

BOLT: Optimizing OpenMP Parallel Regions with User-Level Threads

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OpenMP: the Most Popular Multithreading Model

 Multithreading is essential for exploiting modern CPUs.



- OpenMP is a popular parallel programming model.
 - In the HPC field, OpenMP is most popular for multithreading.
 - 57% of DOE exascale applications use OpenMP [*].
- Not only user programs but also runtimes and libraries are parallelized by OpenMP.

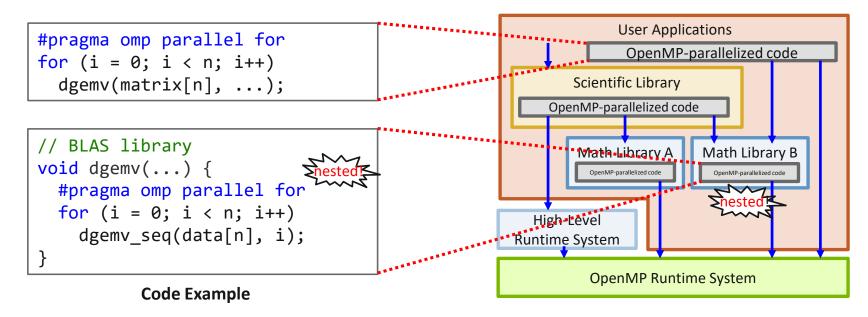
Kokkos, RAJA, OpenBLAS, Intel MKL, SLATE, Intel MKL-DNN, FFTW3, ...

Runtimes that have an OpenMP backend

BLAS/LAPACK libraries

FFTW library

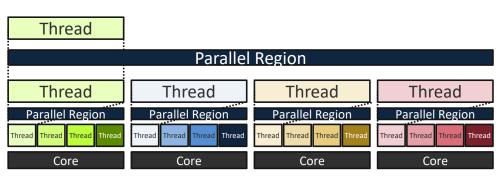
Unintentional Nested OpenMP Parallel Regions



- OpenMP parallelizes multiple software stacks.
- Nested parallel regions create OpenMP threads exponentially.

```
#pragma omp parallel for
for (i = 0; i < n; i++)
  dgemm(matrix[n], ...);

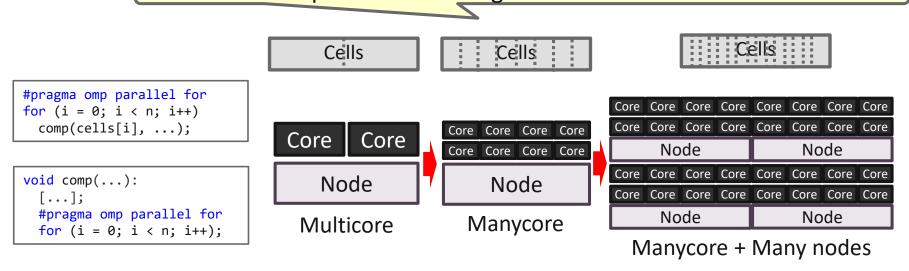
void dgemm(...):
  #pragma omp parallel for
  for (i = 0; i < n; i++);</pre>
```



Can We Just Disable Nested Parallelism?

- How to utilize nested parallel regions?
 - Enable nested parallelism: creation of exponential the number of threads
 - Disable nested parallelism: adversely decrease parallelism
- Example: strong scaling on massively parallel machines

Is the outer parallelism enough to feed work to all the cores???



Two Directions to Address Nested Parallelism

- Nested parallel regions have been known as a problem since OpenMP 1.0 (1997).
 - By default, OpenMP disables nested parallelism^[*].
- Two directions to address this issue:
 - 1. Use several work arounds implied in the OpenMP specification.
 - => Not practical if users do not know parallelism at other software stacks.
 - 2. Instead of OS-level threads, use lightweight threads as OpenMP threads

 User-level threads (ULTs, explained later)
 - => It does not perform well if parallel regions are not nested (i.e., flat).
 - It does not perform well even when parallel regions are nested.
- => Need a solution to efficiently utilize nested parallelism.

BOLT: Lightweight OpenMP over ULT for Both Flat & Nested Parallel Regions

- We proposed BOLT, a ULT-based OpenMP runtime system,
 which performs best for both flat and nested parallel regions.
- Three key contributions:
 - 1. An in-depth performance analysis in the LLVM OpenMP runtime, finding several performance barriers.
 - 2. An implementation of thread-to-CPU binding interface that supports user-level threads.
 - 3. A novel thread coordination algorithm to transparently support both flat and nested parallel regions.

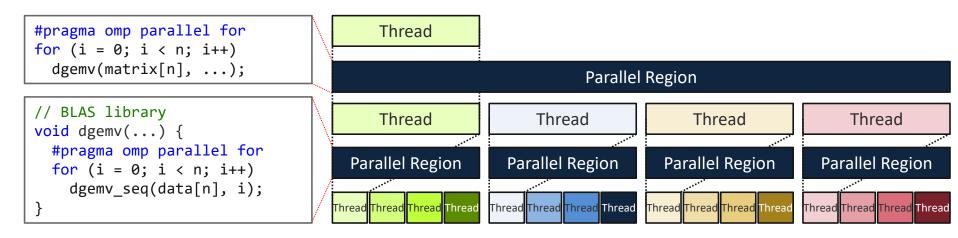
Index

1. Introduction

2. Existing Approaches

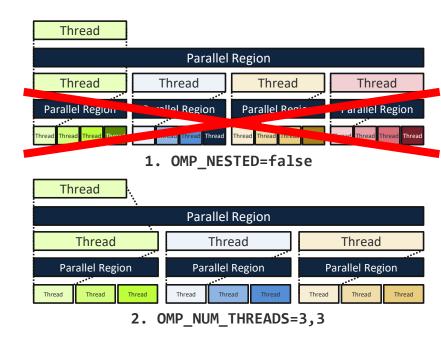
- OS-level thread-based approach
- User-level thread-based approach
 - What is a user-level thread (ULT)?
- 3. BOLT for both Nested and Flat Parallelism
 - Scalability optimizations
 - ULT-aware affinity (proc_bind)
 - Thread coordination (wait_policy)
- 4. Evaluation
- 5. Conclusion

Direction 1: Work around with OS-Level Threads (1/2)



Several workarounds

- Disable nested parallel regions
 (OMP_NESTED=false, OMP_ACTIVE_LEVELS=...)
 - Parallelism is lost.
- Finely tune numbers of threads
 (OMP_NUM_THREADS=nth1,nth2,nth3,...)
 - Parallelism is lost. Difficult to tune parameters.

