Kokkos Port of CoMD Mini-App

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Outline

- Background Motivation
- Molecular Dynamics / CoMD proxy application
- Kokkos Library
- Porting Effort
- Performance Results
- Lessons Learned

Motivation

Background

Motivation

LANL CCS-7 Application Performance Team FY18 Goal

- Explore programming models
- Extensively test on proxy apps and other relevant code
- Educate IC user community

Background

Programming Models

Programming Model	Portable CPU/GPU	Data layout	Approach
RAJA	Yes	Yes	Library
C++ AMP	Yes	No	Language
Thrust	Yes	No	Library
SGPU2	Yes	No	Library
XKAPPI	Yes	No	Library
OpenACC	Yes	No	Directives
OpenHMPP	Yes	No	Directives
StarSs	Yes	No	Directives
OmpSs	Yes	No	Directives
HOMPI	Yes	No	Translator
PEPPHER	Yes	No	Directives
OpenCL	Yes	No	Language
StarPU	Yes	No	Language
Loci	No	Yes	Library
Cilk Plus	No	Yes	Language
TBB	No	No	Library
Charm++	No	No	Library
OpenMP	Almost*	No	Directives
CUDA†	No	No	Language

CoMD Proxy App

CoMD: Molecular Dynamics Proxy Application

CoMD App

- Based on SPaSM, a Gordon Bell Prize winning MD code important to several projects in materials science
  - Essential feature is the emphasis on short-range interactions
  - SPaSM, the go-to code for shaking out new architectures such as Roadrunner, Cielo, and Trinity, among other notable HPC platforms
- Array-of-Structures (AoS) data layout

  $\mathbf{r} = \{x_i, y_i, z_i\}$, i=1..# atoms

  $\mathbf{f} = \{f_{xi}, f_{yi}, f_{zi}, e_i\}$, i=1..# atoms
- Force calculations follow serialized (per rank), nested loop design

```
for all local link cells
   for each atom in local link cell
      for all neighbor link cells
         for each atom in neighbor link cell
```

CoMD: Molecular Dynamics Proxy Application

CoMD App

- Created and maintained by the Exascale Co-Design Center for Materials in Extreme Environments (ExMatEx) group

  http://www.exmatex.org/comd.html

  https://github.com/exmatex/CoMD

- Written entirely in C using a collection of object-oriented
- Makes adding C++ code very simple (Kokkos is C++)
- CoMD exists as several ports to other programming models
  - –pure MPI
  - –OpenCL
  - –CUDA
  - –OpenMP
  - –tuned vector + OpenMP (Toks)

Kokkos Programming Model

Kokkos: Many-core device performance library

Kokkos

- ✓ C++ library, not a new language or language extension
- ✓ Supports clear, concise, thread-scalable parallel patterns
- ✓ Abstracts away commonalities between languages and libraries that run on multiple architectures (*CUDA, OpenACC, OpenCL, OpenMP, Coarray Fortran/Fortran 2008, …)*
- ✓ Supports "*write once, run everywhere*" code development
- ✓ Minimizes the amount of architecture-specific implementation details users must know to leverage mix of simple & complex cores
- ✓ Solves the data layout problem through multi-dimensional arrays with architecture-dependent layouts to handle heterogeneous memory

Kokkos: Many-core device performance library

Fundamental Abstractions

- Devices have ***Execution Spaces*** and ***Memory Spaces***
  - **Execution spaces**: Subset of CPU cores, CPU, PIM, ...
  - **Memory spaces**: host memory, host pinned memory, high-bandwidth memory, GPU global memory, GPU shared memory, GPU UVM memory, ...

  *Dispatch computation to **execution space** accessing data in **memory spaces***

- Multidimensional Arrays on steroids
  - Map multi-index (i,j,k,...) ⇔ memory location in a ***memory space***
  - Map derived from an array *layout*
  - Choose layout for device-specific memory access pattern
  - Make layout changes transparent to user code
  - Users only need to follow the simple API: a(i,j,k) (*Fortran-like*)

  Separates user index space from memory layout

Kokkos: Many-core device performance library

Kokkos

OpenMP

```
#prama omp parallel for
for (int i=0; i< N; i++) {
   y[i] = a*x[i] + y[i];
}
```

Kokkos

```
Kokkos::parallel_for(N, KOKKOS_LAMBDA (const int& i) {
   y[i] = a*x[i] + y[i];
});
```

- Kokkos defines a **library of known pattern types.**
- Computational bodies are passed to the libraries as **C++ lambda functors.**
- **`KOKKOS_LAMDA`** is a macro to hide much of the details from users.
- The above line is a short-hand way to tell Kokkos we want to do a **parallel-for** on the computational body we have given over the declared index **`i`.**

CoMD-Kokkos Porting Effort

CoMD-Kokkos

Porting Effort

- Tuned version of CoMD contained ~6,000 lines of code
- Majority of time is spent calculating inter-atomic forces and time-stepping
  - Kokkos routines added to **ljForce** and **EAM** routines
  - Kokkos used to update velocities, positions, energy, and to redistribute atoms at the end of a time-step
  - Kokkos also used for initialization of data structures
- In all, 15 loops instrumented with Kokkos
  - 10 parallel-for
  - 5 parallel-reduce
- New data structures created to handle multiple-variable reductions
- Minor changes to some data structures to compile under C++11

L-J Force Calculation

Porting Effort

```
// loop over local boxes
for (int iBox=0; iBox<s->boxes->nLocalBoxes; iBox++)
{
   int nIBox = s->boxes->nAtoms[iBox];
   // loop over neighbors of iBox
   ...
   for (int jTmp=0; jTmp<nNbrBoxes; jTmp++)
   {
      int jBox = s->boxes->nbrBoxes[iBox][jTmp];
      ...
      // loop over atoms in iBox
      for (int iOff=MAXATOMS*iBox; iOff<(iBox*MAXATOMS+nIBox); iOff++)
      {
         // loop over atoms in jBox
         for (int jOff=jBox*MAXATOMS; jOff<(jBox*MAXATOMS+nJBox); jOff++)
         {
            compute_sum_of_inter_atomic_potential_energy(...);
         } // loop over atoms in jBox
         ...
      } // loop over atoms in iBox
   } // loop over neighbor boxes
} // loop over local boxes in system
```

L-J Force Calculation

Porting Effort

```
// loop over local boxes
Kokkos::parallel_reduce( s->boxes->nLocalBoxes, KOKKOS_LAMBDA( const int& iBox,
                         real_t& local_ePot)
{
   int nIBox = s->boxes->nAtoms[iBox];
   // loop over neighbors of iBox
   ...
   for (int jTmp=0; jTmp<nNbrBoxes; jTmp++)
   {
      int jBox = s->boxes->nbrBoxes[iBox][jTmp];
      ...
      // loop over atoms in iBox
      for (int iOff=MAXATOMS*iBox; iOff<(iBox*MAXATOMS+nIBox); iOff++)
      {
         // loop over atoms in jBox
         for (int jOff=jBox*MAXATOMS; jOff<(jBox*MAXATOMS+nJBox); jOff++)
         {
            compute_sum_of_inter_atomic_potential_energy(...);
         } // loop over atoms in jBox
         ...
      } // loop over atoms in iBox
   } // loop over neighbor boxes
}, ePot); // loop over local boxes in system
```

Implementing multiple variable parallel reduction

Porting Effort

```
real_t v0 = 0.0;
real_t v1 = 0.0;
real_t v2 = 0.0;
real_t v3 = 0.0;

#pragma omp parallel for reduction(+:v0) reduction(+:v1) reduction(+:v2) reduction(+:v3)
for (int iBox=0; iBox<s->boxes->nLocalBoxes; ++iBox)   {
   for (int iOff=MAXATOMS*iBox, ii=0; ii<s->boxes->nAtoms[iBox]; ++ii, ++iOff)      {
      v0 += s->atoms->p[iOff][0];
      v1 += s->atoms->p[iOff][1];
      v2 += s->atoms->p[iOff][2];
      int iSpecies = s->atoms->iSpecies[iOff];
      v3 += s->species[iSpecies].mass;
   }
}
vcmLocal[0] = v0;
vcmLocal[1] = v1;
vcmLocal[2] = v2;
vcmLocal[3] = v3;
```

Summing momenta and particle mass

Implementing multiple variable parallel reduction

Porting Effort

```
// A struct needed to implement a multiple variable reduction in Kokkos
struct vstruct {
   real_t v0;
   real_t v1;
   real_t v2;
   real_t v3;
   // default constructor
   KOKKOS_INLINE_FUNCTION
   vstruct() {
      v0 = 0.0;
      v1 = 0.0;
      v2 = 0.0;
      v3 = 0.0;
   }
   // operator += (volatile)
   KOKKOS_INLINE_FUNCTION
   vstruct & operator+=( const volatile vstruct & src) volatile {
      v0 += src.v0;
      v1 += src.v1;
      v2 += src.v2;
      v3 += src.v3;
   }
};
```

