

MPI and OpenMP common bottlenecks and how to spot them

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Tutorial on Profiling @ MHPC - ICTP

Size matters

!



How much work 1 worker
can do is limited by his
speed.

A single worker can only
move so fast.



Size matters



Union is strength

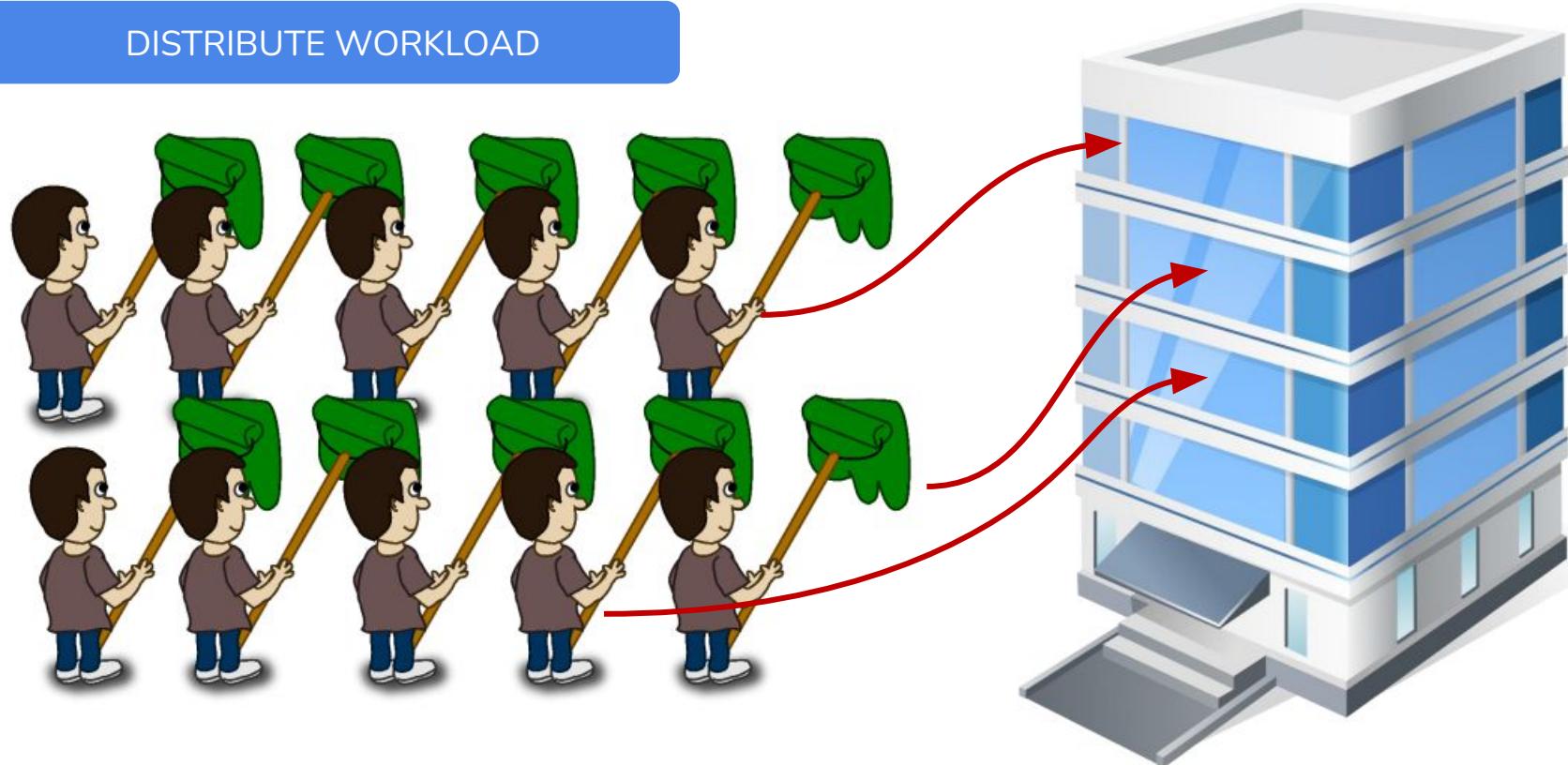


Multiple workers can do more work and share resources, if organized properly.



