# Software Development Environments for Scientific and Engineering Software: A Series of Case Studies

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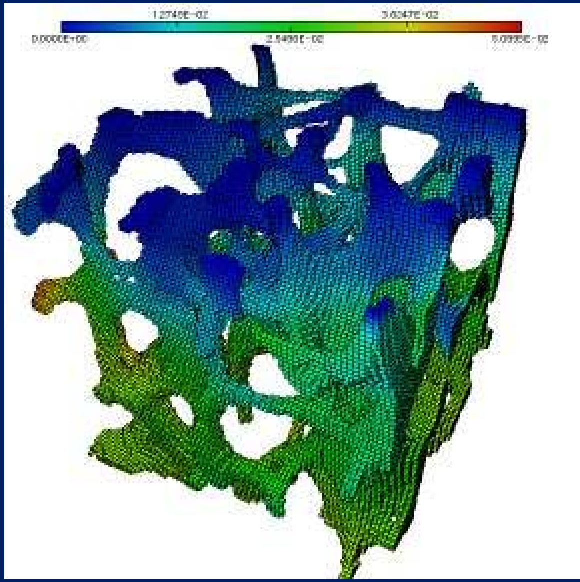
Trilinos User Group Meeting

November 4, 2009



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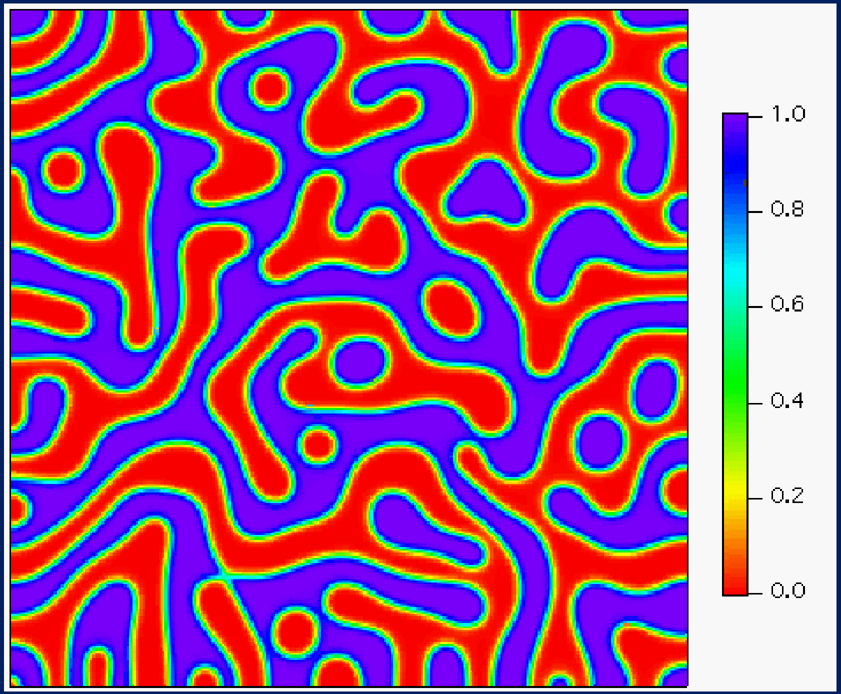
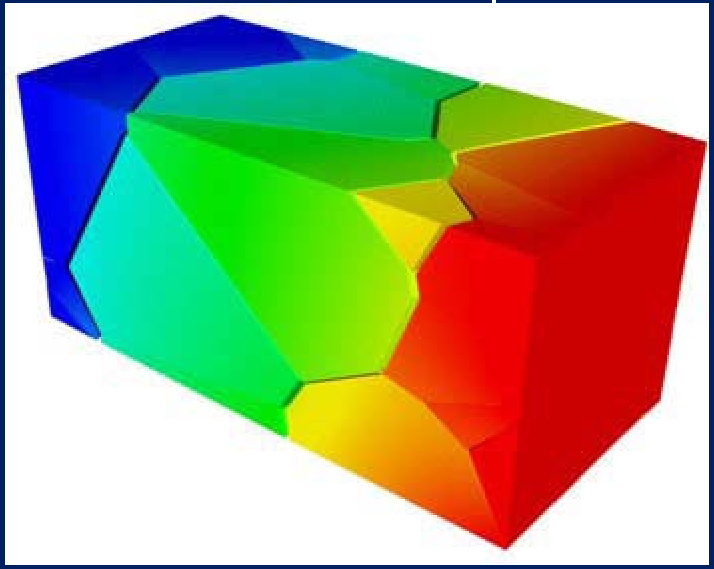



http://www.ctcms.nist.gov/fipy/installation.html



FlexFEM: http://www.cs.sandia.gov/materials_methods/news1.html

# Outline

- Introduction
- Methodology
  - Empirical Software Engineering
  - Case Study
- Projects Studied
- Lessons Learned
- SE-CSE Workshops
- Summary

