A cast of thousands: How the IDEAS Productivity project has advanced software productivity and sustainability

David E. Bernholdt (he/him)
Oak Ridge National Laboratory

On behalf of the entire IDEAS-ECP team

a Best Practices for HPC Software Developers webinar

learn more about IDEAS at https://ideas-productivity.org
and https://doi.org/10.48550/arXiv.2311.02010

This work was supported by the U.S. Department of Energy Office of Science, Office of Advanced Scientific Computing Research (ASCR), and by the Exascale Computing Project (17-SC-20-SC), a collaborative effort of the U.S. Department of Energy Office of Science and the National Nuclear Security Administration
A Brief History of IDEAS

• IDEAS = Interoperable Design of Extreme-Scale Application Software

• First of its kind (in U.S.) with a focus on incubating, curating, and disseminating knowledge and methodologies about the sustainment of scientific software
  – Inspired by UK Software Sustainability Institute

• IDEAS is now a family of related projects
  – Different sponsors, different time frames, different people (but significant overlap), different approaches
  – Common focus on improving developer productivity and software sustainability and trustworthiness

• IDEAS-Classic (2014—2017)
  – Focus: multiscale multiphysics terrestrial ecosystem modeling
  – Sponsors: DOE/ASCR and BER

• IDEAS-ECP (2017—2023)
  – Focus: supporting the ecosystem of applications, libraries, and tools developed by ECP
  – Sponsor: DOE/ECP

• IDEAS-Watersheds (2019—present)
  – Focus: accelerating watershed science through a community driven software ecosystem
  – Sponsor: DOE/BER

Acronyms:
- DOE = U.S. Department of Energy
- ASCR = Office of Advanced Scientific Computing Research
- BER = Office of Biological and Environmental Research
- ECP = Exascale Computing Project
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ECP = Exascale Computing Project
ECP’s holistic approach uses co-design and integration to achieve exascale computing

Application Development (AD)
- Develop and enhance the predictive capability of applications critical to DOE
  - 24 applications
  - National security, energy, Earth systems, economic security, materials, data
  - 6 co-design centers
  - ML, graph analytics, mesh refinement, PDE discretization, particles, online data analytics

Software Technology (ST)
- Deliver expanded and vertically integrated software stack to achieve full potential of exascale computing
  - 70 unique software products developed by 35 teams spanning programming models and runtimes, math libraries, data and visualization, development tools

Hardware and Integration (HI)
- Integrated delivery of ECP products on targeted systems at leading DOE HPC facilities
  - 6 US HPC vendors focused on exascale node and system design; application integration and software deployment to Facilities

80+ R&D teams, 1000 researchers!

Andrew Siegel, AD Director
Erik Draeger, AD Deputy Director
Mike Heroux, ST Director
Lois Curfman McInnes, ST Deputy Director
Richard Gerber, HI Director
Susan Coghlan, HI Deputy Director
### Science and beyond: Applications and discovery in ECP

<table>
<thead>
<tr>
<th>National security</th>
<th>Energy security</th>
<th>Economic security</th>
<th>Scientific discovery</th>
<th>Earth systems</th>
<th>Health care</th>
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<tr>
<td>Next-generation, stockpile stewardship codes</td>
<td>Turbine wind plant efficiency</td>
<td>Additive manufacturing of qualifiable metal parts</td>
<td>Cosmological probe of the standard model of particle physics</td>
<td>Accurate regional impact assessments in Earth system models</td>
<td>Accelerate and translate cancer research (partnership with NIH)</td>
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<td>Reentry-vehicle-environment simulation</td>
<td>Design and commercialization of SMRs</td>
<td>Reliable and efficient planning of the power grid</td>
<td>Validate fundamental laws of nature</td>
<td>Stress-resistant crop analysis and catalytic conversion of biomass-derived alcohols</td>
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<td>Multi-physics science simulations of high-energy density physics conditions</td>
<td>Nuclear fission and fusion reactor materials design</td>
<td>Seismic hazard risk assessment</td>
<td>Plasma wakefield accelerator design</td>
<td>Metagenomics for analysis of biogeochemical cycles, climate change, environmental remediation</td>
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<td></td>
<td>Subsurface use for carbon capture, petroleum extraction, waste disposal</td>
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<td>Light source-enabled analysis of protein and molecular structure and design</td>
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<td></td>
<td>High-efficiency, low-emission combustion engine and gas turbine design</td>
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<td>Find, predict, and control materials and properties</td>
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<td></td>
<td>Scale up of clean fossil fuel combustion</td>
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<td>Predict and control magnetically confined fusion plasmas</td>
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<td>Biofuel catalyst design</td>
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<td>Demystify origin of chemical elements</td>
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Thank you to Andrew Siegel, Erik Draeger and ECP applications teams

