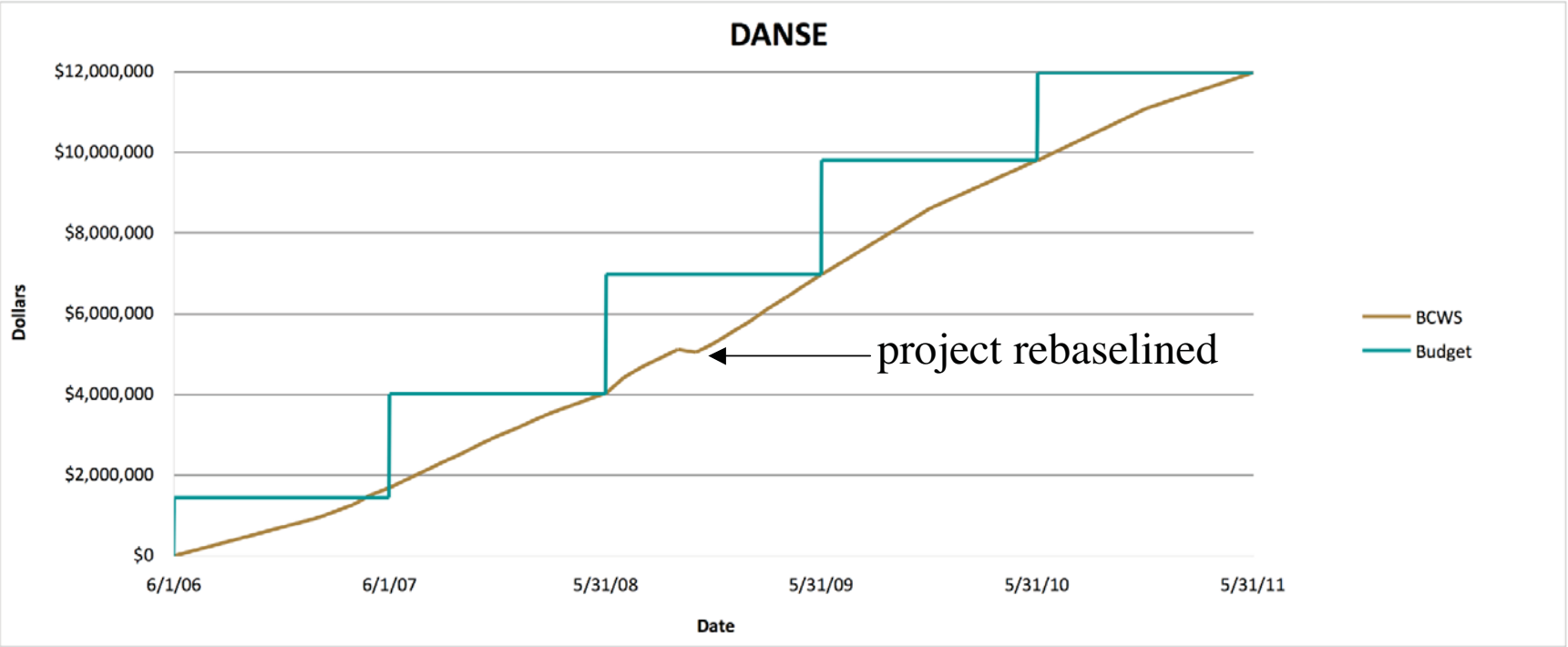
Project Management

Mike McKerns, Caltech

- Project Status
  - Schedule, Cost, and Earned Value
  - Issues and a Path Forward
- Integrated Development and Management
  - Flagship Science Applications
  - Computing Infrastructure
  - Neutron Facility Integration

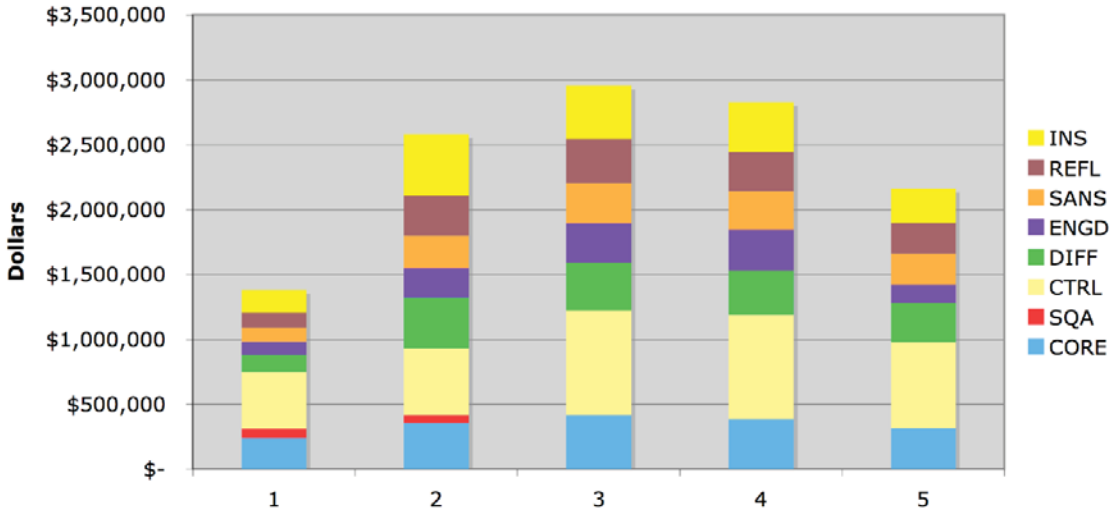
Overview & Project Growth Profile



- year 1: infrastructure and training
- year 2: DANSE application releases
- year 3: project-wide integration
- year 4: DANSE framework releases
- year 5: project robustness

	yearly	cumulative
6/1/06 - 5/31/07	$ 1,441,801	$ 1,441,801
6/1/07 - 5/31/08	$ 2,583,204	$ 4,025,005
6/1/08 - 5/31/09	$ 2,956,169	$ 6,981,174
6/1/09 - 5/31/10	$ 2,827,881	$ 9,809,055
6/1/10 - 5/31/11	$ 2,164,215	$ 11,973,270

