
AMBER CUDA ***The Project***

- A collaboration between NVIDIA and the AMBER Development Team.

San Diego Supercomputer Center

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GPU Support in AMBER

GPU Support

- **Collaboration with NVIDIA to produce CUDA version of AMBER.**
 - PMEMD Engine
 - Implicit Solvent GB
 - Explicit Solvent PME
- **Serial version released as part of AMBER v11.**
- **Parallel version released as an update patch on the AMBER website.**



Supported Features

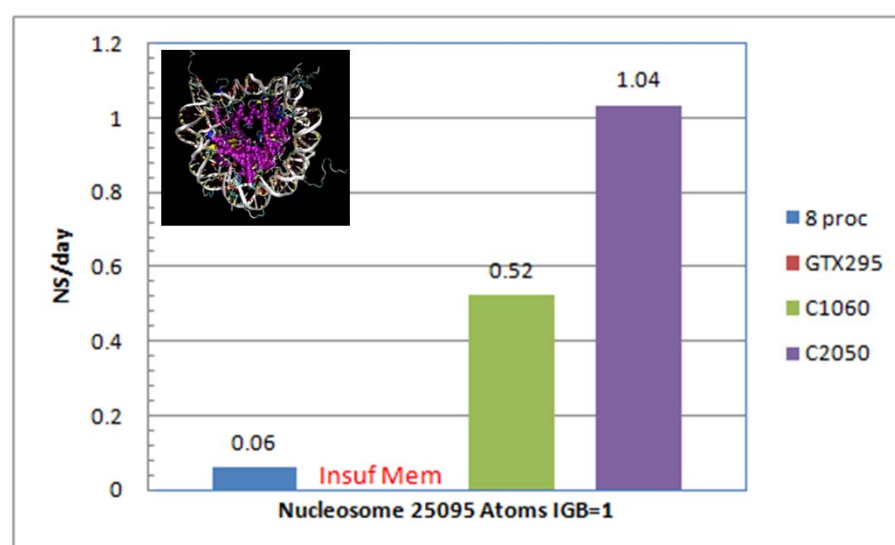
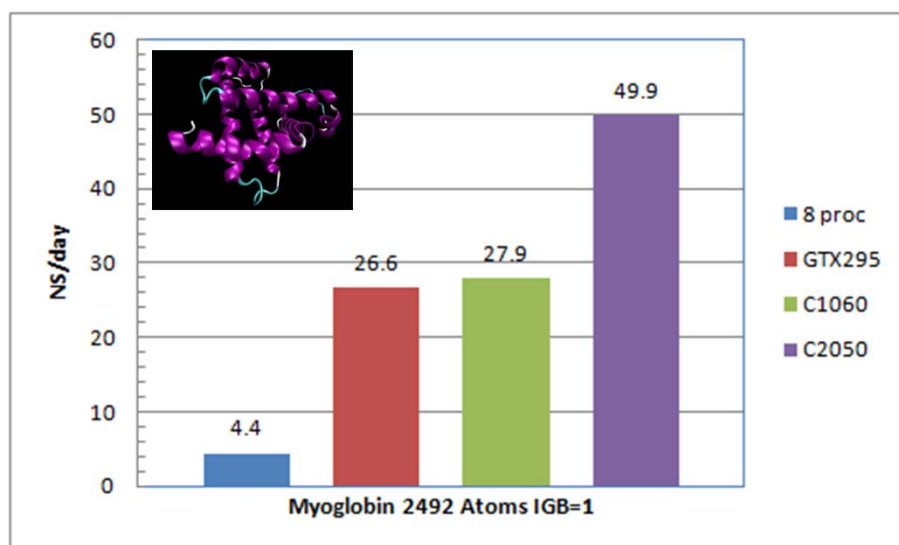
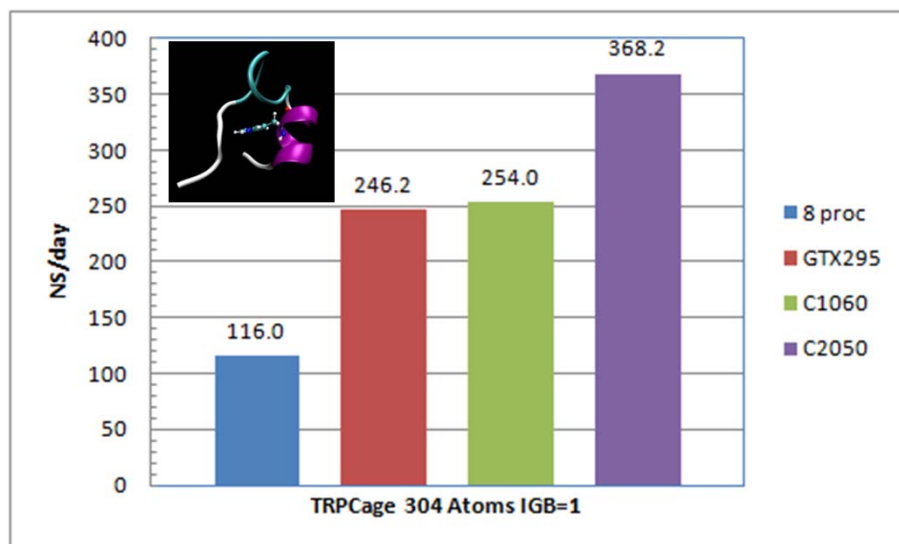
- **Supports ‘standard’ MD**
 - Explicit Solvent (PME)
 - NVE/NVT/NPT
 - Implicit Solvent (Generalized Born)
- **Thermostats**
 - Berendsen, Langevin, Anderson
- **Restraints / Constraints**
 - Standard harmonic restraints
 - Shake on hydrogen atoms

