The SciDAC Center for Technology for Advanced Scientific Component Software (TASCS)

http://tascs-scidac.org

Lead PI: David Bernholdt

Oak Ridge National Lab, *bernholdtde@ornl.gov*

Institution	Institutional Lead PI	Institution	Institutional Lead PI
ANL	Lois McInnes	SNL	Rob Armstrong
Binghamton U	Madhu Govindaraju	Tech-X	Sveta Shasharina
Indiana U	Randy Bramley	U Maryland	Alan Sussman
LLNL	Tom Epperly	U Oregon	Matt Sottile
ORNL	Jim Kohl	Virginia State U	Kosta Damevski
PNNL	Jarek Nieplocha	past participants	LANL, U Utah

General contact point (PIs and technical leads):

tascs-leads@cca-forum.org

Past, Present, Future

- The Common Component Architecture (CCA) is a ***community*** effort, with SciDAC projects in the vanguard
- CCTTSS (SciDAC1) brought the CCA from idea to prototype stage
  - Core ideas well-developed
  - Useful implementations, but not polished
  - Numerous users, but not “standard”
- TASCS is bringing the CCA from prototype to production for general computational science users
  - Robustness of tools
  - Usability of components and component environment
  - Developing an ecosystem (component toolkit) around CCA
  - Providing new features and capabilities for scientific software developers via the component environment
- Still many open issues and opportunities beyond those TASCS is addressing
  - Must gather experience before we can determine appropriate abstractions

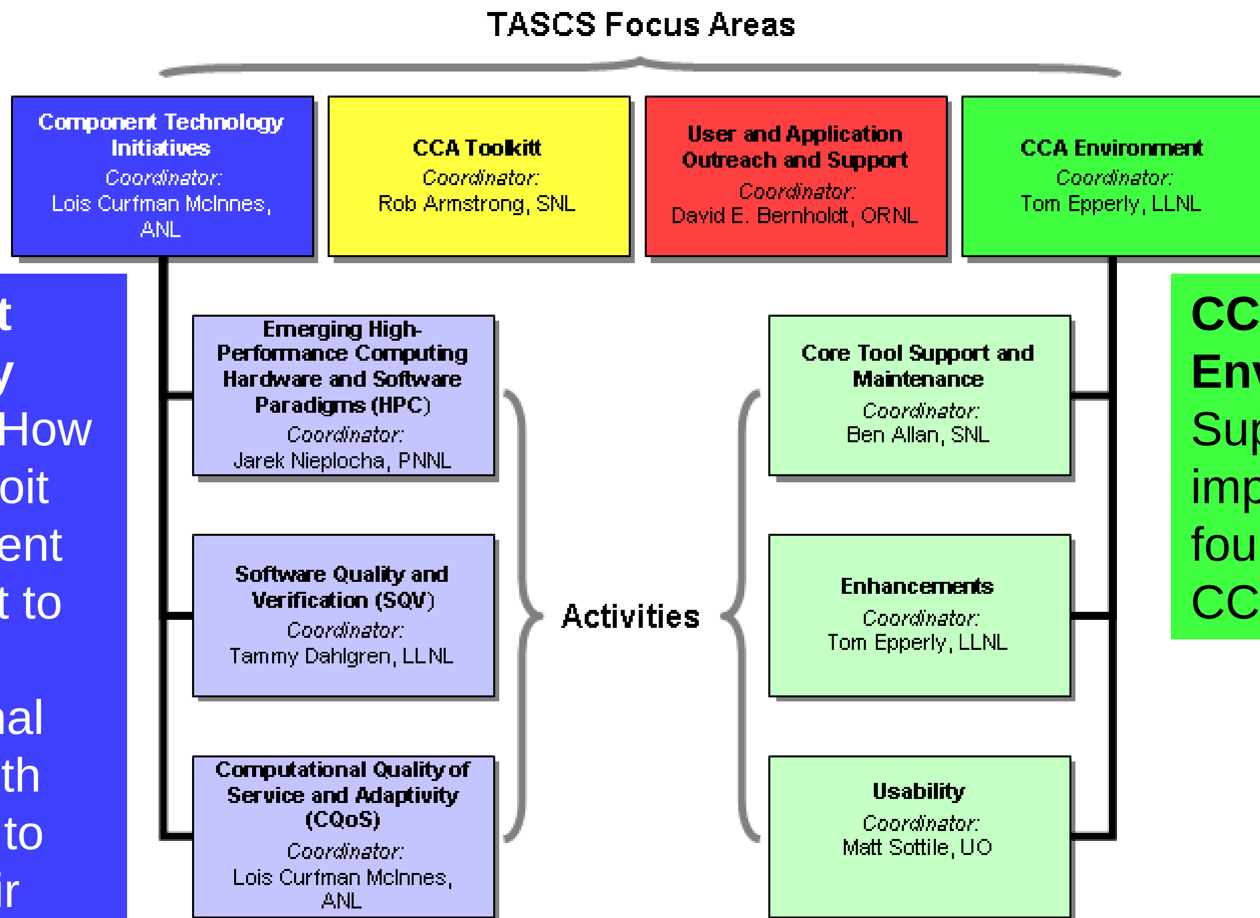
We're Different (from Most SciDAC Projects)