Subgroup-level Budget Profile & Status



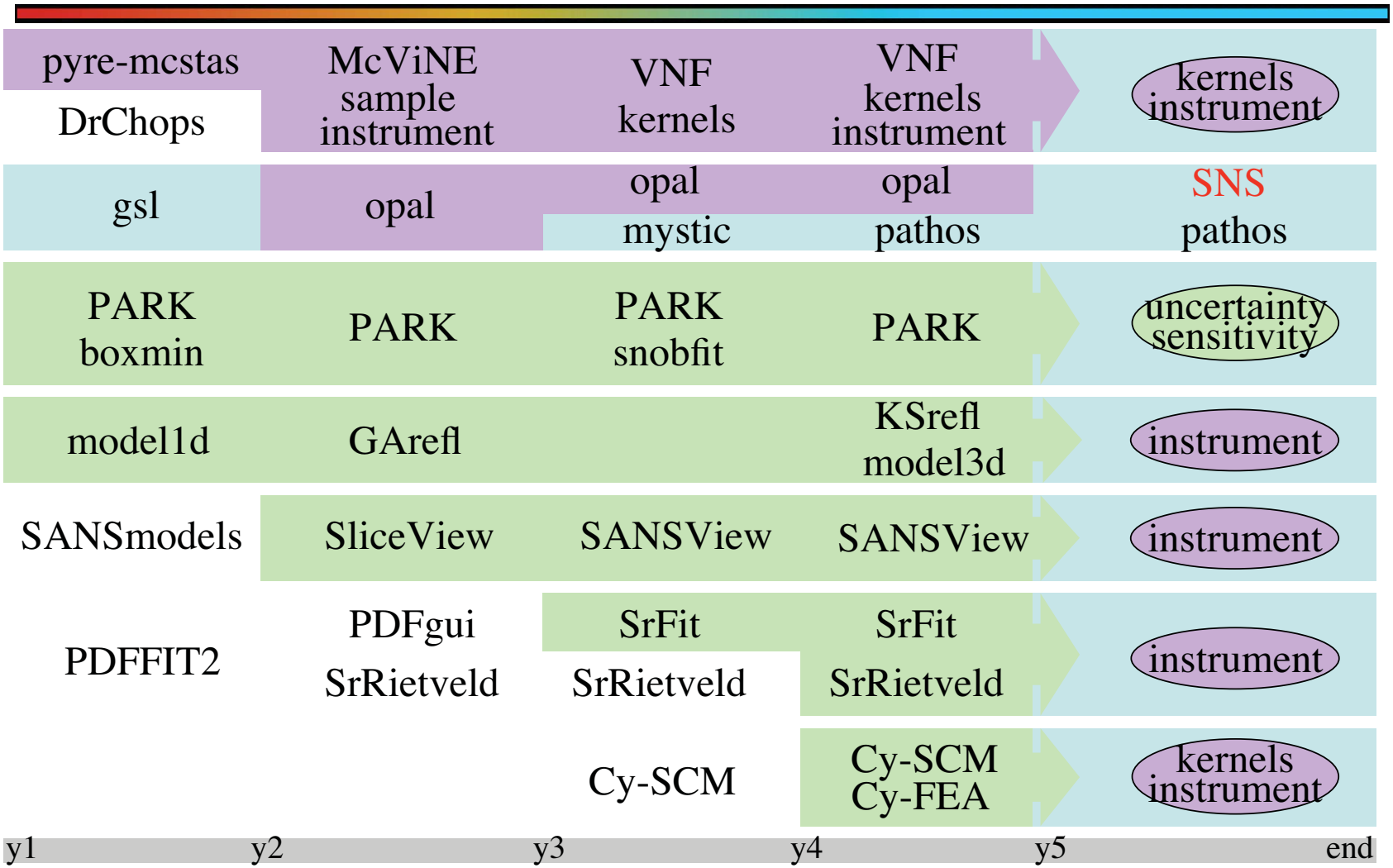
- year 4 has similar funding profile to year 3
- year 5 %increase for DIFF, SANS, & REFL
- y4: focus on frameworks
- y5: focus on robustness

Please inquire to Mike McKerns or Brent Fultz for access to information contained on this slide.

Major Project Deliverables

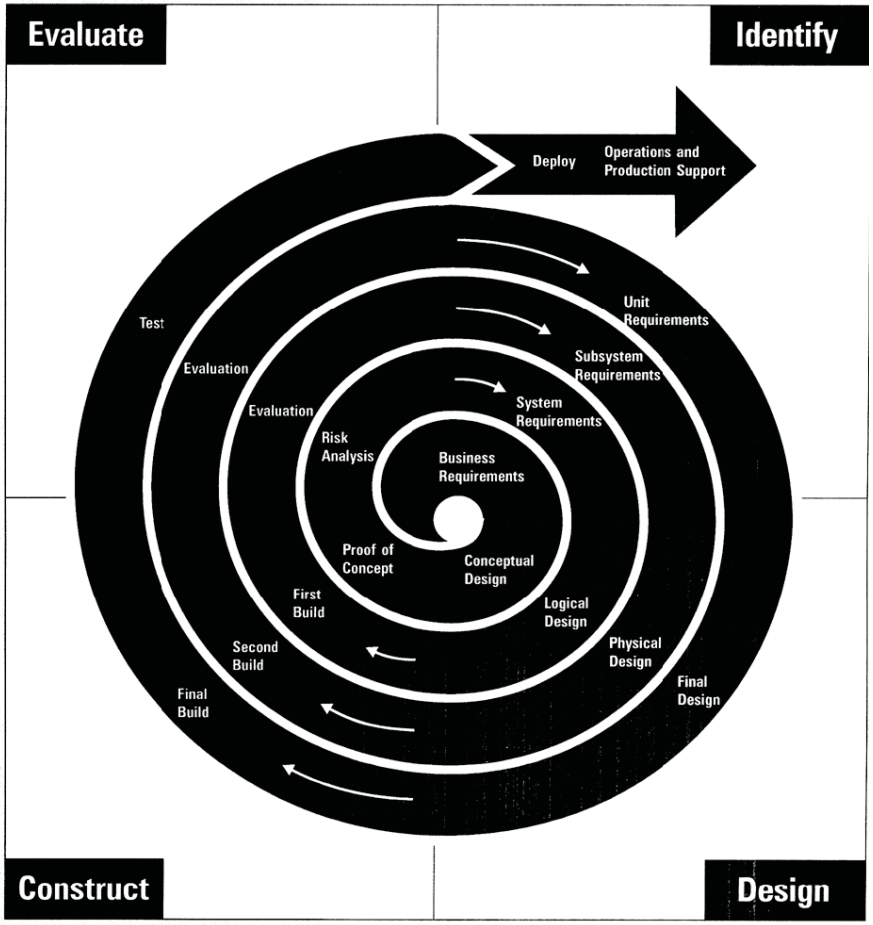
- Flagship Science Applications
  - Rietveld & PDF Refinement; mechanics modeling
  - SANS & Reflectometry model fitting
- Global Optimization Framework (PARK)
  - 'Plug-and-play' model-independent local & global optimization
  - Constrained simultaneous refinements & parameter sensitivity analysis
- Virtual Neutron Facility (VNF) [opal + McViNE]
  - Web portal for Monte-Carlo simulation of neutron experiments
  - Materials theory calculations utilized in Monte-Carlo simulations
- Distributed Service Framework (pathos)
  - Configuration & management of parallel & distributed computing services

