What We Have Learned About Using Software Engineering Practices in Scientific Software

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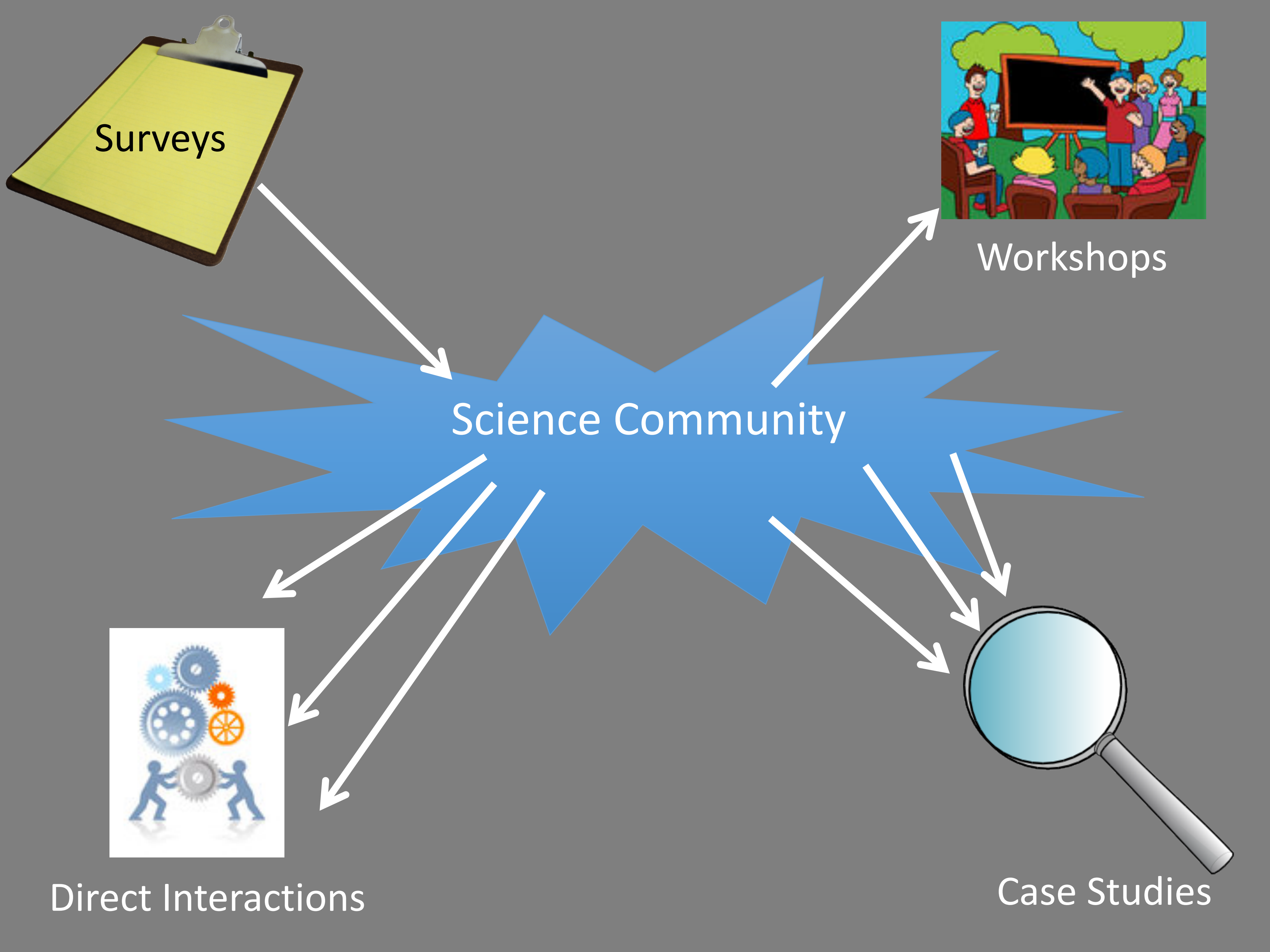
March 1, 2017


Surveys
Workshops
Science Community
Direct Interactions
Case Studies

Community Surveys

Community Surveys:
First Survey

- Sufficiency of SE Knowledge
  - Personally - 92% said yes
  - Science community - 63% said yes

