COMPUTER & COMPUTATIONAL SCIENCES

Continuum Dynamics Group (CCS-2)

John Turner, *Group Leader*
James Sicilian, *Deputy Group Leader*

CCS Division All-Hands Meeting

July 10, 2006

Computer and Computational Sciences Division
Voice: (505) 667 - 4297
Fax: (505) 667 - 4972
turner@lanl.gov
www.ccs.lanl.gov

NNSA

Los Alamos NATIONAL LABORATORY

What We Do

Unifying research interests

- continuum approximations to dynamic physical processes

Common research approach

- simulation of physical processes via numerical solutions of model equations
- verification and validation of simulations, including quantification of sensitivities and uncertainties
- use our simulation tools for *analysis and prediction* where possible

Numerous products and services

- simulation tools, simulation tool analysis and application, numerical algorithms, physical models
- delivery via software, manuals, reports, publications, books, consultation, etc.

We span the theoretical / applied spectrum more completely than peer groups, often serving as a bridge between them.

Research Portfolio (1 of 2)

Physical model formulation

- interface dynamics, high explosives, phase change, chemistry, shock dynamics, instabilities and turbulence
- material response (deformation, fracture, damage, rupture)
- induction heating, convective/conductive/radiative heat transfer

Numerical algorithm development

- PDE discretization
  - *finite difference, finite volume, finite element, and meshless techniques*
- solution techniques for coupled linear and nonlinear PDEs
- parallel algorithm formulation
- uncertainty analysis and quantification
- challenges
  - *coupling multiple physical processes*
  - *balancing of accuracy and robustness*

Research Portfolio (2 of 2)

Applied Math

- data-driven modeling and analysis
- image analysis

Advanced Architectures

- algorithmic opportunities and tradeoffs presented by recent and future hardware architectures

