow$ **volume compatibility of zonal pressure scheme is "inherited" by the subzonal version**

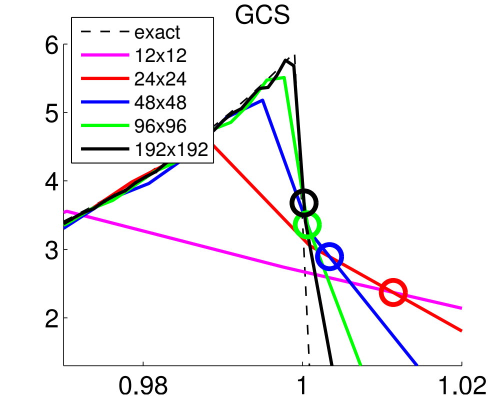
- Our example with quadrilateral subcells, $\mathbf{X}_c = \frac{1}{4}\sum_{p(c)} \mathbf{X}_p$ and $\mathbf{X}_e = \frac{1}{2}(\mathbf{X}_p + \mathbf{X}_{p'})$:

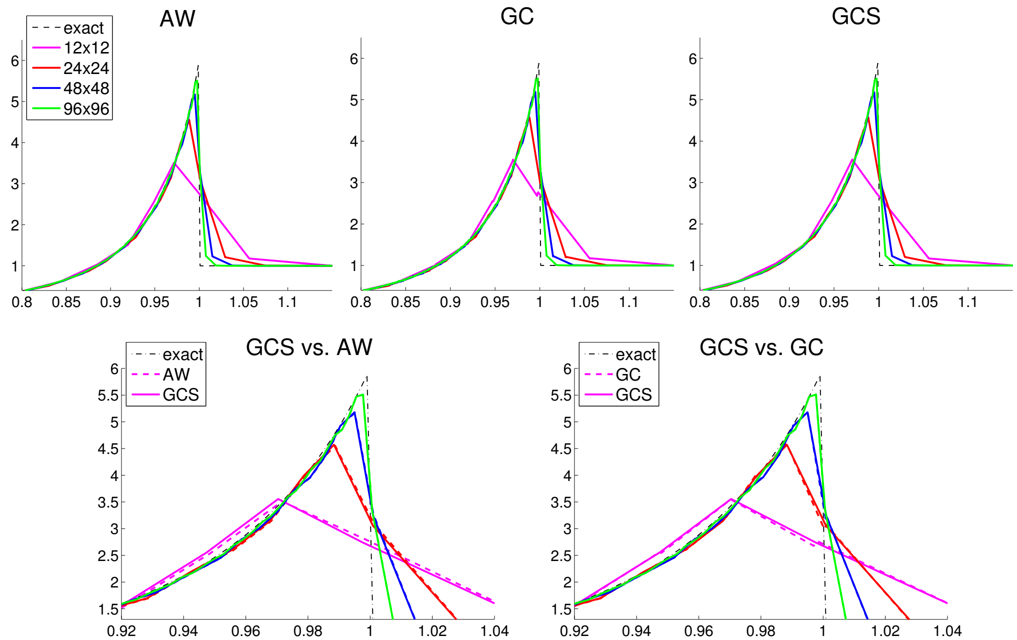


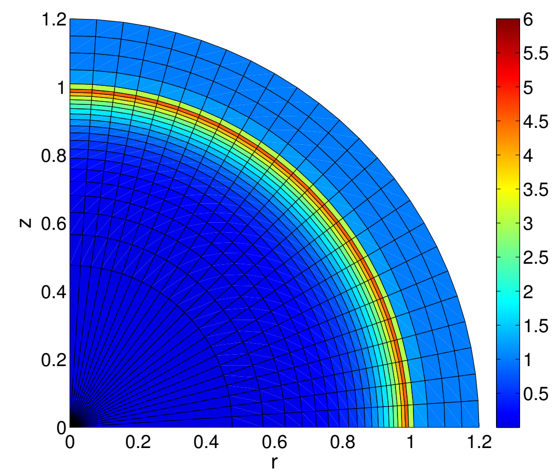
- Other redistribution than (1) and other shapes of subcells are possible
- **GCS symmetry corrections** δ_{as} calculated per subcell and collected: $\delta_p = \sum_{s(c)} \sum_{a(s)} \alpha_{ap}\delta_{as}$.
- **AW:** subcells are standard; **CV:** nodal forces combine from AW and GC forces as before