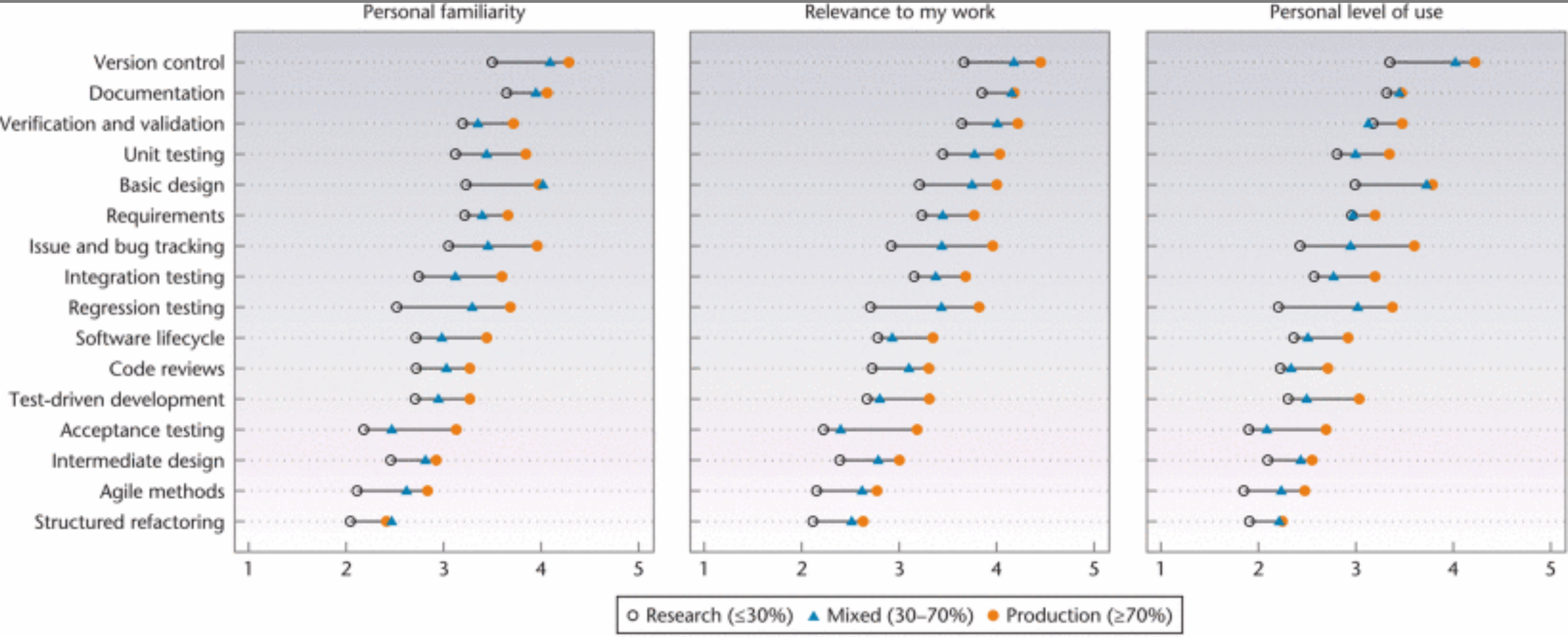
- Research vs. Production

- Reported 4 Key Problems
  - Rework
  - Performance issues
  - Regression
  - Forgetting to fix bugs not tracked

Community Surveys: Second Survey

- Broad subset of CSE audience – 151 responses
- Level of usage of various SE practices
- Generally agreed with our definitions of SE terminology

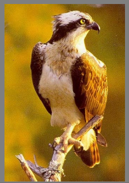
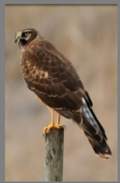
Community Surveys: Second Survey



Carver, J., et al. "Self-Perceptions about Software Engineering: A Survey of Scientist and Engineers." *Computing in Science & Engineering,* 15(1):7-11

Case Studies

Case Studies

	FALCON	**HAWK**	**CONDOR**	**EAGLE**	**NENE**	**OSPREY**	**HARRIER**
Application Domain	Prediction of Product Performance	Predication of Manufacturing Process	Analysis of Product Performance	Signal Processing	Calculate Molecule Properties	Weather Forecasting	Engineering Mesh Generation
Duration (Years)	~ 10	~ 6	~ 20	~ 3	~ 25	~10	~8
# of Releases	9 (production)	1	7	1	?	?	~16
Staffing (FTEs)	15	3	3-5	3	~10 (100's of contributors)	~10	5 primary + students
Customers	< 50	10s	100s	None	~ 100,000	100s	10s
Code Size (LOC)	~ 405,000	~ 134,000	~200,000	< 100,000	750,000	150,000	50,000
Primary Languages	F77 (24%), C (12%)	C++ (67%), C (18%)	F77 (85%)	C++, Matlab	F77 (95%)	Fortran	C++ (50%), Python (50%)
Other Languages	F90, Python, Perl, ksh/csh/sh	Python, F90	F90, C, Slang	Java Libraries	C	C	None
Target Hardware	Parallel Supercomputer	Parallel Supercomputer	PCs to Parallel Supercomputer	Embedded Hardware	PCs to Parallel Supercomputer	Parallel Supercomputer	Linux, Windows