# Introduction

- Scientific and engineering software
  - Simulations of physical phenomena
  - Processing large amounts of data
  - Performing complex calculations

- Unique characteristics
  - Requirements discovery and gathering process
  - Focus on science/engineering not software
  - Developers tend to be “process-averse”

- HPCS High Productivity Computer Systems

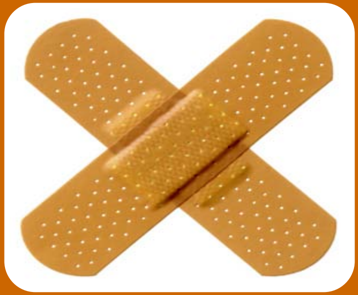
# Areas of Study

## Effort

- How to measure?
- What variables affect?
- Relationship between effort and other variables?
- What activities consume effort?

## Process Flow

- What is the normal process?
- Work vs. rework?
- Can automated data collection be used to measure process steps?
- Which techniques are effective / not effective?

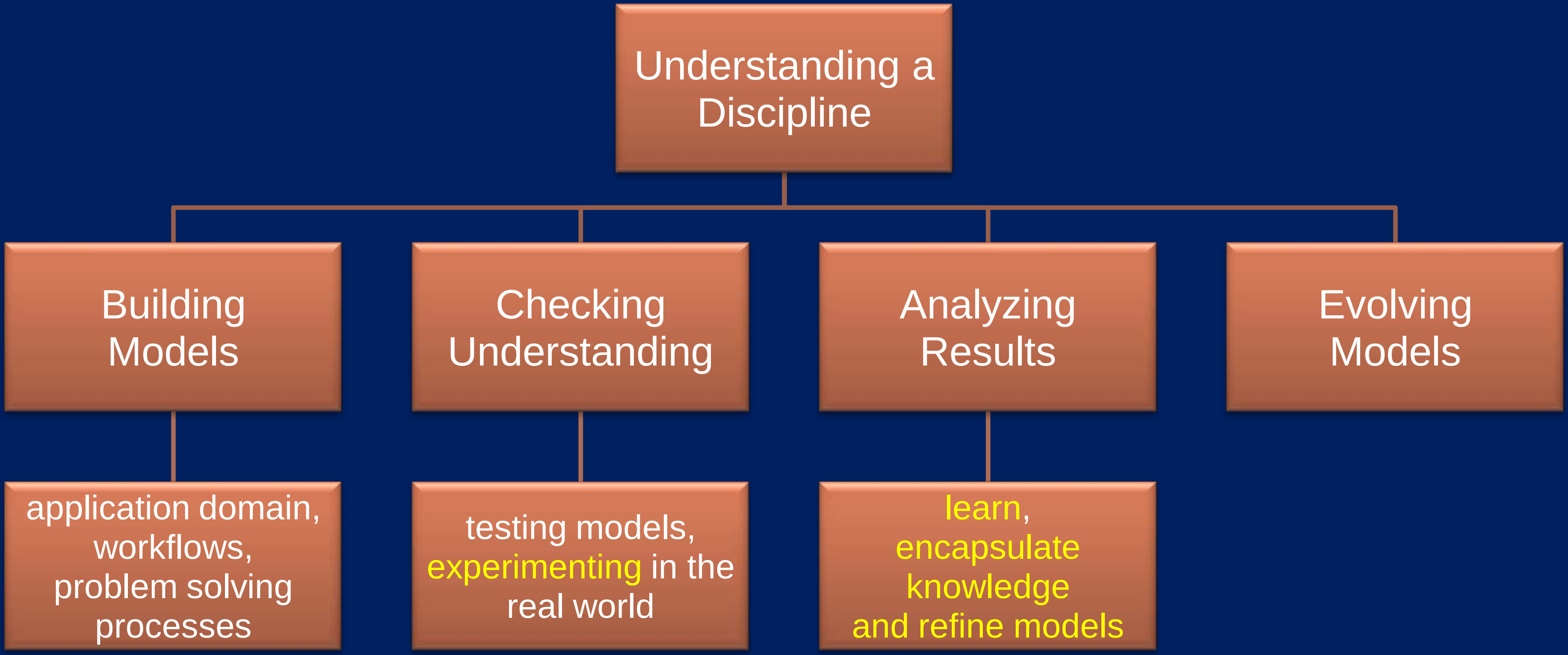


## Defects

- Domain-specific defects?
- Can we identify patterns?
- Can we measure effort to find and fix defects?

# Empirical Studies

**Empirical** → "Based on Observation"



# Empirical Studies: Answer Questions about a Technology

- Does it work better for certain types of people?
