

A photograph of several Anton 3 server racks in a data center. The racks are illuminated with blue light, and the perforated doors are glowing. The text "Anton 3 Capabilities and Enhanced Sampling" is overlaid in white. The name "ANTON 3" is visible on the lower part of the racks.

# Anton 3 Capabilities and Enhanced Sampling

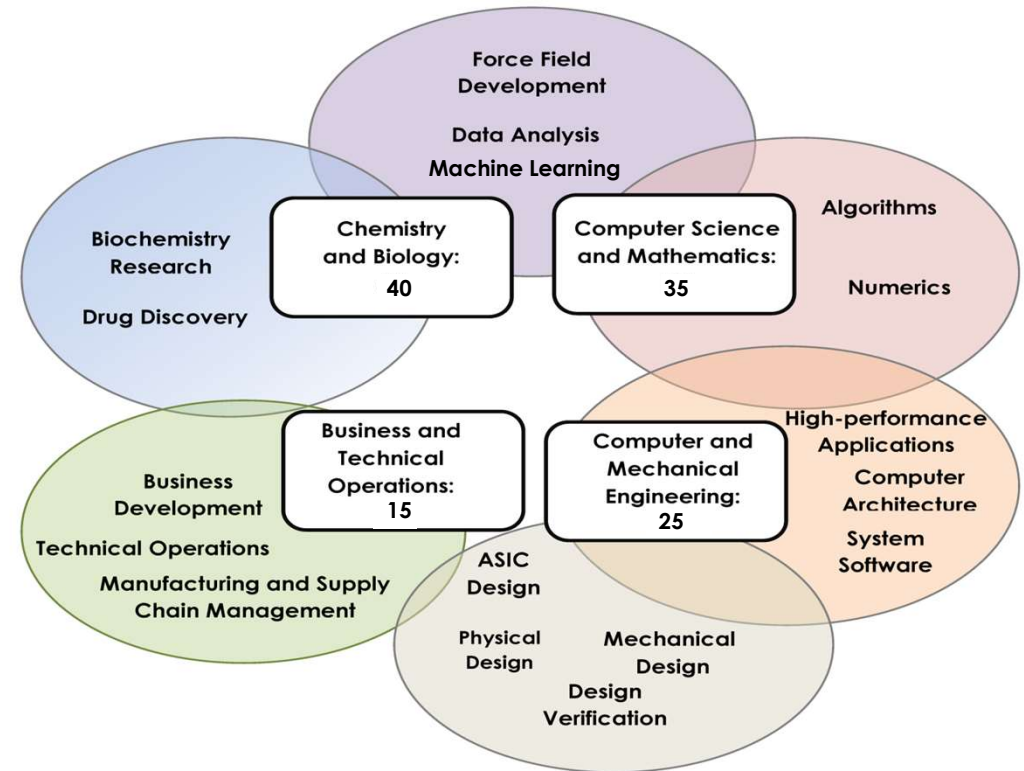
**D E Shaw Research**

Ken Mackenzie  
Avi Robinson-Mosher  
Parker de Waal