Integration Plan for Major Deliverables

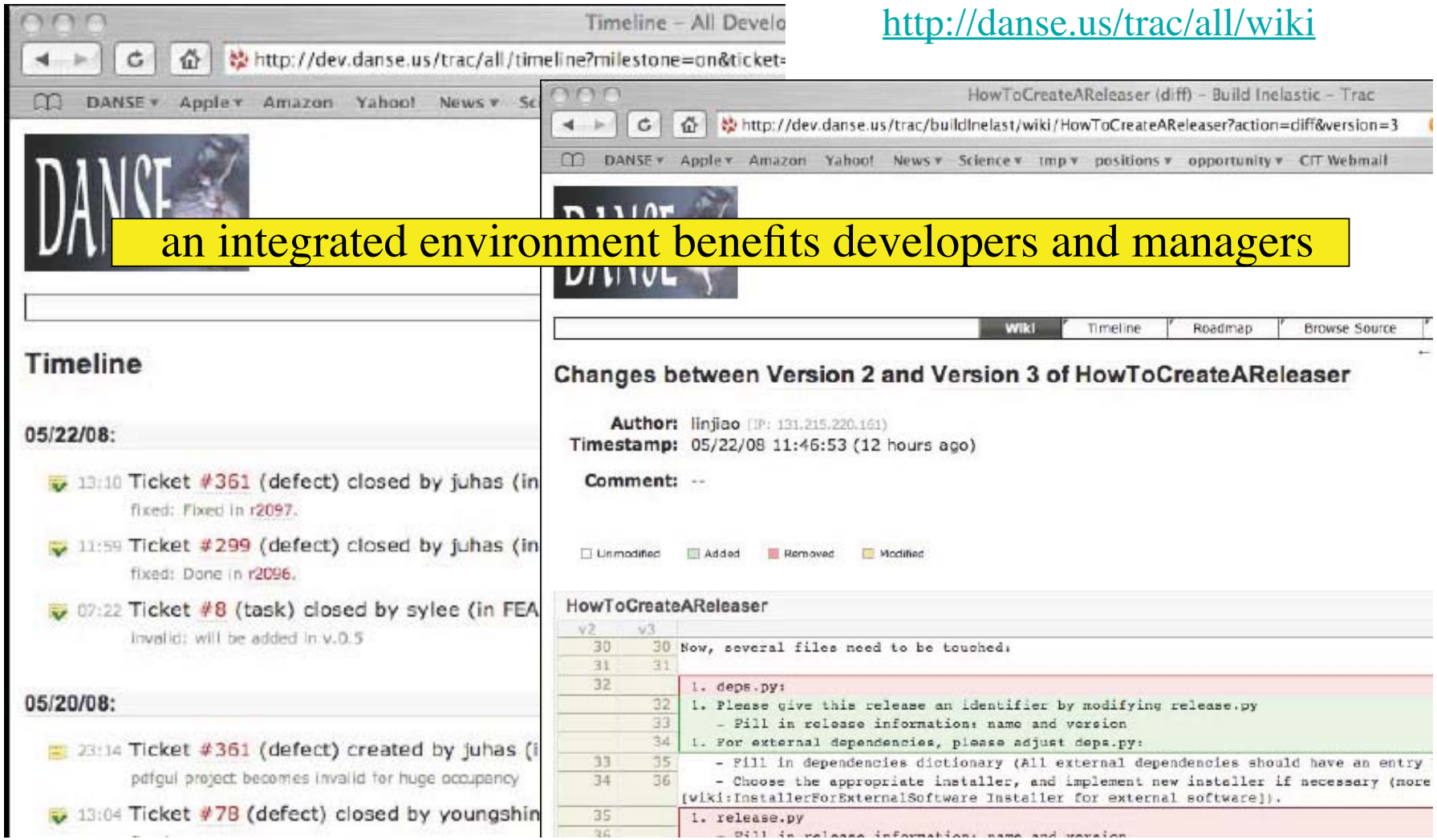


DANSE uses Good Development Practices

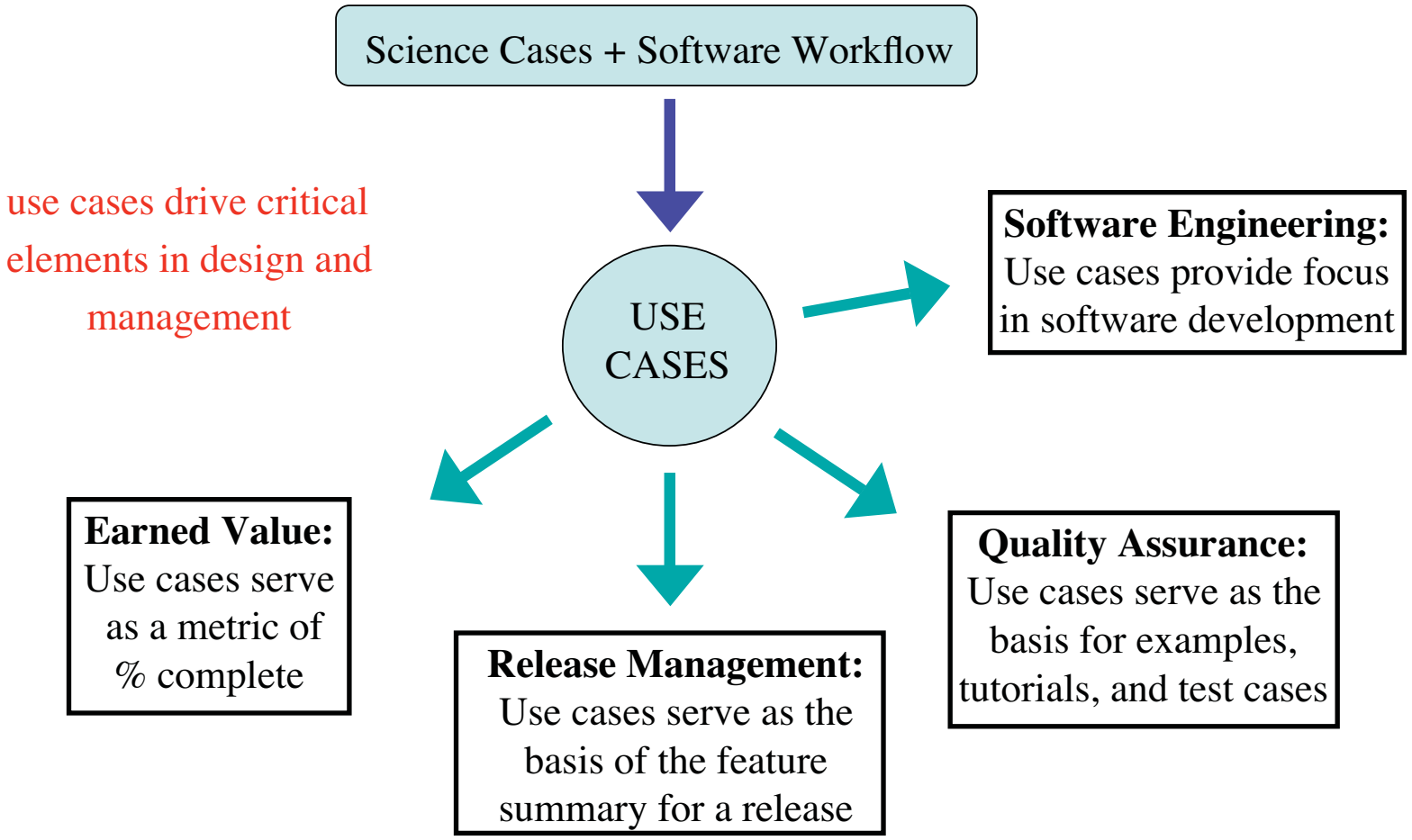
- Early design & definition
- Use cases & workflow
- Prototyping
- Iterative code growth
- Minimize refactoring
- Plan for “plug-in” development
- Utilize abstraction
- Document all interfaces
- Monitor and contribute to 3rd party solutions



Integrated Change Tracking System



Centralized Role of Use Cases



Features Cast as WBS Dictionary Entries

5.3.1.1 Monte-Carlo Instrument Simulation Framework: *In its purest form, a full experiment simulation would track individual neutrons from the moderator, into the instrument, through the sample, and into the detectors. We will produce an instrument simulation framework that provides a stock set of extensible instrument components, and allows the integration of components from common Monte-Carlo simulation packages used to design neutron instruments for optimum combinations of resolution and flux.*

