Hybrid Dataflow Programming on Blue Waters

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http://swift-lang.org
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When do you need parallel scripting?

Typical application: protein-ligand docking for drug screening

- $O(10)$ proteins implicated in a disease
- $O(10^6)$ drug candidates

Tens of fruitful candidates for wetlab & APS

Work of M. Kubal, T.A. Binkowski, and B. Roux
Problem: *How to code such applications?*

```
foreach p, i in proteins {
    foreach c, j in ligands {
        (structure[i,j], log[i,j]) = dock(p, c, minRad);
    }
}

scatter_plot = analyze(structure)
```
Solution: *A compact, portable script*

**Swift code excerpt:**

```swift
foreach p, i in proteins {
    foreach c, j in ligands {
        (structure[i,j], log[i,j]) =
            dock(p, c, minRad, maxRad);
    }
}
scatter_plot = analyze(structure)
```

**To run:**

```
swift --site stampede,trestles \
  docksweep.swift
```
Programming model: all execution driven by parallel data flow

```c
(int r) myproc (int i)
{
    j = f(i);
    k = g(i);
    r = j + k;
}
```

f() and g() are computed in parallel
myproc() returns r when they are done

This parallelism is *automatic*
Works recursively throughout the program’s call graph
Pervasive parallel data flow

Fig. 1: Task and data dependencies in data-driven task parallelism, forming a spawn tree rooted at task $a$. Data dependencies on shared data defer execution of tasks until the variables are finalized.
Swift runs across diverse parallel platforms

Submit host (login node, laptop, Linux server)

Swift script

Apps

Data

http://swift-lang.org
...but centralized evaluation is a bottleneck at extreme scales

Had this:
(Swift/K)

For extreme scale, we need this:
(Swift/T)

Centralized evaluation

Distributed evaluation
ExM – Extreme scale Many-task computing

Compiler Techniques for Massively Scalable Implicit Task Parallelism

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http://swift-lang.org
MPI process architecture for parallel evaluation in Swift/T

Legend:
- □ Process
- → Task flow

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**GeMTC**: GPU-enabled Many-Task Computing

**Motivation**: Support for MTC on all accelerators!

**Goals**:
1) MTC support  
2) Programmability  
3) Efficiency  
4) MPMD on SIMD  
5) Increase concurrency from 15 to 192 (~13x)

**Approach**:
Design & implement GeMTC middleware:
1) Manages GPU  
2) Spread host/device  
3) Workflow system integration (with Swift/T)
GeMTC API

Device Management
- gemtcSetup()
- gemtcCleanup()

Task Management
- gemtcPush()
- gemtcPoll()

Data Movement
- gemtcMemcpyDevToHost()
- gemtcMemcpyHostToDevice()

Memory Management
- gemtcGPUMalloc()
- gemtcGPUFree()
GeMTC AppKernels

- Precompiled into GeMTC Framework
- Optimized for Single Warp Execution
  - (Future: Bond multiple warps for one task)
- Previous AppKernel Work:
  - Molecular Dynamics, Synthetic Benchmarks
- Current AppKernel Work:
  - BLAS functionality, etc.
    - SAXPY, SGEMM, Image processing, Black Scholes
Swift/T + GeMTC Node Layout

Node 0

Server
CPU Worker
CPU Worker
GeMTC Worker
GPU

Node 1

Server
CPU Worker
CPU Worker
GeMTC Worker
GPU

...

Node N

Server
CPU Worker
CPU Worker
GeMTC Worker
GPU

Work Stealing

http://swift-lang.org
Multi Node Scaling (MD proxy app)

Walltime (seconds)

Level of Concurrency

http://swift-lang.org
GeMTC throughput on Blue Waters

http://swift-lang.org
GeMTC + Swift Throughput 10K GPU Workers

http://swift-lang.org
GeMTC Efficiency 86K GPU Workers
One worker per GPU
GeMTC Efficiency: 86K GPU Workers
168 active workers per GPU
Swift/T: scaling of trivial foreach `{ }` loop
100 microsecond to 10 millisecond tasks
on up to 512K integer cores of Blue Waters

Advances in compiler and runtime optimization enable Swift to be applied in new in-memory programming models.
Swift/T application benchmarks on Blue Waters

(a) Sweep weak scaling: 0.2 ms tasks
(b) Sweep weak scaling: 0.5 ms tasks
(c) ReduceTree scaling: 0 s tasks
(d) UTS scaling
(e) Wavefront: 5ms tasks
(f) Annealing strong scaling: 256 annealing processes × 2000 tasks per objective function × 5 parameter updates

Fig. 10: Application speedup and scalability at different optimization levels. X axes show scale in cores. Primary Y axes show application throughput in application-dependent terms. Secondary Y axes show problem size or degree of parallelism where applicable.
Future Work

• Evaluate additional applications
  • Cancer gene detection, glass modelling
• Support other accelerators (Phi, AMD)
• Simplify the development of task kernels (OpenCL, OpenACC?)
• More efficient node utilization (CPU)
• Bond multiple warps for a single worker
• CUDA 6 Enhancements (Unified Memory…)

http://swift-lang.org
Code, docs and downloads

GeMTC:
http://datasys.cs.iit.edu/projects/GeMTC
https://github.com/skrieder/gemtc

Swift:
http://swift-lang.org

Swift/T and Turbine:
http://mcs.anl.gov/exm/local/guides/swift.html
Publications

- Scott J. Krieder, Ioan Raicu - “Early Experiences in running Many-Task Computing workloads on GPUs” - XSEDE 2012 - Chicago, IL (07/2012)
- Scott J. Krieder, Ioan Raicu - “An Overview of Current and Future Accelerator Architectures” - Greater Chicago Area System Research Workshop - Chicago, IL (05/2012)
Conclusions

• More efficient MTC on NVIDIA GPUs
• MPMD on SIMD
• Evaluated synthetic benchmarks and proxy molecular dynamics app on Blue Waters
• Integrated GeMTC with a higher-level programming model (Swift’s implicitly parallel functional dataflow)
• Achieved new scaling breakthroughs for an implicitly-parallel programming model