Hybrid Dataflow Programming on Blue Waters

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Blue Waters Symposium, 2014

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http://swift-lang.org

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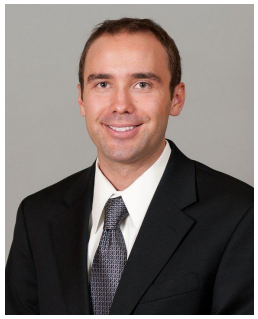
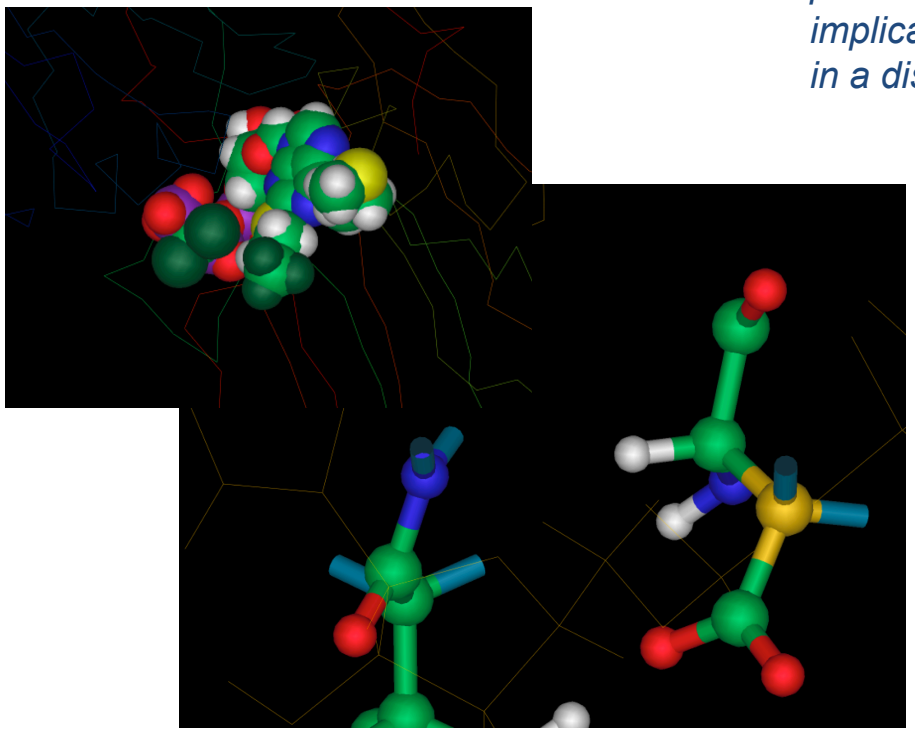
Supported in part by Blue Waters/GLCPC, NSF SI2, and DOE-ASCR X-Stack




When do you need parallel scripting?

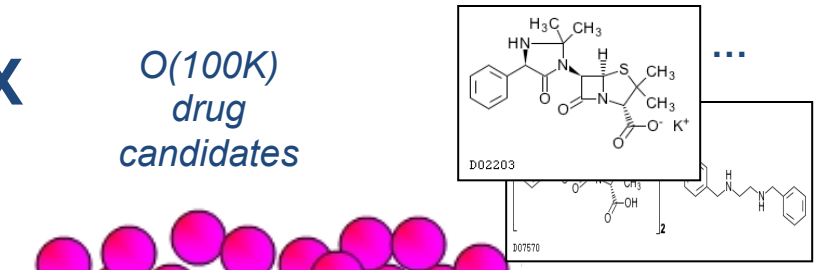
Typical application: protein-ligand docking for drug screening

