



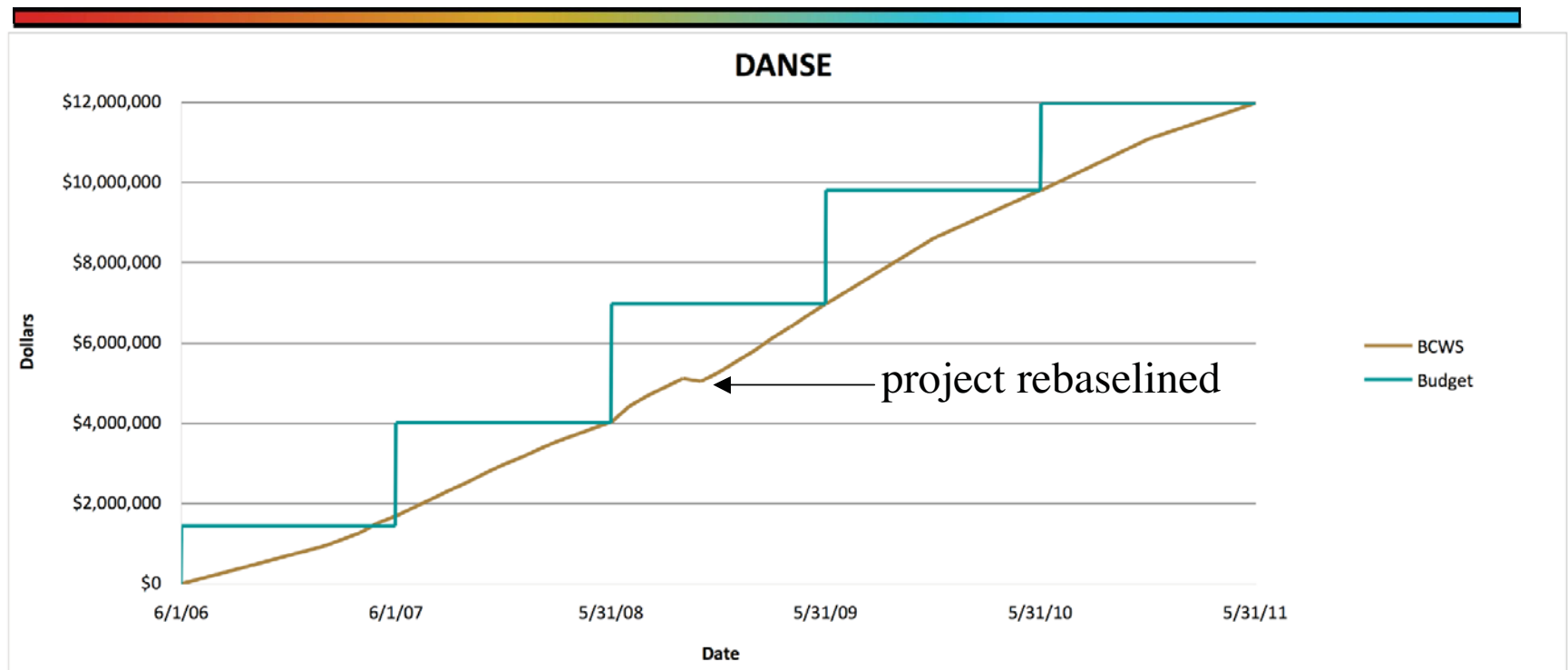
# Project Management

Mike McKerns, Caltech

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

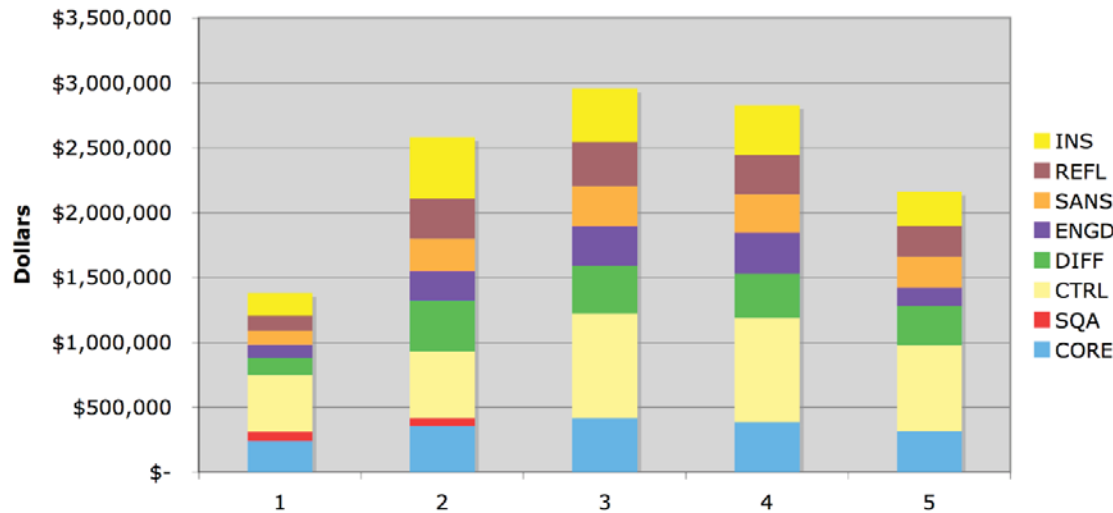
