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LLNL-TR-678283

McCallen Professional Research and Teaching Leave Report

R. McCallen

October 16, 2015

Disclaimer

This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

October 13, 2015

John Knezovich, Ph.D.
Director, University Relations
Lawrence Livermore National Laboratory
7000 East Avenue
Livermore, CA 94550

Subject: Professional Research and Teaching Leave Report

This end of assignment report for a Professional Research and Teaching (PRT) Leave award includes the attached assessment of success by the host organization, University of California Davis (UCD).

The following summarizes the accomplishments and attached are a selection of documented items.

Scope
The PRT at UC Davis involved technical growth, fostering collaborations, and student/faculty interactions, especially with those from under-represented groups in science, engineering, and math.

Technical Growth

- Presented two seminars to faculty and graduate students in the Departments of Chemical Engineering and Materials Science (CHMS) and Mechanical and Aerospace Engineering (MAE). Document provided.
- Constructed and gave lecture for graduate course MAE 219 *Introduction to Scientific Computing in Solid and Fluid Dynamics.* Discussed frames of reference with presentation of Lagrangian and Eulerian formulations, and then introduced ALE methods (Lagrange with Remap and Eulerian with grid motion) with examples and discussion on R&D challenges in mechanics, materials, and chemical engineering. Document provided.
- Reviewer for CHMS graduates research poster competition and ENG 98 *Introduction to Engineering Design* projects (35% of grade) with class populated by first year undergrads from under-represented groups. Also reviewed other formal and informal research and projects.
- Attended weekly CHMS faculty/graduate seminars and a variety of exit seminars and followed up with faculty discussions. I was a member of an MAE qualifying exam committee.
- Attended a special seminar series (~1.5 hrs/wk for Spring Quarter) *California's Research University: The UC System Yesterday, Today, and Tomorrow* with lectures from UC's high level leadership and policy makers, e.g., UC's former VP for Budget and Capital Resources, UCD Chancellor.
- Participated and helped organize workshops at UCD on the topics of big data science and bio medical technology and followed up with faculty discussions.
- Research activity - Objective is to determine effect of numerical methods and parameter choices in single and multiphase simulations. Document provided.
  - Performed literature review on modeling of single and multiphase compressible flow including high-pressure gas or chemical explosions (with and without particles).
  - Performed hand calculations for stoichiometric properties of reactants, products, and air mixtures, and compared to explosive reference manual and online resources.
  - Reviewed training material, course exercises, and software manual with special focus on hydro, chemistry, and grid generation and exercised options.
  - Constructed a range of input files (from scratch) for a high-pressure gas expansion and explosion simulations for various grids investigating source of numerical features.
  - Documented suggestions and identified errors.

Fostering collaborations

- Invited to present to UCD's Council of Deans. The presentation included an outline of the PRT objectives, current activities, and success in establishing LLNL and UCD collaborations.
- Presented at and lead a discussion session with Dr. Dimitri Kusnezov, DOE's Chief Scientist and Senior Advisor to the Secretary of Energy on topic of "Collaborations with Universities and Industry for Cutting-Edge Simulation Capability". Document provided.
- Developed and executed a strategic approach for identifying research areas of mutual UCD/LLNL interest and attracting faculty through student engagements. For example, established and led weekly graduate student discussion sessions and followed-up by meeting with their major research advisors.
- Organized seminars and visits by UCD faculty to LLNL and by LLNL researchers to UCD.
- Consulted in the NASA funded UCD/LLNL/NASA collaborative effort in Uncertainty Quantification (UQ) for Additive manufacturing (AM). Connected UCD faculty and student to LLNL's UQ efforts in WCI (UQpipeline), HEAF (PSUADE), and Engineering (DAKOTA).
- Meso-scale experiments and modeling with LANL
    - Connected with LANL's Dr. Irene Beyerlein to discuss collaborative efforts in meso-scale modeling and experiments with UCD
    - Helped organize LANL visit by Dr. John Sarrao and participated in breakout group discussions on LANL/UCD collaborations in meso-scale modeling.
- Made UCD and LLNL/WCI connection in the area of remapping methods and wrote initial draft of research motivation and scope that matured into an LDRD white paper by the LLNL PIs.
- Longer-term strategic planning
    - Working with a faculty advisor to the UCD Chancellor, Prof. Bob Powell, I assisted in the construction of a white paper titled *Strategic Engagement with UC-Affiliated National Laboratories: Science and Engineering in the National Interest Center (SENIC)*. Working with the UCD and WCI manager, Frank Graziani, we condensed ideas into a high level briefing, and met with LLNL's Program Deputy AD's for input. The SENIC plan includes: Joint solicitation of R&D funding, working groups and seminar series, and faculty engagement with a student-hiring pipeline. Briefing document provided.
    - Met with WCI AD, to discuss his interest in UCD/LLNL collaborations and was given direction to identify and pursue areas of innovation where UCD brings something unique that is outside LLNL's current capability or workforce expertise.
    - Invited to present to LLNL's Diversity Committee. LLNL's Diversity Committee has chosen UCD as one of three campuses for a pilot study on methods and approach for collaborating with universities to improve diversity at LLNL. Briefing document provided.
    - Helped organize and guide the first LLNL/UCD Working Group with graduate student leadership (a collaborative think tank and problem solving group).

Student and faculty interactions, especially under-represented groups

- Connected 8 successful internships at LLNL in WCI, NIF, ENG, and PLS from UCD Departments of Chemical Engineering (3), Materials Science (1), Mechanical and Aerospace (3), and Civil (1) – includes female, hispanic, and first-generation students.
- Facilitated successful connection with WCI designer, UCD faculty member, and female graduate student researcher on the topic of metal failure/fracture modeling and simulation for high shock loads.
- One-on-one student mentoring and research guidance with faculty approval
    - Identified a DOE Nuclear Energy fellowship and a female student interested in energy research. With her faculty advisor's approval, I worked with the student in defining a research topic, scope, and technical approach and the student/faculty received the award.
    - Constructed a summary description of DoD's high priority research topics, to help faculty and students applying to DoD fellowships and grants. In addition, per faculty request, I worked with one particular PhD student in constructing a DoD fellowship application.

- As a member of the UCD Advisory Board for the Leadership in Engineering Advancement Diversity and Retention (LEADR) Center, I participated in annual meeting with board members and in developing strategies for retention and success from under-represented groups.

- Other
  - MARS/Wrigley and UCD scientist and engineers were connected with LLNL. MARS has a long-term relationship with UCD and supports the formation of an Innovation Institute.
    - Attended MARS/Wrigley General Advisory Board meeting in Chicago, IL and UCD/MARS/LLNL strategic planning meetings.
    - Invited to be a member of the MARS Computational Science Board and attended meetings in Miami, FL at the US Department of Agriculture facility and Billings, MT.
    - With PLS, helped organize and coordinate MARS LLNL visit.
    - Scoped and constructed draft plans for a UCD/MARS/LLNL collaboration on topic of coating and extrusion efficiency and quality improvements.
  - Invited presentation at CECD/ME Symposium on Computation-Enabled Materials Discovery, University of Maryland.

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Department of Chemical Engineering & Materials Science
Department of Mechanical and Aerospace Engineering
University of California Davis
Davis, CA

Attachments:

- Host Organization's Assessments
  Prof. Robert Powell, Chemical Engineerin and Materials Science Department, UCD
  Prof. JP Delplanque, Mechanical and Aerospace Department, UCD
- Documents
  - *Science and Engineering R&D Challenges at a DOE National Laboratory*, 2015, LLNL-PRES-665786
  - *Arbitrary Lagrangian-Eulerian (ALE) and Multi-Physics Modeling and Simulation*, 2014, LLNL-PRES-663421
  - *Predicting Physics Rather than an Artifact of a Numerical Method*, 2015
  - *Collaborations with Universities and Industry for Cutting-Edge Simulation Capability,* 2015 LLNL-PRES-666413
  - *Science and Engineering in National Interest Center (SENIC)*, 2015
  - *UC Davis Demographics and Strengths*, July 2015

Cc:
Charles Verdon, PhD, Associate Director, WCI
Des Pilkington, PhD, Division Leader, Design Physics Division (DPD), WCI
Brian Pudliner, PhD, Group Leader, DPD/WCI

From: Robert Powell <rlpowell@ucdavis.edu>
Date: Sunday, August 16, 2015 at 11:00 AM
To: Default <pudliner1@llnl.gov>
Cc: Robert Powell <rlpowell@ucdavis.edu>
Subject: Dr. Rose McCallen: Performance Appraisal Input

Dear Dr. Pudliner:

It is my pleasure to offer my comment regarding Dr. Rose McCallen's performance over the last year. Let me begin by noting that Dr. McCallen's work at UC Davis has been transformative. She has breathed new life into the relationship between UC Davis and LLNL. This is demonstrated by the research and education opportunities that she has spearheaded, as well as broader impacts. Eight UC Davis students were placed at LLNL as graduate interns, undergraduate interns and graduate student researchers.

She has collaborated with a UC Davis faculty member to obtain funding from NASA for a project to do predictive modeling of qualifying materials. She has organized a one day meeting with LLNL that has so far led to two graduate students working on LLNL projects. Also, as a result of this, there has been an LDRD proposal submitted with two UCD co-PIs.