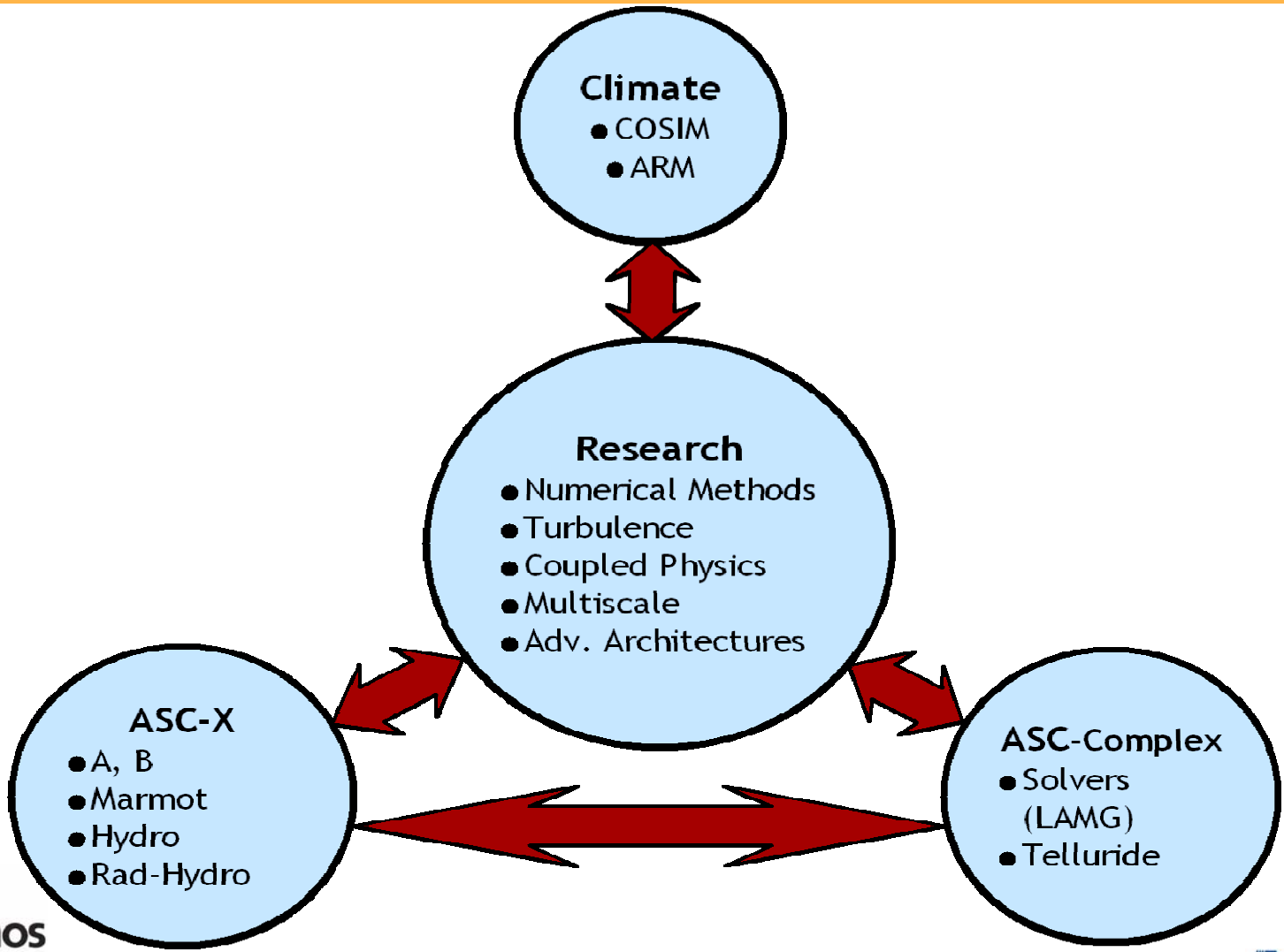
Software engineering

- component-based software design and construction
- testing infrastructure (unit, regression, integral)
- finding reproducible team software processes

Simulation applications and analysis

- using our simulation tools to get answers for customers

CCS-2 Project View



CCS-2: Continuum Dynamics

John Turner, Group Leader

Jim Sicilian, *Deputy Group Leader*

5/18/2006

Group Operations

Frankie Gomez,
Admin. Operations Specialist, CMC
Mary Ann Lynch, *Group Admin.*
Geneva Miera, *Admin. Specialist*

Radiation/Hydrodynamics

Malcolm Andrews, *Nat. Security Fellow*
Andrew Brydon
Ed Caramana
Gary Dilts
John Grove
Yunghee Kang, *Post-Doc*
Larry Libersky
Daniel Livescu
Rob Lowrie, ***Team Leader***
Thomas Masser, *GRA*
Jim Morel, *Contractor*
Nely Padial-Collins
Philip Randles, *Guest Scientist*
John Wohlbier

Climate

Rainer Bleck, *Guest Scientist*
Sumner Dean
Scott Elliott
Matthew Hecht
Jens Lorenz, *Guest Scientist*
Bob Malone, *Lab Associate*
Balu Nadiga
Mark Peterson, *Post-Doc*
Wilbert Weijer
Beth Wingate, **Team Leader**

Scientific Advisor

Darryl Holm, *Laboratory Fellow*
(joint with Imperial College, London)

Telluride

(DGL serves as Team Leader)
Markus Bussmann, *Guest Scientist*
Neil Carlson
Jane Cullum, *Contractor*
Sharen Cummins
Marianne Francois
Roland Glowinski, *Guest Scientist*
Michael Hall
Erin Iesulauro, *Post-Doc*
Doug Kothe, *Guest Scientist*
Larry Schwalbe, *Guest Scientist*
Barry Smith

Advanced Computing and Algorithms

(GL serves as Team Leader)
Tom Asaki
Ben Bergen, *Post-Doc*
Paul Henning
Rudy Henninger, *Lab Associate*
Wayne Joubert, *Contractor*
Bryan Lally
Jamaludin Mohd-Yusof
Collin Powell, *UGS*
Daniel Pruitt, *Network Admin., OCSR, CSO*
Sriram Swaminarayan

Rad-Hydro Team [Rob Lowrie]

Expertise

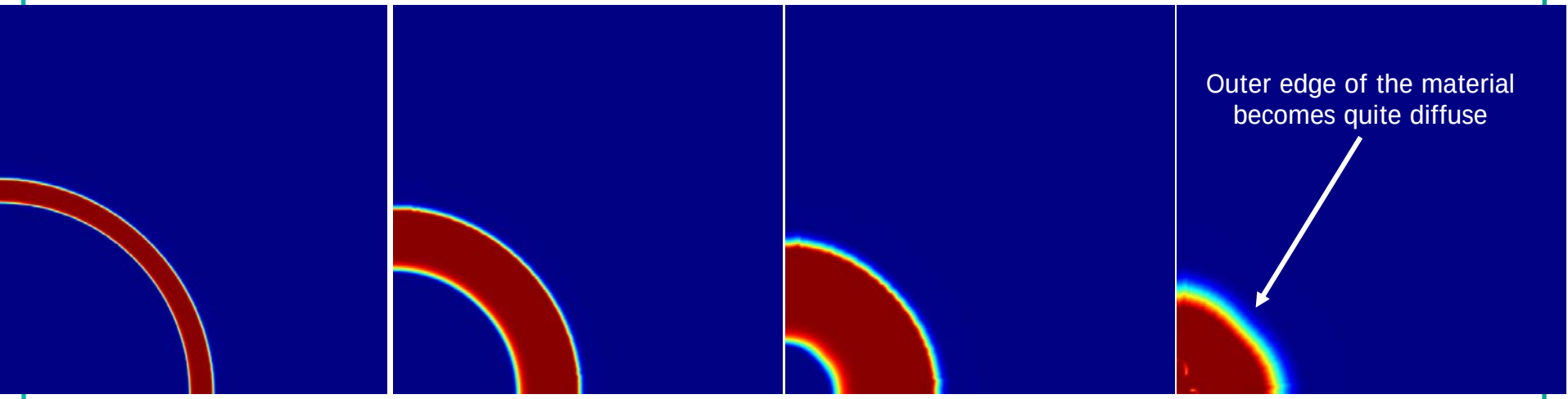
- Development of numerical algorithms and physical models
- Hydrodynamics, Radiation Transport, Coupled-physics issues
- Turbulence
  - *theory, modeling (DNS, LANS-α), experiments*
- Large-scale, multiphysics code development