# Overview & Project Growth Profile



- 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

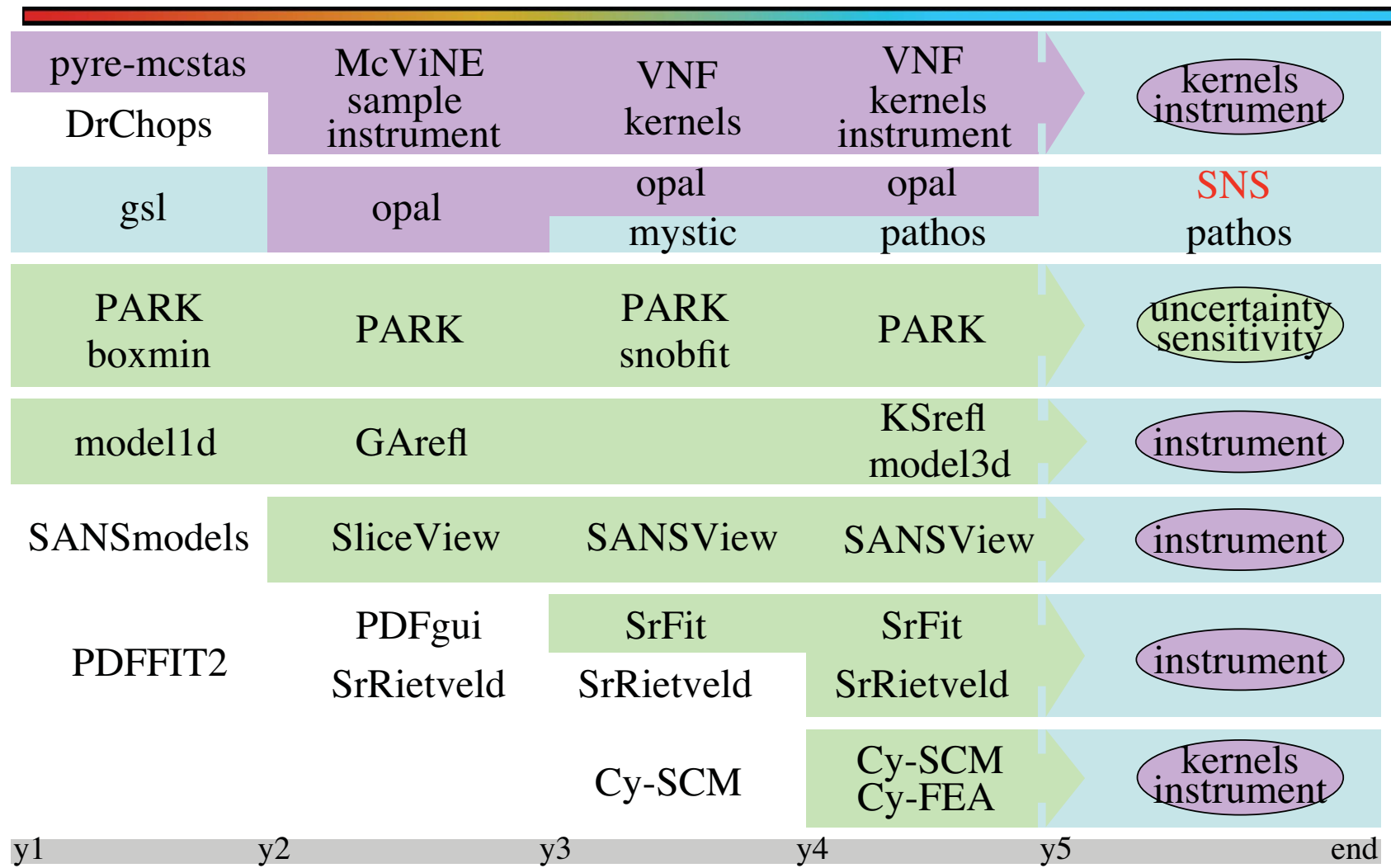
Please inquire to Mike McKerns or Brent Fultz for access to information contained on this slide.