Union is strength

DISTRIBUTE WORKLOAD



Union is strength

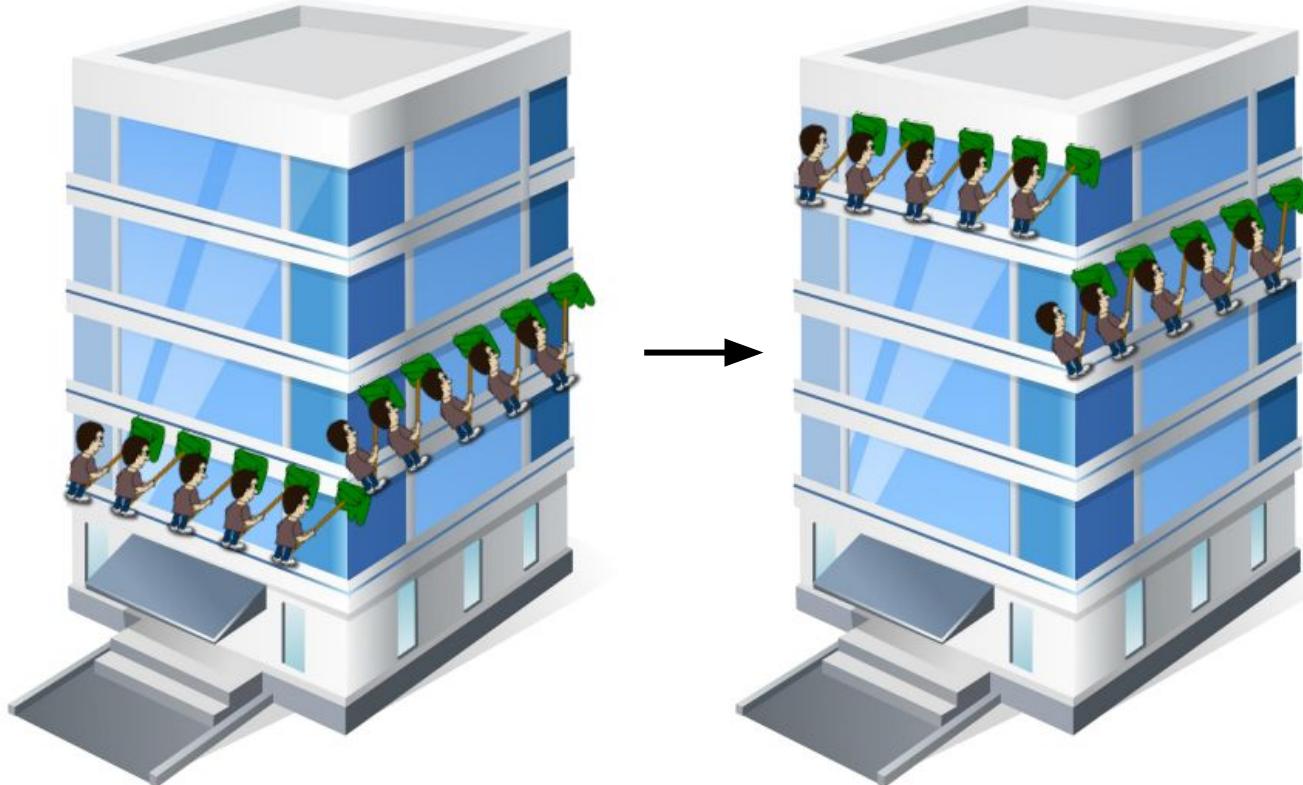


SYNCHRONIZE



EXCHANGE INFORMATION

Union is strength



You need a good team management

Which are the main causes of bottlenecks for an MPI application?



You need a good team management

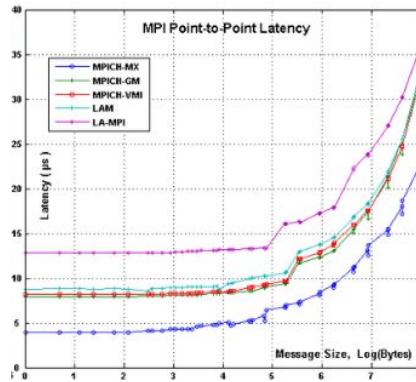
1. DEPENDENCIES
2. MESSAGE TRANSFERS
3. WORKLOAD DISTRIBUTION



Network metrics

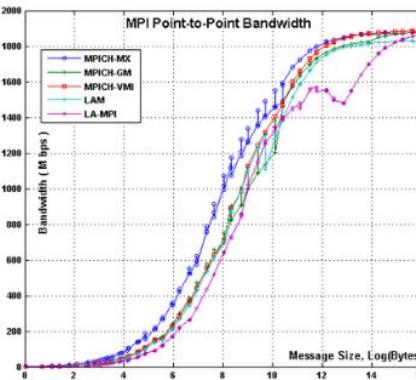
Latency :

The time it takes for a message of size 0 to get to a destination



Bandwidth :

The maximum rate at which data can flow over the network.

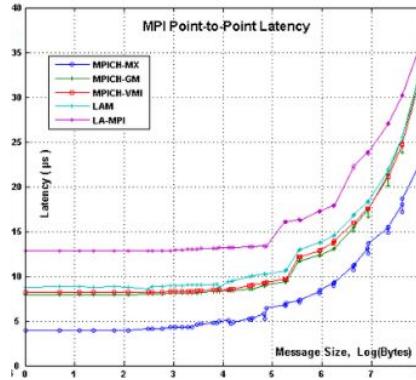


Network metrics

Latency :

The time it takes for a message of size 0 to get to a destination

- Dominates the performance of **small messages**
- Better to **bundle multiple small messages** into larger one

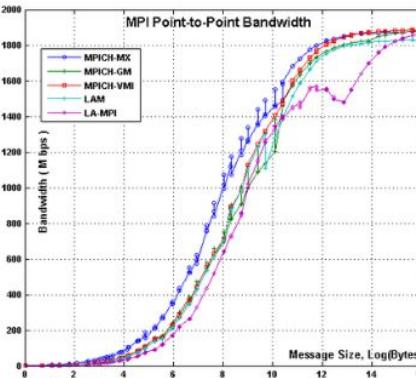


Bandwidth :

The maximum rate at which data can flow over the network.

- Dominates the performance of **large messages**
- Improve **network topology or mapping**

$$T = L + (1/BW) * V$$



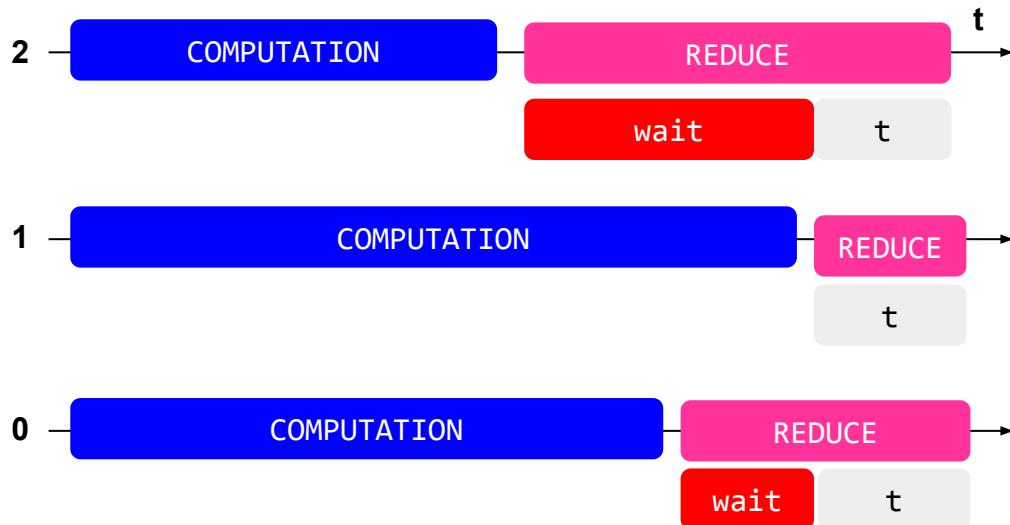
Workload imbalance

MPI procs might spend time in barriers inside MPI calls (“MPI wait time”)