Case Studies: Lessons Learned

- Verification and Validation are difficult
- Performance competes with other goals
- Use of higher-level languages is low
- Developers prefer command line over IDE
- Agile development methods are useful
- Primary language does not change
- External software is risky
- Multi-disciplinary teams are important
- Success/failure depends keeping customers/sponsors satisfied

Lessons Learned:
Validation and Verification

http://dilbert.com/strip/2010-11-07

Lessons Learned: Validation and Verification

- Vary in formality and completeness
  - Core algorithms vs. User Interactions
  - Percentage of code tested
  - Dedicated testers vs. End users
- Required by sponsor?
- Existing verification techniques not useful

“V&V is very hard because it is hard to come up with good test cases”

Lessons Learned:
Validation and Verification

"I have tried to position CONDOR to the place where it is kind of like your trusty calculator – it is an easy tool to use. Unlike your calculator, it is only 90% accurate … you have to understand that then answer you are going to get is going to have a certain level of uncertainty in it. The neat thing about it is that it is easy to get an answer in the general sense <to a very difficult problem>."

"We have a rule of thumb. We plot 2 lines (from Matlab and C++ programs) and if close, then it is ok."

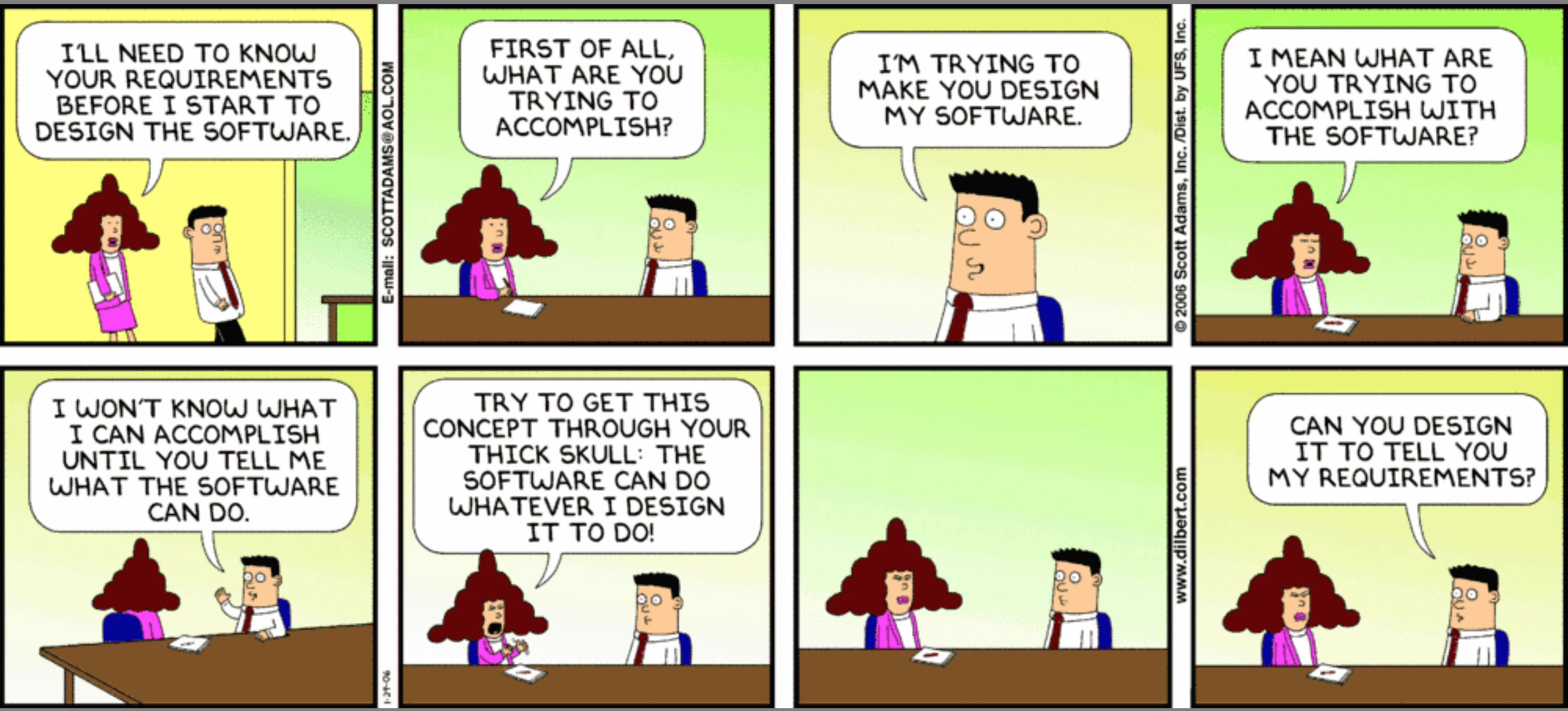
"It is an engineering judgment as to which errors are important and which ones are on the margins"

