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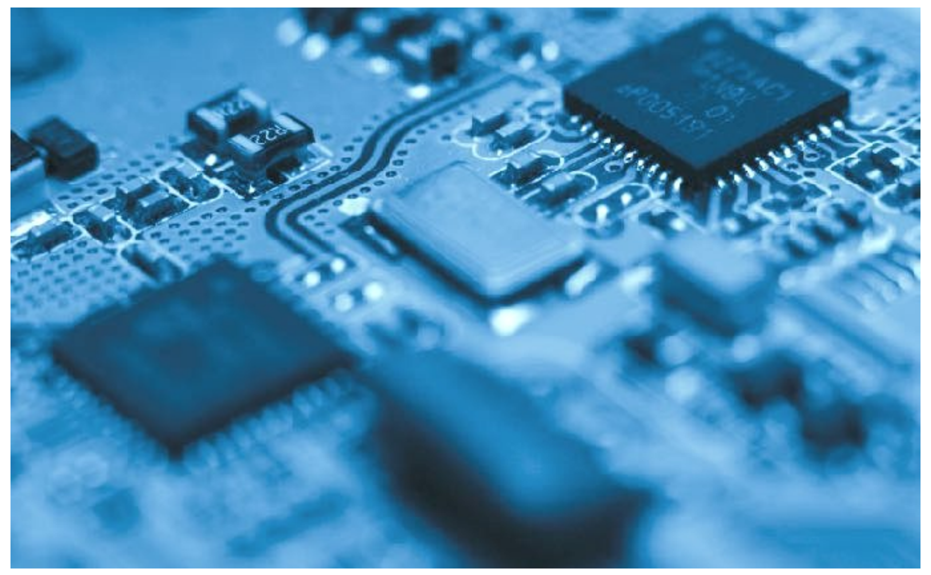

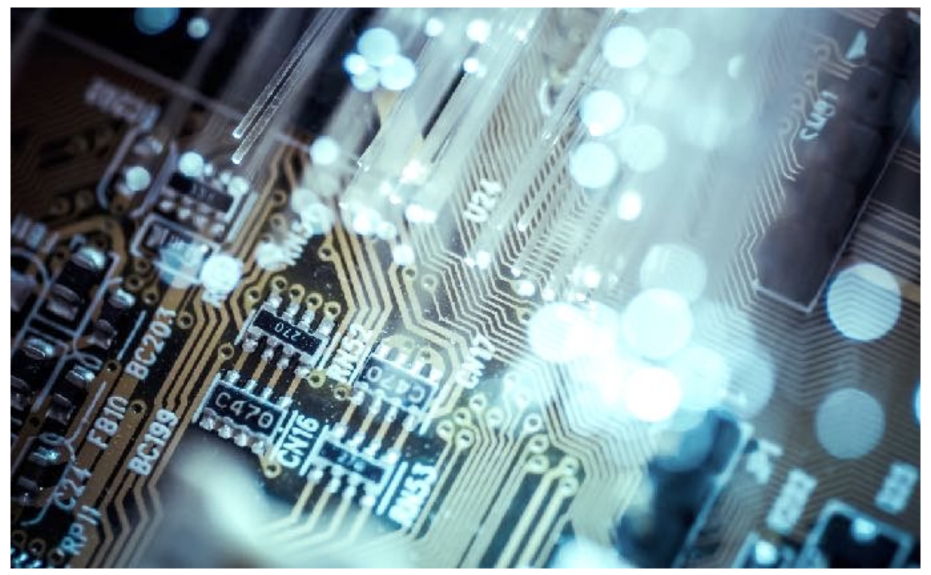

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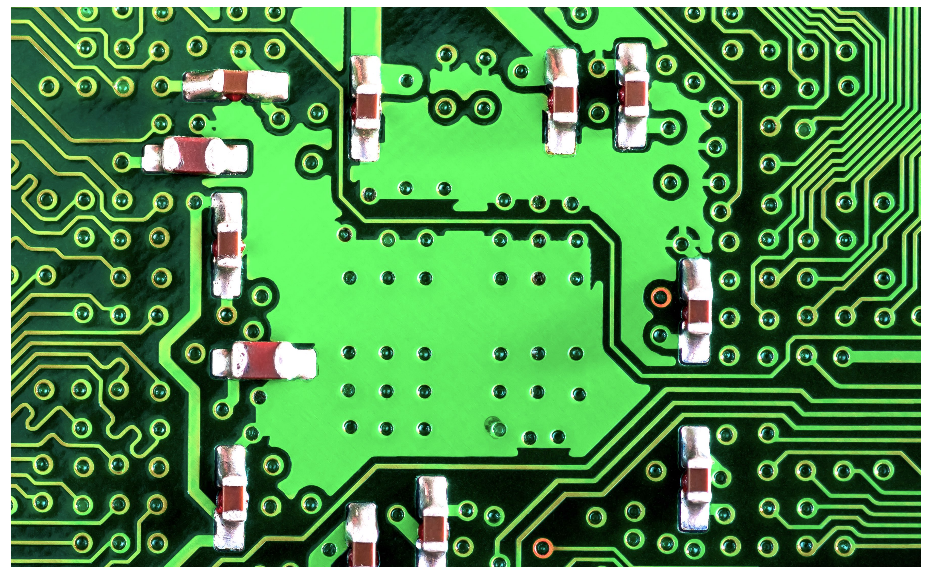
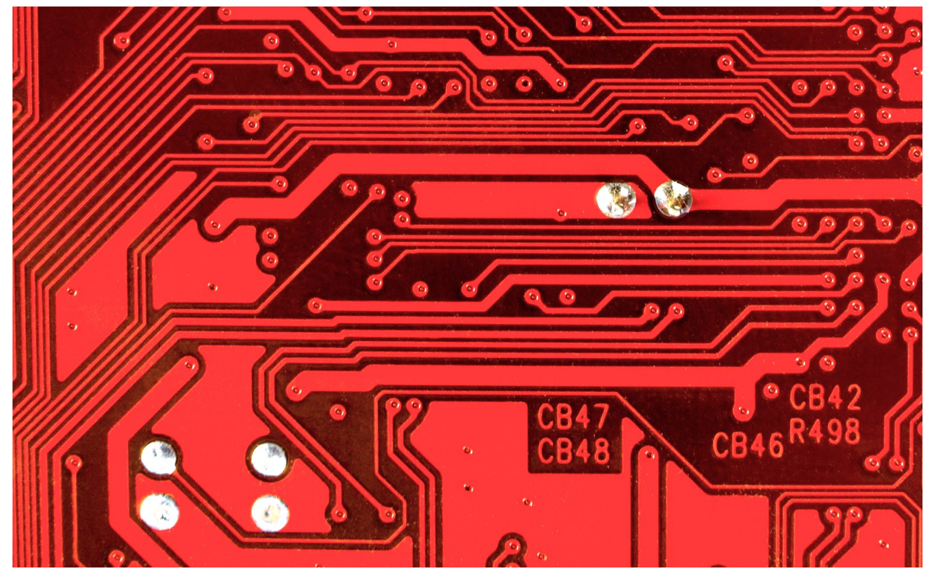


Massively Parallel Computing for NWP and climate



Andreas Mueller

ECMWF DKRZ Deutsches Klimarechenzentrum Max-Planck-Institut für Meteorologie MeteoSwiss Barcelona Supercomputing Center Centro Nacional de Supercomputación cea Loughborough University RMI Politecnico Milano 1863 MOX DMI cmcc Centro Euro-Mediterraneo sui Cambiamenti Climatici Bull atos technologies

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Overview

- Why do scientists need to know so much about computer science?
- What do we need to be aware of to write efficient code?
- How good are we?

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Why do we as scientists need to know so much about computer science?

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Why do we as scientists need to know so much about computer science?

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- Excuse 1: let the computer scientists take care of it
- Response: computer scientists cannot do everything because they do not know about different numerical methods
- Excuse 2: just buy a faster computer if the code is not fast enough
- Response: we (and the environment) cannot afford wasting that much energy!

computer	electricity cost per year
ECMWF	~3 million £
fastest current supercomputer	~15 million $
next generation (exascale)	~20 million $

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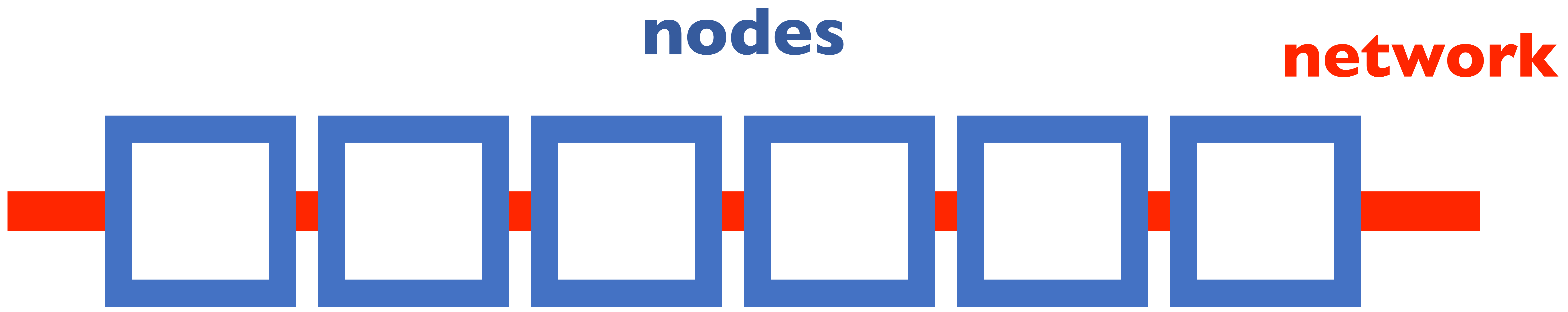
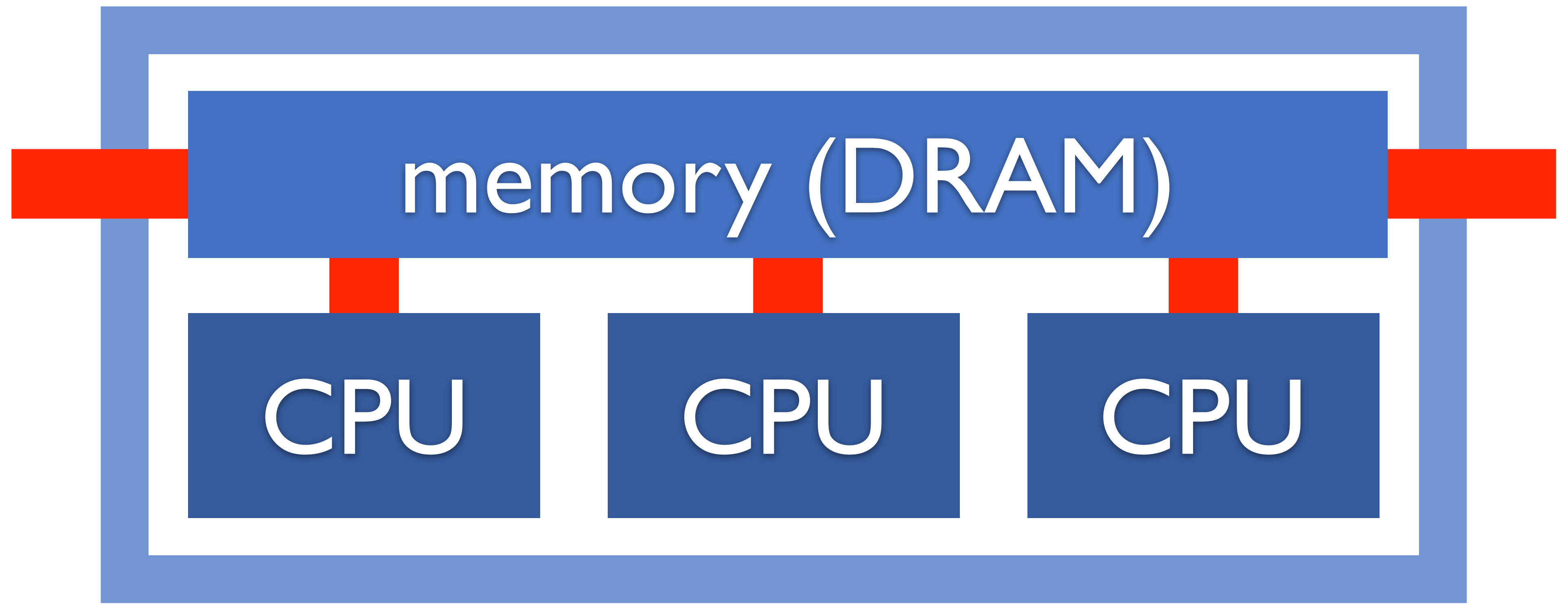
Supercomputer/Cluster



Node



CPU

central processing unit; does one instruction like $c=a+b$ per clock cycle

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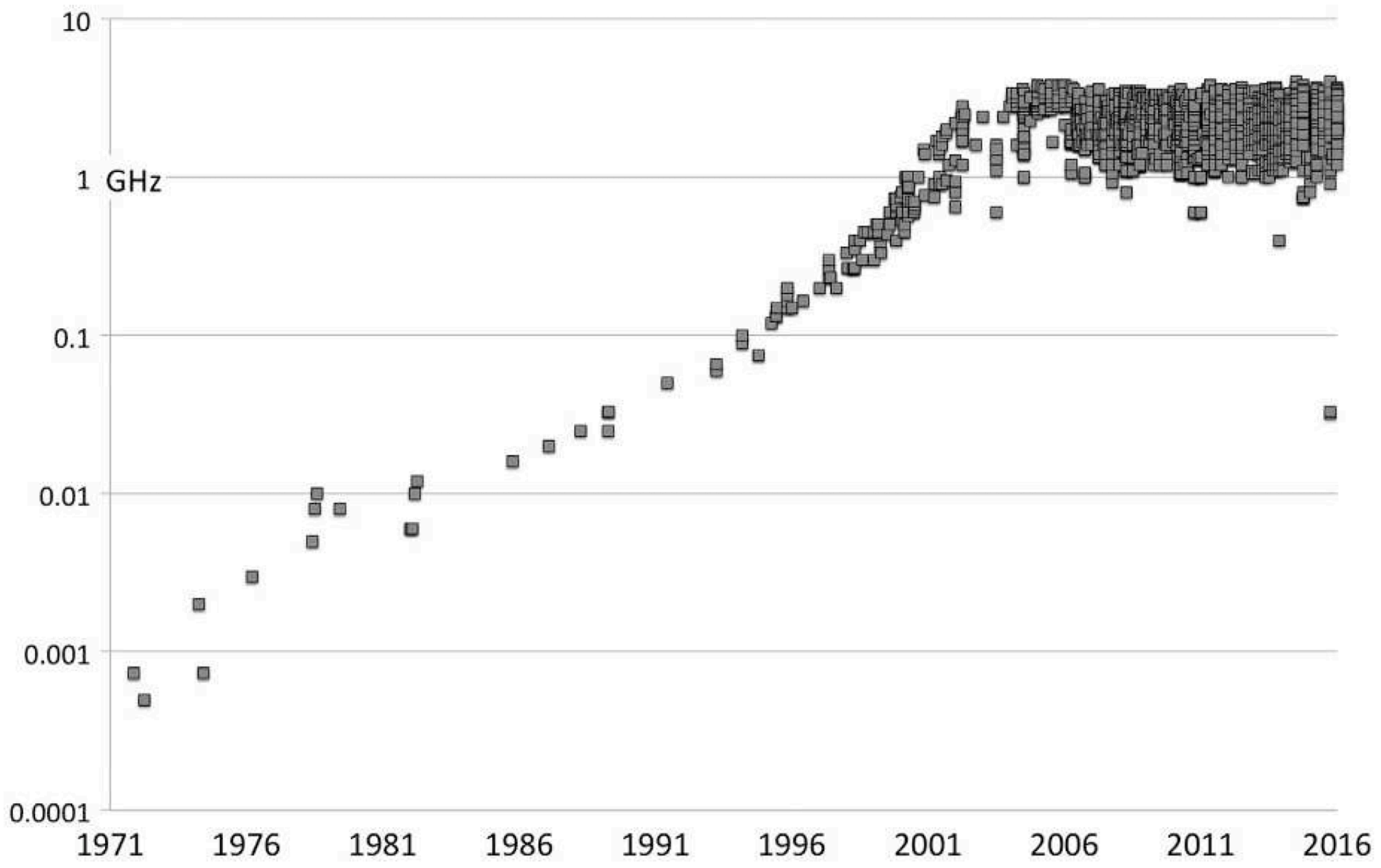
CPU clock rate over time