Performance

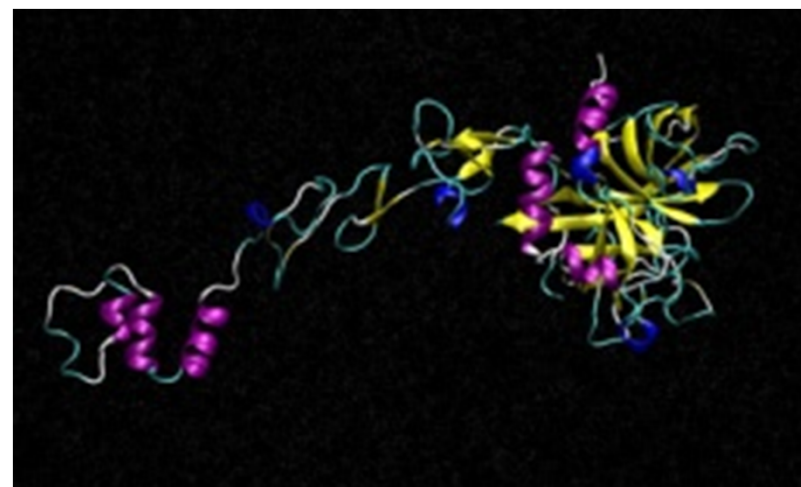
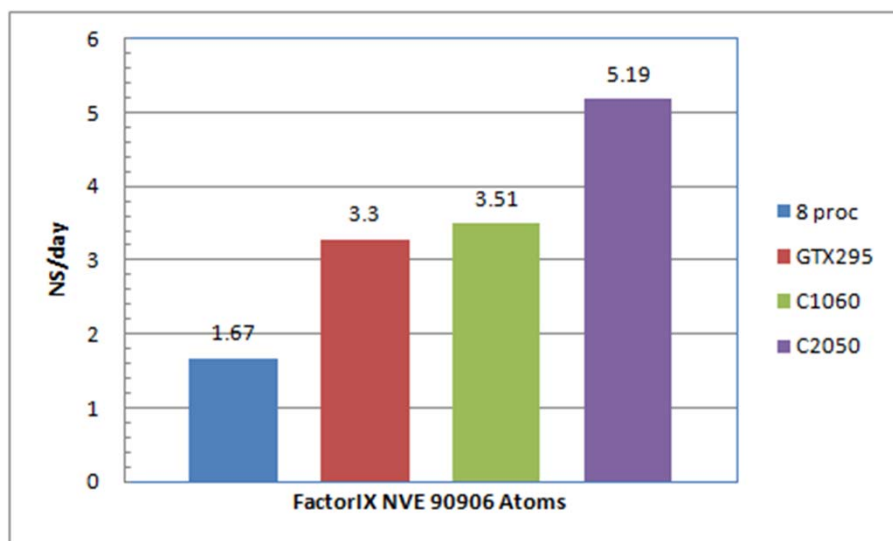
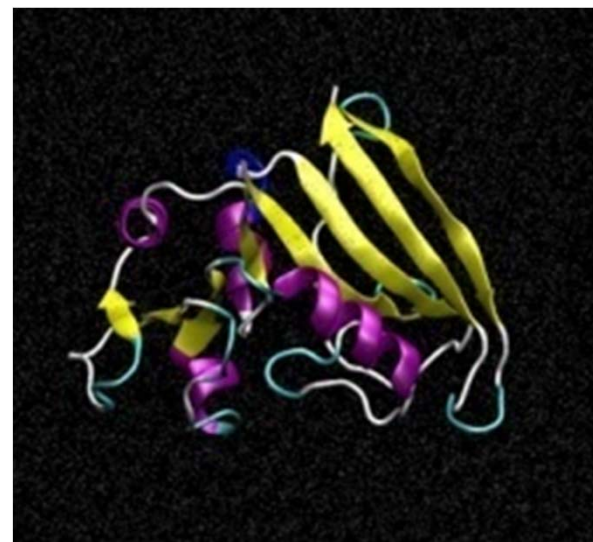
