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Author(s):	Baker, Randal Scott
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An Overview of the Computational Physics and Methods Group at Los Alamos National Laboratory

Randy Baker

Computational Physics and Methods

Computer, Computational, and Statistical Sciences Division

Los Alamos National Laboratory

March 2018

National Nuclear Security Administration

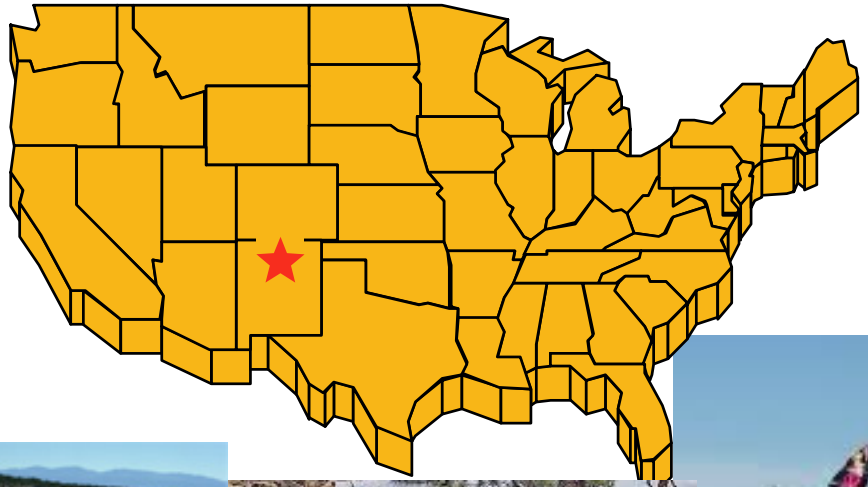
Operated by Los Alamos National Security, LLC for the U.S. Department of Energy's NNSA

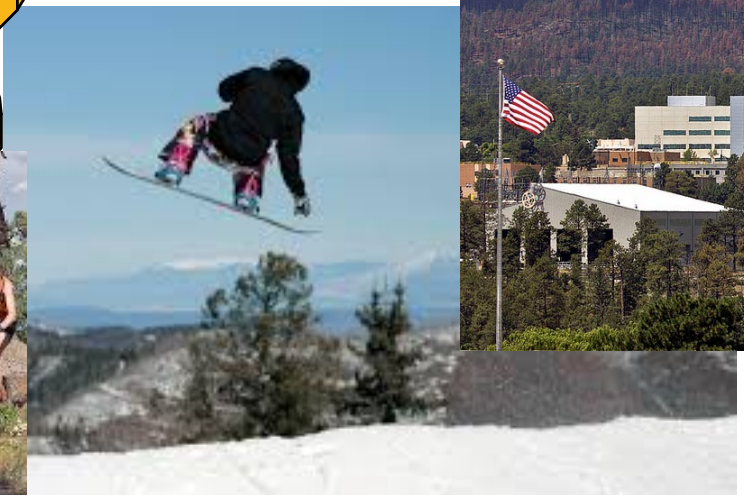
Outline

- **Overviews**
  - Los Alamos National Laboratory
  - Computational Physics and Methods Group CCS-2
- **Scientific Software Development in CCS-2 and at LANL**
  - Numerical Methods
  - History of high performance computing at LANL
  - Mini Apps
  - Modern approaches to scientific software development
- **Research and Production Codes/Libraries in CCS-2 – A tour of practical computational physics and methods**
  - Climate Science – ACME, MPAS-Ocean
  - Astrophysics – SuperNU, Fornax, eblight, xRage
  - Computational Fluid Dynamics – QUINOA, Truchas, CFDNS
  - Multi-Scale – Nambe
  - Transport – CAPSAICIN, JAYENNE, PARTISN

Los Alamos, New Mexico

Los Alamos is located in northern New Mexico, approximately 35 miles northwest of Santa Fe, surrounded by natural beauty ideal for hiking, skiing, and other outdoor sports.





LANL was founded in 1943 as part of the Manhattan Project

Budget

Approx. $2.45 billion

- 65% Weapons programs
- 7% Nonproliferation programs
- 5% Safeguards and Security
- 7% Environmental Management
- 4% DOE Office of Science
- 2% Energy and other programs
- 10% Work for Others

Place

~40 square miles of DOE-owned property

47 technical areas with 8.2 million square feet under roof, including

- 1,000 buildings (13 nuclear facilities)
- 268 miles of roads (100 paved)
- 198 miles of primary and secondary electrical lines
- 57 miles of gas lines
- power plant

Workforce

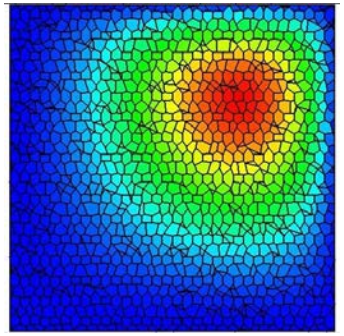
Total employees: 11,200, including approximately:

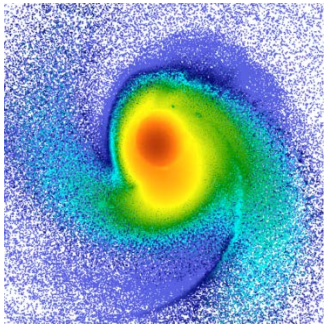
- Los Alamos National Security, LLC: 7,200
- Centerra-LA (Guard Force): 300
- Contractors: 400
- Students: 1,600
- Unionized craft workers: 900
- Post doctoral researchers: 350

LANS and students only:

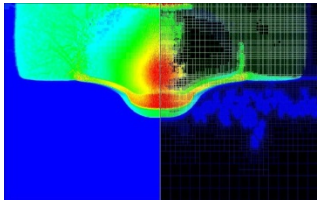
- 28% hold undergraduate degrees
- 17% hold master's degrees
- 21% have earned a PhD

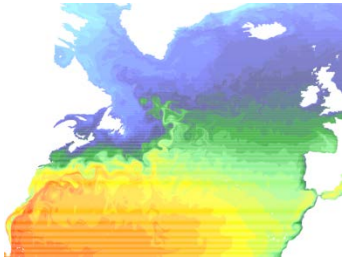
Computational Physics and Methods Group, CCS-2

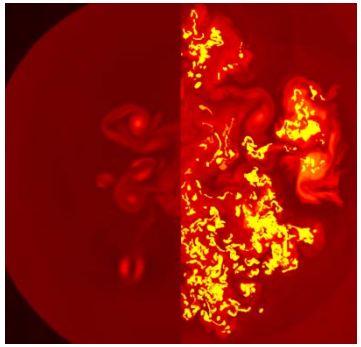


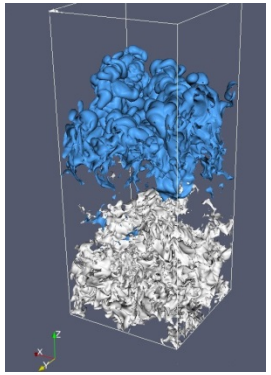


- Evolving Applications & Advanced Architectures
- Transport Methods (MC, Deterministic)
- Radiation Hydrodynamics
- Astrophysics
- Climate
- Materials
- Fluid Dynamics









Computational Physics and Methods Group, CCS-2

“Performing innovative simulations of physics phenomena on tomorrow's scientific computing platforms”

- CCS Division was formed to strengthen the visibility and impact of computer science and computational physics research on strategic directions for the Laboratory.
- Both computer science and computational science are now central to scientific discovery and innovation. They have become indispensable tools for all other scientific missions at the Laboratory.
- CCS Division forms a bridge between external partners and Laboratory programs, bringing new ideas and technologies to bear on today’s important problems and attracting high-quality technical staff members to the Laboratory.
- **The Computational Physics and Methods Group CCS-2 conducts methods research and develops scientific software aimed at the latest and emerging HPC systems.**

Computational Physics and Methods Group, CCS-2

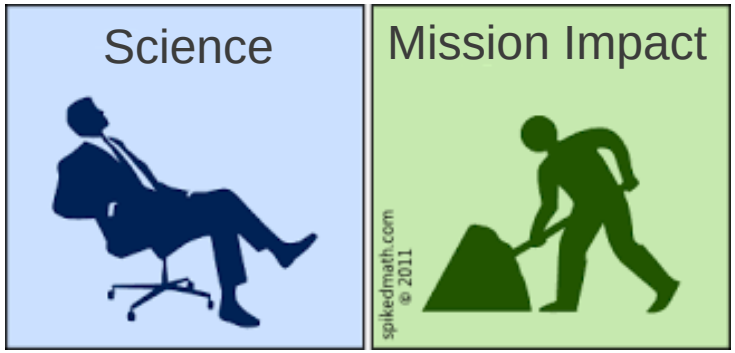
People

- 42 Scientists
- 17 Postdocs
- ~25 students, most in summer
- 2 scientist/managers
- 1 admin

Education

- Physics
- Engineering (Nuclear, Aerospace, Mechanical)
- Climate Science
- Astrophysics
- Applied Mathematics

Budget: ~$25 million/year



Academic Activities

- Publishing – in FY16 ~80 peer reviewed publications by people in CCS-2
- Several staff serve on editorial boards
- Service on review panels
- Several staff are fellows of their academic associations (AIAA, ANS, APS)

as of October 2017

Numerical Methods Expertise in CCS-2

Discretizations
- Finite Elements (spectral, DG, classical)
- Finite Volume
- Finite Difference (mimetic, classical, high order)
- Particle Methods (SPH, MC)

Solvers
- Multigrid (classical, FAC, AMG)
- Nonlinear Solvers (JFNK, Anderson/NKA, Picard)
- Sweeps (e.g. in S_n)
- Physics based preconditioning

Time integration
- Implicit (BDF)
- Semi-implicit (CN)
- Explicit (RK, Euler)

Multi-physics coupling
- Explicit operator splitting
- Nonlinear coupling

Meshes/Meshing
- Unstructured (Cubit, LAGrid, HexPress, Altair)
- Voronoi (2D, 3D)
- Structured, curvilinear
- AMR (patch, element, overset)
- Mesh Smoothing (ALE)

Transport
- S_n
- MC, IMC
- High Order Low Order (HOLO)
- Discrete Diffusion MC Acceleration
- Variance Reduction

Computing at Los Alamos National Laboratory

Since the early 50s LANL has been at the forefront of HPC.

- MANIAC // IBM701 // CDC6600
- Cray 1, XMP, YMP
- CM 2, 5 // Cray T3D
- Blue Mountain // Roadrunner // Cielo // Trinity

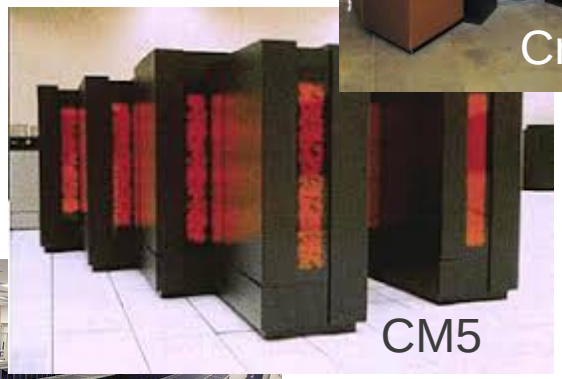
Computing at LANL Today

- Desktop
- TLCC (Tri-Lab Capacity Clusters), ASC and Institutional Computing:
  - Trinity, Fire/Ice, …
  - Trinitite, Snow, …
- Hardware (totals):
  - Processors
    - AMD and Intel CPUs: ~430,000 cores,
    - Xeon Phi (KNL): ~650,000 cores
    - Memory: ~1.62 PB memory.

Radiation Transport!

