

Anton 3 Capabilities and Enhanced Sampling

D E Shaw Research

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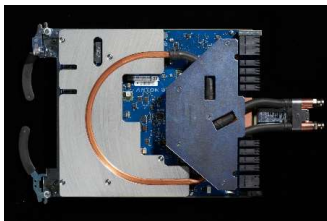
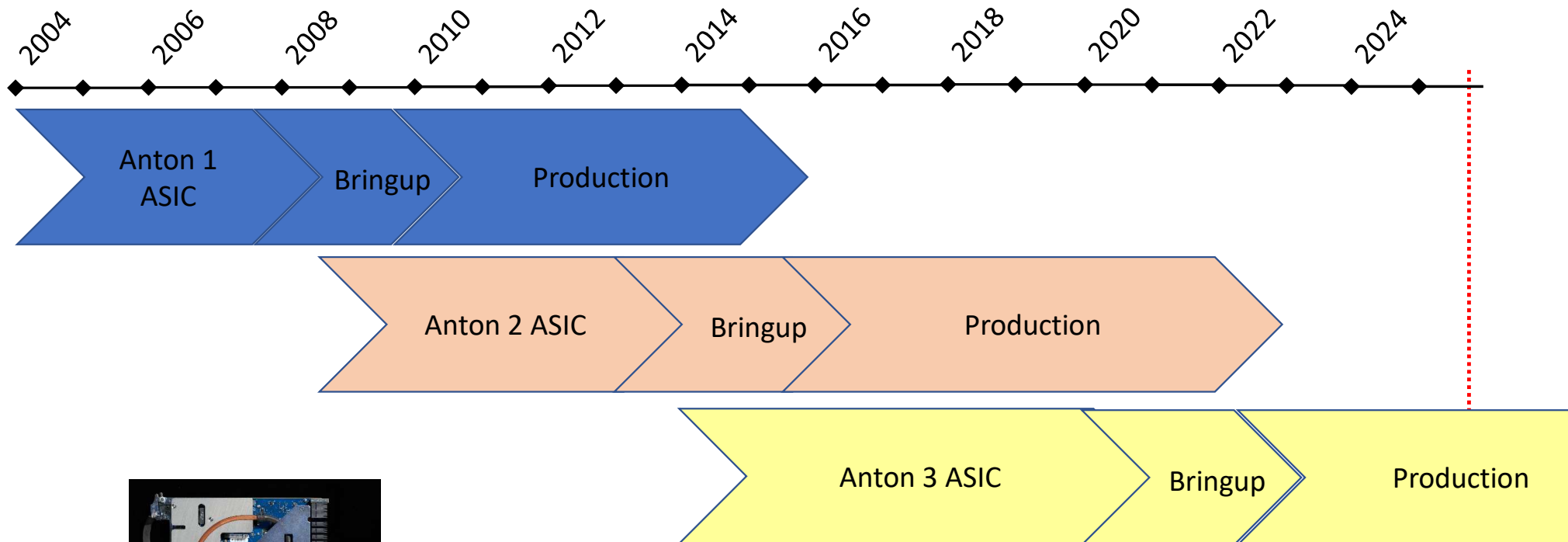
September 22, 2025

A unique collaborative project

- D. E. Shaw Research started in 2002 (midtown Manhattan)
- Founder and Chief Scientist: David E. Shaw
- High-level goal: Transform biochemistry research and the process of drug discovery and development through high-performance computation