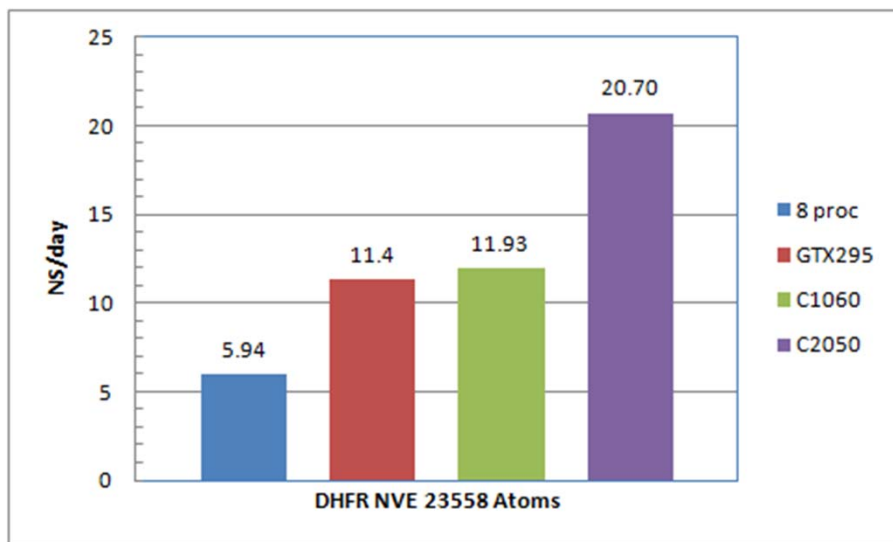
Single GPU

Implicit Solvent Performance

As expected the performance differential is larger for bigger systems.



