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

http://tascs-scidac.org

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Institution	Institutional Lead PI	Institution	Institutional Lead PI
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LLNL	Tom Epperly	U Oregon	Matt Sottile
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PNNL	Jarek Nieplocha	past participants	LANL, U Utah

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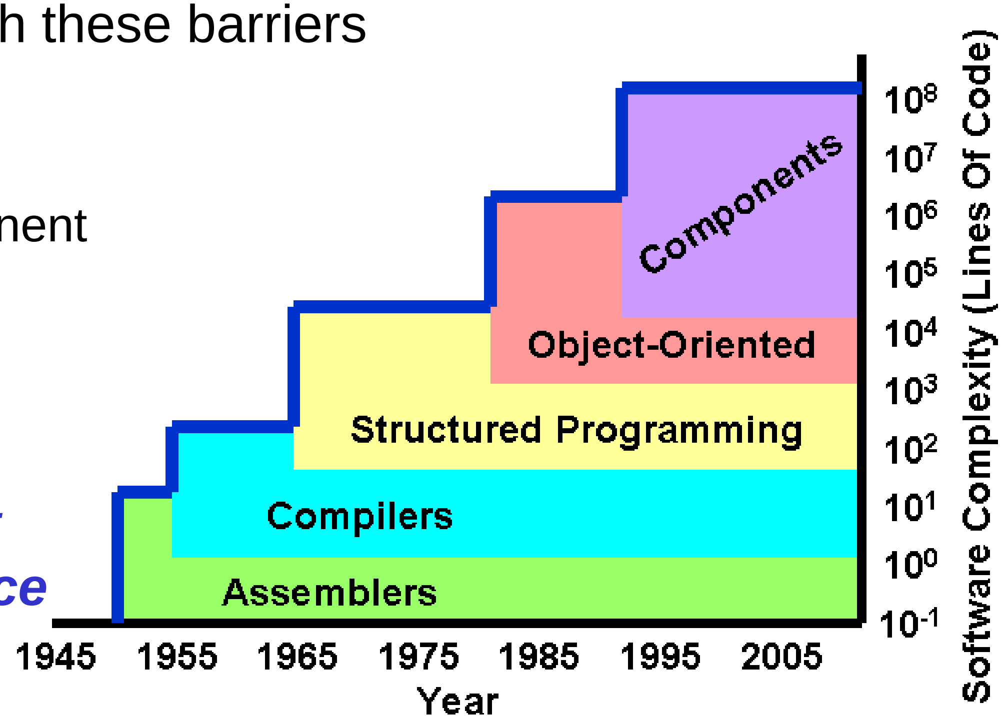
Component Technology for Scientific Discovery

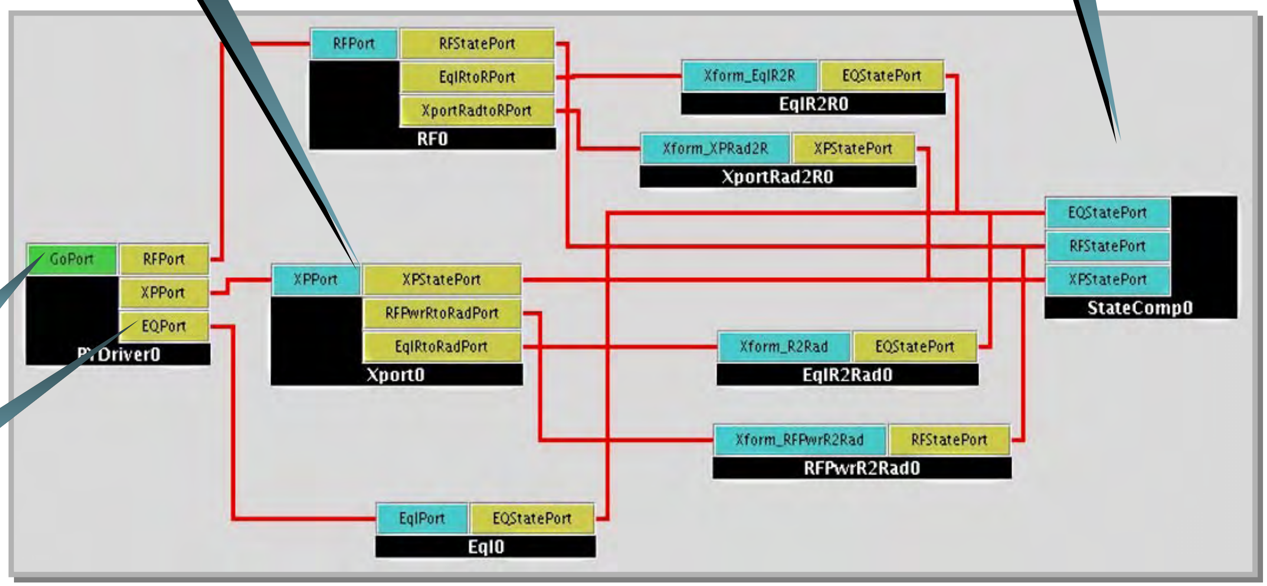
- Scientific discovery in SciDAC hinges on advanced scientific software
  - Software complexity increases with simulation fidelity, multi-physics coupling, computer power → software crisis
- As software developers encounter limitations in their ability to comprehend and manage software, computer scientists develop better approaches to help break through these barriers
- Component technology is well established outside of HPC
  - All enterprise software is component software, but commercial implementations do not support high-performance computing