Maniac

Cray 1


CM5

Roadrunner

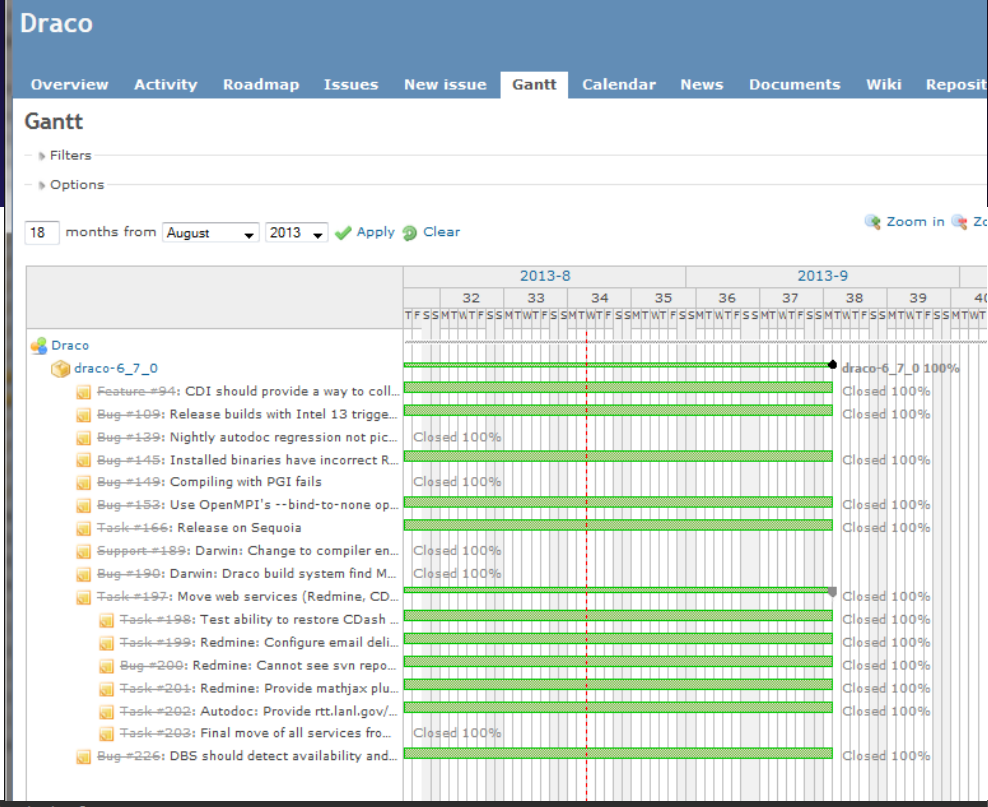
Trinity

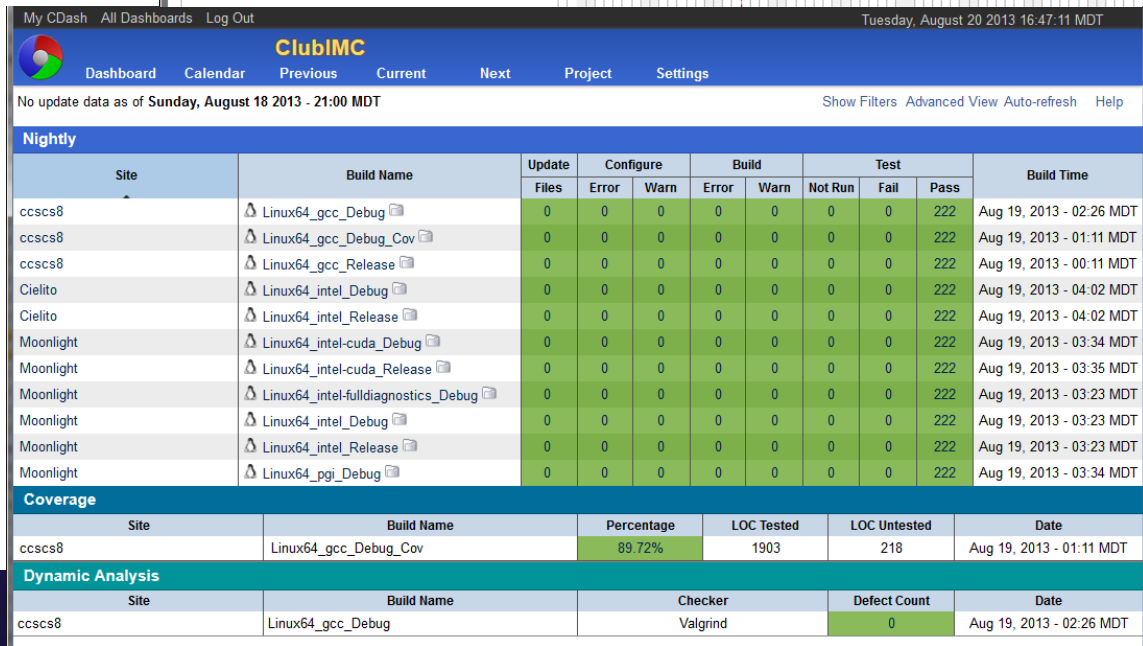
Highly Parallel Scientific Production Software

- **All staff and postdocs in CCS-2 develop code that must run at scale**
- **Our codes/libraries run on the largest computers in the country**
- **Many/most of our codes/libraries**
  - Are highly parallel (MPI)
  - Leverage accelerators (KNL, GPU, …)
- **Code teams utilize various levels of SQA**
  - Version control
  - Continuous testing
  - Code reviews
  - Documentation
- **We program in many languages and paradigms**
  - C, C++, Fortran (various versions), python
  - Charm++, Legion, MPI, MPI+X, CUDA, OpenMP, OpenACC, …

Software Management

- **Software Design**
  - C++ Object-Oriented design
  - Package management
  - Profiling
- **Build systems**
  - Workstations, Unique Systems, Heterogeneous
  - Vendor management
- **Testing**
  - Unit testing
  - Regression testing
  - Memory testing & Code Coverage
- **Dashboards**
- **Documentation**
- **Releases**





CCS-2 is currently helping support a large, high priority calculation for NNSA

- **4,800 dedicated KNL nodes on Trinity**
  - This allows for two “parallel” calculations to explore physics and CS options
- **24 hours/day, 7 days/week**
  - Operator intervention when abnormal job termination detected
- **Expected duration ~3 months**
- **Large, time-dependent 3-D calculation**
- **Restart files ~25 Tbytes**
- **“Burst Buffer” write time ~1 minute!**
  - Cray XC40 Data Warp
  - Flash memory (solid-state drive)
  - 3.7 PBytes
- **75 PByte standard file system**
- **2 MW power**

Our Approach to Porting Codes to New Architectures

- **We develop mini-apps**
  - A mini app is representative of the numerical methods in a large code or library
  - Mini apps are usually open source, not export controlled
  - They can be shared with vendors and collaborators
  - They are used to learn about potential problems early

- **We collaborate with vendors early in the procurement process**
  - Centers of Excellence bring together vendor experts (e.g. from Intel, Cray) and methods developers from LANL and other labs.
  - **Knowledge about new hardware is shared early: our staff have access to pre-production (or earlier!) hardware to test mini-apps**

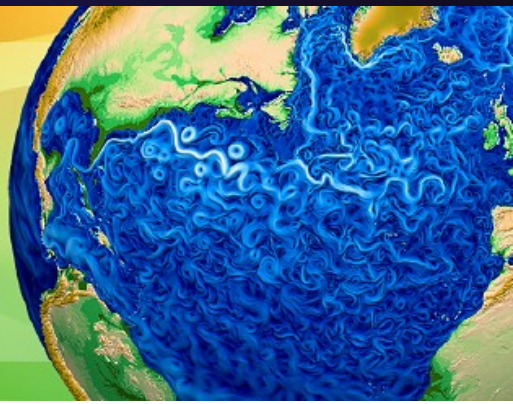
- **Acceptance of a new HPC machine**
  - Procurement of a new machine concludes with acceptance tests
  - Important production codes and libraries are demonstrated to work on the new hardware **(e.g, PARTISN!)**

CCS-2 staff and PD participate in this process in all steps.

Climate Science

Accelerated Climate Model for Energy

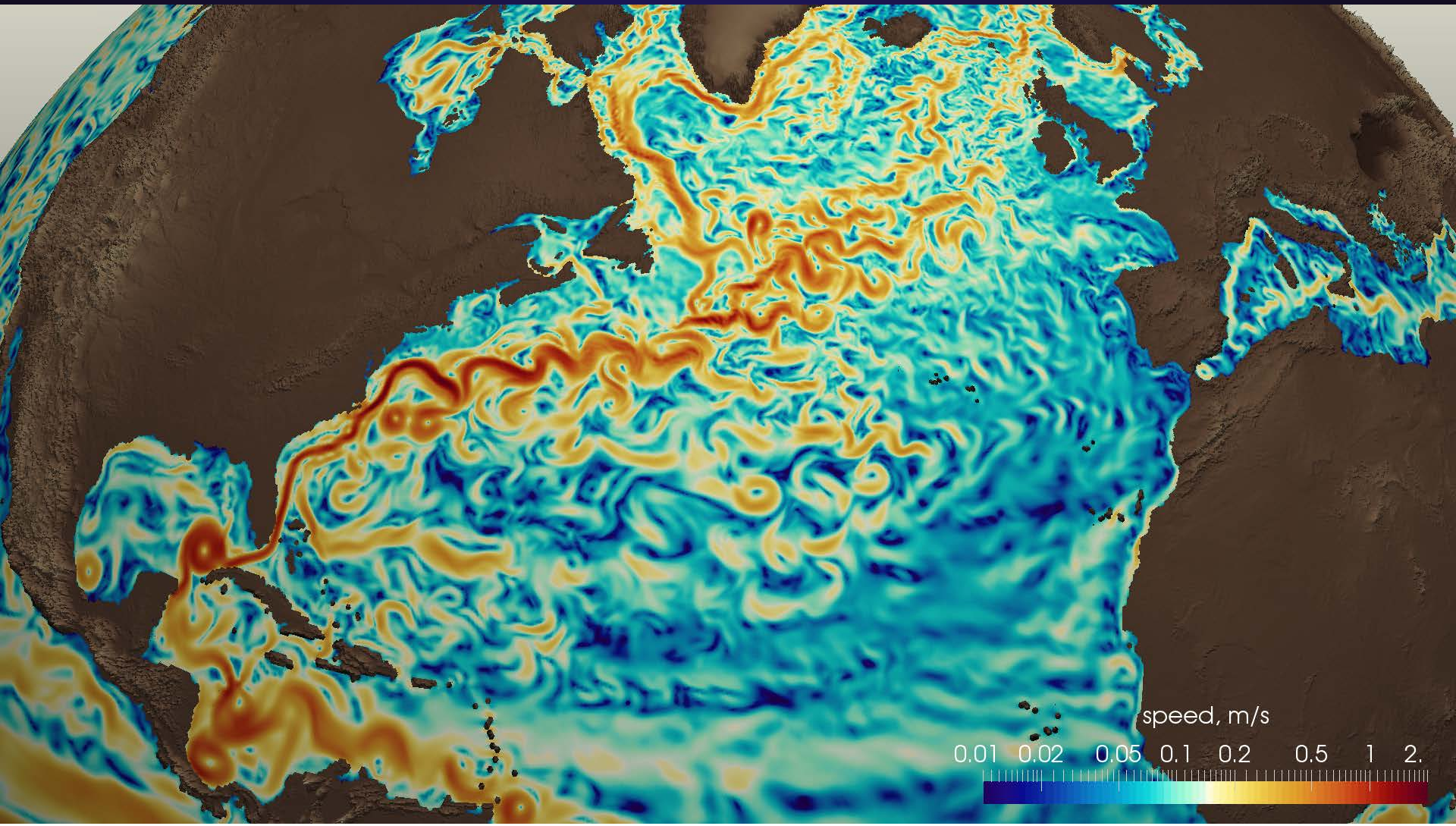
ACME
Accelerated Climate Modeling for Energy



- New coupled climate model by the U.S. Department of Energy
- 120 DOE employees on effort
- Goals:
  - Risk assessment and planning related to climate and extreme weather.
  - Address mission-specific applications from U.S. energy sector vulnerabilities
  - Sea level rise, Antarctic ice sheet instabilities
  - Efficiently utilize DOE leadership computing resources

Point of Contact: Mark Petersen, CCS-2/LANL

Gulf Stream



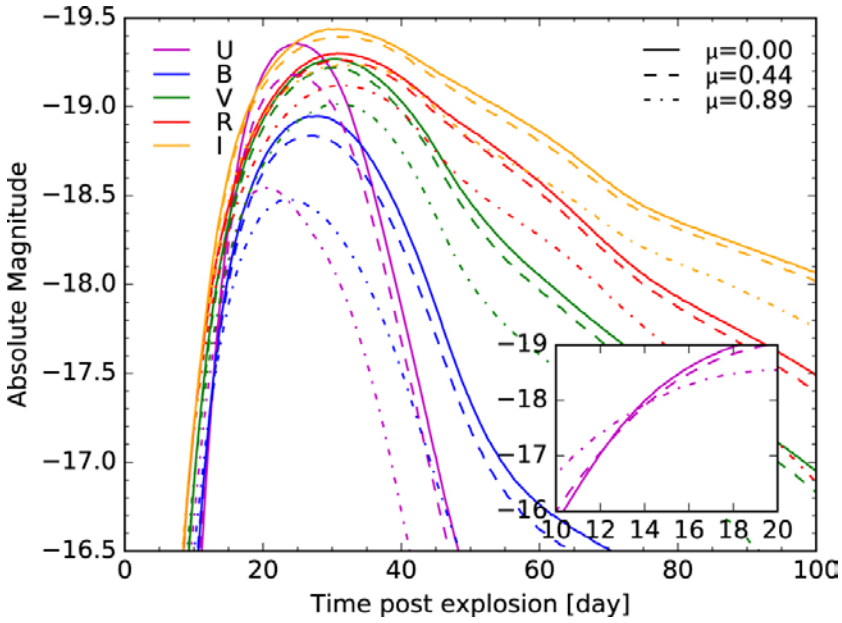
Point of Contact: Mark Petersen, CCS-2/LANL

Astrophysics

SuperNu

SuperNU is a parallel code that our former postdoc and now staff-scientist Ryan Wolleager wrote and still develops.