Explicit Solvent Performance



Performance

Multi GPU

PME Benchmarks

*Note: All runs are NVE, use 2fs time step, shake and evaluate the long range electrostatics (PME, FFT) on **every** time step.*

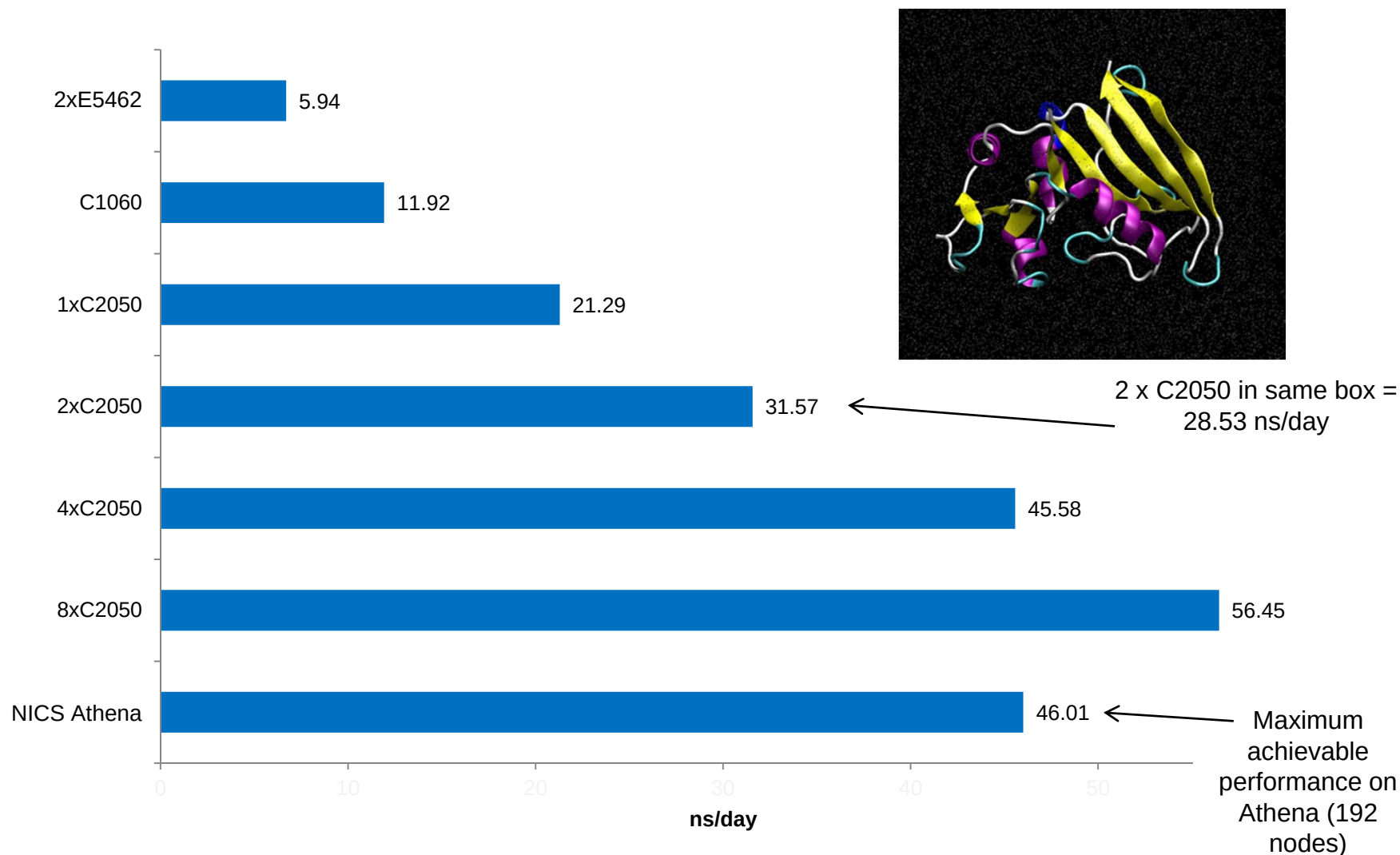
Dual x Quad Core Intel E5462 @ 2.8GHz