- Simulation Engine
- Neutron Buffer
- Neutron Storage
- Geometers
- Instrument Factories
- Generic Instrument Components
- Basic Sample Components

5.3.1.2 Bindings to McStas: *We will provide*
simulation software.

5.3.1.3 Bindings to NISP: *We will provide p*
simulation software. [This task has been rem

5.3.1.4 Bindings to VITESS: *We will provi*
simulation software.

- Over 300 level 4 tasks, based on engineering design

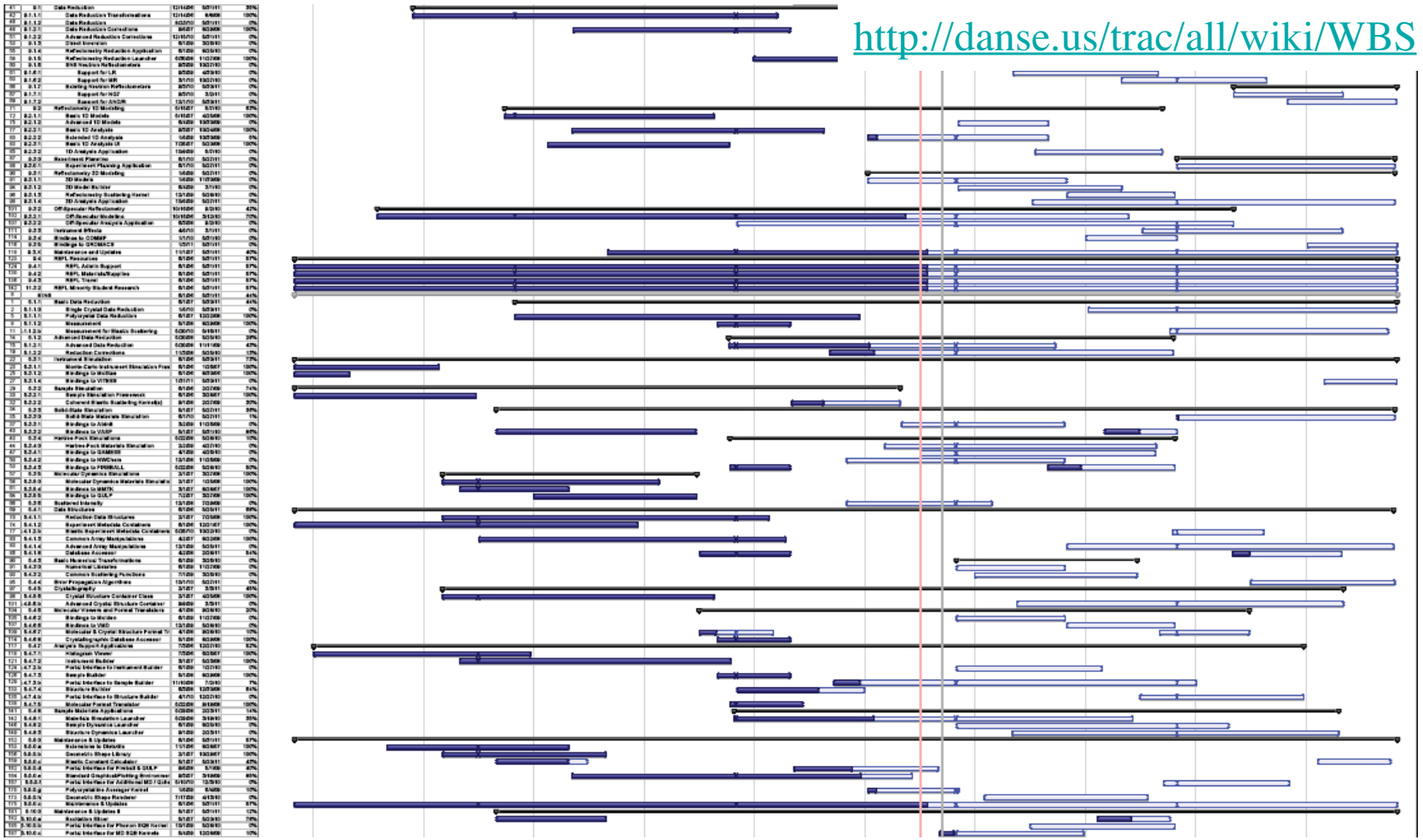
5.3.2.1 Sample Simulation Framework: *A goal of the DANSE project is to integrate the structure and dynamics of the sample into Monte-Carlo instrument simulations, and calculate the scattering from the sample into the detectors. More traditional scattering kernels from geometric shapes will also be supported. Sample components are fully extensible to simulate an arbitrarily complex sample and sample environment.*