Numerics: Sedov Test, Zonal Pressure Forces

- **Serves as a sanity check that**
  - the symmetry correction (CG→GCS) does not compromise the shock speed
  - AW, GCS and CVS preserve symmetry (unlike GC and CV)







- **Viscosity dominates (LapEdge used here)**

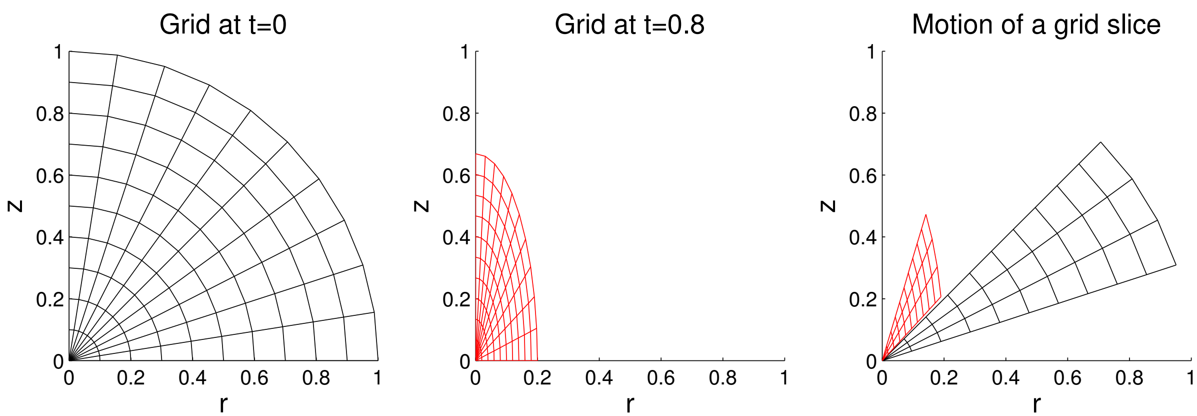
  ⇒ **most schemes** (press. force types) **perform similarly** (visually same except for small resol.)

The Coggeshall Test Problem

- **A simple adiabatic compression problem that becomes singular at $t = 1.0$.**
- **A sphere of radius 1 is filled with a perfect gas with $\Gamma = 5/3$ and is collapsing with cylindrical (but not spherical) symmetry so, that the exact solution at a given time t is**

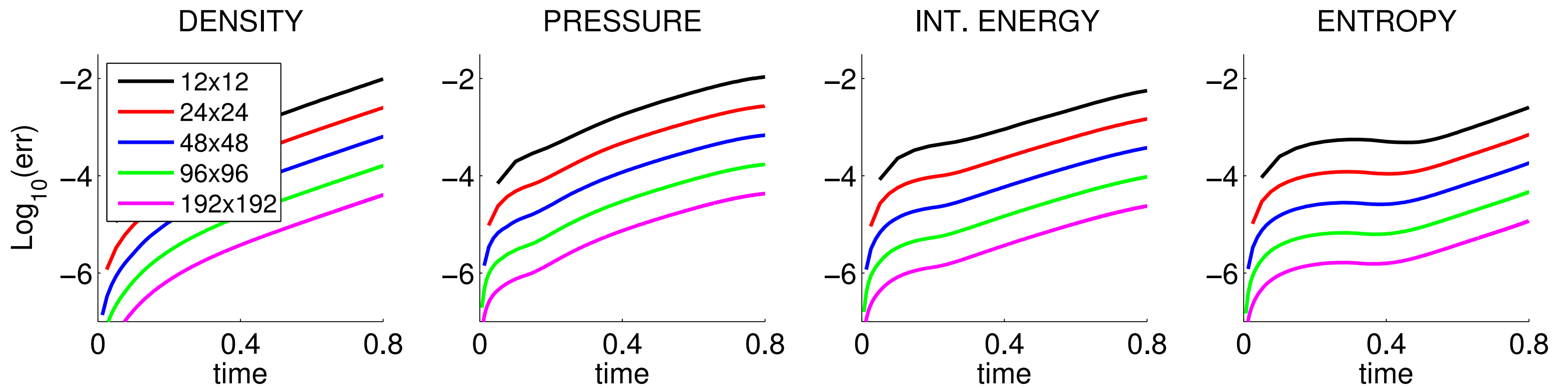
$$u^{\text{ex}}(t)= \frac{-\,r(t)}{1-t}, \quad v^{\text{ex}}(t)= \frac{-\,z(t)}{4(1-t)}, \quad \rho^{\text{ex}}(t)= (1-t)^{-9/4}, \quad \varepsilon^{\text{ex}}(t)= \left(\frac{3\,z(t)}{8(1-t)}\right)^2$$