Funding from multiple projects

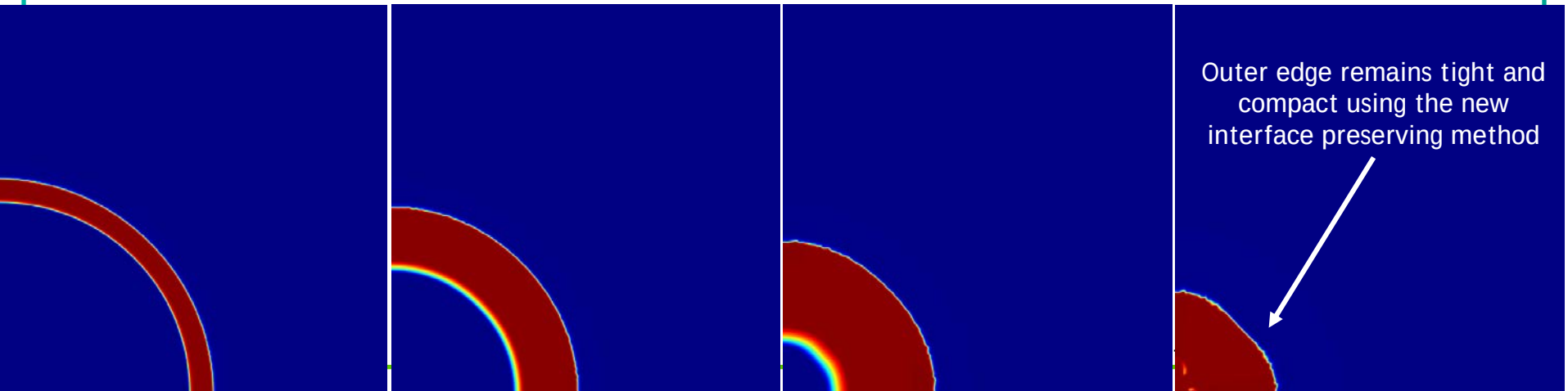
- ASC – hydro methods, transport, turbulent mixing
- WSR – mesh-free hydro methods, rad-hydro, interface treatments
- LDRD – adv. architectures (GPU), turbulent mixing
- DoD - mesh-free hydro methods