  - Novices: It's a good solution for training
  - Experts: Users need certain background knowledge...
- Does it work better for certain types of systems?
  - Static/dynamic aspects, complexity
  - Familiar/unfamiliar domains
- Does it work better in certain development environments?
  - Users [did/didn't] have the right documentation, knowledge, amount of time, etc... to use it

Shull, 2004

# Empirical Studies: Types

### Controlled Experiments

**Typically**:
- high cost
- small projects
- good basis for strong quantitative analysis and stronger statistical confidence in conclusions

**Example**
- comparing the effect of a new drug to a placebo

### Case Studies

**Typically**:
- reasonable cost
- larger projects
- ability to simulate the effects of treatment variables in a realistic environment

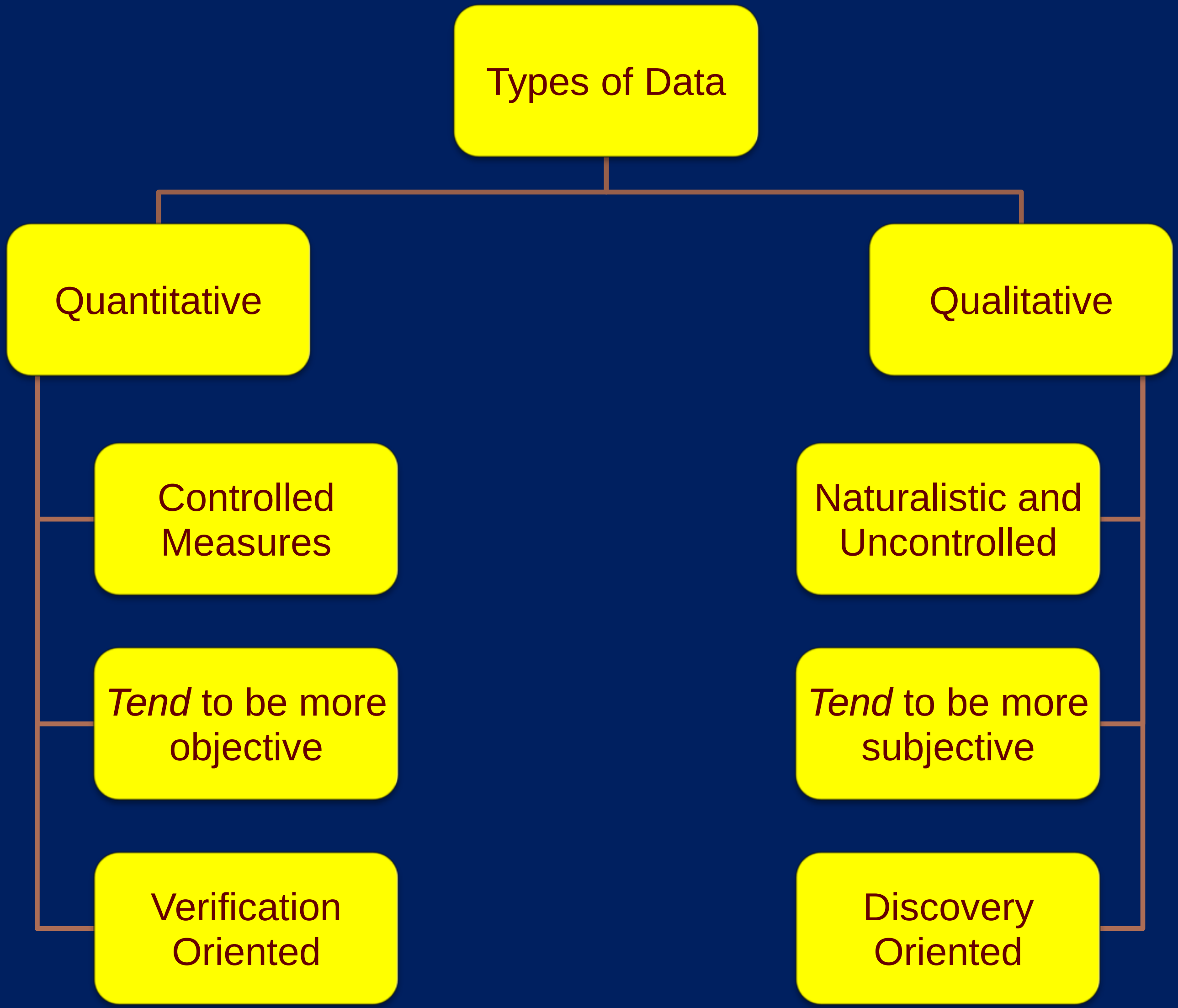
**Example**
- Introducing a new development process and measuring the impact

