How the Common Component Architecture (CCA) Advances Computational Science

Presented by

The CCA Forum

and the

Center for Technology for Advanced Scientific Component Software (TASCS)

See companion presentation:
An Overview of the Common Component Architecture (CCA)

SC07

Office of Science
U.S. DEPARTMENT OF ENERGY

SciDAC
Scientific Discovery through Advanced Computing

CCA's impact is as diverse as the applications in HPC

A recent survey found 25 applications using CCA in a variety of ways.

1. CCA in single codes for extra flexibility
2. CCA to combine incompatible codes
3. CCA to develop community standards (and deliver interchangeable codes)
4. CCA a la carte: using parts of CCA technology
5. CCA to bridge frameworks
6. CCA's conceptual impact

> "There are a b'jillion references to CCA at this HPDC/Compframe workshop… These are all Europeans we haven't met before."
>
> -- Rob Armstrong, Paris

Ask a CCA team member for more information about the projects mentioned in the following slides

CCA Common Component Architecture

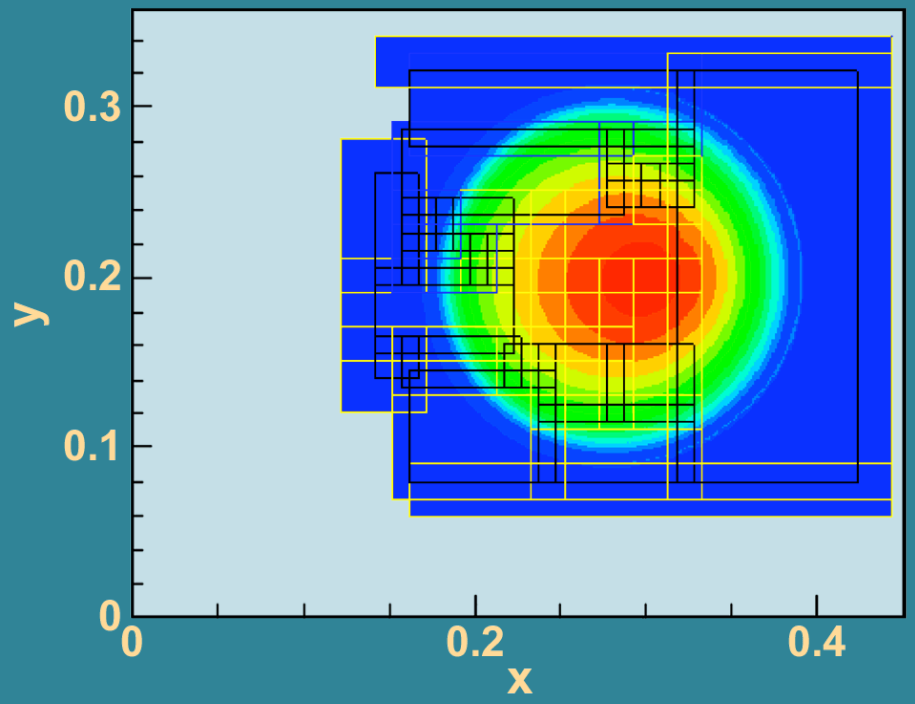
CCA in single codes for increased flexibility

Application	Project	Contact
Combustion	CFRFS	Jaideep Ray, Sandia
Chemistry	NWChem and global arrays	Theresa Windus, Iowa State U.
Subsurface transport	PSE compiler	Jan Prins, UNC Chapel Hill
Geomagnetics	–	Shujia Zhou, NASA Goddard
Performance monitoring	TAU	Sameer Shende, U. Oregon
Sparse linear algebra	Sparskit-CCA	Masha Sosonkina, Ames Lab

Example: CCA in combustion

- Toolkit of 60+ components for flexible simulation of chemically reacting flow problems
- Novel high order (4th and 6th) discretization for SAMR
- Extended stability R-K-C integrator developed for ADR on SAMR
- Five refereed science papers
- Eight refereed software papers
- Quantitative study of how components affected their code

OH concentration in advective-diffusive-reactive simulation using 4th order Runge-Kutta-Chebyshev integrator on 4 levels of AMR



