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Corner gradient reconstruction (CGR) and the reduction of dissipation in Lagrange cell-centered hydrodynamics (CCH)

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LANL ASC & LDRD programs

Our principal goals are to reduce dissipation in cell-centered hydro (CCH) and to improve accuracy in ALE schemes

Motivation:

Cell centered hydro (CCH) schemes produce excellent results on many test problems, but appear too dissipative on others

Similarly, swept face advection is satisfactory for many problems, but it performs poorly on others

We wish to:

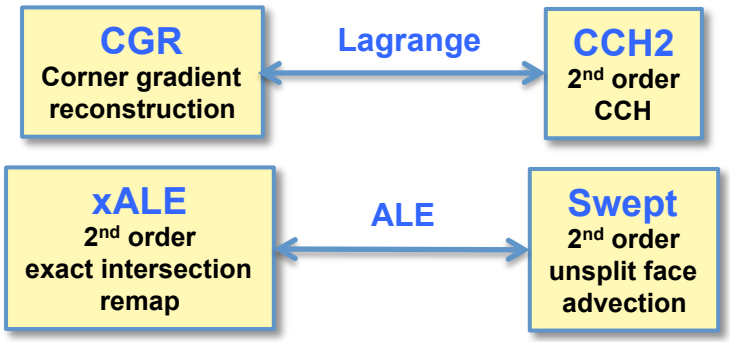
Reduce dissipation in CCH by introducing a new variation called Corner Gradient Reconstruction (CGR**)

Improve smooth flow solutions without degrading those with shocks

Achieve higher order accuracy within the framework of linear cell faces

Although we focus on our particular implementation (CCH2*), the method should be beneficial in other CCH formulations

We will contrast CGR & xALE* with previous methods:**



* C&F 2012
** JCP 2015
*** MultiMat 2013

Motivation: CCH2 dissipates kinetic energy in shockless problems such as an elastic bending plate

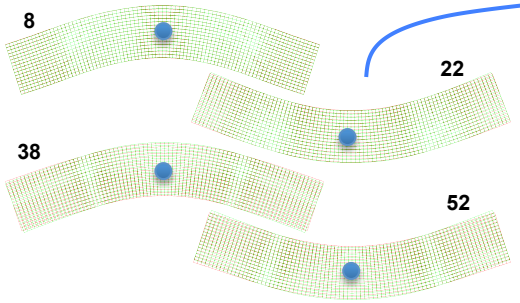
Large deformation of an elastic Be Plate
Initial velocity field activates only first flexural mode
80x16 cells
Times are near maxima of displacement

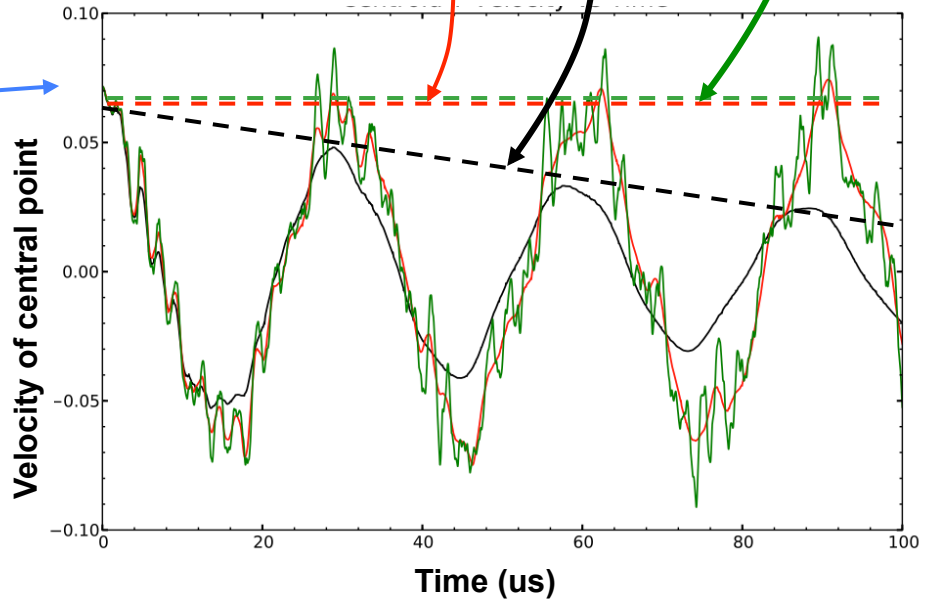
Reference: SGH with Q artificially set to 0 – impractical, but possible for smooth flow. Noisy, but does not dissipate kinetic energy

CCH2: Loses amplitude and is clearly more dissipative

CGR: Free of excess dissipation Amplitude essentially constant

The amplitude should not decrease





Weseloh, Pagosa Sample Problems, 2011

Lagrange CCH overview: There are three steps of interest - Note that "conservation" has 2 different contexts

Finite volume method: Cell averages are found by integrating surface fluxes

$$M_z \dot{\mathbf{u}}_z = \oint_z d\mathbf{N} \cdot \sigma \rightarrow \sum_i^z \mathbf{N}^i \cdot \sigma_p^i$$

The challenge in CCH is the determination of the surface fluxes $\mathbf{u}_p \,\&\, \sigma_p$

Conservative reconstruction: Finite volume provides no information about the distribution of quantities within a cell.

Infer a distribution by fitting to adjacent cells & requiring conservation within the cell

$$V_z \mathbf{u}_z = \oint_z \mathbf{u}(\mathbf{x}) dV$$
$$V_z \sigma_z = \oint_z \sigma(\mathbf{x}) dV$$

This yields discontinuous values of at the cell surface $\mathbf{u}_c \,\&\, \sigma_c$

CGR differs from traditional CCH2 only in the reconstruction

Flux conservation requires the sum of the fluxes at nodes to vanish

$$\sum_i^p \mathbf{N}^i \cdot \sigma_p^i = 0$$
$$\sum_i^p \mathbf{N}^i \cdot \mathbf{u}_p^i = 0$$

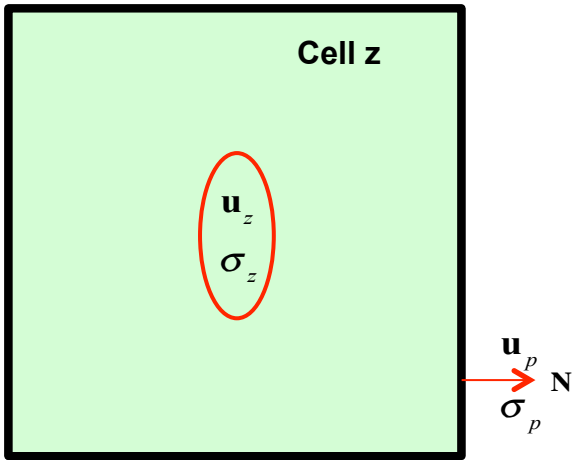
A dissipation relation enforces the 2nd law

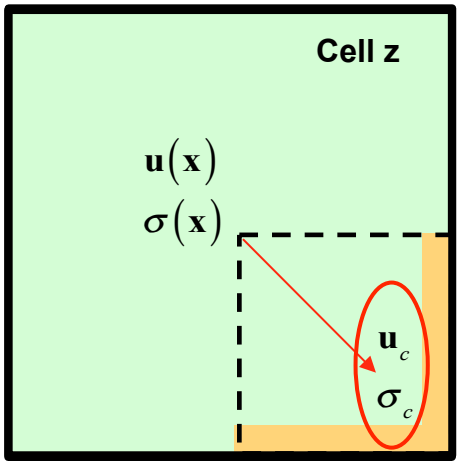
$$\mathbf{N} \cdot (\sigma_p - \sigma_c) \cdot (\mathbf{u}_p - \mathbf{u}_c) \geq 0$$

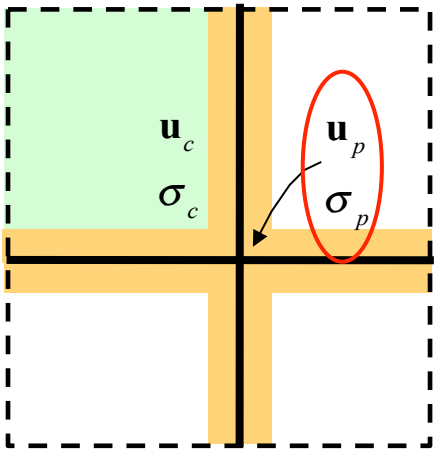
An approximate Riemann solution determines the fluxes

$\mathbf{u}_p \,\&\, \sigma_p$

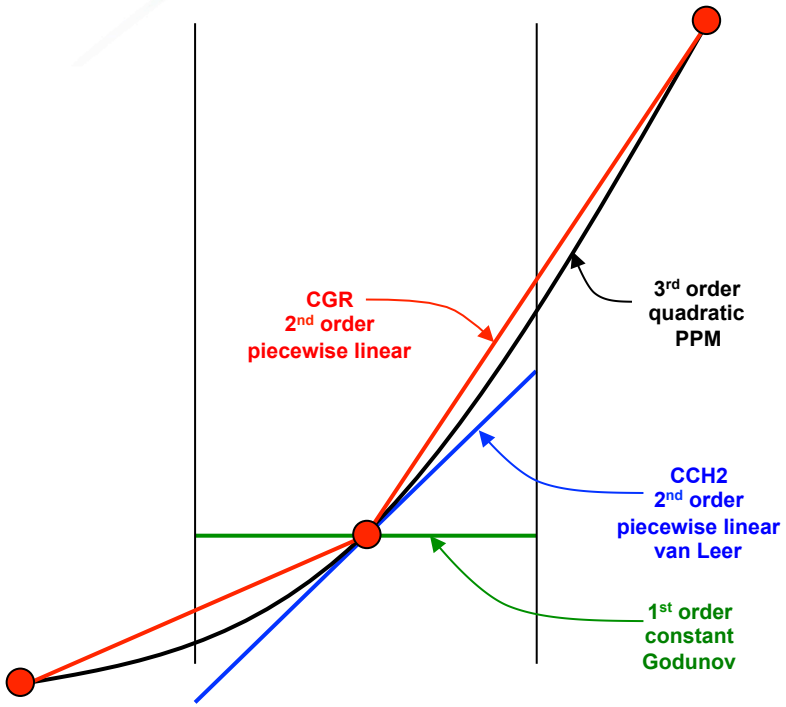
& completes the cycle







Now consider some alternative polynomial reconstructions for the Lagrange phase*



PPM-like (black) is 3rd order and the most accurate

However, 3D requires an expensive solution to a 10 equation system for each of 3 velocity components and 6 stress components

$$u^k(\mathbf{x}) = u_o^k + a_1^k\delta x + a_2^k\delta y + a_3^k\delta z + a_{11}^k\delta x^2 + a_{22}^k\delta y^2 + a_{33}^k\delta z^2 + a_{12}^k\delta x\delta y + a_{13}^k\delta x\delta z + a_{23}^k\delta y\delta z$$

CCH2 (blue) uses the traditional 2nd order reconstruction

Requires only Cramer's rule.

