UCRL-PRES-150024

# Practical Approaches to Advection Difficulties in a Multi-material, Multi-physics Code

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Presented to workshop on

Numerical Methods for Multimaterial Compressible Fluid Flows

Paris

September 25, 2002

This work was performed under the auspices of the U.S. Department of Energy by the University of California, Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.

# Goals

Extend utility of ALE techniques without fundamental changes to underlying algorithms

- Code features
- Motivation
- Slide Surfaces
- Reactive Flow
- Summary

# Code Features

- 3D
- Unstructured Grid (arbitrarily structured hexahedra)
- ALE (Lagrange plus remap)
  - Equipotential relaxation with nodal weights
  - 2nd order Van Leer monotonic advection in pure zones
  - 1st order upwind for mixed zones
- Multiple material zones
- Discontinuous slide surfaces
- Thermal diffusion
- Chemical reactions
- Deflagration models

# Motivation

- HE Tests
  - Cylinder tests, Bigplate, Steven test
  - Used to investigate detonation speed and front shape
- Los Alamos annular confinement test
  - Deflagration in a 3D geometry

# Los Alamos annular confinement test

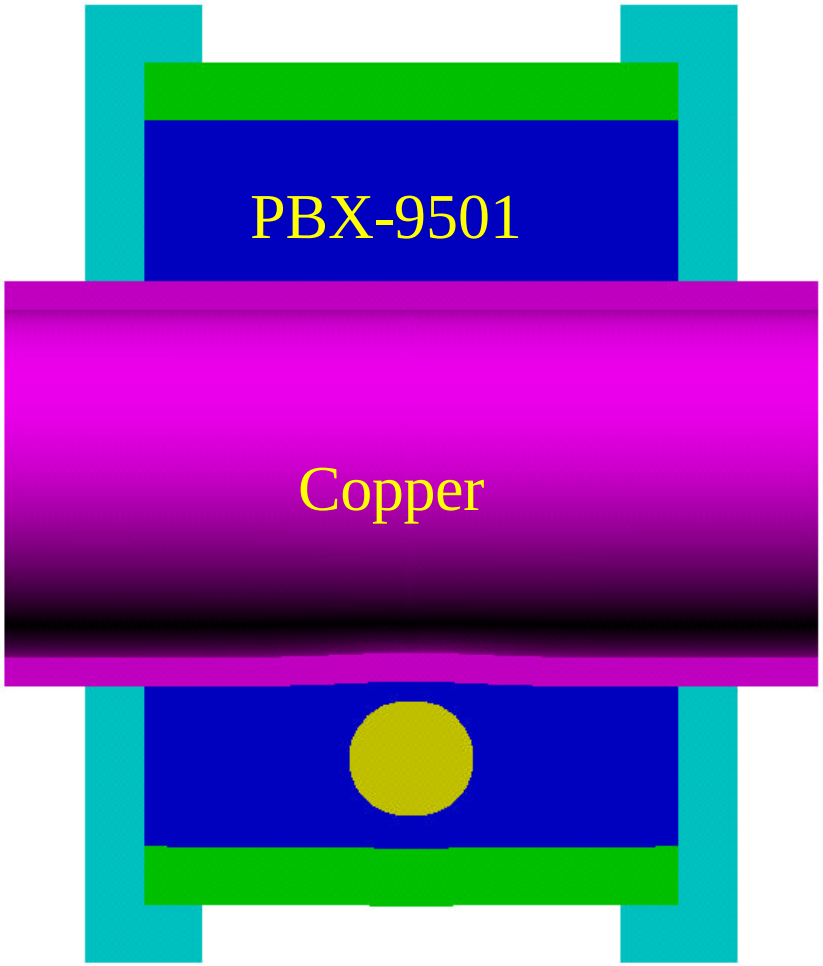
Initiation of burn (deflagration) of HE, and tracking burn front between reactants and products

Advection issues:

Level set propagates burn between ALE zones

Reaction front is treated as a true discontinuity

Slide surface between copper and HE requires deletion



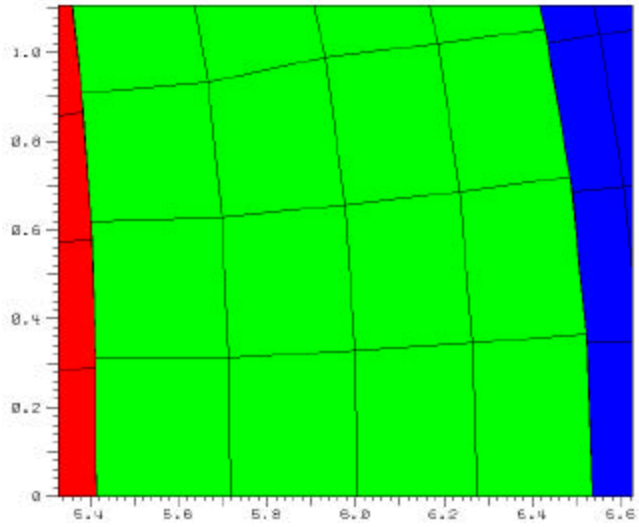
# Slide Surfaces

- Discontinuous mesh slide surfaces
- Master/Slave
- Slave Relaxation methods
  - Projection
  - Parametric
  - Migration
- Master Relaxation
- Slide deletion

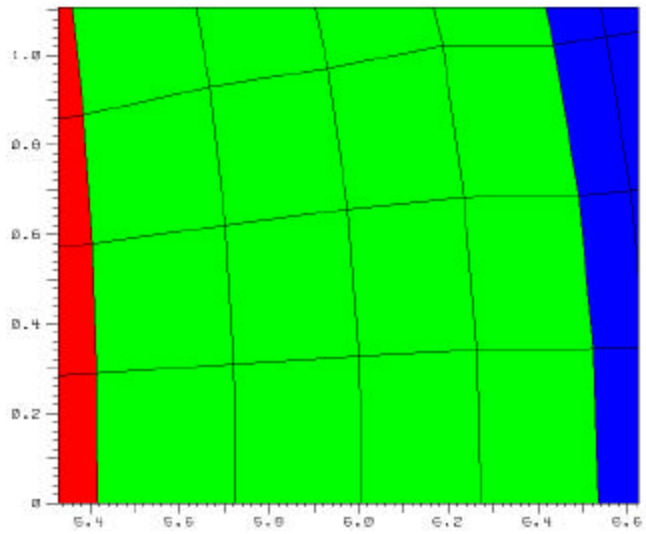
# Parametric Slide Relaxation

- “Slave” node returns to same parametric coordinate on nearest “master” face every cycle

