

Introduction to Parallel Programming with MPI

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Odds and Ends – what we have left out



What we have left out

- **Point-to-point** bells and whistles
 - Persistent communication (more efficient PtP)
 - Message probing: `MPI_Probe`,... (is there a message waiting?)
 - One-sided communication: `MPI_Put`, `MPI_Get`, `MPI_Accumulate`,... (only one rank necessary to get data across)
 - Partitioned communication (better communication of threads are present)
- **Collectives** bells and whistles
 - `MPI_Reduce_scatter`, `MPI_Scan`, neighborhood collectives, ...
- **MPI I/O** (reading and writing files through MPI, in parallel)
- **Virtual topologies** (make known to MPI who communicates with whom)
- **MPI shared memory** (more efficient intra-node communication)

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Computer Architecture and Performance issues
In MPI programming



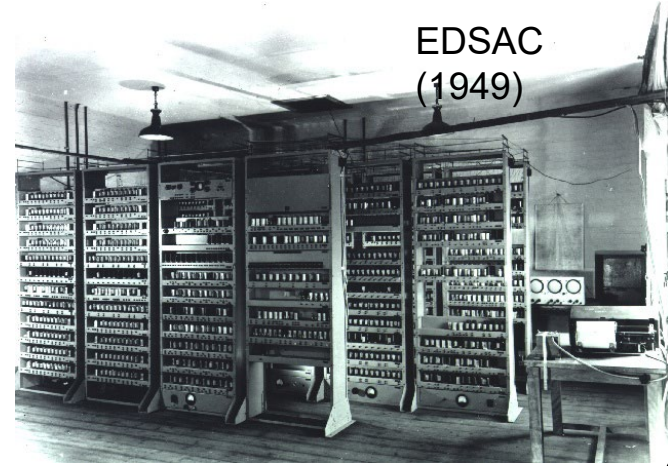
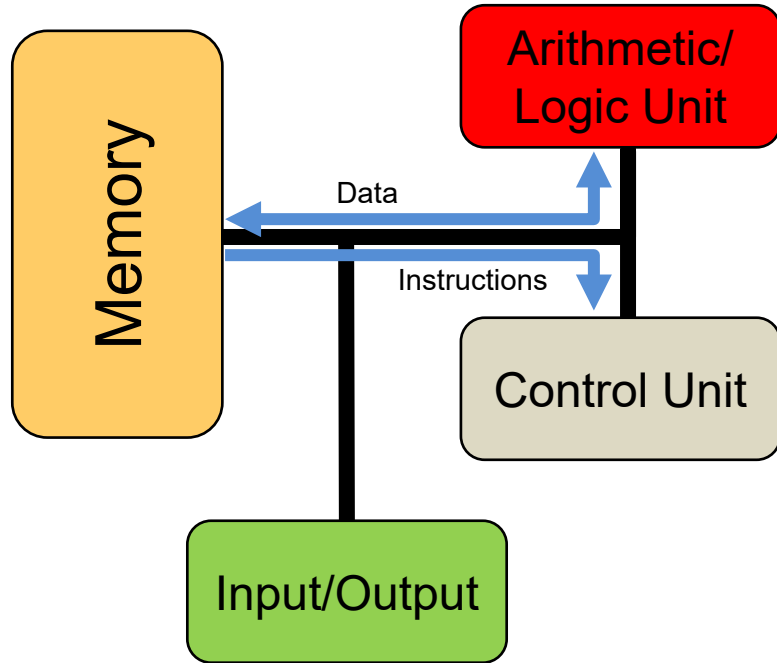
Performance issues – overview

- Basics of parallel computer architecture
- Affinity and pinning
- Simple scaling laws
- Benchmarking and performance assessment
- Tracing tools

Basics of parallel computer architecture



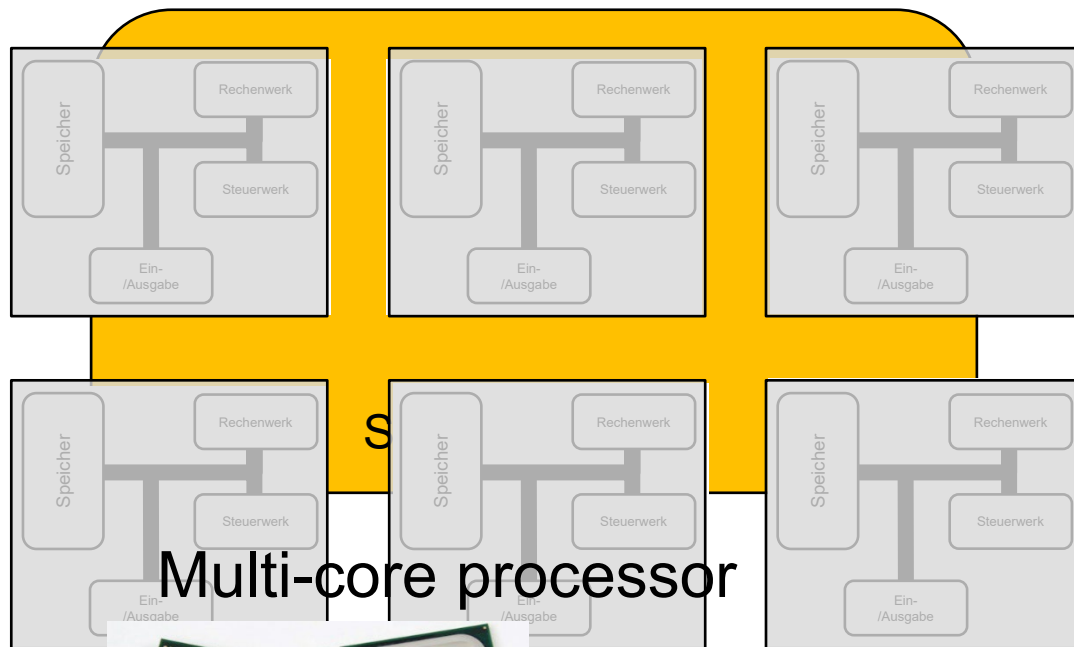
At the core: the stored-program computer



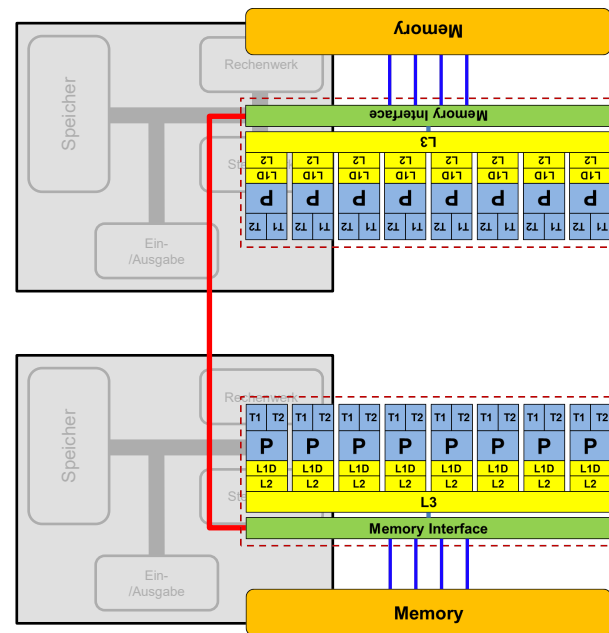
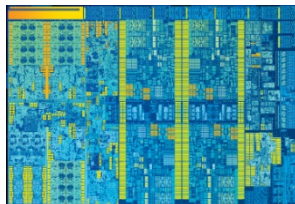
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Shared memory: a single cache-coherent address space

