



STEP

SUSTAINABLE TOOLS
ECOSYSTEM PROJECT

What is STEP & Why are we here

August 16, 2023

Terry Jones, STEP Principal Investigator

WELCOME to the STEP West Coast Town Hall!



- Provide some Backstory on Software Sustainability
- Describe the Tools Ecosystem and Why It's Special
- Introduce the Sustainable Tools Ecosystem Project (STEP)
- Community informed solution to a challenging puzzle

DOE/ASCR's Software Sustainability Program

What's New: The Exascale Computing Project sunsets Dec-31-2023

| Fiscal Year | Exascale Computing Project Budget |
|-------------|-----------------------------------|
| 2017 | \$164.0M |
| 2018 | \$162.9M |
| 2019 | \$232.7M |
| 2020 | \$188.7M |
| 2021 | \$168.9M |
| 2022 | \$129.0M |
| 2023 | \$77.0M |
| 2024 | \$14.0M* |




* President's request

Software Sustainability Program – Building On ECP Successes

- Program managers
Hal Finkel & Bill Spotz
- Phase I: Six Funded Seedlings in FY23
 - 3 Service focused seedlings
 - 3 Functional area seedlings
- Leads to a Phase II Software Sustainability Program in FY24

DEPARTMENT OF ENERGY (DOE)
OFFICE OF SCIENCE (SC)



FY 2023 CONTINUATION OF SOLICITATION FOR THE OFFICE
OF SCIENCE FINANCIAL ASSISTANCE PROGRAM

FUNDING OPPORTUNITY ANNOUNCEMENT (FOA) NUMBER:
DE-FOA-0002844

FOA TYPE: 000001
CFDA NUMBER: 81.049

Amendment 000001 is issued with a number of minor revisions as detailed on the following page.

| | |
|---|---|
| FOA Issue Date: | September 30, 2022 |
| Submission Deadline for Pre-Applications: | A Pre-Application is optional/encouraged |
| Submission Deadline for Applications: | Not Applicable This FOA will remain open until September 30, 2023 or until replaced by a successor FOA. Applications may be submitted any time during that period. |

Seedlings Focused on *Functional Areas*

STEP : Sustainable Tools Ecosystem Project

- *Lead PI: Terry Jones (ORNL)*
- Software for performance tools, correctness, debugging
- Co-design with hardware vendors

S4PST : Sustainability for Node Level Programming Systems and Tools

- *Lead PI: Keita Teranishi (ORNL)*
- Software for compilers, abstractions, libraries, and tools for node level programming
- Vendor and Third Party engagement

SWAS – Center for Sustaining Workflows and Application Services

- *Lead PI: Rafael Ferreira da Silva (ORNL)*
- Software and services for complex workflows
- Similar to STEP



Seedlings Focused On *Providing Services*

PESO: Toward a Post-ECP Software-Sustainability Organization

- *Lead PI: Mike Heroux (SNL)*
- ECP revised for software sustainability program --- promotes a “hub and spoke” as a possible structure
- Cover libraries and tools under ECP. E4S, xSDK, SPACK
- Conduit of funding to projects

OSSF: Open Scientific Software Foundation

- *Lead PI: Greg Watson (ORNL)*
- Additional Services, Marketing/sponsorship/fundraising activities, Sustainability funding for projects
- FAIR data and DOI minting
- Badging and incentives, legal and IP advice

COLABS: Collaboration for Better Software (for Science)

- *Lead PI: Anshu Dubey (ANL)*
- Matrixed Research Software Engineering, include embedding personnel
- Common Sustainability Services, Infrastructure (such as CI/CD)
- Software engineering training and education, Standards and guidelines

Delving into STEP – Sustainable Tools Ecosystem Project



GOALS:

- a) Develop a community strategy for HPC tool ecosystem sustainability
- b) Plan for a STEP Codesign Center follow-on proposal to scale the project activities beyond year 1 and ensure long-term coordination and engagement.

Introducing STEP – Sustainable Tools Ecosystem Project



GOALS:

- a) Develop a community strategy for HPC tool ecosystem sustainability
- b) Plan for a STEP Codesign Center follow-on proposal to scale the project activities beyond year 1 and ensure long-term coordination and engagement.

