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Enhancing Productivity on Heterogeneous Supercomputers with Task-based Programming Model

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SIAM CSE, Amsterdam
February 28, 2023
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?)

**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 ($\rightarrow$ saturate GPU cores)
- and the working set ($\rightarrow$ bounded GPU memory)

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

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

variation dataset input size

Relate the two metrics

Extrapolate application behavior

GPU Porting
Contents

1. Introduction

2. Application Characterization Method

3. Proxy Applications Analysis

4. Porting Proxy App to GPU: LULESH

5. Conclusion
2. Application Characterization

Method
Maximizing FFMA throughput ("floating point fused multiple add")

\[ RP = \#\text{cores} \times L \]

where

- \( L \) : 32 bits FFMA instruction latency

Targeted GPU Characterization

Characterization

Required Parallelism (RP)

RAM (GB)

#cores

Targeted GPU

L2 Cache

DRAM

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
- Parallelism Degree \( P(L) \)

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

- \( WS_{malloc}(L) \)
- \( WS_{cache\ line}(L) \)

- # independent Iterations (i.e., tripcount)
Extrapolation Methodology

Extract most time-consuming loops

∀ L ∈ S, n ∈ \{n_1, n_2, \ldots\} → measure
- working set WS(L)
- parallelism degree P(L)

∀ L ∈ S, WS(L) = f(P(L))
P(L) = g(n)

For each loop

\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 \\
\ldots & \ldots & \ldots & \ldots \\
\hline
\end{tabular}
Extrapolation Methodology

\[ \forall L \in S, \ n \in \{n_1, n_2, \ldots\} \]

\[ \rightarrow \text{measure} \]

- working set \( WS(L) \)
- parallelism degree \( P(L) \)

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

projection

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

LULESH, miniFE
Experimental Protocol

- Evaluation Machine

<table>
<thead>
<tr>
<th>processor</th>
<th>Intel Xeon E5-2680</th>
</tr>
</thead>
<tbody>
<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>
</tr>
<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

<table>
<thead>
<tr>
<th>target GPU</th>
<th>$s_{\text{max}}$</th>
<th>$\rho$ (loop 1773)</th>
<th>$\rho$ (other loops)</th>
<th>$s_{\text{max}}$</th>
<th>$\rho$ (loop 1773)</th>
<th>$\rho$ (other loops)</th>
</tr>
</thead>
<tbody>
<tr>
<td>V100 16 GB</td>
<td>285</td>
<td>19.2</td>
<td>1130.3</td>
<td>289</td>
<td>19.4</td>
<td>1178.6</td>
</tr>
<tr>
<td>A100 40GB</td>
<td>387</td>
<td>19.3</td>
<td>2099.4</td>
<td>393</td>
<td>19.6</td>
<td>2195.4</td>
</tr>
<tr>
<td>A100 80GB</td>
<td>487</td>
<td>24.3</td>
<td>4198.7</td>
<td>495</td>
<td>24.7</td>
<td>4386.8</td>
</tr>
<tr>
<td>MI100 32GB</td>
<td>359</td>
<td>16.1</td>
<td>1511.5</td>
<td>365</td>
<td>16.4</td>
<td>1586.6</td>
</tr>
</tbody>
</table>

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
#pragma omp parallel for
for (int i = 0; i < n_nodes; i++)
  work_on_nodes(mesh->nodes[i]);

#pragma omp parallel for
for (int i = 0; i < n_cells; i++)
  work_on_cells(mesh->cells[i]);
```

```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]);
  }
}
```
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
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], buffer[i]);
    }
    buffer = cudaMallocHost(…);
    […]
}
```

```c
for (int j = 0 ; j < n_nodes; j += BS)
{
    # pragma omp target update to(buffer[j:BS]) \ 
        depend(out : mesh->nodes[j])
    
    # pragma omp target 
        teams distribute parallel for nowait \ 
        depend(iterator(i=0:N_BS), out: mesh->nodes[j+i*BS])
    {
        for (int i = j ; i < j + N_BS * BS ; ++i)
            work_on_nodes(mesh->nodes[i], buffer[i]);
    }
    # pragma omp target update from(buffer[j:BS]) \ 
        depend(out: mesh->nodes[j])
}
```
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>

### MPC

- MPC-OpenMP (No Offloaded part): 4.1.0
- LLVM (Offloaded part): 16.x
- Open MPI: 4.0.5
LULESH Performance Evaluation

- **Problem size**
  - $264^3$ 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>Number of MPI ranks</th>
<th>Median Time (s)</th>
<th>parallel-for</th>
<th>no-offloading</th>
<th>offloading</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>565.84</td>
<td>325.02</td>
<td>209.31</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>572.45</td>
<td>331.09</td>
<td>209.43</td>
<td></td>
</tr>
<tr>
<td>27</td>
<td>581.26</td>
<td>333.98</td>
<td>212.78</td>
<td></td>
</tr>
</tbody>
</table>
5. Conclusion
Conclusion

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

- **complementary** to existing work (analysis of several application runs $\rightarrow$ 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?