Experiences with OpenMP in tmLQCD

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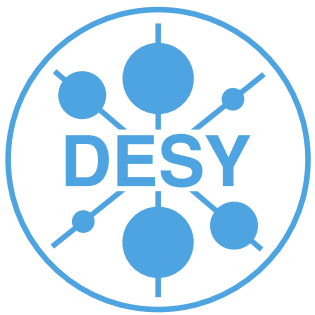


Overview

Experiences from adding OpenMP to tmLQCD

Introduction

OpenMP

Shared memory parallel programming models

- Data shared between execution units (e.g. threads)
- No explicit communication (usually)
  - $\Rightarrow$ synchronization built into programming model
  - $\Rightarrow$ lower memory requirements (usually)
  - **!** need for "locking" when data is modified concurrently

OpenMP

- Simple syntax through pragmas with "directives":
  `#pragma omp parallel`
  - can be specialized with parameters, even runtime conditionals
- Most common scenarios are addressed
- Strong focus on loops
- No provision for complicated models before OpenMP 3.0
  - $\Rightarrow$ e.g.: no possiblity (within syntax) to launch independent "I/O thread"

Introduction

Basic Example

```
su3 function(args) {
  su3 accum;
  su3 U0, U1, U2;
  #pragma omp parallel for private(U0,U1,U2) shared(args,accum)
  for(int x = 0; x < VOLUME; ++x) {
    for(int mu = 0; mu < 4; ++mu) {
      U0 = get_staples(x,mu);
      [...]
    }
  }
  return accum;
}
```

+ **explicit mention of private/shared**
− **nightmare to maintain → updating private/shared prone to mistakes**

Introduction

Improved Basic Example

- **Use scoping rules to automate private / shared:**

```
su3 function(args) {
  su3 accum;
#pragma omp parallel
{
  su3 U0, U1, U2;
  #pragma omp for
  for(int x = 0; x < VOLUME; ++x) {
    for(int mu = 0; mu < 4; ++mu) {
      U0 = get_staples(x,mu);
      [...]
    }
  }
} /* OpenMP parallel closing brace */
  return accum;
}
```

+ **private/shared automatic, less overhead for multiple for loops**
− **private/shared less explicit**

Subtleties

working set size, performance, execution order

Setting up threads and assigning work has overhead

- maximize work, reduce relative size of overhead

Debugging can be challenging

- execution order not fixed (e.g.: summations) $\rightarrow$ difficult to differentiate bug and rounding
- some bugs may only show 'in production' and with very high statistics

  $\Rightarrow$ add debugging code with explicit ordering

  ! even then, errors might only show in high statistics

Subtleties

Amdahl & co.

Amdahl's law

- many threads $\rightarrow$ 2% serial function can easily turn into 25%
  - $\Rightarrow$ need to add OpenMP almost everywhere

Barriers can have substantial overhead

- Slow: computationally simple loops
- Slow: unbalanced thread workload
  - $\Rightarrow$ Use tools to find problematic areas
    - $\star$ Example: scalar product
      - $\star$ simple function $\rightarrow$ large barrier overhead
      - $\star$ scheduling: 'static' $\rightarrow$ 'guided' leads to 50% reduction in loop barrier overhead
      - $\star$ however, total time spent reduced only by 10%
  - $\Rightarrow$ Combine operations to increase workload

Subtleties

Data concurrency and race conditions

- Concurrent data access requires locking
  - ! `#pragma omp critical` is very slow

- Use `#pragma omp atomic`

```
[...]
#pragma omp atomic
derivative.d4 += [...]
[...]
```

  - ! Operation must compile into single instruction
  - ! Safety guaranteed only if multiple threads read, one thread writes
  - ! Conflicts may be unnoticeable in test programs
  - ! Conflict probability depends on total thread number

