Intro to HPC

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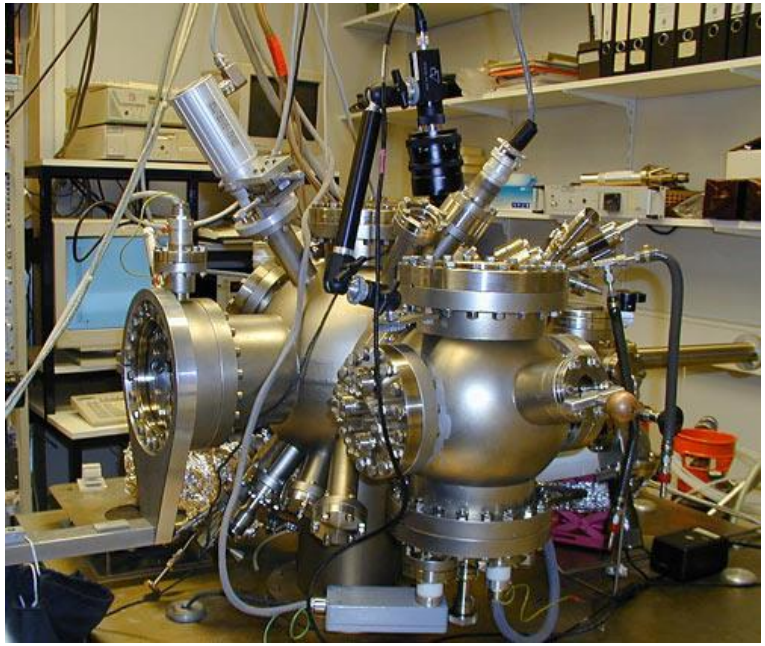
IT4Innovations

Computer - Scientific instrument

Computers are instruments of research, just like microscope

Supercomputer - Scientific instrument



Supercomputers are instruments of research, just like STM microscope

Supercomputing - a phenomenon

Supercomputing is no science by itself

Supercomputing is what happens when scientists
(physicists, chemists, engineers, medical doctors,
linguists, mathematicians etc.)
do research on supercomputer

Skills are needed to acquire to use
supercomputers efficiently

- Codes need to be ported
- Algorithms need to be modified and adapted
- Techniques are to be learned
- Nobody will do it all for you

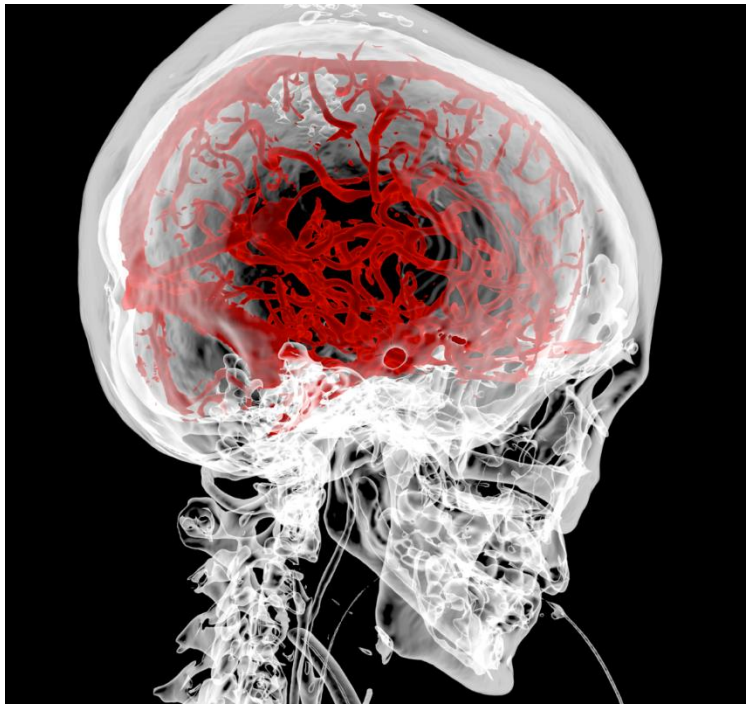
Simulation: The Third Pillar of Science

- Traditional scientific and engineering paradigm:
  - 1) Do theory or paper design.
  - 2) Perform experiments or build system.
- Limitations:
  - Too difficult - build large wind tunnels.
  - Too expensive - build a throw-away passenger jet.
  - Too slow - wait for climate or galactic evolution.
  - Too dangerous - weapons, drug design, climate experimentation.
- Computational science paradigm:
  - 3) Use high performance computer systems to simulate the phenomenon
    - Base on known physical laws and efficient numerical methods.

