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RECFMM: Recursive Parallelization of the Adaptive Fast Multipole Method for Coulomb and Screened Coulomb Interactions

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Abstract. We present RECFMM, a program representation and implementation of a recursive scheme for parallelizing the adaptive fast multipole method (FMM) on shared-memory computers. It achieves remarkable high performance while maintaining mathematical clarity and flexibility. The parallelization scheme signifies the recursion feature that is intrinsic to the FMM but was not well exploited. The program modules of RECFMM constitute a map between numerical computation components and advanced architecture mechanisms. The mathematical structure is preserved and exploited, not obscured nor compromised, by parallel rendition of the recursion scheme. Modern software system—CILK in particular, which provides graph-theoretic optimal scheduling in adaptation to the dynamics in parallel execution—is employed. RECFMM supports multiple algorithm variants that mark the major advances with low-frequency interaction kernels, and includes the asymmetrical version where the source particle ensemble is not necessarily the same as the target particle ensemble. We demonstrate parallel performance with Coulomb and screened Coulomb interactions.

AMS subject classifications: 15A06, 31C20

Key words: Fast multipole method, recursive parallelization, dynamic scheduling, Coulomb interaction, screened Coulomb interaction.

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Program summary

Program title: RECFMM

Nature of problem: Rapid evaluation of interactions among charged particles in 3D space, in terms of potential and force field, governed by low-frequency kernels such as for the Coulomb and screened Coulomb interactions.

Software licence: GPL 2.0

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

Distribution format: .gz

Programming language(s): C with CILK and Fortran

Computer platform: Any quipped with that described in the next three items.

Operating system: Linux, Cygwin, Mac OS X

Compilers: Intel compilers `icc` and `ifort` (15.0.4 or newer); GNU compilers (5.3.0 or newer); LLVM compiler `Cilk Plus` (3.4.1 or newer).

RAM: 32KB of storage per 1000 particles; 1.5KB (5.6KB) for each multipole or local expansion of 3-digit (6-digit) accuracy; 0.9KB (4.5KB) for each exponential expansion of 3-digit (6-digit) accuracy.

External routines/libraries: Fortran subroutines for accurate evaluation of Gamma and Bessel functions used for computing the screened Coulomb interaction.

Running time: Problem-size and computer-resource dependant.

Restrictions: 3-digit or 6-digit accuracy; low-frequency interaction kernels.

Supplementary material and references:

Additional Comments: The subroutines for multipole expansions and translated expansions can be customized to different accuracy, or replaced according to a different interaction kernel.

1 Introduction

We present RECFMM, a program representation and implementation of a recursive scheme for parallelizing the adaptive fast multipole method (FMM) on shared-memory computers. RECFMM expedites the computation of the potential ϕ and force field $\nabla\phi$ at M target locations $\{\mathbf{t}_i | i = 1,2,\cdots,M\} \subset \Omega_t$ due to charges q_j of N source particles located at $\mathbf{s}_j$, $\{\mathbf{s}_j, | j = 1,2,\cdots,N\} \subset \Omega_s$,

$$\phi_i = \sum_{j=1}^{N} K(\|\mathbf{t}_i - \mathbf{s}_j\|_2) q_j, \qquad \nabla\phi_i = \sum_{j=1}^{N} \nabla K(\|\mathbf{t}_i - \mathbf{s}_j\|_2) q_j, \tag{1.1}$$

where the target domain Ω_t and source domain Ω_s are in the 3D space $\mathbb{R}^3$, the kernel function $K(t,s)$ describes the potential at location t due to a unit charge at location s. In