### Qualitative/Quantitative Analysis

**Typically**:
- a set of variables for observation
- identified *a priori*

**Example**
- Observing professional developers to record their reaction to different types of defects in their software

# Types of Data



# Types of HPCS Studies

### Controlled experiments

Study programming in the small under controlled conditions to:
Identify key variables, check out methods for data collection, get professors interested in empiricism

E.g., compare effort required to develop code in MPI vs. OpenMP

### Observational studies

Characterize in detail a realistic programming problem in realistic conditions to:
validate data collection tools and processes

E.g., build an accurate effort data model

### Case studies and field studies

Study programming in the large under typical conditions

E.g., understand multi-programmer development workflow

### Surveys, interviews & focus groups

Collect “folklore” from practitioners in government, industry and academia

e.g., generate hypotheses to test in experiments and case studies

# Case Study Methodology

- Environment
  - Computational Science and Engineering projects
- Goals
  - Understand and document software development practices
  - Gather initial information about which practices are effective / ineffective
- Approach
  - Series of retrospective case studies

# Case Study Methodology

# Projects Studied:
# FALCON

GOAL: Develop a predictive capability for a product whose performance involves complex physics to reduce the dependence of the sponsor on expensive and dangerous tests.

DURATION: ~10 years

STAFFING: 15 FTEs

USERS: External; highly knowledgeable product engineers

LANGUAGE: OO-FORTRAN

CODE SIZE: ~405 KSLOC

TARGET PLATFORM:
- Shared-memory LINUX cluster (~2000 nodes)
- Vendor-specific shared-memory cluster (~1000 nodes)

Post, 2005

# Projects Studied:
# HAWK

GOAL: Develop a computationally predictive capability to analyze the manufacturing process allowing the sponsor to minimize the use of time-consuming expensive prototypes for ensuring efficient product fabrication.

DURATION: ~ 6 Years

STAFFING: 3 FTEs

USERS: Internal and external product engineers; small number

LANGUAGE: C++ (67%); C (18%); FORTRAN90/Python (15%)

CODE SIZE: ~134 KSLOC

TARGET PLATFORM:
- SGI (Origin 3900)
- Linux Networx (Evolocity Cluster)
- IBM (P-Series 690 SP)
- Intel-based Windows platforms

Kendall, 2005a

# Projects Studied:
# CONDOR

GOAL: Develop a simulation to analyze the behavior of a family of materials under extreme stress allowing the sponsor to minimize the use of time-consuming expensive and infeasible testing.

DURATION: ~ 20 Years

STAFFING: 3-5 FTEs

LANGUAGE: FORTRAN77 (85%)

CODE SIZE: ~200 KSLOC

USERS: Internal and external; several thousand occasional users; hundreds of routine users

TARGET PLATFORM:
- PC – running 106 cells for a few hours to a few days (average)
- Parallel application – 108 cells on 100 to a few 100s of processors

Kendall, 2005b

# Projects Studied:
# EAGLE

GOAL: Determine if parallel, real-time processing of sensor data is feasible on a specific piece of HPC hardware deployed in the field