Improved interface treatment for Crestone Project

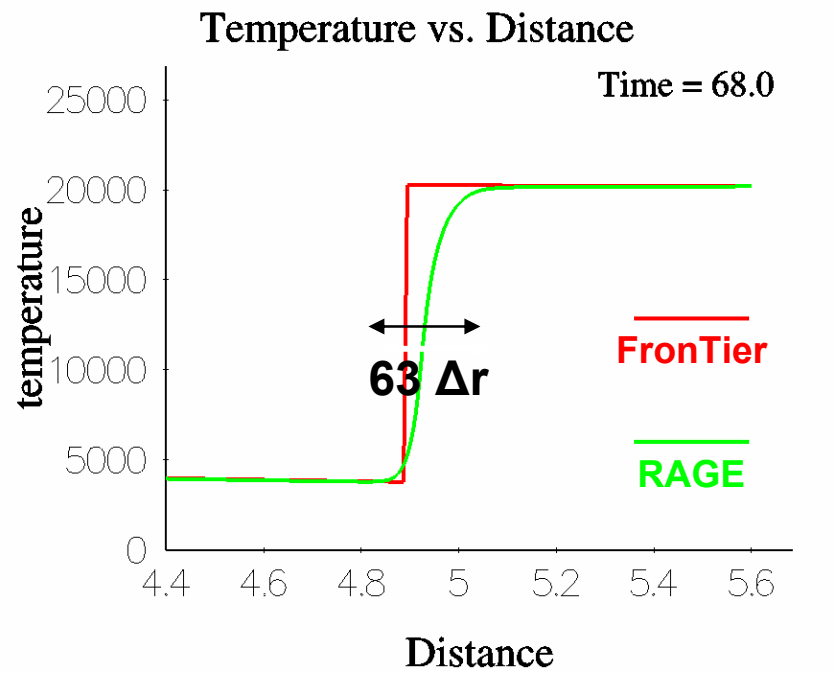
Base Reconstruction Technique

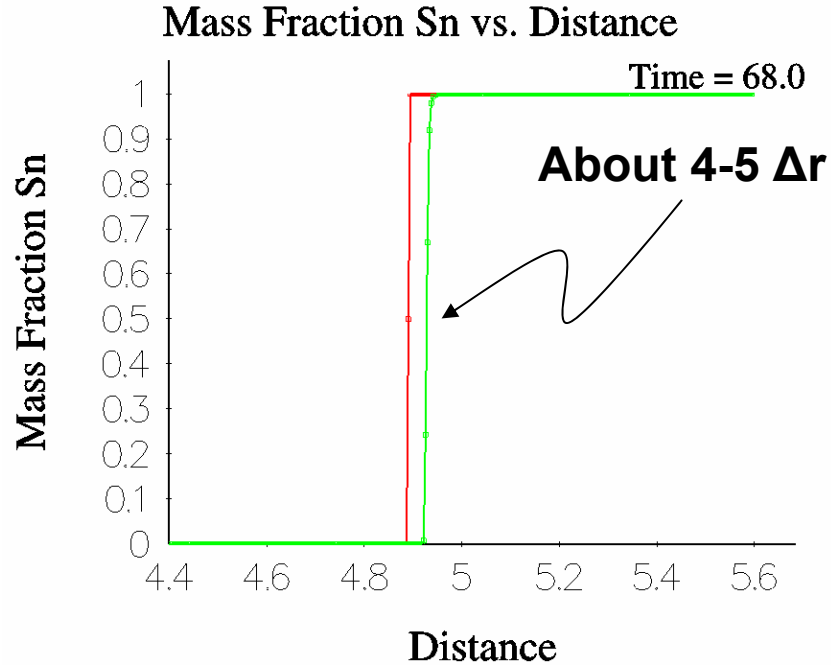


Interface Preserving Reconstruction Technique



Temperature Diffusion Greatly Exceeds Mass Diffusion





- *256 zones/cm*
- *Mass fraction width ≈ 5 zones*
- *Thermal width ≈ 50-75 zones at time 68 μsec*
- *Thermal width increases with each refraction*

John A. Turner, CCS-2, turner@lanl.gov

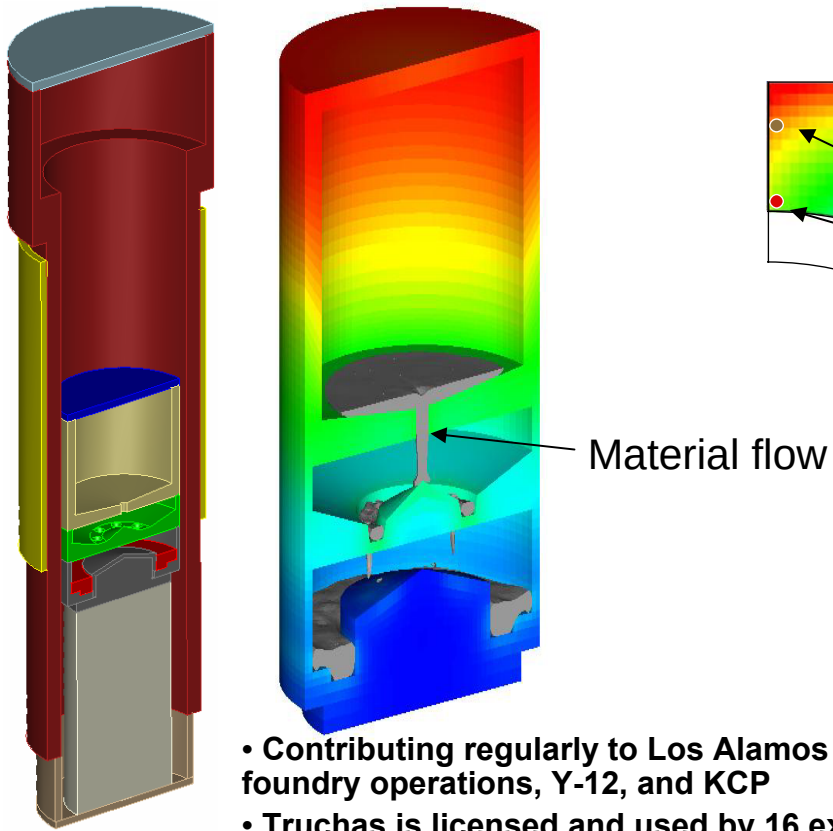
Telluride Team/Project [Jim Sicilian]

LANL weapons certification and stockpile stewardship missions require manufacturing expertise