Courtesy of Jaideep Ray, Sandia National Laboratories

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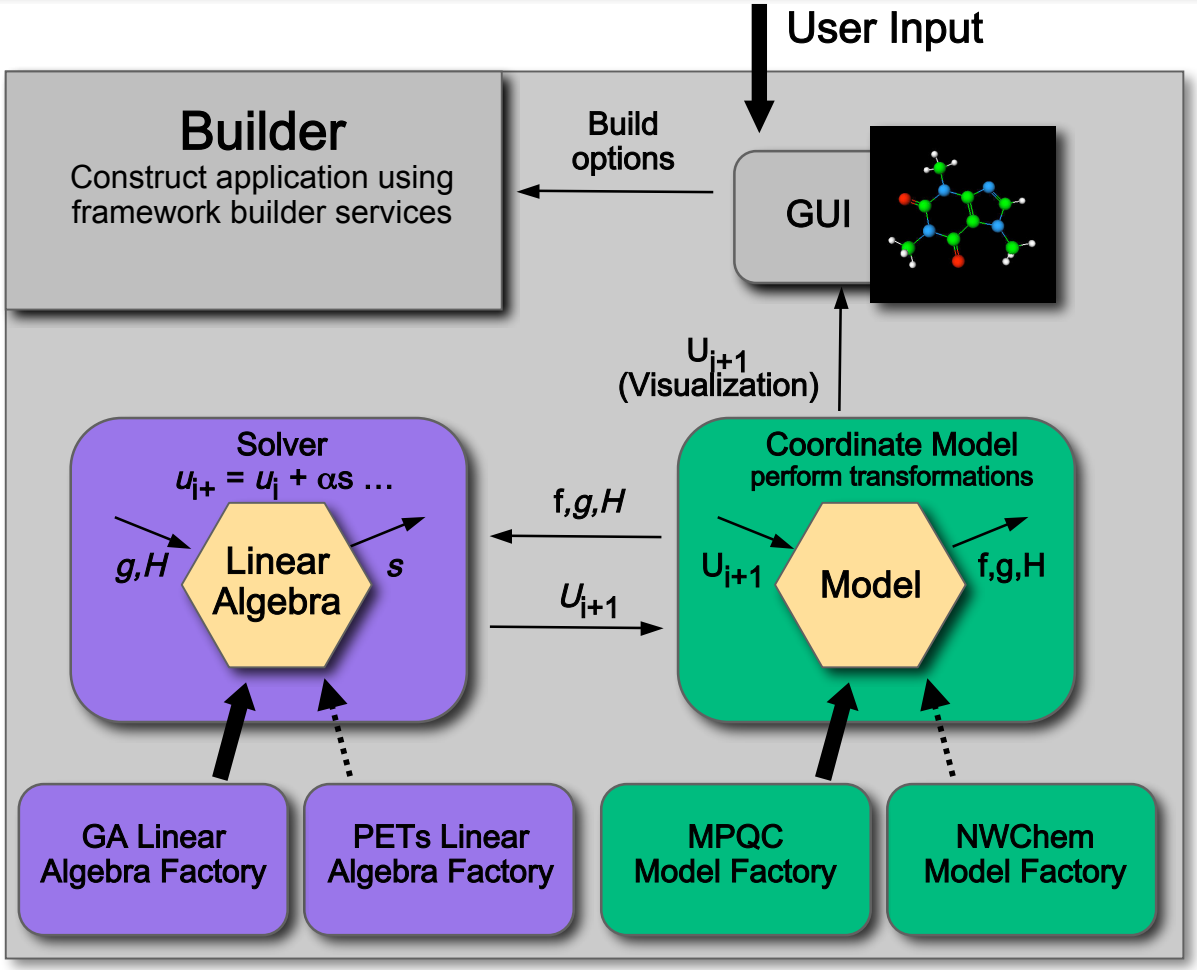
CCA to combine previously incompatible codes

Application	Project	Contact
Quantum chemistry	GAMESS, MPQC, and NWChem Interoperability	Curtis Janssen, Sandia Mark Gordon or Theresa Windus, Iowa State U.
Nuclear power plant training simulation	–	M. Diaz, U. Malaga, Spain
Fusion	DistComp	Nanbor Wang, Tech-X Corp.
Radio astronomy	eMiriad	Athol Kemball, UIUC

Example: Quantum chemistry

Building better instruments for scientific inquiry by integrating best-in-class software packages