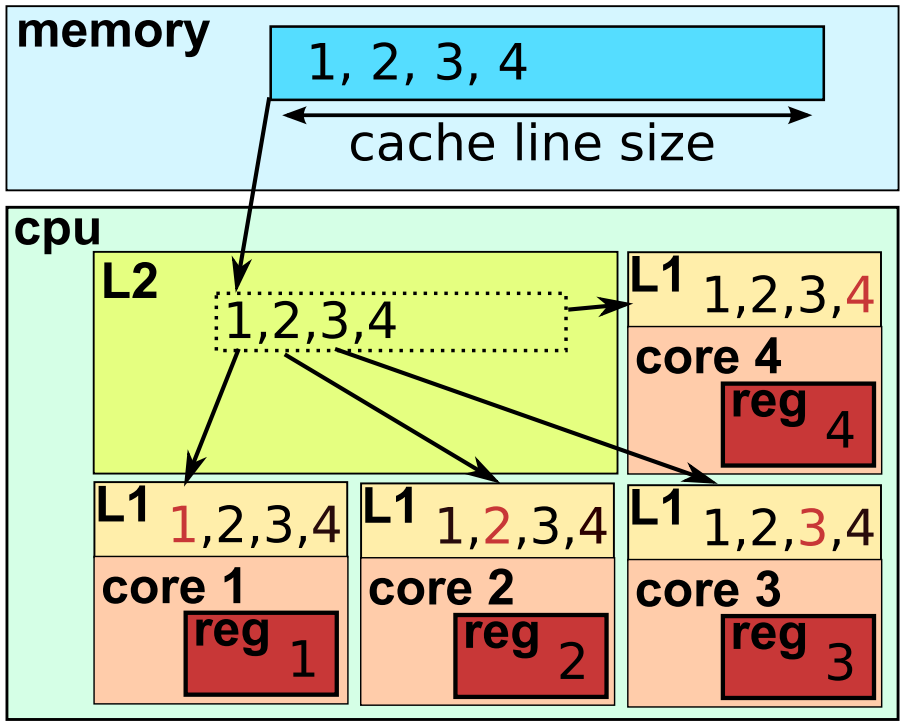
- In macros, use this syntax:

```
_Pragma("omp atomic")
```

Subtleties

False sharing

- threads update independent data, but on same cache line



- threads will invalidate each other's cache lines

! can slow multi-threaded program to less than sequential speed

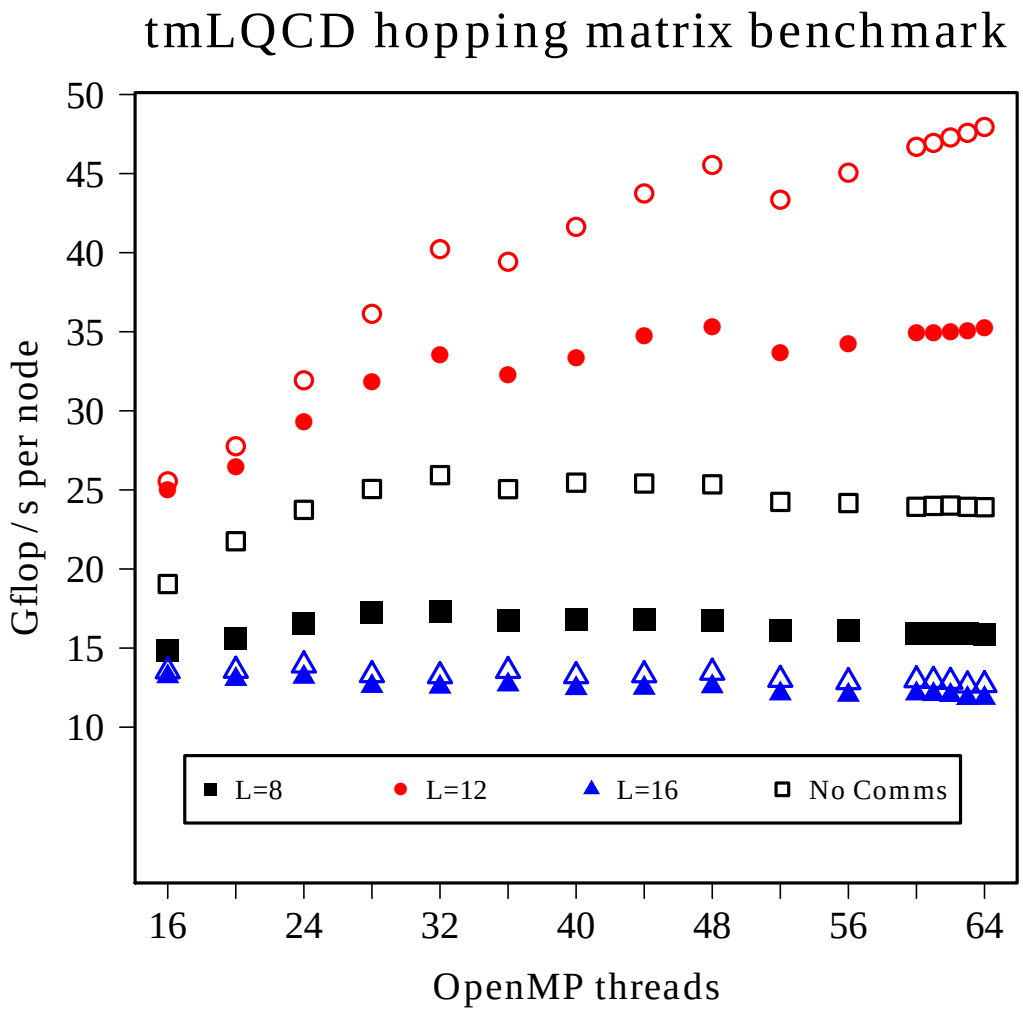
$\Rightarrow$ Add padding to ensure separate cache-lines, but total no. of cache lines limited!