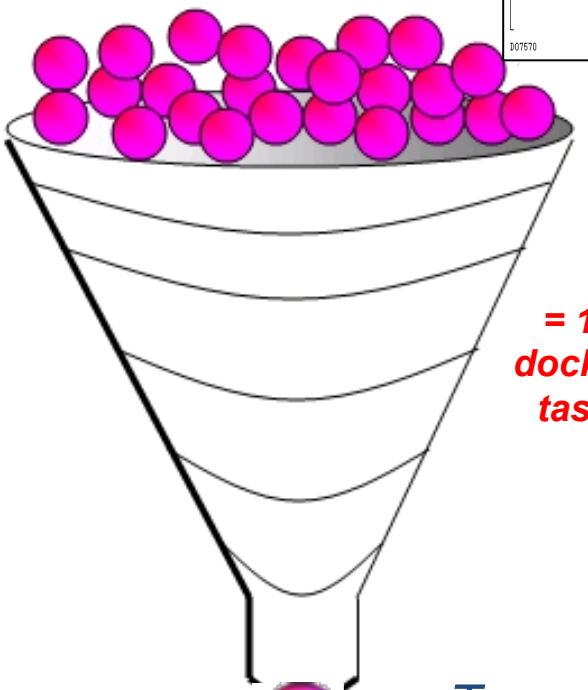


O(10) proteins implicated in a disease

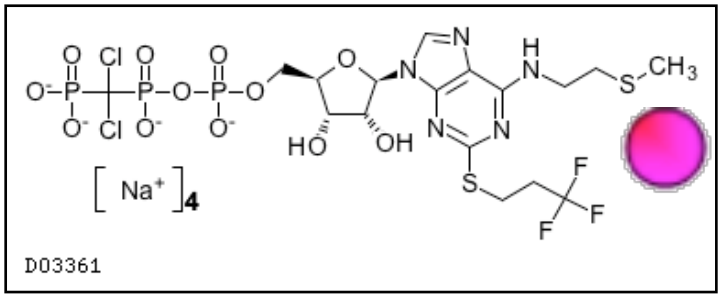
X

O(100K) drug candidates





= 1M docking tasks

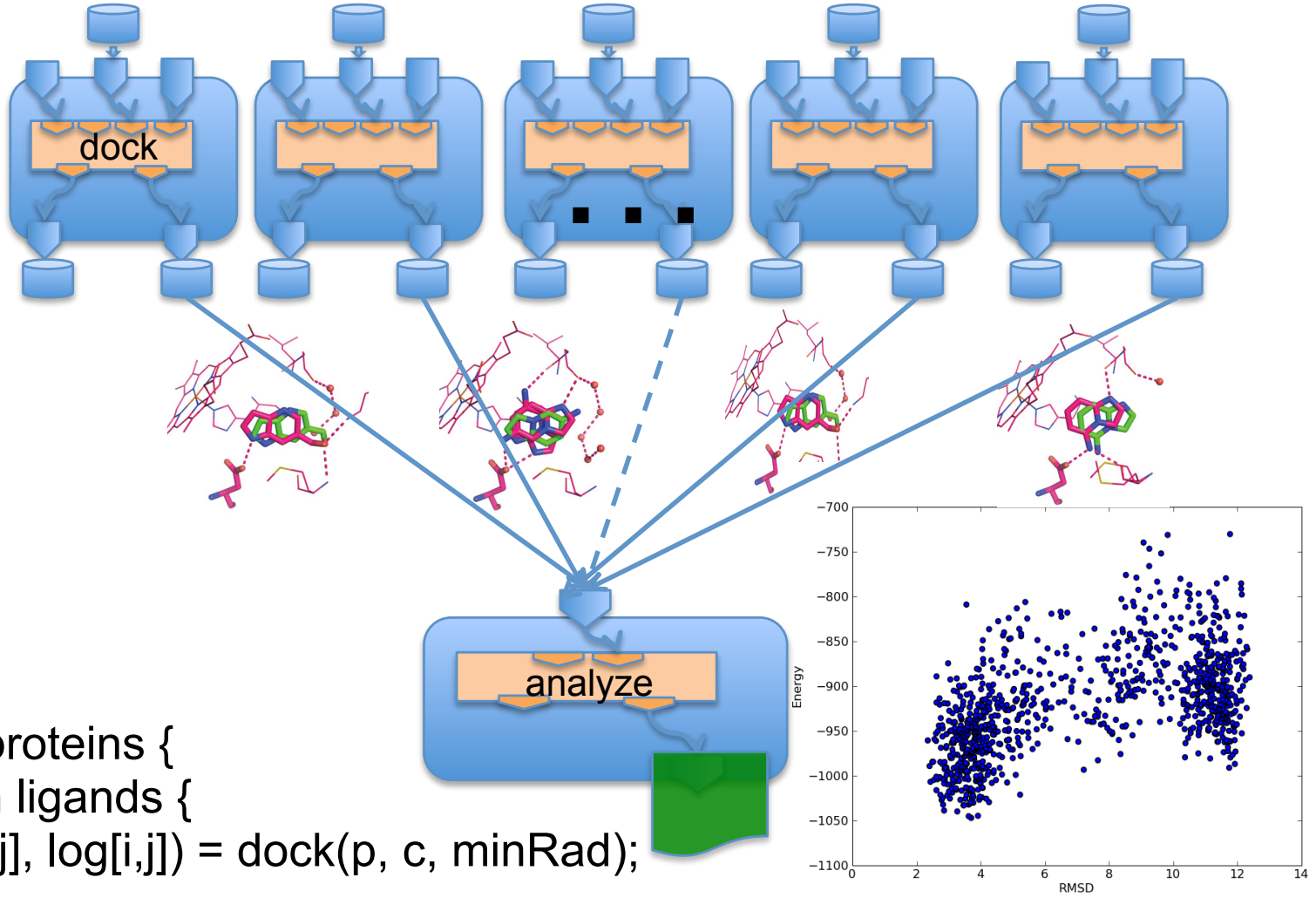


Tens of fruitful candidates for wetlab & APS

Work of M. Kubal, T.A.Binkowski, and B. Roux

Problem: *How to code such applications?*

1,000,000 runs of the "dock" application




```
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:

```
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

```
(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

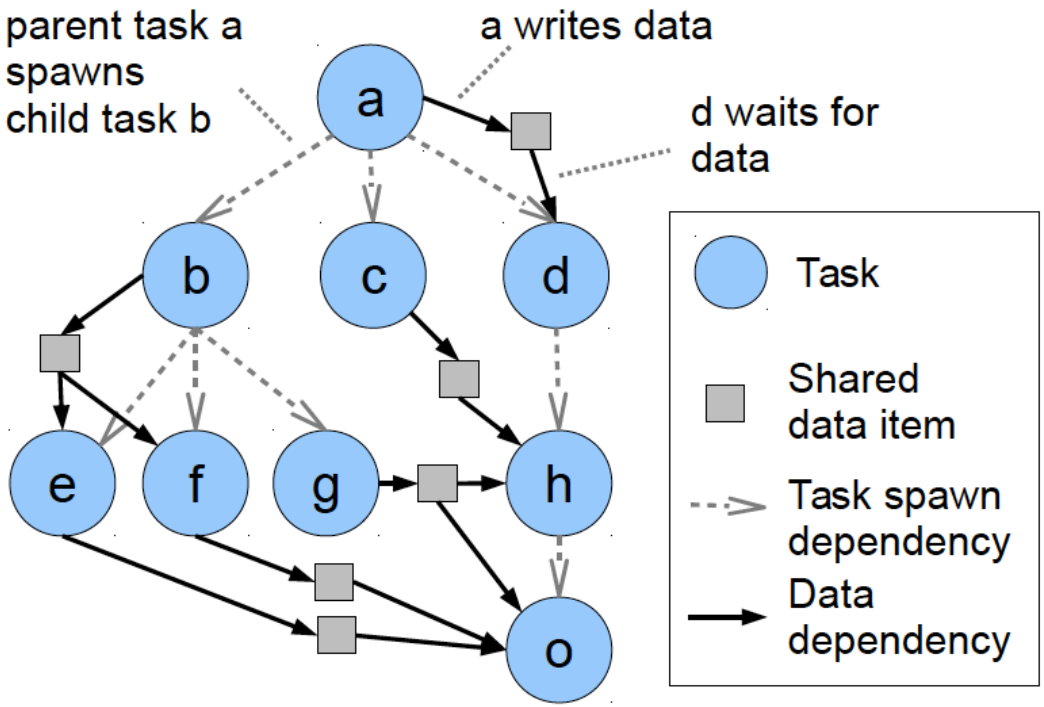
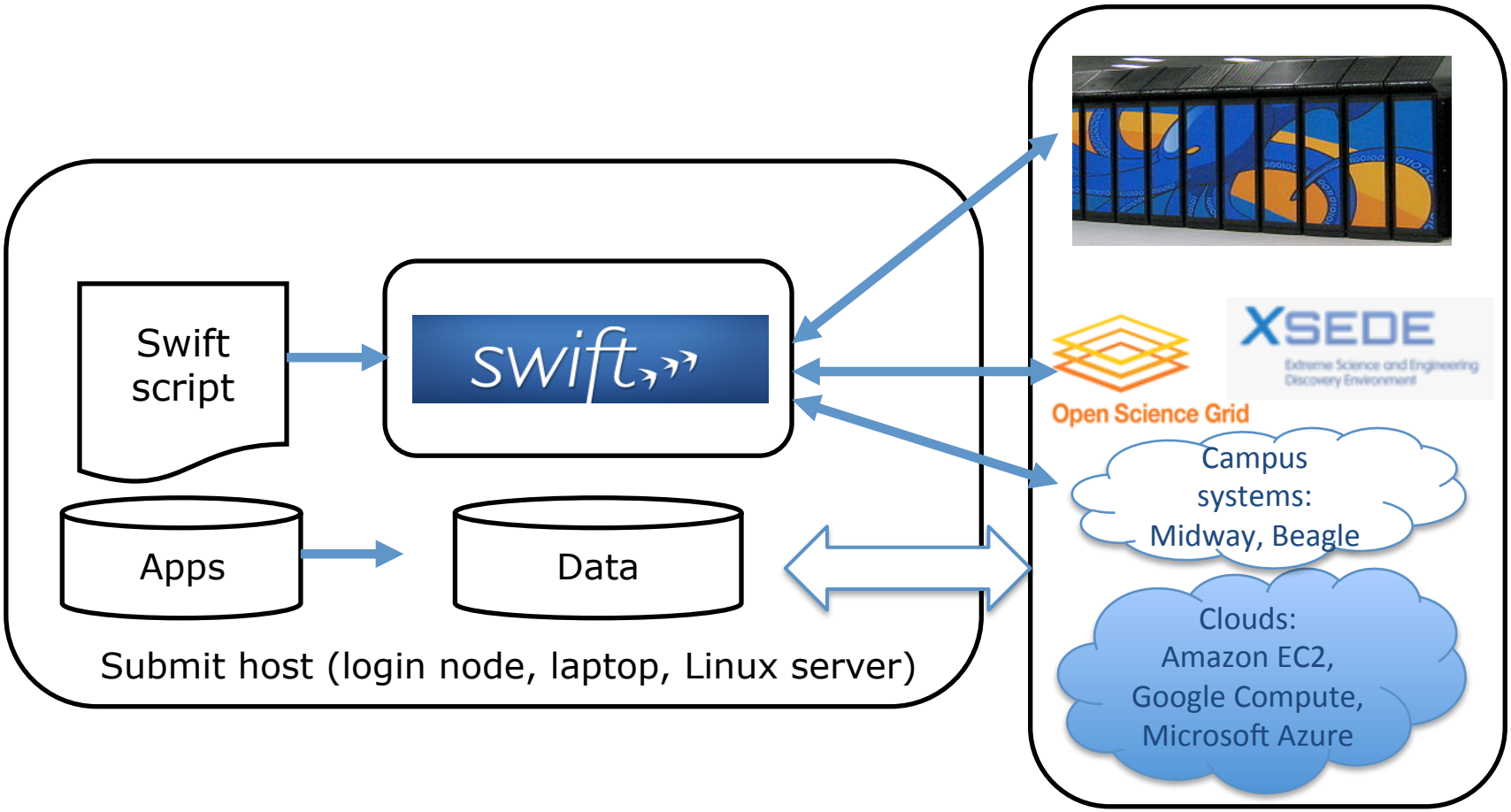
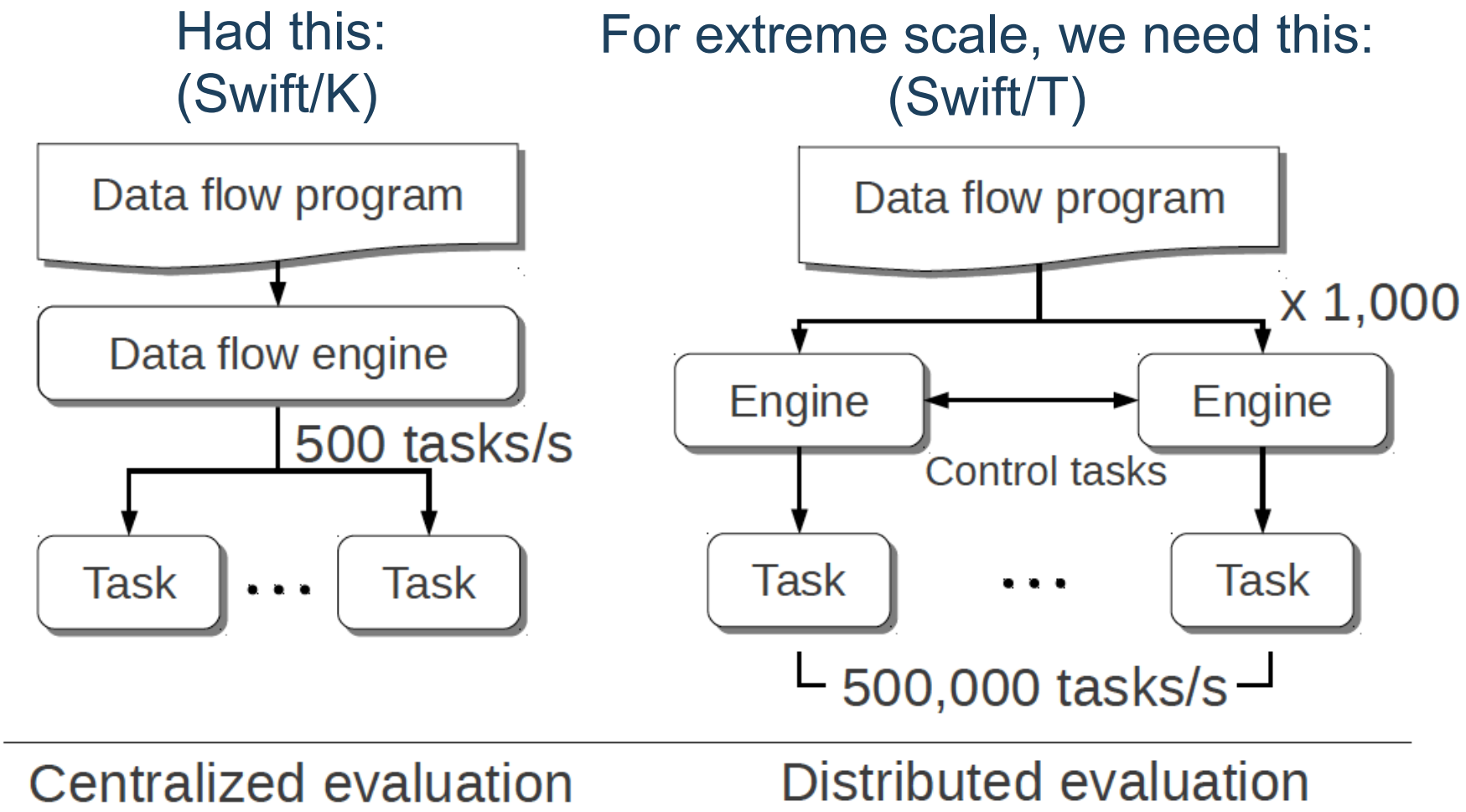


Fig. 1: Task and data dependencies in data-driven task parallelism, forming a spawn tree rooted at task a. Data dependencies on shared data defer execution of tasks until the variables are finalized.

Swift runs across diverse parallel platforms