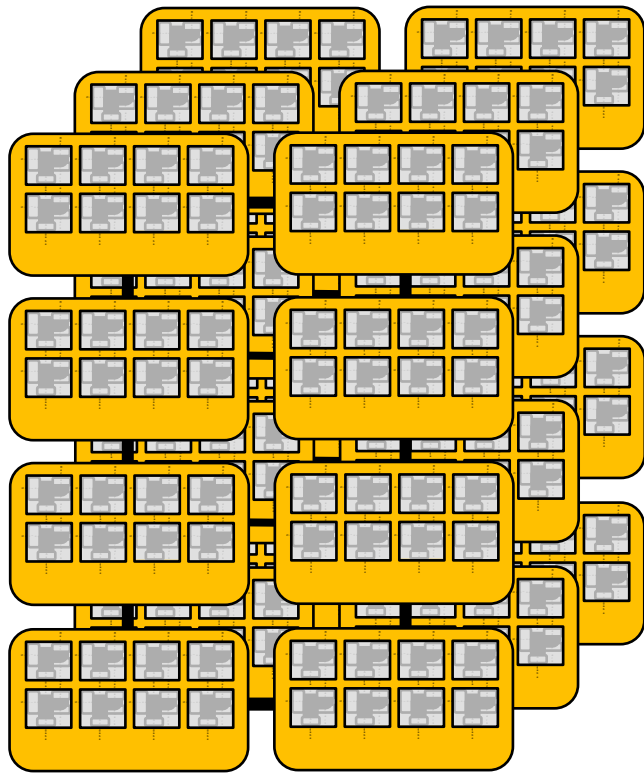


Multi-core processor



Multiple CPU chips per node

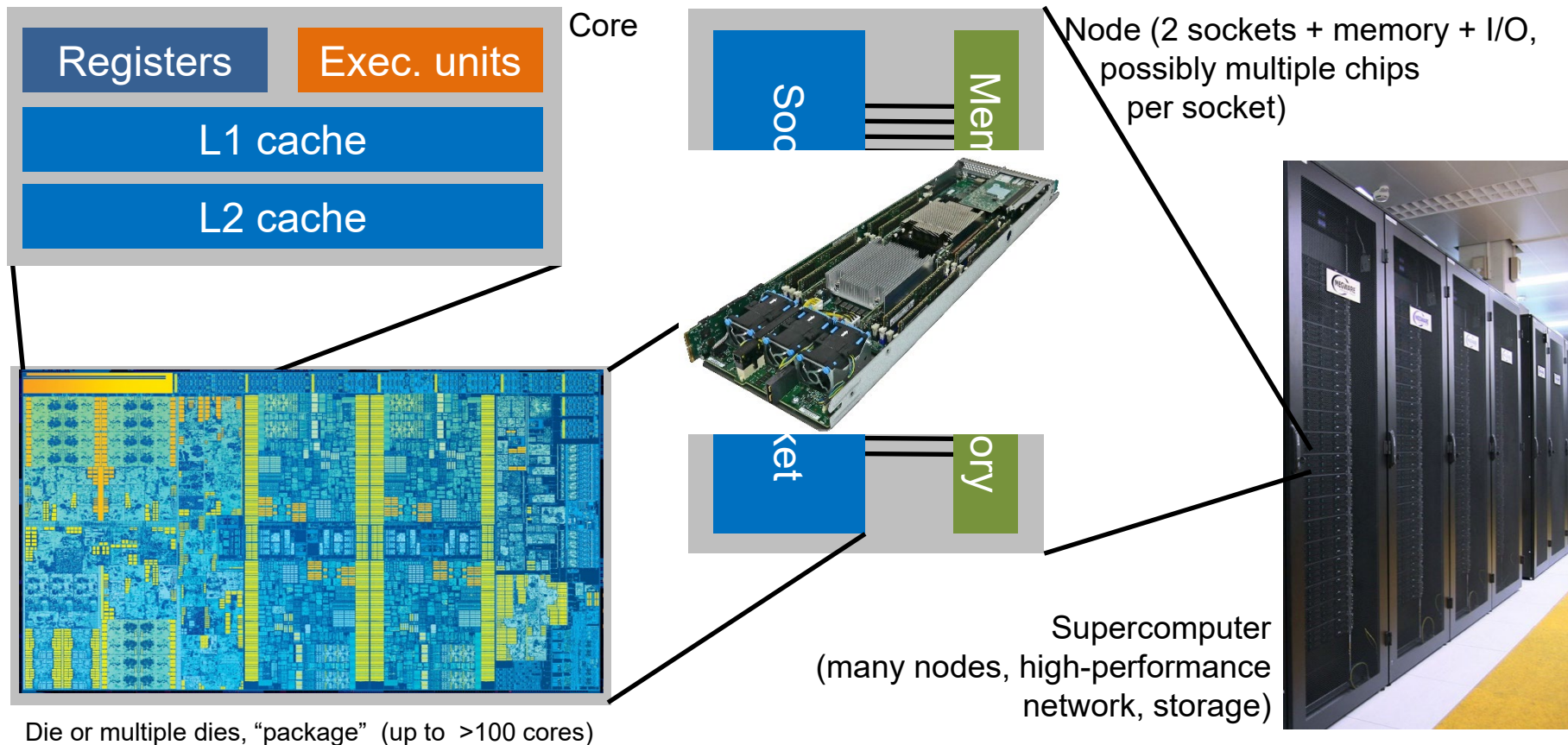
Distributed memory: no cache-coherent single address space



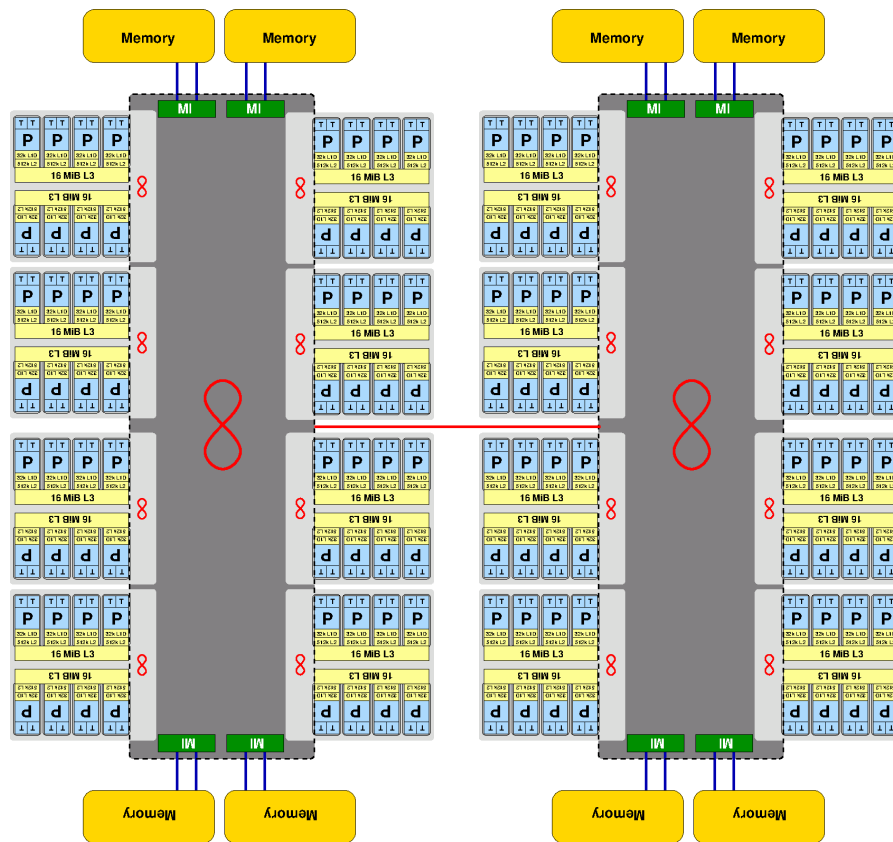
Cluster/
supercomputer

Modern supercomputers are
shared-/distributed-memory hybrids

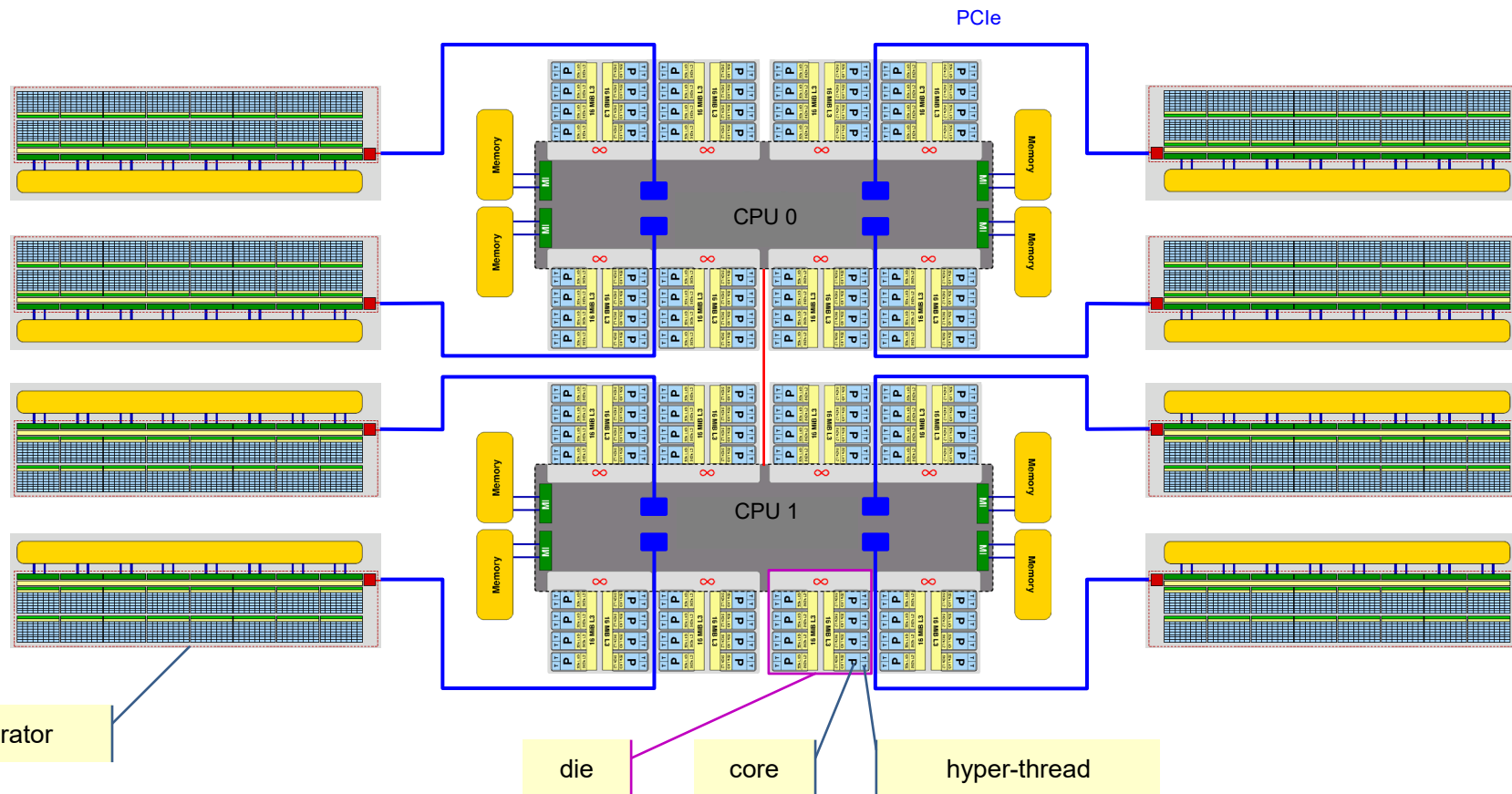
Parallelism in modern computers



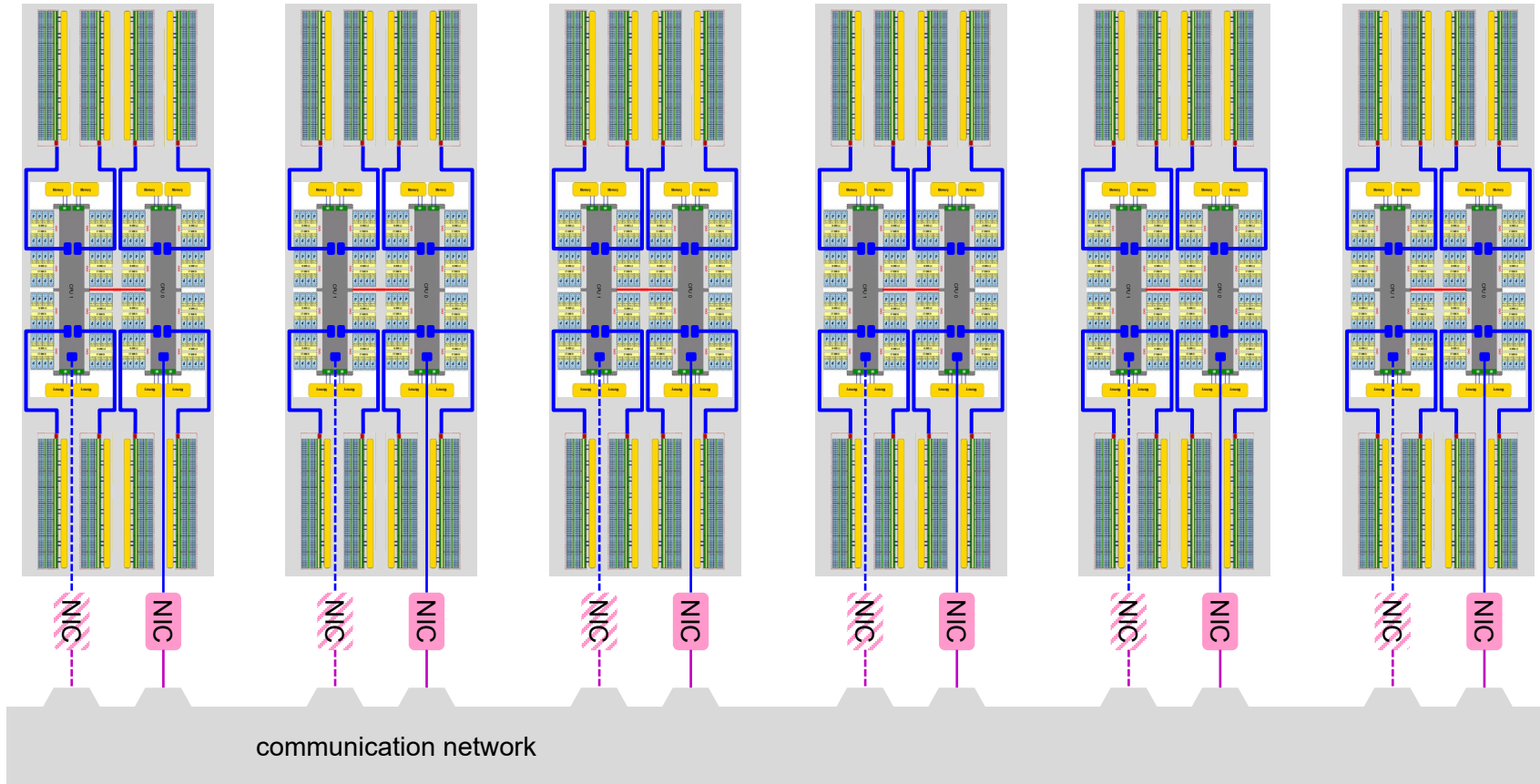
A modern CPU compute node (AMD Zen2 “Rome”)