Courtesy of Curtis Janssen and Joe Kenny, SNL

f	energy
u	catesian coordinates
u	internal coordinates
g	gradient in cartesians
g	gradient in internals
H	Hessian in cartesians
H	Hessian in internals
s	update in internals

Chemistry Components

Mathematics Components

Infrastructure

SIDL Classes

CCA Common Component Architecture

CCA to develop community standards

Application	Project	Contact
Meshing	TSTT	Lori Diachin, LLNL
Solvers	TOPS	Barry Smith, Argonne

… and applications using these interfaces		
Cell biology	VMCS (using TSTT)	Harold Trease, PNNL
Fusion	FACETS	Stefan Muszala, Tech-X Corp.
Chemistry	GAMESS-CCA (NWChem and MPQC)	Masha Sosonkina, Ames Lab

CCA Common Component Architecture

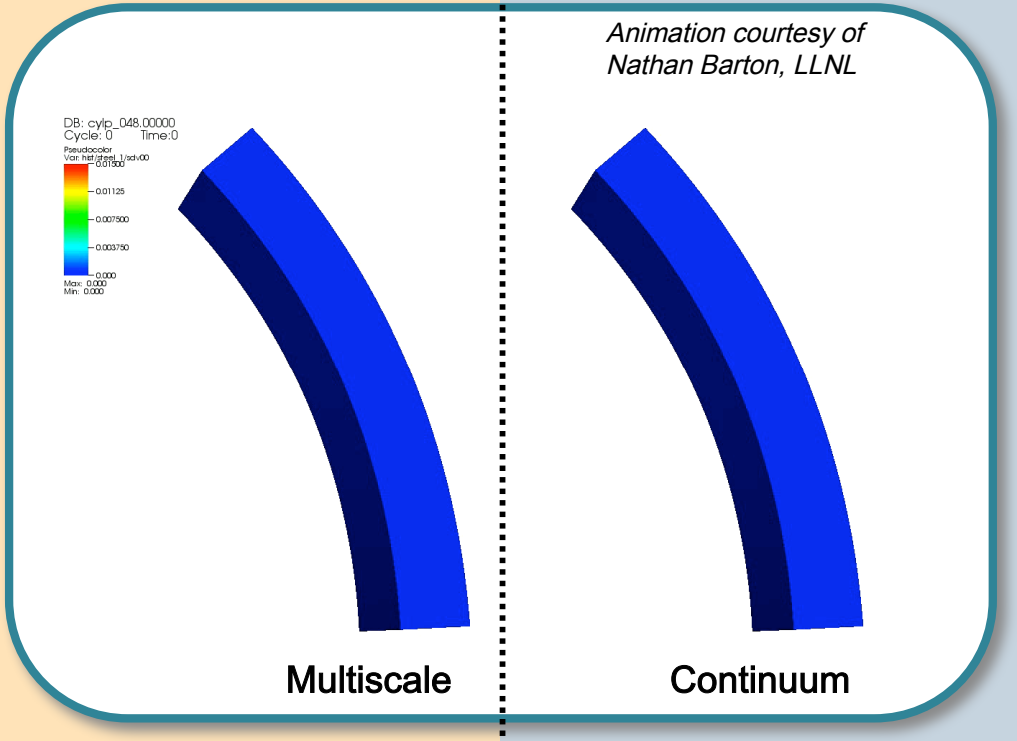
CCA a la carte: Using parts of CCA technology

Application	Project	CCA Aspect	CCA Tools	Contact
Combustion	CFRFS	Parallel framework	Ccaffeine	Jaideep Ray, Sandia
Electron effects	CMEE	Language interoperability	Babel	Peter Stoltz, Tech-X Corp.
Material science	PSI	RMI framework	Babel	John May, LLNL
Computer-assisted source refactoring	CASC	Language interoperability	Babel	Dan Quinlan, LLNL
Fusion	FMCFM	Language interoperability	Babel	Johann Carlsson, Tech-X Corp.
Solvers	Hypre	Language interoperability	Babel	Jeff Painter, LLNL

Example: Multiscale materials science using Babel RMI

Massively parallel simulation of strain localization on idealized shock-driven cylinders

- ***Multiscale model*** consisting of **continuum model at macroscale** coupled with a farm of **microscale polycrystal plasticity models** running independently on same cluster.
- The intricate cross-hatching that appears at macroscale is due to the additional microscale physics.



