High-Impact Modeling and Simulation:
Realizing the Potential for the Applied DOE Offices and Industry

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Workshop: Responding to the Software Crisis in DOE Scientific Computing
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http://energy.ornl.gov/
Two projects with integrated modeling and simulation components and strong industry connections...

- Consortium for Advanced Simulation of Light-Water Reactors (CASL)
  - http://www.casl.gov/
  - U.S. DOE Innovation Hub
- Batteries
  - multiple agencies, programs, and institutions
  - http://batterysim.org/

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Omitting due to time constraint – contact me about it if interested
Overview

• Brief description of CASL
• Lessons learned from CASL
  – challenges
  – what has worked
• Provocative statements on the software crisis
• What I won’t emphasize:
  – nuclear energy
  – HPC
  – GPUs
Consortium for Advanced Simulation of Light-Water Reactors (CASL)

Objectives and Strategies

- DOE Innovation Hub on Modeling & Simulation for Nuclear Energy Systems
- Develop “Virtual Reactor” to assess fuel design, operation, and safety criteria
- Virtual Environment for Reactor Applications (VERA)

Computational Science Areas

- Advanced numerical methods
- Increased coupling of physics
- Increased use of mechanistic models of lower length-scale phenomena
- Large-scale software development
  — geographically-dispersed, multi-institutional

Results and Impact

- Advance understanding of key reactor phenomena
- Improve performance of today’s commercial power reactors
- Evaluate new fuel designs to further enhance safety margins
CASL was the first DOE Innovation Hub

A Different Approach

• “Multi-disciplinary, highly collaborative teams ideally working under one roof to solve priority technology challenges” – Steven Chu

• “Create a research atmosphere with a fierce sense of urgency to deliver solutions.” – Kristina Johnson

• Characteristics
  – Leadership – Outstanding, independent, scientific leadership
  – Management – “Light” federal touch
  – Focus – Deliver technologies that can change the U.S. “energy game”

Contributing Partners
ASCOMP GmbH
CD-adapco
City College of New York
Florida State University
Imperial College London
Rensselaer Polytechnic Institute
Texas A&M University
Pennsylvania State University
University of Florida
University of Wisconsin
University of Notre Dame
Anatech Corporation
Core Physics Inc.
G S Nuclear Consulting, LLC
University of Texas at Austin
University of Texas at Dallas
University of Tennessee – Knoxville
Pacific Northwest National Laboratory

Core partners
Oak Ridge National Laboratory
Electric Power Research Institute
Idaho National Laboratory
Los Alamos National Laboratory
Massachusetts Institute of Technology
North Carolina State University
Sandia National Laboratories
Tennessee Valley Authority
University of Michigan
Westinghouse Electric Company
Example VERA Application: Coupled Flow-Neutronics-Fuel Response

- Standalone components run in their own MPI process space in unified executable
  - reduces collisions and improves algorithm performance - can overlap if desired
- PIKE (Physics Integration Kernels) drives nonlinear solve (part of Trilinos)
- Data transfers are handled through DataTransferKit (DTK) with MPI sub-communicators
  - Based on rendezvous algorithm developed by SNL SIERRA team
  - https://github.com/ORNL-CEES/DataTransferKit
CASL has addressed challenges in four specific ways.

Challenges

- Geographically-dispersed team
- Wide range of experience / motivation / priorities
- Deciding when to build and when to leverage existing software
- Leveraging software components with lives outside CASL
- Tension between currently-available industry hardware and HPC
- Domain scientists “vs.” computational scientists “vs.” computer scientists
- Maintaining software quality in a high-visibility, milestone-driven project
- Intellectual property agreements and software licensing
- Export control and proprietary data, software, and models
- Regulatory environment

What has worked?

1. Challenge problem-driven development
2. Agile development processes (augmented by videoconferencing technology)
3. Near-obsessive dedication to testing
4. Test Stand concept (getting code into hands of users/analysts)
Challenge-problem driven development

- CASL has followed a challenge-problem driven plan
  - use specific relevant problems to drive development of broadly-applicable simulation capability
  - progressively more challenging
- essentially large-scale iterative development
- sort of a large-scale version of Test-Driven Development
- seems to work well for programs with significant R&D components
- feedback from customers / users on priorities is critical
Lean Software Development

- Motivation for Lean Software Methods: Lean Manufacturing (e.g. Toyota)
- Seven Principles of Lean:
  1. eliminate waste
     - for software, waste is partially completed work, churn due to changing requirements, extra features, etc.
  2. build quality in
     - test-driven development, continuous integration and automated testing
  3. amplify learning through iterative development
     - sketch design, prototype, assess, customer feedback, refine
  4. defer commitment
     - delay irreversible decisions and/or follow multiple paths
  5. deliver fast
     - short release cycles, limit work in progress
  6. respect people
     - team should design and refine processes
     - no single “Best Way”
  7. optimize the whole

Great principles, but...
- must be translated into a specific process and implemented
- must be customized for each team
The VERA Physics Simulation Suite builds on a foundation of mature, validated, and widely-used software (this is a slide from the beginning of CASL).