- **SuperNU solves radiative transfer in supernovae, for light curves and spectra.**
  - Results can be compared to observations.
- **Typical time scales simulated are days to months**

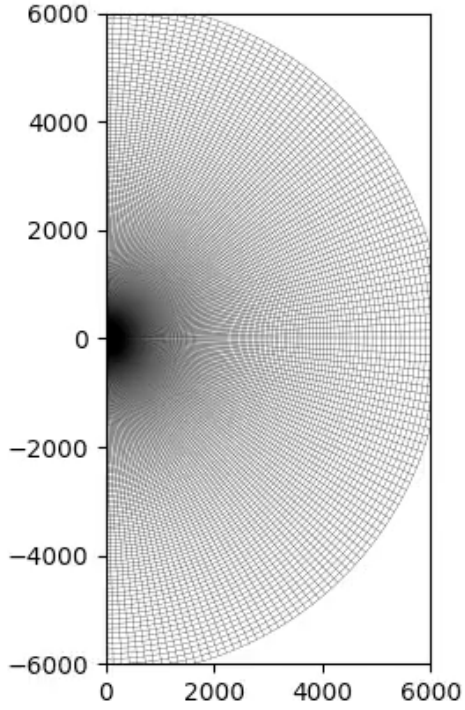


- Light curves for different viewing angles of a White Dwarf merger (van Rossum et al (2016))

The Fornax Supernova Code

- **1-D, 2-D, 3-D neutrino radiation hydrodynamics**
- **Metric-based formalism makes it “easy” to change geometries and coordinates**
- **Dendritic mesh avoids severe CFL limit at small radii**
- **Geometrically correct parabolic reconstruction**
- **3-species, multi-group M1 transport**
- **All O(v/c) terms included**
- **Multipole gravity**
- **“Relativistic corrections” for monopole gravity, and transport (e.g. redshifts)**
- **Support for complex, tabulated equations of state**
- **Fast and highly scalable**
  - 2D CCSN simulations in ~2-3 days
  - 3D shows **excellent** *strong* scaling

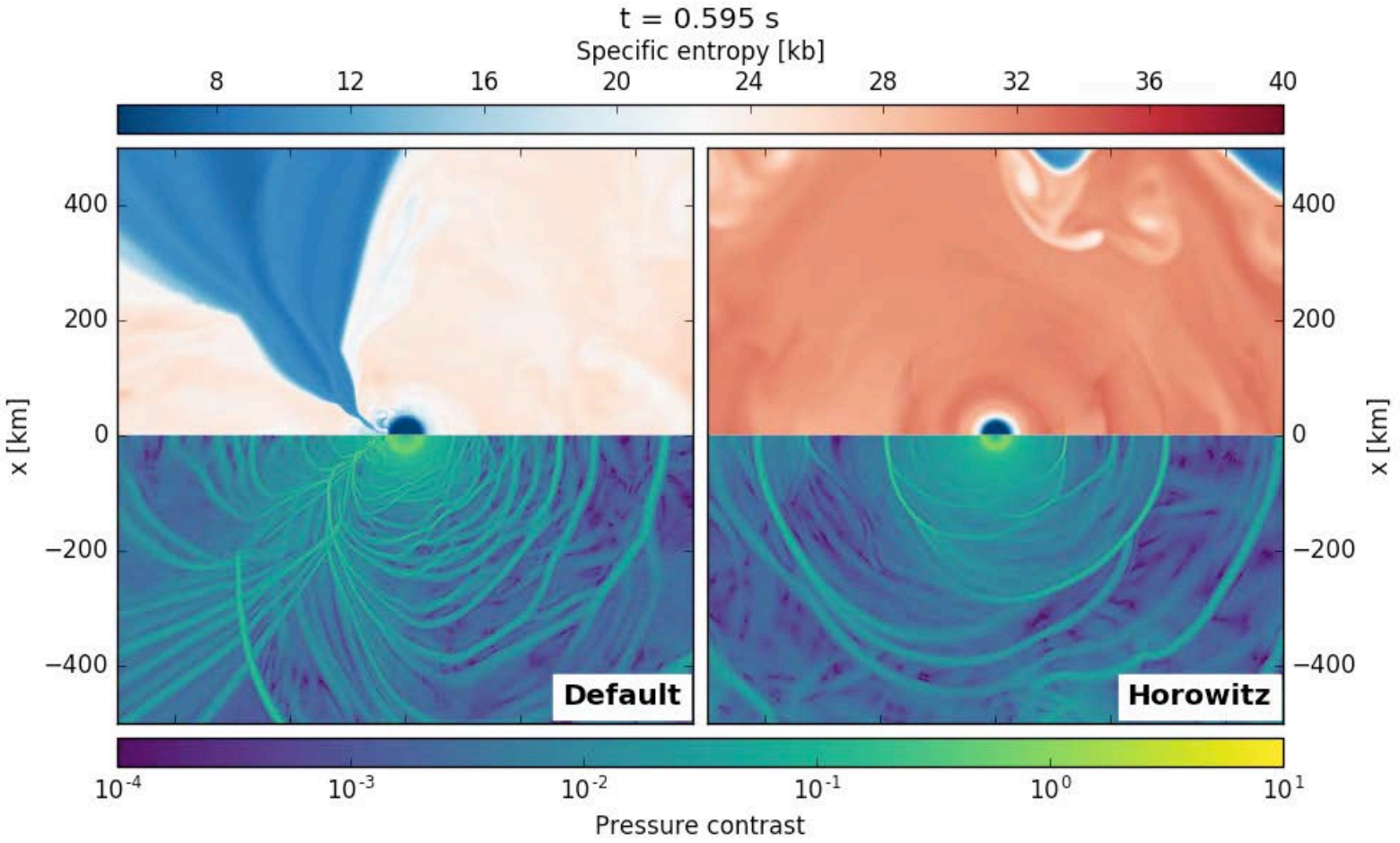
Fornax and eblight were developed/co-developed by our former postdoc and now staff-scientist Joshua Dolence.



Point of Contact: Joshua Dolence, CCS-2/LANL

The Fornax Supernova Code

Fornax is used primarily to understand how massive stars explode

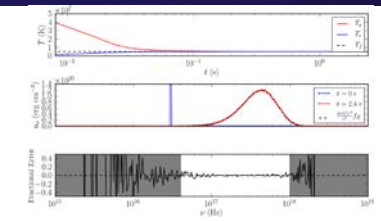


Default vs. Horriwitz: Difference in neutrino opacities

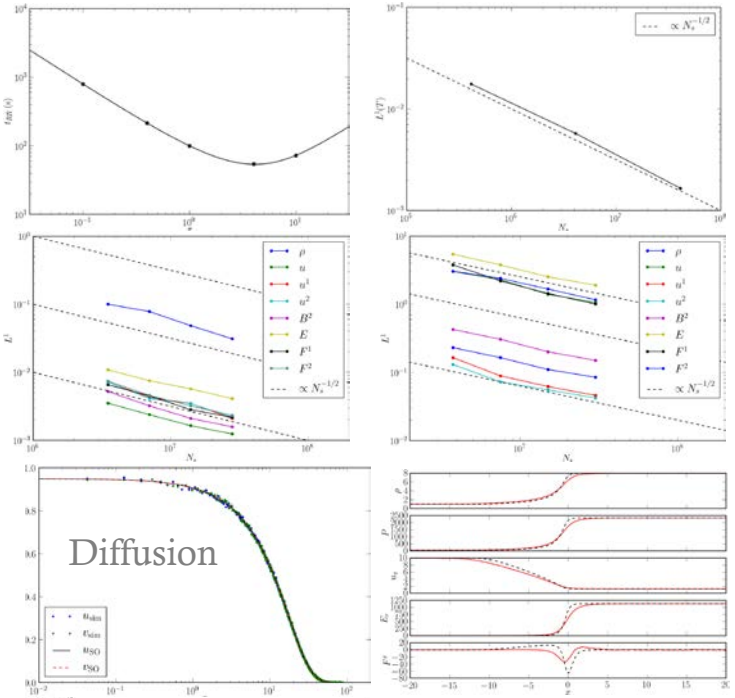
Point of Contact: Joshua Dolence, CCS-2/LANL

ebhlight: General Relativistic Radiation MHD with Monte Carlo Transport and Electron Thermodynamics

- Ideal GRMHD
- Full solutions of the relativistic transport equation --- no ad hoc or approximate closures
- Anisotropic emission and scattering
- Inelastic (Compton) scattering
- Separate evolution of ion and electron thermodynamics with input from detailed plasma physics models
- Conservative coupling
- Limitations: Monte Carlo noise and stiff source terms



Comptonization



Linear Modes

Shocks

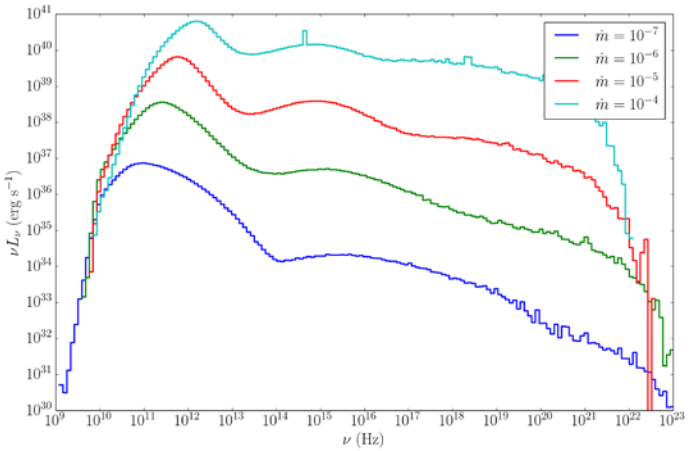
Relativistic Equilibria

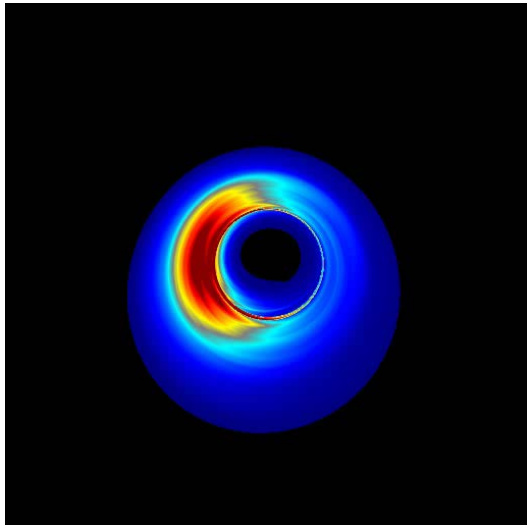
Point of Contact: Joshua Dolence, CCS-2/LANL

ebhlight studies the dynamics of radiating MHD flows around black holes

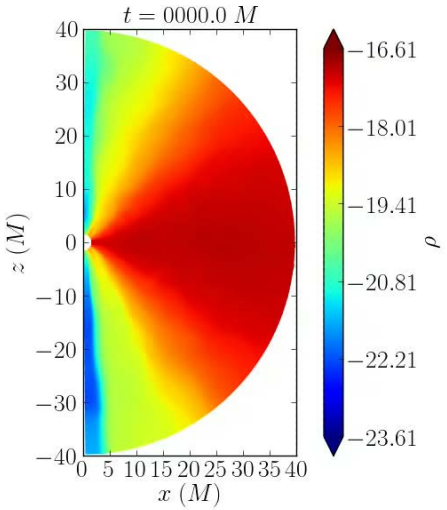
Results can be compared with observations…(→event horizon telescope)

Simulated spectra

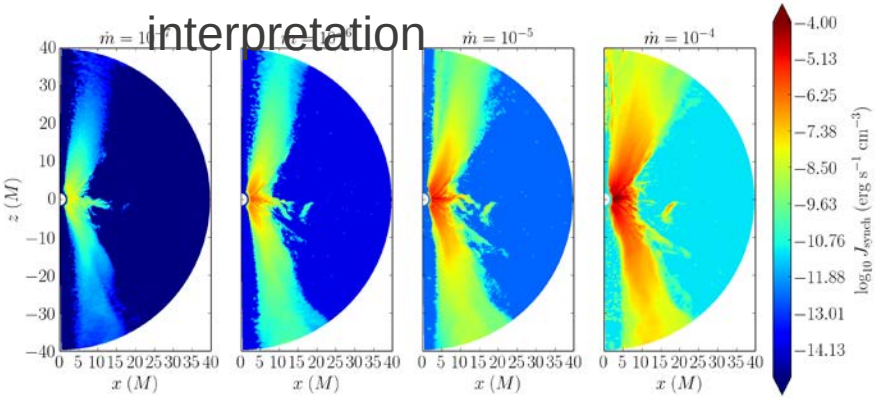




Simulated images



…and used to facilitate interpretation

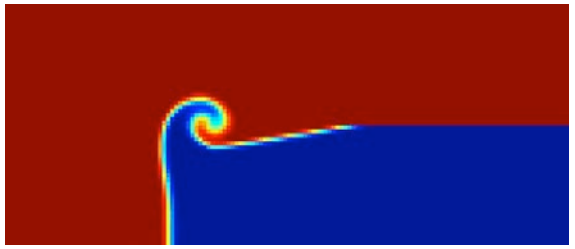


Point of Contact: Joshua Dolence, CCS-2/LANL

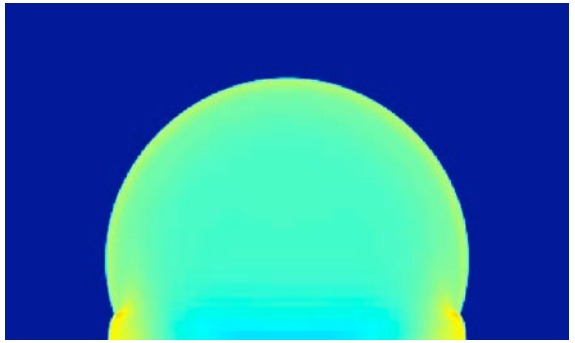
xRage – A Large-Scale Multi-Physics Hydro Code