Lessons Learned:
Validation and Verification

- Implications
  - Traditional software testing methods are not sufficient
  - Need methods that ensure the quality and limits of software

- Suggestions
  - Inspections
  - Formal planning
  - Use of regression test suites

Lessons Learned:
Agile vs. Traditional Methodologies



Lessons Learned:
Agile vs. Traditional Methodologies

- Requirements constantly change as scientific knowledge evolves

- "Agile" software development methods
  - Tend to be more adaptable to change
  - Favor individuals and practices over process and tools

- Teams operate with agile philosophy by default

- Implications
  - Appropriate, flexible SE methodologies need to be employed for CSE software development
  - Agile-inspired approaches may be most appropriate

SE4Science Workshops

SE4Science Workshop Series
http://SE4Science.org

- Facilitate interaction between SE and Computational Scientists

- Held at ICSE, ICCS, and SC

- Discussion Topics
  - Testing scientific software
  - Trade-offs between quality goals
  - Research Software vs. IT Software
  - Crossing the communication chasm
  - Measuring impact on scientific productivity
  - Reproducibility of results

SE4Science Workshop Series
Testing Scientific Software

- Stakes not high enough to make testing important
- Needs differ across domains
- Focus on process transparency
- Guaranteed not to give an incorrect output

SE4Science Workshop Series
Scientific Impact

- Need to evaluate impact
- Scientific productivity ≠ Software productivity
- Need results in a relatively short time
  - Self-assessments
  - Word of mouth