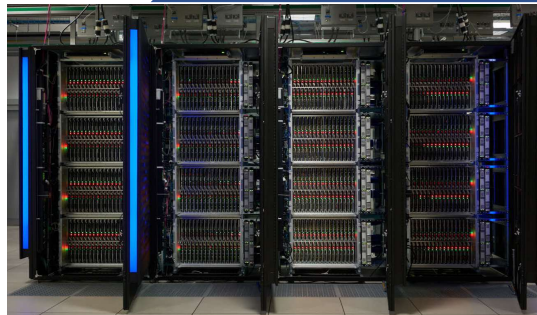


Anton Timeline



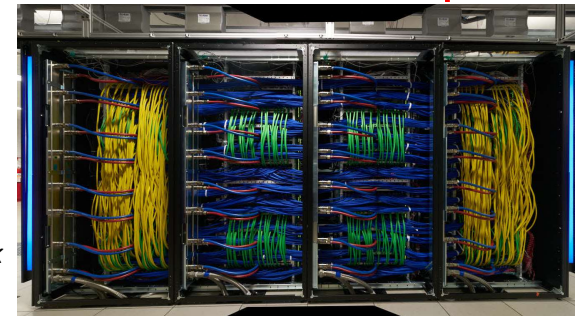
Anton 3 node board

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512-node
Anton 3

front

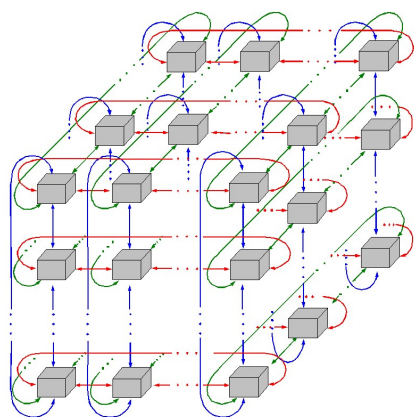


back

Anton 3 Architecture

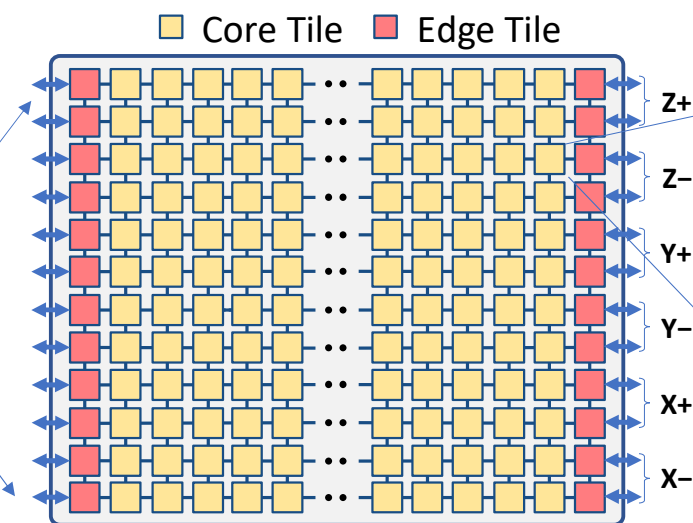
Massively parallel, specialized to molecular dynamics

3D torus of "nodes":



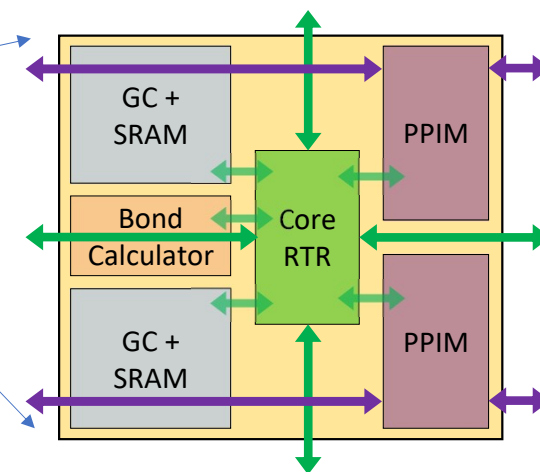
power-of-two sizes,
e.g. 2x2x2, 4x4x8

A node is basically one chip ("ASIC"):



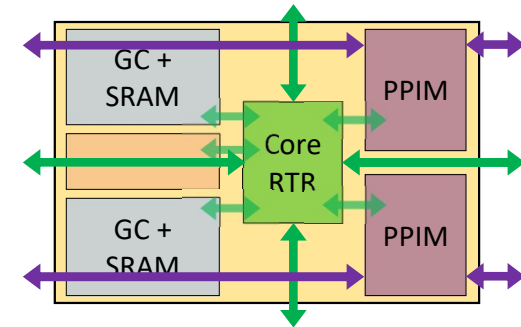
12 rows by up to 24 columns
(working columns vary from 22-24)

The ASIC is composed of "tiles"



