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Accelerating Scientific Workflow Applications with GPUs

DataSys
Data-Intensive Distributed Systems Laboratory

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Abstract

This work analyzes the performance increases gained from enabling Swift applications to utilize the GPU through the GeMTC Framework. By identifying computationally intensive portions of Swift applications, we can easily turn these code blocks into GeMTC microkernels. Users can then call these microkernels throughout the lifetime of their Swift application. The GeMTC API handles task overlap and data movement, providing transparent GPU acceleration for the user. This work highlights preliminary performance results from the scientific application MDProxy. This application determines the energy of particles in a modeled universe as they move around in space.

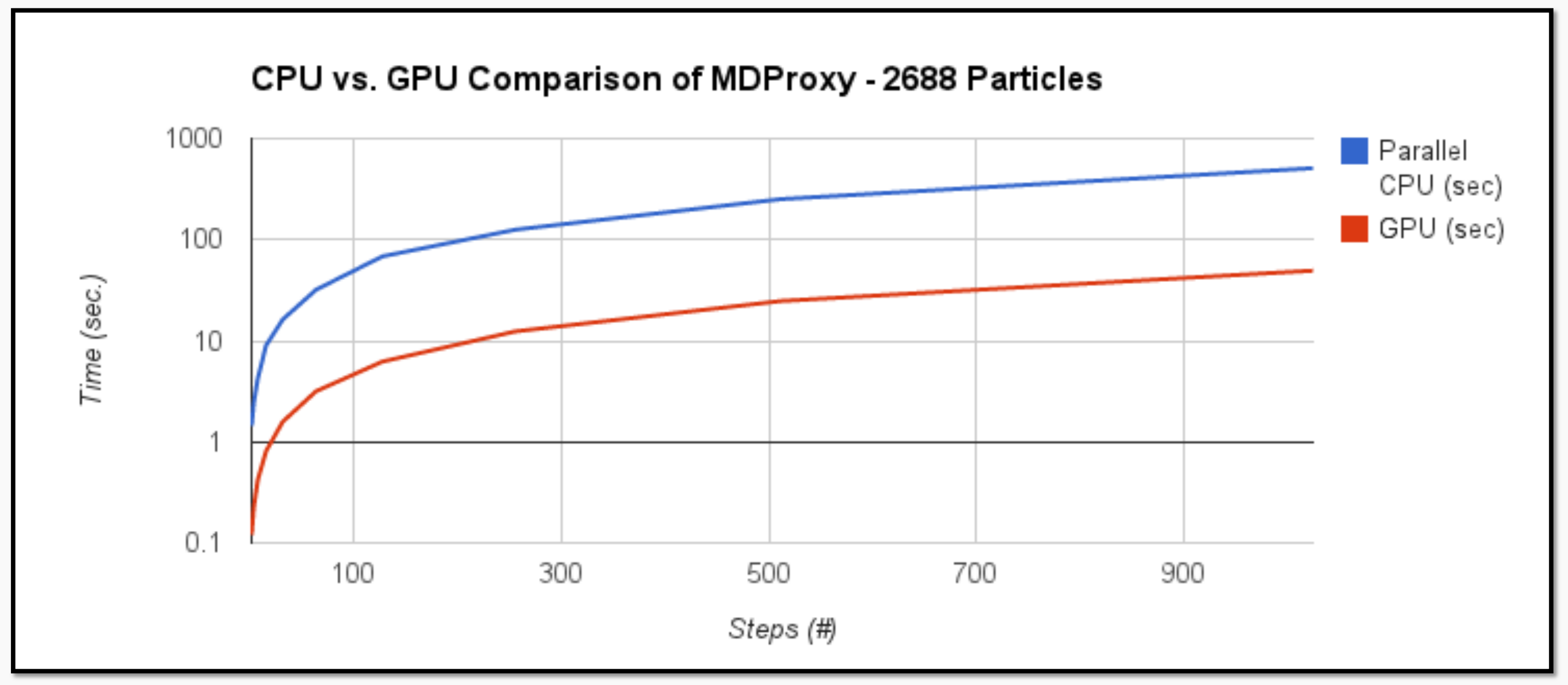
What is GeMTC?