24 applications + 6 co-design projects
62 separate codes!
ECP ST has six technical areas

**Programming Models & Runtimes**
- Enhance and get ready for exascale the MPI and OpenMP programming models (hybrid programming models, deep memory copies).
- Develop performance portability tools (e.g., Kokkos and Raja).
- Support alternate models for potential benefits and risk mitigation: PGAS (UPC++/GASNet), task-based models (Legion, PaRSEC).
- Libraries for deep memory hierarchy and power management.

**Development Tools**
- Continued, multifaceted capabilities in portable, open-source LLVM compiler ecosystem to support expected ECP architectures, including support for F18.
- Performance analysis tools that accommodate new architectures, programming models, e.g., PAPI, Tau.

**Math Libraries**
- Linear algebra, iterative linear solvers, direct linear solvers, integrators and nonlinear solvers, optimization, FFTs, etc.
- Performance on new node architectures; extreme strong scalability.
- Advanced algorithms for multi-physics, multiscale simulation and outer-loop analysis.
- Increasing quality, interoperability, complementarity of math libraries.

**Data and Visualization**
- I/O via the HDF5 API.
- Insightful, memory-efficient in-situ visualization and analysis.
- Data reduction via scientific data compression.
- Checkpoint restart.

**Software Ecosystem**
- Develop features in Spack necessary to support ST products in E4S, and the AD projects that adopt it.
- Develop Spack stacks for reproducible turnkey software deployment.
- Optimization and interoperability of containers for HPC.
- Regular E4S releases of the ST software stack and SDKs with regular integration of new ST products.

**NNSA ST**
- Open source NNSA Software projects.
- Projects that have both mission role and open science role.
- Major technical areas: New programming abstractions, math libraries, data and viz libraries.
- Cover most ST technology areas.
- Subject to the same planning, reporting and review processes.

Area Leads:
- Rajeev Thakur
- Jeff Vetter
- Sherry Li
- Jim Ahrens
- Todd Munson
- Kathryn Mohror

35 projects 70 software products
IDEAS-ECP Had to Be Different

- The ECP environment and needs were very different from IDEAS-Classic
  - Stringent deliverable set for performance and capability
  - Requirement to utilize new exascale hardware platforms
    - Actual exascale hardware available only late in the project
    - Strong likelihood of encountering bugs or inadequacies in developing software environment
    - Extensive exploration and experimentation with code
  - Impossible to do 1:1 interactions with every ECP software team
    - 80+ software teams, 100+ software products, ~1000 people
- So, we had to develop a different approach for IDEAS-ECP, focusing on…
  - Fostering software communities,
  - Broadly applicable methodologies and resources, and
  - Disseminating knowledge broadly
Diffusion of Innovations via Teams, Teams of Teams, and Communities

- Accelerating design space exploration
- Advancing quality, usability and interoperability, while respecting team autonomy
- Software community policies
- Software Development Kits (SDKs) and E4S
  - xSDK, CAT-SDK, DAV-SDK, SWAS, etc
- Webinar Series:
  - HPC Best Practices
  - HPC Workforce Development and Retention
  - Tutorials on Practices for Better Scientific Software

- Incubating and curating methodologies and resources
- Fostering software communities
- Disseminating knowledge to advance developer productivity and software sustainability

- Productivity and Sustainability Improvement Planning (PSIP)
- Team of teams concepts
- Better Scientific Software (BSSw.io) website
- Webinar Series:
  - HPC Best Practices
  - HPC Workforce Development and Retention
  - Tutorials on Practices for Better Scientific Software

- BSSw Fellowship Program
- Panel Series:
  - Strategies for Working Remotely
  - Performance Portability
  - Events: BOFs, workshops, and more
Fostering Software Communities