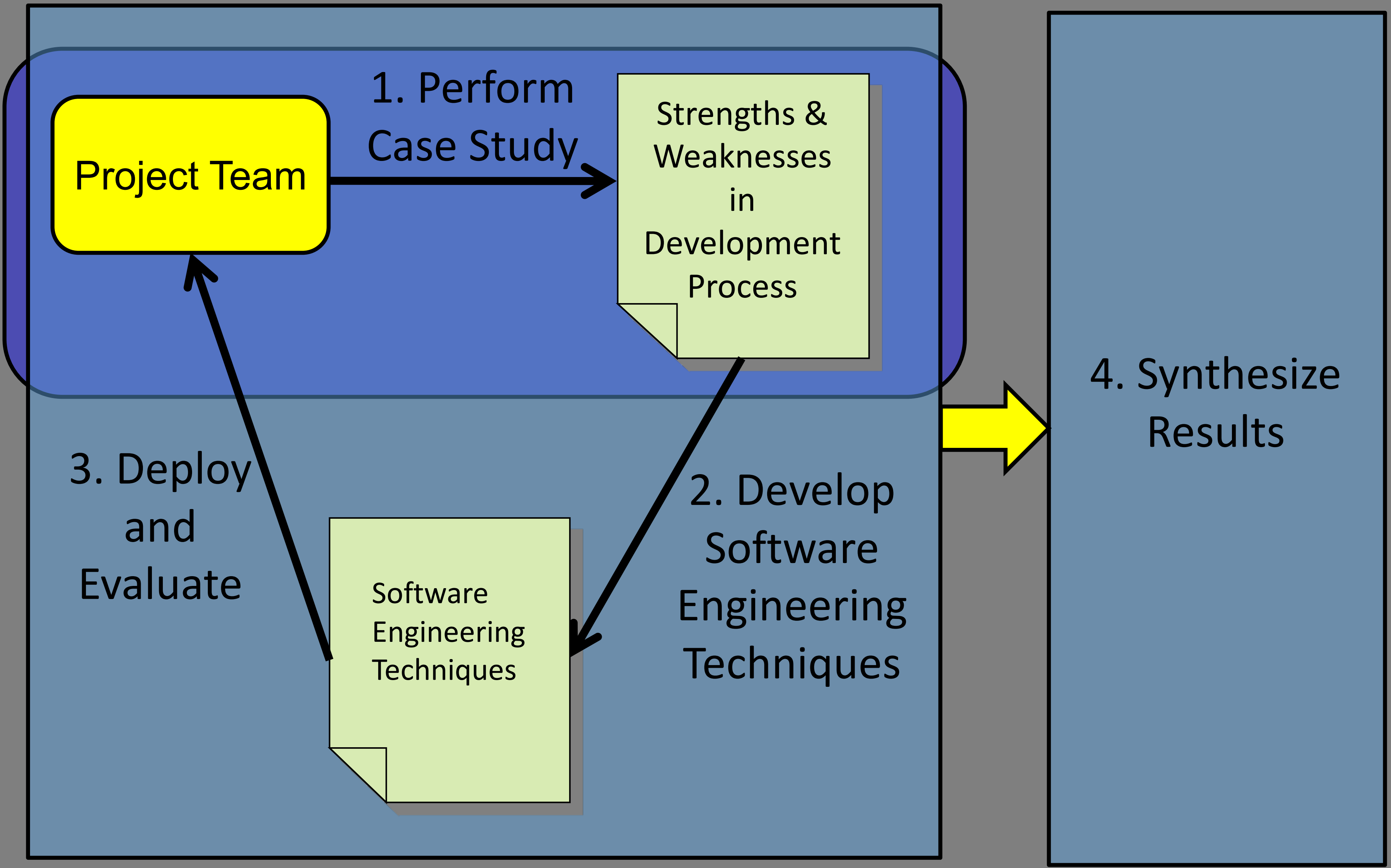
SE4Science Workshop Series
http://SE4Science.org

- May 22 – during ICSE'17
- Buenos Aires
- Please consider submitting papers and attending