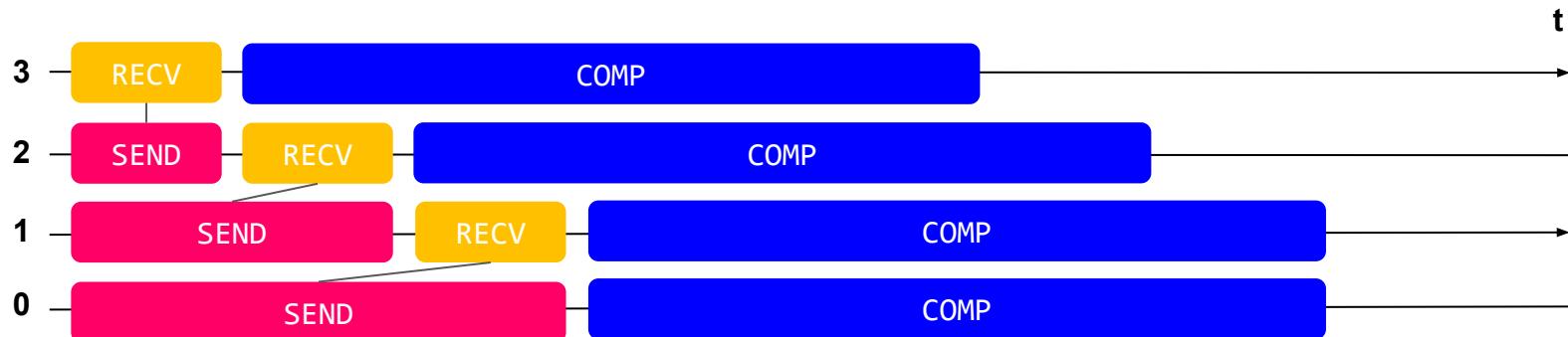
Workload imbalance

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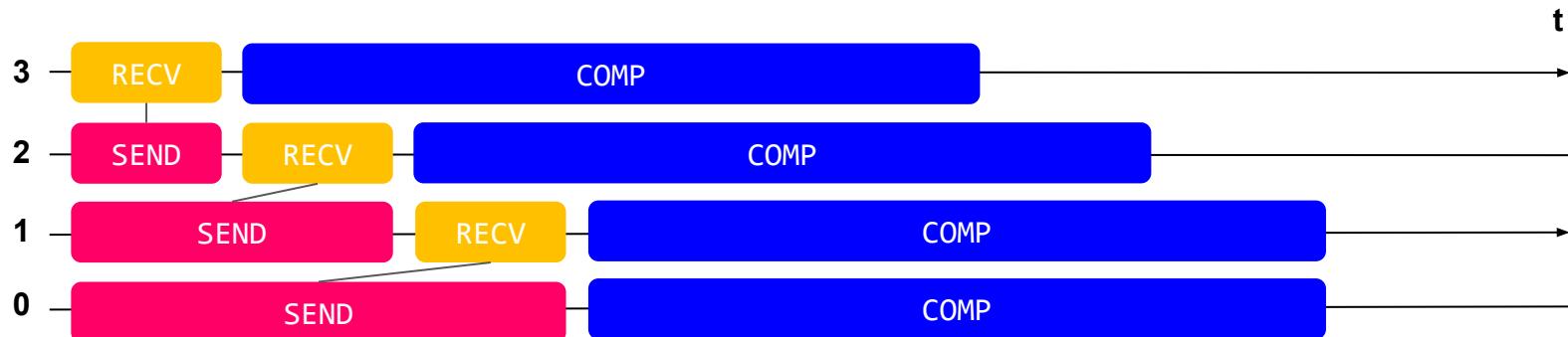
Dependencies

```
MPI_Recv(&token, 1, MPI_INT, rank - 1, 0, MPI_COMM_WORLD, MPI_STATUS_IGNORE);  
MPI_Send(&token, 1, MPI_INT, rank + 1, 0, MPI_COMM_WORLD, MPI_STATUS_IGNORE);
```



Dependencies

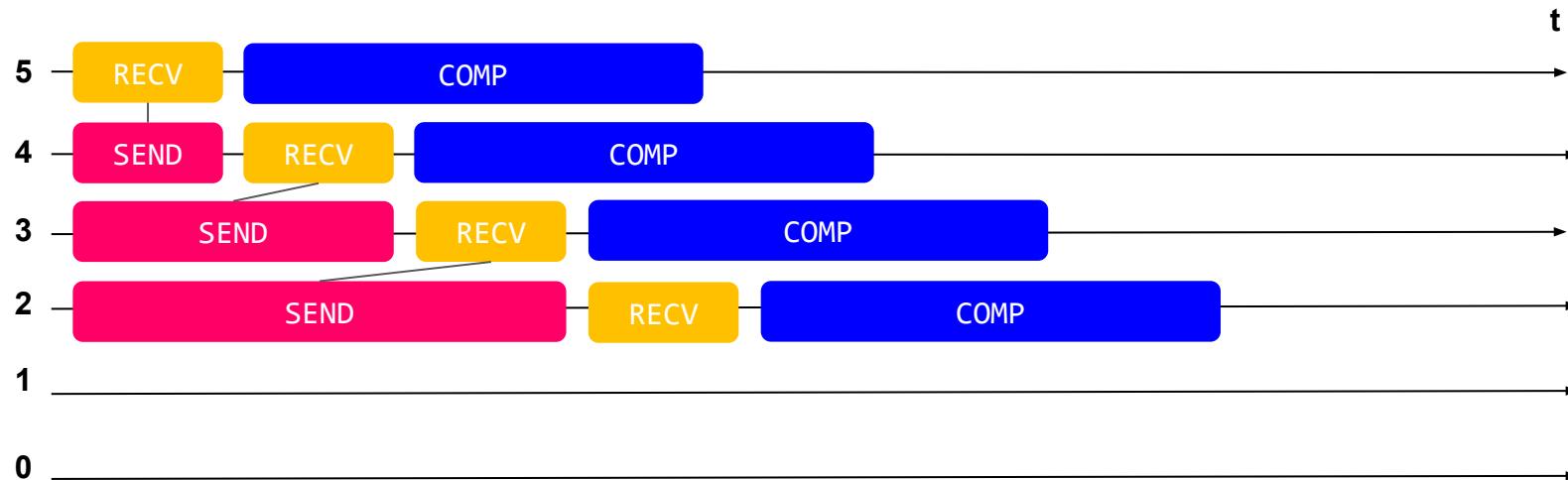
```
MPI_Recv(&token, 1, MPI_INT, rank - 1, 0, MPI_COMM_WORLD, MPI_STATUS_IGNORE);  
MPI_Send(&token, 1, MPI_INT, rank + 1, 0, MPI_COMM_WORLD, MPI_STATUS_IGNORE);
```



What happens if the number of MPI ranks increases?

