Introduction to Parallel Computing

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ECMWF

Outline

- Parallel computing?
- Types of computer
- Parallel Computers today
- Challenges in parallel computing
- Parallel Programming Languages
- OpenMP/OpenACC and MPI

What is Parallel Computing?

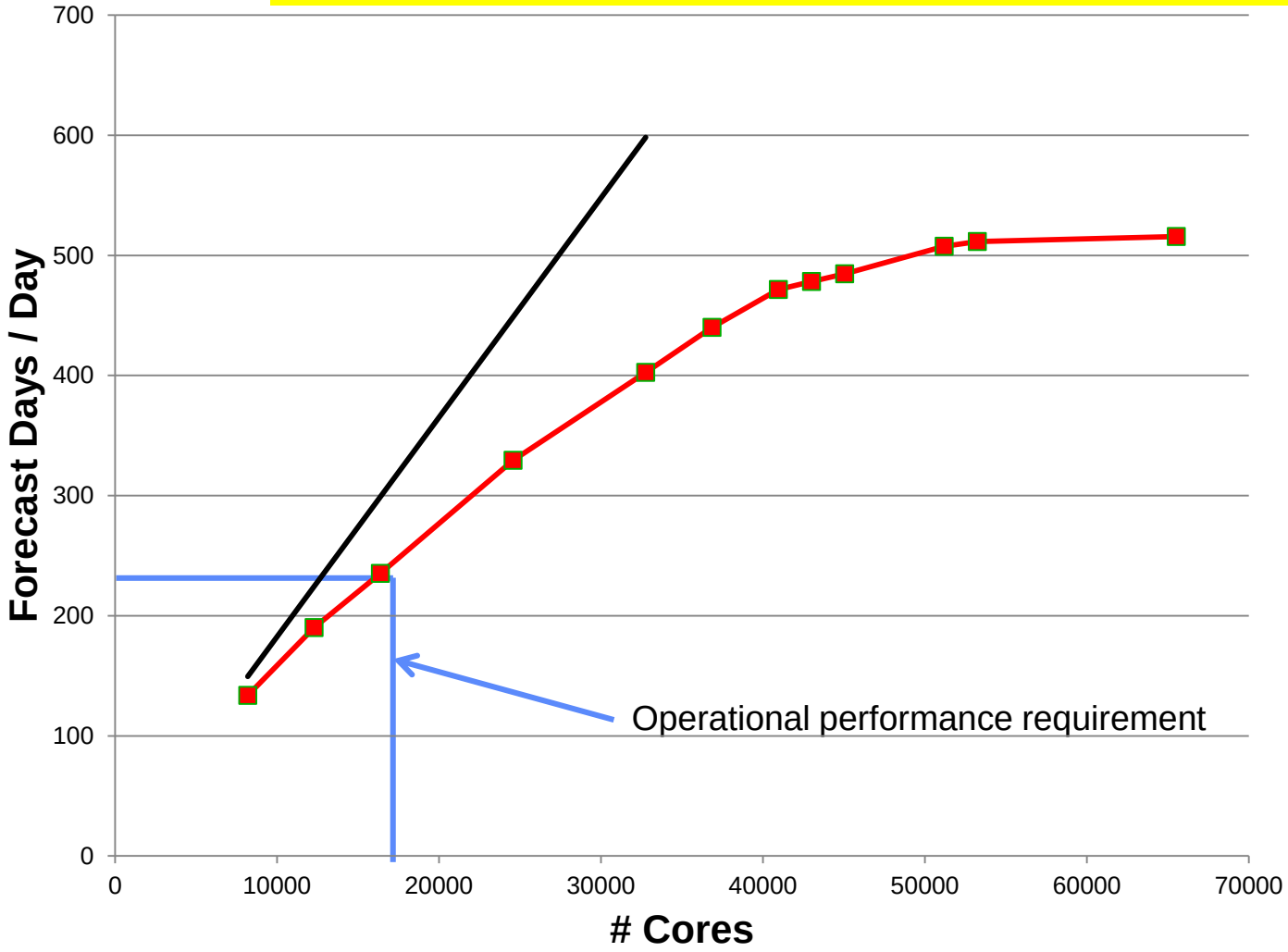
The simultaneous use of more than one processor or computer to solve a problem

Why do we need Parallel Computing?

- **Serial computing is too slow**
- **Need for large amounts of memory not accessible by a single processor**

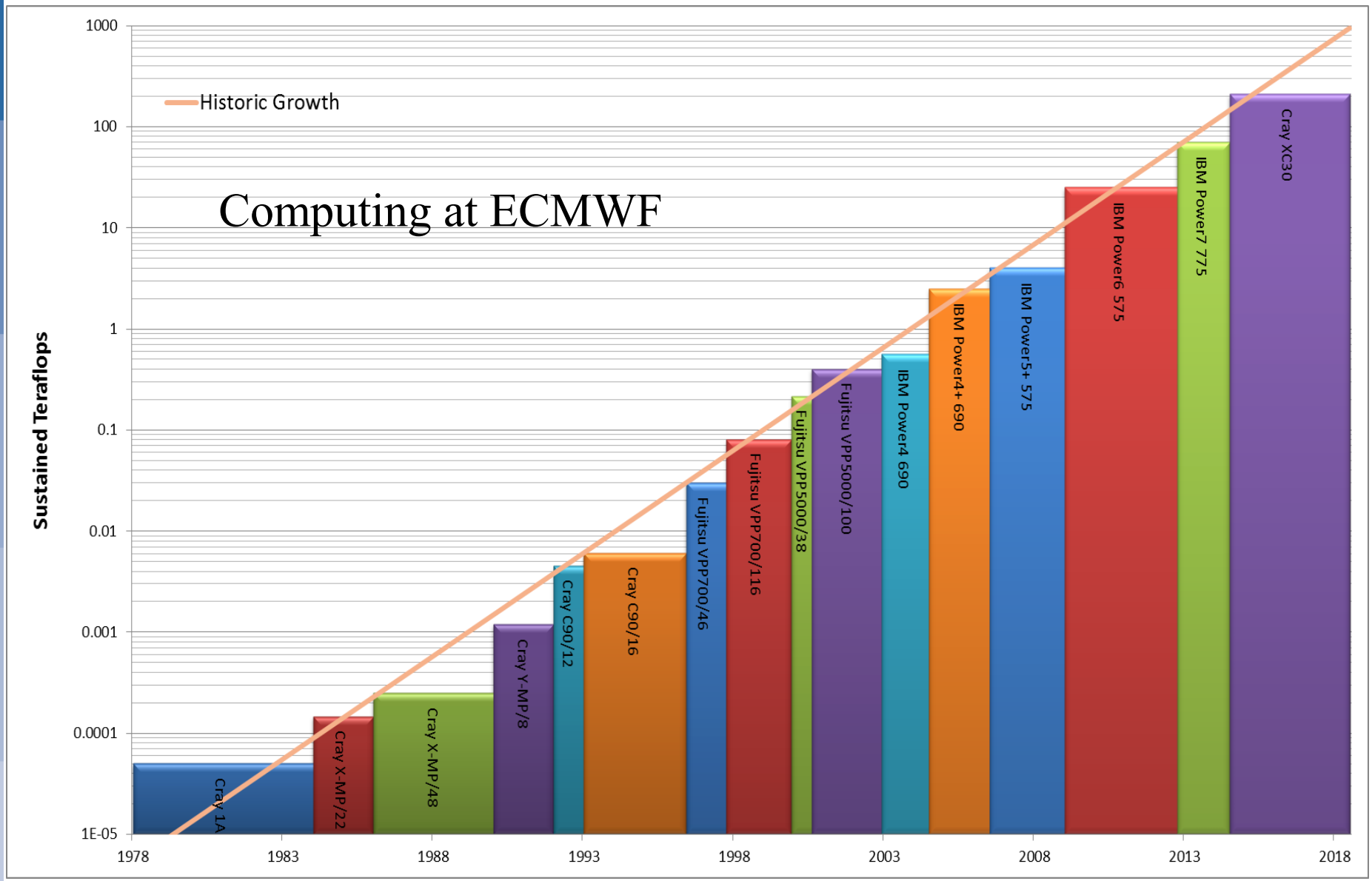
T2047 IFS global model (10 km) performance on CRAY XE6, 2012

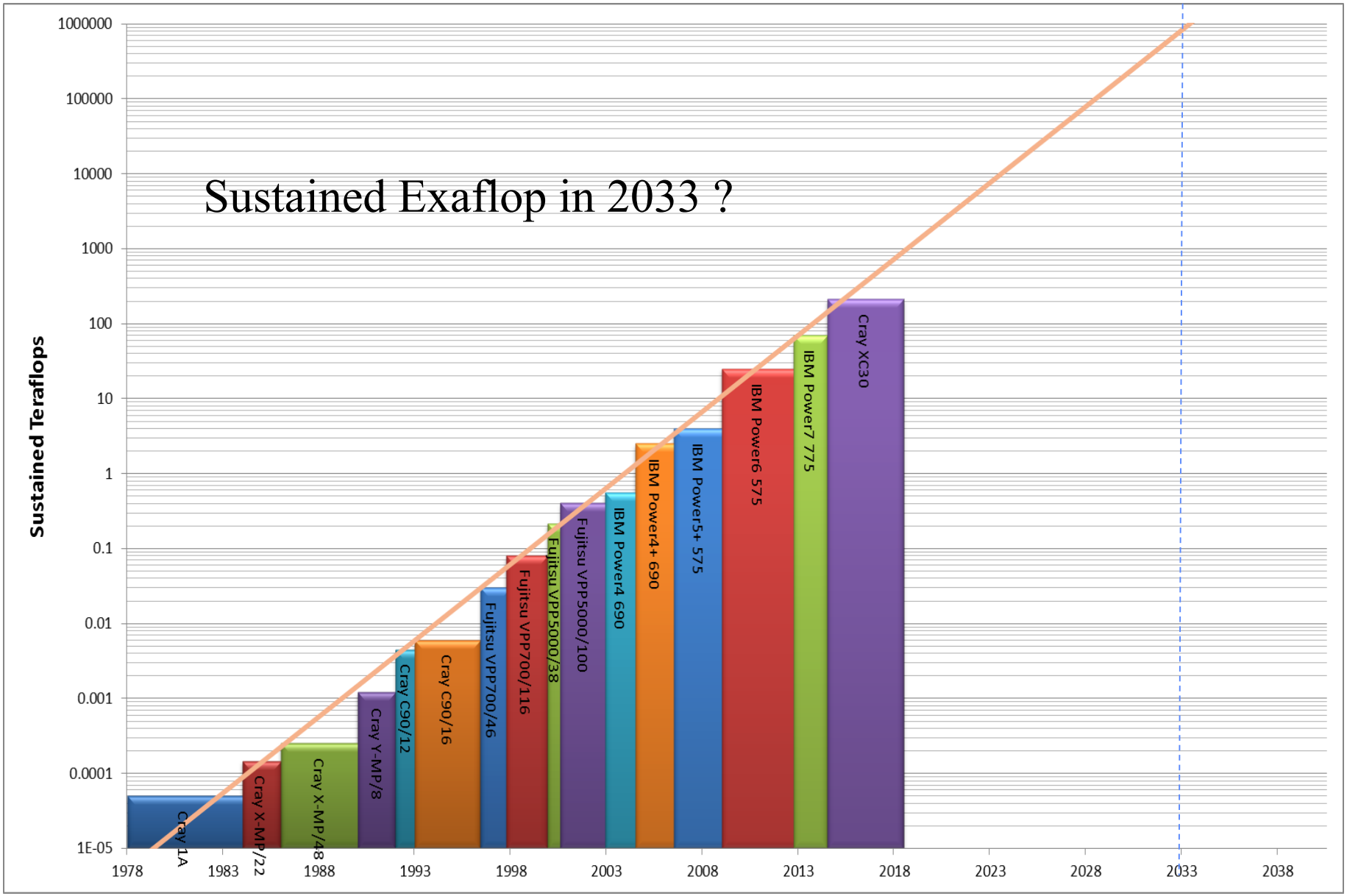
10 day forecast in 1 hour = 240 forecast days / day