Benefits and Overheads

Scaling

OpenMP scaling

- 1 process per node
- Variable number of hardware threads
- Overlapping MPI Communication (no SPI!)



- Scaling seems quite linear
- When local volume too small $\rightarrow$ use fewer threads?

Benefits and Overheads

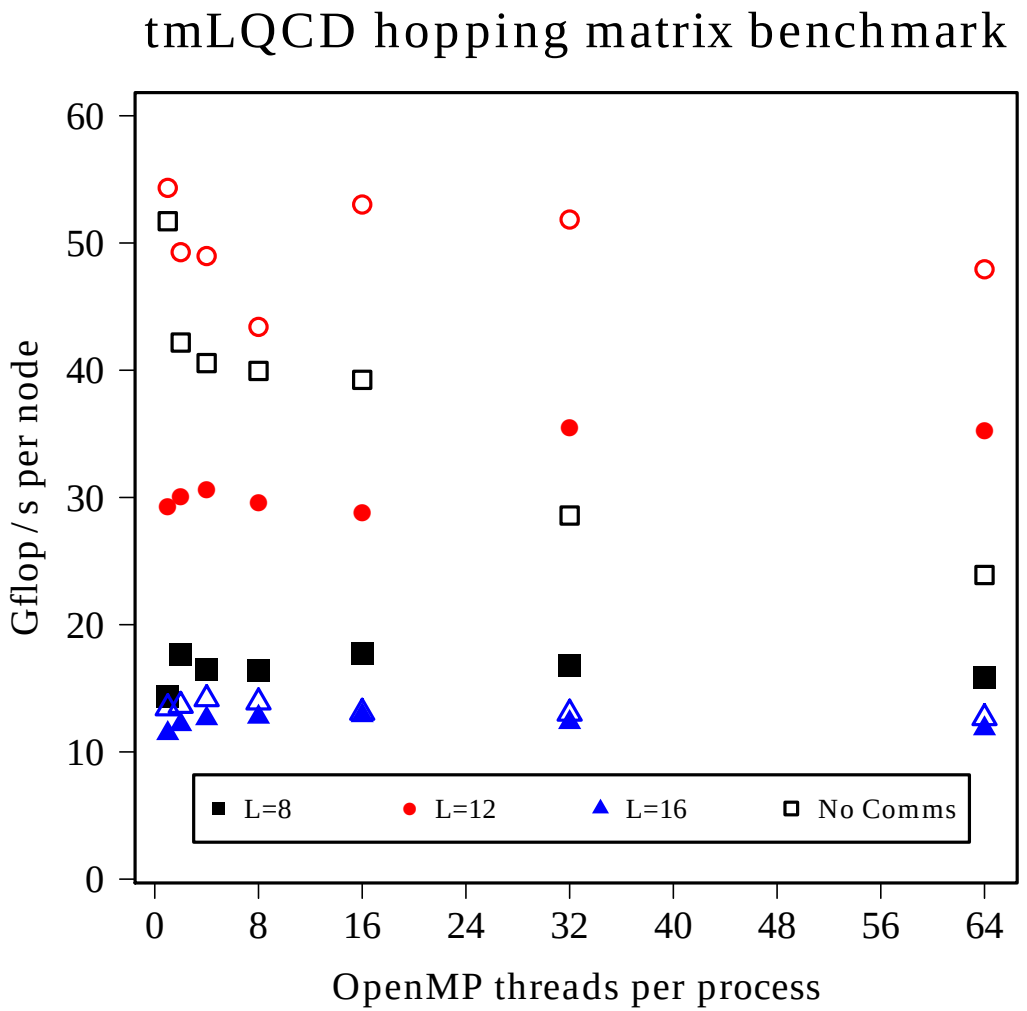
What's the point?