• Accelerating design space exploration
• Advancing quality, usability, interoperability, and sustainability, while respecting team autonomy
• Software community policies
• Software Development Kits (SDKs) and E4S
  – xSDK, CAT-SDK, DAV-SDK, etc.
xSDK: Primary delivery mechanism for ECP math libraries’ continual advancements

As motivated and validated by the needs of ECP applications:

ECP Math libraries

- Performance on new node architectures
- Extreme strong scalability
- Interoperability, complementarity: xSDK
- Optimization, UQ, solvers, discretizations
- Advanced, coupled multiphysics, multiscale

Next-generation algorithms

Toward predictive scientific simulations

Advances in data structures for new node architectures

Increasing performance, portability, productivity

Improving library quality, sustainability, interoperability

Timeline:
- xSDK release 1
- xSDK release 2
- xSDK release n

Refs: xSDK: Building an Ecosystem of Highly Efficient Math Libraries for Exascale, SIAM News, Jan 2021; Building Community through xSDK Software Policies, HPC-BP webinar, Dec 2019
**Mandatory Policies**

1. Support portable installation through Spack
2. Provide a comprehensive test suite
3. Packages using MPI must not directly use `MPI_COMM_WORLD`
4. Package must support common platforms
5. Must provide a reliable way to contact developers
6. Respect decisions by other previously called packages about system resources (e.g., exception and signal handlers)
7. Permissive open-source licence
8. Runtime API call to return library version
9. Must not pollute namespaces
10. Must have a public repository
11. Must be able to turn off/off and redirect I/O
12. If a package embeds externally developed, it must be buildable against an outside copy of that software
13. Installations must conform to certain conventions for names and locations of header and library files
14. Must be buildable with 64-bit pointers
15. xSDK compatibility changes go into the regular development/release versions, not special branches
16. Build options must include a “debug” mode
17. Packages must provide sufficient documentation

**Recommended Policies**

1. Should have at least one “smoke” test
2. Should be possible to run test suite under Valgrind
3. Adopt and document a consistent system for handling error conditions
4. Free all resources acquired
5. Ability to export an ordered list of library dependencies
6. Document the versions of packages it works with or depends upon
7. Include README, SUPPORT, LICENSE, and CHANGES files
8. Provide preprocessor macros to allow for version comparisons
Extreme-scale Scientific Software Stack (E4S)

- **E4S**: HPC software ecosystem – a curated software portfolio
- A **Spack-based** distribution of software tested for interoperability and portability to multiple architectures
- Available from **source, containers, cloud, binary caches**
- Leverages and enhances SDK interoperability thrust
- Not a commercial product – an open resource for all
- Growing functionality: E4S 23.08 – 115 packages

**Community Policies**
Commitment to software quality

**Curated collection**
The end of dependency hell

**Turnkey stack**
A new user experience

**DocPortal**
Single portal to all E4S product info

**Quarterly releases**
Release 23.08 – August

**Portfolio testing**
Especially leadership platforms

**Build caches**
10X build time improvement

**E4S Strategy Group**
US agencies, industry, international

**https://e4s.io**
E4S lead: Sameer Shende (U Oregon)

**https://spack.io**
Spack lead: Todd Gamblin (LLNL)

Also includes other products, e.g.,
**AI**: PyTorch, TensorFlow, Horovod
**Co-Design**: AMReX, Cabana, MFEM
E4S Community Policies: A commitment to quality improvement

- Purpose: Enhance sustainability and interoperability
- Will serve as membership criteria for E4S
  - Membership is not required for inclusion in E4S
  - Also includes forward-looking draft policies
- Modeled after xSDK community policies
- Multi-year effort led by SDK team
  - Included representation from across ST
  - Multiple rounds of feedback incorporated from ST leadership and membership

SDK lead: Jim Willenbring (SNL)

Policies: Version 1
https://e4s-project.github.io/policies.html

- **P1: Spack-based Build and Installation**
- **P2: Minimal Validation Testing**
- **P3: Sustainability**
- **P4: Documentation**
- **P5: Product Metadata**
- **P6: Public Repository**
- **P7: Imported Software**
- **P8: Error Handling**
- **P9: Test Suite**