…but centralized evaluation is a bottleneck at extreme scales



ExM – Extreme scale Many-task computing

Compiler Techniques for Massively Scalable Implicit Task Parallelism

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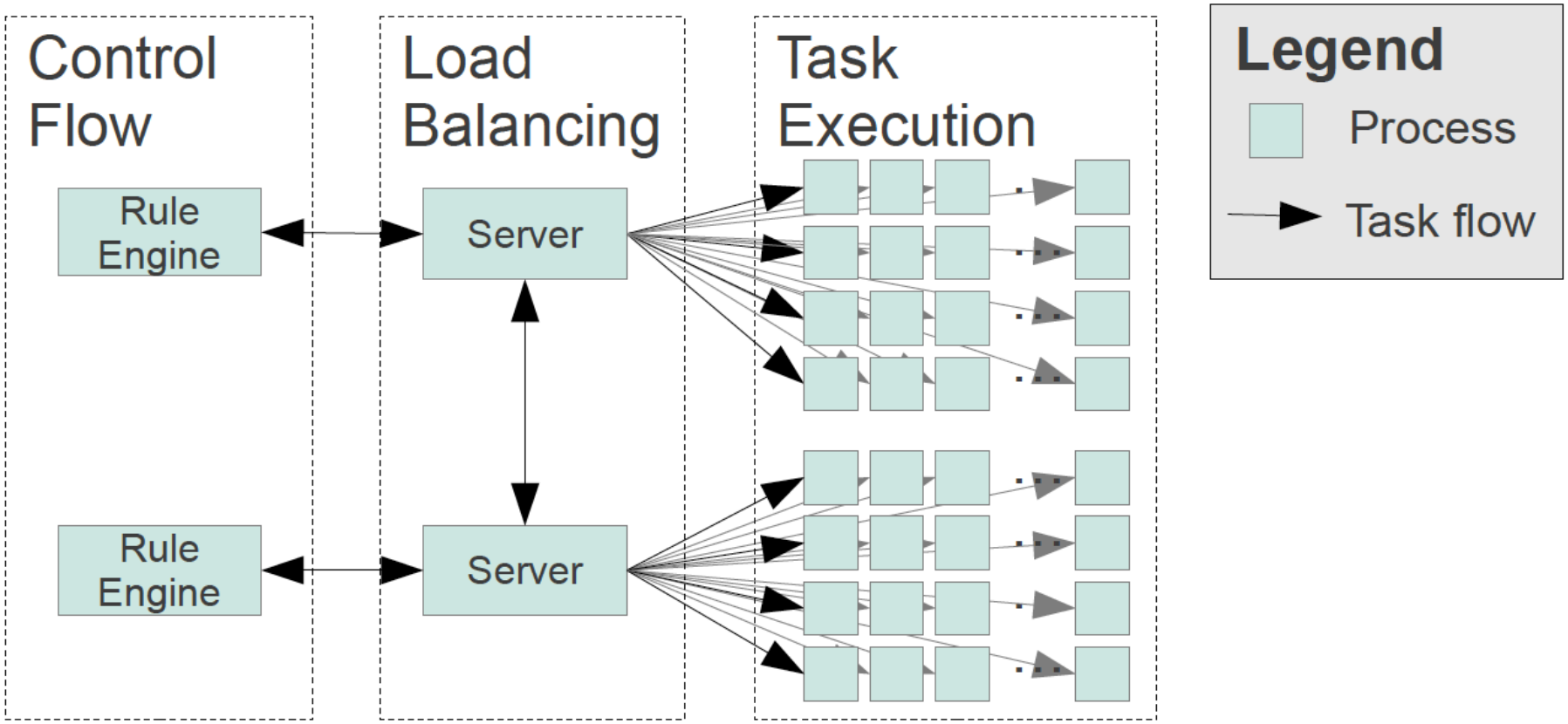
http://people.cs.uchicago.edu/~tga/pubs/stc-preprint-apr14.pdf

MPI process architecture for parallel evaluation in Swift/T



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

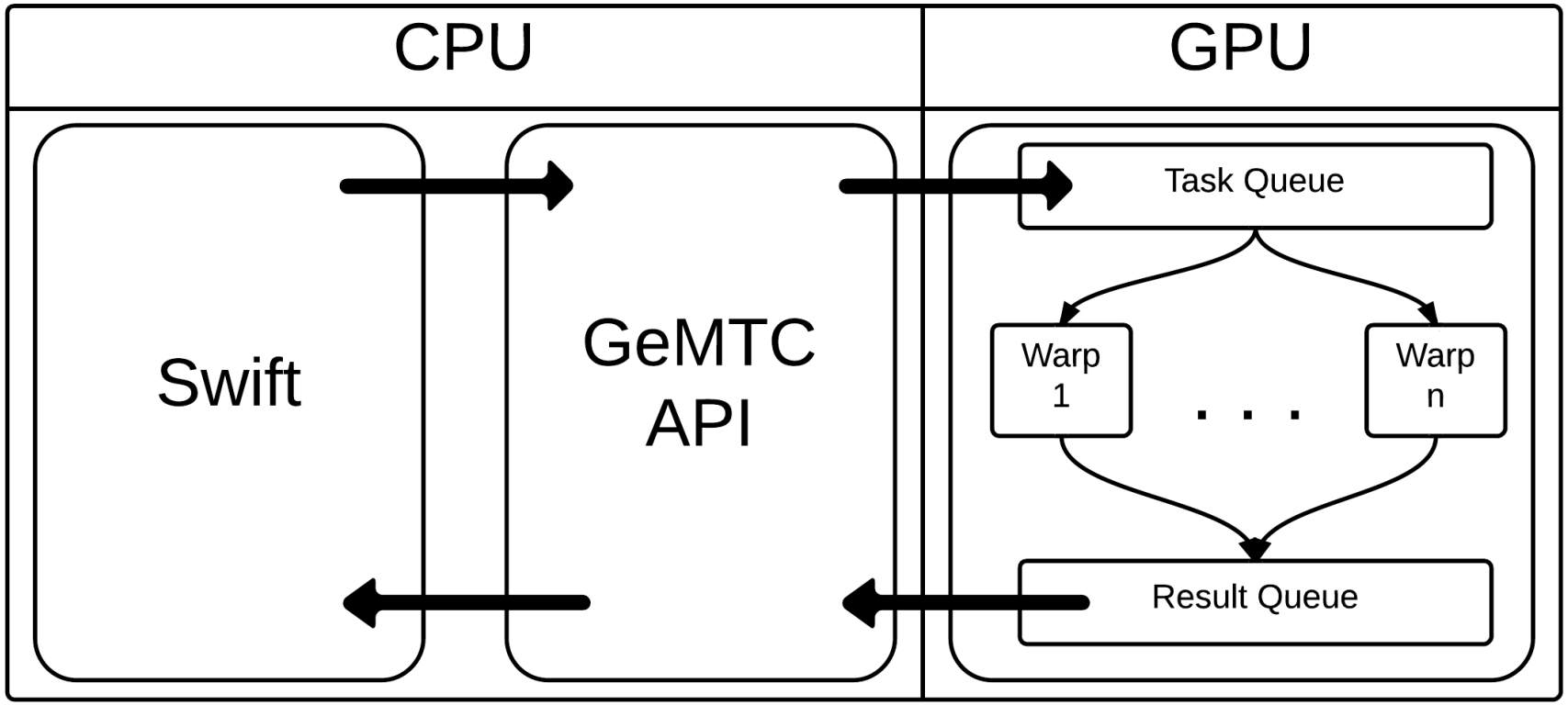