- **xRAGE is a multi-material, multi-physics Eulerian AMR code**
- **Application Areas: Inertial Confinement Fusion, Astrophysics**
- **Problem Size: Up to… many billions of cells in computational domain, multiples of 10,000 processors, multiple weeks of simulation time**
- **xRage employs finite volume discretizations with mostly explicit time-integration for conservative-by-construction algorithms**
- **Some reliance on third-party libraries, mostly for numerical linear algebra (e.g. HYPRE, Trilinos); also, interpolators and ODE integrators**

Triple point problem



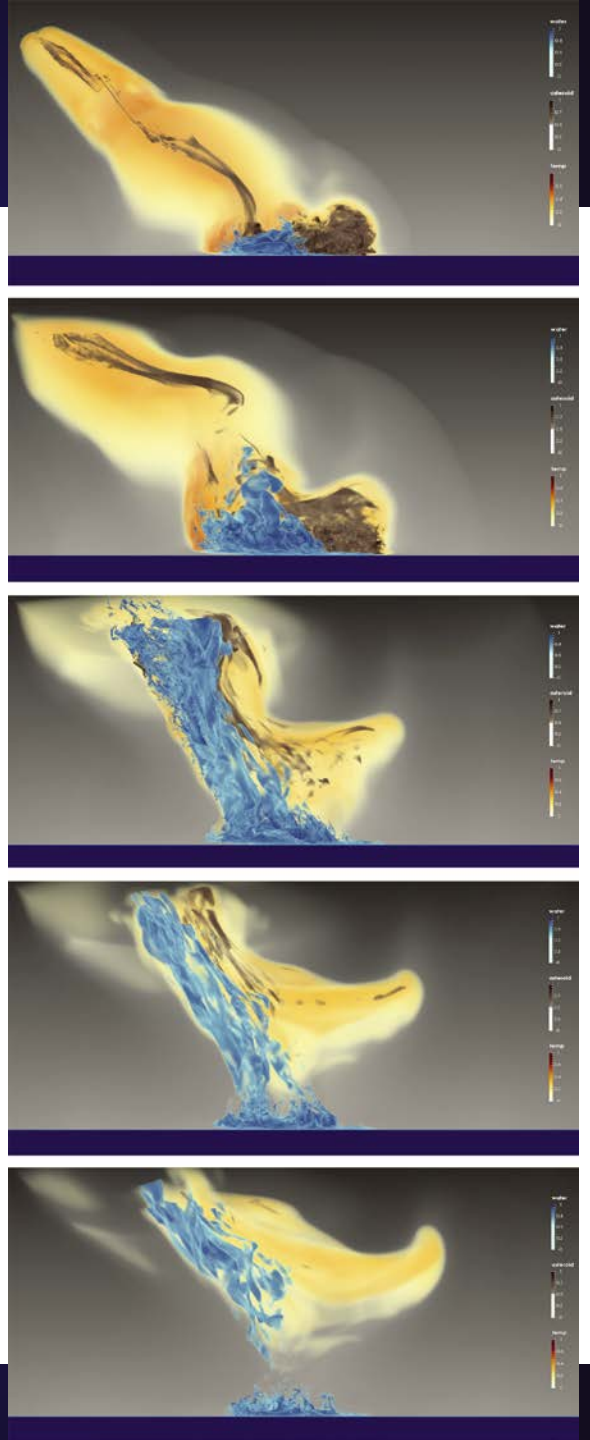
Ground interacting blast



LANL's xRAGE code is being developed by the ASC Eulerian Applications Project (Leads: Joann Campbell XCP-2, Galen Shipman CCS-7)

xRage – all the physics

- Multi-dimensional hydrodynamics (inviscid Euler Equations)
- Material interface reconstructions
- Constitutive models (Equations of State, Strength models)
- Cell-based Adaptive Mesh Refinement (AMR)
- Grey radiation diffusion
- Heat conduction
- Plasma physics (electron, ion heat conduction, electron-ion coupling)
- Lasers (ray-tracing)
- Isotopes
- Thermonuclear burn
- Engineering Turbulence Models
- Gravity (uni-directional, and self-gravity)
- High Explosives models



xRage asteroid Impact calculation – visualization by John Patchet, CCS-7/LANL

Computational Fluid Dynamics

CFDNS is a petascale code framework for Direct Numerical Simulations of fluid turbulence

BACKGROUND & MOTIVATION

- Almost all fluid systems of practical relevance have some turbulence component.
- Yet after decades of research, turbulence and turbulent mixing still remain unsolved problems in physics; this due in part to the very large range of spatio-temporal, dynamically relevant scales.

DESCRIPTION

- Large scale computing is beginning to allow accurate simulations of ever more complex turbulent flows at practically relevant parameter ranges.
- Such simulations (called DNS), using higher order methods and resolving all the dynamically relevant scales, without subgrid modeling, artificial dissipation or other numerical stabilization algorithms, complement physical experiments in elucidating the physics of the flow and providing data for the development of turbulence models.

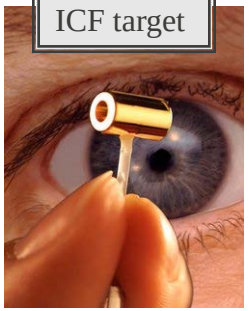
➢ Unlike the physical experiments, there is a complete control of the initial and boundary conditions as well as measuring quantities of interest.

➢ A large variety of synthetic test problems can be designed to isolate and investigate specific physical effects.

➢ *Limitations:*
need the largest supercomputers available;
most practical flows still out of reach

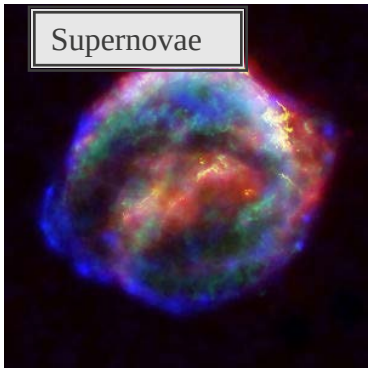
Examples of instabilities driven turbulence from small to large size systems

ICF target



Mammatus clouds

Supernovae

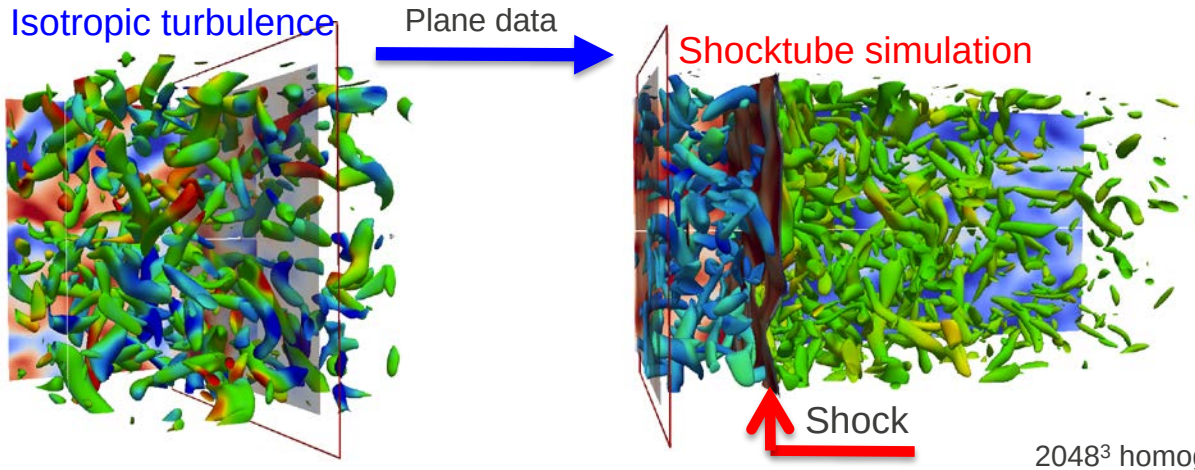


Point of Contact: D. Livescu, CCS-2/LANL

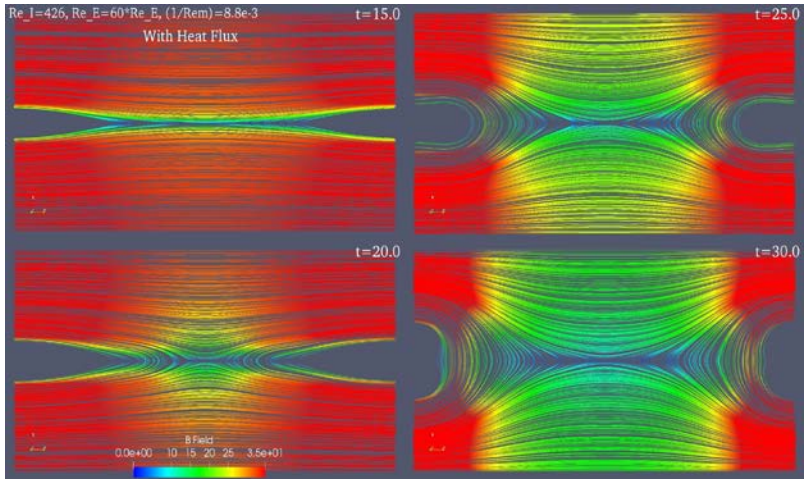
CFDNS scales well to > 1,500,000 cores, was used to perform some of the largest turbulence simulations to date in a variety of configurations.

More examples

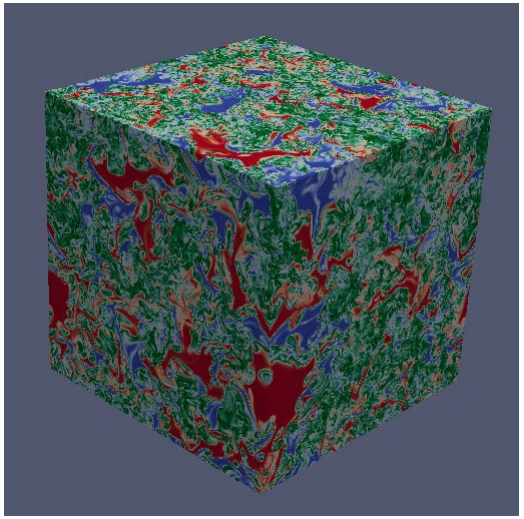
Shock-resolving DNS of shock- isotropic turbulence interaction with comprehensive coverage of the parameter space: data from 1024^3 forced compressible isotropic turbulence is fed through the inlet of a 4096×1024^2 shock tube



Fully resolved magnetic reconnection with finite transport



2048^3 homogeneous buoyancy driven turbulence at high density ratio



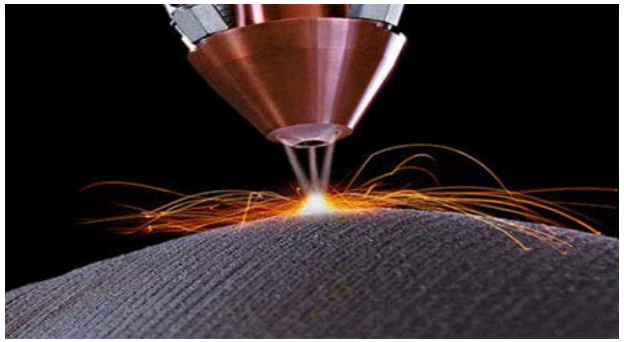
Point of Contact: D. Livescu, CCS-2/LANL

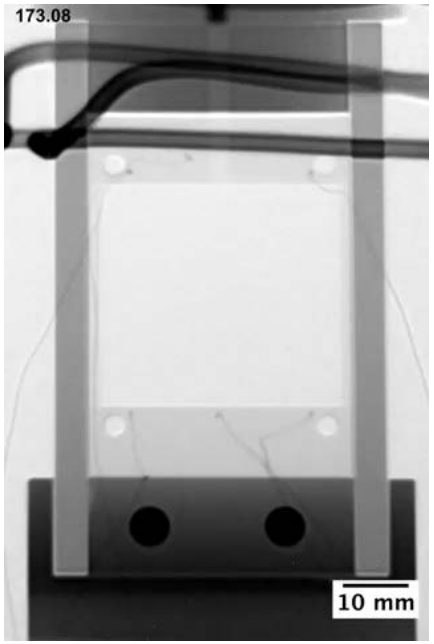
Truchas - Metal Casting and Advanced Manufacturing

Truchas is software for 3D physics-based modeling and simulation of manufacturing processes.

- Primary application areas:
  - Metal casting
  - Emerging capabilities: Additive manufacturing (AM) and welding
- General multi-physics tool with wide range of possible applications
- Open source: https://gitlab.com/truchas
- Typical problem sizes < 10M cells, scaling up to several thousand cores.
- Need is for quick turn around of many modest-sized problems.

Laser powder feed AM process





Proton radiography (pRad) of casting/solidification experiment. A. Clarke, et al

Truchas is funded under the ASC Program and has been around for almost 20 years.