DURATION: ~ 3 Years

STAFFING: 3 FTEs

LANGUAGE: C++

CODE SIZE: < 100 KSLOC

USERS: Demonstration project – no users

TARGET PLATFORM:
- Specialized computer that can be deployed on military platforms
- Developed on – SUN Sparcs (Solaris) and PC (Linux)

Kendall, 2006

# Projects Studied:
# NENE

GOAL: Calculate the properties of molecules using a variety of computational quantum mechanical models

DURATION: ~25 Years

LANGUAGE: FORTRAN77 subset of FORTRAN90

STAFFING: ~10 FTEs (Thousands of contributors)

CODE SIZE: 750 KSLOC

USERS: 200,000 installations and estimated 100,000 users

TARGET PLATFORM: All commonly used platforms except Windows-based PCs

# Projects Studied:
# OSPREY

GOAL: One component of a large weather forecasting suite that combines the interactions of large-scale atmospheric models with large-scale oceanographic models.

DURATION: ~10 years (predecessor > 25 years)

STAFFING: ~10 FTEs

USERS: Hundreds of installations – some have hundreds of users

LANGUAGE: FORTRAN

CODE SIZE: 150 KLOC (50 KLOC Comments)

TARGET PLATFORM: SGI, IBM, HP, and Linux

Kendall, 2008

# Projects Studied: Summary

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

# Lessons Learned

# Lessons Learned: Validation and Verification

## Validation

- Does the software correctly capture the laws of nature?
- Hard to establish the correct output of simulations *a priori*
  - Exploring new science
  - Inability to perform experimental replications

## Verification

- Does the application accurately solve the equations of the solution algorithm?
- Difficult to identify problem source
  - Creation of mathematical model
  - Translation of mathematical model into algorithm(s)
  - Implementation of algorithms in software

# 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>.*

- Implications
  - Traditional methods of testing software then comparing the output to expected results are not sufficient
  - Need to develop methods that ensure quality and limits of software

# Lessons Learned: Language Stability

- Long project lifecycles require code that is:
  - Portable
  - Maintainable
- FORTRAN
  - Easier for scientists to learn than C++
  - Produces code that performs well on large-scale supercomputers
- Users of the code interact frequently with the code
- Implications
  - FORTRAN will dominate for the near future
  - New languages have to have benefits of FORTRAN plus some additional benefits to be accepted

# Lessons Learned:
# Use of Higher-Level Languages

*I'd rather be closer to machine language than more abstract. I know even when I give very simple instructions to the compiler, it doesn't necessarily give me machine code that corresponds to that set of instructions. If this happens with a simple do-loop in FORTRAN, what happens with a monster object-oriented thing?*

- MATLAB
  - Code is not efficient or fast enough
  - Used for prototyping

- C++
  - Used by some newer teams
  - Mostly used the C subset of C++

- Implications
  - CS&E domain places more constraints on the language that traditional IT domain
  - A language has to
    - Be easy to learn
    - Offer reasonably high performance
    - Exhibit stability
    - Give developers confidence in output of compiler

# Lessons Learned: Development Environments

*They all [the IDEs] try to impose a particular style of development on me and I am forced into a particular mode*

- Developers prefer flexibility of the command line over an Integrated Development Environment (IDE). They believe that:
  - IDEs impose too much rigidity
  - They are more efficient when typing commands than when navigating menus
- Implications – developers do not adopt IDEs because:
  - They do not trust the IDE to automatically perform a task in the same way they would do it manually
  - They expect greater flexibility than is currently provided
  - Prefer to use what they know rather than change

# Lessons Learned:
# External Software

- Projects view external software as a risk
  - Long duration
  - Fear that software may disappear or become unsupported
  - Prefer to develop tools in-house or use open-source

- Exception – NENE
  - Employed a librarian to thoroughly test code before integrating into code base
  - Designed the project so that it was not dependent on external software to meet its commitments

- Implication - Tool problem
  - Very few quality tools for this environment
  - Catch-22 situation

# Lessons Learned:
# Development Goals

- Multiple goals are important
  - Performance – software is used on supercomputer
  - Portability and Maintainability – platforms change multiple times during a project

- Success of a project depends on the ability to port software to new machines

- Implications
  - The motivation for these projects may be different than for traditional IT projects
  - Methods must be chosen and tailored to align with the overall project goals