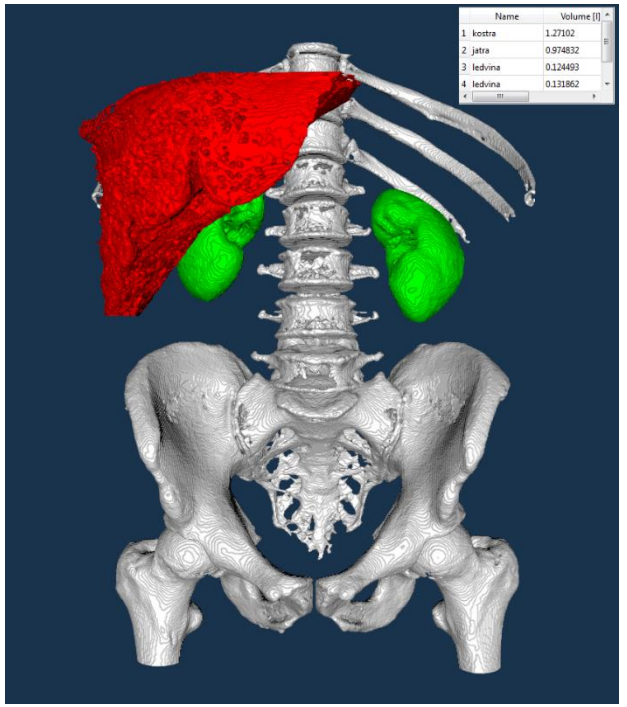
Source : V. Sarkar – Rice University

Image Analysis and Processing

- Rendering
- Creating 3D models from CT and MR scans

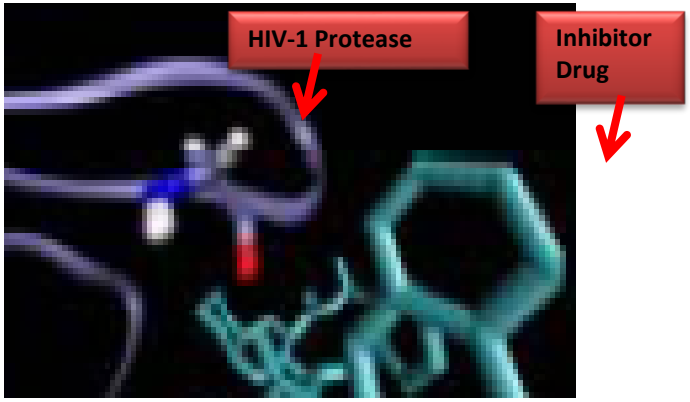


- Bio CFD and CSM simulations
- Virtual Reality Lab



Why is HPC Important?

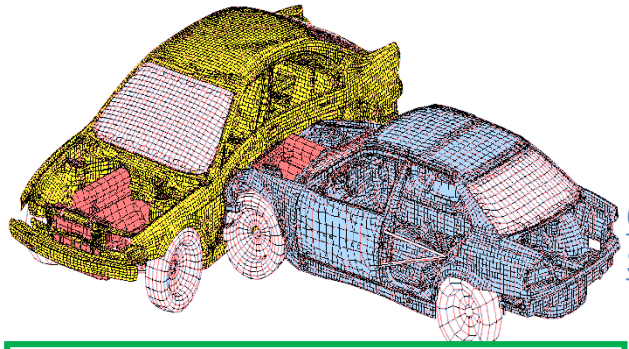
Molecular Dynamics



Simulation for 2ns:
- **2 weeks on a desktop**
- **6 hours on a supercomputer**

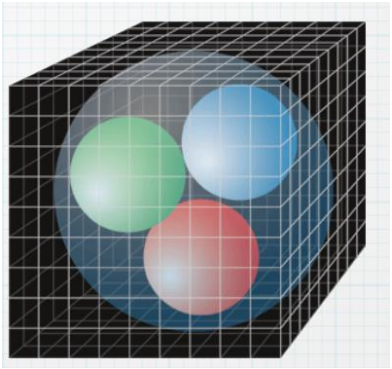
Gene Sequence Alignment

Phylogenetic Analysis:
- **32 days on desktop**
- **1.5 hrs supercomputer**



Car Crash Simulations

2 million elements simulation:
- **4 days on a desktop**
- **25 minutes on a supercomputer**