Measuring Performance

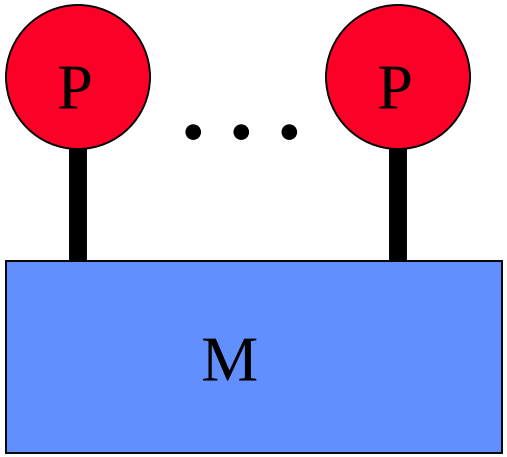
- **Wall Clock**
- **Floating point operations per second (FLOPS or FLOP/S)**
  - **Peak (Hardware), Sustained (Application)**
- **SI prefixes**
  - **Mega Mflops 10**6**
  - **Giga Gflops 10**9**
  - **Tera Tflops 10**12**
  - **Peta Pflops 10**15 ECMWF: 2 * 1.79 Pflops peak (XC-30)**
  - **Exa, Zetta, Yotta**
- **Instructions per second, Mips, etc,**
- **Transactions per second (Databases)**


Computing at ECMWF
Historic Growth
Sustained Teraflops
1000
100
10
1
0.1
0.01
0.001
0.0001
1E-05
1978
1983
1988
1993
1998
2003
2008
2013
2018
Cray 1A
Cray X-MP/22
Cray X-MP/48
Cray Y-MP/8
Cray C90/12
Cray C90/16
Fujitsu VPP700/46
Fujitsu VPP700/116
Fujitsu VPP5000/38
Fujitsu VPP5000/100
IBM Power4 690
IBM Power4+ 690
IBM Power5+ 575
IBM Power6 575
IBM Power7 775
Cray XC30

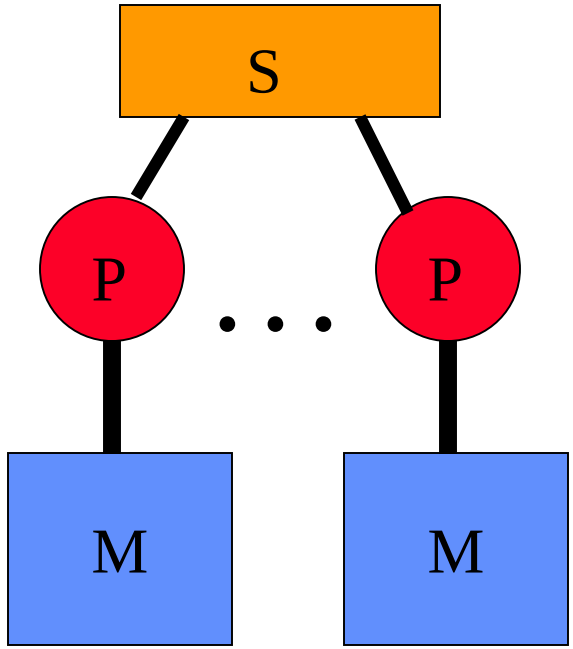

Sustained Exaflop in 2033 ?
Sustained Teraflops
1000000
100000
10000
1000
100
10
1
0.1
0.01
0.001
0.0001
1E-05
1978
1983
1988
1993
1998
2003
2008
2013
2018
2023
2028
2033
2038
Cray 1A
Cray X-MP/22
Cray X-MP/48
Cray Y-MP/8
Cray C90/12
Cray C90/16
Fujitsu VPP700/46
Fujitsu VPP700/116
Fujitsu VPP5000/38
Fujitsu VPP5000/100
IBM Power4 690
IBM Power4+ 690
IBM Power5+ 575
IBM Power6 575
IBM Power7 775
Cray XC30

Types of Parallel Computer

P=Processor
M=Memory
S=Switch



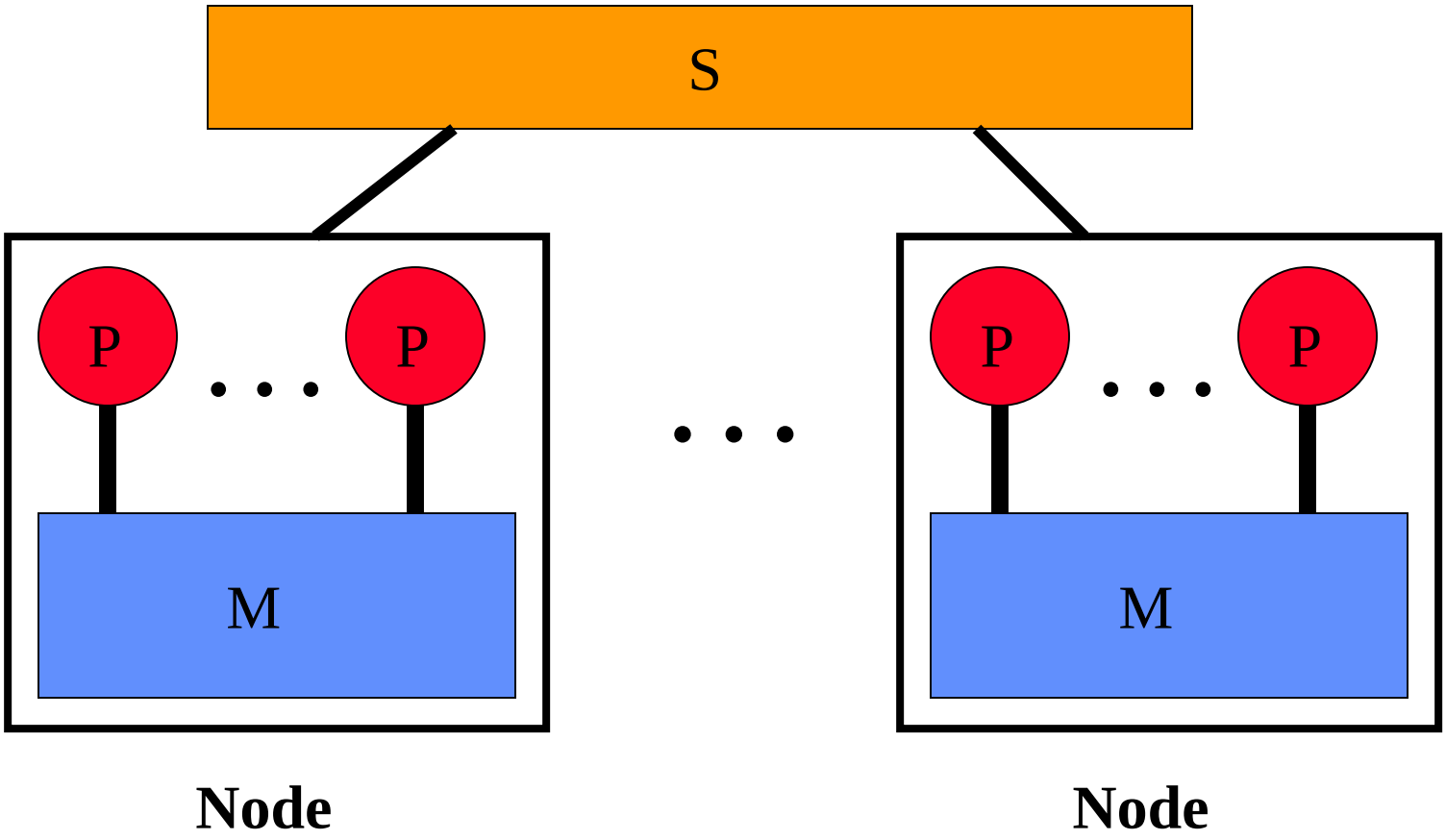
Shared Memory



Distributed Memory

IBM/CRAY Cluster
(Distributed + Shared memory)

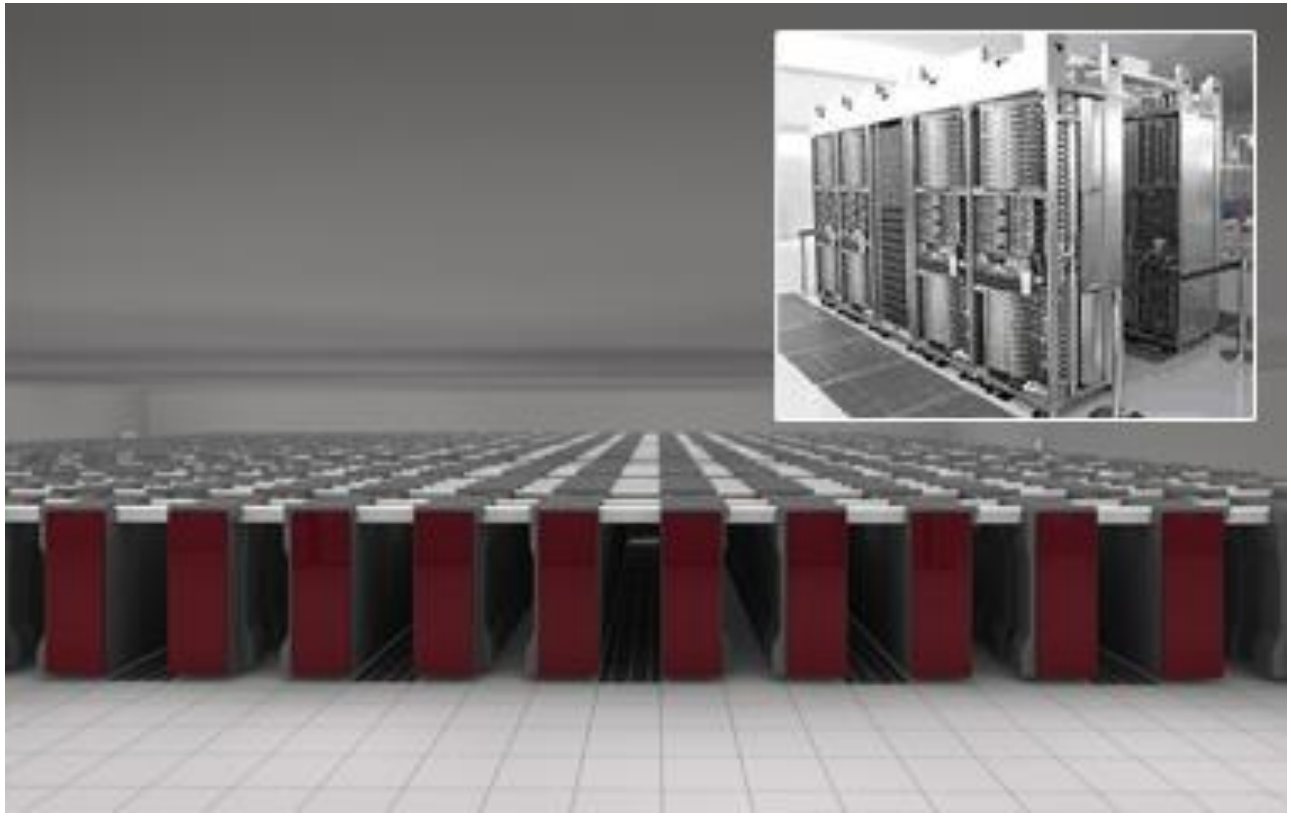
P=Processor
M=Memory
S=Switch



CRAY XC-30 clusters at ECMWF

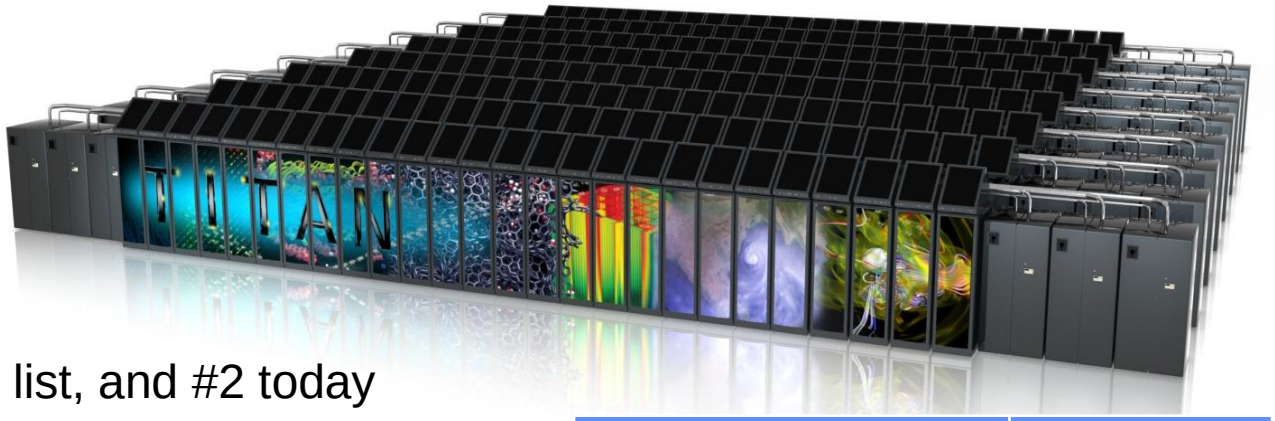
One of the TWO identical XC-30 clusters

…and one the world's fastest (#4) and largest supercomputers – Fujitsu K computer