Three Key points:

1. Not **_just_** replacing ECP
2. Focus on **_sustainability_**
3. We want involvement from stakeholders in tool developer, facility, vendor, and application teams.

STEP Specifically Targets *Tools*

- WHAT ARE *TOOLS*?
 - We define Tools to mean “the collection of tools and utilities for analyzing and optimizing application performance, identifying correctness problems, and debugging.”
 - These tools interact with hardware features, compilers, communication libraries, programming model runtime systems, and operating systems capabilities that support HPC Tools, as well as the many applications that use these tools.

What's So Important about *Tools?*

- *As computers have increased in complexity and scale, using them effectively has become much more difficult.*
- In addition to their role in enabling supercomputer performance (a decisive determinant of scientific discovery), these tools provide essential feedback to users, operations staff, and system and application software developers.

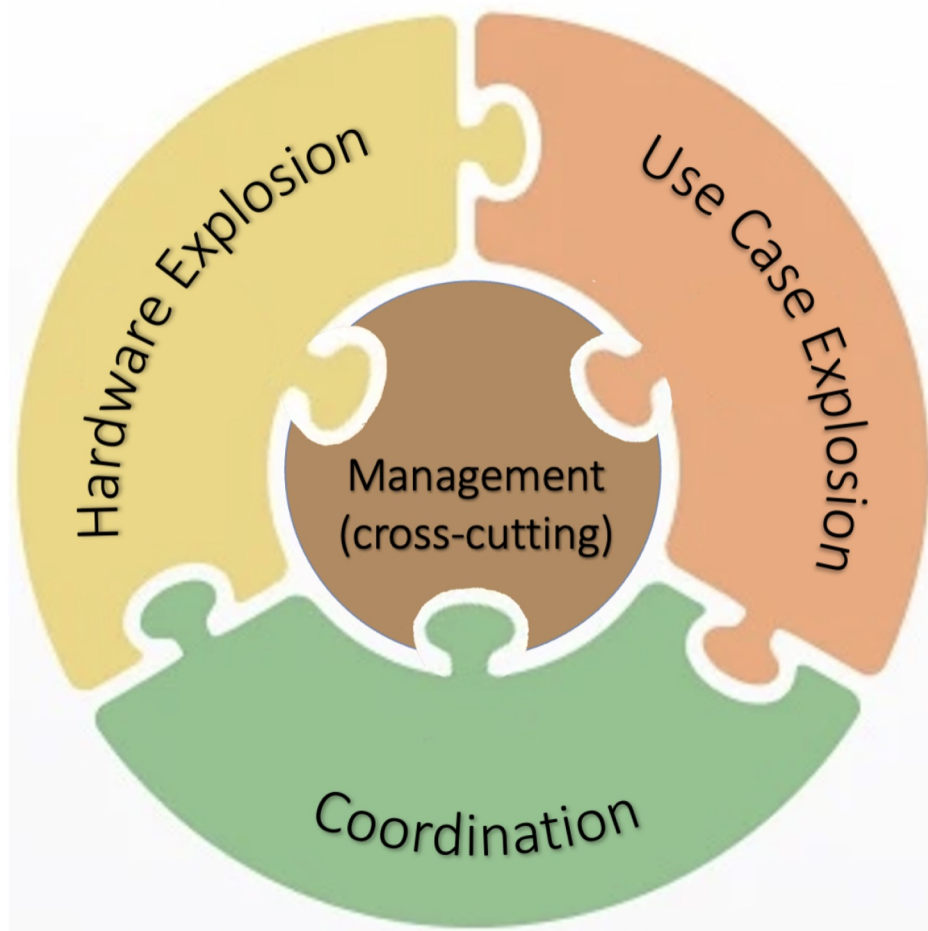
How Are Tools Unique?

- Tools are closely bound to architectures and system software in ways that other types of software, such as libraries and scientific applications, are not.
- For example, a tool that tracks how an application uses computing resources must be able to measure low-level architectural events and metrics and relate them to program progress and source code.
- The need for tools is most acute for understanding code performance on systems that push the boundaries of technology and scale, but these systems' novelty makes them extremely difficult for tool developers to support when first deployed.