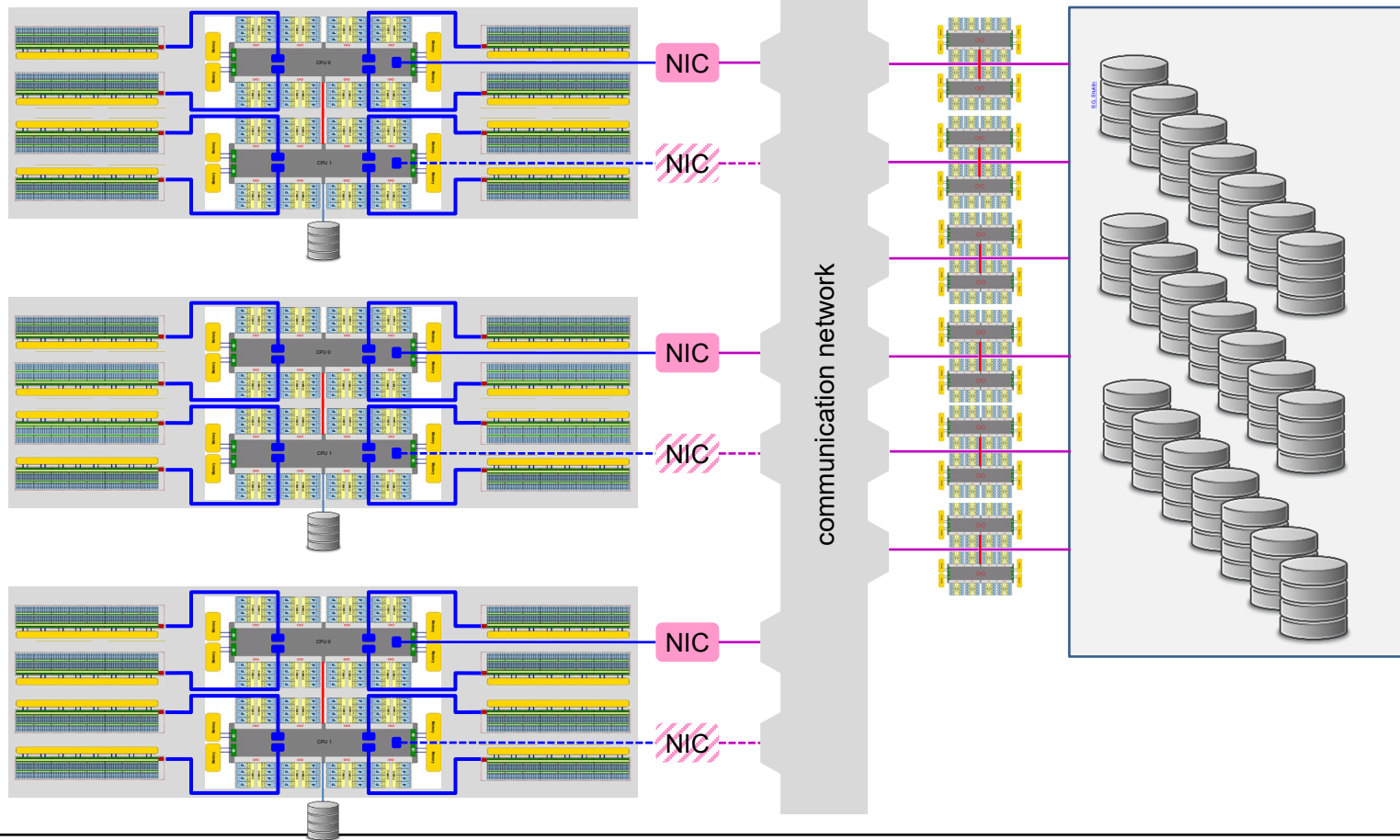
Adding accelerators to the node



Turning it into a cluster



Adding permanent storage



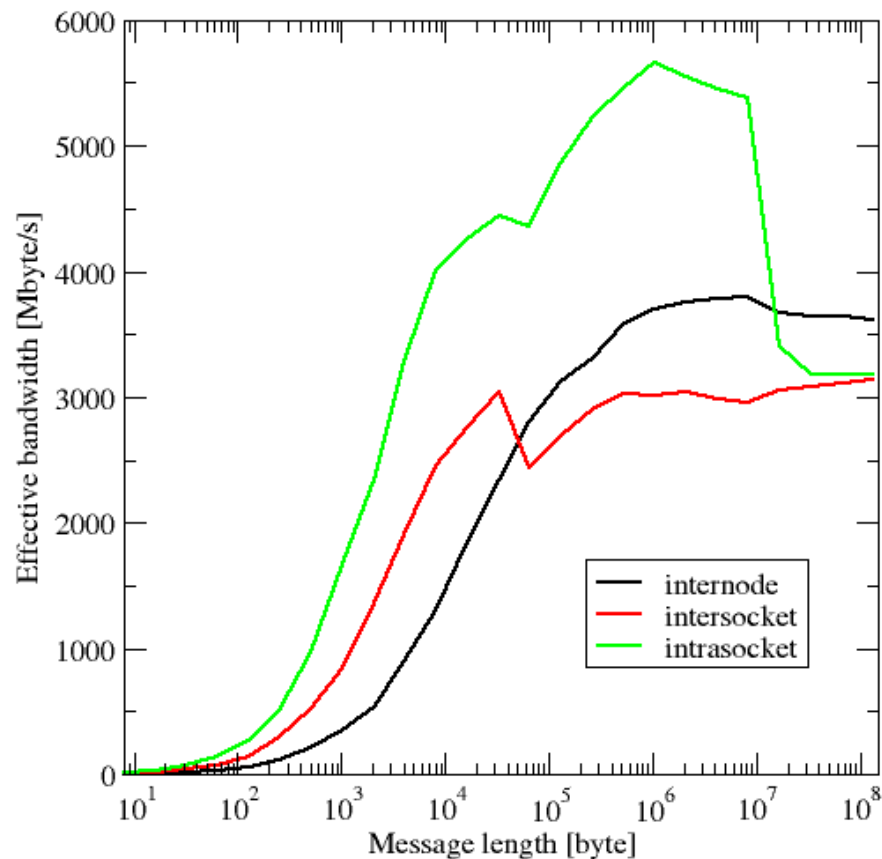
Point-to-point data transmission performance

- Simple “Hockney model” for data transfer time

$$T_{comm} = \lambda + \frac{V}{b}, \quad B_{eff} = \frac{V}{T_{comm}}$$

λ : latency, b : asymptotic BW

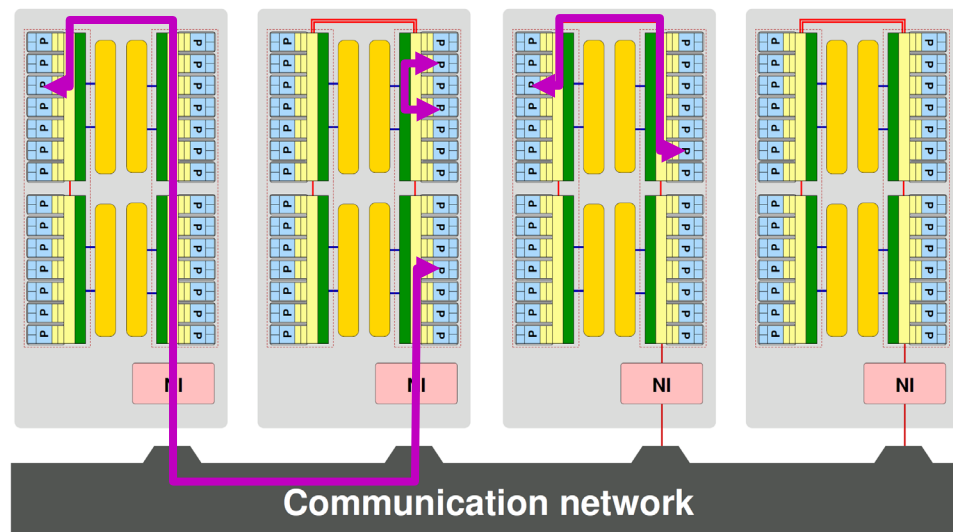
- Reality is more complicated
 - System topology
 - Caching effects
 - Contention effects
 - Protocol switches
 - Collective communication



Distributed-memory systems today

“Hybrid” distributed-/shared-memory systems

- Cluster of networked shared-memory nodes
 - ccNUMA architecture per node
 - Multiple cores per ccNUMA domain
-
- Expect strong topology effects in communication performance
 - Intra-socket, inter-socket, inter-node, all have different λ and b
 - On top: Effects from network structure

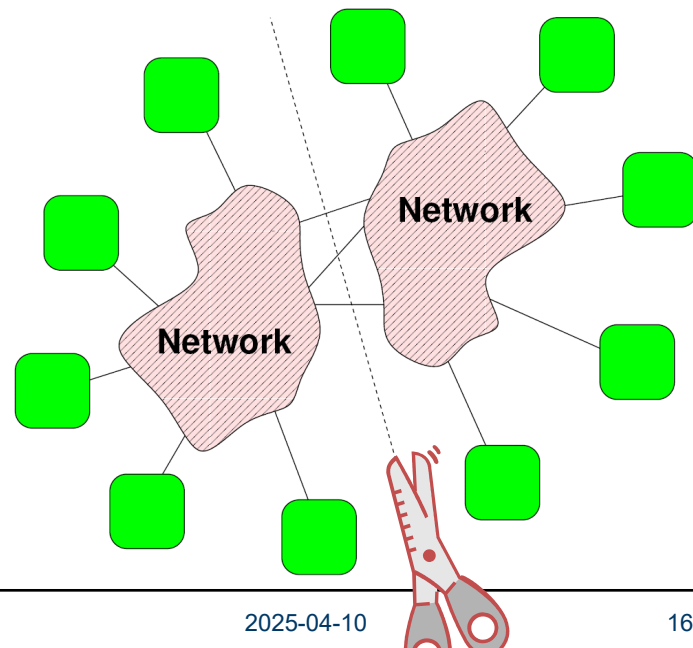


Characterizing communication networks

- Network **bisection bandwidth** B_b is a general metric for the data transfer “capability” of a system:

Minimum sum of the bandwidths of all connections cut when splitting the system into two equal parts

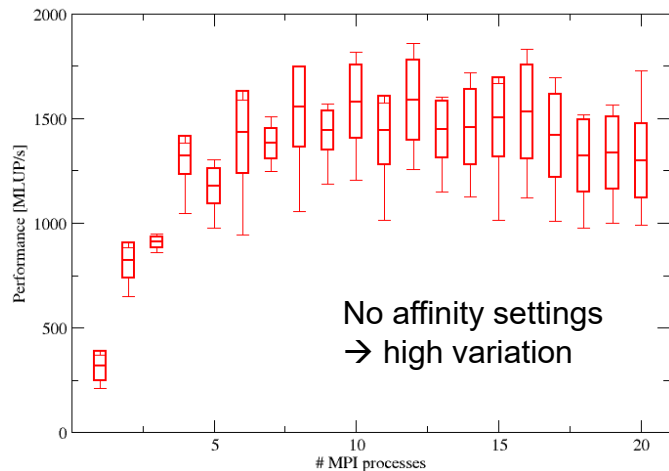
- More meaningful metric for system scalability: bisection BW **per node**: B_b/N_{nodes}
- Bisection BW depends on
 - Bandwidth per link
 - Network topology



Affinity control (pinning) of processes

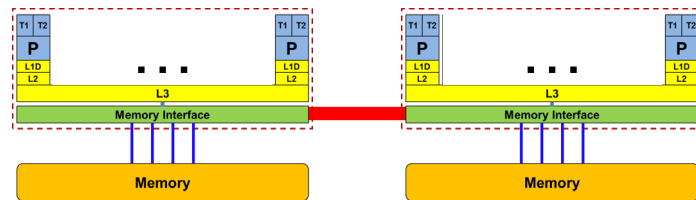


Anarchy vs. affinity with a heat equation solver

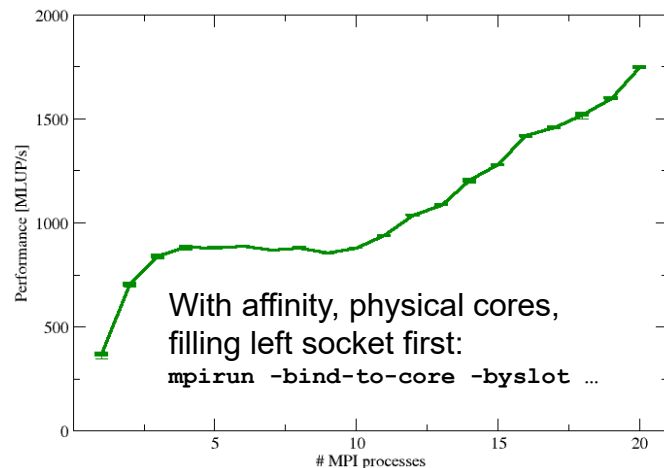


Reasons for caring about affinity:

- Eliminating performance variation
- Making use of architectural features
- Avoiding resource contention



2x 10-core Intel Ivy Bridge, OpenMPI



Pinning of MPI processes

- Highly implementation and system dependent!
- **Intel MPI**: env variable `I_MPI_PIN_PROCESSOR_LIST` (MPI only) or `I_MPI_PIN_DOMAIN` (MPI+OpenMP)
- **OpenMPI**: choose between several mpirun options, e.g.,
-bind-to-core, -bind-to-socket, -bycore, -byslot ...
- Cray's **aprun**
- Platform-independent tools: `likwid-mpirun`
(`likwid-pin`, `numactl`)

Simple example (Intel MPI)

- MPI-only code: `I_MPI_PIN_PROCESSOR_LIST`
- Many options
- Straightforward use:

```
$ mpirun -genv I_MPI_PIN_PROCESSOR_LIST=0-71 -np 144 ./a.out
```

pins one process on each physical core

Limits of parallelism: simple scaling laws



Metrics to quantify the efficiency of parallel computing

- $T(N)$: execution time of some fixed workload with N workers
- How much faster than with a single worker?

→ parallel speedup: $S(N) = \frac{T(1)}{T(N)}$

- How efficiently do those N workers do their work?

→ parallel efficiency: $\varepsilon(N) = \frac{S(N)}{N}$

Can we
predict
 $S(N)$? Are
there limits
to it?

- **Warning:** These metrics are not performance metrics!

Assumptions for basic scalability models

- **Scalable hardware:** N times the iron can work N times faster
- Work is either **fully parallelizable** or **not at all**
- For the time being, assume a **constant workload**



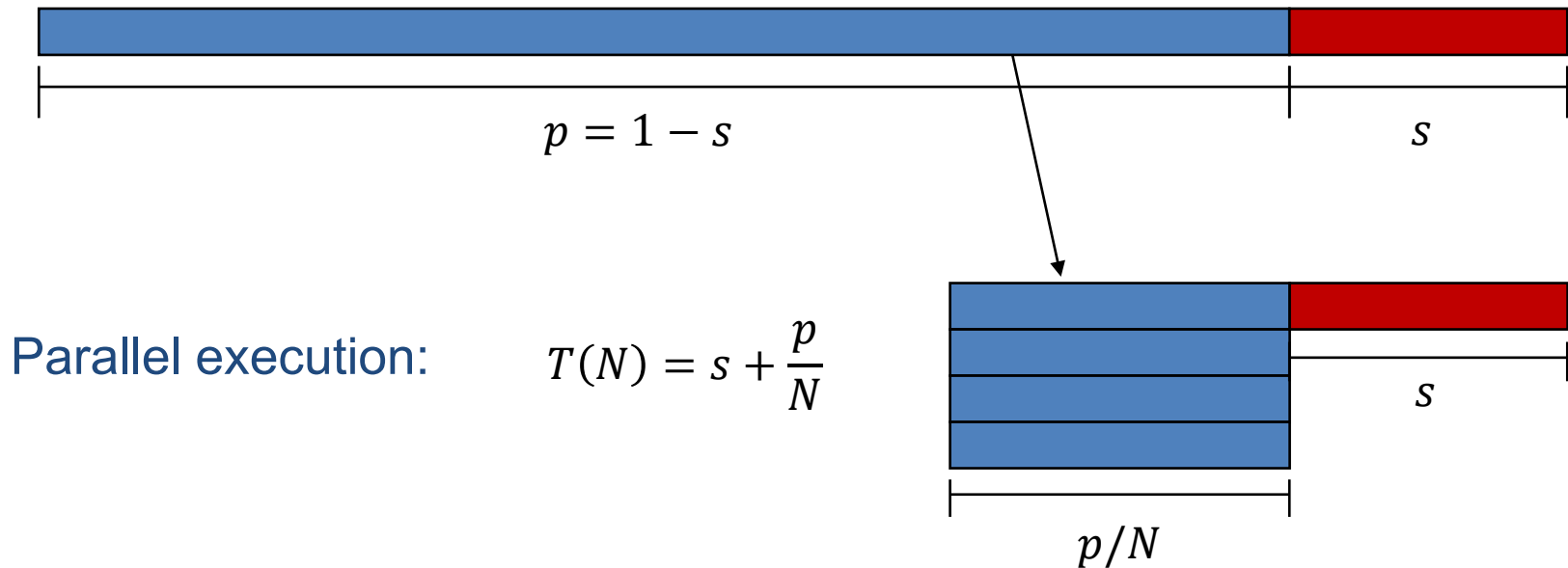
Ideal world:
All work is perfectly parallelizable
$$S(N) = N, \quad \varepsilon = 1$$

A simple speedup model for fixed workload

One worker normalized execution time: $T(1) = s + p = 1$

s : runtime of purely serial part

p : runtime of perfectly parallelizable part

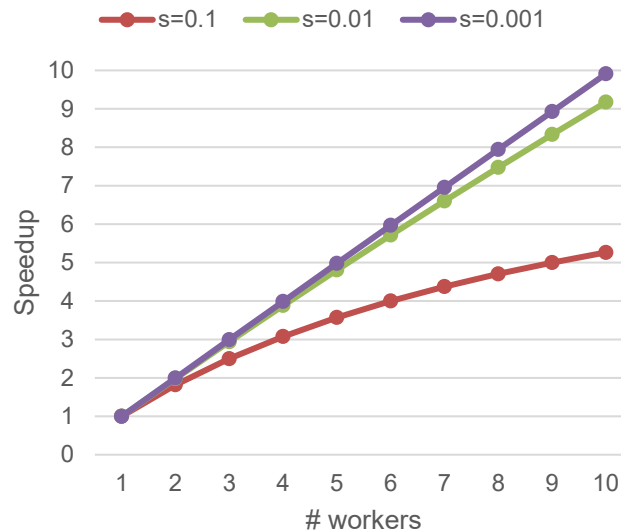


Amdahl's Law (1967) – “Strong Scaling”

- **Fixed workload** speedup with s being the fraction of nonparallelizable work

$$S(N) = \frac{T(1)}{T(N)} = \frac{1}{s + \frac{1-s}{N}}$$

- **Parallel efficiency:** $\varepsilon(N) = \frac{1}{s(N-1)+1}$



Gene M. Amdahl: *Validity of the single processor approach to achieving large scale computing capabilities*. In Proceedings of the April 18-20, 1967, spring joint computer conference (AFIPS '67 (Spring)). Association for Computing Machinery, New York, NY, USA, 483–485. [DOI:10.1145/1465482.1465560](https://doi.org/10.1145/1465482.1465560)

Fundamental limits in Amdahl's Law

- Asymptotic speedup

$$\lim_{N \rightarrow \infty} S(N) = \frac{1}{s}$$



- Asymptotic parallel efficiency

$$\lim_{N \rightarrow \infty} \varepsilon(N) = 0$$



→ Asymptotically, nobody is doing anything except the worker that gets the serial work!

- In reality, it's even worse...

Strong scaling plus overhead

- Let $c(N)$ be an overhead term that may include communication and/or synchronization

$$\rightarrow T(N) = s + \frac{p}{N} + c(N)$$

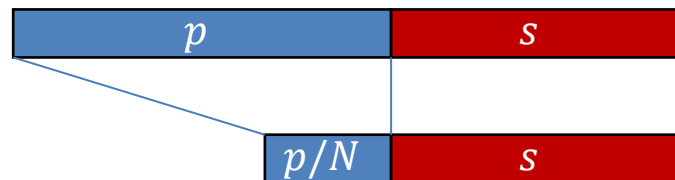
- What goes into $c(N)$?
 - Communication pattern
 - Synchronization strategy
 - Message sizes
 - Network structure
 - ...

