Application Skeletons: Constructing and Using Abstract Many Task Applications in eScience

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Motivation

- Computer scientists who build tools and systems need to work on real scientific applications to prove the effectiveness of their tools and systems
  - And often vary them – change problem size, etc.
- However, accessing and building real applications can be hard (and isn’t really the core of their work)
  - Some applications (source) are privately accessible
  - Some data is difficult to access
  - Some applications use legacy code and are dependent on out-of-date libraries
  - Some applications are hard to understand without domain science expertise
  - Real applications may be difficult to scale or modify to demonstrate system trends and characteristics
Part of the AIMES Project

AIMES: Abstractions and Integrative Middleware for Extreme Scales

- **Goal**
  - Improve principles and practice of distributed dynamic resource federation

- **Motivation**
  - Identify abstractions; implement to study & support federation
  - Improve dynamic and distributed execution on heterogeneous distributed computing infrastructure (DCI)
    - “How will my application perform on this DCI?”
    - “How can I best adapt my application to a DCI?”
    - “How can the set of resources DCI best adapt to my application?”
    - “Why did the system allocate this DCI to my application?”
    - “What “variables” matter most ... matter least?
  - Understand how distributed workload execution can be managed
    - Hypothesis: Using middleware that supports the integration of application-level and resource-level information
    - Questions: What are the relevant decisions, and at what level should they be made?
AIMES Approach

- Use abstractions that can be flexibly composed and support a range of experiments, including
  - **Skeletons** represent primary DCI application characteristics
  - **Resource Bundles** provide real-time info on state of diverse resources
  - **Pilot Jobs** enable dynamical distributed resource federation & management
  - **Execution strategy**: temporally ordered set of decisions that need to be made when executing a given workload

- Experiment to understand requirements & trade-offs
We want to build a tool so that

- Users can quickly and easily produce a synthetic distributed application that represents the key distributed characteristics of a real application
  - The synthetic application should have task type (serial or parallel), runtime, I/O buffer, I/O quantity, computation and I/O interleaving pattern and intertask communication that are similar to those of the real application
- The synthetic application is easy to run in a distributed environment: grids, clusters, and clouds
- The synthetic application should be executable with common distributed computing middleware (e.g., Swift and Pegasus) as well as the ubiquitous Unix shell
Classes of Distributed Applications

- Bag of Tasks: a set of independent tasks
- MapReduce: a set of distributed application with key-value pairs as intermediate data format
- Iterative MapReduce: MapReduce application with iteration requirement
- Campaign: an iterative application with a varying set of tasks that must be run to completion in each iteration
- Multi-stage Workflow: a set of distributed applications with multiple stages that use POSIX files as intermediate data format
- Concurrent Tasks: a set of tasks that have to be executed at the same time (not supported by current work)

Note that most/all of these are many-task applications
Contributions

• An application abstraction that gives users good expressiveness and ease of programming to capture the key performance elements of distributed applications
• A versatile Skeleton task implementation that is configurable (number of tasks, serial or parallel tasks, amount of I/O and computation, I/O buffer size, computation and I/O interleaving options)
• An interoperable Skeleton implementation that works with mainstream workflow frameworks and systems (Swift, Pegasus, and Shell)
• The usage of Skeleton applications to simplify system optimization implementation and highlight their impacts
Challenge

- Balance the ease of programming and usage with the performance gap between Skeleton applications and real applications.
An Multi-Stage Application Example

• Applications have stages
• Each stage has tasks
  – Tasks have types (serial/parallel)
  – Tasks have computation lengths
  – Input/Output files have sizes
  – I/O is through buffers
  – Input files can be (pre) existing files or Output files from previous stages
  – Computation and I/O can be interleaved
• Each stage has input/output files
  – Input files map to tasks with patterns
Skeleton Abstraction

