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Sierra Thermal Fluids use of Trilinos

Trilinos User Group meeting, October 29, 2015

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U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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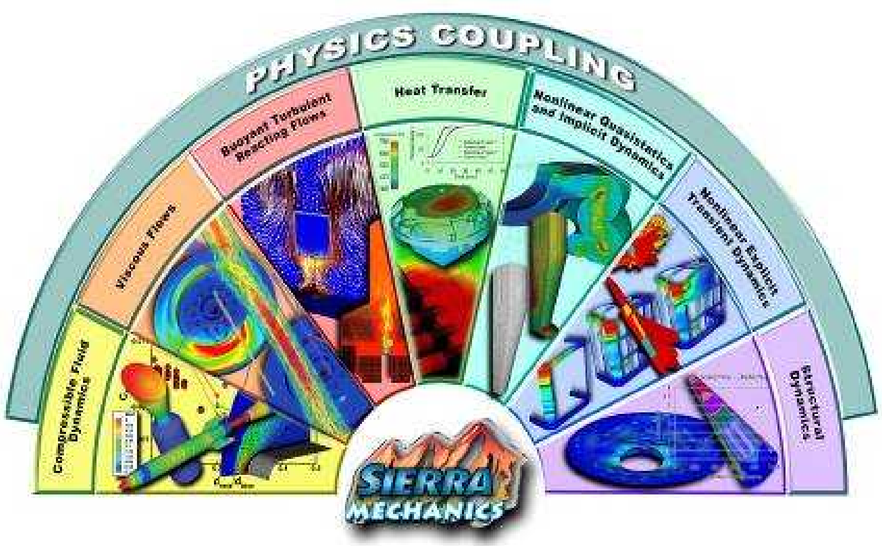
Discussion outline

1. What are the Sierra/TF codes and what are they used for?
2. Sierra/TF TPLs
3. What are the current successful collaboration areas between Sierra/TF and Trilinos?
4. What are the current problem areas with Sierra/TF use of Trilinos?
5. Sierra/TF prioritized wish list for Trilinos development
6. Organic material decomposition needs
7. Laser welding and additive manufacturing needs
8. Path forward

Sierra is the engineering mechanics simulation code supporting the NW mission, as well as other customers

- Distinguishing strengths
  - "Application aware" development
  - Scalable
  - SQA and V&V
  - Multiple scales
  - Coupling



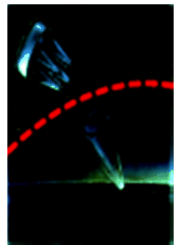
- Explicit tie to SNL workflow, including
  - Geometry and meshing
  - Visualization
  - Design and optimization

- Partner applications at Sandia include
  - CTH and ALEGRA for shock physics simulations
  - RAMSES suite for radiation effects, electrical and electronics simulations

The Nuclear Weapons program is the principal driver for Sandia's Computational Simulation efforts