Understanding Fundamental Structure of Matter

Requires a billion-billion calculations per second

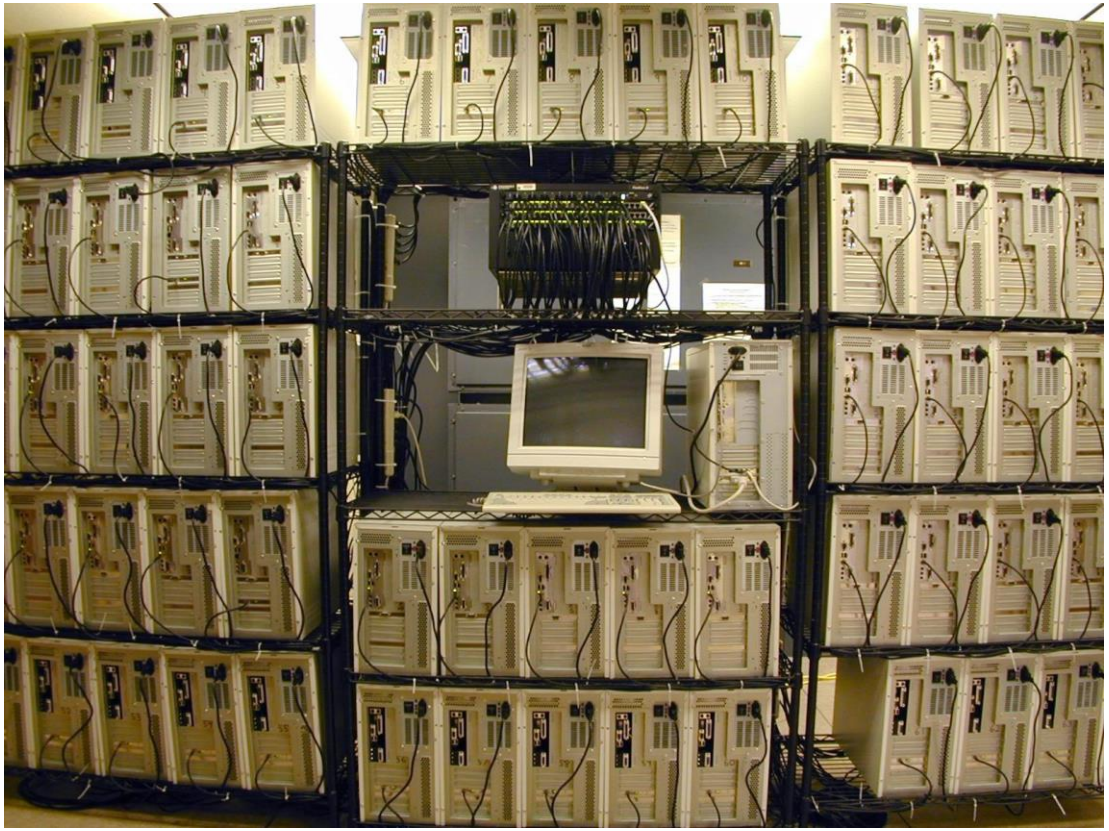
HPC in Everyday Products

- **Industrial competitiveness**
- **Not only for the design of NASA space shuttles, but according to Proctor and Gamble, it is also for the**
  - **Pringles Potato Chips**
  - **Clorox Bottles**
  - **…**