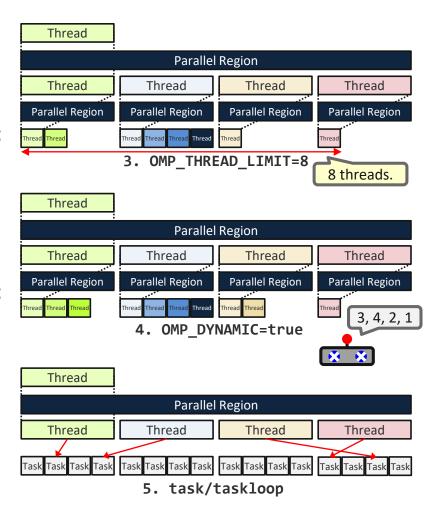


Direction 1: Work around with OS-Level Threads (2/2)

- Workarounds (cont.)
 - 3. Limit the total number of threads (OMP_THREAD_LIMIT=nths)
 - Can adversely serialize parallel regions;
 doesn't work well in practice.
 - Dynamically adjust # of threads (OMP_DYNAMIC=true)
 - Can adversely serialize parallel regions;
 doesn't work well in practice.
 - 5. Use OpenMP task

(#pragma omp task/taskloop)

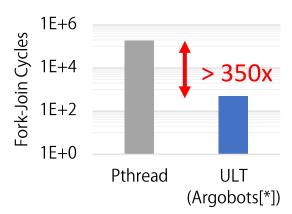
Most codes use parallel regions.
 Semantically, threads != tasks.



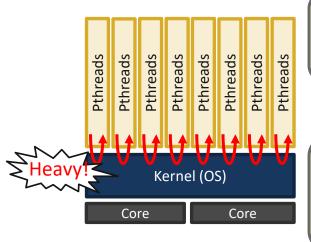
How about using lightweight threads for OpenMP threads?

Direction 2: Use Lightweight Threads => User-Level Threads (ULTs)

- User-level threads: threads implemented in user-space.
 - Manages threads without heavyweight kernel operations.



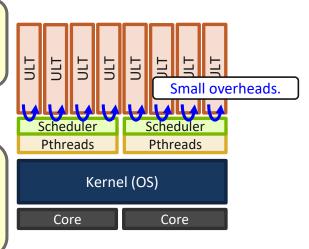
Fork-Join Performance on KNL



Naïve Pthreads

Thread scheduling (= context switching) involves heavy system calls.

User-level threads (ULTs) are running on Pthreads; scheduling is done by user-level context switching in user space.



User-level threads

Solution 2: Use User-Level Threads

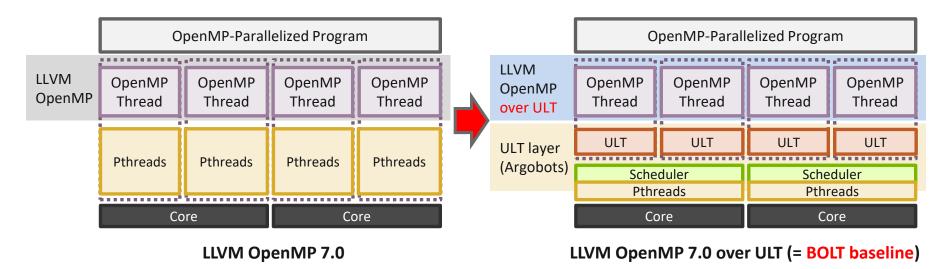
The idea of ULTs is not new (back to <90s).</p>



- and more.
- Several ULT-based OpenMP systems have been proposed.
 - NanosCompiler [1], Omni/ST [2], OMPi [3], MPC [4], ForestGOMP [5],
 OmpSs (OpenMP compatible mode) [6], LibKOMP [7] ...
 - [1] Marc et al., NanosCompiler: Supporting Flexible Multilevel Parallelism Exploitation in OpenMP. 2000
 - [2] Tanaka et al., Performance Evaluation of OpenMP Applications with Nested Parallelism. 2000
 - [3] Hadjidoukas et al., Support and Efficiency of Nested Parallelism in OpenMP Implementations. 2008
 - [4] Pérache et al., MPC: A Unified Parallel Runtime for Clusters of NUMA Machines. 2008
 - [5] Broquedis et al., ForestGOMP: An Efficient OpenMP Environment for NUMA Architectures. 2010
 - [6] Duran et al., A Proposal for Programming Heterogeneous Multi-Core Architectures. 2011
 - [7] Broquedis et al., libKOMP, an Efficient OpenMP Runtime System for Both Fork-Join and Data Flow Paradigms. 2012
- However, these runtimes do not perform well for several reasons.
 - Lack of OpenMP specification-aware optimizations
 - Lack of general optimizations

For apples-to-apples comparison, we will focus on the ULT-based LLVM OpenMP.

Using ULTs is Easy



- Replacing a Pthreads layer with a user-level threading library is a piece of cake.
 - Argobots^[*] we used in this paper has the Pthreads-like API
 (mutex, TLS, ...), making this process easier.

 Note: other ULT libraries (e.g., Qthreads, Nanos++, MassiveThreads ...) also have similar threading APIs.
 - The ULT-based OpenMP implementation is OpenMP 4.5-compliant (as far as we examined)
- Does the "baseline BOLT" perform well?