# Major Project Deliverables

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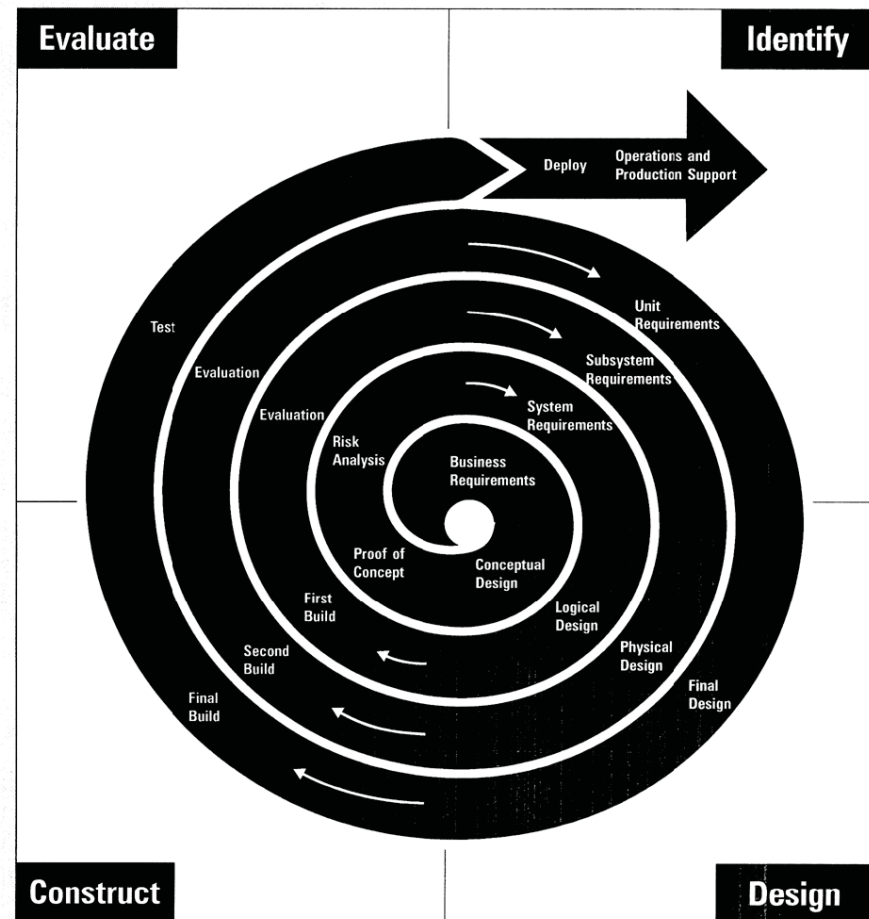
- **Flagship Science Applications**
  - Rietveld & PDF Refinement; mechanics modeling
  - SANS & Reflectometry model fitting
- **Global Optimization Framework (PARK)**
  - ‘Plug-and-play’ model-independent local & global optimization
  - Constrained simultaneous refinements & parameter sensitivity analysis
- **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

<http://danse.us/trac/all/wiki>

an integrated environment benefits developers and managers

The screenshot displays two browser windows from the Trac system. The left window shows a 'Timeline - All Develop' page with a 'DANSE' logo and a list of tickets. The right window shows a 'HowToCreateAReleaser (diff) - Build Inelastic - Trac' page with a diff view of code changes between version 2 and version 3.