- Generic Sample Component
- Scattering Path Calculation through Geometric Shapes
- Couple Scattering Probability Function to Scattering Path

5.3.2.2 Coherent Elastic Scattering Kernels: *We will provide a mechanism for representing coherent elastic scattering from crystals and polycrystals from arbitrarily complex geometric shapes.*

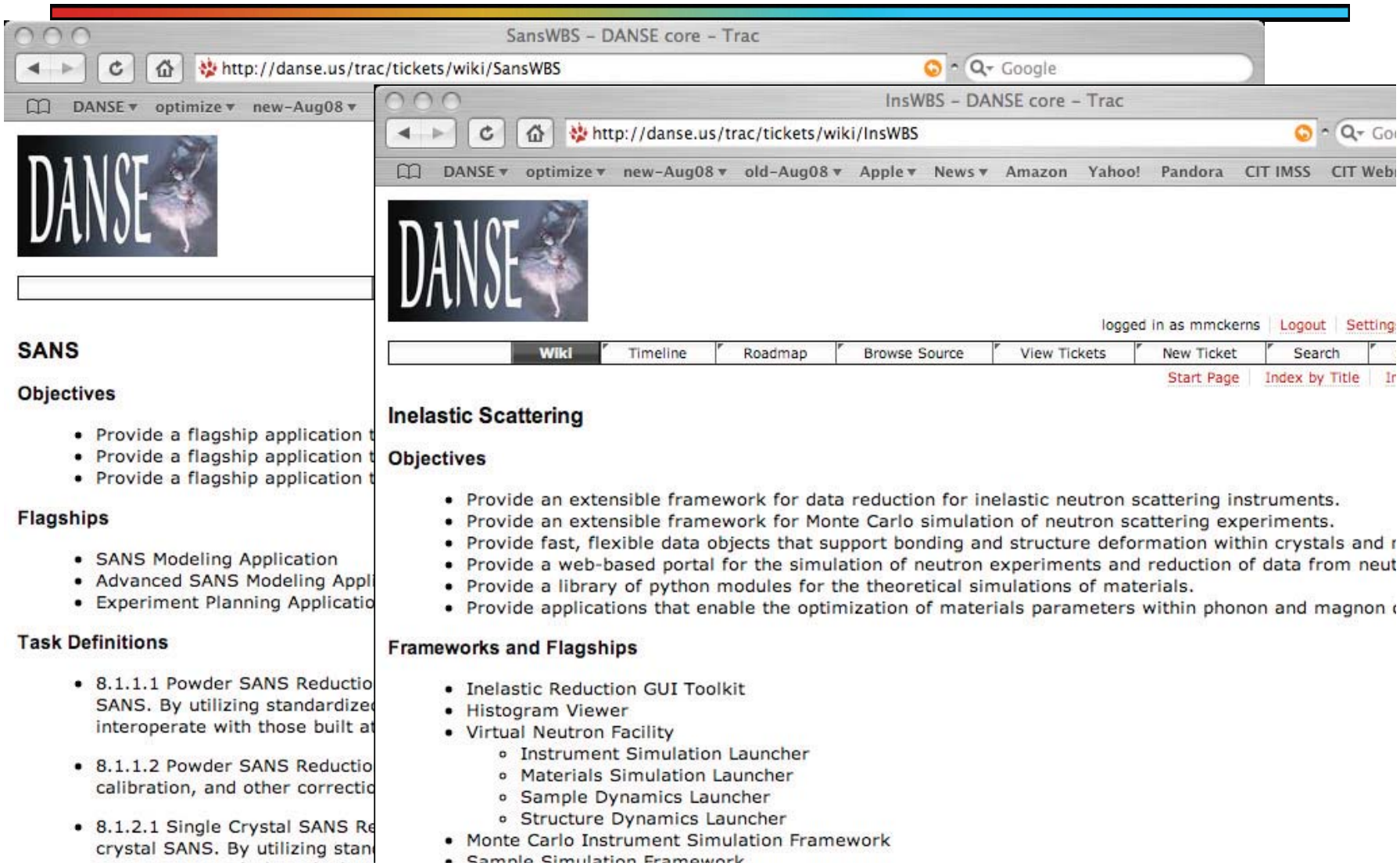
5.3.3.0 Solid-State Materials Simulations: *Ab initio solid-state calculations of electronic structure are practical on systems with 100 atoms or so in a periodic unit cell. These quantum mechanical calculations provide electron wavefunctions within the local density approximation and its extensions. At minimum, we will support calculations of optimized atom positions, electron densities, densities of state, dynamical matrices, and total energy and forces.*