- ***Continuum model*** only
- Material "rings" uniformly

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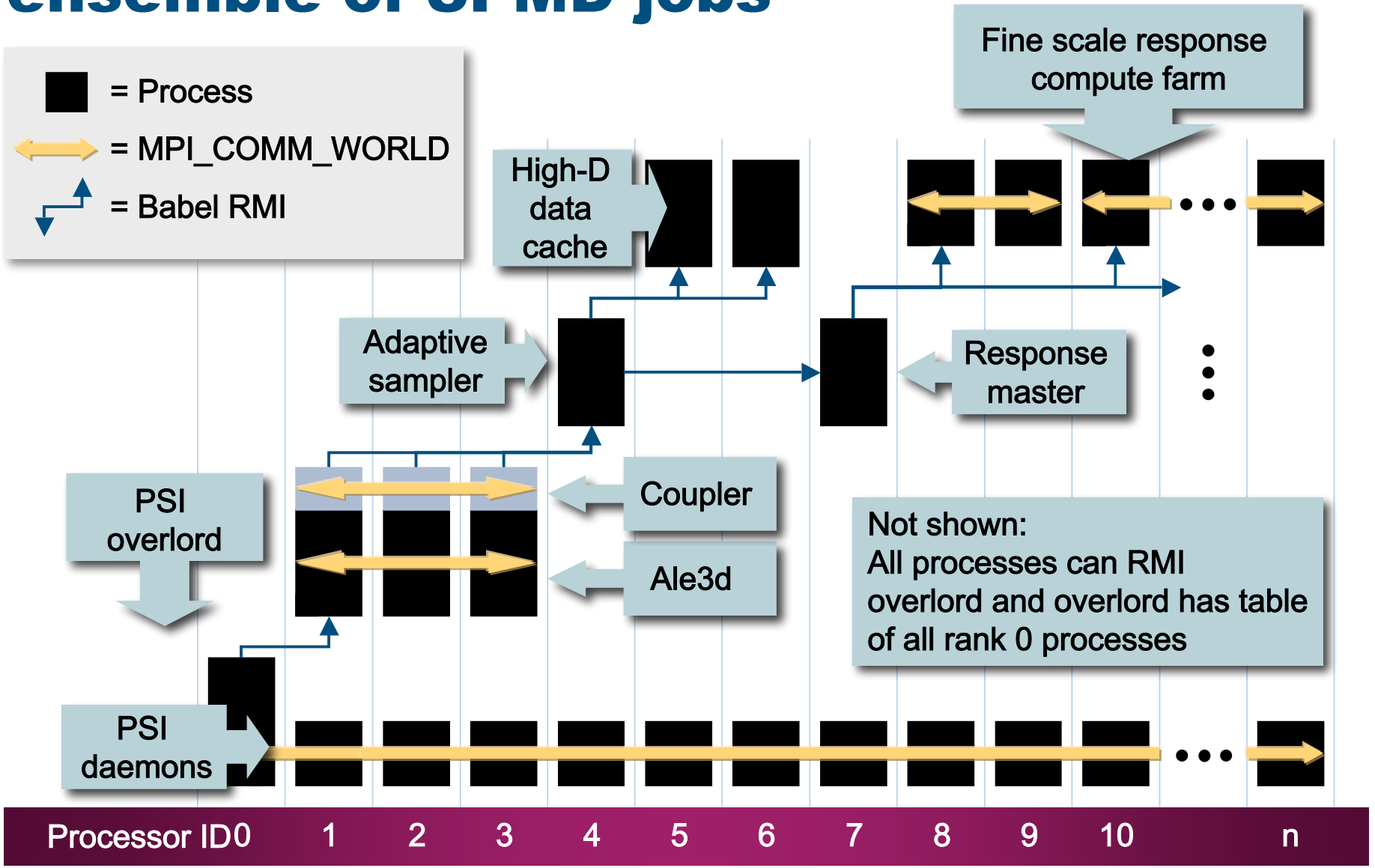
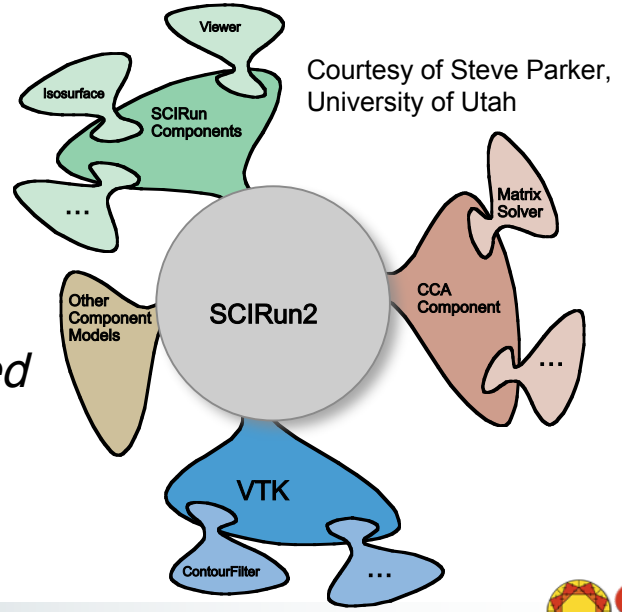
Vision: Petascale computing as an ensemble of SPMD jobs