Summing momenta and particle mass

Implementing multiple variable parallel reduction

Porting Effort

Summing momenta and particle mass

```
vstruct Vvals;

Kokkos::parallel_reduce(s->boxes->nLocalBoxes, KOKKOS_LAMBDA( const int& iBox,
                        vstruct& local_v) {
   for (int iOff=MAXATOMS*iBox, ii=0; ii<s->boxes->nAtoms[iBox]; ++ii, ++iOff)
   {
      local_v.v0 += s->atoms->p[iOff][0];
      local_v.v1 += s->atoms->p[iOff][1];
      local_v.v2 += s->atoms->p[iOff][2];
      local_v.int iSpecies = s->atoms->iSpecies[iOff];
      local_v.v3 += s->species[iSpecies].mass;
   }
}, Vvals);

vcmLocal[0] = Vvals.v0;
vcmLocal[1] = Vvals.v1;
vcmLocal[2] = Vvals.v2;
vcmLocal[3] = Vvals.v3;
```

Performance Results

Performance Results

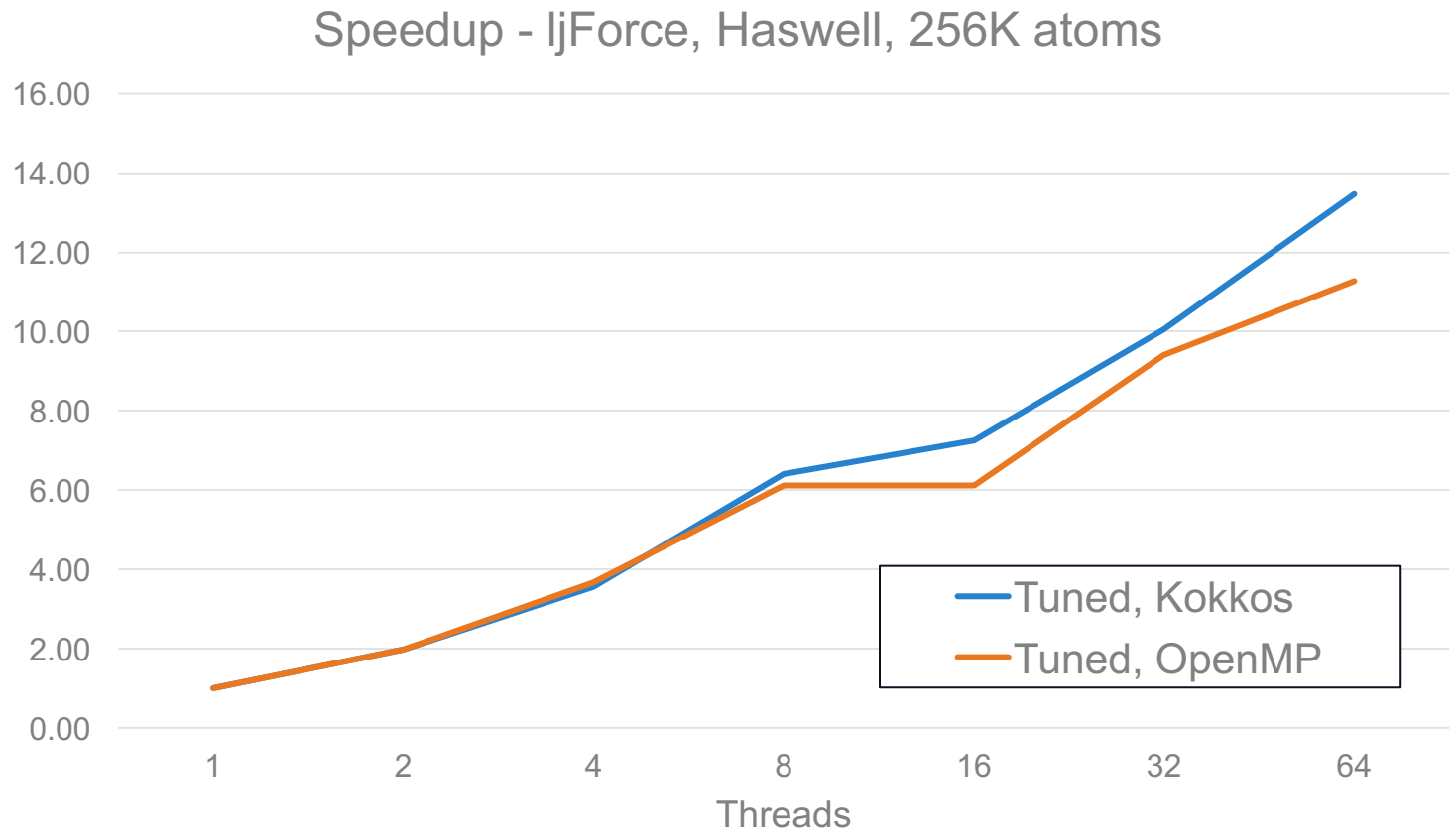
Benchmarks

The benchmark problem

- Single-node (1 MPI rank)
- 256K & 2,048K atoms
- 100 time steps
- Varied number of threads
- KNL and Haswell nodes of Trinity
- *Still working on GPU compilation...*
- Metrics
  - Walltime
  - Strong Scaling, speedup
  - Time (μs) per atom over solution