Lagrange



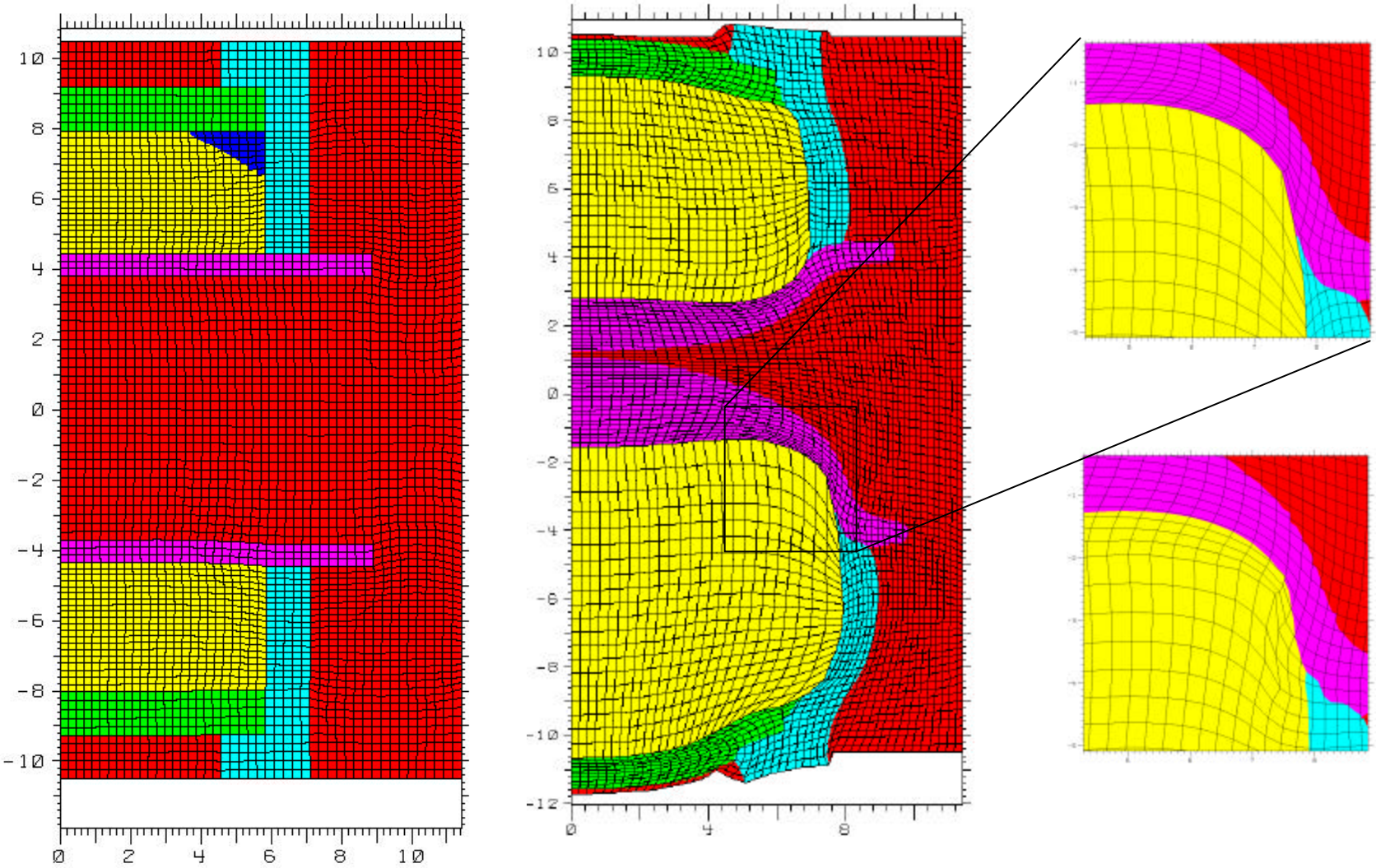

Advection



# Slide Deletion

- If master and slave nodes perfectly align, slide surface (or part of it) can be deleted if necessary to allow advection normal to the sliding interface
- Parametric relaxation ensures the alignment of master and slave nodes
- Automatic deletion possible with an activity criterion (i.e. speed) and a grace time

# Slide Deletion



# Lee-Tarver I&G Reactive Flow

- Treat HE as reactant and product with a reaction rate (see below) for the transition
- Both Reactant and Product treated with JWL EOS

$$dF/dt = I \cdot (1-F)^{r} \cdot \left(r/r_0 - 1 - C^*\right)^{h} \quad \textbf{Ignition}$$

