Many-core Programming with OpenMP* 4.x

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Notice revision #20110804
Outline

• Very brief Introduction to OpenMP
• OpenMP for Many-core Processors
• OpenMP SIMD Constructs
• Task-generating loops
• Affinity Control
Brief Introduction to OpenMP
OpenMP API

- De-facto standard, OpenMP 4.0 out since July 2013
- API for C/C++ and Fortran for shared-memory parallel programming
- Based on directives (pragmas in C/C++)
- Portable across vendors and platforms
- Supports various types of parallelism
OpenMP History

1997
- In spring, 7 vendors and the DOE agree on the spelling of parallel loops and form the OpenMP ARB. By October, version 1.0 of the OpenMP specification for Fortran is released.

1998
- First hybrid applications with MPI* and OpenMP appear.

1999
- cOMPurity, the group of OpenMP users, is formed and organizes workshops on OpenMP in North America, Europe, and Asia.

2000
- Minor modifications.

2001
- The merge of Fortran and C/C+ specifications begins.

2002
- Unified Fortran and C/C++: Bigger than both individual specifications combined. The first International Workshop on OpenMP is held. It becomes a major forum for users to interact with vendor.

2003
- Incorporates task parallelism. A hard problem as OpenMP struggles to maintain its thread-based nature, while accommodating the dynamic nature of tasking.

2004
- Support min/max reductions in C/C++.

2005
- Incorporates task parallelism. A hard problem as OpenMP struggles to maintain its thread-based nature, while accommodating the dynamic nature of tasking.

2006
- Incorporates task parallelism. A hard problem as OpenMP struggles to maintain its thread-based nature, while accommodating the dynamic nature of tasking.

2007
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2010
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2011
- Incorporates task parallelism. A hard problem as OpenMP struggles to maintain its thread-based nature, while accommodating the dynamic nature of tasking.

2012
- Incorporates task parallelism. A hard problem as OpenMP struggles to maintain its thread-based nature, while accommodating the dynamic nature of tasking.

2013
- Incorporates task parallelism. A hard problem as OpenMP struggles to maintain its thread-based nature, while accommodating the dynamic nature of tasking.

2014
- Incorporates task parallelism. A hard problem as OpenMP struggles to maintain its thread-based nature, while accommodating the dynamic nature of tasking.

2015
- Incorporates task parallelism. A hard problem as OpenMP struggles to maintain its thread-based nature, while accommodating the dynamic nature of tasking.

2016
- Incorporates task parallelism. A hard problem as OpenMP struggles to maintain its thread-based nature, while accommodating the dynamic nature of tasking.

2017
- Incorporates task parallelism. A hard problem as OpenMP struggles to maintain its thread-based nature, while accommodating the dynamic nature of tasking.

SOFTWARE AND SERVICES
- Permanent ARB
- Auxiliary ARB

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## OpenMP Platform Features

<table>
<thead>
<tr>
<th>Feature</th>
<th>Description</th>
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</thead>
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<td>Cluster</td>
<td>Group of computers communicating through fast interconnect</td>
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<tr>
<td>Coprocessors/Accelera</td>
<td>Special compute devices attached to the local node through special interconnect</td>
</tr>
<tr>
<td>Node</td>
<td>Group of processors communicating through shared memory</td>
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<td>Socket</td>
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<td>Core</td>
<td>Group of functional units communicating through registers</td>
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<td>Sequence of instructions sharing functional units</td>
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<tr>
<td>Vector</td>
<td>Single instruction using multiple functional units</td>
</tr>
</tbody>
</table>
OpenMP 3.0 in Three Slides

```c
#pragma omp parallel
{
    #pragma omp for
    for (i = 0; i<N; i++)
    {...}

    #pragma omp for
    for (i = 0; i<N; i++)
    {...}
}
```

SOFTWARE AND SERVICES
OpenMP 3.0 in Three Slides /2

double a[N];
double l,s = 0;
#pragma omp parallel for reduction(+:s) private(l) \ 
schedule(static,4)
for (i = 0; i<N; i++)
{
    l = log(a[i]);
    s += l;
}

SOFTWARE AND SERVICES
OpenMP 3.0 in Three Slides /3

```c
#pragma omp parallel
#pragma omp single
for(e = l->first; e; e = e->next)
    #pragma omp task
    process(e);
```

fork

join
OpenMP for Many-core Processors
Intel Xeon Phi Tile Architecture

x4 DMI2 to PCH
36 Lanes PCIe* Gen3 (x16, x16, x4)

