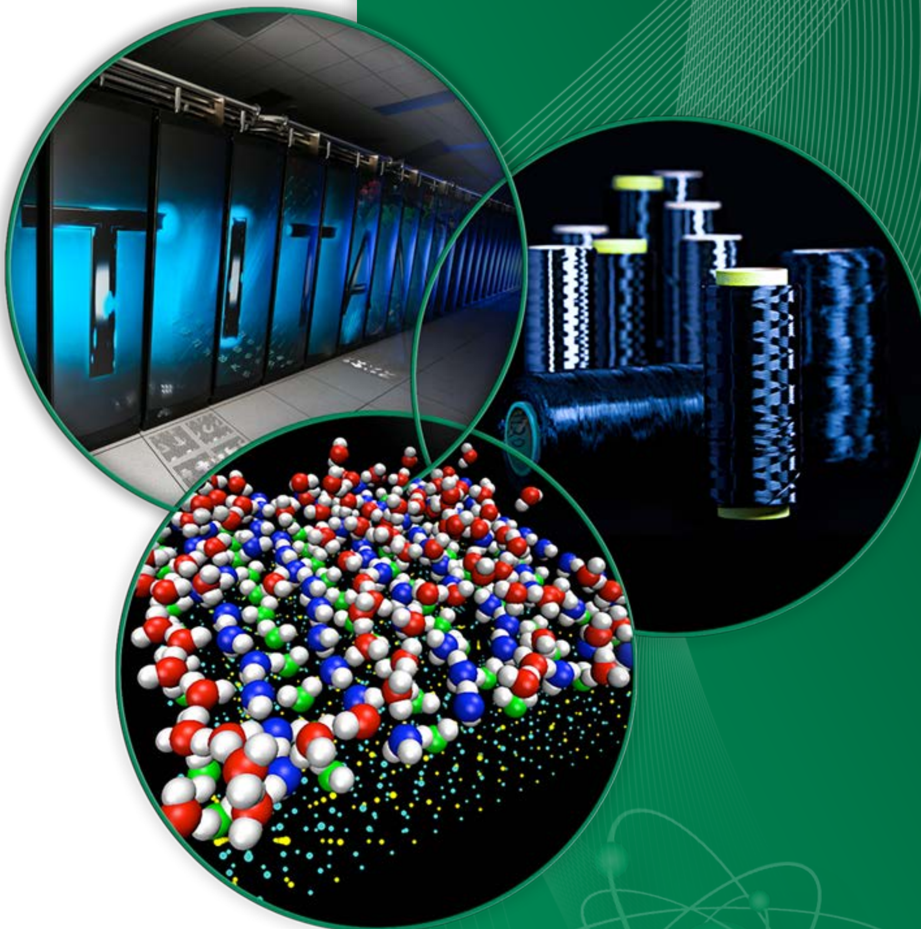
Industry Interactions in Three Programs

John A. Turner

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



HPC User Forum
Apr 7-9, 2014, Santa Fe, NM

Brief Introduction…

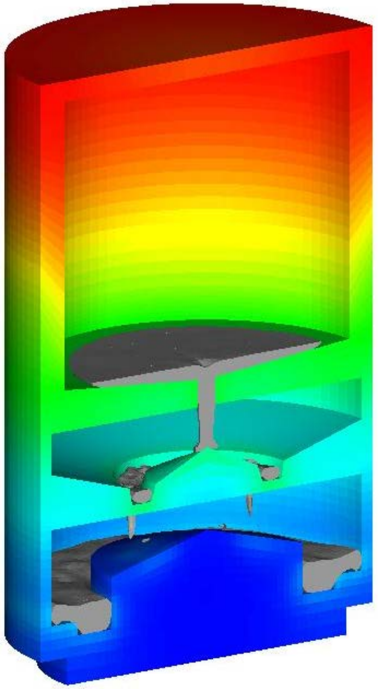
- degrees in Nuclear Engineering

- 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



Simulation of metal casting (Telluride Project)

http://www.imdb.com/title/tt0268380/

http://www.lanl.gov/roadrunner/

http://www.casl.gov/

CASL

Consortium for Advanced Simulation of LWRs

Three Projects with Strong Industry Connections...

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

	NE	Batt	AM
Community acceptance of simulation			
Community acceptance of HPC			
Maturity of physics models			
Maturity of software			
State of funding landscape			