Delivery

Separation shock/ Aerodynamic Heating

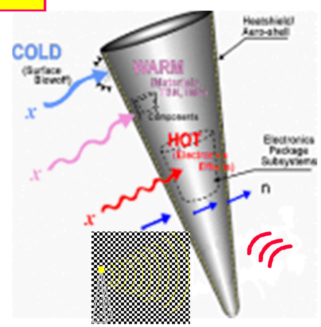


Staging shock

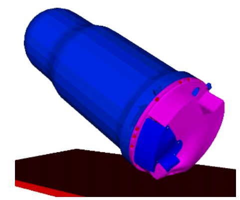
Random vibration

Survivability

Radiation Effects

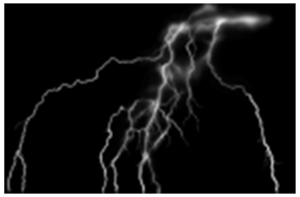


Assured Safety and Security



Mechanical Insult

Thermal Insult



Electromagnetic Insult

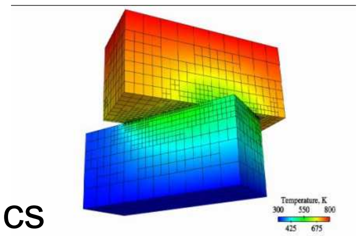
Security Components

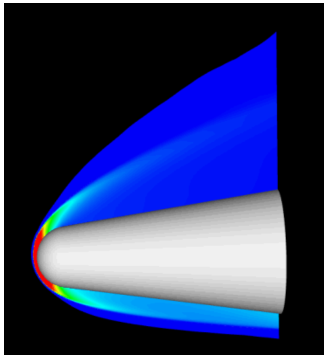
Assured Performance & Manufacturing

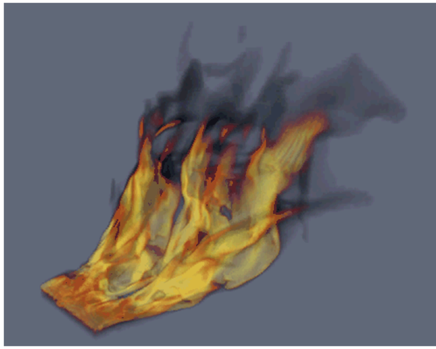
Safe & Secure Transport

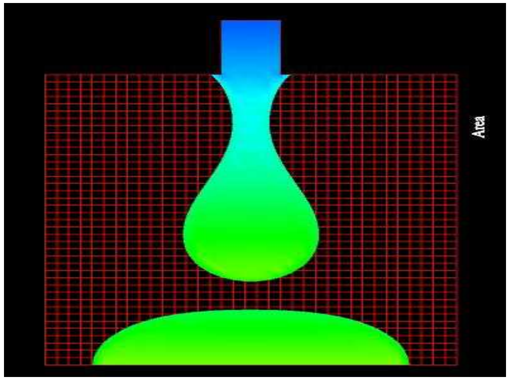
Computational Thermal & Fluid Mechanics

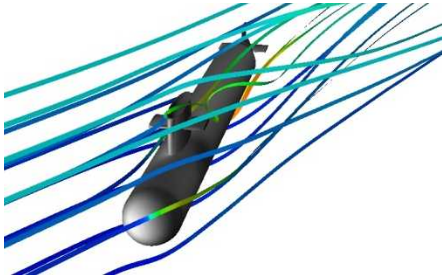
- **Thermal** – Heat Transfer, Enclosure Radiation and Chemistry
  - Dynamic enclosures
  - Element birth death
  - Contact
- **Aero** – Compressible Fluid Mechanics
  - Subsonic through hypersonic
  - Laminar and turbulent
  - Unstructured mesh
- **Multiphase** – Non-Newtonian, Multi-physics, and Free Surface Flows
  - Complex material response
  - Level sets for surface tracking
  - Flexible coupling schemes
- **Fire/Combustion** – Low Speed, Variable Density, Chemically Reacting Flows
  - Eddy dissipation and mixture fraction reaction models
  - RANS and LES based turbulence models
  - Unstructured Mesh
  - Pressurization models



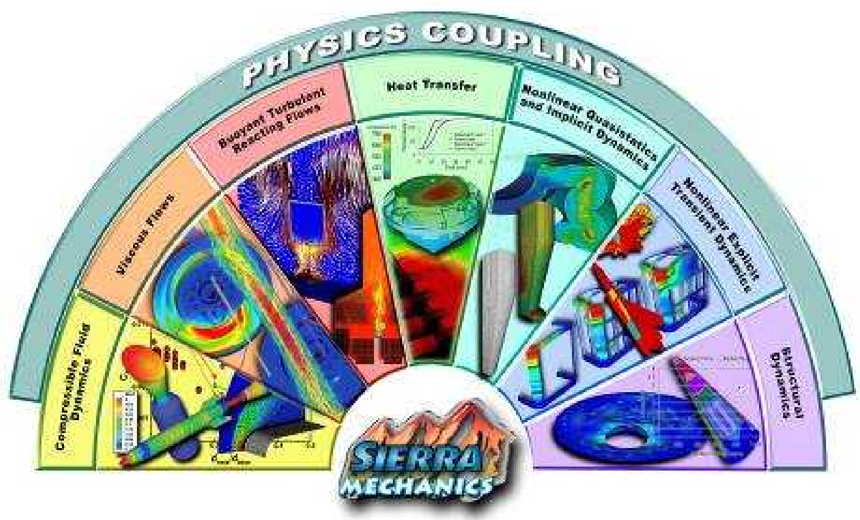








What are the Sierra/TF codes and what are they used for?