What do we mean by *Sustainability*?

- We define sustainability to be the “**ongoing** support and processes needed for tools to **thrive**.”
- **In Scope:** Applied *targeted* work on a software tool that is currently utilized or will be utilized in an HPC context. Research on how to accomplish a specific need is also in scope.
 - ASCR envisions supporting targeted work under Software Sustainability Phase II
- **Out of Scope:** Research and proof of principle work that is *exploratory* in nature. To build knowledge for the sake of knowing or investigating, rather than to solve a problem.
 - ASCR envisions supporting exploratory work with the traditional FOA mechanism

Four Key Challenge Areas Faced by the Tools Ecosystem



The Novelty Conundrum:
Can Tools Transition from Reactive to Proactive?



How STEP Can Be Transformative for Tools

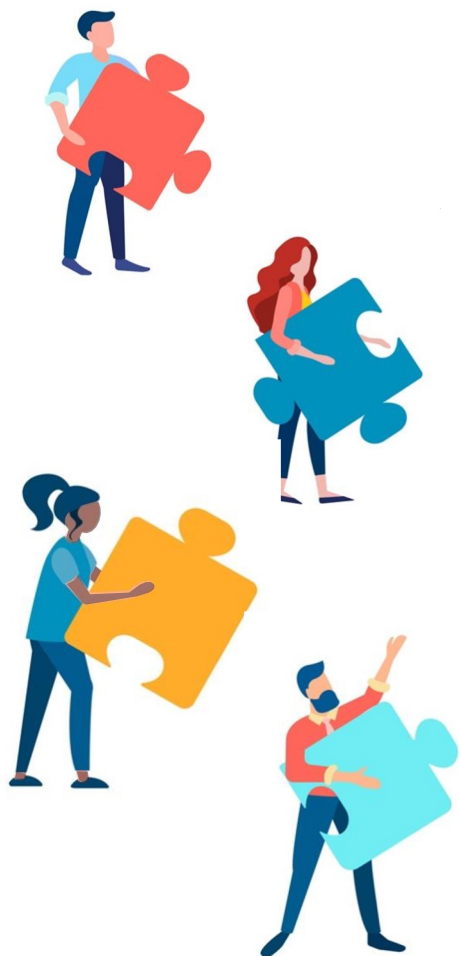
Building An Enduring Ecosystem for Vital Tools



- “STEP will bring together a diverse community of High Performance Computing (HPC) tools developers and stakeholders to **develop plans for the sustainability of the HPC tools ecosystem.**”
- The outcome of the one year proposal should be a **compelling plan** for a center (follow on proposal) for “**the long-term coordinated community-driven development directions necessary to sustain the HPC tools ecosystem.**”
- “Further, many collaborative efforts lose steam when internal priority directions outweigh collaborative gain. Our approach **increases the collaborative gain by bringing together communities to address challenges caused by their dependencies.**”

Sustainable Tools Ecosystem Project (STEP) Team

| NAME | PERSPECTIVE | NAME | ORGANIZATION |
|-----------|--------------|---------------------|--------------------------------|
| Lead PI | Tools | Terry Jones | Oak Ridge National Lab |
| Deputy PI | Tools | Philip Carns | Argonne National Lab |
| Co-PI | Tools | James Brandt | Sandia National Laboratories |
| Co-PI | Vendors | James Custer | Hewlett Packard Enterprise |
| Co-PI | Vendors | Kshitij Doshi | Intel Corporation |
| Co-PI | Tools | Ann Gentile | Sandia National Laboratories |
| Co-PI | Facilities | Richard Gerber | Lawrence Berkeley National Lab |
| Co-PI | Facilities | Kevin Harms | Argonne National Lab |
| Co-PI | Tools | Heike Jagode | University of Tennessee |
| Co-PI | Tools | Mike Jantz | University of Tennessee |
| Co-PI | Tools | Matthew Legendre | Lawrence Livermore Natl Lab |
| Co-PI | Vendors | John Linford | NVIDIA |
| Co-PI | Vendors | Keith Lowery | Advanced Micro Devices |
| Co-PI | Tools | John Mellor-Crummey | Rice University |
| Co-PI | Tools | Barton Miller | University of Wisconsin |
| Co-PI | Vendors | José Moreira | IBM |
| Co-PI | Applications | Erdal Mutlu | Pacific Northwest Natl Lab |
| Co-PI | Facilities | Phil Roth | Oak Ridge National Lab |
| Co-PI | Tools | Sameer Shende | University Oregon |
| Co-PI | Tools | Shane Snyder | Argonne National Lab |
| Co-PI | Tools | Galen Shipman | Los Alamos National Laboratory |
| Co-PI | Tools | Devesh Tiwari | Northeastern University |
| Co-PI | Applications | Theresa Windus | Ames National Lab |