- We're trying to fundamentally change the way scientific software is developed and used
- Current "culture" of computational science emphasizes short-term heroism over long-term sustainability
  - CCA impact on performance, simulation size is second-order
- CCA (and most software engineering) requires a significant initial investment (intellectual and in software)
  - Longer-term payback
  - Significant social and sociological issues
- Groups choosing to make the investment in CCA tend not to be the ones issuing press releases for the fastest/biggest/*-est
  - PR challenge

Project Organization

CCA Toolkit: Making it easier to create components, and making available a suite of real, useful components

User Outreach & Application Support: Broaden awareness and adoption of component technology and the CCA



Component Technology Initiatives: How can we exploit the component environment to provide computational scientists with better ways to develop their software?

CCA Environment:: Supporting and improving the foundation of the CCA environment

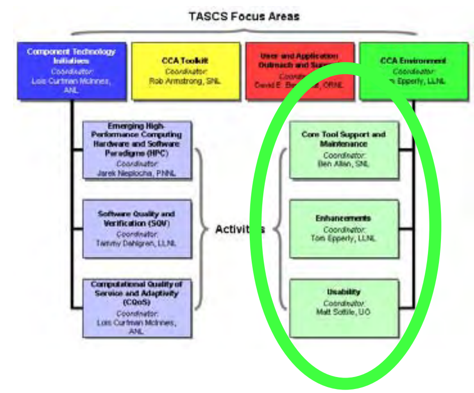
Institutional Involvement

	ANL	BU	IU	LLNL	ORNL	PNNL	SNL	Tech-X	UM	UO	VSU
Initiatives	C			3	3	3	3				
HPC					3	C					
SQV				C	3						
CQoS	C						3				
Environment	3	3		C	3		3			3	3
Support	3			3	3		C				
Enhance ments		3		C	3		3				3
Usability				3	3		3			C	
Toolkit	3		3	3	3	3	C	3	3		3
Outreach	3		3	3	C	3	3	3			

C = Coordinator 3 = Participant

CCA Environment Activities

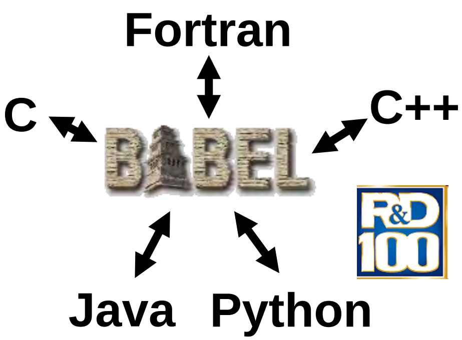
Supporting and improving the foundation of the CCA environment

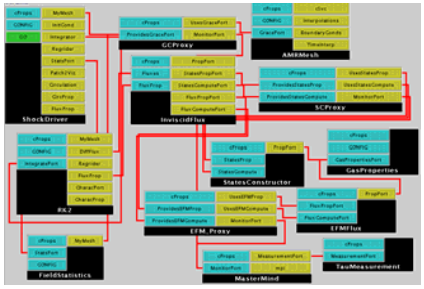


- **Core Tool Support and Maintenance**
  - Keeping the core software tools running in the face of change
- **Enhancements**
  - Extending the CCA environment (specification, core tools) with additional features/capabilities required by customers and other activities in TASCS
- **Usability**
  - Making HPC component technology more accessible to users through automatic wrapping, testing tools, better debugging support

CCA Tool Chain

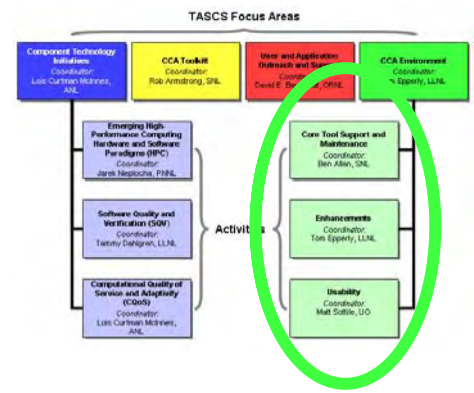
- Onramp
  - (Semi-) automatic componentization of legacy code
  - Under development
- Bocca
  - Component development tool ("command line IDE")
  - Initial release, additional development planned
- Babel
  - Language interoperability & component middleware
  - In production
- CCA-Spec-Babel
  - Implementation of CCA spec functionality using Babel
  - In production
- Ccaffeine
  - HPC framework with optional GUI
  - In production