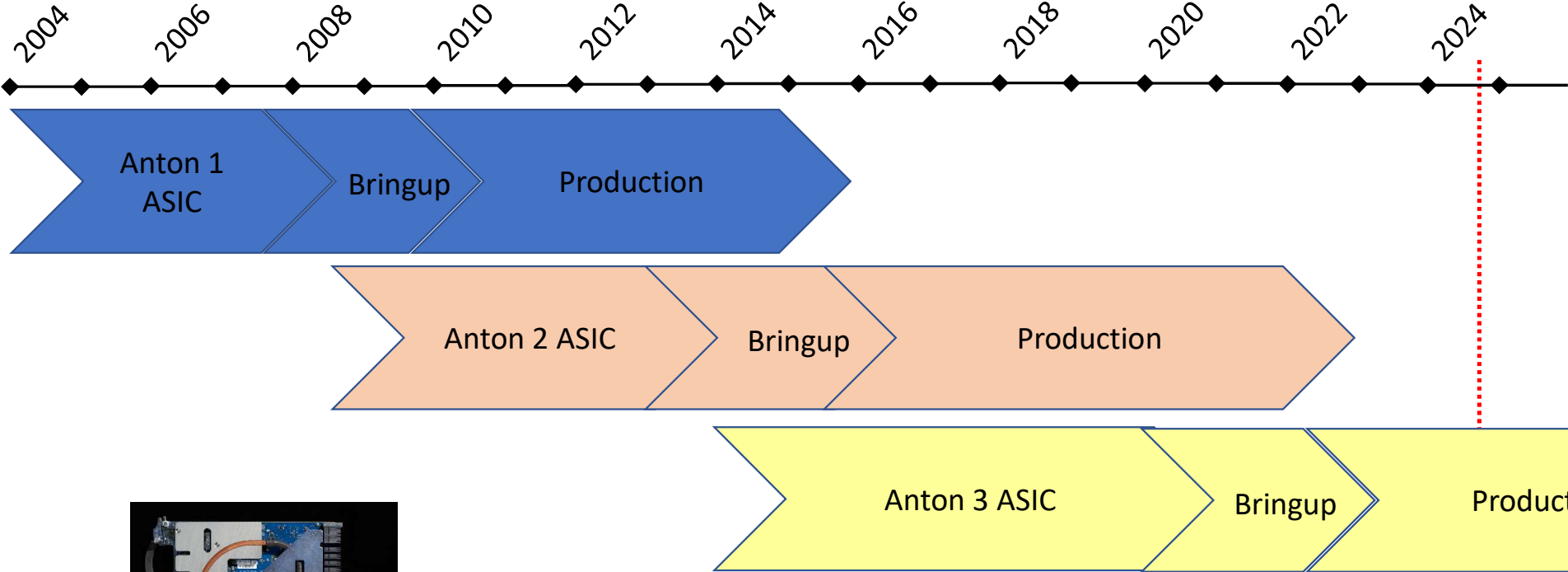
September 23, 2024

# 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



# Roadmap



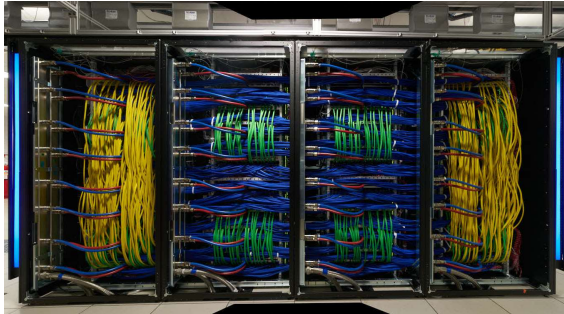
Anton 3 node board

D E Shaw Research



512-node  
Anton 3

front

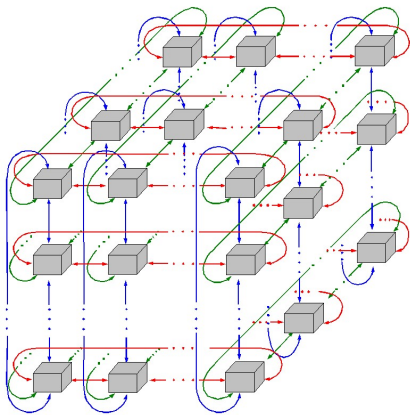


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# Anton 3 Architecture

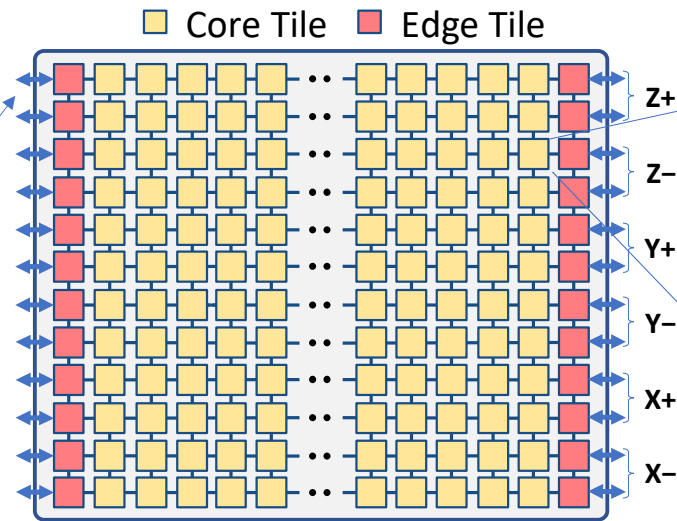
Massively parallel, specialized to molecular dynamics

