Xpert Network Panel: Best practices for Computational and Data-intensive (CDI) Research

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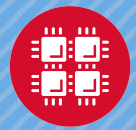
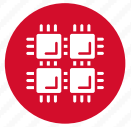


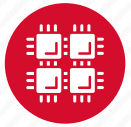
Best Practices

- Build a strong foundation
  - Computing: computer organization, operating systems, programming languages, software engineering, AI
  - Math: linear algebra, numerical analysis, statistics
  - The scientific method: computational science or data analytics
- Be curious
  - Learn about
    - New technologies, tools, languages and standards
    - What others are doing
  - Try things, experiment
    - How does this work? Is a faster or is b? etc.
- Be disciplined / methodical
  - Particularly important for debugging
  - Tools can help with this



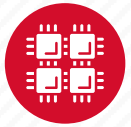
For RSE work specifically

- Communicate
  - Expectations / project goals
  - Ask questions
  - Meet regularly
- Corral the code
  - What version of the code am I starting with?
  - How do I build and run it?
  - How do I know if it's running correctly?
  - Choose a license (if there isn't one)
- Use modern tools
  - Source code repos (branch, merge, …)
  - Build systems / package managers
  - Compilers, debuggers, profilers
  - CI pipelines
- Automate frequent tasks
  - Regression & benchmark tests
  - Debugging runs
  - Treat scripts as code, they are
- Document …
  - The code (including scripts)
  - The install procedures
  - Issues and what you've tried and learned
- Nudge, don't push
  - Introduce new tools and processes gradually
  - Don't make code unrecognizable to the science team (without consent)
- Get a quick win (if you can)
  - Performance gain or bug fix

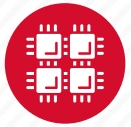


Training new team members

- Foundation gaps
  - Direct to resources (classes, tutorials, books, …)
  - Provide time for learning
- HPC specific skills
  - Direct to tutorials, bootcamps or online learning
- RSE mentoring
  - Coaching with respect to communication
  - Encourage use of appropriate tools
  - Guidance during debugging & troubleshooting
  - Be a resource (e.g. Fortran, netlib)
- Support participation in the RCD community by encouraging …
  - joining mailing lists and slack channels
  - attending seminars, webinars, community chats
  - attending workshops, tutorials, and conferences

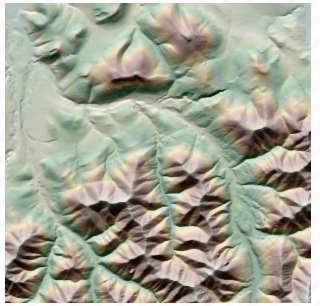


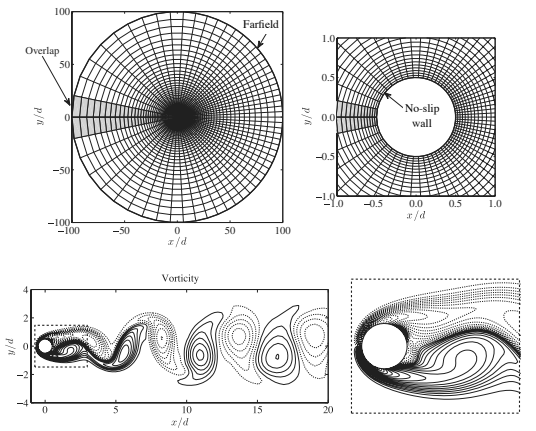
Backup Slides



Current RSE Project Portfolio

- SETSM Terrain Generation Code
  - C/C++, MPI+OpenMP
  - Code is in active development and used in a production environment
  - Software engineering, performance improvement
- FDL3DIv2 CFD software
  - Fortran, MPI+OpenMP
  - Performance improvement, modernize for new architectures
- Soil Spectroscopy
  - R
  - Software engineering, parallelization, development
- MVAPICH2 MPI
  - C/C++, Fortran, CUDA, new programming models (PGAS, tasks), Python
  - Performance analysis, case studies
- GPS Gear Simulation
  - Fortran, OpenMP
  - Port to Linux, add MPI parallelization





Tools we currently use

- Git / Gitlab, Cmake/make
- Docker and singularity
- Compiler reports and diagnostics: Intel, Gnu, Cray
- Debuggers: gdb, DDT
- Memory Debuggers: Valgrind, Asan (via gcc)
- Performance Analysis: Intel Advisor & ITAC, ARM Map & Performance reports, Tau, mpiP
- Manual Instrumentation: timing, dumping variables, checking memory use
- Reframe test framework, test scripts