U.S. DEPARTMENT OF ENERGY

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SOFTWARE PRODUCTIVITY FOR EXTREME-SCALE SCIENCE WORKSHOP

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Extreme–Scale Computational Science Productivity

Extreme-Scale Science Productivity

- Extreme-scale science productivity is a measure of the effective and efficient use of all resources in extreme-scale computational science ecosystem.

Productivity Stakeholders

- Taxpayers & policymakers
- Domain scientists
- Computational scientists (Applied Math & CS)
- Computational facility operators

Extreme–Scale Computational Science Productivity- Why Now?

Looming computational science productivity crisis:

- As supercomputers *get faster and bigger, they become more difficult to use efficiently in order to exploit their full capability.*

High-Performance computing beyond Moore's Law

- From Moore's Law to multicore – unprecedented parallelism
- Hybrid architectures – multicore, many-core, GPUs, FPGA accelerators
- New concerns for *energy and massive data sets*

Trends towards more complex physics

- From single physics to *multiscale and multi-physics*
- From scientific programming to *computational science software engineering*
- *Rapidly changing machine architectures* and programming models

Extreme–Scale Computational Science Productivity –Vision & Scope

Vision:

- **Develop a framework and research agenda to *identify and remove or ameliorate productivity bottlenecks* in the extreme-scale computing ecosystem from application software development to program execution.**

Approach

Explore the challenges issues of extreme-scale system productivity in three separate workshops:

1. ***Software productivity for extreme-scale science workshop - (current workshop)***
2. **Execution-time productivity for extreme-scale systems *(workshop TBD)***
3. **Reliability and availability modeling of extreme-scale computing systems**

Current Workshop Scope

Focus on the processes, methodologies, infrastructures, human factors, and tools to develop software that has the following features:

- **Software that is easy to use, maintain, refactor, and port to rapidly changing machine architectures**
- **Software that can readily exploit the full capabilities and deal with challenges of emerging hybrid architectures (multicore, manycore, GPUs, and accelerators)**

Extreme–Scale Computational Science Productivity: Contributors

Productivity discussion contributors:

- Productivity is a cross-cut issue that demands the collaboration of experts working in related disciplines (domain scientists, applied math, computer scientists, system engineers, etc.)

- **Office of Advances Scientific Computing Research (ASCR)**
  - **Randall Laviolette** - (SciDAC & Science Partnerships)
  - **Karen Pao** - (Applied mathematics & Exascale Co-Design)
  - **Sonia Sachs** – (Computer Science)

- **Office of Biological and Environmental Science (BER)**
  - **Dorothy Koch** – Climate and Environmental Sciences
  - **David Lesmes** – Climate and Environmental Sciences

- **Office of Fusion Energy Sciences (FES)**
  - **John Mandrekas – Fusion Theory, Modeling, Simulation, and & SciDAC**

End

Q & A