**Timeline - All Develop**

05/22/08:

- 13:10 Ticket #361 (defect) closed by juhas (in pefgul project becomes invalid for huge occupancy)  
fixed: Fixed in r2097.
- 11:59 Ticket #299 (defect) closed by juhas (in pefgul project becomes invalid for huge occupancy)  
fixed: Done in r2096.
- 07:22 Ticket #8 (task) closed by sylee (in FEAT)  
Invalid: will be added in v.0.5

05/20/08:

- 23:14 Ticket #361 (defect) created by juhas (in pefgul project becomes invalid for huge occupancy)
- 13:04 Ticket #78 (defect) closed by youngshin

**HowToCreateAReleaser (diff) - Build Inelastic - Trac**

Changes between Version 2 and Version 3 of HowToCreateAReleaser

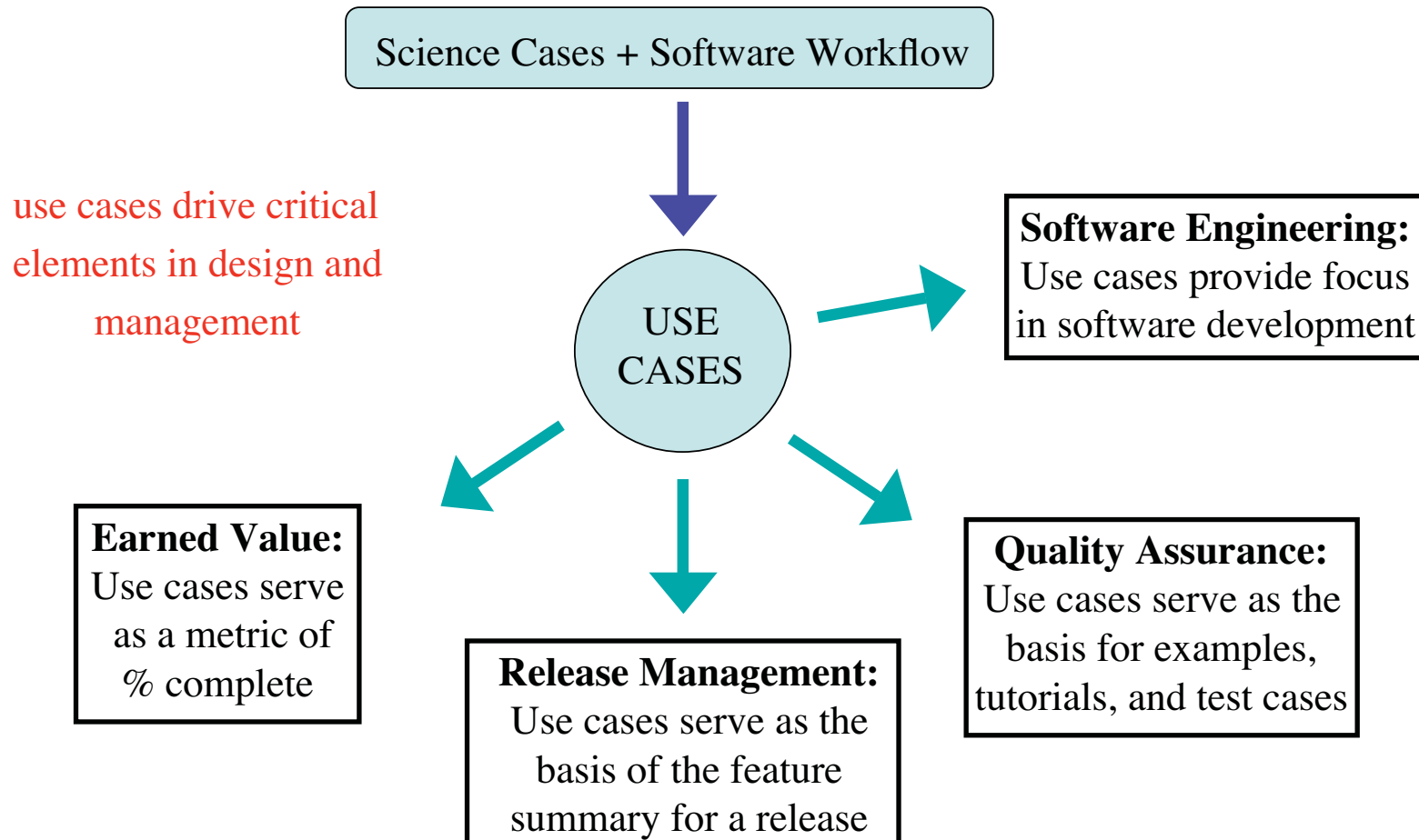
Author: linjiao (IP: 131.215.220.161)  
Timestamp: 05/22/08 11:46:53 (12 hours ago)  
Comment: --

