Performance-Portability:
Case Studies of NIM and FV3 Models

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## Comparison

<table>
<thead>
<tr>
<th>NIM</th>
<th>FV3</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Weather Prediction</strong></td>
<td><strong>Weather &amp; Climate Prediction</strong></td>
</tr>
<tr>
<td><strong>Non-hydrostatic</strong></td>
<td><strong>Hydrostatic, non-hydrostatic</strong></td>
</tr>
<tr>
<td>~4K lines of code</td>
<td>~28K lines of code</td>
</tr>
<tr>
<td>– ESRL, Spire Global</td>
<td>– GFDL, NWS, NASA, NCAR</td>
</tr>
<tr>
<td>– Designed for GPU, MIC, CPU</td>
<td>– Designed for CPU</td>
</tr>
<tr>
<td><strong>Icosahedral grid</strong></td>
<td><strong>Cube-sphere grid</strong></td>
</tr>
<tr>
<td>– All cells treated identically</td>
<td>– Special cases for edges, corners</td>
</tr>
<tr>
<td>– Lookup table for neighbors</td>
<td>– I – J index for Latitude, Longitude</td>
</tr>
<tr>
<td><strong>Simple time-step</strong></td>
<td><strong>Complex time-step</strong></td>
</tr>
<tr>
<td><strong>Arakawa – A grid</strong></td>
<td><strong>Arakawa – C &amp; D grid</strong></td>
</tr>
<tr>
<td>– All data in cell centers</td>
<td>– Data in cell centers, edges, corners</td>
</tr>
<tr>
<td></td>
<td>– Transformations between grids</td>
</tr>
</tbody>
</table>
Model Grids

Cube-Sphere Grid
FV3, EndGame, ...

Icosahedral Grid
NIM, MPAS, ICON, ...
Indirect Addressing Scheme
Used in NIM, Adopted by MPAS

- Single horizontal index
- Store number of sides (5 or 6) in “nprox” array
  - $\text{nprox}(34) = 6$
- Store neighbor indices in “prox” array
  - $\text{prox}(1,34) = 515$
  - $\text{prox}(2,19) = 3$
- Place directly-addressed vertical dimension fastest-varying for speed
- Very compact code
- Indirect addressing costs <1%

(slide courtesy Tom Henderson)
## Code Structure & Parallelism

<table>
<thead>
<tr>
<th>NIM</th>
<th>FV3</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Fortran:</strong> ~21 routines</td>
<td><strong>Fortran:</strong> ~165 routines</td>
</tr>
<tr>
<td>1-2 deep call tree</td>
<td>3-4 deep call tree</td>
</tr>
<tr>
<td>Small routines</td>
<td>Large routines</td>
</tr>
<tr>
<td>K - I ordering</td>
<td>I – J - K ordering</td>
</tr>
<tr>
<td>OMP, openACC, SMS - MPI</td>
<td>OMP, openACC, MPI</td>
</tr>
</tbody>
</table>

### Parallelism

<table>
<thead>
<tr>
<th>NIM</th>
<th>FV3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Vectorization in “K”</td>
<td>Vectorization on “I”or “J”</td>
</tr>
<tr>
<td>– Except vertical remapping</td>
<td>– Limited by horiz dependencies</td>
</tr>
<tr>
<td>Small OMP regions over “I”</td>
<td>Large OMP loops over “K”</td>
</tr>
<tr>
<td>– ~100 – 200 lines</td>
<td>– ~1000-5000 lines</td>
</tr>
</tbody>
</table>

10% of peak on Haswell
NIM Performance
10242 horizontal columns
96 vertical levels

Runtime (sec)

Year Intel CPU (cores) NVIDIA GPU (cores) Intel MIC (cores)
2010/11 Westmere (12) Fermi (448)
2012 SandyBridge (16) Kepler K20x (2688)
2013 IvyBridge (20) Kepler K40 (2880) Knights Corner (61)
2014 Haswell (24) Kepler K80 (4992)
2016 Broadwell (30) Pascal P100 (3672) Knights Landing (68)
FV3: Fine-Grain Parallelization

- Increased parallelism needed for GPU
  - Push vertical “k” dimension into routines

Original: $I - J$

```
do k = 1, npz
  call c_sw(a(:,:,k), )
call riem_solver( ...
call update_dz( ...
call d_sw( ...
enddo
```

```
subroutine c_sw (a, )
  real a(isd:ied,jsd:jed)
  do j
    do i
```

Transformed: $I - J - K$

```
call c_sw_3D(a(:,:,:,:), )
call riem_solver_3D ( ...
call update_dz_3D ( ...
call d_sw_3D ( ...
```

```
subroutine c_sw_3D (a, )
  real a(is:ie,js:je,npz)
  do k
    do j
      do i
```
FV3: Shallow Water Kernel