source: James Reinders, Intel Xeon Phi

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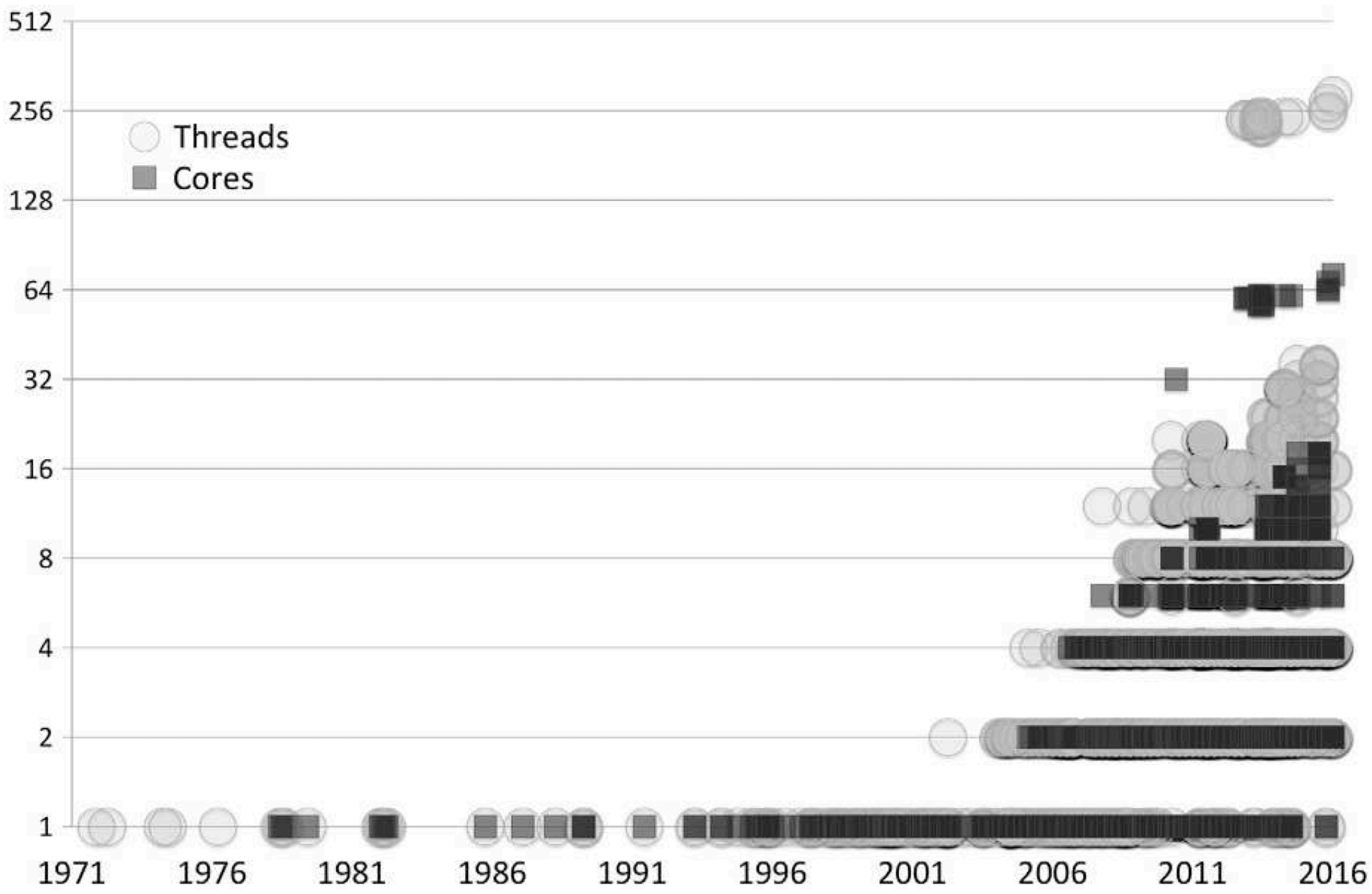
Number of cores per chip over time



source: James Reinders, Intel Xeon Phi

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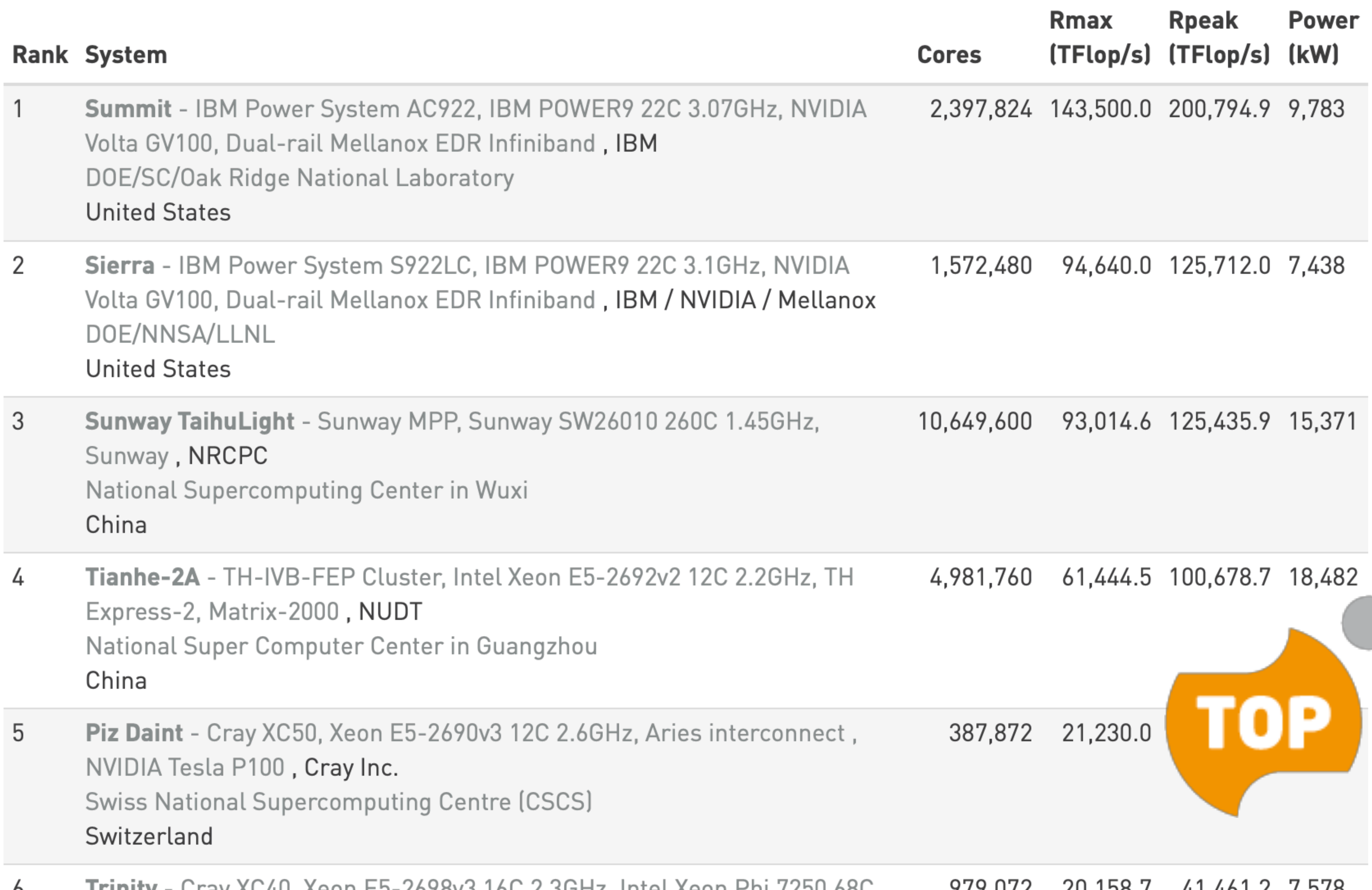
http://top500.org



Rank	System	Cores	Rmax (TFlop/s)	Rpeak (TFlop/s)	Power (kW)
1	**Summit** - IBM Power System AC922, IBM POWER9 22C 3.07GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband , IBM DOE/SC/Oak Ridge National Laboratory United States	2,397,824	143,500.0	200,794.9	9,783
2	**Sierra** - IBM Power System S922LC, IBM POWER9 22C 3.1GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband , IBM / NVIDIA / Mellanox DOE/NNSA/LLNL United States	1,572,480	94,640.0	125,712.0	7,438
3	**Sunway TaihuLight** - Sunway MPP, Sunway SW26010 260C 1.45GHz, Sunway , NRCPC National Supercomputing Center in Wuxi China	10,649,600	93,014.6	125,435.9	15,371
4	**Tianhe-2A** - TH-IVB-FEP Cluster, Intel Xeon E5-2692v2 12C 2.2GHz, TH Express-2, Matrix-2000 , NUDT National Super Computer Center in Guangzhou China	4,981,760	61,444.5	100,678.7	18,482
5	**Piz Daint** - Cray XC50, Xeon E5-2690v3 12C 2.6GHz, Aries interconnect , NVIDIA Tesla P100 , Cray Inc. Swiss National Supercomputing Centre (CSCS) Switzerland	387,872	21,230.0		
6	**Trinity** - Cray XC40, Xeon E5-2698v3 16C 2.3GHz, Intel Xeon Phi 7250 68C	979,072	20,158.7	41,461.2	7,578

TOP 500 The List.

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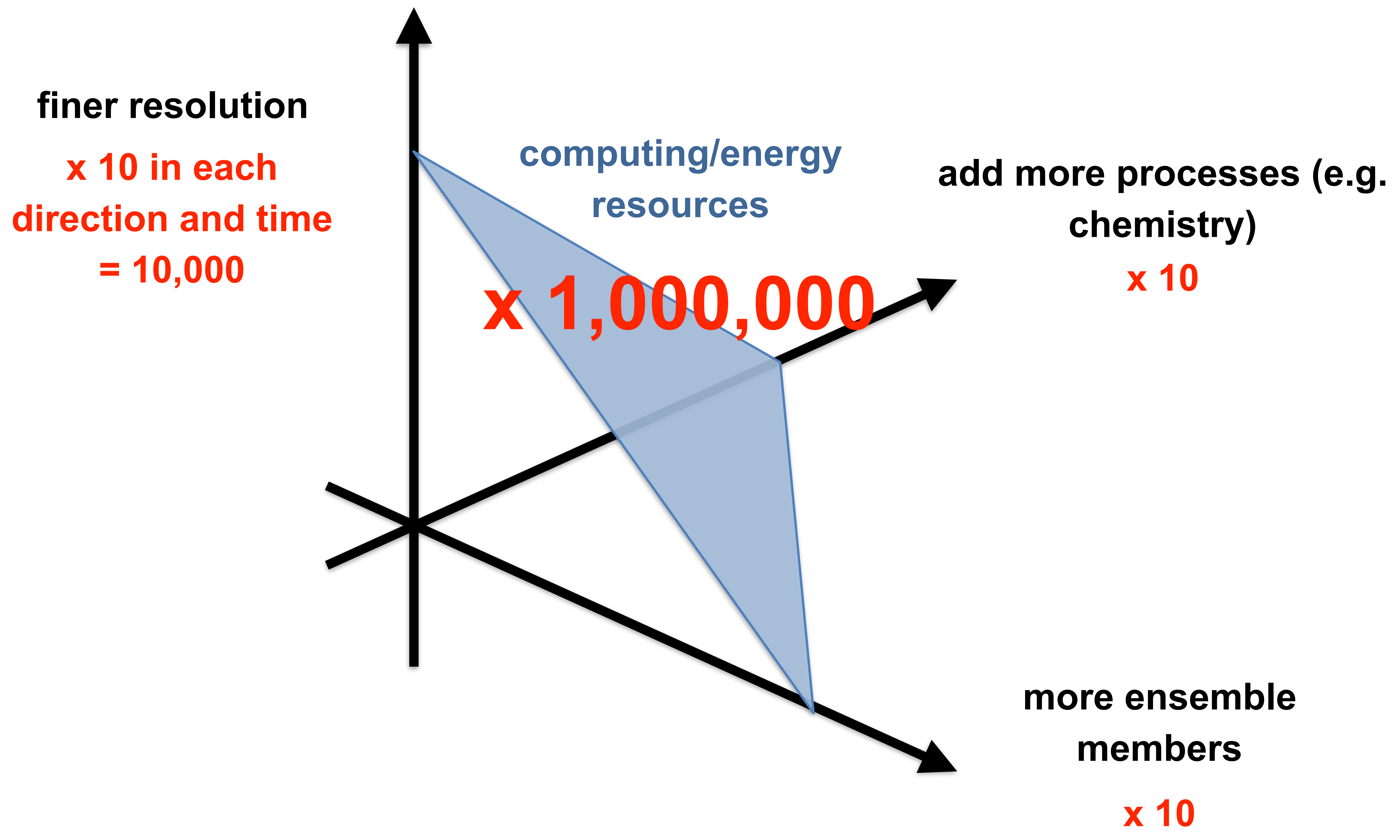
What comes next?


finer resolution
x 10 in each direction and time = 10,000
computing/energy resources
x 1,000,000
add more processes (e.g. chemistry)
x 10
more ensemble members
x 10

Computing at ECMWF

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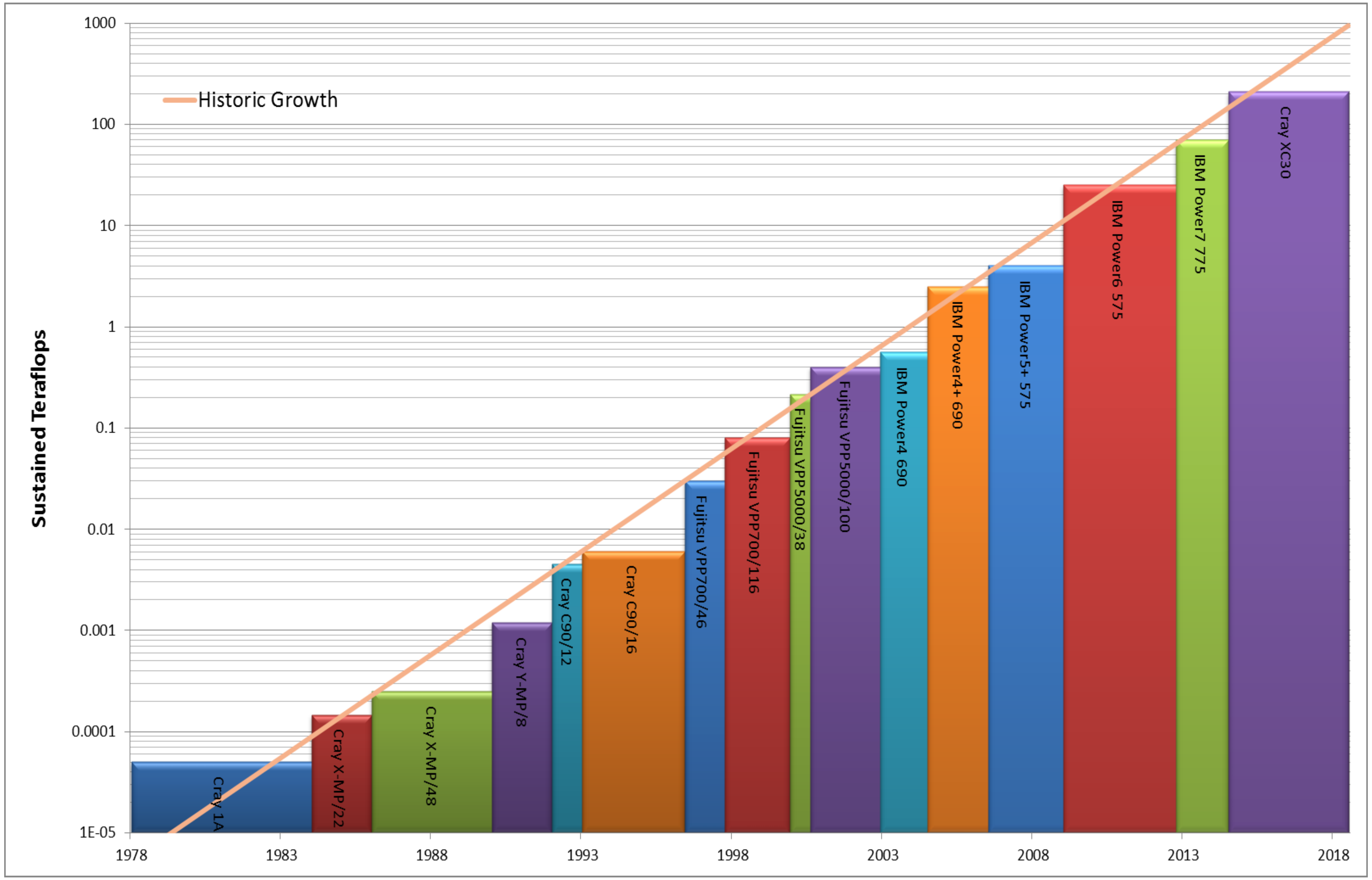