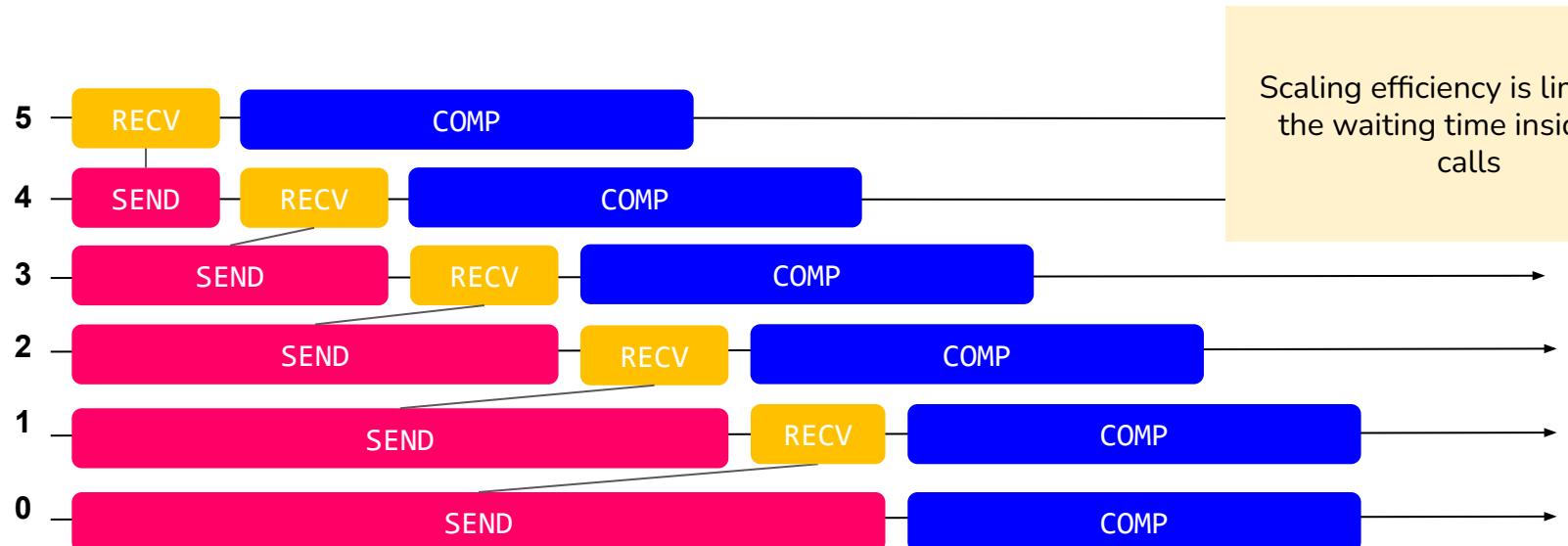
Dependencies

```
MPI_Recv(&token, 1, MPI_INT, rank - 1, 0, MPI_COMM_WORLD, MPI_STATUS_IGNORE);  
MPI_Send(&token, 1, MPI_INT, rank + 1, 0, MPI_COMM_WORLD, MPI_STATUS_IGNORE);
```