TASCS is bringing component technology to high-performance scientific computing



Simple but Powerful Basic Concepts

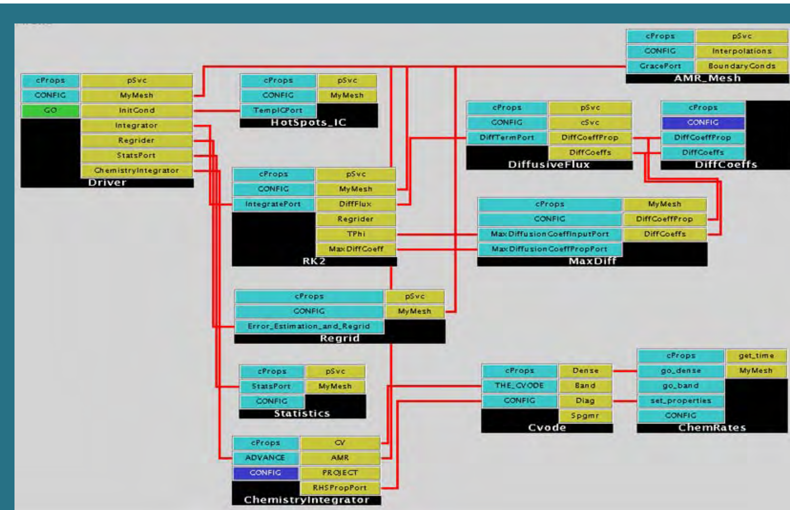
- ***Components***
  - Are units of software development/ functionality
  - Interact only through well-defined interfaces
  - Can be composed into applications based on their interfaces
- ***Ports***
  - Are the interfaces through which components interact
  - Follow a provides/uses pattern
    - Provided ports are implemented by a component
    - Used ports are functionality a component needs to call
- ***Frameworks***
  - Hold components while applications are assembled and executed
  - Control the connections of ports
  - Provide standard services to components

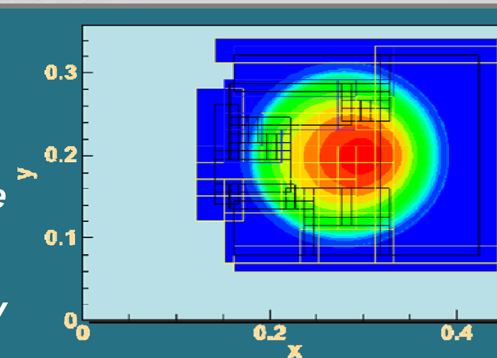


Screenshot of application in the Ccaffeine framework's GUI

Computational Facility for Reacting Flow Science (CFRFS)

- A toolkit to perform simulations of combustion and shock hydrodynamics
- Solve the Navier-Stokes with detailed chemistry
  - Various mechanisms up to ~50 species, 300 reactions
  - Structured adaptive mesh refinement
- CFRFS today:
  - 100+ components
  - 8 external libraries
  - 13 contributors
  - 5 journal papers in CFD/Numerics
  - 4 software-oriented journal papers, 1 book chapter
  - Over 15 conference papers, including best paper award
  - Over 60 presentations
  - 1 MS and 2 PhD theses
  - 6 test applications