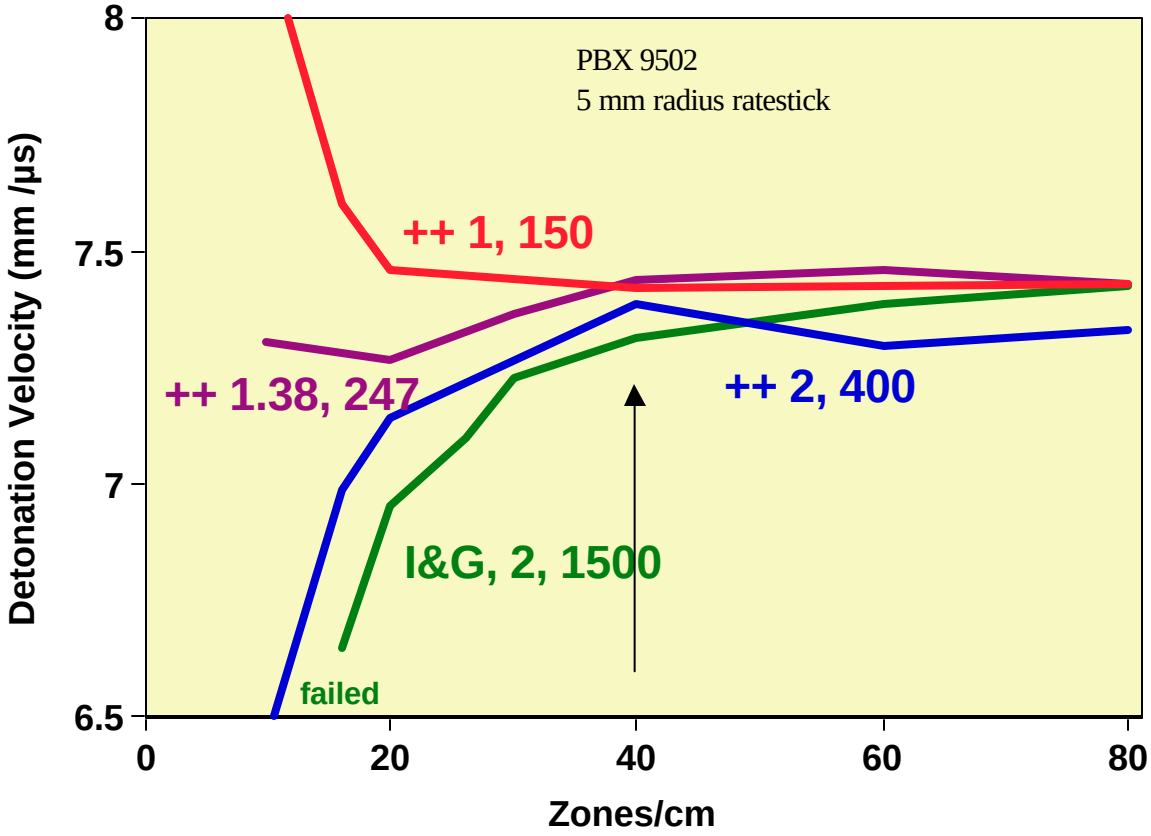
$$+ G_1 \cdot (1-F)^{h_1} \cdot F^{a_1} \cdot p^{m} \quad \textbf{Growth}$$

$$+ G_2 \cdot (1-F)^{h_2} \cdot F^{a_2} \cdot p^{n} \quad \textbf{Completion}$$

# Convergence of Reactive Flow (Clark Souers)

JWL++, alternative reactive flow model

Different curves indicate different pressure exponents and rate constants




"Edge of convergence" is where curves come together and approach right answer

# Reactive Flow and ALE

- If 80 zones/cm are required, a 3D simulation of the “Steven test” (HE cylinder driven by off-axis impact) would require ~ 100 million zones
- Need  a way to get more elements in reaction zone without the code infrastructure changes required by AMR

# What Can be Done with ALE?

- Use nodal relaxation weights to pull mesh elements into the reaction zone
- Migrate mesh back behind reaction front, so slave nodes line up with master
- Delete parts of slide surface if necessary

