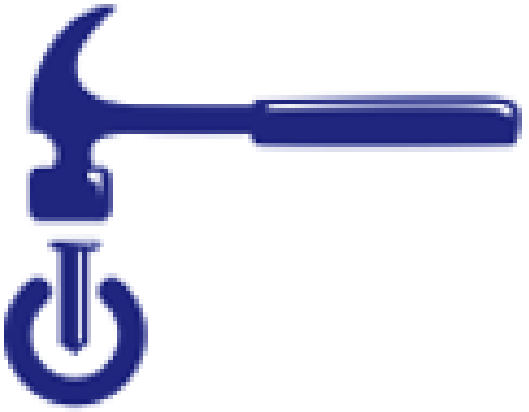
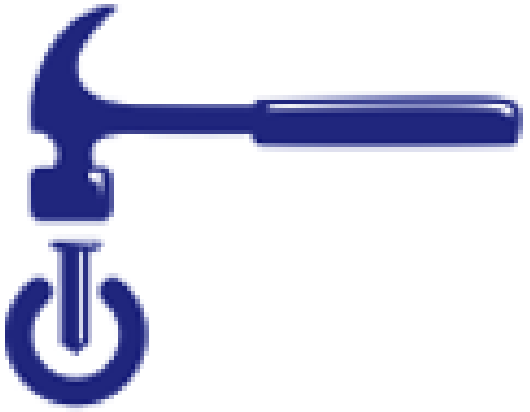


Welcome to Software Carpentry!
January 13-16, 2015

Instructors:

Matt Gidden
Steve Goldstein
Lauren Michael
Danielle Nielsen
Cliff Rodgers
Paul Wilson

ACI
Advanced Computing
Infrastructure

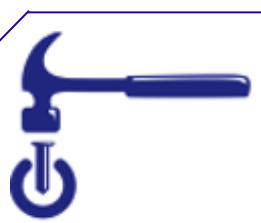


If You Can't Reproduce It, Is It Still Science?

And how long will it take?

Paul Wilson

Inspired by Greg Wilson
Software Carpentry



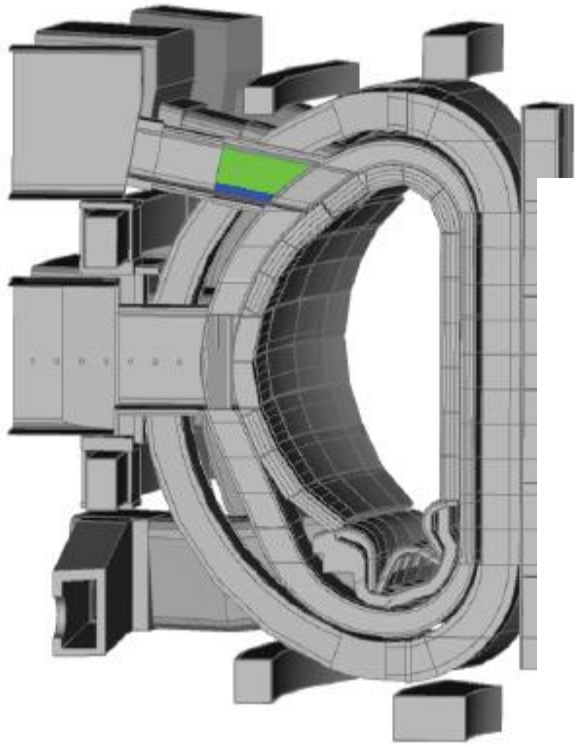
Reality of Research Computing

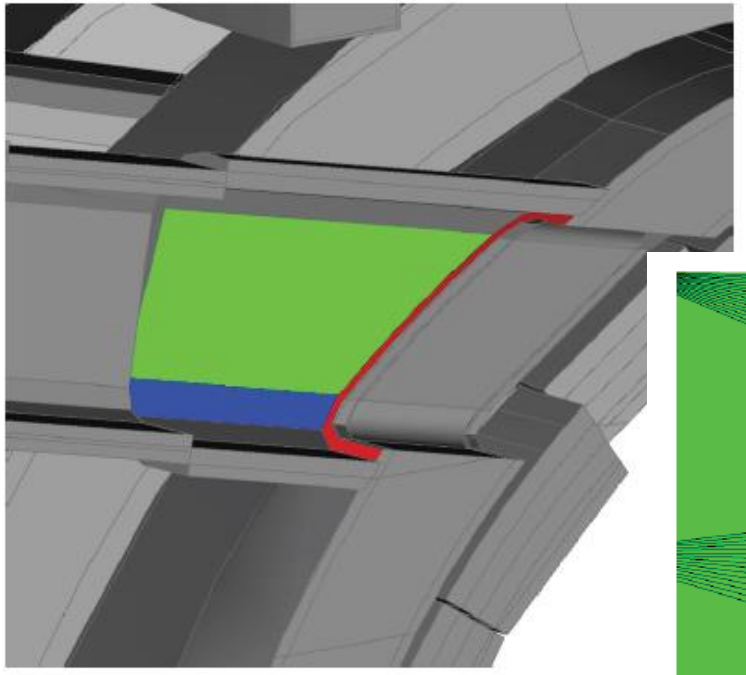
- Many scientists spend most of their time developing, maintaining, or running software
  - Most don’t consider themselves software engineers
  - Few have ever been taught how
    - Learned on-the-job
    - Communal knowledge