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

Consortium for Advanced Simulation of LWRs

- 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

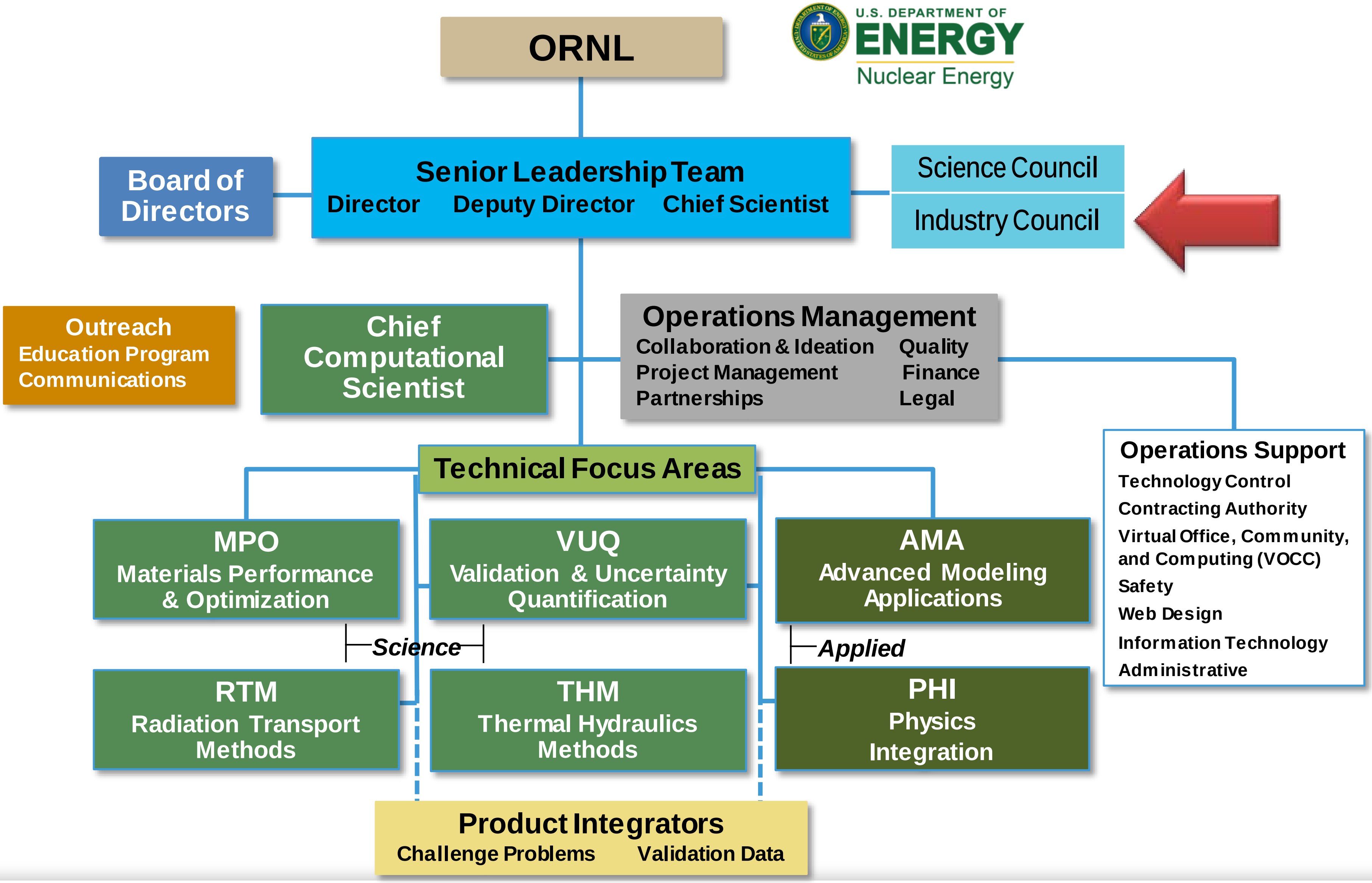
University of Michigan

Westinghouse Electric Company

Contributing Partners

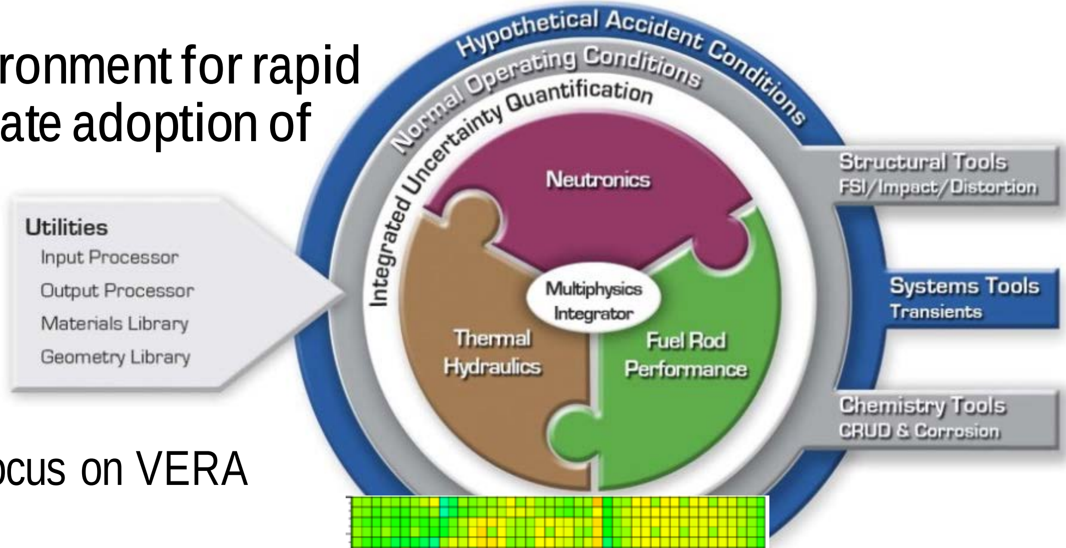
ASCOMP GmbH
CD-adapco
City College of New York
Florida State University
Imperial College London
Rensselaer Polytechnic Institute
Texas A&M University
Pennsylvania State University
University of Florida
University of Wisconsin
University of Notre Dame
Anatech Corporation
Core Physics Inc.
G S Nuclear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

