



U.S. DEPARTMENT OF
ENERGY

Office of Science

Mini-Symposium on Scientific Software Engineering

**Office of Advanced Scientific
Computing Research (ASCR)**

POC: Thomas Ndousse-Fetter

**Office of Biological and Environmental
Research (BER)**

POC: David Lesmes

Software Productivity

Application software development at extreme-scale: challenges and opportunities

- ***“While computer performance has improved dramatically, real productivity in terms of the science accomplished with these ever-faster machines has not kept pace. Indeed, scientists are finding it increasingly costly and time consuming to write, port, or rewrite their software to take advantage of the new hardware.”***

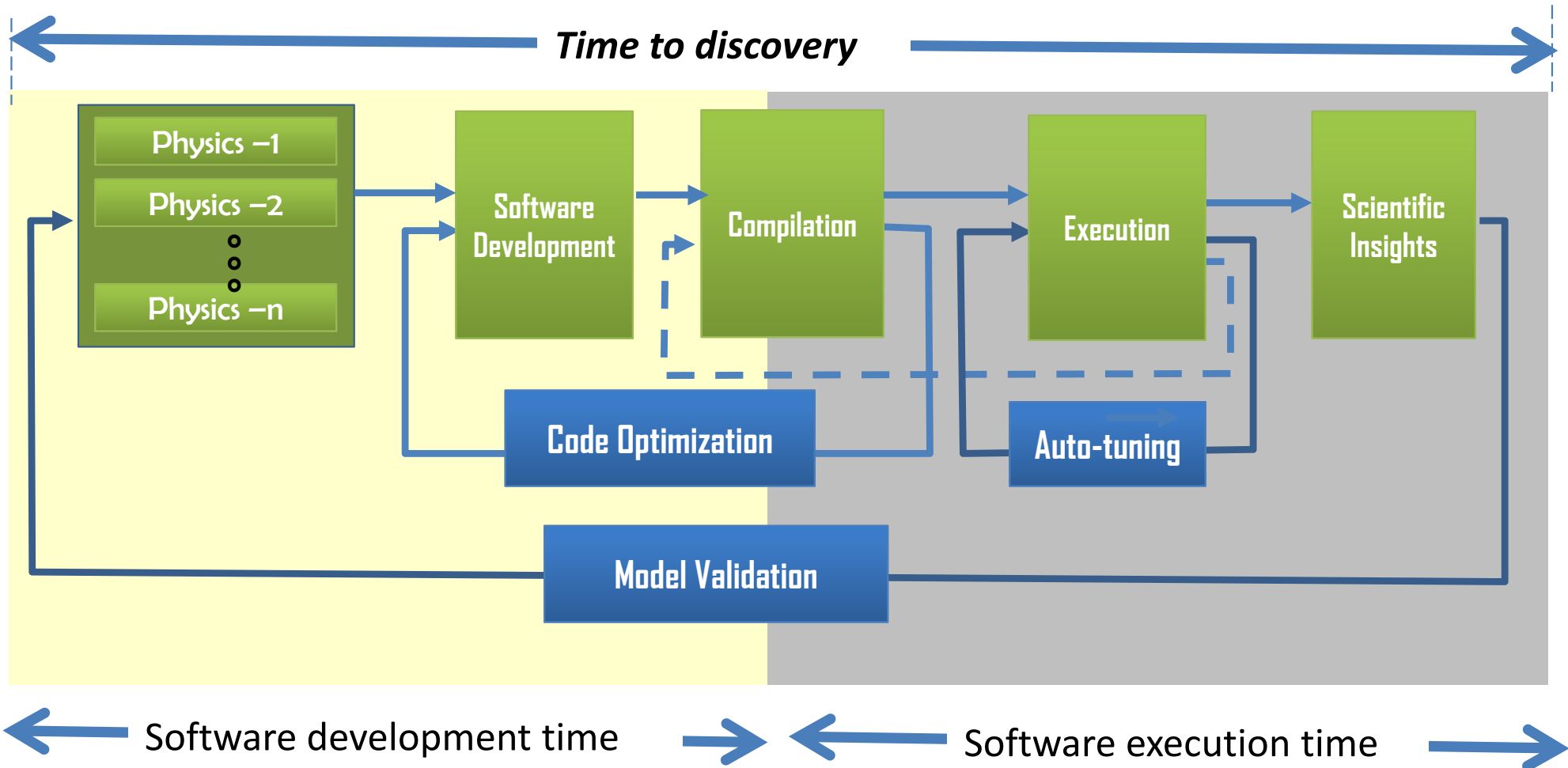
Stuart Faulk – productivity gridlock

Where are the productivity bottlenecks?

