David Shaw: The Neutral Territory Algorithm and Anton

Miranda Fluharty

The Neutral Territory Algorithm

- calculates forces of particles on other particles
- “neutral” because the calculation happens between the particles

- how it works
  - each particle sends its information out on a horizontal plane (“plate”) up to a certain distance
  - also sends it up and down in a “tower” up to the same distance
  - whenever a tower meets a plate, the force of the plate particle on the tower particle is calculated

The Neutral Territory Algorithm

- calculates forces of particles on other particles
- “neutral” because the calculation happens between the particles

- how it works
  - each particle sends its information out on a horizontal plane (“plate”) up to a certain distance
  - also sends it up and down in a “tower” up to the same distance
  - whenever a tower meets a plate, the force of the plate particle on the tower particle is calculated

The Neutral Territory Algorithm

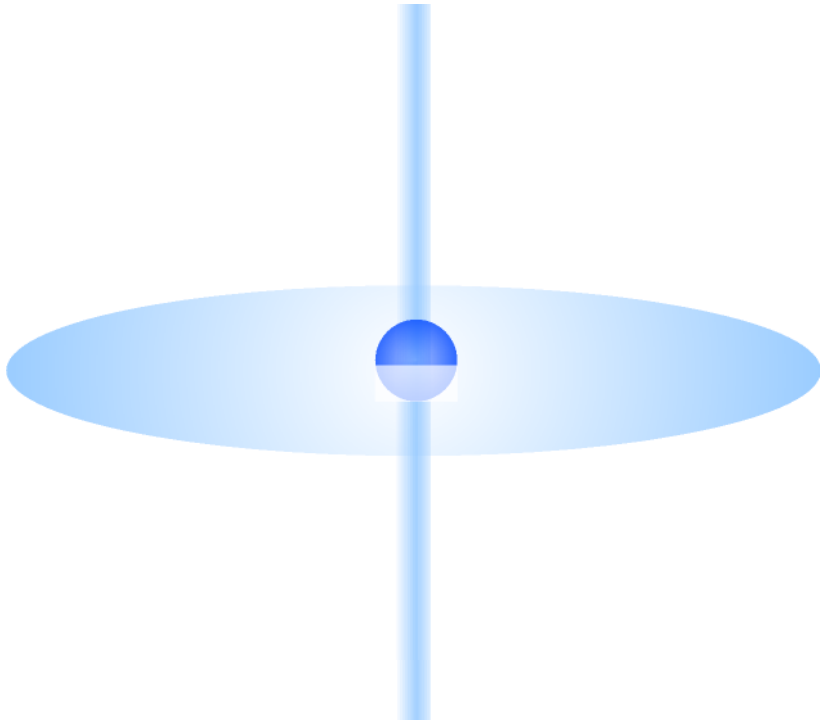
- calculates forces of particles on other particles
- “neutral” because the calculation happens between the particles

- how it works
  - each particle sends its information out on a horizontal plane (“plate”) up to a certain distance
  - also sends it up and down in a “tower” up to the same distance
  - whenever a tower meets a plate, the force of the plate particle on the tower particle is calculated

The Neutral Territory Algorithm

- calculates forces of particles on other particles
- “neutral” because the calculation happens between the particles