Corner gradient reconstruction (CGR - red) uses a piecewise linear fit between cell averages

Also requires only Cramer's rule

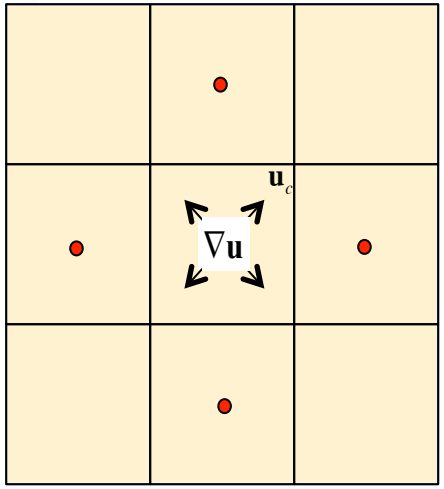
Although formally 2nd order, CGR is a much closer representation of the 3rd order function

CGR captures a 3rd order characteristic: differing slopes within a cell

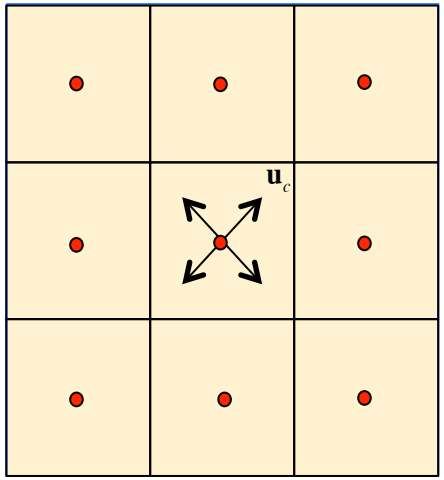
* The notion of "reconstruction" is common in Eulerian advection, but seldom thought about in the Lagrange step

For regular grids in 2D, the stencils for the reconstruction polynomials reduce to:

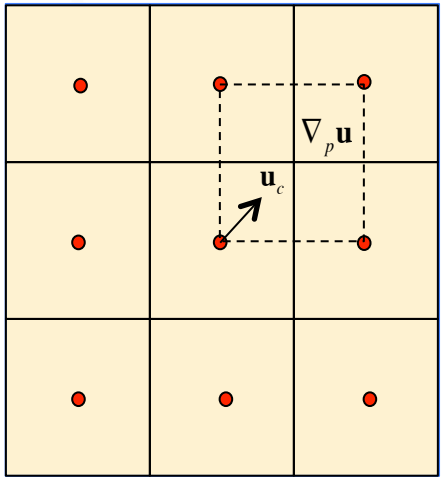
CCH2 uses a 4 point stencil and is inaccurate at the corners

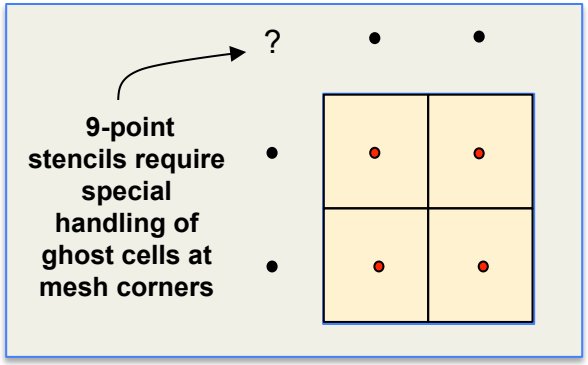


3rd order uses a 9-point stencil is more accurate at the corners than 2nd order



CGR stencil is effectively 9-point and is more accurate at the corners than 2nd order





When should dissipation occur?
Smooth flows should not dissipate

Our goal is the reduction of dissipation, not necessarily the most accurate polynomial reconstruction

We need a numerical notion of "smooth flow"

Consider velocity

Fit a polynomial across a cell and its neighbors (red) such that the integral is conserved:

$$V_z \mathbf{u}_z = \oint_z \mathbf{u}(\mathbf{x}) dV$$

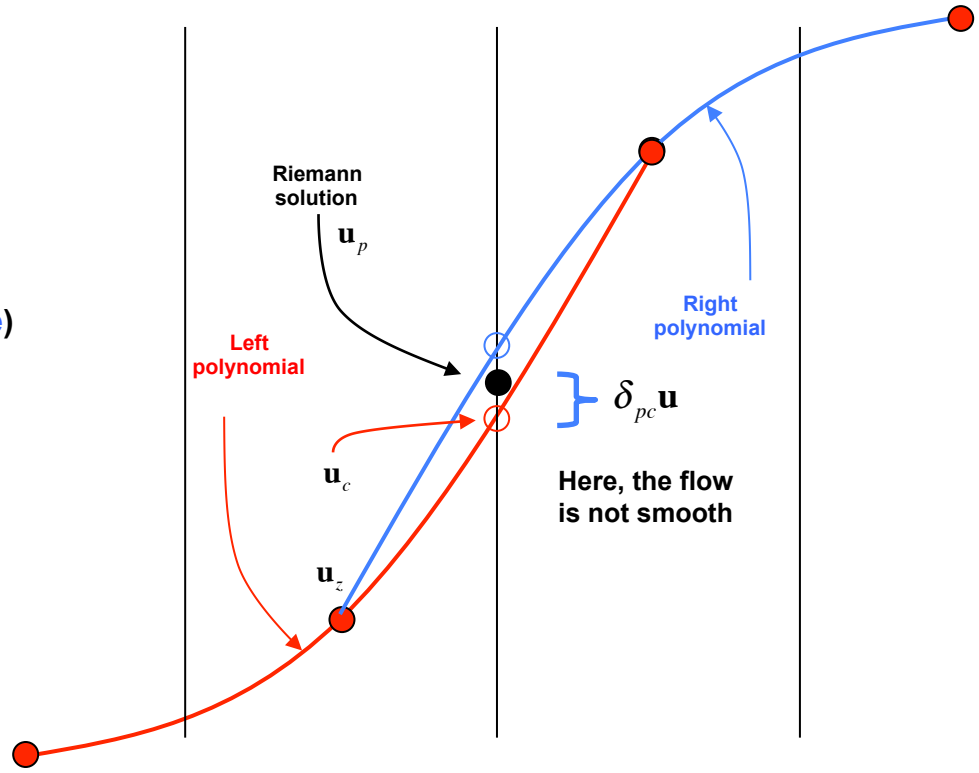
Then do the same for an adjacent cell (blue)

If the polynomials are coincident at the interface,
the flow is locally smooth

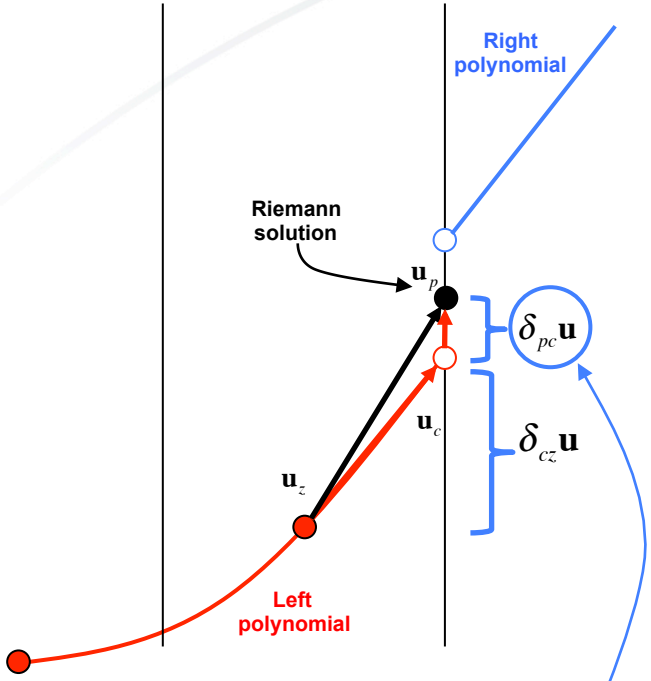
and there should be no dissipation

If not, the discontinuity
is the source of dissipation

and is resolved by an approximate Riemann solution that yields $\delta_{pc}\mathbf{u}$



How does the discontinuity affect the total energy and the decomposition into kinetic and internal energy?



The surface fluxes can be decomposed into a reconstruction and a discontinuity

$$\mathbf{u}_p = \mathbf{u}_z + \delta_{cz}\mathbf{u} + \delta_{pc}\mathbf{u}$$
$$\sigma_p = \sigma_z + \delta_{cz}\sigma + \delta_{pc}\sigma$$

With this substitution,

the total energy rate equation can then be exactly decomposed into a sum of kinetic $\dot{K}_z$ & internal $\dot{E}_z$ contributions

$$\dot{T}_z = \oint_z \mathbf{dN}\cdot\left(\sigma_p\cdot\mathbf{u}_p\right) = \dot{K}_z + \left[\dot{W}_z + \dot{R}_z + \dot{D}_z\right]$$

in which

Kinetic energy	$\dot{K}_z = \left[\oint_z \mathbf{dN}\cdot\sigma_p\right]\cdot\mathbf{u}_z = \dot{\mathbf{U}}_z\cdot\mathbf{u}_z$
Reversible work due to average stress	$\dot{W}_z = \sigma_z : \left[\oint_z \mathbf{dN}\,\mathbf{u}_p\right] = \sigma_z : \dot{\Gamma}_z$
Work due to the reconstruction	$\dot{R}_z = \oint_z \mathbf{dN}\cdot\left(\delta_{cz}\sigma\cdot\delta_{pc}\mathbf{u} + \delta_{cz}\mathbf{u}\cdot\delta_{pc}\sigma\right)$
Irreversible dissipation	$\dot{D}_z = \oint_z \mathbf{dN}\cdot\mu\hat{\mathbf{n}}\left(\delta_{pc}\mathbf{u}\right)^2 \geq 0$

The source of dissipation lies in the $\dot{D}_z$ & $\dot{R}_z$ terms

Reconstruction reduces the dissipation by reducing the discontinuity $\delta_{pc}\mathbf{u}$

In CGR, discontinuity & dissipation occur only when "curvature" requires a shift to guarantee conservative reconstruction

In each cell corner

$$\mathbf{u}(\mathbf{x}) = \mathbf{u}_0 + \beta(\mathbf{x} - \mathbf{x}_z) \cdot \nabla_p \mathbf{u}$$

The left and right polynomials are initially coincident (black), corresponding to no dissipation

However, a change in slope within the cell ("curvature") requires a shift to guarantee conservation

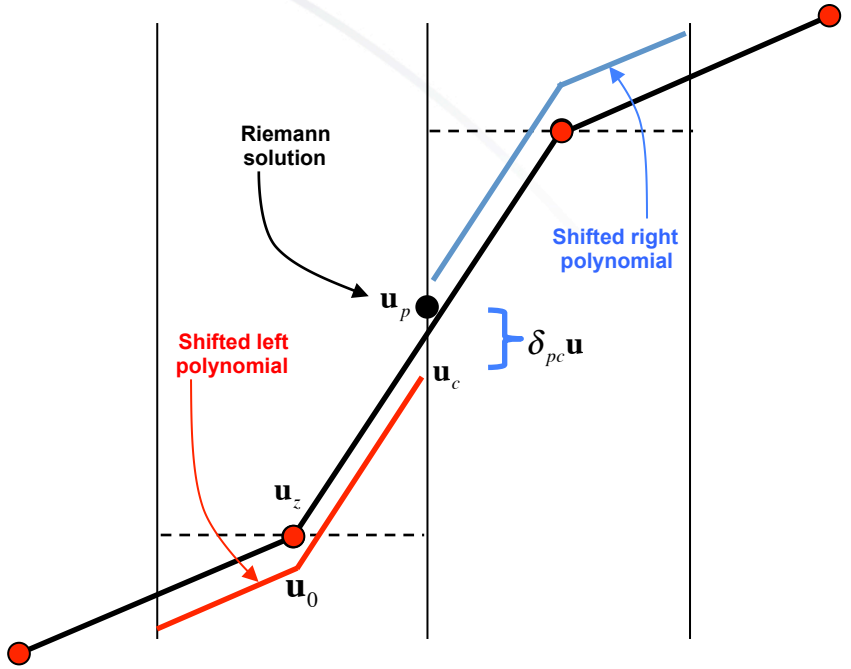
$$V_z \mathbf{u}_z = \oint_z \mathbf{u}(\mathbf{x}) dV$$

This results in a discontinuity at the interface and therefore dissipation

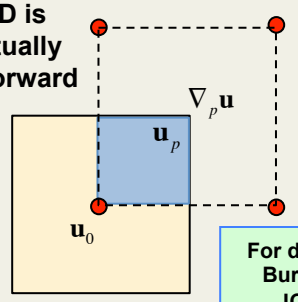
No shift occurs when the slopes within the cell are identical

Monotonicity is enforced by limiting the gradient with a Barth-Jespersen scheme.