Productive Extreme-scale Computing

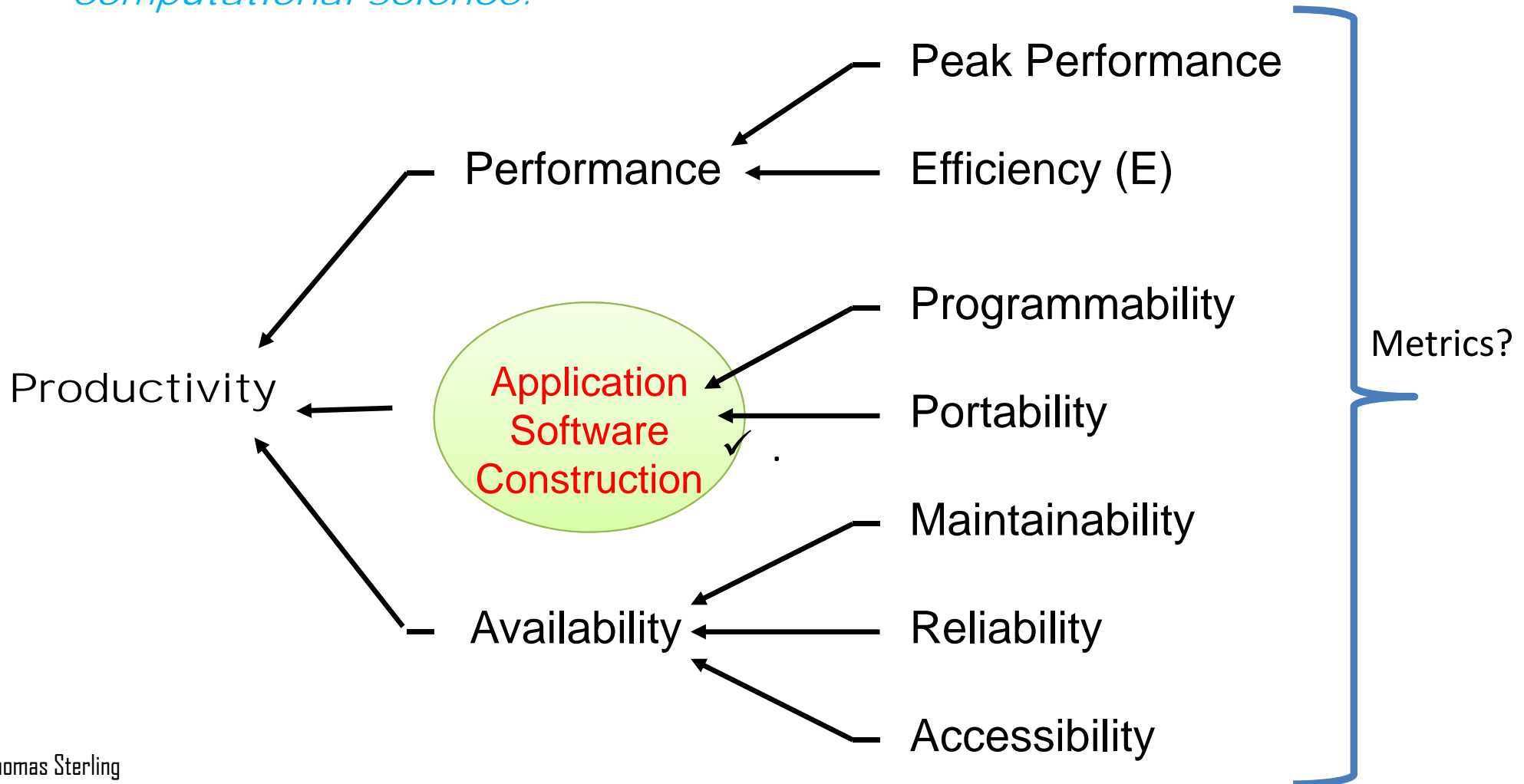
Productive Computing Goal

- **Maximizing the value, reducing the cost, and minimizing the effort needed to achieve the solution to a complex problem through the application of modern supercomputing.**

