LA-UR-17-25129

Arbitrary Lagrangian-Eulerian Hydrodynamics

Recent Development and Test Problems

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Acknowledgments

- Jimmy Fung
- Brandon Smith
- Nick Denissen
- Jim Hill
- Marc Charest
- Paul Henning
- Dave Montoya
- Lagrangian Applications Project members, past and present

Outline

- Introduction
- FLAG, an ALE Multi-Physics Code
- Test Problems
- State of the Art
- Closing Thoughts

Introduction

```
% whoami
gaber

% module list
1) modules/3.2.10.5      14) craype-mic-knl                 27) rca/2.1.8_g6cd9a1b-3.1
2) eproxy/2.0.14-4.3     15) craype-network-aries           28) atp/2.0.5
3) cray-mpich/7.5.2      16) craype/2.5.9                   29) PrgEnv-intel/6.0.3
4) slurm/17.02.4-SSE.5   17) cray-libsci/16.11.1            30) papi/5.5.0.2
5) user_contrib          18) udreg/2.3.2-7.54               31) fftw/3.3.4.11
6) friendly-testing      19) ugni/6.0.15-2.2                32) lapdev
7) use.own               20) pmi/5.0.11                     33) cashdsd/16.11.21
8) svn/1.8.13            21) dmapp/7.1.1-39.37              34) dsd/1.0.0beta5
9) ctags/5.8             22) gni-headers/5.0.11-2.2         35) gmp/6.1.1
10) idutils/4.6          23) xpmem/2.1.1_gf9c9084-2.38      36) hdf5-parallel/1.8.17
11) global/6.3.4         24) job/2.1.1_gc1ad964-2.175       37) hypre/2.9.0b
