HPC 4 MATERIALS for Severe Environments

Advancing Innovation in Industry
HPC—Mid-Stream Applications

Jeff Roberts, Director Advanced Energy Technologies

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U.S. DEPARTMENT OF ENERGY | Fossil Energy
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OAK RIDGE National Laboratory
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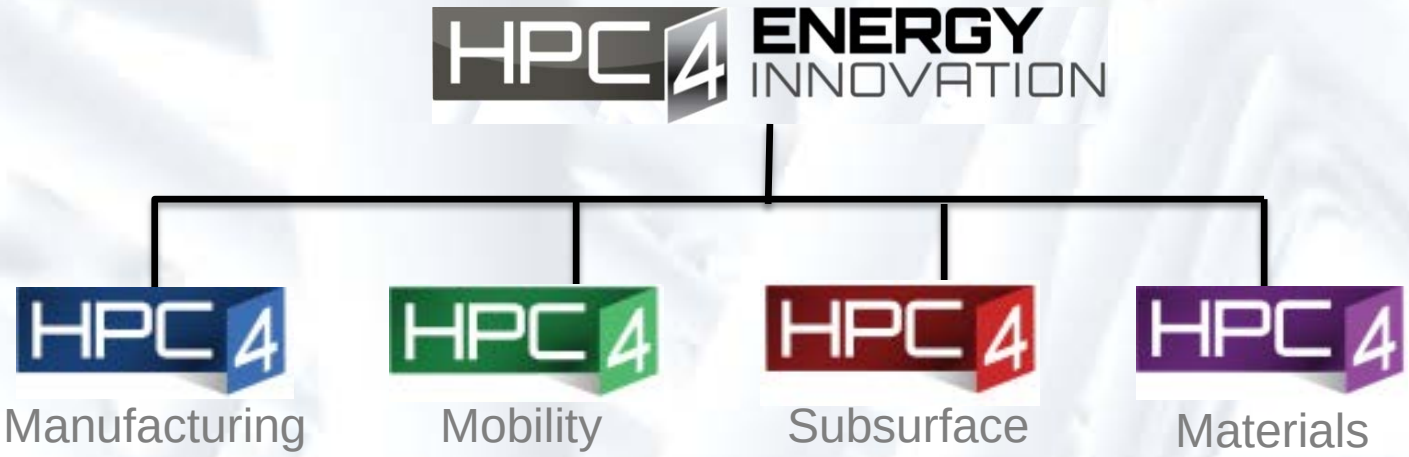
Los Alamos NATIONAL LABORATORY

LLNL-PRES-746208

The HPC4Materials Program is part of a larger program



Each aims to apply high performance computing to private sector challenges.
All DOE Labs are eligible to participate.