3D torus of "nodes":



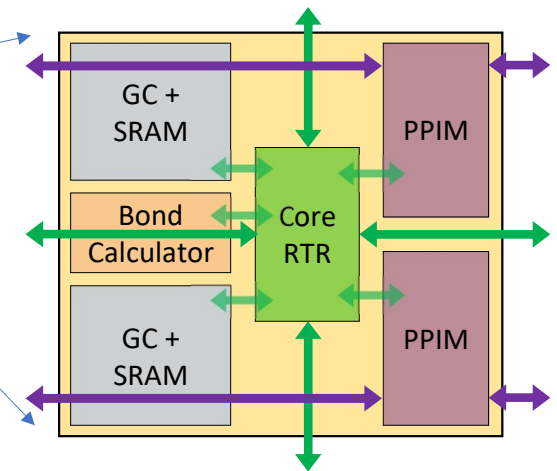
power-of-two sizes,  
e.g. 2x2x2, 4x4x8

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



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

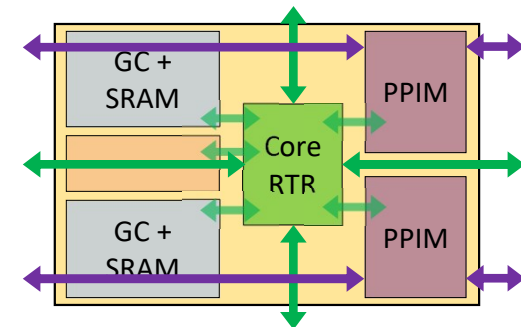
The ASIC is composed of "tiles"



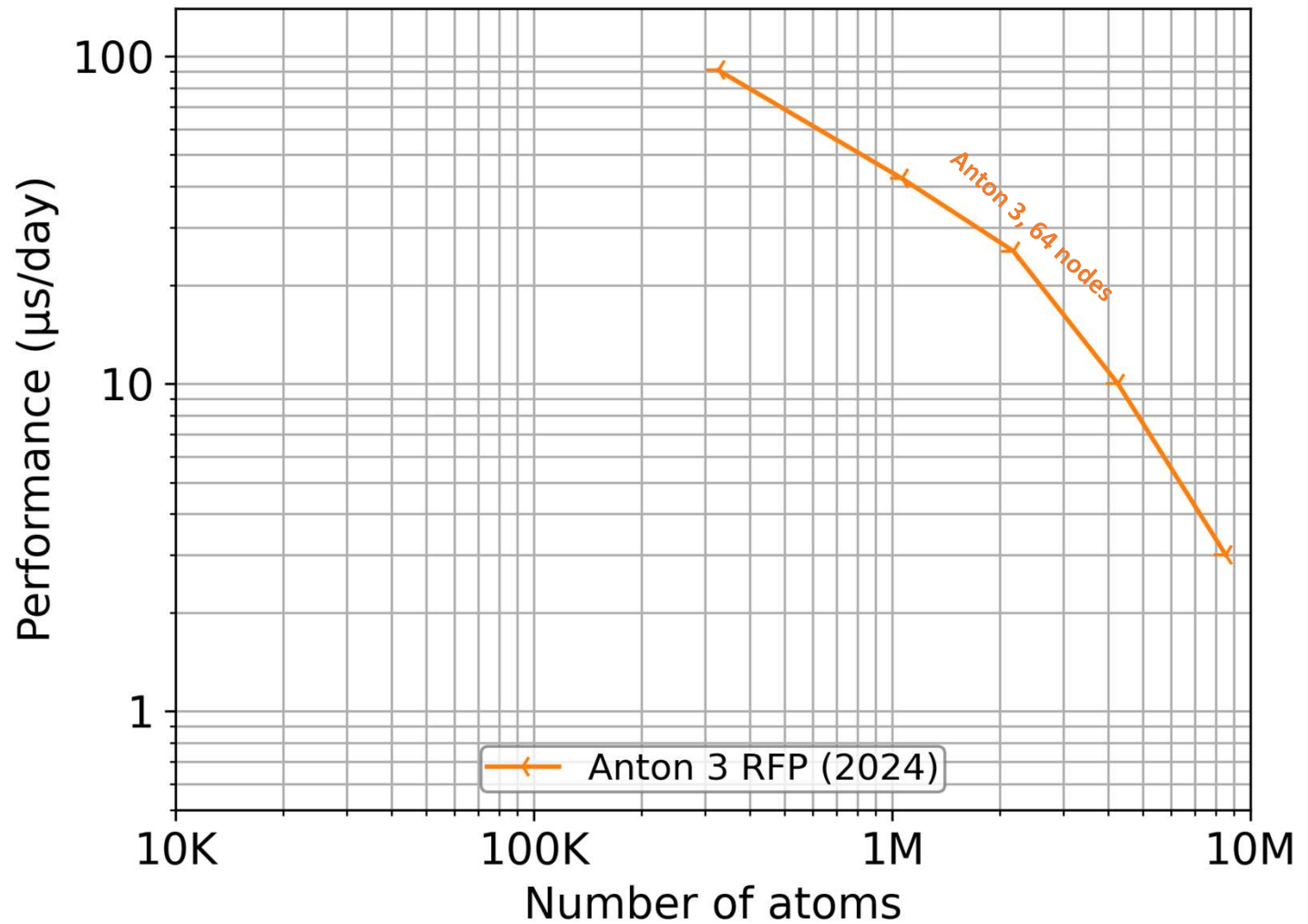
GC = "Geometry Core" (processor core)  
PPIM = "Particle-Particle Interaction Module"

