Future Direction with NAMD

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NAIS: State-of-the-Art Algorithms for Molecular Dynamics
Short-term Outlook

• Important for our software to support GPUs
  – GPU acceleration is being incorporated into new supercomputers
  – GPU-accelerated desktop workstations to replace cluster computing
    • Easier maintenance
    • Improved power consumption

• Both NAMD and GROMACS are in good shape for using GPU computing
Trends in Computing Hardware

- Computing hardware will continue to get “wider”
  - Moore’s Law is still in effect
- Core clock speeds have plateaued
- Memory hierarchies likely to get “deeper”
- Memory bandwidth not increasing at the same rate as compute cores and FLOP/s
- High performance software increasingly more difficult to develop
NAMD and Performance

• Could benefit from single core level performance improvements
  – SSE intrinsics within key computational kernels
• Could make better use of GPUs
• Asynchronous message-driven design is advantageous for large scale parallelization
  – Dynamic load balancing helps with hardware issues (e.g. system noise, recovery from failed nodes)
Molecular Dynamics Challenges

• Extending timescales of simulations
  – NAMD has high performance replica exchange, basis for other enhanced sampling methods

• Improving force fields
  – NAMD supports leading polarizable force field efforts (Drude, FlucQ)
  – Plans to support AMOEBA polarizable force field

• Better scaling methods
  – Multilevel summation method has promise