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COMPUTATIONAL SOFTWARE

Revision of DASHMM: Dynamic Adaptive System for Hierarchical Multipole Methods

J. DeBuhr*, B. Zhang and T. Sterling

Center for Research in Extreme Scale Technologies, School of Informatics and Computing, Indiana University, Bloomington, IN, 47404, USA.

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Abstract. We present version 1.2.0 of DASHMM, a general library implementing hierarchical multipole methods using the asynchronous multi-tasking HPX-5 runtime system. Compared with the previous release [10], this new version: (1) enables execution in both shared and distributed memory architectures; (2) extends DASHMM's infrastructure to support advanced multipole methods [18]; and (3) provides built-in implementations of both the Yukawa [15] potential and Helmholtz [16] potential in the low frequency regime. These additions have not impacted the user interface, which remains simple and extensible.

AMS subject classifications: 15A06, 31C20, 68N19

Key words: Generic multipole methods, Laplace potential, Yukawa potential, Helmholtz potential, distributed computing.

Program summary

Program title: DASHMM version 1.2.0

Nature of problem: Evaluates the Laplace, Yukawa or Helmholtz potentials at N target locations induced by M source points in three dimensions.

Software license: BSD 3-Clause

CiCP scientific software URL: `http://www.global-sci.com/code/dashmm-1.2.0.tar.gz`

Distribution format: .gz

Programming language(s): C++

Computer platform: x86_64

*Corresponding author. *Email address:* `jdebuhr@indiana.edu` (J. DeBuhr)

Operating system: Linux

Compilers: GCC 4.8.4 or newer; icc (tested with 15.0.1)

RAM:

External routines/libraries: HPX-5 4.0.0 or later

Running time:

Restrictions:

1 Introduction

Hierarchical Multipole Methods (HMMs) are a key component of many science applications in a wide range of fields. However, conventional parallel programming practice leaves many of these applications strong-scaling constrained. Asynchronous Many-Tasking (AMT) runtime systems offer some promise as a means to overcome the scaling constraints of HMMs. Many such programming models and runtime systems are difficult to incorporate into existing code, leading to the need to rewrite potentially large applications, a cost which is often not feasible for many groups. What is needed is a system that can provide both ready-made and user-created HMMs, in a form that is easy to use, and which obviates the need to write application code that targets advanced, and often experimental, AMT systems. The Dynamic Adaptive System for Hierarchical Multipole Methods (DASHMM) is a scientific software library that provides easy-to-use, extensible, scalable and efficient parallel implementations of HMMs on both shared and distributed memory architectures.

This paper presents a major update to DASHMM version 0.5.0 [10]. The centerpiece of this update is the ability of the library to operate on distributed memory architectures. The implementation deviates from typical bulk-synchronous executions, which mostly rely on locally essential trees [24–26], in favor of adaptive runtime techniques. DASHMM also differs from previous adaptive runtime implementations of HMMs [2,3,13,22], which were limited to shared memory architectures. DASHMM maintains the simple interface of the earlier version that requires no particular knowledge of the advanced experimental runtime system that provides DASHMM's parallelism. Further, this parallelism requires no explicit specification by the user about where the data is to be placed across the system.

In addition, this update includes a new built-in method, and two new built-in kernels. DASHMM now includes an advanced FMM [7,18], which this paper refers to as the FMM97 method, that uses exponential expansions and the merge-and-shift technique. This method can be applied to the previously supplied Laplace kernel, as well as the two new built-in kernels, Yukawa and low-frequency Helmholtz. The Yukawa kernel is widely used in Brownian dynamics [21], and in the computation of non-bonded interactions [4]. The Helmholtz kernel is has wide applications in computational electromagnetics [8], the scattering of radiation [14] and electromagnetic compatibility/interference, the design of antennas, radar [5], optical and imaging systems, frequency-selective surfaces