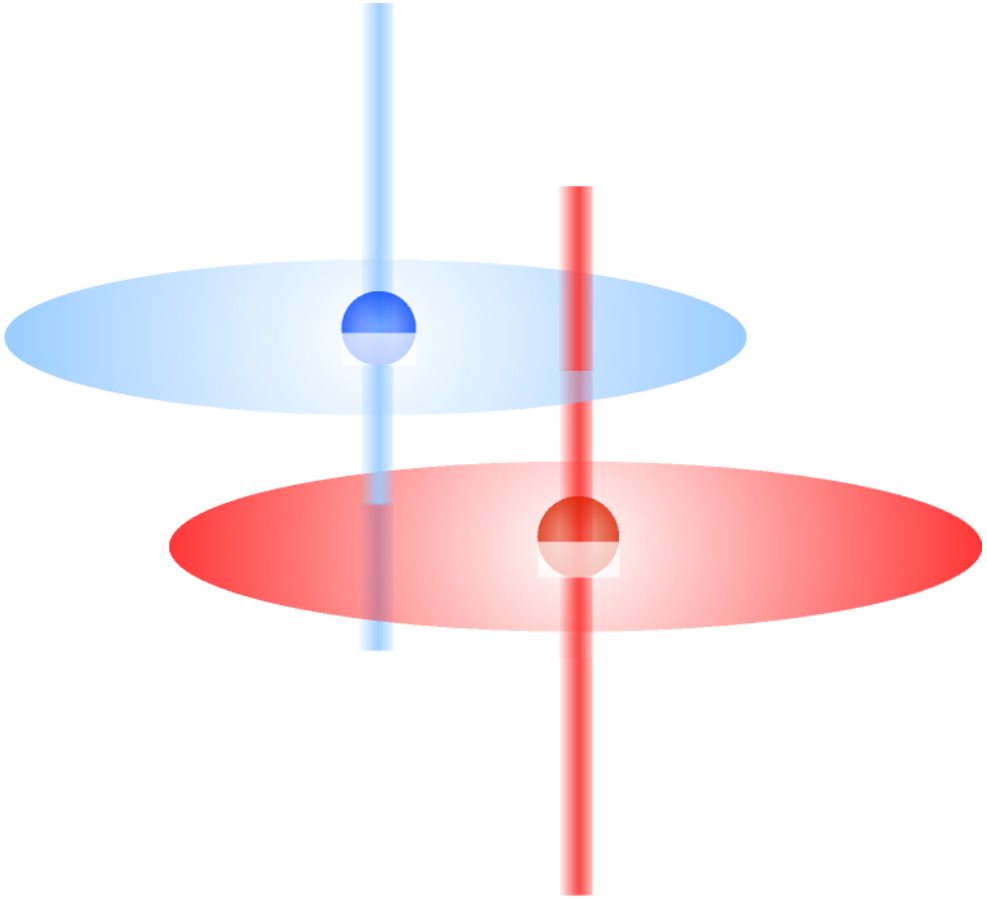
- how it works
  - each particle sends its information out on a horizontal plane (“plate”) up to a certain distance
  - also sends it up and down in a “tower” up to the same distance
  - whenever a tower meets a plate, the force of the plate particle on the tower particle is calculated



The Neutral Territory Algorithm

- calculates forces of particles on other particles
- “neutral” because the calculation happens between the particles

- how it works
  - each particle sends its information out on a horizontal plane (“plate”) up to a certain distance
  - also sends it up and down in a “tower” up to the same distance
  - whenever a tower meets a plate, the force of the plate particle on the tower particle is calculated



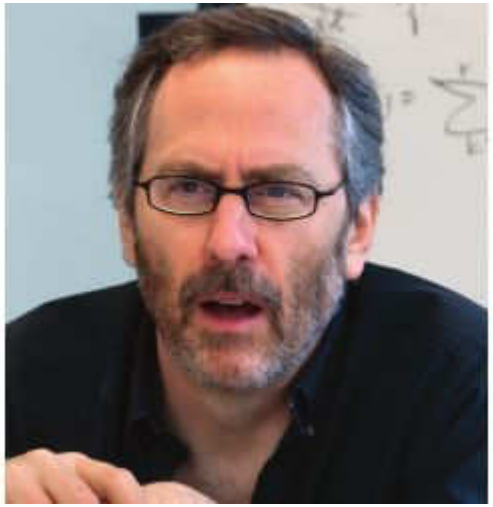
The Neutral Territory Algorithm

- calculates forces of particles on other particles
- “neutral” because the calculation happens between the particles

- how it works
  - each particle sends its information out on a horizontal plane (“plate”) up to a certain distance
  - also sends it up and down in a “tower” up to the same distance
  - whenever a tower meets a plate, the force of the plate particle on the tower particle is calculated

Shaw Says:

“In biological applications like the ones that interest us, the idea is to simulate the motions of large biomolecules, such as proteins or DNA, at an atomic level of detail over a simulated time period during which biologically interesting things happen in real life… During each 'time step' in the integration process, the atoms move a very short distance, after which the forces are recomputed, the atoms are moved again, and so on.”