She has been absolutely critical in fostering a new collaboration among UC Davis, LLNL and Mars, Inc., She has become key in planning the Mars HPC strategy. She has been building bridges that promise to touch upon LLNL's additive manufacturing efforts as well as the Forensic Science Center. I am quite hopeful that this collaboration could be a cornerstone of the new UC Davis - Mars Institute for Innovation in Food and Heath.

Finally, and perhaps most importantly in the long run, Dr. McCallen has advocated for strong connections between the LLNL Programs and UCD. During the recent visit of UC Davis Chancellor to LLNL this was manifested by the engagement of the Program heads at the meeting. Dr. McCallen was absolutely critical in ensuring that the meeting was an overall success. During her remaining time at UCD, I expect that Dr. McCallen will develop a concrete set of opportunities for the future that will be critical in fleshing out the UCD LLNL relationship.

I cannot overemphasize the enormous impact that Dr. McCallen has had. Please let me know if I can provide any more information.

Bob

Robert Louis Powell III
Distinguished Professor
Chemical Engineering & Materials Science and Food Science & Technology
University of California Davis

Chair, Science and Technology Committee
Los Alamos National Security & Lawrence Livermore National Security

Science Advisor
Secretary of California Natural Resources Agency

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From: Jean-Pierre Delplanque <delplanque@ucdavis.edu>
Date: Tuesday, September 1, 2015 at 11:29 PM
To: Default <pudliner1@llnl.gov>
Subject: Input for the Performance Appraisal of Dr. Rose McCallen's PRT Leave at UC Davis

Dear Dr. Pudliner:

The purpose of this letter is to provide input for the Performance Appraisal of Dr. Rose McCallen's Professional Research and Teaching (PRT) Leave at UC Davis. I am a professor of mechanical and aerospace engineering at UC Davis. My main area of expertise is computational and theoretical fluid dynamics, heat transfer, and transport phenomena with interdisciplinary applications. I have been teaching and conducting research in that area for about twenty years. During most of Dr. MacCallen's PRT leave at UC Davis I was also serving as Associate for Undergraduate studies in the College of Engineering. I now serve as Associate Dean for Graduate Students in the campus Office of Graduate Studies.

I met Dr. McCallen when she reached out to my department (Mechanical and Aerospace Engineering, MAE) two years ago regarding an open position for a post-doctoral researcher. These discussions lead to the organization, by Dr. McCallen, of a visit by faculty members from MAE at LLNL to identify potential areas of collaboration. That effort was immediately fruitful resulting in two, still on-going, collaborations. I am directly involved in one of these. One of my graduate students, Brian Weston, has been working at LLNL since June 2014, benefitting from the mentoring of Lab staff members. This relationship formed the nucleus for the successful submission of a grant proposal to NASA on the topic of Uncertainty Quantification of Selective Laser Melting Processes. Drs. McCallen and Anderson are collaborators on that grant. Since Dr. McCallen arrived on campus a year ago, she successfully endeavored to stimulate similar opportunities and collaborations with several other units on campus (e.g. biomedical engineering, Chemical Engineering and Materials Science). Her keen knowledge of the administrative processes at the lab have been an invaluable resource in surmounting obstacles to the establishment of research collaborations that would have otherwise deterred many faculty members. She proved to be a true problem-solver and was always able to find a solution to make things happen.

Dr. McCallen also dedicated her efforts to undergraduate and graduate student mentoring. In January 2014, I was appointed Associate for Undergraduate studies in the College of Engineering. The portfolio of that position includes a program called LEADR (Leadership in Engineering Advancement Diversity and Retention) that aims at improving the retention of undergraduate engineering majors. Dr. McCallen serves on the advisory board of that program and I also had several opportunities to interact with her in that context. After arriving on campus last year she starting holding office hours for students interested to learned about internship opportunities at LLNL and the application process. She also mentored graduate students. She guided one of my graduate student through the process of the NEUP fellowship application. That student was awarded the fellowship and will start this coming Fall. Dr. McCallen also helped her identify interlocutors at LLNL to define the details of her fellowship research. She patiently provided advice for graduate students looking for a postdoctoral or career position; reviewing CVs and offering interview advice.
Dr. McCallen's interactions with students during her PRT also involved lecturing. For example, she guest lectured in my graduate course on computational methods last Fall and gave several seminars while on campus. She also facilitated the organization of seminars by LLNL staff members (e.g. Dr. Nourgaliev).

In summary, I genuinely believe that our campus and, more specifically, the students and faculty in the college of engineering have tremendously benefitted from the hard work of Dr. McCallen while she was with us. She has directly contributed to opening up opportunities that have already made a difference in the lives of several of our students, graduates and undergraduates. The research collaborations that she catalyzed will undoubtedly form the foundation for a renewed, strengthened relationship between UC Davis and LLNL. I intend to keep working with Dr. McCallen on such activities. Her motivation, resolve, and enthusiasm are contagious.

Please do not hesitate to contact me if I can provide any further information. Please also let me know if you would prefer receiving this input on letterhead.

Best Regards,

-jp
Jean-Pierre Delplanque
Professor of Mechanical and Aerospace Engineering
Associate Dean, Graduate Studies
University of California • One Shields Avenue • Davis, CA 95616-5294 • (530) 754-6950

Science and Engineering R&D Challenges at a DOE National Laboratory

January 8, 2015

Rose McCallen, Ph.D.
ALE3D Research and Development Team

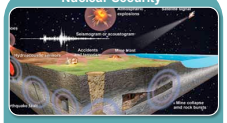
Lawrence Livermore National Laboratory

LLNL-PRES-665786

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC

Department of Energy (DOE) National Laboratories' mission spans national security, energy, and environment

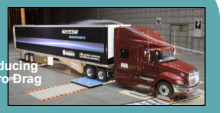
Nuclear Security



International & Domestic Security

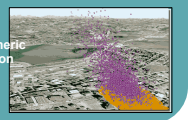
Energy

Reducing Aero Drag

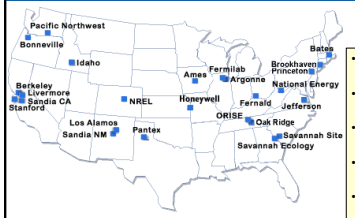


Environment

Atmospheric Dispersion



Department of Energy (DOE) National Laboratories: Leading institutions for innovation for sixty years



- Tackle critical scientific challenges
- Unique instruments and facilities
- Address large scale, complex challenges
- Utilize a multi-disciplinary approach
- Emphasis on translating basic science to innovation

http://energy.gov/about-national-labs

Lawrence Livermore National Laboratory (LLNL) managed by DOE's National Nuclear Security Administration (NNSA)

Livermore branch of the University of California Radiation Laboratory (UCRL) opened in 1952

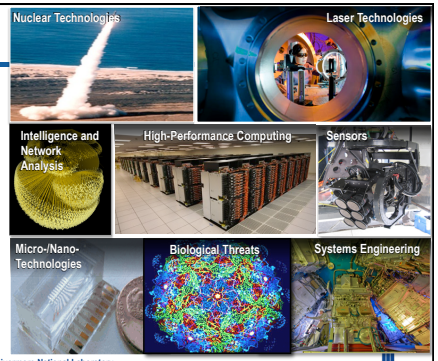
1952

- 123 employees
- Annual budget: ~ $3.5 million
- 1 square mile main site

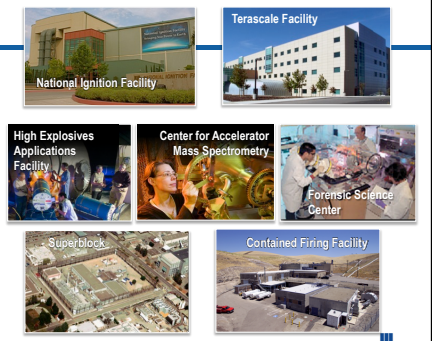
Today

- Over 6,000 employees
- Annual budget ~ $1.5 billion
- 1.3 square mile main site

Broad scientific and technical capabilities



Outstanding scientific and technical facilities

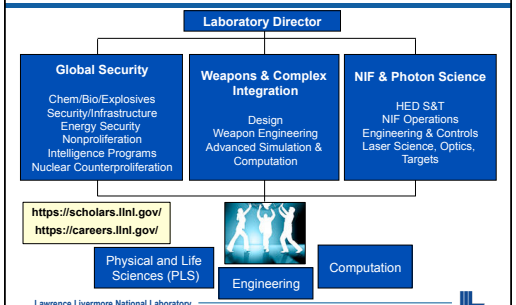


A key objective is to ensure the next generation of skilled personnel

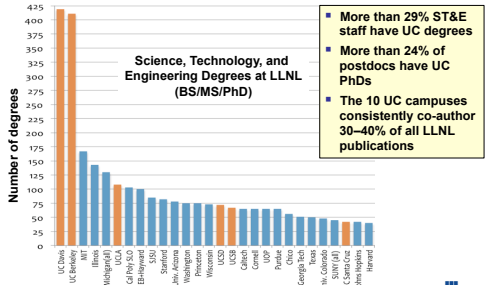
https://www.llnl.gov

Internships
https://scholars.llnl.gov/
Career
https://careers.llnl.gov/

Job postings reflect the integration of personnel across organizational boundaries