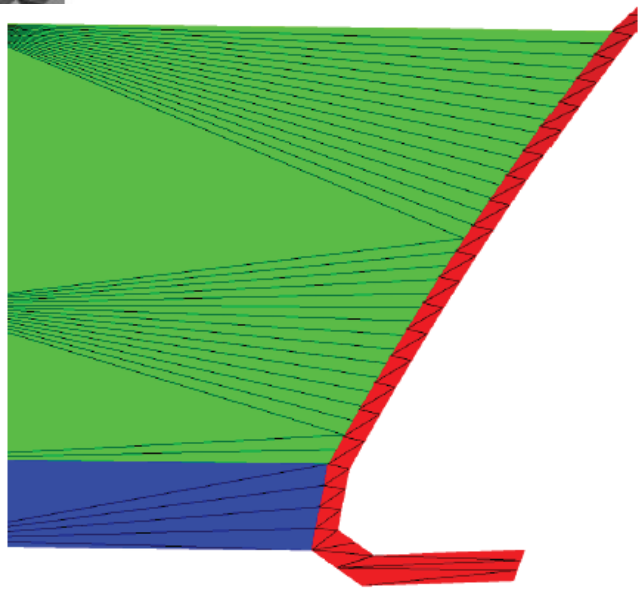
So What…

- Most results take longer to produce than they need to
  - Not because of a lack of computers
- Difficult to assess quality
  - Often measured by reproducibility
  - “System” doesn’t care

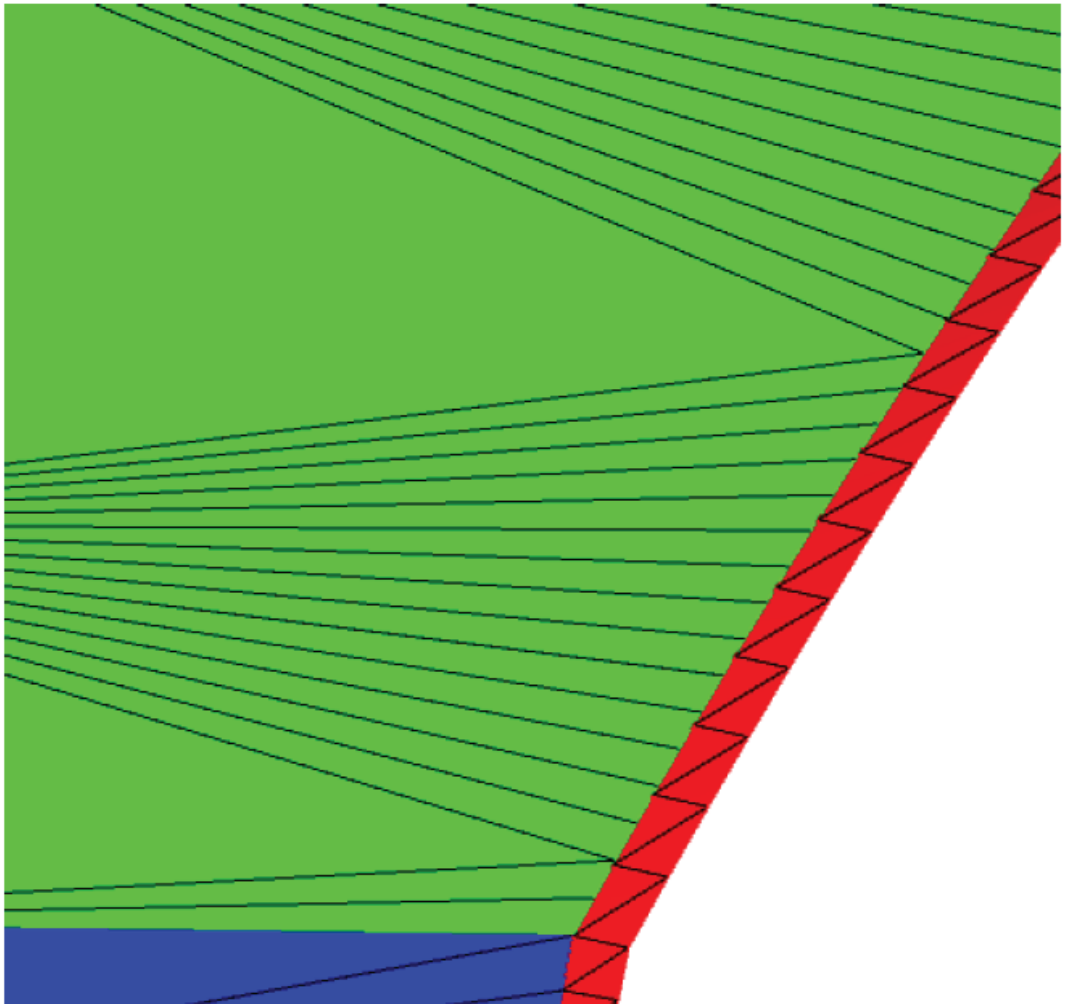
A Recent Story:
Sealing a Faceted Geometry