STEP Activities in Software Sustainability Phase I

- Currently developing a *Plan of Action Narrative*.
- Community Driven: Bottom-up driven Narrative will utilize Three Town Halls.
 - **East Coast Town Hall** – HW Challenge, Use Case Challenge, Coordination
 - **Midwest Town Hall** – Based on input from the first town hall, propose a structure for how to organize STEP into discrete components and discuss how to best manage those components
 - **West Coast Town Hall** – Refine plan
- Agile and Codesign-based

Structuring Effective Town Halls

- Each Town Hall focuses on specific challenges to realizing a sustainable tools ecosystem. We will utilize a three-component process to capture comments and recommendations:
 - A presentation or panel discussion to set the stage and provide context on issues facing the tools ecosystem
 - Randomized breakout group working sessions to gather information and explore solutions in cross-cutting subtopics, recorded in google docs
 - Report-out sessions to share key outcomes from breakout sessions
- Solicit feedback on how to improve the town hall process for future events
- (post-event) Publish artifacts and solicit public feedback



Guiding Principles (1 of 2)

- **Bottom-up planning:** We intend to employ a "bottom-up" approach by collecting information, clarifying challenges, and identifying paths forward rather than starting with a presumed structure. The eventual STEP center will be an agile organization in keeping with the needs of the rapidly-evolving, cutting-edge tools ecosystem.
- **Community-oriented solutions:** our individual experiences with tool sustainability are crucial reference points, but we should leverage these experiences to inform broad solutions that will help sustain the ecosystem as a whole (i.e. improving coordination, communication, and integration across the field rather than advocating for specific technical solutions).
- **Inclusive viewpoints:** We can only ensure the sustainability of the ecosystem as a whole by considering experiences and incorporating feedback from the full breadth of stakeholders in the community: tool developers, vendors, users, and facilities.

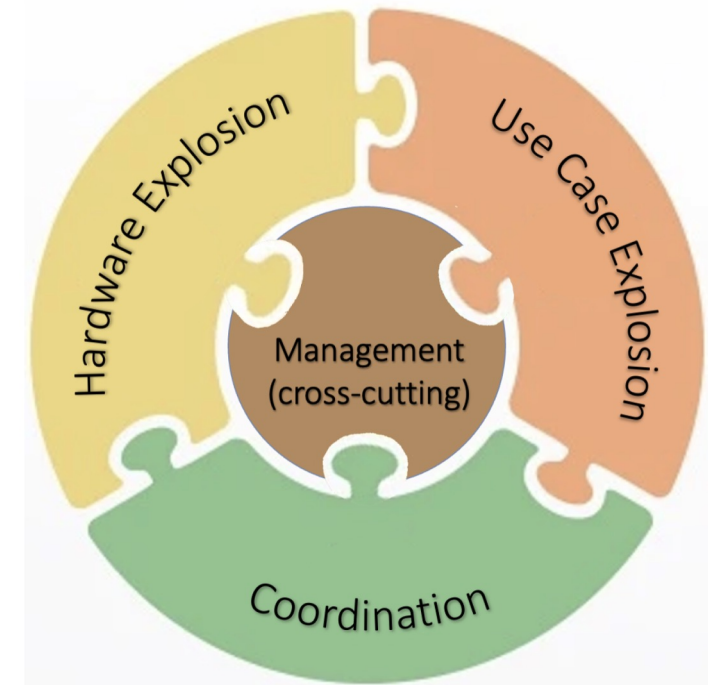


Guiding Principles (2 of 2)