MCDRAM

DDR4

MCDRAM

MCDRAM

Thr. 0  Thr. 1  Thr. 2  Thr. 3

2VPU  HUB  1MB  L2  2VPU

Core

Core

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SIMD on Intel® Architecture

SSE
- 128 bit
- 2 x DP
- 4 x SP

AVX
- 256 bit
- 4 x DP
- 8 x SP

AVX-512
- 512 bit
- 8 x DP
- 16 x SP
Good News and Bad News!

- **Goods news are:**
  - OpenMP has already everything you need to get to good many-core performance
  - You can combine individual OpenMP features to match your code with the underlying hardware structure

- **Bad news are:**
  - Simplistically adding pragmas to loops does no longer cut it!
  - You need to think about parallelism at much higher levels
  - My above statement was a bit of a lie...
    - Memory allocation still missing from OpenMP
    - Still requires use of non-OpenMP APIs
OpenMP SIMD Constructs
Why Auto-vectorizers Fail

- Data dependencies
- Other potential reasons
  - Alignment
  - Function calls in loop block
  - Complex control flow / conditional branches
  - Loop not “countable”
    - E.g. upper bound not a runtime constant
  - Mixed data types
  - Non-unit stride between elements
  - Loop body too complex (register pressure)
  - Vectorization seems inefficient
- Many more ... but less likely to occur
Data Dependencies

• Suppose two statements S1 and S2
• S2 depends on S1, iff S1 must execute before S2
  • Control-flow dependence
  • Data dependence
  • Dependencies can be carried over between loop iterations

• Important flavors of data dependencies

FLOW
s1: \(a = 40\)

\[b = 21\]

s2: \(c = a + 2\)

ANTI

\(b = 40\)

s1: \(a = b + 1\)

\(s2: b = 21\)
Loop-Carried Dependencies

- Dependencies may occur across loop iterations
  - Loop-carried dependency
- The following code contains such a dependency:

```c
void lcd_ex(float* a, float* b, size_t n, float c1, float c2) {
    size_t i;
    for (i = 0; i < n; i++) {
        a[i] = c1 * a[i + 17] + c2 * b[i];
    }
}
```

- Some iterations of the loop have to complete before the next iteration can run
  - Simple trick: Can you reverse the loop w/o getting wrong results?
Loop-Carried Dependencies

- Can we parallelize or vectorize the loop?
  - Parallelization: no (except for very specific loop schedules)
  - Vectorization: yes (if vector length is shorter than any distance of any dependency)
Example: Loop not Countable

• “Loop not Countable” plus “Assumed Dependencies”

```c
typedef struct {
    float* data;
    size_t size;
} vec_t;

void vec_eltwise_product(vec_t* a, vec_t* b, vec_t* c) {
    size_t i;
    for (i = 0; i < a->size; i++) {
        c->data[i] = a->data[i] * b->data[i];
    }
}
```
In a Time before OpenMP 4.0

• Programmers had to rely on auto-vectorization...
• ... or to use vendor-specific extensions
  • Programming models (e.g., Intel® Cilk™ Plus)
  • Compiler pragmas (e.g., #pragma vector)
  • Low-level constructs (e.g., _mm_add_pd())

```c
#pragma omp parallel for
#pragma vector always
#pragma ivdep
for (int i = 0; i < N; i++) {
    a[i] = b[i] + ...;
}
```

You need to trust the compiler to do the “right” thing.
OpenMP SIMD Loop Construct

• Vectorize a loop nest
  • Cut loop into chunks that fit a SIMD vector register
  • No parallelization of the loop body

• Syntax (C/C++)
  #pragma omp [for] simd [clause[,[,] clause],...] for-loops

• Syntax (Fortran)
  !$omp [do] simd [clause[,[,] clause],...] do-loops
Example

```c
void sprod(float *a, float *b, int n) {
    float sum = 0.0f;
    #pragma omp simd reduction(+:sum)
    for (int k=0; k<n; k++)
        sum += a[k] * b[k];
    return sum;
}
```

vectorize
Example: Worksharing w/ SIMD

```c
void sprod(float *a, float *b, int n) {
    float sum = 0.0f;
    #pragma omp for simd reduction(+:sum)
    for (int k=0; k<n; k++)
        sum += a[k] * b[k];
    return sum;
}
```

**parallelize**

**vectorize**

**Thread 0**

**Thread 1**

**Thread 2**

**Remainder Loop**

**Peel Loop**
Data Sharing Clauses

• **private**(var-list):  
  Uninitialized vectors for variables in var-list

  x: 42  ➔  ? | ? | ? | ?

