FEN ZI: GPU-Enabled MD Simulations Based on CHARMM Force Field and PME
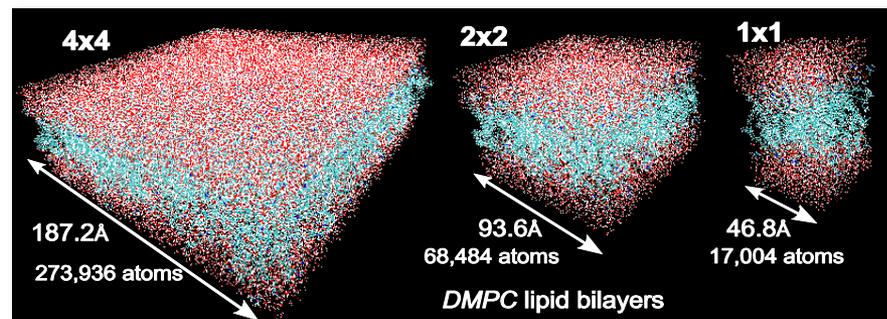
M. Taufer and S. Patel
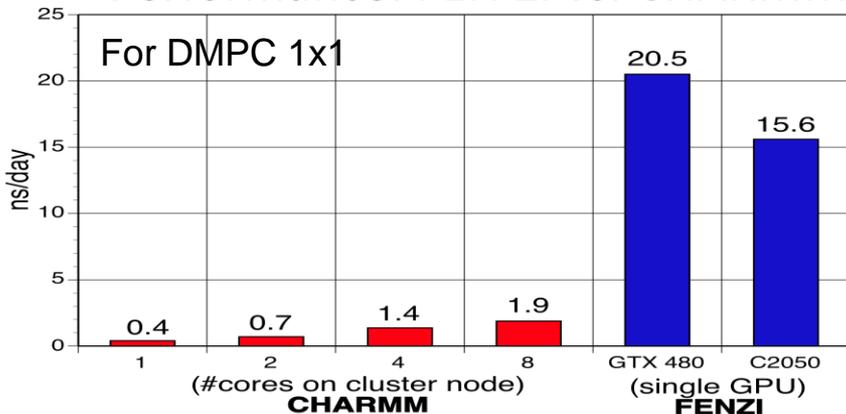
UNIVERSITY OF DELAWARE

- Use FEN ZI, a MD GPU-based code for NVT, NVE, and NTP ensembles including PME, to study:
  - Structural and electrostatic properties of DMPC lipid bilayers membranes
  - Pathological conditions and behaviors of protein-membrane interactions (**work in progress on Keeneland**)
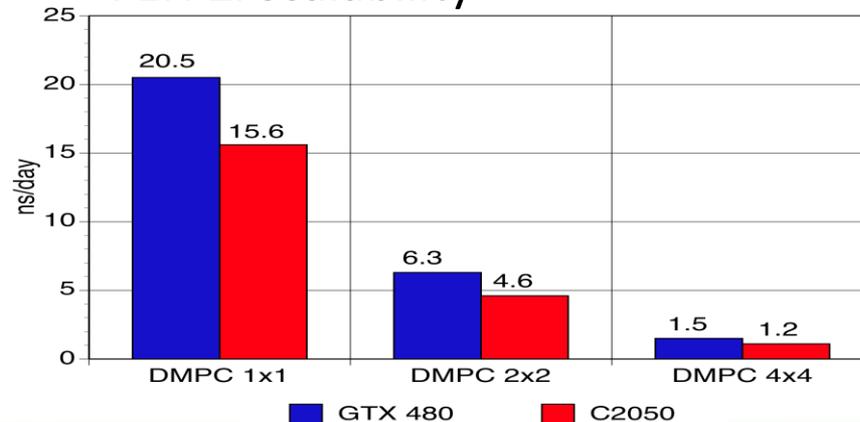
URL: http://gcl.cis.udel.edu/projects/fenzi/

- GPUs enable fast simulations of larger membranes over longer simulated times (>100ns)

4x4 — 187.2A 273,936 atoms
2x2 — 93.6A 68,484 atoms
1x1 — 46.8A 17,004 atoms
DMPC lipid bilayers

- Performance: FEN ZI vs. CHARMM

For DMPC 1x1

CHARMM: 1 → 0.4, 2 → 0.7, 4 → 1.4, 8 → 1.9 (#cores on cluster node)
FENZI: GTX 480 → 20.5, C2050 → 15.6 (single GPU)

- FEN ZI scalability

DMPC 1x1: GTX 480 → 20.5, C2050 → 15.6
DMPC 2x2: GTX 480 → 6.3, C2050 → 4.6
DMPC 4x4: GTX 480 → 1.5, C2050 → 1.2

- GTX 480
- C2050

Georgia Tech   NICS   THE UNIVERSITY of TENNESSEE   OAK RIDGE National Laboratory   NVIDIA   hp   NSF