<u>Sierra/TF primary codes</u>

- Aria
- Fuego
- Aero
- Nalu

Thermal/fluids/aerodynamics

- Compressible fluid mechanics with subsonic through hypersonic flows
- Non-newtonian reacting flow with free surfaces and complex material response
- Low mach number turbulent reacting flow participating media radiation
- Heat transfer with limited convection, chemistry, and enclosure radiation

Third party libraries used by Sierra/TF

Aria

Trilinos packages:

- STK
- Kokkos
- Tpetra
- Epetra
- Various linear solvers

Other packages:

- Sierra
- Sierra Utilities
- Framework
- Apublic
- Equation solver
- Contact

Fuego

Trilinos packages:

- STK
- Kokkos
- Various linear solvers
- SEACAS

Other packages:

- Sierra
- Sierra Utilities
- Framework
- Apublic
- Cantera
- Encore
- Math Toolkit
- Netflow
- Aria
- Syrinx
- Tabular Props

Aero

Trilinos packages:

- STK
- Kokkos
- Tpetra
- Ifpack2
- Belos
- Muelu
- Sacado

Other packages:

- FETI
- Krino
- Percept
- Geometry Toolkit

Nalu

Trilinos packages:

- STK
- Kokkos
- Tpetra
- Epetra
- ML
- MueLu
- AztecOO
- Belos
- Ifpack2
- Amesos2
- Zoltan2
- SEACAS

Other packages:

- Boost
- HDF5
- netCDF
- YAML_cpp
- zlib

What are the current (or recent) successful collaboration areas between Sierra/TF and Trilinos?

1. Sierra/TF successfully using many Trilinos TPLs.
2. Kokkos / Sierra/TF team members meeting regularly on Kokkos-izing Sierra/TF codes.
3. FY12 and FY13 L2 joint milestones.
4. Trilinos libraries "productionized": MueLu, Tpetra, Ifpack2, Belos
5. Kokkos tutorial Sept 1 – 2.
6. Paul Lin's help with Trinity CoE and Trinity acceptance.
7. Ray Tuminaro's help with multiphysics solver development for Sierra/TF.
8. Sierra/Algs discussions, every week.
9. Trilinos – Sierra/TF meetings, every 3 weeks.
10. Bug fix in crucial solver than enabled much better Nalu scaling.
11. Eric Phipps's work with Victor Brunini in identification of Sacado-related issue.
12. Other recent bug fixes.
13. Help from Carter Edwards, Si Hammond, Mike Heroux, Rob Hoekstra, Mark Hoemmen, Jonathan Hu, Paul Lin, Andrey Prokopenko, Chris Siefert, Christian Trott, et al. …

Thank you!

What are the current problem areas with Sierra/TF use of Trilinos?