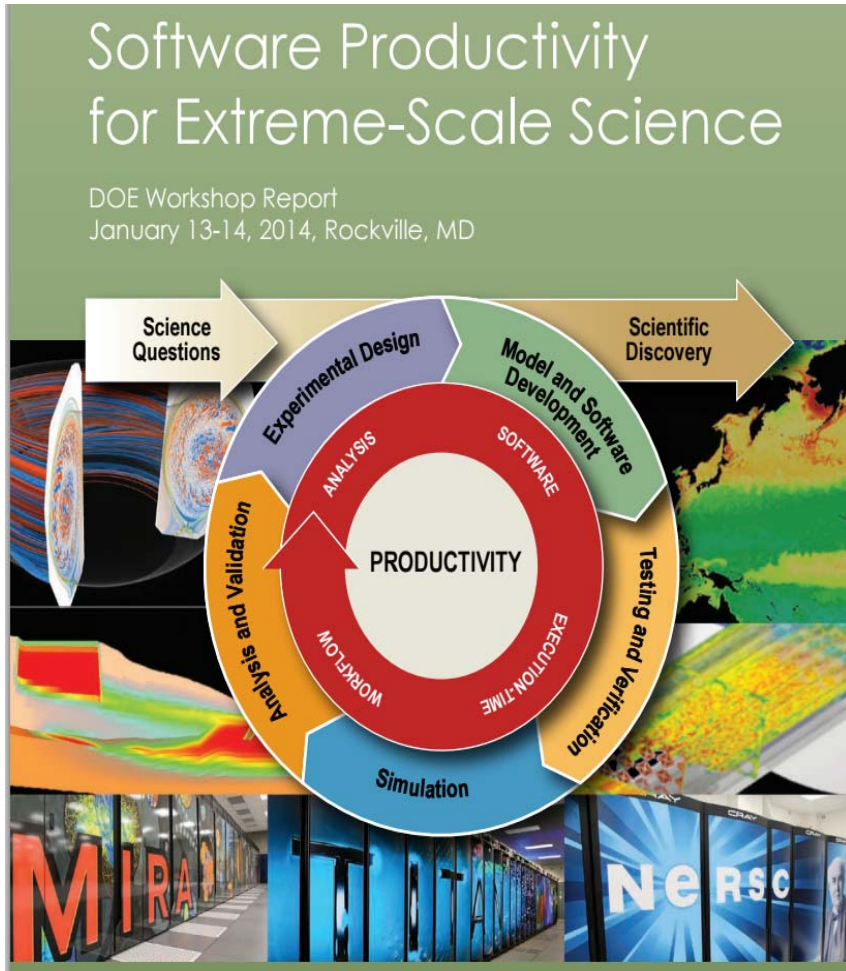


HPC Computing Ecosystem Productivity

The time and effort needed to specify, develop, test, tune, execute, and maintain large community-based application software greatly impact the overall productivity of computational science.



IDEAS Project Background



Workshop Finding

- **Scientific software engineering R&D**
- **Software performance productivity metrics**
- **Software as a scientific virtual facility**
- **Easy to use software tools to support reusability, portability, and inter-operability**
- **Strategies for scientific sustainability**
- **Tools for legacy code understanding and transformation**
- **Easy to use software development tools**
- **Community code development/management**