Unmodified  Added  Removed  Modified

v2	v3	
30	30	Now, several files need to be touched:
31	31	
32		1. deps.py:
	32	1. Please give this release an identifier by modifying release.py
	33	- Fill in release information: name and version
	34	1. For external dependencies, please adjust deps.py:
33	35	- Fill in dependencies dictionary (All external dependencies should have an entry
34	36	- Choose the appropriate installer, and implement new installer if necessary (more
		[wiki:InstallerForExternalSoftware Installer for external software]).
35		1. release.py
36		- Fill in release information: name and version

# Centralized Role of Use Cases

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# 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 bindings to McStas simulation software.*

**5.3.1.3 Bindings to NISP:** *We will provide bindings to NISP simulation software. [This task has been removed]*

**5.3.1.4 Bindings to VITESS:** *We will provide bindings to VITESS 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

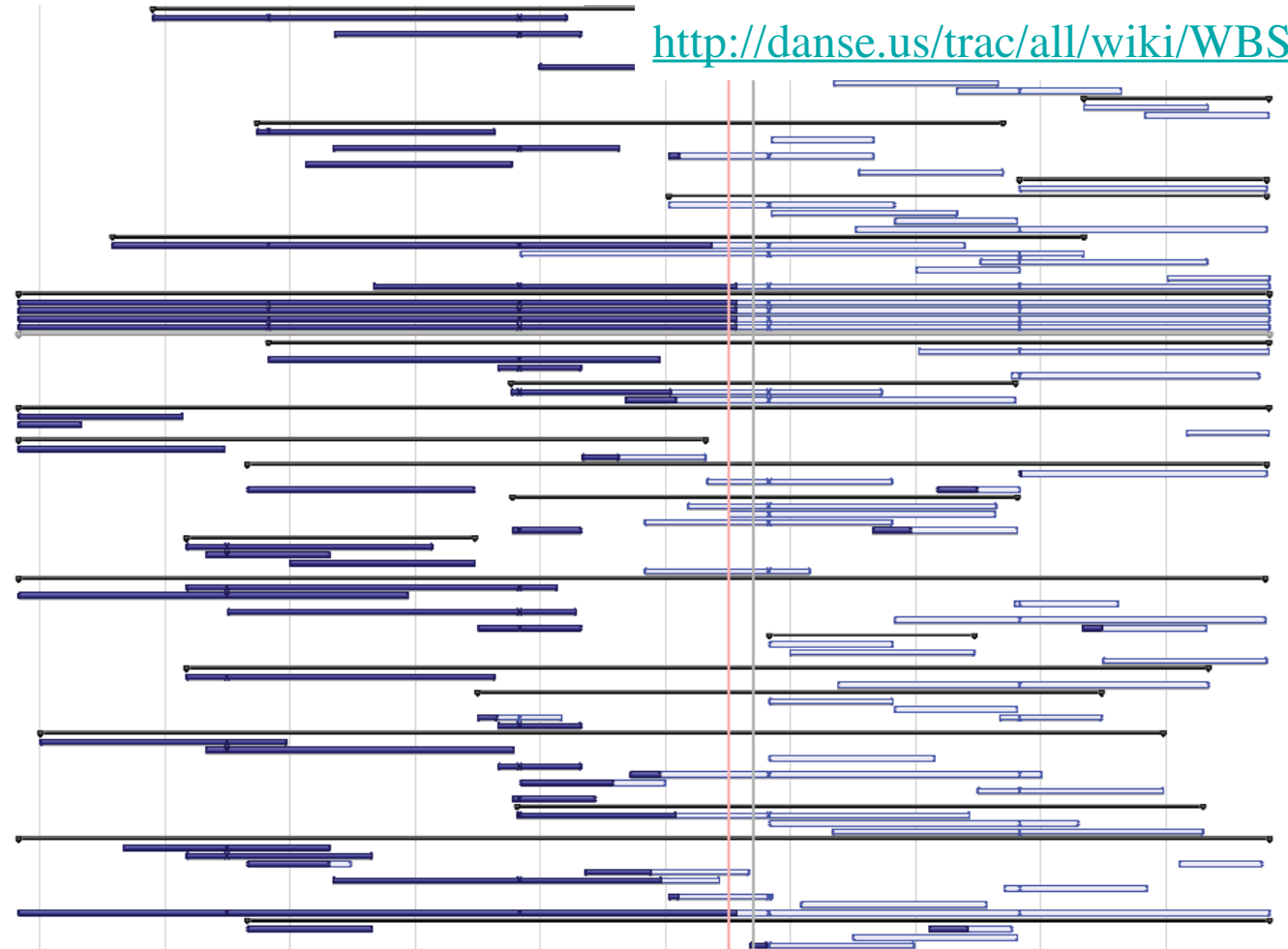
**5.3.2.2 Coherent Elastic Scattering Kernels:** *We will provide a mechanism for representing coherent elastic scattering from crystals and polycrystals from arbitrarily complex geometric shapes.*