Five Year Software Construction Plan



http://danse.us/trac/all/wiki/WBS

Highlight Objectives and Deliverables



Iterative Improvements in Release Strategy

- **Original:** project release of plug-in libraries & packages
  - initial DANSE 1.0 releases scheduled in year 4
  - moving to an iterative release plan enables better quality software

- **Better:** standalone "flagship application" releases in year 2
  - PRO: provides experience with release process; allows community feedback
  - PRO: provides focal point for use cases and feature development
  - CON: major rescheduling of (CTRL) tasks to support early release
  - CON: framework development slowed; subgroups support own UI / build

- **Best:** framework-supported releases scheduled for year 4
  - good software engineering allows separation of library from UI & app
  - ***subgroup apps leverage framework middleware as it becomes available***

Rebaseline around Release of Deliverables

- Completed rebaseline in October 2008
  - Each subgroup WBS (level 1) lists major deliverables & objectives
  - Major project deliverables also listed in appendix of Project Plan
- Rebaselined with little overall change in scope
  - Releases become implicit within estimate of task % complete
  - No credit for subgroup UI / build work outside of original scope
  - Rebaseline thus reduces to task reorganization and refinement
  - Larger budgets for “maintenance and updates” tasks
- Recovery of earned value from future-scheduled work
  - BCWS fixed (yearly) by NSF funding profile
  - BCWP increases as tasks are refined to support completed portions of work
  - Tasks now mirror feature addition through release & integration cycles

WBS & Earned Value Reporting

- subgroups fill out monthly reports on scheduled WBS tasks
- report cost per task and *report % complete at a near functional level*
- provides a detailed picture of what is complete and what is to be completed
- earned value derived from reported cost and activity

WBS	Task	Type	Account	Year / Month	Direct Costs	Indirect Costs
7.2.1.1	Modular integration of finite element analysis (FEA) software – Al	LA	ENGDIF	2007/04	$ 1,402	$ 423
7.2.1.2	Input/output parameters for FEA	LA	ENGDIF	2007/04	$ 1,402	$ 423
7.2.2	Self-Consistent Modeling	LA	ENGDIF	2007/04	$ 1,261	$ 270
7.2.3	Inverse Problem Analysis	LA	ENGDIF	2007/04	$ 1,261	$ 270
7.3.2	Microstructure Simulation	LA	ENGDIF	2007/04	$ 2,200	$ 467
7.3.X	Maintenance and Updates	LA	ENGDIF	2007/04	$ 961	$ 254
7.4.1	Local administrative support	LA	ENGDIF	2007/04		
7.4.2	Computing hardware and software	MS	ENGDIF	2007/04	$ 147	$ 69
7.4.3	Travel	TR	ENGDIF	2007/04		
7.4.4	Communications	MS	ENGDIF	2007/04		
7.4.X	Subawards	SA	ENGDIF	2007/04		
11.3.5	Minority Student Research Position	LA	ENGDIF	2007/04		

Budget Period: Jun 1, 2006 to May 31, 2007 (NCE)
Reporting Period: Apr 1, 2007 to Apr 30, 2007

TOTALS $ 8,634 $ 2,176

SOW

WBS	Task	Account	Baseline Start Date	Baseline End Date	Projected % Complete at End y2p1	Prior Reported % Complete	Actual % Complete
7.2.1.1	Modular integration of finite element analysis (FEA) software – Al	ENGDIF	09/02/10	10/28/10	100%	69%	70%
7.2.1.2	Input/output parameters for FEA	ENGDIF	10/02/10	12/13/10	100%	65%	68%
7.2.2	Self-Consistent Modeling	ENGDIF	09/22/10	04/26/12	70%	29%	32%
7.2.3	Inverse Problem Analysis	ENGDIF	12/31/10	04/10/12	65%	19%	21%
7.3.2	Microstructure Simulation	ENGDIF	05/02/11	02/23/14	18%	0%	7%

Budget Period: Jun 1, 2006 to May 31, 2007 (NCE)
Reporting Period: Apr 1, 2007 to Apr 30, 2007

Measures of Earned Value

- Two measures of earned value are tracked each month
  - provide estimate of maximum and minimum earned value due to ACWP
- "Instantaneous" Actual Cost of Work Performed (ACWP)
  - costs reported by subgroups in monthly reports
  - tracks expenses before they hit the Caltech books
  - directly ties earned value to cost at the task level
  - a better way to monitor subgroup expenditures
- Actual Cost Expended (ACE) or "invoiced" ACWP
  - this is the standard definition of ACWP
  - subgroups often bill irregularly; can lag expenditures by several months
  - granularity is at subcontract level
  - only better for project-level earned value reporting

Project-level Earned Value

Please inquire to Mike McKerns or Brent Fultz for access to information contained on this slide.

Issue: ENGD Earned Value & Performance

Please inquire to Mike McKerns or Brent Fultz for access to information contained on this slide.

Planned Resolution: ENGD + THEORY

- Changes are still required for ENGD subcontract
  - subcontract scope cannot be completed at present progress rate
  - issues in staffing and subproject management remain, but are improving

- In Jun 2009, transfer PI to R. LeSar (E. Ustundag as Co-PI)
  - LeSar has staffing in place to support required software engineering effort
  - LeSar brings experience and leadership in Materials Theory
  - LeSar originally targeted for collaboration on Texture & Microstructure tasks
  - summary of relevant research at http://web.mac.com/rlesar
- Shift in ENGD focus toward Materials Theory
  - provide much needed support on existing year 4-year 5 VNF kernel tasks
  - WBS details (level 3) are presently being worked out
  - will slightly decrease project scope… but enable greater science impact

the Change Control Process

- All changes require approval through a change request
  - changes activate only after PCR / TCR is complete
  - to date, ***we have required ~30 TCRs and 5 PCRs*** (ENGD: 3/5 PCRs)

