Thoughts on Software Sustainability from OLCF

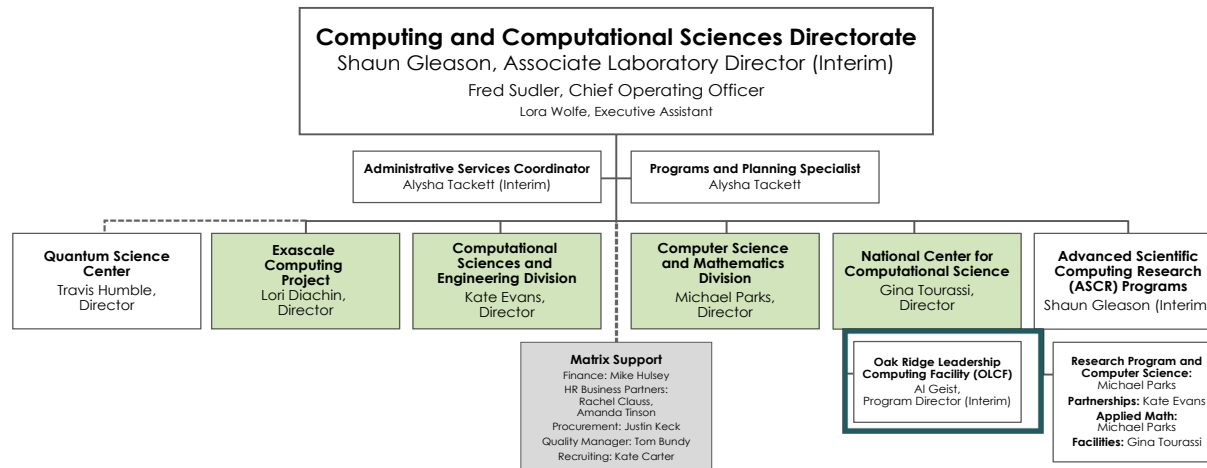Bálint Joó (joob AT ornl.gov) – *Oak Ridge Leadership Computing Facility, Oak Ridge, USA*

PESO Community Meeting

Argonne National Laboratory, June 8-9, 2023

ORNL is managed by UT-Battelle LLC for the US Department of Energy

About OLCF

- OLCF operates the worlds largest computer systems
  - Frontier (HPE/AMD) #1 on Top500 (1.19 EF HPL)
  - Summit (IBM/NVIDIA) #5 on Top500 (148 PF HPL)

- Primarily support INCITE and ALCC projects
  - 37 INCITE projects in 2022, 42 in 2023 (+/-1 due to me miscounting)
  - 24 ALCC projects in 2022-23 period

- OLCF liaisons
  - Assist in porting, optimizing, application workflows for users
  - Advocate for user needs
  - Collaborate scientifically with the users (as appropriate)

- Our place in the directorate org chart:

OLCF Frontier

OLCF Summit

Computing and Computational Sciences Directorate
Shaun Gleason, Associate Laboratory Director (Interim)
Fred Sudler, Chief Operating Officer
Lora Wolfe, Executive Assistant

Administrative Services Coordinator
Alysha Tackett (Interim)

Programs and Planning Specialist
Alysha Tackett

Quantum Science Center
Travis Humble, Director

Exascale Computing Project
Lori Diachin, Director

Computational Sciences and Engineering Division
Kate Evans, Director

Computer Science and Mathematics Division
Michael Parks, Director

National Center for Computational Science
Gina Tourassi, Director

Advanced Scientific Computing Research (ASCR) Programs
Shaun Gleason (Interim)

Matrix Support
Finance: Mike Hulsey
HR Business Partners: Rachel Clauss, Amanda Tinson
Procurement: Justin Keck
Quality Manager: Tom Bundy
Recruiting: Kate Carter

Oak Ridge Leadership Computing Facility (OLCF)
Al Geist, Program Director (Interim)

Research Program and Computer Science:
Michael Parks
Partnerships: Kate Evans
Applied Math:
Michael Parks
Facilities: Gina Tourassi