- Application Skeletons abstract an application using a top-down approach: an application is composed of stages, each of which is composed of tasks.
- An application can be defined by a configuration file containing:
  - Number of stages
  - For each stage
    - Task types (serial/parallel)
    - Tasks (number and computation length)
    - Number of processes for each task
    - Input files (number, sizes, and mapping to tasks)
    - Output files (number, sizes)
    - I/O buffer size
    - Computation and I/O interleaving option
The Skeleton tool is implemented as a parser.
Task Executable

- All tasks implemented as one standalone C program via parameters
- C program can be compiled as serial with GCC, as parallel with MPICC compiler.
- An execution example:
  - task serial 1 5 65536 65536 1 1 0
    Stage_1_Input/Stage_1_Input_0_1
    Stage_1_Output/Stage_1_Output_0_1 4200000
  - Path_to_Task Task_Type Num_Processes Task_Length
    Read_Buffer Write_Buffer Num_Input Num_Output
    Interleave_Option [Input_File] [Output_File Output_Size]
A Bag of Task Application Example

1. Num_Stage = 1
2. 
3. Stage_Name = Bag
4. Task_Type = serial
5. Num_Processes = 1
6. Num_Tasks = 4
7. Task_Length = uniform 5
8. Read_Buffer = 65536
9. Write_Buffer = 65536
10. Input_Files_Each_Task = 1
11. Input_1.Source = filesystem
12. Input_1.Size = uniform 2100000
13. Output_Files_Each_Task = 1
14. Output_1.Size = uniform 4200000
15. Interleave_Option = 0

https://github.com/applicationskeleton/Skeleton/blob/master/src/sample-input/bag.input
A Bag of Task Application Example

- **Other options**
  - Task_Type can be parallel
    - Task_Type = parallel
  - Task_Length can be a statistical distribution
    - Task_Length = normal [20, 3]
  - Task_Length can be a polynomial function of input file size
    - Task_Length = polynomial [20, 3] Input_1
      - 20*Input_1.Size^3
  - Output size can be a polynomial function of Task_Length
    - Output_1.Size = polynomial [10, 2] Length
      - 10*Length^2
  - Interleaving_Option can be ...
A Bag of Task Application Example

- Interleaving Option can be

<table>
<thead>
<tr>
<th></th>
<th>read</th>
<th>sleep</th>
<th>write</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Interleave-nothing:

Interleave-read-compute:

Interleave-compute-write:

Interleave-all:

Time
A Multi-stage Workflow

- Num_Stage = 3
- Stage_Name = Stage_1
  - ...
- Stage_Name = Stage_2
  - ...
- Write_Buffer = 65536
- Input_Files_Each_Task = 2
  - Input_Task_Mapping = combination Stage_1.Output_1 2
  - ...
- Stage_Name = Stage_3
  - ...
- Input_Files_Each_Task = 6
  - Input_Task_Mapping = combination Stage_2.Output_1 6
  - ...

https://github.com/applicationskeleton/Skeleton/blob/master/src/sample-input/multi-stage.input
Input_Task_Mapping

- Specify Input_Task_Mapping:
  - Input_Task_Mapping = combination Stage_1_output_1 2
  - Equivalent to “N choose k” mathematically
  - 4 files, 6 tasks =>
    o file0, file1 : task0
    o file0, file2 : task1
    o file0, file3 : task2
    o file1, file2 : task3
    o file1, file3 : task4
    o file2, file3 : task5

https://github.com/applicationskeleton/Skeleton/blob/master/src/sample-input/multi-stage.input
Input_Task_Mapping

- If Input_Task_Mapping is not specified
  - Input_Files_Each_Task = 2
  - Input_1.Source = Stage_1.Output_1
  - Input_2.Source = Stage_1.Output_1

- Files are mapped to tasks in a natural order
  - file0, file1 : task0
  - file2, file3 : task1
  - file4, file5 : task2
  - file6, file7 : task3
• External mapping option
  – Input_Task_Mapping = external sample-input/mapping.sh
  – cat sample-input/mapping.sh
    o echo Stage_1_Output_0_1  Stage_1_Output_0_2
    o echo Stage_1_Output_0_1  Stage_1_Output_0_3
    o echo Stage_1_Output_0_1  Stage_1_Output_0_4
    o echo Stage_1_Output_0_2  Stage_1_Output_0_3
    o echo Stage_1_Output_0_2  Stage_1_Output_0_4
    o echo Stage_1_Output_0_3  Stage_1_Output_0_4
  – The ith line maps to the ith task

https://github.com/applicationskeleton/Skeleton/blob/master/src/sample-input/external-mapper.input
A Single Stage Iterative Application