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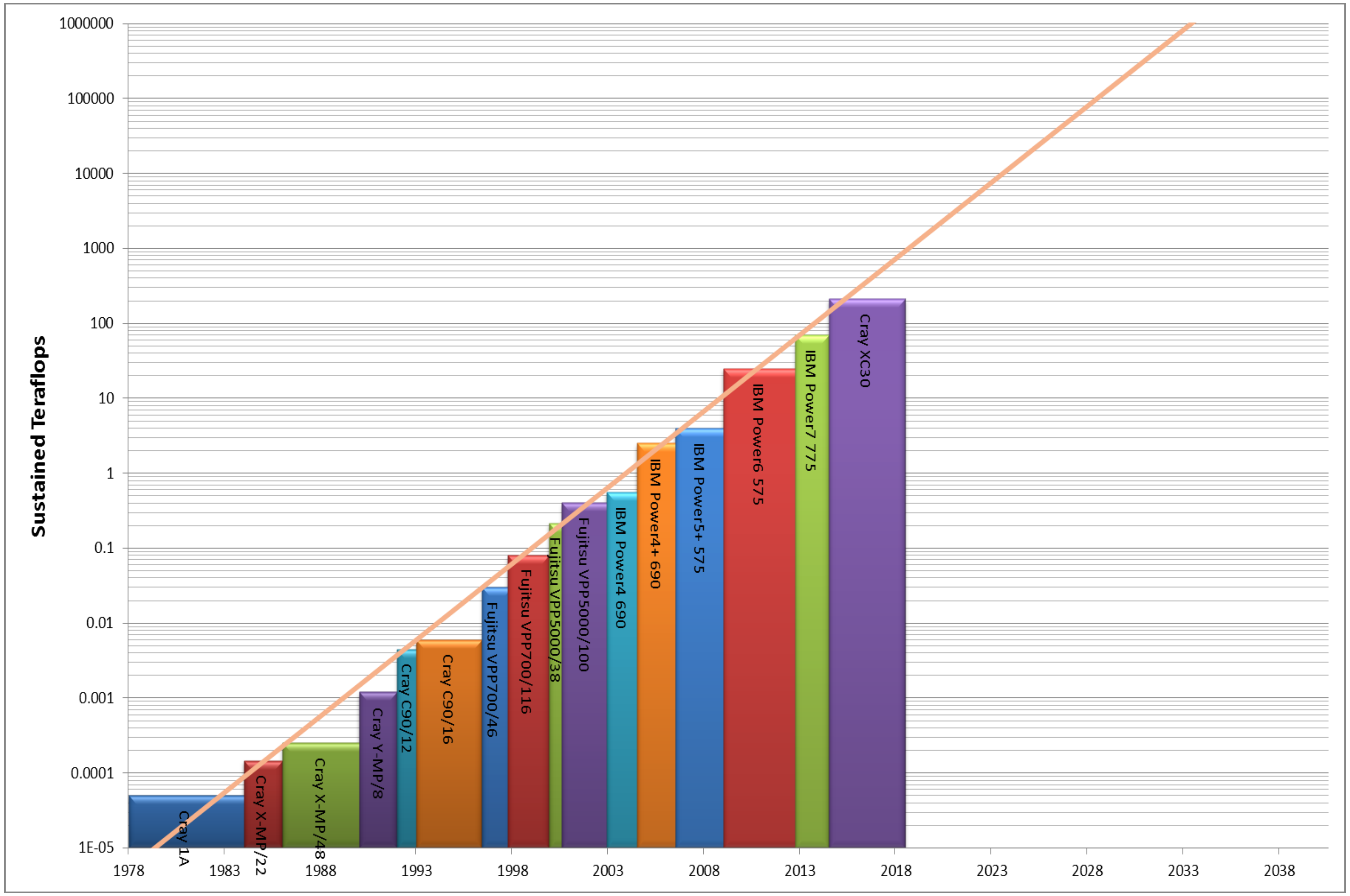
Sustained Exaflop in 2033 ?



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What do we need to be aware of to write efficient code?

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Recommendations

-
-
-

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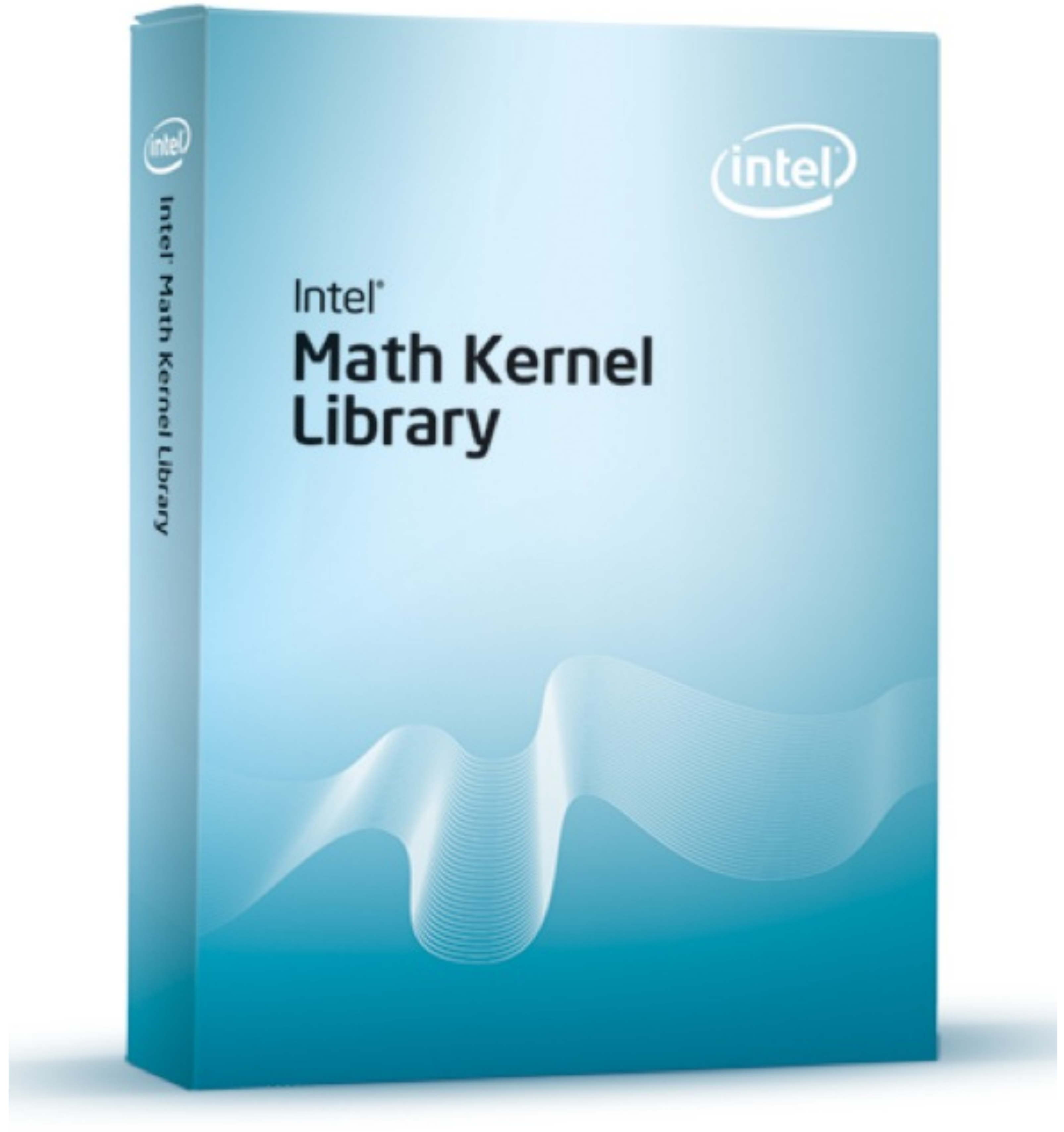
Libraries

- there are well optimised libraries for many tasks
- BLAS for vector-matrix product or matrix-matrix product (if matrices are large)
- Lapack for matrix factorisation (e.g. LU decomposition)
- some hardware vendors have special math libraries, e.g. MKL by Intel
- there are some cases in which libraries are fairly slow (e.g. BLAS with very small matrices)



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Recommendations

- **try if using libraries is fast enough**

Compiler optimisation

- compilers have optimisation flag -On (O0: no optimisation, O3: strong compiler optimisation)
- O3 is usually much faster than O2, but it can also be slower than O2
- O3 can produce completely wrong results!
- you can use different compiler flags for different files
- different compiler versions can have very different performance
- check compiler messages (Intel: ifort -O2 -qopt-report=2 code.f90 -o program)
- make sure that your code runs correctly with different compilers

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Recommendations

- try if using libraries is fast enough
- **try to use compiler optimisation (be careful!)**

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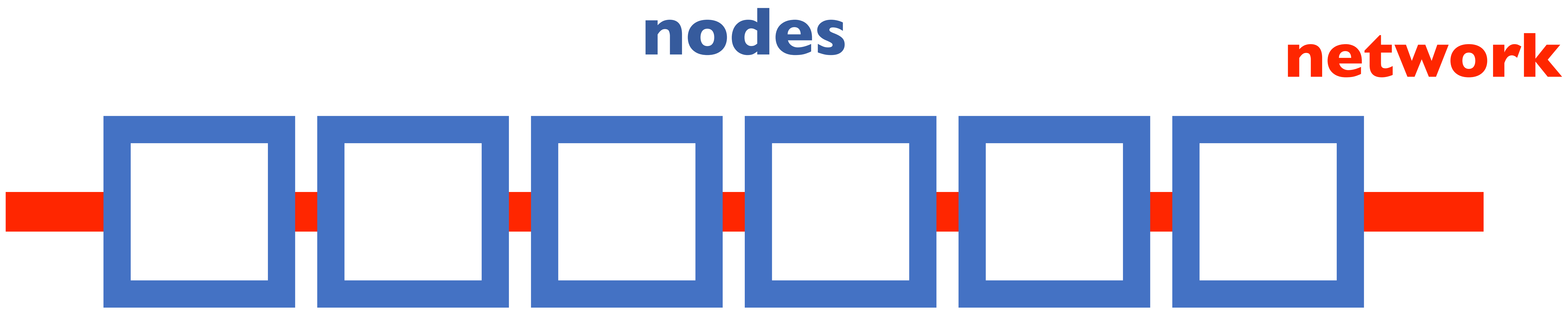
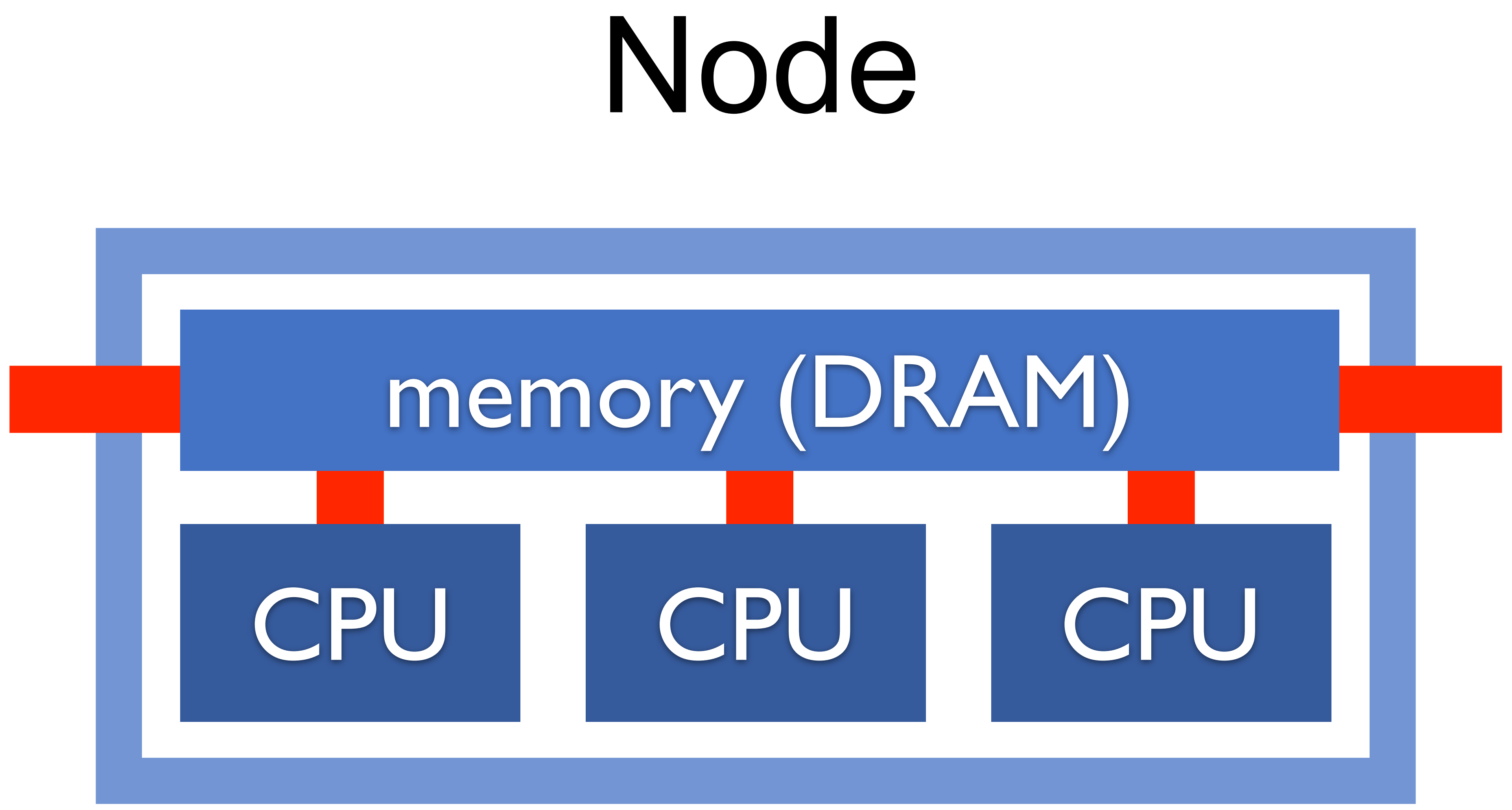
Supercomputer/Cluster





Bottlenecks

- network (connection between nodes)
- connection between DRAM and processor

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Recommendations

- try if using libraries is fast enough
- try to use compiler optimisation (be careful!)
- **avoid unnecessary computation and communication**

ESCAPE 2

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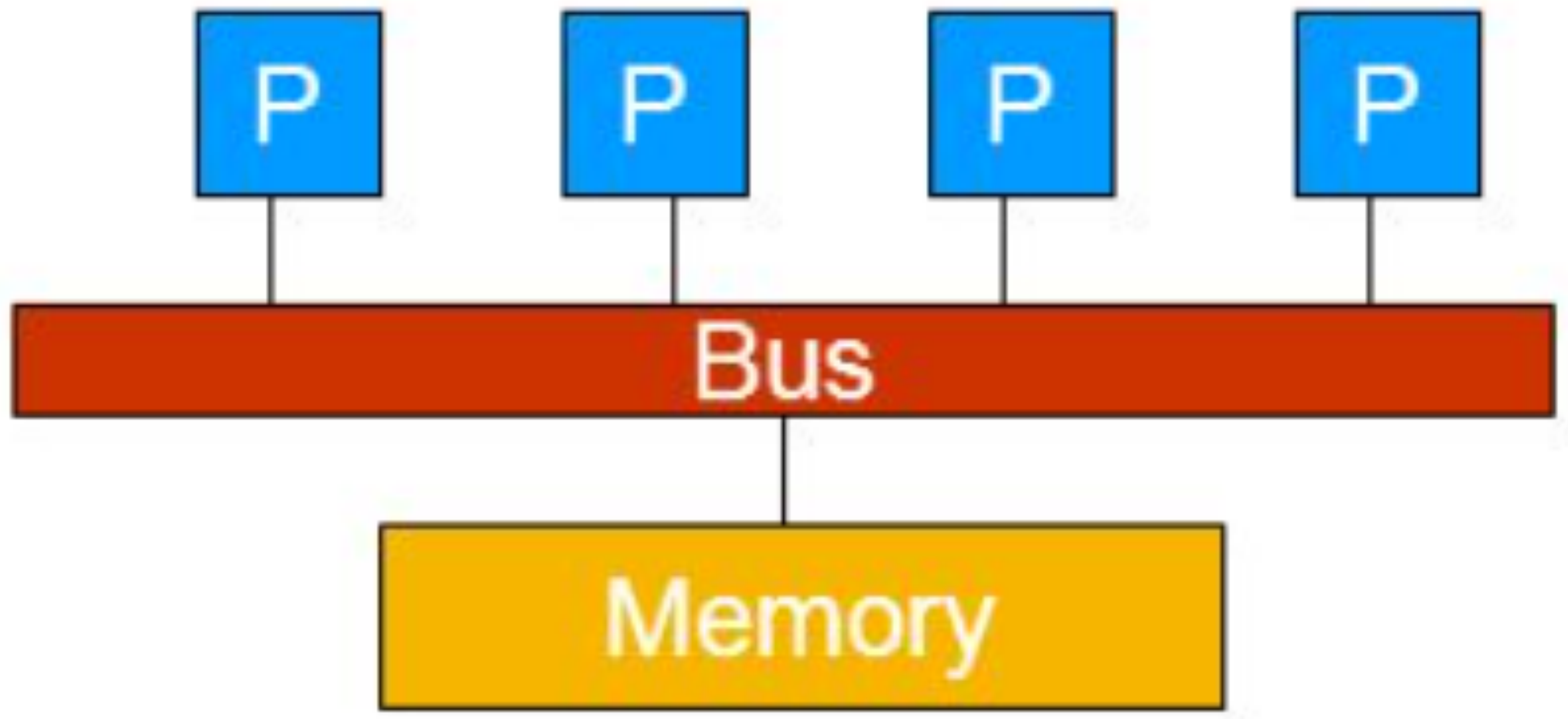
Shared memory: OpenMP