Feedback welcome. What policies make sense for your software?
Incubating and Curating Methodologies and Resources

- Productivity and Sustainability Improvement Planning (PSIP)
- Team of teams concepts
- Better Scientific Software (BSSw.io) resource portal
PSIP: Productivity and Sustainability Improvement Planning
Continual, Incremental Software Process Improvement

1. Identify your team’s “pain points” in your software development processes
   - Help: RateYourProject assessment tool: https://rateyourproject.org/

2. Set a goal for something to improve
   - Target processes and behaviors, not just tasks
   - Pick something that you can address in a few months that will give you a noticeable benefit

3. Agree on a plan to address it, identify markers of progress and what is “done”
   - Write them down
   - Help: Progress tracking card examples: https://bssw-psip.github.io/ptc-catalog/catalog

4. Work your plan, track your progress

5. When you are done, celebrate…
   …then pick a new pain point to address

https://bssw.io/psip

Target: your project should include “just enough” software engineering so that you can meet your short-term and longer-term scientific goals effectively

Lead: Elaine Raybourn (SNL)
PSIP multi-pronged, socio-technical strategy

**EDUCATION**
Share knowledge via tutorials, paper publications, and seminars to engender a culture of productivity by engaging PSIP liaisons, early adopters, and champions.

**TEAM ENGAGEMENT**
By directly working with ECP teams, PSIP facilitators help software teams to **IDENTIFY** opportunities to iteratively and incrementally **IMPROVE** software team practices and processes.

**RESEARCH**
Conduct Team of Teams data-driven research (data mining + interviews) to characterize ECP organization, draw general conclusions about observable behaviors that contribute to team productivity, collaboration, and success.

**METHOD & TOOL DEVELOPMENT**
Develop tools that automate PSIP to support ECP teams, scientific software quality, and developer productivity. Development of PSIP tools based on needs and salient issues identified during Team of Teams research and ECP team engagement.
Examples of Who’s using PSIP

The HDF Group

Improvements to documentation, setting code style standards, transition to GitHub (blog article)

The PSIP project had an immediate impact on our community. With the GitHub move we see increasing amounts of small but very valuable contributions to make HDF5 code and documentation better.” – Elena Pourmal, Director of Engineering, The HDF Group

Flash5

Improve testing and verification, transition development workflow to GitHub

ALPINE/ZFP

Created a VTK-m filter for APLINE in situ algorithm users

Revamp build system, implement a CTest-based testing framework, implement a basic CI pipeline

EXAALT

OAK RIDGE

National Laboratory

Using a more detailed version for internal project assessment

Completed PSIP tutorial, investigating how it can be used in academic context

Sandia National Laboratories

Using internally for reproducibility LDRD research, and for large projects updating version control systems, and updating documentation to support better onboarding

IDEAS productivity

ECP EXAScale Computing Project
Collaboration via Teams of Teams

• The “team of teams” concept (ToT) was popularized by Stanley McChrystal’s 2015 book
  – IDEAS efforts are an offshoot of PSIP, led by Elaine Raybourn (SNL)
  – Using tools from the CAT-SDK software community for repository analysis

• ToT provides a powerful lens through which to better understand the ECP, as well as many other software ecosystems, and to improve their effectiveness
  – Strengthen community partnerships
  – Scaling productivity typically experienced in small teams (where it’s easy), to larger groups via the team of teams paradigm

• ToT principles facilitated contributions of the HDF5 team to the E4S and Data & Viz SDK
  – Supported applications in modeling earthquakes, electronic structures, subsurface flow, reacting flow, stellar explosions, wind plants, and cosmology

• Distributed, Interconnected Teams through the Lens of Team of Teams Principles
  – Panel discussion with members of PETSc, Trilinos, xSDK, and E4S ECP projects

• Scaling productivity and innovation on the path to exascale with a “team of teams” approach
  – Case study of the ASC Ristra ECP project
A central hub for sharing information on practices, techniques, experiences, and tools to improve developer productivity and software sustainability for computational science & engineering (CSE)

- **Find information** on scientific software topics
- **Contribute new resources** based on your experiences
- Editor-in-chief: Rinku Gupta (ANL)