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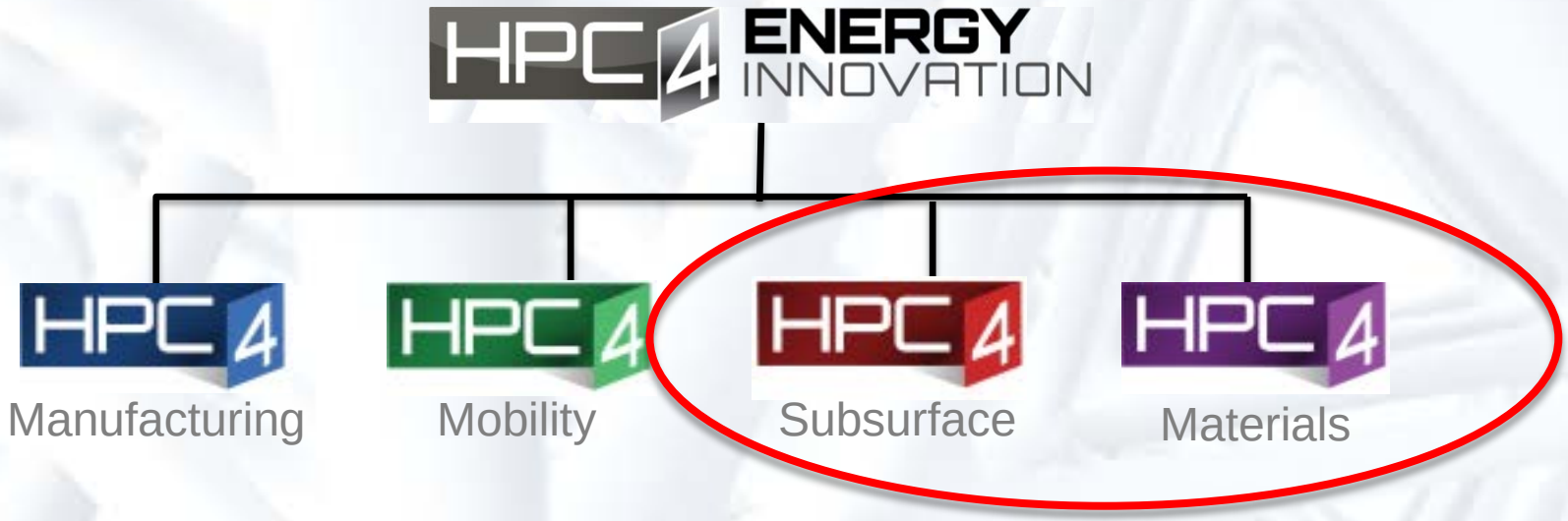
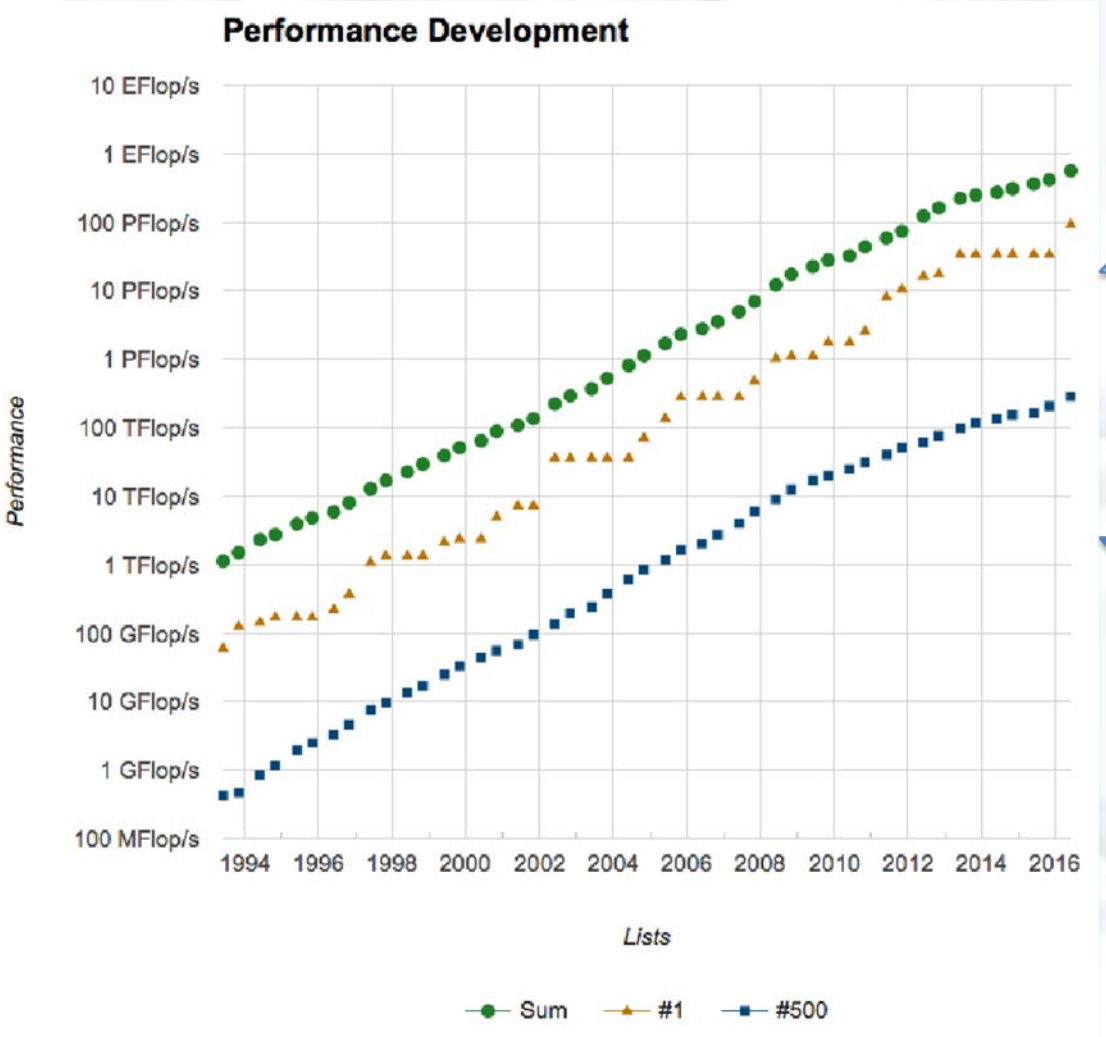
Today we'll focus on Mid-stream needs, and solutions—your hardest problems are welcome!



