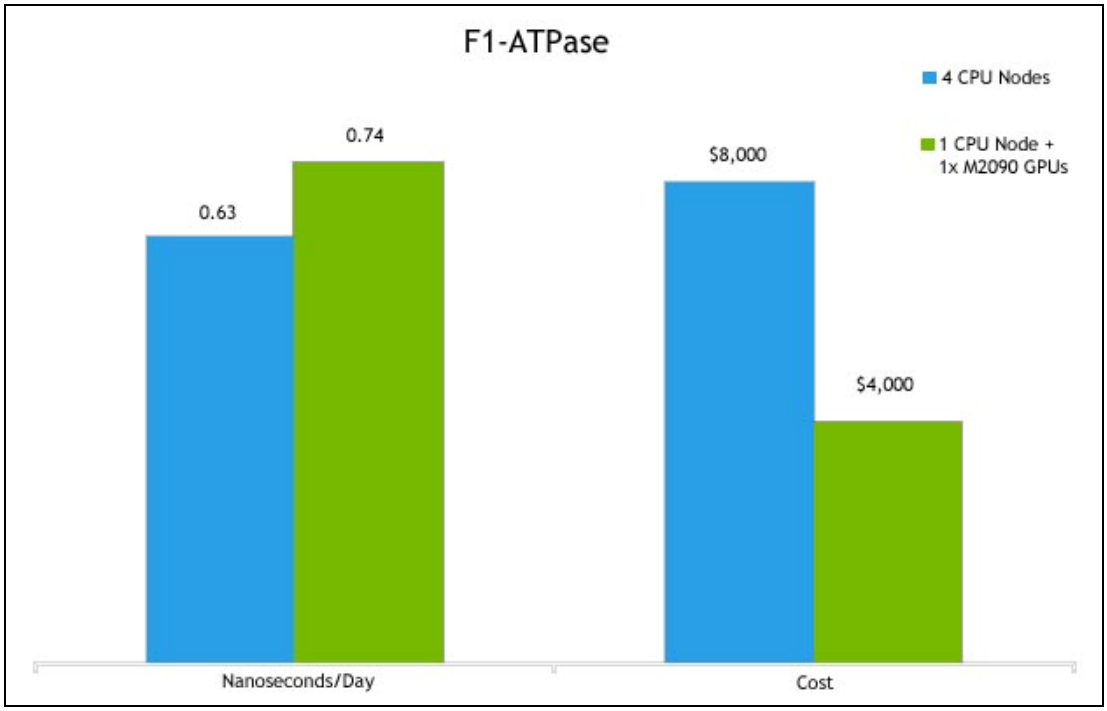
NAMD 2.8 and 2.9 Benchmark Report

Benefits of GPU Accelerated Computing

- Faster than CPU only systems in all tests
- Large performance boost with marginal price increase
- Energy usage cut in half or less
- GPUs scale very well within a node and over multiple nodes
- New Tesla K10 GPU board contains 2 of our fastest single precision GPUs to date

Replace 3 Nodes with 1 GPU Board

Speedup of 1.2x for 50% less money



Running NAMD version 2.9

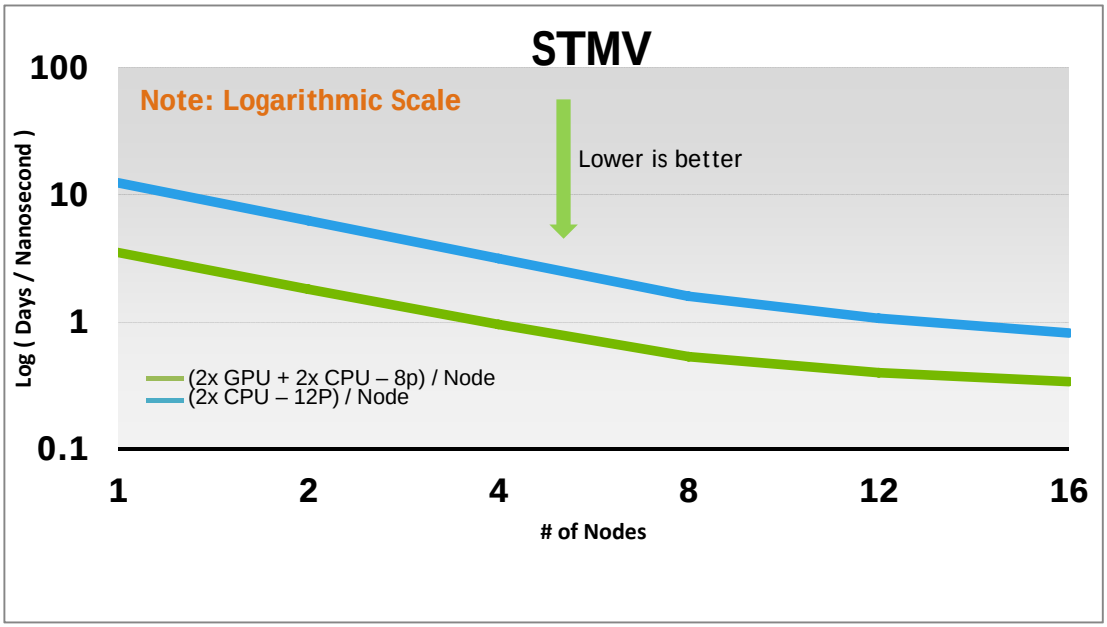
Each **blue node** contains 2x Intel Xeon X5550 CPUs