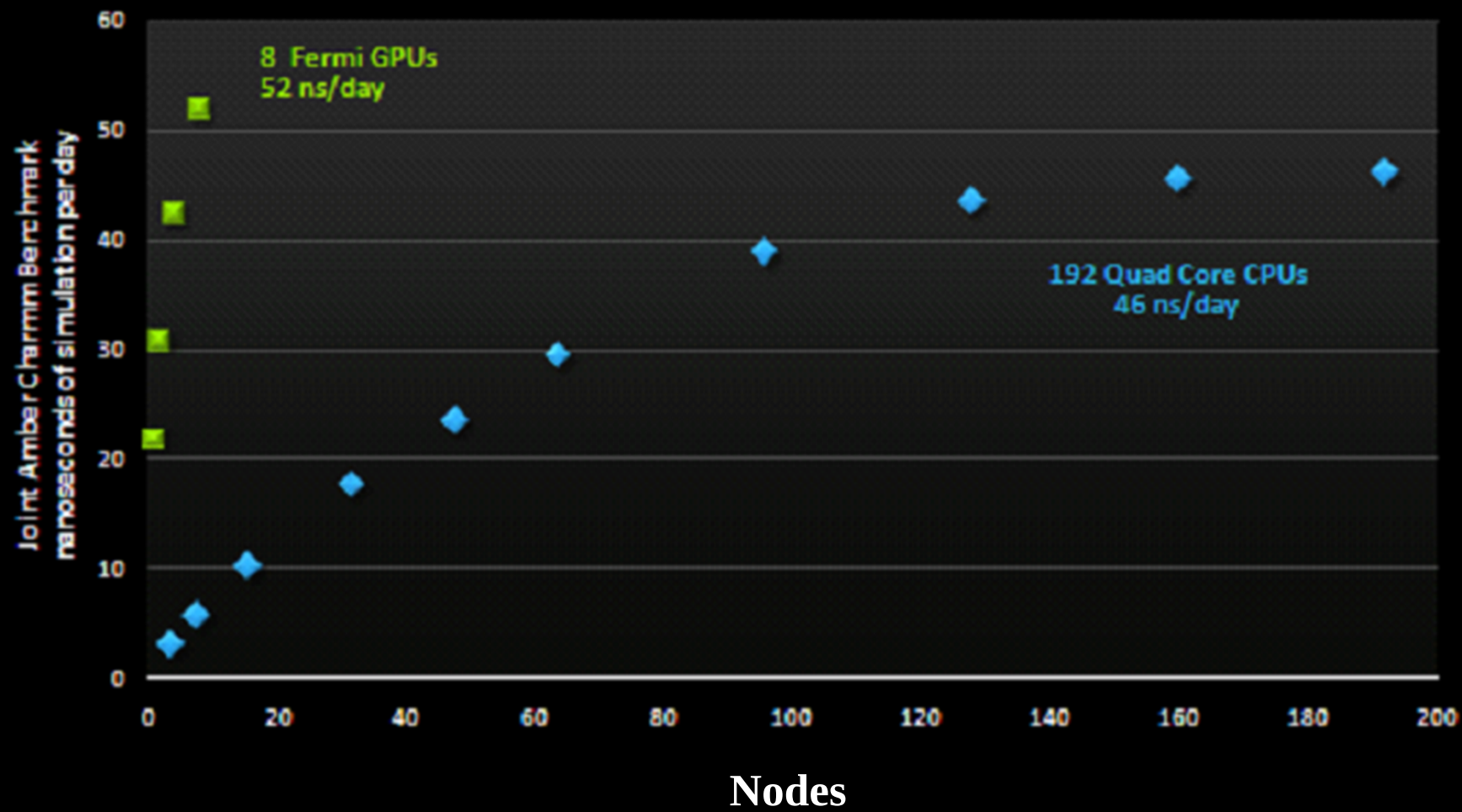
1 NVIDIA C1060

1, 2, 4, and 8 NVIDIA C2050s x QDR
Infiniband

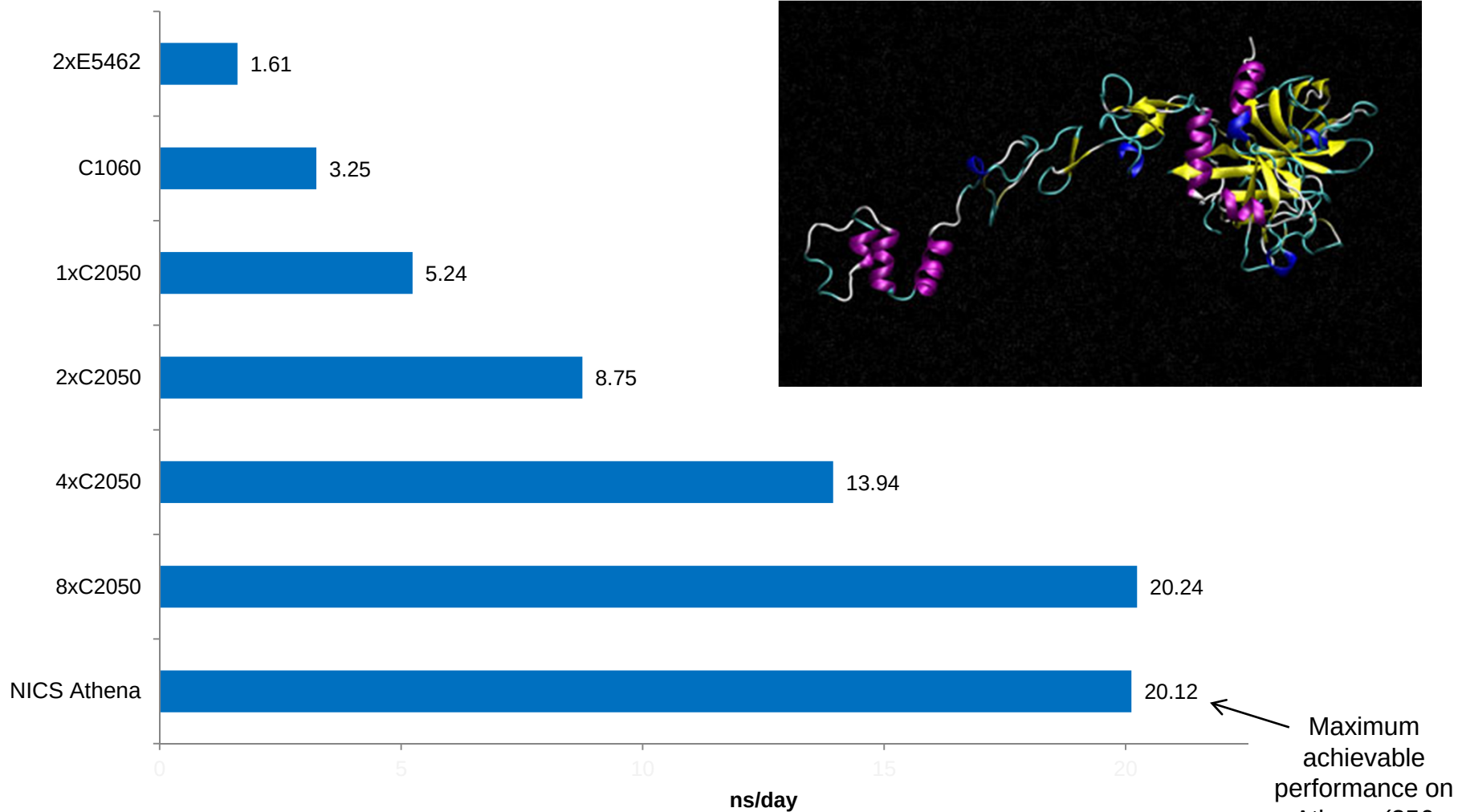
256 nodes of NICS Athena (Cray XT4)
(Up to 1024 cores)

DHFR NVE Performance (ns/day)





Factor IX NVE Performance



Acknowledgements

San Diego Supercomputer Center

University of California San Diego

National Science Foundation

NSF Strategic Applications Collaboration (AUS/ASTA) Program

NSF SI2-SSE Program

NVIDIA Corporation

Hardware + People

People

Mark Williamson

Scott Le Grand

Andreas Goetz

Duncan Poole

Dong Xu