- many threads of a process run on a single node
- all threads can access the same data
- data may be physically distributed, but logically shared



without OpenMP:

```
real, dimension(N) :: a,b
integer :: i,N
do i=1,N
 a(i) = a(i) + b(i)
end do
```

with OpenMP:

```
real, dimension(N) :: a,b
integer :: i,N
!$omp parallel do private(i)
do i=1,N
 a(i) = a(i) + b(i)
end do
!$omp end parallel do
```

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Shared memory: OpenMP

faster for bigger codes:

```
real, dimension(N) :: a,b
integer :: i, N, iStart, iEnd,
 myid, numthreads
!$omp parallel private(i,iStart,iEnd)
myid = omp_get_thread_num()
numthreads = omp_get_num_threads()
iStart = ...
iEnd = ...
do i=iStart,iEnd
 a(i) = a(i) + b(i)
end do
!$omp end parallel
```

without OpenMP:

```
real, dimension(N) :: a,b
integer :: i,N
do i=1,N
 a(i) = a(i) + b(i)
end do
```

with OpenMP:

```
real, dimension(N) :: a,b
integer :: i,N
!$omp parallel do private(i)
do i=1,N
 a(i) = a(i) + b(i)
end do
!$omp end parallel do
```

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Recommendations

- try if using libraries is fast enough
- try to use compiler optimisation (be careful!)
- avoid unnecessary computation and communication
- **give each thread as much work as possible**

ESCAPE 2

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Shared memory: OpenMP

Example 2: race conditions

without OpenMP:

```
real, dimension(N) :: a
real :: sum
integer :: i,N
do i=1,N
 sum = sum + a(i)
end do
```

with OpenMP (wrong!):

```
real, dimension(N) :: a
real :: sum
integer :: i,N
!$omp parallel do private(i)
do i=1,N
 sum = sum + a(i)
end do
!$omp end parallel do
```

working, but slow:

```
real, dimension(N) :: a
real :: sum
!$omp parallel do private(i)
do i=1,N
 !$omp atomic
 sum = sum + a(i)
end do
!$omp end parallel do
```

faster:

```
real, dimension(N) :: a
real :: sum
!$omp parallel do private(i
 reduction (+: sum )
do i=1,N
 sum = sum + a(i)
end do
!$omp end parallel do
```

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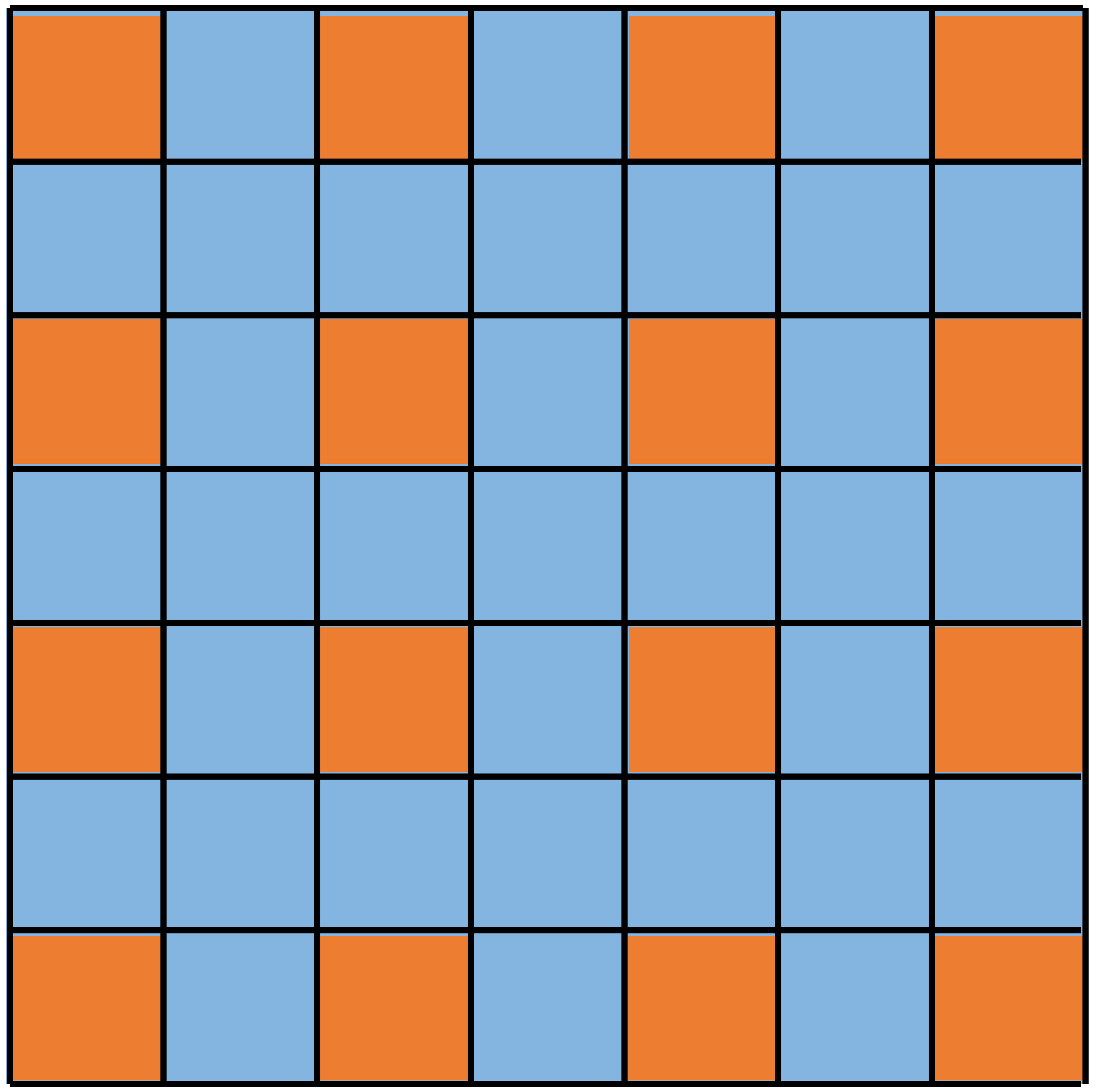
Shared memory: OpenMP

Example 2: race conditions

best: arrange work such that different threads work on different data



example: spectral element, start with orange (non-adjacent) elements

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Recommendations

- try if using libraries is fast enough
- try to use compiler optimisation (be careful!)
- avoid unnecessary computation and communication
- give each thread as much work as possible
- **let the threads do work that does not affect others**

ESCAPE 2

Distributed memory: MPI

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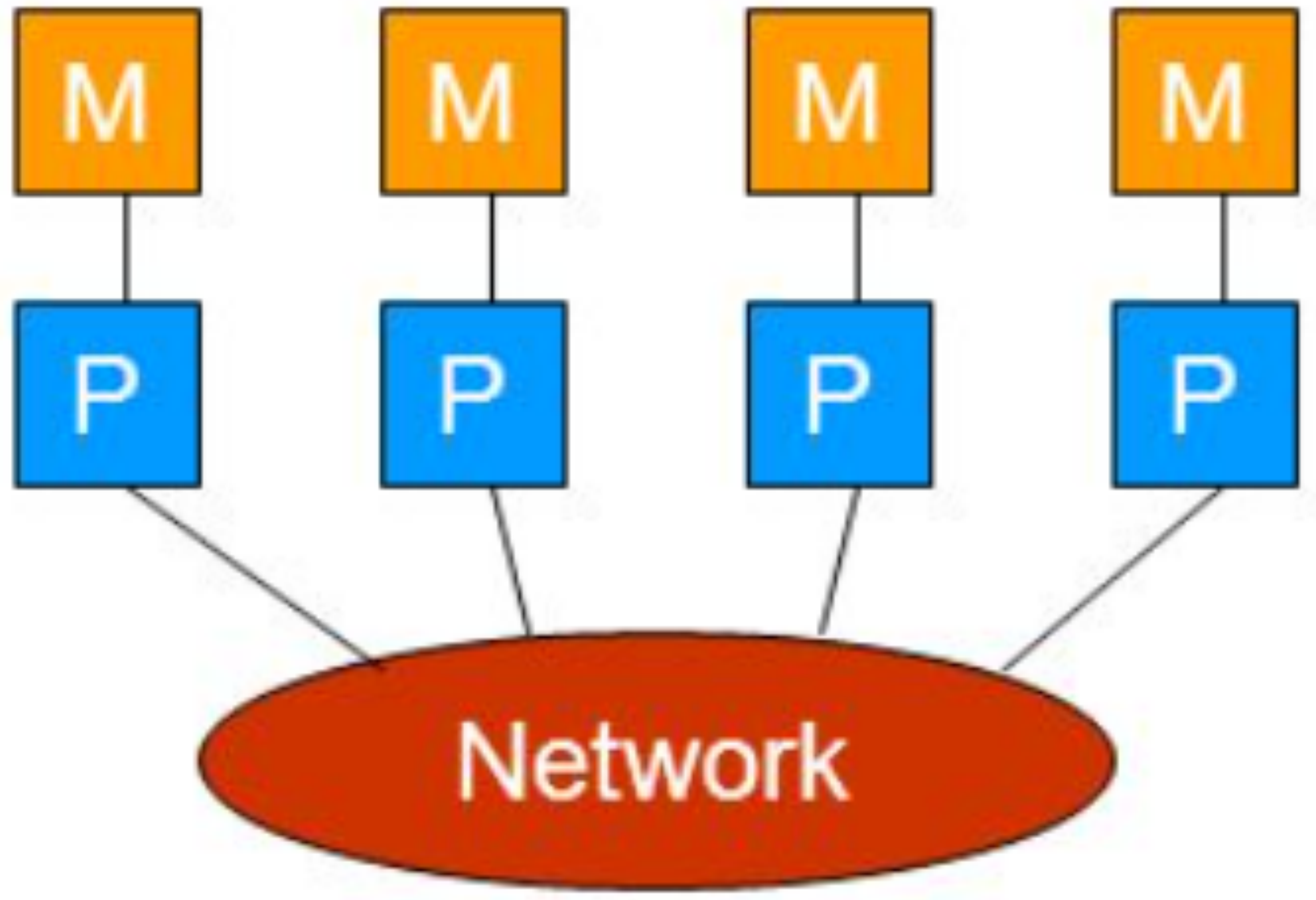
- many processes run on multiple nodes
- process can access only data on the node it is running
- use communication library MPI (Message Passing Interface) to access data on other nodes



```
integer :: len, destination, tag, nreq
comm = mpi_comm_world
call mpi_init(ierr)
call mpi_comm_rank(comm, myid, ierr)
call mpi_comm_size(comm, numproc, ierr)
nreq = 0
...
do i=1,N ! loop over processors with which we
    want to communicate
 destination = ...
 nreq = nreq + 1
 call mpi_irecv(recvdata, len, mpi_real,
     destination, tag, comm, request(nreq), ierr)
 nreq = nreq + 1
 call mpi_isend(senddata, len, mpi_real,
     destination, tag, comm, request(nreq), ierr)
end do
... do some work ...
call mpi_waitall(nreq, request, status, ierr)
call mpi_finalize(ierr)
```

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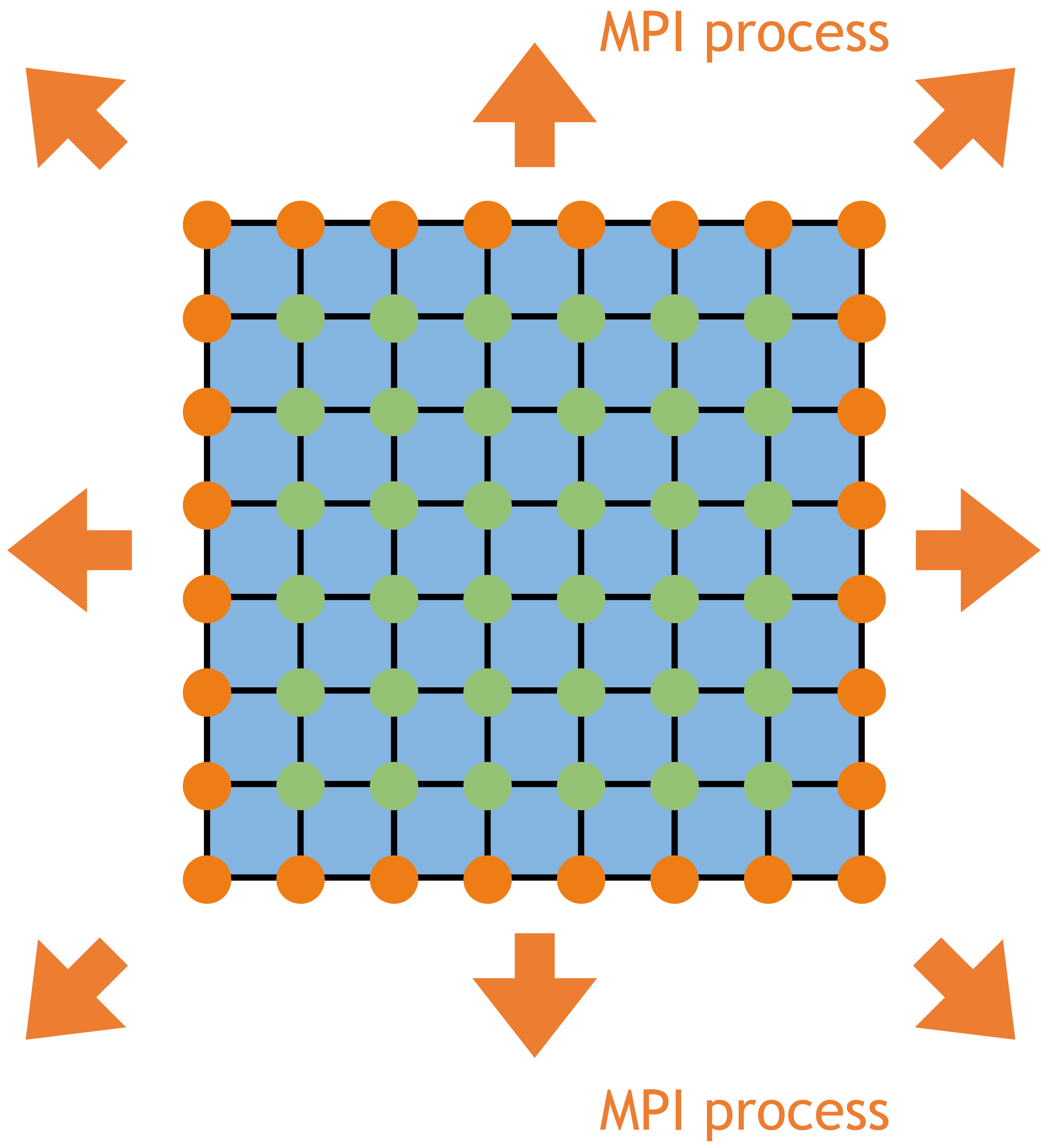
Overlap communication and computation