The **green node** contains 2x Intel Xeon X5550 CPUs and 1x NVIDIA M2090 GPU board

F1-ATPase

Strong Scaling with Single STMV

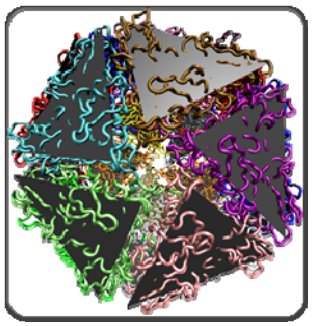
GPU nodes outperform CPU nodes by 5-7x



Running NAMD version 2.8

Each **blue CPU node** contains 2x Xeon X5670
(6 Cores per CPU)

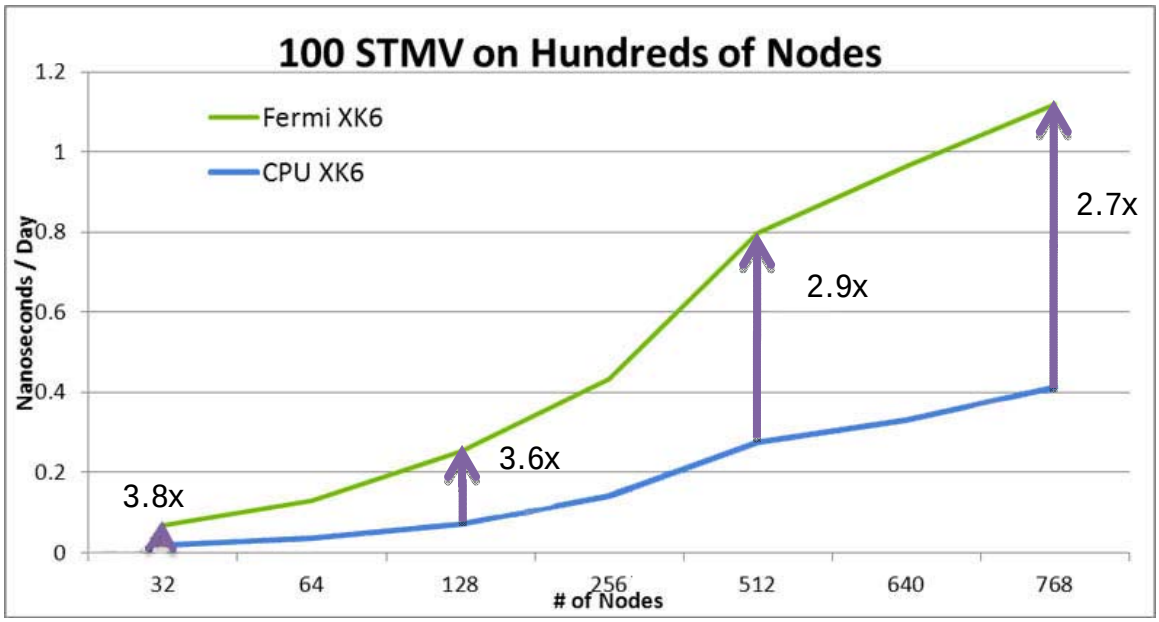
Each **green GPU node** contains 2x Xeon X5670
(6 Cores per CPU) plus 2x Tesla M2070 GPU boards



