

BREAK TIME ACTIVITY

- 1 Create an account on GitHub
- 2 Follow your friends (@rmmilewi and @gonsie)
- 3 Be Social

Modern Software Design, Tools, and Practices

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Outline

1 Mindset & Terms

2 Essential Practices & Common Tools for ...

- The Individual Contributor (Personal Use)
- HPC Software User
- Software Developer
- Scientist: Reproducible & Sustainable Software

Mindset

- Programming is a social activity
- Continue from Reed's talk
- Frame of mind: academic / scientific software.

Terms

Practice The actual application or use of an idea, belief, or method

Repeated performance of an activity so as to acquire or maintain proficiency in it

Best practice A method or technique that has been generally accepted because it produces results that are superior or it has become a standard way of doing things.

Tool An implement used in the practice of a vocation

How to Use These Slides

- You will start a project and work by yourself
- You will start a project and will want to bring other people on board
- You will join an existing project that already has some practices in place

Essential Practices & Common Tools for ...

- The Individual Contributor (Personal Use)
 - Time Management
 - Version Control
 - Continued Education
- HPC Software User
 - Using the Terminal
 - Building Software
 - Running Software
- Software Developer
 - Documentation
 - Testing
 - Issue Tracking
 - Debugging
 - Project Management
- Scientist
 - Licenses
 - Building Community
 - Reproducible Science
 - Sustainability

The Individual Contributor (Personal Use)

Photo by [Vlad Bagacian](#) from Pexels



Time Management in Practice

- Work life balance
- Learn what works for you and when you work best
- Scaling Yourself as a Software Developer

Time Management Tools

Have a system

- 1 Calendar
- 2 To Do List
- 3 Workflow / Time Tracking

Version Control in Practice

Hit 'Save' so I don't lose my work

A series of discrete changes needed to create the current state of the system.

Version Control Tools

- svn
 - git
 - mercurial
 - bazaar
-
- GitHub
 - GitLab
 - BitBucket

Version Control Workflow

Method to work with others.

- Contributing guidelines
- Pull requests
- Forks

Continued Learning in Practice

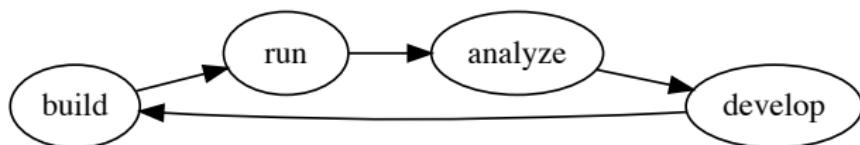
- Social networks and blogs, [dev.to](#) or StackOverFlow
- Conferences & Workshops
- Online Learning
- More school

HPC Software User



HPC in Practice

- Log in to a system, usually through a terminal using SSH
- Must *do work* on the system



Terminal Tools

- bash
- csh
- tsh
- zsh
- fish
- nu shell
- emacs
- vim
- VSCode
- Sublime Text
- atom

Building Software

```
gcc source.c
```

```
gcc source.c -o my_program
```

```
gcc source.c util.c -o my_program -g -O2 -lboost -I/opt/boost
```

Build Tools

- make *Magical Incantation*
- autotools `configure # or ccmake`
- CMake `make`
- Spack `make install`

Running Jobs & Schedulers

- Queuing
- Fair share
- Back fill
- Allocations: batch vs.
interactive
- Slurm
- Moab
- LSF
- PBS
- Flux

Software Developer

Source: #WOCinTech Chat



Types of Documentation

Know your audience

- Users
- Developers
- Academics/Collaborators
- Customers

Documentation Tools

- README.txt file
- Wiki from the hosting platform
- Website
 - built on GitHub/GitLab Pages
- In-source documentation
 - Doxygen
 - Sphinx
 - readthedocs
- Conference & Journal Papers
 - latex

Testing in Practice

Test-Driven Development (TDD) Turn requirements in to very specific test cases.

