How the CCA Advances Computational Science

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with David E Bernholdt, Thomas Epperly, James Kohl, Lois Curfman McInnes, Steven Parker, and Jaideep Ray

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This talk is a survey of how CCA is used in science

Outline:

- Components are important because...
- 25 examples of CCA impact on science
- How CCA will lead future of scientific software technology (next 5 years)
Human Beings Do Not Scale

We write imperfect software

...but we are driven to write more of it.

Program Complexity (C SLOC)

Practical upper bound

Date


Assemblers

Compilers

Structured Programming

Object-Oriented

Components

We write imperfect software

...but we are driven to write more of it.

Practical upper bound

Date


Assemblers

Compilers

Structured Programming

Object-Oriented

Components
In Industry, All Enterprise Software is Component Software

- Components are invented for codes where complexity exceeds the comprehension of a single human mind.

**Object-Oriented (OOP)**
1. Assumes a single language
2. Implementation details pollute the interfaces

**Components**
1. Code generation (language wrappers & stronger interfaces)
2. Additional runtime services to support dynamicism & loose coupling

- Loose coupling and robust interfaces are effective in greater range, including single teams.
Code Reuse is NOT the Reason for Components

Real reasons are robust interfaces & loose coupling, which can be used to great effect…

- Corporate/For Profit
  - Time to Market

- Science/Research
  - Maintaining Correctness in the Face of Change
CCA Delivers Component Technology to Scientific Computing

- **SIDL** – Interface Language
- **Babel** – Reads SIDL, Generates wrapper code in C, C++, Fortran, Java, & Python
- **CCA Specification** – Defines a component, an interface (“port”) and how they interact with frameworks (written in SIDL)
- **CCA Frameworks**
  - Implement the CCA specification & provide services to components
  - Examples: CCaffiene, Uintah, XCAT
CCA’s Impact is as Diverse as the Applications in HPC

25 examples grouped roughly into six categories of impact/use

1. CCA in single codes for extra flexibility
2. CCA to combine incompatible codes
3. CCA to develop community standards (& deliver interchangeable codes)
4. CCA a la carte: Using parts of CCA tech.
5. CCA to bridge frameworks
6. CCA’s impact on competing technologies
1. **CCA in single codes for increased flexibility**

<table>
<thead>
<tr>
<th>Application</th>
<th>Project</th>
<th>POC</th>
</tr>
</thead>
<tbody>
<tr>
<td>Combustion</td>
<td>CFRFS</td>
<td>Jaideep Ray, Sandia</td>
</tr>
<tr>
<td>Chemistry</td>
<td>NWChem &amp; Global Arrays</td>
<td>Theresa Windus, PNNL</td>
</tr>
<tr>
<td>Subsurface Transport</td>
<td>PSE Compiler</td>
<td>Jans 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>Sparsekit-CCA</td>
<td>Masha Sosonkina, Ames Lab</td>
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</tbody>
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Example: CCA in Combustion

- Novel high order (4th & 6th) discretization for SAMR
- Developed an extended stability R-K-C integrator for ADR on SAMR
- 5 refereed science papers
- 8 refereed software papers
- Quantitative study on how components affected their code

Figure courtesy of Jaideep Ray, SNL
2. CCA to combine previously incompatible codes

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<thead>
<tr>
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<tr>
<td>Quantum Chemistry</td>
<td>MPQC &amp; NWChem</td>
<td>Curtis Janssen, Sandia Theresa Windus, PNNL</td>
</tr>
<tr>
<td>Nuclear Power Plant Training Sim</td>
<td></td>
<td>M. Diaz, U. Malaga, Spain</td>
</tr>
<tr>
<td>Fusion</td>
<td>DFC</td>
<td>Nanbor Wang, Tech-X Corp.</td>
</tr>
<tr>
<td>Radio Astronomy</td>
<td>eMiriad</td>
<td>Athol Kemball, UIUC</td>
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</tbody>
</table>
Example: Quantum Chemistry

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

Figure courtesy of Curtis Janssen and Joe Kenny, SNL
3. **CCA to Develop Community Standards**

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<thead>
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<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>
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... and Applications using these interfaces

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<tr>
<td>Cell Biology</td>
<td>VMCS</td>
<td>Harold Trease, PNNL</td>
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<tr>
<td></td>
<td>(using TSTT)</td>
<td></td>
</tr>
<tr>
<td>Accelerator Beam</td>
<td>Beam-SBIR</td>
<td>Douglas Dechow, Tech-X Corp.</td>
</tr>
<tr>
<td>Dynamics</td>
<td>(will use TOPS)</td>
<td></td>
</tr>
<tr>
<td>Chemistry</td>
<td>GAMESS-CCA</td>
<td>Masha Sosonkina, Ames Lab</td>
</tr>
<tr>
<td></td>
<td>(NWChem&amp;MPQC)</td>
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4. **CCA a la carte: using parts of CCA technology**

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</tr>
<tr>
<td>Electron Effects</td>
<td>CMEE</td>
<td>Peter Stoltz, Tech-X Corp.</td>
</tr>
<tr>
<td>Material Science</td>
<td>PSI</td>
<td>David Jefferson, LLNL</td>
</tr>
<tr>
<td>Computer-Assisted Source Refactoring</td>
<td>CASC</td>
<td>Dan Quinlan, LLNL</td>
</tr>
<tr>
<td>Fusion</td>
<td>FMCFM</td>
<td>Johann Carlsson, Tech-X Corp.</td>
</tr>
<tr>
<td>Solvers</td>
<td>Hypre</td>
<td>Jeff Painter, LLNL</td>
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Strain on Shock-Driven Metal Cylinder

Courtesy, Nathan Barton, LLNL.
Vision: The Petascale computer as ensemble of SPMD jobs

= Process
 MPI_COMM_WORLD
 = Babel RMI

Fine Scale Response
Compute Farm

Adaptive
Sampler

High-D
Data
Cache

PSI Overlord

Coupler

Ale3d

Response
Master

Not shown: All processes can RMI Overlord & Overlord has table of all rank 0 processes.

Vision: The Petascale computer as ensemble of SPMD jobs
## 5. **CCA to connect frameworks**

<table>
<thead>
<tr>
<th>Framework</th>
<th>Comment</th>
<th>POC</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, Binghamston University</td>
</tr>
<tr>
<td>MOCCA</td>
<td>Personal Grid Environments (Part of Harness)</td>
<td>Vaiday Sunderam, Georgia Tech</td>
</tr>
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</table>
# 6. CCA's Impact on Competing Technologies

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</thead>
<tbody>
<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

“Gary, 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, last week
Future Directions of CCA: “Adaptivity”

- Computational Quality of Service (CQoS)
  - Tradeoffs: performance, accuracy, robustness
  - Motivated by: Accelerators, Combustion, Quantum Chemistry, Fusion,…
  - In collaboration with: PERC, TSTT, TOPS

- Hybrid Computing
  - Driven by: multi-core/hybrid-core arch.

- Interface Semantics
  - Dynamic enforcement of semantic errors
Conclusion

• Components are serious technology for building large scale codes

• CCA accomplishments include:
  ▶ delivered technology uniquely applicable for HPC
  ▶ Demonstrated broad impact across multiple application domains
  ▶ Demonstrated technical leadership within our own CS discipline

• Vision: build a component ecosystem DoE
  ▶ Researchers spend more time in the 10% of their code that is of scientific interest
  ▶ Share the other 90% necessary for completeness
Thank You

CCA
Common Component Architecture

www.cca-forum.org