705,024 Sparc64 processor cores

ORNL's "Titan" System



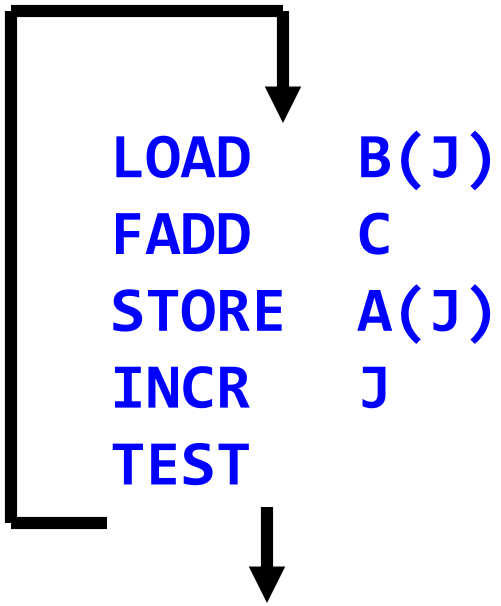
- #1 in Nov 2012 Top500 list, and #2 today
- 7.5X peak perf. of ECMWF's CRAY XC-30 clusters (CCA+CCB=3.6 Petaflops peak)
- Gemini interconnect
  - 3-D Torus
  - Globally addressable memory
- AMD Interlagos cores (16 cores per node)
- Accelerated node design using NVIDIA K20 "Kepler" GPUs
- 600 TB DDR3 mem. + 88 TB GDDR5 mem

Titan Specs	
Compute Nodes	18,688
Login & I/O Nodes	512
Memory per node	32 GB + 6 GB
# of NVIDIA K20 "Kepler" processors	14,592
Total System Memory	688 TB
Total System Peak Performance	27 Petaflops

Source (edited): *James J. Hack, Director,* Oak Ridge National Laboratory

Types of Processor

```
DO J=1,1000
  A(J)=B(J) + C
ENDDO
```



SCALAR PROCESSOR

Single instruction processes one element

```
LOADV   B->V1
FADDV   V1,C->V2
STOREV  V2->A
```

VECTOR PROCESSOR

Single instruction processes many elements

The TOP500 project

- started in 1993
- Top 500 sites reported
- Report produced twice a year
  - EUROPE in JUNE (ISC15)
  - USA in NOV (SC14)
- Performance based on LINPACK benchmark
  - dominated by matrix multiply (DGEMM)
- High performance conjugate gradient (HPCG) benchmark announced at SC13
- http://www.top500.org/

Top500: SC14 top 6 systems

RANK	SITE	SYSTEM	CORES	RMAX (TFLOP/S)	RPEAK (TFLOP/S)	POWER (KW)
1	National Super Computer Center in Guangzhou China	**Tianhe-2 (MilkyWay-2)** - TH-IVB-FEP Cluster, Intel Xeon E5-2692 12C 2.200GHz, TH Express-2, Intel Xeon Phi 31S1P NUDT	3,120,000	33,862.7	54,902.4	17,808
2	DOE/SC/Oak Ridge National Laboratory United States	**Titan** - Cray XK7 , Opteron 6274 16C 2.200GHz, Cray Gemini interconnect, NVIDIA K20x Cray Inc.	560,640	17,590.0	27,112.5	8,209
3	DOE/NNSA/LLNL United States	**Sequoia** - BlueGene/Q, Power BQC 16C 1.60 GHz, Custom IBM	1,572,864	17,173.2	20,132.7	7,890
4	RIKEN Advanced Institute for Computational Science (AICS) Japan	K computer, SPARC64 VIIIfx 2.0GHz, Tofu interconnect Fujitsu	705,024	10,510.0	11,280.4	12,660
5	DOE/SC/Argonne National Laboratory United States	**Mira** - BlueGene/Q, Power BQC 16C 1.60GHz, Custom IBM	786,432	8,586.6	10,066.3	3,945
6	Swiss National Supercomputing Centre (CSCS) Switzerland	**Piz Daint** - Cray XC30, Xeon E5-2670 8C 2.600GHz, Aries interconnect , NVIDIA K20x Cray Inc.	115,984	6,271.0	7,788.9	2,325

ECMWF in Top 500

TFlops

Rank	Site	Computer/Year Vendor	Cores	R_{max}	R_{peak}	Power
28	ECMWF United Kingdom	Cray XC30, Intel Xeon E5-2697v2 12C 2.7GHz, Aries interconnect Cray Inc.	83,160	1,552.0	1,796.3	
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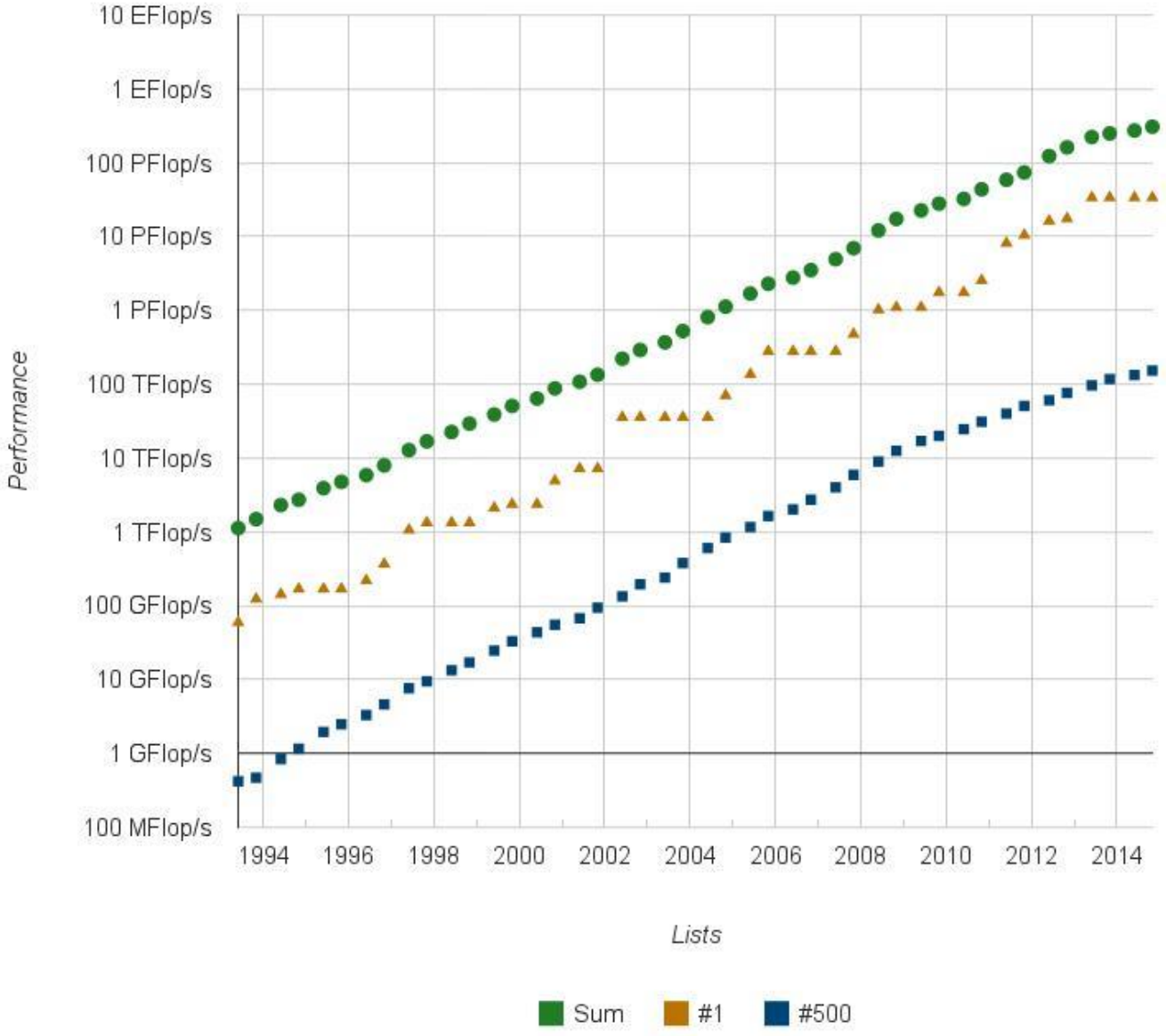
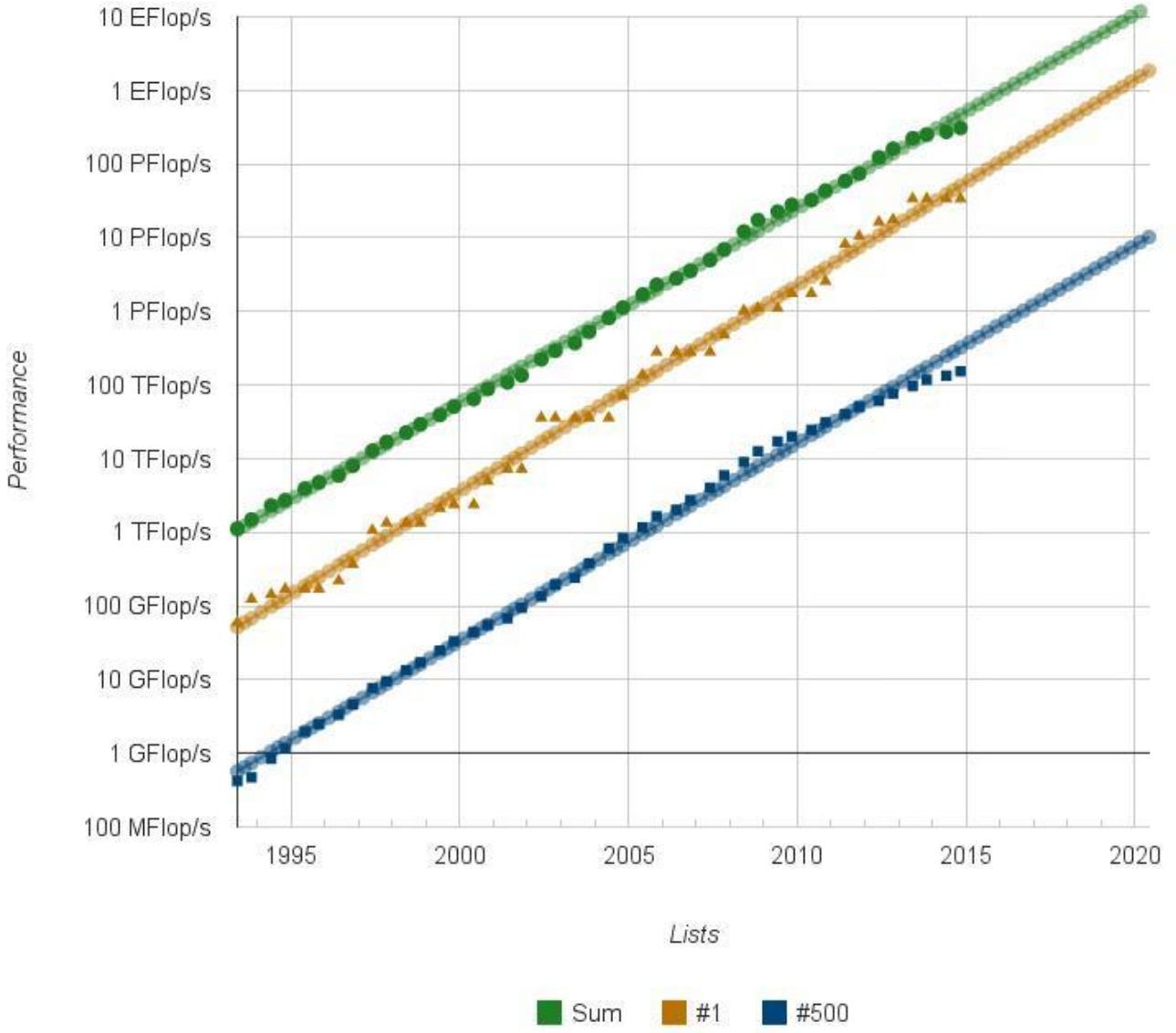
R_{max} – Tflop/sec achieved with LINPACK Benchmark

R_{peak} – Peak Hardware Tflop/sec (that will never be reached!)

