NEMO 3-D Development and Scalability Study

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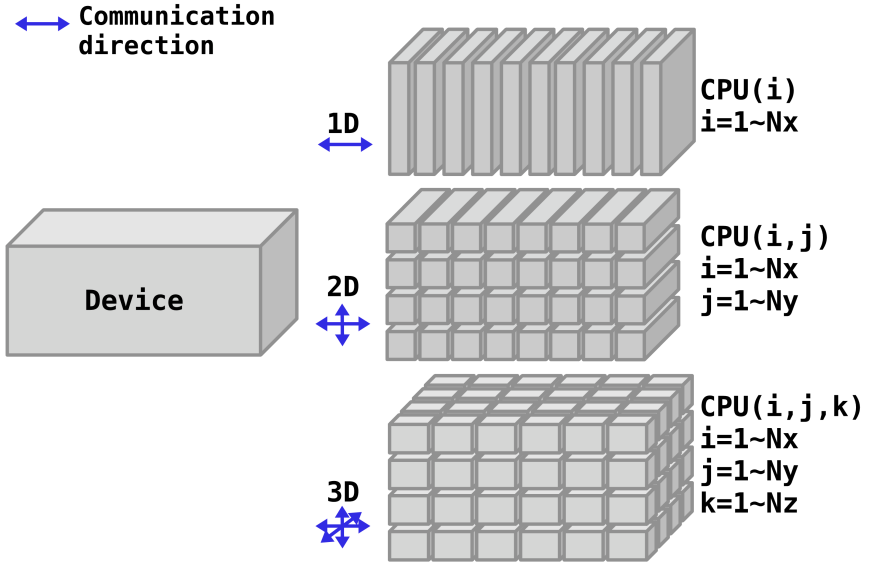
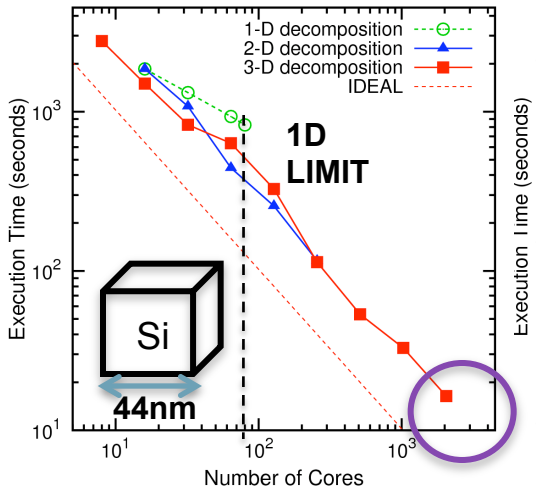
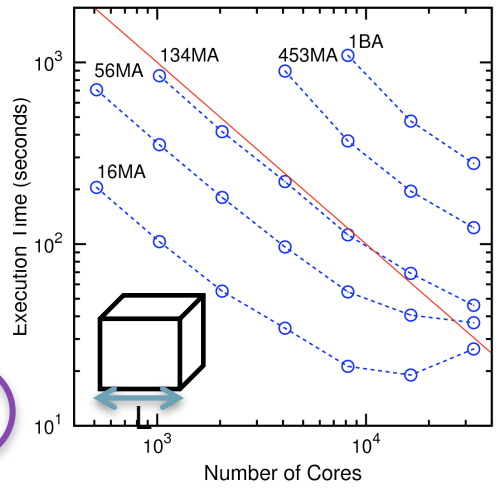
- Objective
  - » Run large atomistic electronic structure simulations in minutes
  - » Represent realistically large structures atomistically
  - » Utilize available peta-scale computers
- Approach
  - » Improve spatial decomposition parallelism
  - » Include self-consistent calculations
- Performance / Impact
  - » Strong scaling of 3D decomposition => have overcome 1D limitation
  - » Utilized over 10,000 cores for realistic simulation domain size
  - » Expecting dramatic reduction of simulation time => 10hours to 20 minutes
  - » Published in SCIDAC proceedings, 2009, Haley, Lee et al.





Tested on Ranger



Tested on Kraken