

# Welcome to Software Carpentry!

## August 25 & 26, 2014

### Instructors:

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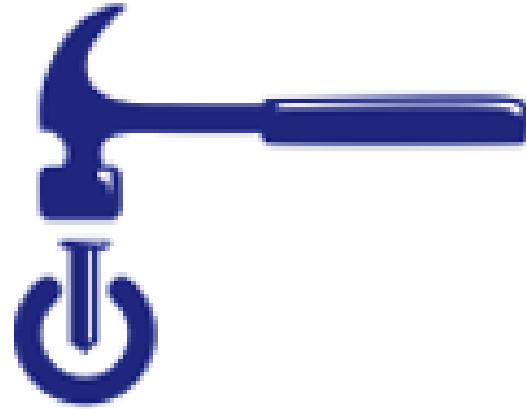
Matt Gidden

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Paul Wilson





# 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
    - Tribal knowledge

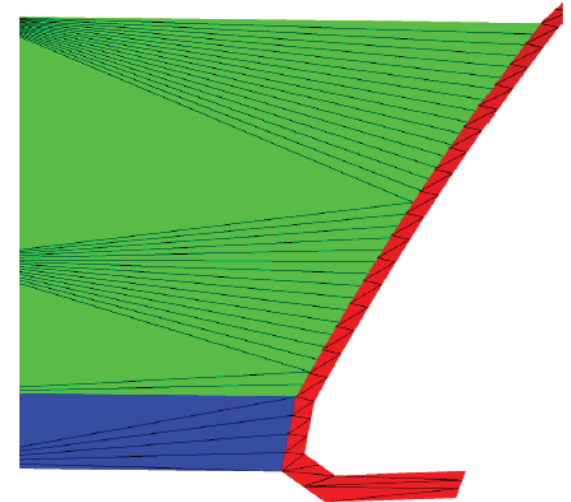
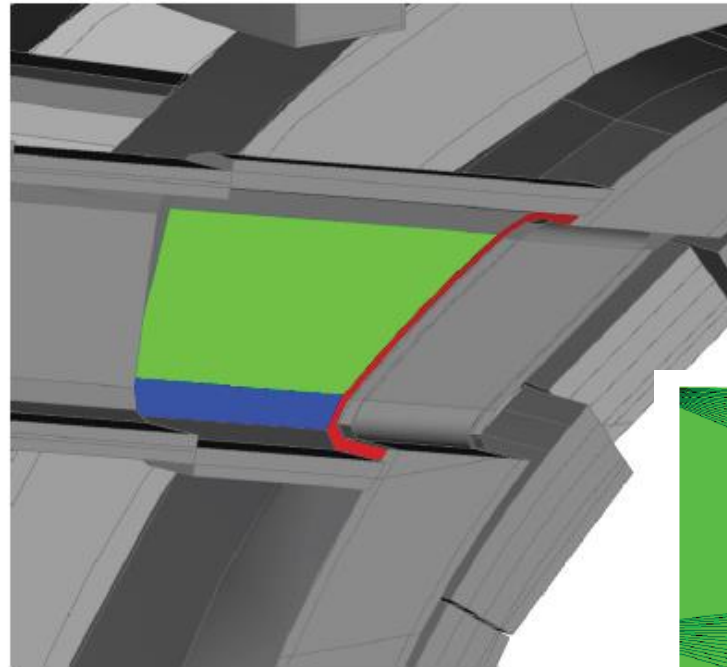
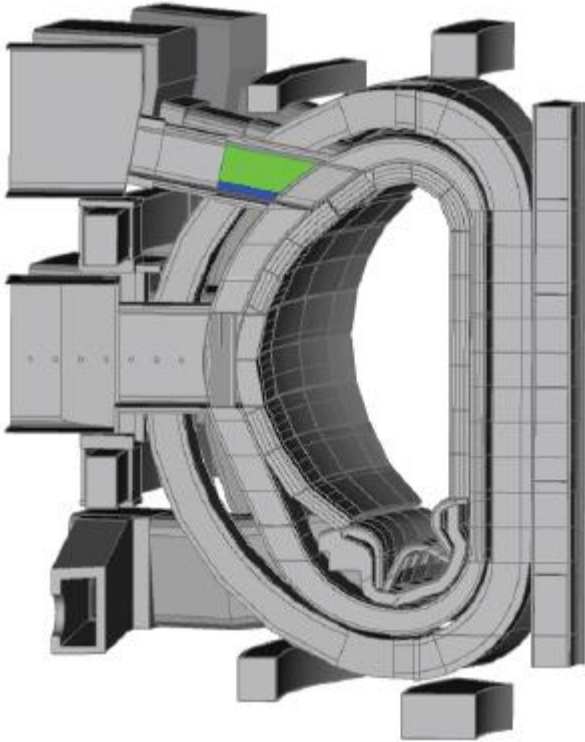