5) Increase concurrency from 15 to 192 (~13x)

Approach:

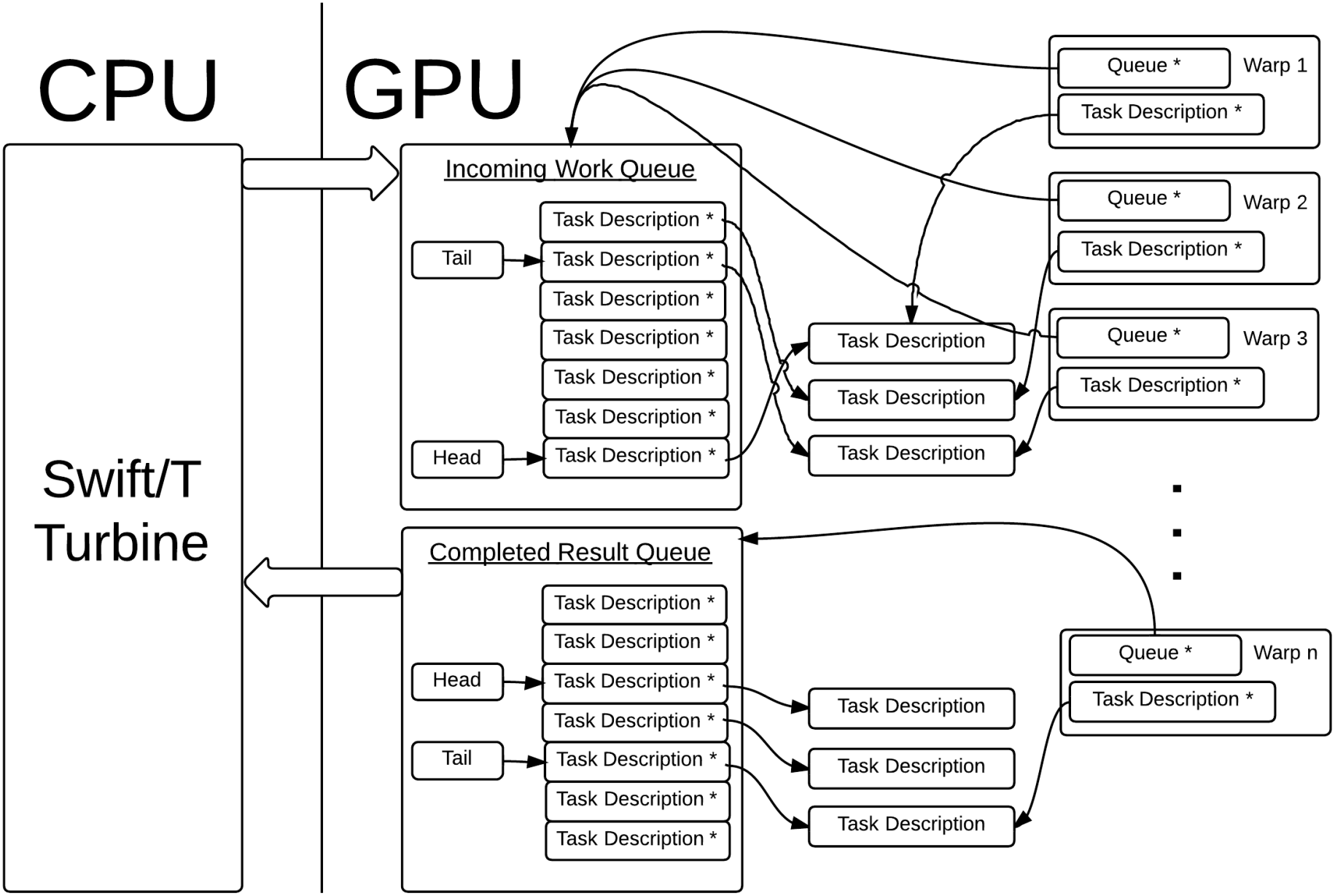
Design & implement GeMTC middleware:

1) Manages GPU 2) Spread host/device

3) Workflow system integration (with Swift/T)



GeMTC Architecture



GeMTC API

Device Management

- gemtcSetup()
- gemtcCleanup()

Data Movement

- gemtcMemcpyDevToHost()
- gemtcMemcpyHostToDev()

Task Management

- gemtcPush()
- gemtcPoll()

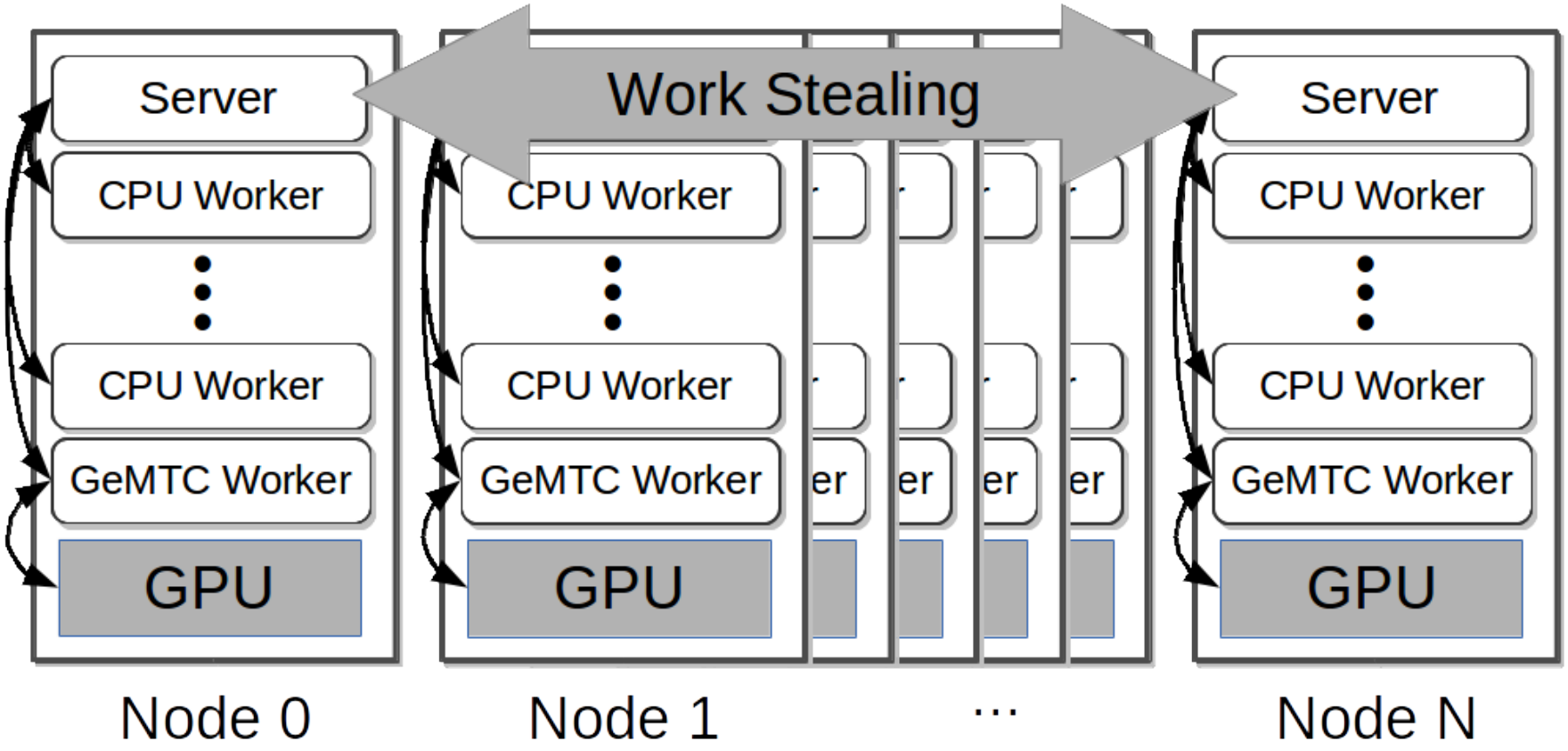
Memory Management

- gemtcGPUMalloc()
- gemtcGPUFree()

