Optimization Strategies for WSM6

1. Motivation
2. Overview of NEPTUNE and WSM6
3. Overview of KNL architecture
4. Methodology
5. Stand alone Experiments
6. WSM6 results
7. Discussion and Conclusion

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User Productivity Enhancement, Technology Transfer, and Training (PETTT)

Intel Parallel Computing Center

The University of Utah
Motivation

- Optimizing Numerical Weather Prediction (NWP) codes leads to faster forecast.
- “Navy Environmental Prediction sysTem Utilizing the NUMA corE” (NEPTUNE)
- This optimization targets intel KNL and potential future architectures because NWP codes port easily to Intel MIC as opposed to GPUs
- Understand how to effectively use OpenMP for portable shared memory parallelism in the context of NEPTUNE.

**NEPTUNE**

- **Dynamics**
  - Uses spectral elements --> high scalability because of small communication.
  - Non-hydrostatic Unified Model of the Atmosphere

- **Physics (WSM6)**
  - Does not Scale Well
  - Comprised of surface flux, boundary layer, shallow convection, warm-rain microphysics, and radiation processes
  - WSM6 is a components of the physics part of NEPTUNE
Physics Optimization Challenges

- WSM6 models various precipitation phenomena within vertical columns, exchanged through dynamics
  - 27 loops over 39 arrays with conditionals, array copies, and subroutine calls.
- Irregularity and complexity of physics between various states makes optimization challenging.

**Grauple Particles**

Like soft hail and about 2-5mm in diameter

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**WRF single-moment 6-class Microphysics Scheme (WSM6)**

- WSM6 models various precipitation phenomena within vertical columns, exchanged through dynamics
  - Irregularity and complexity of physics between various states makes optimization challenging.
Overview of KNL Architecture

- Cores+L2
- MCDRAM (as mem)
- DDR
- MCDRAM (as cache)
- DDR

**Chip:** 36 Tiles interconnected by 2D Mesh  
**Tile:** 2 Cores + 2 VPU/core + 1 MB L2  
**Memory:** MCDRAM: 16 GB on-package; High BW  
**DDR4:** 6 channels @ 2400 up to 384 GB  
**IO:** 36 lanes PCIe* Gen3. 4 lanes of DMI for chipset  
**Node:** 1-Socket only  
**Fabric:** Intel® Omni-Path Architecture on-package (not shown)  
**Vector Peak Perf:** 3+TF DP and 6+TF SP Flops  
**Scalar Perf:** ~3x over Knights Corner  
**Streams Triad (GB/s):** MCDRAM : 400+; DDR: 90+

Physical Addr Space
Methodology

Identify Bottlenecks
- Wall clock time (at each loop)
  Vtune profiler
- Adviser, compiler optrpt. output

Standalone Experiments
- Examine OpenMP, and structures of arrays (SOA) behavior on code’s subsets in controlled setting

Apply Findings to WSM6
- Threads (OMP PARALLEL, DO)
- SIMD (OMP SIMD, DO SIMD)
Structure of Arrays (SOA)

- Simple example of SOA.
- Figure to the right shows actual SOA used in WSM6 optimization.
- Chunk size is chosen to be multiple of vector unit length.
- Top down optimization approach = From “high-level” to “low-level”
Standalone Experiments

• OpenMP functionality with a non-trivial WSM6 loop
  – OMP PARALLEL and OMP DO constructs Using WSM6 loop 12
  – Functionality of conditionals and nested conditionals
  – Functionality of subroutine calls

• Add OpenMP directives to individual loops
  – OMP SIMD, OMP DO SIMD constructs
  – On sample code with conditional and subroutine call

• SOA with 1D and 2D arrays
  – Size and structure of SOA.
Pthreads vs OpenMP (in C)

<table>
<thead>
<tr>
<th>Threads</th>
<th>Pthread</th>
<th>OpenMP</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Thread creation (us)</td>
<td>Context switch (us)</td>
</tr>
<tr>
<td>2</td>
<td>199</td>
<td>0.6</td>
</tr>
<tr>
<td>8</td>
<td>121</td>
<td>1.2</td>
</tr>
<tr>
<td>32</td>
<td>102</td>
<td>1.0</td>
</tr>
<tr>
<td>64</td>
<td>99</td>
<td>1.0</td>
</tr>
</tbody>
</table>