Full oversubscription

- Using maximum number of hardware threads

$\Rightarrow$ $N_{\text{threads}} \times N_{\text{procs}} = 64$

- Overlapping MPI Communication (no SPI!)

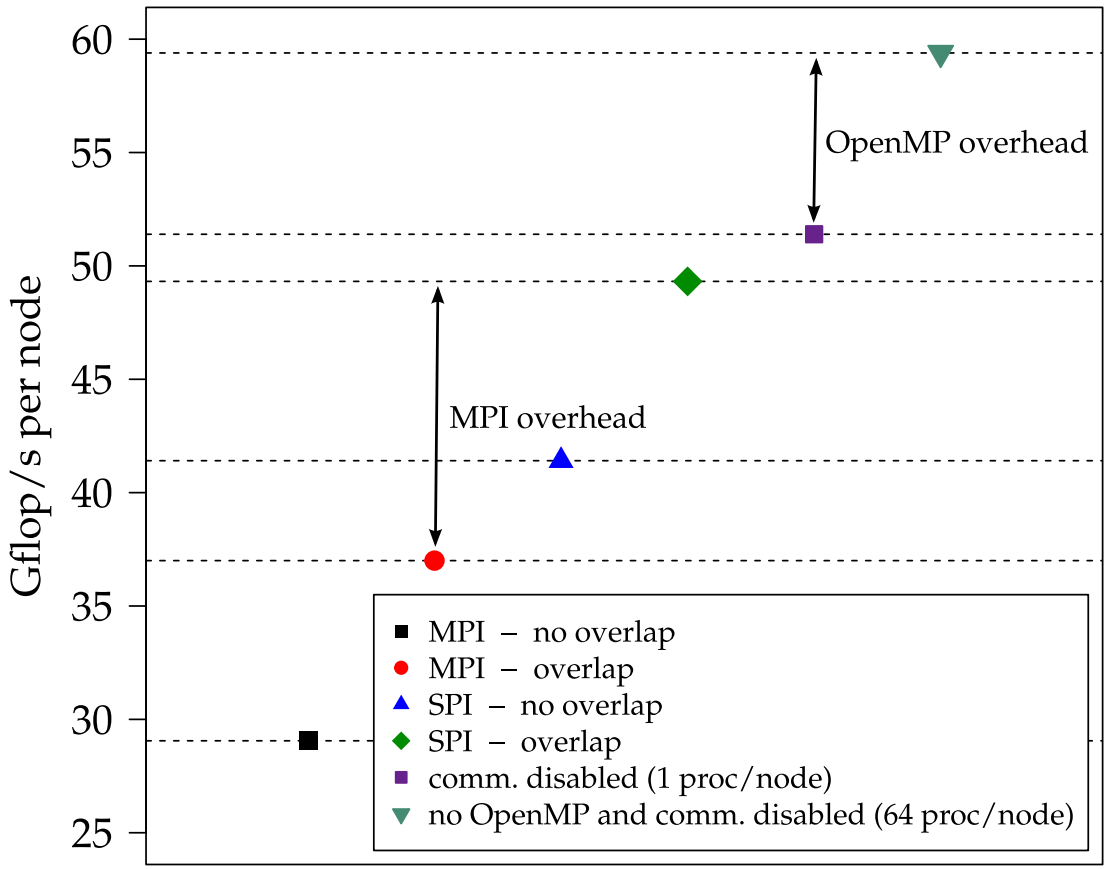


- OpenMP and MPI overheads are comparable on BG/Q
  - Hybrid MPI/OpenMP codes scale to more cores