Anton

- dedicated hardware
- “computational microscope”

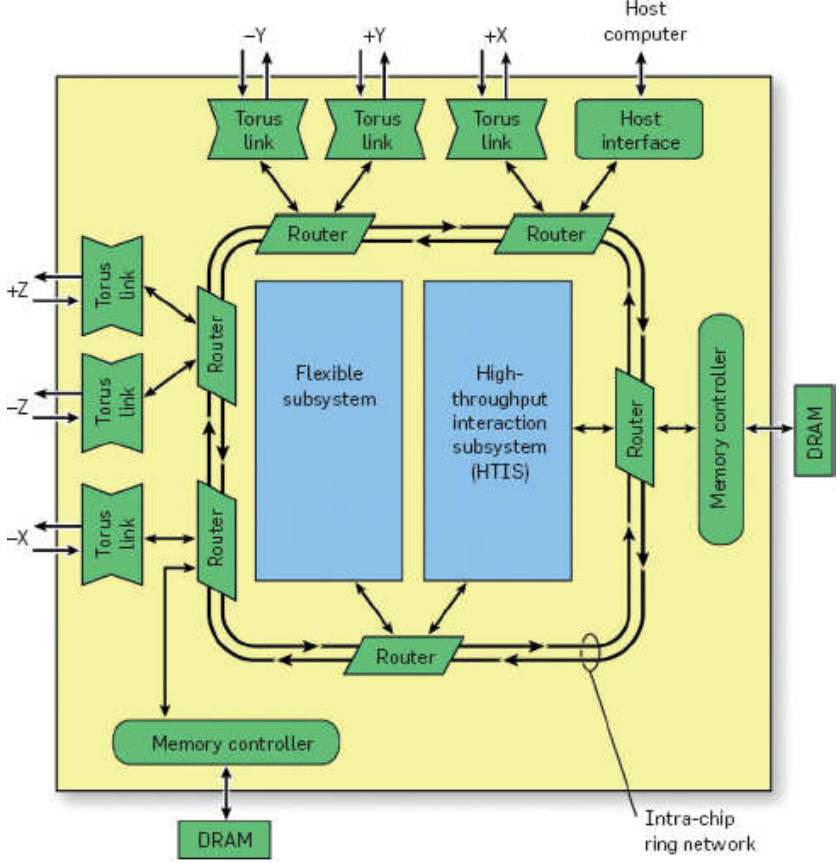
- average computer could simulate a few nanoseconds per day
- Anton can simulate 16,400 nanoseconds per day