- **Tool scope:** the STEP proposal stated the following: We define HPC tools as the collection of tools and utilities for analyzing and optimizing application performance, identifying correctness problems, and debugging. We will use this as our starting point rubric for tool scope.
- **Multiple town halls:** We do not need to cover every single discussion topic in depth at one town hall. They will transition over the summer from information gathering to more detailed planning, with overlapping topic coverage at each town hall. Please suggest future topics if you feel that important issues have been overlooked.
- **Flexibility:** we do not yet know for sure what funding models will be available for the proposed STEP center, so we need to be prepared to be flexible with a range of possible activities to support sustainability of the tool ecosystem.

Why Are We Here?

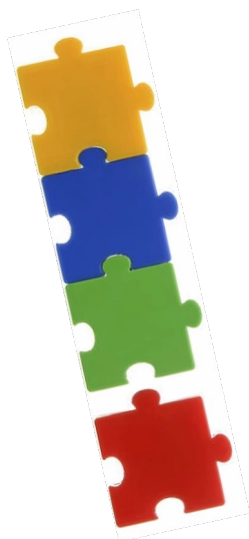
- Prioritizing and refining strategies for key sustainability challenges.
 - Challenge 1: Exploding hardware complexity
 - Challenge 2: Exploding software use cases
 - Challenge 3: Management
 - Challenge 4: Coordination
- Community input on STEP's plan of action and how to organize STEP
- Community input on 3 key Questions
 - How do we build a workforce
 - How do we handle security (esp. open source)?
 - How do we transition from ECP to SS in 2024?



Town Hall Agenda

| Time | Topic – Items marked with blue font will be available online via Zoom for remote observers |
|---------------|---|
| 8:00 – 9:00 | Registration & Badging - <outside Golden Gate Ballroom> |
| 8:00 – 9:00 | Working Breakfast – St. Helena Room |
| 9:00 – 10:00 | Plenary – Opening Comments -- Golden Gate Ballroom or zoom link <ul style="list-style-type: none"> What is STEP and Why Are We Here? [45 mins] (Terry Jones, ORNL) Remarks and Q&A from DOE Headquarters [15 mins] (Bill Spatz, DOE/ASCR) |
| 10:00 - 10:30 | Break – Golden Gate Ballroom |
| 10:30 - 12:00 | Plenary – Review of STEP & Our Goals -- Golden Gate Ballroom or zoom link <ul style="list-style-type: none"> Provisional STEP Structure [10 mins] (Phil Carns, Argonne) Challenge 1: Exploding HW Complexity [20 mins] (breakout lead: Mke Jantz) Challenge 2: Exploding Use Cases [20 mins] (breakout lead: James Custer) Challenge 3: Coordination [20 mins] (breakout lead: Kevin Harms) Challenge 4: Management [20 mins] (breakout lead: Phil Carns) |
| 12:00 - 1:00 | Working Lunch (Provided) – Discussions on morning sessions – St. Helena Room |
| 1:00 - 1:30 | Primer and Desired Outcomes for Breakouts (Terry Jones, ORNL) – Golden Gate Ballroom |
| 1:30 - 3:00 | Breakouts Session 1: Prioritizing & Refining Strategies for Key Sustainability Challenges in Tools <ol style="list-style-type: none"> Challenge 1: Exploding HW Complexity (breakout lead: Mke Jantz) – Mendocino Rm Challenge 2: Exploding Use Cases (breakout lead: James Custer) – Sonoma Rm Challenge 3: Coordination (breakout lead: Kevin Harms) – Monterey Rm Challenge 4: Management (breakout lead: Phil Carns) – Boardroom Rm Virtual Breakout: What Questions Do You Have About STEP? (lead: Terry Jones, ORNL) |
| 3:00 - 3:20 | Break – Golden Gate Ballroom |
| 3:20 - 3:35 | Primer and Desired Outcomes for Breakouts (Terry Jones, ORNL) – Golden Gate Ballroom |
| 3:35 - 5:00 | Breakouts Session 2: Key Components Needed for Phase II Proposal <ol style="list-style-type: none"> Short-term Objectives, Priorities & Risks (lead: John Mellor-Crummey) – Mendocino Rm STEP Roles & responsibilities, processes to staff them (lead: David Montoya) – Sonoma Rm STEP Integration in whole Software Sustainability Landscape (lead: Doshi) – Monterey Rm Charting Technical Directions (lead: John Linford) – Boardroom Rm |
| 5:00 - 5:30 | Closing Guidance / Adjourn day (Terry Jones, ORNL) – Golden Gate Ballroom |