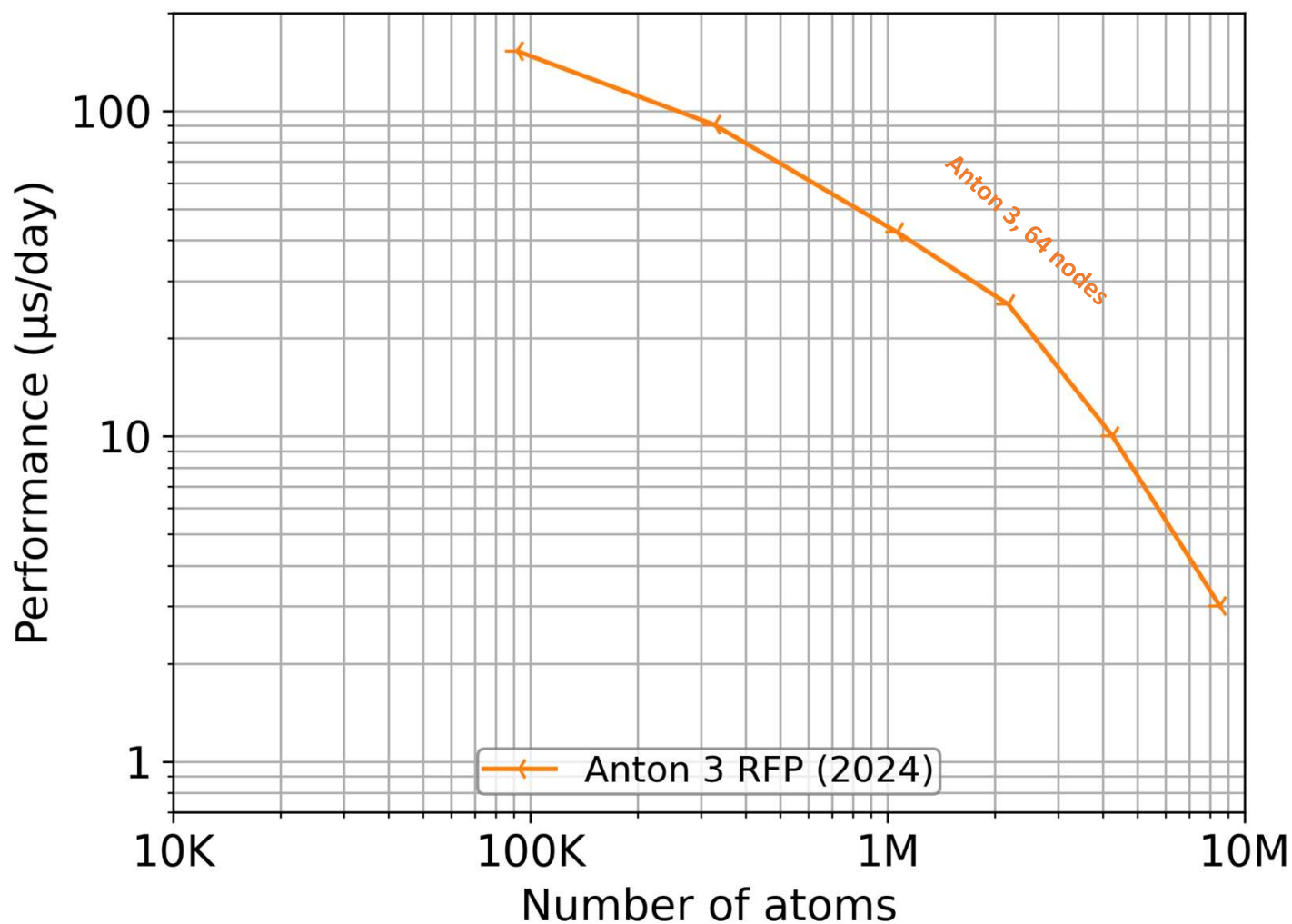
GC = "Geometry Core" (processor core)
PPIM = "Particle-Particle Interaction Module"

