Center of Excellence for Computational Biomolecular Research

The Future of HPC

Exascale and Challenges

Partners

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Outline

- Future hardware & architectures
  - Architectures & exascale
  - Processors
  - Accelerators
  - Memory
  - Impacts on performance
- Software challenges
  - Parallelism and scaling
  - New algorithms
  - What about software that does not scale?
- Other impacts and developments relevant to HPC

Future architectures

What will HPC machines look like?

What will future systems look like?

	2016	2020
System Perf.	100 Pflop/s	1 Eflop/s
Memory	1.3 PB	10 PB
Node Perf.	100 Gflop/s	1-10 Tflop/s
Concurrency	O(1000)	O(10000)
Interconnect BW	40 GB/s	200-400 GB/s
Nodes	10,000	O(10000)
I/O	2 TB/s	20 TB/s
MTTI	Several days	O(1 Day)
Power	15 MW	20 MW

Compare to Top500 list: https://top500.org/

Processors

- More Floating-Point compute power per processor
  - Only exploit this power via parallelism
  - More cores combined in some way – “fatter” nodes (also accelerators)
  - Vectorisation (greater vector width) – software needs to use for good performance

- Memory bandwidth very important
  - Top500 #1 HPC machine “Fugaku”: Fujitsu ARM A64FX processor
  - A64FX designed to have high memory bandwidth to feed its cores

Accelerators

- Accelerators (Nvidia & AMD) increasingly widespread in HPC
  - Offer excellent floating point performance per Watt
  - “Fatter” nodes (more computing power)
    - challenge will be to “feed” these fat nodes fast enough – through communications with other nodes, fetching data from memory, …
- Investment in design & fabrication follows the money
  - expect accelerators increasingly optimised for AI applications
    - e.g. double precision less important
  - Scientific computing needs for HPC overlap → leverage hardware
    - c.f. emergence of GPUs for gaming

Memory

- Moving data to/from places where compute happens costs energy & time (performance)

- Memory hierarchy will become more complex:
  - Memory will be packaged with processor
    - Increases power efficiency, speed and bandwidth…
    - …at the cost of smaller memory per core
    - High bandwidth memory on chip with processor and with accelerator
  - Additional persistent storage layer between disk and RAM
    - NVRAM and/or SSD – faster and smaller than disk but slower and larger than RAM
    - Close to compute nodes
    - Enables low latency, high bandwidth to computing elements
  - Still unclear how this will be exposed to users & software developers