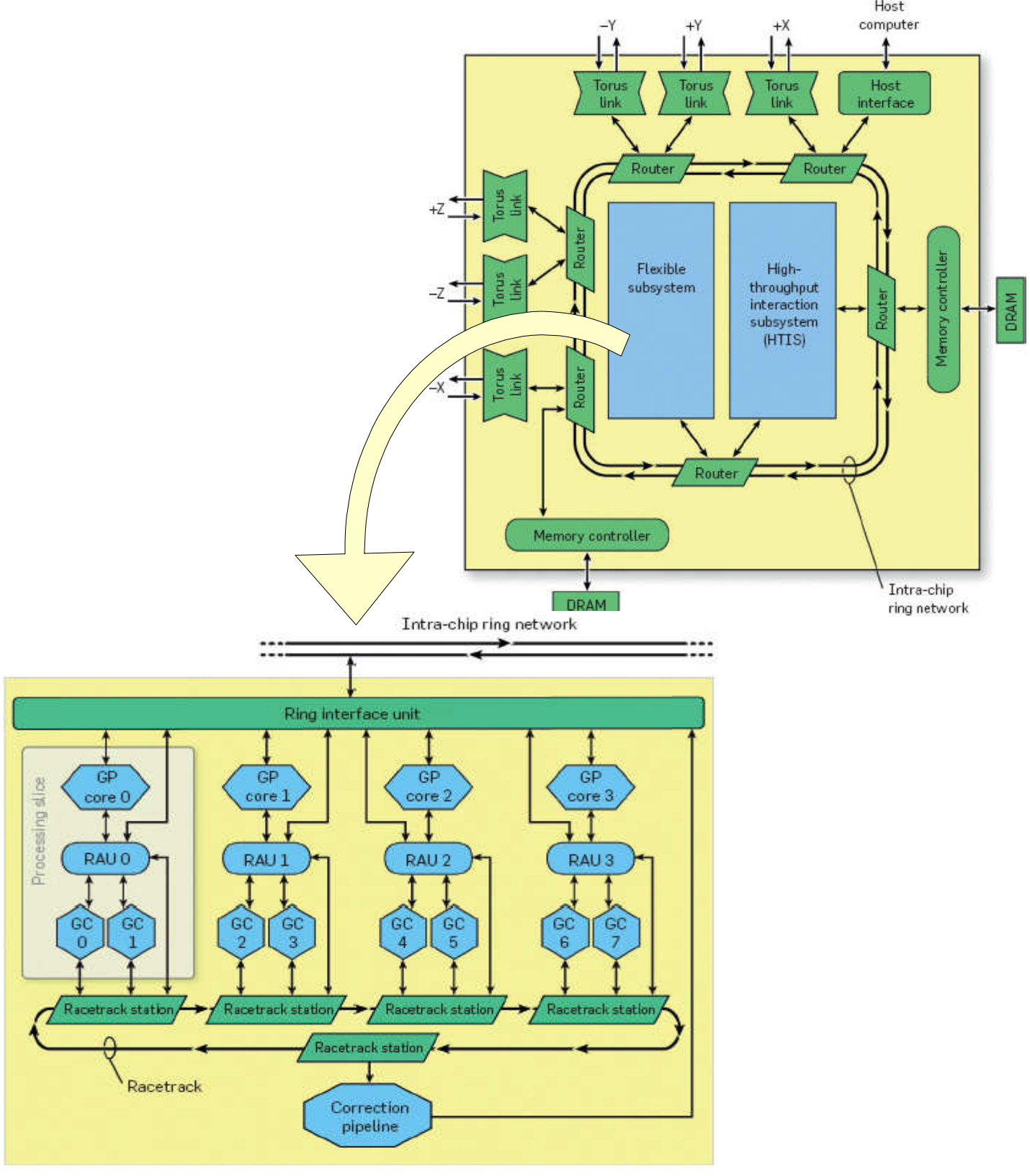
Anton

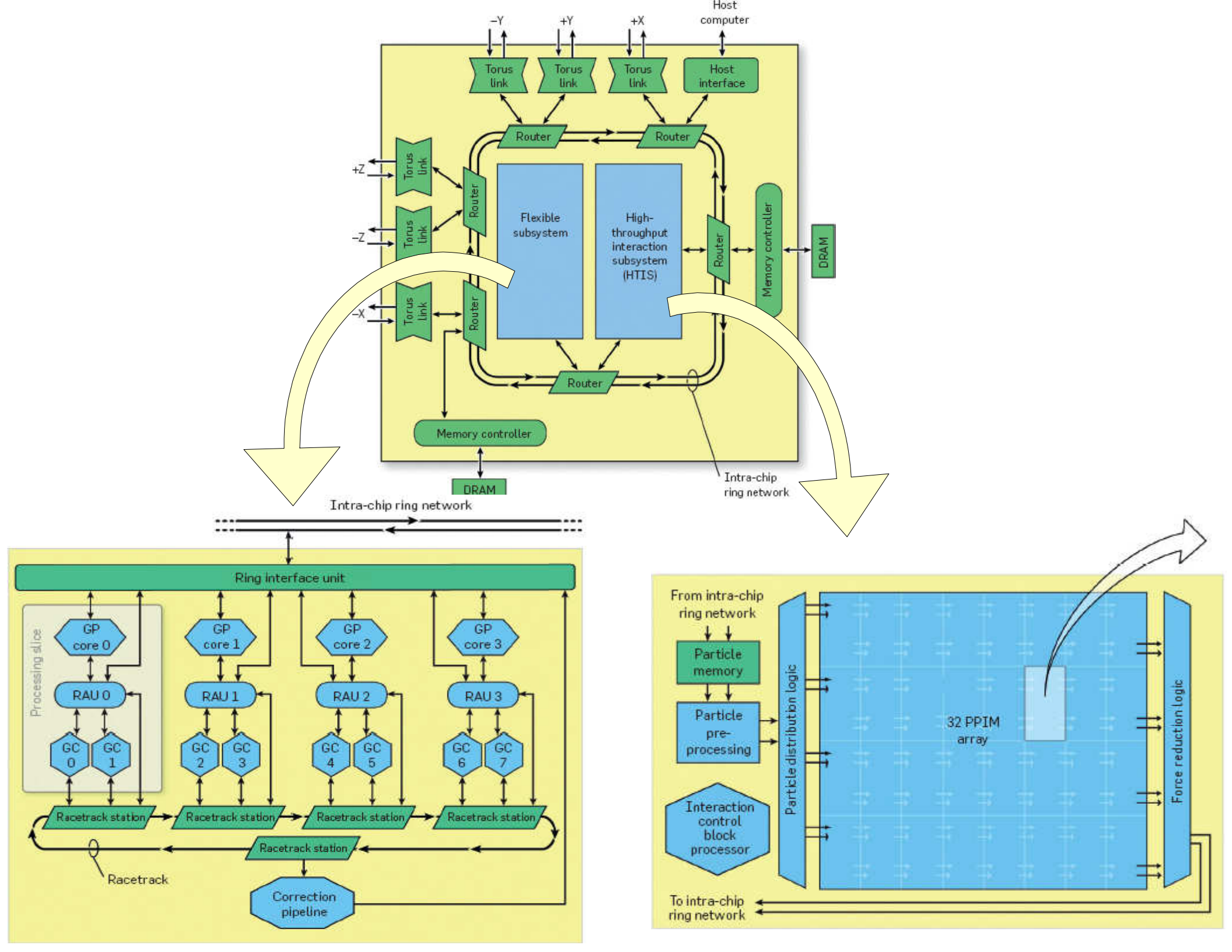
- dedicated hardware
- “computational microscope”