Specialized Hardware

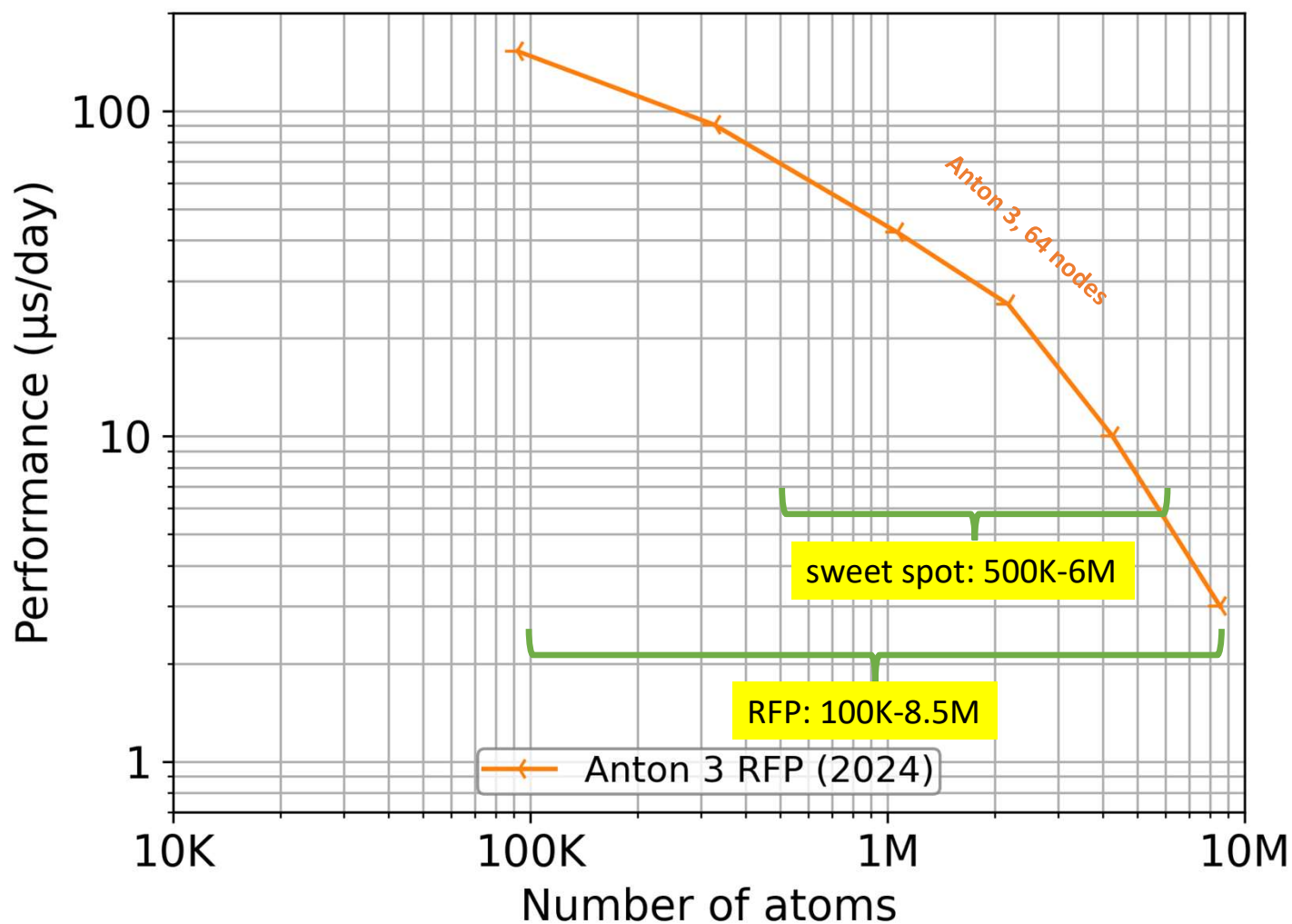


- From-scratch hardware for molecular dynamics
 - Hardware pipelines + embedded processors + integrated network
 - (not a GPU, not an FPGA, not infiniband)
 - No operating system, no virtual memory, no floating-point
- Whole machine is a big coprocessor: load, run, unload
- Why is isn't it all hardware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