# Aggressive Relaxation

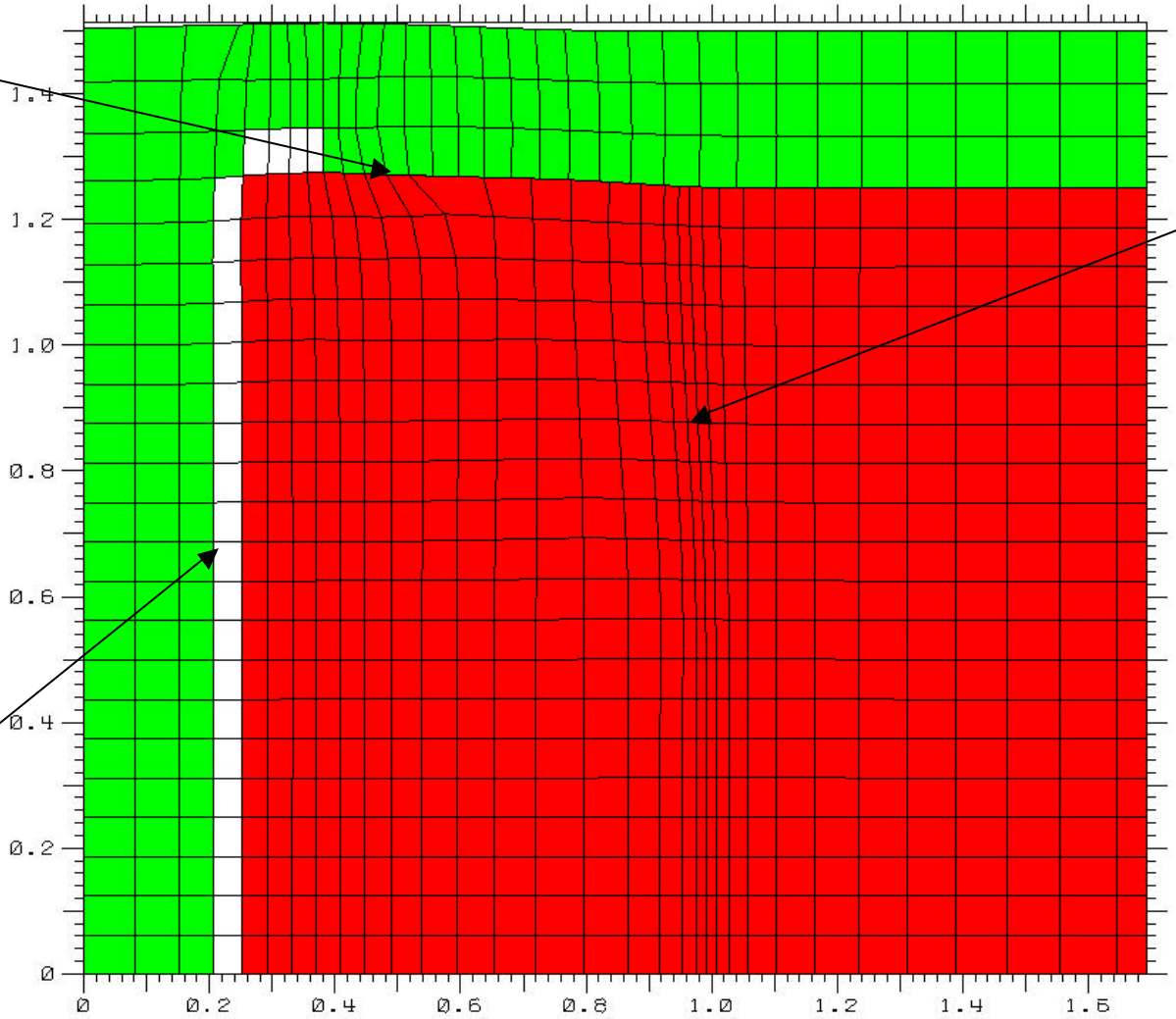
- Assign nodal weights according to the value of the artificial viscosity (in combination with advection sub-cycling)
- Migrate slave nodes back according to the value of the relative volume (for program burn) or the burn fraction (for reactive flow)
- Delete slide surface nodes based on elapsed time since node became “active”