HPC instruments

The supercomputers and supercomputing

1999-2006 Beowulf class



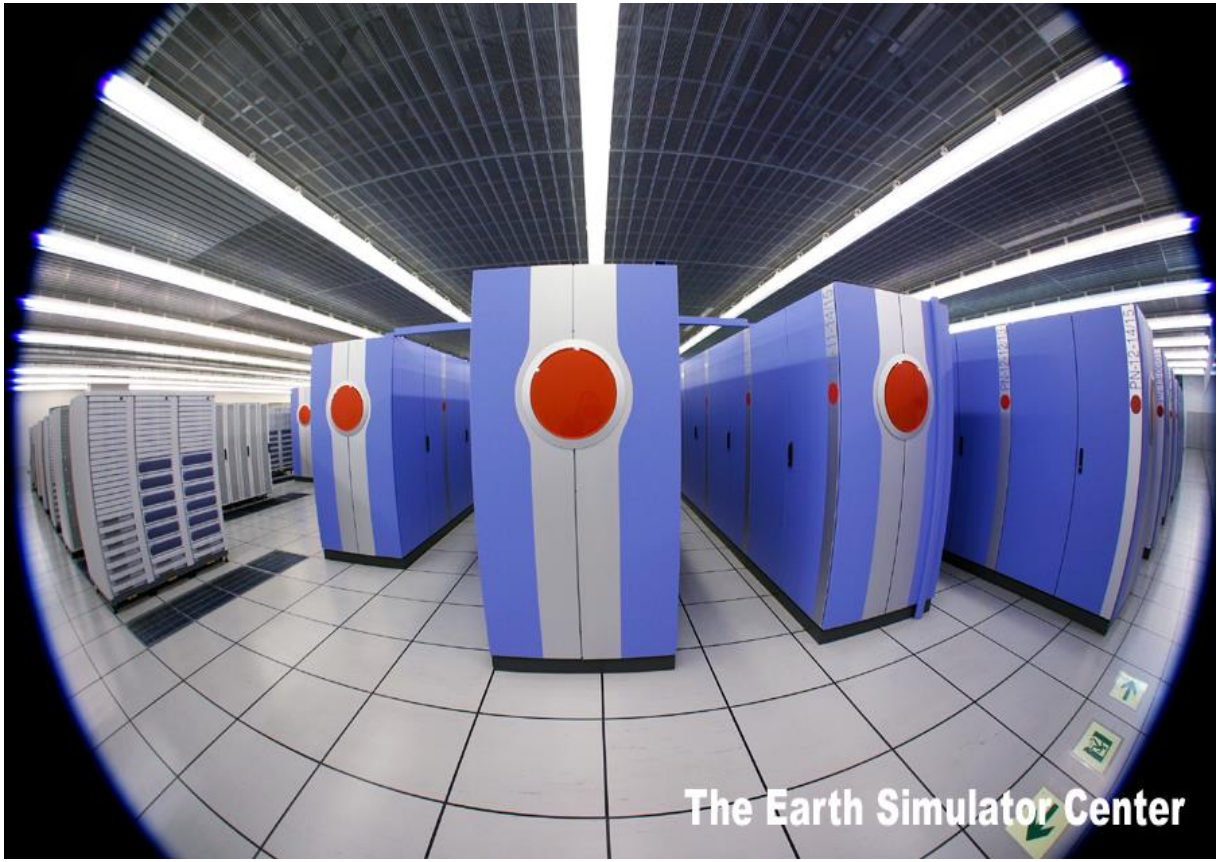
Widespread in 2000-2006

- 32+ nodes

- x86 architecture single chip

- commodity PC hardware, ethernet interconnect

2002: NEC Earth Simulator



Fastest Supercomputer from 2002-2004

- 640 nodes with 16GB memory at each node

- SX-6 node 8 vector processors + 1 scalar processors on single chip

- application - modeling global climate changes

2013: OLCF Titan

Fastest Supercomputer 2013

- 18668 nodes with 32GB memory at each node

- 16 core AMD opternon processors + K20 Kepler GPU

- application – modeling in all areas of science

From Gaming to Scientific Computations

- **Condor Cluster – 1760 PS3s**
  - » **Air Force Research Laboratory**

- first stage
  - 336 PS3 units
- second stage
  - 1760 PS3 units
  - 84 dual CPU (6 core) headnodes
  - 1 headnode coordinates 22 PS3 units
  - 500 Tflops performance
- designed for radar image processing in urban surveillance
- $2 million budget
  - 10x cheaper

2015: IT4I Salomon

#40 on Top500 list in summer 2015

- 1008 nodes with 128GB memory at each node

- 2x12 core Intel Xeon processors + 2x Intel Xeon Phi 7120P accelerators

- application – modeling in all areas of science

-see 3D image!

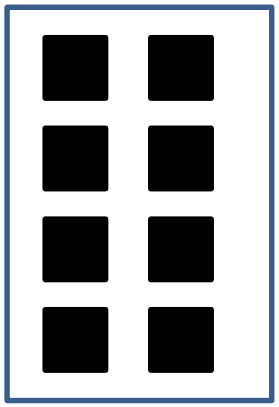
Units of Measure in HPC

- High Performance Computing (HPC) units are:
  - Flop: floating point operation
  - Flops/s: floating point operations per second
  - Bytes: size of data
    - double precision floating point number is 8 Bytes
- Typical sizes are millions, billions, trillions…
  - Mega Mflop/s = 10^6 flop/sec Mbyte = 2^{20} = 1048576 ~ 10^6 bytes
  - Giga Gflop/s = 10^9 flop/sec Gbyte = 2^{30} ~ 10^9 bytes
  - Tera Tflop/s = 10^{12} flop/sec Tbyte = 2^{40} ~ 10^{12} bytes
  - Peta Pflop/s = 10^{15} flop/sec Pbyte = 2^{50} ~ 10^{15} bytes

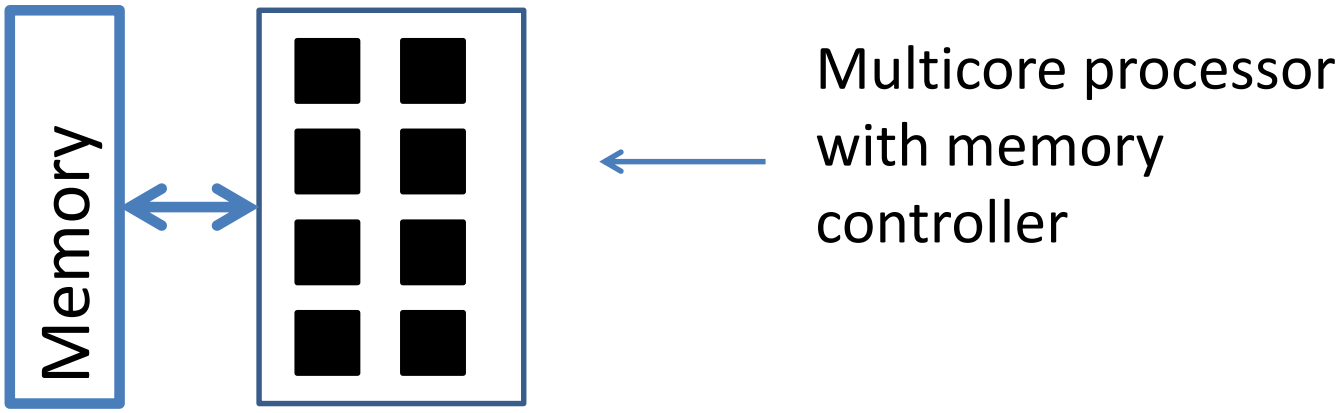
    - Today – 10 PFLOPS (K Computer - Japan)
  - Exa Eflop/s = 10^{18} flop/sec Ebyte = 2^{60} ~ 10^{18} bytes