Because the slope affects the conservation integral, the limiter β and the shift $\mathbf{u}_0(\beta)$ are coupled



Extension to 2D & 3D is conceptually straightforward



For details, see Burton et al, JCP 2015

We tested CGR (& xALE) under a wide variety of conditions

Hydro:
- Lagrange
- Swept face advection
- Exact intersection remap

Geometry:
- 1D (X)
- 2D (XY RZ)
- 3D (XYZ)

Flow:
- Smooth
- Vortical
- Shock

Meshes:
- Rectangular
- Polar
- Skewed

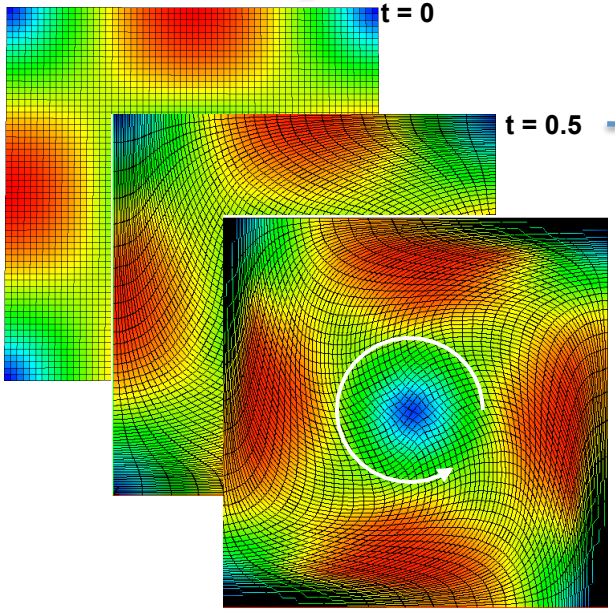
Materials:
- Fluids
- Elastic
- Elastic-plastic solids
- Elastic-plastic hardening

Problem	Dim	Geom	Mesh	Hydro	Material	Flow
Be plate	2D	XY	Square	Lag	Elastic	Smooth
Taylor-Green	2D	XY	Square	Lag	Gas	Smooth+vorticity
Coggeshall	2D	XY	Square	Lag	Gas	Smooth
	3D	XYZ	Square	Lag	Gas	Smooth
Kidder shell	2D	RZ	Polar	Lag	Gas	Smooth
	3D	XYZ	Special	Lag	Gas	Smooth
Kidder ball	2D	RZ	Square	Lag	Gas	Smooth
Howell	2D	XY	Polar	Lag	EP	Smooth
Verney	2D	RZ	Polar	Lag	EP	Smooth
	3D	XYZ	Geo	Lag	EP	Smooth
Taylor Anvil	2D	RZ	Square	Lag	EP+hardening	Shock+smooth
Sod	2D	XY	Rect	Lag	Gas	Shock
Noh	2D	XY	Polar	Lag	Gas	Shock
	2D	RZ	Polar	Lag	Gas	Shock
	2D	XY	Square	Lag	Gas	Shock
	2D	RZ	Square	Lag	Gas	Shock
	3D	XYZ	Square	Lag	Gas	Shock
Sedov	2D	XY	Square	Lag	Gas	Shock
	2D	RZ	Square	Lag	Gas	Shock
	3D	XYZ	Square	Lag	Gas	Shock
Saltzman	2D	XY	Special	Lag	Gas	Shock
	2D	RZ	Special	Lag	Gas	Shock
	3D	XYZ	Special	Lag	Gas	Shock
Adiabatic rel	1D	X	Rect	Lag	Gas	Shock+release
EP piston	1D	X	Rect	Lag	EP	Shock
Triple point	2D	XY	Square	ALE	Gas	Shock+vorticity
He bubble	2D	RZ	Rect	ALE	Gas	Shock+vorticity

SMOOTH & VORTICAL FLOW PROBLEMS

Be Beam (elastic solid)
Taylor-Green (vortical flow)
Coggeshall
Kidder shell & ball
Verney & Howell (elastic-plastic solid)
Taylor anvil (hardening EP solid)

2D Taylor Green is a test of vortical flow: CGR reduces the error & has a convergence rate approaching 3rd order



30x30 mesh

Color represents velocity magnitude

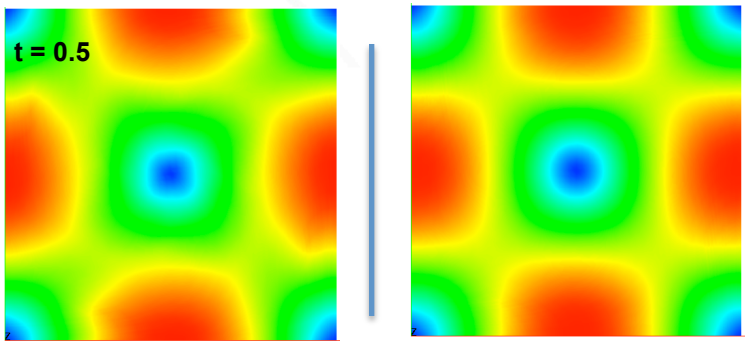
Lagrange mesh is severely deformed at t=0.75

So we look at earlier convergence t=0.25

Velocity contours should remain stationary in time

CCH2

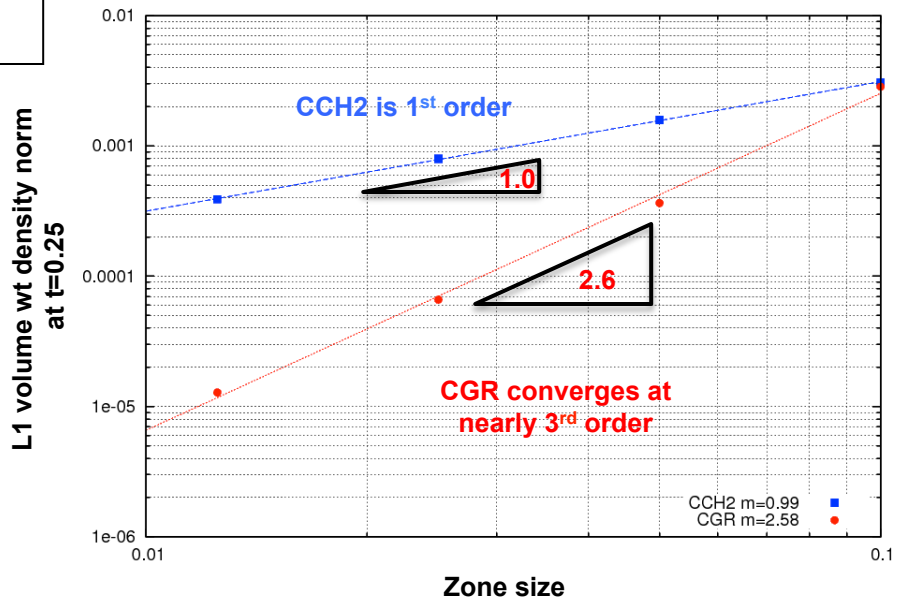
CGR is significantly better



The flow should be incompressible and the velocity field should not change with time

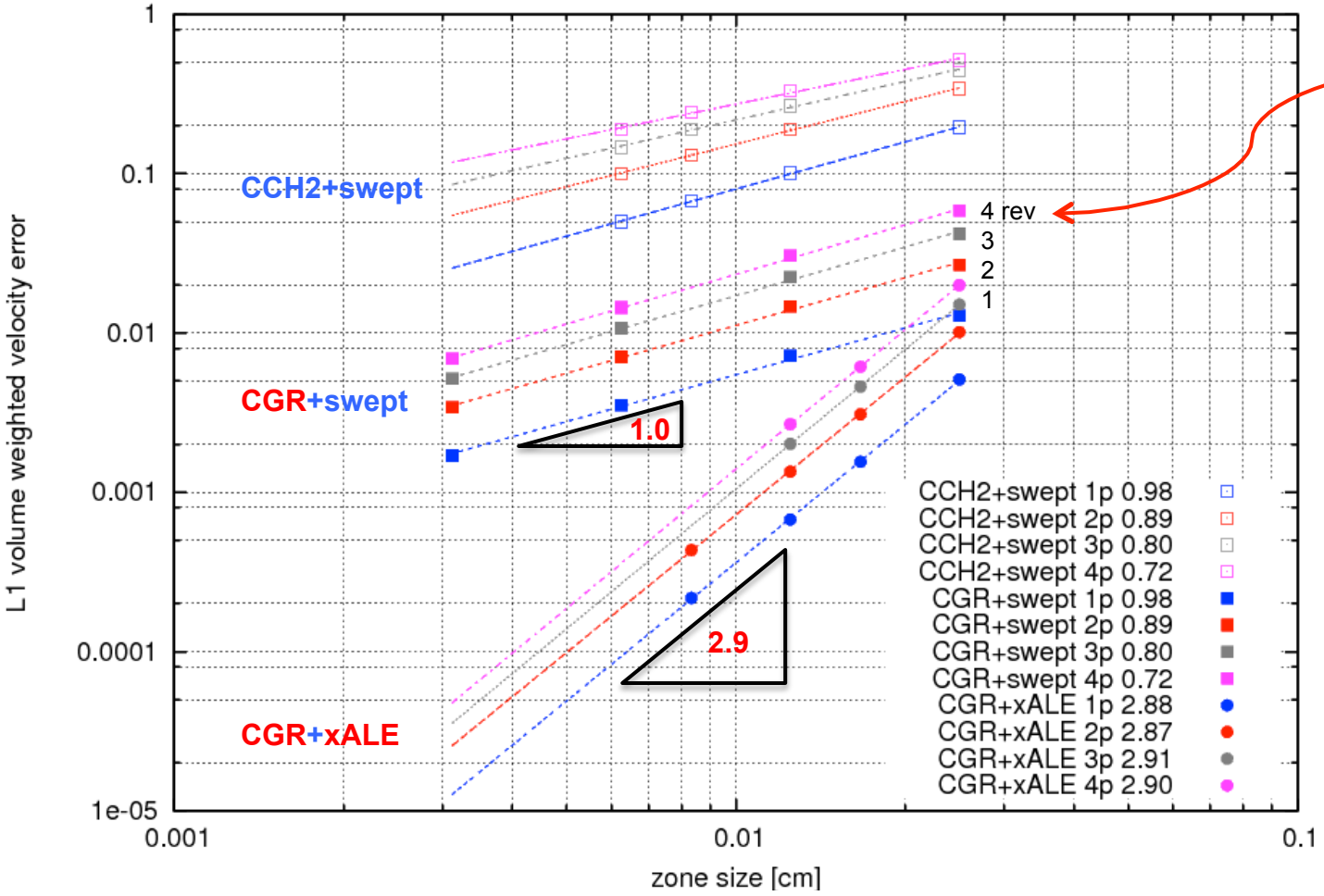
$$\mathbf{u}_0 = \{\sin(\pi x)\cos(\pi y), -\cos(\pi x)\sin(\pi y)\}$$

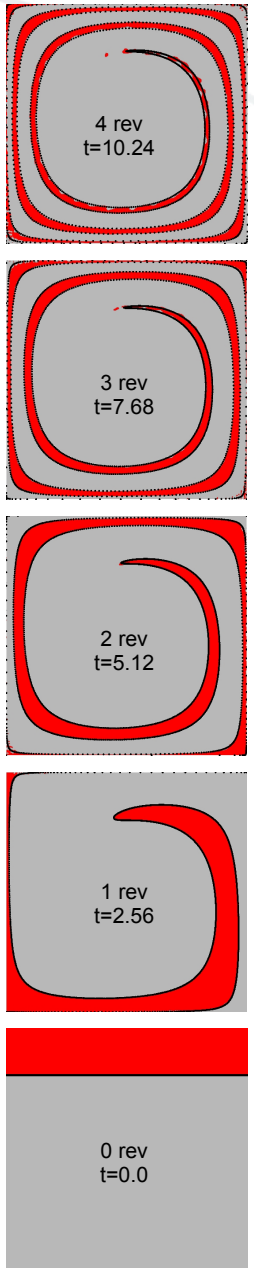
The solution also involves a time dependent energy source from a manufactured solution