- OpenMP thread creation time is significant
  - The first PARALLEL section costs a lot
  - Subsequent PARALLEL sections (with small KMP_BLOCKTIME), or DO constructs within one section – not much worse than pthreads.
- Context switches are in fact slightly cheaper than with Pthreads
Impact of function calls and conditionals in OMP DO construct

- OMP DO With conditionals and subroutine calls: **9.7x speedup** at 64 cores
- OMP DO Without conditionals and subroutine calls: **30x speedup** at 64 cores
- Conditionals and function calls hurt scalability
- This behaves better with SIMD in actual WSM6 results:
  - Loops 12-14: 41x speedup with OMP DO SIMD

Loop 12 from WSM6

do k=kte,kts,-1
  do i=its,ite
    ....
    if(t(i,k).gt.t0c)then
      ....
      work2(i,k)=venfac(p(i,k), t(i,k),den(i,k))
    endif
    if(qrs(i,k,2).gt.0)then
      ....
      psmlt(i,k)= xka(t(i,k),den(i,k)) ....
    endif
  endif
  if(qrs(i,k,3).gt.0)then
    ....
    pgmlt(i,k)= xka(t(i,k),den(i,k)) ....
  endif
endo
OMP DO, SIMD, DO SIMD

- OMP SIMD is beneficial for both conditionals and subroutines
  - Works fine with nested subroutines, when OMP DECLARE SIMD is used
- OMP PARALLEL + OMP SIMD (manual binding) was fastest
  - OMP DO SIMD slower than manual binding, but less so with conditionals

<table>
<thead>
<tr>
<th></th>
<th>Time</th>
<th>Speedup</th>
</tr>
</thead>
<tbody>
<tr>
<td>OMP DO</td>
<td>2.88</td>
<td>24</td>
</tr>
<tr>
<td>Manual binding</td>
<td>0.63</td>
<td>109</td>
</tr>
<tr>
<td>OMP DO SIMD</td>
<td>0.61</td>
<td>112</td>
</tr>
<tr>
<td>manual binding + OMP SIMD</td>
<td>0.23</td>
<td>229</td>
</tr>
</tbody>
</table>

Vector length for vectorization

<i>Thread 0</i> → <i>Thread 1</i> → <i>Thread 2</i> → <i>Thread 3</i>
1D vs 2D Standalone Experiments

1D Case

```
!$OMP SIMD
do  j=2, je -1
  a(j) = 0.1 + c(j)/d(j)
  b(j) = (0.2 + c(j-1) - c(j))/ (c(j) - c(j-1) + 0.5)
enddo
```

2D Case

```
do  i=1s, 1e
  !$OMP SIMD
do  j=2, je -1
  a(i, j) = 0.1 + c(i, j)/d(i, j)
  b(i, j) = (0.2 + c(i, j-1) - c(i, j))/ (c(i, j) - c(i, j-1) + 0.5)
enddo
enddo
```

- Computation similar to some of the computation in WSM6.
- 1D Case: SIMD is applied on the j loop. Along j the access pattern are more involved than 2D.
- 2D Case: SIMD is applied on the i loop. No dependencies even in the case of WSM6.
The table shows results from a standalone experiment with 1D arrays as SOA. SOA yield good results but not the best. The transpose approach performs better - uses more threads than original.