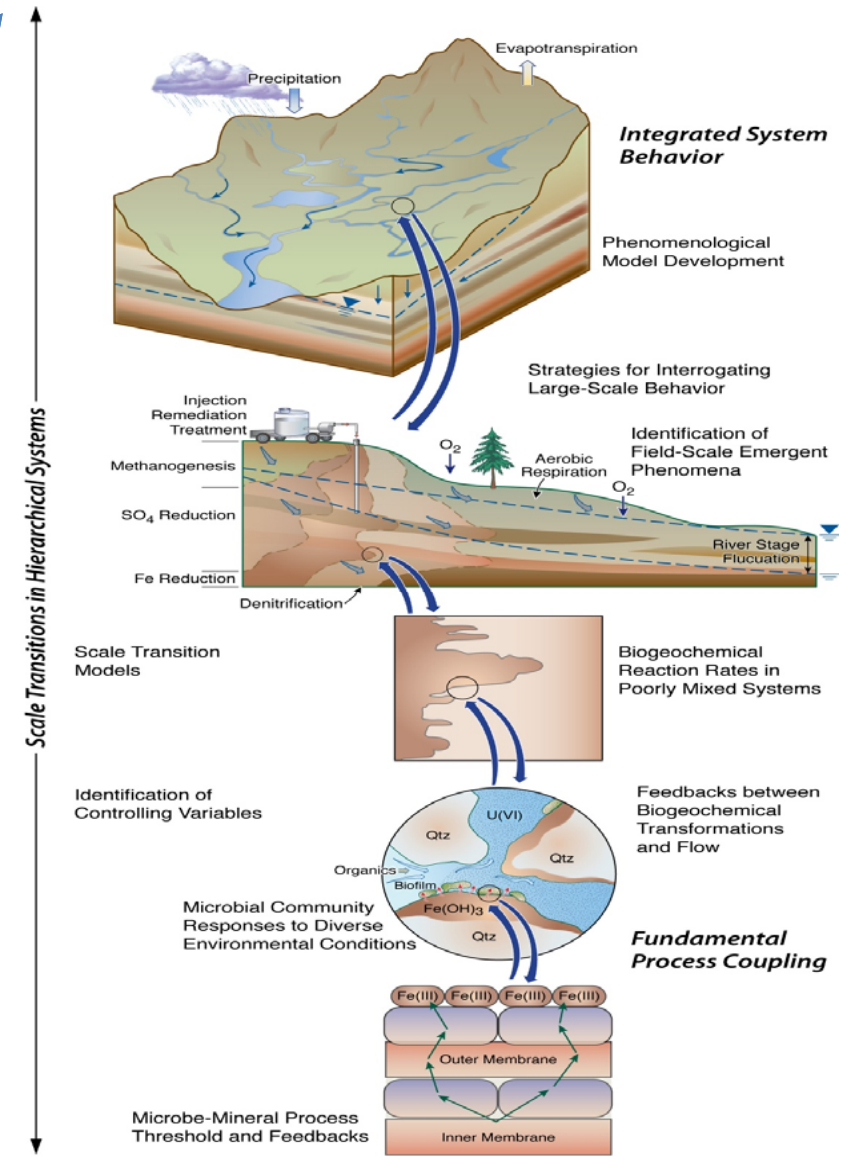
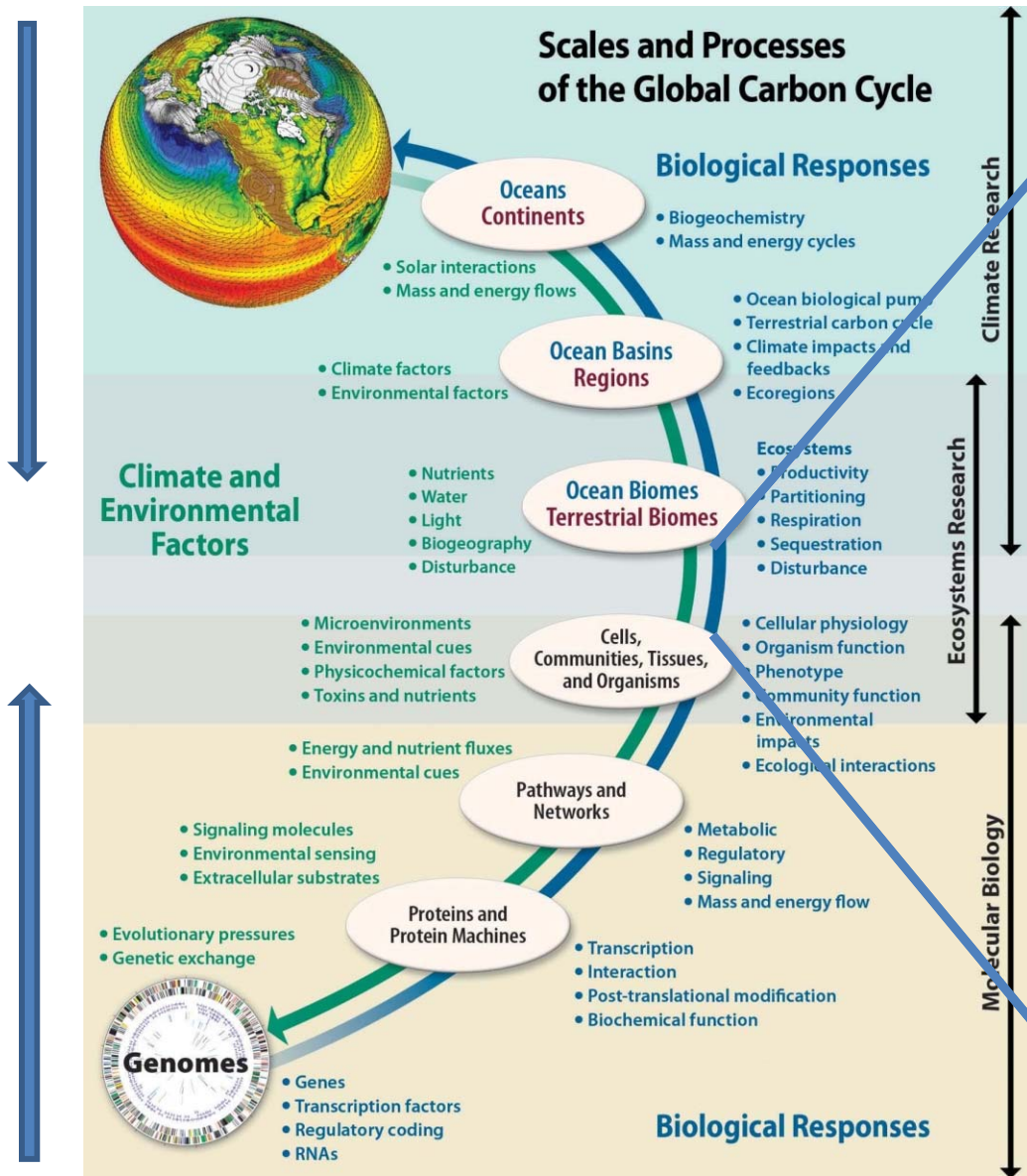
IDEAS Project