Benefits and Overheads

Overlapping communication and computation!

- Standard non-blocking `MPI_Isend/recv` usually communicate in `MPI_WaitAll` $\Rightarrow$ effectively blocking
- One-sided MPI communication difficult and a lot of work
  - $\Rightarrow$ Do `MPI_Isend/recv` and `MPI_Waitall` in the same thread!



Improvements

Overhead reduction

Coarsen parallelism - reduce 'parallel' overhead

- employ 'orphaned' directives [a]

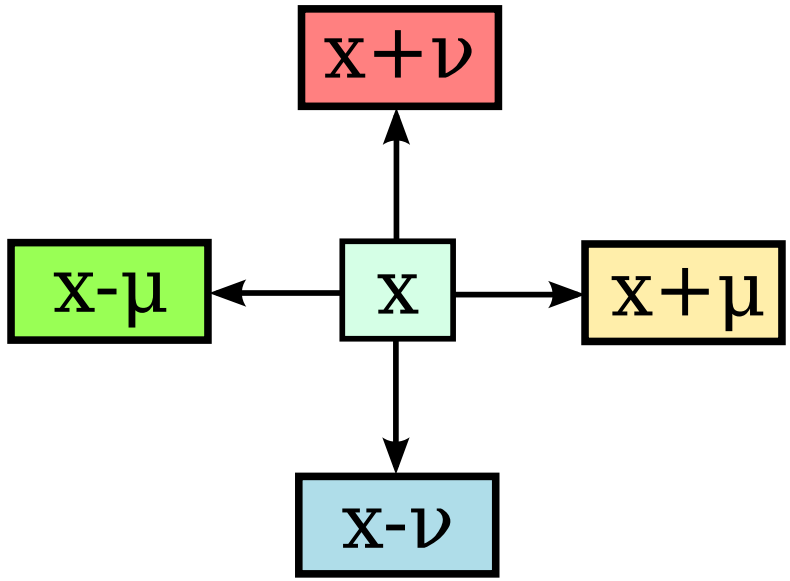
```
void complex_function(output,input) {
  #pragma omp parallel
  {
  operator1(output,input);
  operator2(output,input);
  [...]
  } /* OpenMP parallel section closing brace */
}

void operator1(output,input) {
  #pragma omp for
  for(int x = 0; x < VOLUME; ++x) { [...] }
}
```

[a] thanks to A. Deuzeman for pointing this out

Improvements

Dedicated memory for push algorithms - no locking, no concurrency issues



- \+ No locking overhead or concurrency issues
- \+ 'Obvious' for hopping matrix (half-spinor)
- \+ Keep efficient flop/byte ratio (rather than converting to pull-style)
- – Extra loop to collect the results
- – Higher memory requirements
- – Dedicated function versions and memory layout when using threads

Summary and Concluding Remarks

- Implementing good multi-threaded code is difficult
  - Benchmark and use performance tools
  - Balanced workloads lead to highest performance
  - Exploit scoping rules for maintainability
  - Eliminate false-sharing
  - Fine-tune scheduling
  - Coarse-grained parallelism
  - ...

\+ Pay-offs on CPUs with many cores and efficient threading (BG/Q)

\+ Overlapping communication and computation using usual MPI_Isend/recv

\+ For BG/Q, threading allows very efficient communication with SPI

\– Intel currently lagging behind, overheads LARGE

? Situation on Cray currently unknown

Thank you for your attention!

tmLQCD is an open-source project:
http://github.com/etmc/tmLQCD