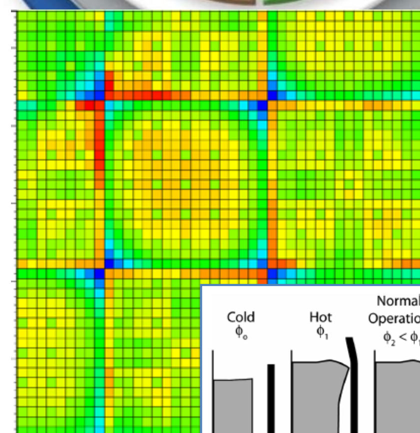
CASL Organization

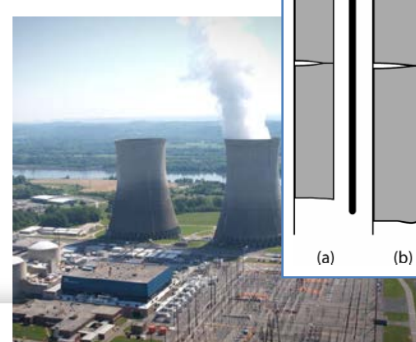


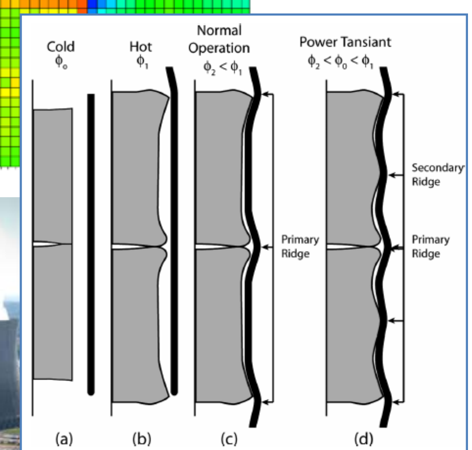
CASL Test Stands: From Plan to Execution

- 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)

2D
- *Single Lattice (20 types)*
- *Multi Lattice (Unrodded and Rodded)*
- ***Core with Reflector** (Various Reflectors)*

3D Assembly
- *Single Assembly (7 types)*
- ***Multi Assembly (Partial Rod Insertion)***

3D Core
- ***HZP Critical Boron***
- ***Rod Worth (11 Banks)***
- ***Boron Worth***
- ***ITC, DTC and MTC***
- ***MSHIM Maneuver Bank Configuration***