Point of Contact: Neil Carlson, CCS-2/LANL

Multi-Scale Methods

Nambe - Summary

- **Hydrodynamics codes can miss important physics**
  - EOS/Opacities/properties of mixtures
  - Kinetic effects (non-equilibrium phenomena)
  - Important and difficult to diagnose in HED experiments
- **Nambe project (collaboration with LLNL, MSU, ORNL, others) looks to examine HED problems at the atomic (molecular dynamics) and kinetic theory level, leveraging atomic level data in a multiscale way**
  - MODMD: a multiscale MD package that can compute in much larger length, time, and temperature scales than previous MD codes.
  - Stanton-Murillo derived kinetic integrated cross sections in a dense plasma regime based on ideas used in defining potentials for MD. They show remarkably good agreement with MD even in moderately coupled regimes, where previous kinetic methods break down.
  - Haack-Hauck-Murillo developed multispecies BGK-type kinetic model. This is the first entropically accurate multispecies relaxation model and directly incorporates the high fidelity Stanton-Murillo cross sections.
  - Scullard-Ellison developed an electron-ion temperature relaxation model based on the quantum Lenard-Balescu equation, which includes degenerate electron statistics and sidesteps Coulomb Logarithm ambiguities. It has been implemented into LANL (Flag) and LLNL (Ares) production codes.

Point of Contact: Jeff Haack, CCS-2/LANL

Radiation Transport

Overview of the Transport Project

- **Delivers radiation transport capabilities software libraries:**
  - CAPSAICIN: X-ray thermal transport using finite-element methods on unstructured meshes
  - JAYENNE: X-ray thermal transport using Implicit Monte Carlo (IMC)
  - PARTISN: Neutron/gamma transport using deterministic methods on structured meshes
- **Each library is massively-parallel and runs on the latest high-performance computing hardware**
- **20 staff, 2 post-docs (2 other post-docs recently converted to staff), and 7 summer students in 2017**
- **Multidisciplinary: Nuclear and other engineering disciplines, physicists, mathematicians, computer scientists.**

We approximate variants of the Boltzmann Transport Equation

Linear radiation transport equation for neutrons

$$\left(\frac{1}{v}\frac{\partial}{\partial t}+\vec{\Omega}\cdot\vec{\nabla}+\Sigma_t\right)\psi(\vec{r},\hat{\Omega},E)=\int_{4\pi}\int_{0}^{\infty}\Sigma_s\left(\hat{\Omega}'\rightarrow\hat{\Omega},E'\rightarrow E\right)\psi' d\Omega' dE'$$

$$+\frac{\chi(E)}{k}\int_{4\pi}\int_{0}^{\infty}\nu\Sigma_f\psi' d\Omega' dE'+Q$$

Nonlinear radiation transport equation for thermal x-rays.

$$\frac{1}{c}\frac{\partial I}{\partial t}+\vec{\Omega}\cdot\nabla I+\sigma(\vec{r},\vec{\Omega},\nu)I(\vec{r},\vec{\Omega},\nu,t)=\sigma B(\nu,T)+\frac{Q_r}{4\pi}$$

coupled with hydrodynamic motion at temperature T

- The seven-dimensional solution domain (space+velocity+time) often results in billions, sometimes trillions, of unknowns.

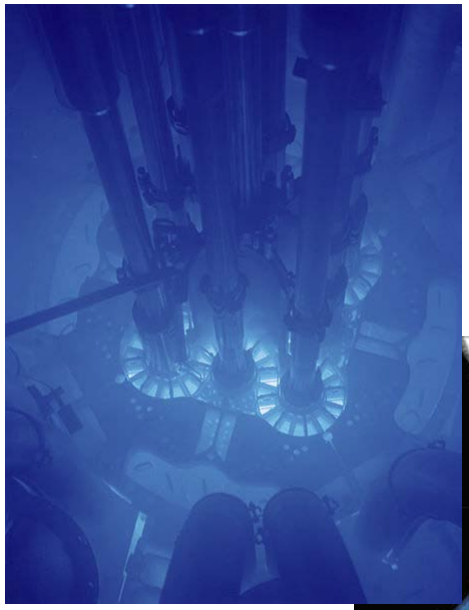
Our radiation transport packages consume ~30% of LANL's computational resources

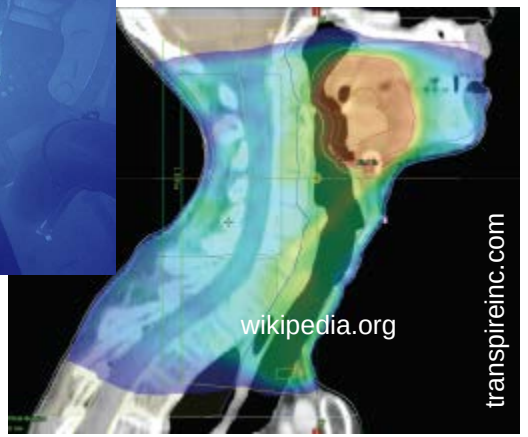
Point of Contact: Rob Lowrie, CCS-2/LANL

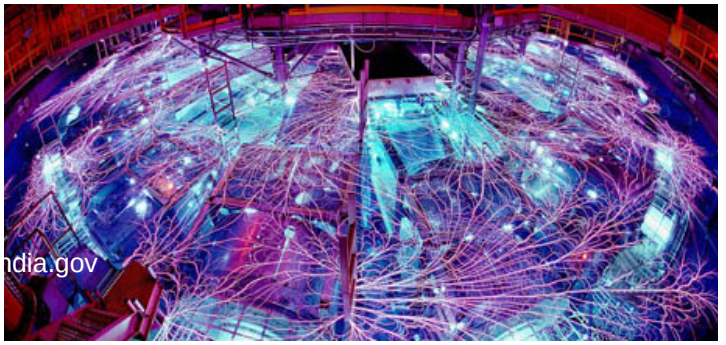
Radiation Transport Applications

- **Neutral particle, linear transport**
  - Nuclear reactor simulations
    - Criticality (k-effective)
    - Isotope depletion
    - Shielding
  - Medical, e.g., brachytherapy
  - Oil well logging
  - Supernova explosion

- **Nonlinear transport of thermal x-rays**
  - Inertial confinement fusion
    - National Ignition Facility (Lawrence Livermore)
    - Laboratory for Laser Energetics (Rochester)
  - Astrophysics (Center for Theoretical Astrophysics, Los Alamos)
  - Z Pulsed-Power machine (Sandia)







CAPSAICIN – X-Ray Thermal Transport

CAPSAICIN is a finite-element transport library for general mesh topologies

- **A collection of object-oriented C++ components.**
- **Components are assembled into packages to provide desired capabilities, including**
  - 3-temperature (ion, electron, radiation), time-dependent radiative transfer
  - Steady-state radiation transport
  - Non-local tensor diffusion
- **We make heavy use of the third-party software libraries; e.g., Trilinos, ParMetis, and SuperLU_DIST. We collaborate with the developers of many of these libraries.**
- **Parallel non-symmetric Krylov iterative method, such as source (Richardson) iteration, GMRES, and BiCGStab**
- **Linear and Non-Linear (JFNK and NKA) solvers are accessed through the Trilinos framework and interface.**

Point of Contact: Jae Chang, CCS-2/LANL

CAPSAICIN – X-Ray Thermal Transport

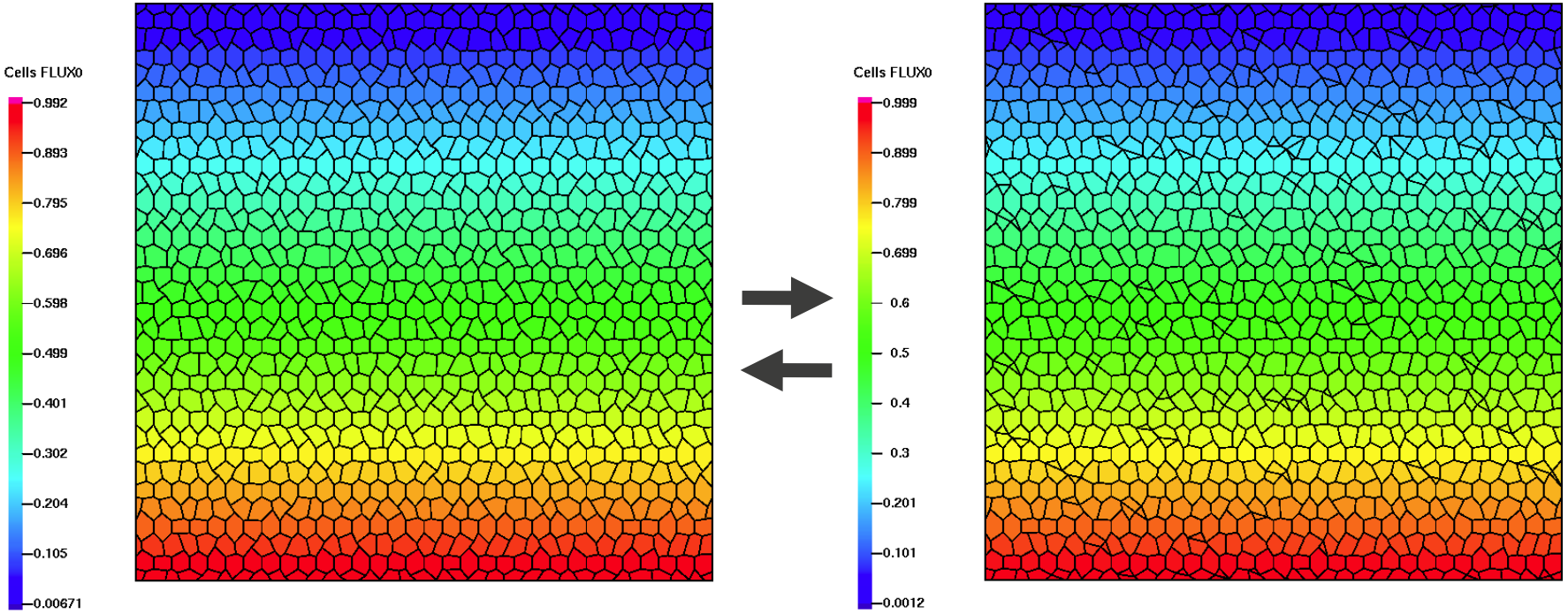
Capabilities

- Discrete ordinates (S_N) angular discretization.
- Backward-Euler time discretization.
- Multigroup energy approximation.
- 1D, 2D, and 3D in Cartesian AMR and unstructured meshes, with curvilinear coordinates.
- Parallel mesh and energy domain decomposition.
- Discontinuous finite elements (DFEM, a.k.a. “Discontinuous Galerkin”)
- Diffusion, tensor diffusion, SPn and Quasi-diffusion options available.

Point of Contact: Jae Chang, CCS-2/LANL

CAPSAICIN – X-Ray Thermal Transport

Detects non-convex mesh (such as from Lagrangian hydrodynamics codes), computes on convex mesh, and then projects back to original non-convex



non-convex mesh

convex mesh

Point of Contact: Jae Chang, CCS-2/LANL

CAPSAICIN – X-Ray Thermal Transport

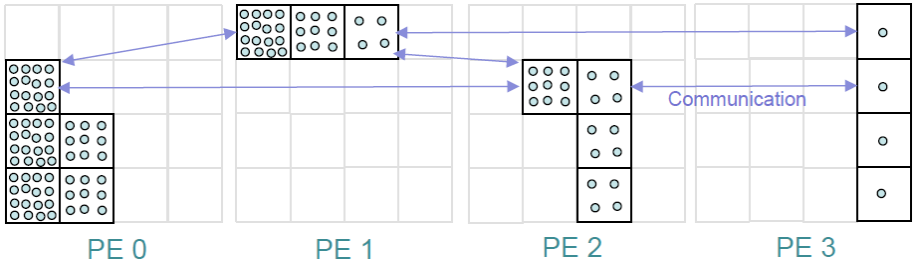
Research Topics

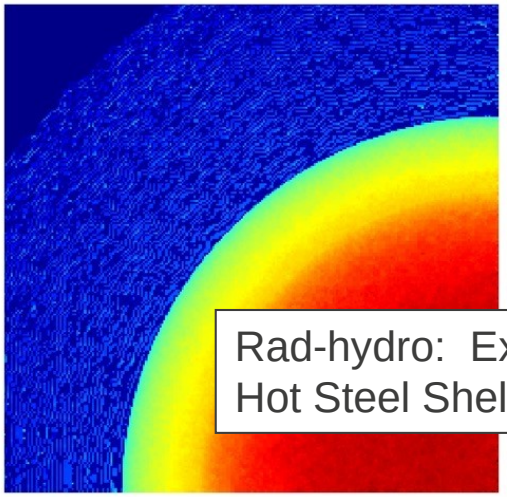
- **Extension to 100K processors using threads with MPI.**
  - Tycho2 mini-app is research platform (open source, https://github.com/lanl/tycho2)
- **Investigating the use of Kokkos, a Trilinos package for many-core performance portability.**
- **Evaluating higher-order accurate finite elements.**
- **Linear and nonlinear solver research.**
- **Improved physics capabilities, such as full Compton nonlinear scattering.**
- **Optimization of energy discretization.**

Point of Contact: Jae Chang, CCS-2/LANL

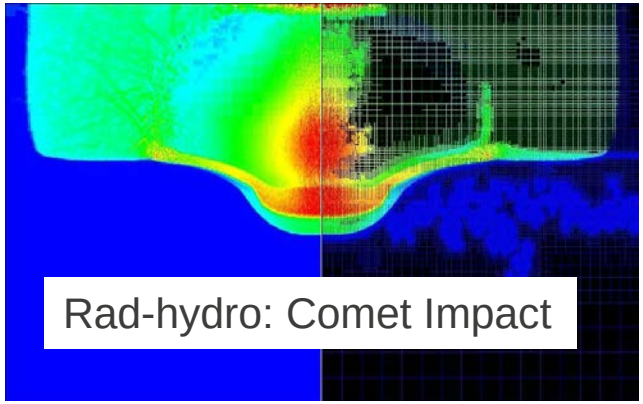
JAYENNE: X-Ray Thermal Transport using IMC