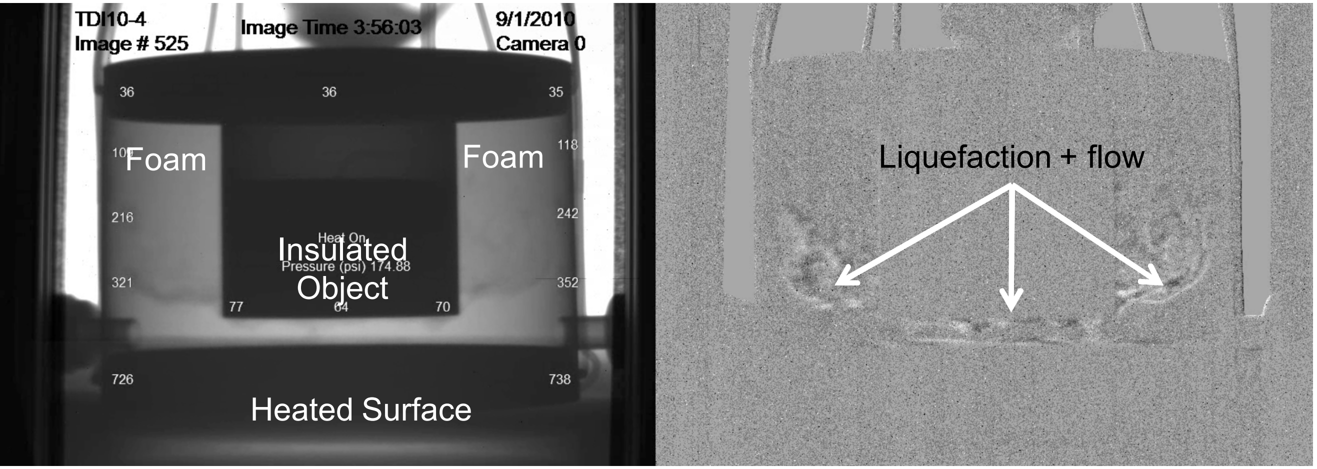
- Sierra / Trilinos / STK integration, building, testing issues
  - Updates too infrequent, leading to major hiccups when they do occur.
  - Brent Pershbacher is the "man caught in the middle" trying to sort this out manually.
  - Rich Drake et al proposed improved Sierra/Trilinos/STK integration, and we're seeing some progress.
  - Public Trilinos repository has not been updated in a month. Moving to GitHub.
  - Improvements occurring: DevOps and iSEMS teams plan to help with these issues soon.
- Trilinos bugs issues
  - Trilinos changes sometimes break Sierra/TF tests.
  - Other bugs slip through, jeopardizing Sierra/TF "production" code status.
  - High churn for Tpetra and Kokkos.
- Culture issues
  - Language barriers.
  - Values mismatches.
- Performance, scaling, and memory footprint issues
  - (See wish list.)
  - Sierra executable file size growth, build times, and ETI.
  - Memory footprint increasing.
- Missing capabilities issues
  - (See wish list.)

Sierra/TF's prioritized wish list for Trilinos development

1. Improved Sierra / Trilinos / STK integration. (POC: Paul Wolfenbarger)
2. Help efficiently & effectively "Kokkos-izing" Sierra/TF and STK. (POCs: Christian Trott, Si Hammond)
3. Improved multi-physics solvers. (POC: Ray Tuminaro)
4. Development of a high-performing BlockCRS matrix linear system and solver stack.
   - Put Kokkos under Tpetra's block CRS linear system to improve it's performance.
   - Thread-parallel matrix vector products using the BlockCRS matrix format.
   - Thread-safe and efficient assembly interface for BlockCRS matrix format.
5. Add a line solver capability to Ifpack2. (POC: Travis Fisher)
6. BiCGSTAB solver
7. Efficient AMG preconditioner set-up time (for simulations where topological changes or matrix smoothness changes over simulation).
8. MueLu improvements:
   - Development of a coarse-matrix correction capability.
   - Thread MueLu kernels to prepare for NGP.
9. ILU improvements:
   - Thread-parallel ILU factorization.
   - Add a minimum discarded fill reordering for block ILU preconditioning in Ifpack2.

Organic material decomposition needs

- Application
  - In fire environments, organic materials liquefy and flow during decomposition
  - Evolved gases can cause pressurization and failure of sealed systems
  - Historical analyses focused on heat transfer to components→ now focus also involves predicting pressurization
- Problem Complexity:
  - Decomposition reaction kinetics
  - Radiative heat transfer through virgin + decomposed foam
  - Variable density porous media and Navier-Stokes flow
  - Conjugate heat transfer to components
  - Foam liquefaction + multi-phase flow