UC is LLNL's partner and pipeline for ST&E talent



- More than 29% ST&E staff have UC degrees
- More than 24% of postdocs have UC PhDs
- The 10 UC campuses consistently co-author 30–40% of all LLNL publications

DOE National Labs address R&D challenges with cutting-edge multi-physics modeling

DOE Laboratories and LLNL
- ✓ R&D activities and facilities
- ✓ Career and internship opportunities

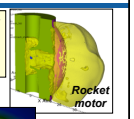
R&D in multi-physics modeling
- Applications (ALE3D code)
- Arbitrary Lagrangian-Eulerian (ALE) methods
  - Accurately capture multi-physics with extreme deformations
  - Material models developed for Lagrange simulation and are mesh dependent
  - Chemical reactive models are computationally intensive and approximate methods are necessary

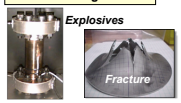
Penetration of a projectile into a structure with subsequent explosion and damage

ALE application space is huge and the multi-physics is challenging

DOE: Stockpile Stewardship and other NNSA Programs

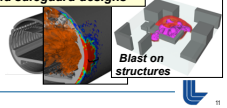
DoD: Munitions and rocket design performance, lethality, vulnerabilities, and safety



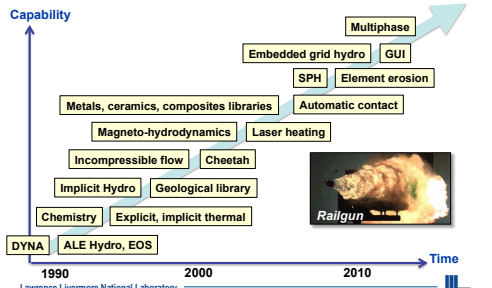


NASA : Launch systems and risk evaluations

DHS : Transit and structures vulnerabilities and safeguard designs



Integrated multi-physics is required

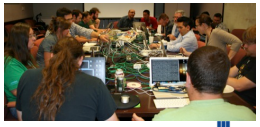


It takes a multi-discipline team, technically challenging work, and some fun

Multi-discipline team

Small groups or individuals work on projects

Bug-fix days



Arbitrary Lagrangian-Eulerian (ALE) methods are a powerful and complicated tool for multi-physics modeling

✓ Applications

- Application space is huge and the coupled physics is challenging
- It takes a multi-discipline team to address the technical challenges

Penetrator

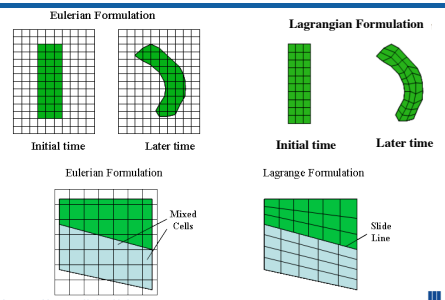
Explosive cookoff

Fragment impacting a composite

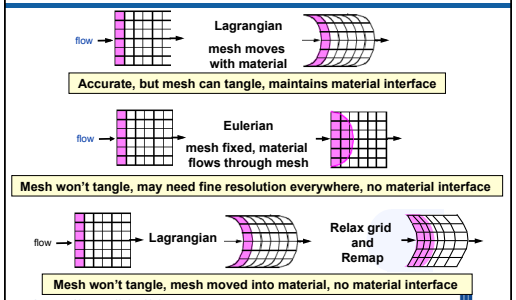
Laser damage

Arbitrary Lagrangian-Eulerian (ALE) Method : Lagrange step, mesh relaxation, and remap

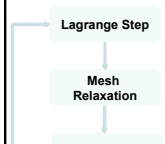
What do we mean by Lagrangian and Eulerian?



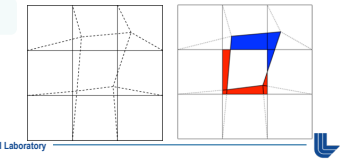
Arbitrary Lagrangian-Eulerian (ALE) combines both methods



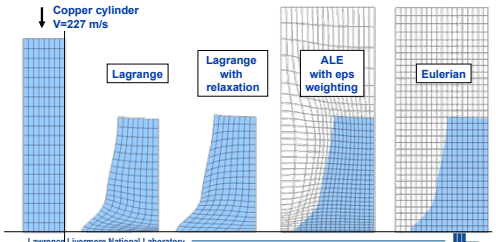
ALE process has several distinct phases



- Mesh Relaxation
  - A revised mesh that smooths or improves the current mesh
  - Various options are available to construct the relaxed mesh
- Remap
  - Remapping the state of the calculation from the mesh at the end of the Lagrange step onto the relaxed mesh



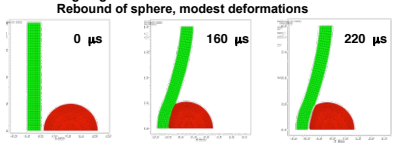
Benefit of ALE is improved accuracy



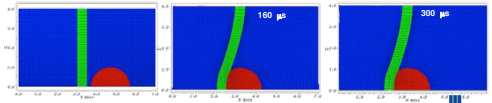
Implications of Lagrange versus ALE for mild deformation

Case 1: Lagrange with slidelines
Rebound of sphere, modest deformations

Copper sphere impacting steel plate (200m/s)



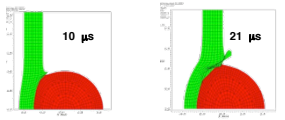
Case 2: ALE without slidelines
No rebound of sphere, no interface, no separation of sphere and plate



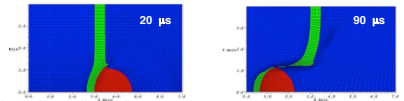
Implications of Lagrange versus ALE for extreme deformation

Case 1: Lagrange with slidelines
Lagrange solution fails

Copper sphere impacting steel plate (500m/s)

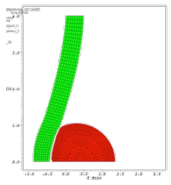


Case 2: ALE without slidelines
ALE handles significant material deformations



Arbitrary Lagrangian-Eulerian (ALE) methods are a powerful and complicated tool for multi-physics modeling

- ✓ ALE Methods
  - ✓ Lagrange step, mesh relaxation, and remap
  - Eulerian with grid motion
- ✓ The benefit of ALE is improved accuracy without mesh tangling



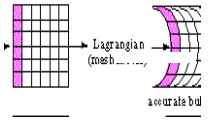
Eulerian with Grid Motion (ALE)

ALE : Eulerian with grid motion

Lagrangian $\left.\frac{\partial \varphi(X,t)}{\partial t}\right|_X = f$

Eulerian $\left.\frac{\partial \varphi(x,t)}{\partial t}\right|_x + u\frac{\partial \varphi}{\partial x} = f$

ALE $\left.\frac{\partial \varphi(\chi,t)}{\partial t}\right|_\chi + (u-\hat{u})\frac{\partial \varphi}{\partial x} = f$



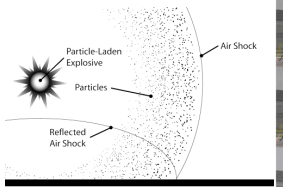
X : Material
x : Spatial
χ : Referential

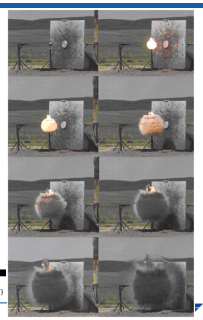
$u = \left.\frac{\partial x}{\partial t}\right|_X$: Material Velocity

$\hat{u} = \left.\frac{\partial x}{\partial t}\right|_\chi$: Ref. Frame Velocity

Multiphase Example : Metal particles in an explosive

Blast-driven shocks with entrained particulate





D.L. Frost, et. al., Particle momentum effects from the detonation of heterogeneous explosives, Journal of Applied Physics, 101, 113529 (2007)

Multiphase for particle and shock interaction

- **Eulerian with grid motion (ALE)**
- **Equation of motion for each material**
- **Continuum representation of particles**
- **Superimposed Lagrange particles**
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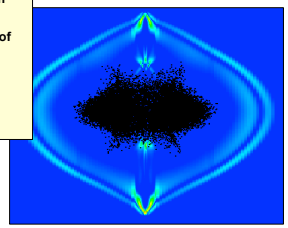
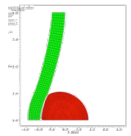
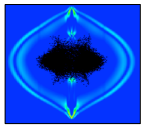


Arbitrary Lagrangian-Eulerian (ALE) methods are a powerful and complicated tool for multi-physics modeling

- ✓ **ALE Methods**
  - ✓ **Lagrange step, mesh relaxation, and advection**
  - ✓ **Eulerian with grid motion**
- ✓ **The benefit of ALE is improved accuracy without mesh tangling**



