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SC'11 Poster: A Highly Efficient MGPT Implementation for LAMMPS; with Strong Scaling

T. Oppelstrup, A. Stukowski, J. Marian

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Tomas Oppelstrup
Lawrence Livermore National Lab
7000 East Avenue
Livermore, CA 94550
+1 (925) 422-2808
oppelstrup2@llnl.gov

Alexander Stukowski
Lawrence Livermore National Lab
7000 East Avenue
Livermore, CA 94550
+1 (925) 423-8168
stukowski1@llnl.gov

Jaime Marian
Lawrence Livermore National Lab
7000 East Avenue
Livermore, CA 94550
+1 (925) 423-7039
marian1@llnl.gov

ABSTRACT

The MGPT potential has been implemented as a drop in package to the general molecular dynamics code LAMMPS. We implement an improved communication scheme that shrinks the communication layer thickness, and increases the load balancing. This results in unprecedented strong scaling, and speedup continuing beyond 1/8 atom/core.

In addition, we have optimized the small matrix linear algebra with generic blocking (for all processors) and specific SIMD intrinsics for vectorization on Intel, AMD, and BlueGene CPUs.

Categories and Subject Descriptors

G.4 [**Mathematical software**]: Parallel and vector implementations, Efficiency; J.2 [**Physical sciences and engineering**]: Physics

General Terms

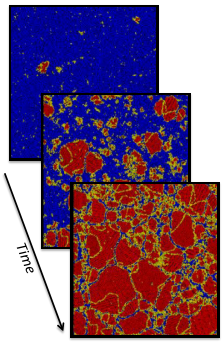
Algorithms, Performance.

Keywords

MGPT, LAMMPS, strong scaling, optimized linear algebra

1. INTRODUCTION

In molecular dynamics (MD), the space-time trajectories of atoms or molecules are computed by evaluating the inter-atomic forces, and using them to integrate Newton's equations of motion in time. Various approximations of the forces can be used, from simple (and computationally cheap) empirical potentials such as Lennard-Jones and EAM, to detailed (and expensive) quantum mechanical forces using density functional theory (DFT). MGPT potentials lies somewhere in between in terms of accuracy and computational expense. It can be derived from DFT using certain approximations (3). The benefit of MGPT is that large scale simulations can be performed, while allowing enough accuracy to model sensitive physical phenomena. For example, solidification from melt in Tantalum and Uranium has been successfully simulated (2), something that requires large scale systems in order for finite size and boundary effects to become negligible.



MGPT simulation of solidification in Ta
Graphics from (2)

In MGPT, matrices are evaluated for each close pair of atoms, and an energy term is calculated for each *n*-tuple (pair, triplet, quadruplet), by taking traces of products of the bond matrices. The MGPT energy for a system of N particles can be written:

$$U = NE_{vol} + \sum_{i>j} \phi(r_{ij}) + \sum_{i<j<k<m} tr(H_{ij}H_{jk}H_{km}H_{mi}) + \sum_{i>j>k} (tr(H_{ij}H_{jk}H_{ki}) + tr(H_{ij}H_{jk}H_{kj}H_{ji}))$$

where H_{ij} is a bond matrix, E_{vol} is a volume dependent constant, and ϕ is a pair-energy function.

2. POSTER CONTENTS

The poster concerns an optimized implementation of the MGPT interatomic forces. In order to be efficient on massively parallel computers, the implementation must achieve high performance on each processor, and distribute the computations evenly across the processors. In addition, communication must be minimized, so that the processors do not spend a significant amount of time waiting for data.

Most of the computational cost of the MGPT potentials lies in linear algebra with small (e.g. 7x7) matrices. The top part of the first page of the poster illustrates the techniques used to reach close to optimal performance of the linear algebra computations. The rest of the first page shows the communication scheme used in our implementation. It is design to reduce communication compared to commonly used schemes, and also achieves very uniform load balancing.

The second page of the poster shows the overall performance and parallel scaling of our MGPT implementation, for BlueGene and x86 architectures. In addition this page has a brief summary and potential future work.

3. ACKNOWLEDGMENTS

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