- Example: grid point method with only next neighbour communication:
    - compute values along processor boundaries first (orange) and send result to neighbours
    - compute interior points while the data is on its way (green)
- try to reduce the physical distance that data needs to travel (difficult)



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Recommendations

- try if using libraries is fast enough
- try to use compiler optimisation (be careful!)
- avoid unnecessary computation and communication
- give each thread as much work as possible
- let the threads do work that does not affect others
- **overlap computation and communication**

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Use data once per time-step

bad example:

```
real, dimension(N) :: a,b
real :: sum
integer :: i,N
sum = 0.0
a = 0.0
b = 0.0
do i=1,N
 b(i) = i
end do
do i=1,N
 a(i) = a(i) + b(i)
end do
do i=1,N
 sum = sum + a(i)
end do
print*,sum
```

good:

```
real, dimension(N) :: a,b
real :: sum
integer :: i,N
sum = 0.0
do i=1,N
 a(i) = 0.0
 b(i) = i
 a(i) = a(i) + b(i)
 sum = sum + a(i)
end do
print*,sum
```

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Recommendations

- try if using libraries is fast enough
- try to use compiler optimisation (be careful!)
- avoid unnecessary computation and communication
- give each thread as much work as possible
- let the threads do work that does not affect others
- overlap computation and communication
- **use data only once per time-step**

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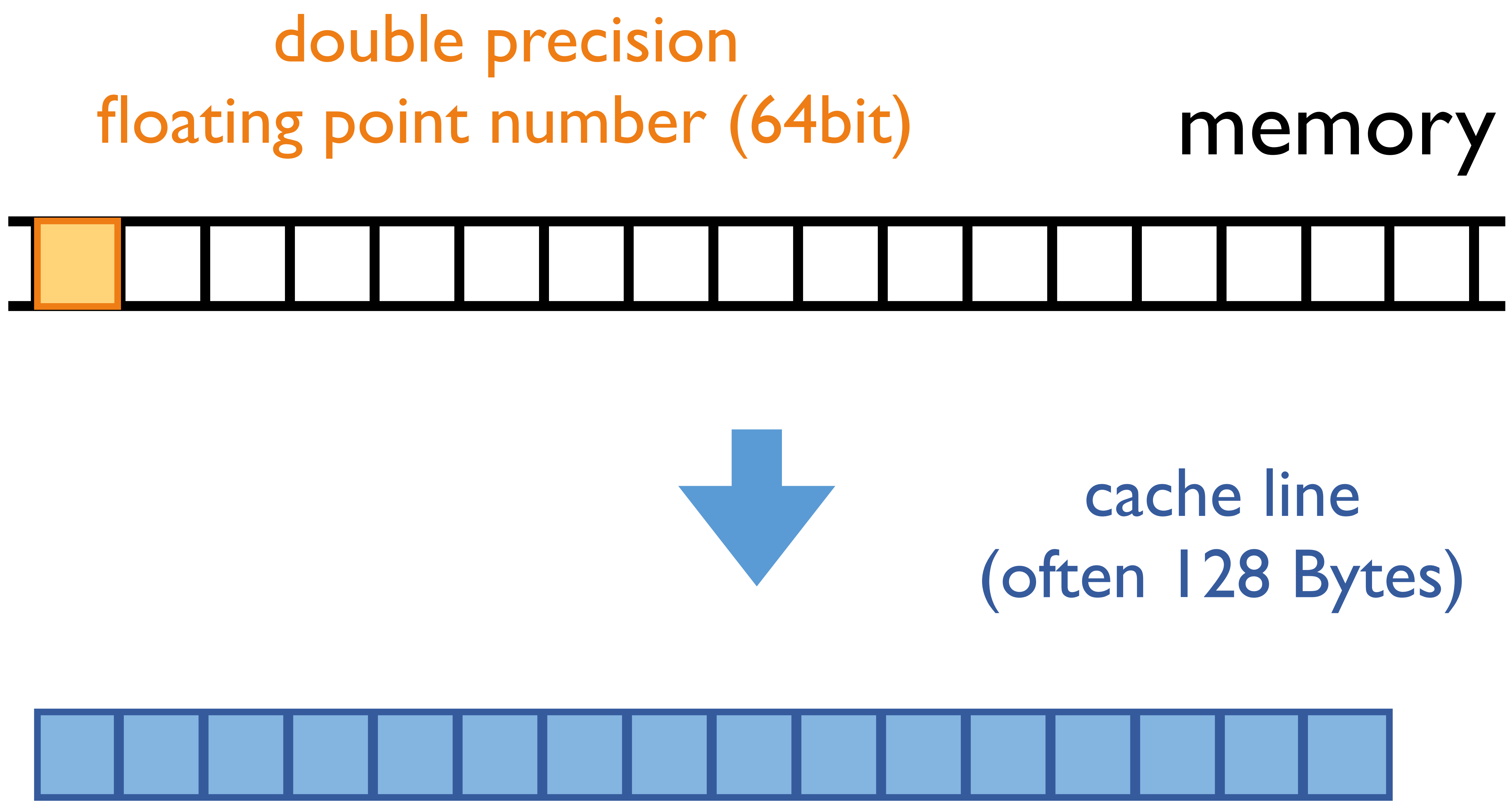
Contiguous memory access



store data in the order in which you need it and use it in this order!

Fortran (column major order):

```
real, dimension(N,M) :: a,b
integer :: i,j,N,M
do j=1,M
 do i=1,N
  a(i,j) = a(i,j) + b(i,j)
  ! fast index should be i
 end do
end do
```

C (row major order):

```
int i,j,N,M;
for (i=0; i<N; i++) {
 for (j=0; j<M; j++) {
  a[i][j] = a[i][j] + b[i][j]
  // fast index should be j
 }
}
```

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Recommendations

- try if using libraries is fast enough
- try to use compiler optimisation (be careful!)
- avoid unnecessary computation and communication
- give each thread as much work as possible
- let the threads do work that does not affect others
- overlap computation and communication
- use data only once per time-step
- **contiguous memory access**

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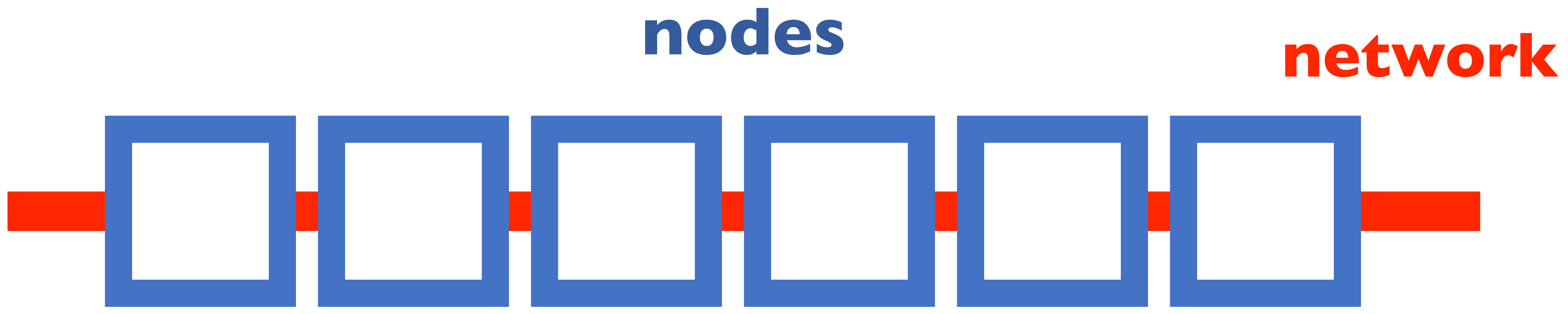
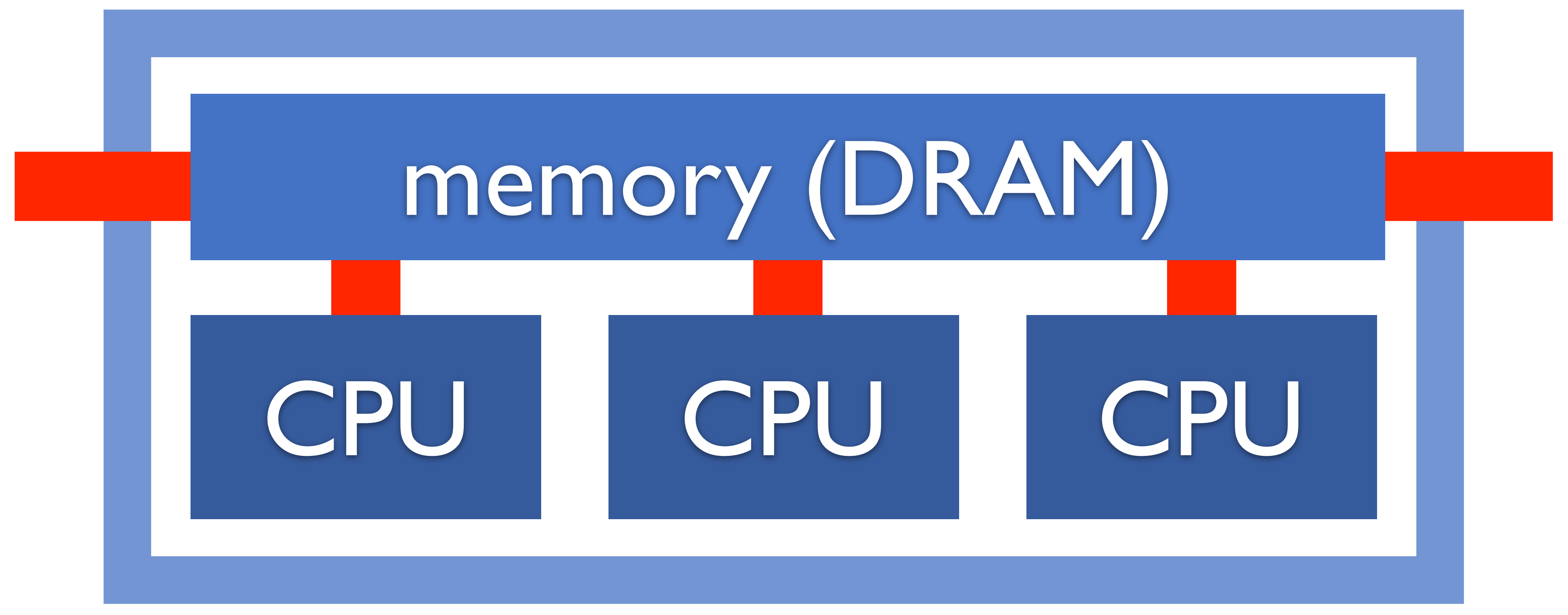
Supercomputer/Cluster



Node



CPU

central processing unit; does one instruction like c=a+b per clock cycle

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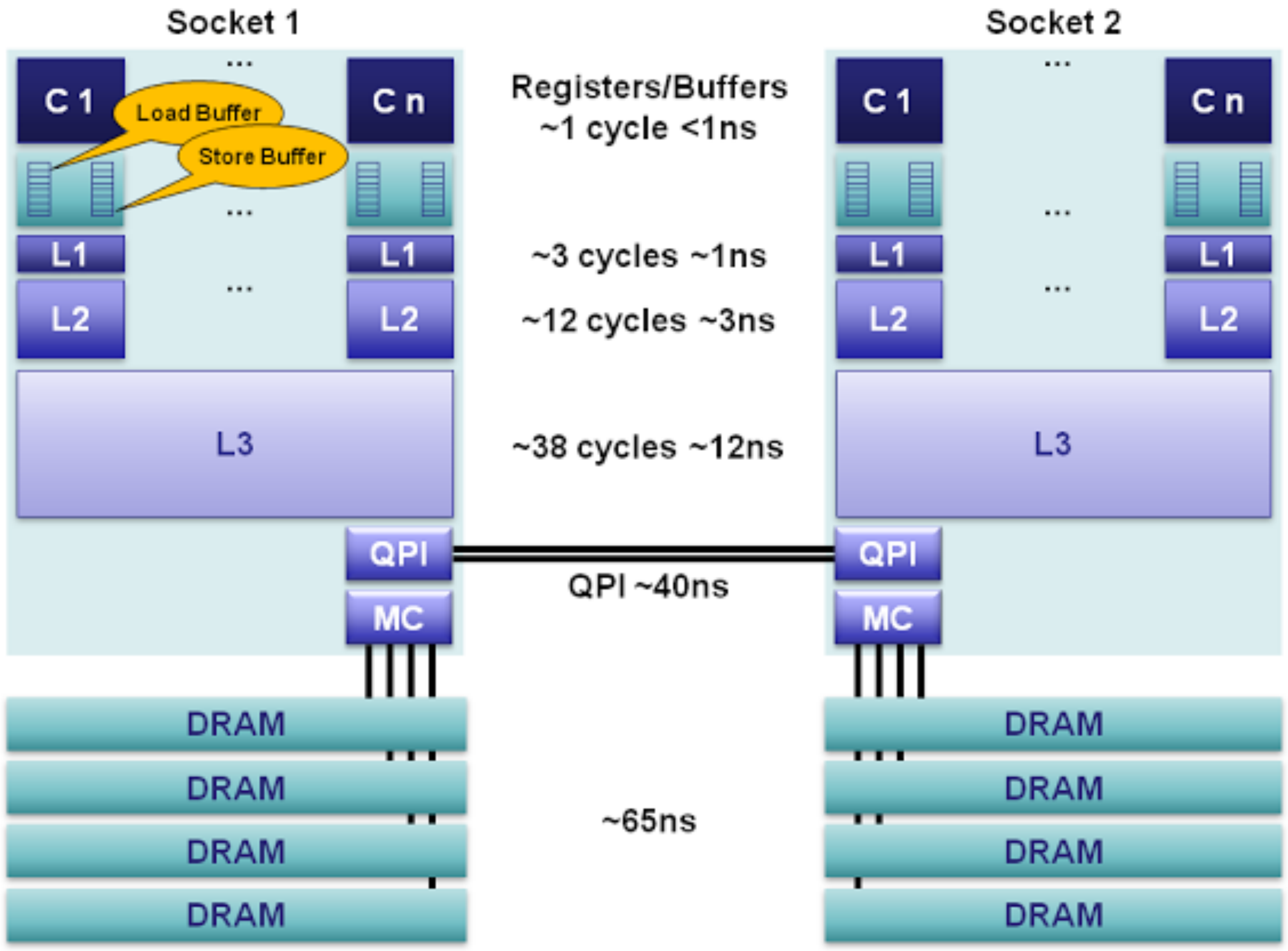
Memory hierarchy inside one node



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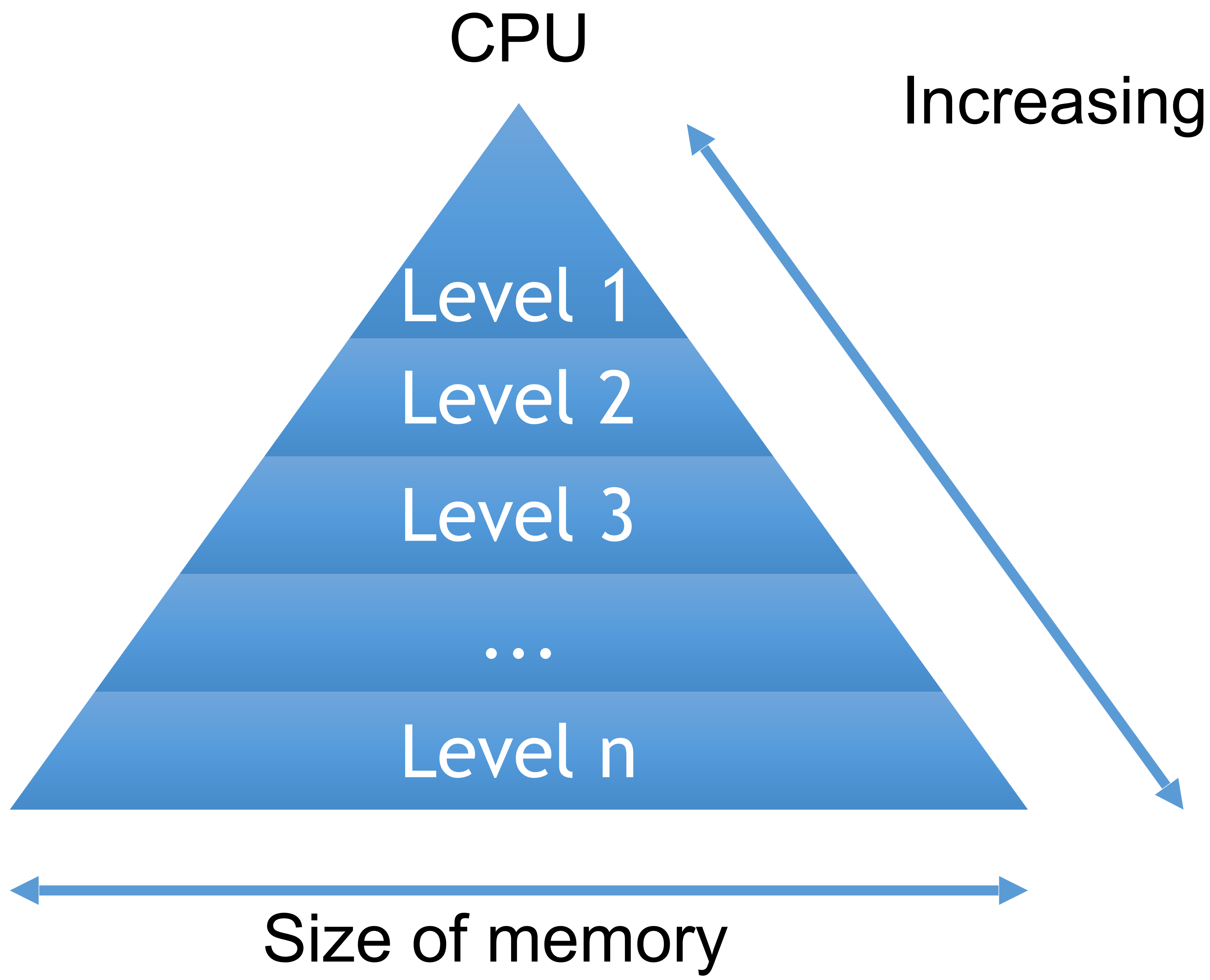
Cache