Simple Replacement Performs Poorly

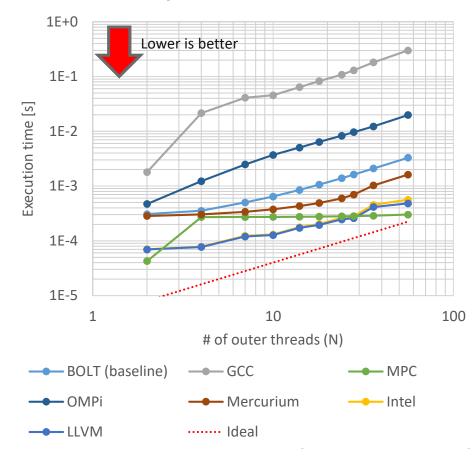
```
// Run on a 56-core Skylake server
#pragma omp parallel for num_threads(N)
for (int i = 0; i < N; i++)
    #pragma omp parallel for num_threads(28)
    for (int j = 0; j < 28; j++)
        comp_20000_cycles(i, j);</pre>
```

Nested Parallel Region (balanced)

- Faster than GNU OpenMP.
 - GCC
- So-so among ULT-based OpenMPs
 - MPC, OMPi, Mercurium
- Slower than Intel/LLVM OpenMPs.
 - Intel, LLVM

Popular Pthreads-based OpenMP

State-of-the-art ULT-based OpenMP



GCC: GNU OpenMP with GCC 8.1
Intel: Intel OpenMP with ICC 17.2.174
LLVM: LLVM OpenMP with LLVM/Clang 7.0

MPC: MPC 3.3.0

OMPi: OMPi 1.2.3 and psthreads 1.0.4

Mercurium: OmpSs (OpenMP 3.1 compat) 2.1.0 + Nanos++ 0.14.1

Index

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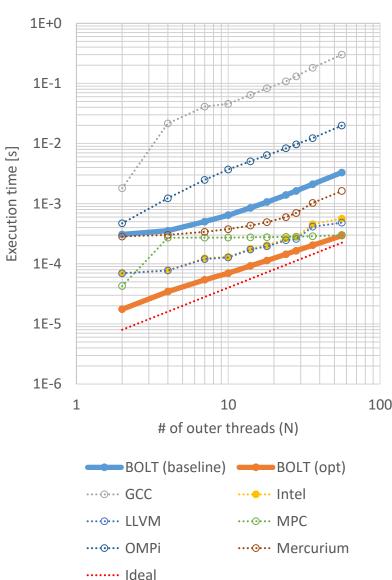
Three Optimization Directions for Further Performance

```
// Run on a 56-core Skylake server
#pragma omp parallel for num_threads(N)
for (int i = 0; i < N; i++)
    #pragma omp parallel for num_threads(28)
    for (int j = 0; j < 28; j++)
        comp_20000_cycles(i, j);</pre>
```

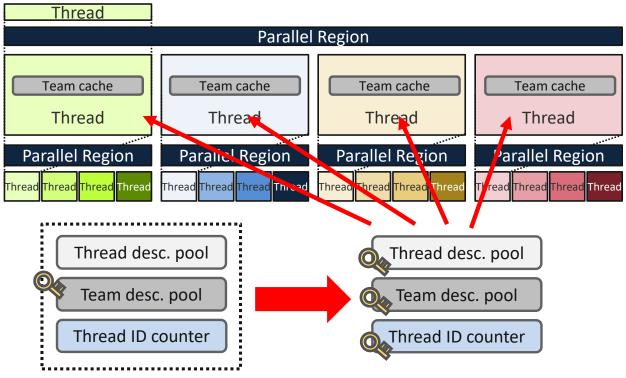
Nested Parallel Region (balanced)

The naïve replacement (BOLT (baseline))
 does not perform well.

- Need advanced optimizations
 - 1. Solving scalability bottlenecks
 - 2. ULT-friendly affinity
 - 3. Efficient thread coordination



1. Solve Scalability Bottlenecks (1/2)

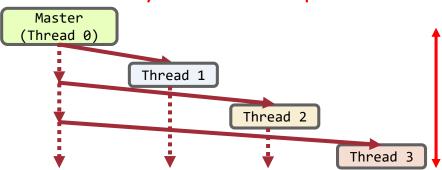


- Resource management optimizations
 - 1. Divides a large critical section protecting all threading resources.
 - This cost is negligible with Pthreads.
 - 2. Enable multi-level caching of parallel regions
 - Called "nested hot teams" in LLVM OpenMP.

1. Solve Scalability Bottlenecks (2/2)

Thread creation optimizations

Binary creation of OpenMP threads.

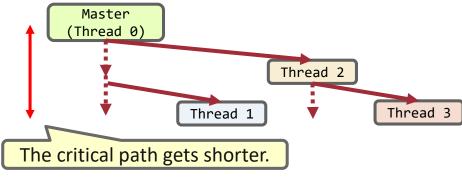


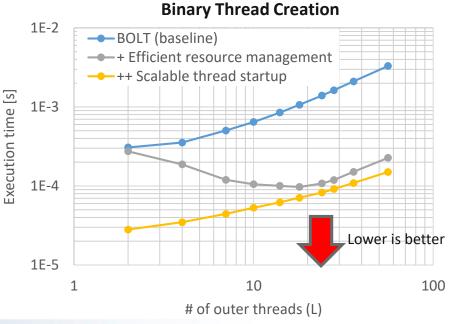
Serial Thread Creation (default LLVM OpenMP)

```
// Run on a 56-core Skylake server
#pragma omp parallel for num_threads(L)
for (int i = 0; i < L; i++)
    #pragma omp parallel for num_threads(56)
    for (int j = 0; j < 56; j++)
        no_comp();</pre>
```

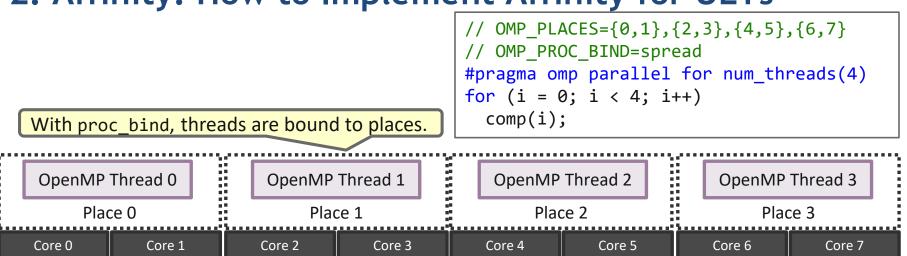
Nested Parallel Regions (no computation)

No computation to measure the pure overheads.