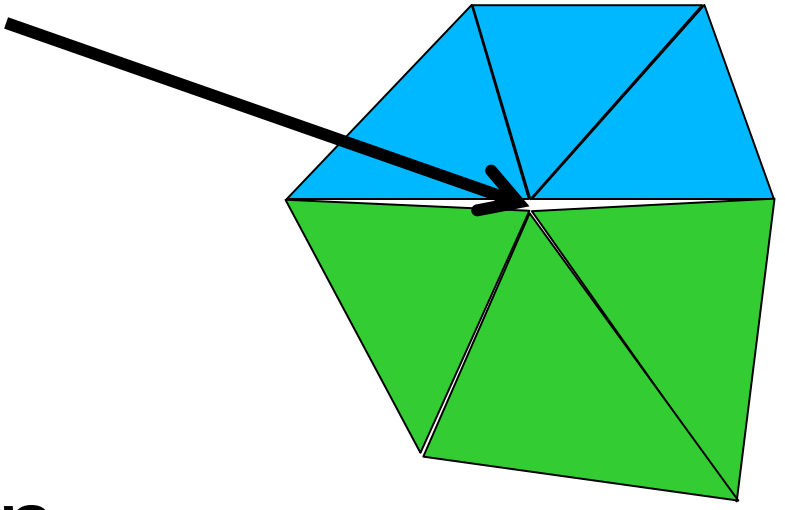


A Recent Story:
Sealing a Faceted Geometry



A Recent Story: Sealing a Faceted Geometry

- Lost particles through “leaks”
- Reduce confidence in solution

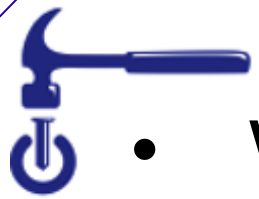


A Recent Story: Sealing a Faceted Geometry

Model	Particles Simulated [millions]	Lost Particles	
		Original	Robust
UW Nuclear Reactor	41	5649 ± 178	0
Advanced Test Reactor	74	141 ± 32	0
40° ITER Benchmark	225	67 ± 39	0
ITER TBM	205	665 ± 184	0
ITER Module 4	59	59 ± 19	0
ITER Module 13	79	450 ± 60	0
FNG Benchmark	1310	31273 ± 989	0
ARIES First Wall	4070	25 ± 18	0
HAPL IFE	286	65 ± 19	0
Z-Pinch Fusion	409	2454 ± 317	0

Software Carpentry to the Rescue

- Best practices used by the best software engineers whose business is development of quality software
  - They don’t always have formal training
  - They don’t always follow all the practices
  - Growing evidence supported by empirical studies



- Write software for people, not computers
- Automate repetitive tasks
- Use the Computer to Record History
- Make Incremental Changes
- Use Version Control
- Don’t Repeat Yourself
- Plan for Mistakes
- First make it correct, then make it fast
- Document Design & Purpose
- Conduct Code Reviews

Two Days ≠ Ten Practices

- Automate repetitive tasks
- Write software for people, not computers
- Don’t Repeat Yourself (or Others)
- Make Incremental Changes/Use Version Control
- Plan for Mistakes
- Conduct Code Reviews