<table>
<thead>
<tr>
<th>Threads</th>
<th>Speed-up</th>
<th>Threads</th>
<th>Speed-up</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Orig.</td>
<td>Transp.</td>
<td>SOA</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>0.61</td>
<td>0.62</td>
</tr>
<tr>
<td>2</td>
<td>1.30</td>
<td>1.05</td>
<td>1.18</td>
</tr>
<tr>
<td>4</td>
<td>2.26</td>
<td>1.43</td>
<td>2.45</td>
</tr>
<tr>
<td>8</td>
<td>3.07</td>
<td>4.12</td>
<td>5.02</td>
</tr>
<tr>
<td>16</td>
<td>3.75</td>
<td>7.92</td>
<td>11.44</td>
</tr>
<tr>
<td>32</td>
<td>3.81</td>
<td>12.12</td>
<td>13.73</td>
</tr>
<tr>
<td>64</td>
<td>2.86</td>
<td>41.20</td>
<td>18.73</td>
</tr>
<tr>
<td>128</td>
<td>2.37</td>
<td>41.20</td>
<td>34.33</td>
</tr>
<tr>
<td>256</td>
<td>1.53</td>
<td>20.60</td>
<td>4.20</td>
</tr>
</tbody>
</table>

1D Case

```c
!$OMP SIMD
do  j = 2, je - 1
   a(j) = 0.1 + c(j)/d(j)
   b(j) = (0.2 + c(j - 1) - c(j))/ (c(j) - c(j - 1) + 0.5)
endo
```
SOA Results 1D with Large Arrays

- The Table shows result of a standalone experiment with increase size of the 1D arrays 16x previous experiment with 1D arrays.
- Transpose still outperforms SOA.
- This indicate that the structure of SOA plays a role in performance.

<table>
<thead>
<tr>
<th>Threads</th>
<th>Speed-up Orig.</th>
<th>Speed-up Transp.</th>
<th>Speed-up SOA</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.00</td>
<td>1.15</td>
<td>0.45</td>
</tr>
<tr>
<td>2</td>
<td>1.25</td>
<td>1.74</td>
<td>0.74</td>
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<tr>
<td>4</td>
<td>2.18</td>
<td>2.51</td>
<td>1.45</td>
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<td>8</td>
<td>3.10</td>
<td>6.64</td>
<td>4.55</td>
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<td>16</td>
<td>3.82</td>
<td>11.35</td>
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<td>32</td>
<td>3.79</td>
<td>12.96</td>
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</tr>
<tr>
<td>256</td>
<td>1.52</td>
<td>15.59</td>
<td>3.53</td>
</tr>
</tbody>
</table>

1D Case

```c
!$OMP SIMD
do j=2,je-1
a(j) = 0.1 + c(j)/d(j)
b(j) = (0.2 + c(j-1)-c(j))/((c(j)-c(j-1)+0.5)
enddo
```
SOA Results 2D with Large Arrays

- The table shows results from a standalone experiment with 1D arrays as SOA.
- SOA outperforms here because we are able to better leverage vector units.

<table>
<thead>
<tr>
<th>Threads</th>
<th>Speed-up</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Orig.</td>
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</tr>
<tr>
<td>1</td>
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</tr>
<tr>
<td>256</td>
<td>1.53</td>
<td>20.60</td>
</tr>
</tbody>
</table>

2D Case

```fortran
do i=2,ie-1
!$OMP SIMD
  do i=is,ie
    a(i,j) = 0.1+c(i,j)/d(i,j)
    b(i,j) = (0.2+c(i,j-1)-c(i,j))/c(i,j)-c(i,j-1)+0.5
  enddo
enddo
```
SOA Results 2D

- The Table shows results from a standalone experiment with an increase in size of the 1D arrays 16x compared to previous experiments with 2D arrays.
- Transpose outperforms the others.
- SOA performs poorly due to cache misses. The size of arrays in the SOA does not fit in cache, resulting in memory access penalties.
- The key to using SOA is structure and size.

<table>
<thead>
<tr>
<th>Threads</th>
<th>Speed-up</th>
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<td>1.36</td>
<td>1.65</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>2.21</td>
<td>2.19</td>
<td>2.34</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>2.68</td>
<td>4.30</td>
<td>4.64</td>
<td></td>
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<td>4.89</td>
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<td>7.73</td>
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<td>16</td>
<td>8.79</td>
<td>16.24</td>
<td>11.59</td>
<td></td>
<td></td>
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1D Case

```c
!$OMP SIMD
do j = 2, je - 1
    a(j) = 0.1 + c(j) / d(j)
    b(j) = (0.2 + c(j - 1) - c(j)) / (c(j) - c(j - 1) + 0.5)
enddo
```
- Chunk size chunk = 32 provides better results.
- The chunk size have to be large enough to provide sufficient work to minimize the overhead related to thread usage.
WSM6 Optimization Effort