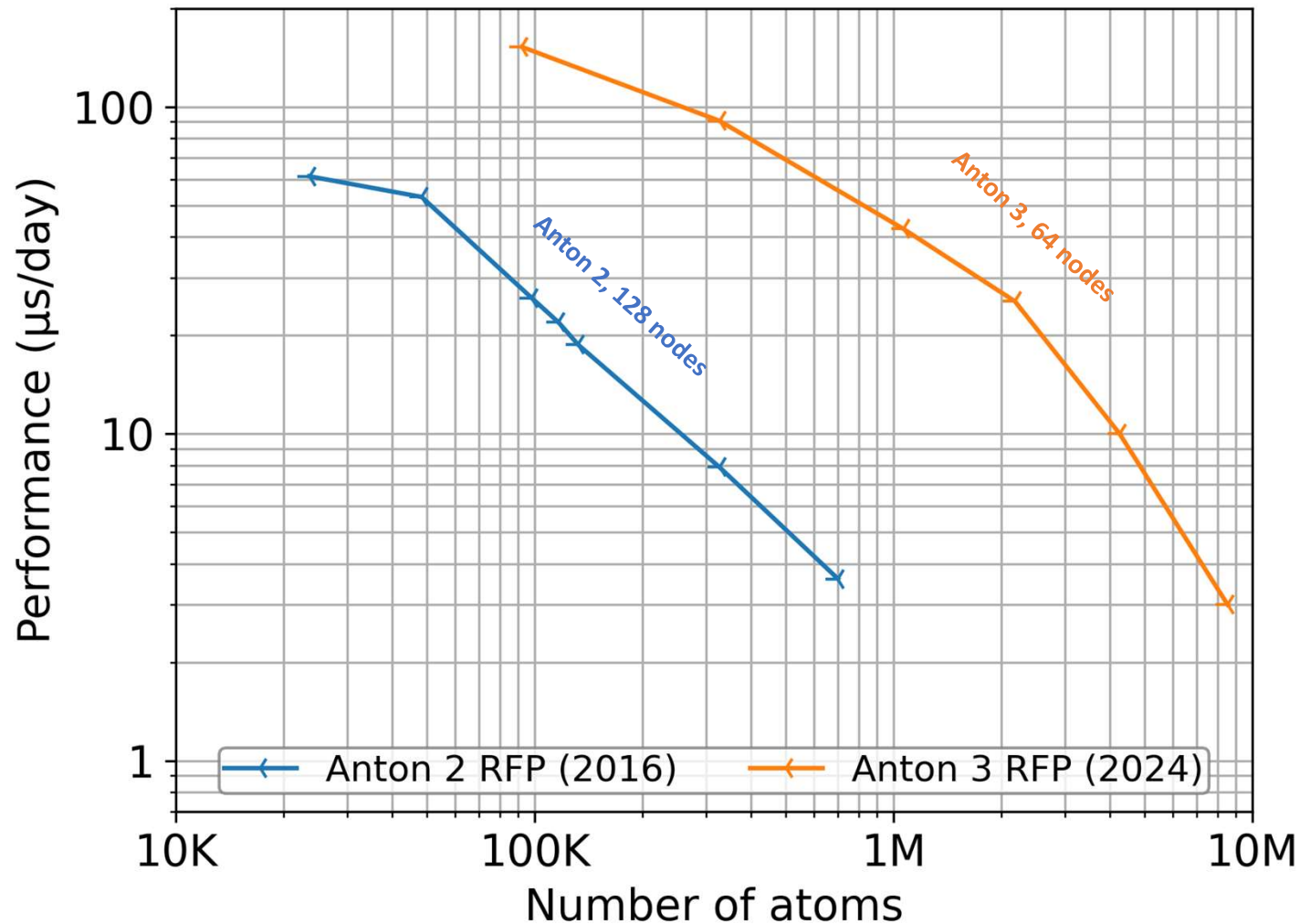
Anton 3 Performance



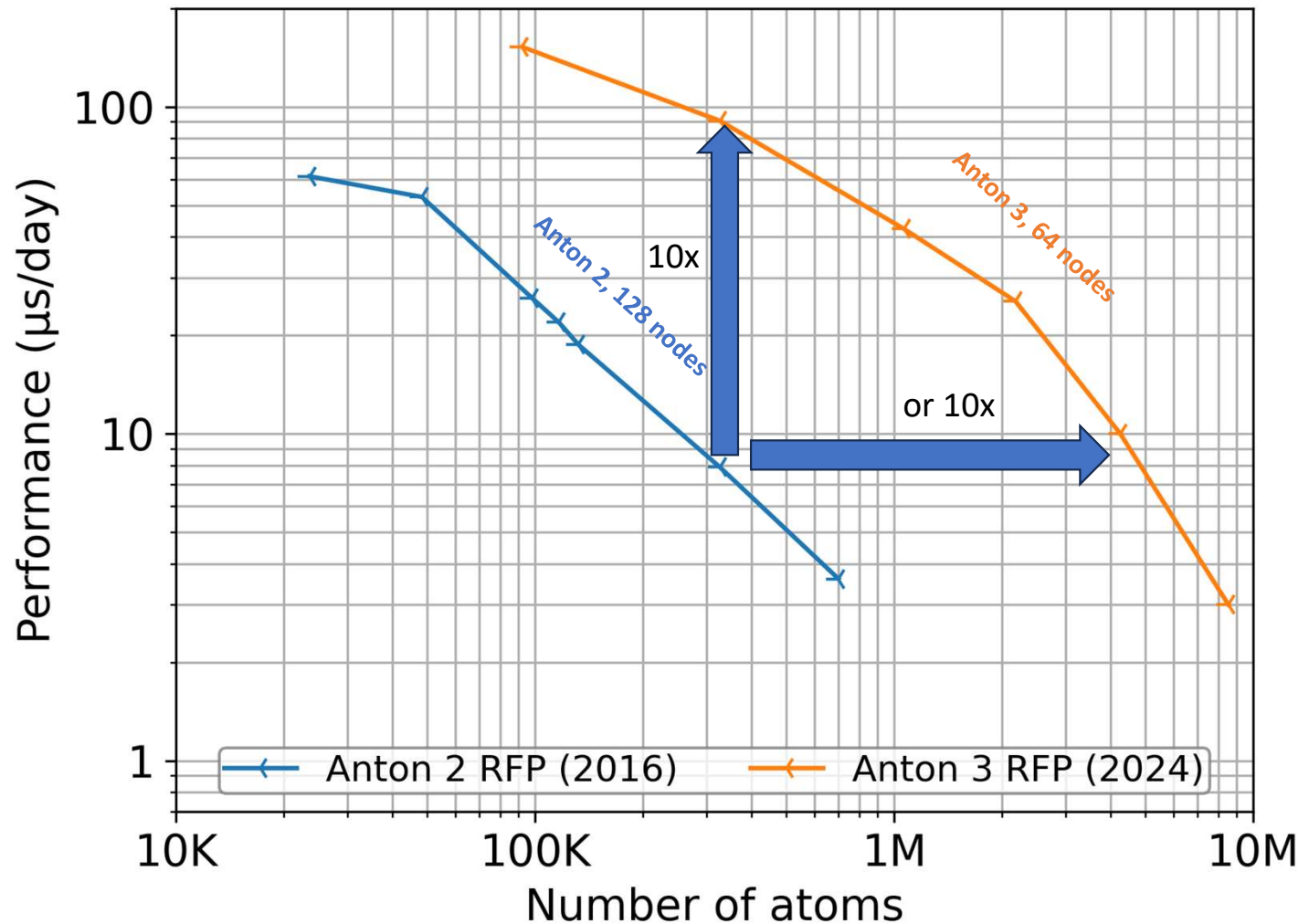