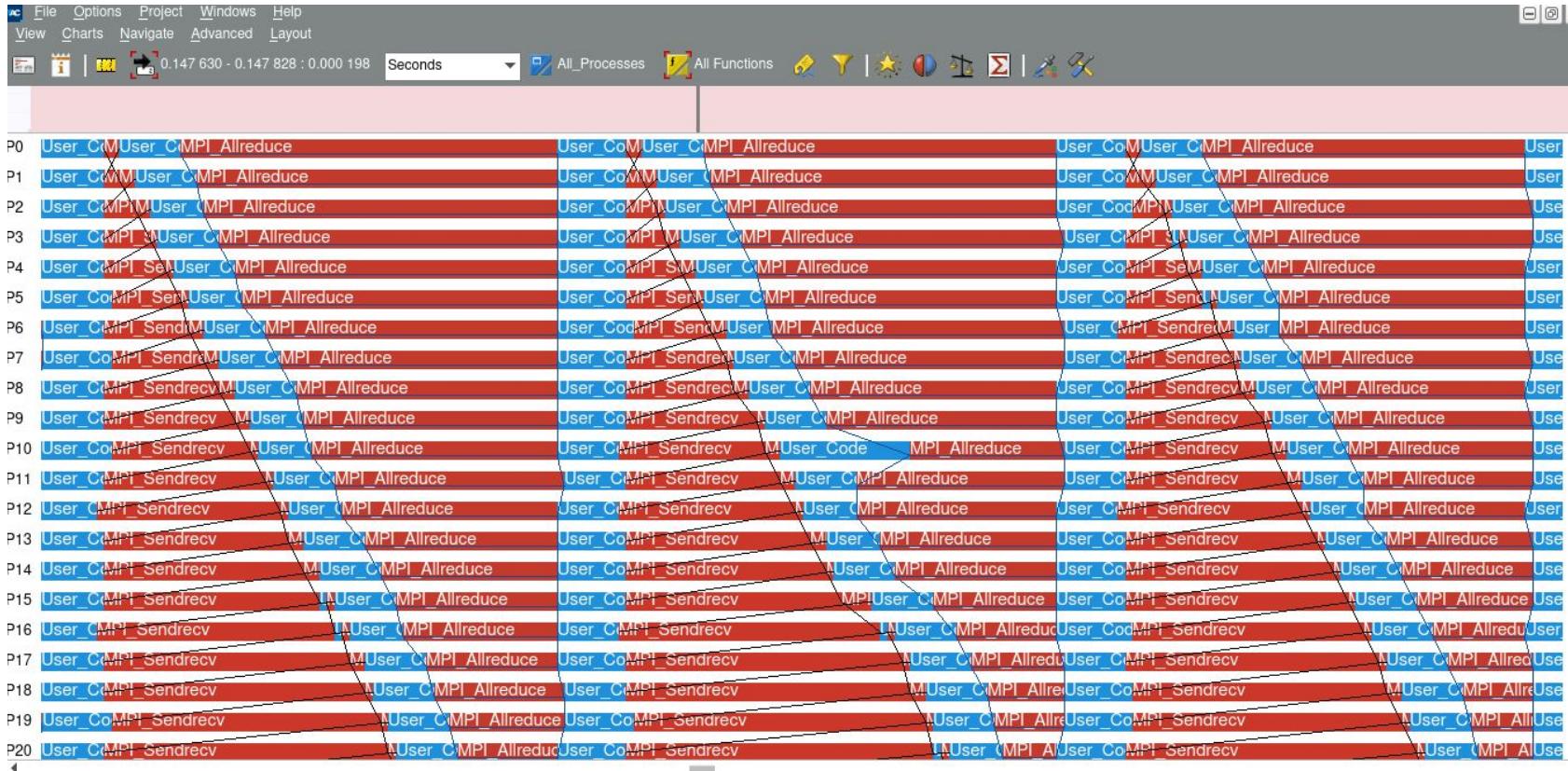


Dependencies

```
MPI_Recv(&token, 1, MPI_INT, rank - 1, 0, MPI_COMM_WORLD, MPI_STATUS_IGNORE);  
MPI_Send(&token, 1, MPI_INT, rank + 1, 0, MPI_COMM_WORLD, MPI_STATUS_IGNORE);
```

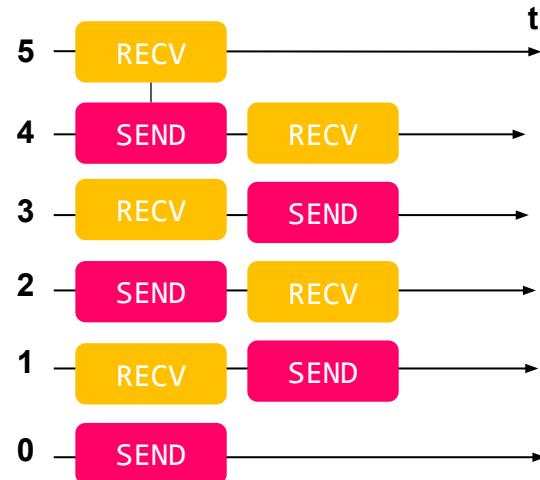


Dependencies

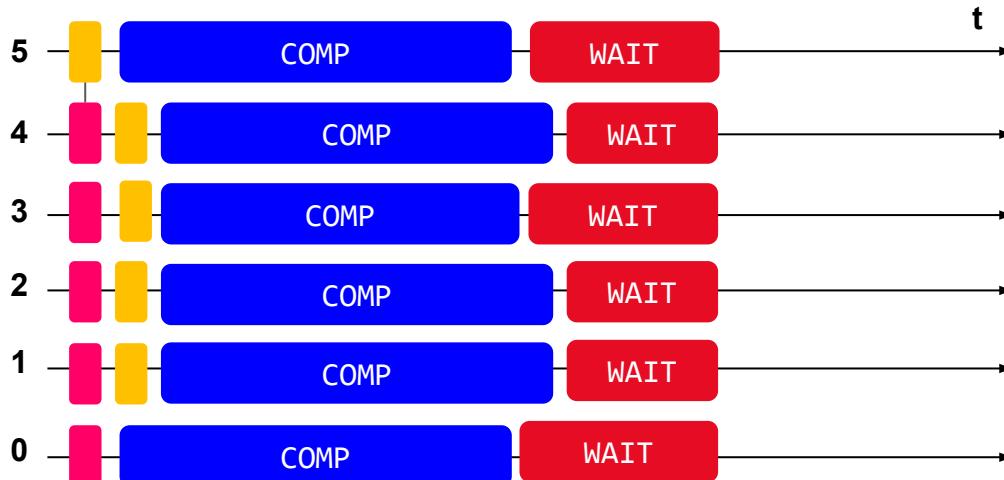


Dependencies

Consider using more efficient patterns or non-blocking operations



Overlap with GPU computing and or data movements

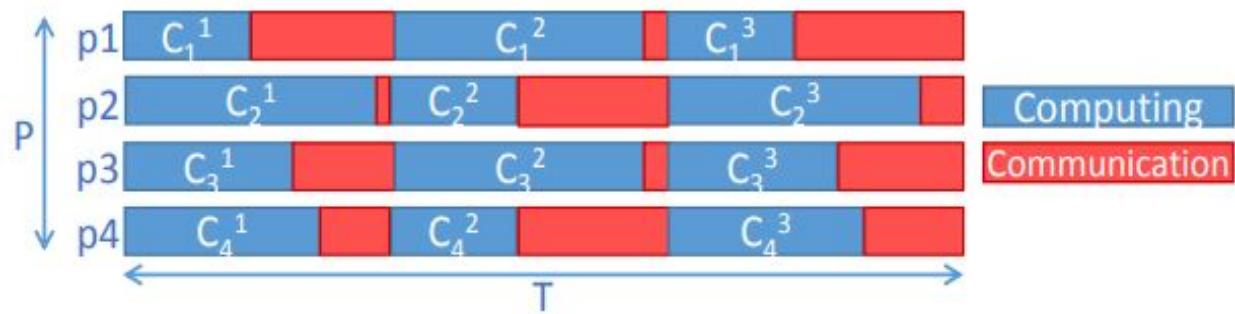
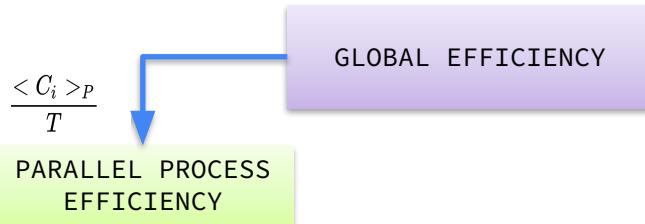


