Future Direction with NAMD

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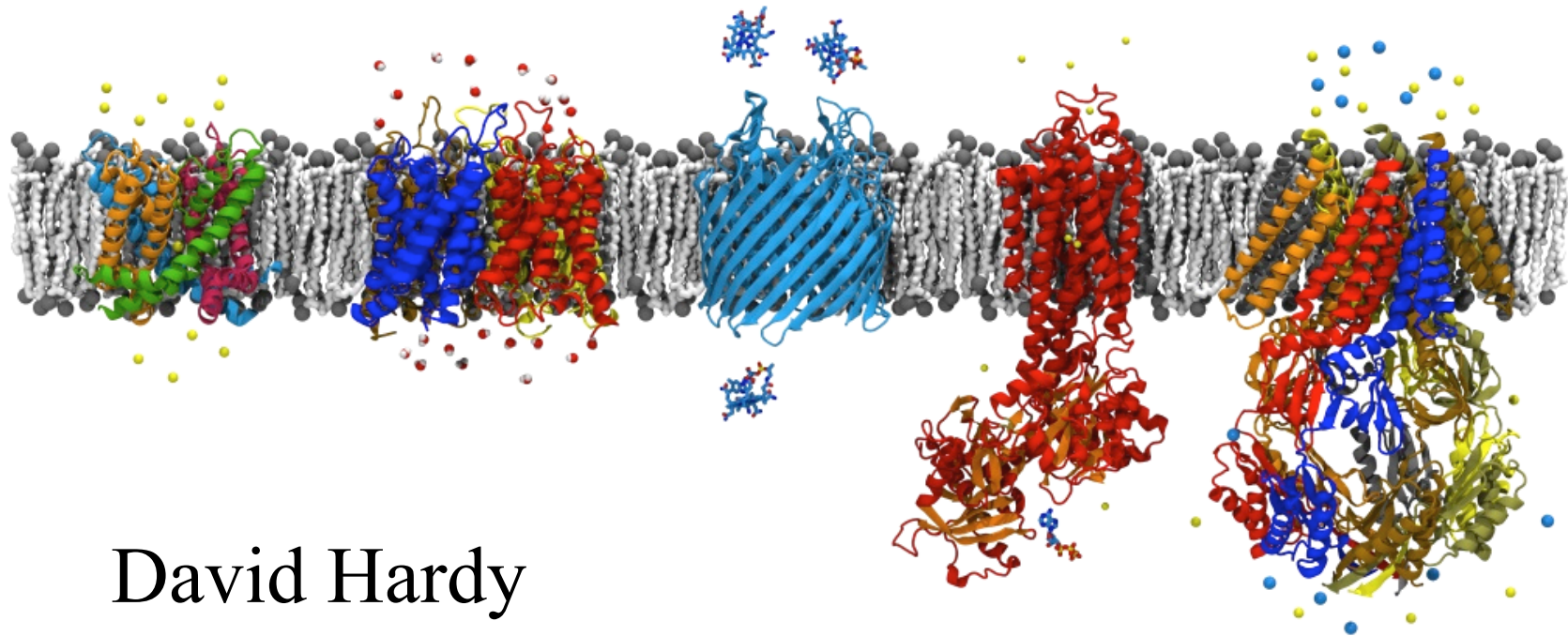
NAIS: State-of-the-Art Algorithms for Molecular Dynamics

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

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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

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