12) git/2.11.0           25) dvs/2.7_2.1.68_g779d71a-[…]    38) silo/4.10.2-bsd
13) intel/17.0.1         26) alps/6.3.4-2.21                39) rewrite/170614
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```
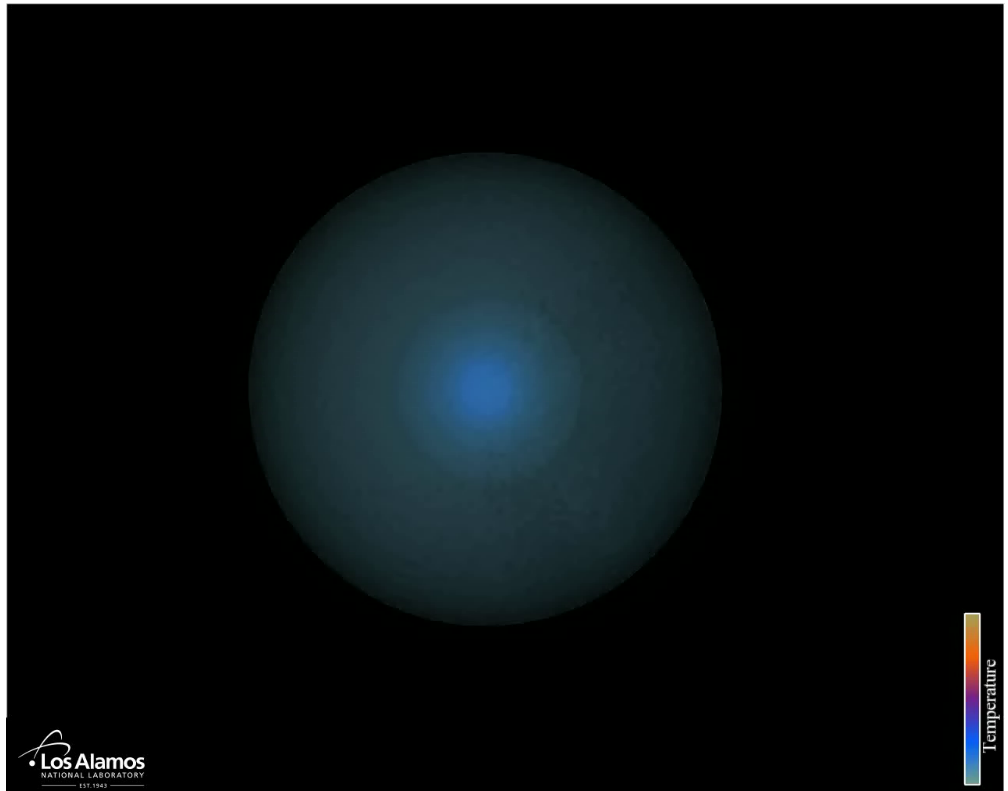
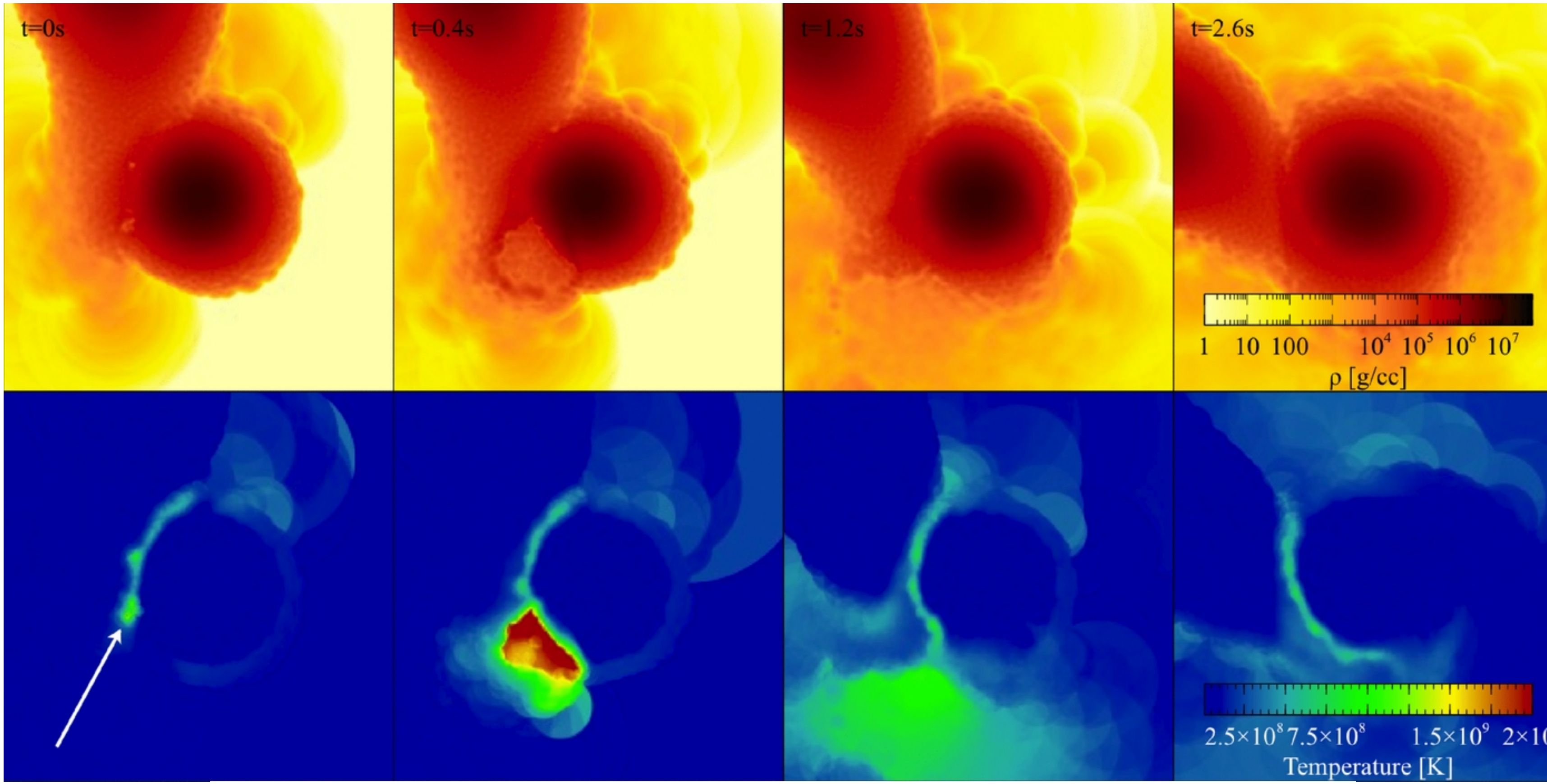

Previous work (SPH): Constraints on the Progenitor of Cassiopeia A



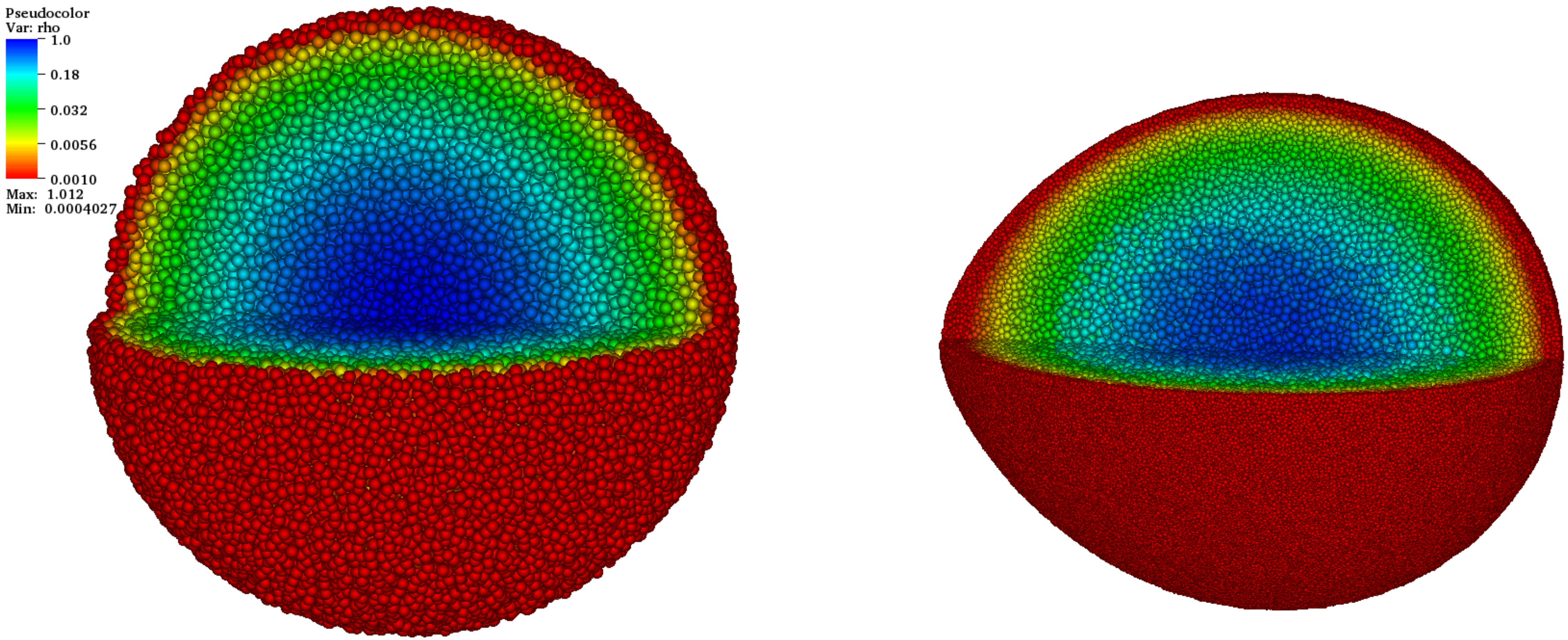
Young, Fryer, Hungerford, Arnett, Rockefeller, Timmes, Voit, Meakin & Eriksen 2006, *Astrophys. J.* 640, 891.

Previous work (SPH): Remnants of Binary White Dwarf Mergers



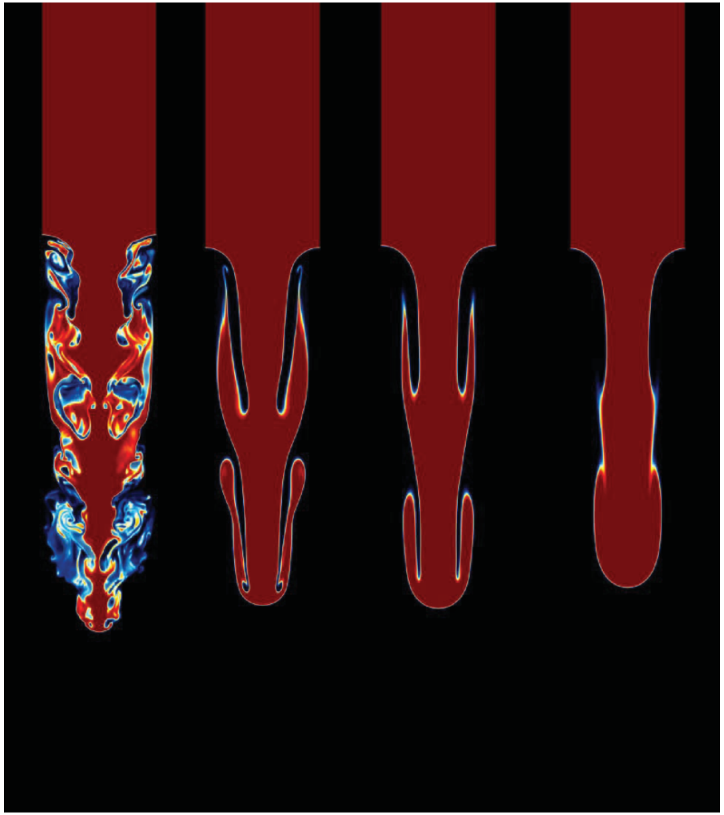
Raskin, Scannapieco, Fryer, Rockefeller & Timmes 2012, *Astrophys. J.* 746, 62.