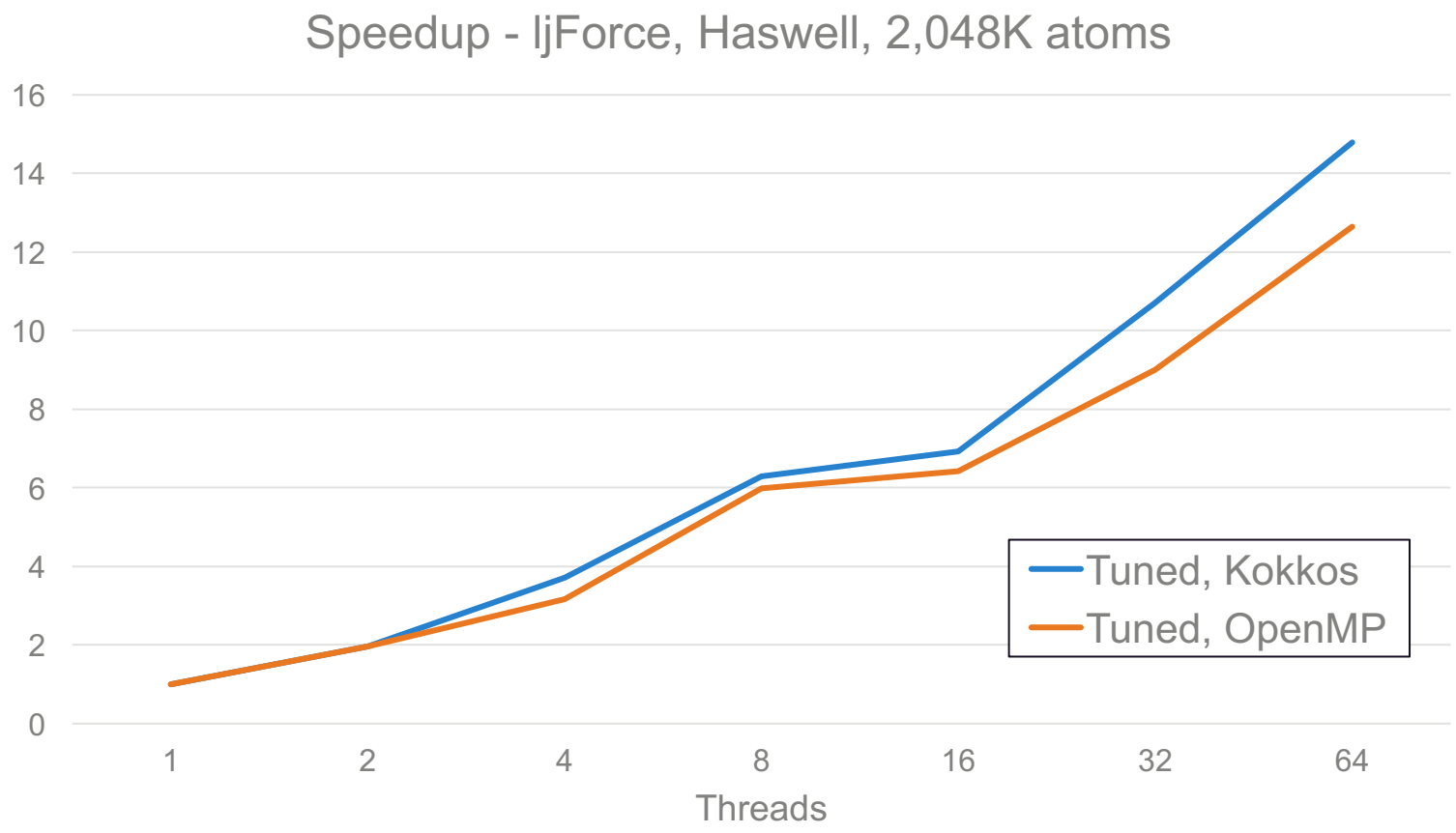
Performance Results

Benchmarks



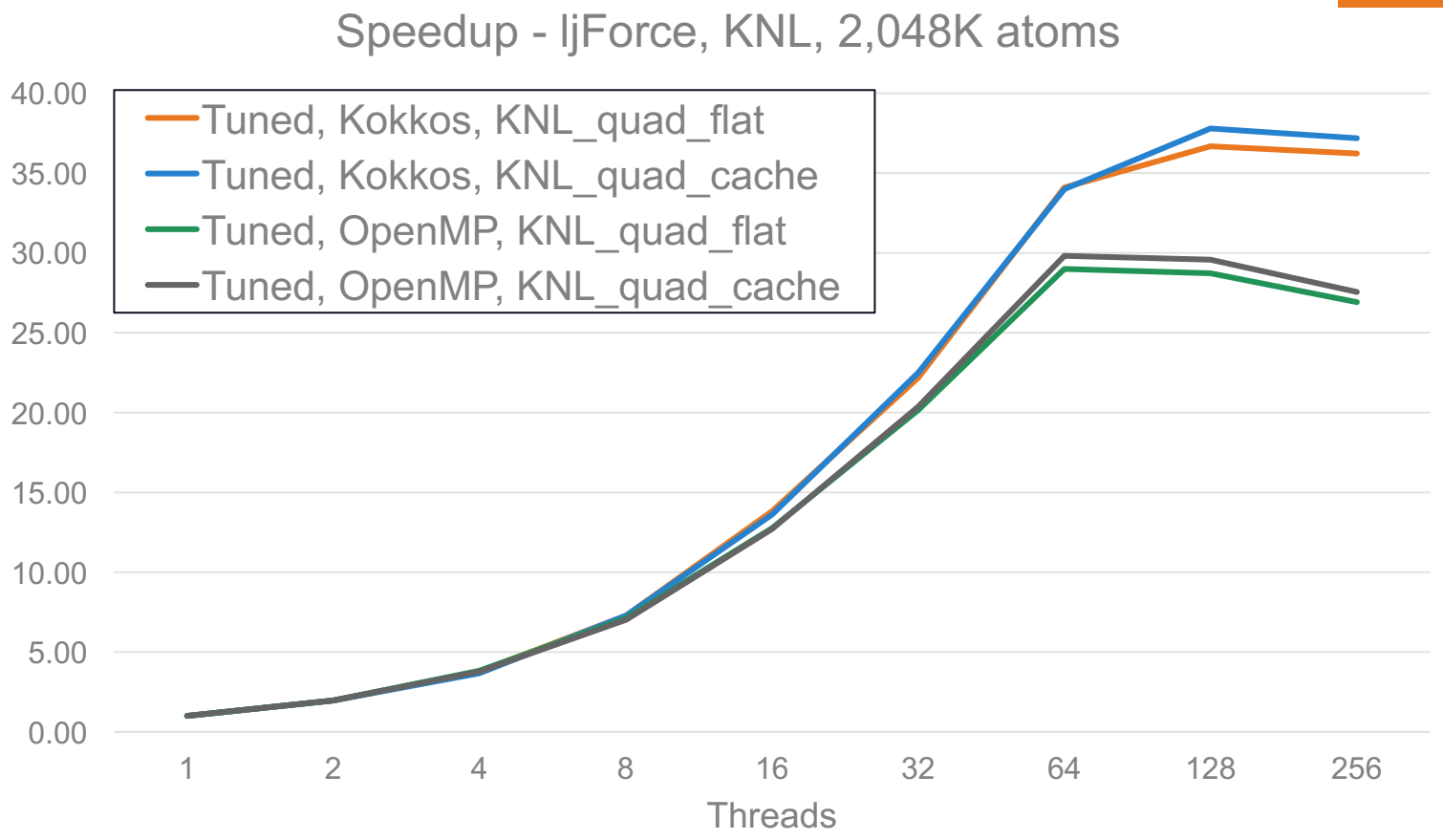
Performance Results

Benchmarks



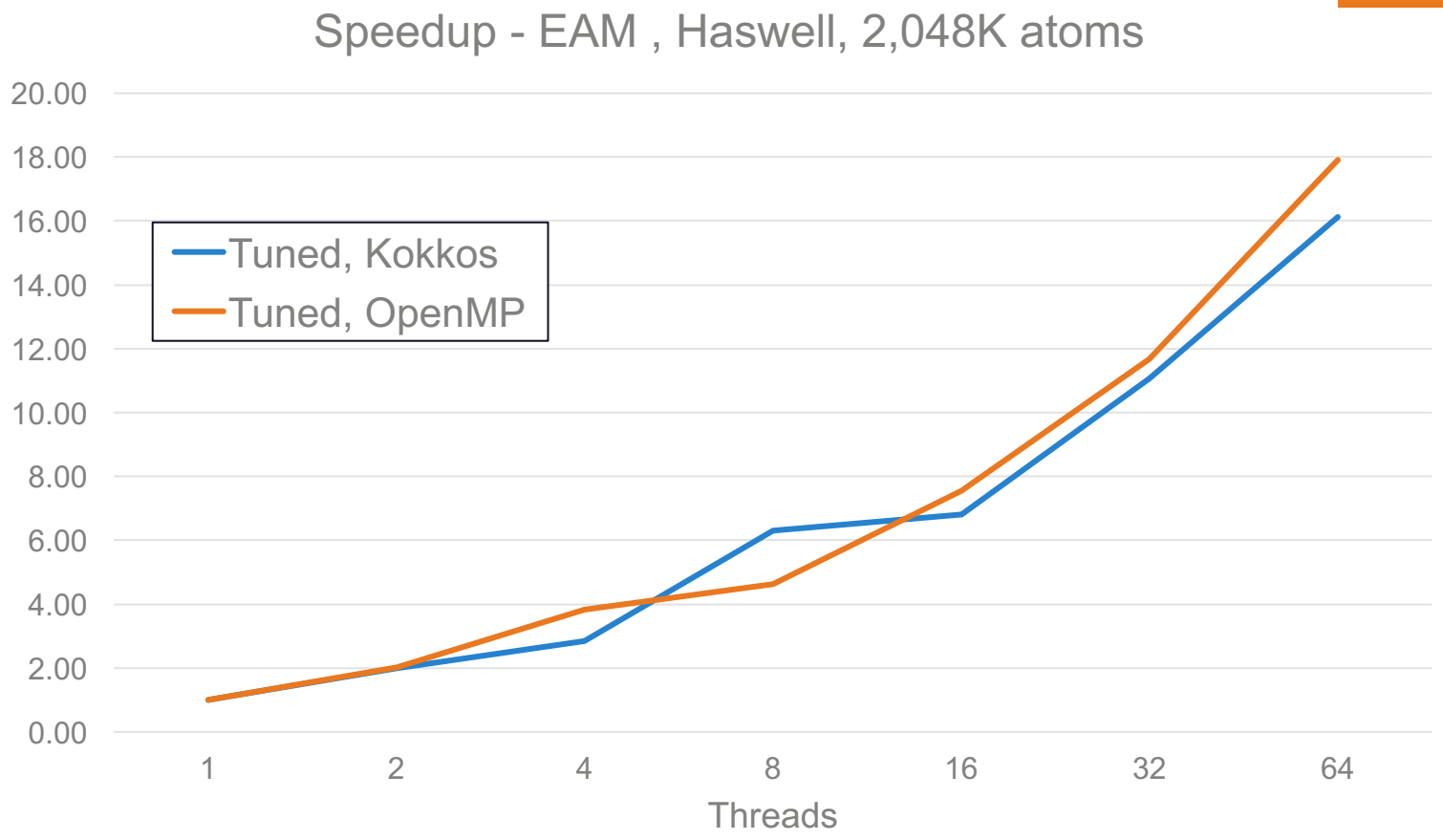
Performance Results

Benchmarks



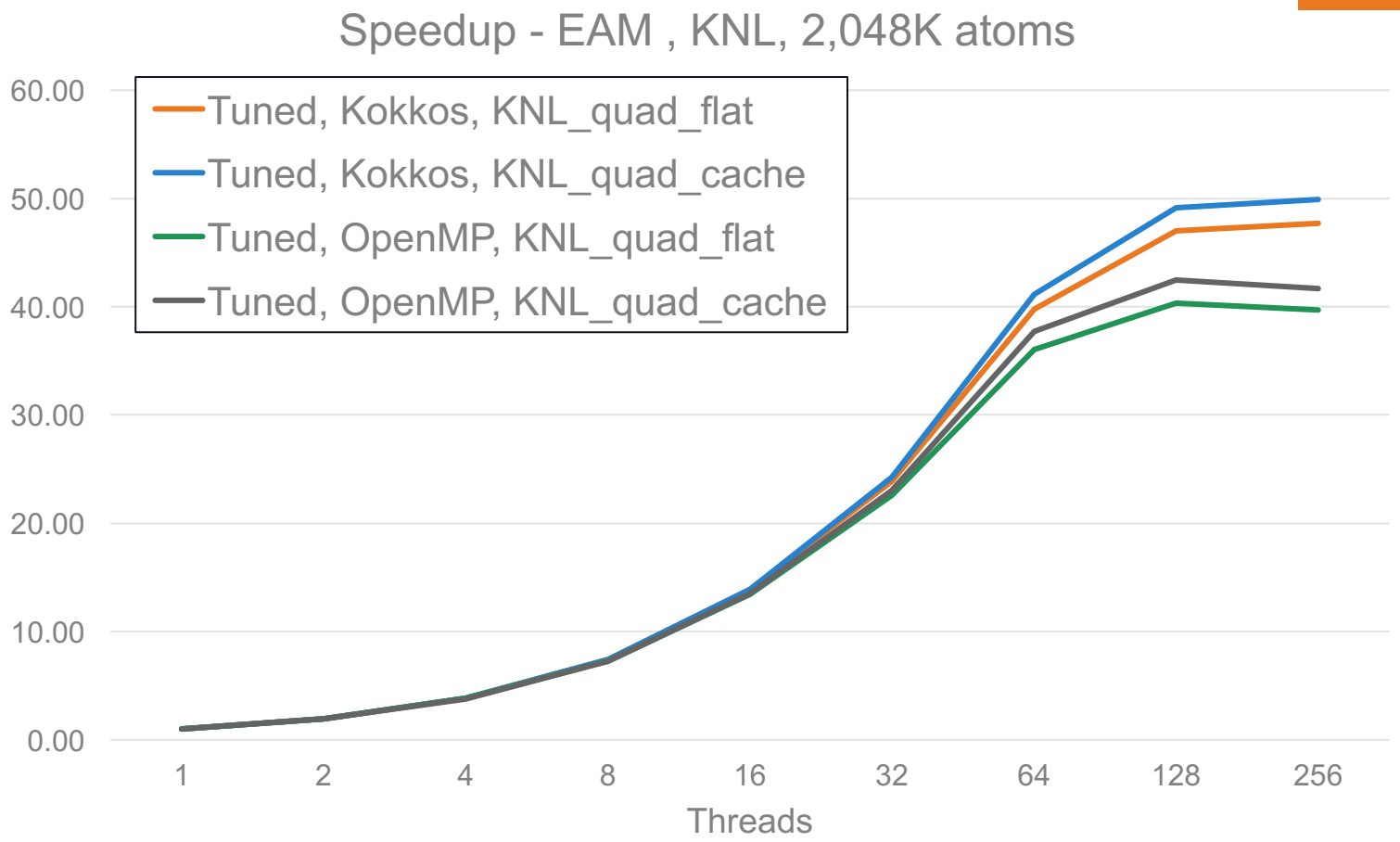
Performance Results

Benchmarks



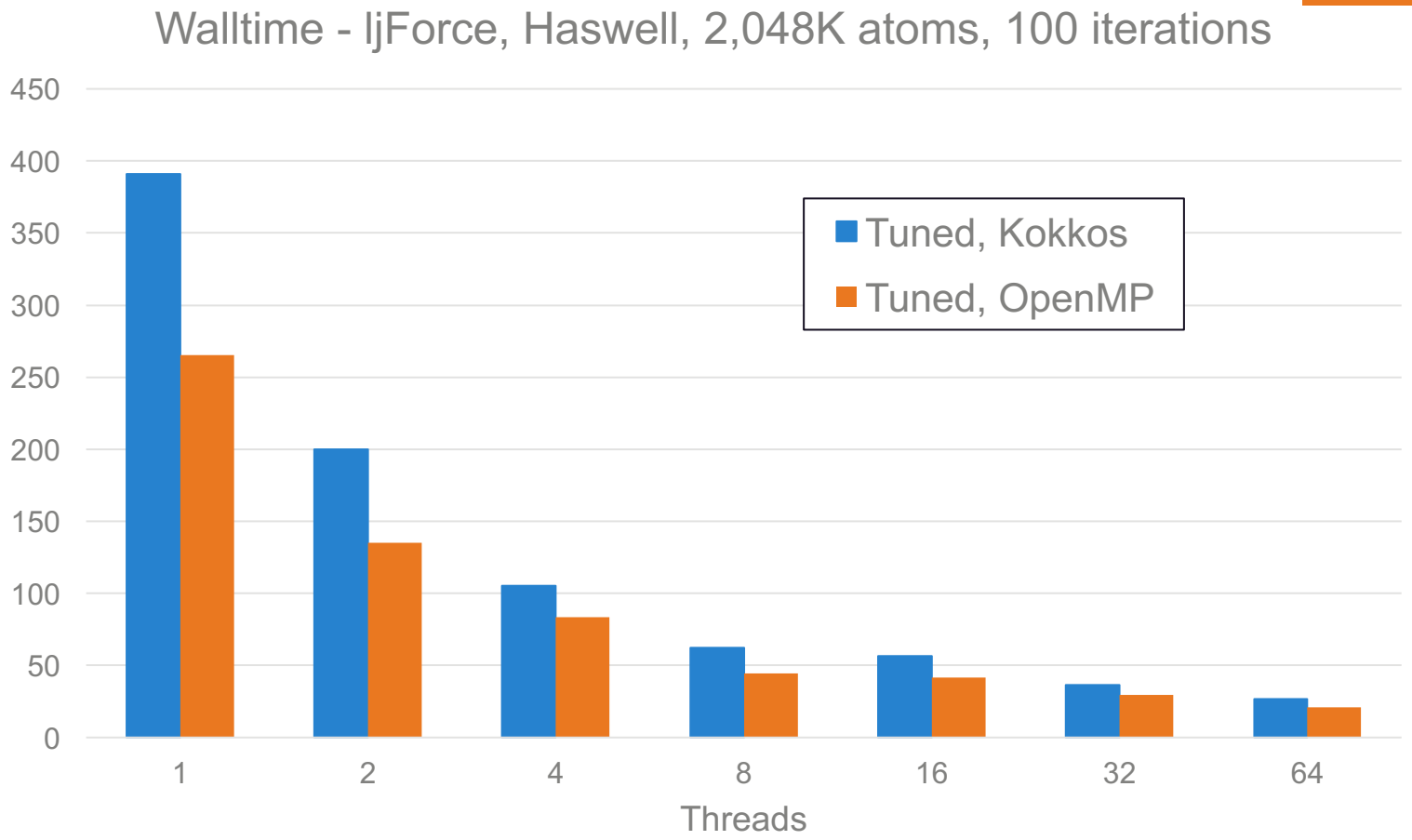
Performance Results

Benchmarks



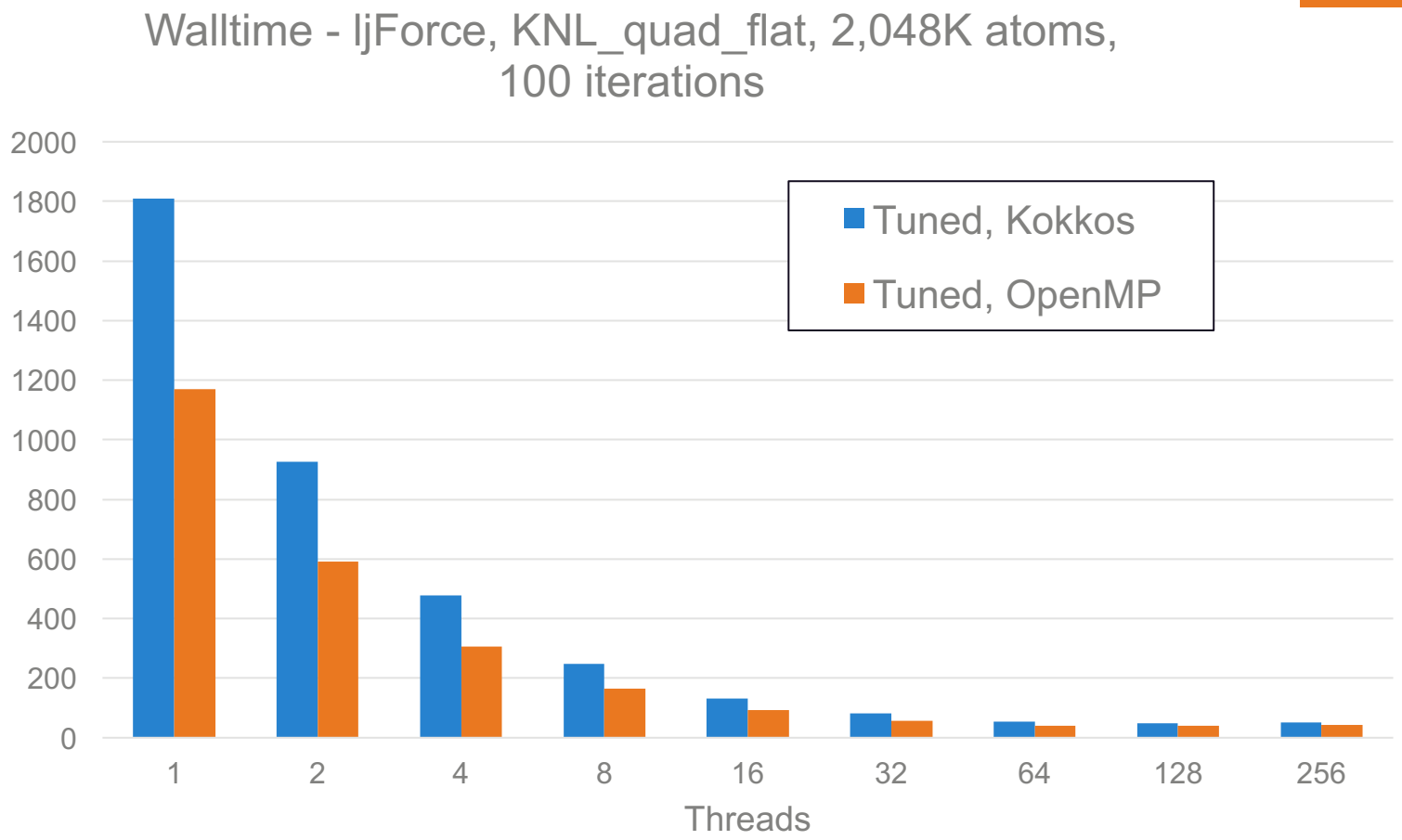
Performance Results

Benchmarks