• **firstprivate**(var-list):  
  Initialized vectors for variables in var-list

  x: 42  ➔  42 | 42 | 42 | 42

• **reduction**(op:var-list):  
  Create private variables for var-list and apply reduction operator op at the end of the construct

  12 | 5 | 8 | 17  ➔  x: 42
SIMD Loop Clauses

- **safelen (length)**
  - Maximum number of iterations that can run concurrently without breaking a dependence
  - In practice, maximum vector length
- **linear (list[:linear-step])**
  - The variable’s value is in relationship with the iteration number
    \[ x_i = x_{orig} + i \times \text{linear-step} \]
- **aligned (list[:alignment])**
  - Specifies that the list items have a given alignment
  - Default is alignment for the architecture
- **collapse (n)**
void sprod(float *a, float *b, int n) {
    float sum = 0.0f;
    #pragma omp for simd reduction(+:sum) \
         schedule(static, 5)
    for (int k=0; k<n; k++)
        sum += a[k] * b[k];
    return sum;
}

• You should choose chunk sizes that are multiples of the SIMD length
  • Remainder loops are not triggered
  • Likely better performance
• In the above example ...
  • and AVX-512, the code will only execute the remainder loop!
  • and SSE, the code will have one iteration in the SIMD loop plus one in the remainder loop!
OpenMP 4.5 Simplifies SIMD Chunks

void sprod(float *a, float *b, int n) {
    float sum = 0.0f;
    #pragma omp for simd reduction(+:sum) \
    schedule(simd: static, 5)
    for (int k=0; k<n; k++)
        sum += a[k] * b[k];
    return sum;
}

• Chooses chunk sizes that are multiples of the SIMD length
  • First and last chunk may be slightly different to fix alignment and to handle loops that are not exact multiples of SIMD width
• Remainder loops are not triggered
• Likely better performance
SIMD Function Vectorization

float min(float a, float b) {
    return a < b ? a : b;
}

float distsq(float x, float y) {
    return (x - y) * (x - y);
}

void example() {
    #pragma omp parallel for simd
    for (i=0; i<N; i++) {
        d[i] = min(distsq(a[i], b[i]), c[i]);
    }
}
SIMD Function Vectorization

• Declare one or more functions to be compiled for calls from a SIMD-parallel loop

• Syntax (C/C++):

```cpp
#pragma omp declare simd [clause[[], clause],...]
[#pragma omp declare simd [clause[[], clause],...]]
[...]
function-definition-or-declaration
```

• Syntax (Fortran):

```fortran
!$omp declare simd (proc-name-list)
```
#pragma omp declare simd
float min(float a, float b) {
  return a < b ? a : b;
}

#pragma omp declare simd
float distsq(float x, float y) {
  return (x - y) * (x - y);
}

void example() {
  #pragma omp parallel for simd
  for (i=0; i<N; i++) {
    d[i] = min(distsq(a[i], b[i]), c[i]);
  }
}

vec8 min_v(vec8 a, vec8 b) {
  return a < b ? a : b;
}

vec8 distsq_v(vec8 x, vec8 y) {
  return (x - y) * (x - y);
}

vd = min_v(distsq_v(va, vb), vc)
SIMD Function Vectorization

- **simdlen** (length)
  - generate function to support a given vector length
- **uniform** (argument-list)
  - argument has a constant value between the iterations of a given loop
- **inbranch**
  - function always called from inside an if statement
- **notinbranch**
  - function never called from inside an if statement
- **linear** (argument-list[:linear-step])
- **aligned** (argument-list[:alignment])
- **reduction** (operator:list)
inbranch & notinbranch

```c
#pragma omp declare simd inbranch
float do_stuff(float x) {
    /* do something */
    return x * 2.0;
}

void example() {
    #pragma omp simd
    for (int i = 0; i < N; i++)
        if (a[i] < 0.0)
            b[i] = do_stuff(a[i]);
}

vec8 do_stuff_v(vec8 x, mask m) {
    /* do something */
    vmulpd x{m}, 2.0, tmp
    return tmp;
}

for (int i = 0; i < N; i+=8) {
    vcmp_lt &a[i], 0.0, mask
    b[i] = do_stuff_v(&a[i], mask);
}
```
SIMD Constructs & Performance