Environment: Core Tool Support & Maintenance

Keeping the core software tools running in the face of change



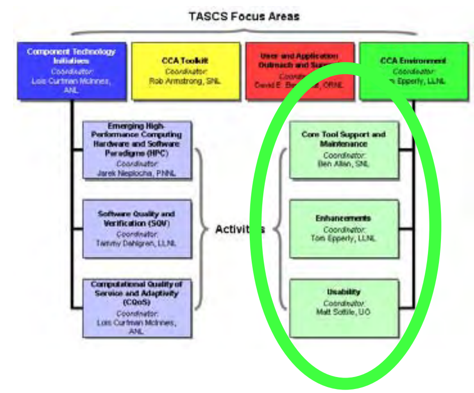
- Helpdesk and bug tracking
- Technical documentation
- Ports for high-end and other platforms
- Continuous integration and regression testing for tools
- Develop CCA (specification) conformance tests
- Automated conformance testing

Environment: Support Recent Accomplishments

- Helpdesk and bug tracking implemented on all tools and tutorial
- Extensive expansion of documentation in tutorial format
- Fully ported to commodity Linux, Mac
- All tools working on Cray, build still “special”
- Partially ported to IBM Blue Gene
- General “static application generator” nearly complete
  - Important on systems that don’t support dynamic linking

Environment: Enhancements

Extending the CCA environment (specification, core tools) with additional features and capabilities required by customers and other activities in TASCS



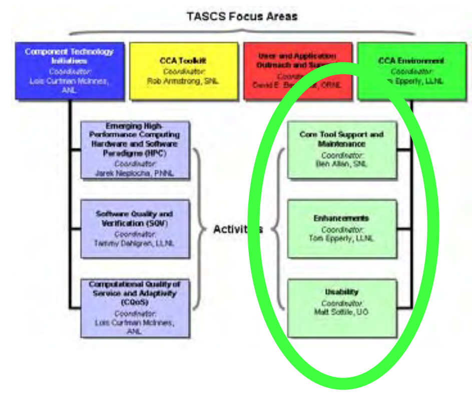
- Filling out the CCA specification with crucial new services
- Building bridges to other related technologies (e.g., Kepler)
- Interoperability and integration of CCA foundational tools

Environment: Enhancements
Recent Accomplishments

- Establish CCA Review Board (CCARB) to ensure rigorous multi-stage specification process
- MPIService & EventServices are nearing CCARB approval
- Babel gains initial F2003 support and multi-language structs in C, C++, Python, & F2003
- Demonstrated CCA/Kepler interoperability (CBHPC 2008)
- Prototype of BabelRMI using Proteus
- New stable Babel 1.4.0 release

Environment: Usability

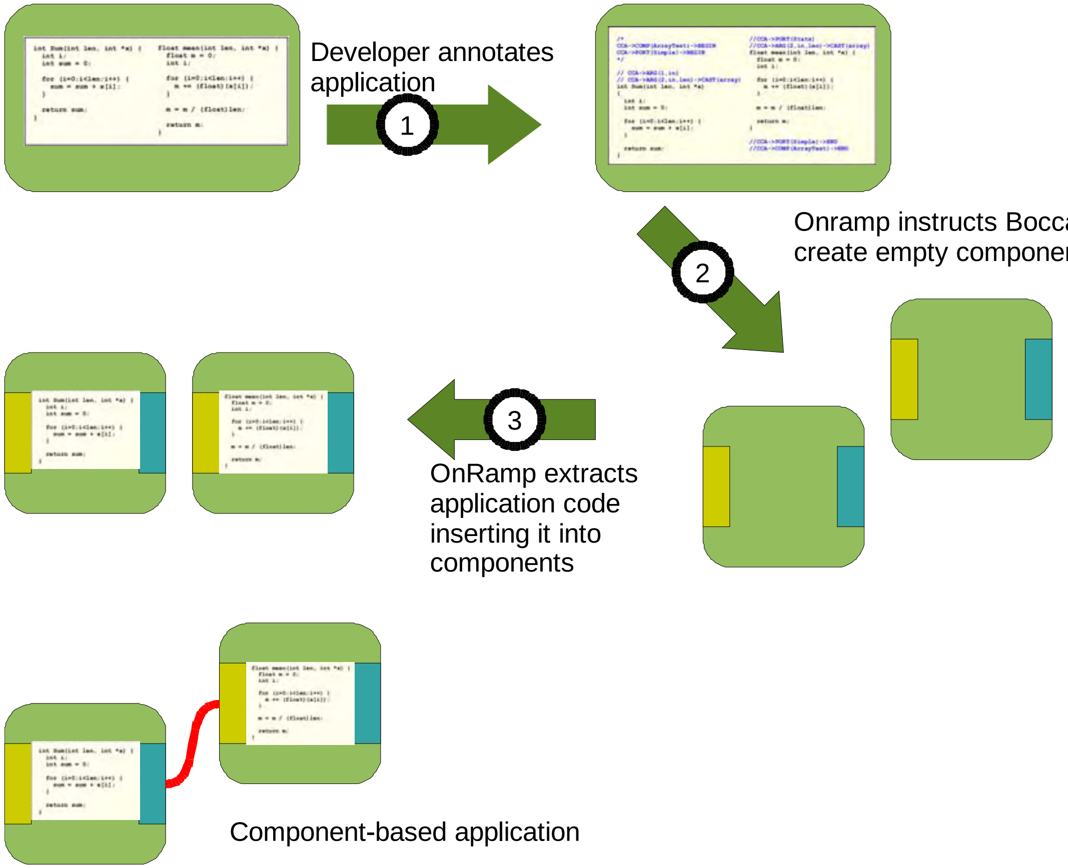
Making HPC component technology more accessible to users through automatic wrapping, testing tools, better debugging support