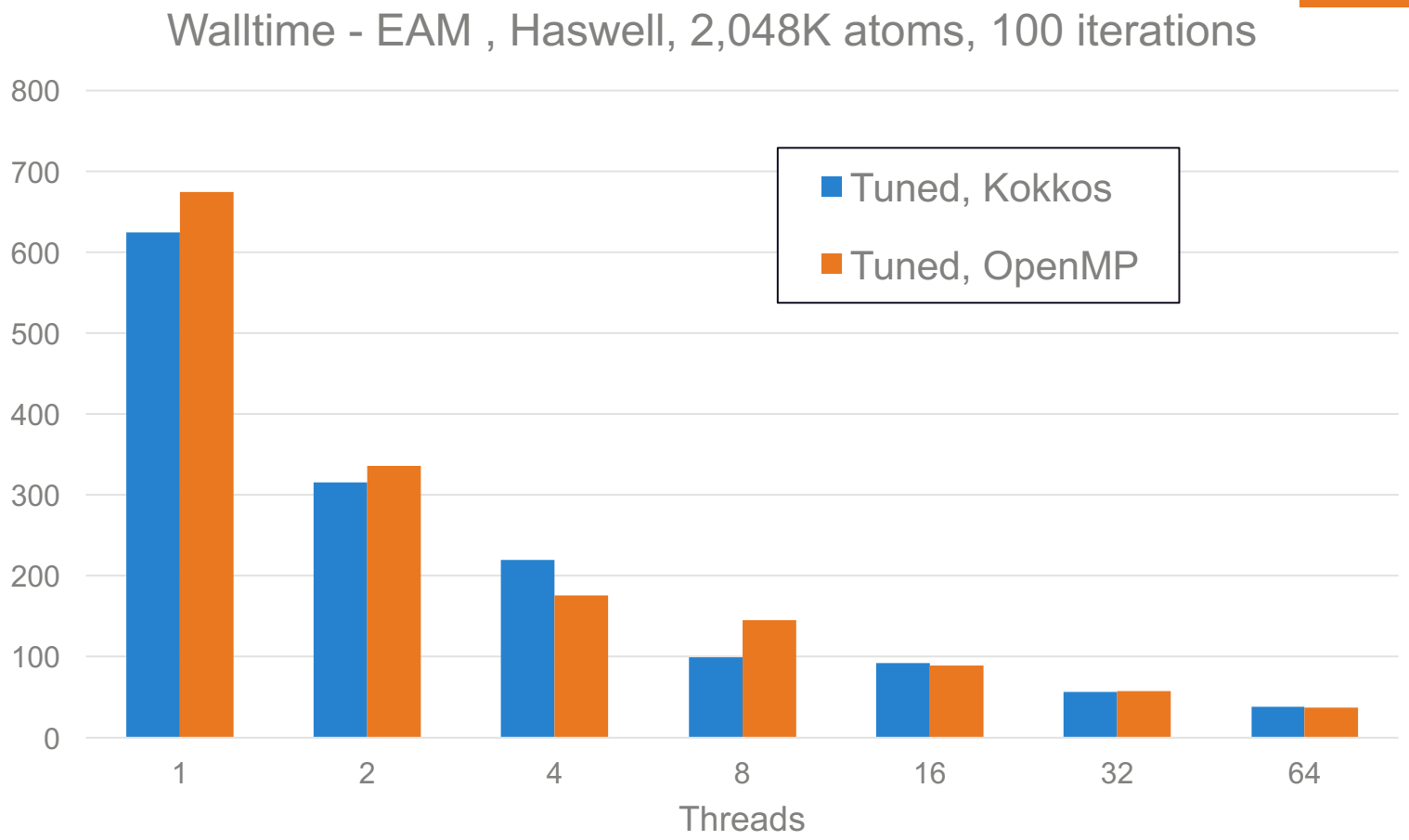
Performance Results

Benchmarks



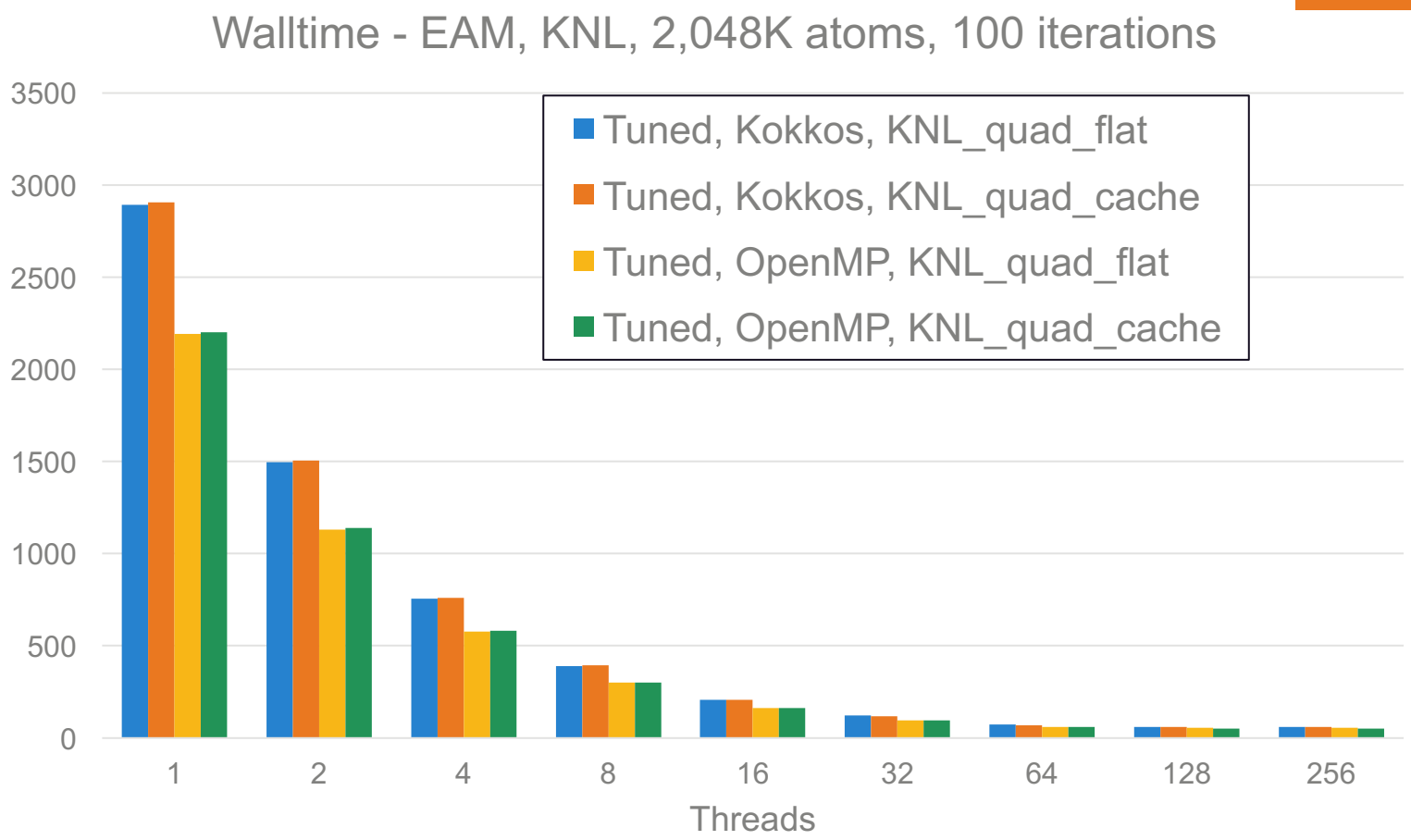
Performance Results

Benchmarks



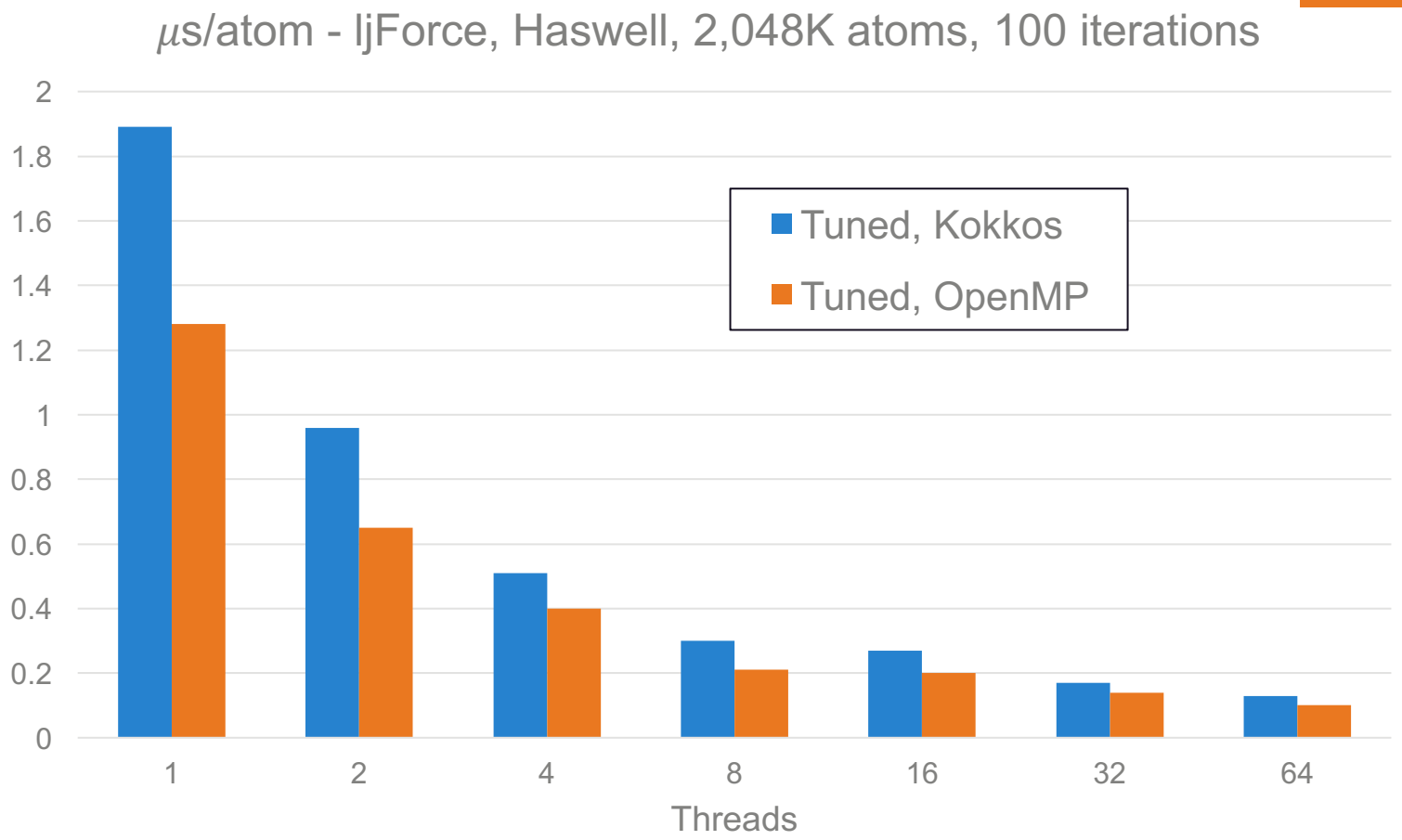
Performance Results

Benchmarks



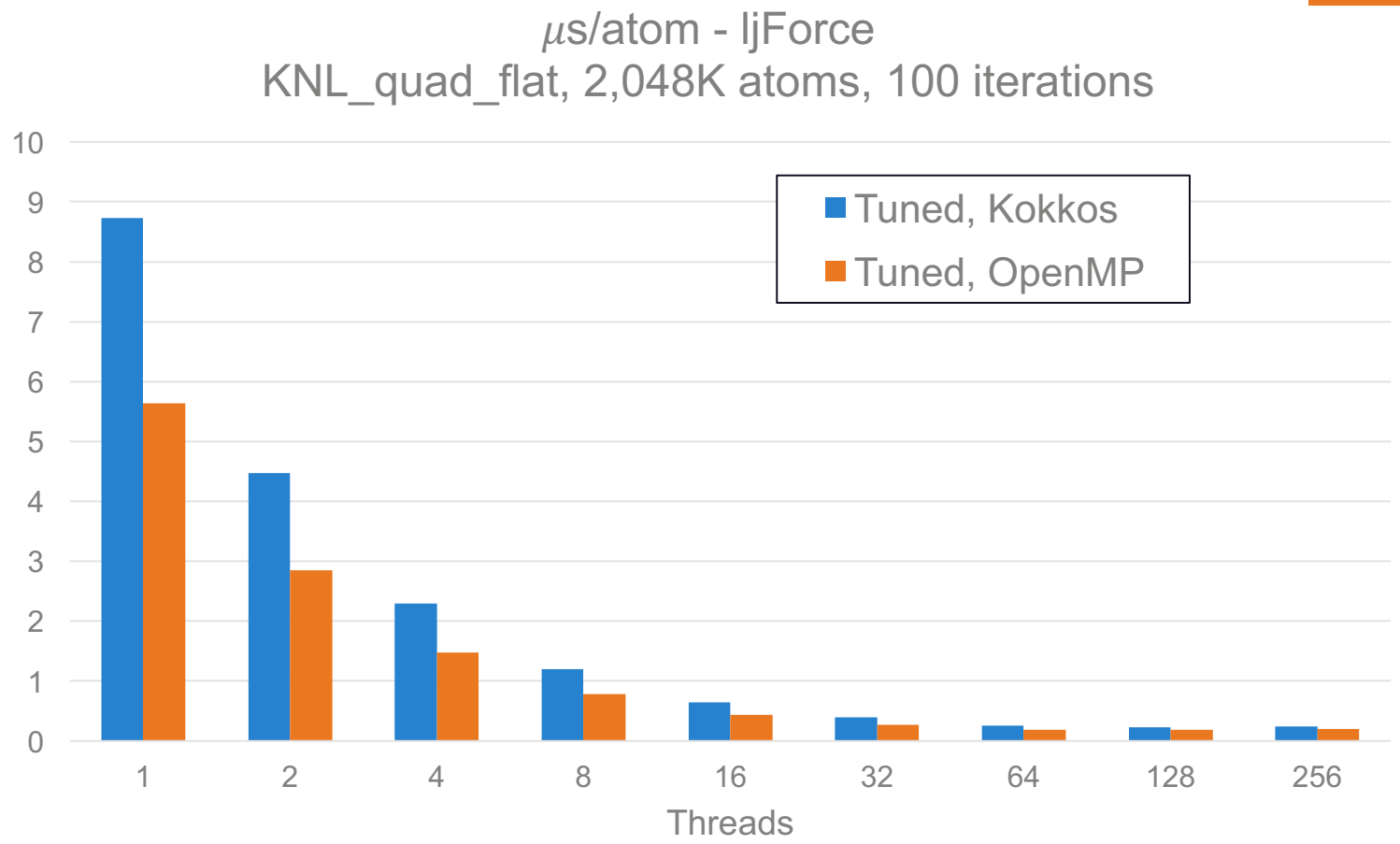
Performance Results

Benchmarks



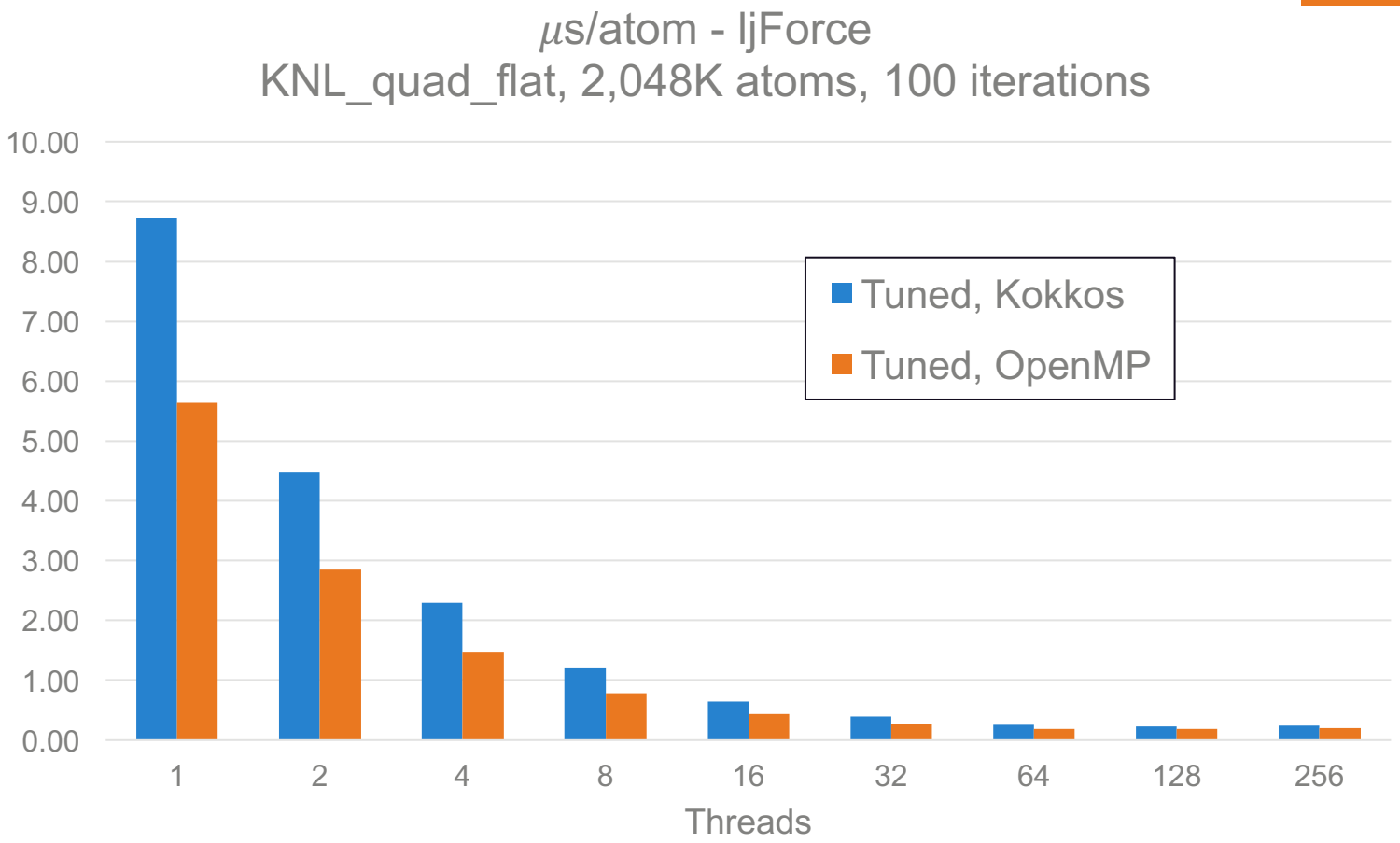
Performance Results

Benchmarks



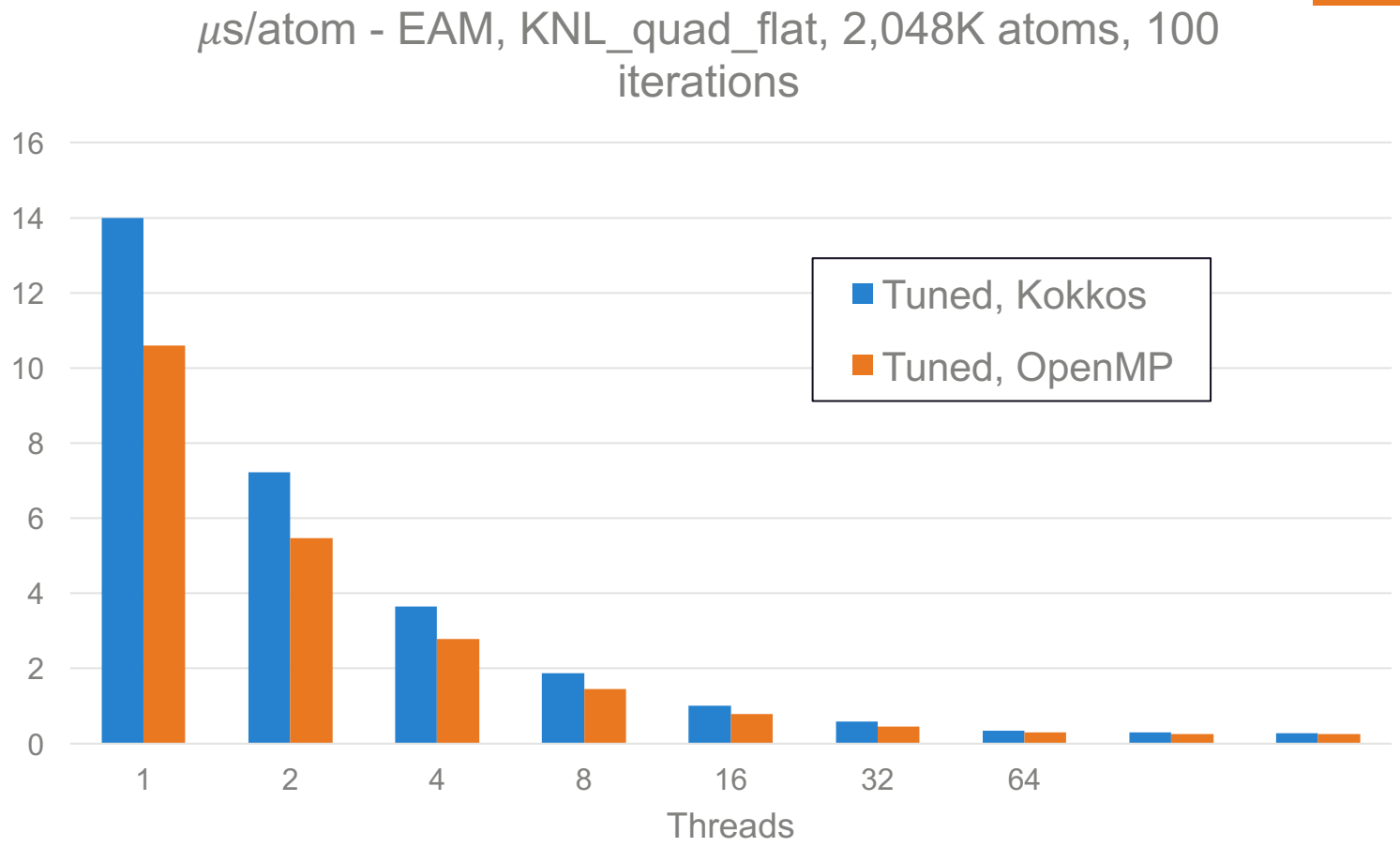
Performance Results

Benchmarks



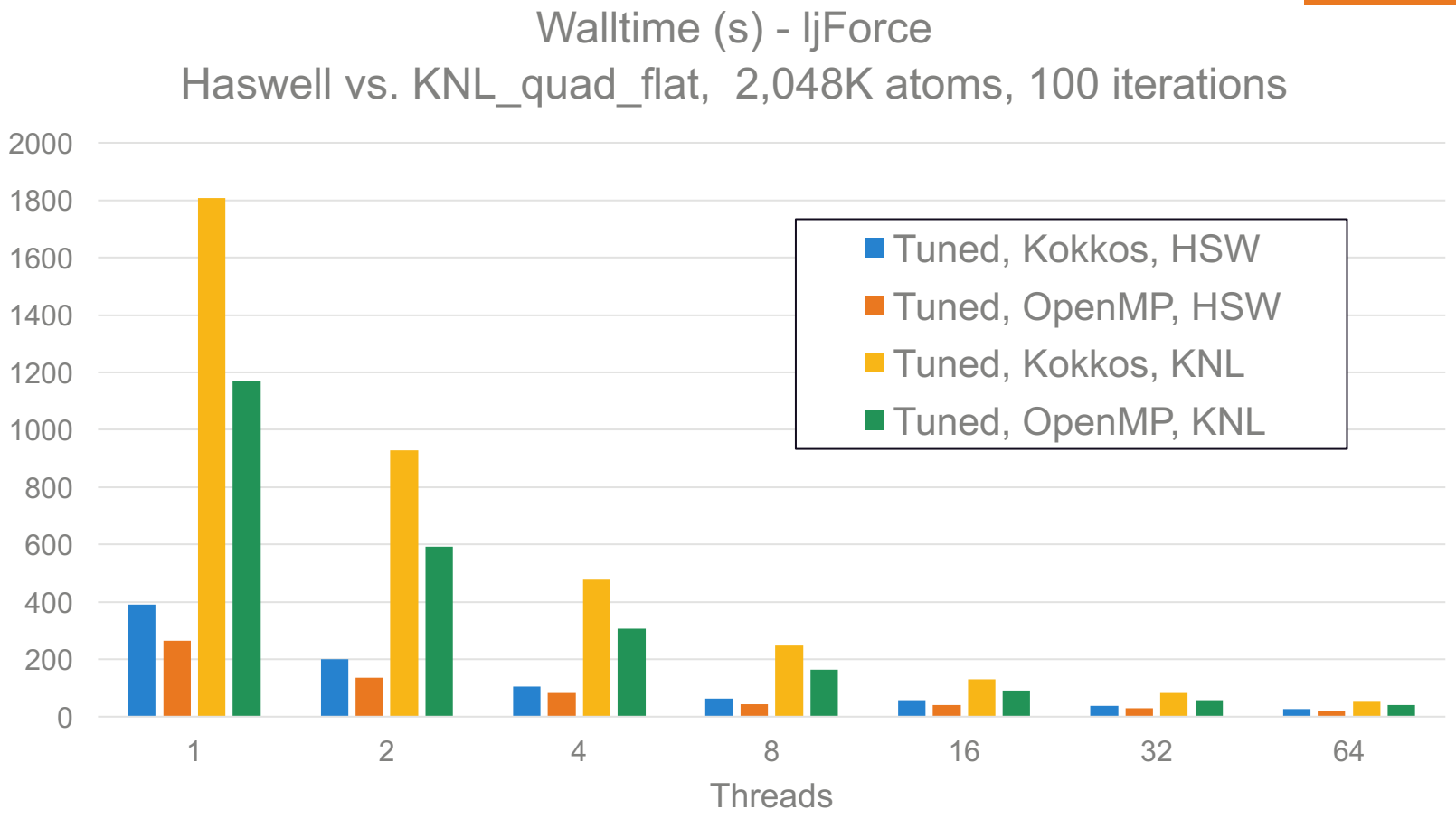