We aim to leverage the vast HPC capabilities at the national labs to partner with industry and address critical challenges

- DOE labs possess 5 of the top 12 HPC systems worldwide and broad expertise in their application: 2 of top 3 in Graph500
- Some larger companies use HPC, but struggle to stay current – few small to medium companies use HPC
- Challenges exist to Industry / National Lab partnerships

This program introduces the power of HPC at low risk to industry.



Benefits of HPC to Industry

- Accelerate innovation
- Lower energy costs
- Environmental benefits
- Reduce testing cycles
- Reduce waste/reduce rejected parts
- Quality processes and Pre-qualify
- Optimize design
- Shorten the time to market

These all enhance economic competitiveness

The DOE/International Data Corp. report on HPC: New results indicate high ROI returns resulting from investments in HPC.

On average, from 329 case studies:

$673 in revenue per dollar of HPC invested

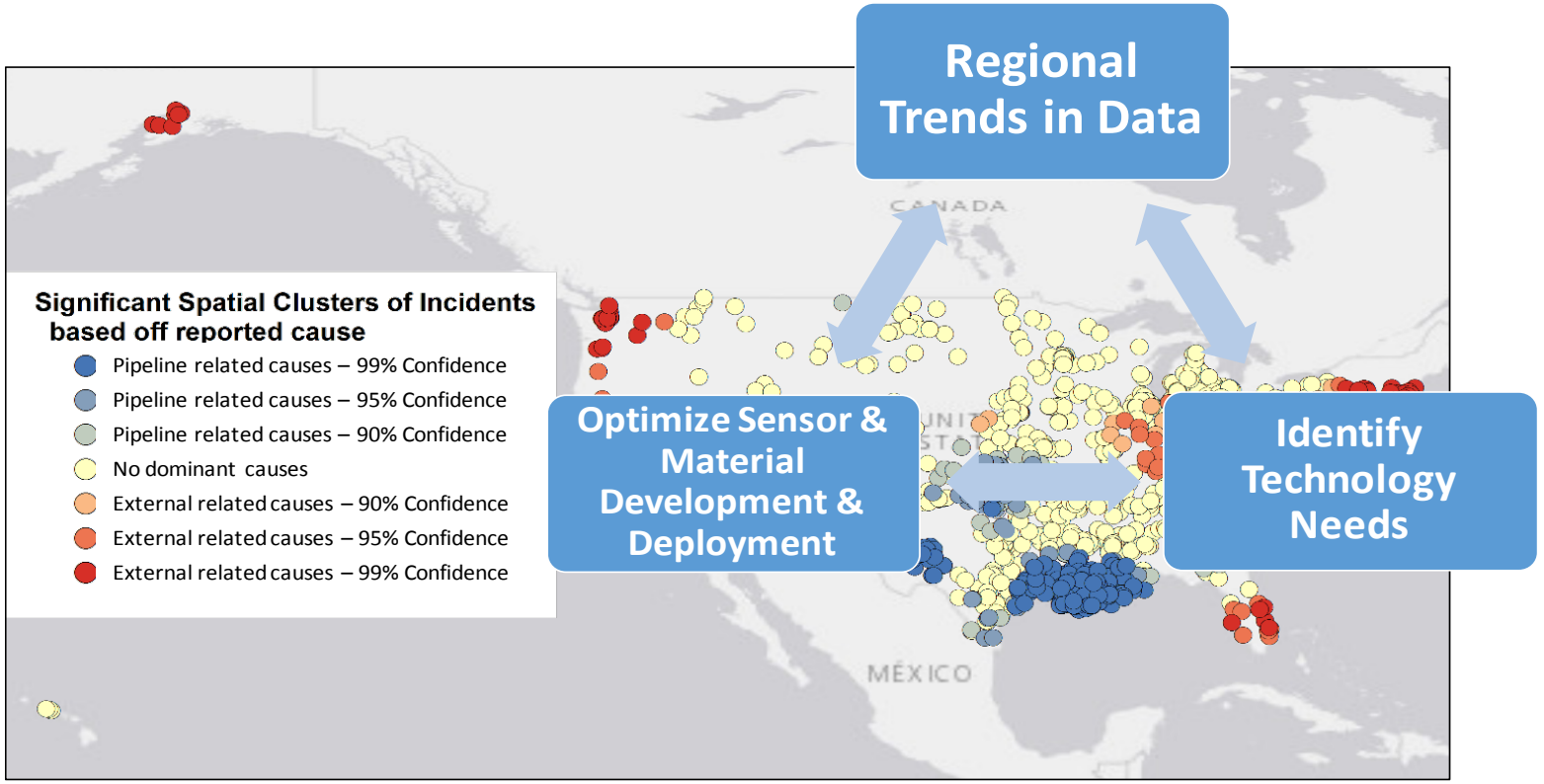
$44 of profits/cost savings per dollar of HPC invested