SOFTWARE AND SERVICES
Task-generating Loops
Issues with Traditional Worksharing

- Worksharing constructs do not compose well
- Pathological example: parallel `dgemm` in MKL

```c
void example() {
    #pragma omp parallel
    {
        compute_in_parallel(A);
        compute_in_parallel_too(B);
        // dgemm is either parallel or sequential
        cblas_dgemm(CblasRowMajor, CblasNoTrans, CblasNoTrans,
                    m, n, k, alpha, A, k, B, n, beta, C, n);
    }
}
```

- Writing such code either
  - oversubscribes the system,
  - yields bad performance due to OpenMP overheads, or
  - needs a lot of glue code to use sequential `dgemm` only for sub-matrixes

SOFTWARE AND SERVICES
Issues with Traditional Worksharing /2

- Worksharing constructs do not compose well
- Pathological example: load imbalance

```c
void load_imbalance() {
    long_running_task() // can execute concurrently

    for (int i = 0; i < N; i++) { // can execute concurrently
        for (int j = 0; j < M; j++) {
            loop_body(i, j);
        }
    }
}
```

- Writing such code requires
  - nested parallelism,
  - manual, non-portable fine-tuning, and
  - a lot of care to get the load balance right.
Ragged Fork/Join

• Traditional worksharing can lead to ragged fork/join patterns

```c
void example() {
    compute_in_parallel(A);
    compute_in_parallel_too(B);
    cblas_dgemm(..., A, B, ...);
}
```
Example: Sparse CG

```c
for (iter = 0; iter < sc->maxIter; iter++) {
    precon(A, r, z);
    vectorDot(r, z, n, &rho);
    beta = rho / rho_old;
    xpay(z, beta, n, p);
    matvec(A, p, q);
    vectorDot(p, q, n, &dot_pq);
    alpha = rho / dot_pq;
    axpy(alpha, p, n, x);
    axpy(-alpha, q, n, r);
    sc->residual = sqrt(rho) * bnrm2;
    if (sc->residual <= sc->tolerance) break;
    rho_old = rho;
}
```

```c
void matvec(Matrix *A, double *x, double *y) {
    // ...
    #pragma omp parallel for \
    private(i,j,is,ie,j0,y0) \
    schedule(static)
    for (i = 0; i < A->n; i++) {
        y0 = 0;
        is = A->ptr[i];
        ie = A->ptr[i + 1];
        for (j = is; j < ie; j++) {
            j0 = index[j];
            y0 += value[j] * x[j0];
        }
        y[i] = y0;
    }
    // ...
}
```
The taskloop Construct

• Parallelize a loop using OpenMP tasks
  • Cut loop into chunks
  • Create a task for each loop chunk

• Syntax (C/C++)
  #pragma omp taskloop [simd] [clause[[,] clause],...]
  for-loops

• Syntax (Fortran)
  !$omp taskloop[simd] [clause[[,] clause],...]
  do-loops
  !$omp end taskloop [simd]
Clauses for taskloop Construct

• Taskloop constructs inherit clause both from worksharing constructs and the task construct
  • shared, private
  • firstprivate, lastprivate
  • default
  • collapse
  • final, untied, mergeable

• grainsize(\textit{grain-size})
  Chunks have at least \textit{grain-size} and max 2*\textit{grain-size} loop iterations