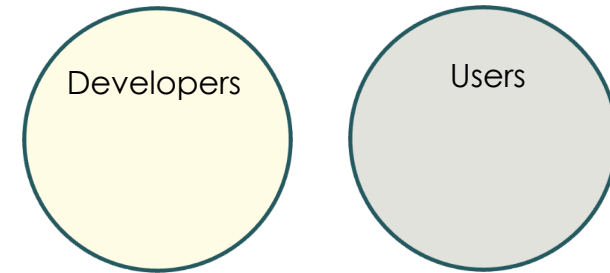OAK RIDGE National Laboratory | FACILITY

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OCLF's General Philosophy

- We want to enable our users to reach their scientific aims
- We want to help them as much as they want us to:
    - Some projects need a lot of help
    - Some projects need none
    - Our general preference is closely coupled, bespoke engagements
- We want to support and sustain software that we or our users need
    - We are reactive in this regard
    - Our liaisons may **suggest solutions**, but we will not proscribe them
- The bulk of software that runs on the system is user applications and dependencies they bring with them
    - OLCF primarily supplies the core programming environment and low level libraries
- OLCF is generally not staffed (time or expertise) to directly support the software used on the system
    - The liaisons and UA staff will help solve problems or find workarounds, but…
    - Real support necessarily comes from vendors or third-party software providers

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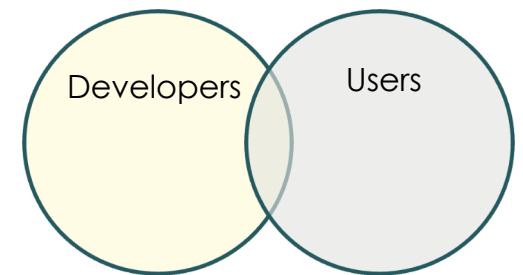National Laboratory | COMPUTING
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We want user software to run well on our systems

- Certain products are important dependencies for a large body of our users
  - Programming models, Profiling packages, build systems, basic libraries (BLAS, etc.)
  - Some we may support through funding (e.g. Kokkos)

- Others we anticipate will be brought along by our applications
  - e.g. Larger math libraries come to mind (PETSc, Trilinos,..)
  - Liaisons provide ECP AppInt-like support for these
    - E.g. Report bugs to and Shepherd resolution of issues with Vendor partners, ...

- We don't want a pre-installation of a library to carry an imprimatur of endorsement by OLCF. Library/App pre-installs are on a pragmatic, user-driven, case-by-case basis
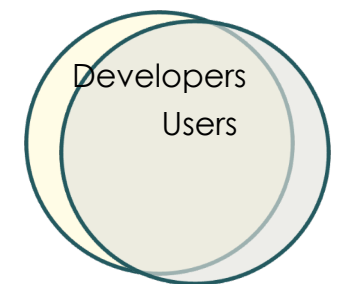 - We do provide User Managed Software areas on request

User Community A:

Developers   Users

User Community B:

Developers   Users

User Community C:

Developers
Users

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Certain things we are passionate about

- Engagement with the Software Sustainability Community
  - **David Rogers** at OLCF leads Software Sustainability WG in SciEng Section.
  - He is an excellent point person: `rogersdm` AT `ornl.gov`
  - He interacts with other groups within ORNL (e.g. CSED), and with IDEAS

- Good User Education and Training
  - tools, software best practices, writing sustainable software, productivity
  - strong engagement in community efforts by our User Engagement Section
  - this includes training on many products (e.g. through hackathons, or directly)
  - Liasons can suggest libraries/technoligies hey feel can help users
    - I am a strong proponent of Kokkos, CMake, Git (de-facto 'standard' tools of the trade)
    - But not all of my suggestions are accepted – and that i s OK.

- I personally strongly want to advocate for CI on LCF hardware
  - Push level CI is industry best practice.
  - Often, our newest hardware is not yet available in the cloud.
  - Even a fully open source stack would do so much for us.

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Acknowledgements

- This research used resources of the Oak Ridge Leadership Computing Facility, which is a DOE Office of Science User Facility supported under Contract DE-AC05-00OR22725.

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