SAND2017-12834R

Project Accomplishment Summary

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Sandia National Laboratories
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Sandia Corporation
Albuquerque, New Mexico

PROJECT ACCOMPLISHMENTS SUMMARY

Cooperative Research and Development Agreement (#SC07/01742.05.00)

between **Sandia National Laboratories** and **ExxonMobil Upstream Research Company**

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 Software Components and Libraries for Large-Scale Reservoir Simulations

Final Abstract:

The objective of this project was for Sandia National Laboratories (SNL) and ExxonMobil Research Company (URC) to collaborate on the development and integration of numerical algorithms and software components for the solution of partial differential equations (PDEs) that address the high fidelity simulation of reservoir flows. SNL's role was to consult and advise URC on the best practices and use of SNL open-source software components as part of URC's work to incorporate these components into their PDE-based URC reservoir simulation code. A desired outcome was for URC to leverage SNL's open-source software components as within their own codes, rather than to have to develop from scratch those same capabilities themselves, and for SNL to harden and mature those software components based on usage and feedback from URC.

Background:

SNL and URC collaborated on agile software components within the Trilinos framework for solving PDEs, including URC's reservoir simulation applications. Traditionally, application codes, such as reservoir simulation codes, would independently develop their own parallel computation capabilities, frequently reproducing common capabilities with each new application code. With the advent of massively parallel numerical libraries, like SNL's Trilinos Project, those common capabilities can be utilized from a library (like Trilinos) and do not have to be developed independently. Trilinos is large project supporting the development and integration of numerical algorithms for solving mathematical equations posed by computational methods.

Trilinos includes core numerical kernels and data models for solving systems of equations, as well as providing software and tool infrastructures for developing algorithm packages. Trilinos packages can be written to be extremely modular, and the software interfaces provided enable a high degree of interoperability. With these characteristics, Trilinos is a viable platform for developing PDE algorithm components that can be vertically integrated, together with application-specific physics constituents, to quickly develop lightweight simulation applications. Furthermore, advanced algorithm packages, such as optimization and automatic differentiation, can be integrated into new as well as existing applications to add embedded, transformational capabilities such as error estimation, uncertainty quantification, and optimization.

Description:

The objective of this project was for SNL and URC to collaborate on the development and integration of numerical algorithms and software components for the solution of partial differential equations (PDEs) that address the high fidelity simulation of reservoir flows. SNL's role was to consult and advise URC on the best practices and use of SNL open-source software components as part of URC's work to incorporate these components into their PDE-based URC reservoir simulation code. A desired outcome was for URC to leverage SNL's open-source software components as within their own codes, rather than to have to develop from scratch those same capabilities themselves, and for SNL to harden and mature those software components based on usage and feedback from URC.

Several mutually-beneficial interactions of this nature took place during the project. Partitioning algorithms from Trilinos were used in the simulator, and the lead developer consulted on algorithmic choices. Ideas and experience were exchanged on the prospects of using GPU accelerators for the project. Nonlinear solver algorithms from Trilinos were implemented in the URC code. Feedback to Trilinos developers was given on apparent computational overhead in calling the Trilinos solvers. The use of automatic differentiation technologies from Trilinos was adopted in the URC code, and ideas on whether automatic differentiation can be compatible with sparse gradients were discussed. SNL's experience in component-based software design, testing infrastructure, and scalability were shared, influencing design decisions in the URC code base.

Benefits to the Department of Energy:

URC's early use of SNL's agile components technology explored new use cases for that capability, identifying some shortcomings and helping to identify opportunities for improvement. Agile Components are central to the Advanced Technology Development and Mitigation (ATDM) program within SNL's Advanced Simulation and Computing (ASC) program, which provides state-of-the-art computer simulation capabilities as part of NNSA's mission to extend the lifetime of nuclear weapons in the stockpile without underground testing.

Economic Impact:

This work was geared at the evaluation of component software libraries for the solution of partial differential equations (PDEs) within URC's reservoir simulation code. High fidelity simulation of reservoirs is driven by the economic importance of economic extraction of subsurface energy resources.

Project Status:

This project has been completed.

ADDITIONAL INFORMATION

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

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Company Size and Points of Contact

Exxon Mobil Corporation is an American multinational oil and gas corporation with 75,300 employees. Its 2016 revenue was $218.6 billion.

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CRADA Intellectual Property

No new intellectual property was created under this PTS.

Technology Commercialization

As this work is exploratory, there is no commercialization plan.

Project Examples

Technical staff from URC visited SNL for the Trilinos Users Group meeting, shared their experiences, and learned about many promising technologies that were being developed within Trilinos.

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This summary has been approved for public release by Sandia and ExxonMobil Upstream Research Company.

Sandia National Laboratories

By Michael S. Parks _____ 11/1/2017
Michael Parks — Date
Principal Investigator

Sandia National Laboratories

By _____ 10/23/17
Manager — Date
WFO/CRADA Agreements

ExxonMobil Upstream Research Company

By _____ _____
Title: — Date

In order to expedite the process, if we do not receive your signed reply by 11/9/17 we will assume your concurrence for the release of this document to the public.