Westinghouse

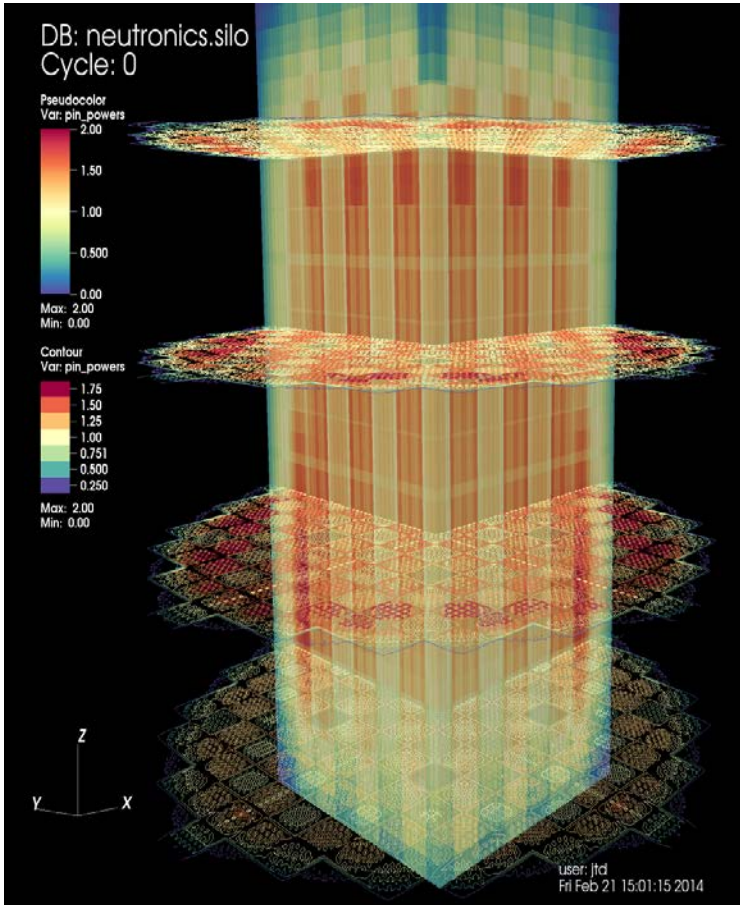
CASL

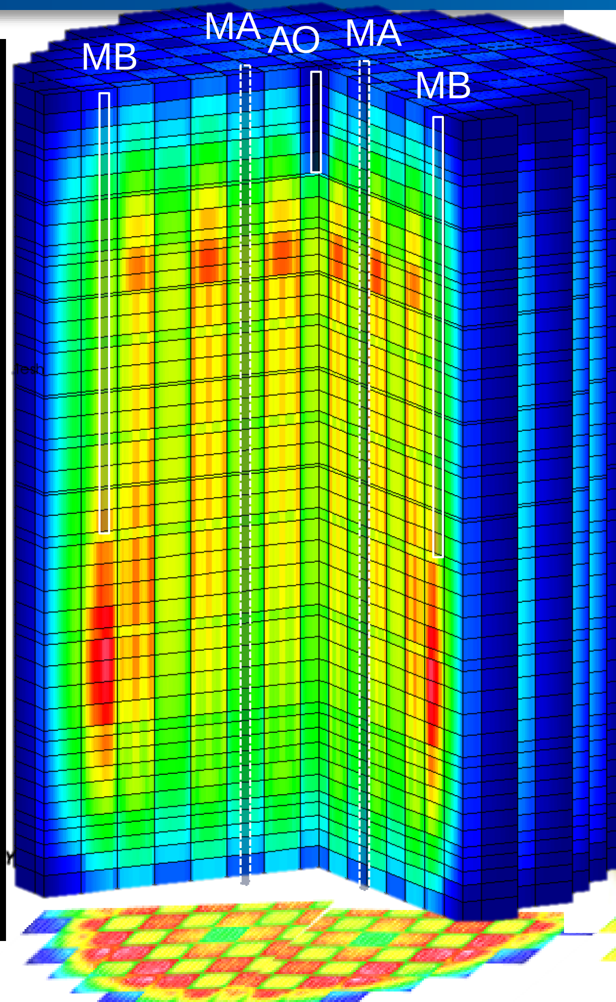
3D Core Power Distribution

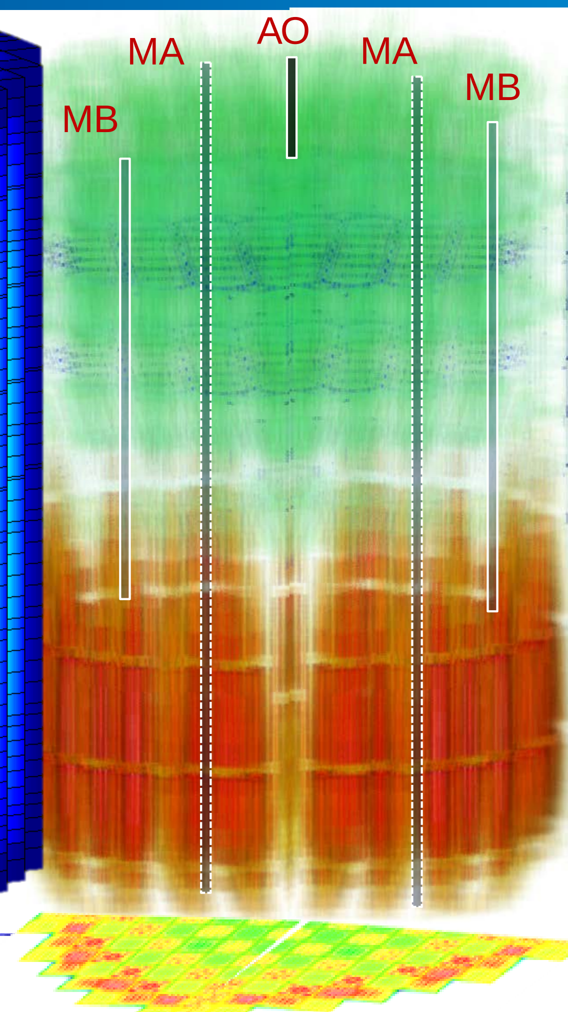
(AO and M-Banks Inserted)

3D Core ΔPower

100x(VERA-SHIFT)







Δk-eff = -81 +/- 2 pcm Hot Spot ΔP = 1% ΔAO = -0.9%

RMS ΔP = 1.2% Max ΔP = 5.9%

Westinghouse

CASL

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

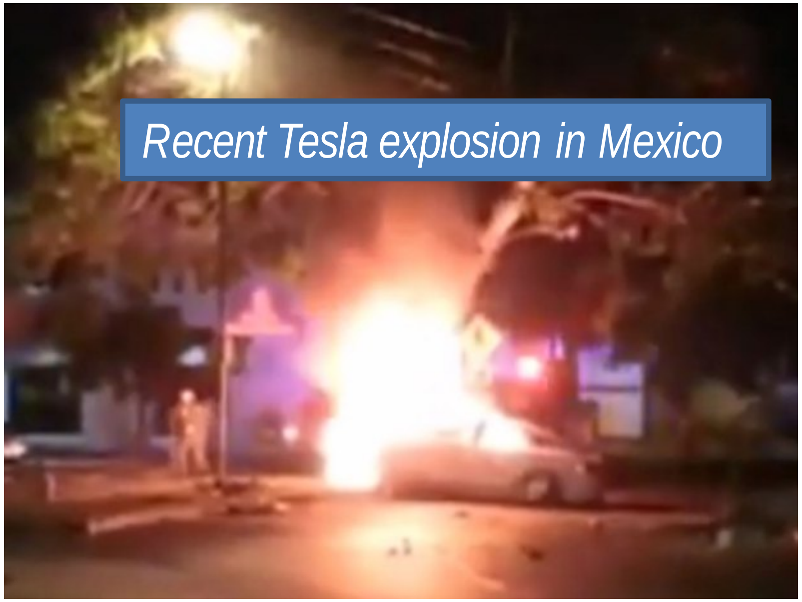
- Relevant and engaging application of VERA to an advanced PWR first-core
- Very positive and useful experience
- Enhances confidence in first-core start-up prediction