- CCA Onramp
  - (Semi-) automatic wrapping of existing code into the CCA environment based on source code annotations
  - Allows “mixed use” of code in both original form and as components
  - Refactor application into componentized domain-specific framework
- Debugging and testing
  - CCA abstractions and capabilities simplify designing, developing software but can make it harder to debug, test
  - Capturing and documenting multi-language debugging approaches, developing testing tools

CCA Onramp

- Source code annotations to specify componentization (components, interfaces)
- Generate SIDL for interfaces, components
- Use bocca to generate component skeleton
- Generate code to adapt between existing code and Babel bindings

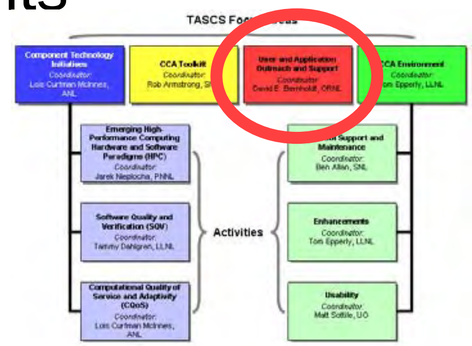


Environment: Usability Recent Accomplishments

- Onramp created and released for C-based codes.
  - Fortran and C++ support in near-term plan.
- Source annotation specification draft available for public comment and contribution.
  - Reference implementation in Onramp tools.
- Distribution of Onramp through SciDAC outreach site.
  - As of October 2008, third most downloaded project
- New versions of PDToolkit static source analysis tools to support CCA efforts (e.g. new query interface)
- Evaluation of automated build and test harnesses (e.g. CruiseControl)
- Establishment of routine tools testing on Cray

CCA Toolkit

Making it easier to create components, and making available a suite of real, useful components



- Provides instant application prototyping
  - Scientists can try out ideas quickly in a parallel HPC setting.
  - Develop those ideas incrementally, concentrating on particular components to increase performance or fidelity
- Provide tools to make componentry easy
  - Bocca automatically generates a CCA component template as easy as giving them a name

Simple Bocca Example

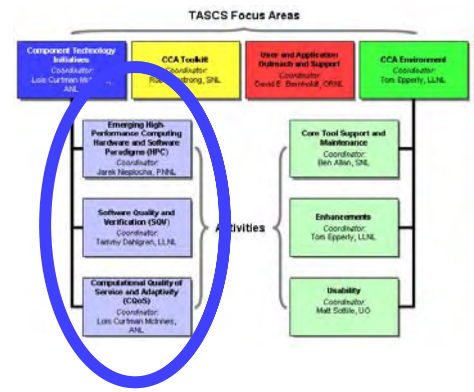
```
# create an empty but buildable CCA skeleton
bocca create project myproj
cd myproj
./configure

bocca create port myJob
bocca create component myWorker –provides=myJob:job1

# fill in public functionality
bocca edit port myJob

# fill in implementation
bocca edit component –i myWorker

# compile application
make
```

CCA Toolkit
Recent Accomplishments

- Components ready to use for:
  - Linear Algebra, Equation Solvers, Optimization, MPI
    - PETSc, SPARSEKIT2, and more
  - Parallel decomposed meshes
- More components being packaged to meet Toolkit requirements
- Initial release of bocca
  - Incorporated into tutorial
  - Significant productivity gains

Component Technology Initiatives

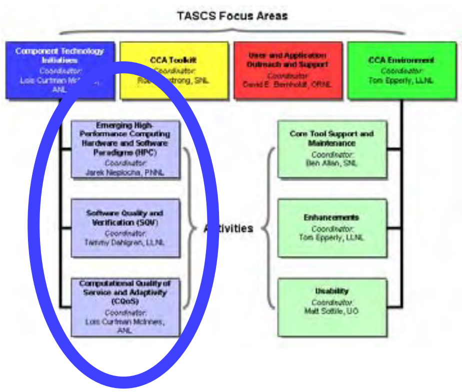
How can we exploit the component environment to provide computational scientists with better ways to develop their software?



