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Enabling New Approaches to Simulation Software and New Science with the Common Component Architecture

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Summary

The Center for Component Technology for Terascale Simulation Software (CCTTSS) develops tools and techniques for component-based high-performance scientific computing. Many application groups have adopted the CCA as their software design paradigm in order to exploit the productivity and performance enhancements afforded by component-based design. Applications are already realizing benefits from this approach, as they better utilize externally developed software, achieve better performance, and even perform simulations that they would not have considered feasible before they began using the CCA.

Combustion

The SciDAC CFRFS[1] project is developing a component-based toolkit for flame simulations to facilitate the creation and execution of simulations by researchers with minimal knowledge of the underlying software. As an early adopter of the CCA component design paradigm, the CFRFS has been a driving force in the incorporation of diverse software (often from other SciDAC centers) into its toolkit, and has engendered new fields of research (e.g., performance evaluation in a component environment). The CCA approach has enabled unprecedented software collaboration, allowing the CFRFS to take advantage of state-of-the-art software developed outside of their project. Currently, high-order numerical software developed in by Sandia mathematicians is being evaluated, and a parameter set suitable for combustion simulations is under development (Figure 1). CFRFS researchers are also investigating the use of elliptic solvers for APDEC's[2] Chombo framework. Common interfaces and a prototypical data-exchange mechanism, jointly developed by CFRFS and CCTTSS, facilitated the effort.

Climate Modeling

Computational climate modeling is critical for our understanding of global processes and the consequences of human impact. Recent work on climate applications has proceeded in several areas. We have leveraged the CCA's Babel language-interoperability technology to enhance the Model Coupling Toolkit (MCT), on which the coupler for the SciDAC-supported Community Climate System Model (CCSM) is based, and we have demonstrated a CCSM prototype that has been

[1] *Computation Facility for Reacting Flow Science*, PI: H. Najm, http://cfrfs.ca.sandia.gov/

[2] *Algorithmic and Software Frameworks for Applied Partial Differential Equations*, PI: P. Colella, http://davis.lbl.gov/APDEC

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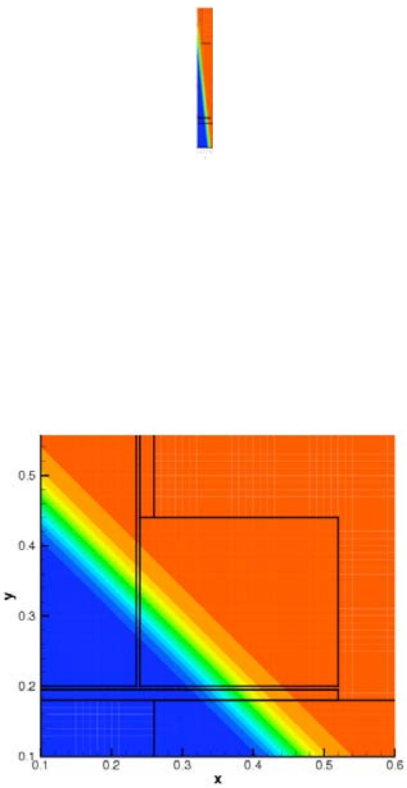

Figure 1. A Fitzhugh-Nagumo equation being solved on a block-structured adaptively refined mesh. The top image illustrates Runge phenomena at coarse-fine interfaces (dashed ovals) when using high-order schemes (6^{th} order interpolations with 4^{th} order discretizations). Filtering them with an 8^{th} order filter removes them (bottom).

componentized at the top level. We are also developing climate-related components to be included in the CCA Toolkit, including a component interface to netCDF, a popular data format in the geosciences.

Computational Chemistry

Quantum chemistry (QC) is a major tool in the simulation of chemical phenomena. Two groups of researchers working with NWChem and MPQC devised common interfaces and a componentization strategy that has enabled them to exploit the state-of-the-art optimization and linear algebra algorithms in TAO, Global Arrays and PETSc. Recent work has moved beyond package-level interchangeability to delve deeper into the componentization and sharing of algorithmic components, in particular the evaluation of high dimensional molecular integrals. Such a finer grained decomposition facilitates the creation of new algorithms and capabilities with components drawn from *both* chemistry packages, thus enhancing the scientific capabilities of users. Another stunning success has been the use of component hierarchies to implement a hybrid parallelization approach for a time-consuming method in NWChem, which resulted in an order of magnitude improvement in scalability. The hybrid algorithm would have been impractical to implement in a reasonable time without the use of the CCA.

Additional Application Areas

While we have space here to highlight only a few CCA-based applications, an increasing number of projects are turning to the CCA to help them better manage and use their software, produce new coupled simulation capabilities, and move toward community-based standards to facilitate collaboration through software. In addition to APDEC, we collaborate closely with the SciDAC TSTT[3] and TOPS[4] Centers on community interfaces for mesh-based scientific data management and linear solvers. The CCA is also being used in such diverse areas as nanoscience, biology, nuclear power plant simulation, astronomy, and real-time data collection.

For further information on this subject contact:

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3 *Terascale Simulation Tools and Technologies Center*, PIs: Jim Glimm, David Brown, and Lori Freitag Diachin, http://www.tstt-scidac.org

4 *Terascale Optimal PDE Simulations Center*, PI: David Keyes, http://tops-scidac.org