Industry Interactions in Three Programs

John A. Turner

Group Leader
Computational Engineering and Energy Sciences
Chief Computational Scientist
Consortium for Advanced Simulation of Light-Water Reactors (CASL)

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Brief Introduction...

- **degrees in Nuclear Engineering**

- **1990-1997: Los Alamos National Laboratory (LANL)**
  - numerical solution of linear systems
  - radiation transport, fluid flow

- **1997-2001: Blue Sky Studios**
  - computer animation
  - physics-based rendering, some fluid flow

- **2001-2008: LANL**
  - led computational physics group
  - led applications team for Roadrunner supercomputer

- **2008-now: Oak Ridge National Laboratory (ORNL)**
  - advanced simulation for energy applications
  - focus on nuclear energy systems and batteries

[http://energy.ornl.gov/]
[http://www.imdb.com/title/tt0268380/]
[http://www.lanl.gov/roadrunner/]
[http://www.casl.gov/]
Three Projects with Strong Industry Connections...

- Nuclear energy
- Batteries
- Additive manufacturing (3D printing)

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<th>NE</th>
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<td>Community acceptance of simulation</td>
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Nuclear Energy

• Consortium for Advanced Simulation of Light-Water Reactors (CASL)
  – http://www.casl.gov/
  – U.S. DOE Innovation Hub
  – presentation at Sept. 2010 HPC User Forum in Seattle

• Center for Exascale Simulation of Advanced Reactors (CESAR)
  – http://cesar.mcs.anl.gov/
  – U.S. DOE Office of Science Co-Design Center
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”

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

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

http://energy.ornl.gov/
CASL Test Stands: From Plan to Execution

• Early deployment into industrial environment for rapid and enhanced testing, use, and ultimate 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 planned for Q2 2014; lower plenum flow anomaly

• Early Test Stand deployment is already producing dividends for CASL and users
  - Better code installation processes
  - Input processing for heterogeneous cores
  - Reductions in user problem setup times
  - Core tilt analysis
  - Analysis of new design features (e.g., tungsten rods)
Timeline for CASL Westinghouse Test Stand

- Test Stand discussion (early 2013)
- Scope proposed in Westinghouse memo (April 2013)
- VERA deployment at Westinghouse (June 2013)
- Technical analysis (July-Nov 2013)
- Analysis completed and documented (Jan 2014, Rev. 1 in Mar 2014)
$\Delta k^{-\text{eff}} = -81 +/- 2 \text{ pcm}$

Hot Spot $\Delta P = 1\%$ $\Delta AO = -0.9\%$

RMS $\Delta P = 1.2\%$ Max $\Delta P = 5.9\%$
Benefits

• Enhanced confidence in AP1000 PWR start-up predictions
• Generated high-quality benchmarks for code comparison
• Expanded application of VERA to an advanced core
• Provided key feedback to guide future developments
• Provided framework for VERA build and update

Recommendations

• Mitigate computational resources
• Cycle depletion and shuffling
• Expand capabilities
  – Thermal expansion
  – General reflector
  – Other fuel lattice configurations
• Improve output
• Improve documentation

• Relevant and engaging application of VERA to an advanced PWR first-core
• Very positive and useful experience
• Enhances confidence in first-core start-up prediction
Electrical Energy Storage

- primarily batteries, but also supercapacitors and fuel cells
Electric Vehicles (EVs) need cheaper, lighter, and safer batteries

• EVs will have greater penetration with reduced cost
  – Better performing, long life, higher energy density, etc.

• EV adoption will be severely impacted by safety incidences
  – Every day 100s of gasoline vehicles catch fire
  – However any EV fire (even without any casualties) makes headlines

• Modeling is critical not only to reduce cost but also to identify and mitigate these events
  – just like crashworthiness simulations improved vehicle safety

Goal is full virtual crash simulation.

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Vehicle crash simulation

- Models validated against deformation of crashed vehicles
- Deformation is more difficult to match than accelerometer signals

Design optimization includes vehicle crash compatibility performance.

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DOE / EERE / VT CAEBAT Program

- U.S. Department of Energy (DOE)
  - Office of Energy Efficiency and Renewable Energy (EERE)
    - Vehicle Technologies (VT) Program Office
- Computer-Aided Engineering for Batteries (CAEBAT)
  - started April, 2010
  - Goal: Predictive battery design tools for optimizing cost, performance and life
  - barriers
    - lack of computational standards for battery modeling
    - no common software framework for integrating battery modeling efforts
  - partners
    - NREL (lead), ORNL, INL
    - three industry teams
      - EC Power / PSU / Ford / JCI
      - GM / ANSYS / Esim
      - CD-adapco / Battery Design / JCI / A123Systems