    ~2018 – Exascale

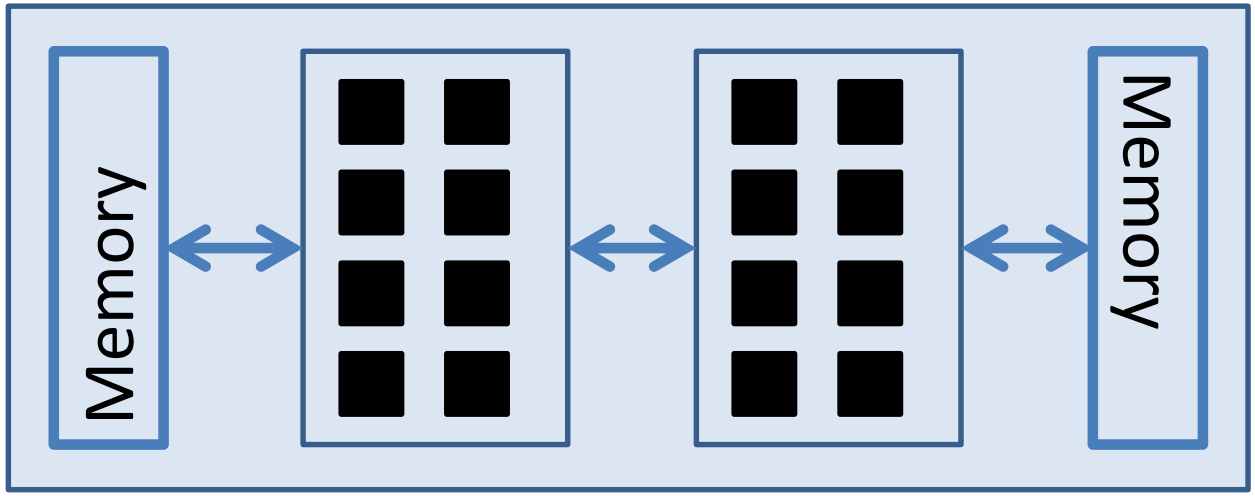
SIMD core, capable of SSE and AVX instructions