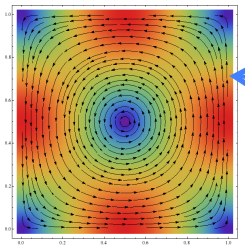


Taylor & Green, 1937
Drikakis et al, 2007
Dobrev et al 2012
Burton et al 2015

Using ALE, we can run Taylor-Green through multiple revolutions: CGR + xALE improves accuracy and convergence to near 3rd order







Related TG calculation with material interfaces to illustrate rotation.
Black is the analytic solution

Brown & Morgan 2015

Spherical Coggeshall problem on a box grid: CCH2 has large perturbations not present in CGR

Shock-free spherical compression of polytropic gas with initial linear velocity field $u_0(r)=-r_0$

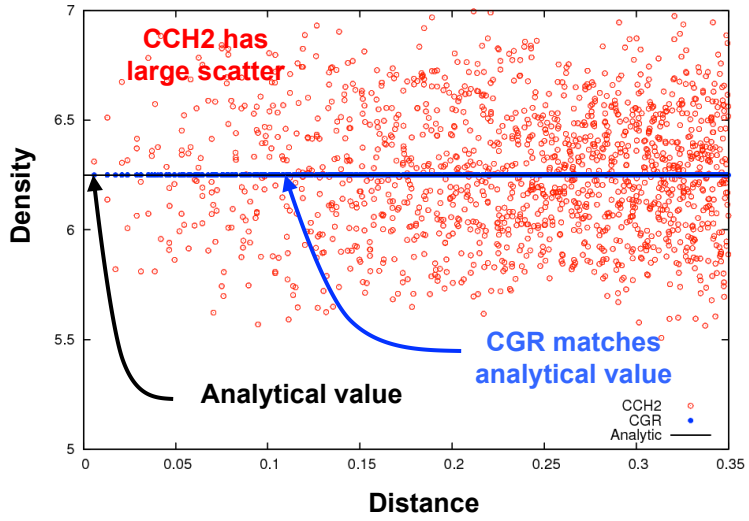
The problem is characterized by high specific kinetic energy (~1) and low internal energy (~1e-6).

Relatively small velocity perturbations give rise to large error in thermodynamic variables.

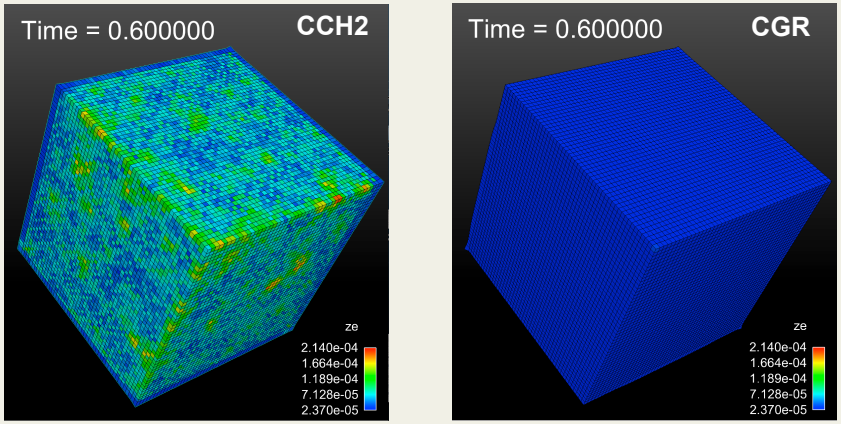
Scatter plots: one dot per cell

Exact solutions in black

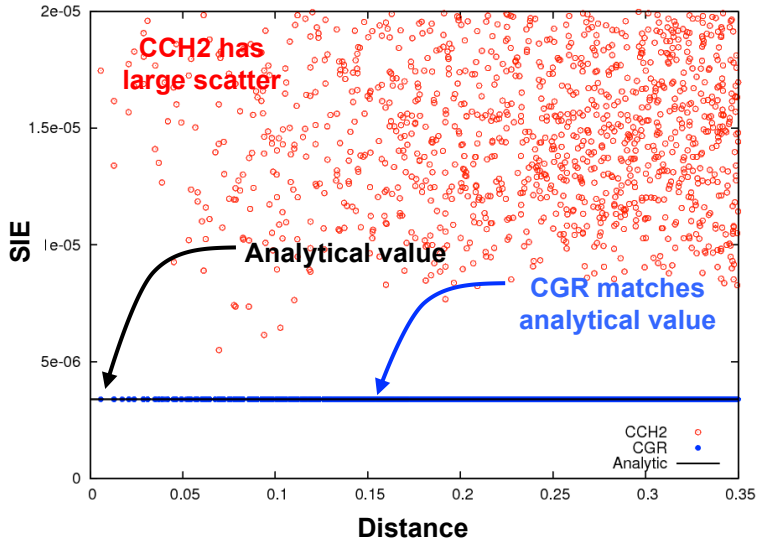
SIE = specific internal energy



3D results are similar



Mesh and SIE at t=.6 50x50x50

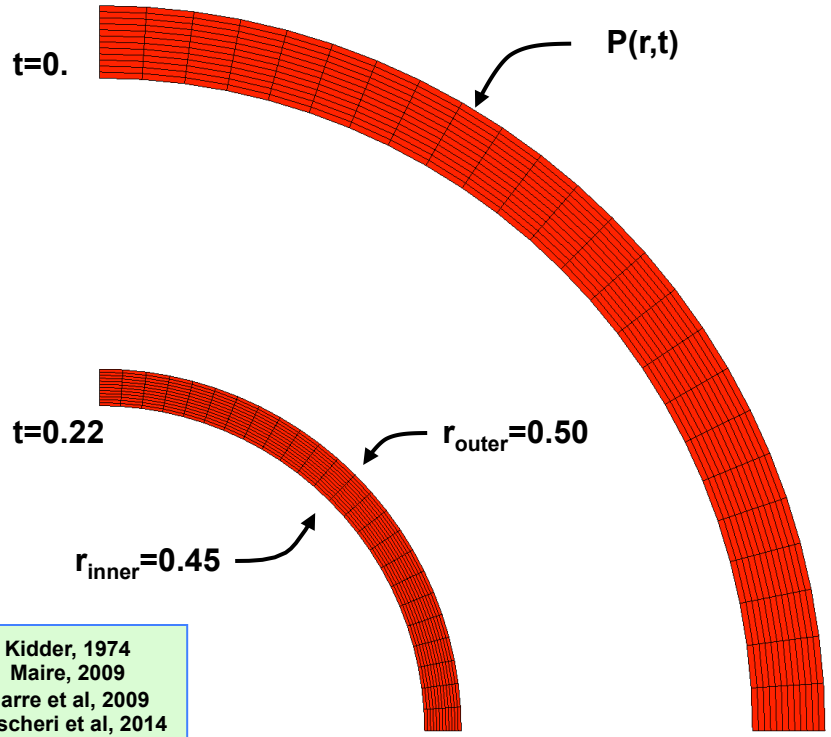


Coggeshall & Meyer ter Vehn, 1992

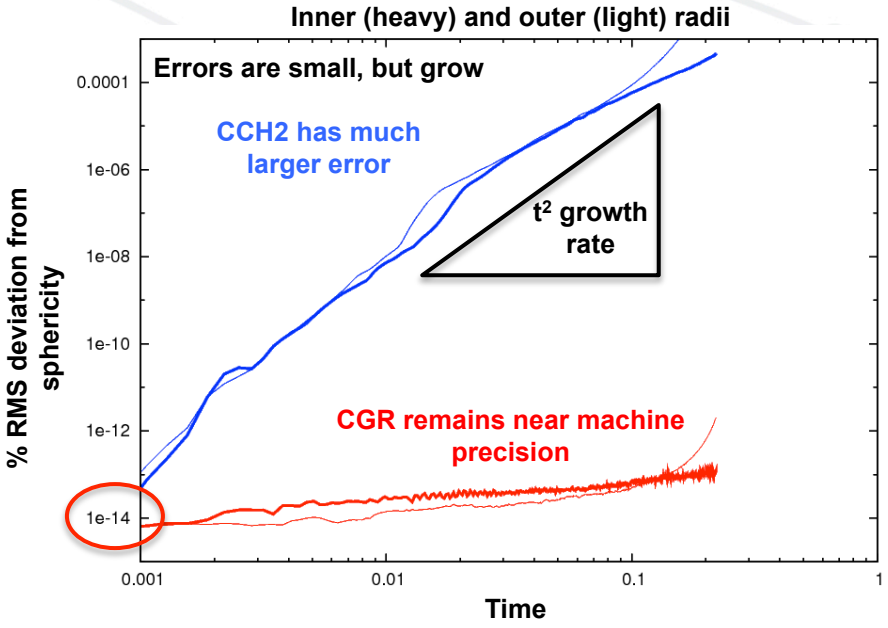
2D Kidder shell tests symmetry: Given P(r,t) at outer surface compare with analytic r(t)

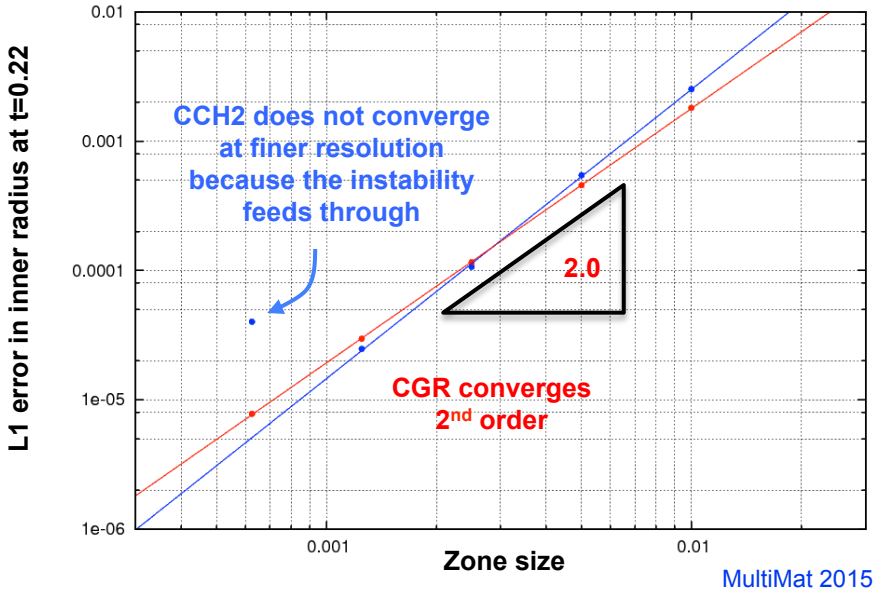
Because the surface has an Atwood number of unity, it is hydrodynamically unstable, and therefore sensitive to numerical perturbations

In 2D, near perfect grids mitigate the error



Kidder, 1974
Maire, 2009
Carre et al, 2009
Boscheri et al, 2014
Villar et al, 2014
Morgan et al, 2015
Burton et al, 2015