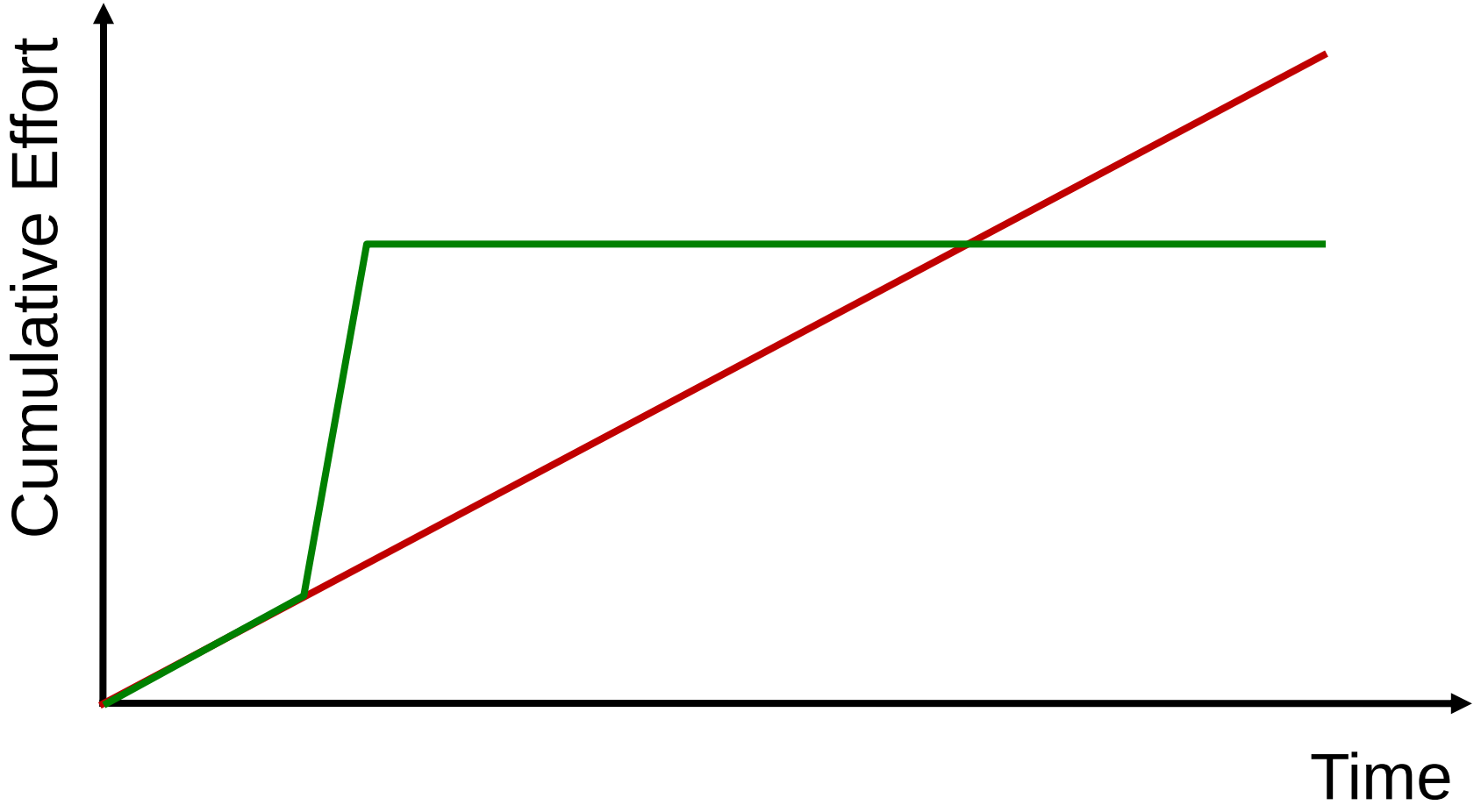
Make Incremental Changes Redux

- This applies to HOW you work
- Choose one practice
  - Implement it in your work
  - Share it with your lab group
  - Allow it to sink in
- Repeat

How to Choose Where to Start?

- It will depend on the nature of your work
- Consider the purpose:
  - Improve productivity
  - Improve quality

Thoughts on Productivity and Automation



Thoughts on Productivity and Automation

HOW LONG CAN YOU WORK ON MAKING A ROUTINE TASK MORE EFFICIENT BEFORE YOU'RE SPENDING MORE TIME THAN YOU SAVE?
(ACROSS FIVE YEARS)