Typical examples: $c(N) =$

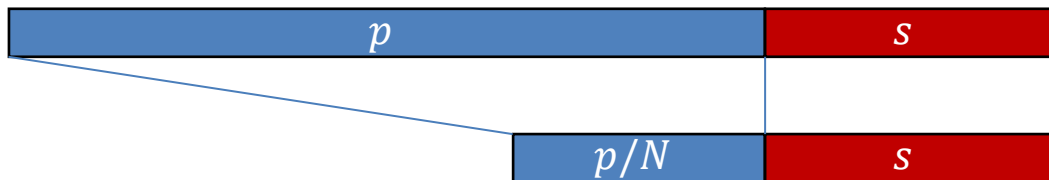
- kN^2 (all-to-all on bus network)
- $k \log N$ (optimal synchronization)
- kN (one sends to all)
- $\lambda + kN^{-\frac{2}{3}}$ (Cartesian domain decomposition, nonblocking network)

A simple speedup model for scaled workload

- What if we could **increase the parallel part** of the work only?
→ the larger p , the larger the speedup



- This is not possible for all applications, but for some



- “Weak scaling”**

A simple speedup model for scaled workload

- Parallel workload grows linearly with N

→ $T(N) = s + \frac{pN}{N} = s + p$, i.e., runtime stays constant

- Scalability metric?

→ How much more **work** per **second** can be done with N workers than with one worker?

$$S(N) = \frac{(s + pN)/(s + p)}{(s + p)/(s + p)} = s + (1 - s)N$$

Gustafson's Law
("weak scaling")

John L. Gustafson: *Reevaluating Amdahl's law*. Commun. ACM 31, 5 (May 1988), 532–533.

[DOI:10.1145/42411.42415](https://doi.org/10.1145/42411.42415)

Gustafson's Law for weak scaling

- Linear speedup (but not proportional unless $s = 0$) with N :

$$S(N) = s + (1 - s)N \rightarrow \text{unbounded speedup!}$$

- Weak scaling is the solution to the Amdahl dilemma: Why should we build massively parallel systems if all parallelism is limited by the serial fraction?
- Extension to communication?

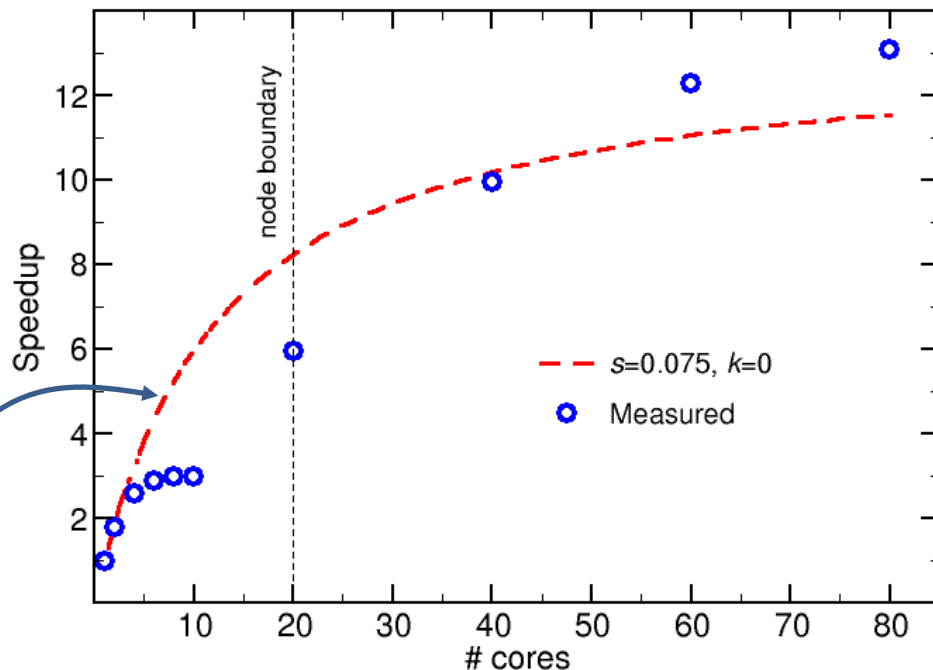
$$\rightarrow T(N) = s + \frac{pN}{N} + c(N) = 1 + c(N)$$

$$\rightarrow S(N) = \frac{(s+pN)/(1+c(N))}{(s+p)/1} = \frac{s+(1-s)N}{1+c(N)}$$

Much more relaxed
conditions on $c(N)$

How can we determine the model parameters?

- **Manual analysis:** Requires in-depth knowledge of hardware and program
- **Curve fitting:** Less insight, but also less cumbersome
- Example: Strong scaling of hypothetical code on “Meggie” node @FAU (10 cores per socket, 2 sockets per node)
- Use “extended Amdahl’s” with kN overhead
- Result:
Best fit is not a good fit at all

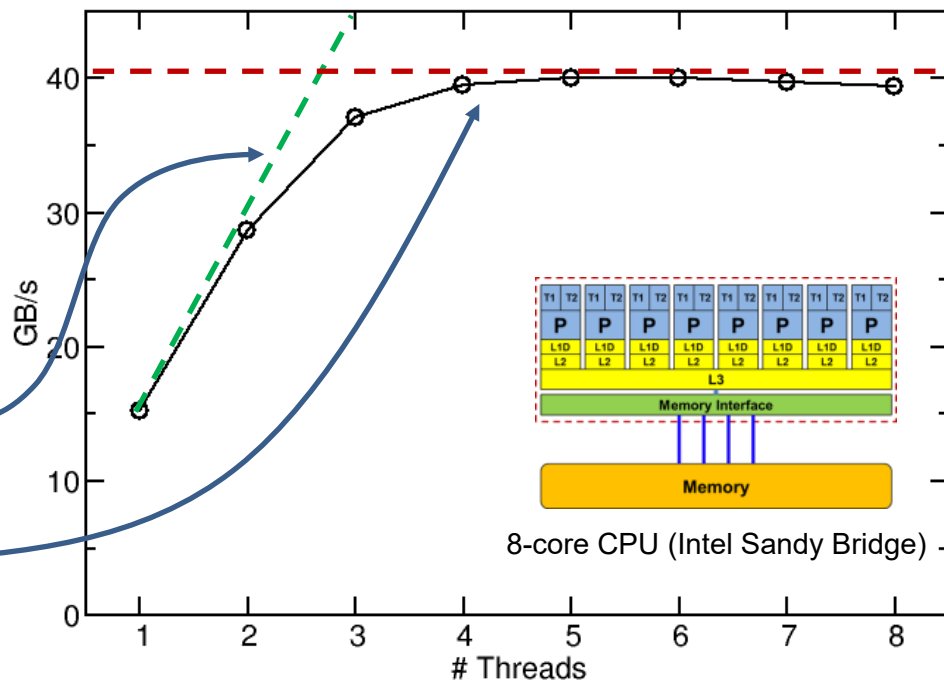


Resource bottlenecks

- Amdahl's Law assumes perfect scalability of resources
- Reality: Computer architecture is plagued by bottlenecks!
- Example: array update loop

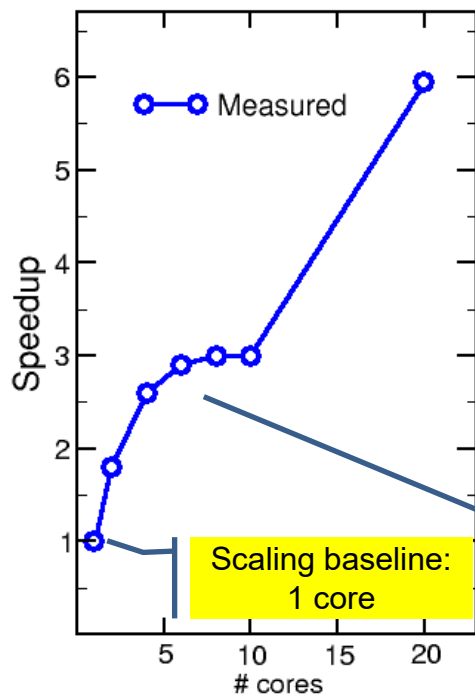
```
// MPI-parallel
for(i=0; i<100000000; ++i)
    a[i] = a[i] + s * c[i];
```

- Amdahl's: $s = 0$, $c(N) = 0$
 - Perfect speedup? No!
 - Saturation because of memory bandwidth exhaustion



Separation of scaling baselines is key!

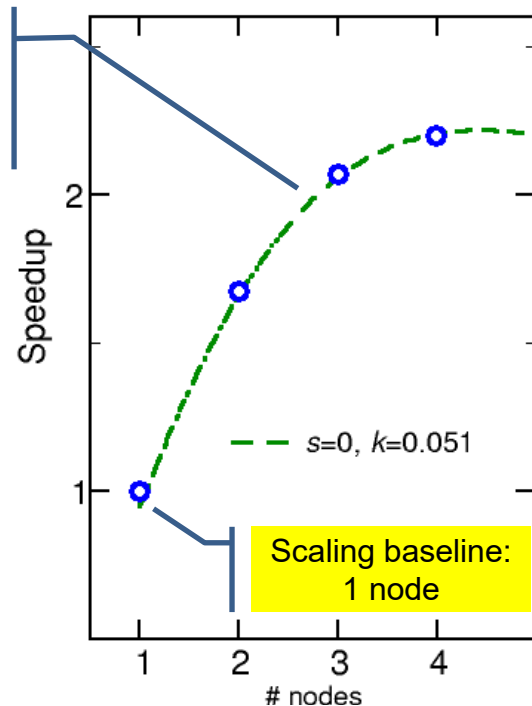
- Intra-socket scaling is often not covered by the model
 - Model assumes “scalable resources”



Model well suited
for internode
scaling!

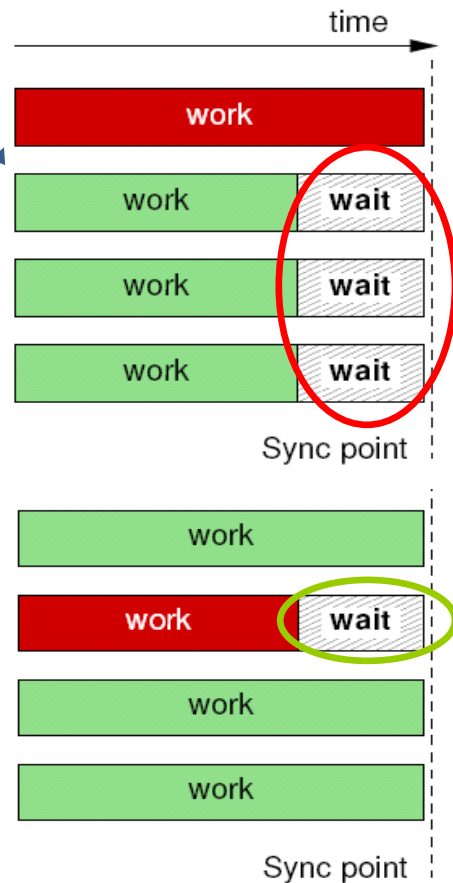
Separating scaling baselines
is important in modeling!