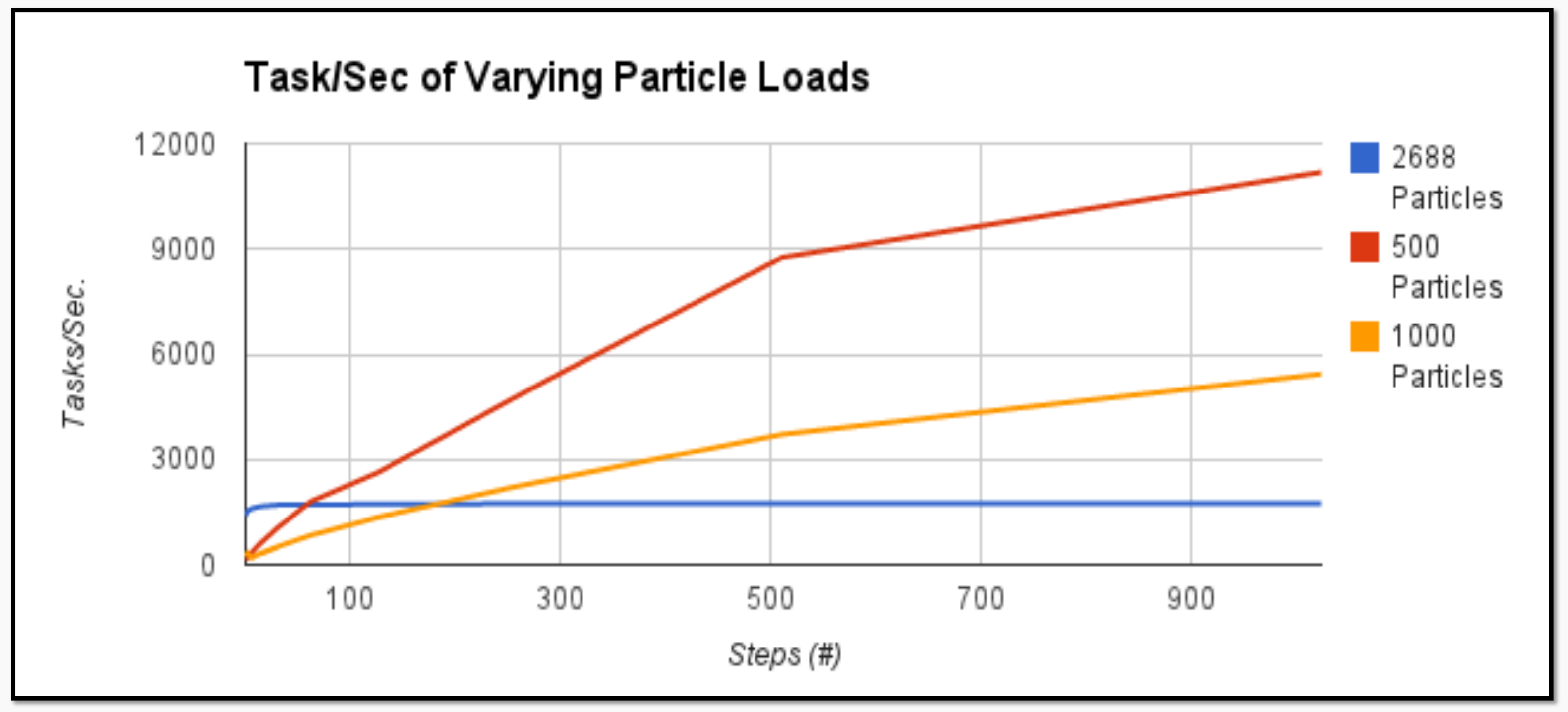
GeMTC (GPU enabled Many-Task Computing), is a CUDA-based framework which provides efficient support for Many-Task Computing workloads on accelerators. The GeMTC framework has been integrated into Swift/T, a parallel programming framework from Argonne National Laboratory and the University of Chicago, providing GPU functionality for the Swift language.

What is a microkernel?