**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>

ID	Task Name	Start	End	Progress
01	01	01/01/00	01/01/01	100%
02	02	01/01/00	01/01/01	100%
03	03	01/01/00	01/01/01	100%
04	04	01/01/00	01/01/01	100%
05	05	01/01/00	01/01/01	100%
06	06	01/01/00	01/01/01	100%
07	07	01/01/00	01/01/01	100%
08	08	01/01/00	01/01/01	100%
09	09	01/01/00	01/01/01	100%
10	10	01/01/00	01/01/01	100%
11	11	01/01/00	01/01/01	100%
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13	13	01/01/00	01/01/01	100%
14	14	01/01/00	01/01/01	100%
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97	97	01/01/00	01/01/01	100%
98	98	01/01/00	01/01/01	100%
99	99	01/01/00	01/01/01	100%
100	100	01/01/00	01/01/01	100%



# Highlight Objectives and Deliverables

The image shows two overlapping browser windows. The top window is titled 'SansWBS - DANSE core - Trac' and displays the 'SansWBS' wiki page. The bottom window is titled 'InsWBS - DANSE core - Trac' and displays the 'InsWBS' wiki page. Both pages feature a 'DANSE' logo and a navigation menu. The 'SansWBS' page lists 'Objectives' and 'Flagships' under the 'SANS' section. The 'InsWBS' page lists 'Objectives' and 'Frameworks and Flagships' under the 'Inelastic Scattering' section.

**SansWBS - DANSE core - Trac**  
http://danse.us/trac/tickets/wiki/SansWBS

DANSE optimize new-Aug08

**DANSE**

logged in as mmckerns | [Logout](#) | [Setting](#)

[Wiki](#) | [Timeline](#) | [Roadmap](#) | [Browse Source](#) | [View Tickets](#) | [New Ticket](#) | [Search](#)

[Start Page](#) | [Index by Title](#) | [Ir](#)

**SANS**

**Objectives**

- Provide a flagship application t
- Provide a flagship application t
- Provide a flagship application t

**Flagships**

- SANS Modeling Application
- Advanced SANS Modeling Appl
- Experiment Planning Applicatio

**Task Definitions**

- 8.1.1.1 Powder SANS Reductio  
SANS. By utilizing standardized  
interoperate with those built at
- 8.1.1.2 Powder SANS Reductio  
calibration, and other correctio
- 8.1.2.1 Single Crystal SANS Re  
crystal SANS. By utilizing stan

**InsWBS - DANSE core - Trac**  
http://danse.us/trac/tickets/wiki/InsWBS

DANSE optimize new-Aug08 old-Aug08 Apple News Amazon Yahoo! Pandora CIT IMSS CIT Web

**DANSE**

logged in as mmckerns | [Logout](#) | [Setting](#)