Performance Results

Benchmarks



Performance Results

Benchmarks



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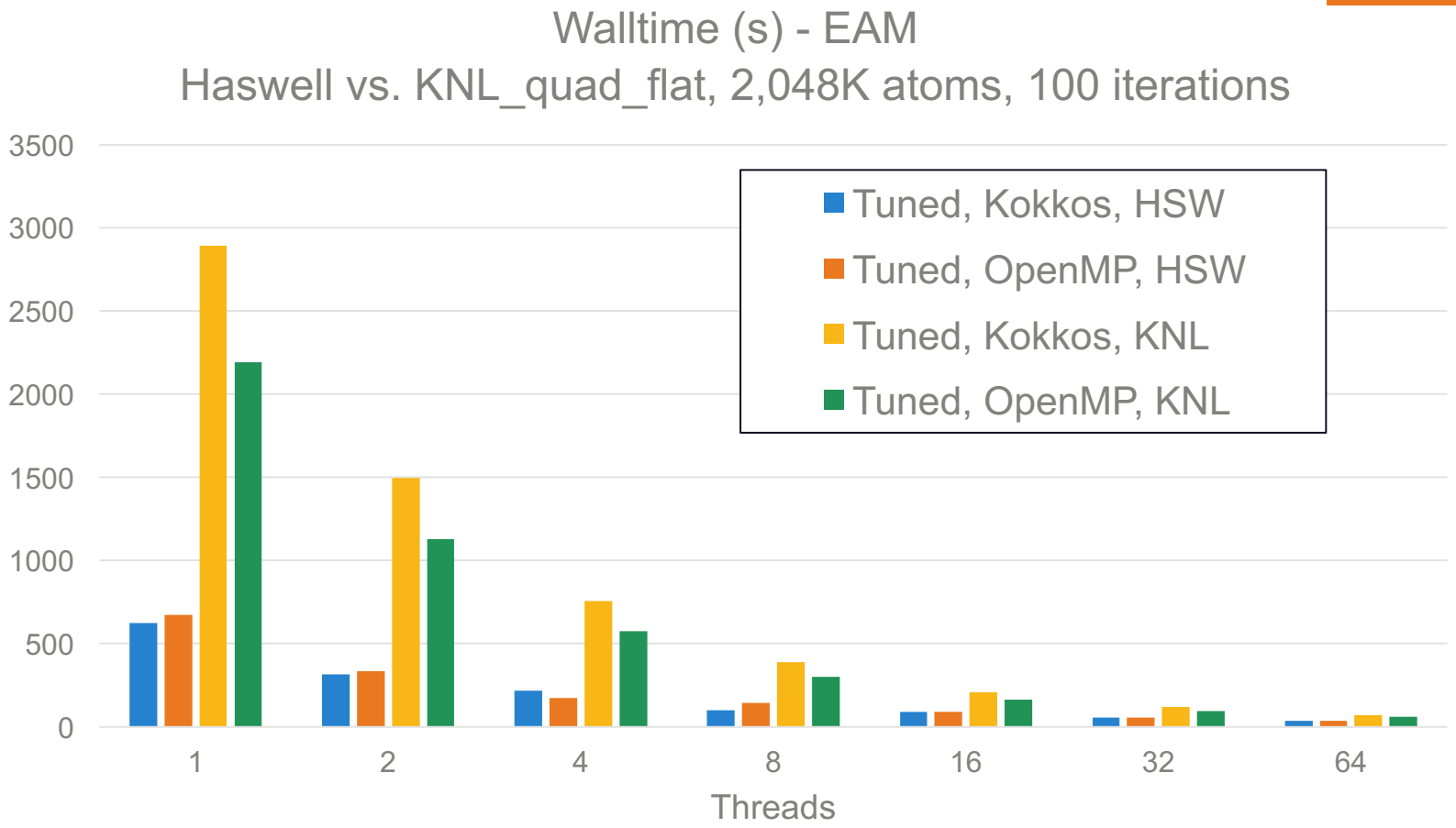

Performance Results

Benchmarks

Kokkos impairs some vector performance

```
// Compute Embedding Energy
// loop over all local boxes
Kokkos::parallel_reduce( s->boxes->nLocalBoxes, KOKKOS_LAMBDA( const int& iBox, real_t&
local_etot) {
   int nIBox =  s->boxes->nAtoms[iBox];
   // loop over atoms in iBox