Previous work: Generating Optimal Initial Conditions for Smoothed Particle Hydrodynamics Simulations

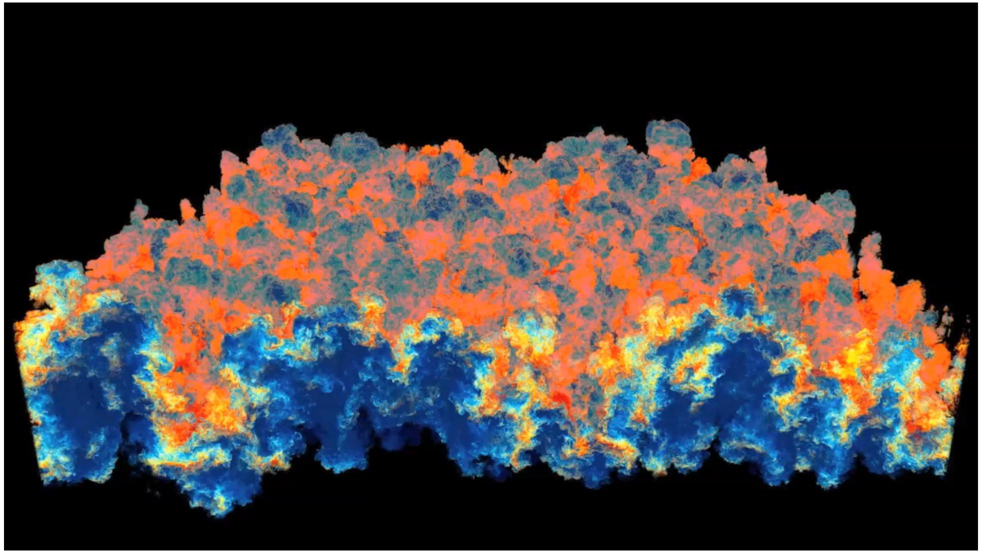


Diehl, Rockefeller, Fryer, Riethmiller & Statler 2015, *PASA* 32, e048.

Previous work (Woodward's Multifluid PPM+PPB)



Ramaprabhu, Dimonte, Woodward, Fryer, Rockefeller, Muthuraman, Lin & Jayaraj 2012, *Phys. Fluids* 24, 074107.



Dimonte, Woodward, Lin, Jayaraj, Fryer & Rockefeller.

FLAG, an ALE Multi-Physics Code

Arbitrary Lagrangian-Eulerian (ALE) methods for multi-material, multi-physics simulation attempt to combine the material-modeling strengths of Lagrangian techniques with flexible, robust strategies for advection and other mesh optimizations. The Lagrangian Applications Project (LAP) at Los Alamos National Laboratory develops the FLAG ALE radiation hydrodynamics code, including staggered-grid and cell-centered hydrodynamics, radiation diffusion, magnetohydrodynamics, and a wide variety of material models, on unstructured meshes that support relaxation, remapping, reconnection, and slide surfaces.

Nick Denissen: “One of the most challenging aspects of FLAG for new users is mesh management.”

- **When feasible, a completely Lagrangian approach has many benefits**
  - Accuracy
  - Speed
  - Well-preserved material interfaces
- **But a tangled mesh more than offsets those**

Nick Denissen: "The goal is to combine the best aspects of both [Lagrangian and Eulerian frames] where appropriate."

- **Mesh optimization**
  - ALE relaxation and remapping (advection)
  - FixMesh
  - Reconnection (Free Lagrange)
  - Refinement (AMR)
  - Stiffening
  - "Stupid mesh tricks"
- **Data optimization**
  - Renumbering
  - Repartitioning

Mesh Optimization

- **ALE relaxers**
  - Vertex-based: maintain relative position, maintain fixed displacement
  - Edge-based: displace to average position
  - Surface-based: displace to average position or area bound
  - Volume-based: adaptation, averaging, condition number, feasible set, etc.
- **ALE relaxation controllers**
  - Angle, time, condition number, timestep, edge length, edge strain, slide removal, etc.
- **ALE boundary conditions, subcycling**
- **ALE remapping (advection)**
  - “A great many of the advection variables you can set should not be mucked around with.”

Mesh Optimization

- **FixMesh**
  - More aggressive than ALE, which helps avoid excessive diffusion of problem state that can occur using ALE with subcycling
  - Several ALE volume relaxers can be used
- **Reconnection (Free Lagrange)**
  - Points remain fixed; connectivity changes
  - Effectively superceded by ALE
- **Refinement (AMR)**
  - Isotropic or anisotropic
  - Based on zone aspect ratio, an error estimate derived from a point- or zone-centered variable, or at a specified time

Mesh Optimization

- **Stiffening**
  - Side-based anti-hourglassing
  - Margolin-Pyun velocity-based anti-hourglassing (LA-UR-87-439)
  - Temporary Triangular/Quadrilaterial Subzoning
- **“Stupid mesh tricks”**
  - noboomerang, to violate energy and momentum conservation and force chevron zones back to triangles
    - “You should not use this in your own problems. Just don’t. There are better ways of addressing a tangling mesh.”

Data Optimization

- **Renumbering**
  - Logical renumbering, for block-structured meshes
  - Advancing-wavefront renumbering
- **Repartitioning**
  - Multilevel Kernighan-Lin partitioning, from Zoltan-ParMETIS (PartKway)
  - Recursive Coordinate Bisection
  - 1D partitioning in a user-specified coordinate direction

Test Problems

"A potential outcome of the discussion in this minisymposium could be a small selection of test problems that could, in principle, be addressed by both approaches. Problems along the lines of "I bet you can't do this" would be fun, but only if they actually could be set up in the opposite approach without huge investments of time and effort."