Top500: Performance Development



Top500: Projected Performance Development



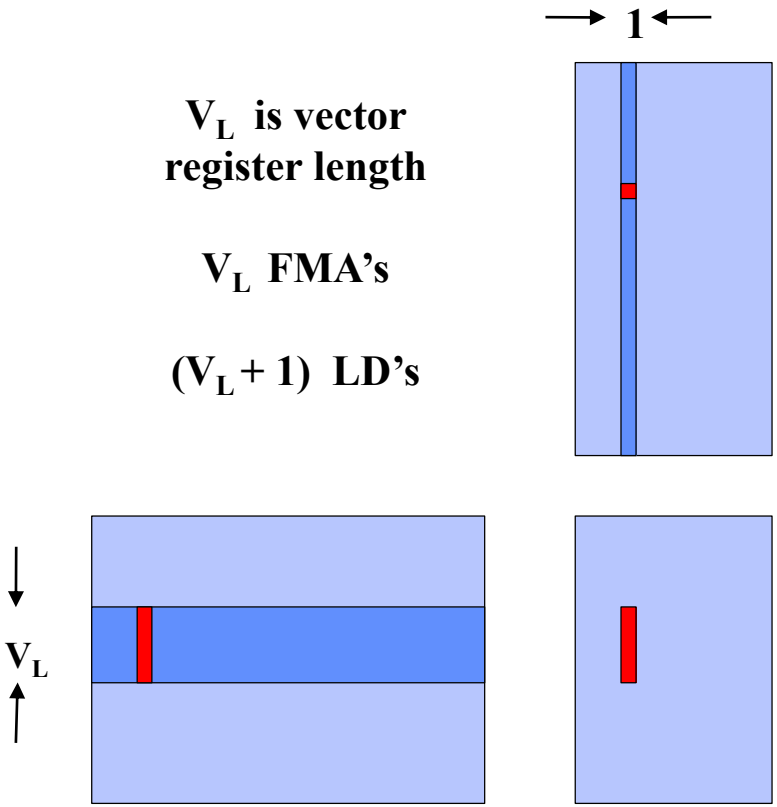
Why is Matrix-Matrix Multiply (DGEMM) so efficient?

VECTOR

V_L is vector register length

V_L FMA's

$(V_L + 1)$ LD's



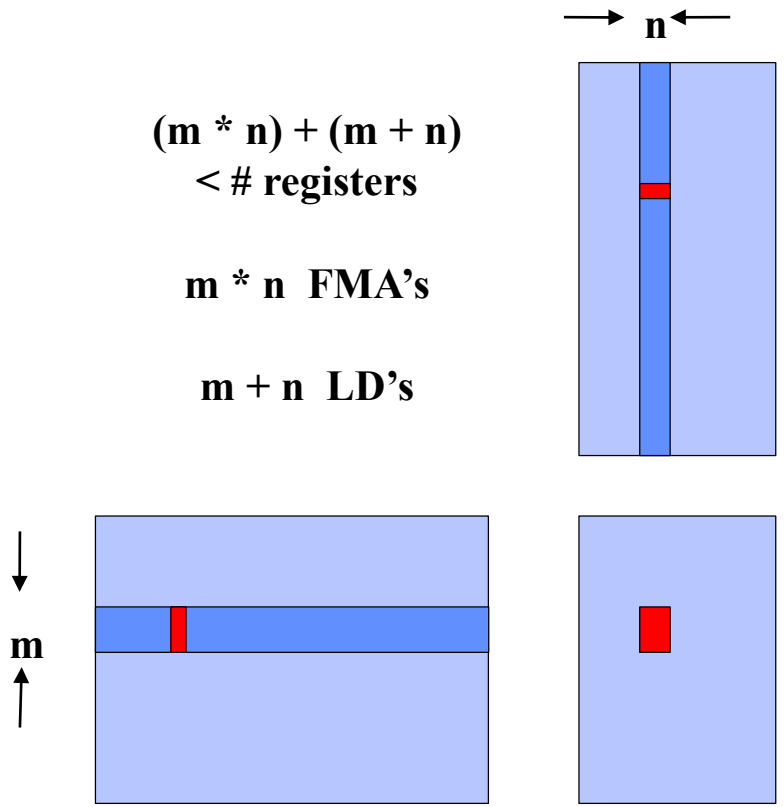
FMA's ~= LD's

SCALAR / CACHE

(m * n) + (m + n) < # registers

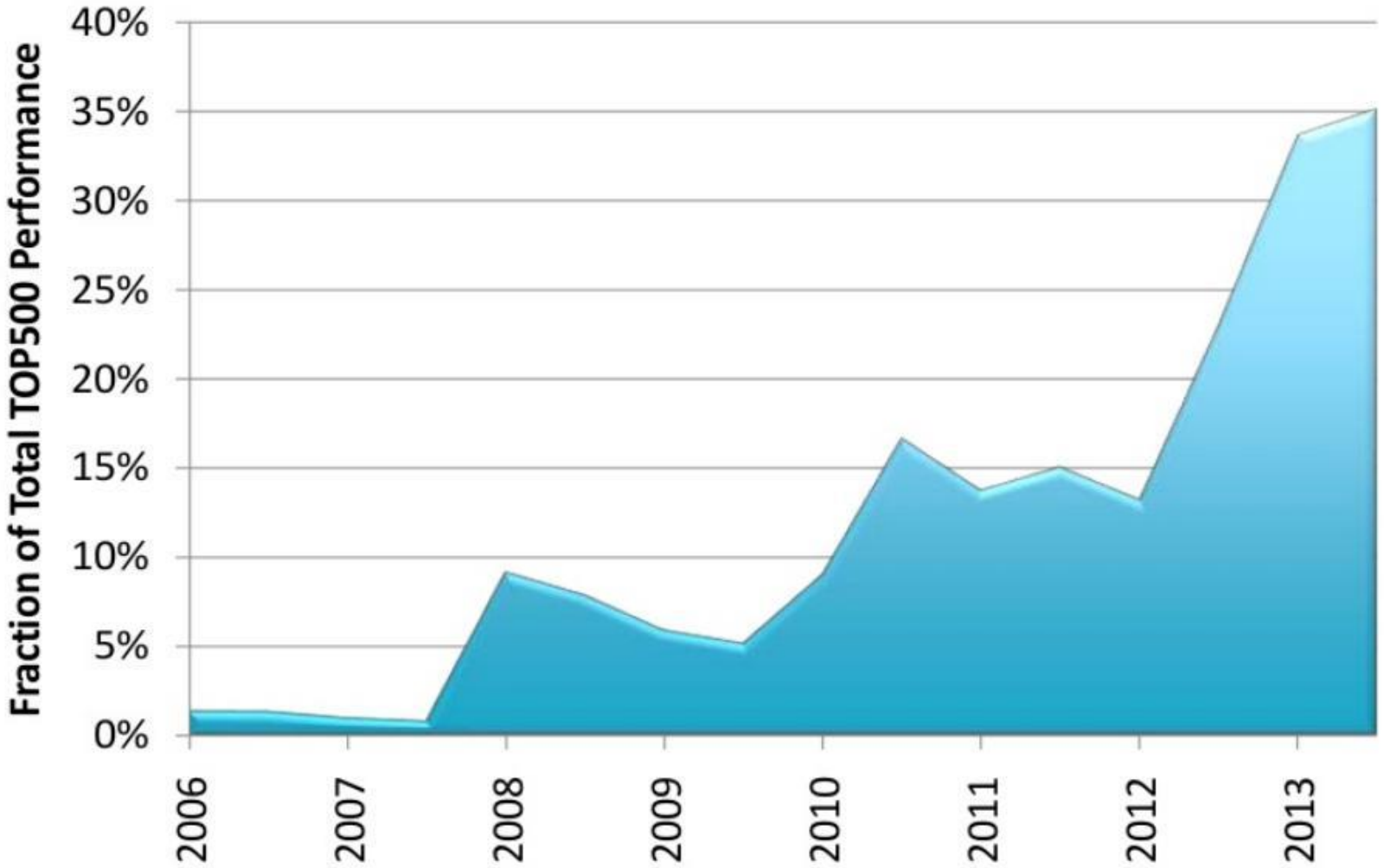
m * n FMA's

m + n LD's

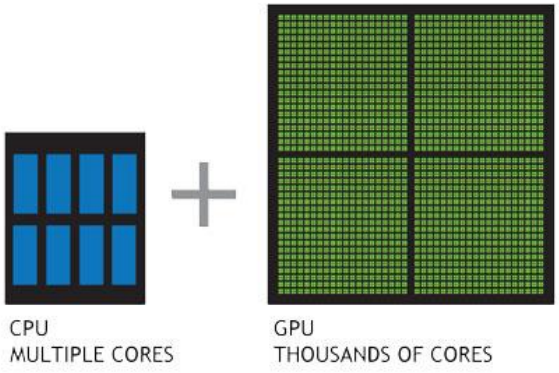


FMA's >> LD's

Performance Share of Accelerators

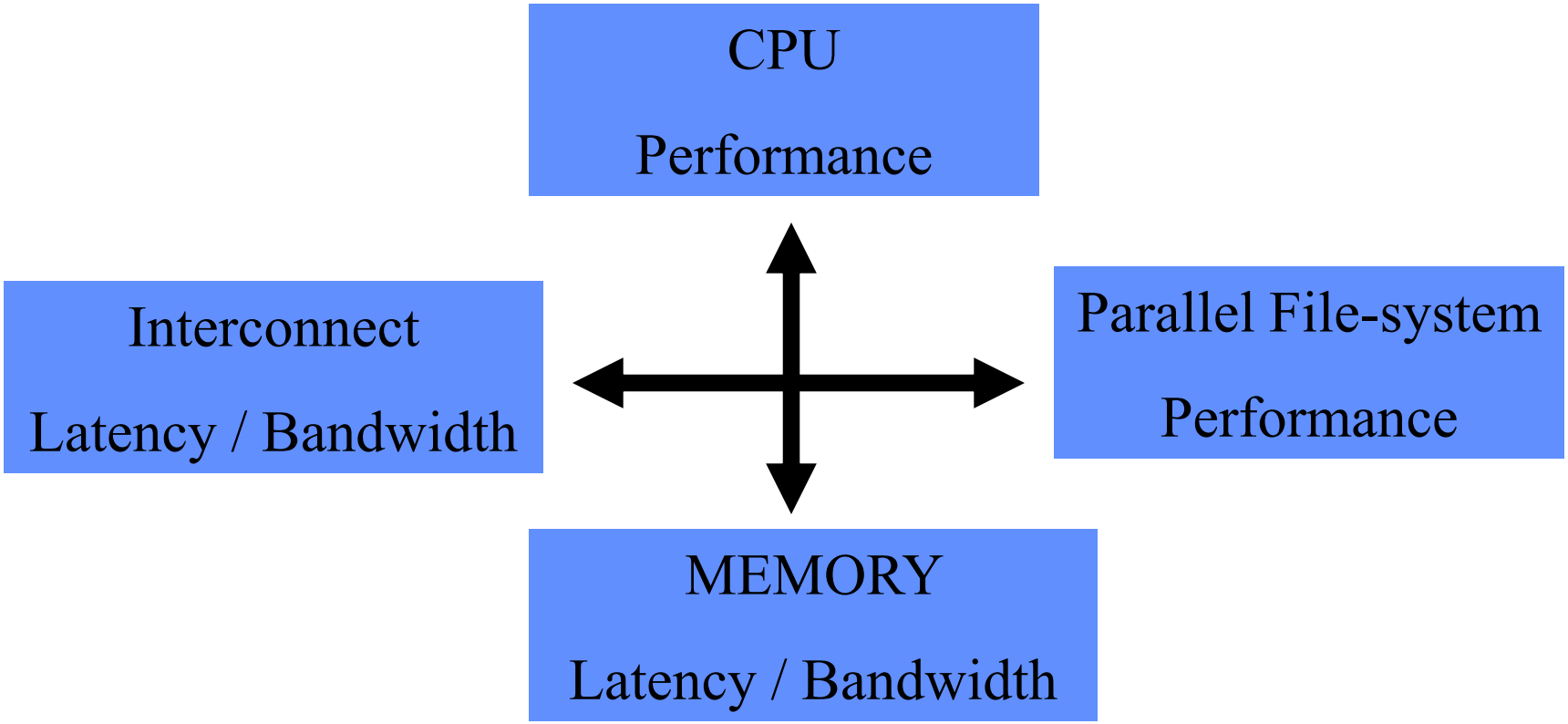


Accelerators



- **GPU – Graphics Processing Unit**
  - **High performance, low power, but 'challenging' to program for large applications, separate memory, GPU/CPU interface (PCIx 8GB/sec)**
  - **Expect GPU technology to be more easily useable on future HPCs**
- **http://gpgpu.org/developer**
- **GPU hardware today mainly supplied by NVIDIA**
- **INTEL (Xeon Phi, aka "MIC")**
  - **"Knights Corner" requires CPU host (via PCIx connector)**
  - **"Knights Landing" available 2016, does not require CPU host**