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

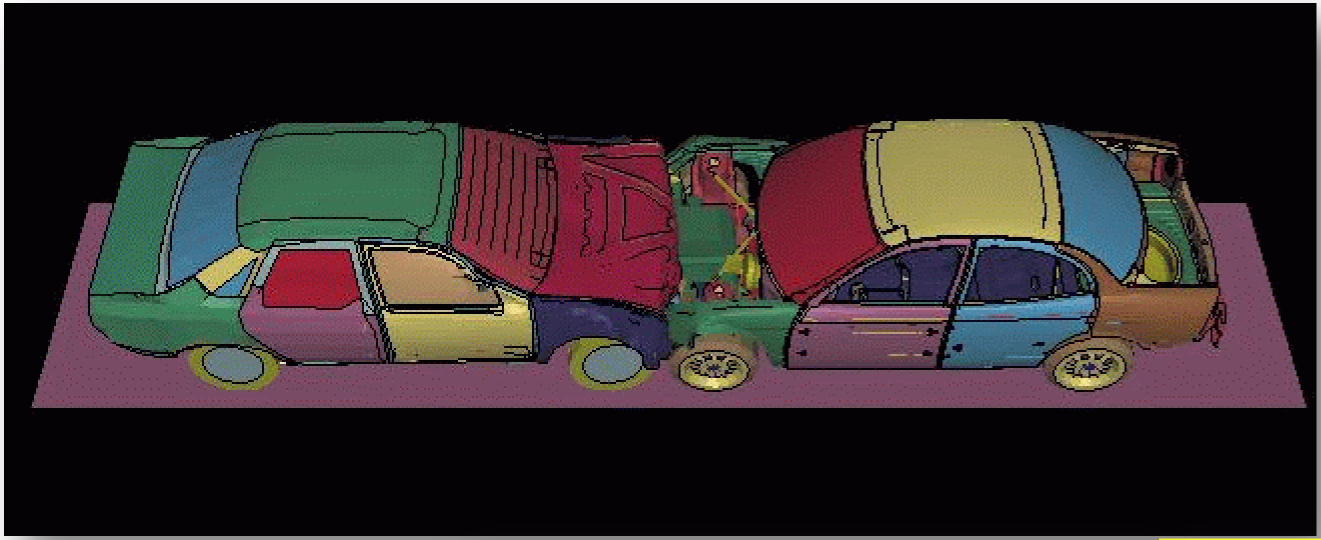


Recent Tesla explosion in Mexico

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

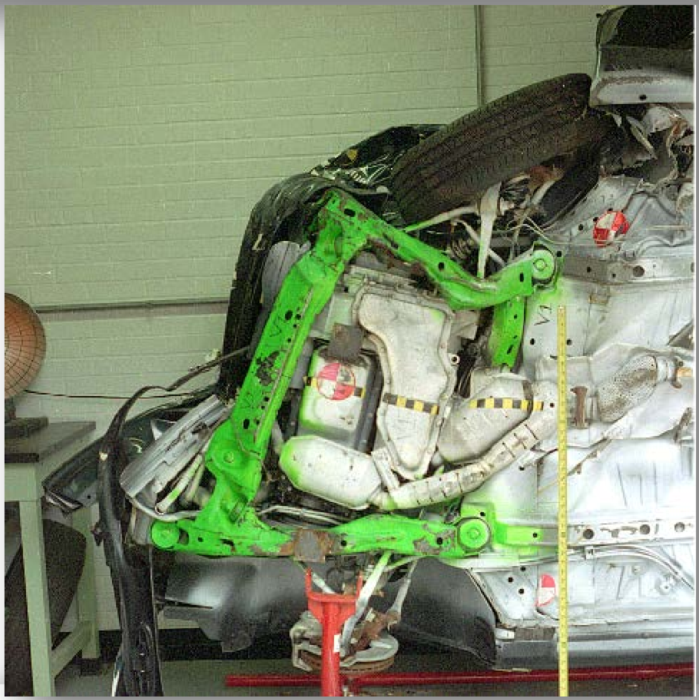
Goal is full virtual crash simulation.