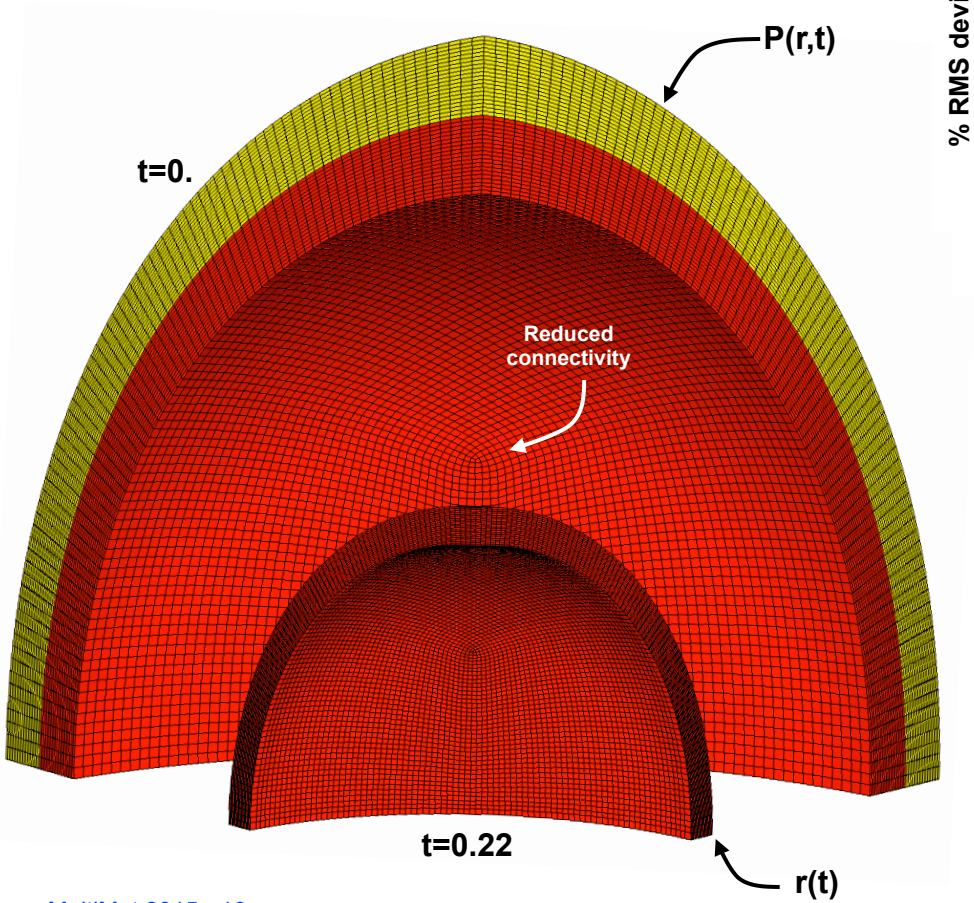


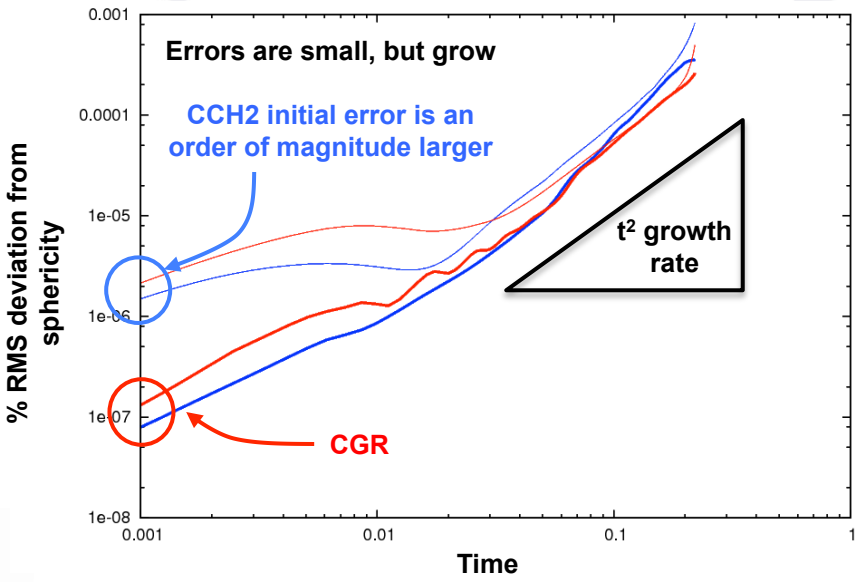


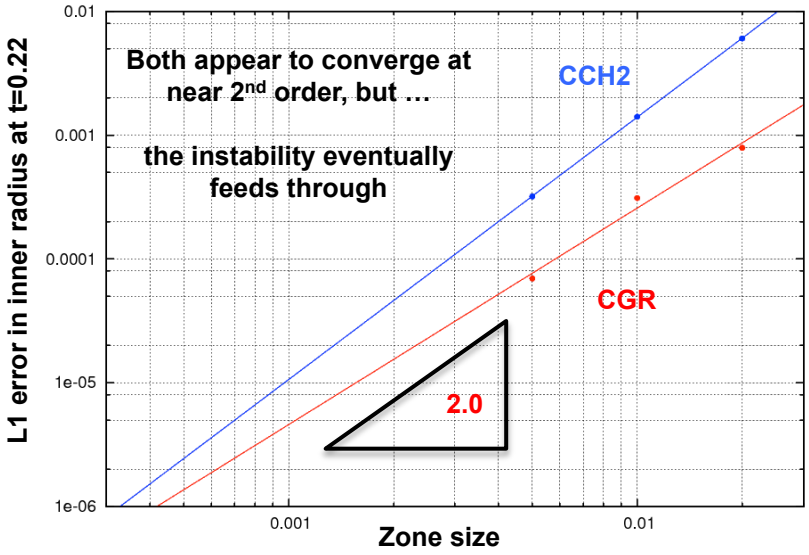
3D Kidder shell: Near perfect grids cannot be generated in 3D, resulting in much greater sensitivity to numerical error

As there exists no completely symmetrical tessellation of a sphere, numerical errors are larger in 3D

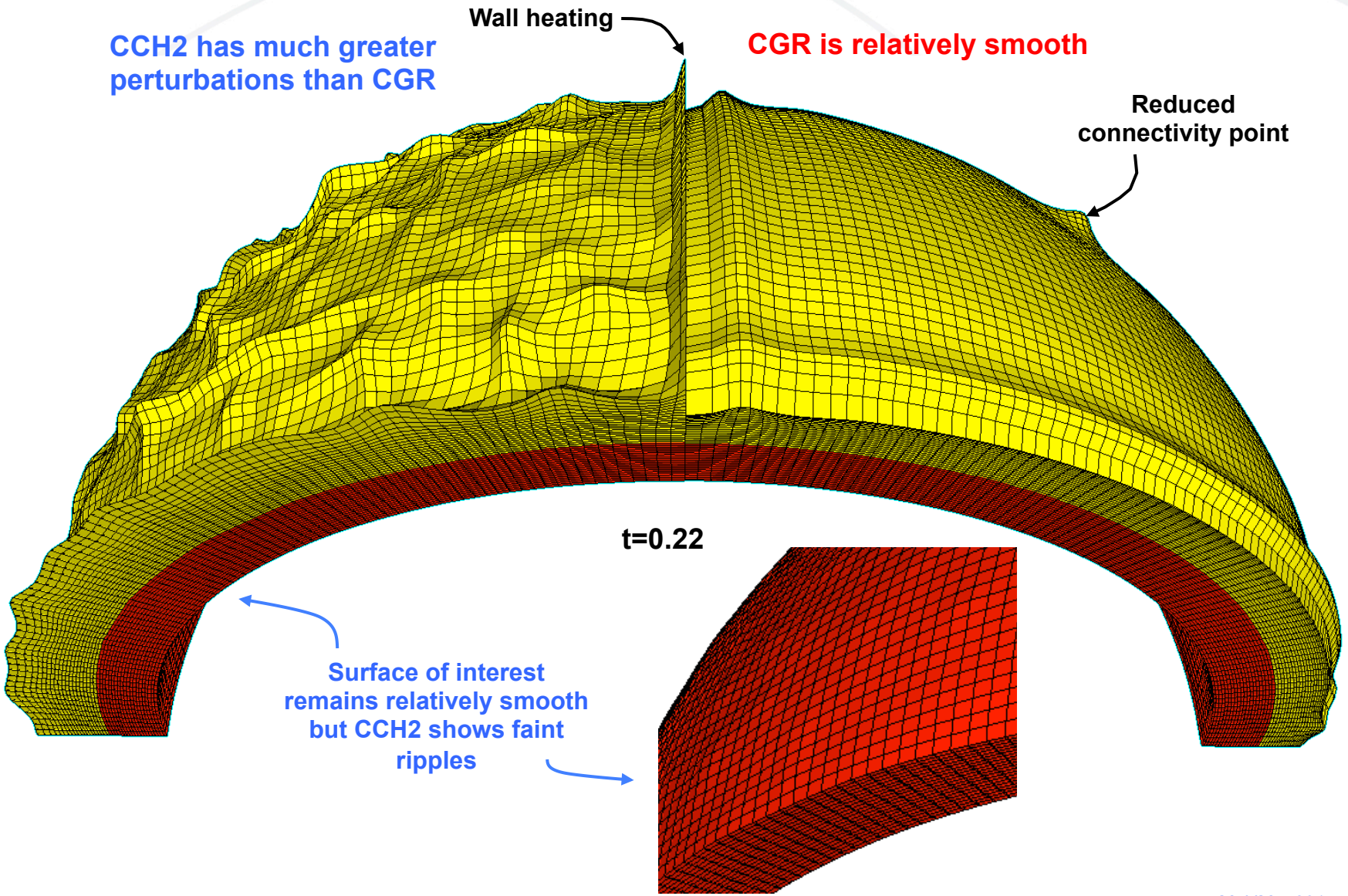
Pressure is applied at larger radius, so that the perturbations propagate inward







The outer surface is hydrodynamically unstable and is especially sensitive to the numerical perturbations of CCH2



SHOCK PROBLEMS

Sod

Noh

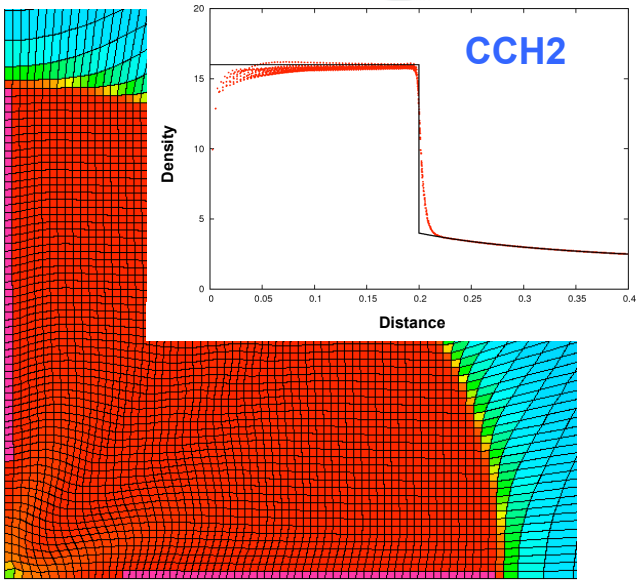
Sedov

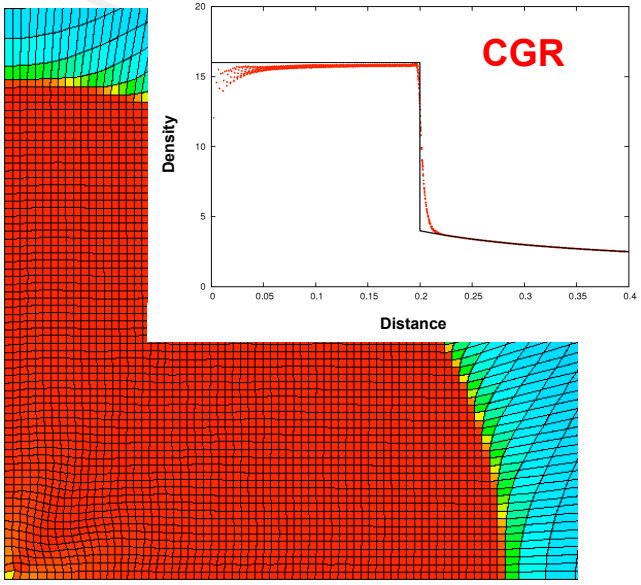
Saltzman

Elastic-plastic piston (solid)