Socket saturation
due to memory
bandwidth



Amdahl generalized: load imbalance

- Load imbalance at **sync points**
 - More specifically, **execution time imbalance**
 - p/N assumption no longer valid in general
- Hard to model in general, but two corner cases:
 - A few “**lagers**” waste lots of **resources**
 - Single lagger → Amdahl’s Law
 - A few “**speeders**” might be **harmless**
- **Tuning advice**
 - Avoid sync points
 - Turn lagers into speeders



Benchmarking and performance assessment

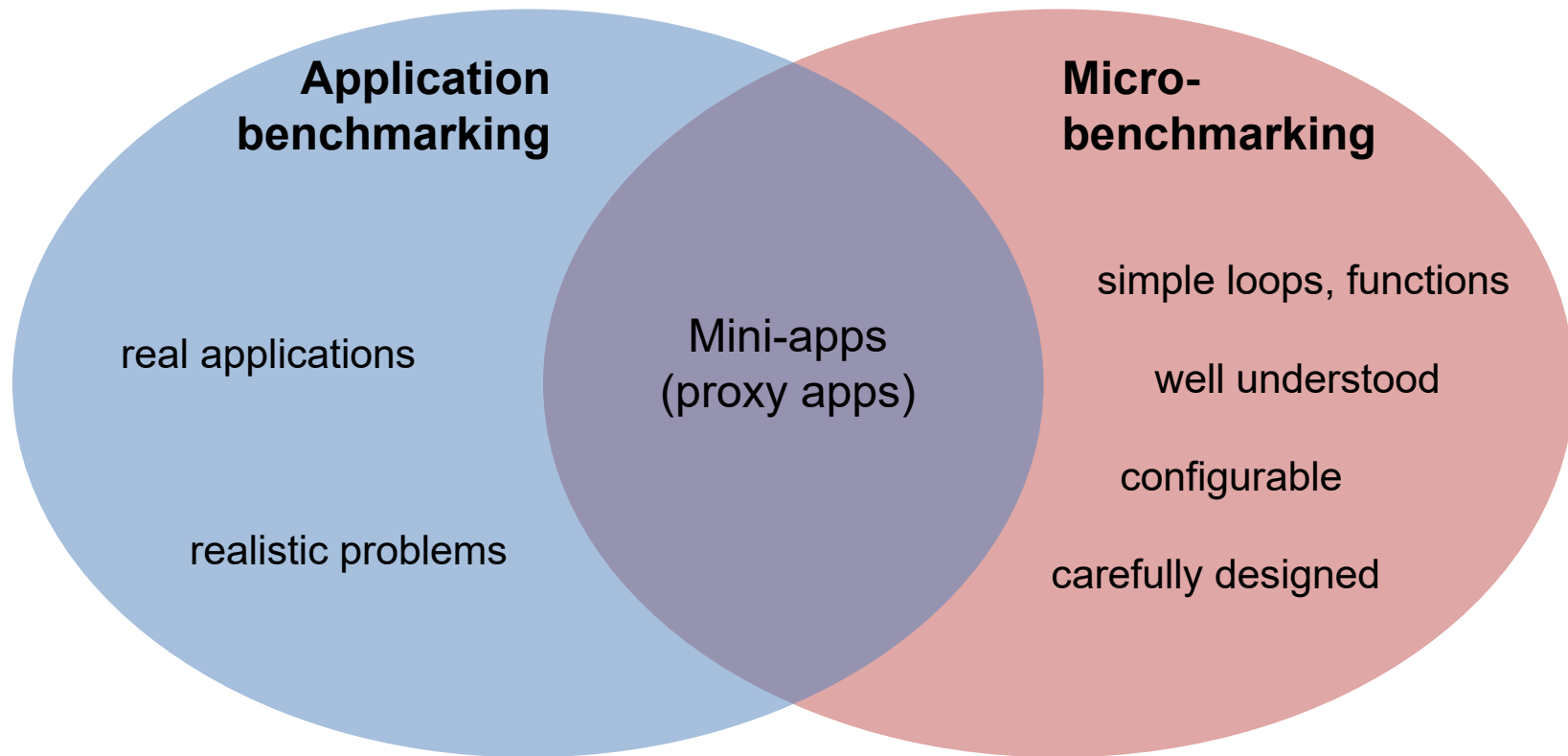
More info:

Lecture “Experiments and Data Presentation in High Performance Computing”

<https://youtu.be/y1n0IJZiPuw>



Benchmarking: two kinds (and a half)



Proper definition of benchmark cases

Benchmarking is a vital part of development and performance analysis

1. Define **proper benchmark case(s)** (input data sets)
 - Reflect(s) “production” workload
 - Tolerable runtime (minutes at most)
2. Document system **settings** and execution **environment**
 - Software: compilers, compiler options, library versions, OS version, ...
 - Hardware: CPU type, network, [... many more ...]
 - Runtime options: Threads/processes per node, affinity, large pages, [... many more ...]
3. Document **measurement methodology**
 - Number of repetitions, statistical variations, ...

Performance and time

- **Performance** is a “higher is better” metric: $P(N) = S(N) \times P(1)$
 - How much work can be done per time unit?
- Work: flops, iterations, “the problem,” ...
- Time: **wall-clock time**

- Measuring performance:

```
double s = get_walltime();  
// do your work here  
double e = get_walltime();  
double p = work / (e - s);
```

Return
time
stamp

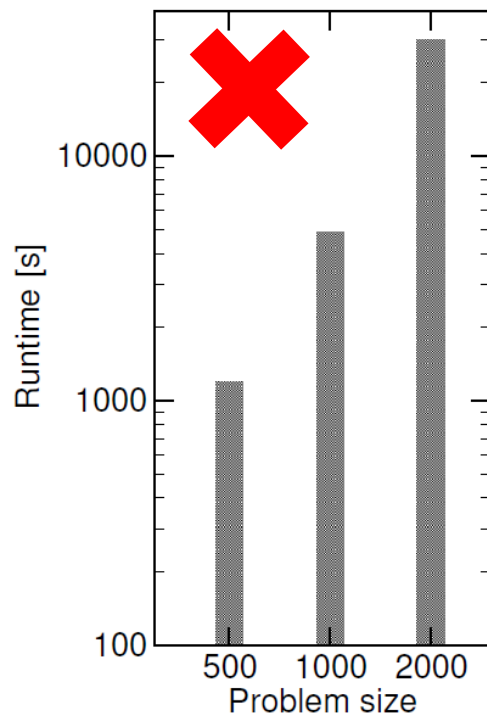
- **Caveat:**
Timer resolution is finite!

For
Fortran

```
#if !defined(_POSIX_C_SOURCE)  
#define _POSIX_C_SOURCE 199309L  
#endif  
  
#include <time.h>  
  
double get_walltime() {  
    struct timespec ts;  
    clock_gettime(CLOCK_MONOTONIC, &ts);  
    return (double)ts.tv_sec +  
           (double)ts.tv_nsec * 1.e-9;  
}  
  
double get_walltime_() {  
    return get_walltime();  
}
```

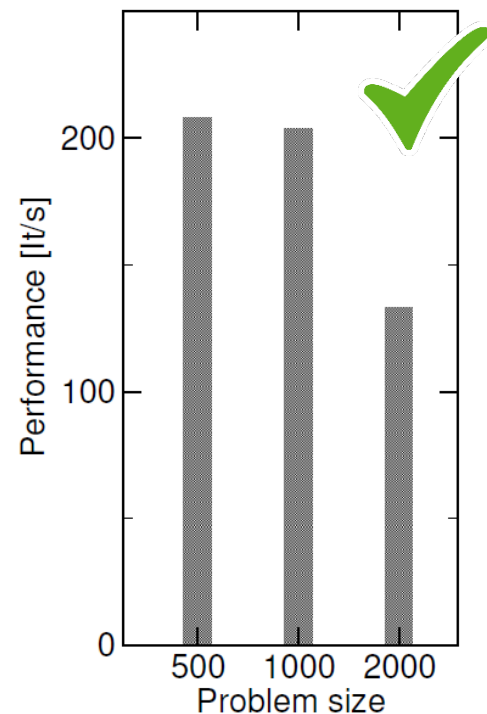
Popular blunders: runtime != performance

- Just presenting **runtime** is almost always a **bad idea!**



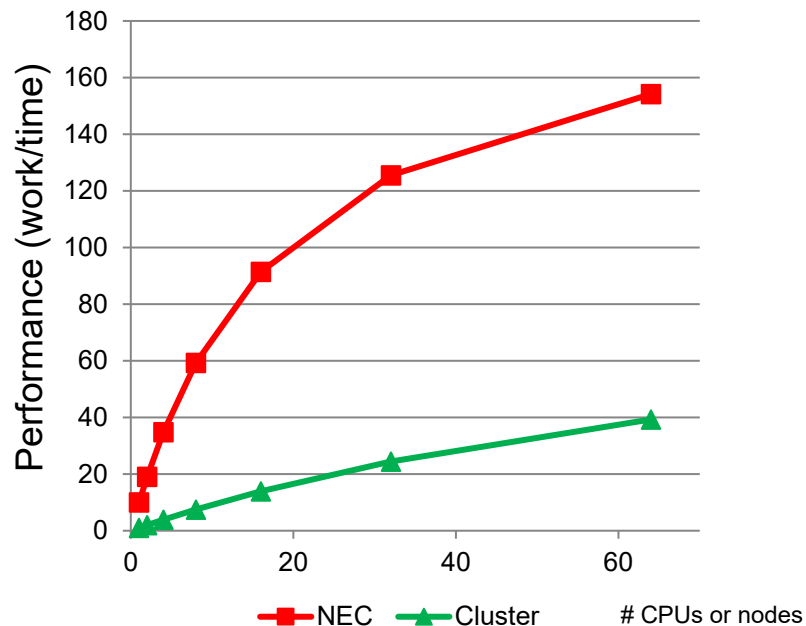
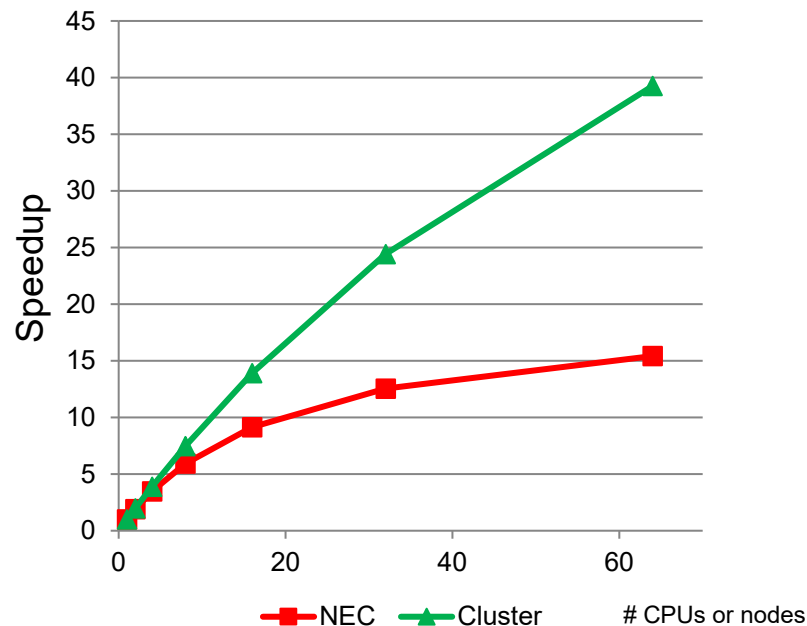
Insights hidden by trivial dependency: “larger problems need more time”

Performance metric reveals interesting behavior worth investigating!