- **Exact BC applied on the outer boundary (spherical outer shell)**
- **On the z-axis, all the presented schemes have a simple, problem independent BC**
- **Entropy is constant on particle paths: $S^{\text{ex}}(r(t), z(t), t) = S^{\text{ex}}(r(0), z(0), 0)$ at every time t**

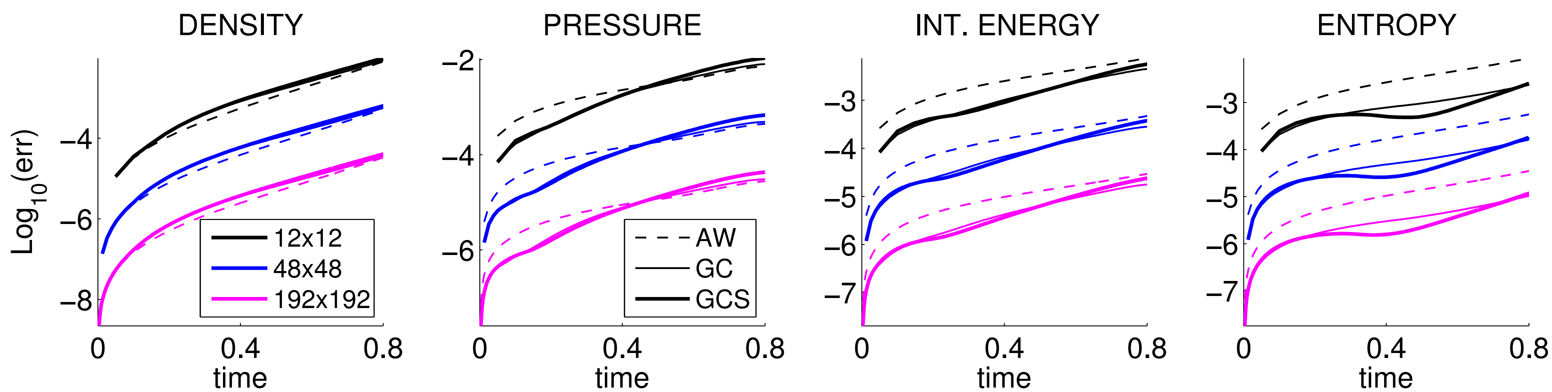


Numerics: Coggeshall - comparison of AW, GC, GCS

- **Evolution of $\log_{10}$ of L_1 error in time. GCS by thick lines**



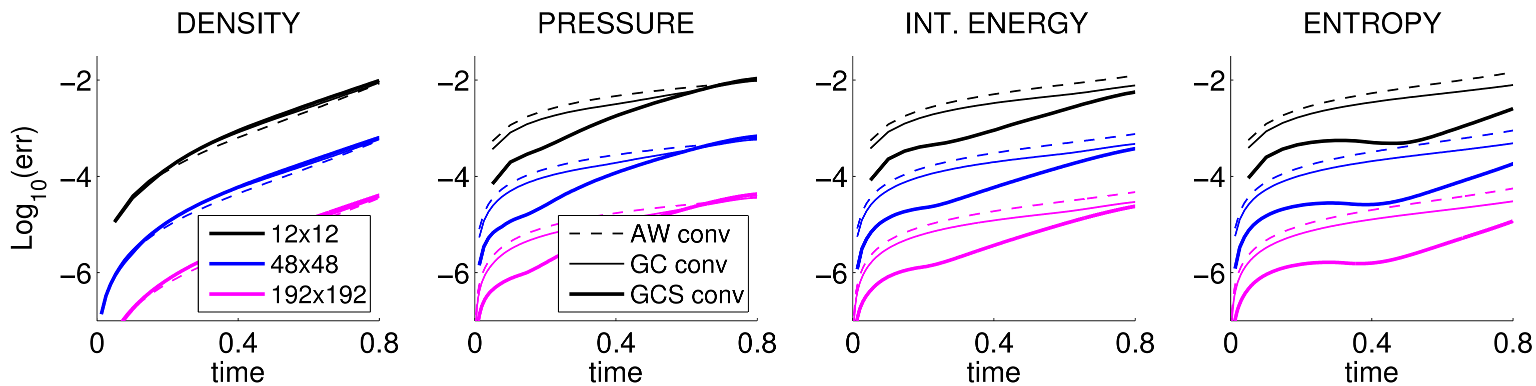
- **Comparison to AW (dashed) and GC (thin solid)**