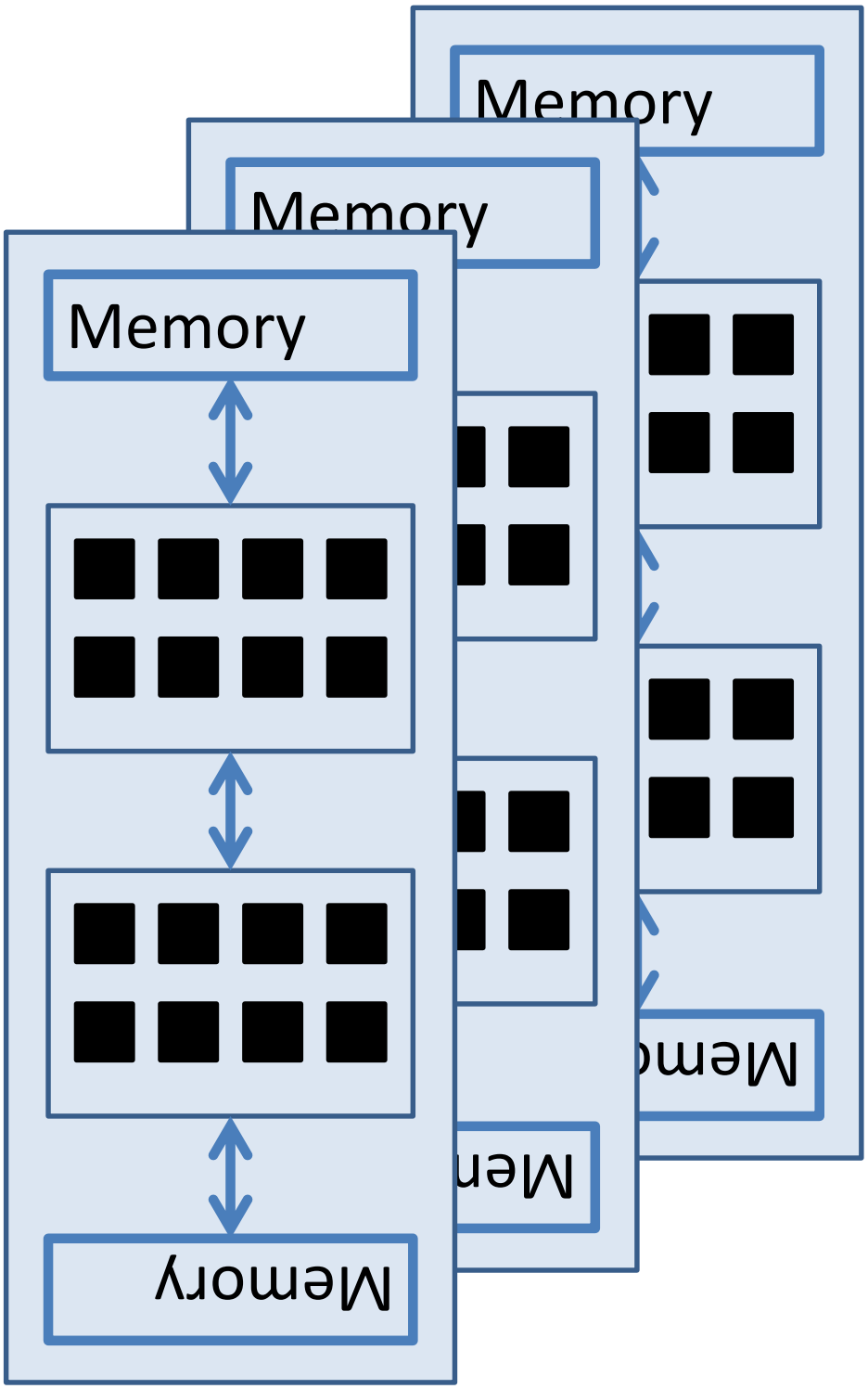


Multicore processor


Memory
Multicore processor
with memory
controller

NUMA board – Full blown multicore computer

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