Anton 2
Enhanced Sampling

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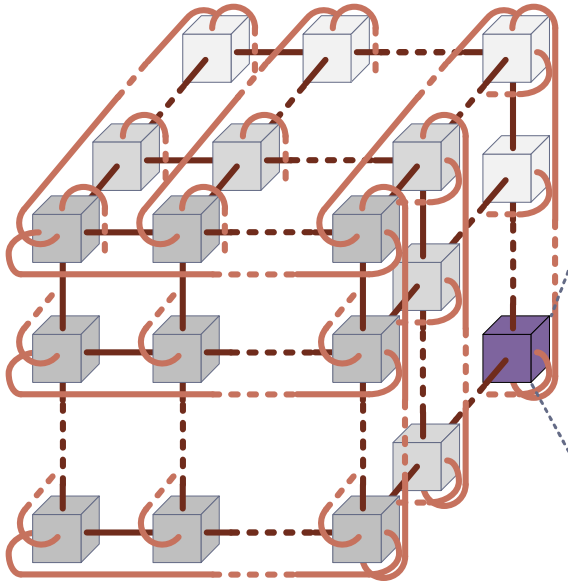
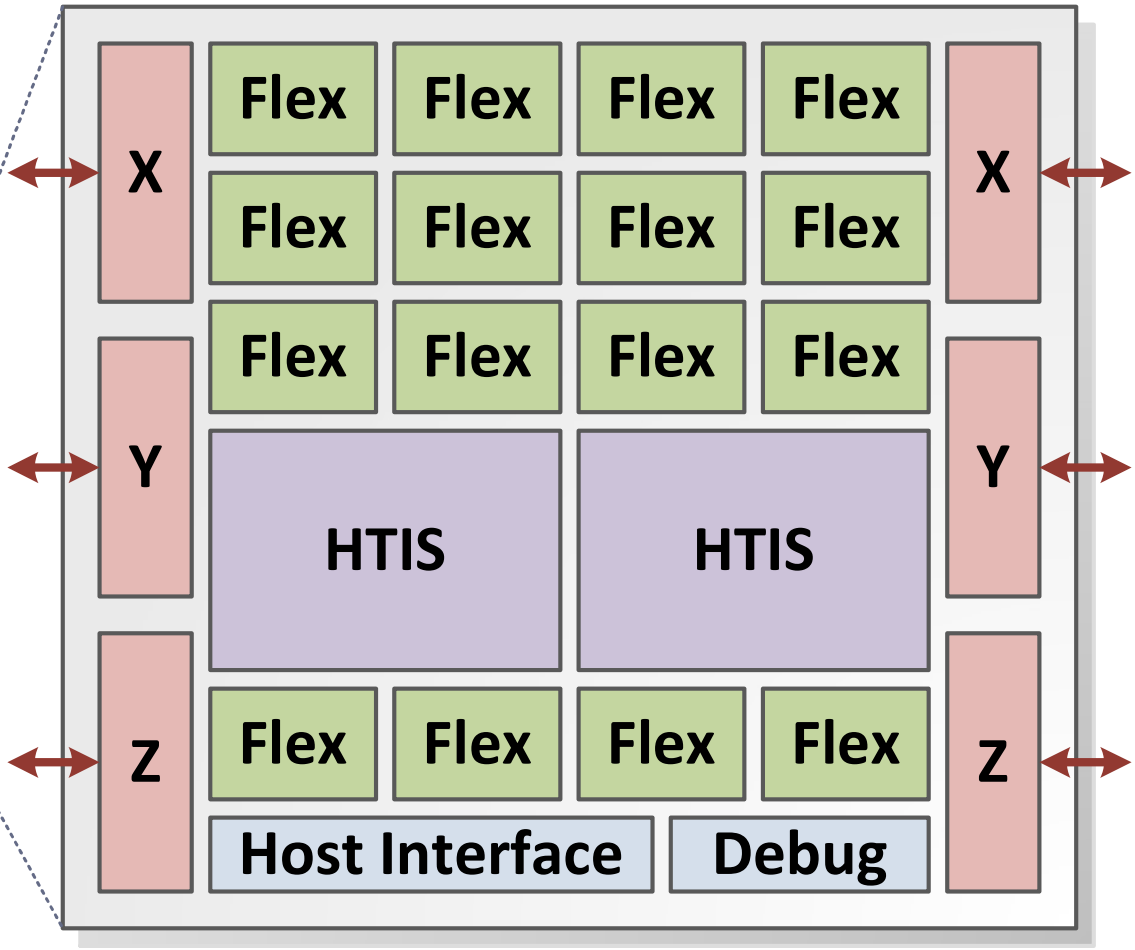
Anton 2 Architecture