**Types of content on BSSw**

- **Blog articles**: success stories, perspectives, opportunities, technical deep-dives, and more
- **Curated content**: short pointers to useful material already hosted elsewhere
- **Events**: increase awareness of events related to better scientific software
Disseminating Knowledge

• BSSw Fellowship Program
• Better Scientific Software tutorials
• Best Practices for HPC Software Developers webinar series
• Panel Series:
  – Strategies for Working Remotely
  – Performance Portability
• Events: BOFs, workshops, and more

IDEAS dissemination and outreach activities have always targeted the general scientific software community
Better Scientific Software (BSSw) Fellowship Program

Meet Our Fellows

The BSSw Fellowship program gives recognition and funding to leaders and advocates of high-quality scientific software. Meet the Fellows and Honorable Mentions and learn more about how they impact Better Scientific Software.

Goal: Foster and promote practices, processes, and tools to improve developer productivity and software sustainability of scientific codes. #somycodewillseethefuture

Also supported by the National Science Foundation since 2021

BSSw Fellowship Coordinator: Elsa Gonsiorowski (LLNL)
Deputy Coordinator, Community Building: Erik Palmer (LBNL)
Better Scientific Software Tutorials

- Covering issues of developer productivity, software sustainability and reliability, with a special focus on the challenges of complex, large-scale HPC
  - software design, agile methodologies, Git workflows, reproducibility, software testing, continuous integration testing, refactoring, and more

- https://bssw-tutorial.github.io

- Lead: David Bernholdt (ORNL)

- 32 tutorials since 2016
  - Presentations (all) and recordings (some) available

- Topics and content under continuous refinement

- Frequent venues
  - Supercomputing (2016-2023)
  - ATPESC (2016-2023)
  - ISC (2018-2019, 2021-2023)

Webinar Series: Best Practices for HPC Software Developers (HPC-BP)

- Covering topics in software development and HPC

- https://ideas-productivity.org/resources/series/hpc-best-practices-webinars/

- Lead: Osni Marques (LBNL)

- Presented by the community to the community

- Monthly series, since May 2016 (offered live and archived)
  - To date: 80 webinars, >12,000 registrations, >5,300 attendees
  - 84 attendees per webinar, on average
Panel Series: Performance Portability & ECP

- Lead: Anshu Dubey (ANL). Refs:
  - SIAM CSE21 minisymposium: https://doi.org/10.6084/m9.figshare.c.5321441
  - ECCOMAS 2022 minisymposium

Panel Series: Strategies for Working Remotely

- Exploring strategies for working remotely, with emphasis on how HPC teams can be effective and efficient in long-term hybrid settings
- https://www.exascaleproject.org/strategies-for-working-remotely
- Lead: Elaine Raybourn (SNL)
- Quarterly series, since April 2020 (offered live and archived)

Technical Meetings and Birds of a Feather Sessions

- Creating opportunities to talk about software development, productivity, and sustainability
- https://ideas-productivity.org/resources/series/technical-sessions-and-meetings/

Minisymposia
  - Ref: A Look at Software-Focused Topics at SIAM CSE21, March 2021

Thematic poster sessions

BOF sessions
- Software Engineering and Reuse in Modeling, Simulation and Data Analytics for Science and Engineering

Collegeville Workshop Series on Scientific Software
- Ref: Software Team Experiences and Challenges, K. Beattie et al, Oct 2021
Promoting Culture Change

- In all of our work, IDEAS promotes a change in the culture around scientific software
  - Recognizing and valuing the software professionals who are increasingly contributing to the development and maintenance of research software
  - Recognizing and valuing the software itself as a first-class product of compute-intensive research

- Engagement with sponsors

- Support for the developing research software engineer (RSE) community
  - Many IDEAS team members are also members of, and leaders in, US-RSE

- HPC Workforce Development and Retention Action Group
  - Part of the ECP Broadening Participation Initiative to expand the pipeline and workforce for DOE high-performance computing
  - HPC-WDR website and webinar series
    - Topics have included ally skills, diversifying computing, mentoring, and normalizing inclusion by embracing difference

Lead: Suzanne Parete-Koon (ORNL)
IDEAS-ECP Impacts

• Feedback underscores IDEAS’s role in **enhancing software quality, promoting best practices, and expanding awareness** of the importance of software development

• Curating best practices for software development and team productivity has **empowered teams** to build new practices into their workflows and increase cross-project collaboration
  – Many community members express a desire for additional resources

• Software communities have proven to be a **source of inspiration** for building shared foundations for software ecosystems while respecting team autonomy

• IDEAS outreach mechanisms have enabled innovators in scientific software practices to **share knowledge** with the community

• **Model for other multi-institutional software ecosystems**
Moving Forward

We believe that IDEAS has been an important catalyst for the scientific software community in ECP and beyond, but two further elements are essential for continued qualitative growth...

