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Enhancing Productivity on Heterogeneous Supercomputers with Task-based Programming Model

Adrien Roussel, Mickael Boichot, Manuel Ferat, Romain Pereira
CEA, DAM, DIF

SIAM CSE, Amsterdam
February 28, 2023
Introduction

- Most of the time, scientific applications are already parallelized for **CPU** (or partly for GPU)

- To take advantage of **GPUs**, developers have to **rewrite** their codes (in part? in whole?)

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**Goals:**
- Build a **preliminary analysis** to determine the **potential** of the application for a **GPU port**
- Port mini-application to **heterogeneous architectures** with this information
Contributions

**Goal**: Inform the user

- that there exists a **test case** of the application **suitable** for a **GPU port**
- about the **strengths** and **weaknesses** of the application for a **GPU port**

- We analyzed the variations of two **metrics**:
  - the **degree of parallelism** (→ saturate GPU cores)
  - and the **working set** (→ bounded GPU memory)

- Porting app. To GPU Computing
  - Using Task based prog. Model
    - MPI+OpenMP (tasks + target)

```c
int main(...)
{
    /* parallel CPU code */
}
```

- Relate the two metrics
- Extrapolate application behavior
- GPU Porting

- varying dataset input size
Contents

1. Introduction

2. Application Characterization Method

3. Proxy Applications Analysis

4. Porting Proxy App to GPU: LULESH

5. Conclusion
2. Application Characterization Method
Targeted GPU Characterization

Maximizing FFMA throughput ("floating point fused multiple add")
→ \( RP = \#\text{cores} \cdot L \)
where
- \( L : 32 \) bits FFMA instruction latency

Characterization

**Required Parallelism (RP)**

- \( \#\text{cores} \)
- L2 Cache
- DRAM

**RAM (GB)**

Already known (GPU documentation)
Metrics to Characterize the Application

Applications analyzed at Loop Granularity (already parallelized with OpenMP)

L: for (i = 0; i < N; ++i)
compute;

Set of data necessary to run the loop
Working Set

measured at two Granularities, i.e., the size of smallest accessed memory element (using DynamoRIO)

Parallelism Degree P(L)

# independent Iterations (i.e., tripcount)

WS\text{malloc}(L) \quad WS\text{cache\ line}(L)
Extrapolation Methodology

For each loop

\[
\forall L \in S, n \in \{n_1, n_2, \ldots\} \rightarrow \text{measure}
\]
- working set \( WS(L) \)
- parallelism degree \( P(L) \)

\[
WS(L) = f(P(L))\]
\[
P(L) = g(n)\]

Extract most time-consuming loops

\[
\text{pre-selection} \quad . / \text{app -input } n \rightarrow S \text{ - working set WS(L) - parallelism degree } P(L) \text{ - inference}
\]

\begin{tabular}{|c|c|c|c|}
  \hline
  loop & working set & parallelism degree & input size \\
  \hline
  L & WS(L) & P(L) & n_1 \\
  L & WS(L) & P(L) & n_2 \\
  ... & ... & ... & ... \\
  \hline
\end{tabular}
Extrapolation Methodology

Extract most time-consuming loops

∀ L ∈ S, n ∈ {n1, n2, ...} → measure
- working set WS(L)
- parallelism degree P(L)

∀ L ∈ S, WS(L) = f(P(L))
P(L) = g(n)

projection

Test cases fitting target GPU memory and exposing enough parallelism
3. Proxy Applications Analysis

LULESH, miniFE
Experimental Protocol

▶ Evaluation Machine

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>processor</td>
<td>Intel Xeon E5-2680</td>
</tr>
<tr>
<td>#sockets</td>
<td>2</td>
</tr>
<tr>
<td>#cores/socket</td>
<td>8</td>
</tr>
<tr>
<td>RAM (GB)</td>
<td>128</td>
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<tr>
<td>OS</td>
<td>Linux 3.10</td>
</tr>
<tr>
<td>Compiler</td>
<td>Intel 20.0.0</td>
</tr>
</tbody>
</table>

▶ Evaluated mini-applications

- **LULESH** (hydrodynamic simulation)
- **MiniFE** (finite element problem)
- Quicksilver (Monte Carlo particle transport)
- XSBench (Monte Carlo particle transport kernel)

*All these applications have CPU OpenMP, GPU CUDA and HIP versions.*

▶ Considered targeted GPUs

<table>
<thead>
<tr>
<th>GPU</th>
<th>RAM</th>
<th>#cores</th>
<th>minimal required parallelism RP</th>
</tr>
</thead>
<tbody>
<tr>
<td>V100</td>
<td>16 GB</td>
<td>5120</td>
<td>20480</td>
</tr>
<tr>
<td>A100 40GB</td>
<td>40 GB</td>
<td>6912</td>
<td>27648</td>
</tr>
<tr>
<td>A100 80GB</td>
<td>80 GB</td>
<td>6912</td>
<td>27648</td>
</tr>
<tr>
<td>MI100</td>
<td>32 GB</td>
<td>7680</td>
<td>30720</td>
</tr>
</tbody>
</table>
LULESH

Working set of LULESH selected loops as a function of their tripcount

Projection of dataset input size $s_{\text{max}}$ saturating GPU memory and corresponding $\rho$ ratio ($\rho(L) = P(L) / RP$)