● “Low-level” OpenMP approach based on standalone experiments:
  – Initialize all threads in an OMP PARALLEL section in wsm6init()
  In main WSM6 body wsm62d()
  – OMP PARALLEL, and DO SIMD directives
  – Merged loops to hide latency, removed redundant assignments

● Compare KNL and Haswell
  – Haswell = Intel Xeon 2.5 GHz, 72 cores with 2 threads per core
  – Haswell has a higher clock frequency than KNL
  – KNL has high higher bandwidth and larger L3/MCDRAM

● “Low level and high-level” Optimization with OpenMP and SOA
  – SOA at a higher level in call stack
  – SIMD at the lower level for vectorization
  – Merged loops, and removed keywords (exit, cycle goto)
### Speedup per Loop

- slope_wsm6 has different speed-ups for the same routine. Thread invocation time and memory access impact runtime.
- Loop 22 and 23 are simple with no complex logic.
- Overall, good scalability to 64 cores on KNL.
- Includes loop 12 (from standalone example). OMP SIMD enables 41x speedup, including nested conditionals, subroutines.
- Final copy of the result arrays shows significant thrashing.

<table>
<thead>
<tr>
<th>Loop</th>
<th>KNL</th>
<th>Haswell</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>14</td>
<td>4.9</td>
</tr>
<tr>
<td>2-4</td>
<td>19</td>
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</tr>
<tr>
<td>5-6</td>
<td>36</td>
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<td>7</td>
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<td>4.2</td>
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<td>3.7</td>
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<td>9-11</td>
<td>6.9</td>
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<td>4.2</td>
</tr>
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<td>5.6</td>
</tr>
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<td>13</td>
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<tr>
<td>23</td>
<td>100</td>
<td>5.5</td>
</tr>
<tr>
<td>24-26</td>
<td>57</td>
<td>12</td>
</tr>
<tr>
<td>27</td>
<td>.77</td>
<td>0.80</td>
</tr>
</tbody>
</table>
Removal of Fortran Keywords

```fortran
sum_precip: do k=1,km
  if(condition1)
    update precip
    cycle sum_precip
  elseif(condition2)
    update precip
    exit sum_precip
  end if
  exit sum_precip
end do sum_precip

sum_mask = 1

sum_precip: do k=1,km
  if(condition1 .and. sum_mask)
    update precip
  elseif(condition2 .and. sum_mask)
    update precip
    sum_mask = 0
  else
    sum_mask = 0
  end do sum_precip

100 continue
  .
  .
  if(n .le. inter)
    goto 100
end if

Do n=1,iter
  .
  .
end do
```
WSM6 Results

- The plot to the left clearly show that using flat mode outperform the cache mode.
- These results are similar to the what we observe in the community.
- 70x Speed-up on WSM6

- The plot to the right clearly show that SOA outperform the Transpose approach.
- The Rain routines are part of the WSM6 Module itself.
Conclusion

- “Low-level” OpenMP with OMP DO SIMD achieves ~50x speedup over the 25 parallelized loops of WSM6.
  - Restructure non-trivial logic with nested conditionals, subroutine calls, and unaligned memory access to enable performance
  - Vtune suggests 5.6% of peak in these sections
  - Including bottlenecks, WSM6 within NEPTUNE is 3x faster than serial on KNL

- “High-level and low-level”
  - Restructure of non-trivial loops
  - SOA at top level call in WSM6 and SIMD at the lower level
  - This approach led to 70x on WSM6
Future Work

- Apply these methodologies to GFS operational physics in NEPTUNE
- Investigate the impact from translation between dynamics and physics
- Investigate behavior and scalability on large system i.e OpenMP + MPI
- Investigate other optimization Strategies
  - lightweight runtime system for weather physics codes
  - Other approaches for data reorganizations

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THANK YOU

Questions?