NumStage = 1

Stage_Name = Stage_1
Task_Type = serial
Num_Tasks = 4
Task_Length = uniform 10
Num_Processes = 1
Read_Buffer = 65536
Write_Buffer = 65536
Input_Files_Each_Task = 1
  Input_1.Source = filesystem
  Input_1.Size = uniform 1048576
Output_Files_Each_Task = 1
  Output_1.Size = uniform 1048576
Interleave_Option = 0
Iteration_Num = 3
Iteration_Stages = Stage_1
Iteration_Substitute = Stage_1.Input_1, Stage_1.Output_1

Stage_1.Input_1 and Stage_1.Output_1 should have IDENTICAL number of files

https://github.com/applicationskeleton/Skeleton/blob/master/src/sample-input/single-stage-iterative.input
A Multi Stage Iterative Application

Stage_Name = Stage_3
Task_Type = serial
Num_Tasks = 6
Task_Length = uniform 32
Num_Processes = 1
Read_Buffer = 65536
Write_Buffer = 65536
Input_Files_Each_Task = 1
  Input_1.Source = Stage_2.Output_1
Output_Files_Each_Task = 1
  Output_1.Size = uniform 1048576
Interleave_Option = 0
Iteration_Num = 3
Iteration_Stages = Stage_3, Stage_4
Iteration_Substitute = Stage_3.Input_1, Stage_4.Output_1

Stage_Name = Stage_4
Task_Type = serial
Num_Tasks = 6
Task_Length = uniform 32
Num_Processes = 1
Read_Buffer = 65536
Write_Buffer = 65536
Input_Files_Each_Task = 1
  Input_1.Source = Stage_3.Output_1
Output_Files_Each_Task = 1
  Output_1.Size = uniform 1048576
Interleave_Option = 0

Stage_3.Input_1 and Stage_4.Output_1 should have IDENTICAL number of files

https://github.com/applicationskeleton/Skeleton/blob/master/src/sample-input/multiple-stage-iterative.input
Determining Skeleton Parameters Manually

- **Steps**
  - Place I/O files on RAM disk, use Unix `time` command to measure run time
  - Use Unix `strace` command to find number of reads and writes, total data read and written
  - Align I/O calls in sequence order\(^1\) to determine I/O concurrency, I/O buffer size, and interleaving option

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Determining Skeleton Parameters Automatically

- Wrap task in a profiler (uses Linux `perf`, hardware and kernel counters, system tools)
  - Measure resource consumption over time as profile: timed sequence of CPU cycles, memory and disk I/O operations
  - Dependencies between compute and I/O implicitly captured in profile in order of the sequence

- Profiles are system independent
  - Assuming comparable optimization at software and hardware levels

- Profile metrics are suitable as input for emulation
Skeleton Apps vs. Real Apps

- Applications:
  - Case 1: a 6x6 degree image mosaic in Montage
  - Case 2: the first 256 queries of NRxNR test in BLAST
  - Case 3: partial seismic study of CyberShake postprocessing on site Test

- Platform configuration:
  - 64 compute nodes on IBM Blue Gene/P
  - Tasks are launched with AMFORA[1]
  - Each task stages input file from GPFS, execute the task, then writes the output files to GPFS

