An Introduction to the HPC4Materials in Severe Environments Program

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Today’s Agenda

2:30-2:40 EDT Welcome and webinar instructions
2:40 – 2:50 EDT Overview of program Needs
2:50-3:20 EDT  Overview of program including DOE resources and steps to writing a good proposal
3:20 – 4:00   EDT Q&A

Participant instructions

- Please turn off video and mute your phone
- Questions will be answered at the end of the briefing
  - Send to "Everyone" via Chat
The HPC4Mtls program is designed to enable a step change in the cost, development time, and performance of materials in severe environments through high performance computing.

- Longer lasting components in difficult environments, e.g., high temperature turbines and nuclear cores
- Lower cost, more reactive catalysts
- Coatings to improve thermal and environmental barriers
- Materials for supercritical CO2 power cycles, chemical looping combustion
- New alloys—lightweight materials
High performance computing is...

...leveraging “supercomputers” to advance our study of that which is otherwise too big (e.g., stars and galaxies), too small (e.g., atomic to nano-scale), too fast (e.g., nuclear fusion), too slow (e.g., cosmology), too dangerous/expensive (e.g., destructive testing)
Applied high performance computing includes…

- **Discovery**
  - Using a supercomputer to explore new material possibilities

- **Model Reduction**
  - Using a supercomputer to create/validate a reduced-order model

- **Concurrent System/Device/Plant Simulation**
  - Using a supercomputer in real time on the shop floor

- **Post-design and operational optimization**
  - Using a supercomputer in energy systems optimization
The benefits of HPC to industry can be extraordinarily high

- 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

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


These all enhance economic competitiveness!
The HPC4Mtls program will lower the barriers to bringing the power of HPC to this community at low risk

- **Industry Status:**
  - Some larger companies use HPC, but struggle to stay current
  - Few small to medium companies use HPC

- **DOE Status:**
  - DOE labs possess 5 of the top 10 HPC systems worldwide; 2 of top 4 in Graph500
  - Broad expertise in the application HPC
  - Can be a challenge for industry to understand the best way to partner with DOE

**HPC4Mtls will create partnerships that leverage DOE lab expertise and compute resources to address critical problems in the manufacturing sector**
The HPC4Mtls program will build an ecosystem to support HPC adoption by industry

- Showing what is possible with HPC through **demonstration projects**
  - DOE program office funds < $300k to laboratories (like a voucher program)
  - Industry funds at least 20% in-kind support w/ optional cash contribution
  - Project duration < 1 year

- Encouraging the adoption of HPC through **capability projects**
  - Execution mechanisms and funding source varies
  - Larger cash share from industry expected
  - Project duration: multiple year

- Building the HPC4Mtls community
  - Student intern programs
  - Workshops
The HPC4Mtls program is governed by a consortium of partner laboratories

- Partner laboratories:
  - Technical review committee participation
  - Compute cycle providers
  - Governance policy determination
- All DOE national laboratories are eligible to be project participants
Our unique approach for building teams in the solicitation process helps ensure each project is successful.

**Engage industry**

Industry submits challenges

**Match challenge to PI**

DOE approval; Feedback to industry

**Sign agreements**

**Inform industry**

Concept paper ➔ Full proposal ➔ Award

Technical Review Committee

**Technical Merit Review Committee**

- Partner labs and DOE representatives
- *Topical focus areas determined in part by this workshop!*

Execution streamlined through the required use of the DOE short form.
The related HPC4Mfg program has been extremely successful using this model

- $>13M technical portfolio
  - Executing on 41 projects with 33 industry partners and 6 labs
  - 40 demonstration; 1 capability
  - Seedling project funded by Office of Transportation

- Spring 2017 Solicitation currently underway
  - $3M available
  - Initial foray into HPC4Mtls research areas
  - Other DOE offices informally involved
Industry is interested in simulations at many levels

- New alloy design: **Alcoa, Arconic**
- Junction design: **Samsung**
- Membrane design for dehumidification air-conditioning: **7AC Technologies**
- Catalyst design for lignin denature: **Agenda 2020 (paper manufacture consortium)**
- Microstructure for additive manufacture, casting, welding: **GE, Eaton, UTRC, GM, Arconic**
- Predict stress-strain curves for ne material: **LIFT (light-weighting consortium)**
- Engine/turbine tolerancing: **Ford, GE**
- Turbine CFD: **GE, Rolls Royce**
- Semiconductor deposition: **Applied Materials, SORAA**
Early success stories from HPC4Mfg demonstration projects

- GE: larger, higher fidelity turbine design
- ZoomEssence: new food particle dryer configuration
- Vitro Glass: real time control of glass furnace using deep-learning
- P&G: faster modeling of paper towel process
Modeling and simulation tools are needed at all steps of additive manufacturing process flow.