• Increasing focus on research software science
  – Applying our experience with hypothesis-driven science to improve our understanding of how scientific software is developed and used
  – Social-, cognitive-, hard-science, and engineering viewpoints needed

• Changing the prevailing attitude that scientific software productivity, sustainability, and trustworthiness are not just “nice to have” but “must-have”
  – Innovators and early adopters are there
  – But many still prioritize more scientific results at the expense of beneficial investments in the software behind them
What’s Next?

• As part of the ECP project, IDEAS-ECP ends at the end of 2023
  – IDEAS-Watersheds continues, with focus on watershed modeling

• **BSSw Fellowship** class of 2024 to be announced soon
  – Thanks to support from DOE/ASCR, DOE/NNSA, and NSF

• **Next Generation Scientific Software Technologies (NGSST)** initiative is emerging to help address scientific software stewardship needs across the ASCR software ecosystem
  – Focus is different than IDEAS-ECP
  – But you can see IDEAS influence in some of the planned work

• Looking for increased engagement from the community to continue some IDEAS legacy activities

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**Acronyms**

NNSA = National Nuclear Security Administration

NSF = National Science Foundation
Next Generation Scientific Software Technologies (NGSST)

• Seven teams submitted interlocking proposals for a **Scientific Software Stewardship Consortium (S3C)** with distinct but complementary foci

• Focus on the ASCR scientific software ecosystem, which includes software products from
  – Exascale Computing Project (ECP) Software Technologies
  – ECP Co-Design Centers
  – Other ASCR-supported products

• At anticipated funding levels, the NGSST will be able to support only a subset of the eligible projects

• Phase 2 proposals under review, most awards expected to start in January 2024
Continuing the IDEAS Legacy in NGSST

• Fostering software communities
  – Extreme-Scale Scientific Software Stack (E4S)
  – Some of the other community-focused NGSST organizations may pursue SDKs

• Incubating and Curating Methodologies and Resources
  – Software quality assurance (emphasis on ecosystem integration)
  – And possibly in other areas
  – BSSw.io resource portal

• Disseminating knowledge
  – Best Practices for HPC Software Developers webinar series
  – Better Scientific Software tutorials
    • Complemented by trainings from other NGSST organizations

• Promoting culture change
  – HPC Workforce Development and Retention
  – Building a community of practice for research software engineers in the DOE national labs

Items in green are specific IDEAS activities that we plan to continue in NGSST – with additional help from the larger community!
You Can Help Change the Culture around Scientific Software!

• IDEAS (or NGSST) can’t do it alone!

• If you’re a developer or user of scientific software (or a manager), you have a role to play in making scientific software better
  – Be thoughtful about the stewardship of your own software
  – Work with your team to learn about and implement better software development practices
    • Focus on incremental, but continual software process improvement, tailored to your needs

• Share your software development knowledge, experience, and resources with others

• Engage with communities relevant to your work and interests (see also doi: 10.1109/MCSE.2018.2883051)

• Talk with your sponsors about the importance of software stewardship, what you’re doing, the benefits, and how they can help

• Remember: Science through computing is, at best, as credible as the software that produces it!
Acknowledgements: The IDEAS-ECP Team and the ECP

Alumni: Satish Balay (ANL), Lisa Childers (ANL), Todd Gamblin (LLNL), Judy Hill (ORNL), Steve Hudson (ANL), Christoph Junghans (LANL), Alicia Klinvex (SNL), Shannon Lindgren (ANL), Lena Lopatina (LANL), Jared O'Neal (ANL), Michele Rosso (SNL), Jean Shuler (LLNL), Barry Smith (ANL), Louis Vernon (LANL), Paul Wolfenbarger (SNL)