Satellite Tobacco Mosaic Virus

Outstanding Strong Scaling with Multi-STMV

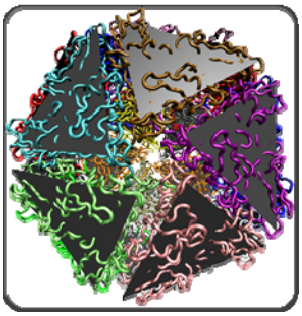
Accelerate your science by 2.7-3.8x when compared to CPU-based supercomputers



Running NAMD version 2.9

Each **blue XE6 CPU node** contains 1x AMD 1600 Opteron (16 Cores per CPU)

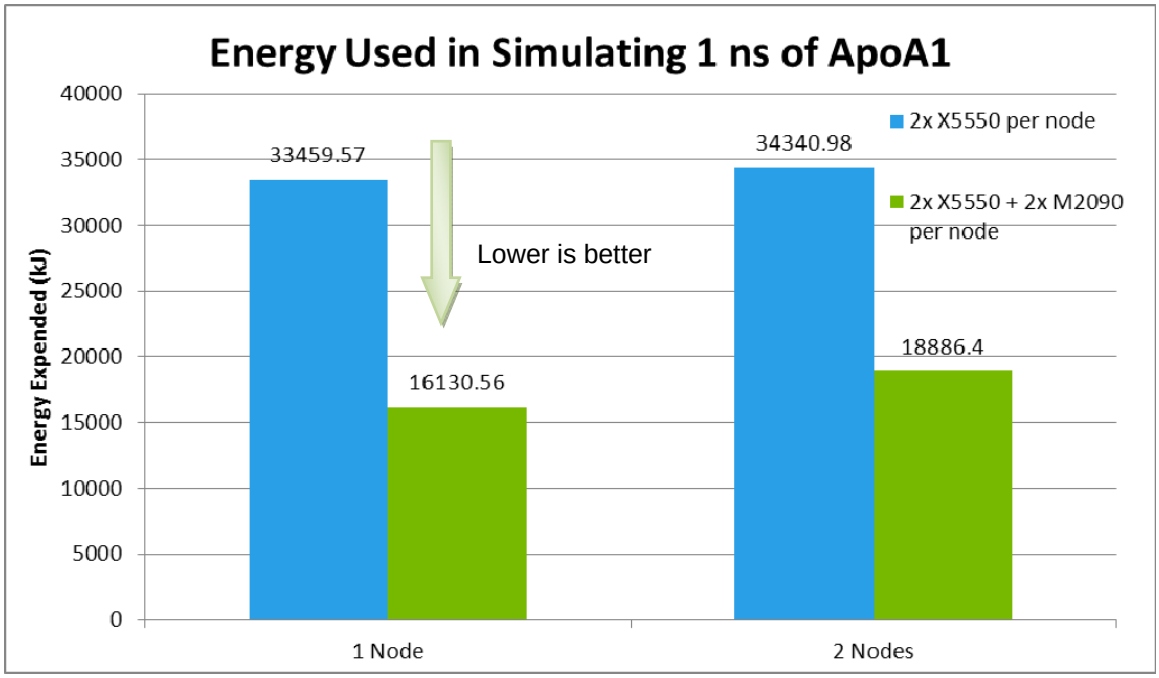
Each **green XK6 CPU+GPU node** contains 1x AMD 1600 Opteron (16 Cores per CPU) and an additiona 1x NVIDIA X2090 GPU board