2. Affinity: How to Implement Affinity for ULTs

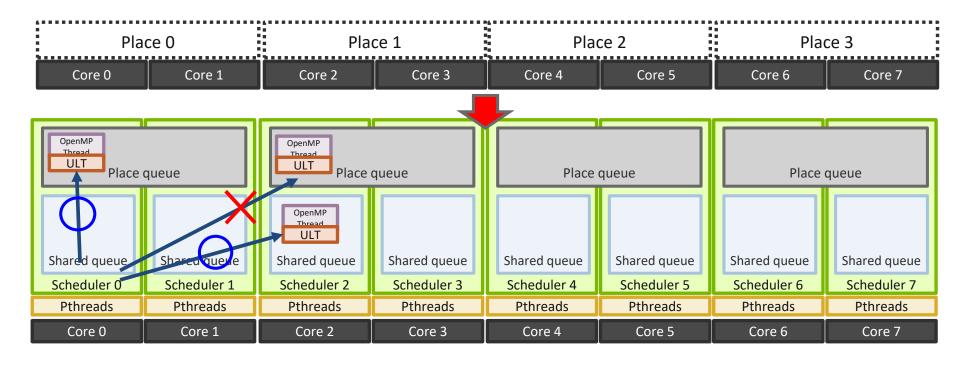


- OpenMP 4.0 introduced place and prod_bind for affinity.
 - OS-level thread-based libraries (e.g., GNU OpenMP) use CPU masks.
- BOLT (baseline) ignored affinity (still standard compliant).
- However, affinity should be useful to
 - 1. improve locality and 2. reduce queue contentions.
 - Note: ULT runtimes use shared queues + random work stealing.
- How to implement place over ULTs?

Implementation: Place Queue

Place queues can implement
 OpenMP affinity in BOLT.

```
// OMP_PLACES={0,1},{2,3},{4,5},{6,7}
// OMP_PROC_BIND=spread
#pragma omp parallel for num_threads(4)
for (i = 0; i < 4; i++)
   comp(i);</pre>
```



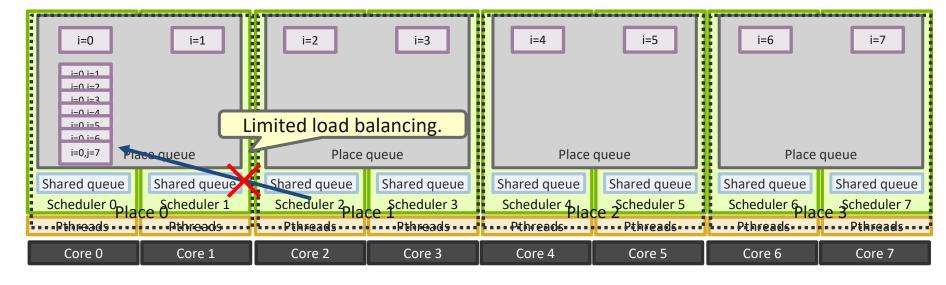
Problem: OpenMP affinity setting is too deterministic.

OpenMP Affinity is Too Deterministic

 Affinity (or bind-var) is once set, all the OpenMP threads created in the descendant parallel regions are bound to places.

```
// OMP_PLACES={0,1},{2,3},{4,5},{6,7}
// OMP_PROC_BIND=spread
#pragma omp parallel for num_threads(8)
for (int i = 0; i < 8; i++)
    #pragma omp parallel for num_threads(8)
    for (int j = 0; j < 8; j++)
        comp(i, j);</pre>
```

The OpenMP specification writes so.



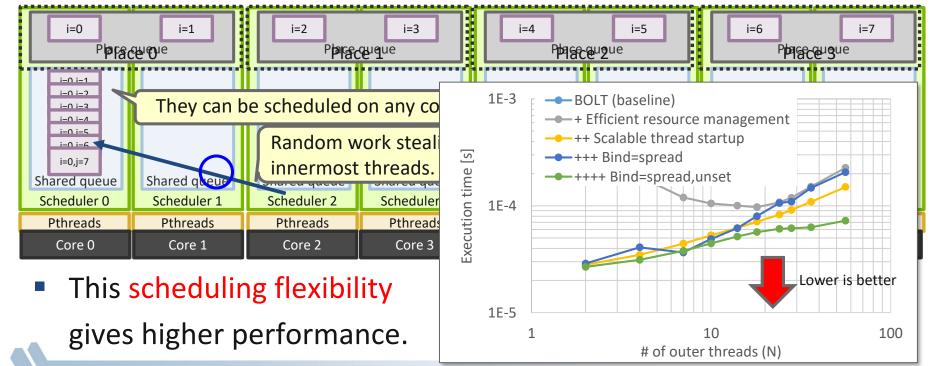
 Promising direction: scheduling innermost threads with unbound random work stealing.

Proposed New PROC_BIND: "unset"

OMP_WAIT_POLICY=unset: reset the affinity setting of the specified parallel region.

(Detailed: The unset thread affinity policy resets the bind-var ICV and the place-partition-var ICV to their implementation defined values and instructs the execution environment to follow these values.)

```
// OMP_PLACES={0,1},{2,3},{4,5},{6,7}
// OMP_PROC_BIND=spread
#pragma omp parallel for num_threads(8)
for (int i = 0; i < 8; i++)
    #pragma omp parallel for num_threads(8)
    for (int j = 0; j < 8; j++)
        comp(i, j);</pre>
// OMP_PLACES={0,1},{2,3},{4,5},{6,7}
// OMP_PROC_BIND=spread,unset
#pragma omp parallel for num_threads(8)
for (int i = 0; i < 8; i++)
    #pragma omp parallel for num_threads(8)
    for (int j = 0; j < 8; j++)
        comp(i, j);
```

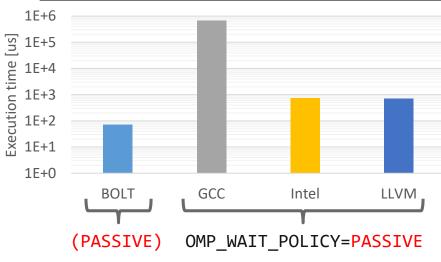


3. Flat Parallelism: Poor Performance

BOLT should perform as good as the original LLVM OpenMP.

