DASHMM Overview

Multipole methods are a key computational kernel for a large class of scientific applications spanning multiple disciplines. Yet many of these applications are strong scaling constrained when using conventional programming practices. This project explores the use of dynamic adaptive runtime techniques to improve the scalability and efficiency of multipole method computations. The result, the Dynamic Adaptive System for Hierarchical Multipole Methods (DASHMM) allows application scientists to rapidly create custom, scalable, and efficient multipole methods.

Project Goals

- Provide a flexible, scalable, and efficient multipole method library.
- Provide widely used kernels and methods.
- Ease the use of multipole methods from end-science users.
- Broaden user-community of the multipole methods.
- Take advantage of ParalleX execution model to bring parallel computing out of the ‘assembly era’.
- Foster next generation scientists.

DASHMM Features

- Dynamic adaptive techniques: DASHMM resides in an active global address space (AGAS). Dots or shaded regions in the figure stand for various local control objects (LCOs). Arrows represent parcels (actions) in the form of lightweight threads.
- Abstraction layers: (1) Handle general multipole methods. (2) HPX-5 hidden from users, but the ability to use HPX-5 directly is made available through the advanced API.

Project Accomplishments

- REU program summer 2015
  - Two participants: one from small liberal arts college and one woman.
  - Ten-week intensive research on
    - Mathematical verification of kernels scheduled for future releases;
    - Exploration of abstractions to facilitate the development of general multipole method library.
  - Comments from participants:
    - “Now that I have done this REU program I feel more confident about my coding and programming abilities and plan to pursue a career that is more computationally based than I had previously decided.” — A.T.
    - “I gained a greater understanding about research as a field, and the subject matter makes me believe I understand more about various fields in physics.” — V.T.
- DASHMM v0.5 release
  - BSD 3-clause license.
  - x86_64 or Xeon Phi (host) running Linux. Compiled with GCC/Intel compilers.
  - OOP implementation in C++ that provides abstraction to encompass both Barnes-Hut (BH) and the Fast Multipole Method (FMM), as well as many variations on those themes.
  - Provide first built-in kernel: Laplace potential.
  - Extensibility—both new methods and new expansions can be defined by users through class inheritance.
  - HPX-5 oblivious—parallelization details are hidden from users. Users need not to learn HPX-5 nor write parallel code to use or extend the capacity of the library.
  - Good SMP scaling for both BH and FMM.
- DASHMM & HPX-5 runtime codeign: user-defined LCO
  - Local Control Objects (LCOs) are event driven conditional structures that causes a thread or some other action to be instantiated once a condition is met.
  - LCOs encode the dependency structure of the data-flow computation in DASHMM.
  - User-defined LCO encodes data and task in one unique handle that enables (i) easy control of computation granularity and (ii) efficient (data, task) migration in an active global address space.

Current Research

- Move towards C++ templates for added flexibility and generality.
- Introspection to assist in data distribution and dynamic load balancing.
- Second built-in kernel: Yukawa potential.
- Visualization of execution to examine:
  - The quality of the initial data distribution.
  - The scheduled tasks, and which are along the critical path of the execution.
  - The quality of the adaptation, how frequent data is moved and how fast are said moves.
- Advanced API exposing more detailed control of library to users enabling:
  - Multiple kernels with the same data.
  - DAG reuse for multipole methods used as accelerators in iterative solve.
  - More efficient time-stepping.
- Applying funding for REU program in 2016.
- Collaborate with established community users:
  - Dr. Jiang from NJIT on Rotne-Prager-Y amakawa (RPY) tensor kernel for Brownian dynamics of DNA molecules with hydrodynamic interactions.
  - Dr. Chen from ORNL on Laplace and Yukawa kernels in the context of membrane biology simulations at biologically relevant time and length scales.
  - Dr. Jiang from NJIT on Rotne-Prager-Y amakawa (RPY) tensor kernel for Brownian dynamic simulations of DNA molecules with hydrodynamic interactions.

Reference

Website: https://www.crest.iu.edu/projects/dashm/