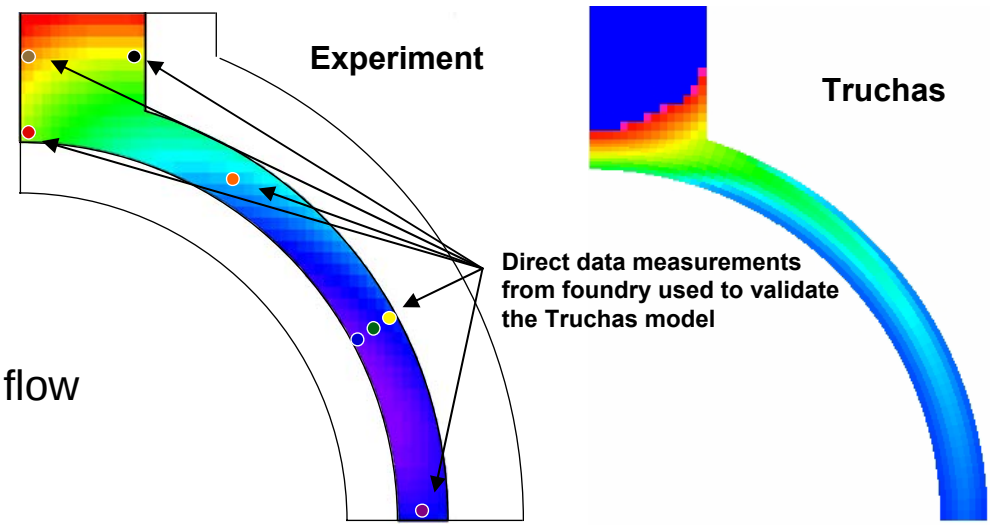
- Significant manufacturing capabilities were lost with the closure of Rocky Flats
- CTB Treaty means we cannot test remanufactured weapons
- Computational simulation is one means to assist certification of different manufacturing methods
- New methods and hardware capabilities make this a feasible goal

Telluride Project: casting and material science capability for the DOE Complex

Sandia pulsed reactor fuel rings



Pit casting and mold design



- Contributing regularly to Los Alamos foundry operations, Y-12, and KCP
- Truchas is licensed and used by 16 external organizations (many uses, manufacturing, coastal water interactions with coastline, etc)
- CCS and three other LANL divisions involved in project

Coupled physics models and numerics:

- ✓Inductive heating (electromagnetic modeling)
- ✓Radiative energy exchange between surfaces
- ✓Fluid flow and interface tracking and voids
- ✓Multiple phase change models and solidification
- ✓Heat transfer by conduction and convection
- ✓Modern linear solver techniques
- ✓Unstructured hex mesh (incl. degenerate cells)

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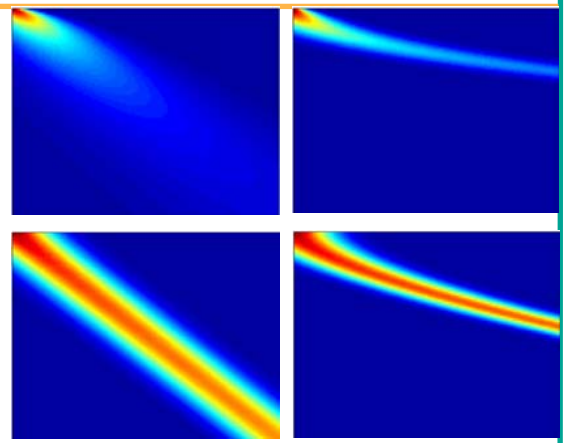
Advanced Computing and Algorithms

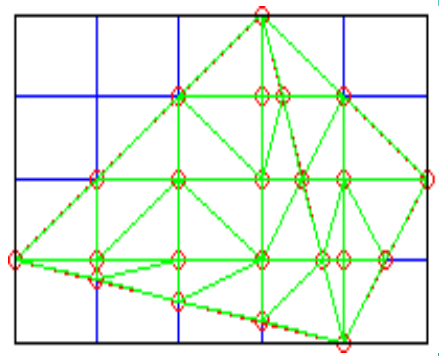
[John Turner (temporary)]

from applied math to high-performance computing

- Data-Driven Modeling and Analysis (DDMA)
  - *understanding data through models and approximation schemes which exploit domain understanding and advanced geometrical, analytical, and statistical insights*
  - *understanding the differences between simulations and data through quantification of model differences and noise-like differences*
- Advanced Architectures
  - *understanding algorithmic opportunities presented by recent and future hardware architectures (e.g. Roadrunner)*
- Scalable solution of linear systems of equations
  - *algebraic multigrid methods (LAMG)*