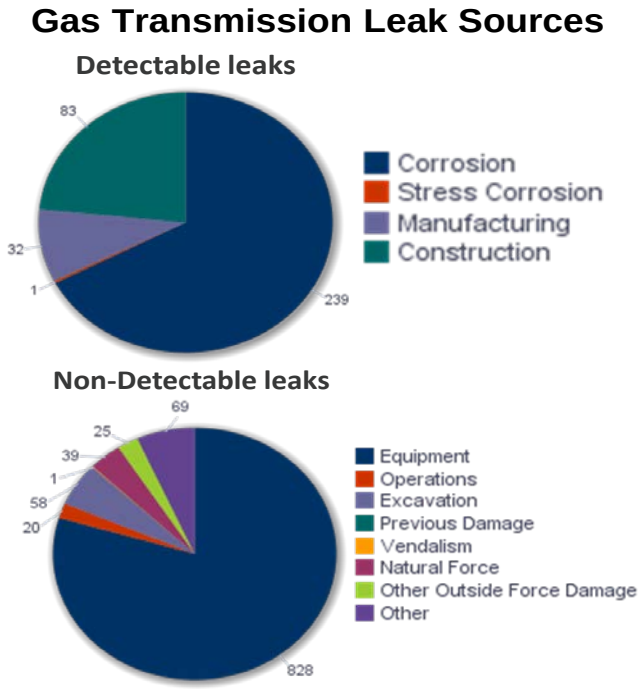
2016 update: http://www.hpcuserforum.com/ROI

Data Analytics, Sensors & Materials Technology

NATIONAL ENERGY TECHNOLOGY LABORATORY

Goal = Optimized Sensor Selection and Placement





Analytics Methodologies can Be Developed and Applied in Parallel with New Sensor and Materials Research and Development Efforts to Impact Infrastructure Risks and Resiliency.

Credit: Paul Ohodnicki

The HPC4Materials Program partners the national labs and the manufacturing industry

- Demonstration projects: HPC impact demonstration
  - AMO funds < $300k to laboratories
  - Industry funds at least 20% in-kind support w/ optional cash contribution
  - Project duration < 1 year
- Multiple follow-on opportunities
- Build HPC community
  - Industry Day
  - Student intern and professor programs

Lori Diachin,
Director
HPC4Materials

HPC4EnergyInnovation is an ecosystem to support HPC industry adoption

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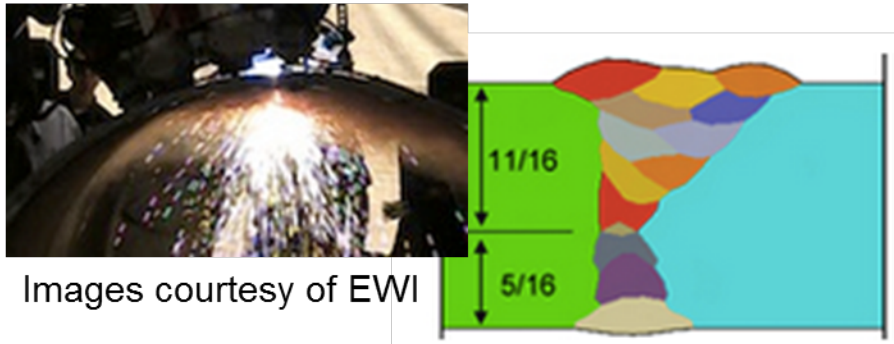
Vacuum Process Engineering—SNL. **Extend Mechanical Lifetime Performance of Compact Microchannel Heat Exchangers (MCHEs)**

Weld Predictor Tool

Goal: Develop an improved online welding software modeling application using advanced 3D models, more material hardening laws, and open source parallel codes