[Wiki](#) | [Timeline](#) | [Roadmap](#) | [Browse Source](#) | [View Tickets](#) | [New Ticket](#) | [Search](#)

[Start Page](#) | [Index by Title](#) | [Ir](#)

**Inelastic Scattering**

**Objectives**

- Provide an extensible framework for data reduction for inelastic neutron scattering instruments.
- Provide an extensible framework for Monte Carlo simulation of neutron scattering experiments.
- Provide fast, flexible data objects that support bonding and structure deformation within crystals and r
- Provide a web-based portal for the simulation of neutron experiments and reduction of data from neut
- Provide a library of python modules for the theoretical simulations of materials.
- Provide applications that enable the optimization of materials parameters within phonon and magnon c

**Frameworks and Flagships**

- Inelastic Reduction GUI Toolkit
- Histogram Viewer
- Virtual Neutron Facility
  - Instrument Simulation Launcher
  - Materials Simulation Launcher
  - Sample Dynamics Launcher
  - Structure Dynamics Launcher
- Monte Carlo Instrument Simulation Framework
- Sample Simulation Framework

# Iterative Improvements in Release Strategy

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- **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

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- 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 – AI	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 – AI	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

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- 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

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

## Issue: ENGD Earned Value & Performance

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information contained on this slide.

# Planned Resolution: ENGD + THEORY

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- 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

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- 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

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- **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

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- 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

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- 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

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

# Lessons Learned, so far

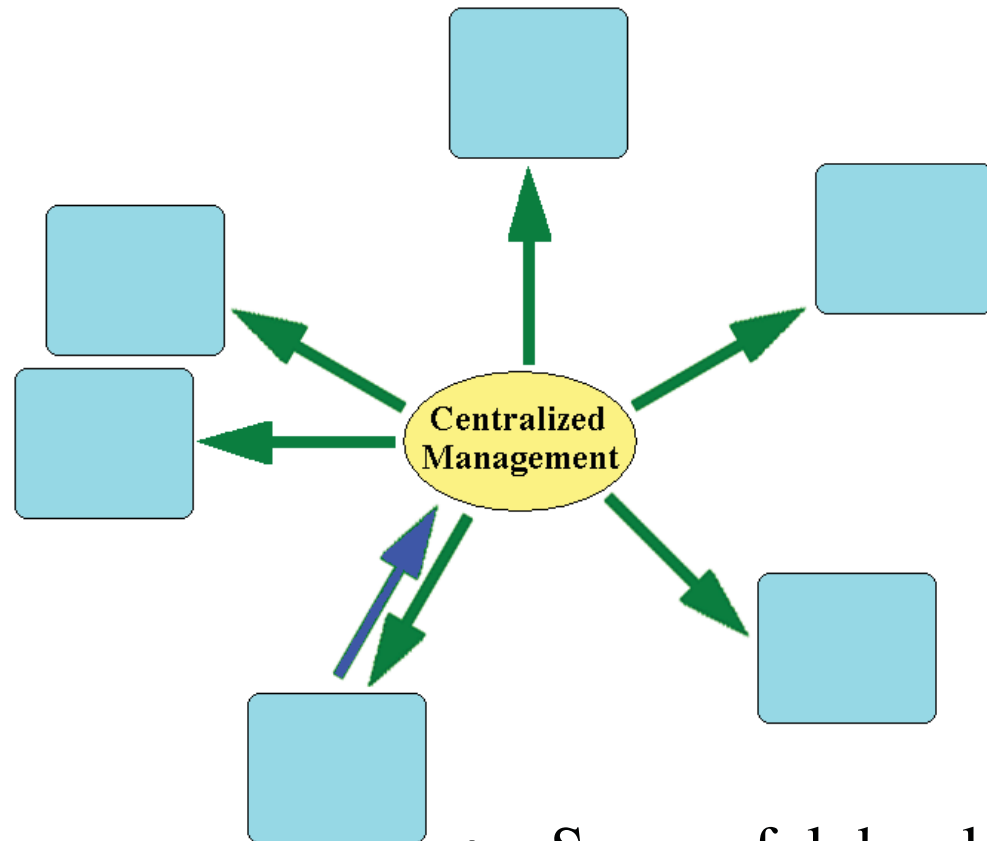
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- Managing Expectations
  - scientific software deliverables are twofold: “the science” & “the software”
  - *software in (trusted) users’ hands as early as possible produces better software*
  - reusable, extensible software for new science takes 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