- **Computational Quality of Service**
  - Adaptation of running component applications in response to changing conditions (performance, accuracy, etc.)
- **Software Quality and Verification**
  - Extend component interface definitions to express contracts, extra-functional characteristics, with automatic verification
- **Support for Emerging HPC Hardware and Software Paradigms**
  - Use CCA interfaces to manage MCMD applications on massively parallel systems
  - Integrate software on hardware accelerators into CCA applications

Initiatives: Computational Quality of Service (CQoS)

Adaptation of running component applications in response to changing conditions (performance, accuracy, etc.)

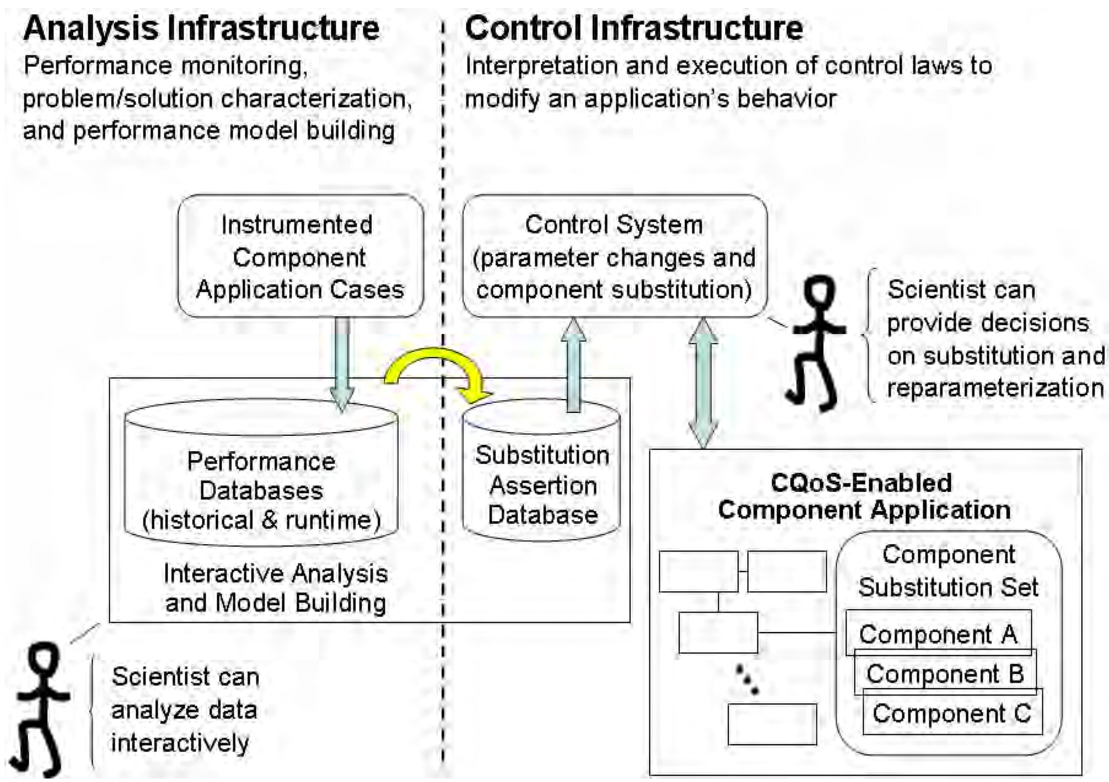


Collaborators: Teaming with TASCS Software Quality and Verification (SQV) Initiative, University of Oregon TAU team, PERI, TOPS. Close interactions with SciDAC scientific applications teams to motivate and validate this work:

- **Combustion:** parallel mesh partitioning in combustion
  - (BES) CFRTS SciDAC project (H. Najm PI)
- **Quantum Chemistry:** resource management in quantum chemistry
  - (BES) SciDAC project (M. Gordon PI)
- **Fusion and Accelerators:** efficient, robust, and scalable linear solvers (with TOPS)
  - (FES) FACETS SciDAC project (J. Cary PI) - Newton-Kryov solvers in parallel edge plasma simulations
  - (HEP) COMPASS SciDAC accelerator project (P. Spentzouris PI) - solvers in beam dynamics simulations