- **FALCON**: Current 1D/2D workhorse (EPRI)
- **BISON**: Advanced 2D/3D capability (INL)
- **AMP FY10**: Initial 3D capability (NEAMS)
- **BOA**: Current CRUD and corrosion workhorse (EPRI)

**Neutronics** (diffusion, transport)
- Lattice physics + nodal diffusion: Current workhorse (Westinghouse)
- Deterministic transport: PARTISn (LANL), Denovo (ORNL), DeCART (UMichigan)
- Monte Carlo transport: MCNP5 (LANL), SCALE/KEO (ORNL)

**Fuel Performance** (thermo-mechanics, materials models)
- Lattice physics + nodal diffusion: Current workhorse (Westinghouse)
- Deterministic transport: PARTISn (LANL), Denovo (ORNL), DeCART (UMichigan)
- Monte Carlo transport: MCNP5 (LANL), SCALE/KEO (ORNL)

**Chemistry** (crud formation, corrosion)
- **FALCON**: Current 1D/2D workhorse (EPRI)
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**Mesh Motion/Quality Improvement**
- Lattice physics + nodal diffusion: Current workhorse (Westinghouse)
- Deterministic transport: PARTISn (LANL), Denovo (ORNL), DeCART (UMichigan)
- Monte Carlo transport: MCNP5 (LANL), SCALE/KEO (ORNL)

**Multi-resolution Geometry**
- **VYPRE-W**: Current subchannel flow workhorse (Westinghouse)
- ARIA (SNL), Charon/Drekar (SNL), NHASE (RPI): Initial 3D flow capability
- STAR-CCM+, TransAT: commercial capabilities

**Multi-mesh Management**
- **SIERRA** (SNL)

**LIME Multiphysics Integrator**
- **(RETRAN (EPRI)**
- **RELAP5 (INL)**

**LIME RAVE Numerical Nuclear Reactor**
- **Sandia National Laboratories**
  - Lightweight Integrating Multiphysics Environment
- **Westinghouse suite of integrated capabilities**
  - RETRAN
  - VIPRE-W
  - PARAGON / ANC

- **Univ. of Michigan**
  - STAR-CD
  - DeCART
VERA was in danger of looking becoming the software equivalent of this....
We absolutely had to downselect.

• Financial and staffing realities.

• Painful process
  – institutionally – at times the partnership was at risk
  – personally – every piece of code is some developer’s precious, beautiful baby
    • I’ve developed my own precious, perfect software babies… which were sometimes beautiful only to me
    • no one likes to hear that their work isn’t the right fit

• If I had it to do over, I would institute a rigorous, formal review of all software to be leveraged.
  – documentation (user? developer? methods? design/architecture?)

I have the most respect for developers who are skeptical of their own code.
“Obsessive” testing

• Consider… what would happen if I went into your code and…
  – set all random numbers to 0.5
  – switched the speed of light and the radiation constant
  – switched sin(θ) and sin(φ) in scattering
  – change value of π
  – switch scattering and absorption opacities
  – inserted a unit conversion error
  – shifted a mesh index by 1 in a broadcast

• Would your testing reveal the error? How long would it take you to realize the answers are wrong? How long would it take you to fix them?
Continuous and obsessively paranoid testing is the backbone of good software.

Current status and needs for each testing category:

- **Pre-Push CI Tests**: Good adoption and usage
- **Post-Push CI Tests**: Catches lots of problems; Need faster feedback
- **Nightly Regression Tests**: Only GCC 4.6.1; Need better coverage and more platforms
- **Weekly Coverage Tests**: Not yet
- **Weekly Memory Tests**: Currently being set up
- **Performance Testing**: Not yet
- **Scalability Tests**: Not supported by TriBITS yet, need CTest/CDash support
CASL Test Stands provide early deployment to industry.

- Early deployment into industrial environment for testing, use, and adoption of VERA to support real-world LWR applications
- Status of initial deployment to core industry partners
  - WEC: Deployment during June 2013; focus on VERA simulation of AP1000 first core startup
  - EPRI: Deployment Dec 2013; fuel performance
  - TVA: Deployment in progress; lower plenum flow anomaly
- Early Test Stand deployment benefited both CASL and users
  - Improved code installation processes
  - Input processing for heterogeneous cores
  - Reduction in problem setup times
  - Core tilt analysis
  - Analysis of new design features (e.g., tungsten rods)
Summary of Software Challenges Faced by CASL, and our Solutions

• Challenges
  – Many codes assume they are the “master”
  – Conflicting dependencies and build systems
  – Existing codes that have a life of their own outside CASL
  – Multiple languages (primarily Fortran and C++)
  – Disparate input and output formats and conventions
  – Different meshes and discretizations

• CASL Solutions
  – Common build system that extends widely-used standards
    • Support for distributed multi-repository integration
    • Improved support for continuous integration, etc.
  – Continuous integration and hierarchical testing
    • Catch and fix issues and conflicts as early as possible
  – Standardize input / output (and restart)
  – Develop infrastructure components as necessary (e.g. DTK for solution transfer)
  – Deploy early and often via Test Stands in order to get feedback from users
The crisis I see has little to do with HPC, hybrid/multicore, etc.

- Developers too quick to believe their code
- Analysts/users too quick to concoct “science” reasons to explain results that are actually numerical artifacts
- Difficult to reproduce published results
  - Claims made are increasingly difficult to verify
  - Large effort, little reward, no one wants to fund
- Imprecise and overloaded terminology (“model”, “coupled”, etc.)
- Lack of standardized test problems and validation data
  - Proprietary/protected data hinders both
- Struggle for funding leads to emphasis on “marketing”
  - Good results hyped, shortcomings / limitations hidden
- Effort required to support infrastructure, testing, developer training is underestimated, underappreciated, and usually hidden
- Bifurcated views of modeling and simulation by applied offices and industry
  - Simulations are less useful than experiments
  - Commercial tools provide all the simulation capability needed
Questions?
e-mail: turnerja@ornl.gov

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