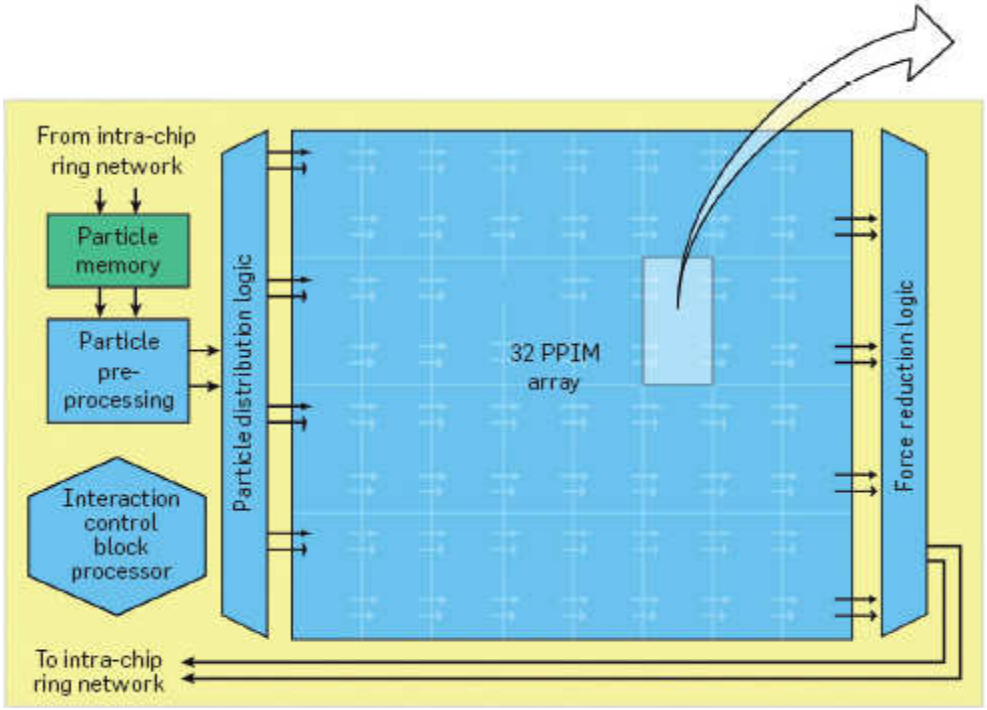
- average computer could simulate a few nanoseconds per day
- Anton can simulate 16,400 nanoseconds per day

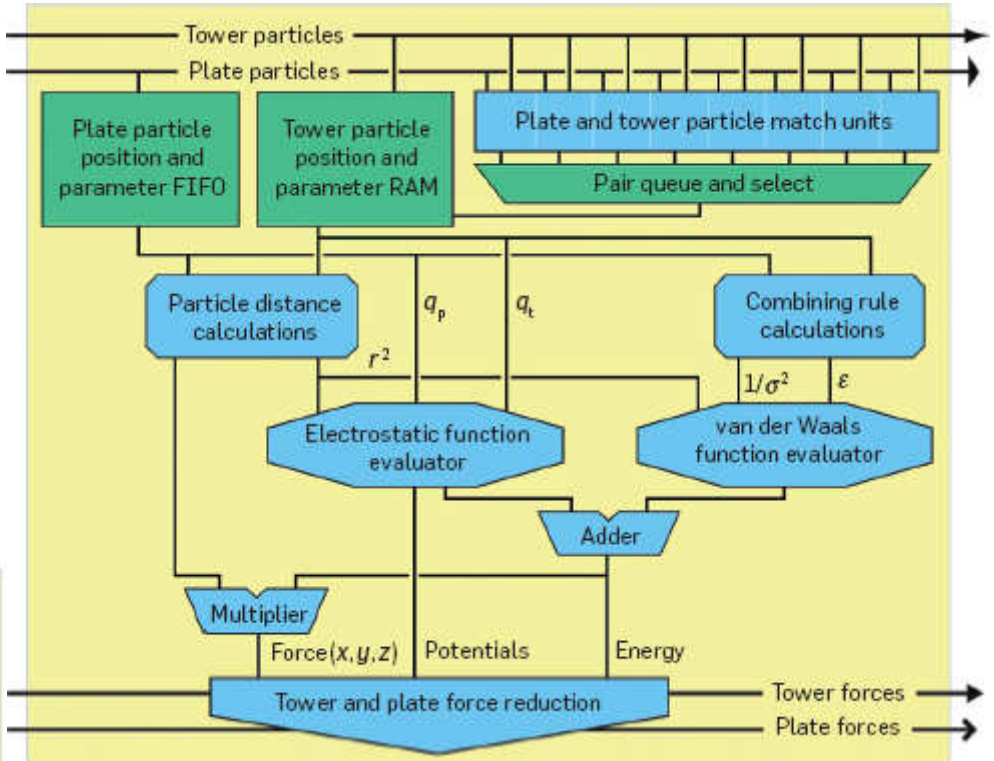
- 512 parallel chips, each containing 32 specialized 28-stage non-programmable arithmetic pipelines designed for calculating inter-particle interactions
- each pipeline gives a result per clock cycle, which would take 50 in a normal processor
- 650 trillion operations per second
- tries not to use any memory outside of the chip, and when it does it uses choreographed “push”-based communication