Key Architectural Features of a Supercomputer



"a balancing act to achieve good sustained performance"

Challenges in parallel computing

- **Parallel Computers**
  - **Have ever increasing processors, memory, performance, but**
  - **Need more space (new computer halls = $)**
  - **Need more power (MWs = $)**
- **Parallel computers require/produce a lot of data (I/O)**
  - **Require parallel file systems (GPFS, Lustre) + archive store**
- **Applications need to scale to increasing numbers of processors, problems areas are**
  - **Load imbalance, Serial sections, Global Communications**
- **Debugging parallel applications (totalview, ddt)**
- **We are going to be using more processors in the future!**
- **More cores per socket, little/no clock speed improvements**

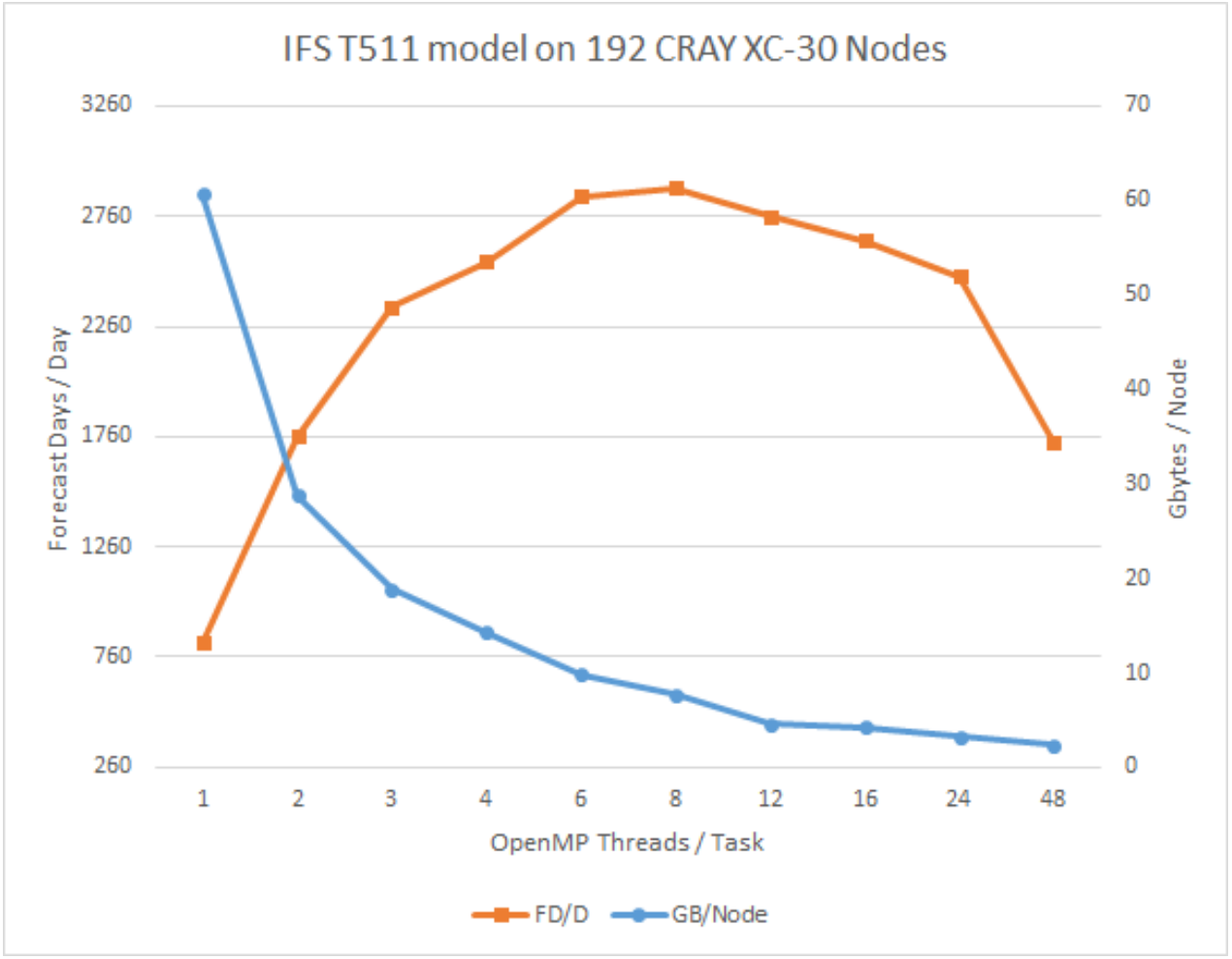
Parallel Programming Languages

- **OpenMP**
  - **directive based (www.openmp.org)**
  - **support for Fortran and C/C++**
  - **shared memory programming only**
- **OpenACC**
  - **directive based (www.openacc.org)**
  - **support for Fortran and C**
  - **GPU programming (e.g. NVIDIA)**
- **PGAS (Partitioned Global Address Space)**
  - **UPC, Fortran 2008 Coarrays**
  - **One programming model for inter and intra node parallelism**
  - **One-sided communication**

OpenMP example

```
!$OMP PARALLEL DO SCHEDULE(STATIC,1)&
!$OMP& PRIVATE(JMLOCF,IM,ISTA,IEND)
      DO JMLOCF=NPTRMF(MYSETN),NPTRMF(MYSETN+1)-1
        IM=MYMS(JMLOCF)
        ISTA=NSPSTAF(IM)
        IEND=ISTA+2*(NSMAX+1-IM)-1
        CALL SPCSI(CDCONF,IM,ISTA,IEND,LLONEM,ISPEC2V,&
         &ZSPVORG,ZSPDIVG,ZSPTG,ZSPSPG)
      ENDDO
!$OMP END PARALLEL DO
```

Why OpenMP? Ans: For performance and memory



Testing combinations 9216Tx1t, 4608Tx2t, 3072Tx3t, 1536Tx6t, 768Tx12t, 384Tx24t and 192Tx48t

OpenACC example

```
!$acc parallel loop copyin(dt,rmass), &
!$acc private(i,j), present(pos,vel,f,a,np,nd)
do i = 1,np
  do j = 1,nd
    pos(j,i) = pos(j,i) + vel(j,i)*dt + 0.5*dt*dt*a(j,i)
    vel(j,i) = vel(j,i) + 0.5*dt*(f(j,i)*rmass + a(j,i))
    a(j,i) = f(j,i)*rmass
  enddo
enddo
!$acc end parallel loop
```

http://www.ecmwf.int/sites/default/files/HPC-WS-Mozdzynski.pdf

Link includes results of a port of IFS spectral transform kernel to GPU using OpenACC

Fortran2008 coarray (PGAS) example

```
!$OMP PARALLEL DO SCHEDULE(DYNAMIC,1) PRIVATE(JM,IM,JW,IPE,ILEN,ILENS,IOFFS,IOFFR)
DO JM=1,D%NUMP
  IM = D%MYMS(JM)
  CALL LTINV(IM,JM,KF_OUT_LT,KF_UV,KF_SCALARS,KF_SCDERS,ILEI2,IDIM1,&
    & PSPVOR,PSPDIV,PSPSCALAR ,&
    & PSPSC3A,PSPSC3B,PSPSC2 , &
    & KFLDPTRUV,KFLDPTRSC,FSPGL_PROC)
  DO JW=1,NPRTRW
    CALL SET2PE(IPE,0,0,JW,MYSETV)
    ILEN = D%NLEN_M(JW,1,JM)*IFIELD
    IF( ILEN > 0 )THEN
      IOFFS = (D%NSTAGT0B(JW)+D%NOFF_M(JW,1,JM))*IFIELD
      IOFFR = (D%NSTAGT0BW(JW,MYSETW)+D%NOFF_M(JW,1,JM))*IFIELD
      FOUBUF_C(IOFFR+1:IOFFR+ILEN)[IPE]=FOUBUF_IN(IOFFS+1:IOFFS+ILEN)
    ENDIF
    ILENS = D%NLEN_M(JW,2,JM)*IFIELD
    IF( ILENS > 0 )THEN
      IOFFS = (D%NSTAGT0B(JW)+D%NOFF_M(JW,2,JM))*IFIELD
      IOFFR = (D%NSTAGT0BW(JW,MYSETW)+D%NOFF_M(JW,2,JM))*IFIELD
      FOUBUF_C(IOFFR+1:IOFFR+ILENS)[IPE]=FOUBUF_IN(IOFFS+1:IOFFS+ILENS)
    ENDIF
  ENDDO
ENDDO
!$OMP END PARALLEL DO
SYNC IMAGES(D%NMYSETW)
FOUBUF(1:IBLEN)=FOUBUF_C(1:IBLEN)[MYPROC]
```