Particle-laden explosive
- ***Multiphase ALE***
- ***Lagrange particles***



Material and Chemistry Considerations in ALE Applications

A significant number of material models are available in ALE3D code

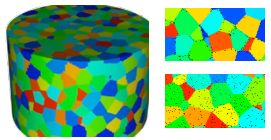
Steinberg-Guinan	Fiber composite unit cell
Steinberg-Lund	Fiber composite with damage
Sack	
MTS	
PTW	
Johnson-Cook	
Zerilli-Armstrong	
Bilinear	
Power Law	
Bilinear w/ tabular Te	
Kelly Limestone	
Power-law rate	
Dislocation Drag (We	
Lesuer	HERMES non-prompt ignition
Garafalo	Mulliken-Boyce polymer
Hyperbolic sine w/ solidification	Visco-SCRAM(LANL)
Radiation Damage	Visco-DCA(LANL)
MSM; MSM with twinning	TEPLA(LANL)
Mooney-Rivlin	BCJ(SNL)
Anisotropic plasticity	MossFrac(LLNL)
Crystal Plasticity	Dfract(SRI)
Crystal plasticity w/phase change	Non Associative flow(UPENN)
Phase change model with kinetics	GeoModel Library(SNL)
	GeoDyn Mat Library(LLNL)

Wide range of

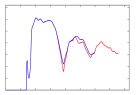
- **Model types, focusing on various aspects of material physics, levels of detail**
- **Material state: pressure, temperature, strain rate**

Models are being used to assess influence of micro-structural features on failure

Effects of nucleation site distribution



Free surface velocity is dependent on number or pattern of nucleation sites



time

Free surface **Movie**

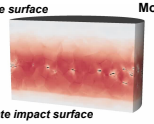
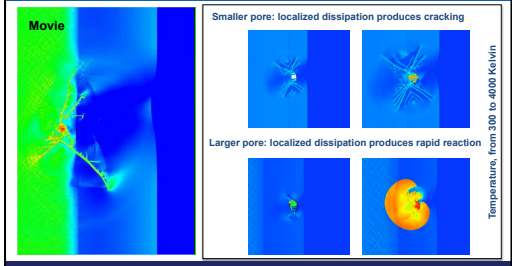


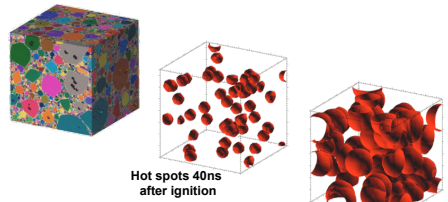
Plate impact surface

Multi-physics modeling bring together mechanics and explosive reactivity



Simulations both test and suggest hypotheses about physics interactions

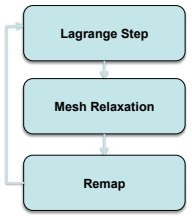
The grain-scale simulations provide insight for approximate full-scale reactive models



Macro-scale

Statistical "Hot-Spot" model for reaction initiation and growth

Fracture and failure models are common in Lagrange codes but can be poorly suited for ALE



Fracture and failure models are usually developed and calibrated with Lagrangian calculations

Extreme deformation problems require mesh relaxation and remap but the models are often poorly suited to standard remap methods

Post remap "fixup" routines are available for each material but cannot fix all the problems

DOE National Labs address R&D challenges with cutting-edge multi-physics modeling

DOE Laboratories and LLNL

- ✓ R&D activities and facilities
- ✓ Career and internship opportunities

R&D in multi-physics modeling

- ✓ Applications (ALE3D code)
- ✓ ALE methods
  - ✓ Accurately capture multi-physics with extreme deformations
  - ✓ Material models developed for Lagrange simulation and are mesh dependent
  - ✓ Chemical reactive models are computationally intensive and approximate methods are necessary

Penetration of a projectile into a structure with subsequent explosion and damage

Lawrence Livermore National Laboratory

Arbitrary Lagrangian-Eulerian (ALE) and Multi-Physics Modeling and Simulation

October 28, 2014

Rose McCallen, Ph.D.
ALE3D Research and Development Team

Lawrence Livermore National Laboratory

LLNL-PRES-663421-DRAFT

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC.

Arbitrary Lagrangian-Eulerian (ALE) methods are a powerful and complicated tool for multi-physics modeling

Part 1 – Applications *
- Application space is huge and the coupled physics is challenging
- It takes a multi-discipline team to address the technical challenges

Part 2 – ALE Intro
- ALE Methods
  - Lagrange step, mesh relaxation, and advection
  - Eulerian with grid motion
- ALE multi-phase and Lagrange particles
- The benefit of ALE is improved accuracy without mesh tangling

Part 3 – Materials
- Fracture and failure models are typically developed and calibrated with Lagrangian calculations
- Models are mesh resolution dependent

* Examples are with a code called ALE3D developed at LLNL

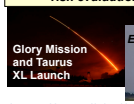
ALE3D's application space is national security

DOE: Stockpile Stewardship and other NNSA Programs

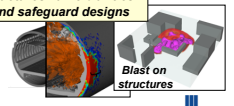
Explosive cookoff
Violence of reaction
Fracture & failure

DoD: Munitions and rocket design performance, lethality, vulnerabilities, and safety

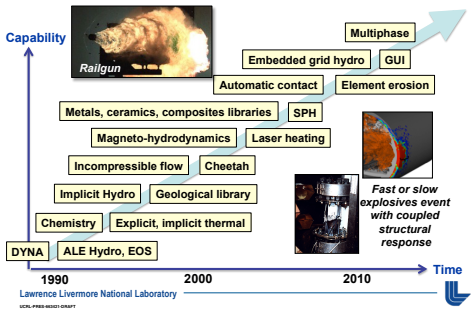
NASA : Launch systems and risk evaluations



DHS : Transit and structures vulnerabilities and safeguard designs



Integrated multi-physics is required

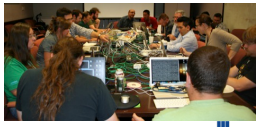


It takes a multi-discipline team, technically challenging work, and some fun

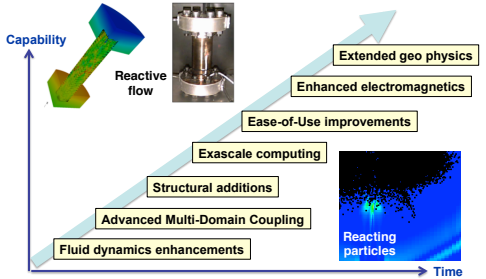
Multi-discipline team

Small groups or individuals work on projects

Bug-fix days



The future brings new challenges



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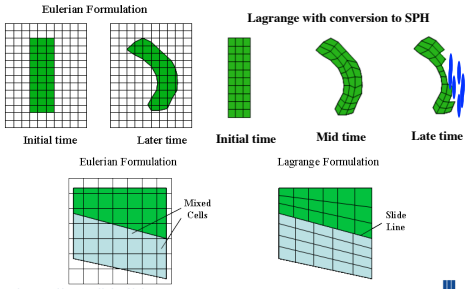
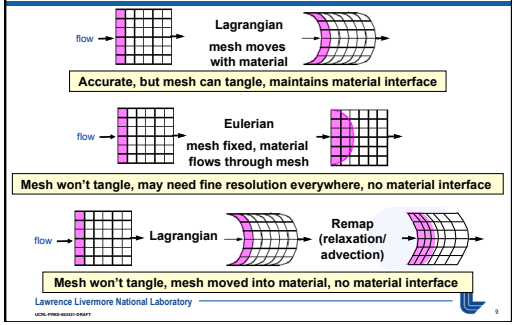
What do we mean by Lagrangian and Eulerian?



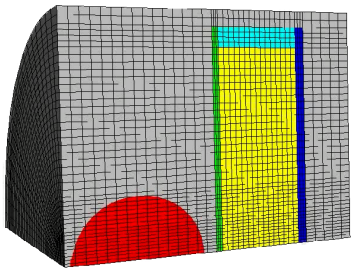
Arbitrary Lagrangian-Eulerian (ALE) combines both methods



What can be done with an ALE simulation

Lexan ball impacting confined explosive cylinder

Movie



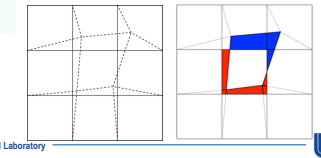
ALE process has several distinct phases

Lagrange Step

Mesh Relaxation

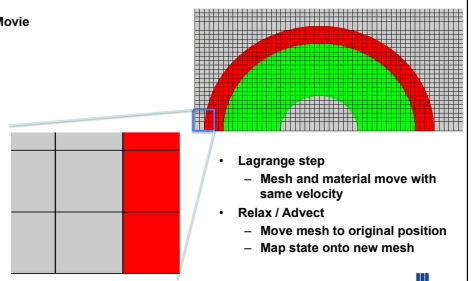
Advection/ Remap

- **Mesh Relaxation**
  - A revised mesh that smooths or improves the current mesh
  - Various options are available to construct the relaxed mesh
- **Advection**
  - Remapping the state of the calculation from the mesh at the end of the Lagrange step onto the relaxed mesh



What do we mean by Eulerian?