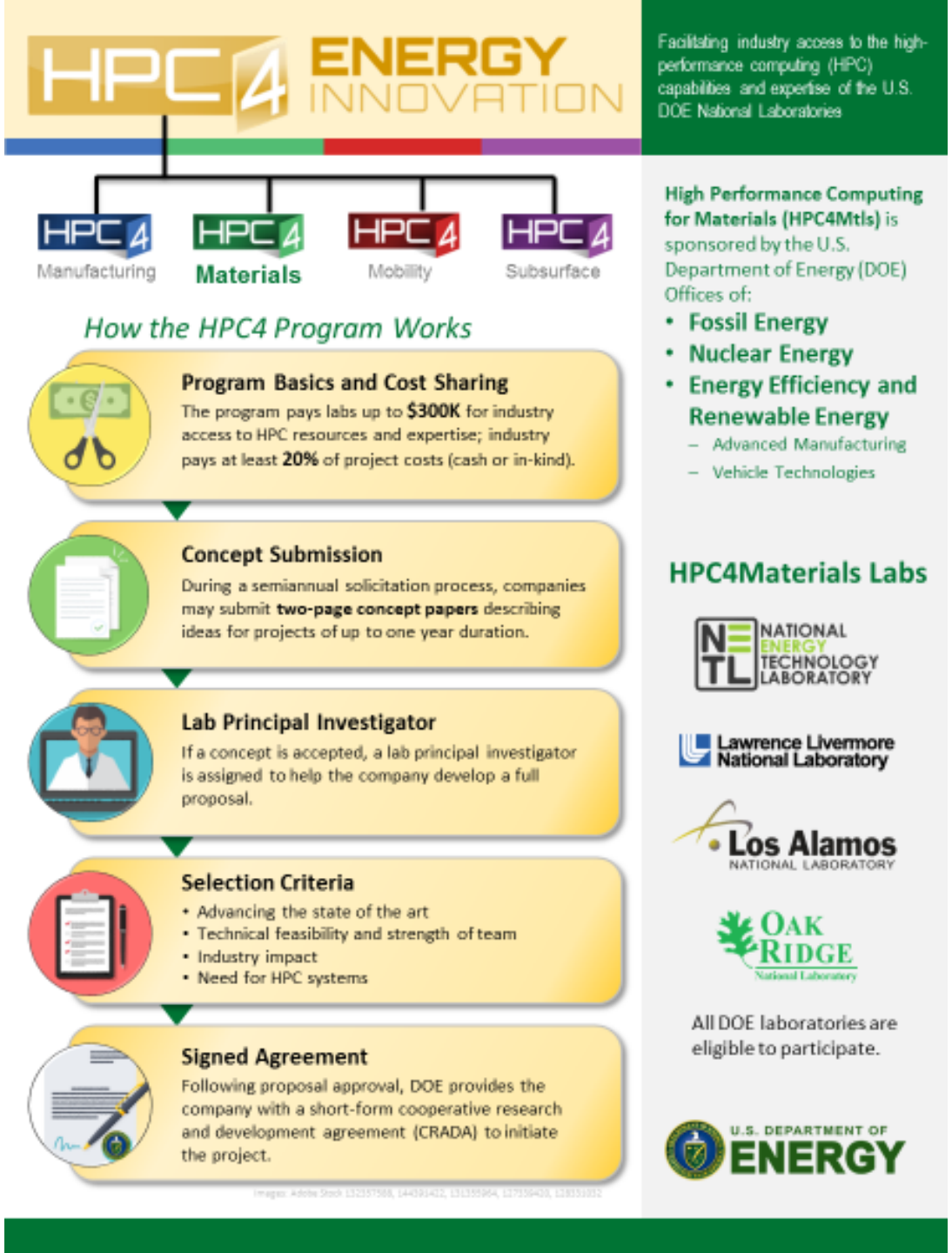


Images courtesy of EWI

Results to date: Developed new front end interface and automated meshing tools; working on new parallel simulation tools for thermal analysis, microstructure prediction, and mechanical analysis

Team: Edison Welding Institute with ORNL/OSU

ARCONIC—ORNL &LLNL. **Multiscale Modeling of Microstructure Evolution During Rapid Solidification for Additive Manufacturing**



- First solicitation expected March 1st, 2018
- Webinars and FAQ
- Email list and website: https://hpc4mtls.llnl.gov/
- Questions: Jeff Roberts; jjr@llnl.gov
- Other topics?

- Advanced sensor networks
- Data Analytics
- Machine Learning
- New alloys
- New, advanced coatings

- ??

HPC4Materials First Solicitation Topics of Interest

Topics of particular interest to FE in this solicitation include:

- predicting material behavior in specific severe environments, such as high temperature or corrosive environments, found in fossil fuel power plants
- the kinetics of materials behavioral degradation,
- improved performance of alloys, e.g., ferritic alloys by 50° C
- overcoming the barriers to the scale up of new material production from grams to kilograms, and from kilograms to tonnes
- better understanding of detailed processes in critical focus areas such as oxidation, corrosion, electrochemical interactions,
- overcoming barriers to the manufacture of components with High Entropy Alloys (HEA), and
- modeling and simulation tools that will reduce the time to qualification and certification of materials, e,g., ASME code materials.