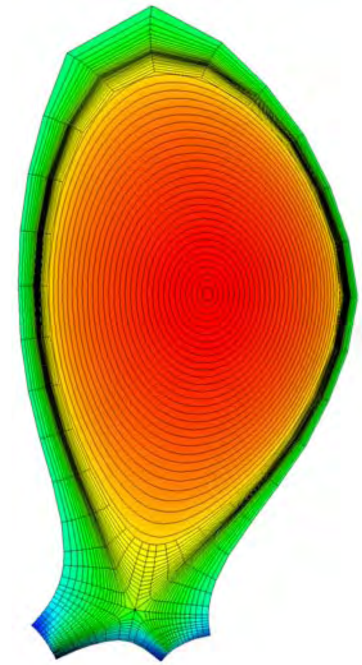


CCA-based simulation of OH concentration in advective-diffusive-reactive simulation using 4th order Runge-Kutta-Chebyshev integrator on 4 levels of adaptively refined mesh

Graphics courtesy of J. Ray, Sandia National Laboratories

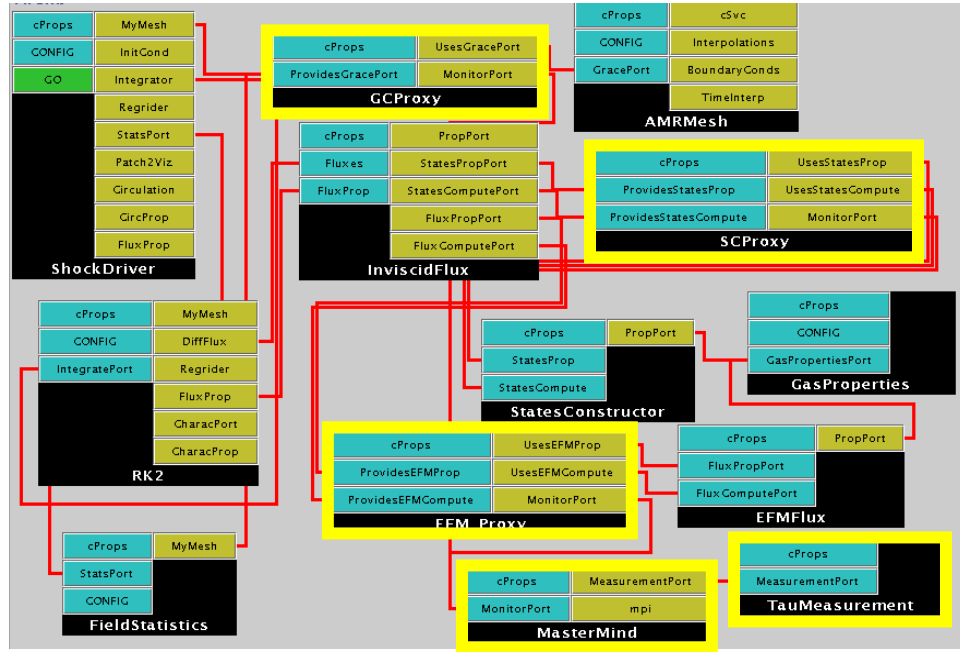
Framework Application for Core-Edge Transport Simulations (FACETS)

- Integrated modeling of plasma core, edge, and wall: prototype for Fusion Simulation Project (FSP)
- Complex physics with different dimensionalities
- Use SIDL to express interfaces between components (core, edge, wall)
- Use Babel to integrate UEDGE code into custom FACETS framework
- Result: FACETS combines physics components using Babel to achieve the first tightly coupled core-edge fusion plasma model. This is a proof of concept run that opens the door to further scientific discovery, parallelization research, and additional performance optimization

