CCA Infrastructure and Enabling Technologies

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Summary

The Center for Component Technology for Terascale Simulation Software (CCTTSS) delivers component technology to terascale simulations, where component-based software promises to be easier to use, compose, specialize, share, and evolve than conventional approaches. Commercial component frameworks are not practical in this context. The CCTTSS is providing vital infrastructure through the Common Component Architecture (CCA), spanning a range of scientific computing architectures, conducting novel research, and deploying production frameworks, components, and tools.

Software Integration Frameworks

CCA frameworks enable the composition of terascale, team-based applications from software components conforming to the CCA specification, which is designed for maximum interoperability. Scientific computing applications require multiple, sometimes conflicting, types of software parallelism and must also run in diverse and evolving parallel hardware and networking environments. Commercial component standards, such as CORBA and Web Services, must be accommodated in new applications. The CCTTSS supports production and experimental frameworks that span modern scientific computing and component software architectures.

The parallel, open-source CCA reference framework, Ccaffeine, and the SCIRun2 framework now support meta-component technology, thereby allowing the integration of existing software component systems, such as the visualization toolkit (VTK). This bridging of component models provides greater reuse of code from existing domain-specific frameworks. The Distributed CCA Architecture (DCA) framework explores data redistribution in a distributed, MPI-based setting and addresses parallel remote method invocation (PRMI) semantics. The DCA approach complements that of SCIRun2.

The XCAT framework has been developed to bring CCA component concepts to wide-area distributed "Grid" applications based on Web Services – the new industry standard for distributed systems. XCAT supports event-driven component models and workflow compositions, as well as simple software configurations. XCAT-C++ is being developed to support the efficient transfer of very large data sets among components deployed in wide area networks via the high-performance, multi-protocol Proteus library. The best communication protocol is chosen for each pair of interacting components. The CCAIN (CCA Integration) framework has been created to

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assess the potential of the Fortran 2003 C interoperability standard to simplify component development. Contributors outside the CCTTSS are also developing CCA-compliant frameworks to satisfy other special needs.

CCA Toolkit
The benefits of the CCA infrastructure and frameworks can be best realized when combined with a practical suite of reusable components, such as those provided by the *CCA Toolkit*. It is crucial for each scientific community to embrace the component-based paradigm to develop their own specialized software interfaces and capabilities. However, general-purpose numerical components can be reused to expedite common computational tasks across communities. The CCA toolkit provides a single repository site for such components. A growing collection of components supports key technologies, including parallel visualization, distributed arrays and meshes, linear solvers, optimizers, and input/output for common data file formats.

"MxN" Parallel Data Coupling
Moving massive amounts of simulation data within and between parallel machines during execution is referred to as the *MxN problem*. Emerging component solutions will soon incorporate new and improved MxN tools into the CCA toolkit, enabling more powerful generalized parallel model coupling. These enhanced components will provide scalable tools for parallel and distributed data management among disparate independent codes. This work is based on the Model Coupling Toolkit (MCT), developed for use with climate modeling, and on an MPI-based extension of the CUMULVS system for visualization, steering, and model coupling, with run-time messaging system selection. The MetaChaos system also continues to expand MxN capabilities in a flexible way using computational Grids, and so will soon be incorporated into the ongoing CCA toolkit effort.

Software Interoperability
The Babel high-performance language interoperability tool has been improved through the addition and enhancement of a number of production-quality features. We have completed full support for Java, enhanced and efficient array passing capabilities, and better support for object-oriented languages such as C++ and Python. The CHASM Fortran Array-Descriptor Library has been expanded to include support for new GNU, 64-bit Intel, and Cray compilers, enabling SIDL and CCA tools to support applications in these new environments.

Other experimental Babel extensions to improve software productivity are being developed in cooperation with the Babel open source community. Research on programming-by-contract with run-time data and behavior validation focuses on enabling run-time verification of plug-and-play scientific software assemblies. Remote method invocation facilitates distributed computing and enables interoperability among CCA-compliant frameworks. Automated configuration management reduces the burden of maintaining and using portable software build tools in high-performance environments.

Conclusion
The CCTTSS, through its research and CCA frameworks, is providing the infrastructure for improving the productivity, efficiency, and quality of terascale applications.

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