





Rinku Gupta (she/her)
Argonne National Laboratory



Better Scientific Software tutorial @ SC21

Contributors: Rinku K. Gupta (ANL), Michael A. Heroux (SNL), James M. Willenbring (SNL)





License, Citation and Acknowledgements

License and Citation

• This work is licensed under a CC BY 4.0).



- The requested citation the overall tutorial is: David E. Bernholdt, Anshu Dubey, Patricia A. Grubel, Rinku K. Gupta, and Gregory R. Watson, Better Scientific Software tutorial, in the International Conference for High-Performance Computing, Networking, Storage, and Analysis (SC21), St. Louis, MO, USA and online, 2021. DOI: 10.6084/m9.figshare.16556628
- Individual modules may be cited as Speaker, Module Title, in Better Scientific Software tutorial...

Acknowledgements

- This work was supported by the U.S. Department of Energy Office of Science, Office of Advanced Scientific Computing Research (ASCR), and by the Exascale Computing Project (17-SC-20-SC), a collaborative effort of the U.S. Department of Energy Office of Science and the National Nuclear Security Administration.
- This work was performed in part at the Argonne National Laboratory, which is managed by UChicago Argonne, LLC for the U.S. Department of Energy under Contract No. DE-AC02-06CH11357.
- This work was performed in part at the Oak Ridge National Laboratory, which is managed by UT-Battelle, LLC for the U.S. Department of Energy under Contract No. DE-AC05-00OR22725.
- This work was performed in part at the Lawrence Livermore National Laboratory, which is managed by Lawrence Livermore National Security, LLC for the U.S. Department of Energy under Contract No. DE-AC52-07NA27344.
- This work was performed in part at the Los Alamos National Laboratory, which is managed by Triad National Security, LLC for the U.S. Department of Energy under Contract No.89233218CNA000001
- This work was performed in part at Sandia National Laboratories. Sandia National Laboratories is a multi-mission laboratory managed and
 operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for
 the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.





Outline

- Refining our Epic
- PSIP: Productivity and Sustainability Improvement Planning





More on Epic, Story, Task

- Definition of Done
- Refining Issues
- Agile Estimation





Epic, Story, Task Review

- Break down and refine when and as needed
 - Close to when the work will be done
 - Only for work that will take place
 - Can be valuable for estimating
 - There is no "correct" level of granularity
- Epics are very high level objectives
- Stories should represent an increment of value to the customer
 - "Definition of Done" understandable to user
- Tasks are the steps necessary to complete a story
 - May not individually provide value to the customer





Definition of Done

- Simplified definition: When all acceptance criteria are met
- Acceptance criteria
 - "Conditions that a software product must satisfy to be accepted by a user, customer or stakeholder." – Microsoft Press
 - "Pre-established standards or requirements a product or project must meet."
 - Can include functional, non-functional, and performance requirements.





Definition of Done

- Important to establish for a story before estimating or beginning a task
- Defined by the team, acceptable to customer
 - Customer language
- Should not specify an implementation unnecessarily





Refining Our Epic

- Epic: Refactor code for enhanced modularity
 - Description: The heat equation code needs refactoring to improve modularity.
 Specifically, there are utilities that could be generalized and used with for other applications. Also, the integration function is currently hard-coded. In the future, we want to use alternative integration functions, so we should generalize the interface for this function.
 - Story 1: Separate out utilities
 - Definition of Done
 - Task list
 - Story 2: Separate out integration function
 - Definition of Done
 - Task list





Refining Our Epic

- Story 1: Separate out utilities
 - Definition of Done
 - Unit tests pass
 - Code review completed
 - Integration/system tests pass
 - Utility performance is at least 95% of pre-separation performance
 - Utility usability demonstrated outside of heat equation application
- Story 2: Separate out integration function
 - Task 1: Add testing for integration function to protect functionality during refactor
 - Needed testing should be specified
 - Task 2: Generalize interface to allow alternative implementations
 - Task 3: Expose current integration function through the new interface & run tests





Agile Estimation

- Estimating is hard
 - Requires practice
 - With practice, it is still hard
- Stories are estimated using "story points"
 - Relative estimate
 - Many estimating techniques
 - Should NOT map to hours, days, etc
 - Definition of done needed, tasking not required
- Tasks are estimated in hours
 - Absolute estimate
- Useful for planning schedules

Key concept:

It is easier to accurately estimate many small tasks than to estimate a large epic.

Epic: Huge refactor effort

Tasks:

- Add tests
- Generalize interface
- Expose existing interface





How To Get Better

"Use iteration and incrementation only for projects you want to succeed."

- Adaptation of Martin Fowler quote





Strategy for Incremental Productivity Improvements

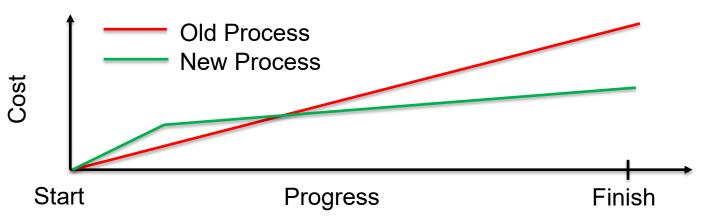
• Identify, analyze, prototype, test, revise, deploy. Repeat.

Realistic: There is a cost.

Startup: Overhead

Payoff: Best if soon, clear

Productivity and Sustainability Improvement Planning (PSIP): <u>https://bssw.io/psip</u>



- Working model:
 - Reserve acceptable time/effort for improvement.
 - Improve how you do your work on the way to getting it done.
 - Repeat.





Productivity and Sustainability Improvement Planning (PSIP) Examples: EXAALT & MPICH



MPICH PSIP: Onboarding new team members

Practice: Create Centralized Training Resources
Score Description Tracking

O Initial Status: No training process in place.

1 Understand MPICH requirement for developers and typical challenges for new hires
2 Review and gather specific training materials
3 Design "MPICH Training Base" website
4 Solicit feedback, improve, add and prune content to ensure effectiveness

PSIP workflow helps a team create user stories, identify areas for improvement, select a specific area and topic for a single improvement cycle, and then develop those improvements with specific metrics for success.