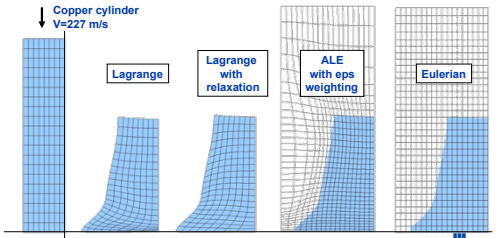
Movie



- **Lagrange step**
  - Mesh and material move with same velocity
- **Relax / Advect**
  - Move mesh to original position
  - Map state onto new mesh

Benefit of ALE is improved accuracy

- Reducing mesh distortion – part Lagrangian, part relaxed (advection)
- Improve accuracy - weighted material relaxation



ALE3D has several methods for mesh relaxation

Relaxer	Description
Equipotential	Global mesh smoothing with weights, tries to generate uniform spaced mesh
Modified Equipotential	Equipotential with corrections for spherical meshes
Condition number	Local optimization to correct aspect ratios and angles
Eulerian	Restores the mesh to its original locations
Programmed Relax	A set of specific controls over mesh movement

Equipotential smoothing is commonly used

- Equipotential (Winslow) smoothing is based on minimizing the objective functional

$$I = \frac{1}{2}\int W(\boldsymbol{x})(\nabla x)^2 d\xi^3$$

- Where the mesh coordinate lines are regarded as functions of parametric coordinates and W is a weighting function.
- The minimizer is the solution to the elliptic PDE

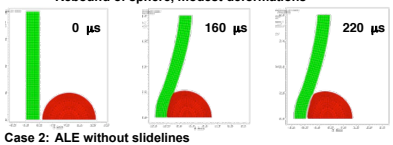
$$\nabla \cdot (\boldsymbol{W}\,\nabla \boldsymbol{x}) = \boldsymbol{0}$$

- The weight function is chosen to be the locally weighted Jacobian – the relaxer tries to obtain equal volume elements.
- An element level weight is equivalent to locally scaling the element volume. The actual calculation will depend on the ratio of element weights.

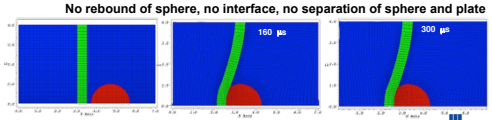
Implications of Lagrange versus ALE

Case 1: Lagrange only with slidelines
Rebound of sphere, modest deformations

Copper sphere impacting steel plate (200m/s)



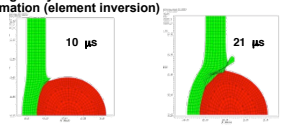
Case 2: ALE without slidelines
No rebound of sphere, no interface, no separation of sphere and plate



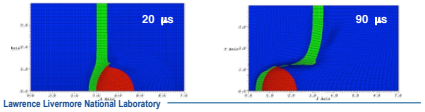
Implications of Lagrange versus ALE (cont.)

Case 3: Lagrange only with slidelines
Lagrange only solution fails due to too much deformation (element inversion)

Copper sphere impacting steel plate (500m/s)



Case 4: ALE without slidelines
ALE handles significant material deformations because portions of the mesh relax when needed



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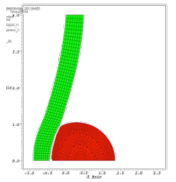
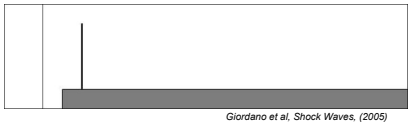


Blast shock impinging on steel plate with Eulerian flow and Lagrange material interface

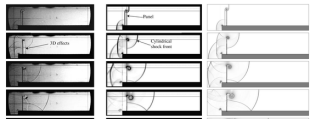
Ma 1.2 shock

Movie



Giordano et al, Shock Waves, (2005)

Giordano Exp | Giordano Calc | ALE3D Grid

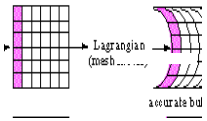


ALE : Eulerian with grid motion

Lagrangian $\left.\frac{\partial \varphi(X,t)}{\partial t}\right|_X = f$

Eulerian $\left.\frac{\partial \varphi(x,t)}{\partial t}\right|_x + u\frac{\partial \varphi}{\partial x} = f$

ALE $\left.\frac{\partial \varphi(\chi,t)}{\partial t}\right|_\chi + (u-\hat{u})\frac{\partial \varphi}{\partial x} = f$



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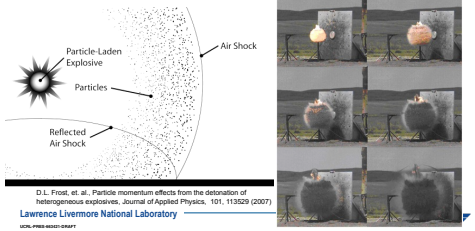
Blast-driven shocks with entrained particulate



D.L. Frost, et. al., Particle momentum effects from the detonation of heterogeneous explosives., Journal of Applied Physics, 101, 113529 (2007)

Reference

Particle momentum effects from the detonation of heterogeneous explosives

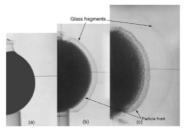


FIG. 9. Radiographs of particle dispersal for an 11.8 cm diameter spherical glass-cased charge containing iron beads; 275 μm diameter particles in frame (b) and 463 μm in frame (c). Time of radiographs, relative to initiation of charge detonation: (a) 0, (b) 43, and (c) 75 μs.

Multi-phase ALE : Each material has its own equation of motion

$\Delta u_{gj} = u_{gj} - u_{mesh,i}$

Eulerian with grid motion

$$\left(\alpha_g \rho_g\right)_t + \sum_j \left(\alpha_g \rho_g \Delta u_{gj}\right)_{x_j} = 0$$

$$\left(\alpha_g \rho_g u_{gi}\right)_t + \sum_j \left(\alpha_g \rho_g \Delta u_{gj} u_{gi}\right)_{x_j} + \left(\alpha_g P_g\right)_{x_i} - P_{\text{int}}\left(\alpha_g\right)_{x_i} = 0$$

$$\left(\alpha_g \rho_g E_g\right)_t + \sum_j \left(\alpha_g \rho_g \Delta u_{gj} E_g\right)_{x_j} + \sum_j \left(\alpha_g P_g u_{gj}\right)_{x_j} + \sum_j P_{\text{int}} V_{\text{int},x_j} \alpha_{gx_j} = 0$$

Allows for a continuum representation of particles

x_g, α_g, u_g, e_g
x_s, α_s, u_s, e_s

Multiphase for particle and shock interaction

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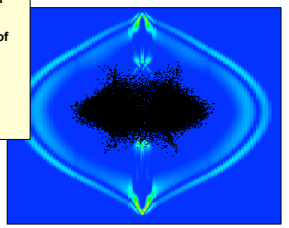
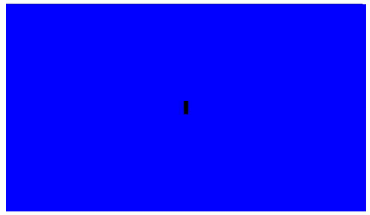
- **Equation of motion for each material**
- **Continuum representation of particles**
- **Superimposed Lagrange particles**
- **Lagrange interface with standard ALE hydro**



Explosive blast ALE simulation with Lagrange particles

Movie



Time=0.0001

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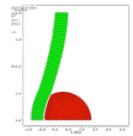
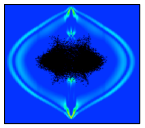




A significant number of material models are available in ALE3D

Steinberg-Guinan
Steinberg-Lund
Sack
MTS
PTW
Johnson-Cook
Zerilli-Armstrong
Bilinear
Power Law
Bilinear w/ tabular Te
Kelly Limestone
Power-law rate
Dislocation Drag (Wolfer)
Lesuer
Garafalo
Hyperbolic sine w/ solidification
Radiation Damage
MSM; MSM with twinning
Mooney-Rivlin
Anisotropic plasticity
Crystal Plasticity
Crystal plasticity w/phase change
Phase change model with kinetics

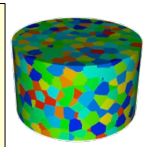
Fiber composite unit cell
Fiber composite with damage
Johnson-Holmquist improved (JH2)
SWRI glass
HERMES non-prompt ignition
Mulliken-Boyce polymer
Visco-SCRAM(LANL)
Visco-DCA(LANL)
TEPLA(LANL)
BCJ(SNL)
MossFrac(LLNL)
Dfract(SRI)
Non Associative flow(UPENN)
GeoModel Library(SNL)
GeoDyn Mat Library(LLNL)

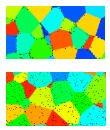
Wide range of pressure, temperature, strain rate, internal state

Wide range of model types, focusing on various aspects of material physics, levels of detail

Models are being used to assess influence of microstructural features on failure

- **Prediction of failure behavior under conditions that are challenging to probe experimentally**
- **More rapid assessments as processing conditions are changed**
- **Example : Focus is on effects of nucleation site distribution**

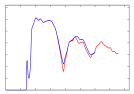




Movie

Free surface

Free surface velocity is dependent on number or pattern of nucleation sites



time

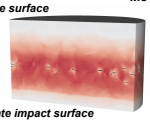
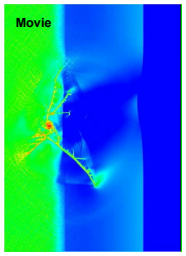


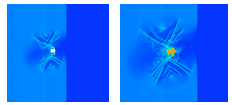
Plate impact surface

Multi-physics efforts bring together crystal mechanics and explosive reactivity

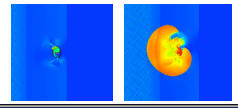
Movie



Smaller pore: localized dissipation produces cracking



Larger pore: localized dissipation produces rapid reaction

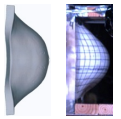


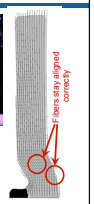
Temperature, from 300 to 4000 Kelvin

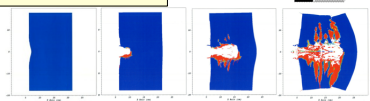
Simulations both test and suggest hypotheses about interactions among various aspects of the physics