Curvature Warping examples



Mass-conserving interpolation

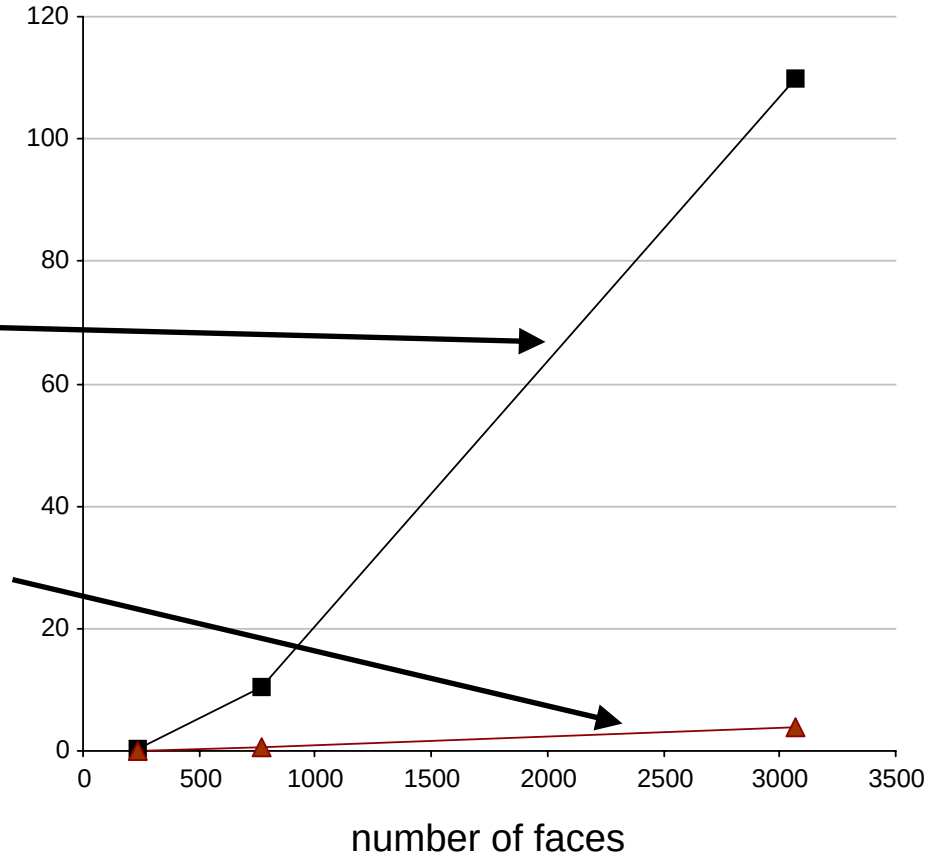
LDRD-DR: Advanced Computational Architectures (viewfactor GPU results)

time (seconds) to compute viewfactors within Truchas

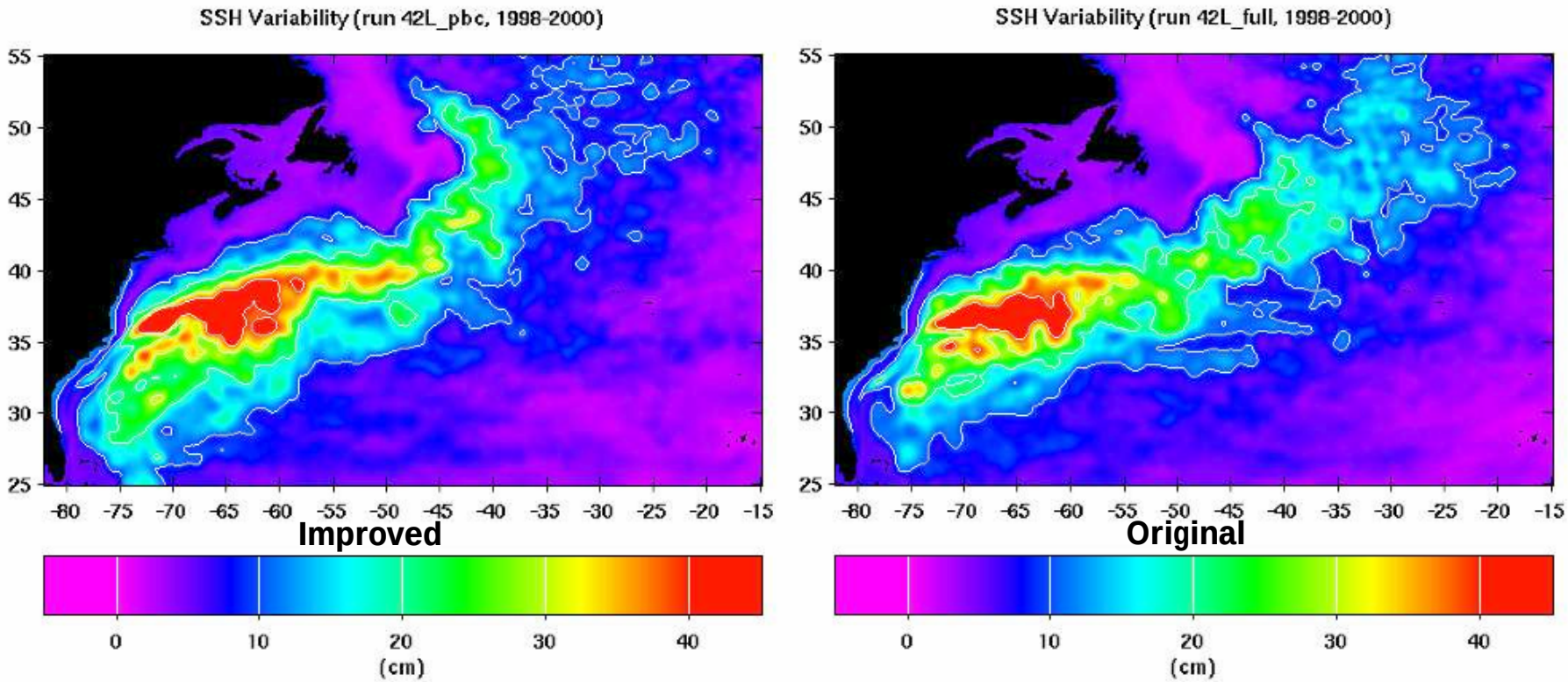
- lower is better
- hemi-cube
  - *3.4 GHz 64-bit Xeon*
  - *Chaparral (from SNL)*
- plane projection
  - *NVIDIA Quadro FX 1400 GPU*