• num\_tasks(num\_tasks)
  Create \textit{num\_tasks} tasks for iterations of the loop
Example: **task** and **taskloop**

```c
void load_imbalance() {
#pragma omp taskgroup
{
#pragma omp task
  long_running_task() // can execute concurrently

#pragma omp taskloop collapse(2) grainsize(500) nogroup
  for (int i = 0; i < N; i++) { // can execute concurrently
    for (int j = 0; j < M; j++) {
      loop_body(i, j);
    }
  }
}
}
```
Example: Sparse CG, taskloop

```c
#pragma omp parallel
#pragma omp single
for (iter = 0; iter < sc->maxIter; iter++) {
    precon(A, r, z);
    vectorDot(r, z, n, &rho);
    beta = rho / rho_old;
    xpay(z, beta, n, p);
    matvec(A, p, q);
    vectorDot(p, q, n, &dot_pq);
    alpha = rho / dot_pq;
    axpy(alpha, p, n, x);
    axpy(-alpha, q, n, r);
    sc->residual = sqrt(rho) * bnrm2;
    if (sc->residual <= sc->tolerance)
        break;
    rho_old = rho;
}
```

```c
void matvec(Matrix *A, double *x, double *y) {
    // ...

#pragma omp taskloop private(j,is,ie,j0,y0) grain_size(500)
    for (i = 0; i < A->n; i++) {
        y0 = 0;
        is = A->ptr[i];
        ie = A->ptr[i + 1];
        for (j = is; j < ie; j++) {
            j0 = index[j];
            y0 += value[j] * x[j0];
        }
        y[i] = y0;
    }
    // ...
```

SOFTWARE AND SERVICES
Performance of Sparse CG w/ Tasks

X. Teruel, M. Klemm, K. Li, X. Martorell, S.L. Olivier, and C. Terboven. A Proposal for Task-Generating Loops in OpenMP. In A.P. Rendell et al., editor, International Workshop on OpenMP, pages 1-14, Canberra, Australia, September 2013. LNCS 8122
NUMA is here to Stay...

• (Almost) all multi-socket compute servers are NUMA systems
  • Different access latencies for different memory locations
  • Different bandwidth observed for different memory locations
• Example: Intel® Xeon E5-2600v2 Series processor
Thread Affinity – Why It Matters?

STREAM Triad, Intel® Xeon E5-2697v2

GB/sec [higher is better]

# of threads/cores

- compact, par
- scatter, par
- compact, seq
- scatter, seq
#pragma omp parallel for num_threads(32)
for (…)
#pragma omp parallel for num_threads(8)
for (…) {}

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Thread Affinity – Processor Binding

Binding strategies depend on machine and the app

• Putting threads far, i.e. on different packages
  • (May) improve the aggregated memory bandwidth
  • (May) improve the combined cache size
  • (May) decrease performance of synchronization constructs

• Putting threads close together, i.e. on two adjacent cores which possible share the cache
  • (May) improve performance of synchronization constructs
  • (May) decrease the available memory bandwidth and cache size (per thread)
Thread Affinity in OpenMP* 4.0

• OpenMP 4.0 introduces the concept of places...
  • set of threads running on one or more processors
  • can be defined by the user
  • pre-defined places available:
    • threads one place per hyper-thread
    • cores one place exists per physical core
    • sockets one place per processor package

... and affinity policies...
  • spread spread OpenMP threads evenly among the places
  • close pack OpenMP threads near master thread
  • master collocate OpenMP thread with master thread

• ... and means to control these settings
  • Environment variables OMP_PLACES and OMP_PROC_BIND
  • clause proc_bind for parallel regions
Thread Affinity Example

• Example (Intel® Xeon Phi™ Processor): Distribute outer region, keep inner regions close

```
OMP_PLACES=cores(8); OMP_NUM_THREADS=4,4
#pragma omp parallel proc_bind(spread)
#pragma omp parallel proc_bind(close)
```

![Diagram of thread affinity example](image-url)
We’re Almost Through

• There are so many things in OpenMP today
  • Can’t cover all of them in 90 minutes!

• OpenMP 4.0 and 4.5 have more to offer!
  • Improved Fortran 2003 support
  • User-defined reductions
  • Task dependencies
  • Cancellation
  • “doacross” Loops

• We can chat about these features in 1:1s, FTFs, phone calls, or in emails 😊
The last Slide...

- OpenMP 4.5 is not only a bugfix release
  - Task-generating loops
  - Locks with hints
  - Improved support for offloading (if it matters to you)

- Work on OpenMP 5.0 has already been started
  - Expected release during Supercomputing 2018
  - OpenMP 5.0 Beta is scheduled for Supercomputing 2017
  - Features being discussed:
    - Bugfixes 😊
    - Futures
    - Error handling
    - Transactional memory
    - Extensions to tasking
    - Fortran 2008 support
    - C++1x support
    - Data locality and affinity