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)
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 in single codes for increased flexibility

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

Courtesy of Jaideep Ray, Sandia National Laboratories
## CCA to combine previously incompatible codes

<table>
<thead>
<tr>
<th>Application</th>
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</tr>
</thead>
<tbody>
<tr>
<td>Quantum chemistry</td>
<td>GAMESS, MPQC, and NWChem Interoperability</td>
<td>Curtis Janssen, Sandia Mark Gordon or Theresa Windus, Iowa State U.</td>
</tr>
<tr>
<td>Nuclear power plant training simulation</td>
<td>–</td>
<td>M. Diaz, U. Malaga, Spain</td>
</tr>
<tr>
<td>Fusion</td>
<td>DistComp</td>
<td>Nanbor Wang, Tech-X Corp.</td>
</tr>
<tr>
<td>Radio astronomy</td>
<td>eMiriad</td>
<td>Athol Kemball, UIUC</td>
</tr>
</tbody>
</table>
Example: Quantum chemistry

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

Builder
Construct application using framework builder services

Solver
\[ u_{i+1} = u_i + \alpha s \ldots \]

Linear Algebra

f, g, H

Coordinate Model
perform transformations

Model

f, g, H

User Input

Build options

GUI

Build options

U_{i+1}

(Visualization)

f, g, H

U_{i+1}

f, g, H

f, g, H

GA Linear Algebra Factory

PETs Linear Algebra Factory

MPQC Model Factory

NWChem Model Factory

Chemistry Components

Mathematics Components

Infrastructure

SIDL Classes

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

Courtesy of Curtis Janssen and Joe Kenny, SNL
# CCA to develop community standards

<table>
<thead>
<tr>
<th>Application</th>
<th>Project</th>
<th>Contact</th>
</tr>
</thead>
<tbody>
<tr>
<td>Meshing</td>
<td>TSTT</td>
<td>Lori Diachin, LLNL</td>
</tr>
<tr>
<td>Solvers</td>
<td>TOPS</td>
<td>Barry Smith, Argonne</td>
</tr>
</tbody>
</table>

... and applications using these interfaces

<table>
<thead>
<tr>
<th>Category</th>
<th>Project</th>
<th>Contact</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cell biology</td>
<td>VMCS (using TSTT)</td>
<td>Harold Trease, PNNL</td>
</tr>
<tr>
<td>Fusion</td>
<td>FACETS</td>
<td>Stefan Muszala, Tech-X Corp.</td>
</tr>
<tr>
<td>Chemistry</td>
<td>GAMESS-CCA (NWChem and MPQC)</td>
<td>Masha Sosonkina, Ames Lab</td>
</tr>
</tbody>
</table>
## CCA a la carte: Using parts of CCA technology

<table>
<thead>
<tr>
<th>Application</th>
<th>Project</th>
<th>CCA Aspect</th>
<th>CCA Tools</th>
<th>Contact</th>
</tr>
</thead>
<tbody>
<tr>
<td>Combustion</td>
<td>CFRFS</td>
<td>Parallel framework</td>
<td>Ccaffeine</td>
<td>Jaideep Ray, Sandia</td>
</tr>
<tr>
<td>Electron effects</td>
<td>CMEE</td>
<td>Language interoperability</td>
<td>Babel</td>
<td>Peter Stoltz, Tech-X Corp.</td>
</tr>
<tr>
<td>Material science</td>
<td>PSI</td>
<td>RMI framework</td>
<td>Babel</td>
<td>John May, LLNL</td>
</tr>
<tr>
<td>Computer-assisted source refactoring</td>
<td>CASC</td>
<td>Language interoperability</td>
<td>Babel</td>
<td>Dan Quinlan, LLNL</td>
</tr>
<tr>
<td>Fusion</td>
<td>FMCFM</td>
<td>Language interoperability</td>
<td>Babel</td>
<td>Johann Carlsson, Tech-X Corp.</td>
</tr>
<tr>
<td>Solvers</td>
<td>Hypre</td>
<td>Language interoperability</td>
<td>Babel</td>
<td>Jeff Painter, LLNL</td>
</tr>
</tbody>
</table>
Example: Multiscale materials science using Babel RMI

- **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

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

Animation courtesy of Nathan Barton, LLNL
Vision: Petascale computing as an ensemble of SPMD jobs

- Black = Process
- Orange = MPI_COMM_WORLD
- Green = Babel RMI

Fine scale response compute farm

Adaptive sampler

High-D data cache

Response master

Not shown: All processes can RMI overlord and overlord has table of all rank 0 processes

Processor ID0 1 2 3 4 5 6 7 8 9 10 n

CCA Common Component Architecture
## CCA to connect frameworks

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

Schematic of framework and component interoperability enabled by the SCIRun2 framework
### CCA’s conceptual impact

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<tr>
<td>Climate</td>
<td>ESMF</td>
<td>Nancy Collins, NCAR</td>
</tr>
<tr>
<td>Astrophysics</td>
<td>TSI</td>
<td>Doug Swesty, SUNY Stony Brook</td>
</tr>
</tbody>
</table>

"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

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