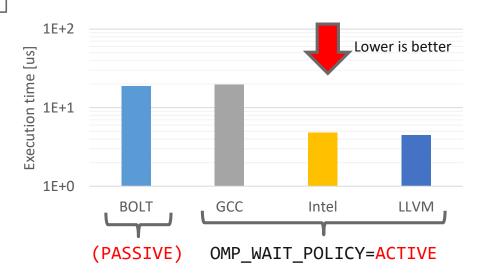
Nested Parallel Regions (no computation)

```
#pragma omp parallel for num_threads(56)
for (int i = 0; i < 56; i++)
   #pragma omp parallel for num_threads(56)
   for (int j = 0; j < 56; j++) no_comp(i, j);</pre>
```



Flat Parallel Region (no computation)

```
#pragma omp parallel for num_threads(56)
for (int i = 0; i < 56; i++)
  no_comp(i);</pre>
```

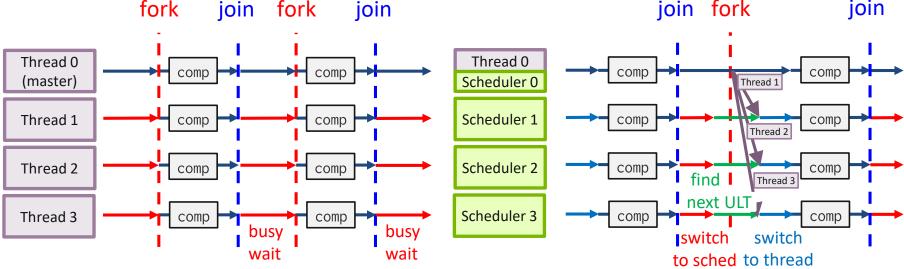


 Optimal OMP_WAIT_POLICY for GCC/Intel/LLVM improves performance of flat parallelism.

Active Waiting Policy for Flat Parallelism

```
for (int iter = 0; iter < n; iter++) {
    #pragma omp parallel for num_threads(4)
    for (int i = 0; i < 4; i++)
        comp(i);
}</pre>
```

- Active waiting policy improves performance of flat parallelism by busy-wait based synchronization.
- If active, Pthreads-based OpenMP
 busy-waits for the next parallel region.
- BOLT on the other hand yields to a scheduler on fork-and-join (~ passive).

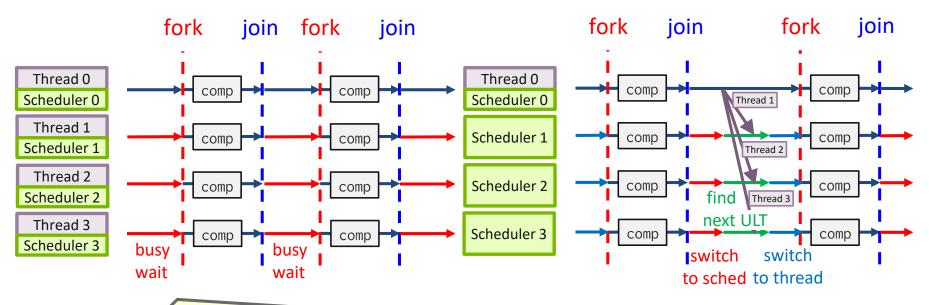


* If passive, after completion of work, threads sleep on a condition variable.

Busy wait is faster than lightweight user-level context switch!

Implementation of Active Policy in BOLT

- If active, busy-waits for next parallel regions.
- If passive, relies on ULT context switching.

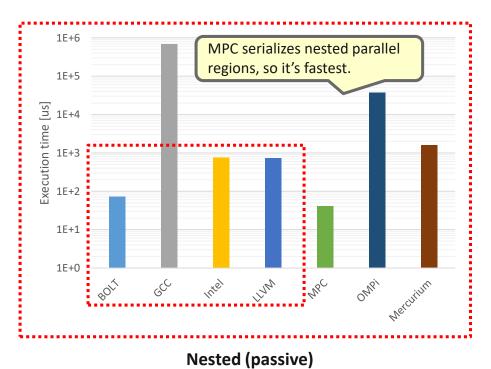


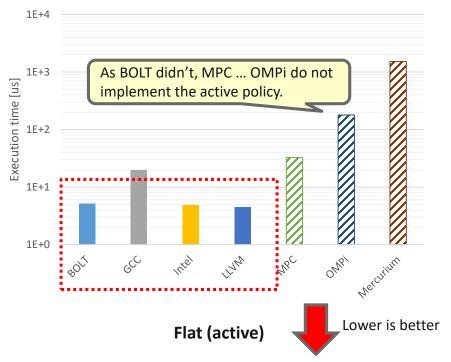
ULT threads are not preemptive, so BOLT periodically yields to a scheduler in order to avoid the deadlock (especially when # of OpenMP threads > # of schedulers).