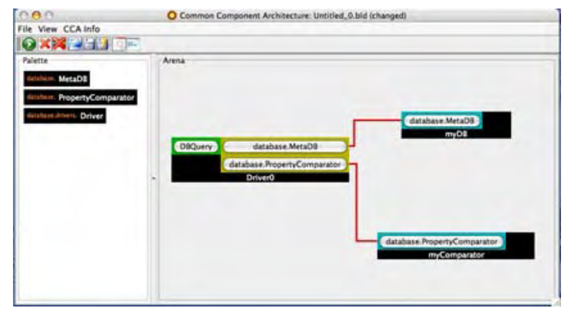
Initiatives: CQoS Approach

- **Analysis:** performance monitoring, problem/solution characterization, and performance model building
- **Control:** Interpretation and execution of control laws to modify an application's behavior
- **CQoS database components:** Manage interactions with performance and runtime databases to facilitate analysis and decision making
- **Leverage external tools** where appropriate, e.g., Anamod (Eijkhout et al.)



Initiatives: CQoS Recent Accomplishments

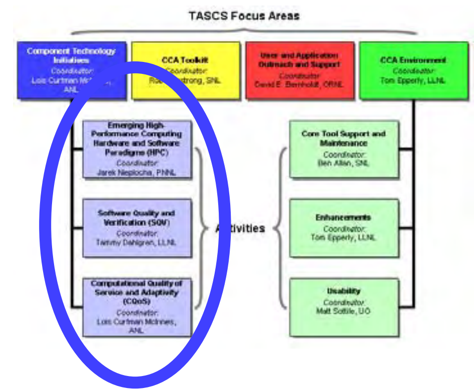
- Collected requirements from four motivating applications
  - Initial implementation focus: component composition and configuration for quantum chemistry and combustion
    - See, e.g., http://wiki.mcs.anl.gov/cqos/index.php/Quantum_Chemistry_CQoS_Activities
- Designed initial CQoS API and software suite testbed
  - Initial API focus on CQoS database query and management
  - Testbed applications for parallel nonlinear solvers, mesh partitioning in combustion, quantum chemistry



- Implemented performance database query and management components
- Determined overall strategy for CQoS software
- Developed prototype models and control laws
  - Preliminary version for combustion, in progress for quantum chemistry
- In progress: running base performance experiments

Initiatives: Software Quality and Verification (SQV)

Extend component interface definitions to express contracts, extra-functional characteristics, with automatic verification



- **Collaborators:** Working in conjunction with CQoS activity
- **Approach**
  - Identify and define relevant component characteristics and constraints
  - Pursue suitable semantic representations leveraging work on interface contract enforcement capabilities integrated into Babel middleware toolkit

Enforcable Contracts for SIDL Interfaces

- Current component architectures define syntax of interfaces
- Extend interface to include semantics (behavior) for more complete definition
  - "Design by contract"
  - Help ensure component performs correctly
  - Help ensure component is used correctly
- Selective enforcement to control impact

```
package vector version 1.0 {
  class Utils { …
    static double norm(in array<double> u,
                       in double tol,
                       in int badLevel)
      require    /* Preconditions */
        not_null : u != null;
        u_is_1d : dimen(u) == 1;
        non_negative_tolerance : tol >= 0.0;
      ensure    /* Postconditions */
        no_side_effects : is pure;
        non_negative_result : result >= 0.0;
        nearEqual(result, 0.0, tol)
          iff isZero(u, tol);
 … }
}
```

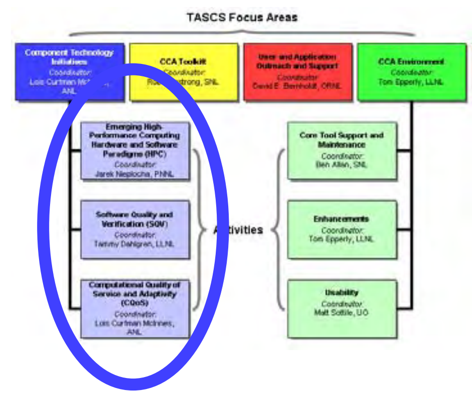
Initiatives: SQV
Recent Accomplishments

- Integrated refactored version of latest prototype enforcement approach into the Babel source code repository
- Developed example implementations of a specification with contracts in C++, FORTRAN 77, Fortran 90, Java, and Python
- Developed example client for the above implementations in C++
- Demonstrated in regression tests for **Babel Release 1.4.0**:
  - C or C++ client → C, C++, FORTRAN 77, Fortran 90, Java, and Python implementations

Initiatives: Support for Emerging HPC Hardware and Software Paradigms (HPC)

Enable effective use of CCA on emerging HPC architectures

- **Multiple-Component-Multiple-Data (MCMD) CCA Technology** to support apps based on multiple levels of parallelism for massively parallel systems
  - Motivated by multiple apps: chemistry, climate, materials modeling, fusion, etc.
  - Used in NWChem