Increasing distance from CPU = larger access time

Example:

L1: 32 kB, latency 3 cycles
L2: 256 kB, latency 10 cycles
L3: 8MB, latency 40 cycles
DRAM: 16GB, latency 200 cycles
DISK: 1TB, latency 1.000.000 cycles

Cache hit – data found in cache
Cache miss – data not found in cache, thus must be copied from lower memory level
Capacity miss – cache runs out of space for new data
Conflict miss – more that one item is mapped to the same location in cache

ESCAPE 2

IFS: divide work into blocks with length NPROMA

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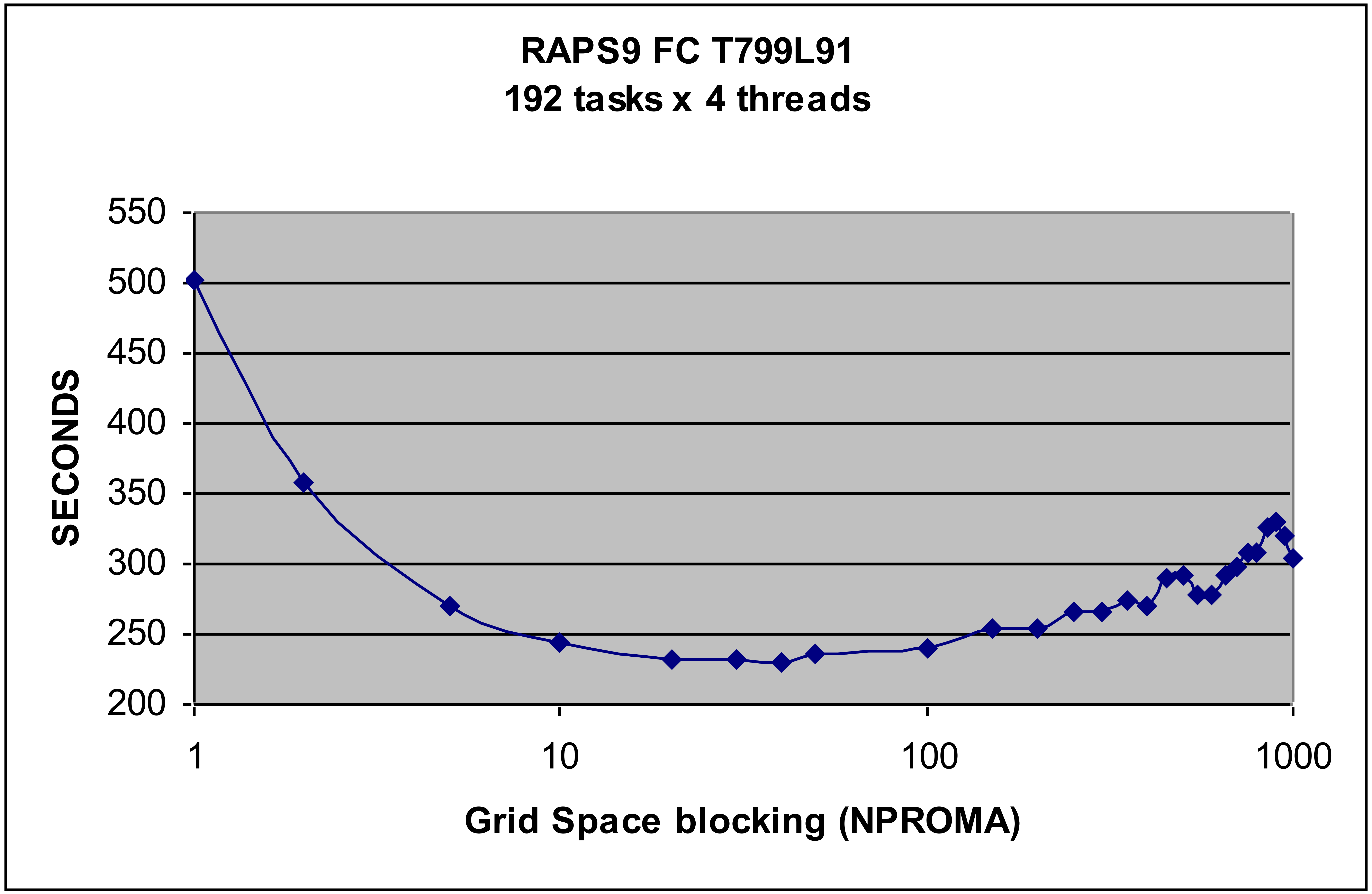

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Recommendations

- try if using libraries is fast enough
- try to use compiler optimisation (be careful!)
- avoid unnecessary computation and communication
- give each thread as much work as possible
- let the threads do work that does not affect others
- overlap computation and communication
- use data only once per time-step
- contiguous memory access
- **try to fit data into cache**

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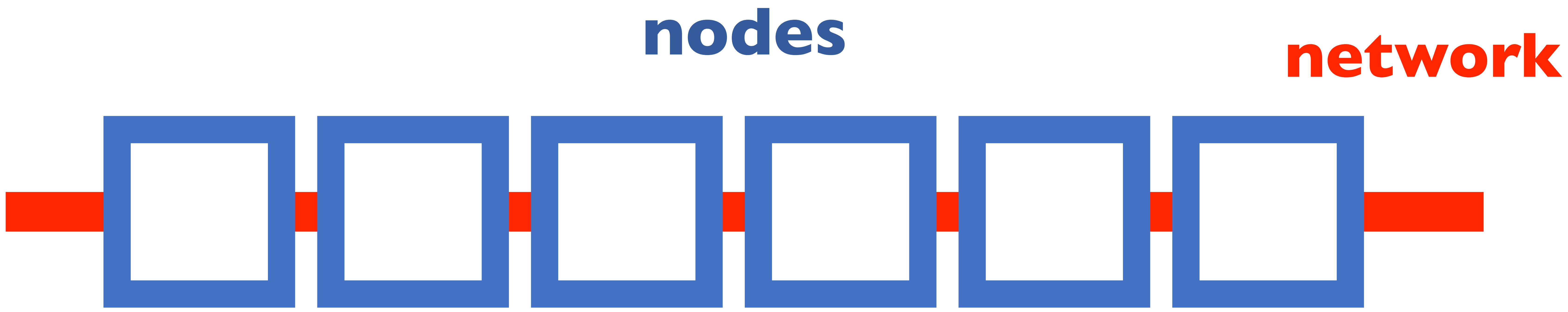
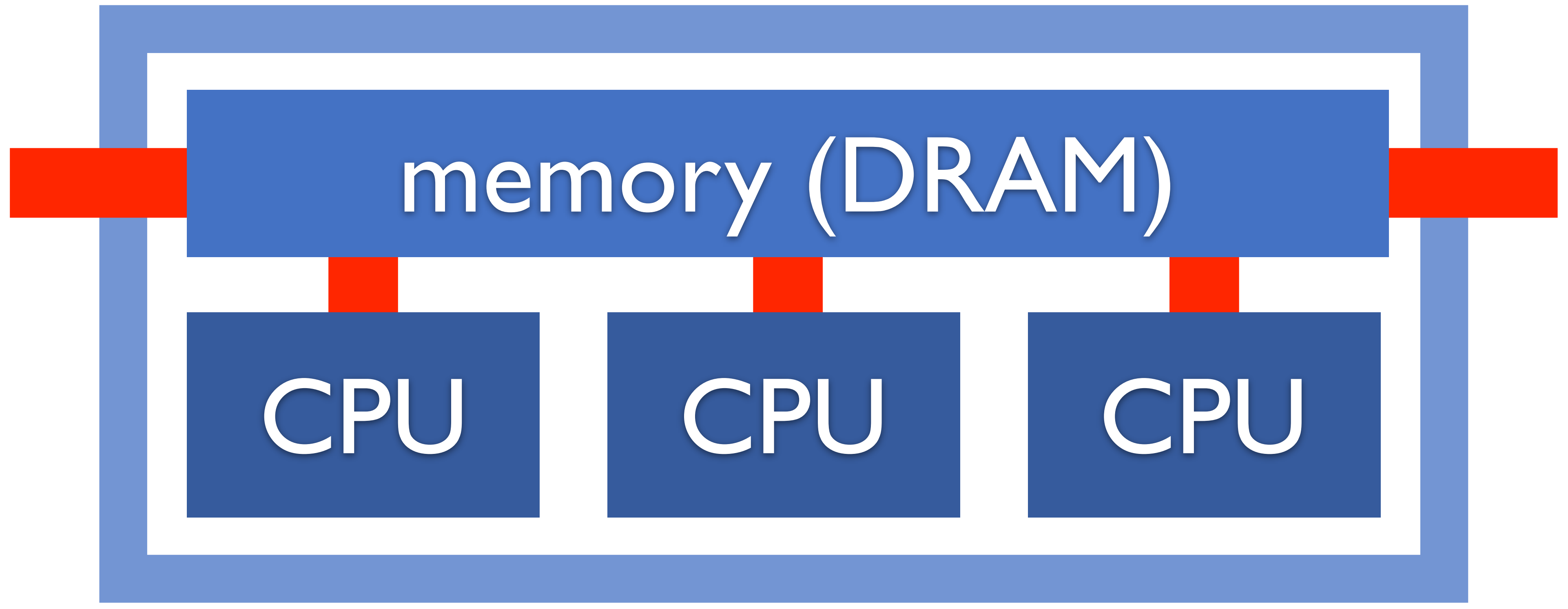
Supercomputer/Cluster



Node



Bottlenecks

- network (connection between nodes)
- connection between DRAM and processor

Fast and slow operations

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- In terms of cost
- Fast and inexpensive: add, multiply, sub, fma (fused multiply add)
- Medium: divide, modulus, sqrt
- Slow: power, trigonometric functions

- try linear algebra (BLAS, LAPACK) and math libraries (Intel MKL)

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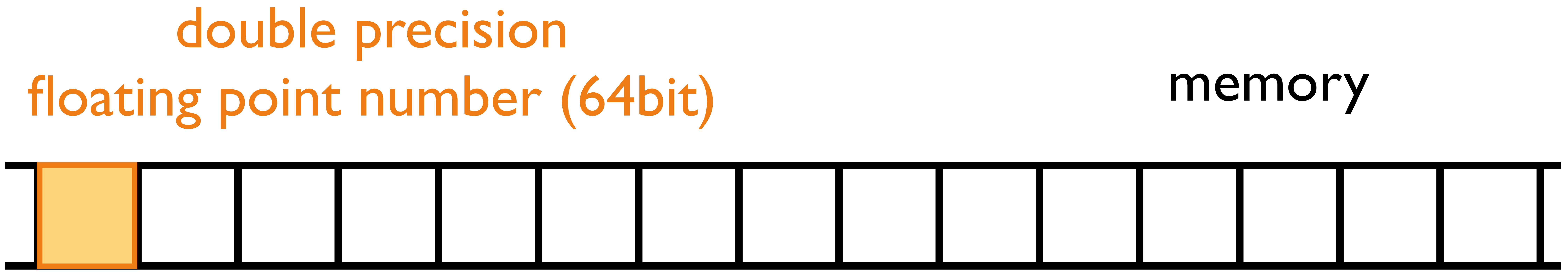
Vectorisation



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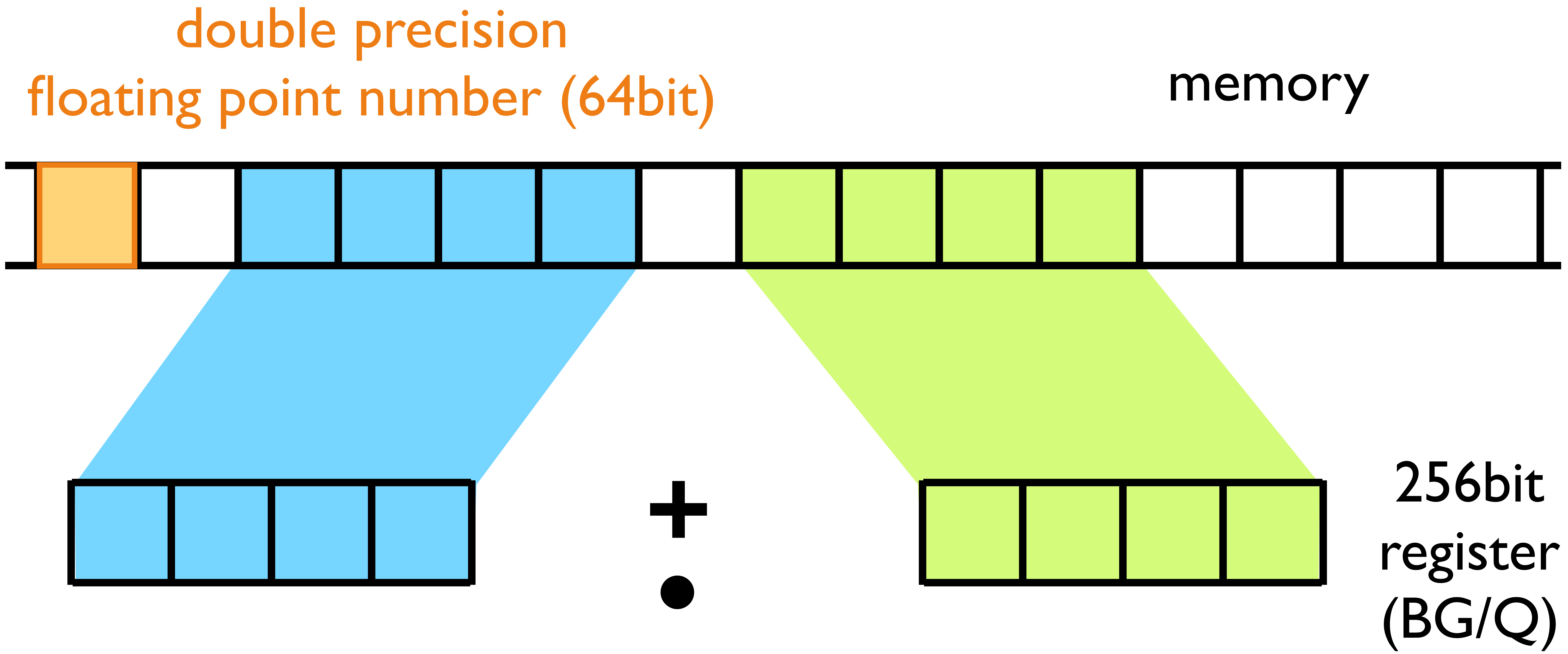
Vectorisation



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Vectorisation

initial version:

```
real :: rho, rho_x, rho_y, rho_z, u, v, w, rhs
do e=1,num_elem ! loop through all elements
   do i=1,num_points_e ! loop through all points of
     the element e
      ... ! compute derivatives rho_x, rho_y, rho_z
      rhs = u*rho_x + v*rho_y + w*rho_z + ...
   end do !i
end do !e
```

optimised for compiler vectorisation:

```
real, dimension(num_points_e) :: rho, rho_x, rho_y, &
   rho_z, u, v, w, rhs
do e=1,num_elem ! loop through all elements
   ... ! compute derivatives like rho_x, rho_y, rho_z
   rhs = u*rho_x + v*rho_y + w*rho_z + ...
end do !e
```