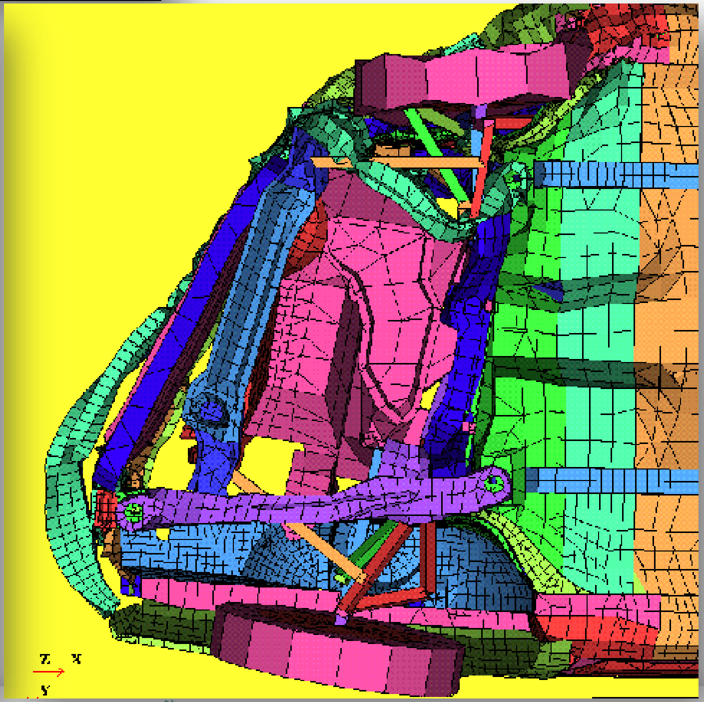
Vehicle crash simulation



Design optimization includes vehicle crash compatibility performance.

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





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DOE / EERE / VT CAEBAT Program

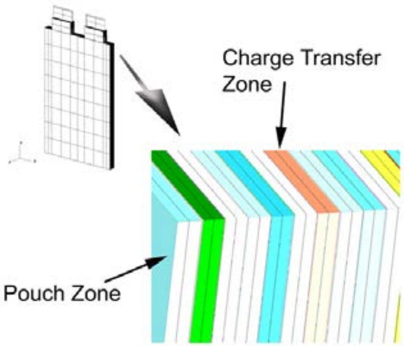
- U.S. Department of Energy (DOE)
  - Office of Energy Efficiency and Renewable Energy (EERE)
    - Vehicle Technologies (VT) Program Office
- Computer-Aided Engineering for Batteries (CAEBAT)
  - started April, 2010
  - **Goal**: Predictive battery design tools for optimizing cost, performance and life
  - 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

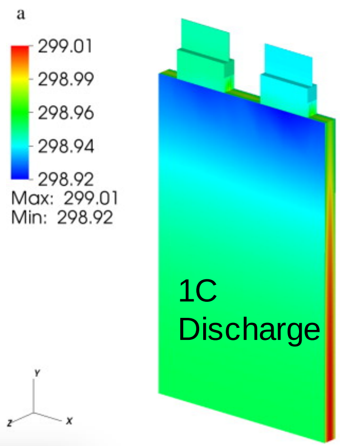
4 software suites for use in cell/pack modeling

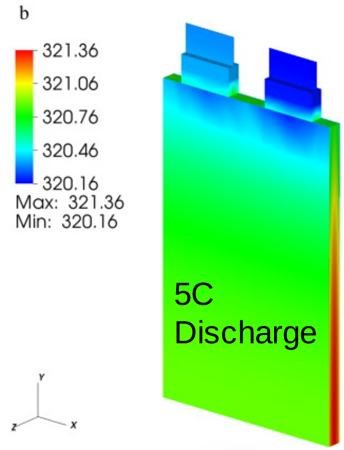
- 1 from each RFP team – may contain (or require) proprietary / commercial components
- additional tool integrates modules from RFP teams as well as Lab and University efforts beyond the RFP teams – community R&D platform - Virtual Integrated Battery Environment (VIBE)

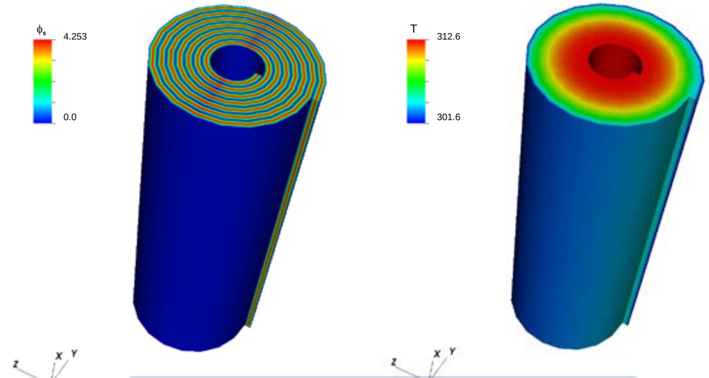
CAEBAT: Current status

Detailed 3D Modeling

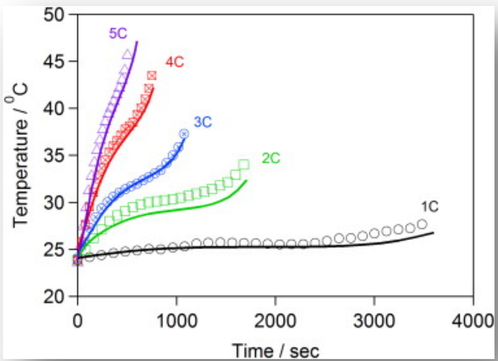




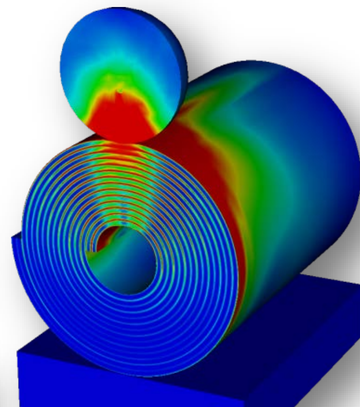




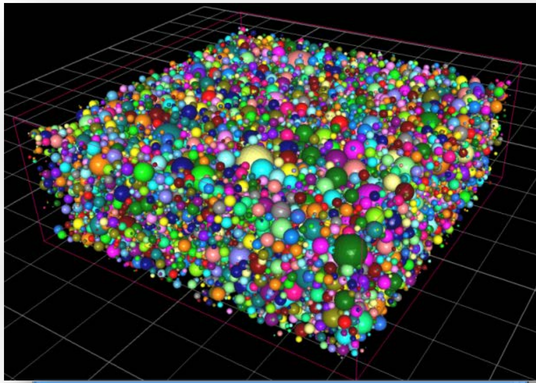
Cylindrical Cell with Resolved Current Collectors (Electrochemical – Thermal - Electrical)