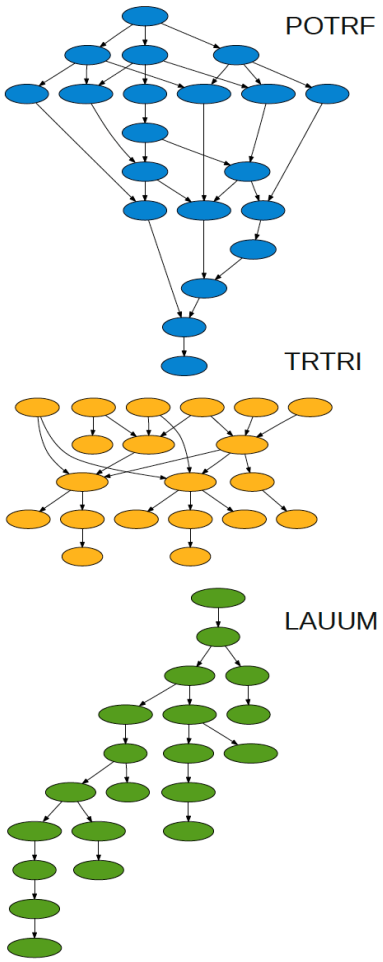
Parallel Programming Libraries

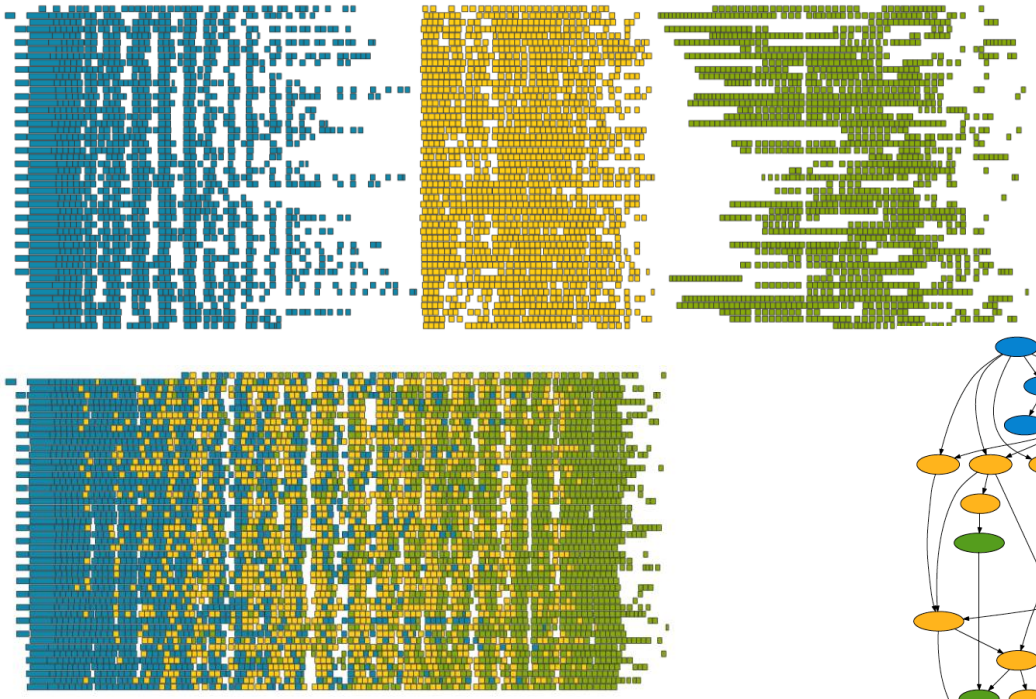
- **MPI**
  - **Most widely used since mid-90's (www.mpi-forum.org)**
  - **MPI-3.0 standard is 852 pages!**
  - **MPI-2.2 is the default MPI on most systems**
  - **Most users will use a small subset of MPI facilities**
  - **Use collectives (e.g. MPI_alltoallv) and non-blocking calls for performance**
  - **MPI-only application scaling issues?**
- **GASPI/GPI**
  - **PGAS one-sided programming (www.gpi-site.com/gpi2)**
  - **Interoperable with MPI**

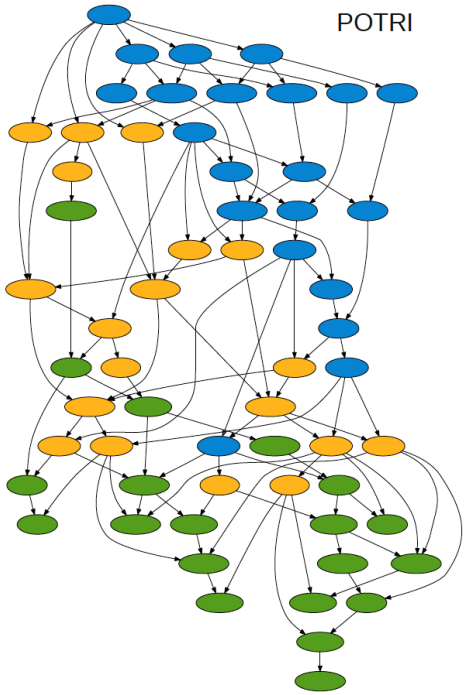
Parallel Programmers use…

- **Fortran, C/C++ with MPI for communicating between tasks**
  - **works for applications running on shared and distributed memory systems**
- **Fortran, C/C++ with OpenMP**
  - **For applications that need performance that is satisfied by a single node (shared memory)**
- **Hybrid combination of MPI/OpenMP**
  - **ECMWF's IFS uses this approach (over 15 years now)**
- **Hybrid combination of MPI/OpenACC (for GPU)**
  - **Meteo-Swiss have ported COSMO to NVIDIA GPU**
- **Early years for DAGs (e.g. MPI + OmpSs)**

DAG example: Cholesky Inversion







DAG = Directed Acyclic Graph

Can IFS use this technology?

Source: Stan Tomov, ICL, University of Tennessee, Knoxville

Topics in Parallel Computing …

Cache, Cache line

Domain decomposition

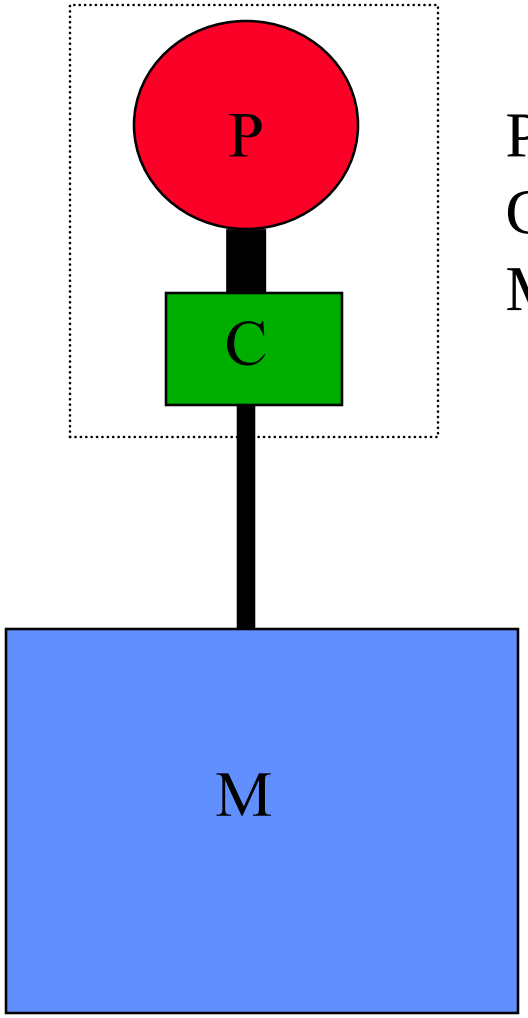
Halo, halo exchange

Load imbalance

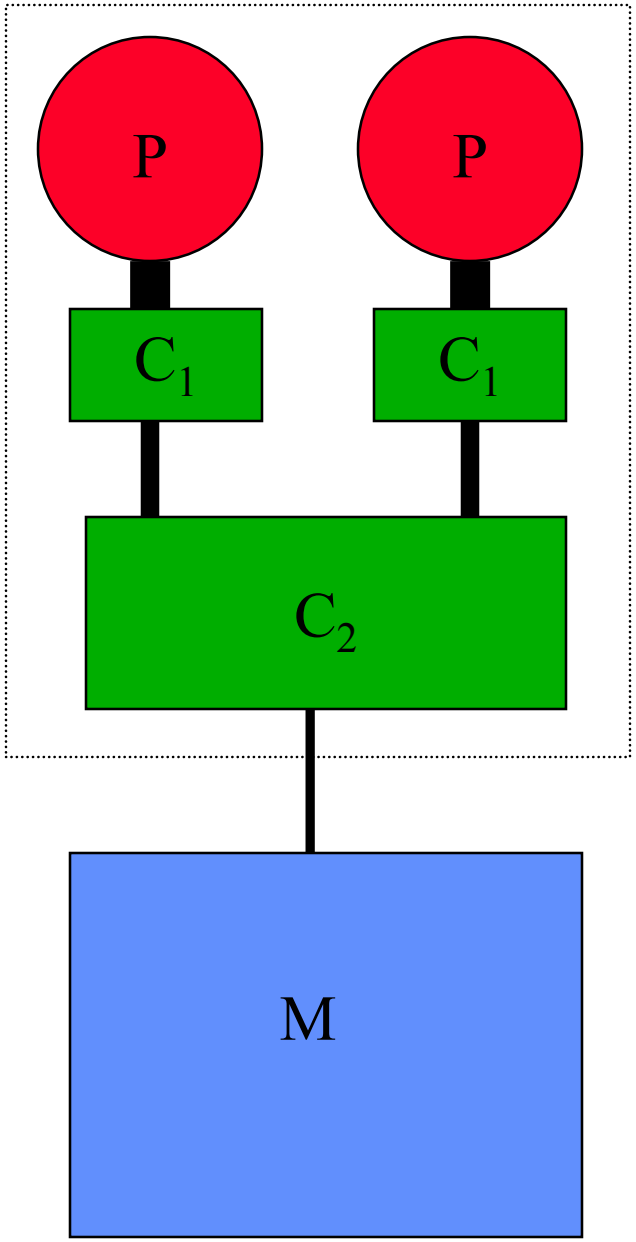
Synchronization

Barrier

Cache



P=Processor
C=Cache
M=Memory



Cache on scalar systems

- **Processors are 100's of cycles away from Memory**
- **Cache is a small (and fast) memory closer to processor**
- **Cache line typically 128 bytes**
- **Good for cache performance**
  - **Single stride access is always the best**
  - **Over inner loop leftmost index (fortran)**

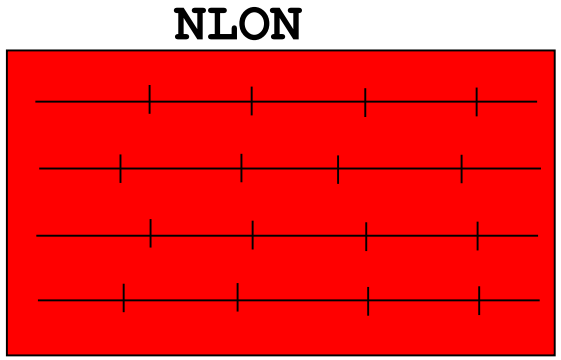
BETTER

```
DO J=1,N
  DO I=1,M
    A(I,J)= . . .
  ENDDO
ENDDO
```

WORSE

```
DO J=1,N
  DO I=1,M
    A(J,I)= . . .
  ENDDO
ENDDO
```

IFS Grid-Point Calculations (cache blocking example)



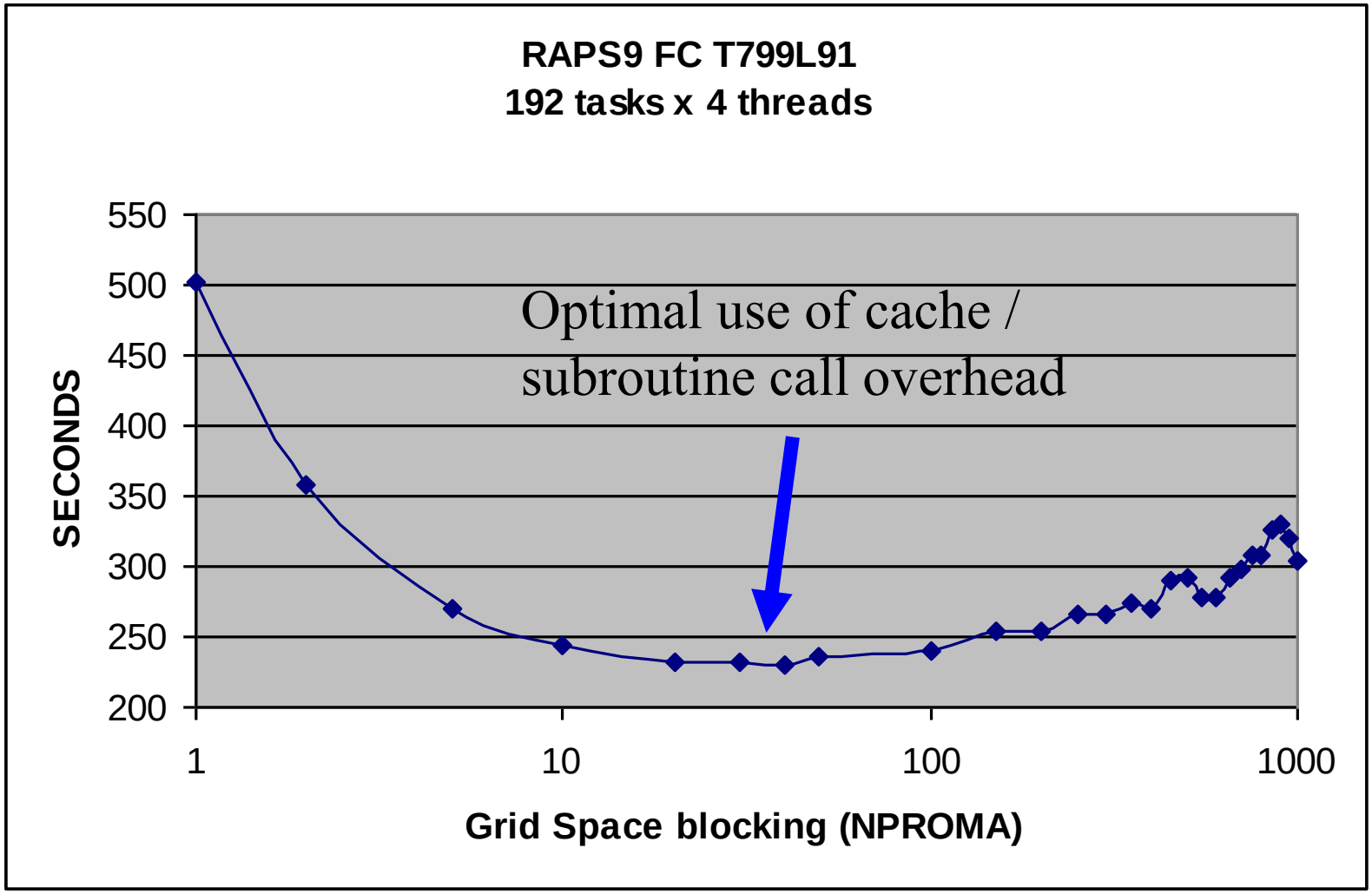

```
U(NGPTOT,NLEV)

NGPTOT = NLAT * NLON
NLEV = vertical levels
```

```
DO J=1, NGPTOT, NPROMA
  CALL GP_CALCS
ENDDO
```