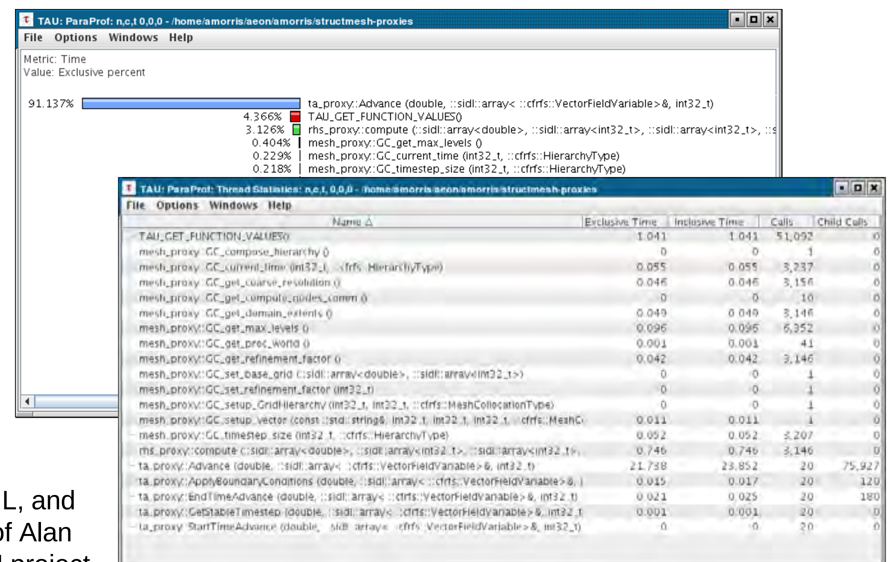


FACETS uses Babel to combine software components written in multiple languages to produce the first integrated core-edge simulation. **Image produced with VisSchema (Tech-X) plugin for VisIt, courtesy of John Cary (Tech-X)**

Semi-Automatic Component-Level Performance Instrumentation



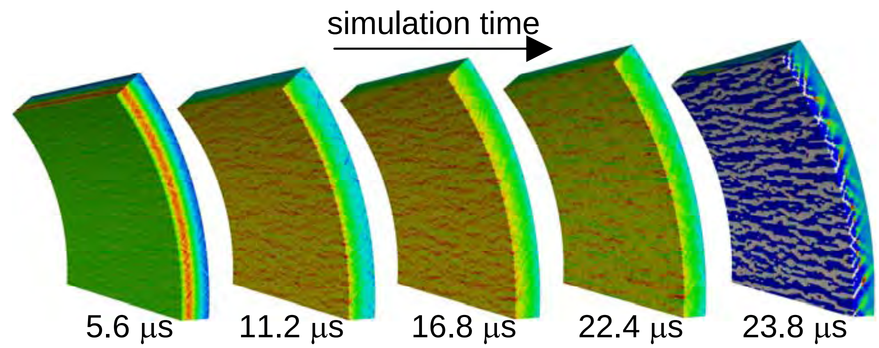
- Tuning and Analysis Utilities (TAU, U Oregon)
- Automatically generate proxies for CCA interfaces
- Proxies use TAU to capture performance data
  - Can store to a performance database
- To use, simply insert proxy between caller and callee
  - No instrumentation or recompilation of application components needed
- Analyze with ParaProf



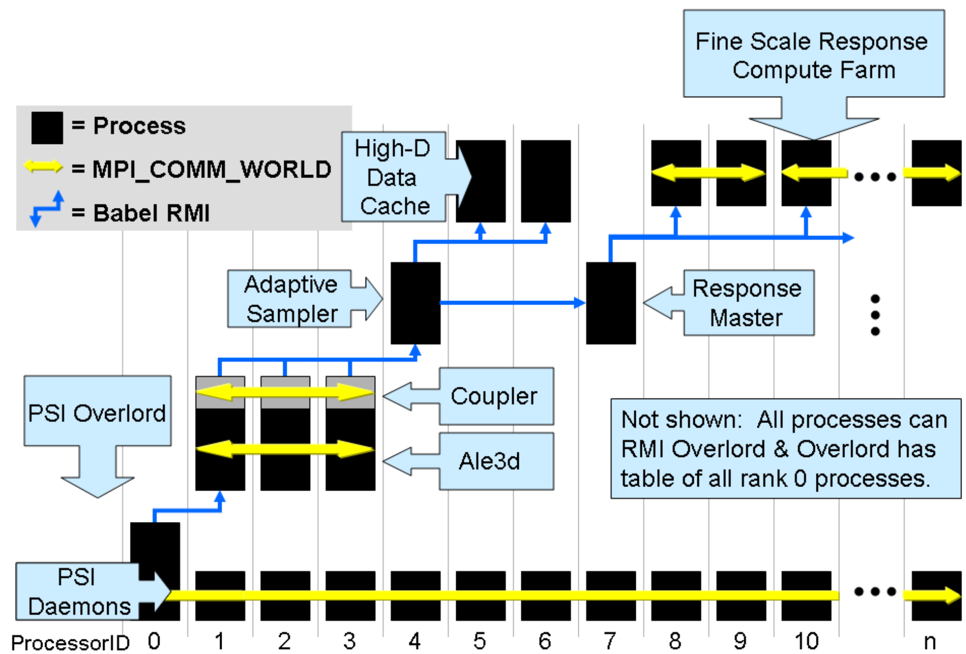
Application wiring diagram courtesy Jaideep Ray, SNL, and the CFRFS project. ParaProf screenshots courtesy of Alan Morris and Sameer Shende, U. Oregon, and the TAU project.