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Weseloh et al. 2005, *PAGOSA Sample Problems*; LA-UR-05-6514

Test Problem	1D	2D	3D
Blowoff	X		
Shock Formation	X		
Shock Tube	X		
JWL Equation of State	X		
Accelerating Piston		X	
Rod Penetrator			X
Be Shell			X
Jump Off			X
Exploding Shell			X
Shaped Charge			X
Taylor Anvil			X

Brock et al. 2006, *Verification test suite for physics simulation codes*; LA-UR-06-8421, UCRL-TR-226984

Test Problem	Gas Dynamics	Non-Linear Heat Conduction	Non-Equilibrium Radiation Diffusion	Neutron Transport	High Explosives
Noh	X				
Sedov	X				
Reinicke/ Meyer-ter-Vehn	X	X			
Coggeshall-8	X		X		
Su-Olson			X		
Sood				X	
HE	X				X

https://e-reports-ext.llnl.gov/pdf/342063.pdf

Kamm et al. 2008, *Enhanced verification test suite for physics simulation codes*; LA-14379, SAND2008-7813

Test Problem	Gas Dynamics	Material Response	Radiation Transport	Heat Conduction
Riemann	X			
Guderley	X			
Cook/Cabot	X			
Woodward-Colella Blast Wave	X			
Shu-Osher	X			
Taylor-Green Vortex	X			
Richtmyer-Meshkov	X			
Rayleigh-Taylor	X			
Mach Reflection	X			

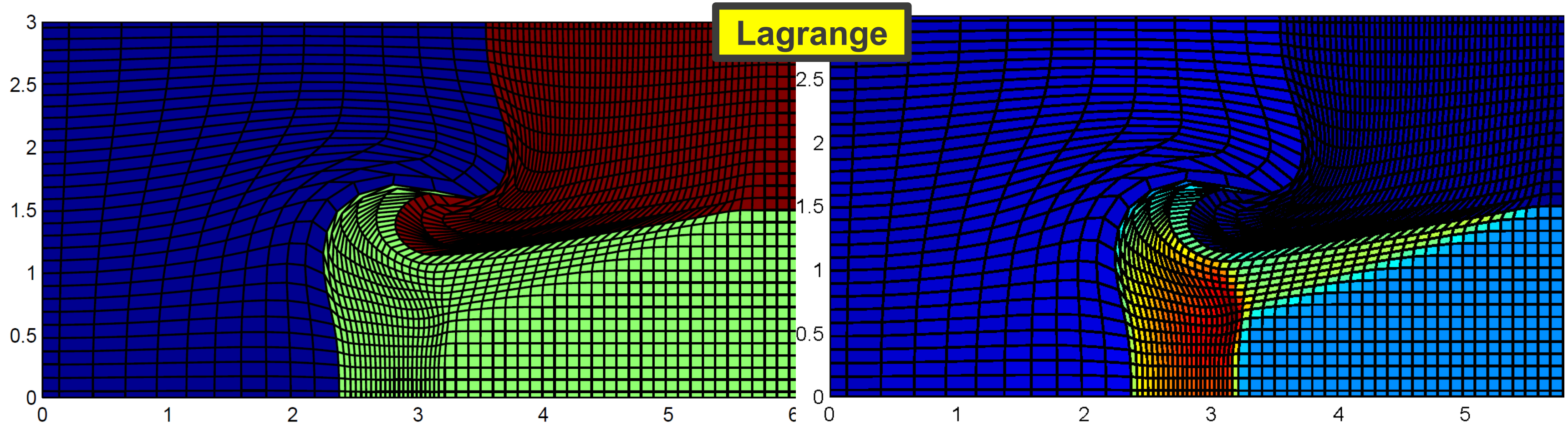
http://permalink.lanl.gov/object/tr?what=info:lanl-repo/lareport/LA-14379

Kamm et al. 2008, *Enhanced verification test suite for physics simulation codes*; LA-14379, SAND2008-7813

Test Problem	Gas Dynamics	Material Response	Radiation Transport	Heat Conduction
Hunter		X		
Bleich & Nelson		X		
Verney		X		
Enhanced Dynamic Sphere		X		
Lowrie/Rauenzahn EDRS	X		X	
Lowrie NEDRS	X		X	
Radiation-Acoustics	X		X	
Top-hat/Crooked-pipe			X	
Shestakov/Bolstad			X	
Miller/Hutchens				X

http://permalink.lanl.gov/object/tr?what=info:lanl-repo/lareport/LA-14379

State of the art: Reconnection-Based ALE (ReALE)



Loubère, Maire, Shashkov, Breil, & Galera 2010, ReALE: A reconnection-based arbitrary-Lagrangian-Eulerian method, *J. Comp. Phys.* 229, 12.
Charest, Burton, Pouderoux, Shaskov, & Kenamond 2016, A regional reconnection-based arbitrary Lagrangian Eulerian method.