- GE
- Applied Materials
- UTRC
- Eaton
- UTRC
- GE
The current status of the HPC4Mtls program

- Fourth HPC4Mfg solicitation contained a new ‘materials in severe environments’ topical area
  - 15 proposals deemed appropriate for review in this category
  - 5 full proposals requested
  - Reviewed on Oct 26; expect 2-3 to be funded by Office of Fossil Energy
- Program officially announced on September 19 by DOE Secretary Perry
- Kickoff workshop held Oct 12, 2017 in Pittsburgh, sponsored by Fossil Energy, EERE, and Office of Nuclear Energy
  - Discussed program guidelines, DOE national lab capabilities, panels by industry, posters from the HPC4Mfg program and national lab capabilities, sponsor presentations
  - About 80 attendees from government, labs, industry and academia
- Solicitation expected in January 2018
The first solicitation will likely focus on...

- Behavior of materials in severe environments
- Scale up of materials from grams to kilograms
- Detailed processes such as oxidation, corrosion, matter-matter interaction, irradiation damage, etc.
- Lightweight materials
- Others: TBD Your input welcome!
Overview DOE National Laboratory Resources
Resources available to you at the DOE National Laboratories
All good projects will be a function of the systems that are available, the expertise, and the application codes used

- **Systems**
  - HPC systems are the computing machines that can drive your science faster.
  - More on these in the next slide. Systems come and go every 3-5 years.

- **Experts**
  - People who scale algorithms, software, and workflows to run on HPC systems.
  - Many are focused on CS and basic science, but applications are interesting.

- **Apps**
  - HPC apps are the software which must exist already or be newly developed to enable a project. Running on XYZ code on HPC is not free.
  - New app development requires real investment. Leverage prior art.
The HPC systems at the four principal laboratories are diverse

<table>
<thead>
<tr>
<th>System: Joule, 24,192 Cores, 9 Petabytes of storage, Quad Data Infiniband, 76 TB memory</th>
<th>Capabilities: Fluid Dynamics, Materials, Chemistry, MFIX.</th>
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</thead>
<tbody>
<tr>
<td>System: Titan, Cray XK7, 18K nodes, 300K CPUs, 18K GPUs,</td>
<td>Capabilities: Computational Biology, Chemistry, Engineering, Earth, Energy, GIS, Technology and Materials.</td>
</tr>
<tr>
<td>System: Vulcan, 24K nodes Power7IBM 1.6 GHz, 393,216 compute cores, 400 TB compute memory</td>
<td>Capabilities: Scaling vendor codes to run on HPC platforms, Expanding software capabilities, algorithm development and multi-physics integration.</td>
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<tr>
<td>System: Trinity, Cray XC30, 19K nodes, Intel Haswell and Intel KNL, 2PB DRAM, unique NVRAM capabilities.</td>
<td>Capabilities: In situ, dynamic measurements, simultaneous imaging and modeling of well-controlled and characterized materials advanced synthesis and characterization in extreme environments.</td>
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Above are HPC4Materials Principals. All DOE Labs are eligible.
Expertise in HPC computing is a critical part of each partnership

- Applied mathematicians capable of delivering new algorithms in areas of interest
- Data scientists capable of analyzing very large amounts of data to understand and improve your processes
- HPC engineers and technicians who can executing your HPC agenda
- Engineers and application scientists with established track records of developing and using HPC solutions in a wide variety of fields
- Established mechanisms for postdoc, visiting faculty and entrepreneur-in-residence programs
- An R&D community concerned with durable solutions in HPC software and capable of leveraging computing advances between fields
Unique software capabilities have been developed that provide solutions no one else is capable of

- Software and algorithms that are cutting edge and scale to hundreds of thousands of cores allowing for high fidelity simulations
- Well-defined methods-of-scale in simulation science and data analysis. Matrix, PDE, and machine learning libraries provide and on ramp for new problems seeking massive computing
- A broad variety of scalable research application codes that can be repurposed to solve applied HPC challenge. Leverage existing HPC software by adapting it
What are the key steps in the process to writing a good proposal?
US industry eligibility and funding

