SAND2015-10596R

Project Accomplishment Summary

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Sandia National Laboratories

Operated for the U.S. Department of Energy by
Sandia Corporation
Albuquerque, New Mexico

PROJECT ACCOMPLISHMENTS SUMMARY

Cooperative Research and Development Agreement (#1789.02.00)

between **Sandia National Labs** and GE Global Research

Note: This Project Accomplishments Summary will serve to meet the requirements for a final abstract and final report as specified in Article XI of the CRADA.

Title: Agile Components for Modeling Internal Flows

Final Abstract:

The purpose of this project was to rapidly demonstrate the capabilities of Sandia's Agile Components toolkit by building a prototype simulator for modeling internal fluid flows and similar technologies of interest to GE Global Research. In doing so, this allowed the CRADA partner to learn about the Agile Components from the Sandia experts that designed and developed the toolkit. Sandia and DOE benefited from the application of Agile Components to another type of modeling and simulation application that helped to further generalize and harden the Agile Components software. As per the CRADA/PTS agreement, the resulting demonstration application can now be distributed under an open source license so that it can be made available for others to also learn from.

Background:

The state of the art prior to initiation of this project was a highly specialized, custom in-house code designed and used solely by the CRADA partner for their internal applications. While this custom application is state-of-the-art for its intended application, it does not incorporate the latest in computational simulation capabilities as represented in Sandia's Agile Component toolkit. The purpose of this project was to work with CRADA partner staff to co-develop a prototype application that would leverage and demonstrate the advantages of the Agile Components toolkit including embedded optimization and uncertainty quantification, performance portability, automatic differentiation and Jacobian construction, and fully unstructured finite-element discretizations. This project leveraged both the current Agile Components as deployed in Sandia open source libraries including Trilinos, Dakota, and Albany.

Description:

The purpose of this project was to work with CRADA partner staff to co-develop a prototype application that would leverage and demonstrate the advantages of the Agile Components toolkit including embedded optimization and uncertainty quantification, performance portability, automatic differentiation and Jacobian construction, and fully unstructured finite-element discretizations. This project leveraged both the current Agile Components as deployed in Sandia open source libraries including Trilinos, Dakota, and Albany. The project was conducted over an intense 1.5 week collaboration in which CRADA partner staff was in residence at Sandia's Computer Science Research Institute (CSRI) and worked daily with CSRI staff to co-develop a prototype application for hyperbolic fluid flow using Sandia's Agile Component/Albany toolkit. A new application called turbo was developed that solved the multi-dimensional Burger's equation for viscous fluid flow using an unstructured finite element method. Unique to this application, we demonstrated: automatic Jacobian construction using automatic differentiation, steady and transient sensitivity analysis, parameter optimization, and parametric uncertainty quantification. This was accomplished using a high-order finite element method on fully unstructured meshes. The prior participant

remarked that “he couldn’t believe how rapid the progress was on this new simulation capability” and that it was one of his most productive times.

Benefits to the Department of Energy:

While the specific Burger’s simulator is not of direct relevance to Defense Programs, the Agile Components themselves are a key element in our NNSA ASC strategy to rapidly build next generation computational simulation capabilities that support advanced analysis capabilities and achieve performance portability for next generation computer architectures. This project enabled Sandia to apply its Agile Component toolkit in a new context with a new collaboration that helped to further improve, harden and enhance the Agile Components for our DP applications. We are now using the Agile Components as part of a new ASC program called Advanced Technology Development and Mitigation (ATDM) and are therefore benefiting from the work of this CRADA project.

Economic Impact:

One of the lessons from the CRADA partner is that Sandia’s Agile Component software infrastructure, while very powerful, also has a steep learning curve and requires software developers with high expertise in advanced C++ object oriented and template programming. While the CRADA participant had this knowledge, the broader developer community is primarily Fortran based. This made direct use of Agile Components untenable for the partner, but there were specific technologies (automatic differentiation) and approaches (object oriented design) that the partner directly learned from and intends to adopt for their next generation software. At this point, it is impossible to directly assess what the benefit will be to the partner. The benefits to the taxpayer are largely associated with the benefits to the Agile Components that are now a key part of Sandia’s DP work for stockpile stewardship.

Project Status:

Completed

ADDITIONAL INFORMATION

Laboratory/Department of Energy Facility Point of Contact for Information on Project

Dr. S. Scott Collis, Sr. Manager, Computational Science & Math, Sandia National Labs,

sscoll@sandia.gov Company Size and Points of Contact

Dr. Brian Mitchell, GE Global Research, GE Corporation, mitchellb@ge.com

CRADA Intellectual Property

Turbo, v1.0, prototype application for solving the multi-dimensional Burger's equation

Technology Commercialization

No intention to commercialize at this time

Project Examples

The Turbo v1.0 software can be made available under open source license per PTS agreement. However, we have not yet exercised this via copyright assertion with DOE.

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This summary has been approved for public release by Sandia and GE Global Research

Sandia National Laboratories

By _____ 1/30/2015
Scott Collis — Date
Principal Investigator

Sandia National Laboratories

By _____ 11.26.14
Manager — Date
WFO/CRADA Agreements

GE Global Research

By Global Tech Leader _____ 2/10/15
Title: — Date

In order to expedite the process, if we do not receive your signed reply by 03/02/2015 we will assume your concurrence for the release of this document to the public.