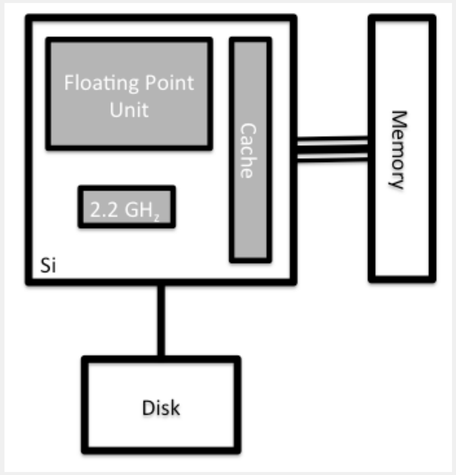
System on a chip

- Instead of separate:
  - Processor
  - Memory
  - Network interface

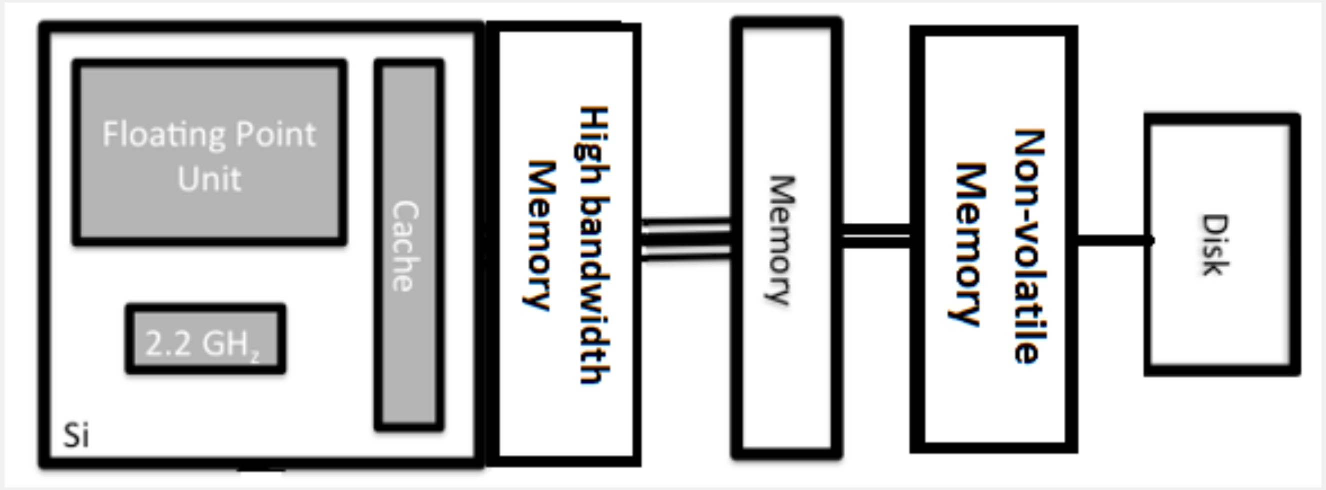
- Will combine these components on a single chip
  - This is what happened to processors in the 70s/80s!
    - Floating point, ALU units used to plug into motherboards directly
  - Reduces latency between components
  - Improves power efficiency (see e.g. Apple Silicon M1)
  - Less scope for customisation
  - If you need more memory than in package you will have to have levels of memory hierarchies

Memory hierarchies

- Moving from:



- To something like:



Software challenges

What does software need to do to exploit future HPC?

What does this mean for applications?

- The future of HPC (as for everyone else):
  - Lots of cores per node (CPU + co-processor)
  - Less memory per core than now
  - Lots of compute power via network interface
  - Increased complexity in memory and IO hierarchy
- Balance of compute to communication power and compute to memory different to now
- Must exploit parallelism at all levels
- Must exploit memory/IO hierarchy efficiently

Algorithms

- New algorithms will be needed to exploit hardware
- Prefer algorithms that run slower on few cores but ultimately contain more scope for parallelisation
- Mixed-precision will become more important
- Try to develop and use numerical libraries that exploit upcoming high-performance energy-efficient accelerators optimised for AI

Applications that do not scale

- If no need for large-scale tightly coupled individual jobs, will still benefit from more of the current size of resources
  - But may be caught out by decrease in memory per core!
  - Options to scale in trivial-parallel way: increase sampling (e.g. ensemble / swarm / replica methods in MD), use more sophisticated statistical techniques
    - This may well be the best route for many simulations

All computing will be (even more) parallel

- All current computers are parallel
  - From supercomputers all the way down to mobile phones
  - Often task-based on 4-8 cores – each application (task) runs on an individual core.

- In the future:
  - More hardware parallelism per device – 10s to 100s cores running at lower clock speeds
  - All applications will have to be parallel
  - Parallel programming skills will be required for all application development.

Cloud Computing (v.s.) HPC

- Cloud computing (AWS, Azure, etc.) has grown in use
- On-demand and flexible
- Not ideal for frequent transfer of very large amounts of data
  - Likely to be a bottleneck
  - On-site computing likely to remain important
- Suitable for high throughput
- Cloud computing historically not had the quality interconnect performance of HPC machines – changing (e.g. Microsoft Azure)

Software Containers & HPC

- Newer HPC machines provide support for software containers (Docker, Singularity)
- Allows more freedom for user customisation of the environment, installed software, etc.
- Facilitate:
  - Management of environments and dependencies (e.g. libraries)
  - Sharing reproducible workflows
  - Portability to different platforms