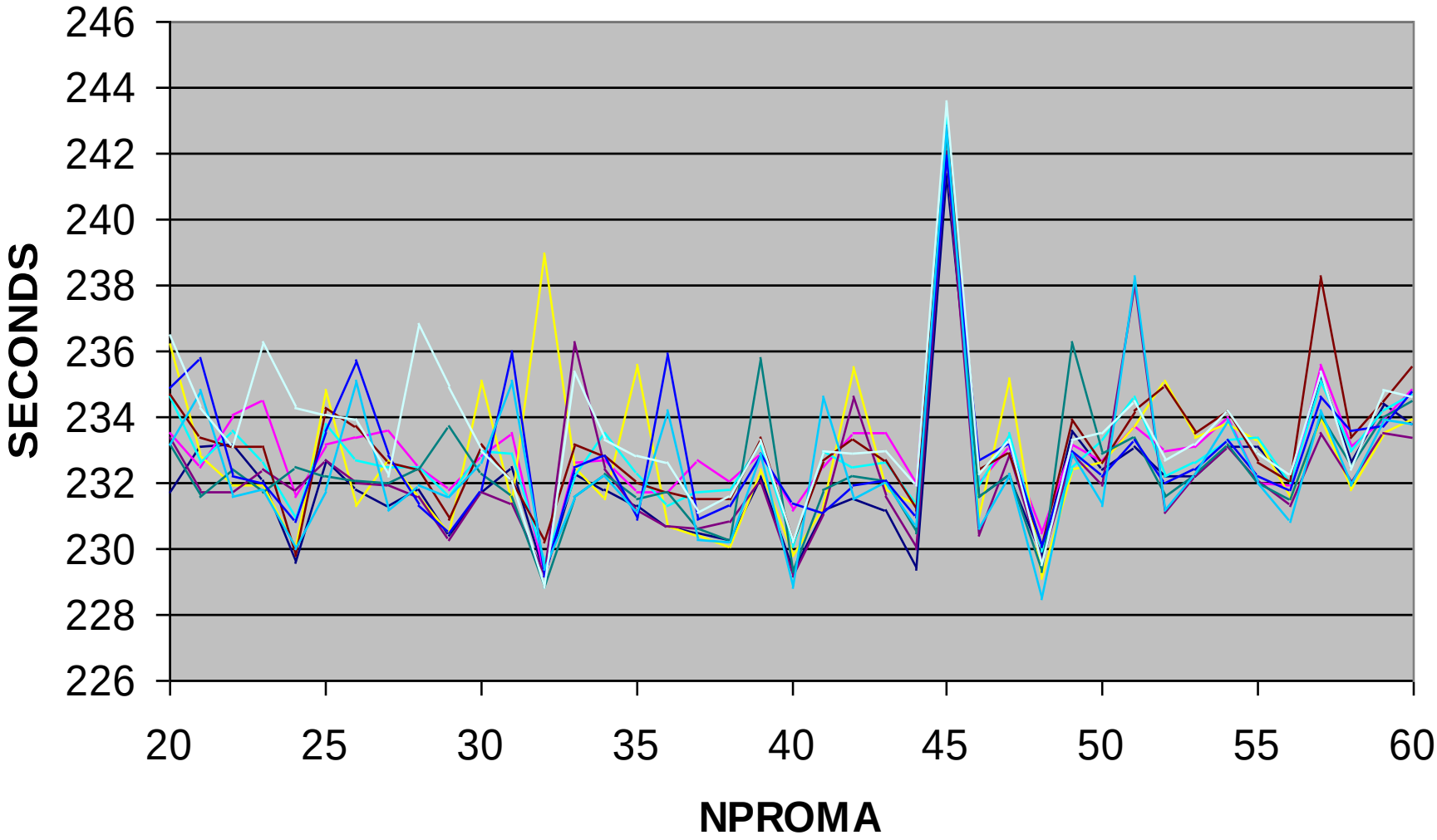
Lots of work
Independent for each J

```
SUB GP_CALCS

DO I=1,NPROMA
ENDDO

END
```

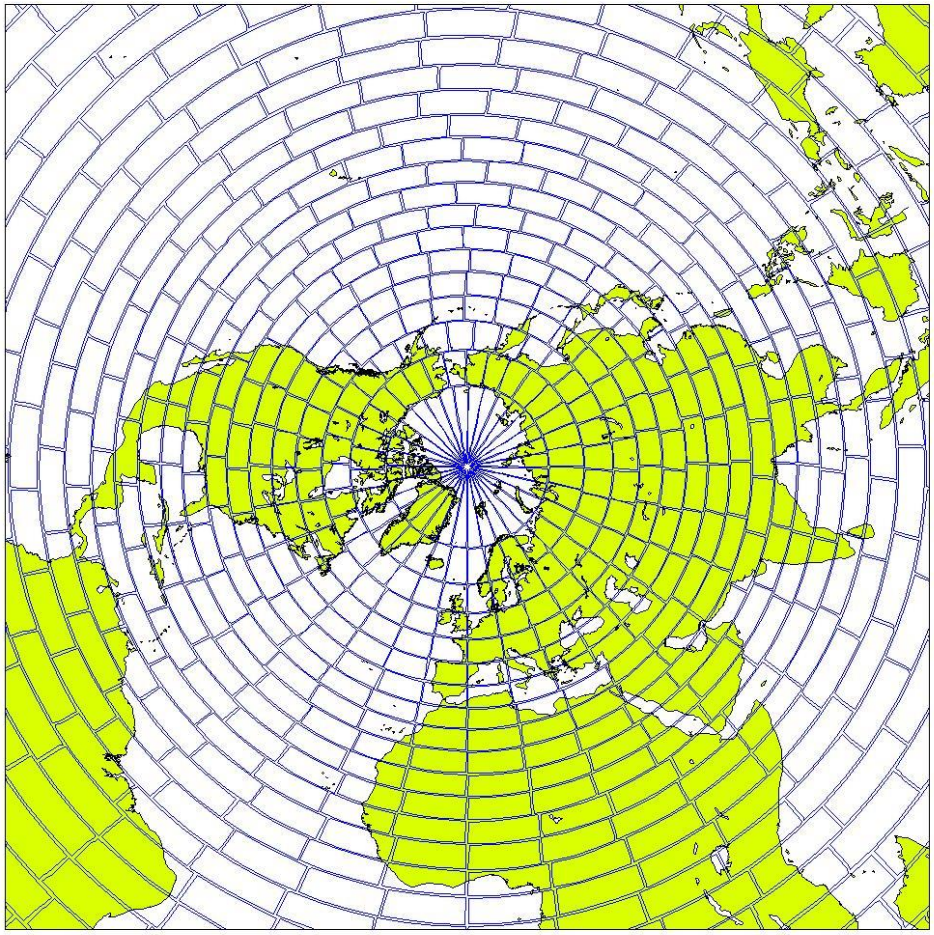
Grid point space blocking for Cache



T799 FC 192x4 (10 runs)

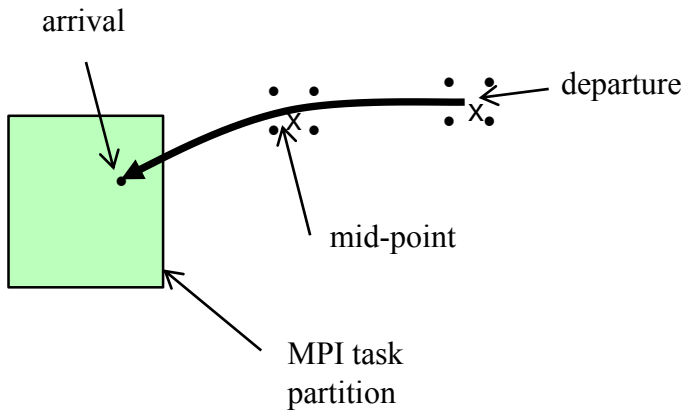


T_L799 1024 tasks 2D partitioning (used in past)



2D partitioning results in non-optimal Semi-Lagrangian comms requirement at poles and equator!

Square shaped partitions are better than rectangular shaped partitions.



eq_regions partitioning algorithm (used in IFS)

FIG. 1.1. *Partition* EQ(2, 33)

where $e(x, y)$ *is the* $\mathbb{R}^{d+1}$ *Euclidean distance* $\|x - y\|$.

The following definitions are specific to the main theorems stated in this paper.

DEFINITION 1.3. *A set* Z *of partitions of* $\mathbb{S}^d$ *is said to be* diameter-bounded *with* diameter bound $K \in \mathbb{R}_+$ *if for all* $P \in Z$, *for each* $R \in P$,

$$\operatorname{diam} R \leqslant K |P|^{-1/d}.$$

DEFINITION 1.4. *The set of recursive zonal equal area partitions of* $\mathbb{S}^d$ *is defined as*

$$\mathrm{EQ}(d) := \{\mathrm{EQ}(d, N) \mid N \in \mathbb{N}_+\}. \tag{1.2}$$

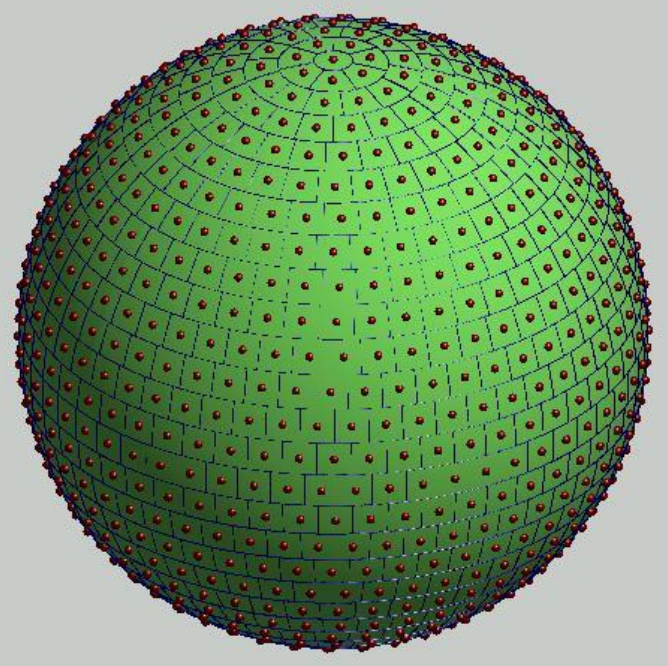
where $\mathrm{EQ}(d, N)$ *denotes the recursive zonal equal area partition of the unit sphere* $\mathbb{S}^d$ *into* N *regions, which is defined via the algorithm given in Section 3.*

This paper claims that the partition defined via the algorithm given in Section 3 is an equal area partition which is diameter bounded. This is formally stated in the following theorems.