# Aggressive Relaxation: Program Burn

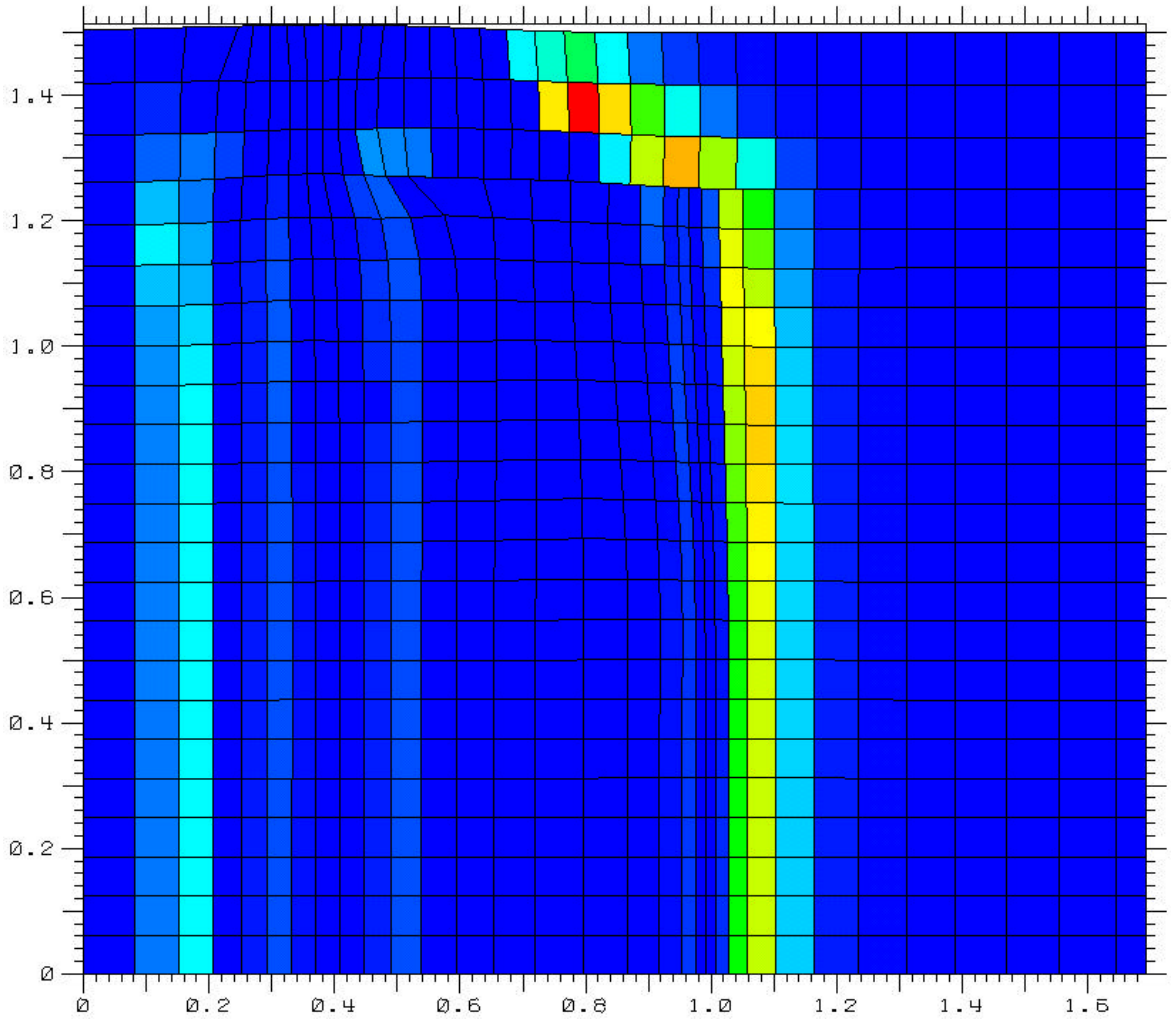
Slave nodes migrating back to home master node