- Project Change Request (PCR) for project-level changes
  - alter scope / cost / schedule across project "funding boundaries"
  - complete upon analysis and vote by Change Control Board (CCB)
  - NSF Program Manager is informed of CCB decision

- Task Change Request (TCR) for task-level changes
  - changes do not alter overall project scope / cost / schedule
  - modify WBS tasks within a single subproject; can alter the SOW
  - (usually) complete upon agreement between subproject leader and PM

Year 4: Science Subgroups

- Diffraction
  - Joint Model Refinement; Magnetic Refinement; Support for POWGEN
- Eng. Diffraction
  - Texture Analysis; Real-time Data Analysis; Support for VULCAN
- SANS
  - Simulation of SANS Experiments; Experiment Planning Tools
- Reflectometry
  - Off-Specular Modeling & Analysis; 3D Modeling
- Inelastic
  - Multiple & Multiphonon Scattering, Solid-State & Hartree-Fock Simulation

- Flagship apps leverage PARK & VNF for new science

Year 4: Computing Infrastructure

- New release of optimization framework (PARK)
  - extend PARK to distributed computing
  - extend parallel mapping infrastructure
  - begin parameter sensitivity and uncertainty quantification
- New release of virtual neutron facility (VNF)
  - add instruments and samples from each subgroup
  - extensive kernel development
  - extend data, instrument, sample, and model visualization
  - extend instrument, sample, and kernel builders
- Initial release of distributed services framework (pathos)
  - PARK & VNF leverage pathos for increased computing capabilities
  - Test integration and deployment within SNS infrastructure

Year 4: Integration at Facilities

- Collaboration with Instrument Scientists
  - increase support for data analysis / instruments: SNS, HFIR, LANSCE, NIST
  - facilitate capture of critical user requirements
- Facility hosting of Flagship Applications
  - stronger role in instrument support, as instruments are added to DANSE
  - install DANSE build tools to update flagship applications in SNS Portal
- Computing services hosted at ORNL & Caltech
  - initial build of DANSE code interacting with SNS portal authentication
  - cyberinfrastructure / cybersecurity policy issues being worked out with SNS
  - targeting installation of VNF (& PARK) at SNS in open research zone
  - transition to production-level integration at SNS in year 5

A Look Forward at Project Completion

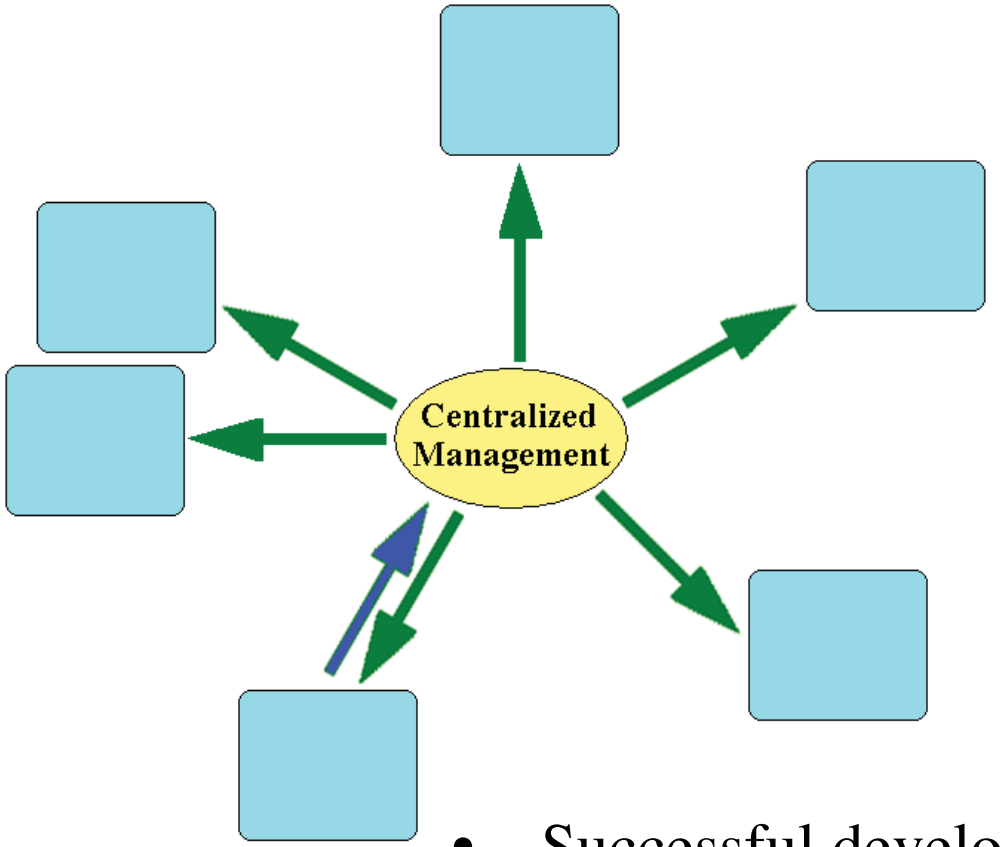
Please inquire to Mike McKerns or Brent Fultz for access to information contained on this slide.

Lessons Learned, so far

- Managing Expectations
  - scientific software deliverables are twofold: “the science” & “the software”
  - ***software in (trusted) users’ hands as early as possible produces better software***
  - reusable, extensible software for new science takes time & infrastructure
  - DANSE, unlike instruments, is ***expected to make an impact far before completion***
  - ***other communities have begun to leverage DANSE in often unexpected ways***
- Project Infrastructure
  - software engineering ***training is a key educational component for project success***
  - management & development must be tightly coupled at all levels and tools
  - management “at the interface” is critical for collaboration
  - scope management must be strict… ***and must be very agile at a technical level***
- Hiring and Retention
  - harder to find and retain people than expected [1 strong dev/group is essential]
  - postdoc-developers tend to be more efficient when partially (science) funded

