

# 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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## 1 Mindset & Terms

## 2 Essential Practices & Common Tools for ...

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

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



**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*

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*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

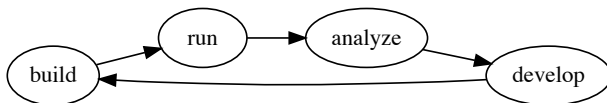
# Continued Learning in Practice

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

# HPC Software User



- 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

```
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
- autotools
- CMake
- Spack

## *Magical Incantation*

```
configure # or cmake  
make  
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

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

*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

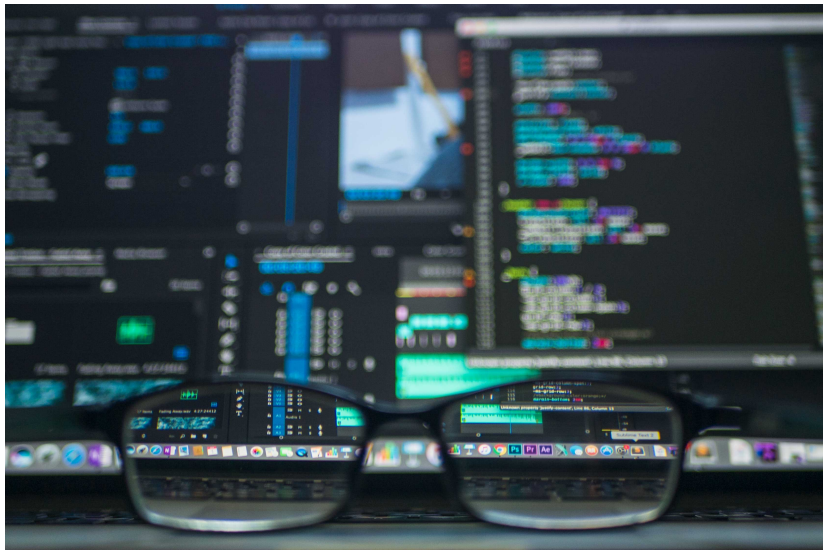


# Project Management

- Waterfall
- Agile
- Scrum
- Systems engineering

# Scientist: Reproducible & Sustainable Software

Photo by [Kevin Ku](#) from Pexels



- 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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