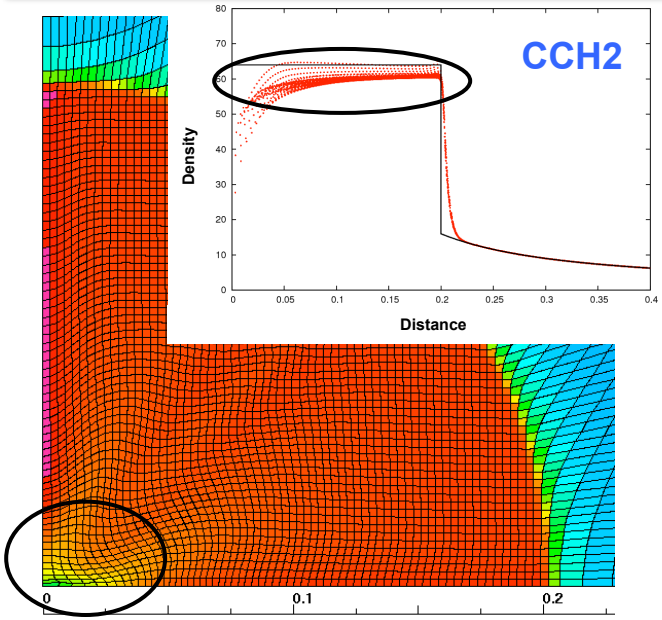
Adiabatic release

2D Noh on a box grid: results are comparable in XY, but CGR is clearly superior in RZ

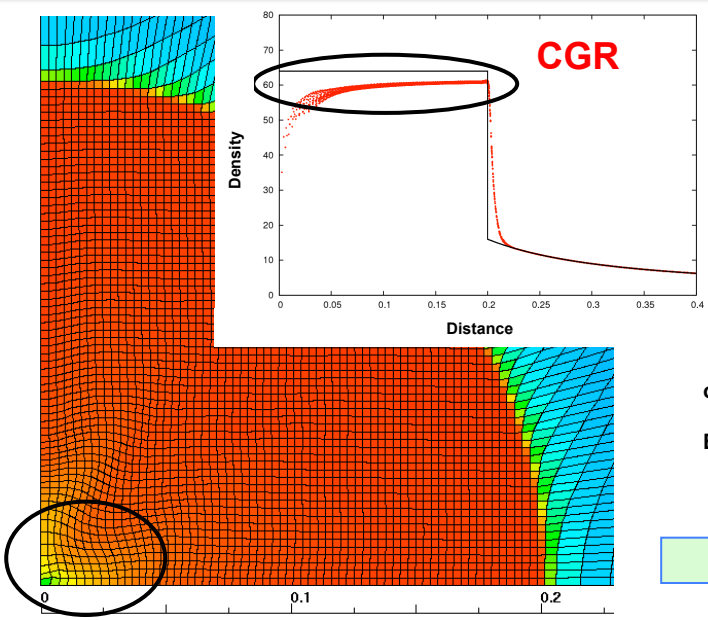




XY



RZ



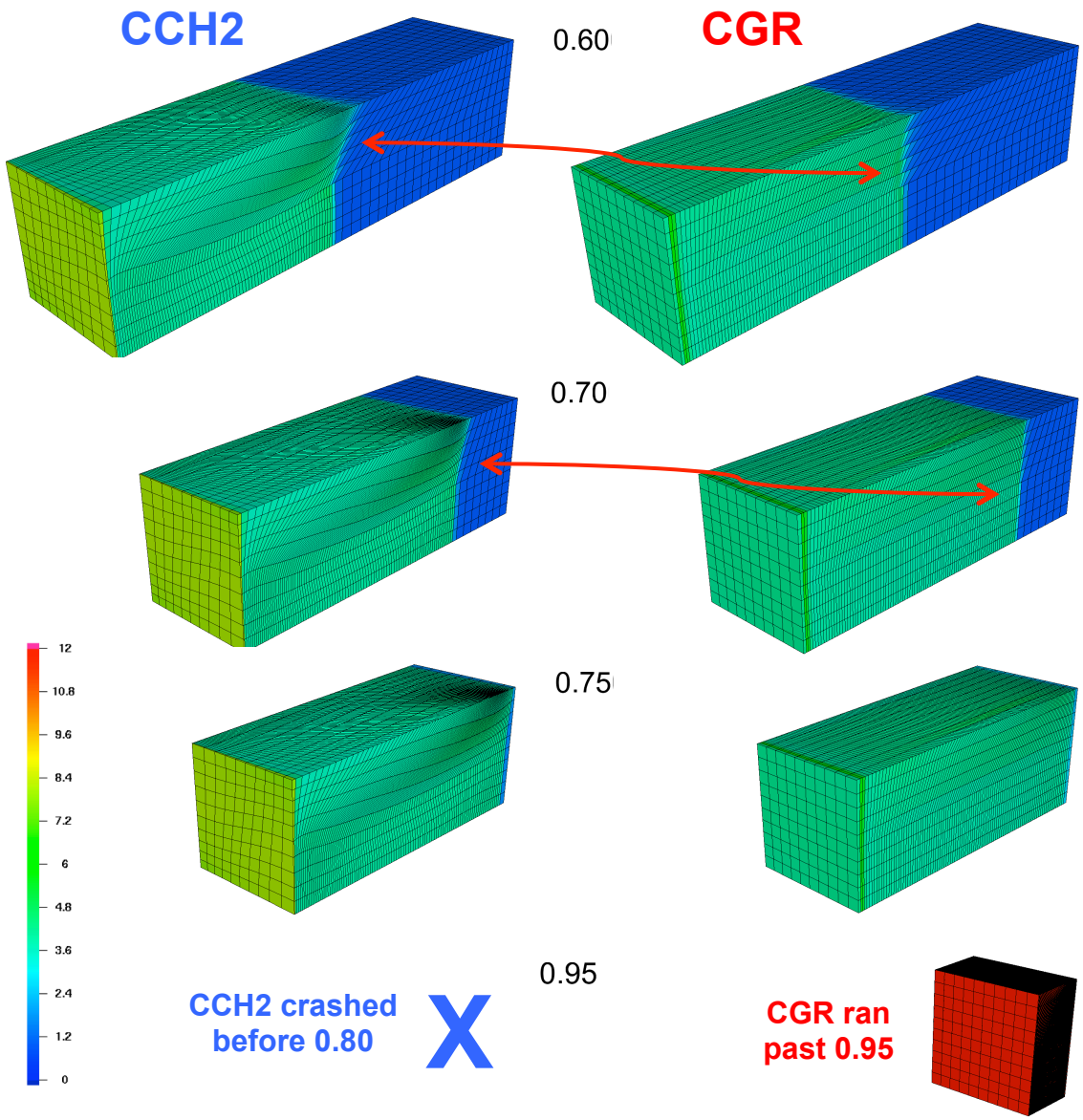
Scatter plots: one dot per cell

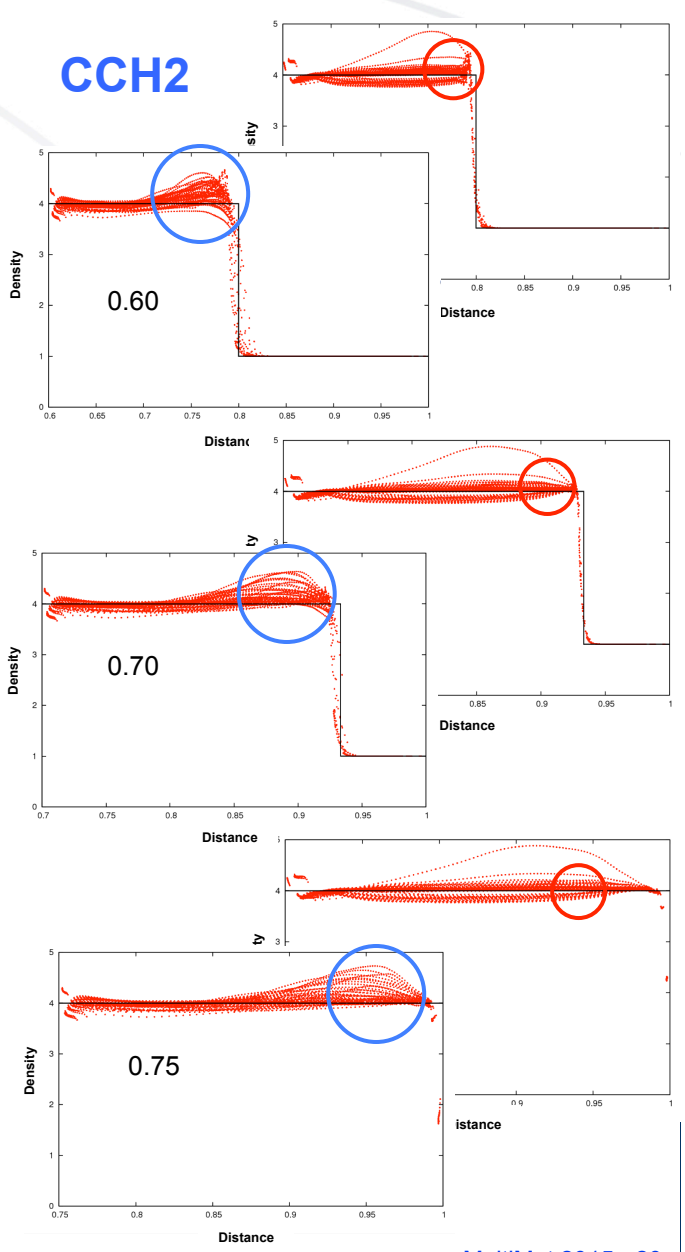
Exact solutions in black

Noh 1987

The 3D skewed Saltzman mesh causes spurious vorticity: CGR results are far superior to CCH2