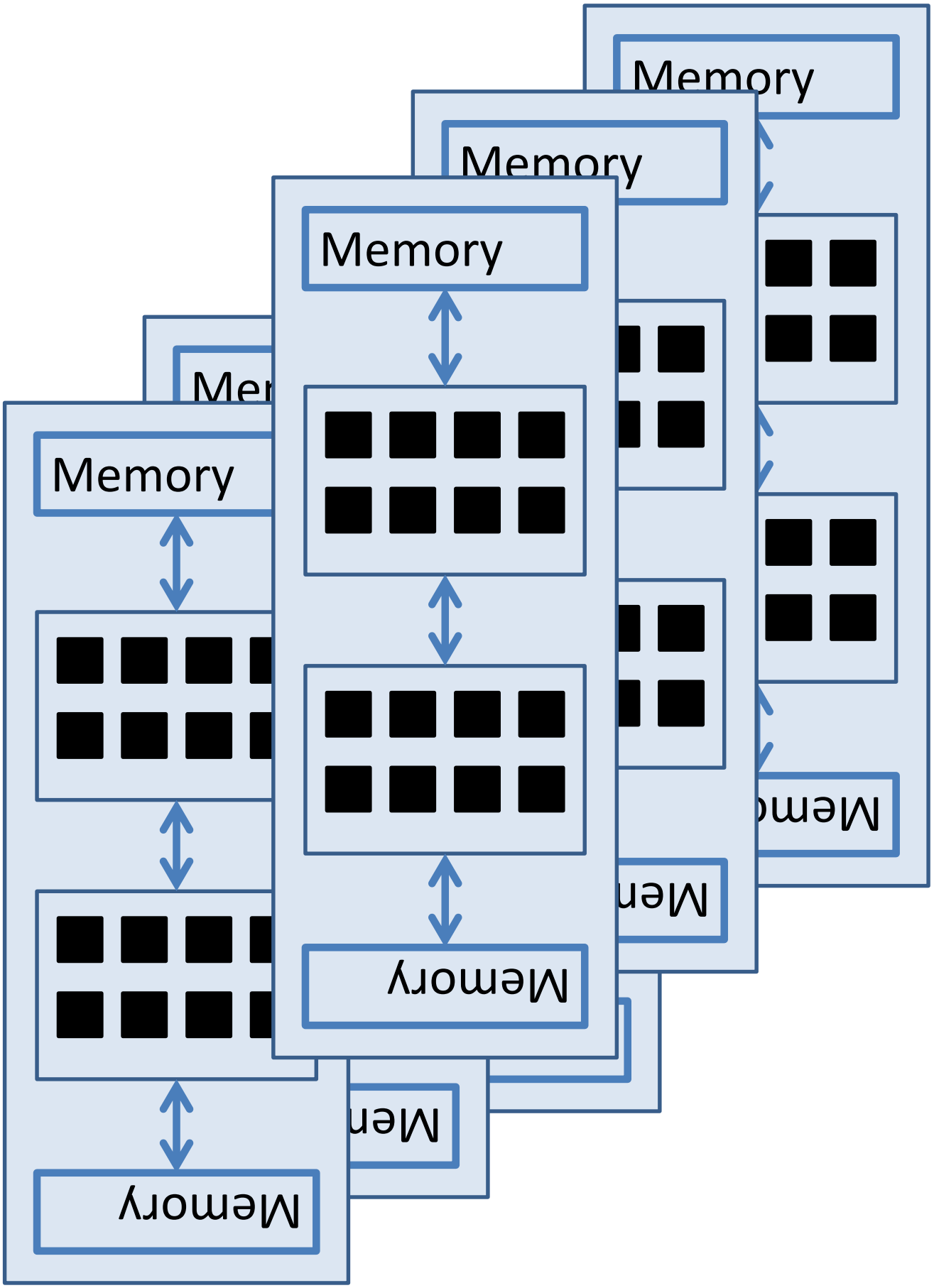
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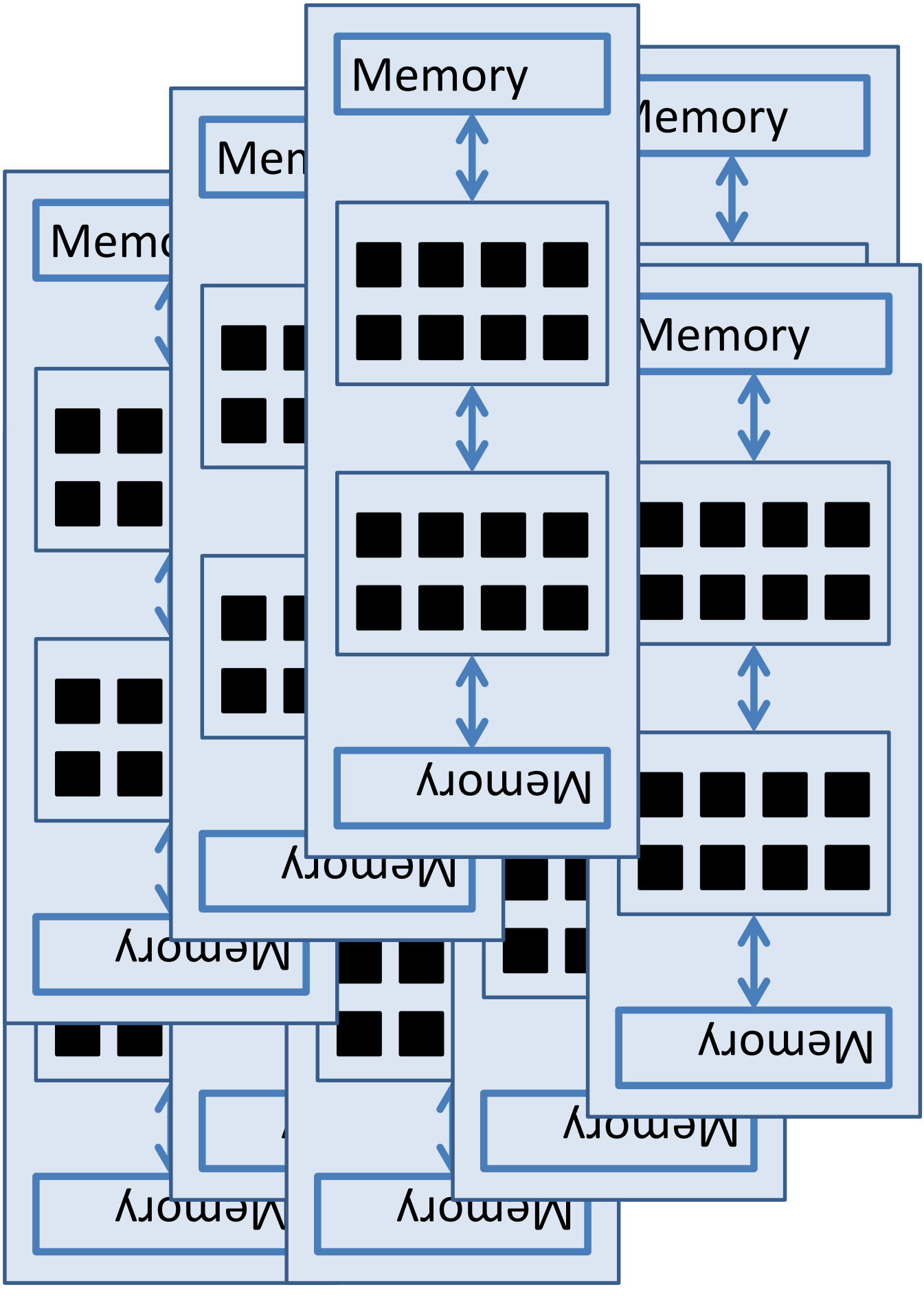
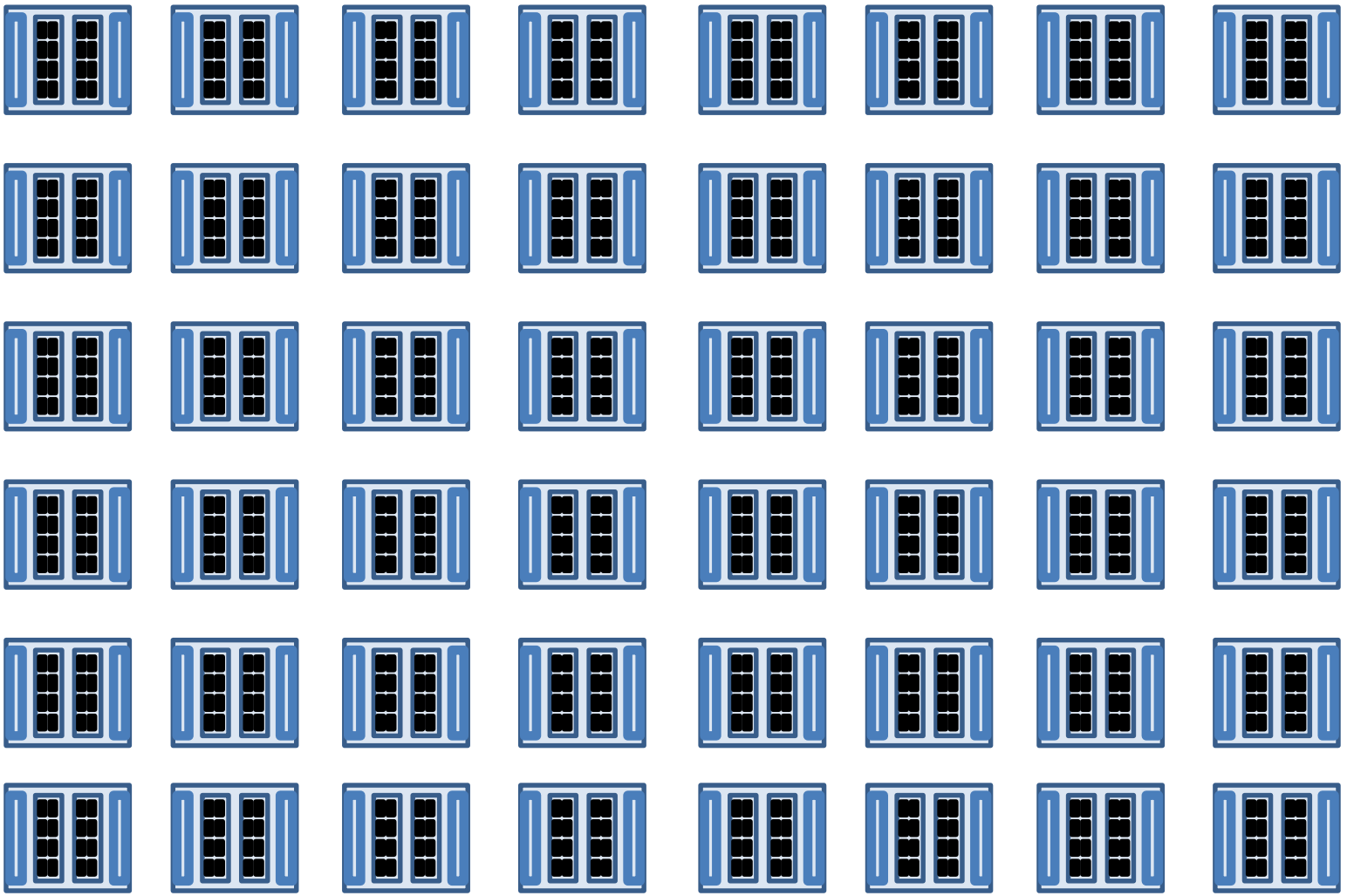