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- 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

<p>Overall Change Impact:  <input type="checkbox"/> High <input type="checkbox"/> Medium <input type="checkbox"/> Low</p> <p>Overall Change Priority:  <input type="checkbox"/> High <input type="checkbox"/> Medium <input type="checkbox"/> Low</p>		<p><b>Detailed Change Description</b>                  Transfer remaining task budget</p>		<h2>DANSE</h2> <h3>Project Change Request</h3>																	
<p><b>Final Review Results</b>                  CCB votes approval: 3-0.</p> <p><b>Actions</b></p> <table border="1"> <thead> <tr> <th>ID</th> <th>Action Item</th> </tr> </thead> <tbody> <tr><td> </td><td> </td></tr> <tr><td> </td><td> </td></tr> <tr><td> </td><td> </td></tr> </tbody> </table>		ID	Action Item							<p><b>Initial Review of Request</b>                  Action (select one)  <input type="checkbox"/> Require Impact Analysis  <input type="checkbox"/> Reject  <input type="checkbox"/> Defer  <input type="checkbox"/> Immediate Approval</p>		<p><b>Change Justification</b>                  The SQA subcontract to Tom S MGMT.</p>		<p><b>Initiating Task Name:</b> 3.1.3 Software Integration and Certification</p> <p><b>Initiating Subproject Leader:</b> Brent Fultz (PI)</p> <p><b>Date:</b> 08/05/08</p> <p><b>Change Control #:</b> 2</p> <p><b>Associated Risk ID #:</b></p>							
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<p><b>Comments</b>                  [Replace this text with comments]</p>		<p><b>Alternatives to Implementing Project</b>                  None.</p>		<p><b>Prepared By</b></p> <table border="1"> <thead> <tr> <th>Document Owner(s)</th> <th>Project Role</th> </tr> </thead> <tbody> <tr> <td>Mike McKerns</td> <td>Project Manager</td> </tr> <tr><td> </td><td> </td></tr> <tr><td> </td><td> </td></tr> </tbody> </table>		Document Owner(s)	Project Role	Mike McKerns	Project Manager												
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<p><b>Approvals</b></p> <p>Board Reviewer: <u>Brent Fultz</u></p> <p>Board Reviewer: _____</p> <p>Board Reviewer: _____</p> <p>Subproject Leader: _____</p>		<p><b>Impact of Implementing Project</b>                  SQA tasks are placed under control of MGMT.</p>		<p><b>Summary of Requested Change</b></p> <table border="1"> <thead> <tr> <th>Area (select all)</th> <th>Change Description</th> </tr> </thead> <tbody> <tr> <td>Scope</td> <td>All remaining SQA tasks transfer to MGMT</td> </tr> <tr> <td>Schedule</td> <td>None</td> </tr> <tr> <td>Budget</td> <td>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.</td> </tr> <tr> <td>Quality</td> <td>None</td> </tr> </tbody> </table>		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						
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<p><b>Impact Analysis for Project</b></p> <table border="1"> <thead> <tr> <th>Impact</th> <th>Project</th> </tr> </thead> <tbody> <tr><td>Task Scope</td><td> </td></tr> <tr><td>Task Schedule</td><td> </td></tr> <tr><td>Task Budget</td><td> </td></tr> <tr><td>Task Quality</td><td> </td></tr> <tr><td>Task Risk</td><td> </td></tr> <tr><td>Project Scope</td><td> </td></tr> <tr><td>Project Schedule</td><td> </td></tr> </tbody> </table>		Impact	Project	Task Scope		Task Schedule		Task Budget		Task Quality		Task Risk		Project Scope		Project Schedule		<p><b>Impact of NOT Implementing Project</b>                  WBS is less accurately reflecting</p>		<p><b>Requested Implementation</b>                  Grants Manager to activate transfer of funds to MGMT.                  Project Manager to adjust contract budgets for SQA and MGMT.</p>	
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# A Look at Existing Project Metrics

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- 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?