



Best Practices for Research Software Engineers

- The Xpert Network -

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4 Main Points of Today

1. The Xpert Network
2. The driving motivation (and ECSS' role)
3. Initial results (best practices)
4. What's next (and what's in it for you)

1. The Xpert Network

- Activities: Monthly webinars on
 - Best practices for computational experts (Xperts)
 - Tools/environments to enhance Xpert productivity

In-person meetings (currently on hold)

- Website sites.udel.edu/xpert-cdi
- Who is invited:
 - Xperts from large sponsored projects (ECSS, CyVerse, Software Institutes, OSG,...)
 - National organizations (US-RSE, Car)
 - Campus RSE teams
 - Individual Xperts on computational science
 - Computational (and data) researchers

What are Xperts ?

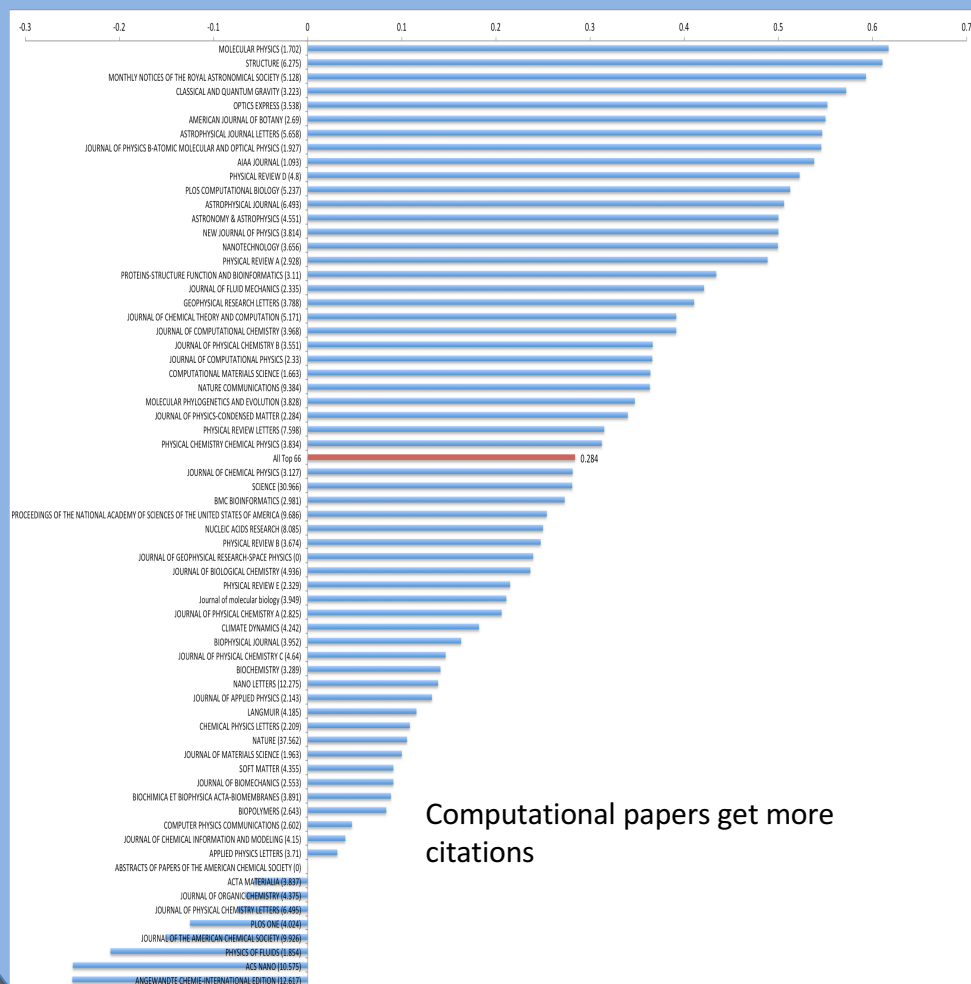
- Support computational and data-intensive research
- Research Software Engineers
- Research Facilitators
- Computational experts
- Research programmers

Bring together,
Create synergy !

2. The Driving Motivation

HPC&D is Pushing the Forefront of Science – Is there evidence?

CDS&E is higher-impact science



Investment in HPC infrastructure means higher impact

“Appearance on the Top 500 list is associated with a contemporaneous increase in NSF funding levels as well as a contemporaneous increase in the number of publications”

-- Ahalt, Apon et al., Journal of Information Technology Impact, Vol. 10, No. 2, pp. 87-98, 2010

2. The Driving Motivation

Where is ECSS' Role in All This?