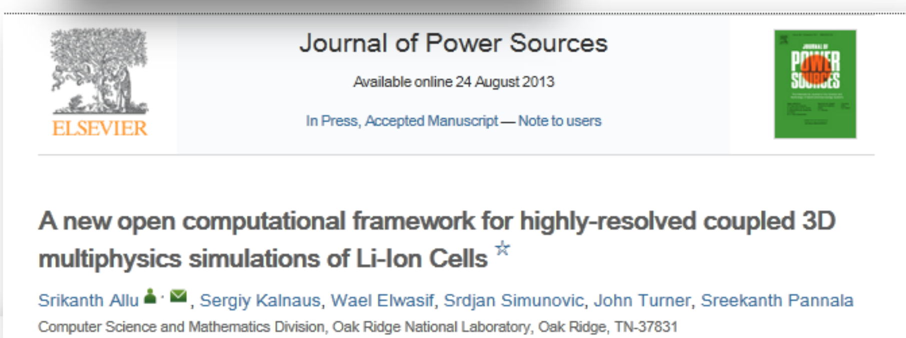
Discharge Curves (Validation with IR Imaging)



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



ELSEVIER
Journal of Power Sources
Available online 24 August 2013
In Press, Accepted Manuscript — Note to users

A new open computational framework for highly-resolved coupled 3D multiphysics simulations of Li-Ion Cells ☆

Srikanth Allu, Sergiy Kalnaus, Wael Elwasif, Srdjan Simunovic, John Turner, Sreekanth Pannala
Computer Science and Mathematics Division, Oak Ridge National Laboratory, Oak Ridge, TN-37831

Industry interactions and impacts

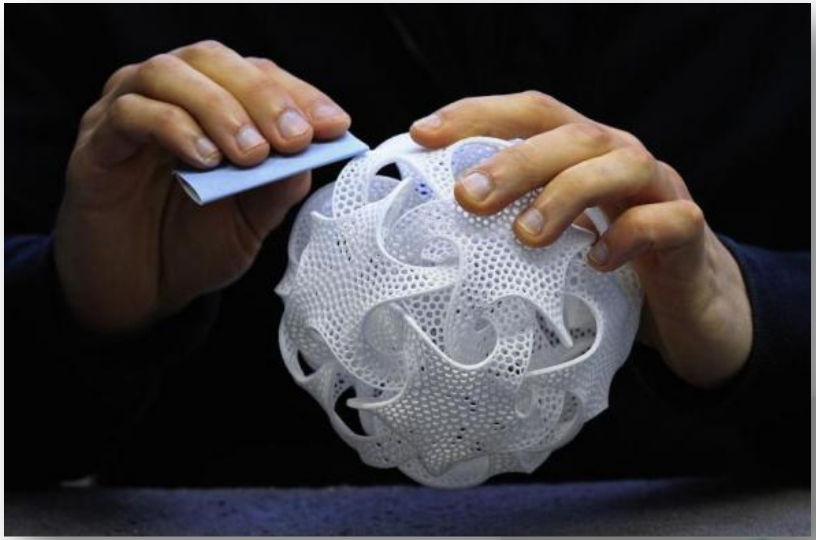
- Working closely with three industrial partners on input standardization and coupling
  - BatML v11 - XML schema, defines battery components from electrode to packs
  - battery “state” standard that encapsulates information for transfer between components for cell simulation
- Input translators to and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