Concatenation of 100 Satellite Tobacco Mosaic Virus

Greener: Twice the Science Per Watt

Cut down energy usage by ½ with GPUs



Running NAMD version 2.9

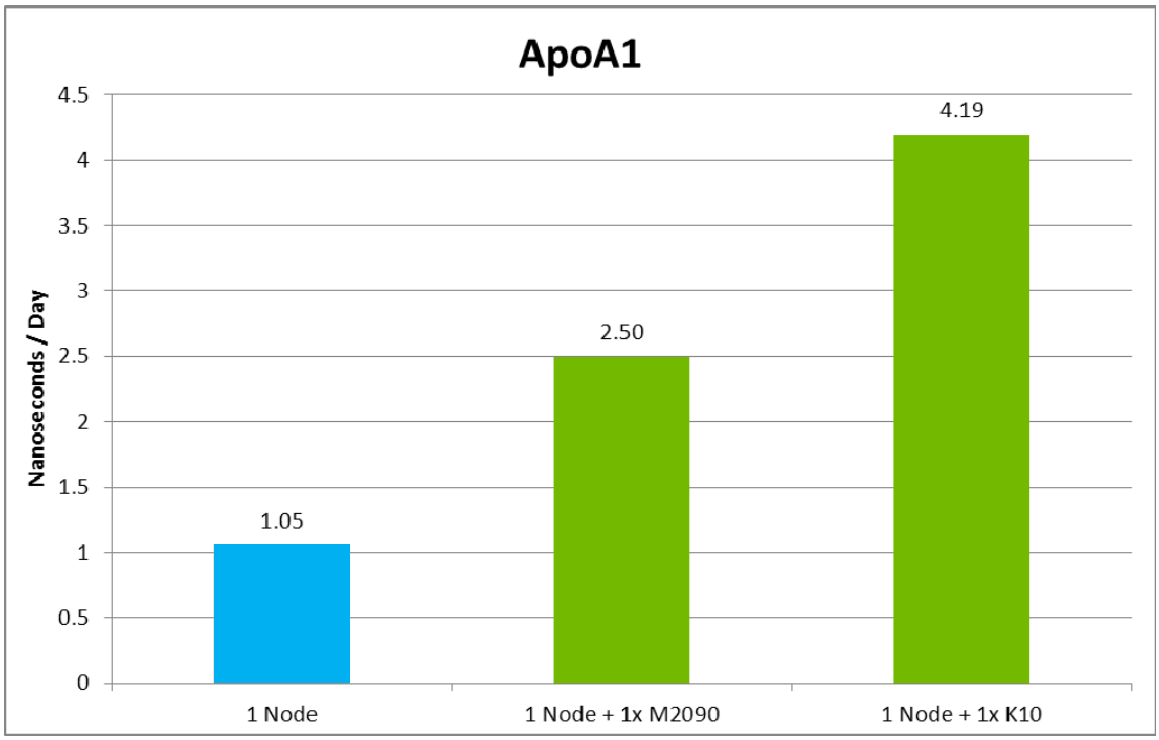
Each **blue node** contains 2x Intel Xeon X5550 CPUs (95W, 4 Cores per CPU)

Each **green node** contains 2x Intel Xeon X5550 CPUs (95W, 4 Cores per CPU) and 1x-4x NVIDIA M2090 GPU boards (225W per GPU)

Energy Expended = Power x Time

K10 - Our Fastest Single Precision GPU

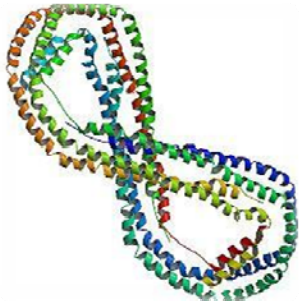
GPU speedup increased from 2.4x (with M2090) to 4x (with 1x K10 board) when compared to a CPU only node



Running NAMD version 2.9

The **blue node** contains 2x Intel Xeon X5690 CPUs (6 Cores per CPU)

The **green nodes** contain 2x Intel Xeon X5690 CPUs (6 Cores per CPU) and either 1x NVIDIA M2090 or 1x K10 for the GPU board



Apolipoprotein A1

Recommended GPU Node Configuration for Computational Chemistry

Workstation or Single Node Configuration	
# of CPU sockets	2
Cores per CPU socket	6+
CPU speed (Ghz)	2.66+
System memory per socket (GB)	32
GPUs	Kepler K10, Fermi M2090, M2075, C2075
# of GPUs per CPU socket	1-2
GPU memory preference (GB)	6
GPU to CPU connection	PCIe 2.0 or higher
Server storage	500 GB or higher
Network configuration	InfiniBand

Scale to multiple nodes with same single node configuration

Summary/Conclusions

Benefits of GPU Accelerated Computing

- Faster than CPU only systems in all tests
- Large performance boost with small marginal price increase
- Energy usage cut in half or less
- GPUs scale very well from 1 to 4, and beyond
- New Tesla K10 GPU board contains 2 of our fastest single precision GPUs to date

GPU Test Drive- Your Science Apps 5x Faster
Take a Free and Easy Test Drive Today

Run your computational chemistry simulations 5x faster. Take a free test drive to try NAMD on a remotely hosted cluster loaded with the latest GPU-accelerated applications and accelerate your results. Simply log on and run your application as usual, no GPU programming expertise required. Try it now and see how you can reduce simulation time from days to hours.

Register for the test drive today at http://www.nvidia.com/object/gpu-test-drive.html#s=namd.