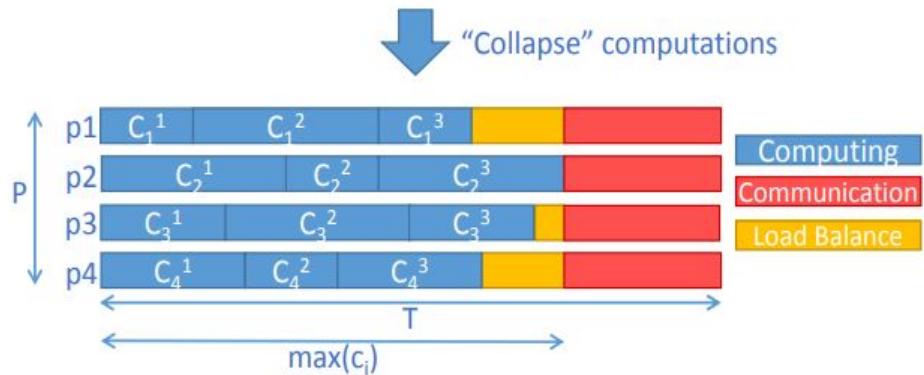
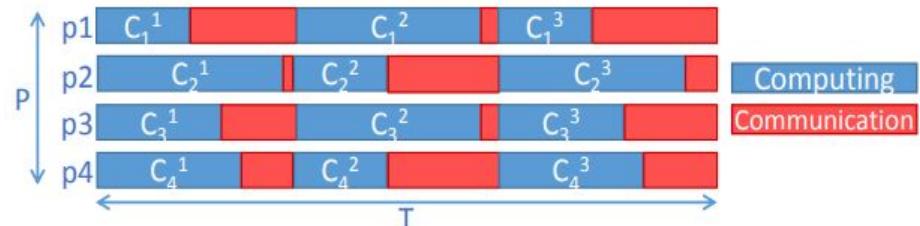
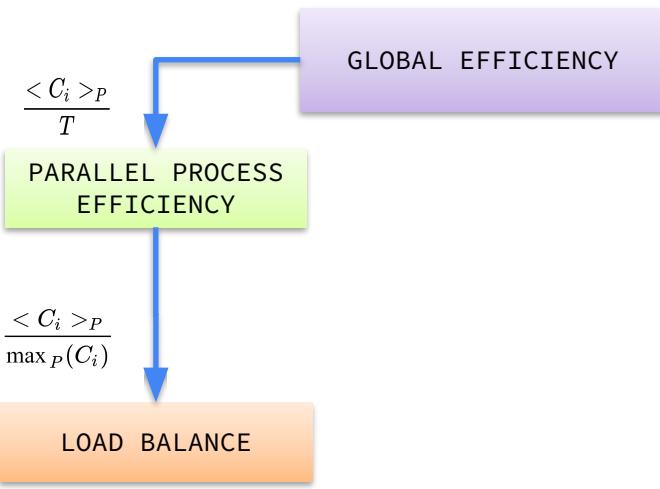
POP metrics for MPI

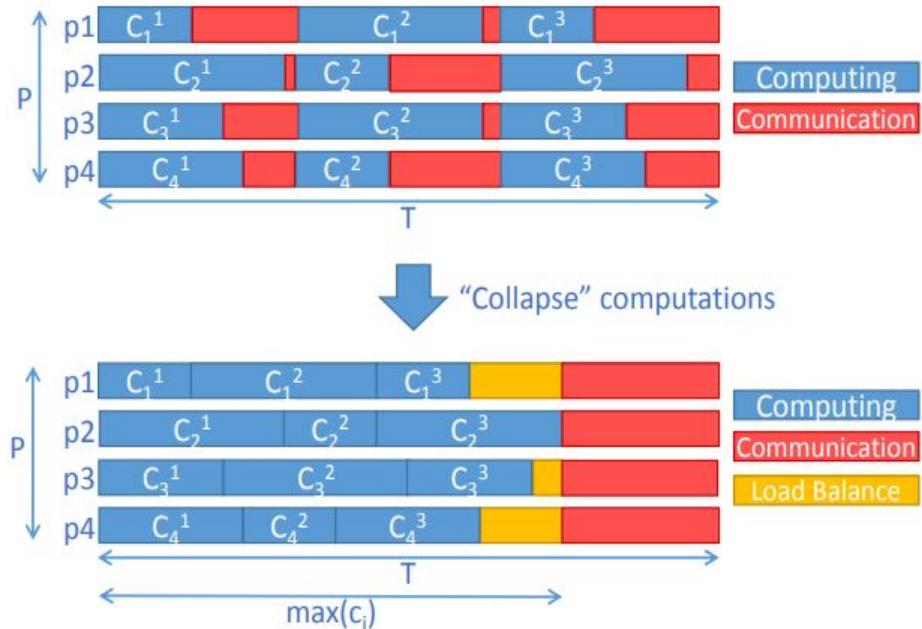
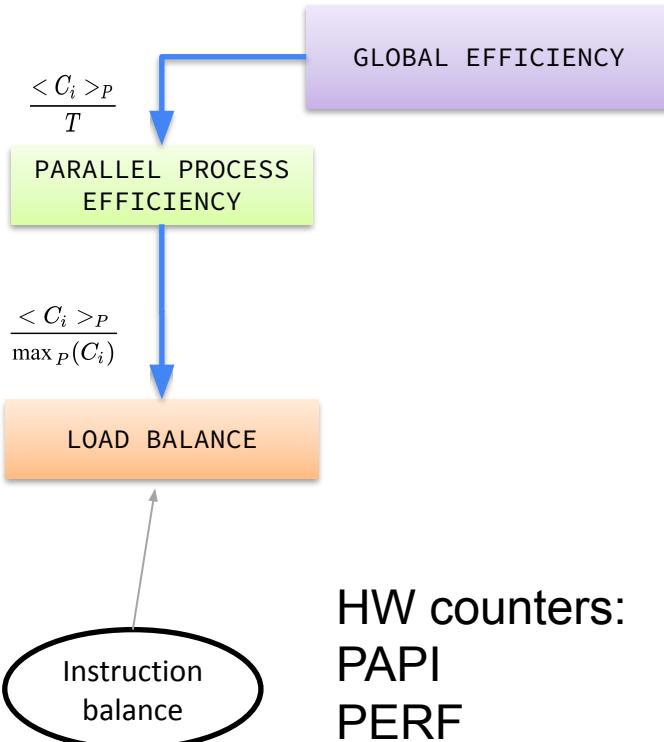
How to measure performance of an MPI application?