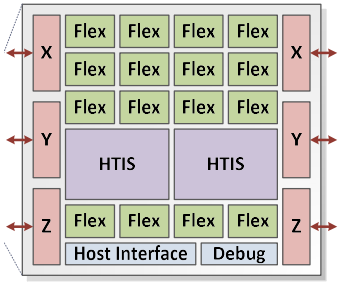
1-4096 nodes/machine
(128 nodes/cabinet)



Each node is one ASIC

David E. Shaw *et al.*, "Anton 2: Raising the Bar for Performance and Programmability," in *Proc. SC14*, Nov. 2014.

Specialized Hardware

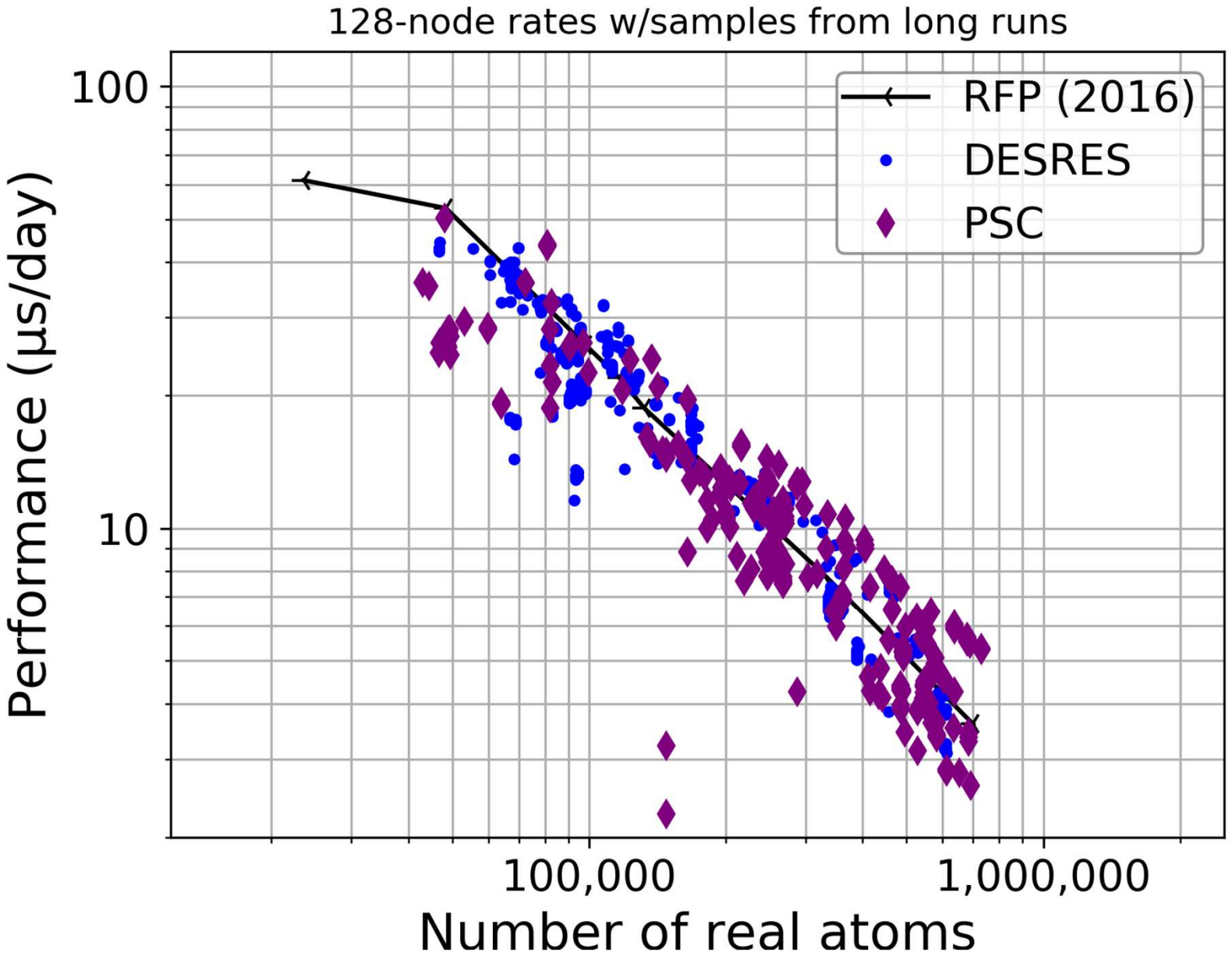


- From-scratch hardware for MD
  - Hardware pipelines + embedded processors + integrated network
  - (not an x86, not an FPGA, not a GPU, not infiniband)
  - No operating system, no virtual memory
- Whole machine is a big coprocessor: load, run, unload
- Why is isn't it all hardware (why embed processors)?
  - Hedge against algorithmic uncertainty (including bugs)
  - Actually a good abstraction around an ALU + memory (e.g. FFT)
  - Lots of housekeeping tasks

User's View of Anton: An Appliance

- Provide a chemical system: atoms, force field
- Specify a few critical options
  - Ensemble (NVE/NVT/NPT), output intervals
- Prep: create a working directory with the initial state
  - "choosers" compute unspecified chemical parameters (e.g. grid and cutoffs) plus a slew of performance-only parameters (e.g. buffer sizes) based on the chemical system characteristics
  - prep tool generates and compiles embedded code.
- Submit: pass the job to a batch scheduler
  - Sends the job to a machine and says "go"
  - Output trajectory frames start appearing on disk...