GPU implementation of new algorithm 30x faster

- can now consider re-computing viewfactors during fill!



Climate Team [Beth Wingate]



primarily COSIM Project

- Climate, Ocean and Sea Ice Modeling
- biogeochemistry
- turbulence

Mark Petersen

Ocean Models in Climate Change Assessment

Major New Areas

(for both CCS-2 and CCS Division in general…)

Roadrunner

- a.k.a. "the earmark machine"

GNEP

- Global Nuclear Energy Partnership

Roadrunner

also known as "the earmark machine"

- primary goal is 1 PFlop/s LINPACK in CY07
  - *restore LANL position in Top500 list (http://top500.org/)*
  - *$41M this FY, $60M in FY07, $20M in FY08*
- Office of Science going after 1 PF also
  - *"Supercomputer set for an upgrade at Oak Ridge National Laboratory", KnoxNews, 6/15/2006*
    - http://nccs.gov/news/pr2006/news_20060615_knoxnews.html
- both logistical (procurement) and technical challenges
  - *timescale for RFP, bids, delivery*
  - *heterogeneous architecture*
  - *software (OS, compilers, etc.)*

Roadrunner Algorithms Project

performance on problems of interest to LANL

- not LINPACK
- this is a challenge tailor-made for CCS
  - *neither CCN nor X can / will do this*
- beyond porting of current software
- leverage experience from Adv. Arch. LDRD-DR
  - *algorithms in the context of architecture*
  - *compiler / tool development (Scout)*

Renaissance of Nuclear Power

first began to think nuclear power might re-emerge when pro-nuclear article appeared in Wired:

- *Nuclear Now! How clean, green atomic energy can stop global warming*, by Peter Schwartz and Spencer Reiss (Wired 13.02, Feb. 2005)
  - *http://www.wired.com/wired/archive/13.02/nuclear.html*

Global Nuclear Energy Partnership

GNEP (http://www.gnep.energy.gov/)

- big announcement expected in State of the Union address, but President backed away and rolled out much more quietly
  - *As part of President Bush's Advanced Energy Initiative, the Global Nuclear Energy Partnership (GNEP) seeks to develop worldwide consensus on enabling expanded use of economical, carbon-free nuclear energy to meet growing electricity demand. This will use a nuclear fuel cycle that enhances energy security, while promoting non-proliferation. It would achieve its goal by having nations with secure, advanced nuclear capabilities provide fuel services — fresh fuel and recovery of used fuel — to other nations who agree to employ nuclear energy for power generation purposes only. The closed fuel cycle model envisioned by this partnership requires development and deployment of technologies that enable recycling and consumption of long-lived radioactive waste.*