Performance of Flat and Nested

```
#pragma omp parallel for num_threads(56)
for (int i = 0; i < 56; i++)
   #pragma omp parallel for num_threads(56)
   for (int j = 0; j < 56; j++) no_comp(i, j);</pre>
```

```
#pragma omp parallel for num_threads(56)
for (int i = 0; i < 56; i++)
  no_comp(i);</pre>
```

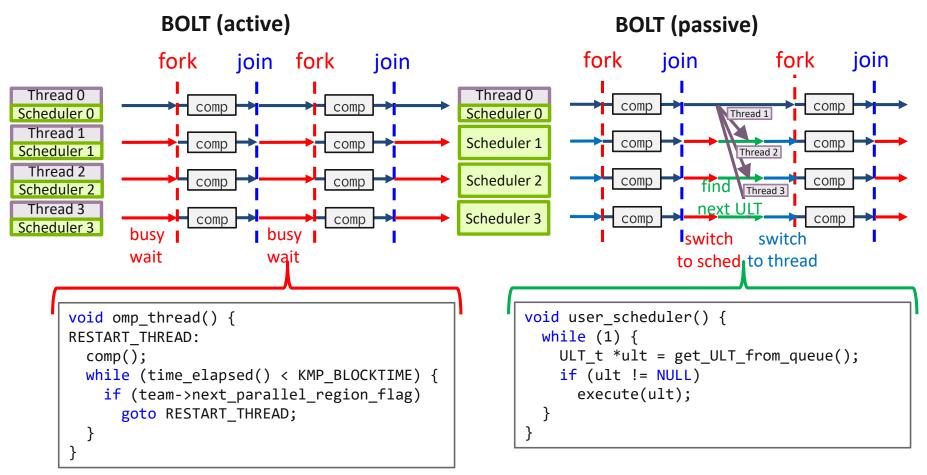




Penalty of the Opposite Wait Policy Lower is better ~650,000 150 1E+4 60 Excution time [us] Execution time [us] 1E+3 23x 1E+2 1E+1 1E+0 **BOLT** GCC **LLVM BOLT** GCC Intel Intel **LLVM** Flat ■ active ■ passive ■ active ■ passive **Nested** #pragma omp parallel for num threads(56) #pragma omp parallel for num threads(56) for (int i = 0; i < 56; i++) for (int i = 0; i < 56; i++) #pragma omp parallel for num threads(56) no comp(i); for (int j = 0; j < 56; j++) no comp(i, j);

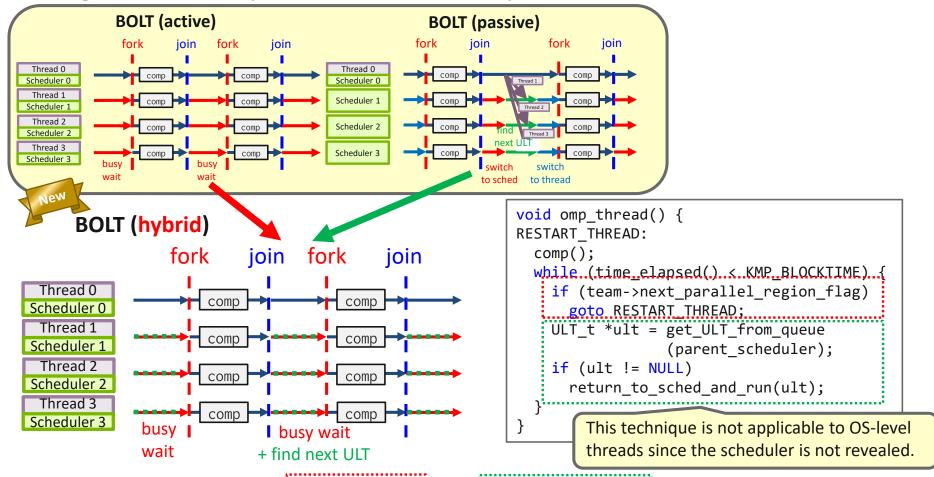
- How to coordinate threads significantly affects the overheads.
 - Large performance penalty discourages users from enabling nesting.
- Is there a good algorithm to transparently support both flat and nested parallelism?

Busy Waiting in Both Active/Passive Algorithms



- Though in both active and passive cases, they enter busywaits after the completion of threads.
 - Can we merge it to perform both scheduling and flag checking?

Algorithm: Hybrid Wait Policy



- Hybrid: execute flag check and queue check alternately.
 - [flat]: a thread does not go back to a scheduler.
 - [nested]: another available ULT is promptly scheduled.

Performance of Hybrid: Flat and Nested Lower is better ~650,000 150 1E+4 60 Execution time [us] 1E+3 1E+2 1E+1

LLVM

Flat

1E+0

BOLT

```
#pragma omp parallel for num_threads(56)
for (int i = 0; i < 56; i++)
  #pragma omp parallel for num threads(56)
  for (int j = 0; j < 56; j++) no_comp(i, j);</pre>
```

■ active ■ passive ■ hybrid

GCC

BOLT

Excution time [us]

BOLT (hybrid wait polocy) is always most efficient in both flat and nested cases.

Intel

 We suggest a new keyword "auto" so that the runtime can choose the implementation.

```
#pragma omp parallel for num threads(56)
for (int i = 0; i < 56; i++)
 no comp(i);
```

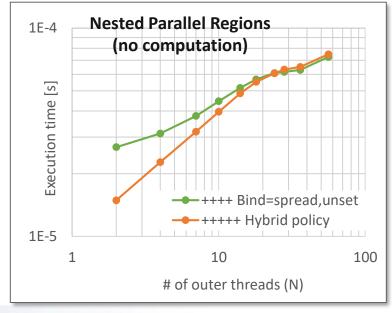
Intel

LLVM

Nested

GCC

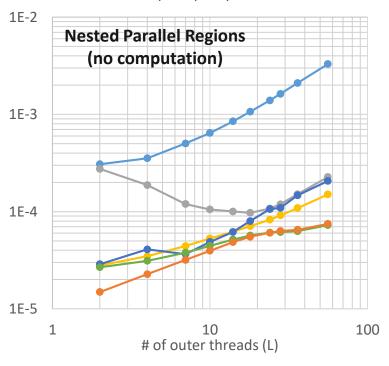
■ active ■ passive ■ hybrid



Summary of the Design

- Just using ULT is insufficient.
 - => Three kinds of optimizations:
 - 1. Address scalability bottlenecks
 - 2. ULT-friendly affinity
 - 3. Hybrid wait policy for flat and nested parallelisms
- Our work solely focuses on OpenMP,
 while some of our techniques are generic:
 - Place queues for affinity of ULTs
 - Hybrid thread coordination for runtimes that have parallel loop abstraction.

```
// Run on a 56-core Skylake server
#pragma omp parallel for num_threads(L)
for (int i = 0; i < L; i++)
    #pragma omp parallel for num_threads(56)
    for (int j = 0; j < 56; j++)
        no_comp();</pre>
```