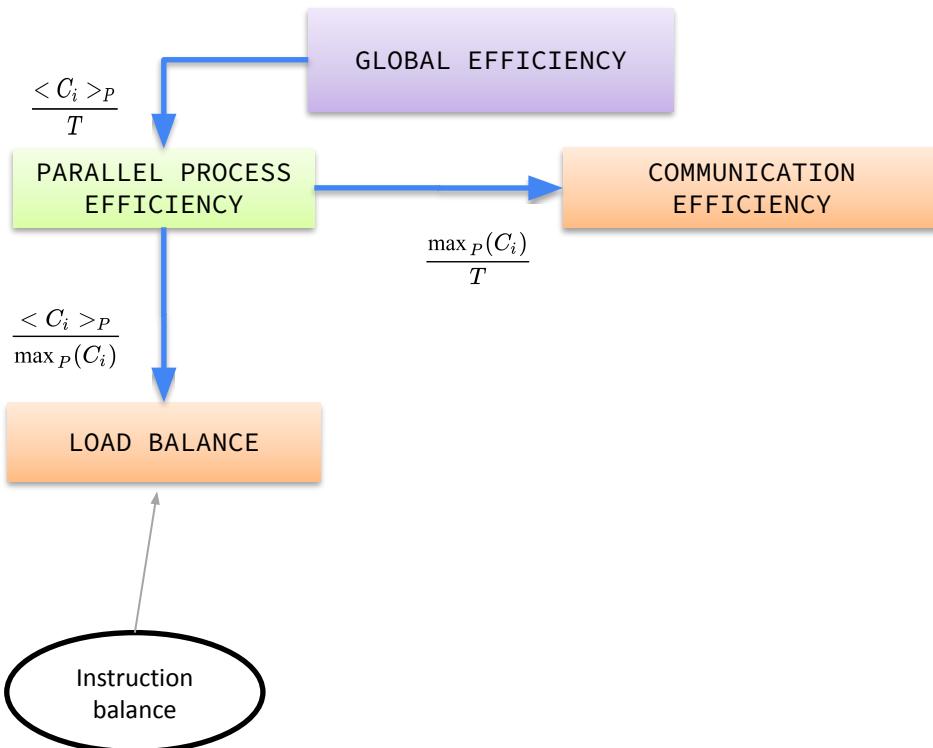
<https://pop-coe.eu/>

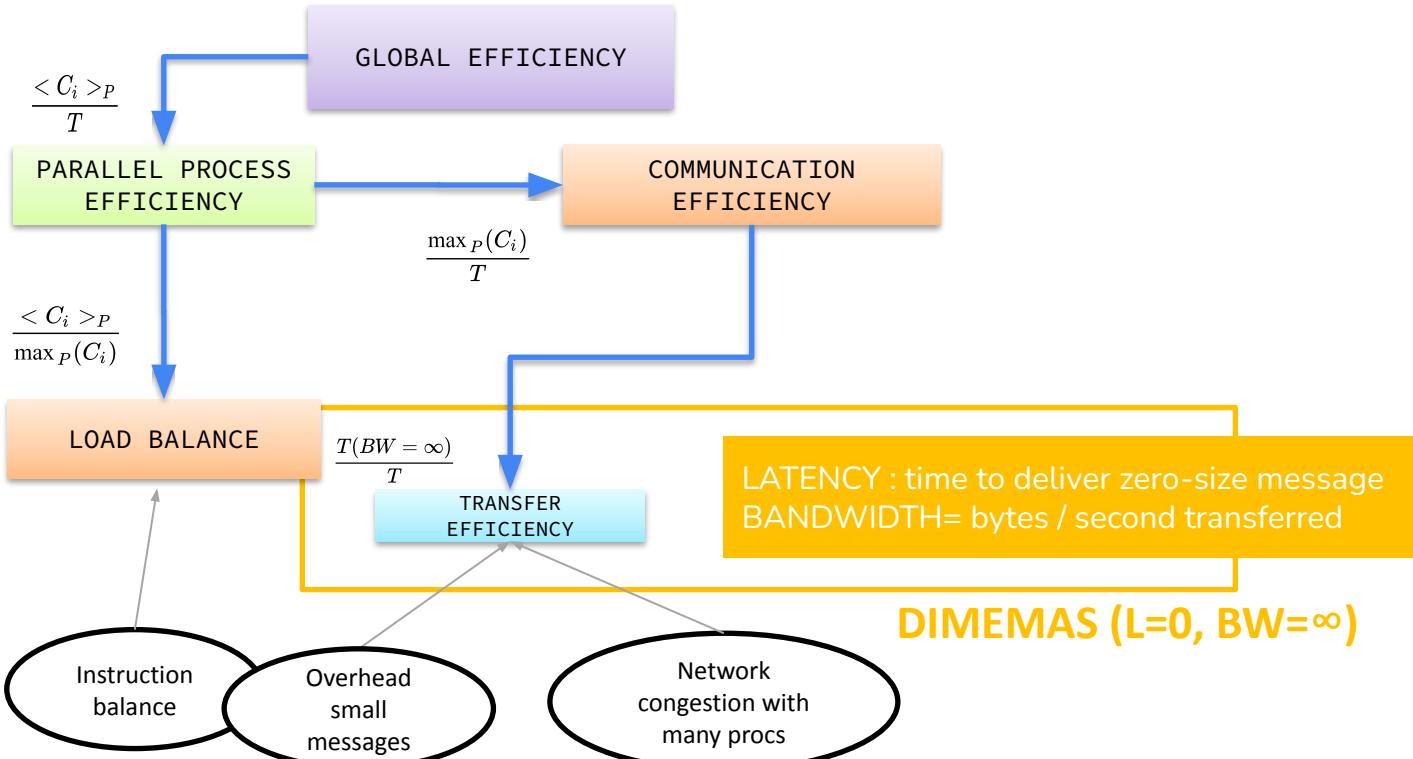


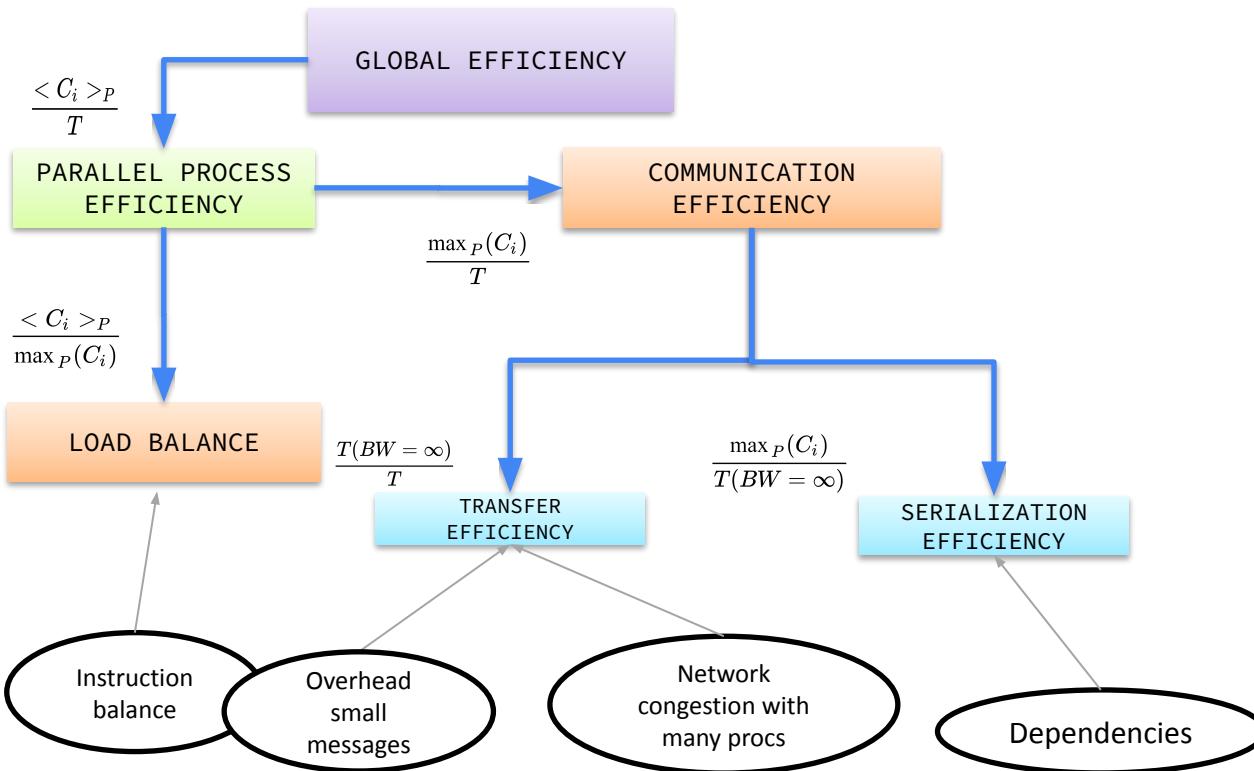


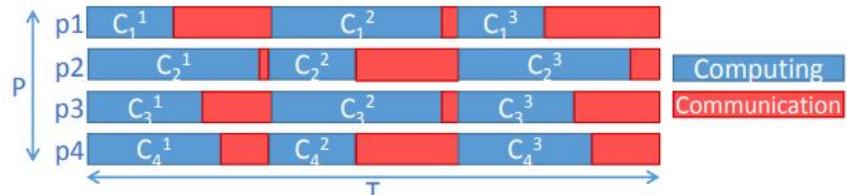