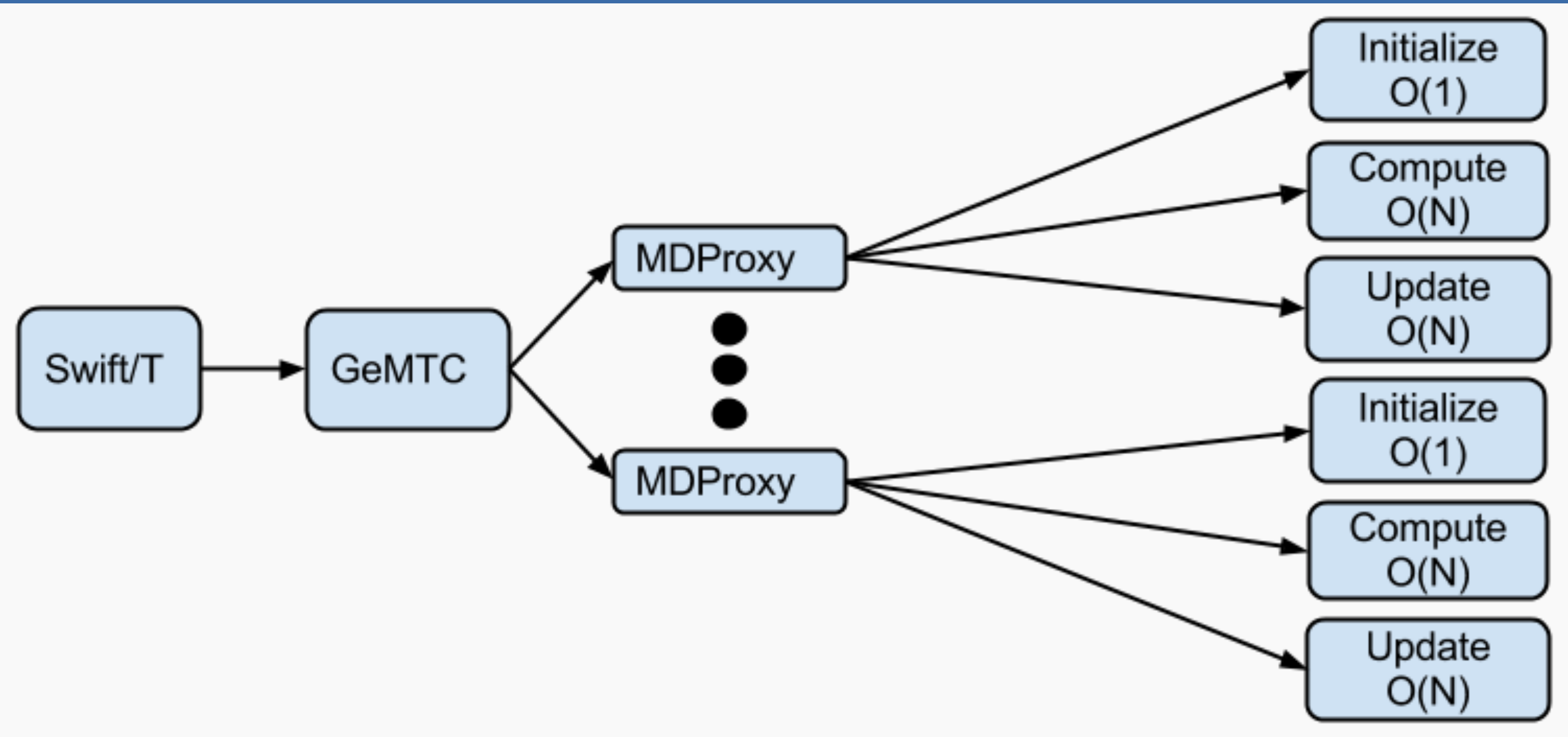
A microkernel is a traditional CUDA kernel that is modified to run in the GeMTC framework. A CUDA kernel is a user-defined function that runs on a NVIDIA GPU.

MDProxy Benchmarks





MDProxy Architecture



GeForce GTX 670

- 7 SMXs
- 84 Warps
- 1344 CUDA Cores
- 2GB DDR5

Conclusions

- Evaluate Science Application
- MDProxy highlights GeMTC potential
- GeMTC 10x faster than threaded CPU

Future Work

- Improve MD algorithm
- Enable Multi-Node Performance
- Investigate optimal MD Task Size
- Compare performance against other GeMTC-enabled accelerators
- Develop high level abstractions for the Swift/T + GeMTC stack
- Expand library of GeMTC microkernels

References

NVIDIA - http://www.nvidia.com/object/nvidia-kepler.html
GeMTC– http://www.datasys.cs.iit.edu/projects/GeMTC