| Time | Topic – Items marked with blue font will be available online via Webex for remote observers |
|---------------|--|
| 8:00 – 9:00 | Registration & Badging - <outside Golden Gate Ballroom> |
| 8:00 – 9:00 | Working Breakfast - St. Helena Room |
| 9:00 - 9:10 | Introduction and Day 2 Logistics (Terry Jones, ORNL) – Golden Gate Ballroom or zoom link |
| 9:10 - 10:40 | Report out summaries from Breakout Session 1: Prioritizing & Refining Strategies for Key Sustainability Challenges in Tools – Golden Gate Ballroom or zoom link <ol style="list-style-type: none"> Challenge 1: Exploding HW Complexity (breakout lead: Mke Jantz) Challenge 2: Exploding Use Cases (breakout lead: James Custer) Challenge 3: Coordination (breakout lead: Kevin Harms) Challenge 4: Management (breakout lead: Phil Carns) Virtual Breakout: What Questions Do You Have About STEP? (lead: Terry Jones) |
| 10:40 - 11:00 | Break – Golden Gate Ballroom |
| 11:00 - 12:30 | Report out summaries from Breakout Session 2: Key Components of Phase II Proposal – Golden Gate Ballroom or zoom link <ol style="list-style-type: none"> Short-term Objectives, Priorities & Risks - What we want to do (breakout lead: John Mellor-Crummey) STEP Roles & responsibilities, processes to staff them (breakout lead: David Montoya) STEP Integration in whole Software Sustainability Landscape (breakout lead: Kshitij Doshi) Charting Technical Directions (lead: John Linford) |
| 12:30 - 1:30 | Working Lunch (Provided) – Discussions on morning sessions – St. Helena Room |
| 1:30 - 2:45 | Plenary 3: Workforce, Security & Survey – Golden Gate Ballroom or zoom link <ol style="list-style-type: none"> Establishing a Workforce [30 mins] (Dorian Arnold, Emory Univ.) Practices Related to the Security & Integrity of Software & Data [30 mins] (Ryan Adamson, ORNL) Survey Results and Primer for Breakout Sessions [15 mins] (Terry Jones, ORNL) |
| 2:45 - 3:45 | Breakouts Session 3: Additional Challenges: Governance, Workforce and Organizational Challenges <ol style="list-style-type: none"> DEI & Workforce Development (breakout lead: Mke Jantz) – Mendocino Rm Security and Integrity of Software and Data (breakout lead: Barton Miller) – Sonoma Rm Exercise: What would we want new HPC Users to see from an aspirational viewpoint? (breakout lead: James Custer) – Monterey Rm Bootstrapping STEP in 2024 - How to “Bridge” Tasks in a Flexible way (breakout lead: Kevin Harms) – Boardroom Rm |
| 3:45 - 4:00 | Break – Golden Gate Ballroom |
| 4:00 - 5:30 | Report out summaries for Breakout Session 3: Golden Gate Ballroom or zoom link <ol style="list-style-type: none"> DEI & Workforce Development (breakout lead: Mke Jantz) Security and Integrity of Software and Data (breakout lead: Bart Miller) Exercise: What would we want new HPC Users to see from an aspirational viewpoint? (lead: James Custer) Bootstrapping STEP in 2024 - How to “Bridge” Tasks in a Flexible way (lead: Kevin Harms) |
| 5:30 - 5:35 | Closing Remarks / Adjourn Town Hall (Terry Jones, ORNL) – Golden Gate Ballroom or zoom link |



Questions?

*Thank you for helping STEP to deliver a sustainable computing **TOOLS ECOSYSTEM** in support of scientific discovery.*

Tools codesigned with

- *Tool Developers*
- *Applications*
- *Facilities*
- *Vendors*