Testing Tools

Make testing easy to do.

- make test
- TravisCI
- Gitlab runners, Bamboo Agents
- Codecov

Issue Tracking

User Get help when the software
doesn't work as expected

Suggest changes

Developer Keep a shared list of things to
work on

Outsider Get involved with a project

- Bug tracker
- Jira
- Github/Gitlab issues

Debugging: Challenges in HPC

- Hit bugs only at scale
- `printf` can get munged
- Launch multiple tasks from debugger

Debugging Tools

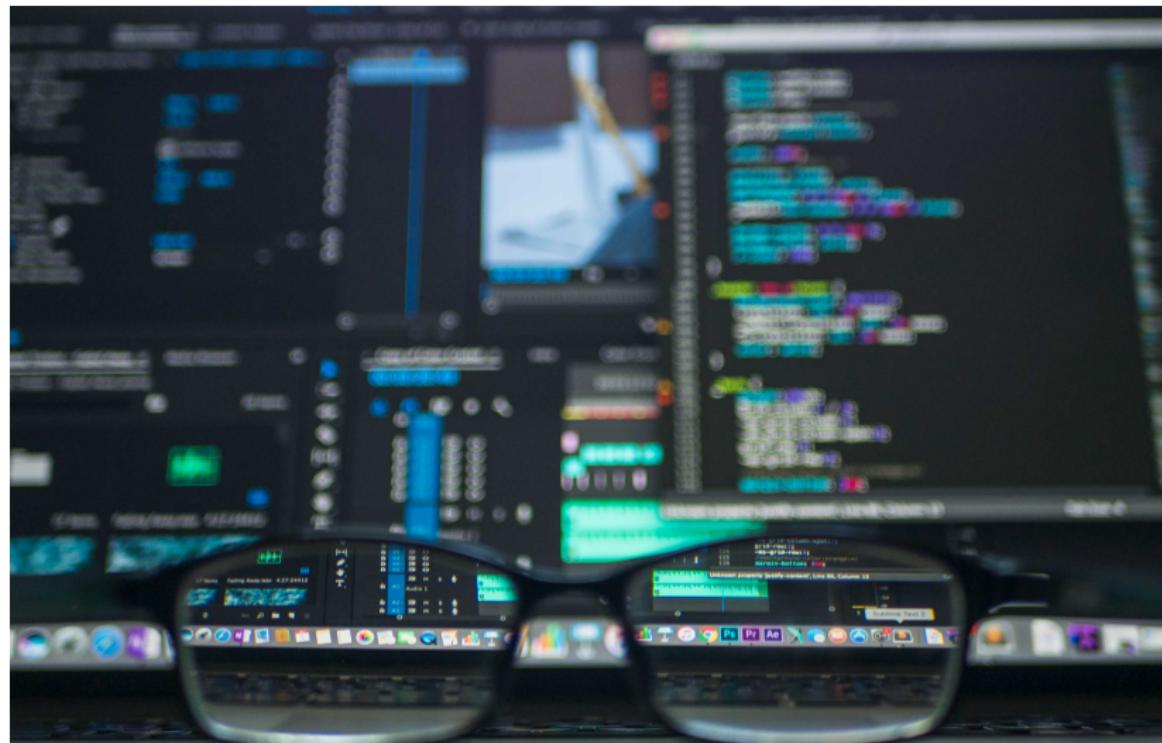
- printf
- gdb / lldb
- TotalView
- Stat, Archer, MPI Replay

Project Management

- Waterfall
- Agile
- Scrum
- Systems engineering

Scientist: Reproducible & Sustainable Software

Photo by [Kevin Ku](#) from Pexels



Scientist

- Licenses
- Community
- Reproducibility
- Sustainability

Resources

- A PhD is Not Enough: A Guide to Survival in Science (goodreads)
- Software Sustainability Institute (SSI)
- CII Best Practices Badge Program
- Better Scientific Software (BSSw)

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