Multiscale Materials Modeling using Adaptive Sampling

- Petascale Simulation Initiative, and DLSMM LDRDs, LLNL
- Exploring multiscale coupling of physics simulations
- Coarse-grain materials model (Ale3d) with fine-grained viscoplastic polycrystal response model
  - Adaptive sampling to reduce fine-scale evaluations
- Uses Babel RMI to manage and execute simulation



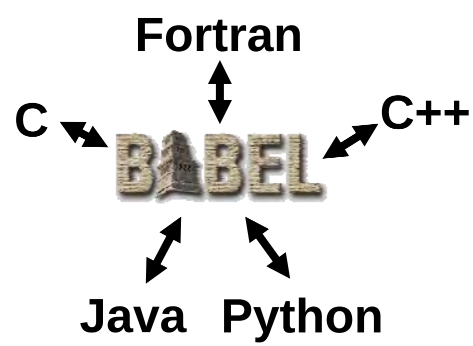
effective plastic strain rate (independent scales)



Graphics courtesy of Nathan Barton and Gary Kumfert, LLNL

Benefits of Components to Scientific Computing

- Components are natural units of decomposition and interaction for both software and developers
  - Manage software complexity
- Tools to formalize and rationalize application software architecture for long-term productivity
- They enable scientists to work together as a cohesive scientific enterprise, across disciplines, geographical boundaries, and technical preferences by facilitating…
  - Collaboration around software development
  - Sharing and exchange of software
  - Community standards for scientific software
  - Coupling of disparate codes



- Integrate code in multiple languages
- Support for both high-performance (parallel) and distributed computing

TASCS Focus Areas and Research Objectives

- **CCA Environment**
  - Supporting and improving the foundation of the CCA environment
  - Coordinator: Tom Epperly, LLNL
- **CCA Toolkit**
  - Making it easier to create components, and making available a suite of real, useful components
  - Coordinator: Rob Armstrong,SNL
- **Component Technology Initiatives**
  - How can we exploit the component environment to provide computational scientists with better ways to develop their software?
  - Coordinator: Lois McInnes, ANL
- **User Outreach & Application Support**
  - Broaden awareness and adoption of component technology and the CCA
  - Coordinator: David Bernholdt, ORNL

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

Component Technology Initiatives

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

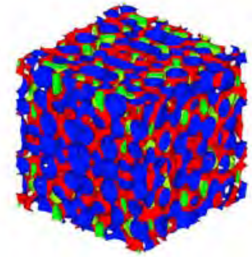
- **Computational Quality of Service**
  - Adaptation of running component applications in response to changing conditions (performance, accuracy, etc.)
- **Software Quality and Verification**
  - Extend component interface definitions to express contracts, extra-functional characteristics, with automatic 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

How We Work with Others

- **R&D Partners**
  - Motivation and testbeds 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.

A Sampling of Our Collaborations



GWACCAMOLE: tracking pollutants entrained in subsurface groundwater. Thanks to: Bruce Palmer, PNNL; Kwan-Liu Ma and Chad Jones at the Ultraviz Institute

- SciDAC Applications and SAPs
  - CFRFS (combustion), COMPASS (accel. phys.), FACETS (fusion), GWACCAMOLE (sub-surface modeling), Quantum Chemistry SAP, SWIM (fusion)
- SciDAC Centers and Institutes
  - CScADS, ITAPS, PERI, SDM, TOPS
- Other Office of Science projects
  - CIFTS (fault tolerance), ROSE, SPARSKIT, TAU (performance), Polygraph (proteomics mass spect. analysis), NWChem (chemistry), Beam dynamics modeling (accel. phys.)
- Others
  - Center for Integrated Space Weather Modeling (NSF), CIMA (NSF), Chapel (Cray), CO-OP (NNSA), GNEP Nuclear Energy Advanced Modeling & Simulation (NE), Community Surface Dynamics Modeling System (NSF)
- See http://tascs-scidac.org/collaborators for more

TASCS Seeks Users and Collaborators…

- Concerned about the long-term evolution of their software
- Especially those who challenge us to develop new and more robust capabilities
- CCA is not all-or-nothing; users obtain different benefits from different aspects
- Often, the ideas are as important as the tools
- **Contacts**
  - **http://tascs-scidac.org**
  - **Leadership team: tascs-leads@cca-forum.org**
  - **Lead PI: David Bernholdt, bernholdtde@ornl.gov**