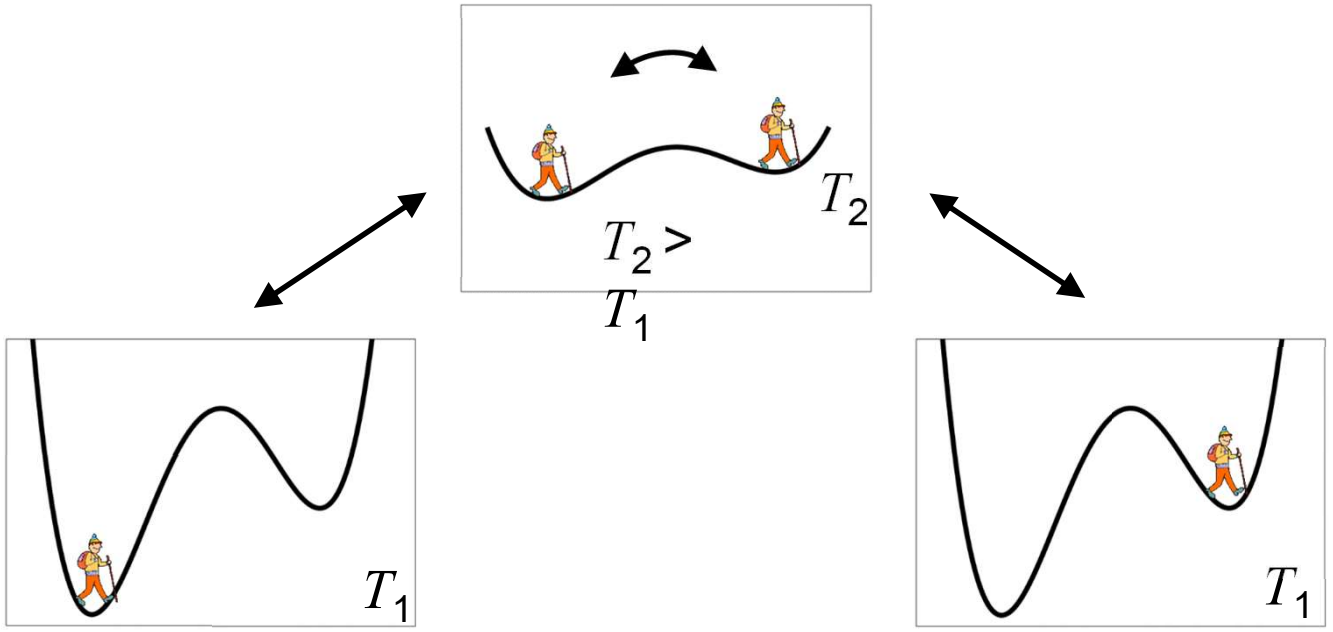
toaster from redbubble.com


128-node rates w/samples from long runs
100
10
Performance (µs/day)
RFP (2016)
DESRES
PSC
100,000
1,000,000
Number of real atoms