- **Implicit Monte Carlo for x-ray transport, nonlinearly coupled with hydrodynamics for high-energy density physics simulations**
- **Object-oriented C++, sharing much code with Capsaicin (via open-source Draco library)**
- **Multiphysics: Jayenne interfaces with rad-hydro application codes**
- **Massively Parallel (MPI; MPI+X)**
  - Mesh replication or decomposition for distributing particle workload
  - Adapted to Roadrunner's IBM Cell chip, NVidia GPU, KNL, etc.
  - *Branson* mini-app (https://github.com/lanl/branson)





Rad-hydro: Exploding Hot Steel Shell



Rad-hydro: Comet Impact

JAYENNE: X-Ray Thermal Transport using IMC

Capabilities

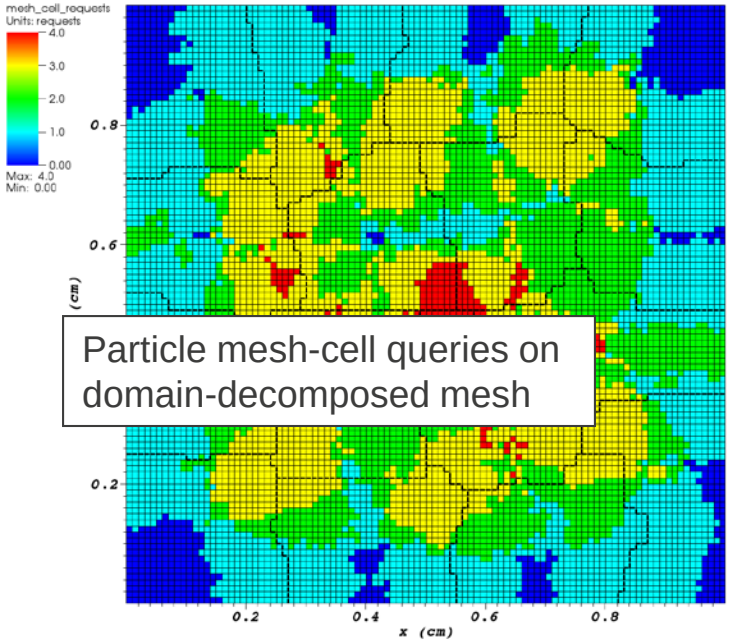
- **Multi-frequency thermal x-ray transport based on the Implicit Monte Carlo (IMC) method (based on Fleck & Cummings).**
- **1D, 2D, and 3D in Cartesian AMR and curvilinear coordinates. Unstructured mesh extension underway.**
- **Parallel options for mesh domain or particle domain decomposition.**
- **Discrete-diffusion Monte Carlo (DDMC) acceleration for optically-thick regions.**
- **Interfaces to radiation hydrodynamics; includes relativistic corrections.**
- **Numerous options for variance reduction.**

Point of Contact: Kelly Thompson, CCS-2/LANL

JAYENNE: X-Ray Thermal Transport using IMC

Current Research Activities

- Optimization for the latest computer architectures; particle load-balancing is a challenge. See open-source *Branson* mini-app (https://github.com/lanl/branson)
- Acceleration for optically-thick regions (extensions to DDMC).
- Variance reduction methods; *e.g.*, dynamic biasing, particle population control, smoothing scattering operators (Compton).
- Nonlinear treatments
- Methods for stochastic media (coupling with turbulent flows).
- Optimization and physics modeling for supernovae simulations.
- Software development for general Monte Carlo codes for particle transport.

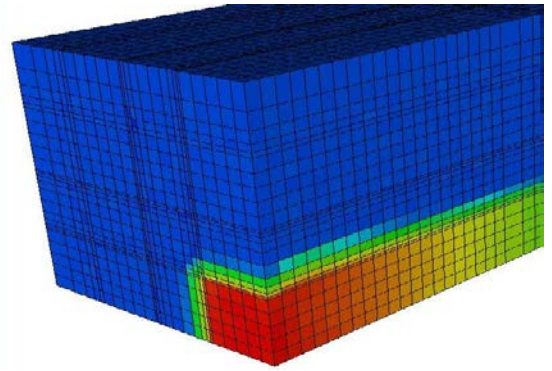


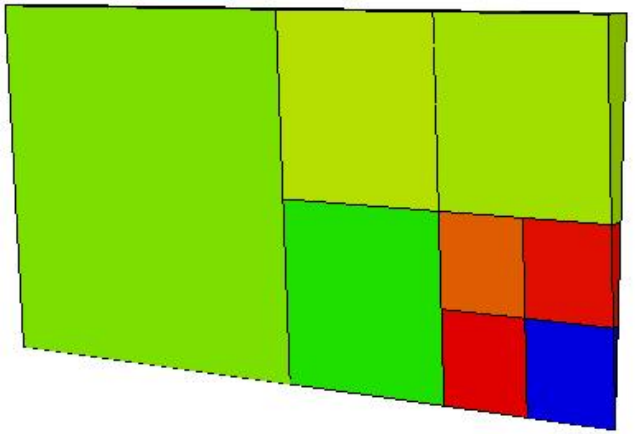
Particle mesh-cell queries on domain-decomposed mesh

PARTISN – Neutron/Gamma Deterministic Transport

The PARTISN team covers a wide variety of research:

- **We focus on providing computational solutions to the linear Boltzmann transport equation for neutral particles using the S_N method.**
- **Our latest research includes novel material-motion discretizations and energy group treatments.**
- **We use traditional structured and block Adaptive Mesh Refinement structured meshes, for static and time-dependent problems.**



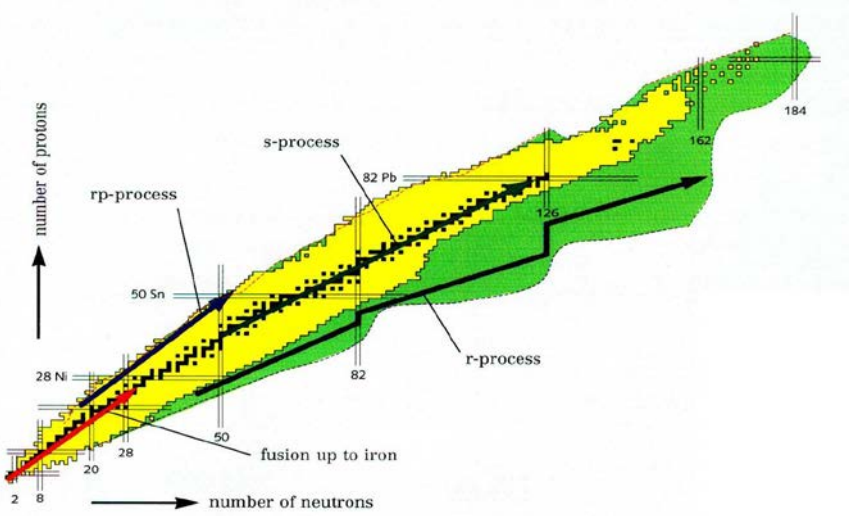


PARTISN – Neutron/Gamma Deterministic Transport

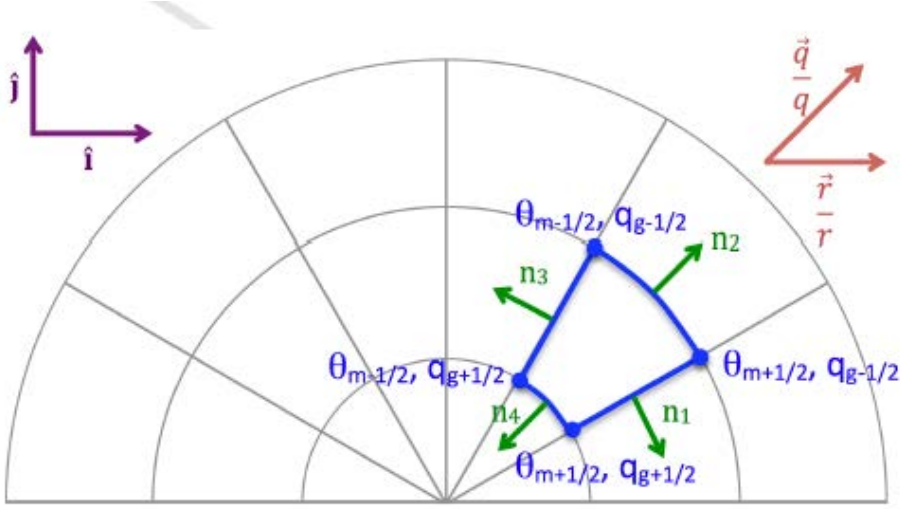
We add new physics, develop better solution methods, translate these into software, and help our users understand their results.

- **Our worldwide users perform a wide variety of 1-D/2-D/3-D calculations, so we require robust and efficient methods for reducing transport solution iterations (e.g., "KBA" sweeps, Diffusion Synthetic Acceleration).**
- **We have long been involved with work and research in nuclear application areas such as criticality safety, reactor engineering/shielding, etc.**
- **We are also applying our methods and solvers to non-traditional areas such as the r-process in core-collapse in supernovae and neutron-star mergers -> material-motion effects.**

Rapid neutron capture in these types of events is believed to account for the creation of roughly half the abundance of materials heavier than Fe

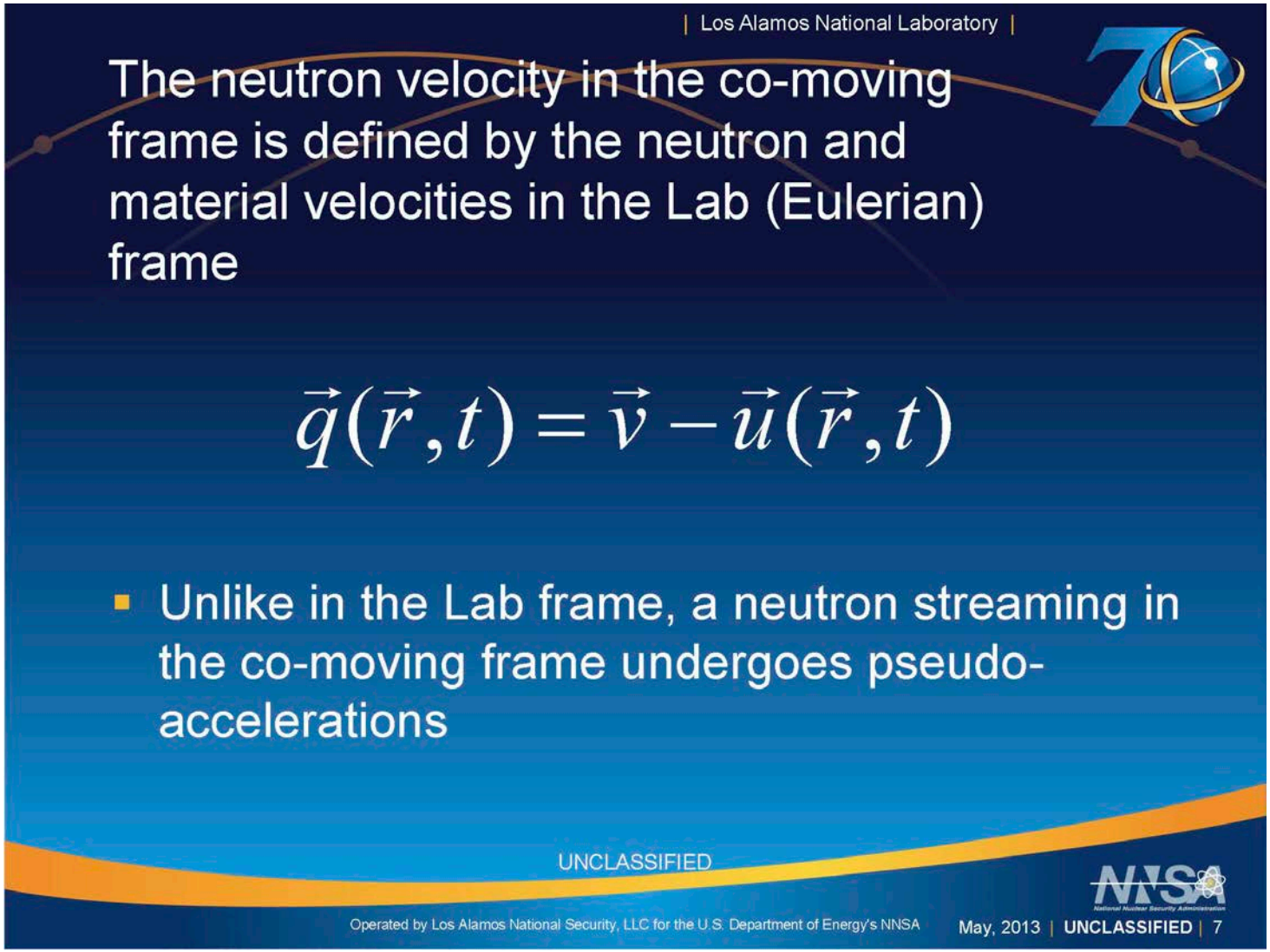


PARTISN – Angles + Energy = Velocity!