Focused efforts lead to improvements for fiber-reinforced composite model with damage

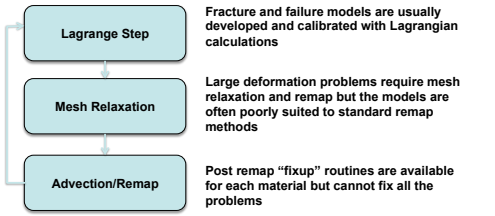
- **Hyper-elastic formulation, non-linear constitutive response**
- **Accurate material response at finite strains**
  - **Large, nonlinear fiber stretching**
  - **Large shearing prior to failure**
- **Multiple damage modes, including fiber damage, matrix damage, and delamination**
- **Fiber directions correctly update in the presence of large rotations and shears**
- **Compatible with advection (ALE)**







Fracture and failure models are common in Lag. codes but can be poorly suited for ALE



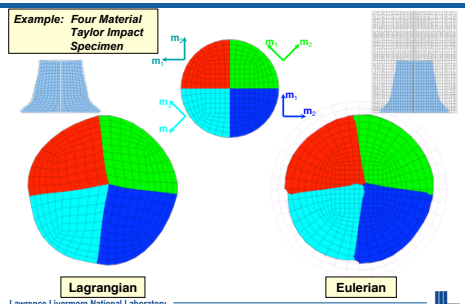
Fracture and failure models are usually developed and calibrated with Lagrangian calculations

Large deformation problems require mesh relaxation and remap but the models are often poorly suited to standard remap methods

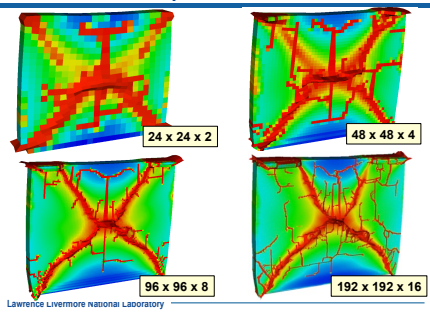
Post remap "fixup" routines are available for each material but cannot fix all the problems

ALE creates additional concerns for material model implementations

Example: Four Material Taylor Impact Specimen



Fracture/failure models are typically mesh and resolution dependent



There is a wide range of active research areas

- Multiple physical mechanisms including reactive materials, phase changes, and complex microstructures
- Balance of model fidelity and cost
- Advection (ALE) of damage and complex state
- Mechanics for mixed material zones
- Mesh convergent treatment for failure and strain softening materials

Arbitrary Lagrangian-Eulerian (ALE) methods are a powerful and complicated tool for multi-physics modeling

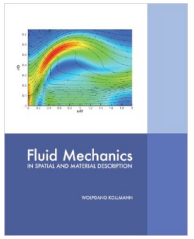
Part 1 – Applications *
- Application space is huge and the coupled physics is challenging
- It takes a multi-discipline team to address the technical challenges

Part 2 – ALE Intro
- ALE Methods
  - Lagrange step, mesh relaxation, and advection
  - Eulerian with grid motion
- ALE multi-phase and Lagrange particles
- The benefit of ALE is improved accuracy without mesh tangling

Part 3 – Materials
- Fracture and failure models are typically developed and calibrated with Lagrangian calculations
- Models are mesh resolution dependent

* Examples are with a code called ALE3D developed at LLNL

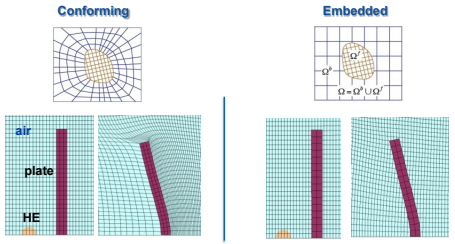
Fundamental equations of fluid dynamics in Lagrangian and Eulerian reference frames, e.g.,



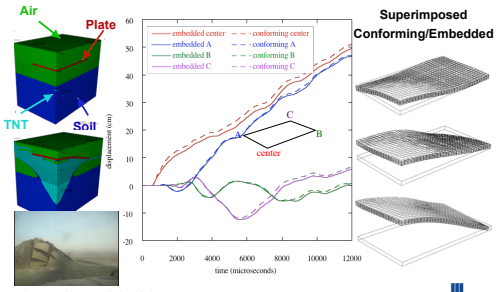
This book … develops the basic tools for the description of flow phenomena and establishes the fundamental equations derived from first principles in spatial and material descriptions. Emphasis is placed on laminar flows of incompressible, viscous and inviscid fluids with significant vorticity. The book consists of two parts, the first covering most of the kinematics, and the second the dynamics of fluid flow with selected applications. …

Embedded grid capability allows for accurate and efficient fluid/structure simulations

Allows coupling of separate meshes without conformal gridding



ALE3D captures buried charge impacting 3D plate with conformal or embedded grid



Lawrence Livermore National Laboratory

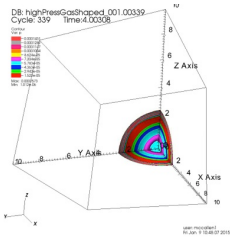
Predicting Physics Rather than an Artifact of a Numerical Method

Rose McCallen, Ph.D.
2015

Objectives

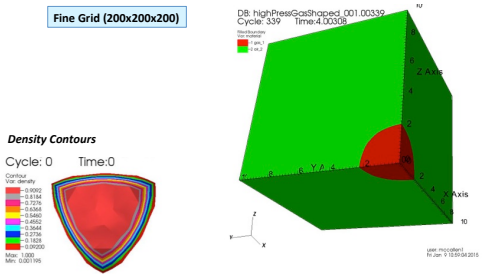
- Determine effect of numerical methods and parameter choices for a known solution
- Exercise a range of options
- Re-familiarize with methods

Spherical high pressure gas expansion



Initial Conditions : High pressure gas ball (.5 cm radius) in low pressure environment (10 cm box)
Solution Method : Fixed Eulerian grid with shaped in high pressure gas
1/8th symmetry and nonreflecting outflow boundaries
Grid : Uniform 100x100x100 and 200x200x200
Observation : Surface of high pressure gas is relatively smooth throughout the simulation for coarse and fine grid

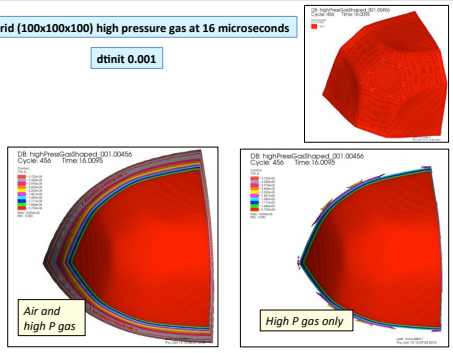
Fine Grid (200x200x200)



Observations : - Planar character of high pressure gas at axis for coarse and fine grid
- Surrounding air is compressed at 16 micro seconds and pushing on high pressure gas material for coarse and fine grid

Coarse Grid (100x100x100) high pressure gas at 16 microseconds

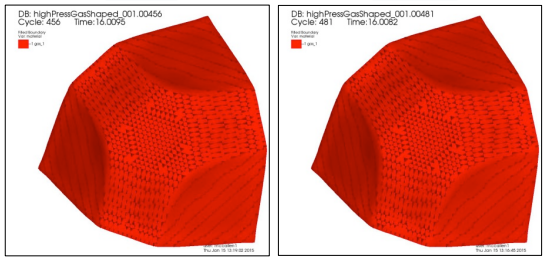
dtinit 0.001



Refinement : Reduce initial time step by two orders of magnitude
Observation : Planar character of high pressure gas material surface persists

Coarse Grid (100x100x100) high pressure gas material surface at 16 microseconds

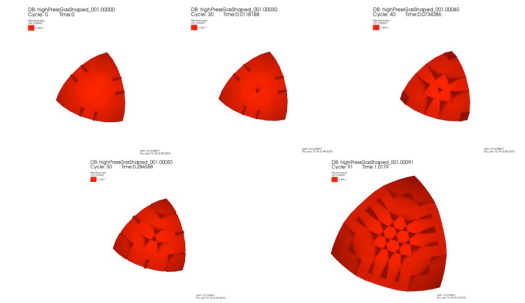
dtinit 0.001 **dtinit 0.00001**



Refinement : Reduce initial time step by two orders of magnitude.
Observation : Planar character is present at early times

Coarse Grid (100x100x100) evolution of surface

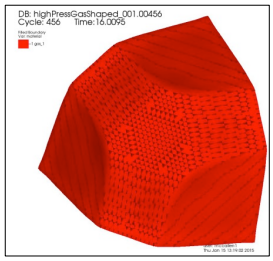
dtinit 0.00001



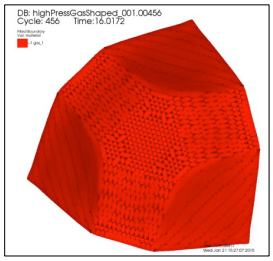
Refinement : Increased value of npics from 6 to 12 (improves volume fraction calculation for shaped-in sphere)
Observation : Planar character of high pressure gas material surface persists.