THEOREM 1.5. *For* $d \geqslant 1$ *and* $N \geqslant 1$, *the partition* $\mathrm{EQ}(d, N)$ *is an equal area partition of* $\mathbb{S}^d$.

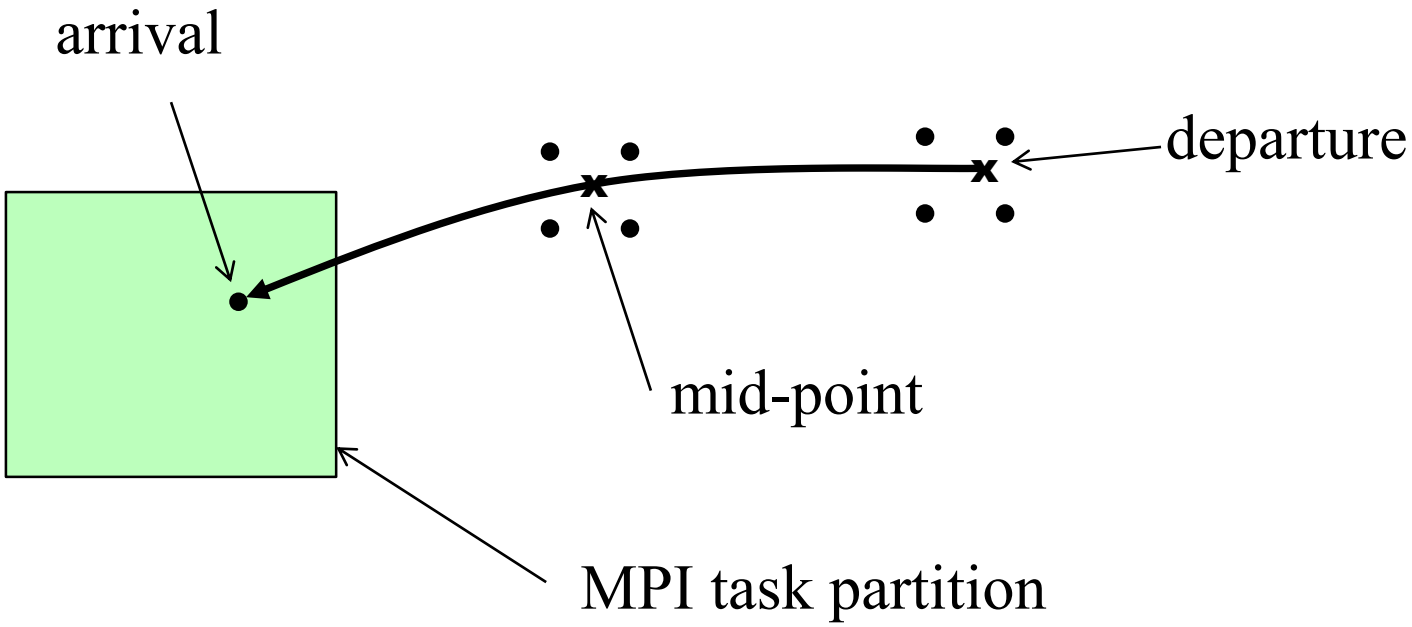
THEOREM 1.6. *For* $d \geqslant 1$, $\mathrm{EQ}(d)$ *is diameter-bounded in the sense of Definition 1.3.*

Recursive zonal equal area partition of S^2 into 1024 regions, showing the center point of each region.

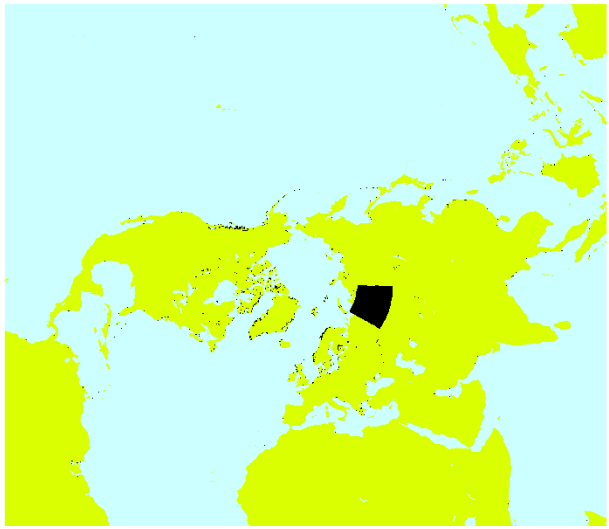


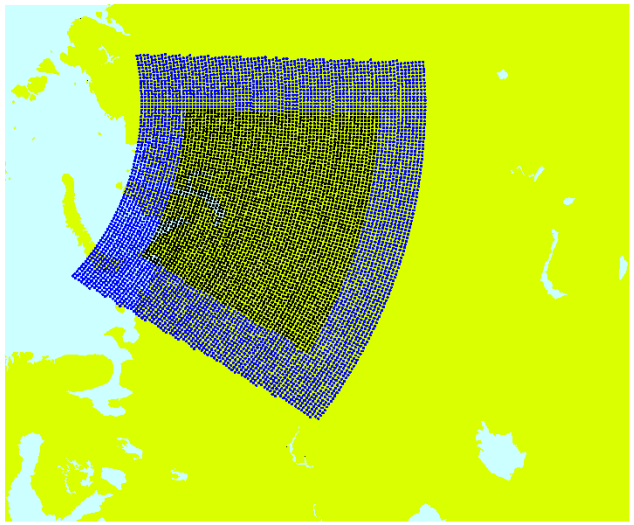
Halo example : IFS Semi-Lagrangian Transport

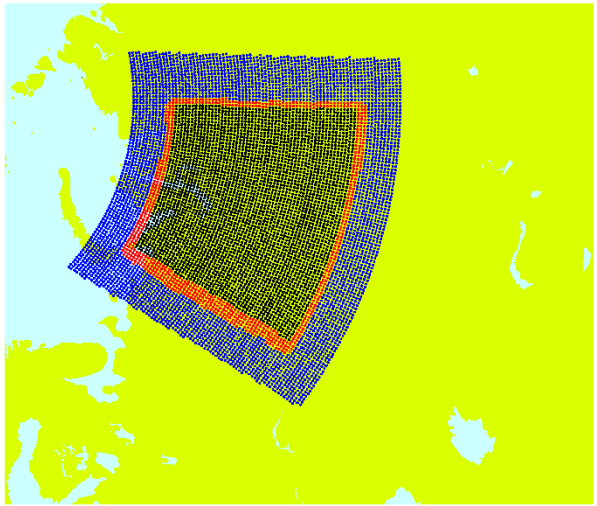
- **Computation of a trajectory from each grid-point backwards in time, and**
- **Interpolation of various quantities at the departure and at the mid-point of the trajectory**

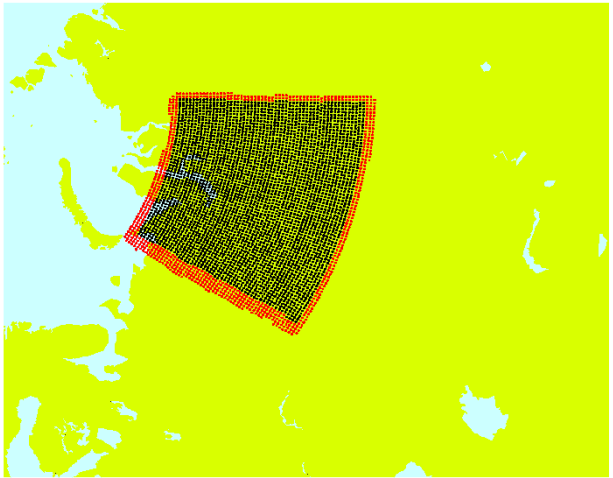


Halo's in IFS (T799 model, 256 tasks, showing task 11)









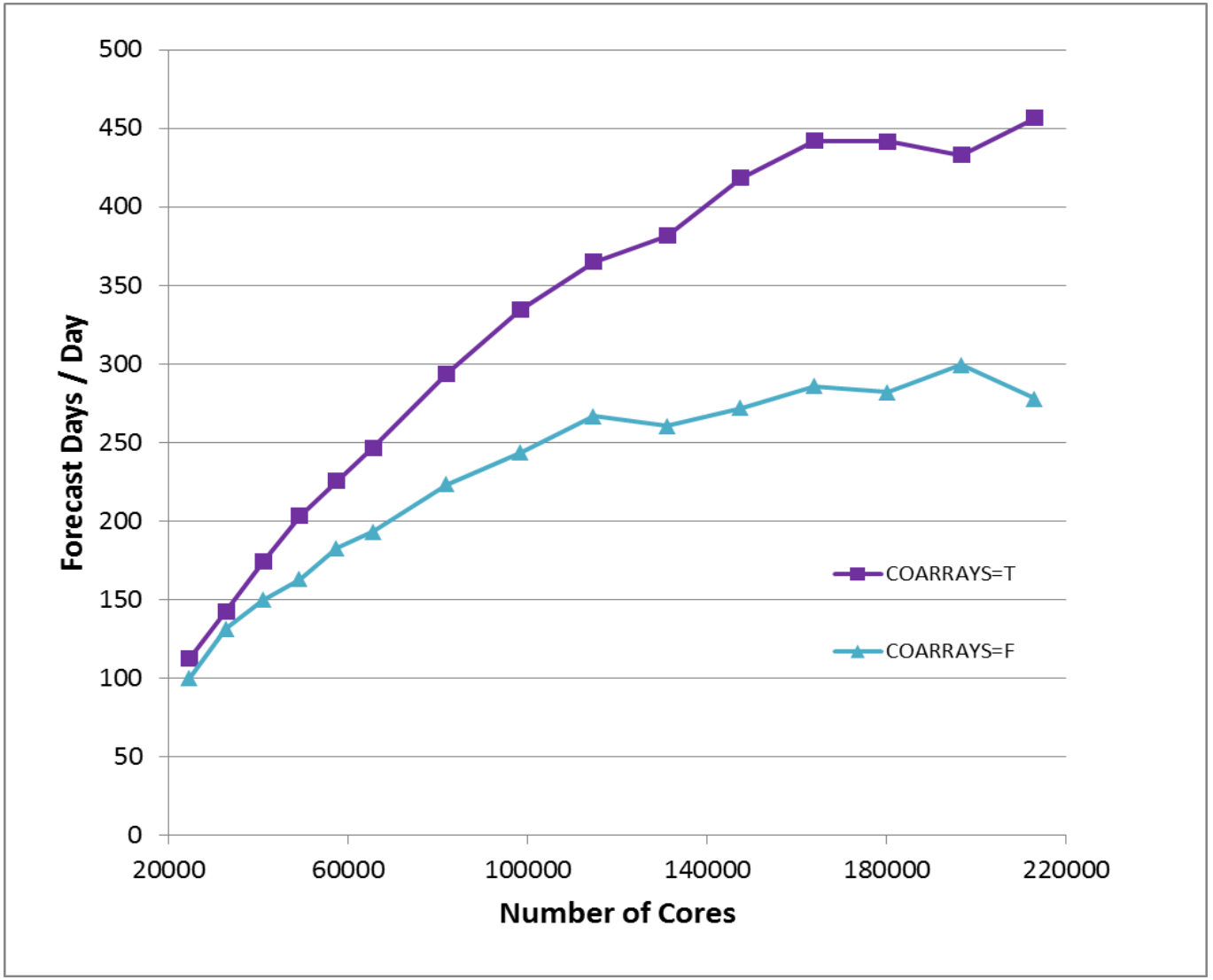
Black – grid points owned by task 11

Blue – halo grid points , max wind x time-step

Red – grid points in halo actually used by task 11

Bottom two graphics
LH – using MPI
RH – using Fortran2008 coarrays (PGAS)

5 km IFS model scaling on TITAN (Fortran2008 coarrays)



Characteristics of codes that will perform well on all parallel computers

- **Computation**
  - **High computational intensity**
  - **Little use of memory bandwidth**
- **Memory**
  - **Locality of reference**
  - **Registers or first level cache**
- **Communication**
  - **Infrequent nearest neighbour or no communication**
- **Input/Output**
  - **Relatively low volume, or**
  - **Parallel implementation (in dedicated nodes)**