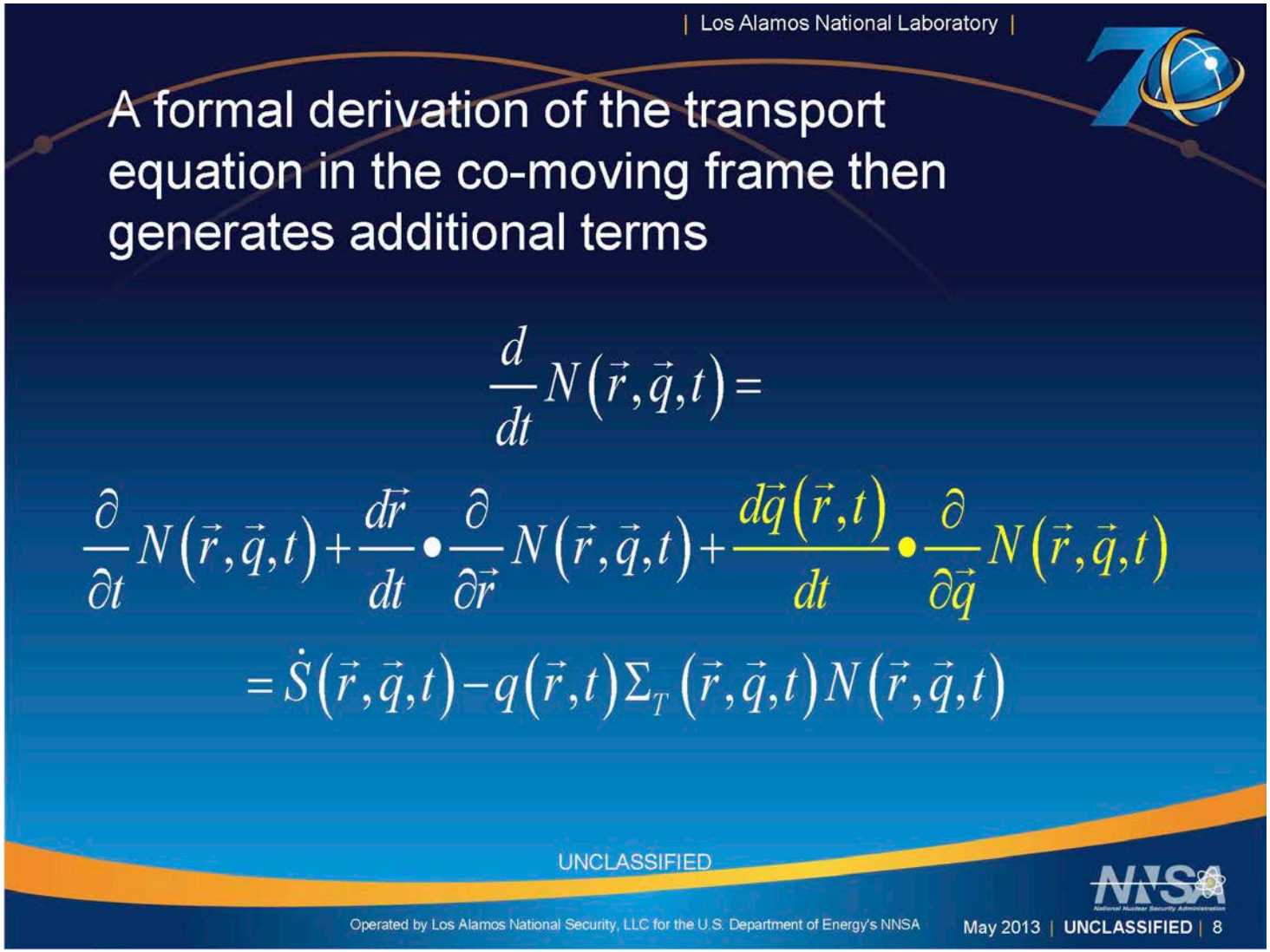


Velocity Mesh

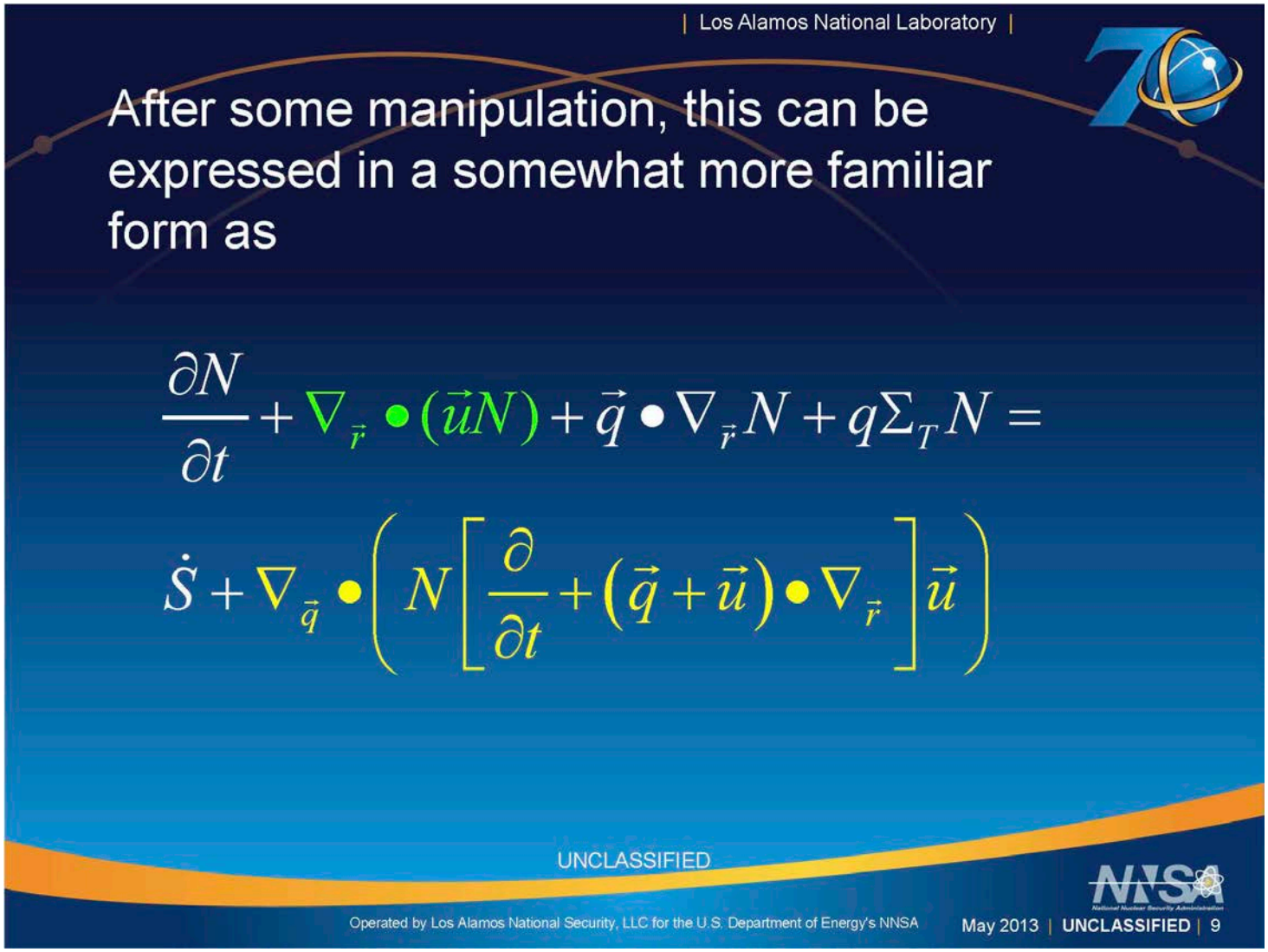
PARTISN – Neutron/Gamma Deterministic Transport



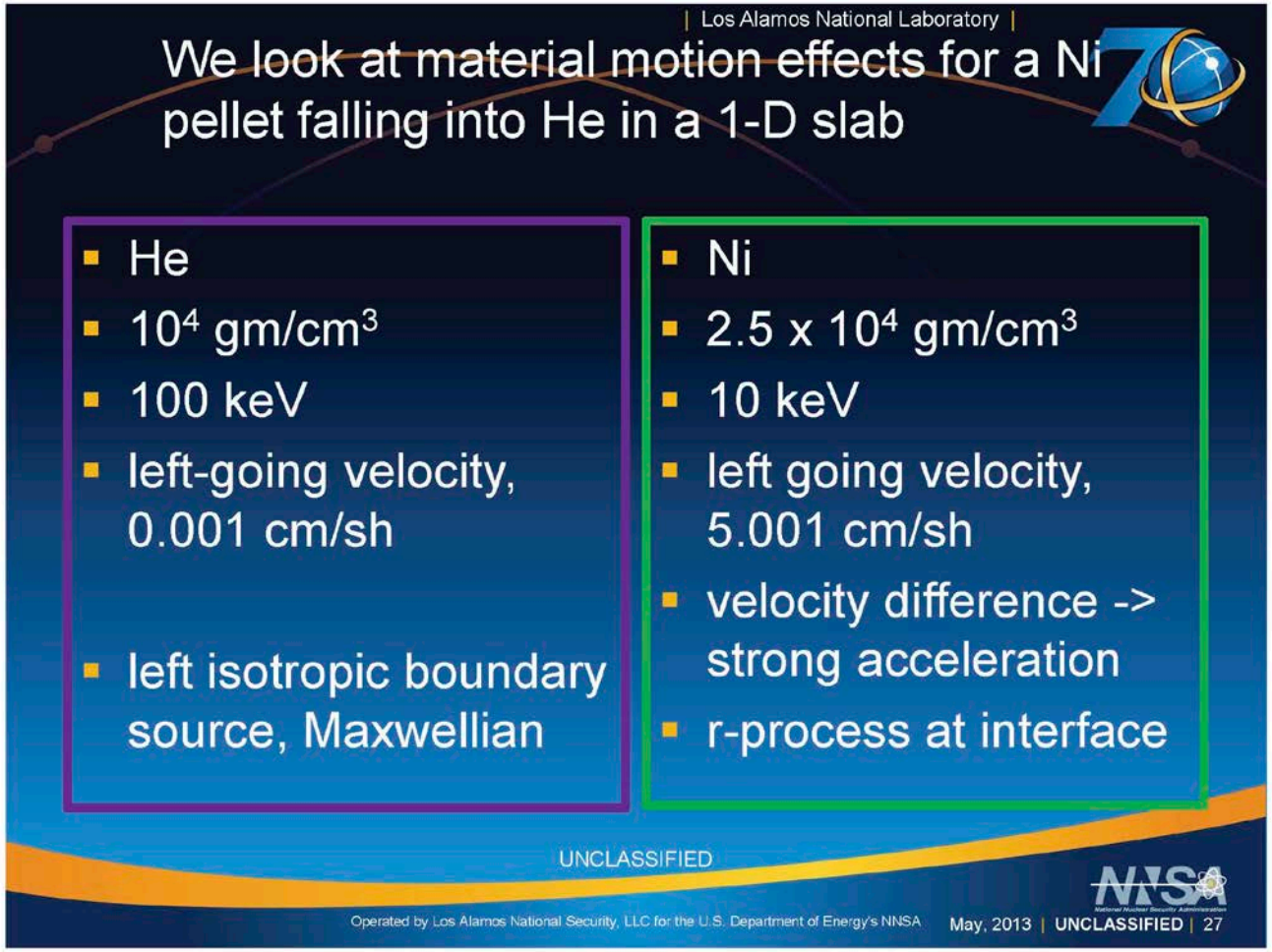
PARTISN – Neutron/Gamma Deterministic Transport



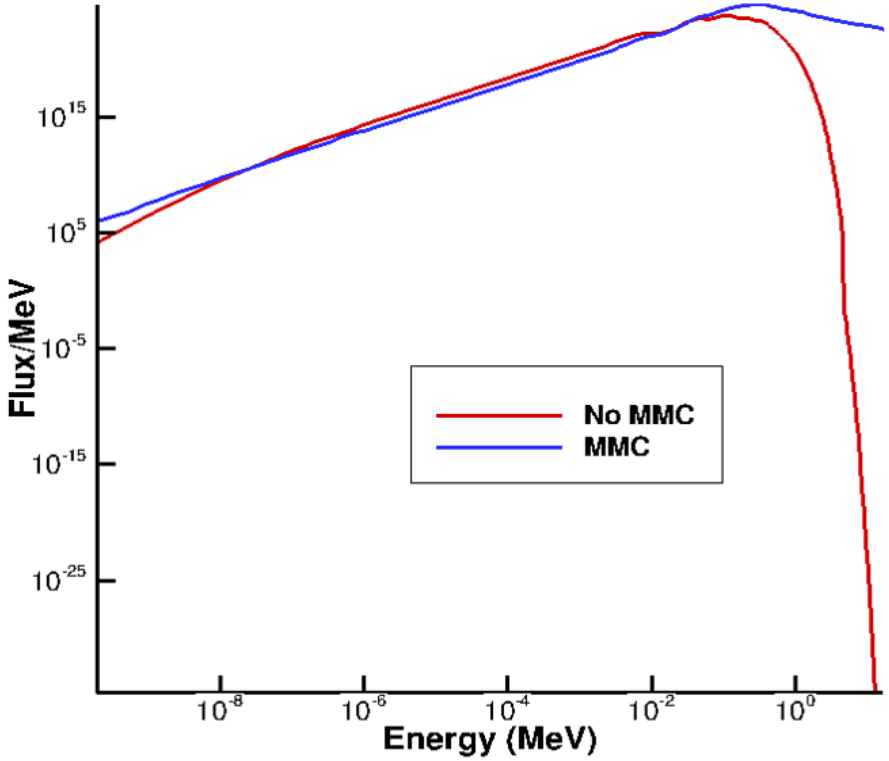
PARTISN – Neutron/Gamma Deterministic Transport