## Montage Statistics

<table>
<thead>
<tr>
<th>Task</th>
<th># Tasks</th>
<th># Inputs</th>
<th># Outputs</th>
<th>Input (MB)</th>
<th>Output (MB)</th>
<th>Skeleton Task Length (uniform)</th>
<th>Interleaving Option</th>
<th>Error in Stage</th>
</tr>
</thead>
<tbody>
<tr>
<td>mProject</td>
<td>1319</td>
<td>1319</td>
<td>2594</td>
<td>2800</td>
<td>10400</td>
<td>11.6</td>
<td>0</td>
<td>-0.2%</td>
</tr>
<tr>
<td>mImgtbl</td>
<td>1</td>
<td>1297</td>
<td>1</td>
<td>5200</td>
<td>0.8</td>
<td>30.1</td>
<td>0</td>
<td>-2.1%</td>
</tr>
<tr>
<td>mOverlaps</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>0.8</td>
<td>0.4</td>
<td>9.1</td>
<td>0</td>
<td>-0.2%</td>
</tr>
<tr>
<td>mDiffFit</td>
<td>3883</td>
<td>7766</td>
<td>7766</td>
<td>31000</td>
<td>487</td>
<td>1.8</td>
<td>0</td>
<td>-3.3%</td>
</tr>
<tr>
<td>mConcatFit</td>
<td>1</td>
<td>3883</td>
<td>1</td>
<td>1.1</td>
<td>4.3</td>
<td>2.1</td>
<td>0</td>
<td>-1.5%</td>
</tr>
<tr>
<td>mBgModel</td>
<td>1</td>
<td>2</td>
<td>1</td>
<td>4.5</td>
<td>0.07</td>
<td>288</td>
<td>0</td>
<td>0.03%</td>
</tr>
<tr>
<td>mBackground</td>
<td>1297</td>
<td>1297</td>
<td>1297</td>
<td>5200</td>
<td>5200</td>
<td>0.4</td>
<td>0</td>
<td>-1.6%</td>
</tr>
<tr>
<td>mAdd</td>
<td>1</td>
<td>1297</td>
<td>1</td>
<td>5200</td>
<td>7400</td>
<td>519</td>
<td>0</td>
<td>-0.9%</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td><strong>-1.3%</strong></td>
</tr>
</tbody>
</table>
## BLAST Statistics

<table>
<thead>
<tr>
<th></th>
<th># Tasks</th>
<th># Inputs</th>
<th># Outputs</th>
<th>Input (MB)</th>
<th>Output (MB)</th>
<th>Skeleton Task Length</th>
<th>Interleaving Option</th>
<th>Error in Stage</th>
</tr>
</thead>
<tbody>
<tr>
<td>split</td>
<td>1</td>
<td>1</td>
<td>64</td>
<td>3800</td>
<td>3800</td>
<td>0</td>
<td>3</td>
<td>-1.9%</td>
</tr>
<tr>
<td>formatdb</td>
<td>64</td>
<td>64</td>
<td>192</td>
<td>3800</td>
<td>4400</td>
<td>uniform 42</td>
<td>3</td>
<td>-0.6%</td>
</tr>
<tr>
<td>blastp</td>
<td>1024</td>
<td>4096</td>
<td>1024</td>
<td>70402</td>
<td>966</td>
<td>normal [109.2, 14.9]</td>
<td>3</td>
<td>1.6%</td>
</tr>
<tr>
<td>merge</td>
<td>16</td>
<td>1024</td>
<td>16</td>
<td>966</td>
<td>867</td>
<td>normal [4.4, 4.1]</td>
<td>3</td>
<td>1.1%</td>
</tr>
<tr>
<td>Total</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>1.4%</td>
</tr>
</tbody>
</table>
## CyberShake PostProcessing Statistics