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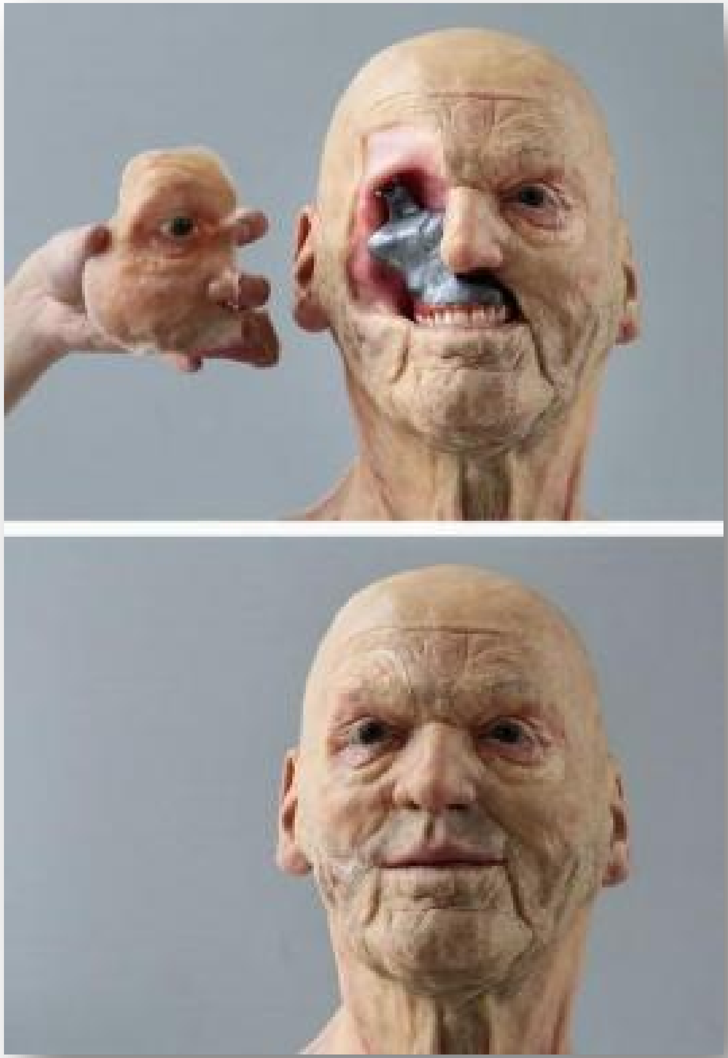
But also serious applications...



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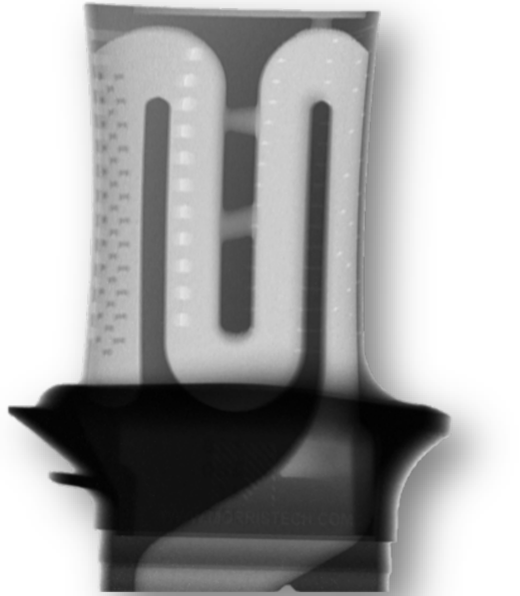
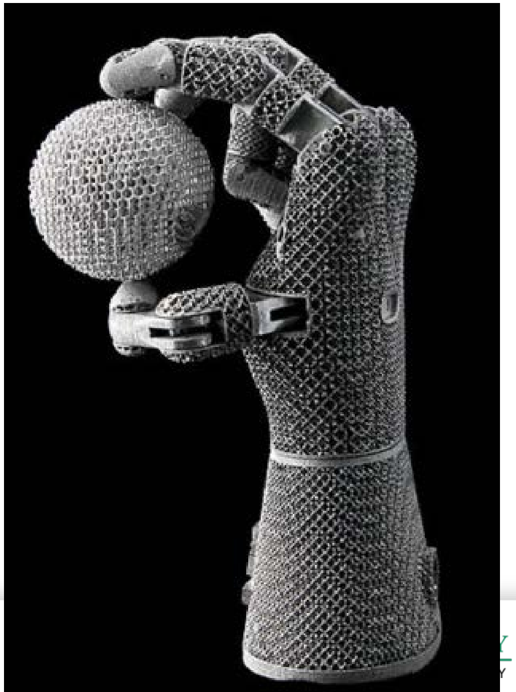
Advantages and Limitations

- 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



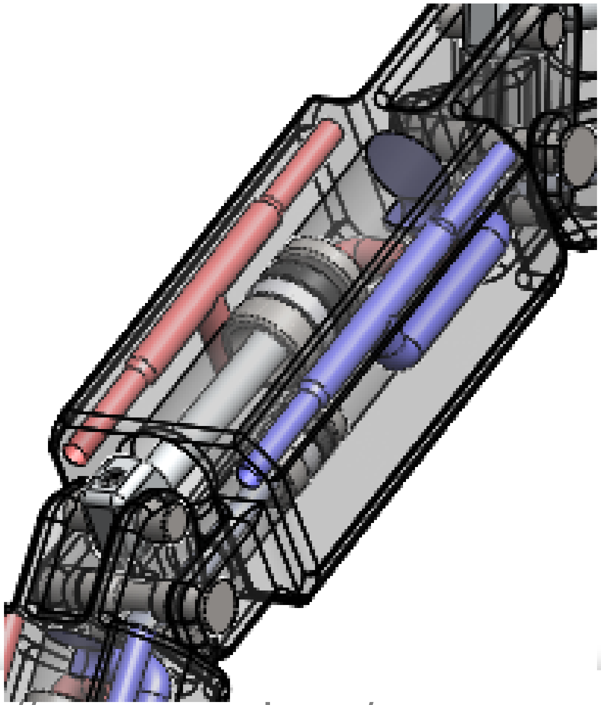
Turbine blade design with complex internal structures



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

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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.

CAD TO METAL®
Arcam AB®

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

U.S. DEPARTMENT OF ENERGY | Advanced Manufacturing

Hardin Valley Campus

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

Process Centric Developments

↓

Design Centric Developments

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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