PARTISN – Neutron/Gamma Deterministic Transport



PARTISN - Ni pellet passing through a He slab with and without moving material corrections

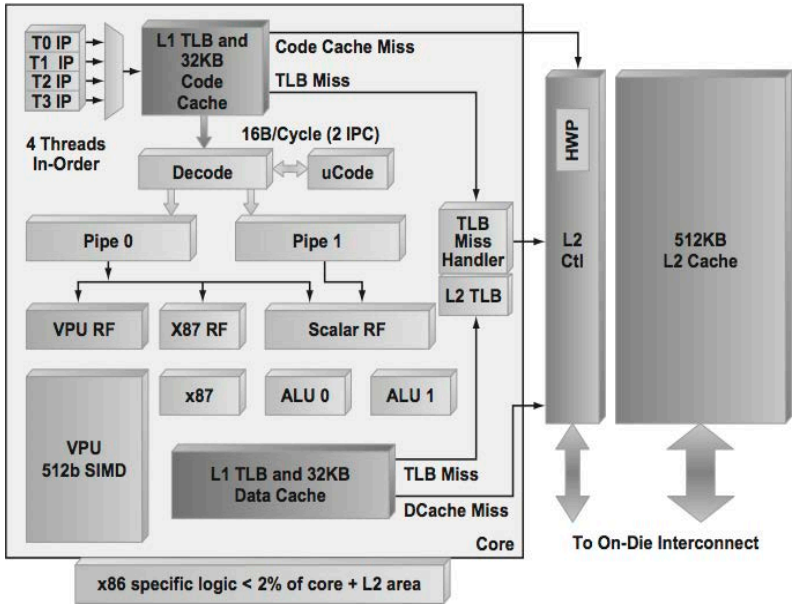


PARTISN – Neutron/Gamma Deterministic Transport

Our computational challenges span the complete gamut and are constantly evolving

- *Platforms*: from a Windows laptop -> desktops -> small clusters -> every type of supercomputer used by NNSA
- 1-D static calculations on a single processor with run times measured in seconds
- We are directly involved with commercial vendors in defining and evaluating tomorrow's exascale platforms
- SNAP is our open-source mini-app for collaborative research on these issues (https://github.com/lanl/SNAP)
- **3-D time-dependent calculations on >100K processors with run times measured in months**

Intel Xeon Phi (KNC) core



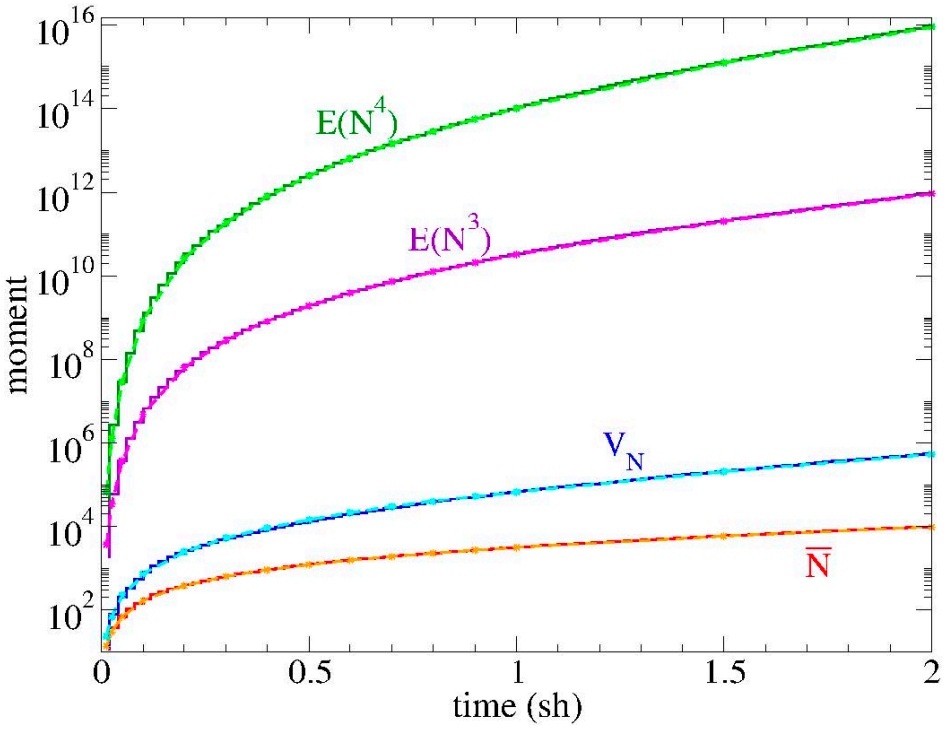
Point of Contact: Randy Baker, CCS-2/LANL

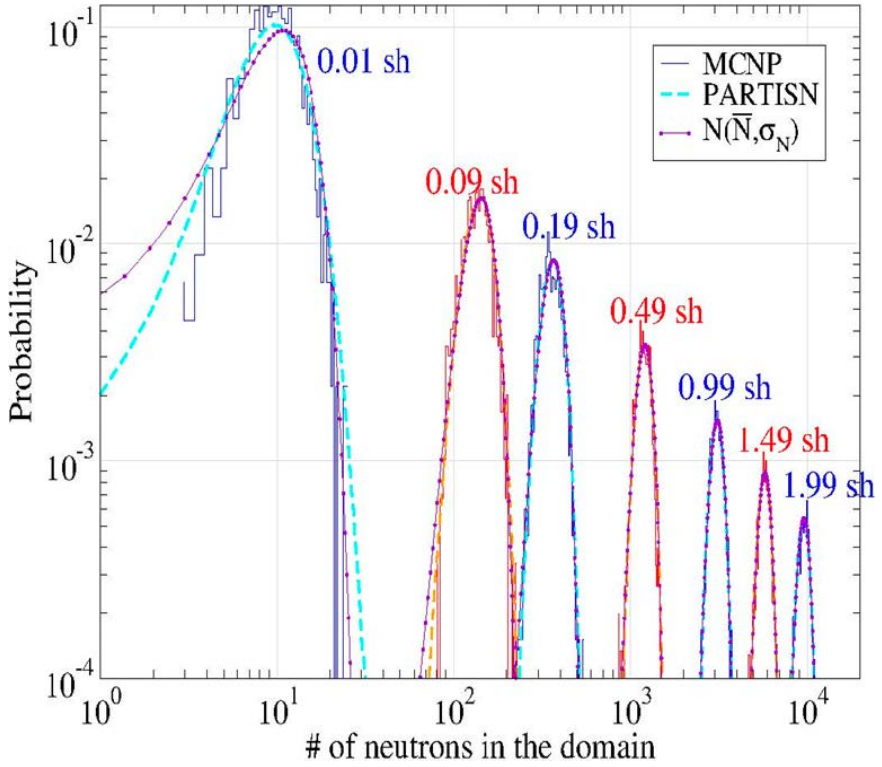
PARTISN – Neutron/Gamma Deterministic Transport

- Fission is an inherently stochastic process
- Backwards Kolmogorov equations, time-dependent adjoint-like transport equations with higher-order source terms (mean is the standard Boltzmann transport equation)
- The P(survival)/P(initiation) equations have been available in PARTISN for some time
- We have recently added the capability to compute the first four moments of the neutron population, allowing us to generate PDFs of the neutron population

- **Results: 6 cm Pu Sphere with = 19.6 g/cm3, keff = 1.165**
- **A uniform volume source emits 1000 neutrons/shake in the energy range 14-14.25 MeV**
- **PARTISN: 618 groups, S32 and P4**
- **MCNP: Continuous energy cross sections from the same data**

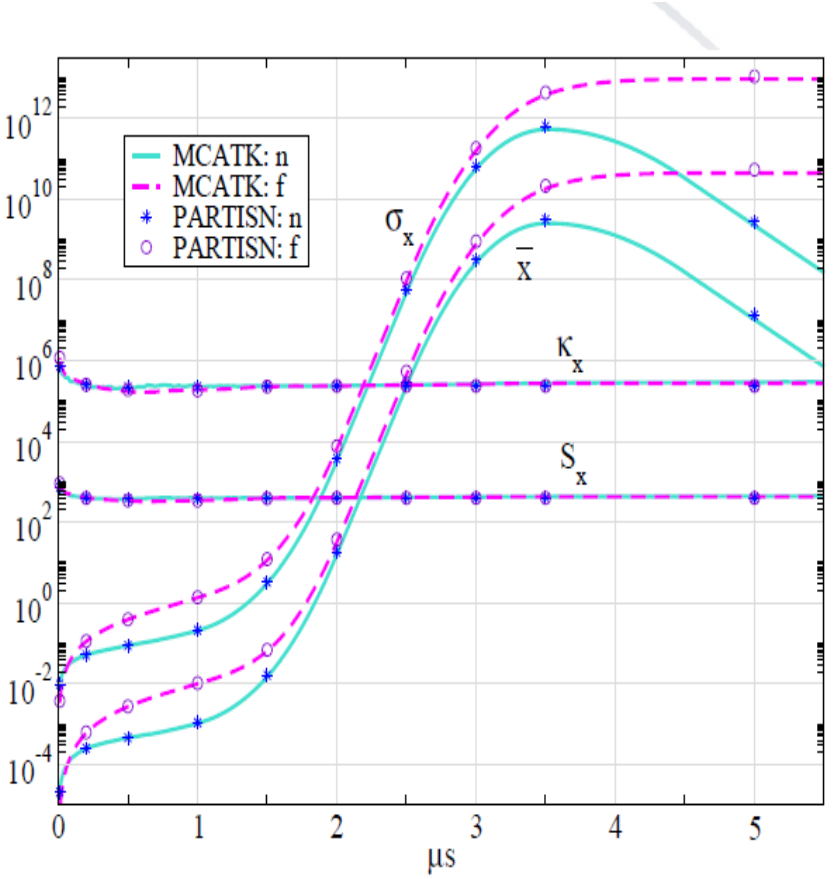
PARTISN – Neutron/Gamma Deterministic Transport





PARTISN – Neutron/Gamma Deterministic Transport

- A similar approach can be used to derive the moments of the fission population
- Here, while *n* is the number of neutrons, *f* is the number of fissions that have occurred
- 1-D sphere with time-varying concentrations of U^{235} and U^{238} (Japanese fissile solution criticality accident)
- MCATK runs were generated from 50 independent runs with 554440 fission chains apiece



PARTISN Research Interests

- **Solution methods for the transport equation with neutron-neutron scattering**
- **Time-dependent multigroup weighting functions**
- **Relativistic moving material corrections**
- **Anisotropic fission**
- **Efficient and scalable computational transport solution methods for massively parallel architectures using a “MPI+X” paradigm**
- **Tool development for the prediction of code performance on future architectures**
- **Sweep-based acceleration methods for the transport equation**

Point of Contact: Randy Baker, CCS-2/LANL

The Transport Project is always looking for exceptional students, post-doc's, and staff

- Expertise in, or a demonstrated aptitude to learn, radiation transport methods and related applications
- A strong desire to
  - learn and apply new physics, numerical methods, computer algorithms, and applications
  - target these skills, along with disciplined software engineering practices, for solving problems on the largest supercomputers in the world
  - work in a multidisciplinary, team environment

Point of Contact: Rob Lowrie, CCS-2/LANL

Summary

Summary

- **CCS-2 is a vibrant group of scientists who bring their skills to bear on important and interesting problems.**
- **Students and postdocs are a very important part of the Laboratory's future.**
  - The Laboratory employs ~1,200 students (most in the summer, some year-round)
  - There are ~350 postdocs employed at the Laboratory
- **The majority of Laboratory staff have been student interns or postdocs at one of the DOE laboratories.**
- **For detailed technical questions please contact the points of contact listed in this presentation.**
- **We are always looking for opportunities to collaborate.**

Contact Information

Los Alamos National Laboratory -- http://www.lanl.gov

Careers at the Laboratory -- http://www.lanl.gov/careers

Computational Physics and Methods Group CCS-2 -- http://ccs2.lanl.gov

CCS-2 Group Leader: James Cooley -- jhcooley@lanl.gov

CCS-2 Deputy Group Leader: Markus Berndt -- berndt@lanl.gov

CCS-2 POCs:

- Transport: Robert Lowrie -- lowrie@lanl.gov
- ACME, MPAS-O: Mark Petersen -- mpetersen@lanl.gov
- xRAGE: Tom Masser -- tmasser@lanl.gov
- Truchas: Neil Carlson -- nnc@lanl.gov
- Fornax, eblight: Joshua Dolence -- dolence@lanl.gov
- SuperNu: Ryan Wollaeger -- wollaeger@lanl.gov
- NAMBE: Jeff Haack -- haack@lanl.gov
- CFDNS: Daniel Livescu -- livescu@lanl.gov