- Compared I-J variant to I-J-K and K-I-J array ordering
- 1.8X faster on the GPU (IVB-20 vs Kepler K40)
  - I-J-K variant minimized code changes, best performance

<table>
<thead>
<tr>
<th></th>
<th>c_sw</th>
<th>divergence_corner</th>
<th>d2a2c_vect</th>
</tr>
</thead>
<tbody>
<tr>
<td>IVB i-j</td>
<td>45</td>
<td>13</td>
<td>20</td>
</tr>
<tr>
<td>IVB k-i-j</td>
<td>67</td>
<td>10</td>
<td>32</td>
</tr>
<tr>
<td>IVB i-j-k</td>
<td>42</td>
<td>7</td>
<td>21</td>
</tr>
<tr>
<td>K40 k-i-j</td>
<td>50</td>
<td>3</td>
<td>50</td>
</tr>
<tr>
<td>K40 i-j-k</td>
<td>29</td>
<td>9</td>
<td>9</td>
</tr>
</tbody>
</table>

Run time (ms)
FV3: Shallow Water Kernel

- 2016 chips: Haswell (24 cores), KNL, Pascal P100
- 1.6X faster on the GPU
Adapting FV3 Dynamics for GPUs

- **dyn_core** (100%)
  - c_sw (13%)
    - d2a2_vect
    - divergence_corner
  - update_dz_c (2%)
  - riem_solver_c (14%)
- d_sw (38%)
  - FV_TP_2D (37%)
    - copy_corners (0.1%)
    - xppm (14%)
    - yppm (14%)
  - xtp_v
  - xtp_u
- update_dz_d (10%)
  - FV_TP_2D (37%)
- riem_solver (1%)
- pg_d (5%)
  - nh_p_grad (5%)
- tracer_2d (6%)
- remapping (6%)

- Minimize changes to the code
- Require bitwise exact results
- Optimize performance
  - Maintain CPU perf
- Update to latest NWS code periodically
- Work with NWS to merge changes into trunk
FV3 Code Changes

• Push “K” loop in, modify array declarations, remove references to array sections, promote temporaries from 2D to 3D
  – Tens of local variables promoted to 3D
  – Break routine into multiple segments for GPU
    • Decrease register pressure
• Work around compiler bugs, derived types, pointers
• Debugging Challenges
  – Extensive use of pointers and array sections that obfuscate meaning, derived types & openACC
• Performance Issues
  – Promotion to 3D blows out cache
  – Increased number of OMP regions may hurt performance
FV3 Performance
- very preliminary results -

• Full model versus standalone kernel
  – Improved CPU performance over standalone
    • Thread pinning, cache reuse
  – 3D variant runs slower than 2D on CPU

• Haswell CPU, Pascal P100 GPU
  – KNL gave ~15% improvement over 2D code

<table>
<thead>
<tr>
<th>Routine</th>
<th>2D Intel</th>
<th>3D Intel</th>
<th>3D GPU</th>
</tr>
</thead>
<tbody>
<tr>
<td>C_SW</td>
<td>0.21</td>
<td>0.34</td>
<td>0.47</td>
</tr>
<tr>
<td>D2A2_vect</td>
<td>0.31</td>
<td>0.95</td>
<td>0.10</td>
</tr>
<tr>
<td>REMAP</td>
<td>1.61</td>
<td>1.55</td>
<td>slower</td>
</tr>
<tr>
<td>D_SW</td>
<td>5.32</td>
<td>7.41</td>
<td>slower</td>
</tr>
<tr>
<td>FV_TP</td>
<td>0.17</td>
<td>0.26</td>
<td>slower</td>
</tr>
</tbody>
</table>
Performance Portability Takeaways
- Code Design -

• Code simplicity
  – Avoid use of pointers, derived types, abstractions, “new” language constructs

• Memory
  – Registers
    • Small kernels reduce register pressure
  – Shared memory
    • FV3 uses none, NIM used extensively

• Compute
  – Stride-1 essential for vectorization, SIMT, memory access
  – Minimize branching
  – Icosahedral grid treats every cell identically
    • FV3 has special cases for edge, and corner cells
  – Use parallel algorithms, avoid complex algorithms
Conclusion

• Performance portability with single source code was achieved with NIM
  – Design targeted GPU
  – Simple language constructs
  – Maximize parallelism

• Adapting FV3 has been difficult
  – Code changes needed for the GPU, run slower on CPU
  – Still digging into FV3 performance issues & resolution
    • Cache, parallelism, kernel size, memory use
    • Cube-sphere grid

• Collaborative design to focus on fine-grain, portability
  – Development by team of scientists, parallelization experts, computer scientists
  – Use language scientists support / accept