# Specialized Hardware

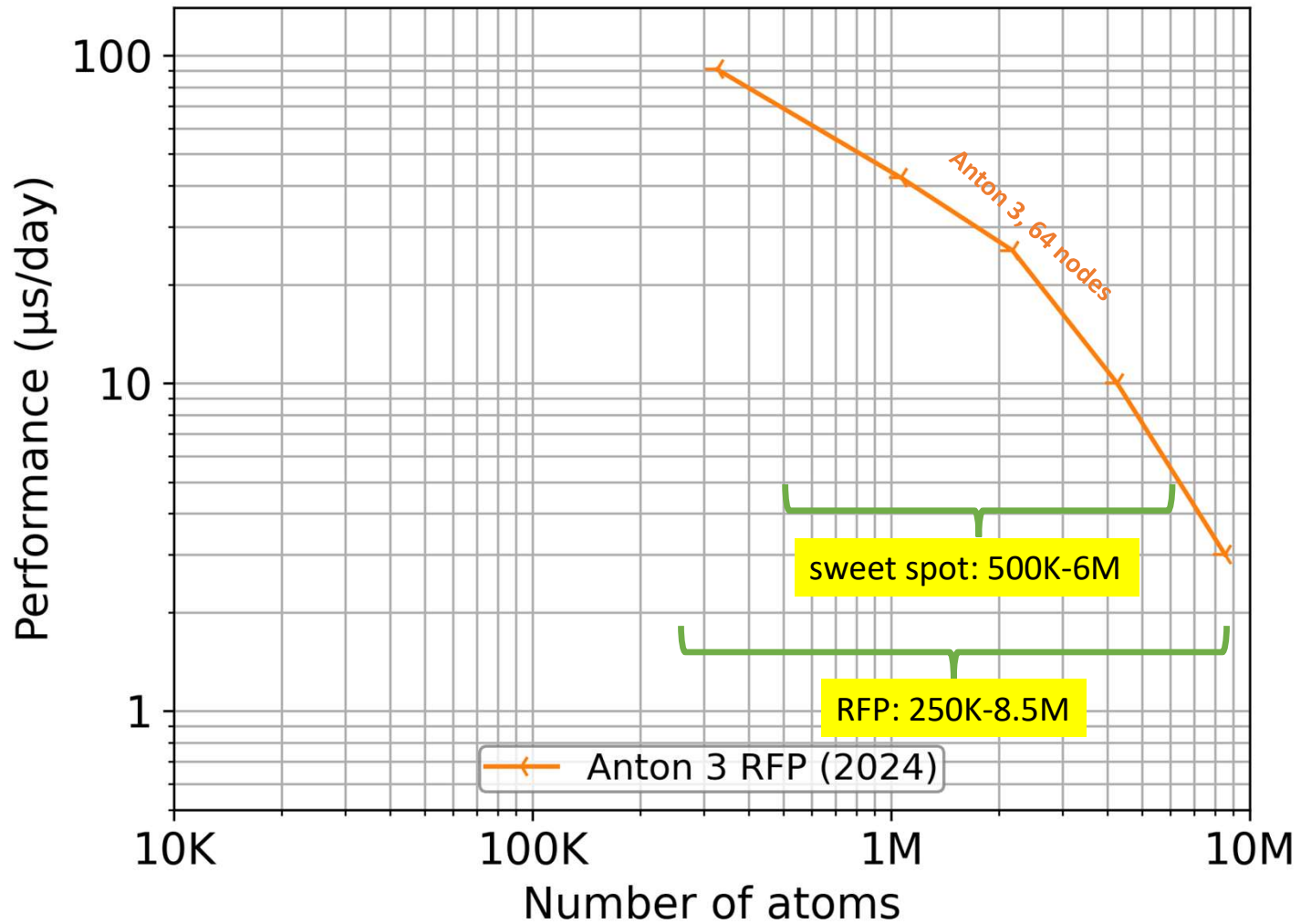
- From-scratch hardware for molecular dynamics
  - Hardware pipelines + embedded processors + integrated network
  - (not a GPU, not an FPGA, not infiniband)
  - No operating system, no virtual memory
- Whole machine is a big coprocessor: load, run, unload
- Why is isn't it all hardware (why embed processors)?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