–Y
+Y
+X
Host computer
Torus link
Torus link
Torus link
Host interface
Router
Router
+Z
–Z
–X
Torus link
Torus link
Torus link
Router
Router
Flexible subsystem
High-throughput interaction subsystem (HTIS)
Router
Memory controller
DRAM
Router
Memory controller
DRAM
Intra-chip ring network


Host computer
−Y
+Y
+X
Torus link
Torus link
Torus link
Host interface
Router
Router
+Z
−Z
−X
Torus link
Torus link
Torus link
Router
Router
Router
Flexible subsystem
High-throughput interaction subsystem (HTIS)
Router
Memory controller
DRAM
Router
Memory controller
DRAM
Intra-chip ring network
Intra-chip ring network
Ring interface unit
Processing slice
GP core 0
GP core 1
GP core 2
GP core 3
RAU 0
RAU 1
RAU 2
RAU 3
GC 0
GC 1
GC 2
GC 3
GC 4
GC 5
GC 6
GC 7
Racetrack station
Racetrack station
Racetrack station
Racetrack station
Racetrack station
Racetrack
Correction pipeline


Host computer
−Y
+Y
+X
Torus link
Torus link
Torus link
Host interface
Router
Router
+Z
−Z
−X
Torus link
Torus link
Torus link
Router
Router
Router
Flexible subsystem
High-throughput interaction subsystem (HTIS)
Router
Memory controller
DRAM
Router
Memory controller
DRAM
Intra-chip ring network
Intra-chip ring network
Ring interface unit
Processing slice
GP core 0
GP core 1
GP core 2
GP core 3
RAU 0
RAU 1
RAU 2
RAU 3
GC 0
GC 1
GC 2
GC 3
GC 4
GC 5
GC 6
GC 7
Racetrack station
Racetrack station
Racetrack station
Racetrack station
Racetrack station
Racetrack
Correction pipeline
From intra-chip ring network
Particle memory
Particle pre-processing
Interaction control block processor
Particle distribution logic
32 PPIM array
Force reduction logic
To intra-chip ring network


From intra-chip ring network
Particle memory
Particle pre-processing
Interaction control block processor
Particle distribution logic
32 PPIM array
Force reduction logic
To intra-chip ring network


Tower particles
Plate particles
Plate particle position and parameter FIFO
Tower particle position and parameter RAM
Plate and tower particle match units
Pair queue and select
Particle distance calculations
q_p
q_t
Combining rule calculations
r^2
$1/\sigma^2$
ε
Electrostatic function evaluator
van der Waals function evaluator
Adder
Multiplier
Force(x,y,z)
Potentials
Energy
Tower and plate force reduction
Tower forces
Plate forces

Sources

CACM Staff. “A Conversation with David E. Shaw.” *Communications of the ACM* 10.1145/1562764.1562782 (2009): 48-54. Web. 12 December 2010.

Shasha, Dennis and Lazere, Cathy. “Anton and the Giant Femtoscope.” *Natural Computing*. New York: W.W. Norton, 2010. Print.

Shaw, David, et al. “Anton, a special-purpose machine for molecular dynamics simulation.” *Communications of the ACM* 10.1145/1364782.1364802 (2008): 91-97. Web. 12 December 2010.