# Lessons Learned:
# Agile vs. Traditional Methodologies

- “Agile” refers to the philosophical approach rather than to any particular Agile method
- Projects are often doing new science -- requirements cannot be known upfront
- Teams have been operating with an agile philosophy before they even knew what it was
  - Favoring individuals and good practices over rigid processes and tools
- Implications
  - Appropriate, flexible SE methodologies need to employed for CS&E software development

# Lessons Learned:
# Team Composition

*In these types of high performance, scalable computing [applications],* in addition to the physics and mathematics*, computer science plays a very major role. Especially when looking at optimization, memory management and making [the code] perform better … You need a multi-disciplinary team. It [C++] is not a trivial language to deal with … You need an equal mixture of subject theory, the actual physics, and technology expertise.*

- Complex problems and domains
  - Too difficult for most software engineers to understand quickly
  - Easier to teach domain scientists/engineers how to program
- Software engineers help with performance and flexibility
- Implication
  - Multi-disciplinary teams are important

# Lessons Learned:
# Key to Success

- Keeping customers (and sponsors) satisfied

- Lesson not unique to this community, but some constraints are important
  - Funding and customers may come from different agencies
  - Success depends on keeping both groups happy
  - HAWK project was suspended due to lack of customer support, even though it was a technical success for the funding agency

- Implication
  - Balancing the needs of these various stakeholders can be challenging

# Software Engineering for Computational Science and Engineering (SE-CSE) Workshops

# SE-CSE Workshops

- Interaction between SE and CS&E
- Held at ICSE – Moving to ICCS (2010)
- Evolved from SE-HPC workshops
- Important Topics
  - Differences between research and IT software
  - CS&E software quality goals
  - Crossing the communication chasm
  - How to measure impact on scientific productivity

# SE-CSE Workshops
## Differences

- Complex domains
- Main focus on science/engineering
- Long lifecycles
- Investigation of unknown introduces risk
- Unique characteristics of developers
  - Deep knowledge of domain – lack formal SE
  - Often the main users of the software

# SE-CSE Workshops
## Quality Goals

- Lack of viable V&V techniques
- Focus on process transparency
- Guaranteed not to give an incorrect output
- Other SE characteristics not as important
  - Testability, reusability, maintainability

# SE-CSE Workshops
## Communication

- SE need to understand CS&E problems
- SE need to learn from CS&E developers
- Describe SE concepts in familiar terms
- Need people with expertise in both SE & CS&E
- CS&E teams have to realize a problem before needed help

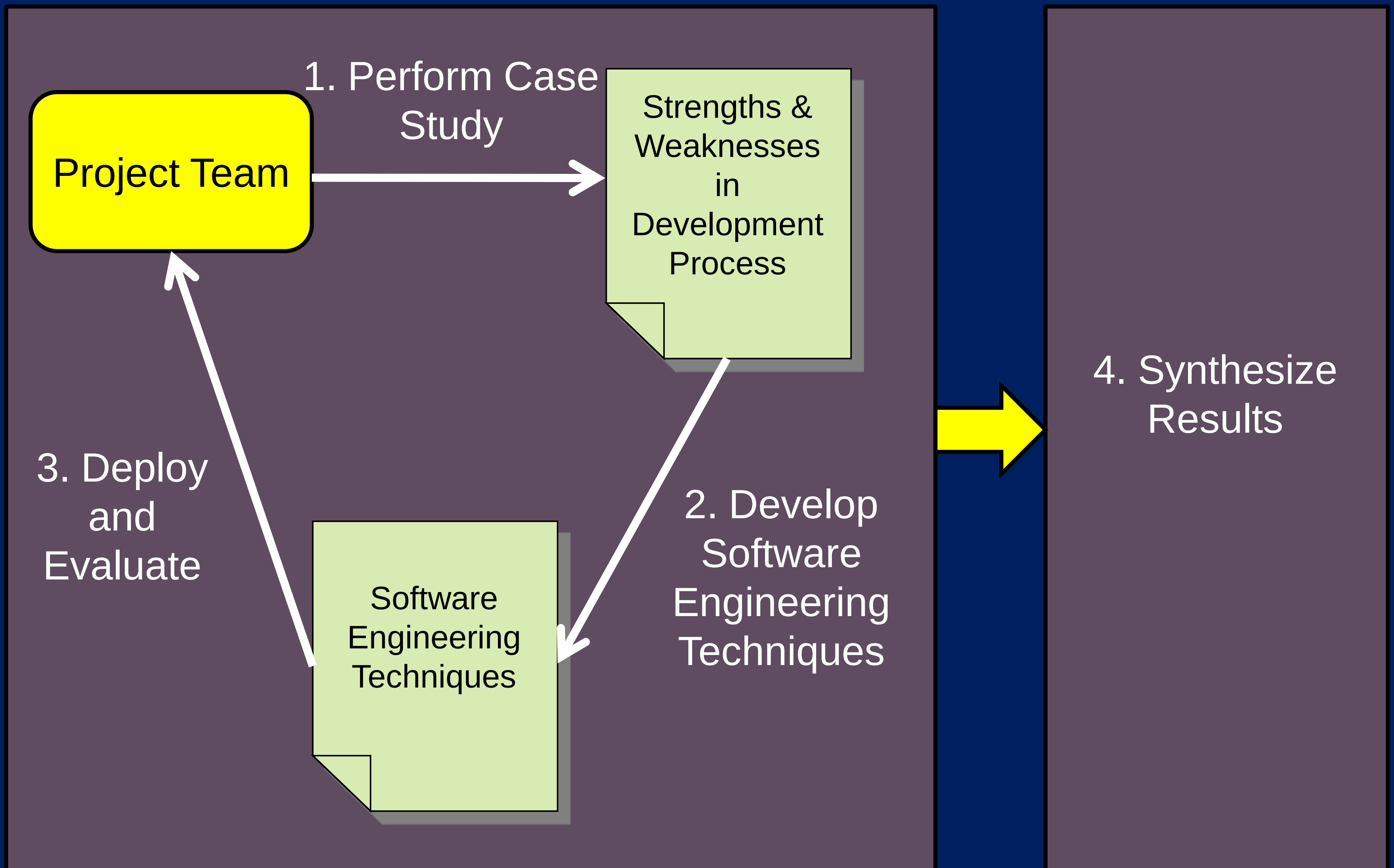
# SE-CSE Workshops
## Scientific Productivity