Popular blunders: speedup != performance

Speedup hides the “higher is better” quality when comparing different systems or cases



MPI tracing tools



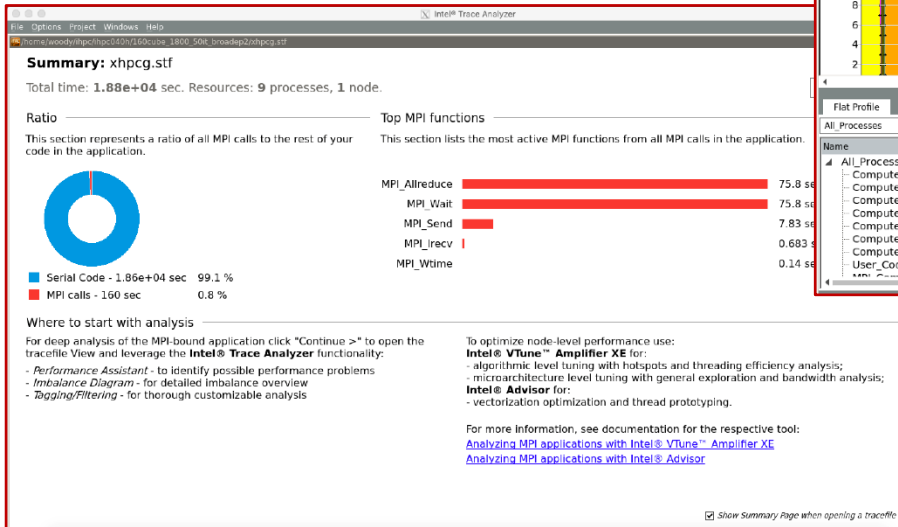
MPI tracing tools

- Allow the user to track events and statistics pertaining to MPI communication and code execution
- Popular tools
 - Intel Trace Analyzer and Collector (ITAC)
 - VAMPIR (commercial)
 - Paraver
- Powerful tools
- Potential to produce massive amounts of data
- Danger of “drowning in data”

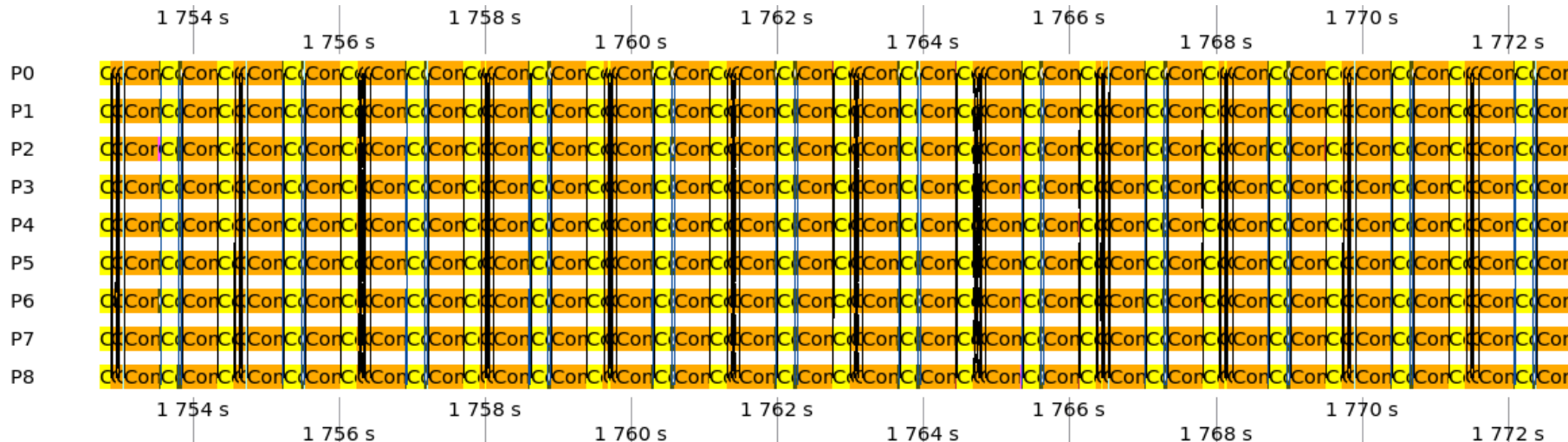
Intel Trace Analyzer and Collector

Event-based tool recording user function calls and MPI communication calls

GUI for advanced visualization

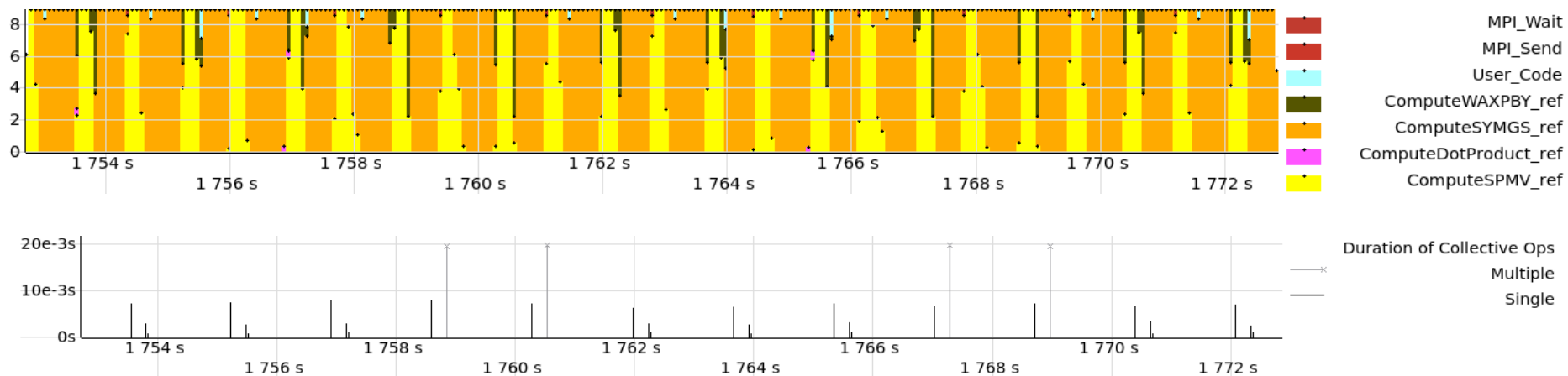


Event timeline view



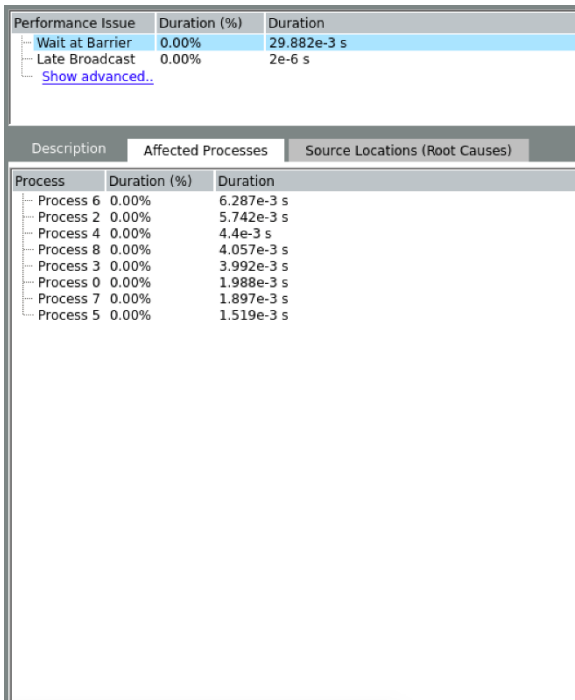
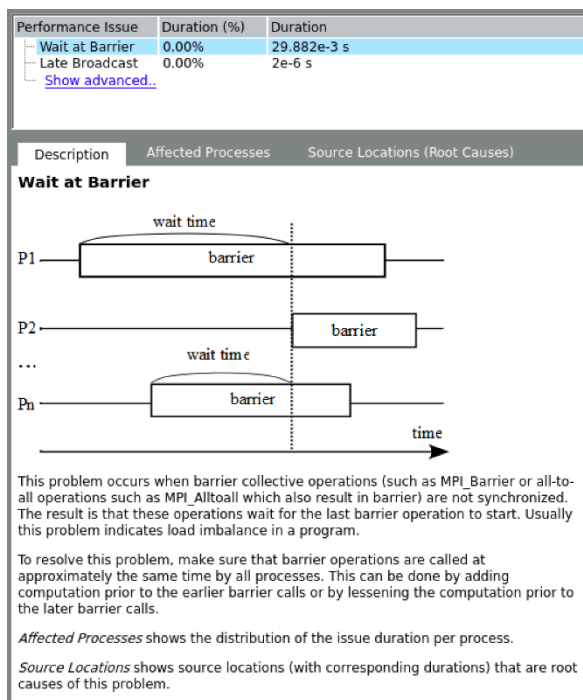
- Timeline of MPI and user function execution
- Message visualization
- Context menu provides details on functions/messages
- Zoom/pan

Quantitative and qualitative timelines



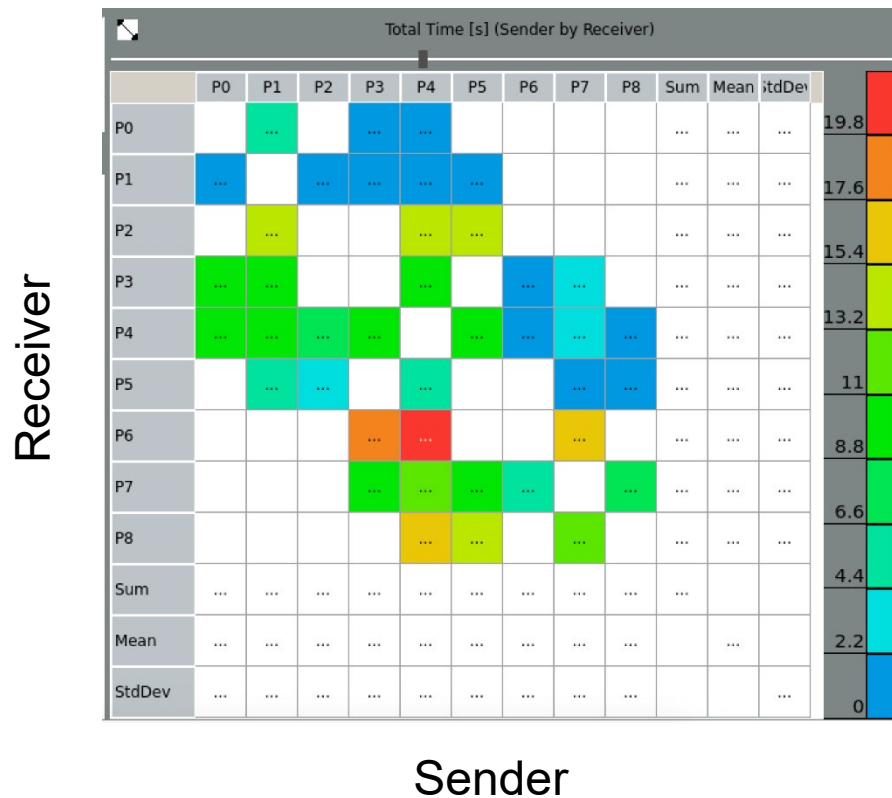
- Time spent in different MPI/user functions across processes
- Duration of certain things (collectives, PtP)

Performance advice



Context-sensitive
advice on typical
performance patterns

Message profile



- Who sends how much to whom?
- How long does it take?
- Effective bandwidth?