Coarse Grid (100x100x100) high pressure gas material surface at 16 microseconds

dtinit 0.001, npics 6

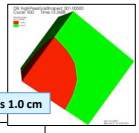


dtinit 0.001, npics 12

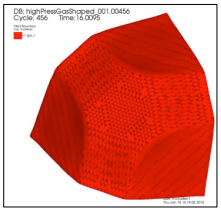


Refinement : Increased radius of high pressure gas from 0.5cm to 1.0 cm
Observation : Some improvement in reducing planar character of high pressure gas material.

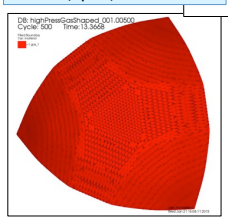
Coarse Grid (100x100x100) high pressure gas material surface at 16 microseconds



dtinit 0.001, npics 6, initial radius 0.5 cm



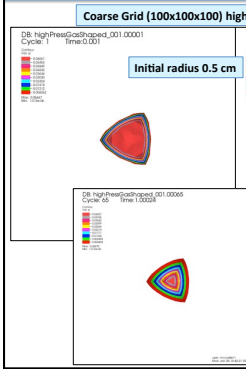
dtinit 0.001, npics 6, initial radius 1.0 cm



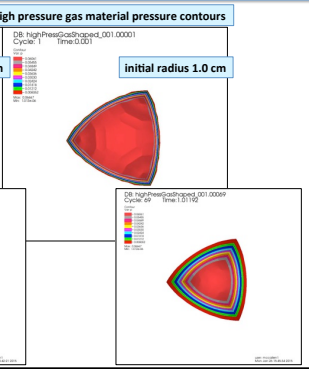
Refinement : Increased radius of high pressure gas from 0.5cm to 1.0 cm
Observation : Comparison of initial pressure condition

Coarse Grid (100x100x100) high pressure gas material pressure contours

Initial radius 0.5 cm

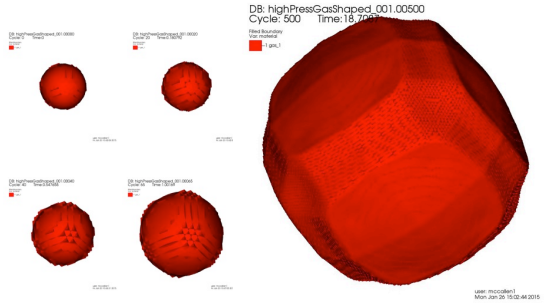


initial radius 1.0 cm



Refinement : Simulate full sphere, rather than 1/8th geometry with symmetry planes.
Observation : Planar character is present at early times

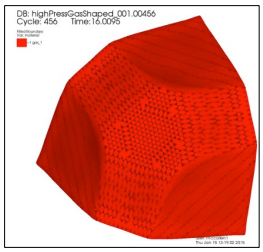
Coarse Grid (100x100x100) evolution of surface



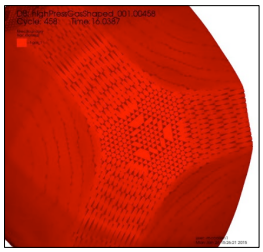
Refinement: Simulate full sphere, rather than 1/8th geometry with symmetry planes
Observations : Same planar character

Coarse Grid (100x100x100) high pressure gas at 16 microseconds

1/8 th geometry with symmetry planes



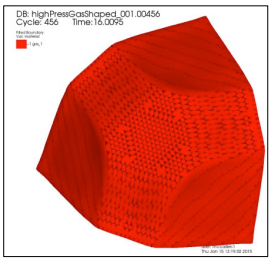
Full geometry simulation



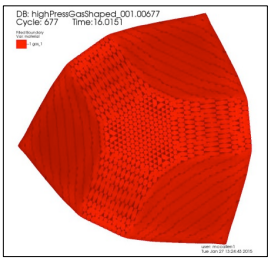
Refinement : Monotonic Q, rather than Bulk Q
Observation : Planar character of high pressure gas material surface persists

Coarse Grid (100x100x100) high pressure gas material surface at 16 microseconds

Bulk Q

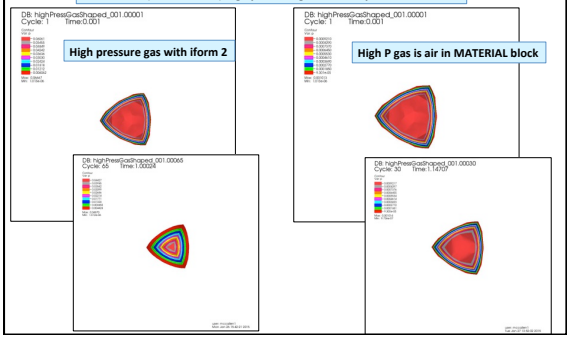


Monotonic Q



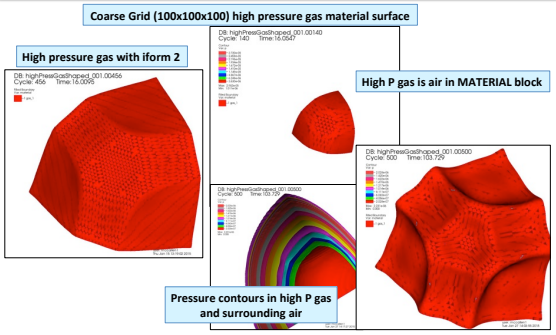
Refinement : Air as the high P gas in MATERIAL block with 2 times t0 and v0 and 3 orders higher p0 and e0 compared to surrounding air
Observation : Comparison of initial pressure condition

Coarse Grid (100x100x100) high pressure gas material pressure contours



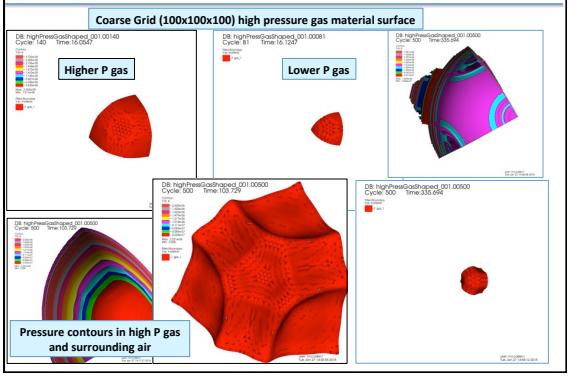
Refinement : Air as the high P gas in MATERIAL block with 2 times t0 and v0 and 3 orders higher p0 and e0 compared to surrounding air
Observation : Planar character of high pressure gas material surface persists and even more extreme

Coarse Grid (100x100x100) high pressure gas material surface



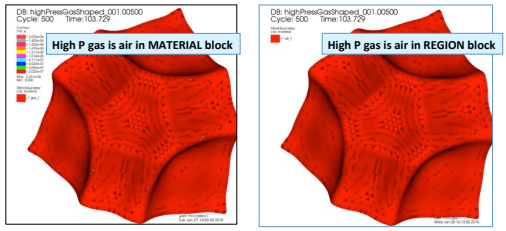
Refinement : Lower pressure difference
Observation : Character of high pressure gas material surface persists

Coarse Grid (100x100x100) high pressure gas material surface



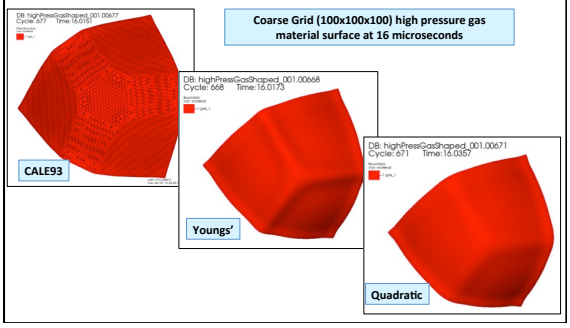
Refinement : Air as the high P gas in REGION versus MATERIAL block
Observation : No change in results (appear to be identical)

Coarse Grid (100x100x100) high pressure gas material surface



Refinement : Mixed zone advection for CALE93 (default) and Youngs' method (linear) and Quadratic method – all with Monotonic Q
Observation : Planar character of high pressure gas material surface persists but with a smooth surface and narrow seam at 45 degrees and on plane of axis

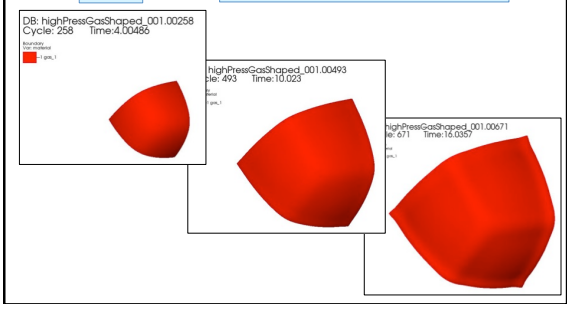
Coarse Grid (100x100x100) high pressure gas material surface at 16 microseconds



Refinement : Mixed zone advection for Quadratic method – with Monotonic Q
Observation : Initial character of high pressure gas material surface is relatively round and smooth

Quadratic

Coarse Grid (100x100x100) high pressure gas material surface at 4, 10, and 16 microseconds