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

# Summary

- Five case studies of CS&E software projects
- Nine lessons learned
- Summary of SE-CSE workshops
- Contributions
  - Reasons why the development process is different for CS&E software
  - Insights into lack of use of traditional SE approaches
  - Ideas to guide the improvement SE for CS&E

# Future Work – Collaboration Ideas



# Acknowledgements

- Doug Post, Richard Kendall (LANL, SEI)
- Susan Squires (SUN)
- Christine Halverson (IBM)
- DARPA HPCS project

# References


- Carver, J., Kendall, R., Squires, S. and Post, D. "  Software Development Environments for Scientific and Engineering Software: A Series of Case Studies." *Proceedings of the 2007 International Conference on Software Engineering*. Minneapolis, MN. May 23-25, 2007. p. 550-559.

- Carver, J., Hochstein, L., Kendall, R., Nakamura, T. Zelkowitz, M., Basili, V. and Post, D. "  Observations about Software Development for High End Computing. *CTWatch Quarterly*. November, 2006. p. 33-37. (Invited Paper).

- Carver, J., Seaman, C., and Jeffery, R. "Using Qualitative Methods in Empirical Software Engineering." Lecture presented at *The International Advanced School on Empirical Software Engineering*. Redondo Beach, CA. 2004.

- Kendall, R.P., Carver, J., Mark, A., Post, D., Squires, S., and Shaffer, D. *Case Study of the Hawk Code Project*. Technical Report, LA-UR-05-9011. Los Alamos National Laboratories: 2005.

- Kendall, R.P., Mark, A., Post, D., Squires, S., and Halverson, C. *Case Study of the Condor Code Project*. Technical Report, LA-UR-05-9291. Los Alamos National Laboratories: 2005.

- Kendall, R.P., Post, D., Squires, S., and Carver, J. *Case Study of the Eagle Code Project*. Technical Report, LA-UR-06-1092. Los Alamos National Laboratories: 2006.

- Post, D.E., Kendall, R.P., and Whitney, E. "Case study of the Falcon Project". In *Proceedings of Second International Workshop on Software Engineering for High Performance Computing Systems Applications (Held at ICSE 2005)*. St. Louis, USA. 2005. p. 22-26

- Shull, F. "Experimental Methods in Software Engineering." Lecture presented at *The International Advanced School on Empirical Software Engineering*. Redondo Beach, CA. 2004.

# Thank You!

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