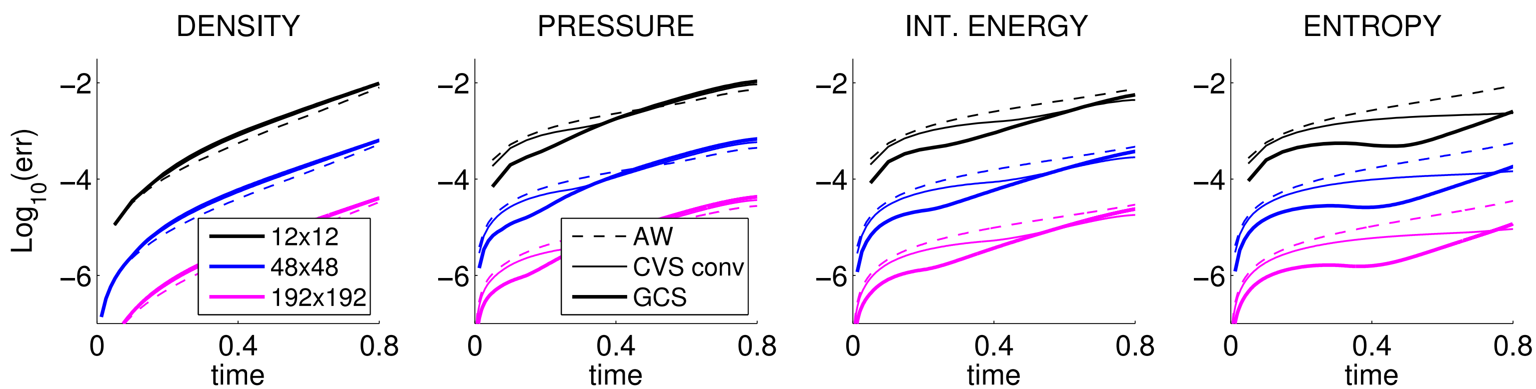
$\Rightarrow$ **From the viewpoint of error evolution, GC is superior to AW and GCS similar to GC**

Numerics: More on Coggeshall

- **NOTE: Outer iterations (predictor-corrector on energy):**
  - For our implementation of AW and GC (but not GCS), doing just 2 iterations instead of iterating until convergence gives smaller errors. Previous pictures showed best of each
  - In our opinion, **pressure should be iterated until convergence.** Then the comparison is

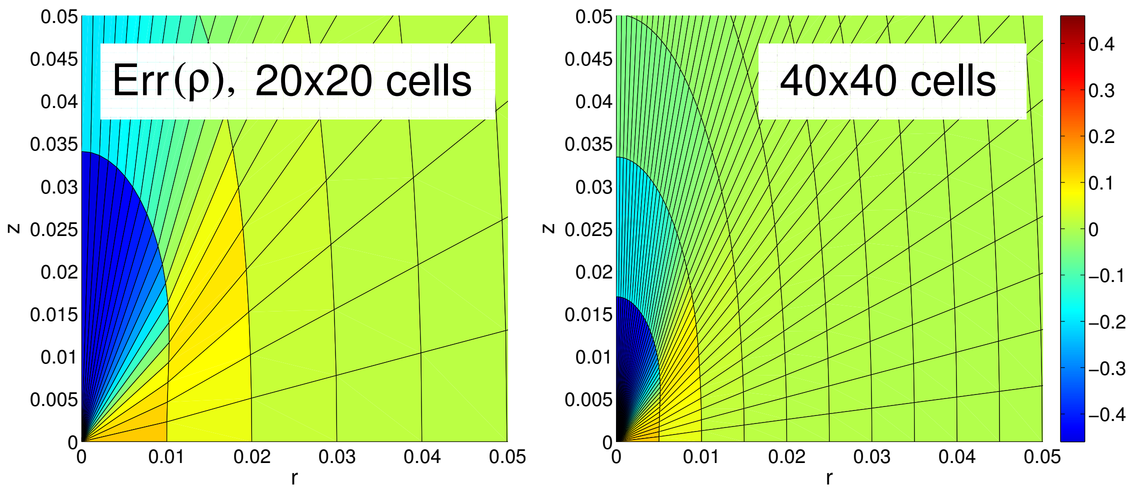


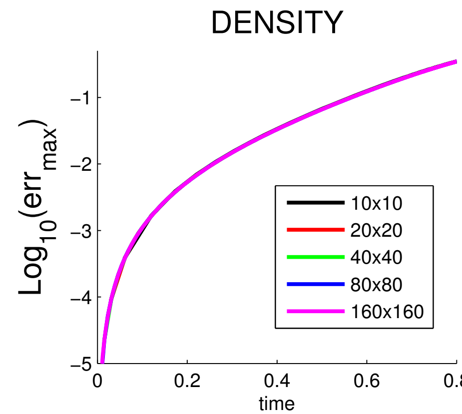
- **Comparison of AW (dashed), CVS (thin solid) and GCS (thick solid)**