- **Co-development effort jointly funded by ASCR and BER**
- **Multidisciplinary team (applied math, computer architecture, domain science)**
- **Use-case to test and validate new software engineering approaches**
- **Outreach to DOE computational science communities**

Biological and Environmental Research

Understanding complex biological, climatic, and environmental systems across vast spatial and temporal scales

Genomes to Watersheds



Institutional Leads (Pictured) Full Team List

Science Use Cases

J. David Moulton

Tim Scheibe

Carl Steefel

Glenn Hammond

Reed Maxwell

Scott Painter

Ethan Coon

Xiaofan Yang



Project Leads

ASCR: M. Heroux and L.C. McInnes

BER: J. D. Moulton

Extreme-scale Scientific Software Development Kit (xSDK)

Mike Heroux

Ulrike Meier Yang

Jed Brown

Irina Demeshko

Kirsten Kleese van Dam

Sherry Li

Daniel Osei-Kuffuor

Vijay Mahadevan

Barry Smith



Hans Johansen

Lois Curfman McInnes

Ross Bartlett

Todd Gamblin*

Andy Salinger*

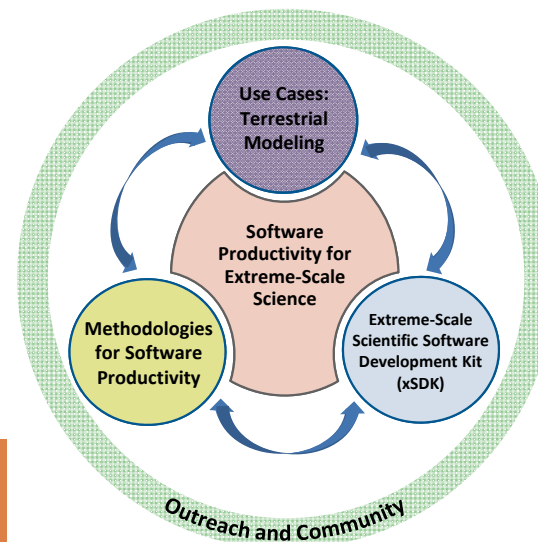
Jason Sarich

Jim Willenbring

Pat McCormick



Methodologies for Software Productivity



*Liaison

Outreach

David Bernholdt

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Lisa Childers*

Judith Hill*⁷