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Vectorisation

initial version:

```
real :: rho, rho_x, rho_y, rho_z, u, v, w, rhs
do e=1,num_elem ! loop through all elements
   do i=1,num_points_e ! loop through all points of
     the element e
      ... ! compute derivatives rho_x, rho_y, rho_z
      rhs = u*rho_x + v*rho_y + w*rho_z + ...
   end do !i
end do !e
```

9.4s
14.4% vector
operations

optimised for compiler vectorisation:

```
real, dimension(num_points_e) :: rho, rho_x, rho_y, &
   rho_z, u, v, w, rhs
do e=1,num_elem ! loop through all elements
   ... ! compute derivatives like rho_x, rho_y, rho_z
   rhs = u*rho_x + v*rho_y + w*rho_z + ...
end do !e
```

2.1s
73.9% vector
operations

measurements: spectral element model NUMA, NPS

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vector intrinsics (here for BG/Q)

```
real, dimension(4,4,4) :: rho, rho_x, rho_y, &
   rho_z, u, v, w, u_x, v_y, w_z, rhs
!IBM* align(32, rho, rho_x, rho_y, rho_z, u, v, w,
     u_x, v_y, w_z, rhs)
! declare variables representing registers: (each
     contains four double precision floating point
     numbers)
vector(real(8)) vct_rho, vct_rhox, vct_rhoy, vct_rhoz
vector(real(8)) vct_u, vct_v, vct_w, vct_rhs
if (iand(loc(rho), z'1F') .ne. 0) stop 'rho is not
     aligned'
... ! check alignment of other variables
do e=1,num_elem ! loop through all elements
   do k=1,4 ! loop over points in z-direction
      do j=1,4 ! loop over points in y-direction
         ... ! compute derivatives rho_x, ...
         ! load always four floating point numbers:
         vct_u = vec_ld(0, u(1,j,k))
         vct_v = vec_ld(0, v(1,j,k))
         vct_w = vec_ld(0, w(1,j,k))
         vct_rhox = vec_ld(0, rho_x(1,j,k))
         vct_rhoy = vec_ld(0, rho_y(1,j,k))
         vct_rhoz = vec_ld(0, rho_z(1,j,k))
         ! rhs = u*rho_x
```

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vector intrinsics (here for BG/Q)

```
         ... ! compute derivatives rho_x, ...
         ! load always four floating point numbers:
         vct_u = vec_ld(0, u(1,j,k))
         vct_v = vec_ld(0, v(1,j,k))
         vct_w = vec_ld(0, w(1,j,k))
         vct_rhox = vec_ld(0, rho_x(1,j,k))
         vct_rhoy = vec_ld(0, rho_y(1,j,k))
         vct_rhoz = vec_ld(0, rho_z(1,j,k))
         ! rhs = u*rho_x
         vct_rhs = vec_mul(vct_u,vct_rhox)
         ! rhs = rhs + v*rho_y
         vct_rhs = vec_madd(vct_v,vct_rhoy,vct_rhs)
         ! rhs = rhs + w*rho_z
         vct_rhs = vec_madd(vct_w,vct_rhoz,vct_rhs)
         ! write result from register into cache:
         call vec_st(vct_rhs, 0, rhs(1,j,k))
         ...
      end do !j
   end do !k
end do !e
```

1.0s
98.6% vector operations

measurements: spectral element model NUMA, NPS

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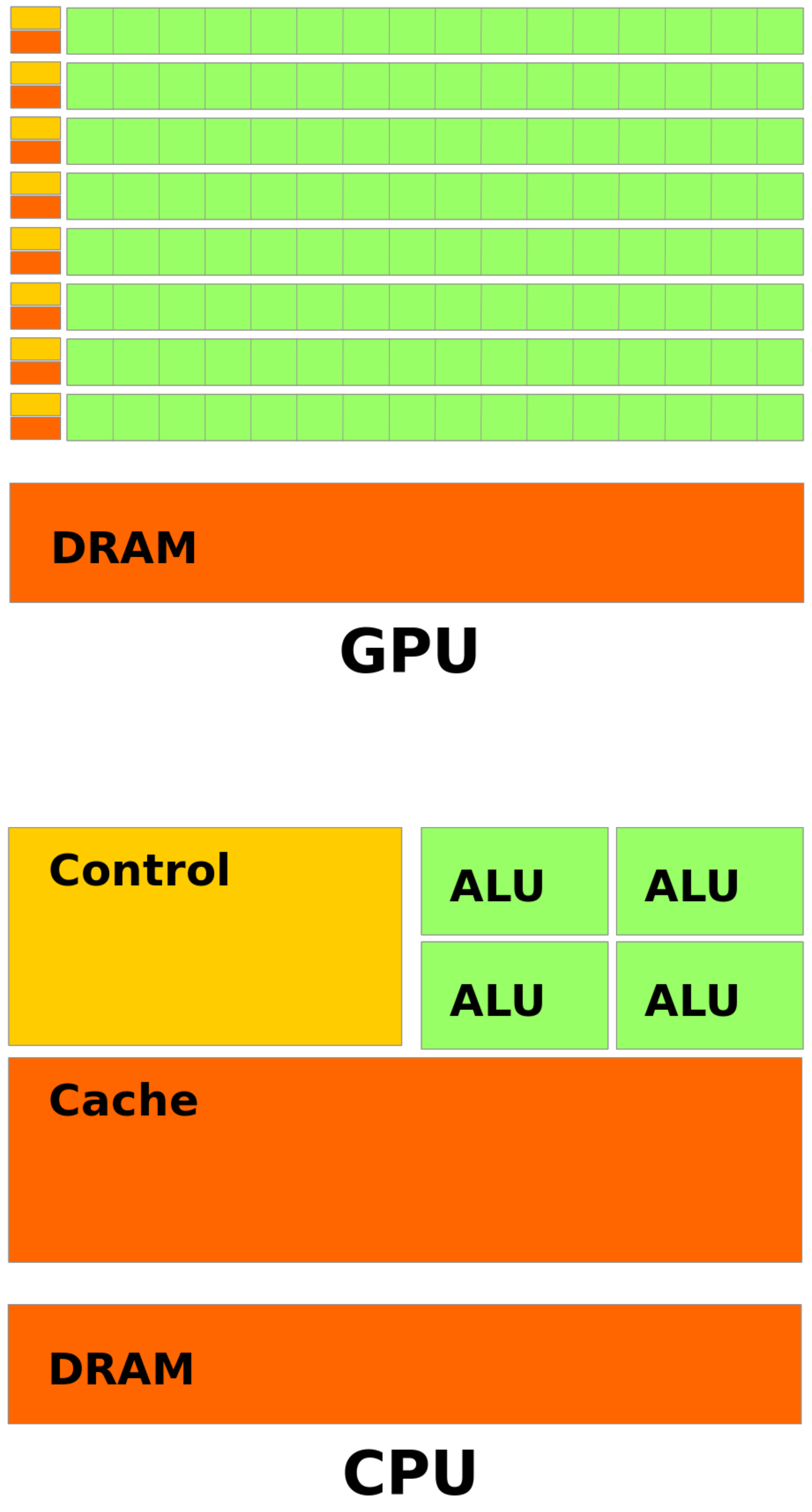
GPU (Graphics Processing Unit)

- small number of instructions => requires host CPU
- GPU/CPU interface (PCIe up to 16GB/sec, NVLINK up to 300GB/sec between GPUs in same node)
- more energy efficient than CPUs
- high performance GPUs today mainly supplied by NVIDIA
- lots of cores share one control unit
- very little memory inside the GPU



Recommendations

- try if using libraries is fast enough
- try to use compiler optimisation (be careful!)
- avoid unnecessary computation and communication
- give each thread as much work as possible
- let the threads do work that does not affect others
- overlap computation and communication
- use data only once per time-step
- contiguous memory access
- try to fit data into cache
- **make good use of vectorisation**

How good are we?

The ESCAPE-2 project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 800897

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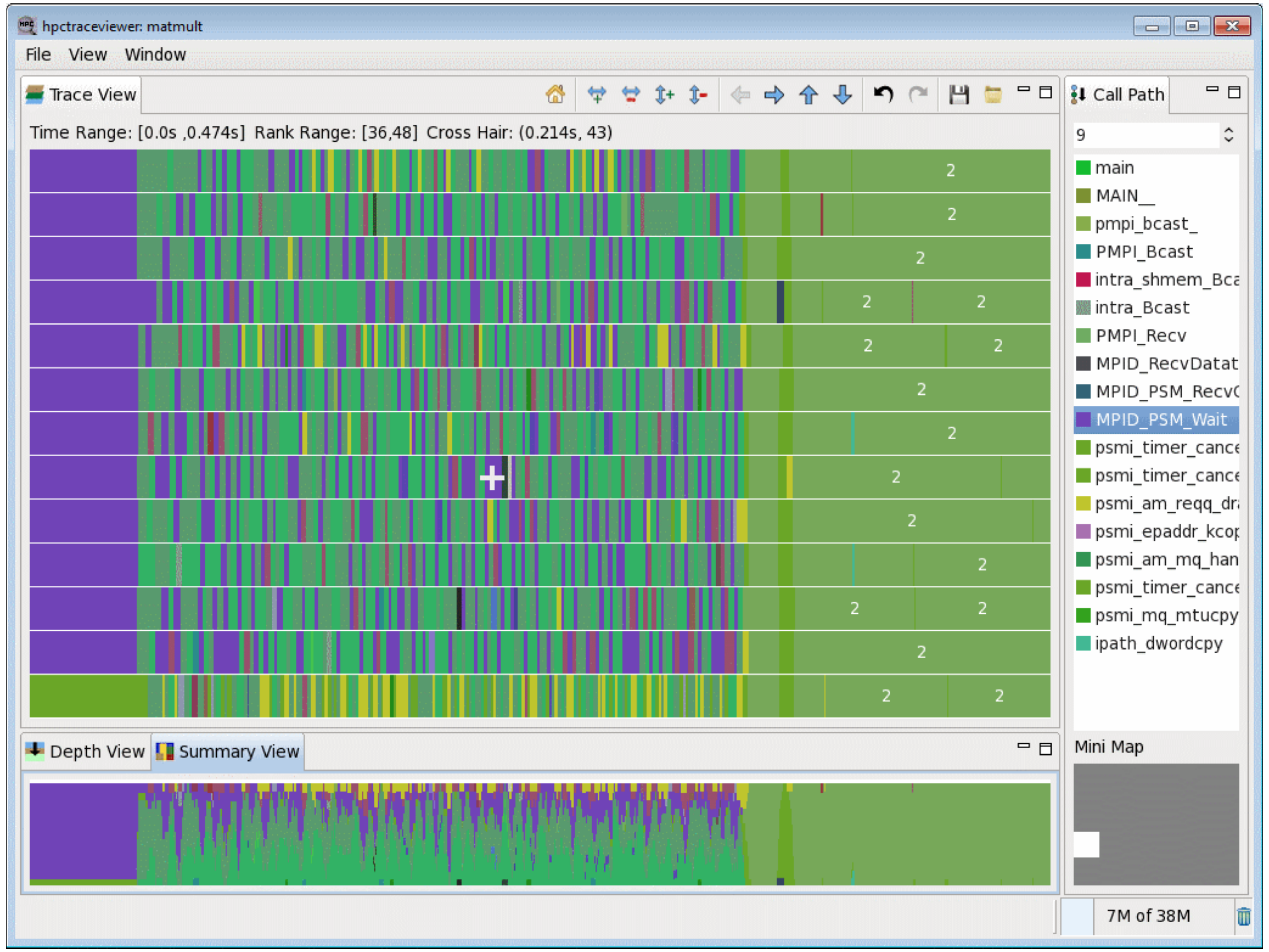
Hardware performance counters

- set of special-purpose hardware registers to store counts of hardware-related activities
- can help in spotting the application bottlenecks
- allow for low-level performance analysis and tuning, though implementation may be somehow difficult
- tools: PAPI, VTUNE, HPCToolkit, ...



Time Range: [0.0s ,0.474s] Rank Range: [36,48] Cross Hair: (0.214s, 43)

main
MAIN__
pmpi_bcast_
PMPI_Bcast
intra_shmem_Bca
intra_Bcast
PMPI_Recv
MPID_RecvDatat
MPID_PSM_Recv(
MPID_PSM_Wait
psmi_timer_cance
psmi_timer_cance
psmi_am_reqq_dr
psmi_epaddr_kcop
psmi_am_mq_han
psmi_timer_cance
psmi_mq_mtucpy
ipath_dwordcpy

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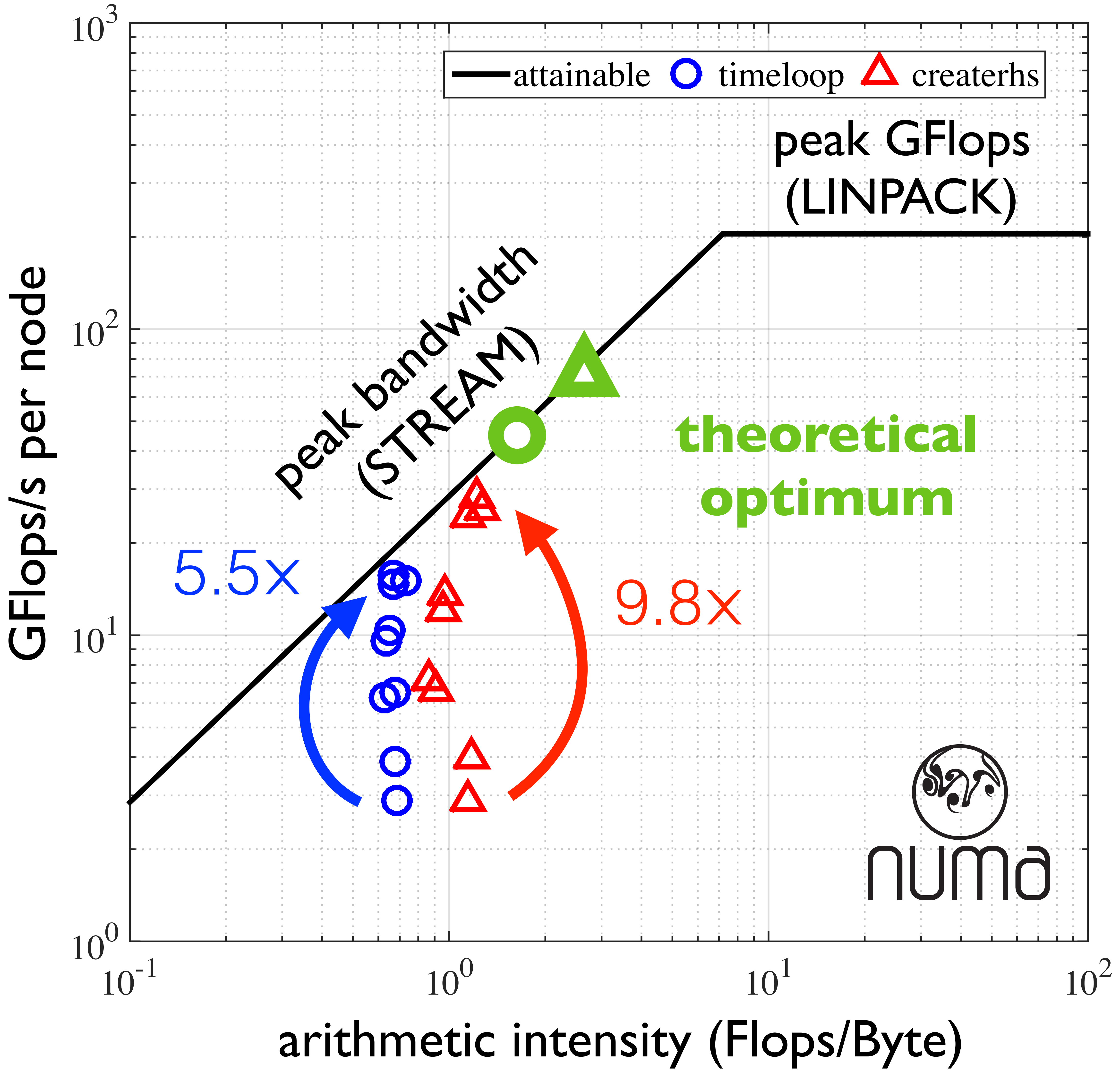
Roofline plot