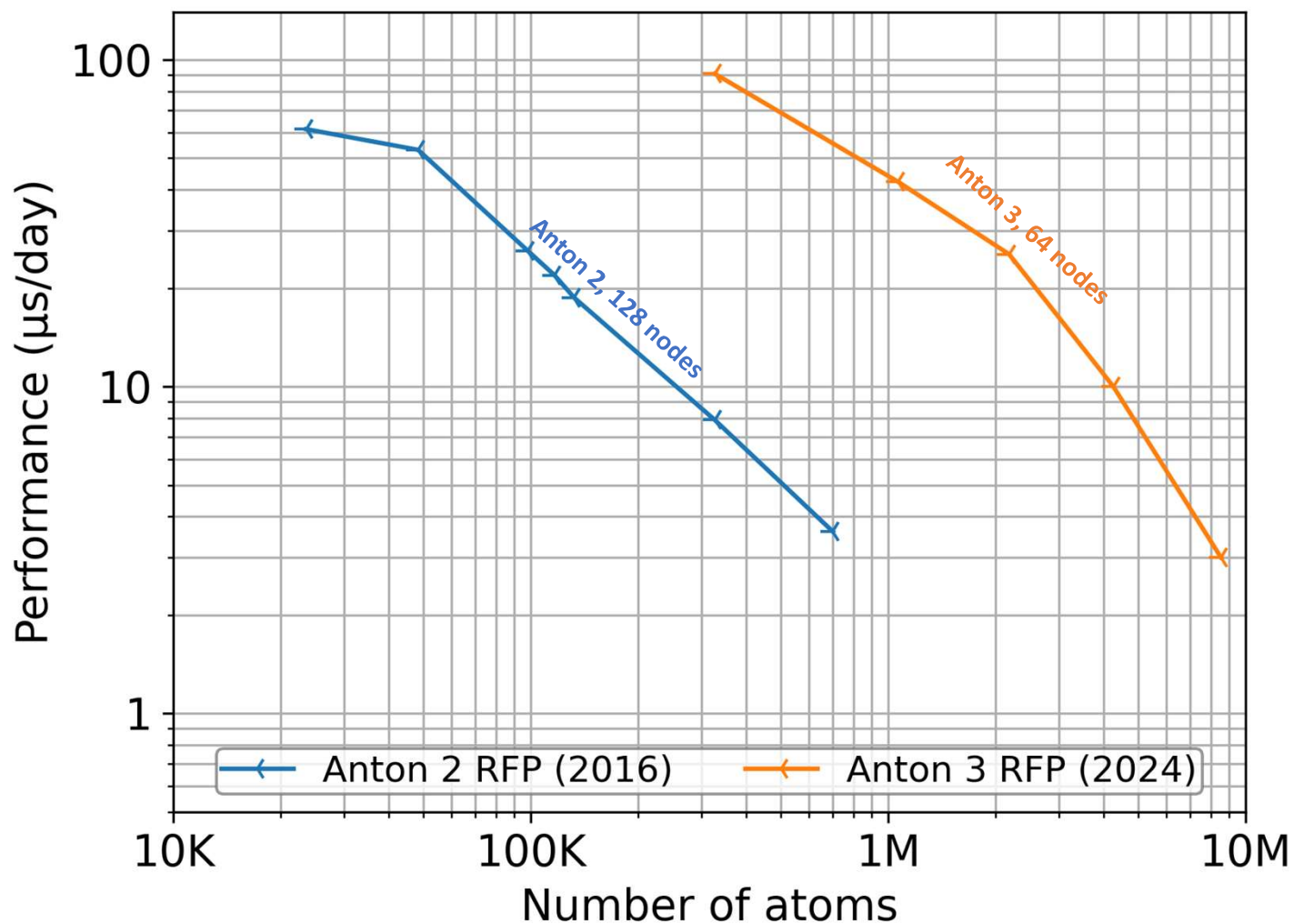
# Anton 3 Performance



# Anton 3 Performance

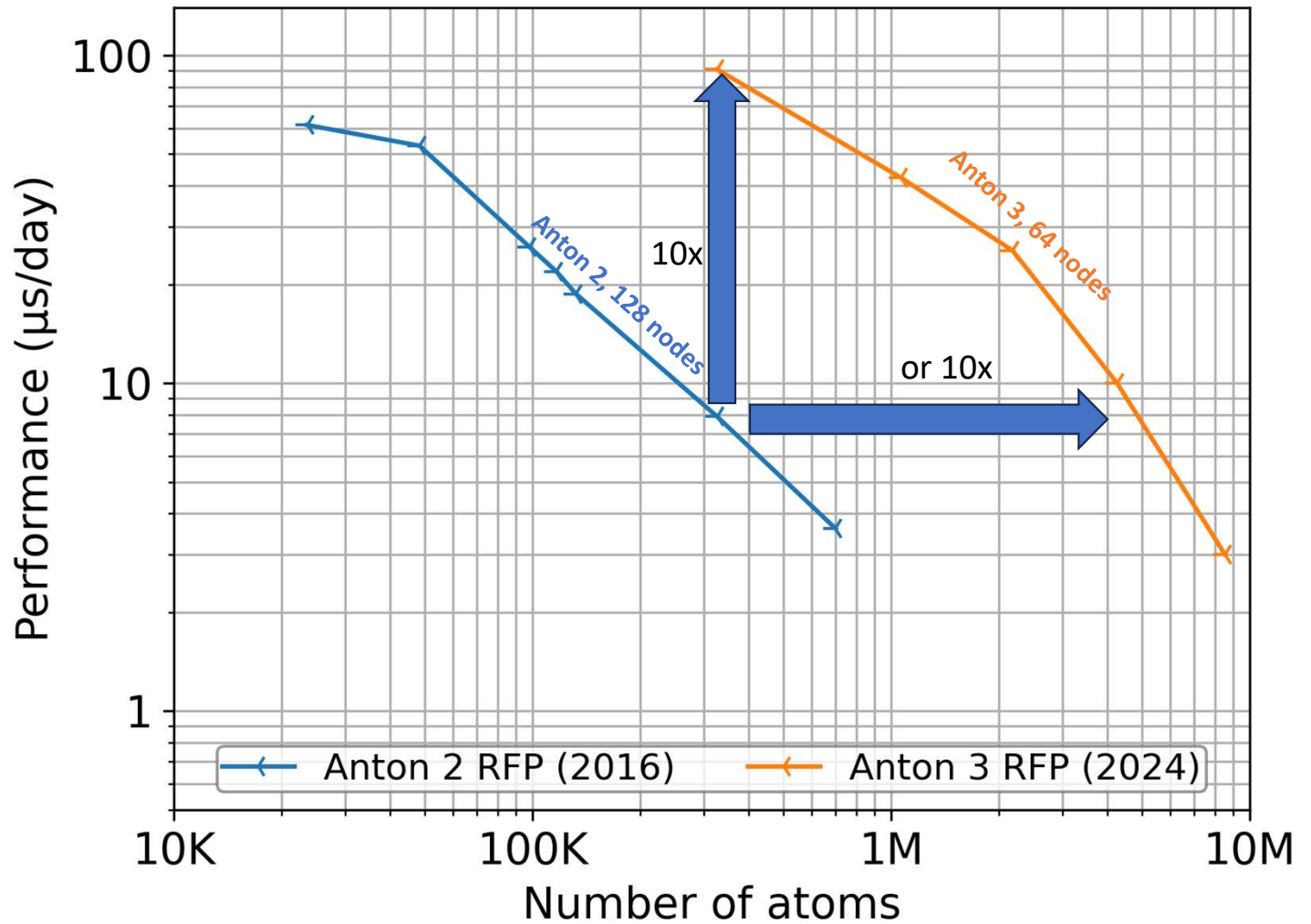