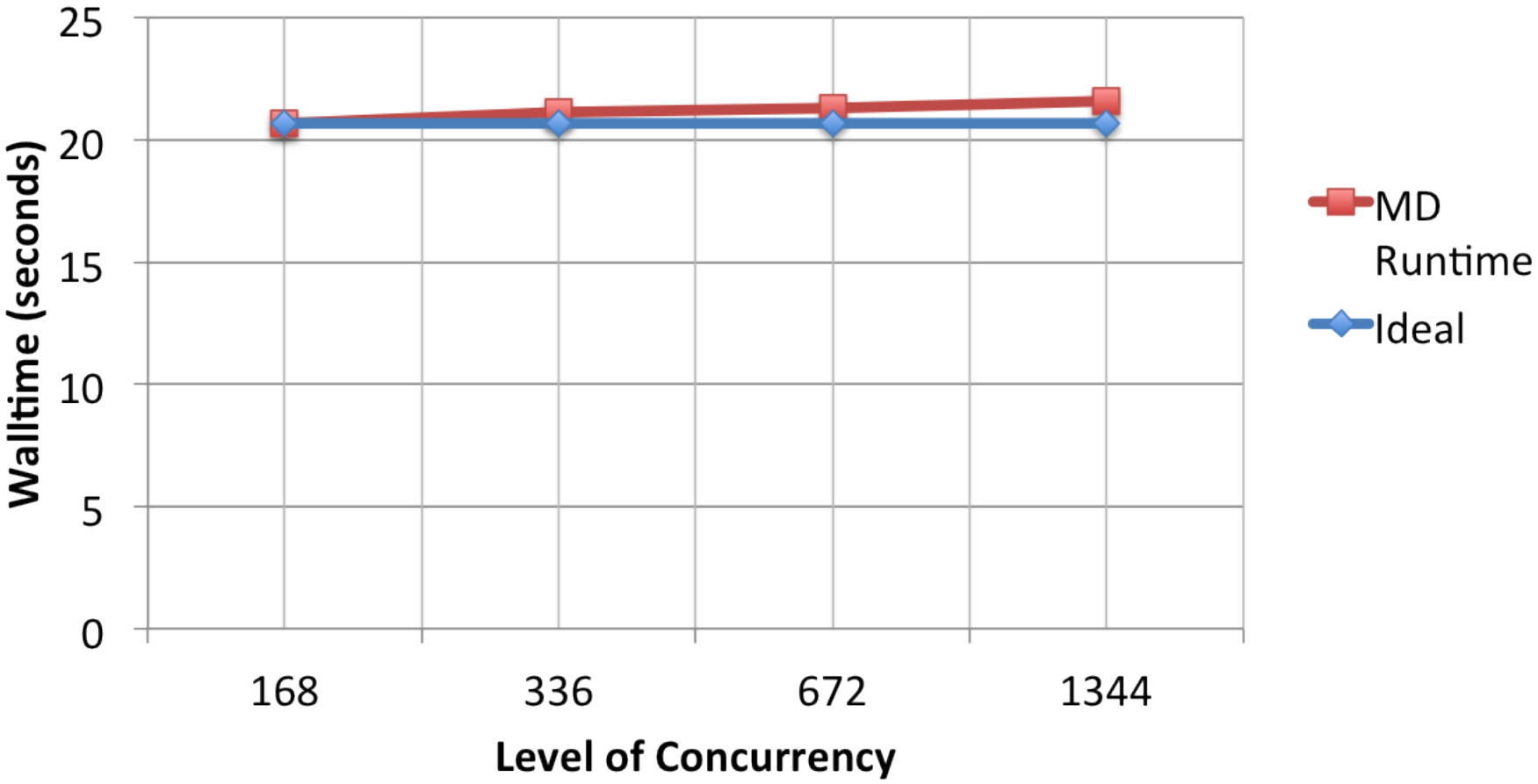
GeMTC AppKernels

- 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

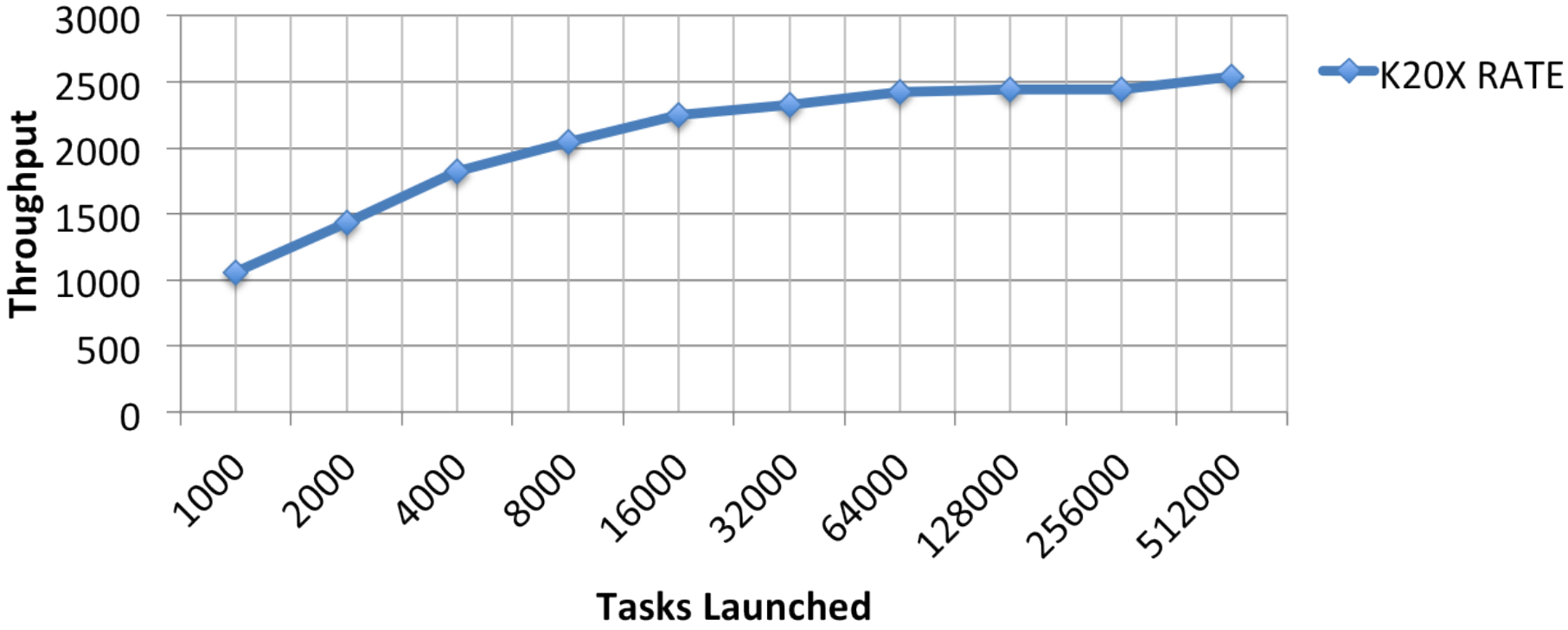
Swift/T + GeMTC Node Layout



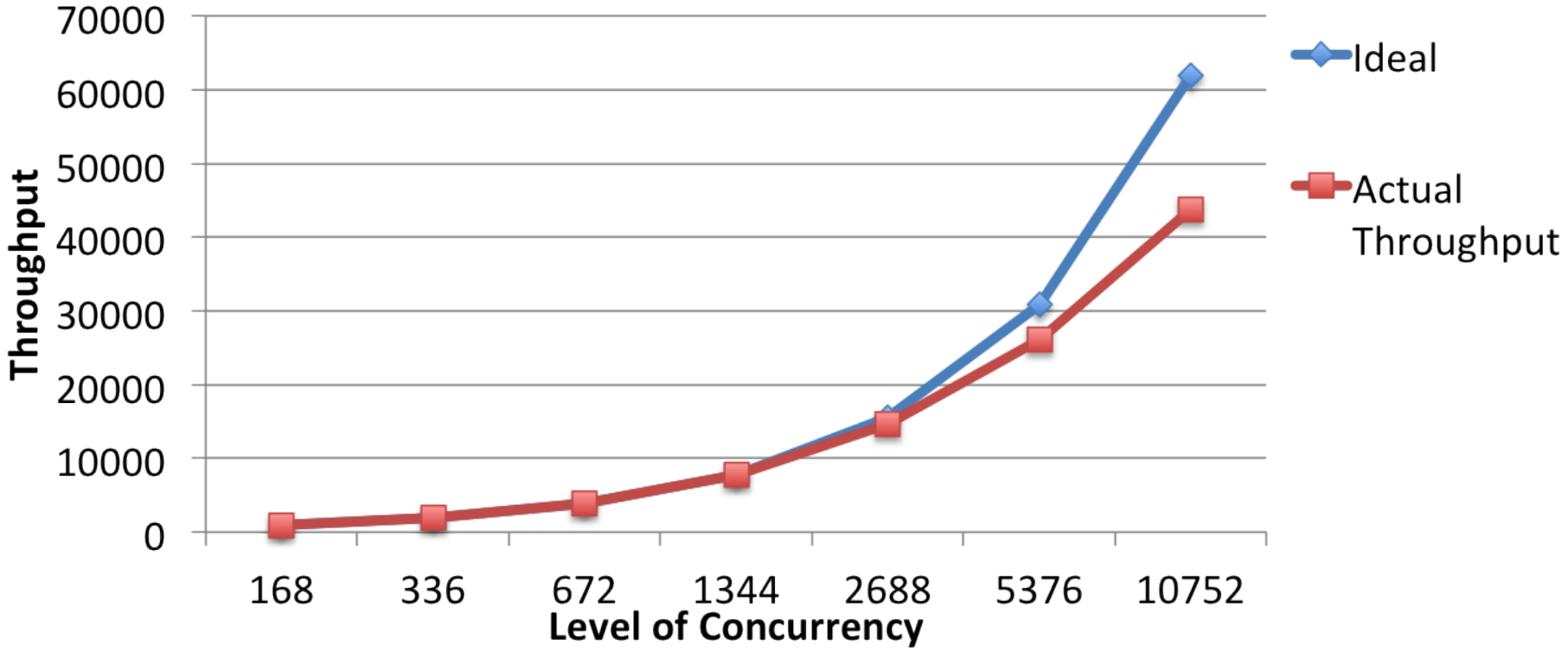
Multi Node Scaling (MD proxy app)



GeMTC throughput on Blue Waters

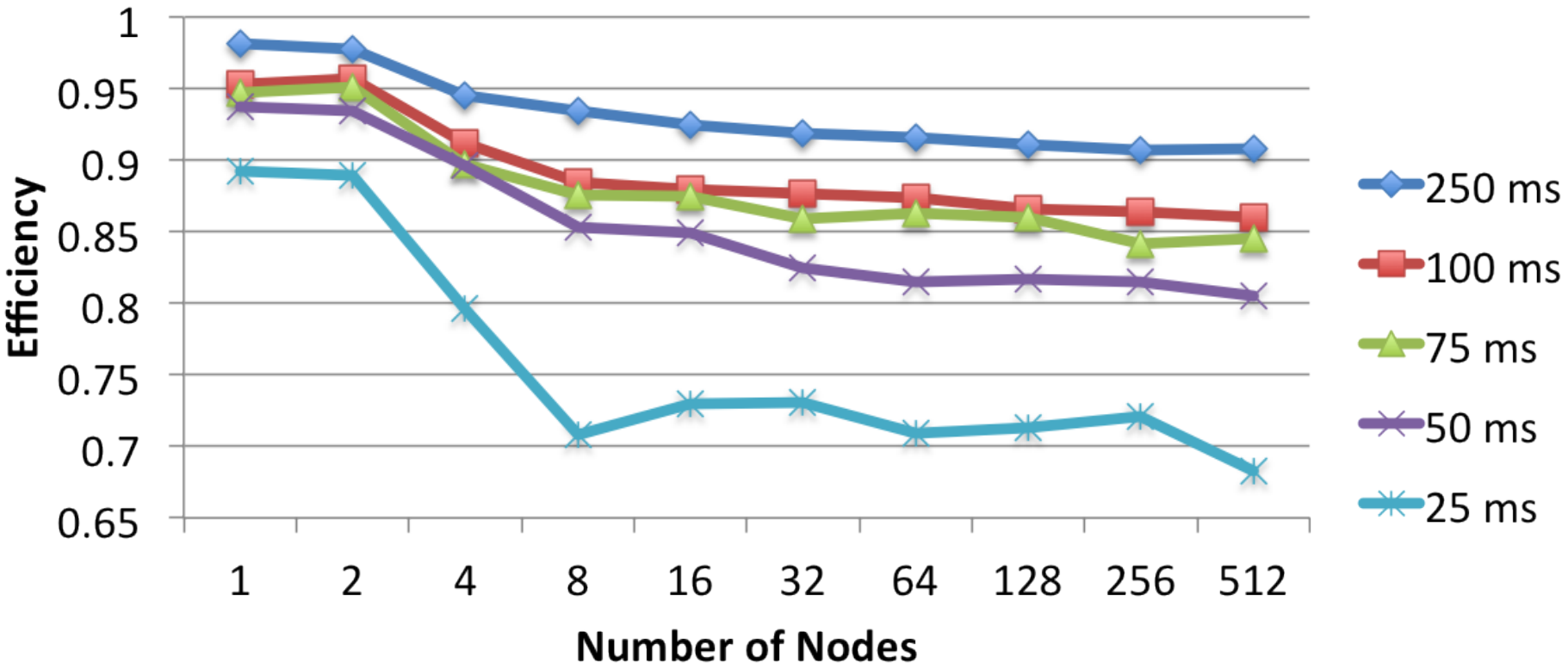


GeMTC + Swift Throughput 10K GPU Workers



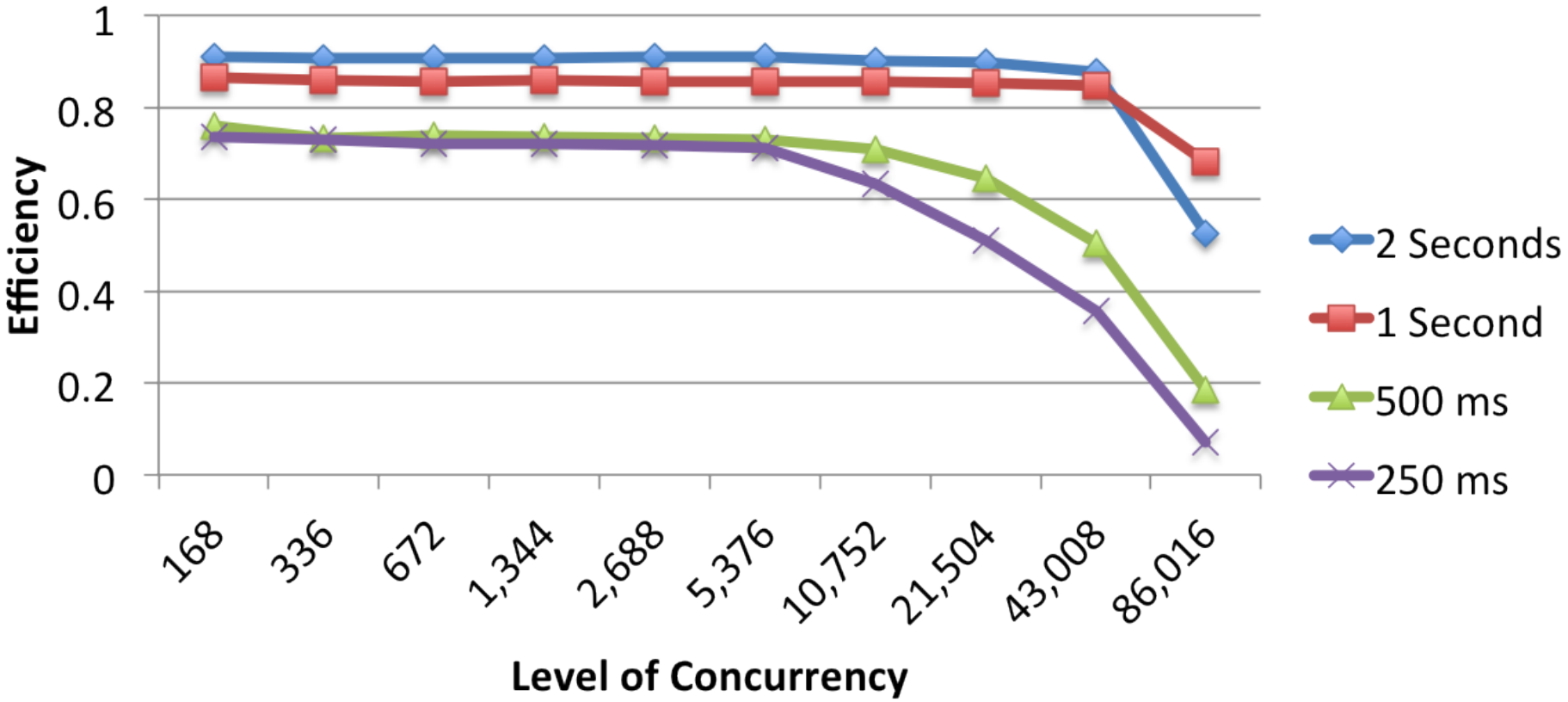
GeMTC Efficiency 86K GPU Workers

One worker per GPU