Anton 3 Performance



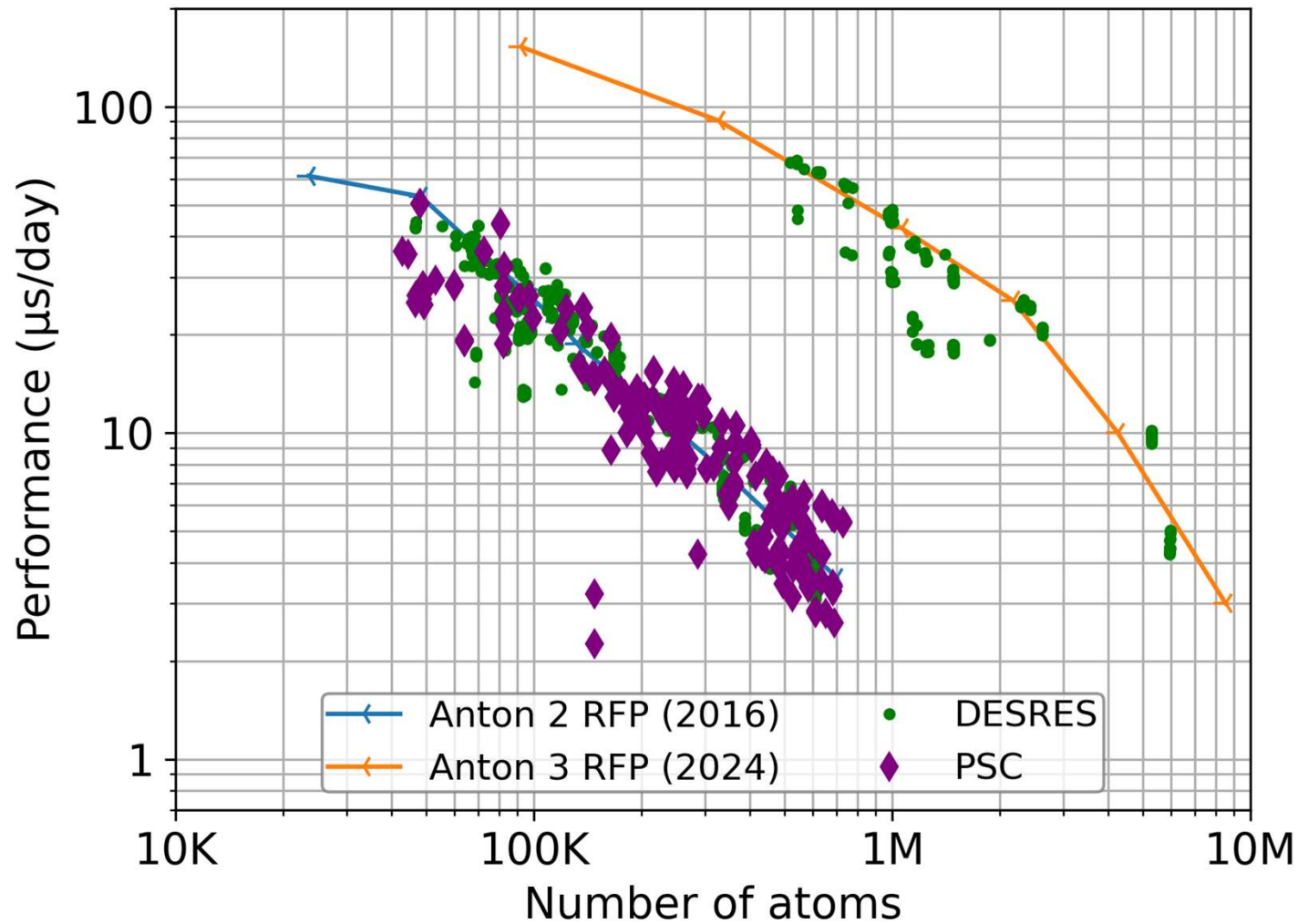
Performance vs Anton 2



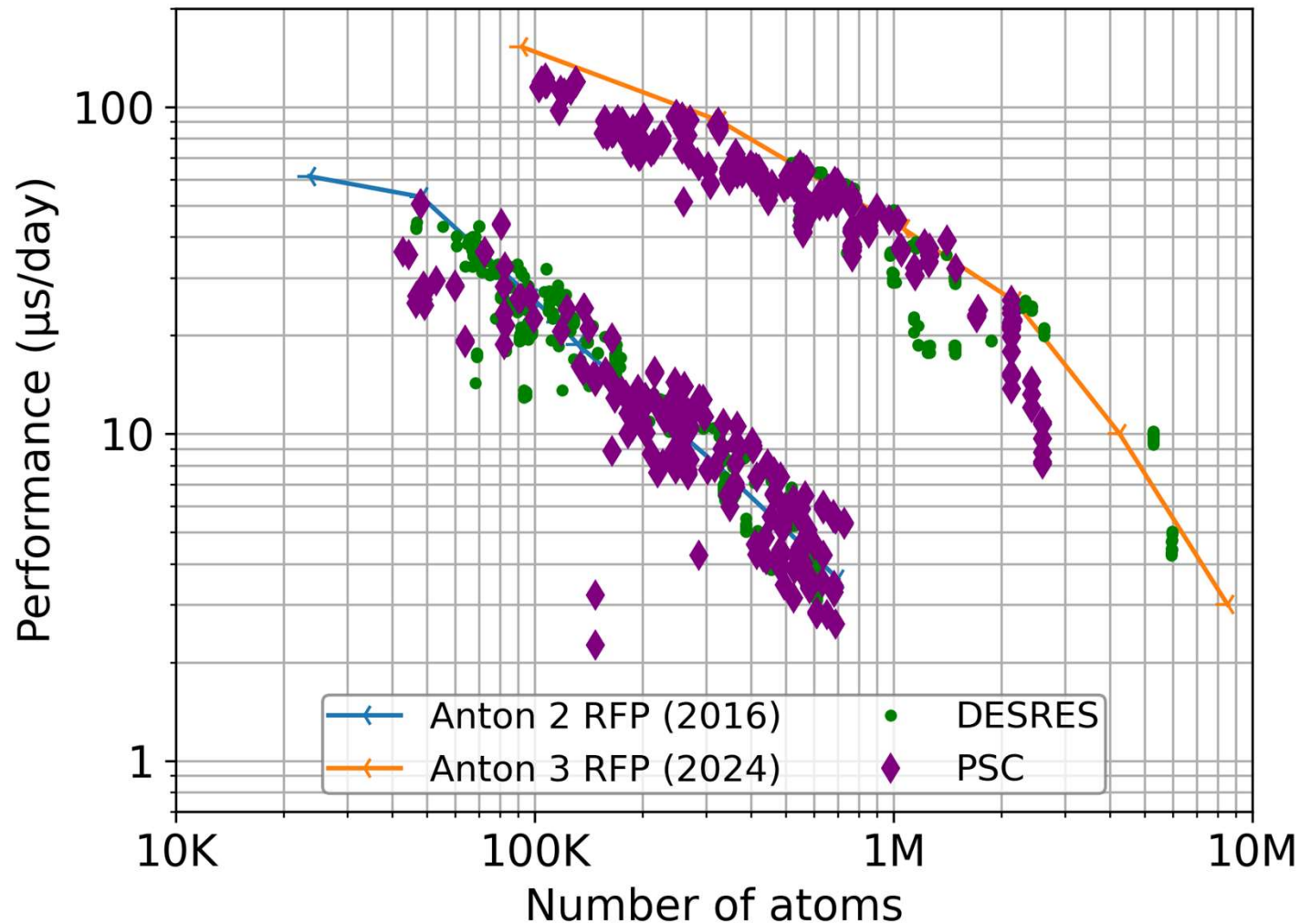