Memory

MPP Cluster



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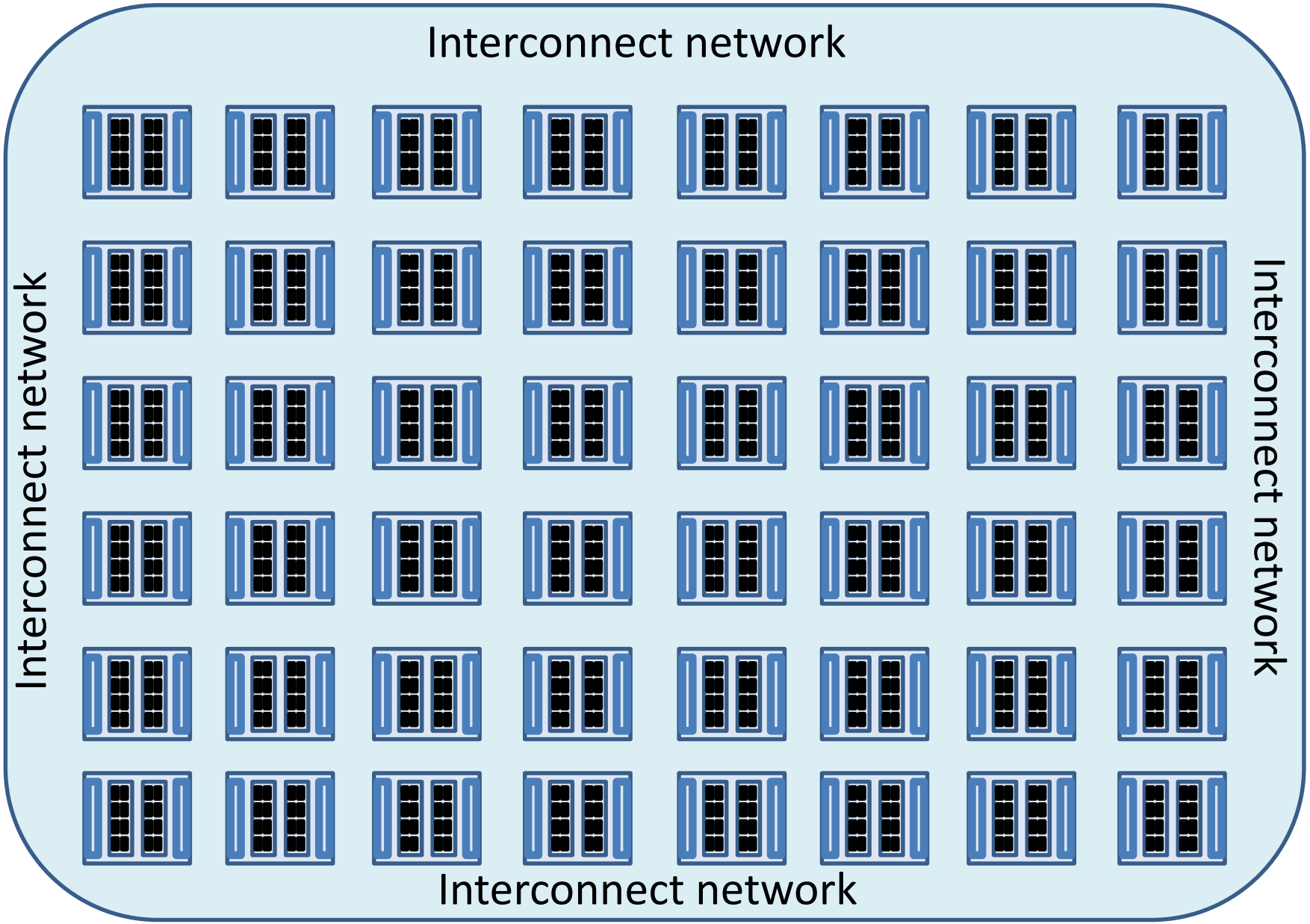
Interconnect network
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