4 software suites for use in cell/pack modeling
- 1 from each RFP team – may contain (or require) proprietary / commercial components
- additional tool integrates modules from RFP teams as well as Lab and University efforts beyond the RFP teams – community R&D platform - Virtual Integrated Battery Environment (VIBE)
CAEBAT: Current status

Detailed 3D Modeling

Discharge Curves
(Validation with IR Imaging)

Cylindrical Cell with Resolved Current Collectors
(Electrochemical – Thermal - Electrical)

Mechanical Abuse of Cylindrical Cell with Resolved Current Collectors
(Electrochemical – Thermal – Electrical – Mechanical)

Detailed particle level simulations to obtain effective mechanical properties of electrodes using DEM / FEM
Industry interactions and impacts

• Working closely with three industrial partners on input standardization and coupling
  – BatML v11 - XML schema, defines battery components from electrode to packs
  – battery “state” standard that encapsulates information for transfer between components for cell simulation

• Input translators to and from:
  – ANSYS
  – EC-Power
  – CD-adapco

• Coupling components
  – EC-Power is using CAEBAT OAS for parameter sweep and optimization
  – Ongoing work to couple electrochemistry, electrical, and thermal components of ANSYS/CD-adapco

• Close and evolving interaction with automotive manufacturers such as Ford Motor Co.
Additive Manufacturing

• also known as 3D printing
  – explosion in low-cost systems based on Fused Deposition Modeling (FDM) technology, a.k.a. Fused Filament Fabrication (FFF)
  – similar trends developing for metals

$500-$2,000
A lot of toys, art, ...
But also serious applications...
Advantages and Limitations

• **Advantages**
  - Energy savings - lightweight redesigns, reduced scrap, remanufacturing
  - Design freedom - complex geometries impossible with conventional processes
  - Cost savings – reduced scrap, avoids high tooling cost of low volume conventional process
  - Shorter leads times from design to product (no wait for tooling manufacture)

• **Current Limitations:**
  - Limited material selection (metals, polymers)
  - Slow – e.g. 32 cm$^3$/hr DMLS build speed
  - Surface roughness – finishing may be required
  - Validation and Certification of materials/processes

Turbine blade design with complex internal structures

Titanium prosthetic hand produced at ORNL
AM Enabled Design:

- Graded Materials, Composites, and Improved Structures for Enhanced Performance
- Advanced Robotics
  - Aluminum finger (65 grams, $6500 to fabricate)
  - Titanium finger (61 grams, $20 worth of material)
- Not possible with conventional technology
- Fast Design Iteration

21.1 g 12.1 g 14.4 g
Electron Beam Melting:

- Electron beam used to melt a powder bed under vacuum
  - similar to welding

- Excellent compositional control with microstructural refinement showing increased mechanical properties

- Precise control of complex geometries

- 2-D Semi Empirical process model to control temperature profile
  - extremely complicated/convoluted process control
  - current, speed, line scan length, thickness, surface temperature, contour, turning point, empirical corrections, scaling factors, hatch, heat time, etc.

Gas Turbine Engine Compressor Support Case
Rocket Engine Impeller
Engine Part with Lattice Structure
Customized Trabecular CMF Implant
DOE’s first Manufacturing Demonstration Facility located at ORNL

Leveraging core capabilities to support advanced manufacturing

- Neutron scattering
- High-performance computing
- Advanced materials
- Advanced characterization

Manufacturing Demonstration Facility (MDF): a multidisciplinary DOE-funded facility dedicated to enabling demonstration of next-generation materials and manufacturing technologies for advancing the US industrial economy

www.ornl.gov/manufacturing
Additive Manufacturing Summary

• Additive manufacturing has the potential to accelerate the dream-design-create-deploy innovation life-cycle.

• Scientific Challenges
  – Mechanical heterogeneity due to spatially (μm to nm) and temporally (<10^{-4} s to 1 min) varying chemical, thermal and mechanical gradients

• Vision & Steps
  – Develop and deploy verified and validated HPC models
  – Leverage ORNL strengths in industry partnerships (MDF) and characterization (SNS, HFIR)

• Expected Breakthrough
  – Fundamental understanding of heterogeneity in all additive manufacturing processes - innovation to mitigate
Three Projects with Strong Industry Connections...

• Common challenges
  – Intellectual property agreements and software licensing
  – Export control and proprietary data, software, and models

• Specific challenges
  – NE: regulatory environment
  – Batt: heavily experimental, fractured funding landscape
  – AM: incomplete understanding of fundamental processes, fractured funding landscape

• What is working...
  – NE: Test Stand concept
  – Batt: development of standards
  – AM: close partnership with equipment manufacturer

• Lessons
  – Begin addressing IP and software licensing EARLY
  – Simulation community needs to listen carefully in order to learn priorities, concerns
Questions?
e-mail: turnerja@ornl.gov

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