Performance vs Anton 2



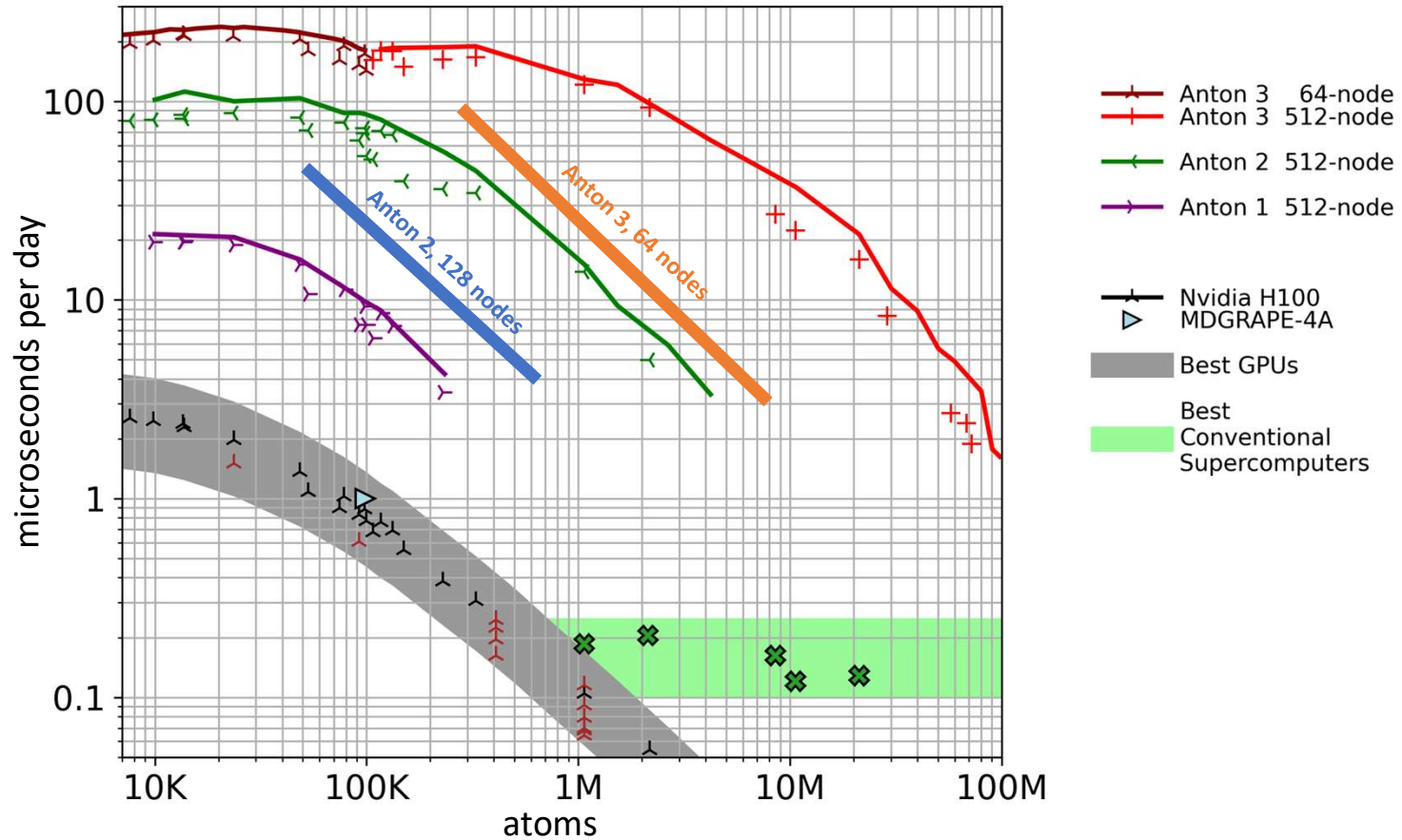
Performance in Practice



Performance in Practice



Performance Universe



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