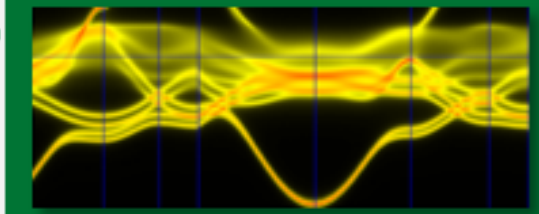
Discussion

HPC4 MATERIALS for Severe Environments

Accelerating industry discovery, design, and development of materials for severe environments through access to computational capabilities and expertise in the DOE laboratories

Challenges

- Discover or design new or improved materials and structures
- Predict material behavior in specific severe environments
- Scale up material from grams to kilograms
- Better understand detailed processes in critical focus areas
  - Oxidation, corrosion, other electrochemical interactions
  - Matter-matter, mater-energy, and matter-plasma interactions, including irradiation damage
  - Behavior under multiple fields (e.g., temperature, stress)



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Discussion


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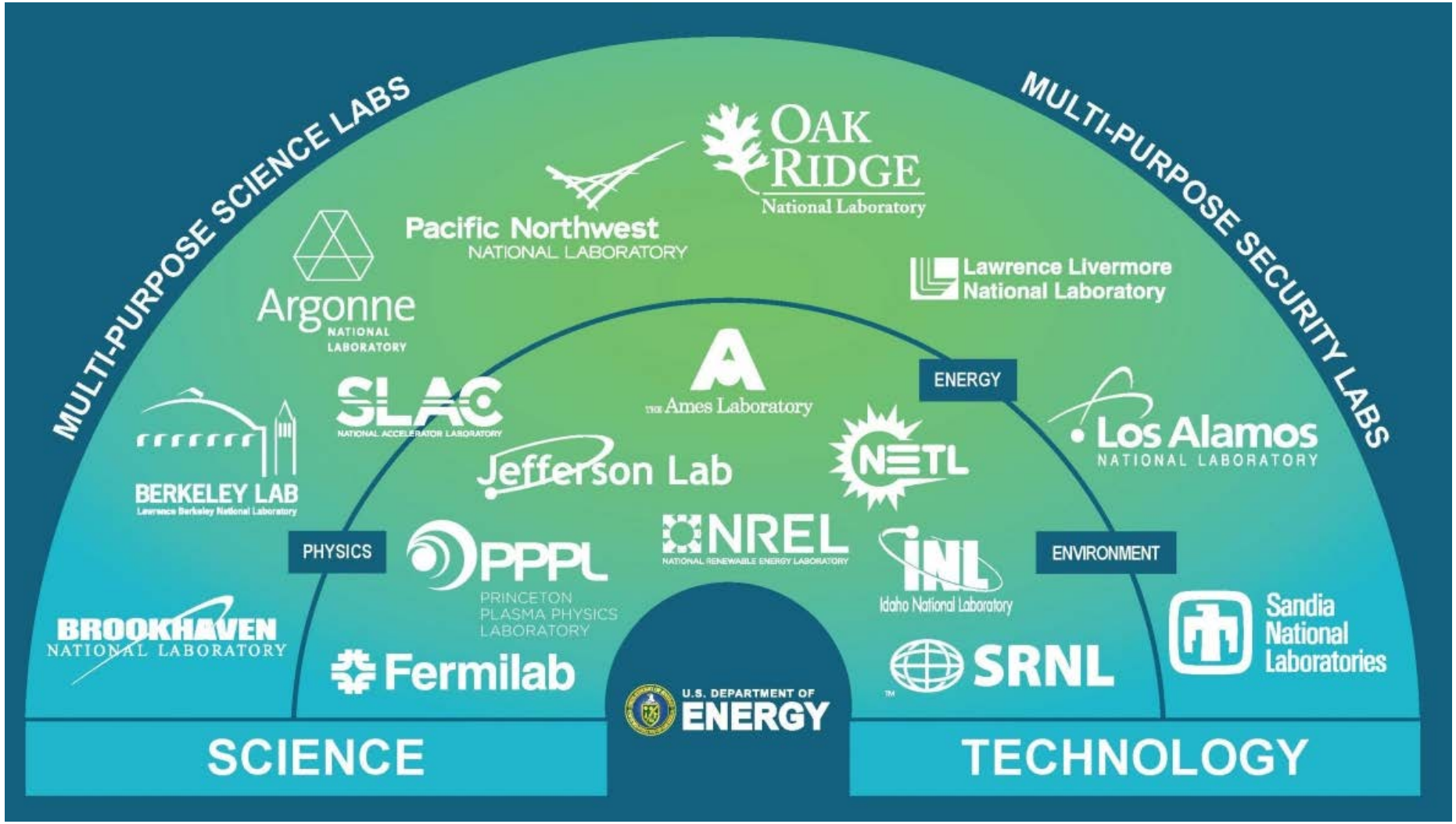
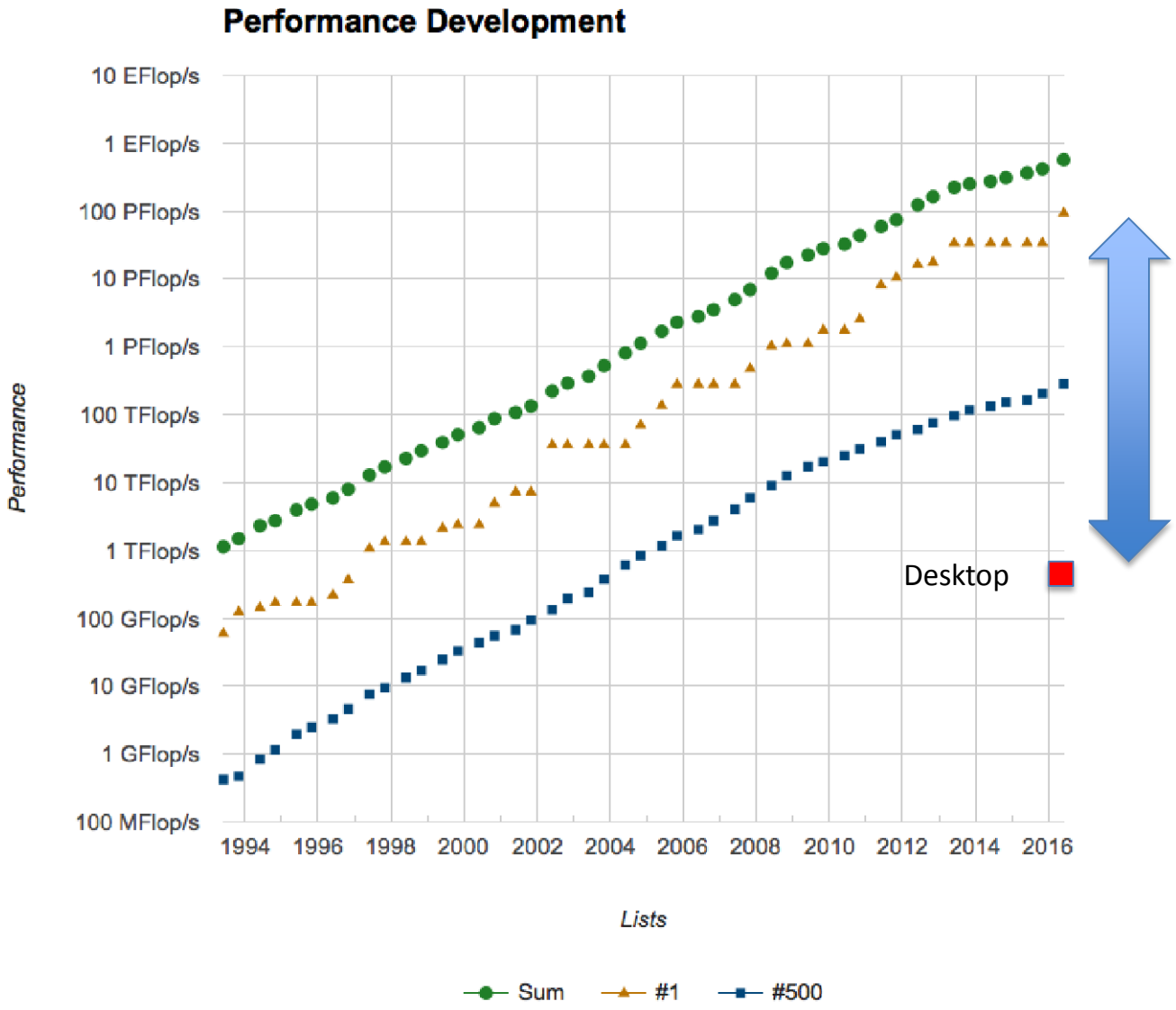
Overview of Lab Capabilities, Expertise & Hardware

David Skinner, Lawrence Berkeley National Laboratory



High performance computing offers an opportunity



Current supercomputers are **5+ orders of magnitude** more powerful than desktop computing

Can we apply this capability to industrial problems?