## So What...

- 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

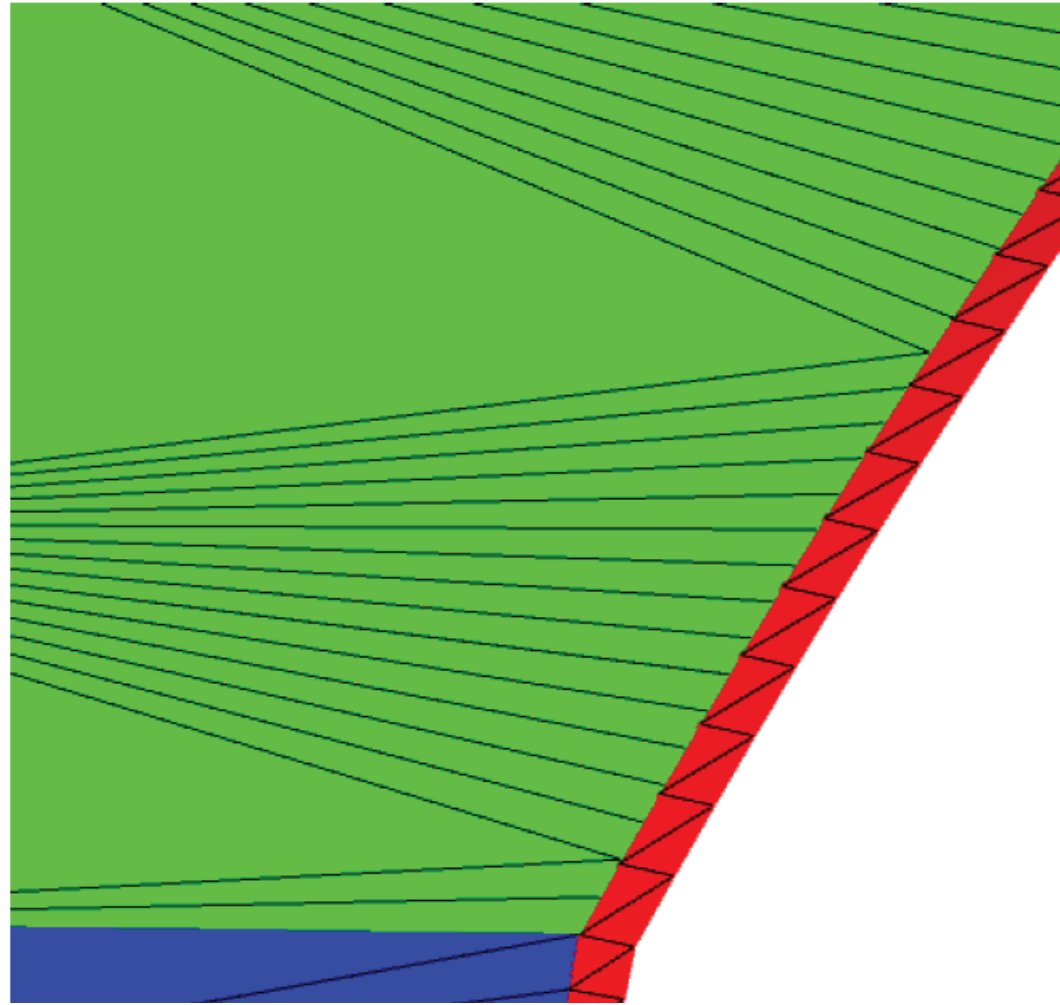


# A Recent Story: Sealing a Faceted Geometry





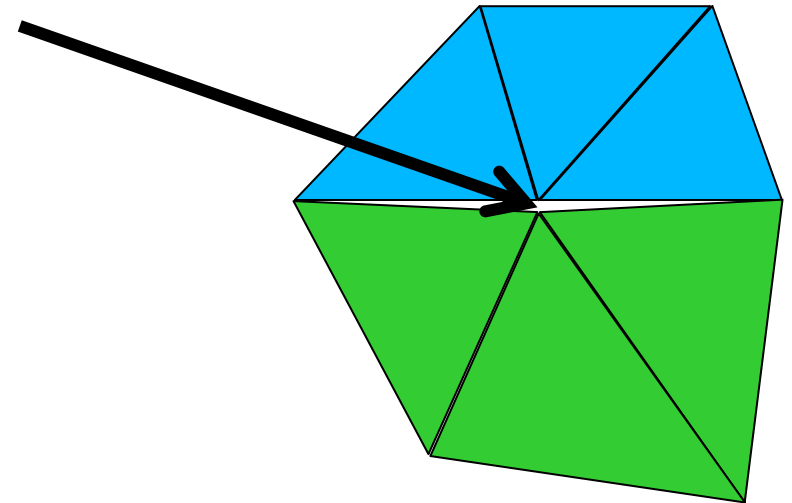
# A Recent Story: Sealing a Faceted Geometry





# A Recent Story: Sealing a Faceted Geometry

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





# A Recent Story: Sealing a Faceted Geometry

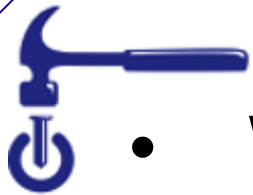
| Model                 | Particles Simulated<br>[millions] | Lost Particles  |        |
|-----------------------|-----------------------------------|-----------------|--------|
|                       |                                   | Original        | Robust |
| UW Nuclear Reactor    | 41     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