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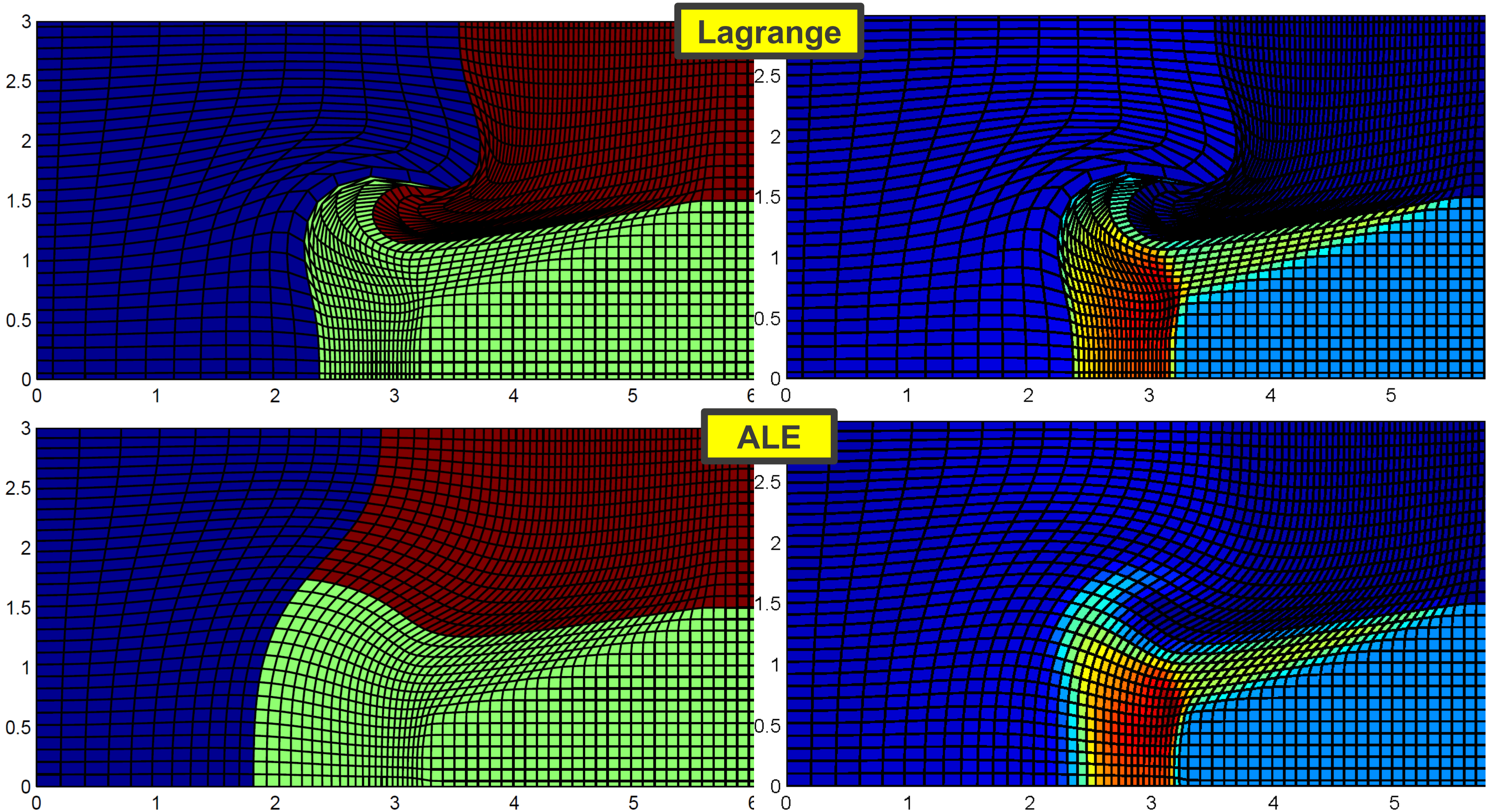

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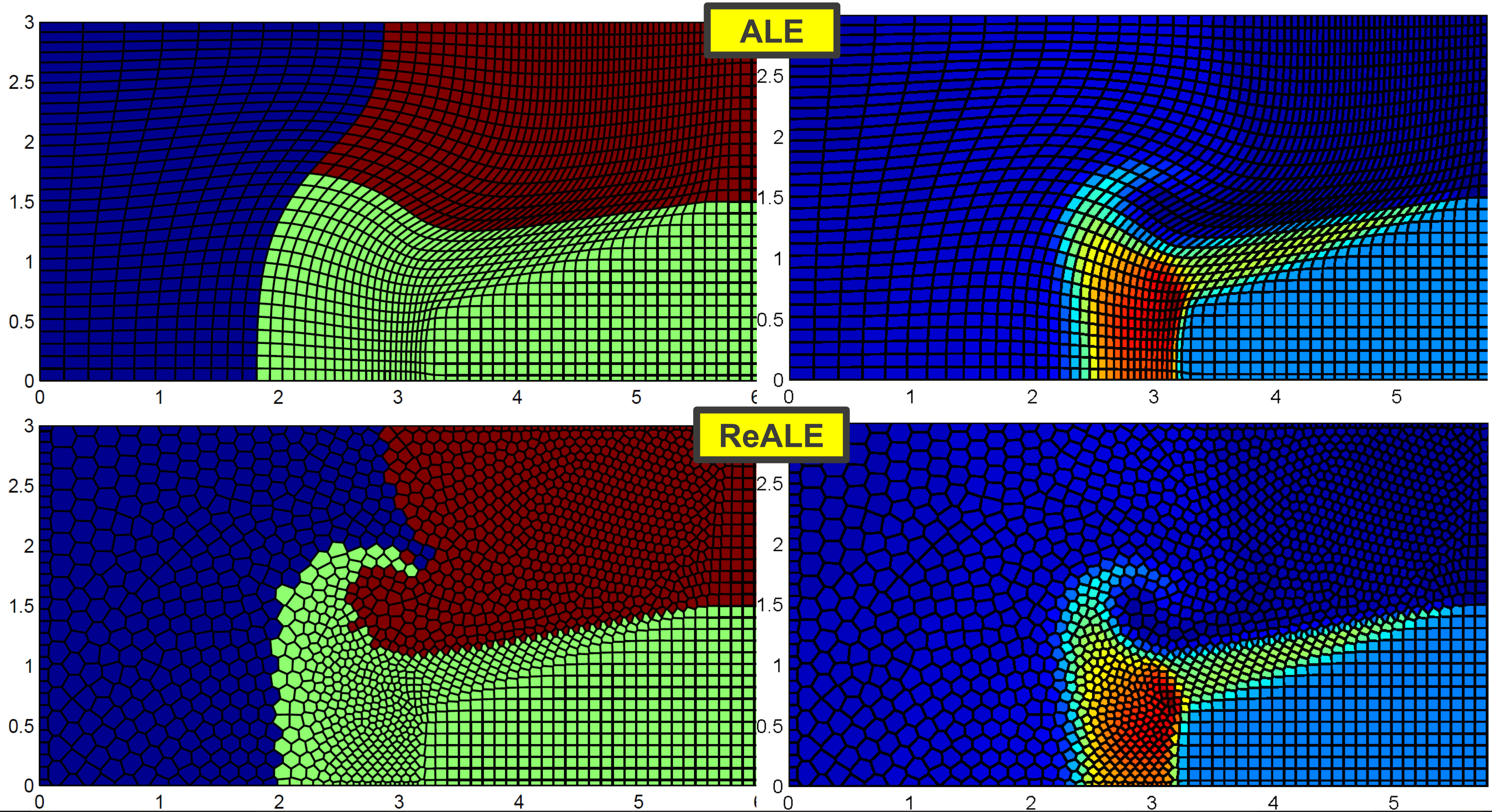
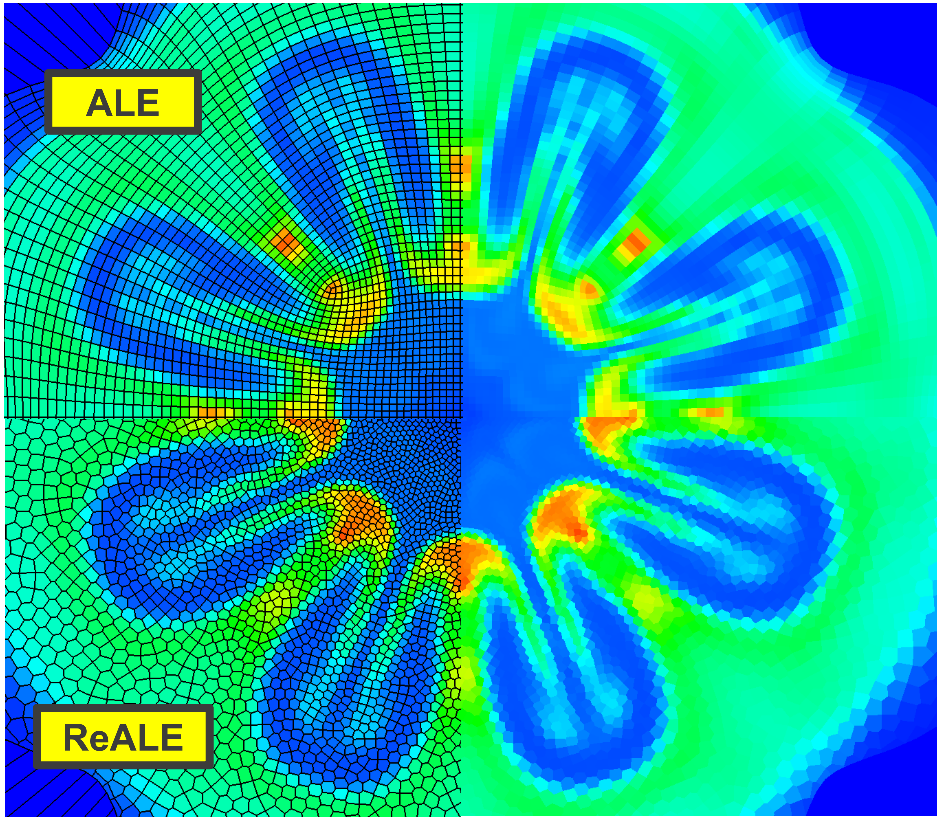


State of the art: Regional ReALE



See also Charest, Shashkov, Burton, Pouderoux, Kenamond, & Fung,
A Regional Reconnection-Based Arbitrary Lagrangian-Eulerian (ReALE) Method for Multiple Materials, MultiMat, 18-22 Sept 2017.