http://SE4Science.org/workshops/se4science17/

Direct Interactions

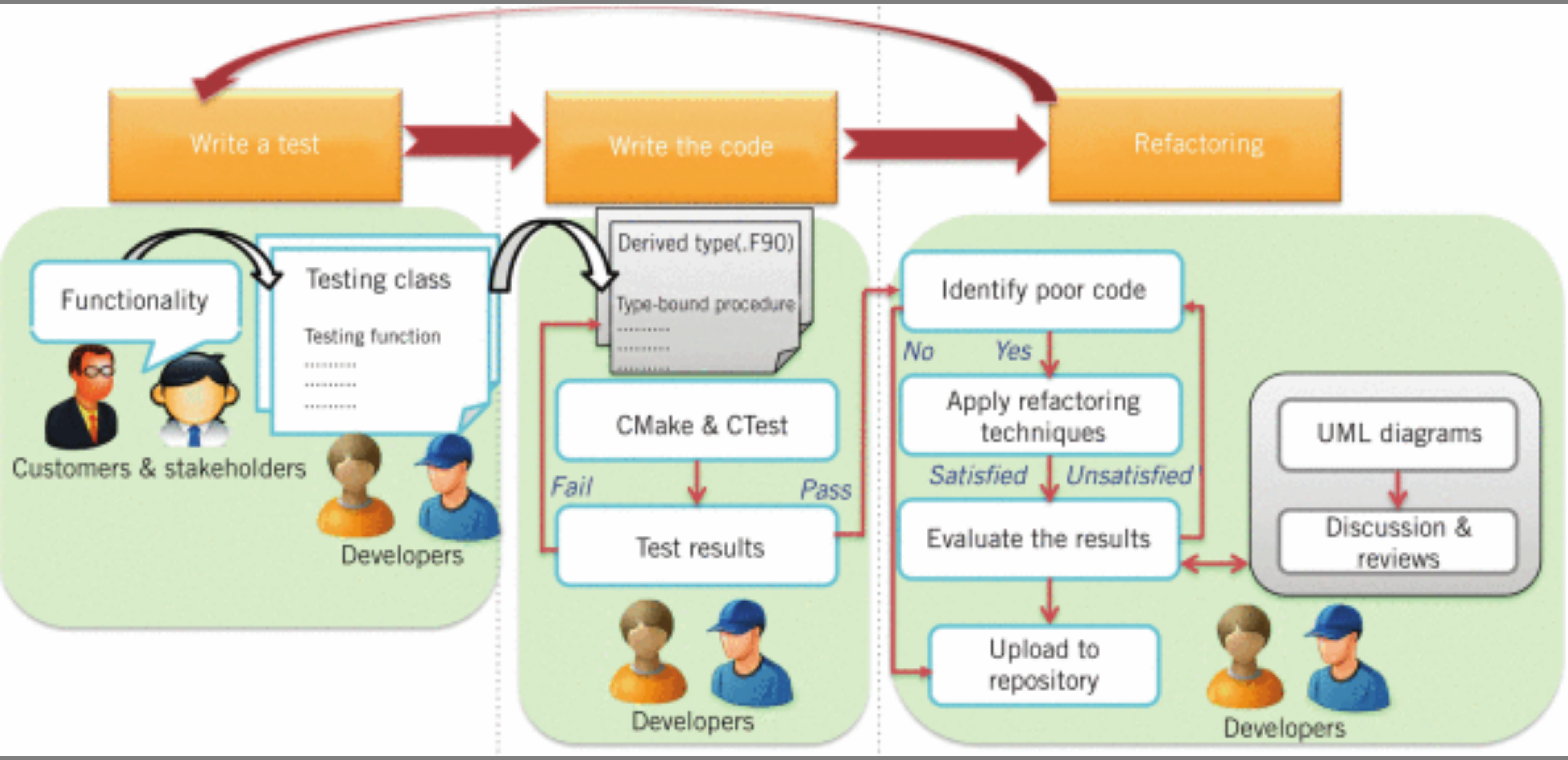
One Possible Methodology



Successful SE/CSE Interactions: TDD - Sandia

- Student spent semester at Sandia
- Taught and modeled TDD on a science code project
- Developed 2 tests for each PDE
  - Small number of steps
  - Whole time evolution
- Lessons Learned
  - Mitigated risks in changing requirements
  - Reduced developer effort
  - Continuous feedback from customer

Successful SE/CSE Interactions: TDD - Sandia



Nanthaamornphong, A. Carver, J., et al. "Building CLiiME via Test-Driven Development: A Case Study." *Computing in Science & Engineering,* 16(3): 36-46

Successful SE/CSE Interactions: Peer Review - ORNL

- Student spent summer with science team at ORNL
- Taught team peer code review process
- Team adopted and continued on own
- Anecdotal Benefits
  - Found faults that would not have been found with traditional testing
  - Adopted coding standard for readability

Ongoing Work

Study of Software Work
Overview

- Choose a domain (e.g. Ecology or Geosciences)
  - Sample a year of papers from a journal

- Goals
  - What does software work look like?
  - How do those in the domain perceive software?

Study of Software Work
Interviews

- Characteristics of:
  - Developers
  - Software development process
  - Domain
  - Funding Model

- Status of software

- Peer-review of code for publication?

- Lessons learned

“Bad By Admission” Code

- Code that is actively recognized as deficient
  - Indicated by TODO or FIX
  - Often not fixed

- Compare Scientific and other software in GitHub
  - Does the frequency differ?
  - How often are these items fixed?

Summary

- Scientific Software Engineering needs:
  - Diverse
  - Deep
- Unique problems that lack simple solutions
- Successful interactions require
  - Time
  - Openness to new ideas

Acknowledgements

- Roscoe Bartlett
- Victor Basili
- Thomas Epperly
- Christine Halverson
- Dustin Heaton – *PhD student*
- Lorin Hochstein
- Jeff Hollingsworth
- Richard Kendall
- Karla Morris
- Aziz Nanthaamornphong - *PhD student*
- Damian Rouson
- Forrest Shull
- Susan Squires
- Doug Post
- Marvin Zelkowitz

Further Readings: Community Surveys

- Carver, J., Heaton, D., Hochstein, L., Bartlett, R. "Self-Perceptions about Software Engineering: A Survey of Scientists and Engineers." *Computing in Science and Engineering*. 15(1): 7-11. Jan/Feb 2013.

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Further Readings:
SE-CSE Workshops

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  - http://secse13.cs.ua.edu/ICSE (ICSE)
  - http://sehpccse13.cs.ua.edu (SC)
- 2011
  - http://SECSE11.cs.ua.edu
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Further Readings:
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Further Readings: Community Interactions

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