Summary

HPC is expanding from the realm of scientific discovery (the lab) to the factory, power plant & shop floor.

HPC models of energy systems can reveal cost savings & deliver confidence in design changes.

HPC is not just simulation. HPC data analytics, e.g. from sensor networks can inform operation of energy systems.

Above: Lowering the risk of HPC adoption in industry.
Below: NERSC's Cori system advances time-to-solution.

The HPC "app store" is growing: materials genomics, turbines, furnaces, metals, PV, batteries, & SUBSURFACE!

HPC software used in discovery science can be re-purposed to solve applied problems. Open source.

HPC algorithms deliver game changing speed-ups. Can change how we think about models. Digital twins, e.g.

VG courtesy David Skinner, LBNL

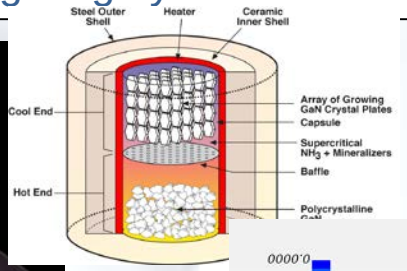
The Program has had significant engagement from a diverse industry through 3 solicitations

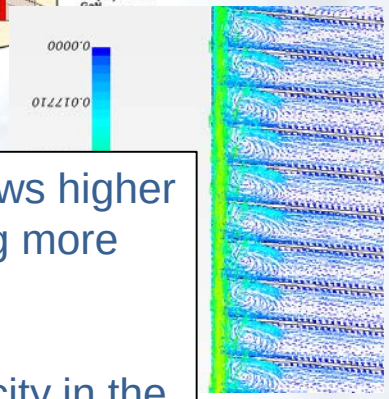
- **Diverse technical portfolio**
  - Executing on 40 projects with 26 industry partners and 6 labs
  - Offices: Advanced Manufacturing, Vehicles Technology, Fossil Energy, Office of Science
- **Fall 2016 Solicitation recently concluded**
- **2017 Solicitation underway**
- **Key benefit** is a direct link to SMEs at each lab—knowledgeable POCs who direct companies to the right group and guide the statement of work.

HPC has been used to design better processes in a variety of industries

More efficient LED lightbulb

Goal: Model ammono-thermal crystal growth of GaN to scale up the process; reduce production costs of LED lighting by 20%



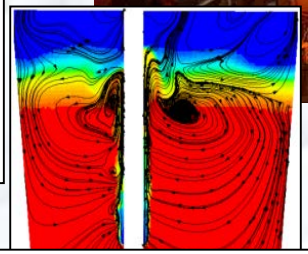


Results to date: HPC allows higher fidelity simulations showing more complicated flow structure, improved predictions of temperature and flow velocity in the reactor; now optimizing uniform growth of crystals

Team: SORAA with LLNL

Reducing Coke Usage in Steel

Goal: Use models of complex reacting flows HPC to optimize blast furnace processes to reduce carbon loads and coke usage; savings up to $80M/yr if successful



Results to date: 1000X improvement in computational speed of parametric studies to examine factors such as CO2 enrichment, wind rate. Scaling code up to 2000 cores

Team: Purdue Calumet with LLNL

Bridging the gap between U.S. Manufacturers and national labs with public-private partnerships

FEDBIZOPPS.GOV Federal Business Opportunities

Engage industry

Industry submits challenges

Match challenge to PI

AMO approval; Feedback to industry

Sign agreements

Inform industry

Concept paper → Full proposal → Award

Technical Review Committee

Technical Merit Review Committee

- Partner labs and AMO representatives
- Heavy focus on **nation-wide** impact to energy efficiency and clean energy technology industry-wide

Execution streamlined through the required use of the DOE short form—An easy way for industry to engage the national lab's HPC expertise at low risk.

CRADA, IP issues and other “best” practices

- Streamlined agreements.
- Industry cost-share.
- Standard IP position: pre-existing kept by company and labs.
  - Proprietary information protected.
  - Reporting requirements.
  - New IP—who invents it ‘owns’ it (can be joint); BUT, company has the right to an exclusive license
- Commercialization desired.
- Early interaction creates best concept papers and proposals. Outreach is key.
- Small- to medium-sized companies might benefit the most, but have the least HPC knowledge and National Lab contacts.

Questions?

Additional information at HPC4Mfg.org

Questions can be sent to HPC4Mfg@llnl.gov

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