<table>
<thead>
<tr>
<th></th>
<th># Tasks</th>
<th># Inputs</th>
<th># Outputs</th>
<th>Input (MB)</th>
<th>Output (MB)</th>
<th>Skeleton Task Length</th>
<th>Interleaving Option</th>
<th>Error in Stage</th>
</tr>
</thead>
<tbody>
<tr>
<td>Extract</td>
<td>128</td>
<td>130</td>
<td>256</td>
<td>5400</td>
<td>11000</td>
<td>uniform 6.39</td>
<td>0</td>
<td>2.6%</td>
</tr>
<tr>
<td>Seis</td>
<td>4096</td>
<td>4352</td>
<td>4096</td>
<td>11000</td>
<td>96</td>
<td>normal [26.9, 13.3]</td>
<td>0</td>
<td>2.4%</td>
</tr>
<tr>
<td>PeakGM</td>
<td>4096</td>
<td>4096</td>
<td>4096</td>
<td>96</td>
<td>1.4</td>
<td>uniform 0.23</td>
<td>0</td>
<td>2.3%</td>
</tr>
<tr>
<td>Total</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>2.4%</td>
</tr>
</tbody>
</table>
Using Application Skeletons

- Data Caching
  - Comparing shared file system (PVFS) and in-memory file system (AMFORA) performance for mProjectPP
  - Using 64 n1-highmem-2 instances on Google Compute Engine (GCE)

<table>
<thead>
<tr>
<th></th>
<th>PVFS</th>
<th>AMFORA</th>
<th>Improvement</th>
</tr>
</thead>
<tbody>
<tr>
<td>mProjectPP-real</td>
<td>285.2 seconds</td>
<td>100.9 seconds</td>
<td>63.0%</td>
</tr>
<tr>
<td>mProjectPP-skeleton</td>
<td>273.7 seconds</td>
<td>101.3 seconds</td>
<td>64.6%</td>
</tr>
</tbody>
</table>
Using Application Skeletons

- Task Scheduling
  - Data-aware scheduling vs. FIFO
  - Using 16 n1-highmem-2 GCE instances

- mProjectPP-real has 0.7% improvement
- mProjectPP-skeleton has 1.6% improvement

- Used skeletons to show: 5x larger input file size => 16.4% time-to-solution improvement with data-aware scheduling
Using Application Skeletons

- I/O Tuning
  - Multiple metadata server vs. Single metadata server
  - Using 16 n1-highmem-2 instances

- mProjectPP-real shows 1.1% improvement
- mProjectPP-skeleton shows 1.2% improvement

- Use skeletons to show: 10x shorter task length => 31.2% improvement for multiple metadata servers
Related Work

- Simplify parallel application code
  - Extract kernels: NAS Parallel Benchmarks, Berkeley Dwarfs/Motifs, CORAL benchmarks, etc.
  - Simplify non-kernel part of app: Kerbyson (SC12), Worley (SC94), miniapps (e.g., Mantevo, MADbench)
- Simplify parallel applications in time
  - Sodhi (Cluster 2008)
- Use system traces in place of applications
  - Chen (VLDB12), Harter (FAST14), Ouserhout (NSDI15)
- Skeleton-like approaches
  - Skel (for I/O), Tigres (distributed app templates), WGL (similar to our work, but simpler)
- Other work that used the term skeleton
- See FGCS paper for comparisons
Conclusion

- Skeleton tool can compose skeleton application in a top-down manner: application, stage, task
- Skeleton task abstraction allows specification of task type, task length, number of processes, I/O buffer, I/O quantity, interleaving option, and file number
- Can create easy-to-access, easy-to-build, easy-to-change, and easy-to-run bag-of-tasks, (iterative) map-reduce, and (iterative) multi-stage workflow applications
- Skeleton applications can be easily shared, making middleware and tool experiments more reproducible
- Skeleton applications have performance close to that of the real applications with an overall error of -1.3%, 1.5%, and 2.4% for Montage, BLAST, and CyberShake PostProcessing
- Skeletons can show the effectiveness of system improvements such as data caching, task scheduling, I/O tuning
Future Work

- Use application trace data to produce skeleton applications
- Determine a way to represent the computational work in a task that when combined with a particular platform can give an accurate runtime for that task
- Support concurrent tasks that need to run at the same time to exchange information
- Test on distributed systems where latencies, particular file usage, and other issues may be more important than on the parallel systems and cloud environments
References

- **Software:**
  - The Skeleton tool is open source at: https://github.com/applicationskeleton/Skeleton
  - Try it! Contribute to it!

- **Papers:**
Acknowledgements

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