Coggeshall: Remark on the choice of norms

- **Maximum density discrepancy** (particularly in the cell $(1,1)$ attached to the origin and to the z-axis) **is the same, regardless mesh resolution**

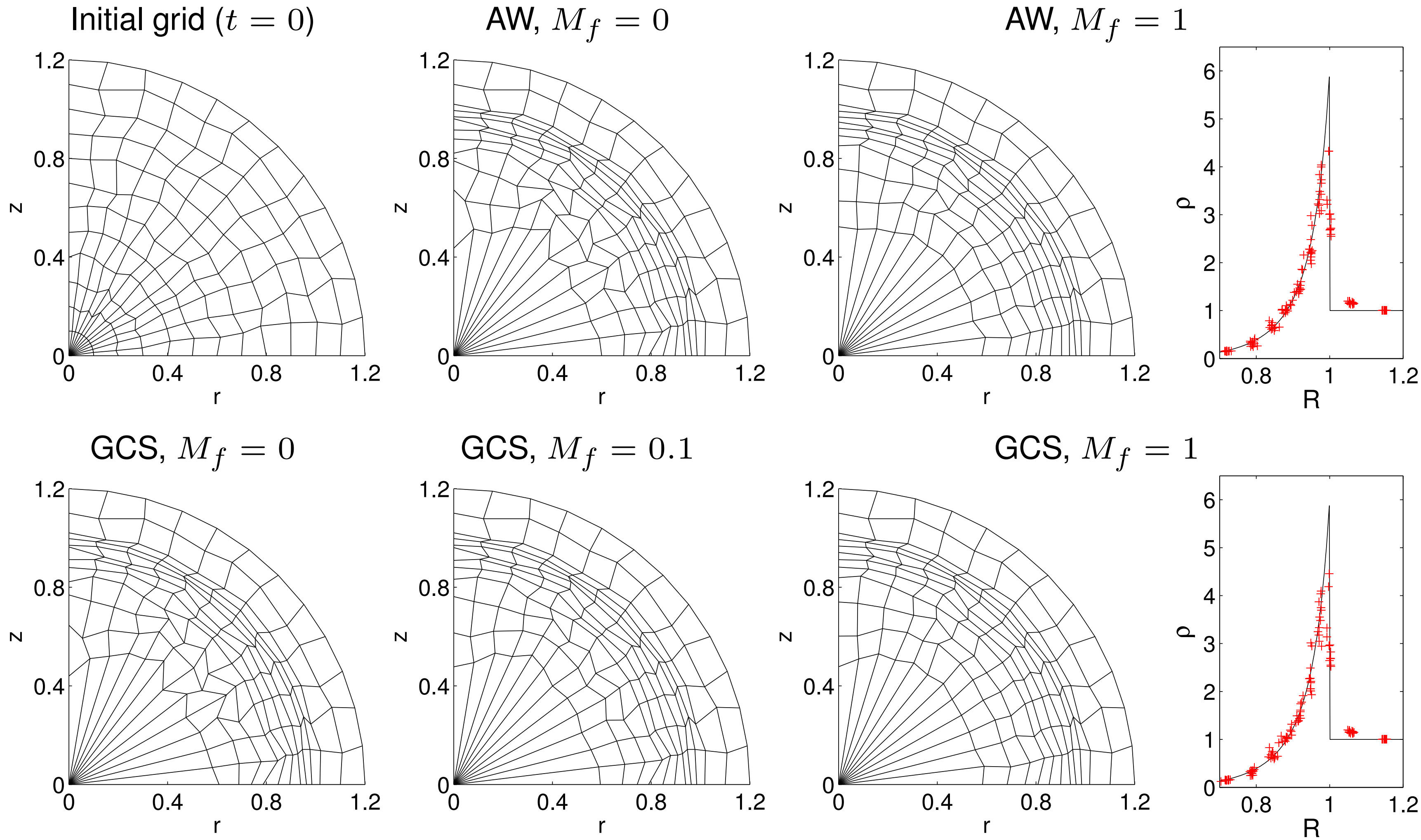




All plots do overlap!