State of the art: Rewrite

Language	files	blank	comment	code
Rewrite	1736	115226	250281	442820
Dictionary	1130	28166	12994	135392
HTML	375	3224	364	63976
C	77	5306	5369	43445
Fortran 77	227	7496	16819	34296
Fortran 90	107	6140	9006	17184
C/C++ Header	105	4040	5939	9725
C++	32	1660	1419	5012
SUM:	3789	171258	302191	751850

- **Code modernization is an ongoing challenge**
- **The LAP has a useful tool at its disposal: source-to-source translation**

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Rewrite

Language	files	blank	comment	code
Fortran 90	1805	128037	273752	997388
HTML	11168	71547	0	848369
C	70	4568	4097	36889
Fortran 77	192	7070	15925	32295
C/C++ Header	70	3348	4561	8068
C++	24	1431	1148	4090
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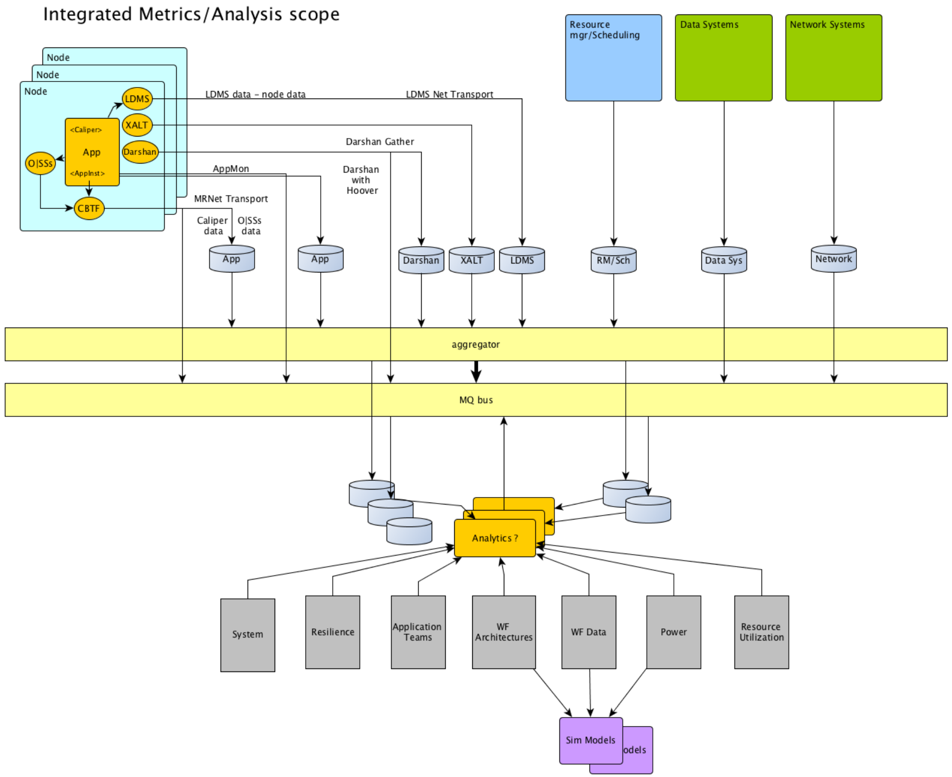
State of the art: IntMAP

- **As a project with production code, we have an obligation to measure and analyze our usage and performance**
  - To quantify our users' evolving workloads
  - To prioritize development effort
  - To identify regressions in our own codebase or elsewhere in the system
  - To provide input to next-generation development
- **Related to/inspired by**
  - The Sonar project at LLNL
  - TACC Stats and similar projects at other centers



Dave Montoya

Closing Thoughts

- **“vi or emacs?” / “big- or little-endian?” / “Lagrangian or Eulerian?”**
- **It seems likely that no single method will be best for all problems (even accounting for improvements and evolution within each class of method over time)**
  - Test problems help motivate such improvements
  - Also of interest: deciding how to compromise when the problem of interest potentially intersects with weakness of different methods (in different regions, or at different times)
- **How often is the decision to use a particular implementation of a particular numerical method based purely on technical suitability?**
  - If less than 100%, what can we do to address those non-technical factors?

Thanks