blue: entire timeloop

red: main computational kernel

data points: different optimization stages

measurements: spectral element model NUMA, NPS

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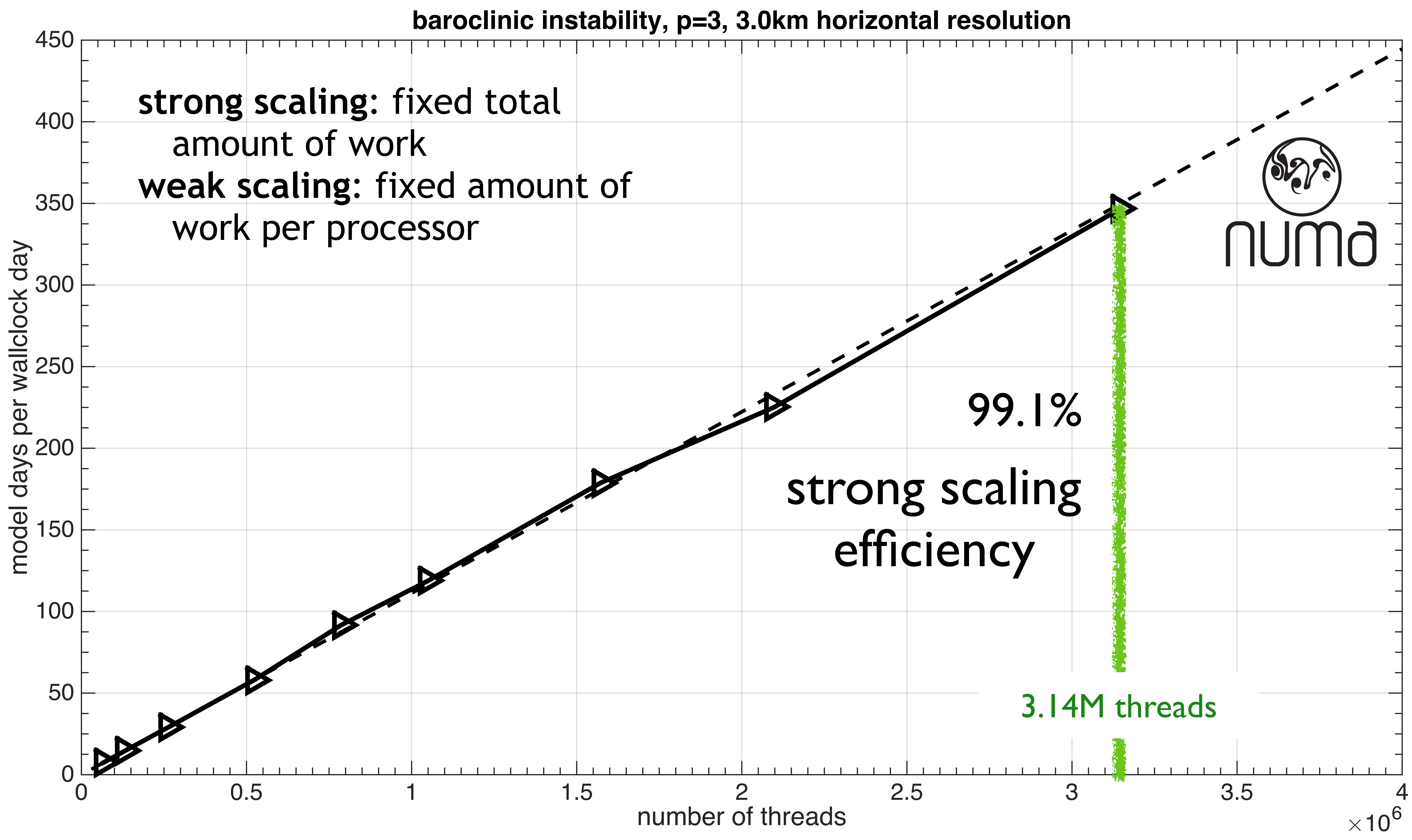
Strong scaling efficiency



measurements: spectral element model NUMA, NPS

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Create performance model

example code:

```
real, dimension(N,M) :: a,b,c
integer :: i,j,N,M
do timestep=1,nstep
 do j=1,M
  do i=1,N
   a(i,j) = a(i,j) + b(i,j) * c(i,j)
  end do
 end do
end do
```

parameters:

parameter	value
N	1E+04
M	1E+05
nstep	100
GB/s	20
GFlops/s	200

floating point operations:

function	operations per step	
main	2*N*M	2E+11
total GFlops for all steps		20000
runtime		100.0

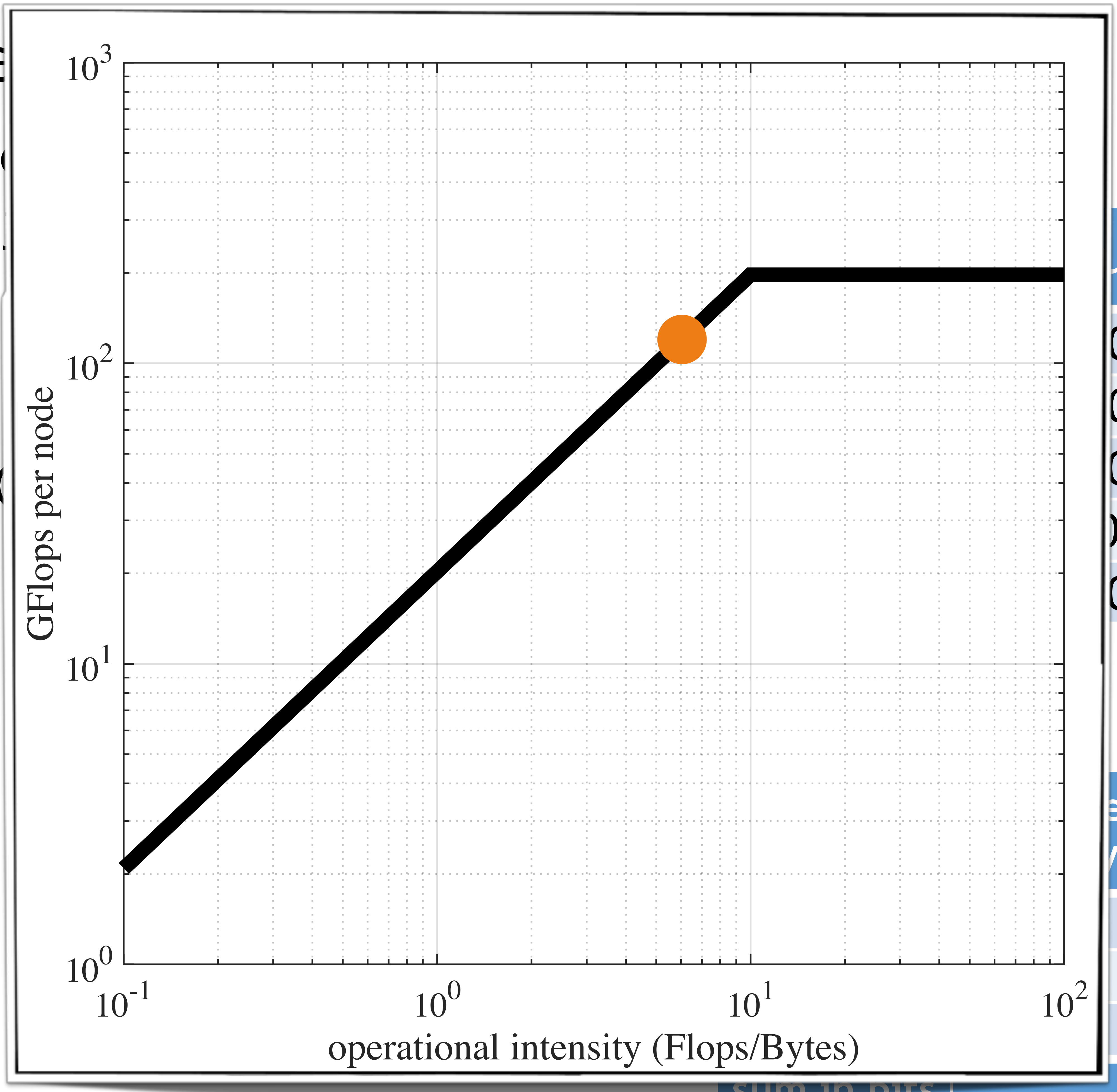
memory:

variable	bits per entry	size	#read per step	#write per step	total bits read	total bits written
a	64	N*M	1	1	6.4E+12	6.4E+12
b	64	N*M	1	0	6.4E+12	0E+00
c	64	N*M	1	0	6.4E+12	0E+00
sum in bits					1.92E+13	6.4E+12
sum in GB					2400	800
intensity	6.25			runtime in seconds		160.0

Create performance model

example code

```
real, dimensi
integer :: i,
do timestep=1
 do j=1,M
  do i=1,N
   a(i,j) = a(
  end do
 end do
end do
```



ue
04
05
0
)
0

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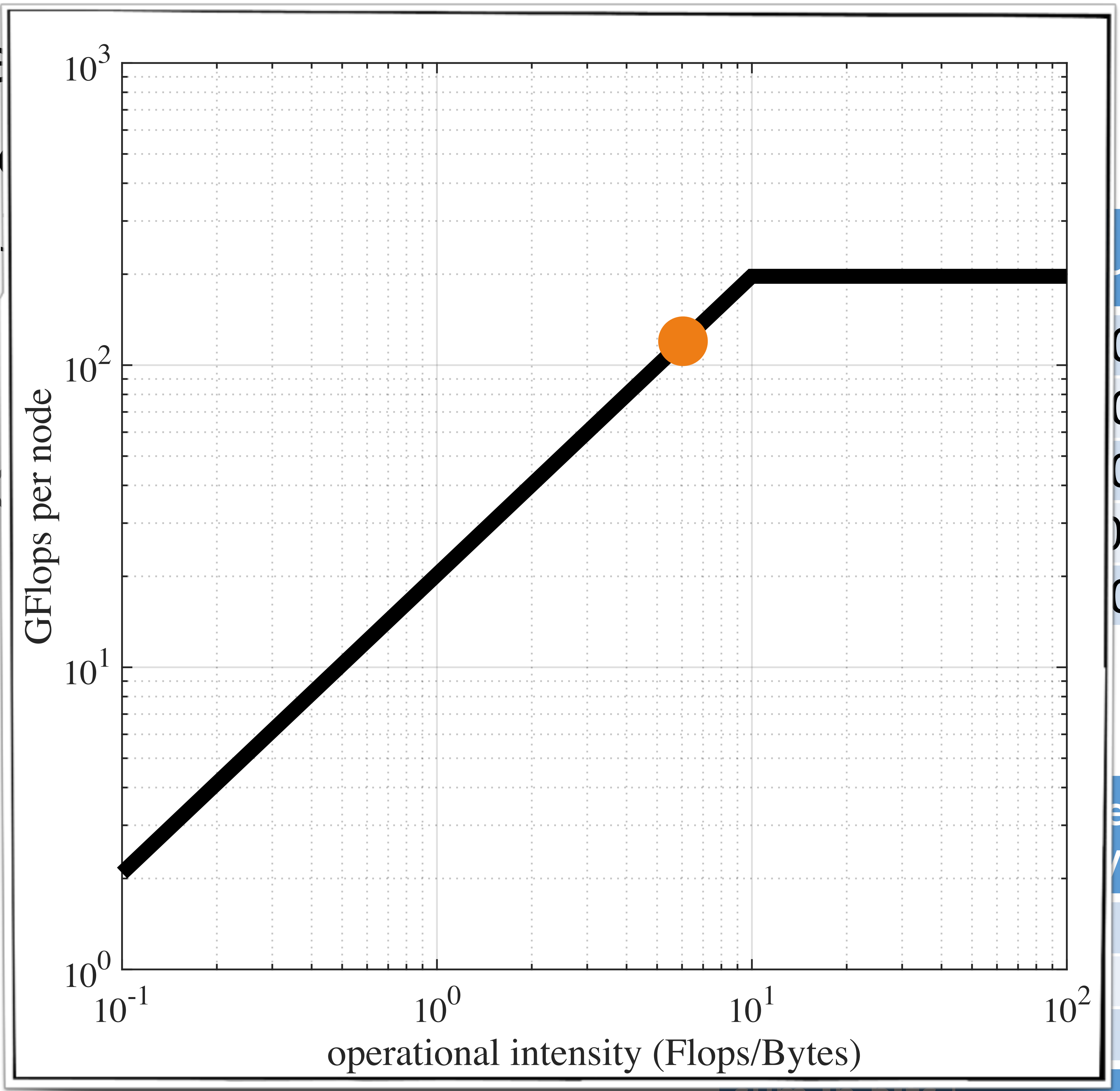

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next step: distinguish between worst case (no data already in cache) and best case (previously used data is still in cache)

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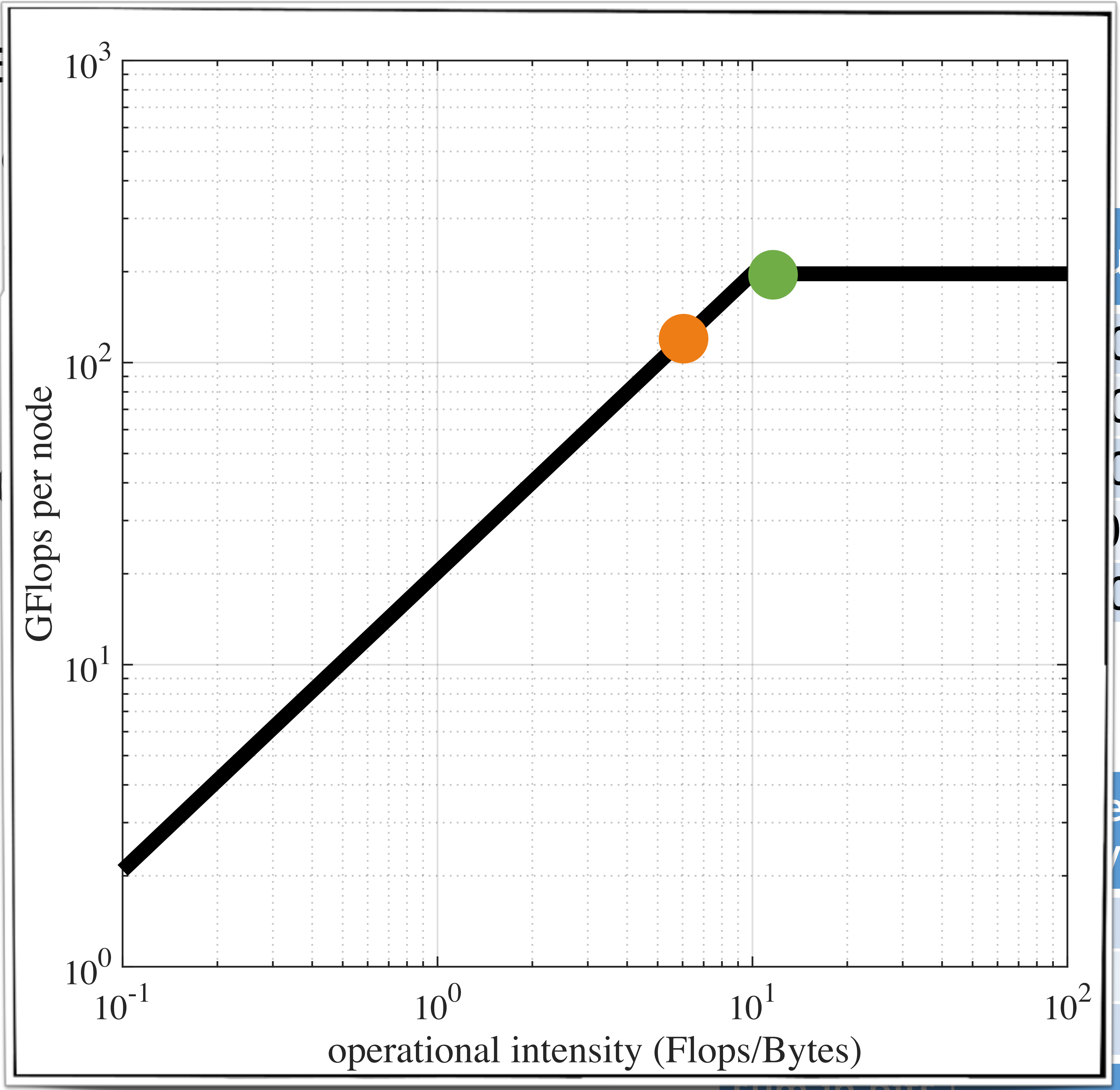

ue
04
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0
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sum in bits				6.4E+12	6.4E+12
sum in GB				800	800
intensity	12.5		runtime in seconds		80.0

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Co-ordinated by ECMWF

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- **compare performance with expectations**

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open question

How to find right compromise between performance and readability, portability, maintainability?

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