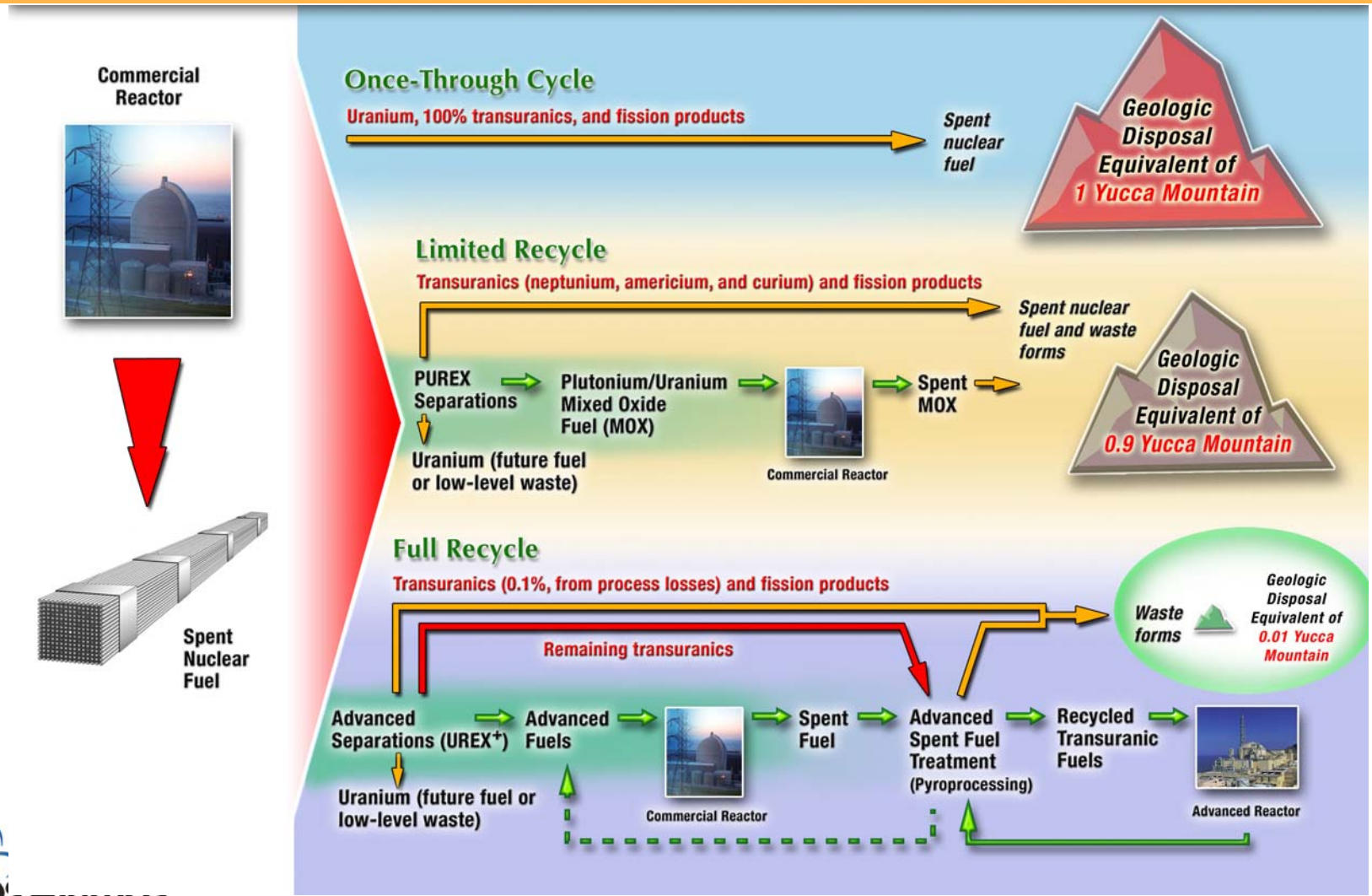
What is GNEP?

This morning, I want to speak to you about one part of this initiative: our plans to expand the use of safe and clean nuclear power. Nuclear power generates large amounts of low-cost electricity without emitting air pollution or greenhouse gases.

….my Administration has announced a bold new proposal called the **Global Nuclear Energy Partnership**. Under this partnership, America will work with nations that have advanced civilian nuclear energy programs, such as France, Japan, and Russia. Together, <u>we will develop and deploy innovative, advanced reactors and new methods to recycle spent nuclear fuel</u>. This will allow us to <u>produce more energy, while dramatically reducing the amount of nuclear waste and eliminating the nuclear byproducts</u> that unstable regimes or terrorists could use to make weapons.

President George W. Bush
Radio Address: February 18, 2006

Spent Nuclear Fuel Management Options



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Broader Scientific Challenges: Closed Fuel Cycle

Materials

- thermodynamic and thermophysical properties
- solid/solid, liquid/liquid and solid/liquid interface interactions
- radiation effects in complex materials

Separations

- behavior of multicomponent fluids
- design, synthesis and characterization of specific receptors for selective separations
- interfacial phenomena and their impact on mass transfer between phases
- understanding and controlling radiation effects
- thermodynamic and transport phenomena of actinides in electrochemical systems

Modeling and Simulation

- nuclear data (e.g., actinide cross sections)
- materials behavior
- design of new separations systems
- reactor performance (e.g., thermal-hydraulics)

Conclusions

CCS-2 represents broad spectrum of computational physics expertise

- spans theory, modeling, algorithms and experiments
- includes software implementation and deployment
- common technical challenges underpin many projects
  - *multiscale physics*
  - *coupling of multiple nonlinear physical processes*
  - *etc.*