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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?)

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)

Porting

- Extending application behavior
- Exposing the strengths and weaknesses of the application for a GPU port

Extrapolate application behavior

Relate the two metrics

varying dataset input size

Parallel computations

working set

projection
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

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

# independent iterations (i.e., tripcount)

Parallelism Degree P(L)

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

WS_{malloc}(L)  \quad WS_{cache\ line}(L)
**Extrapolation Methodology**

For each loop

- Extract most time-consuming loops

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

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

<table>
<thead>
<tr>
<th>loop</th>
<th>working set</th>
<th>parallelism degree</th>
<th>input size</th>
</tr>
</thead>
<tbody>
<tr>
<td>L</td>
<td>WS(L)</td>
<td>P(L)</td>
<td>(n_1)</td>
</tr>
<tr>
<td>L</td>
<td>WS(L)</td>
<td>P(L)</td>
<td>(n_2)</td>
</tr>
<tr>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
</tbody>
</table>

For each loop

- pre-selection
- inference

working set

parallelism degree

Regression
Extrapolation Methodology

pre-selection

Extract most time-consuming loops

S

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

measure

∀ L ∈ S, WS(L) = f(P(L))
P(L) = g(n)

inference

projection

Test cases fitting target GPU memory and exposing enough parallelism

WS(L)

L1

L2

L3

P(L)

P_max(L1) P_max(L2)

M

Ram : M GB

Required Parallelism (RP)

target GPU
Proxy Applications Analysis

LULESH, miniFE
Experimental Protocol

Evaluation Machine

<table>
<thead>
<tr>
<th>Feature</th>
<th>Value</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>
</tr>
<tr>
<td>OS</td>
<td>Linux 3.10</td>
</tr>
<tr>
<td>Compiler</td>
<td>Intel 20.0.0</td>
</tr>
</tbody>
</table>

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>

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.
LULESH

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

Projection of dataset input size $s_{max}$ 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 #pragma omp target update to(buffer[j:BS]) \
                7 depend(out : mesh->nodes[j])
            8 #pragma omp target teams distribute parallel for nowait \
                9 depend(iterator(i=0:N_BS), out: mesh->nodes[j+i*BS])
            10 { 
                11 for (int i = j ; i < j + BS * BS ; ++i)
                    12 work_on_nodes(mesh->nodes[i], buffer[i]);
                13 }
            14 
            15 #pragma omp target update from(buffer[j:BS]) \
                16 depend(out: mesh->nodes[j])
        17 }
```

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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>Median Time (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>ranks</td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>565.84</td>
</tr>
<tr>
<td>8</td>
<td>572.45</td>
</tr>
<tr>
<td>27</td>
<td>581.26</td>
</tr>
</tbody>
</table>
5. Conclusion
Conclusion

- An approach: (int main(...){
  ...
}) \rightarrow \{ \text{test cases such that fit on 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?