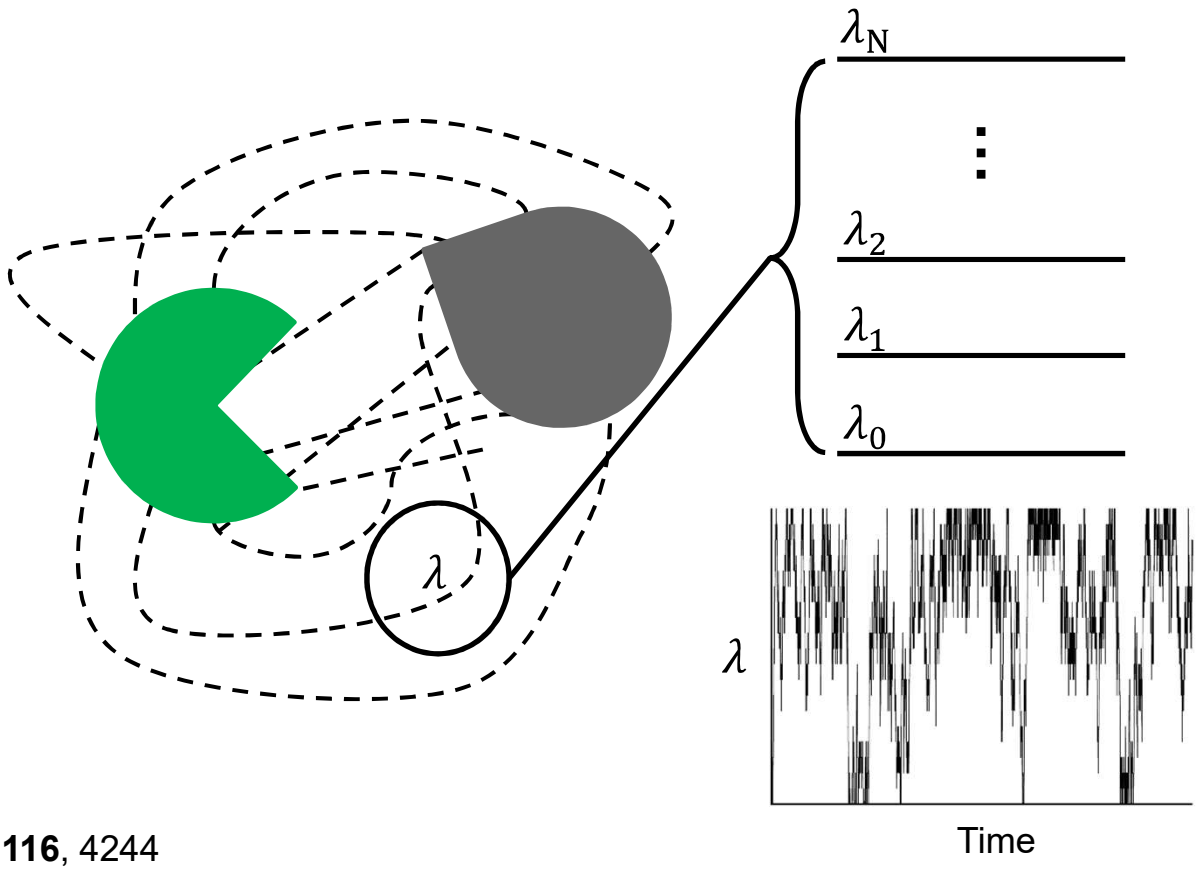

D E Shaw Research
ANTON2
63-00004-01
ECRS600282A-1R
P6N592.00
1343 KOREA
e1

Enhanced sampling with TSS

- Times Square Sampling (TSS) is an enhanced sampling approach related to simulated (Hamiltonian) tempering
- TSS has built-in online free energy estimators

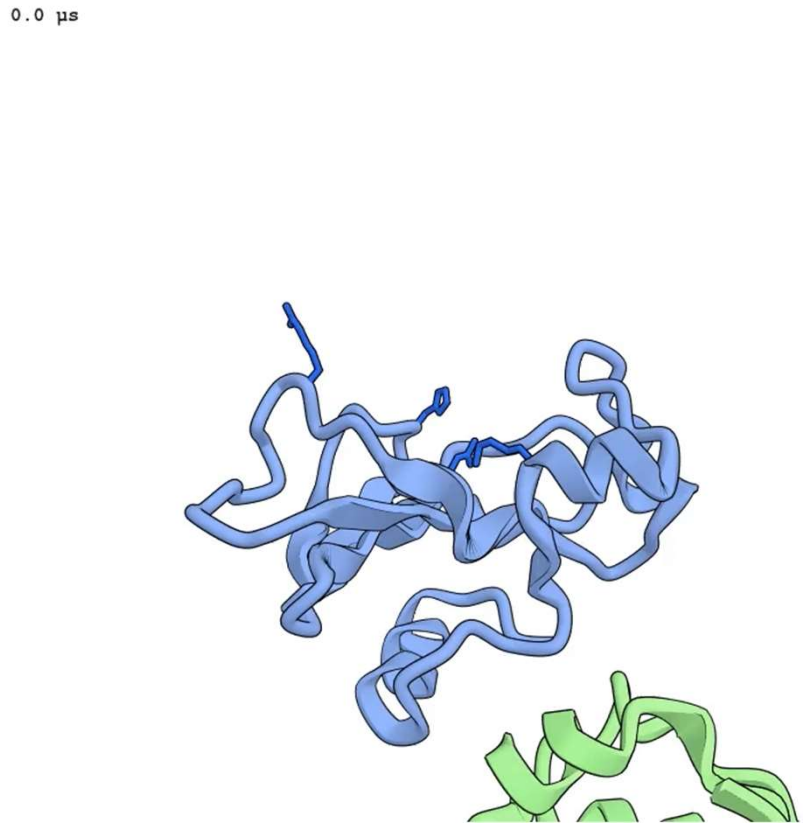


Tempered binding



PNAS (2019), **116**, 4244

Tempered binding speeds up escape from metastable traps



Questions?

- Can apply a uniform constant electric field.
- Position restraints on a per atom basis.
- Enhanced sampling is also available in four forms as follows:
  (i) simulated tempering, including adaptive weighting,
  (ii) application of restraints between the centers of mass of groups of atoms,
  (iii) application of conformational restraints, each based on the calculation of RMSD (root mean squared deviation) with respect to atomic positions of a given reference structure, and
  (iv) tempered binding.

- For restraints in both (ii) and (iii), equilibria and spring constants can be varied during a simulation according to a schedule or adaptively to implement a form of umbrella sampling

Feedback

https://www.psc.edu/survey-enhanced-sampling-techniques-seminar/