$\Rightarrow$ **measuring the density error by the relative L_1 norm**
(and in fact by any norm except for the Maximum norm)
is a bit misleading

Numerics: GCS subcells, Sedov on perturbed grid



Conclusion

- **Developed a new staggered Lagrangian r-z scheme GCS that**
  - **conserves total energy**
  - **preserves spherical symmetry for symmetric problems**
    (unlike the existing GC scheme)
  - **keeps the violation of the Geometric Conservation Law small**
    i.e., has more accurate entropy for a particular adiabatic test problem than AW, GC and CV
- **Demonstrated natural incorporation of subcell pressure forces**
  (to prevent / damp unwanted deformations like hourglassing)
- **Performed standard tests to assess the functionality of the scheme**
- **Studied convergence and error evolution in various quantities**
  on the Coggeshall adiabatic compression problem

BONUS: Wall heating removal by energy exchange

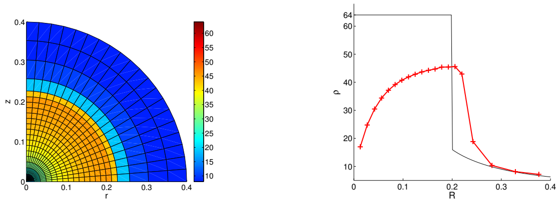
- **Tired of seeing wall heating over and over?**
- **Add a special form of the "heat conduction" as proposed by Noh (seen anywhere else?):**

  The current energy update $\varepsilon_c^{n+1} = \varepsilon_c^n + \frac{\Delta t}{m_c} W_c,$ **with W_c being the viscous work,**

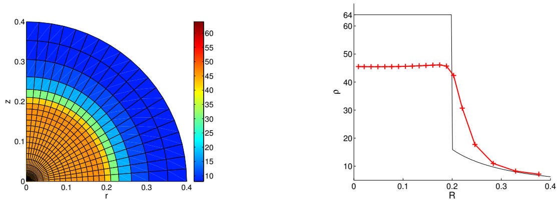
  will be replaced by $\varepsilon_c^{n+1} = \varepsilon_c^n + \frac{\Delta t}{m_c}\left(W_c + L_c\right),$

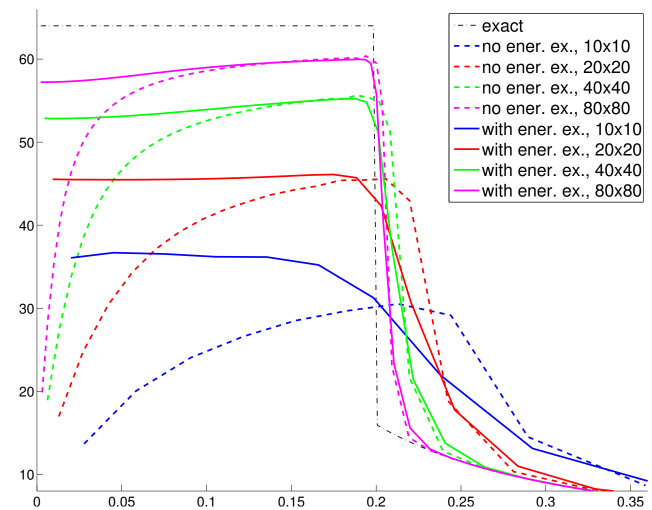
  where $L_c(\varepsilon)$ is a Laplacian type operator on ε: $L_c = \sum_{e(c)} \sigma_e \, r_e \, \|\mathbf{l}_e\| (\varepsilon_{c'} - \varepsilon_c)$.
- Above, $\|\mathbf{l}_e\|$ is the length of the edge tangent vector (and thus also of the edge), and σ has the dimension of ρ times $\mathbf{U}$ (e.g., the average Kuropatenko module of adjac. cells c, c')
- **Noh Problem:**

20×20 cells, NO ENERGY EXCHANGE



20×20 cells, WITH ENERGY EXCHANGE





Acknowledgments

Many fruitful discussions with
Misha Shashkov on AW schemes
and Pierre-Henri Maire on r-z schemes
are highly appreciated

More Info

- First derivation and description of the GCS scheme in **[Proceedings of WCCM XI, ECCM V, ECFD VI, Barcelona 2014]**, also available as **[Los Alamos Technical Report LA-UR-14-21791]**
- Full paper including subcell pressure forces **submitted to [Journal of Computational Physics]**