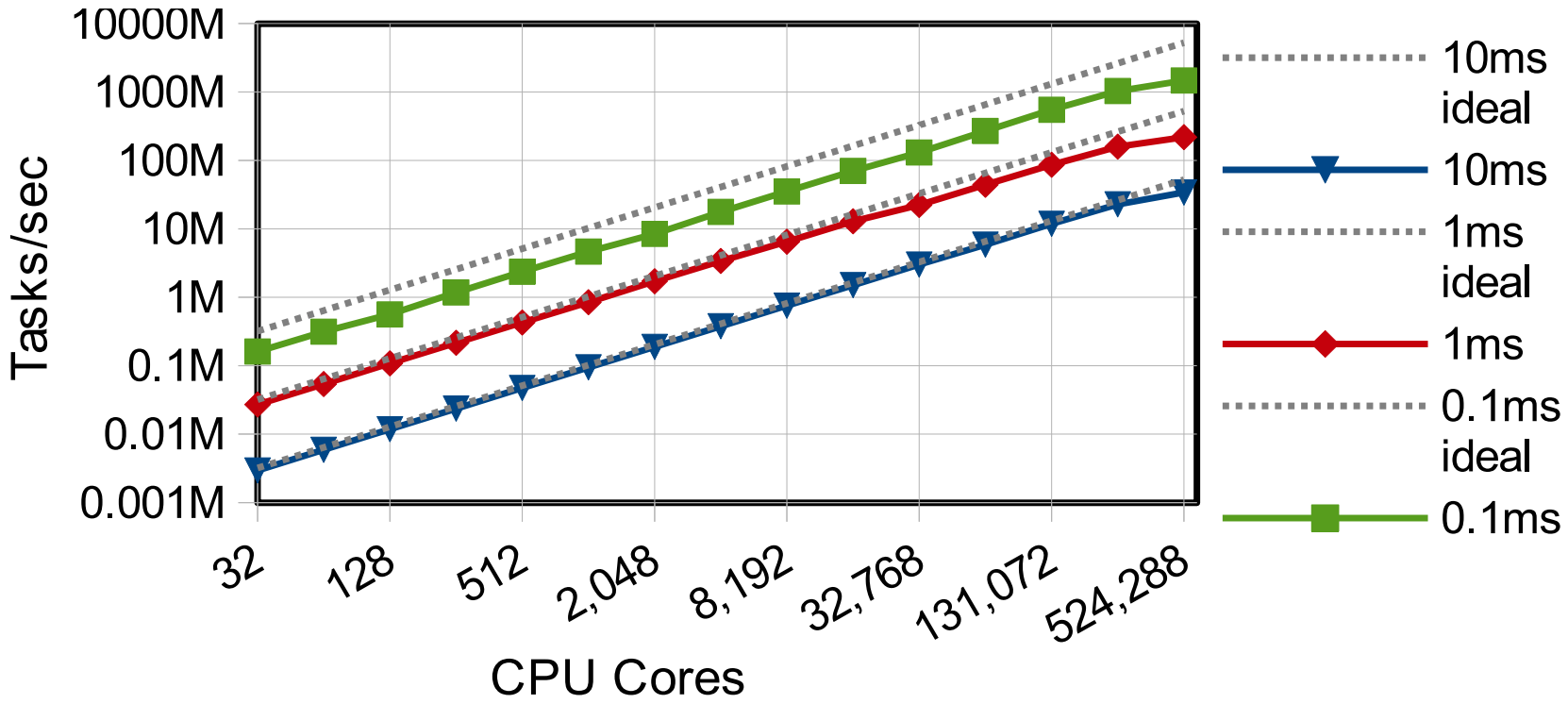
GeMTC Efficiency: 86K GPU Workers

168 active workers per GPU



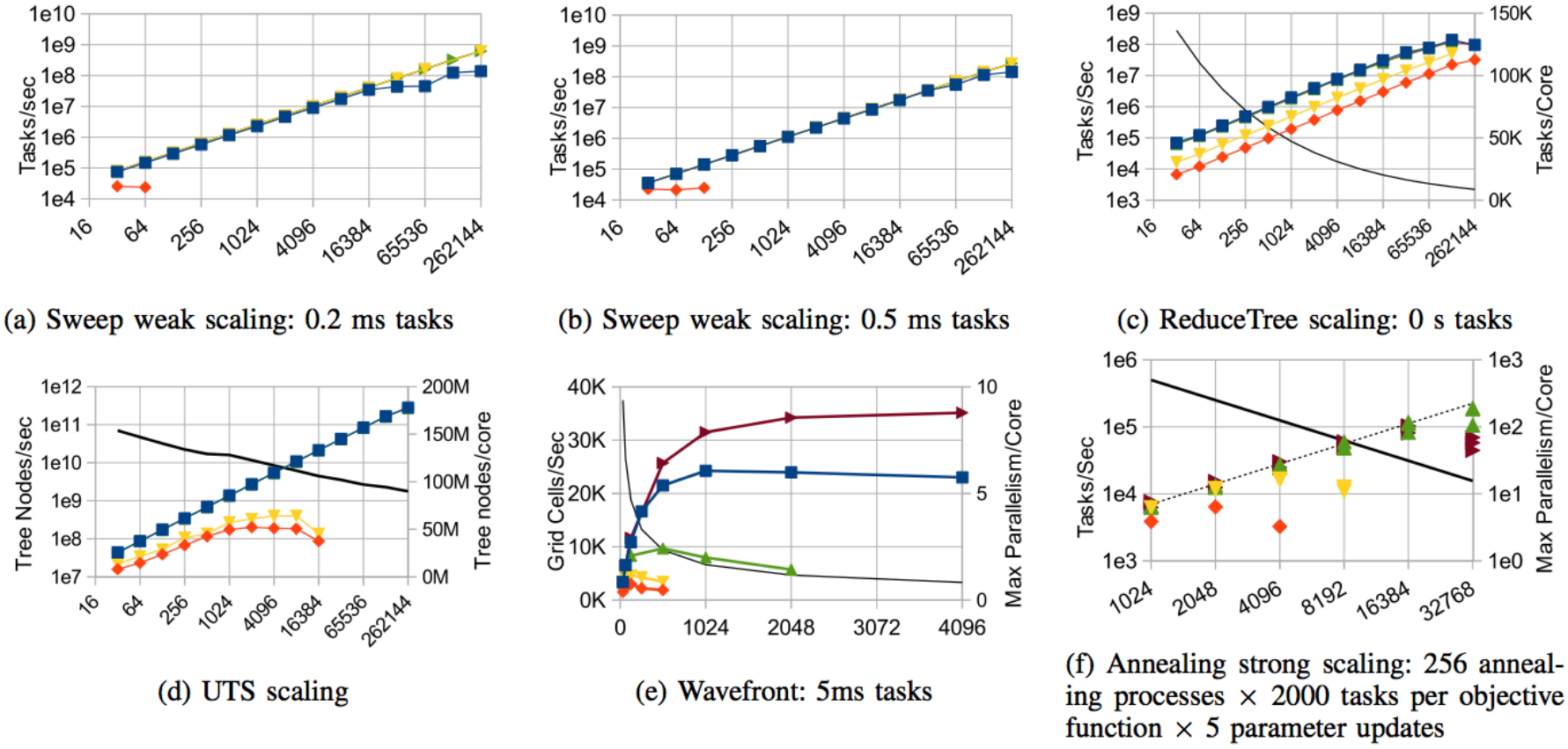
Swift/T: scaling of trivial foreach { } loop

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.
http://people.cs.uchicago.edu/~tga/pubs/stc-preprint-apr14.pdf

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…)

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, Justin M. Wozniak, Timothy Armstrong, Michael Wilde, Daniel S. Katz, Benjamin Grimmer, Ian T. Foster, Ioan Raicu. “ Design and Evaluation of the GeMTC Framework for GPU-enabled Many-Task Computing”, HPDC'14
- Benjamin Grimmer, Scott Krieder, Ioan Raicu. "Enabling Dynamic Memory Management Support for MTC on NVIDIA GPUs", EuroSys 2013 (poster)
- Scott J. Krieder, Ioan Raicu, “ Towards the Support for Many-Task Computing on Many Core Computing Platforms” - IEEE/ACM Supercomputing 2012 (SC’12) - Salt Lake City, UT (11/2012)
- 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