# Performance vs Anton 2

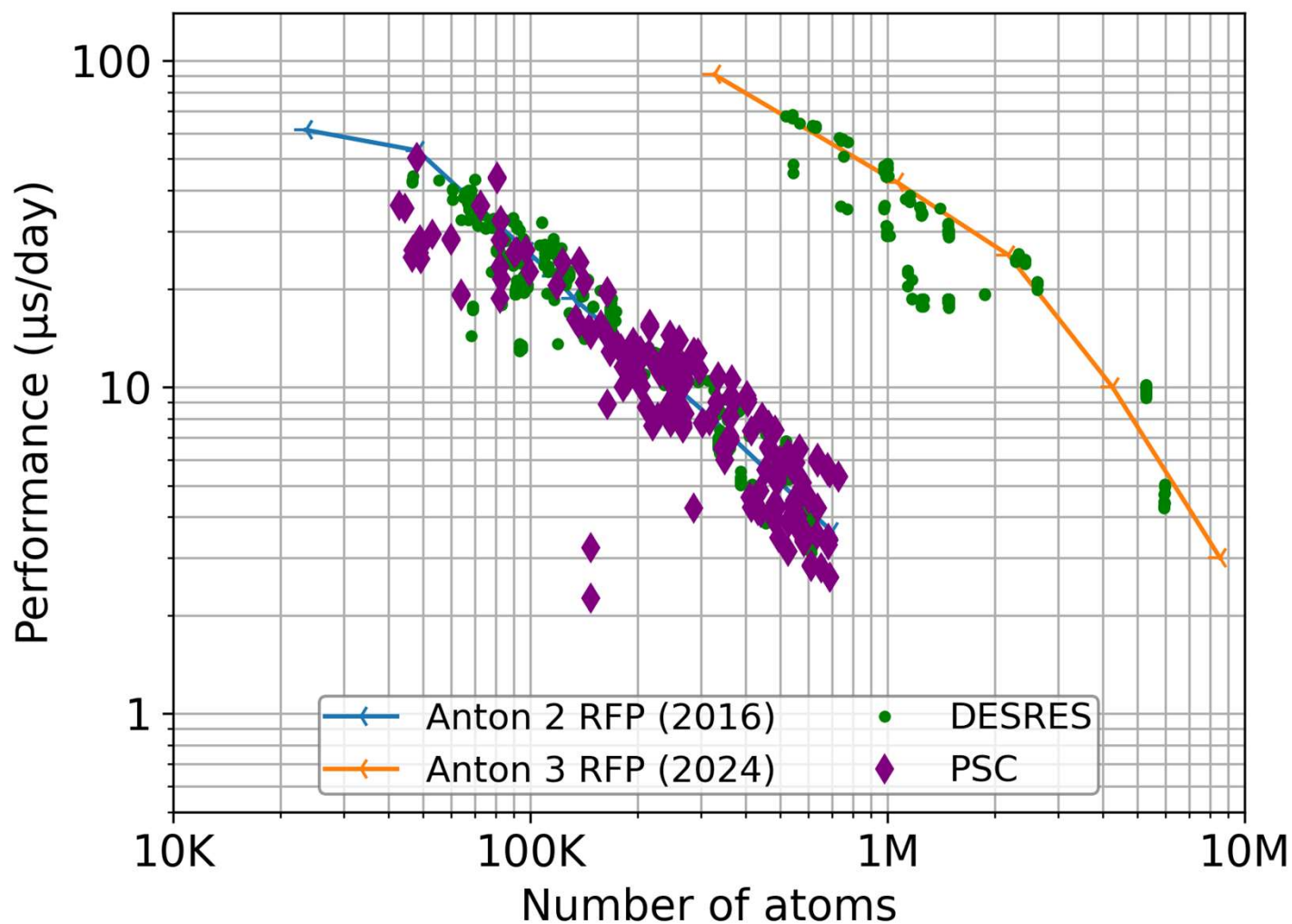




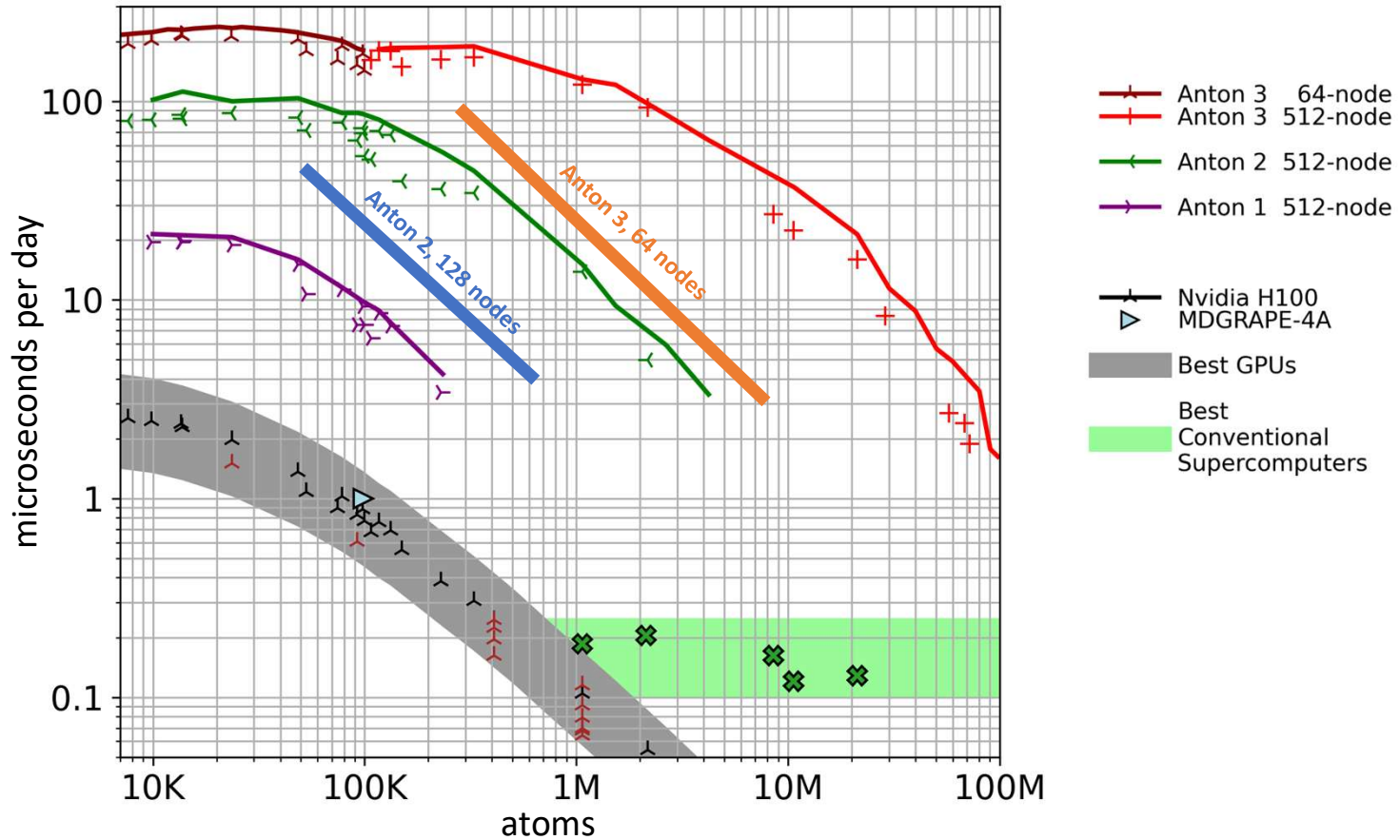
# Performance vs Anton 2



# Performance in Practice



# Performance Universe



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**ANTON 3**

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2PL3-PR11  
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2043 KOREA