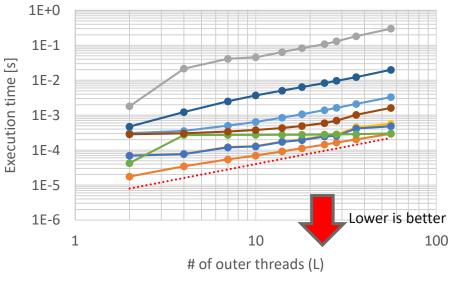


Index

- 1. Introduction
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Microbenchmarks

```
// Run on a 56-core Skylake server
#pragma omp parallel for num_threads(L)
for (int i = 0; i < L; i++) {
    #pragma omp parallel for num_thLreads(28)
    for (int j = 0; j < 28; j++)
        comp_20000_cycles(i, j);
}</pre>
```



─ GCC

─ MPC

······ Ideal

BOLT (baseline) BOLT (opt)

--- Intel

─ OMPi

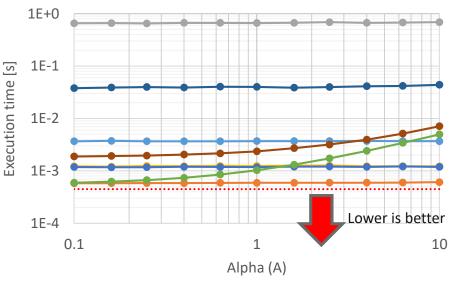
--- LLVM

--- Mercurium

```
alpha makes the computation size random, while keeping the total problem size.
```

Large alpha

```
// Run on a 56-core Skylake server
#pragma omp parallel for num_threads(56)
for (int i = 0; i < 56; i++) {
  int work_cycles = get_work(i, alpha);
  #pragma omp parallel for num_threads(56)
  for (int j = 0; j < 56; j++)
    comp_cycles(i, j, work_cycles);}</pre>
```

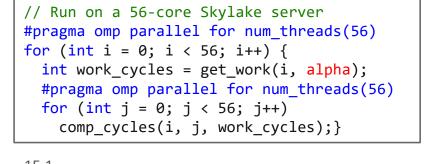


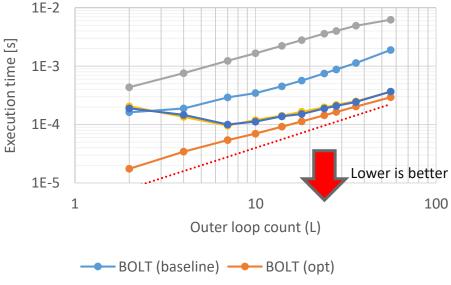
```
→ BOLT (baseline) → BOLT (opt) → GCC
→ Intel → LLVM → MPC
→ OMPi → Mercurium Ideal
```

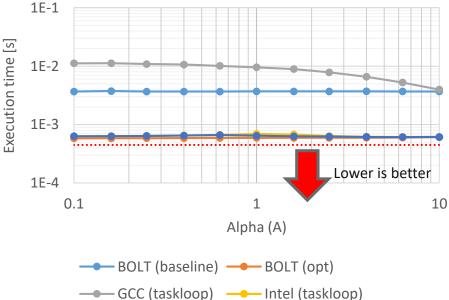
(Ideal): theoretical lower bound under perfect scalability.

Microbenchmarks: vs. taskloop

```
// Run on a 56-core Skylake server
#pragma omp parallel for num_threads(56)
for (int i = 0; i < L; i++) {
    #pragma omp taskloop grainsize(1)
    for (int j = 0; j < 28; j++)
        comp_20000_cycles(i, j);
}</pre>
```







```
BOLT (baseline) BOLT (opt)
GCC (taskloop) Intel (taskloop)
LLVM (taskloop) Ideal
```

LLVM (taskloop) ······· Ideal

Parallel regions of BOLT are as fast as taskloop!

Evaluation: Use Case of Nested Parallel Regions

- The number of threads for outer loops is usually set to # of cores.
 - i.e., if not nested, oversubscription does not happen.
- However, many layers are
 OpenMP parallelized, which can unintentionally result in nesting.

OpenMP-parallelized code

Scientific Library
OpenMP-parallelized code

Math Library A

Math Library B

OpenMP-parallelized code

High-Level
Runtime System

OpenMP Runtime System

:Function call

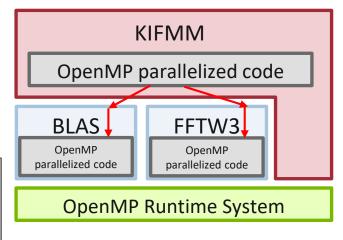
We will show two examples.

Evaluation 1: KIFMM

- KIFMM^[*]: highly optimized N-body solver
 - N-body solver is one of the heaviest kernels in astronomy simulations.
- Multiple layers are parallelized by OpenMP.
 - BLAS and FFT.
- We focus on the upward phase in KIFMM.

```
for (int i = 0; i < max_levels; i++)
  #pragma omp parallel for
  for (int j = 0; j < nodecounts[i]; j++) {
    [...];
    dgemv(...); // dgemv() creates a parallel region.
}</pre>
```

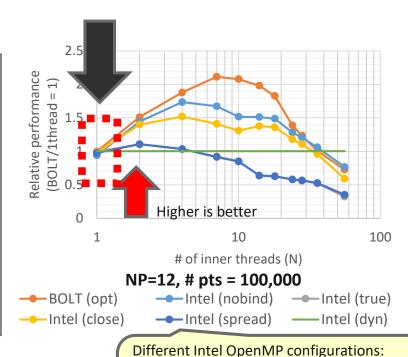




Performance: KIFMM

```
void kifmm_upward():
    for (int i = 0; i < max_levels; i++)
        #pragma omp parallel for num_threads(56)
        for (int j = 0; j < nodecounts[i]; j++) {
            [...];
            dgemv(...); // creates a parallel region.
        }

void dgemv(...): // in MKL
    #pragma omp parallel for num_threads(N)
    for (int i = 0; i < [...]; i++)
        dgemv_sequential(...);</pre>
```



dyn: MKL DYNAMIC=true

(see the paper).