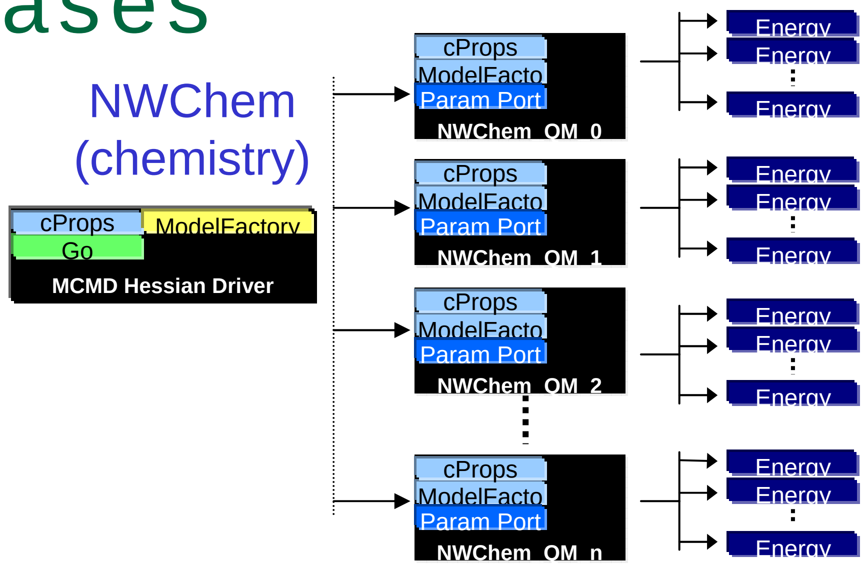


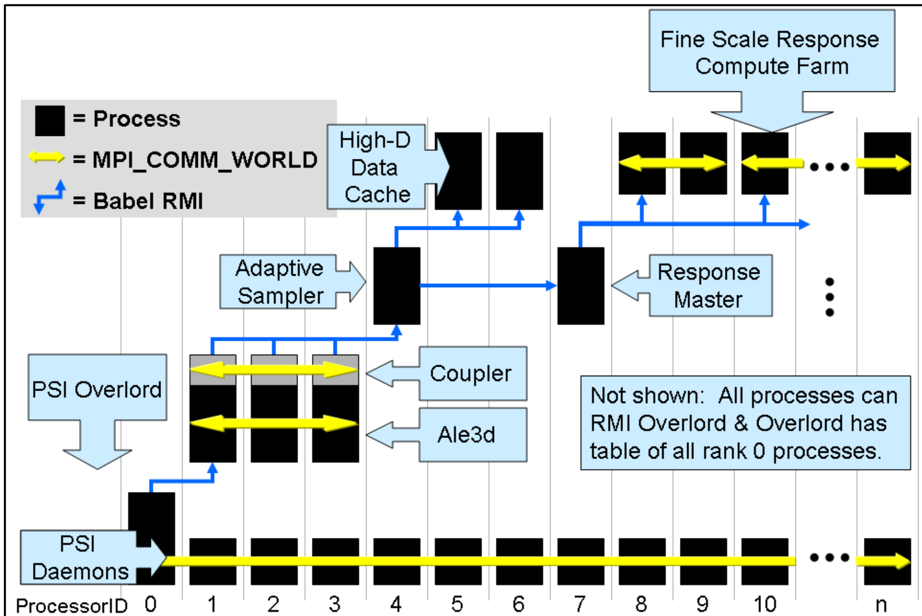
- Simplify use of systems with **heterogenous** node architectures (e.g., IBM RoadRunner)
  - Couple/swap component codes on accelerators and general purpose CPUs
  - bioinformatics/proteomics applications in EMSL Mass Spectrometry facility

- **Fault Awareness** in CCA, in collaboration with CIFTS
  - Bridge between CIFTS Fault Tolerance Backplane (FTB) and CCA Event Service
  - SWIM (fusion) MCMD simulations as initial model application