Caramana et al, 1999
Maire et al, 2009
Boscheri et al, 2014
Burton et al, 2015





ALE PROBLEMS

Triple Point

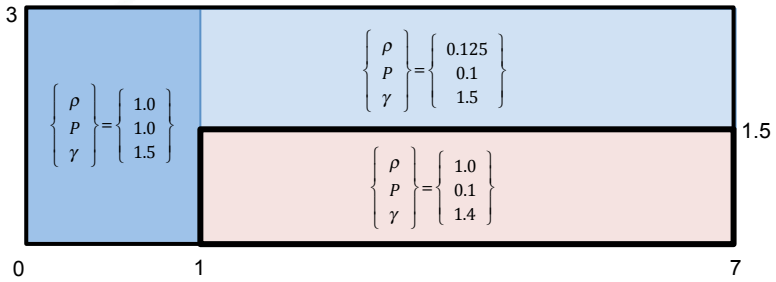
Helium Bubble

xALE is an exact intersection 2nd order remap scheme described at Multimat 2013

Swept is an unsplit 2nd order face advection scheme

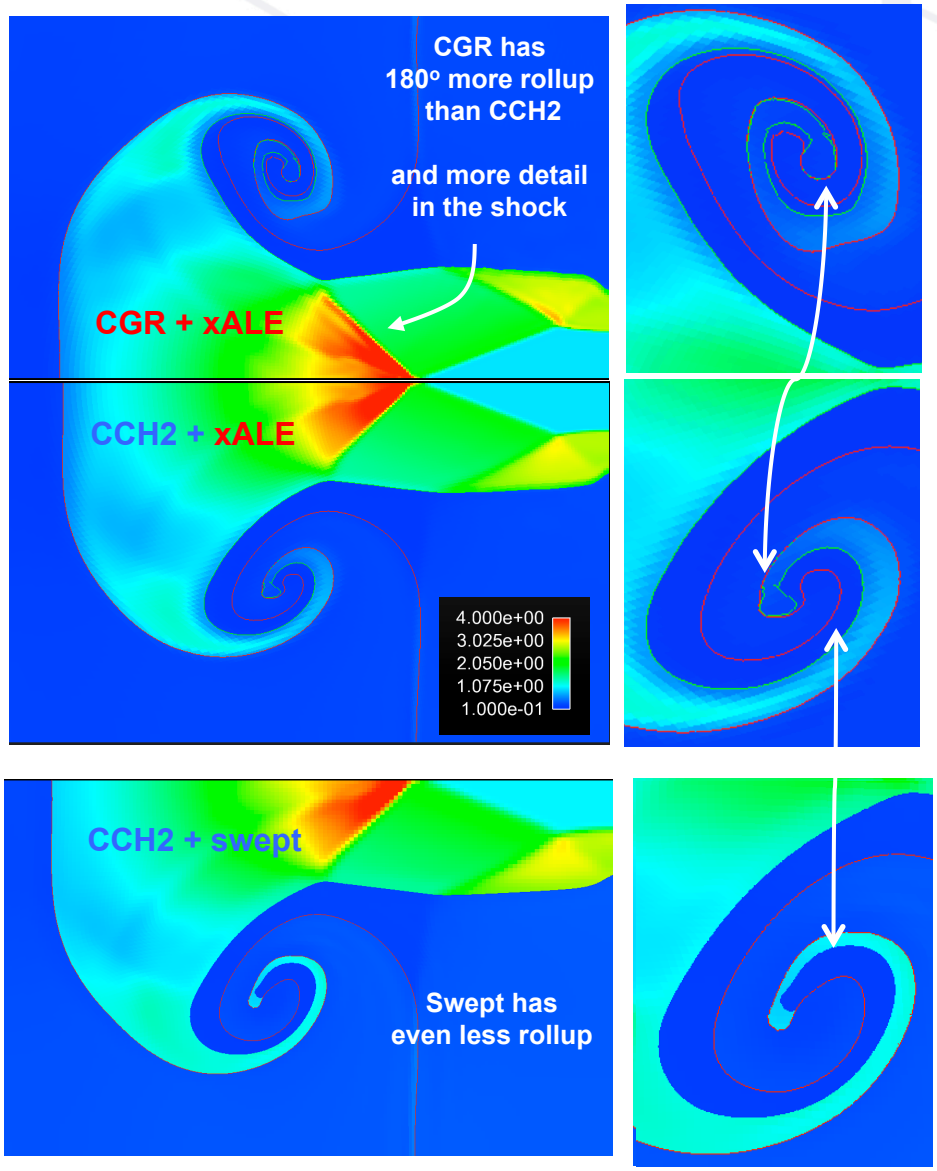
Triple point problem: The combination CGR + xALE is significantly better than CCH2 and swept alternatives

The triple point problem simulates a shock hitting a material discontinuity, producing vortical flow



Although very early flow is self-similar, there is no converged solution at late times

The rollup at t=5.0 should increase with resolution unless perturbed by numerical error, leading to Kelvin-Helmholtz instabilities



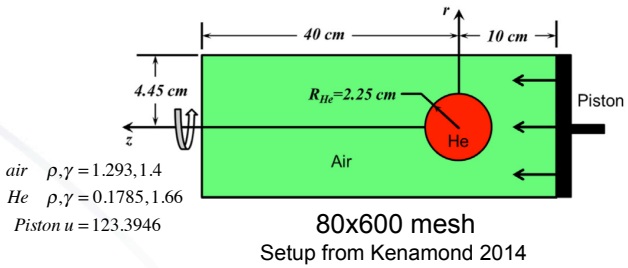
Mesh 200x100
t=5.0 density contours
Red & blue lines are material interfaces

D'yadechko, 1965
Shashkov et al, 1991
Maire, 2009
Galera et al, 2010
Loubere et al, 2010
Burton et al, 2012

Haas-Sturtevant helium bubble experiment: CGR has much less dissipation than CCH2 and a better match to data

Haas & Sturtevant 1987
Quirk & Karni 1996
Galera et at 2010
Loubere et al 2011
Kenamond et al, 2014
Burton et al, 2015

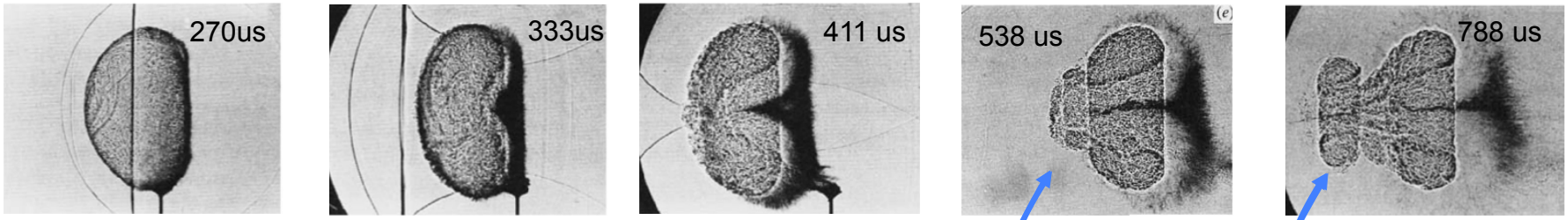
CGR matches Schlieren images much better than CCH2



80x600 mesh
Setup from Kenamond 2014

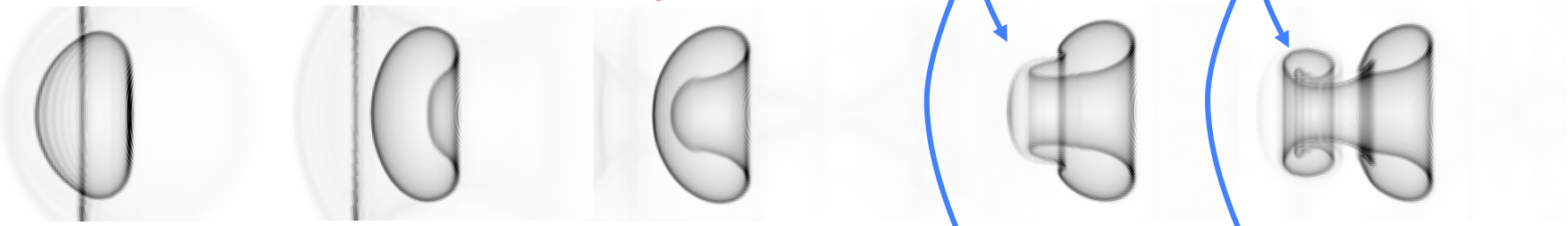
Schlieren images detect density gradient

Haas & Sturtevant JFM 1987, Fig 8

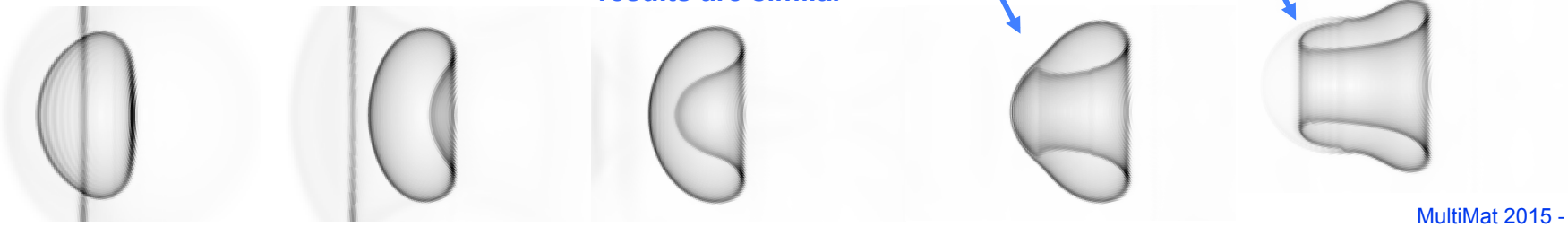


Synthetic Schlieren images

CGR + xALE



CCH2+xALE and CCH2+swept results are similar



Thoughts to take away

Our principal goal was to address excessive dissipation in CCH

- **We have done so**
- **As demonstrated on a wide variety of test problems**
- **With results that are among the best we have seen**

We introduced an extension to CCH called Corner Gradient Reconstruction (CGR)

- **CGR differs from traditional CCH2 only in the reconstruction step**
- **Conceptually simple**
- **Does not require solving large systems of equations in each cell**
- **Multi-dimensional**
- **Applicable to solids and fluids**
- **Potentially beneficial to CCH formulations other than our own**

CGR offers significant advantages over CCH2

- **Improved directional accuracy**
- **Reduction in dissipation, especially for smooth flow problems**
- **Performs comparably or better for shocks**
- **Computational cost is comparable to CCH2**

xALE exact intersection remap

- **Following up on our MultiMat 2013 presentation, we have shown that xALE performs much better than swept face advection for vortical flows such as Taylor-Green**

2D Verney (RZ) problem

Given an initial divergence free velocity field

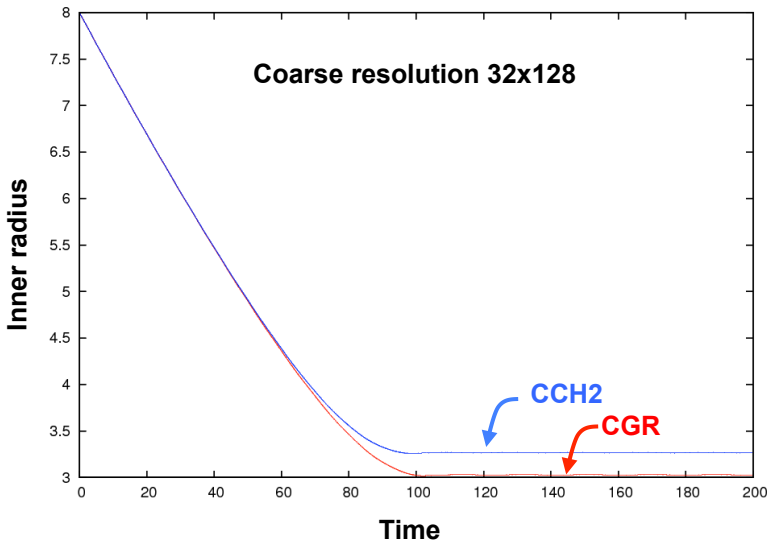
$$u(r) = u_0 \left(\frac{R_{outer}}{r} \right)^{\alpha - 1}$$

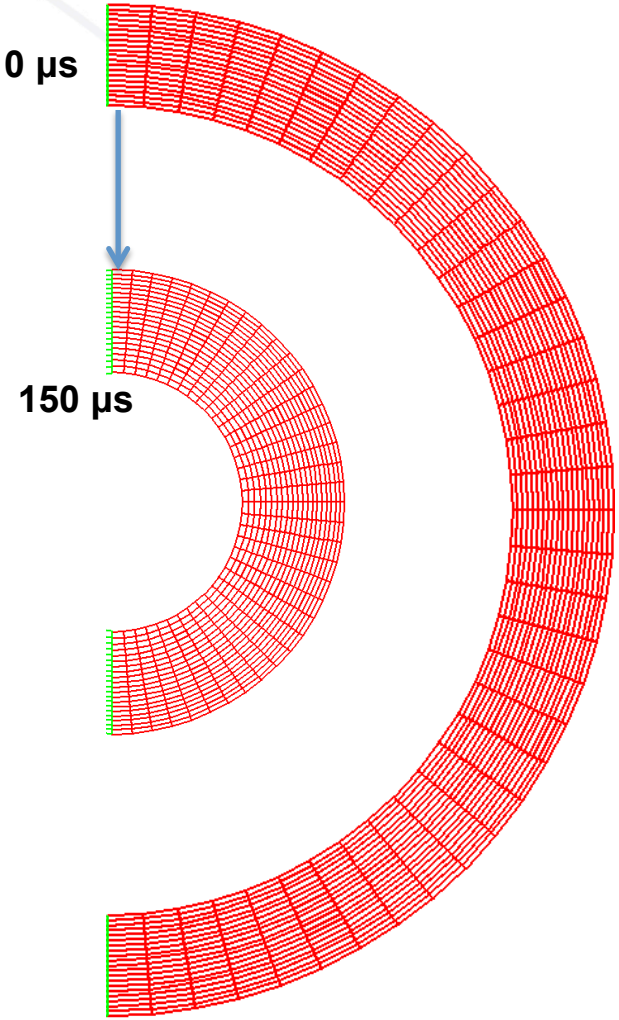
An elastic-plastic shell is initially on the yield surface