Mesh Compressed in reaction zone

White zones indicate mixing where slide was deleted



# Aggressive Relaxation: Artificial Viscosity

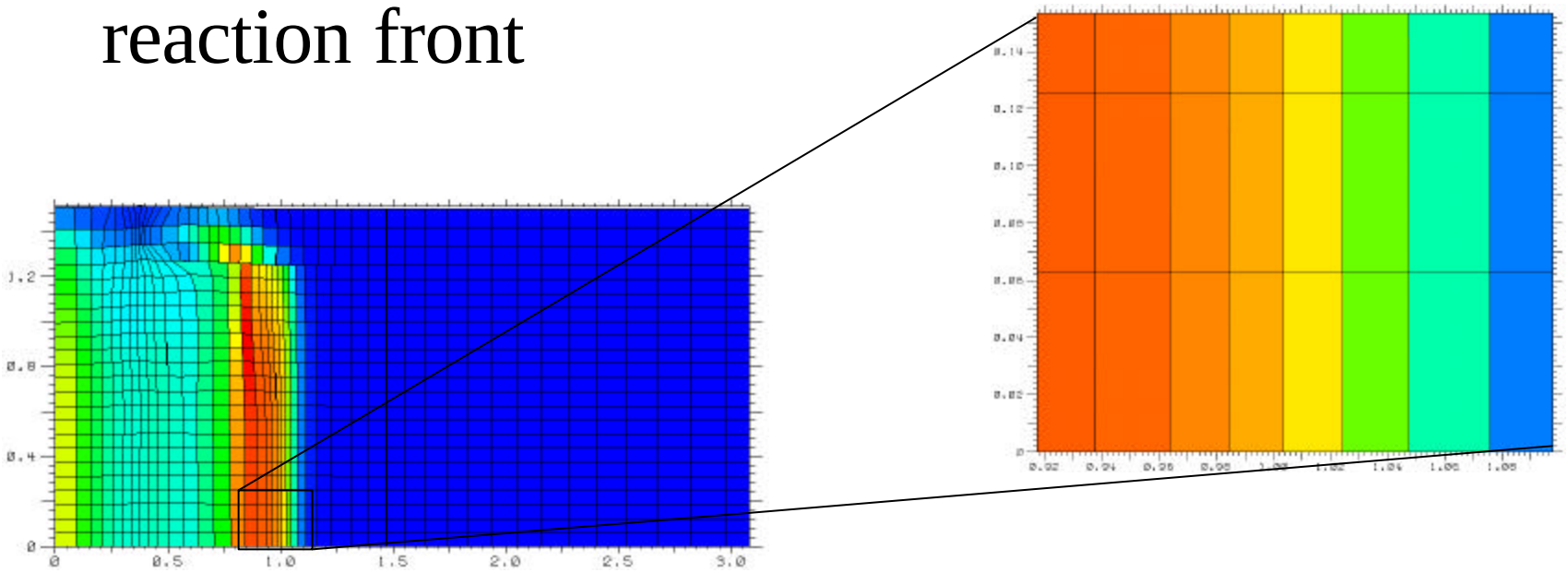


# Additional Useful Techniques

- Relaxation weight propagation
- Relaxation weight smoothing
  - Used in conjunction to smooth regions of disparate relaxation weights
- Prevent relaxation in certain key areas
  - If node has not reached its activity criterion
- Suspend relaxation near discontinuities
  - Rapid variation of chemical species

# Aggressive Relaxation can save many zones

- Beginning with 1 zone/mm, followed by ratio zoning of the initial mesh, aggressive relaxation can pull 8 zones into the 1mm reaction front



# Caveats

- Method works best if initial mesh provides enough zones to get started
- Significant “tuning” required
- Should be possible to mesh confinement and HE separately, as long as the number of slide nodes is equal
- Many aspects of method’s behavior not investigated yet
- Need to try with different reactive flow models

# Conclusions

- Aggressive relaxation can save ~5-10X the total number of zones - more in 3D
- ALE is a very flexible technique, and simple modifications to the basic algorithms can greatly extend its utility

# Acknowledgments


- Al Nichols
- Mike Murphy
- Clark Souers
- Craig Tarver
- Steve Chidester
- Richard Sharp