- XSEDE's Extended Collaborative Support Service has highest "Return on Investment."
- Many projects have similar teams that support computational and data-intensive science. There wasn't a mechanism for exchange of experiences.



2. The Driving Motivation

What Kind of Synergy?



- Best Practices for Xperts/RSEs
- Tools and environments that enhance Xpert productivity
- Coordination

Not our focus: professionalization of RSEs

3. Best Practices

Exchanging Best Practices and Tools for Supporting Computational and Data-Intensive Research, The Xpert Network
[Parinaz Barakhshan](#), [Rudolf Eigenmann](#)
arxiv.org/abs/2102.09373

Summary of Best Practices

Best Practices for Collaborations:

- (1) **Diversity of Xpert Backgrounds**- Be aware of different backgrounds Xperts may bring into a team; configure training so that less-familiar best practices can be acquired as needed.
- (2) **Understanding the Academic Environment**- Be aware of the academic reward system and activities to increase academic standing.
- (3) **Breadth of Xpert Skills Needed**- Prepare for skills needed beyond your current expertise, by networking with other Xperts.
- (4) **Collaborative Assistance**- Help propel new projects though short-term, close collaboration with domain scientists.
- (5) **Overcoming the Terminology Gap**- Carefully identify and resolve terminology gaps. Keep vocabulary to the essentials. Explain using many examples.

Best Practices for Software Development:

- (6) **Developing a Project Plan**- Devote substantial time to understanding the domain problem, turning possibly vague ideas into a feasible solution approach, and developing a project plan.
- (7) **Prioritize Functional Requirements**- Carefully vet all requirements by the application's end users and prioritize aggressively.
- (8) **Issue Tracking**- Track origins as well as implementation status of requirements and bug reports.
- (9) **Source Code Management**- Make use of source code management and version control systems to track your software's evolution.
- (10) **Code Review**- Xpert and domain scientist should review each other's software written.
- (11) **Software Testing**- Define test cases that the application and its components must pass before you begin their implementation.
- (12) **Documentation**- Document your project to ensure long-term success, reproducibility, and obtain proper credit for your work.
- (13) **Continuous Integration**- Integrate new software updates frequently into the application version seen by the end users in their end environments.
- (14) **Reproducibility**- Enable reproducibility and transparency by capturing data and software underlying scientific processes, using available software platforms.
- (15) **Parallelization**- Write serial code first, then parallelize.

Summary of Tools

Tools for CDI Application Development:

- (1) **Project Management** - Jira [8], Kanban boards [16]
- (2) **Documentation** - Doxygen [20] (for C, C++, C#, D, Fortran, Java, Perl, PHP, Python), GhostDoc [33] (for C#, Visual Basic, JavaScript), Javadoc [49] (for Java).
- (3) **Source Code Management** - Git [34], GitHub [35], GitLab [37], Bitbucket [10], Mercurial [58].
- (4) **Issue Tracking** - Jira [8], Trello [86], Github Boards [36], Asana [7]
- (5) **System Build**- CMake [31], GNU Make [39]
- (6) **Compiler Reports and Diagnostics** - Intel [48], Gnu [40], PGI [64], Research Compilers: Cetus [79], Rose [77]
- (7) **Debuggers** - GDB (GNU Project debugger) [73], Arm DDT [5]
- (8) **Memory Debuggers** - Valgrind [88], AddressSanitizer (ASan) [1]
- (9) **Performance Analysis** - Intel Advisor [47], ARM Map [6], Tau [85], HPCtoolkit [22], mpiP [66]
- (10) **Test Frameworks** - Reframe test framework [76]
- (11) **Containers** - Docker [19], Singularity [84]
- (12) **Cloud-based Development Environments** - Eclipse Che [69], Amazon Cloud9 [3], Gitpod [38], Codespaces [15]
- (13) **Continuous Integration** - Travis CI [13], GitLab [37], Jenkins [50]
- (14) **Profiling/Tracing** - GNU Project Profiler (GPROF) [70], TAU [83]
- (15) **User interfaces to HPC resources** -
 - Science Gateways [32]
 - Open OnDemand [63]
 - Rich desktop clients, such as the Eclipse Parallel Tools Platform (PTP) [45]
 - Interactive applications, such as Jupyter [52], RStudio [78], JupyterHub [71], and Jupyter-Lab [52]

4. What's next (and what's in it for you)

- Webinar series
 - Share your experiences, learn from others
- In-person events
 - In-depth discussions
- Extended Best-Practices Report
 - Looking for co-authors
- NSF Cyberinfrastructure Center of Excellence
 - Join us to create a Xpert/RSE Collaboratorium



Thanks for listening !

sites.udel.edu/xpert-cdi



Discussion Time