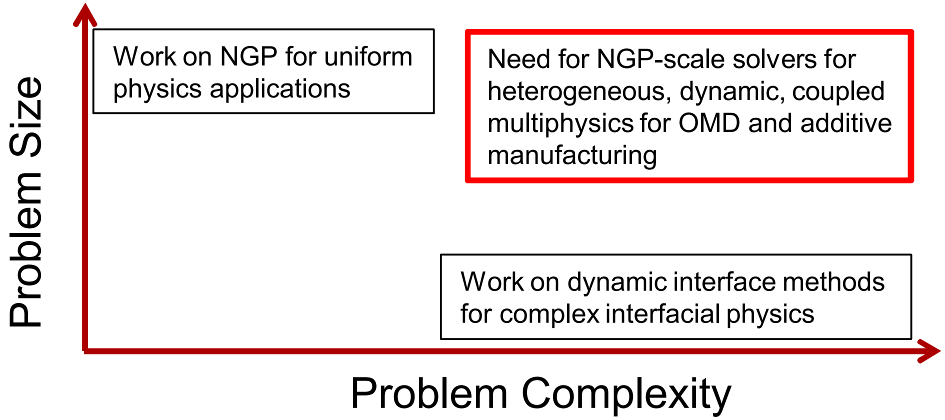
<u>Solver Challenges:</u>

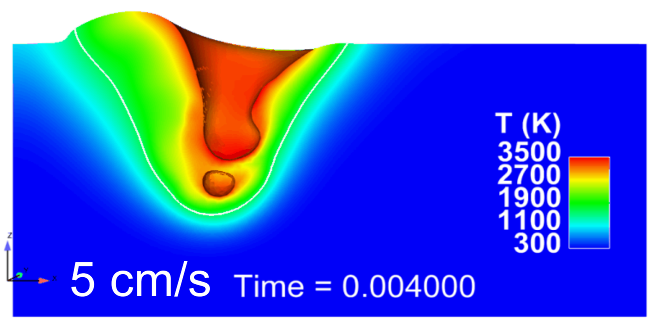
- Tight coupling between different equations with different DOF's at interfaces
- Dynamic discretization as geometry evolves
- Tight coupling between multiple equations within different regions
- System-level calculations could involve O(1B) unknowns for O(100k) time steps

(Slide content courtesy of Mario Martinez, Victor Brunini, David Noble)

Laser welding and additive manufacturing needs

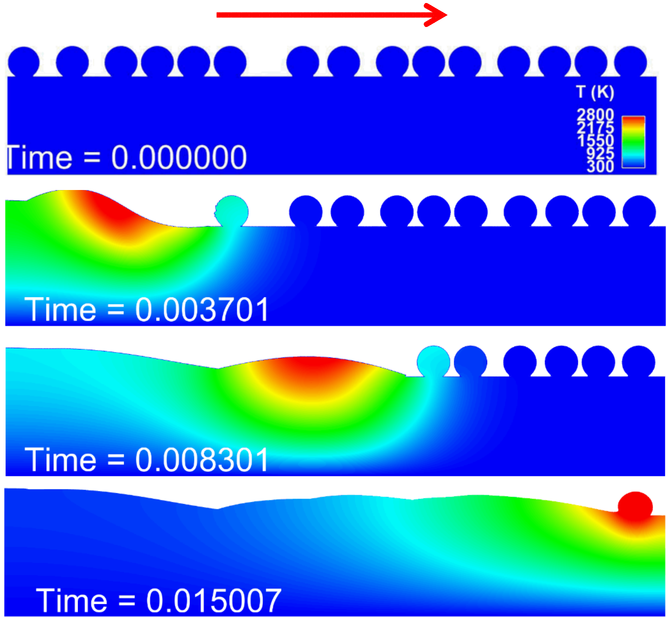
- Applications
  - Both laser welding and additive manufacturing via selective laser melting involve using a laser to apply intense heating over a very small area to metals
  - Complex interfacial transport involving capillarity, laser heating, non-equilibrium vaporization, gives rise to dynamic, discontinuous physics and fields





Laser welding of Stainless 304L

50 micron 304L stainless
6 cm/s scan rate



Additive Manufacturing via selective laser melting

(Slide content courtesy of Mario Martinez, Victor Brunini, David Noble)

Path forward

- Continue and strengthen collaborations between Sierra/TF and Trilinos teams:
  - Continue joint meetings series.
  - Identify and work through issues.
  - Share expertise and lessons-learned.

- Sierra/TF adoption of more Trilinos capabilities, e.g.:
  - Sacado
  - ROL
  - More use of Zoltan-2
  - Catalyst for in-situ viz

- Encourage creation of new Trilinos capabilities that can be used by Sierra/TF, e.g.:
  - Particle library
  - Three-Dimensional Hypersonic Boundary Layer Stability Analysis, like *STABL-3D*
  - Other