"Anton, a Special-Purpose Machine for Molecular Dynamics Simulation"

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Introduction

*"**Do one thing** and do it **well**"*

- Special-purpose logic designed for MD calculations
- Parallel algorithms tuned for the machine to minimize comms

Motivation

- Simulate biochem phenomena that can't be observed in the lab
- Phenomena occur at <u>milli</u>second timescale
- Best simulations do <u>micro</u>second timescale

Hardware Overview

- 512 identical MD-specific ASICs
- Specialized high-speed comms
  - High-speed 3D torus
- Programmable core that directs ASICs
- Balanced system – keep MD ASICs fed
  - Weakness of past MD-specific systems
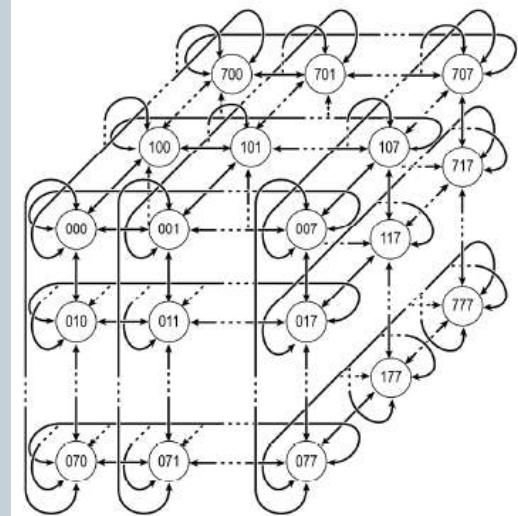
MD Calculations

- Motion of collection of atoms using classical laws of physics
  - Atoms of target molecule
  - Atoms of solvent (usu water)
- Force of every particle on every other
- Integration of all forces to yield new velocity & position
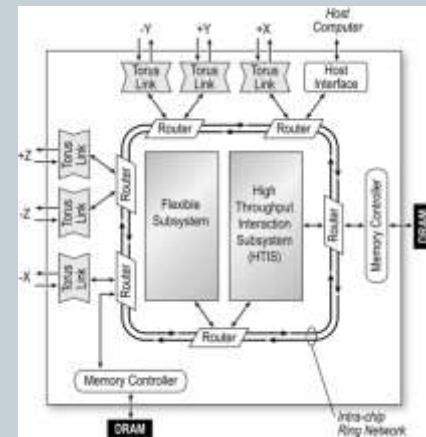
Parallelization

- Break cell up into a grid, much like ocean
  - Each grid box lives on an ASIC
  - Each particle has a home node (ASIC)
- NT method for pairwise non-bonded interactions
  - Each ASIC responsible for its own grid + part of neighboring grids
  - Can calculate the interactions somewhere other than home node – "neutral territory"
  - This allows for more even spread of calculations

MD ASICs

- Don't need large caches

- Devote more chip area to computations

- Pay attention to Amdahl's Law when speeding up particular operations

- Systolic array
  - Each PPIM in the grid does the following: receive, compute, transmit
  - Atoms "flow" through the array and intersect at the various PPIMs

Conclusions

- Special hardware is a big win
  - 80-100x faster than competition
  - Hardware design led to algorithm insights
- …if you can justify it
  - Failure of LISP Machines, database accelerators
  - Must beat Moore's Law

- It works!
  - They built it

Questions/Concerns

- When does a problem domain warrant specialized hardware?
  - They explained the Moore's Law justification for specialized hardware
- Are GPGPUs a more cost-effective option?
  - GPGPUs have become more prevalent since the publication of this paper.
- Would a hierarchy of interconnection structures improve communications?
  - Small collection of nodes = snoopy
  - Large collection of meta-nodes = directory
- Could Anton be used for other classes of problems with similar computational needs?