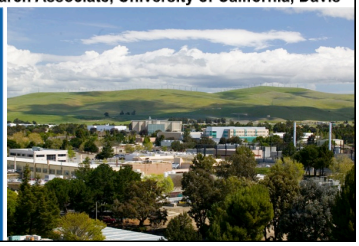


Collaborations with universities and industry for cutting-edge simulation capability

January 2015

Rose McCallen, Ph.D.
Weapons and Complex Integration (WCI), LLNL
Research Associate, University of California, Davis

Lawrence Livermore National Laboratory



LLNL-PRES-666413-DRAFT
This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC

We want expansion of university and industry collaborations with direct impact on cutting-edge simulation capability for DOE

ALE3D
DOE

DoD, DHS, NASA

Increasing demand for use on National Security applications
- Multi-physics
- Production level performance (scalable)
- User support

Universities and Industry

- Open up interactions with a larger pool of sharp people
- Direct spin back of cutting-edge capability into LLNL codes
- Attract top university students to careers at LLNL
- Enhanced computer vendor interactions for new and advanced architectures
- May expand work-for-others (WFO) support

Code modularity and an enhanced build process may provide agility and enhance protection

- Provide a hierarchy of physics modules with identified protection
- A process for customized code builds, testing, and distribution

Control Board
- DOE
- Office of Classification and Export Control (OCEC)
- Industrial Partnership Office (IPO)
- WCI

ALE3D
Full Protection
- Government use on National Security applications

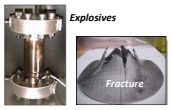
ALE3D-Lite
Appropriate protection
- Industry use on applications of National interest

Solvers, published models, and more
Open Source
- University collaborators

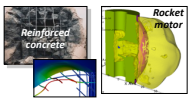
ALE3D's national security application space is broad and the multi-physics is challenging

ALE3D
Full Protection
- Government use on National Security applications

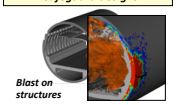
DOE: Stockpile Stewardship and other NNSA Programs



DoD: Munitions and rocket design performance, lethality, vulnerabilities, and safety



DHS : Transit and structures vulnerabilities and safeguard designs



NASA : Launch systems and risk evaluations

Industry use provides simulation challenges outside of national security applications

ALE3D-Lite
Appropriate protection
- Industry use on applications of National interest

Bio- and nano-technology breakthroughs

University collaborations provide opportunities for basic research in numerical methods and physics models

Solvers, published models, and more
Open Source
- University collaborators

Pore collapse with shock loaded explosive using ALE3D

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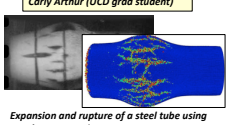

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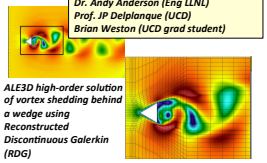


ALE3D high-order solution of vortex shedding behind a wedge using Reconstructed Discontinuous Galerkin (RDG)

Modularity and enhanced processes for customized builds, testing, and distribution

ALE3D
Full Protection

•
•
•

ALE3D-Lite
Appropriate protection

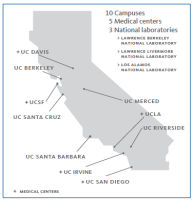
•
•
•

Solvers, published models, and more
Open Source

•
•
•

- **Reduce complexity**
  - **Identify high level operations**
  - **Establish appropriate data dependencies**
  - **Modularize physics packages**
- **Confidence**
  - **Customize builds with (built-in) testing**
  - **Investigate cutting-edge version control and SQA practices**

UC Davis College of Engineering is one of the Top 20 public engineering graduate schools



University of California

Total enrollment	**238,700**
Undergraduate students	**188,300**
Graduate students	**50,400**
Alumni	**1.6 M**
Total operating budget	**$ 25.46 B**

UC Davis College of Engineering

- Ranked **17th** among the Top 20 U.S. public universities, Best Undergraduate Engineering Programs, (US News & World Report 2015)
- Ranked **18th** among the Top 20 public engineering graduate schools, (US News & World Report 2015)
- Ranked **3rd** among top 50 engineering programs for percentage of female faculty, (U.S. News & World Report, 2014)
- **$87.4** million in research expenditures for 2013–14
- Founded in 1962
- 200 faculty
- 4,403 undergraduate students
- 1,159 graduate students
- 23,500 alumni
- 21 current and former faculty elected to national academies
- 50 NSF Faculty Early Career Development Awards (CAREER/PECASE)

Lawrence Livermore National Laboratory

A joint educational and research institute supporting LLNL programs and UCD science excellence

Retention

Energize system

Bring National challenges and encourage strategic relationships through
- Sabbaticals and joint appointments
- HPC resources
- Experiment facilities

UCDAVIS UNIVERSITY OF CALIFORNIA

Top Ranking

Close Proximity

Diversity

Bring scholarly driven inquiry and cutting-edge R&D through
- Faculty sabbaticals, student interns
- Joint proposals, fellowships

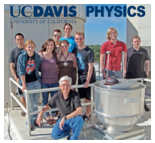
Hiring pipeline

Science and Engineering in National Interest Center (SENIC)

SENIC is a focal point for collaborations and education in support of National Interest

Form working groups and cooperatively solicit support

Connect faculty with LLNL research programs



SENIC
- Leadership
- Strategic planning
- Coordinated effort

Identify focus topics through joint workshops and seminars

MARS WRIGLEY

NASA

Jointly host visits with industry and government funding sources

Promote Joint Research and Coordinate Joint Proposals

Proposing a pilot effort in the development of a model for LLNL's "University Hubs"

SENIC

UCDAVIS UNIVERSITY OF CALIFORNIA
- Historical connection
- Leverage LLNL/UCD MOU
- UCD tops chart of where LLNL employees obtained highest degree

Attract other UC campuses to join in

Attract other National Universities to join in

Science and Engineering in National Interest Center (SENIC)

Requesting support from both LLNL Programs and UCD

SENIC

UCDAVIS UNIVERSITY OF CALIFORNIA

- Encourage participation by researchers
- Support seminars, working groups, and visits
- Establish physical location and visitor offices
- Support Center Lead's time

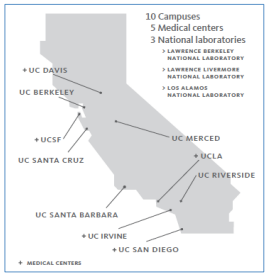
- Encourage participation by faculty and students
- Support seminars, working groups, and visits
- Establish physical location and visitor offices
- Support Center Lead's expenses

Science and Engineering in National Interest Center (SENIC)

UC Davis Demographics and Strengths

Rose McCallen, Ph.D.
July 2015

Nine University of California campuses placed among the top 150 universities in the world



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UC Davis ranks high across the board

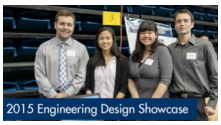
35,415 students in fall 2014

UC Davis Undergraduates		
Total	**27,728**	
Gender		
Women	**15,791**	**57%**
Men	**11,523**	**42%**
International		
	1,985	**7%**

World Ranking
1st for agriculture and forestry
1st in veterinary medicine
1st in the category of research impact in life and earth sciences
National Ranking
Tied **for 1st** among research universities (with UC Berkeley and Penn State) as the top producer of US Fulbright Scholars, 2012-13
7th among public universities, **27th** among public and private universities in 2015 *The Best Colleges*
9th among public research universities and 38th among public and private research universities *2015 US News & World Report's*
9th in granting undergraduate degrees to students of color for 2013-14
9th among U.S. universities in the number of international scholars 2013-14
10th best female-led institutions among the world's top universities for 2015

UC Davis College of Engineering is one of the Top 20 public engineering graduate schools

College of Engineering 2013 Graduate Students		
Total	**1,130**	
Gender		
Women	**303**	**26.8%**
Men	**827**	**73.2%**
International		
	432	**38.2%**



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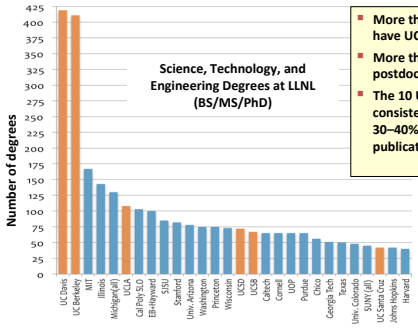
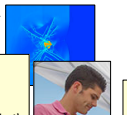
UC is LLNL's partner and pipeline for ST&E talent



- **More than 29% ST&E staff have UC degrees**
- **More than 24% of postdocs have UC PhDs**
- **The 10 UC campuses consistently co-author 30–40% of all LLNL publications**

UC Davis/LLNL collaborations provide opportunities for basic research in numerical methods and physics models



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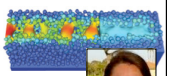

Optimization methods for additive manufacturing

Dr. Dan White (Eng LLNL)
Prof. JP Delplanque (UCD)
Rebecca Barney (UCD grad student)

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Dr. Mike Owen (AX-div/WCI LLNL)
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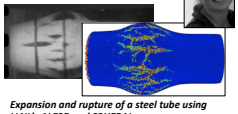

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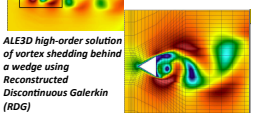

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