   for (int iOff=MAXATOMS*iBox; iOff<(MAXATOMS*iBox+nIBox); iOff++) {
      real_t fEmbed, dfEmbed;
      interpolate(table_F, pot->rhobar[iOff], &fEmbed, &dfEmbed);
      pot->dfEmbed[iOff] = dfEmbed;
      s->atoms->U[iOff] += fEmbed;
      local_etot += fEmbed;
   }
}, etot);
```

unaligned access patterns

Kokkos summary

```
--- begin vector cost summary ---
scalar cost: 291
vector cost: 38.750
estimated potential speedup: 7.000
--- end vector cost summary ---
```

OpenMP summary

```
--- begin vector cost summary ---
scalar cost: 21
vector cost: 2.250
estimated potential speedup: 8.630
--- end vector cost summary ---
```

The Take-Away

Lessons Learned

1. **Difficult finding documentation for building Kokkos libs**
   – especially for GPUs
   – Options like `-DKOKKOS_OPT_RANGE_AGGRESSIVE_VECTORIZATION` hard to find
2. **CoMD relatively easy due to "C++"-like structure of the code**
   – But data structures need much work
3. **Special `structs` required for handling parallel reductions of more than one variable, i.e.**

```
#pragma omp parallel for reduction(+:v0) reduction(+:v1)
reduction(+:v2) reduction(+:v3)
```

4. **Vectorization performance suffers, unclear why**
5. **Code blocks inside Kokkos lambda functors are not optimized by the compiler to the level of the tuned, OpenMP version**

We have a long way to go to show the benefit of Kokkos but we think it is there.