Final Technical Report

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Project Title: Frameworks, Algorithms, and Scalable Technologies for Mathematics (FASTMath) SciDAC Institute

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Abstract

The FASTMath SciDAC Institute addressed two key challenges that application scientists faced at the beginning of SciDAC-3. First, FASTMath helped them continue to improve the quality of their simulations by increasing accuracy and reliability of both their software and algorithms. Second, FASTMath helped them adapt their computations to make effective use of high-end computing facilities acquired by DOE over the past five years. This required the development of new mathematical algorithms that were appropriate for the physics problems being solved, implementations that scaled to million-way parallelism, and software that effectively leveraged both distributed memory and on-node parallelism. The Rensselaer Polytechnic Institute team's efforts focused on the unstructured mesh technologies developed by FASTMath.

Developments/Accomplishments

More complete summaries of the developments listed below appear in the previous progress reports. The publications cited below give more complete technical details.

Unstructured meshes can yield required levels of accuracy using many fewer degrees of freedom (DOF) at the cost of more complex data structures and algorithms to achieve parallel scalability. The ability to take full advantage of unstructured meshes requires an infrastructure for the management, load balancing, adaptation and quality control of the meshes; capabilities that the FASTMath team focused on providing. The unstructured mesh developments have impacted a number of SciDAC applications including ice sheet modeling, atmospheric modeling, edge plasma physics, MHD based plasma physics modeling and accelerator modeling.

Major developments/accomplishments by the Rensselaer Polytechnic Institute team include:

Parallel mesh infrastructures: The PUMI parallel mesh infrastructure was extended to address new capabilities and to more effectively operate on new generation parallel systems. Modifiable array-based procedures compatible with MeshAdapt were introduced into PUMI. Efforts were carried out to improve performance on many core architectures. The ability to perform mesh adaptation on GPUs required a third array-based approach that is part of a new tool, Omega h. A parallel field infrastructure was developed. Methods to perform local solution transfer that satisfy mass and momentum constraints were developed.

Parallel Mesh Adaptation: MeshAdapt has been used on 92B element meshes on 3/4M cores. Fully parallel curved mesh adaptation, including curved boundary layers were developed. Boundary layer mesh adaptation now applies boundary layer theory in the normal direction. Error estimation procedures were extended to support goal-oriented error estimation. A new approach to mesh adaptation, Omega h, that executes most mesh adaptation steps on GPUs was developed.

Dynamic partitioning strategies: The ParMA partition improvement procedure was been extended and used in PHASTA to improve partition quality and yield up to a 28% reduction in total execution times on 256K cores.

Performance and Scalability: PUMI, ParMA, MeshAdapt and PHASTA have been deployed and tested at full machine scale on Mira (3M BGQ processes) and Theta (192K KNL processes). Performance tuning and scaling (weak and strong) were demonstrated in coordination with DOE Early Science Projects on Mira and continue on Theta and Aurora. These tools allowed spatio-temporal independent turbulent flow simulations to be validated at unprecedented scale.

PHASTA-PUMI-PETSc Integration: PETSc and PUMI were coupled to the PHASTA flow solver. This effort identified global equation assembly scaling issues that were addressed to allow strong scaling and in-memory adaptivity to be combined with state-of-the-art preconditioning at full machine scale.

Integration of unstructured meshing technology into simulation workflows: The goal of the unstructured mesh workflow efforts included defining mechanisms and providing tools to support the integration of our unstructured mesh components with existing mesh-based analysis components to produce complete simulation workflows. Methods for the in-memory integration of components included both bulk data transfers based on data streams, and a set of API-based functions. The decisions of when and how to use data streams and/or API integration methods is a function the software implementation of the analysis component and the functions that must be supported. A number of in-memory adaptive simulation workflows have been implemented using the PUMI mesh infrastructure, APF fields, MeshAdapt for mesh adaptation, and Zoltan2 and ParMA for dynamic load balancing. Applications developed using fully in-memory integration of components include electromagnetics (with ACE3P), MHD (with M3D-C1), solid mechanics, including evolving geometry problems, (with Albany), ice sheet modeling (with Albany/FELIX) and fluid mechanics (with PHASTA and FUN3D).

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