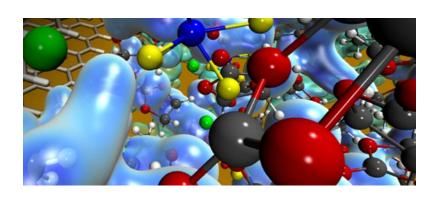
nobind(=false),true,close,spread: proc bind

Note that other parameters are hand tuned

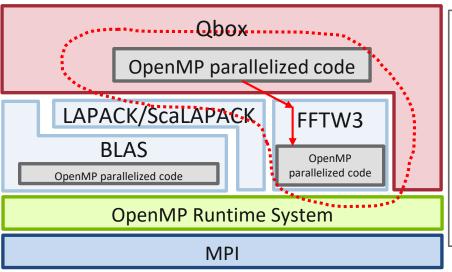
- Experiments on Skylake 56 cores.
 - # of threads for the outer parallel region = 56
 - # of threads for the inner parallel region = N (changed)
- Two important results:
 - N=1 (flat): performance is almost the same.
 - N>1 (nested): BOLT further boosts performance.

Evaluation 2: FFT in QBox

 Qbox^[*]: first-principles molecular dynamics code.



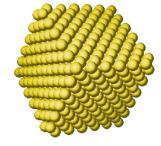
We focus on the FFT computation part.



```
// FFT backward
#pragma omp parallel for
for (int i = 0; i < num / nprocs; i++)
  fftw_execute(plan_2d, ...);

void fftw_execute(...): // in FFTW3
  [...];
  #pragma omp parallel for num_threads(N)
  for (int i = 0; i < [...]; i++)
    fftw_sequential(...);</pre>
```

 We extracted this FFT kernel and change the parameters based on the gold benchmark.



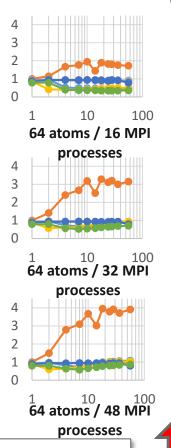
Performance: FFTW3

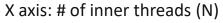
```
// FFT backward
#pragma omp parallel for
for (int i = 0; i < num / nprocs; i++)
  fftw_execute(plan_2d, ...);

void fftw_execute(...): // in FFTW3
  [...];
  #pragma omp parallel for num_threads(N)
  for (int i = 0; i < [...]; i++)
    fftw_sequential(...);</pre>
```

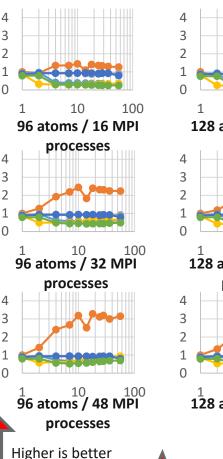
- → BOLT (opt) → Intel (nobind) → Intel (true)

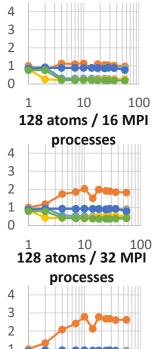
 → Intel (close) → Intel (spread) → Intel (dyn)
- Intel OpenMP configurations: nobind(=false),true,close,spread: proc bind, dyn: OMP DYNAMIC=true
 - nprocs = # of MPI nodes
 - num (and fftw size) is proportional to # of atoms.





Y axis: relative performance (BOLT + N=1: 1.0)







Experiments on KNL 7230 64 cores.

of threads for the outer parallel region = 64 # of threads for the inner parallel region = N (changed)

- N=1 (flat): performance is almost the same.
- N>1 (nested): BOLT further increased performance.

More beneficial for nested parallel regions.

symmetric parallel regions.

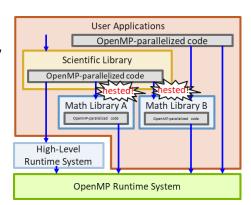
symmetric parallel regions.

Index

- 1. Introduction
- 2. Existing Approaches
 - OS-level thread-based approach
 - User-level thread-based approach
 - What is a user-level thread (ULT)?
- 3. BOLT for both Nested and Flat Parallelism
 - Scalability optimizations
 - ULT-aware affinity (proc_bind)
 - Thread coordination (wait_policy)
- 4. Evaluation
- 5. Conclusion

Summary of this Talk

- Nested OpenMP parallel regions are commonly seen in complicated software stacks.
 - => Demand for efficient OpenMP runtimes to exploit both flat and nested parallelism.



- BOLT: an lightweight OpenMP library over ULT.
 - Simply using ULTs is insufficient:
 - Solve scalability bottlenecks in the LLVM OpenMP runtime
 - ULT-friendly affinity implementation
 - Hybrid thread coordination technique to transparently support both flat and nested parallel regions.
- BOLT achieves unprecedented performance for nested parallel regions without hurting the performance of flat parallelism.

Thank you for listening!

- BOLT: http://www.bolt-omp.org
- Q&A (as a software):
 - What is the goal of the BOLT project?
 - Improve OpenMP by ULTs:
 - 1. enrich OpenMP tasking features with least overheads,
 - 2. minimizing overheads of OpenMP threads, and 3. more.
 - How to use it?
 - BOLT is a runtime library: no special compiler is required. GCC/ICC/Clang + LD LIBRARY PATH+=\${BOLT INSTALL PATH} works.
 - Is BOLT stable?

Much engineering efforts for ABI compatibility and stability.

- Regularly checked with LLVM OpenMP tests (GCC 8.x, ICC 19.x, and Clang 10.x)
- What OpenMP features are supported?

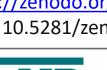
 OpenMP 4.5 including task, task depend, and offloading.

Future work:

- Enhance task scheduling
- MPI+OpenMP interoperability

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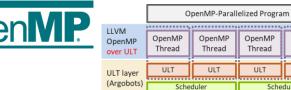
BOLT is part of the ECP SOLLVE project: https://www.bnl.gov/compsci/projects/SOLLVE/



Artifact:



(DOI: 10.5281/zenodo.3372716)



Thread