It coasts inward until the kinetic energy is dissipated by plastic work

For an INCOMPRESSIBLE material, the analytic stopping radius is 3 cm

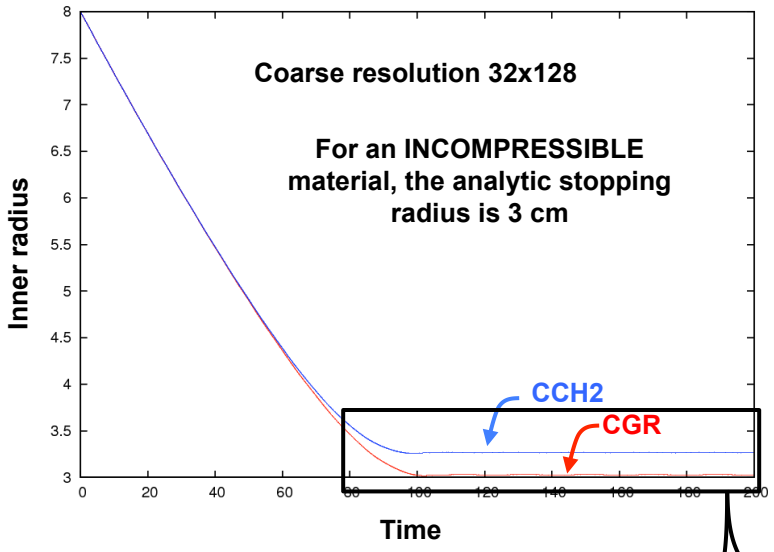
A COMPRESSIBLE material will have acoustic waves and overshoot

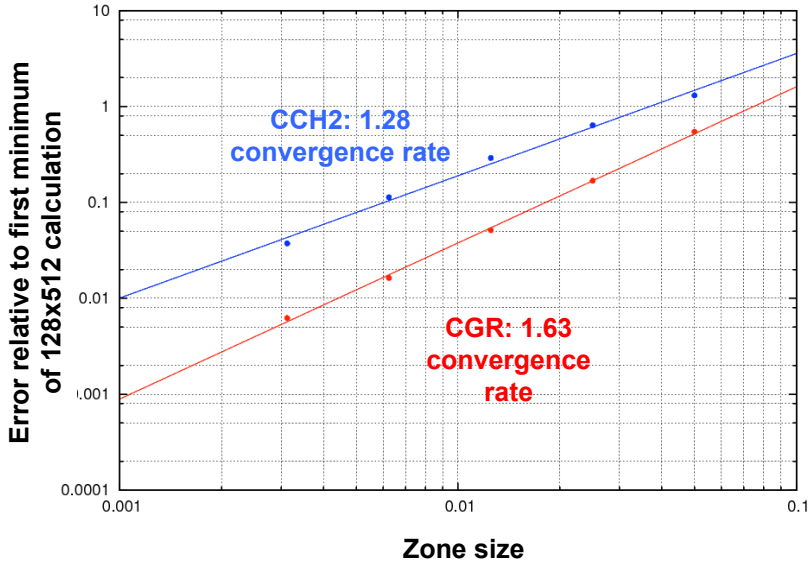


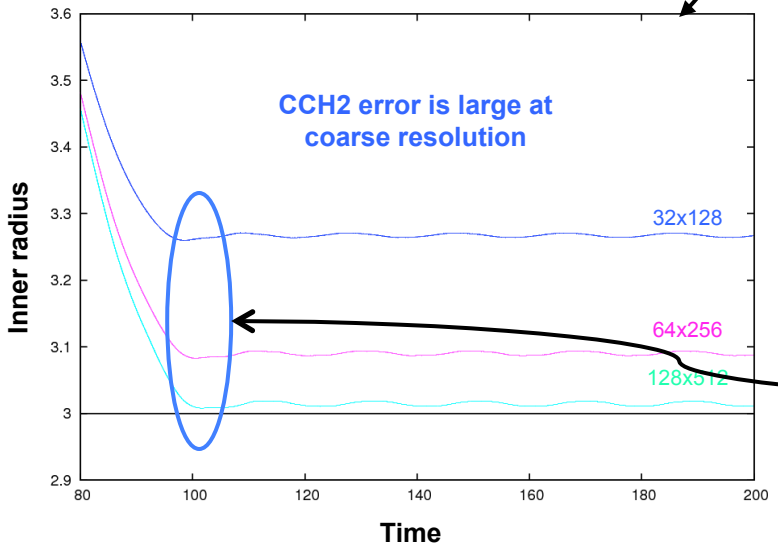


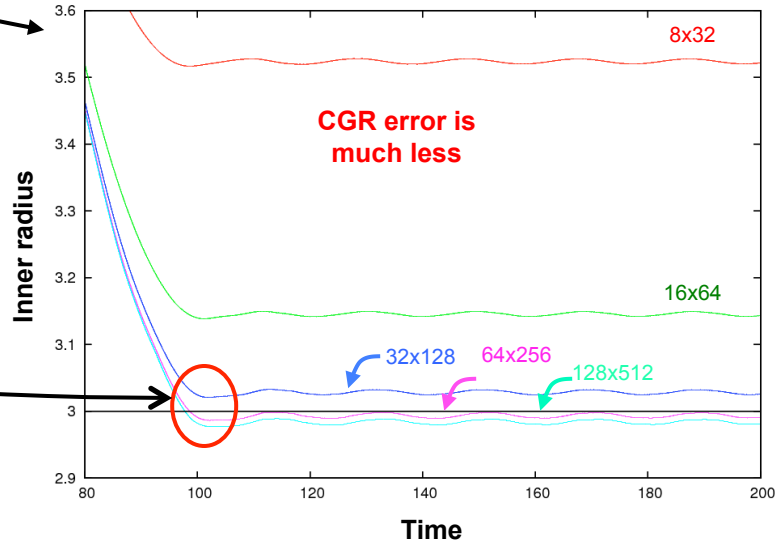
Verney 1968
Howell & Ball 2002

2D Verney
CGR has much smaller error and higher convergence rate



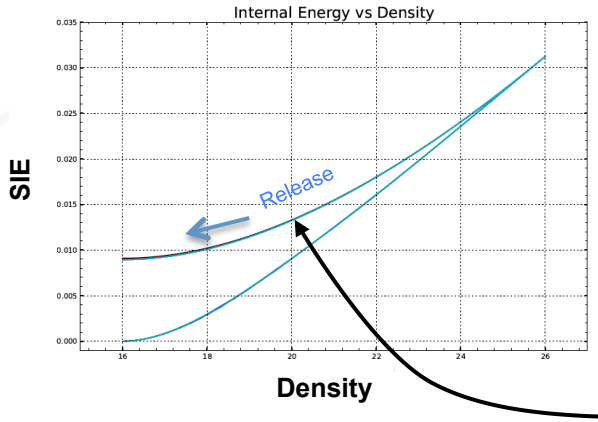






Adiabatic release problem tests the ability to track the adiabat following a shock compression

Base zoning
90 cells
$h=10^{-2}$



$$p(\rho)=\left(\frac{\rho}{\rho_0}-1\right)\rho_0 c_0^2$$

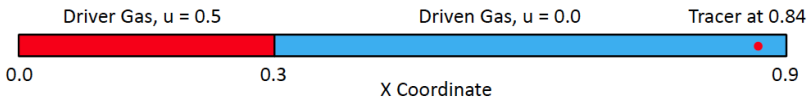
$$u_p=\frac{1}{2}u_L$$

$$p_H=\rho_0 u_p\left(c_0+u_p\right)$$

$$\rho_H=\rho_0\left(1+\frac{u_p}{c_0}\right)$$

$$e_H=\frac{p_H\left(\rho_H-\rho_0\right)}{2\rho_H\rho_0}$$

$$e_A(\rho)=e_H+c_0^2\left[\frac{\rho-\rho_H}{\rho_0}-\ln\left(\frac{\rho}{\rho_H}\right)\right]$$



Bazan & Rieben, LLNL-PRES-463883
Owen et al, LLNL-PRES-557631
Barlow 2011

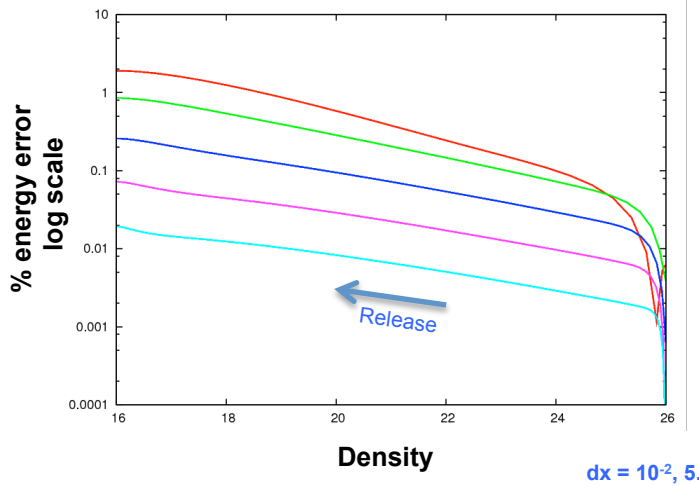
Both are the best Lagrange results we have seen

but CGR is superior to CCH2

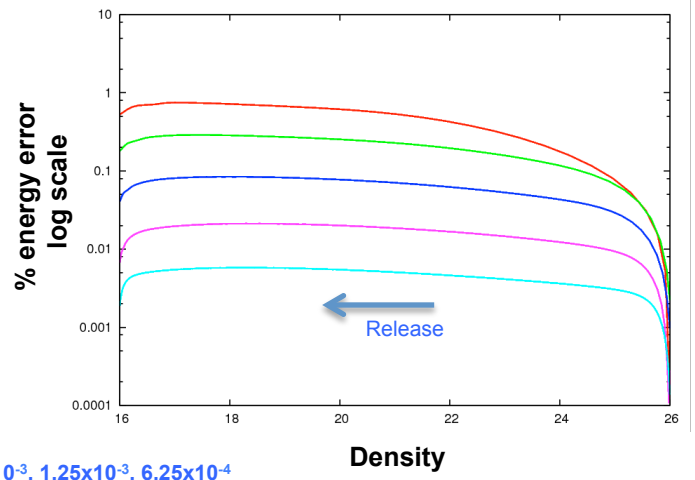
The error is less and more uniform over the release

Percent energy error at tracer location for various resolutions

CCH2



CGR



dx = 10^{-2}, 5.x10^{-3}, 2.5x10^{-3}, 1.25x10^{-3}, 6.25x10^{-4}

The elastic-plastic piston problem tests the strength formulation at the elastic-plastic limit

The objective is to match speed and shape of the elastic precursor

Dissipation can mask the elastic precursor entirely

The CGR results are sharper for both the elastic and plastic waves

Piston velocity 10 cm/s
Aluminum properties:
- density ρ_0=2.79 g/cm^3
- shear modulus G=0.286 Mb
- yield stress Y_0=0.0026 Mb

Gruneisen EOS:
- c_0=0.533
- s=1.34
- Γ=2.0