- Eligibility for call
  - Companies developing and/or manufacturing new materials for severe environments in the US
  - Consortium or other organization supporting development or manufacture of new materials for severe environments in the US

- Who can be funded from the program
  - National laboratories
  - In limited amounts, US Universities, via sub-contract

- Industry participant cost share
  - At least 20% of project funding
  - Can be used to support internal staff
  - Source can not be other federal funding

Required!
The DOE Model Short Form CRADA streamlines execution of new projects

- Standard IP position: pre-existing kept by company and labs.
  - Proprietary information protected
  - Reporting requirements to DOE
  - New IP—who invents it ‘owns’ it (can be joint); BUT, company has the right to an exclusive license

- Objections to terms and conditions can be stated in concept paper; however, this could lead to delays and rejection of proposal

- Standard DOE Short Form CRADA available on the web site
  - Individual labs may have some variances
  - If concept paper is selected to go forward; the specific CRADA for your laboratory will be sent to you
Concept papers will be the first step:

- Two-pages; single spaced; 12 pt. font – Will likely be similar to the template at http://hpc4mfg.org

- Key Elements
  - **Title page**
  - **Abstract** (150 words or less) - must be non-proprietary, publishable summary
  - **Background**
    - Technical challenge to be addressed
    - State-of-the-art in materials in this area; how this program advances that; why national lab HPC resources are required; expertise of industry partners, etc.
  - **Project Plan and Objectives**
    - Technical scope of the work and how this project fits into the overall solution strategy
    - How results will be validated including availability of data;
    - Specific simulation codes that will be used if known
  - **Impact**
    - Assessment of materials in severe environments
    - Ability to scale up production of new materials
    - Specific ability to address issues such as corrosion, oxidation, irradiation, etc.

You do not need to have identified a laboratory partner up front!
Just an interesting and hard problem that HPC can help address!
Six-pages; single spaced; 12 pt. font – Will likely be similar to the template at http://hpc4mfg.org

Key Elements

• Title page
• Abstract (150 words or less) - must be non-proprietary, publishable summary
• Background
  — Similar to concept paper
• Project Plan and Objectives
  — Similar to but more detailed than concept paper with specific tasks; specific simulation codes; modifications to the software needed etc.
• Tasks, Milestones, Deliverables and schedules
  — Goals, timelines and due dates of milestones and deliverables from all partners; responsible party, communication from one partner to another
• Impact
  — Similar to concept paper but more detailed; is this transformational for an industrial sector; what is the enduring impact; how will results be disseminated
• Implementation and adoption
  — How will this be incorporated into company and industry-wide operations; follow on activities to extend this effort to solve the broader problem being addressed
• Various appendices (see next slide)
Appendices provide additional information

- Used in the review process; CRADA development process; compute resource determination, etc.

- Not included in the 6 page limit

- **Appendix A**: Project summary of tasks and schedule (similar to project tasks in main proposal, but used for CRADA development)

- **Appendix B**: Project budget: costs, amount and source for participants, cost share (in-kind or cash); how funding makes a difference relative to existing funding

- **Appendix C**: Computational resources: computational approach, performance of the codes, resources requested (platform and core hours)

- **Appendix D**: Pictures for publication

- **Appendix E**: How the work benefits the laboratory

- **Appendix F**: Resumes of key participants
Elements of a winning proposal

• Impact is key: Why should the sponsor fund this proposal? How does this proposal move the ball forward on the sponsor’s agenda?
  • National-level energy supply/savings
  • National-level competitiveness
  • Serves as an example to solve an important industry-wide problem
  • Serves of an example of key new technology implementation

• Industry partner has application domain, PI will have discipline experience. Can they work together effectively?
  • Does the industry know its domain?
  • Has they chosen a well-posed problem? (importance, scope)
  • Does the industry partner have sufficient expertise to communicate with PI and implement results?

• Working closely with PI on the full proposal is key
  • Reasonable scope for the proposed funding
  • Specific software, specific computer platforms
  • Specific – who does what
For more information on the HPC4Mtls Program

Additional information at http://HPC4Mtls.org

Questions can be sent to HPC4Mtls@llnl.gov

Join the hpc4mtls-info@llnl.gov distribution list via the web to receive program announcements

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