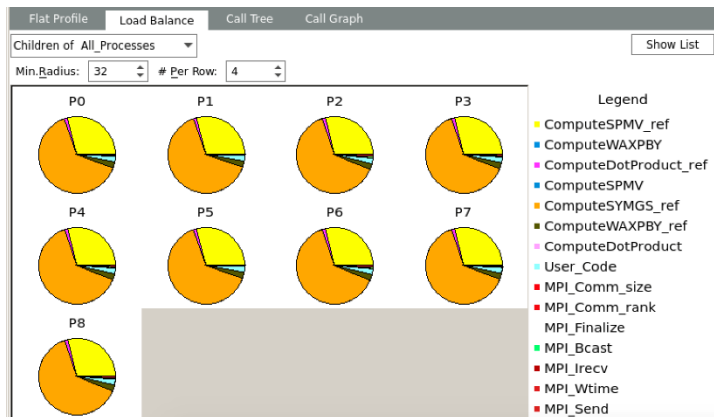
Collective operations profile

	Total Time [s] (Collective Operation by Process)												
	P0	P1	P2	P3	P4	P5	P6	P7	P8	Sum	Mean	StdDev	
MPI_Bcast	5e-6	7e-6	7e-6	7e-6	7e-6	7e-6	6e-6	7e-6	7e-6	60e-6	6.66667e-6	666.667e-9	13.5
MPI_Allreduce	6.98827	2.41008	14.1332	9.46671	9.80818	2.28141	12.1689	7.89127	10.6684	75.8164	8.42405	3.81376	12
Sum	6.98828	2.41009	14.1332	9.46671	9.80818	2.28142	12.1689	7.89127	10.6684	75.8165			10.5
Mean	3.49414	1.20504	7.06659	4.73336	4.90409	1.14071	6.08444	3.94564	5.33422		4.21203		9
StdDev	3.49413	1.20504	7.06658	4.73335	4.90409	1.1407	6.08444	3.94563	5.33422			5.00135	7.5
													6
													4.5
													3
													1.5
													0

- Time spent in collective call
- Data volume sent/received

Functions profile, call tree/graph, load imbalance

Flat Profile					
Load Balance					
Call Tree					
Call Graph					
All_Processes					
Name	TSelf	TSelf	TTotal	#Calls	TSelf /Call
▲ All_Processes					
ComputeSPMV_ref	5.46742e+3 s		5.51519e+3 s	44244	123.574e-3 s
ComputeWAXPBY	53.862e-3 s		475.234 s	31995	1.68345e-6 s
ComputeDotProduct_ref	264.986 s		329.014 s	33408	7.93181e-3 s
ComputeSPMV	15.826e-3 s		2.49945e+3 s	10863	1.45687e-6 s
ComputeSYMGS_ref	11.9892e+3 s		12.0259e+3 s	76608	156.5e-3 s
ComputeWAXPBY_ref	495.263 s		495.263 s	33345	14.8527e-3 s
ComputeDotProduct	31.118e-3 s		315.682 s	32049	970.951e-9 s
User_Code	432.994 s		18.8104e+3 s	9	48.1104 s
MPI_Comm_size	132.739e-3 s		132.739e-3 s	120861	1.09828e-6 s
MPI_Comm_rank	63.288e-3 s		63.288e-3 s	120861	523.643e-9 s
MPI_Finalize	4.043e-3 s		4.043e-3 s	9	449.222e-6 s
MPI_Bcast	60e-6 s		60e-6 s	9	6.66667e-6 s
MPI_Recv	682.73e-3 s		682.73e-3 s	537120	1.27109e-6 s
MPI_Wtime	140.191e-3 s		140.191e-3 s	223353	627.666e-9 s
MPI_Send	7.83291 s		7.83291 s	124	14.5832e-6 s
MPI_Allreduce	75.8164 s		75.8164 s	33534	2.26088e-3 s
MPI_Wait	75.7904 s		75.7904 s	537120	141.105e-6 s



Flat Profile					
Load Balance					
Call Tree					
Call Graph					
All_Processes					
Name	TSelf	TSelf	TTotal	#Calls	TSelf /Call
▲ All_Processes	432.994 s		18.8104e+3 s	9	48.1104 s
User_Code	60e-6 s		60e-6 s	9	6.66667e-6 s
MPI_Comm_rank	1e-6 s		1e-6 s	9	1.11111e-9 s
MPI_Comm_size	3e-6 s		3e-6 s	9	333.333e-9 s
MPI_Wtime	95.84e-3 s		95.84e-3 s	156537	612.251e-9 s
MPI_Allreduce	11.8325 s		11.8325 s	126	93.909e-3 s
ComputeSPMV_ref	2.97267e+3 s		3.01576e+3 s	33381	89.0527e-3 s
MPI_Comm_size	36.969e-3 s		36.969e-3 s	33381	1.10749e-6 s
MPI_Comm_rank	17.688e-3 s		17.688e-3 s	33381	529.882e-9 s
MPI_Recv	175.253e-3 s		175.253e-3 s	148360	1.18127e-6 s
MPI_Send	2.13018 s		2.13018 s	148360	14.3582e-6 s
MPI_Wait	40.7319 s		40.7319 s	148360	274.548e-6 s
ComputeSYMGS_ref	11.9892e+3 s		12.0259e+3 s	76608	156.5e-3 s
MPI_Comm_size	82.736e-3 s		82.736e-3 s	76608	1.07999e-6 s
MPI_Comm_rank	38.209e-3 s		38.209e-3 s	76608	498.76e-9 s
MPI_Recv	420.928e-3 s		420.928e-3 s	340480	1.23628e-6 s
MPI_Send	4.18757 s		4.18757 s	340480	12.299e-6 s
MPI_Wait	31.9995 s		31.9995 s	340480	93.9836e-6 s
ComputeWAXPBY_ref	20.0829 s		20.0829 s	1350	14.8762e-3 s
ComputeDotProduct_ref	10.7614 s		13.3636 s	1359	7.91865e-3 s
MPI_Wtime	1.935e-3 s		1.935e-3 s	2718	711.921e-9 s
MPI_Allreduce	2.60027 s		2.60027 s	1359	1.91337e-3 s
ComputeSPMV	15.826e-3 s		2.49945e+3 s	10863	1.45687e-6 s
ComputeSPMV_ref	2.49475e+3 s		2.49943e+3 s	10863	229.656e-3 s
MPI_Comm_size	13.031e-3 s		13.031e-3 s	10863	1.19958e-6 s
MPI_Comm_rank	7.39e-3 s		7.39e-3 s	10863	680.291e-9 s
MPI_Recv	86.549e-3 s		86.549e-3 s	48280	1.79265e-6 s
MPI_Send	1.51516 s		1.51516 s	48280	31.3828e-6 s
MPI_Wait	3.059 s		3.059 s	48280	63.3595e-6 s
ComputeWAXPBY	53.862e-3 s		475.234 s	31995	1.68345e-6 s

Flat Profile					
Load Balance					
Call Tree					
Call Graph					
All_Processes					
Name	TSelf	TSelf	TTotal	#Calls	TSelf /Call
▲ All_Processes					
Callers					
ComputeSPMV_ref called by ComputeSPMV	2.49475e+3 s		2.49943e+3 s	10863	229.656e-3 s
ComputeSPMV_ref called by User_Code	2.97267e+3 s		3.01576e+3 s	33381	89.0527e-3 s
Callees					
ComputeSPMV_ref calling MPI_Comm_size					
ComputeSPMV_ref calling MPI_Comm_rank					
ComputeSPMV_ref calling MPI_Recv					
ComputeSPMV_ref calling MPI_Send					
ComputeSPMV_ref calling MPI_Wait					

Options for taking traces

- **Caveat:** Tracing can generate vast amounts of data!
- Compiler switches (only works with legacy Intel compiler and wrappers [mpiicc, mpiicpc, mpiifort])
 - `-trace` # record MPI calls (also possible with mpirun/mpiexec)
 - `-tcollect -trace` # record MPI and user code function calls
potential of large overhead and large trace size
 - `-tcollect-filter=func.txt -tcollect -trace` # filter file

func.txt example

```
'.*' OFF
'.*ComputeDotProduct.*' ON
'.*ComputeSYMGS.*' ON
'.*ComputeSPMV.*' ON
'.*ComputeWAXPBY.*' ON
```

More (important) configuration options

Environment variable	Default	Description
VT_FLUSH_PREFIX	... depends	directory for temporary flush files
VT_LOGFILE_PREFIX	current working directory	directory for physical trace information files
VT_LOGFILE_FORMAT	STF	SINGLESTF: rolls all trace files into one file (.single.stf)
VT_LOGFILE_NAME	\${binary}.stf	control the name for the trace file
VT_MEM_BLOCKSIZE	64 KB	trace data in chunks of main memory
VT_MEM_FLUSHBLOCKS	1024	flushing is started when the number of blocks in memory exceeds this threshold
VT_MEM_MAXBLOCKS	1024	maximum number of blocks in main memory, if exceed the application is stopped until AUTOFLUSH/ MEM-OVERWRITE/ stop recording trace info
VT_CONFIG_RANK	0	control the process that reads and parses the configuration file



- **Avoid rapid-fire dumping trace data into shared filesystems!**
- **Your fellow cluster users will hate you for it.**

Alternatives

- **ITAC is deprecated** by Intel and will not be further developed (as of 2025)
 - Intel recommends VTune as a replacement, but this is not competitive
- Other tools with similar functionality
 - **Vampir** (commercial, scalable) <https://vampir.eu/>
 - **Scalasca** (for highly scalable programs, no trace view) <https://www.scalasca.org/>
 - **Paraver** <https://tools.bsc.es/paraver>
 - Jumpshot
Don't even bother.