End Presentation

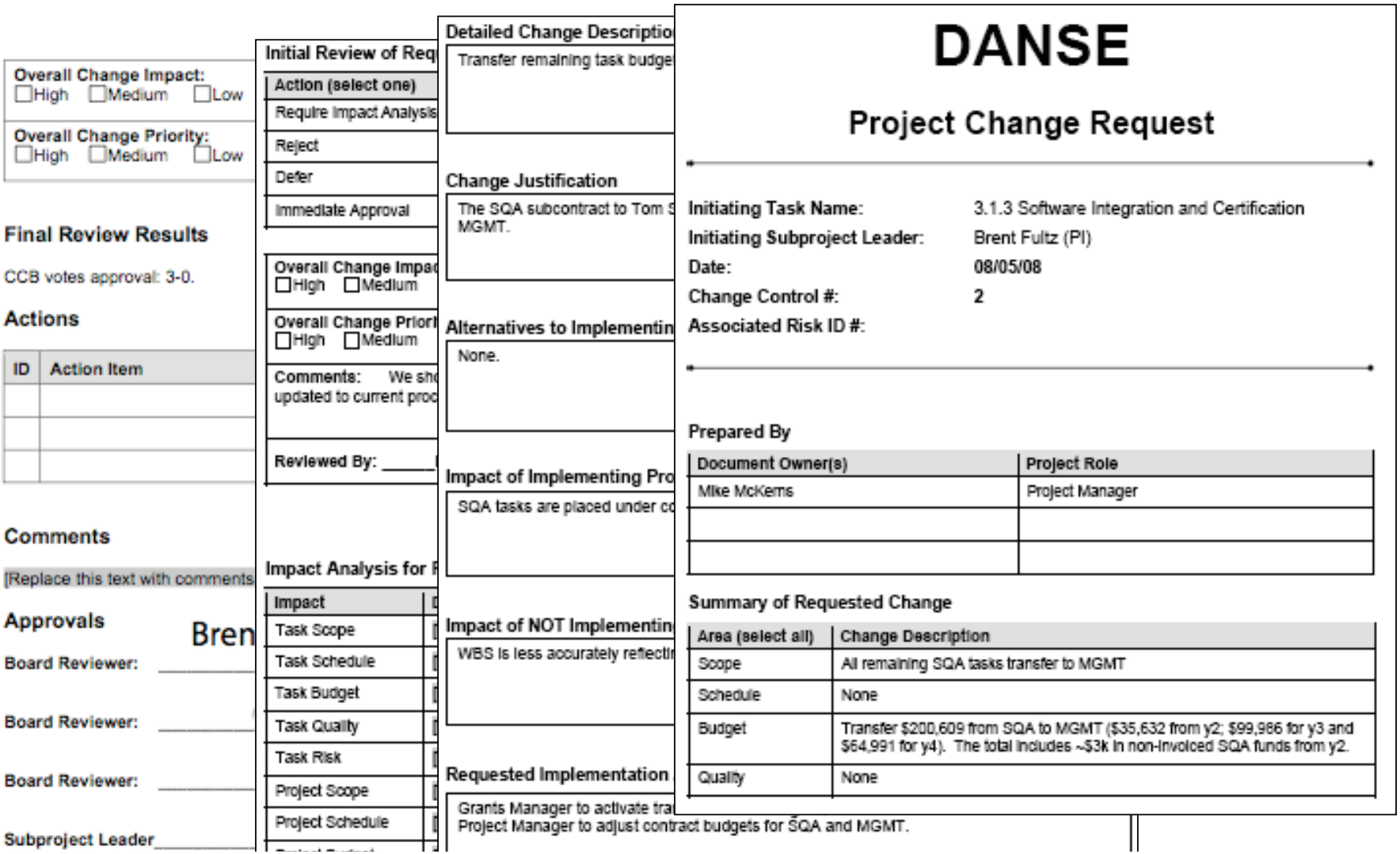
Resource Management Tools



- centralized code repository
- email ticketing system
- systematic tracking
- structured design process
- build/testing infrastructure
- release management
- standardization
- quality assurance
- reporting mechanisms
- review & design steering

- Successful development with distributed resources requires centralized management.

Review & Analysis of Project Change



Overall Change Impact:
☐High ☐Medium ☐Low

Overall Change Priority:
☐High ☐Medium ☐Low

Final Review Results

CCB votes approval: 3-0.

Actions

ID	Action Item

Comments

[Replace this text with comments

Approvals

Board Reviewer: _____

Board Reviewer: _____

Board Reviewer: _____

Subproject Leader_____

Initial Review of Req

Action (select one)
Require Impact Analysis
Reject
Defer
Immediate Approval

Overall Change Impac
☐High ☐Medium

Overall Change Priorit
☐High ☐Medium

Comments: We sh
updated to current proc

Reviewed By: _____

Impact Analysis for

Impact	
Task Scope	
Task Schedule	
Task Budget	
Task Quality	
Task Risk	
Project Scope	
Project Schedule	

Detailed Change Descriptio

Transfer remaining task budge

Change Justification

The SQA subcontract to Tom S
MGMT.

Alternatives to Implementin

None.

Impact of Implementing Pro

SQA tasks are placed under co

Impact of NOT Implementin

WBS is less accurately reflecti

Requested Implementation

Grants Manager to activate tra
Project Manager to adjust contract budgets for SQA and MGMT.

DANSE

Project Change Request

Initiating Task Name: 3.1.3 Software Integration and Certification
Initiating Subproject Leader: Brent Fultz (PI)
Date: 08/05/08
Change Control #: 2
Associated Risk ID #:

Prepared By

Document Owner(s)	Project Role
Mike McKerns	Project Manager

Summary of Requested Change

Area (select all)	Change Description
Scope	All remaining SQA tasks transfer to MGMT
Schedule	None
Budget	Transfer $200,609 from SQA to MGMT ($35,632 from y2; $99,986 for y3 and $64,991 for y4). The total includes ~$3k in non-invoiced SQA funds from y2.
Quality	None

A Look at Existing Project Metrics

- DANSE license requests users to include acknowledgement in all publications resulting from use of DANSE software
  - good metric for flagship applications
  - is this good for other types of DANSE software products?
- DANSE has begun tracking downloads to UIDs
  - DANSE package server counts downloads to UIDs
  - several subgroups have maintained their own download counts
  - few of the more general DANSE packages have 1000s of downloads
- Other possible metrics…
  - DANSE framework user accounts / client logins / job submissions?
  - Search engine records / keyword rankings?