CCA Common Component Architecture

5 CCA to connect frameworks

Framework	Comment	Contact
SCIRun2	Meta-component bridging	Steve Parker, Utah
Legion-CCA	Extended Babel to generate Legion	Michael J. Lewis, Binghamton University
MOCCA	Personal grid environments (part of Harness)	Vaiday Sunderam, Emory University

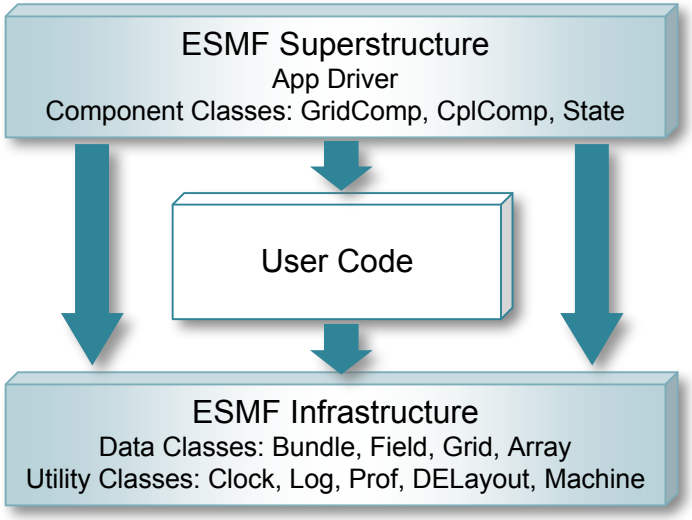


Schematic of framework and component interoperability enabled by the SCIRun2 framework

CCA Common Component Architecture

6 CCA's conceptual impact

Application	Project	Contact
Climate	ESMF	Nancy Collins, NCAR
Astrophysics	TSI	Doug Swesty, SUNY Stony Brook



ESMF high-level architecture
http://www.esmf.ucar.edu

"I have become a complete convert to the idea of component-oriented design and it is now foremost in my mind when it comes to software architecture planning."

-- Doug Swesty, SUNY Stony Brook

CCA Common Component Architecture

Conclusions

- Components are serious technology for building large-scale codes.
- CCA accomplishments include these:
  - Delivered technology uniquely applicable for HPC.
  - **Demonstrated broad, multidisciplinary application impact.**
  - Provided technical leadership in new approaches to large-scale software.
- Vision: build a component ecosystem.
  - Researchers spend more time in the 10% of their code that is of scientific interest.
  - Leverage the other 90% necessary for completeness from other researchers.

For more information

- See companion presentation:
  An Overview of the Common Component Architecture (CCA)
- ORNL booth at SC2007
  - David E. Bernholdt, Wael R. Elwasif, James A. Kohl (ORNL)
  - Tom Epperly, Gary Kumfert (LLNL)
  - Ben Allan, Rob Armstrong, Jaideep Ray (SNL)
- Other booths at SC2007
  - Ames Laboratory (Booth 181)
  - Argonne National Laboratory (Booth 551)
  - Indiana University (402)
  - NNSA/ASC (1617)
  - Pacific Northwest National Laboratory (581)
  - Tech-X Corporation (190)
  - University of Utah (287)
- On the internet
  - http://www.cca-forum.org
  - cca-forum@cca-forum.org