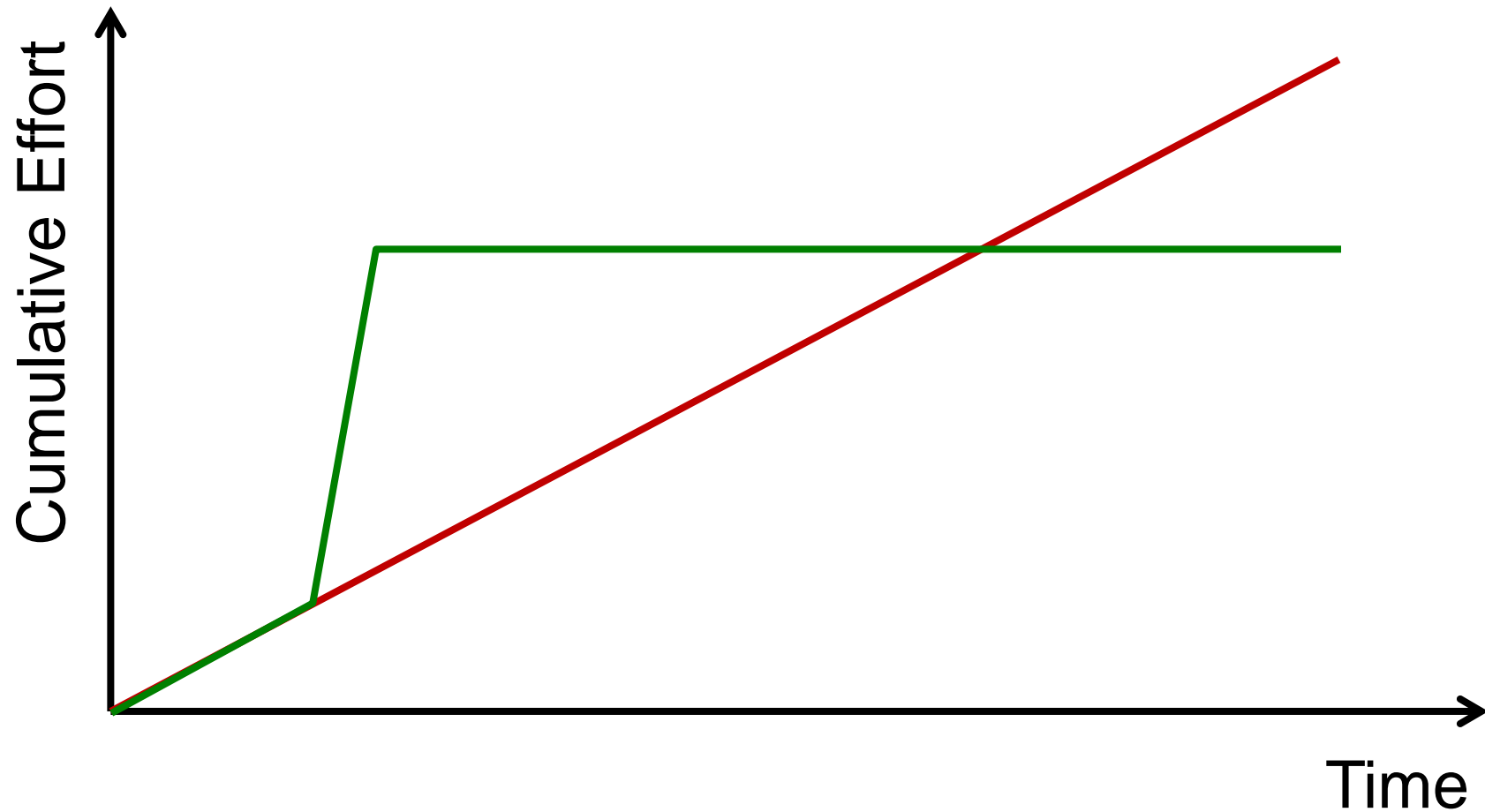


# How to Choose Where to Start?

- 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)

|                             |            | HOW OFTEN YOU DO THE TASK |           |            |            |            |            |
|-----------------------------|------------|---------------------------|-----------|------------|------------|------------|------------|
|                             |            | 50/DAY                    | 5/DAY     | DAILY      | WEEKLY     | MONTHLY    | YEARLY     |
| HOW MUCH TIME YOU SHAVE OFF | 1 SECOND   | 1 DAY                     | 2 HOURS   | 30 MINUTES | 4 MINUTES  | 1 MINUTE   | 5 SECONDS  |
|                             | 5 SECONDS  | 5 DAYS                    | 12 HOURS  | 2 HOURS    | 21 MINUTES | 5 MINUTES  | 25 SECONDS |
|                             | 30 SECONDS | 4 WEEKS                   | 3 DAYS    | 12 HOURS   | 2 HOURS    | 30 MINUTES | 2 MINUTES  |
|                             | 1 MINUTE   | 8 WEEKS                   | 6 DAYS    | 1 DAY      | 4 HOURS    | 1 HOUR     | 5 MINUTES  |
|                             | 5 MINUTES  | 9 MONTHS                  | 4 WEEKS   | 6 DAYS     | 21 HOURS   | 5 HOURS    | 25 MINUTES |
|                             | 30 MINUTES |                           | 6 MONTHS  | 5 WEEKS    | 5 DAYS     | 1 DAY      | 2 HOURS    |
|                             | 1 HOUR     |                           | 10 MONTHS | 2 MONTHS   | 10 DAYS    | 2 DAYS     | 5 HOURS    |
|                             | 6 HOURS    |                           |           |            | 2 MONTHS   | 2 WEEKS    | 1 DAY      |
|                             | 1 DAY      |                           |           |            |            | 8 WEEKS    | 5 DAYS     |