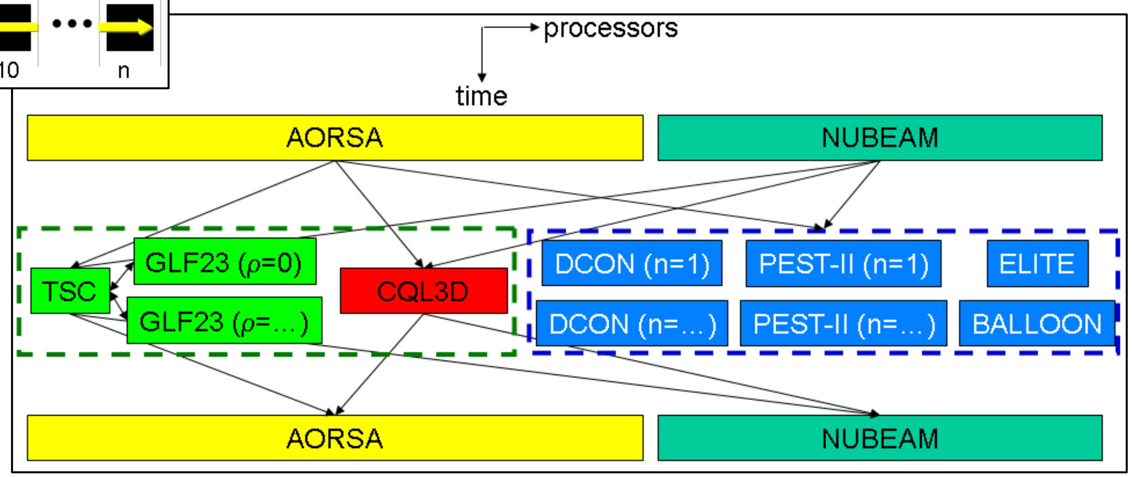
Multiple-Component Multiple-Data Use Cases

NWChem (chemistry)





Co-Op (materials)



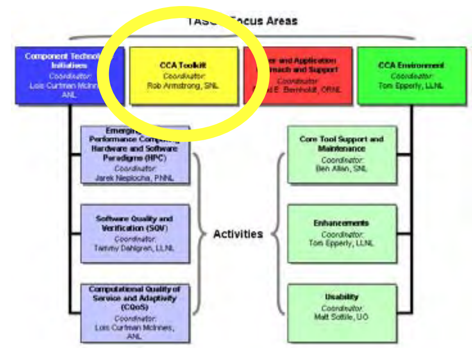
SWIM (fusion)

Initiatives: HPC Recent Accomplishments

- **Multiple-Component-Multiple-Data (MCMD) CCA Technology**
  - Developed processor teams specs and prototype implementation
  - The initial scope extended to support coupling independent jobs in subsurface simulations e.g., hydrology and geophysics
- Simplify use of systems with **heterogenous** node architectures
  - High performance event service developed and demonstrated
  - Coupled component codes on accelerators and general purpose CPUs (e.g. Polygraph on FPGAs)
- **Fault awareness**
  - Prototype fusion demonstration application nearing completion

User Outreach & Application Support

Broaden awareness and adoption of component technology and the CCA



- Application support
  - In tandem with Environment Support activity for tools
- User outreach and support
  - Tutorials, coding camps, etc
- Community outreach
  - Papers, presentations, workshops, collaboration server, etc.

How We Work with Others

- **R&D Partners**
  - Motivation and test beds for specific TASCS R&D activities
  - TASCS support built into *Component Technology Initiatives*
- **Collaborators**
  - Jointly funded w/ partner projects through *Outreach*
- **“Walk-Up” Users**
  - Modest support through *Outreach*
- Help Desk supported through *Environment & Outreach*
- Designated points of contact (often “embedded”), frequent interactions, coding camps, site visits, etc.
- **CCA Forum** (www.cca-forum.org)
  - CCA standards body and user community
- Tutorials, presentations, publications, workshops, etc.

Outreach: Recent Accomplishments

- Many collaborative interactions (23+)
  - See http://tascs-scidac.org/collaborators
- 46+ papers to date (presentations not yet cataloged)
- 6 tutorials
  - ACTS Collection Workshop (annual), Supercomputing 2007, SciDAC 2007, Para’08
- 5 workshops organized
  - HPC-GECO/CompFrame (’06, ’07), CBHPC’08, Para’08, CBC’08
- Host majority of CCA Forum meetings
- Established separate tascs-scidac.org web site
- cca-forum.org collaboration services activities *in progress*
  - Migration from LBNL to ORNL, Improved web site, EPrints server about to go into production

Major New Users and Future Opportunities

New Users

- GWACCAMOLE (groundwater)
- FACETS (fusion)
- COMPASS (accelerator physics)
- Community Surface Dynamics Modeling System (CSDMS)

Future Opportunities

- GNEP Nuclear Energy Advanced Modeling & Simulation (NEAMS)
- DoD CREATE
- HPC Application Software Consortium (HPC-ASC)

Exascale Challenges

- Code complexity!

- Multiphysics code coupling
- Massive parallelism
- Composition of parallel {components, libraries, etc.}
- Exposure and use of extra-functional properties of software components
  - Performance, parallelism, contracts, etc.

- TASCS has some relevant R&D activities and is working with relevant applications
- TASCS will not fully “solve” these problems, but we’re gaining experience

Summary

- TASCS is part of the community developing and using the Common Component Architecture
- Long-range focus on improving the ability to develop, manage, and use increasingly complex high-performance scientific software
- Broad R&D effort
  - Production quality tools
  - Making componentry more accessible
  - Technology initiatives on new capabilities for software developers
- Engaged with many applications, extensive broader outreach