- Sufficient exposed parallelism ($\rho \gg 1$)
- Limiting factor: memory size
- Advised data transfers granularity: malloc

- Similar conclusions for miniFE
4. Porting Proxy App to GPU: LULESH
Porting LULESH to MPI+OpenMP(tasks)

- **LULESH**
  - Hydrodynamic problems solver - Iterative simulation
  - Original code express loop-based parallelism (parallel-for)

- **Porting to MPI+OpenMP (tasks)**
  - Loops splitted into tasks with dependencies
  - Single producer/multi-consumer scheme
  - MPI communications nested within OpenMP tasks
    - Overlap communications by computations

```c
for (int j = 0 ; j < n_nodes; j += BS)
{
    # pragma omp task depend(out : mesh->nodes[j])
    {
        for (int i = j ; i < j + BS ; ++i)
            work_on_nodes(mesh->nodes[i]);
    }
}
for (int j = 0 ; j < n_cells; j += BS)
{
    # pragma omp task depend(in : [...])
    {
        for (int i = j ; i < j + BS ; ++i)
            work_on_cells(mesh->cells[i]);
    }
}
```

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**Concept Generalization for Heterogeneous Architectures with OpenMP Target**

- **Porting to MPI+OpenMP (tasks + GPU target)**
  - GPU « super-tasks » merging several CPU tasks
  - From CPU tasks to GPU offloading while enhancing asynchronism
    - Sending/Retrieving data to/from GPU with ‘update’ clause
    - Executing GPU kernels through ‘nowait’ clause
  - Offloading 6 loops given by application characterization
    - IntegrateStressForElems, CalcKinematicsForElems, CalcAccelerationForNodes, CalcFBHourglassForceForElems1, CalcHourglassControlForElems, CalcMonotonicQGradientsForElems

- **Use of cudaMallocHost for the GPU buffers**
  - Pinned memory to enable asynchronous execution

```c
1 buffer = cudaMallocHost(...);

[...]
2 for (int j = 0 ; j < n_nodes; j += BS)
3 {
4     # pragma omp task depend(out: mesh->nodes[j])
5     {
6         for (int i = j ; i < j + BS ; ++i)
7             work_on_nodes(mesh->nodes[i], buffer[i]);
8     }
9 # pragma omp target update to(buffer[j:BS])
10     depend(out: mesh->nodes[j])
11 # pragma omp target teams distribute parallel for nowait 
12     depend(iterator(i=0:N_BS), out: mesh->nodes[j+i*BS])
13 {
14     for (int i = j ; i < j + N_BS * BS ; ++i)
15         work_on_nodes(mesh->nodes[i], buffer[i]);
16 }
17 # pragma omp target update from(buffer[j:BS])
18     depend(out: mesh->nodes[j])
```

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Experimental Protocol

<table>
<thead>
<tr>
<th>Processor</th>
<th>AMD EPYC 7H12</th>
</tr>
</thead>
<tbody>
<tr>
<td>#sockets</td>
<td>2</td>
</tr>
<tr>
<td>#cores/socket</td>
<td>64</td>
</tr>
<tr>
<td>GPU</td>
<td>NVIDIA A100</td>
</tr>
<tr>
<td>#GPU/socket</td>
<td>2</td>
</tr>
<tr>
<td>RAM (GB)</td>
<td>256</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>MPC-OpenMP (No Offloaded part)</th>
<th>4.1.0</th>
</tr>
</thead>
<tbody>
<tr>
<td>LLVM (Offloaded part)</td>
<td>16.x</td>
</tr>
<tr>
<td>Open MPI</td>
<td>4.0.5</td>
</tr>
</tbody>
</table>
LULESH Performance Evaluation

- **Problem size**
  - 264³ elements
  - 80% of the NUMA domain memory capacity
  - 20% of the GPU memory capacity
  - 128 iterations

- **Placement**
  - Per MPI Process:
    - 16 threads (on 16 cores)
    - + 1 GPU

- **Weak scaling**
  - Median runtime of 10 runs
  - Each version scale very well
  - **OpenMP tasks** version significantly improves performances due to cache reuse
  - Significant performance gain with **GPU offloading**

<table>
<thead>
<tr>
<th></th>
<th>ranks</th>
<th>parallel-for</th>
<th>no-offloading</th>
<th>offloading</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1</td>
<td>565.84</td>
<td>325.02</td>
<td>209.31</td>
</tr>
<tr>
<td></td>
<td>8</td>
<td>572.45</td>
<td>331.09</td>
<td>209.43</td>
</tr>
<tr>
<td></td>
<td>27</td>
<td>581.26</td>
<td>333.98</td>
<td>212.78</td>
</tr>
</tbody>
</table>
5. Conclusion
Conclusion

- An approach: \( \text{int main(...)} \{ \text{...} \} \mapsto \{ \text{test cases such that int main(...)} \{ \text{...} \} \text{fit on } \text{RAM and do not lack parallelism} \} \)

- **complementary** to existing work (analysis of several application runs → extrapolation)

- We have **evaluated** our approach and shown that we can **qualitatively guide developer** in their GPU porting.

- We have **ported** LULESH on heterogeneous machine with a **task-based programming model**
  - Significant gains are observed
Thank you!

Questions?