HW counters:
PAPI
PERF
LIKWID

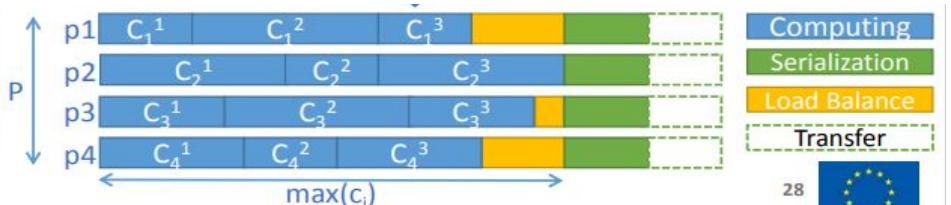
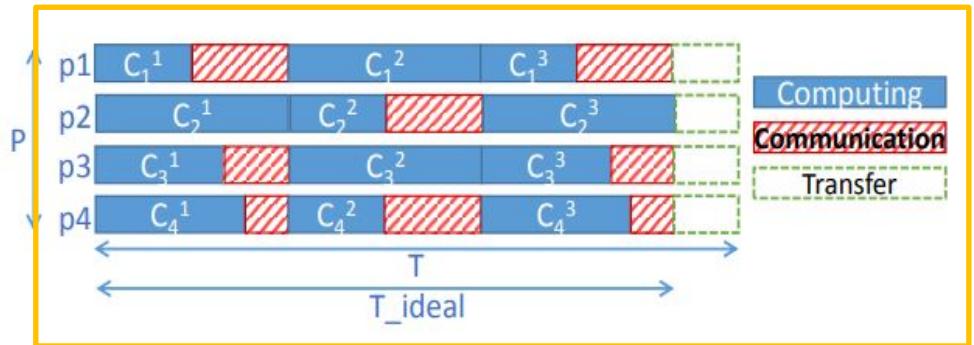
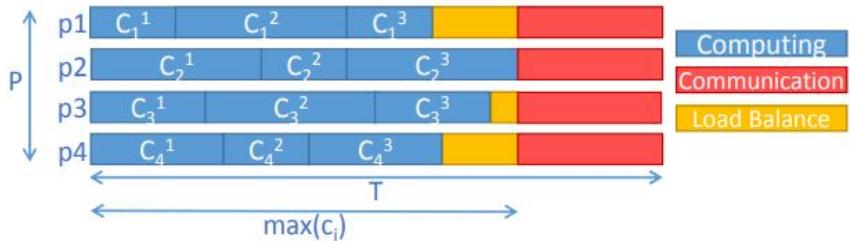


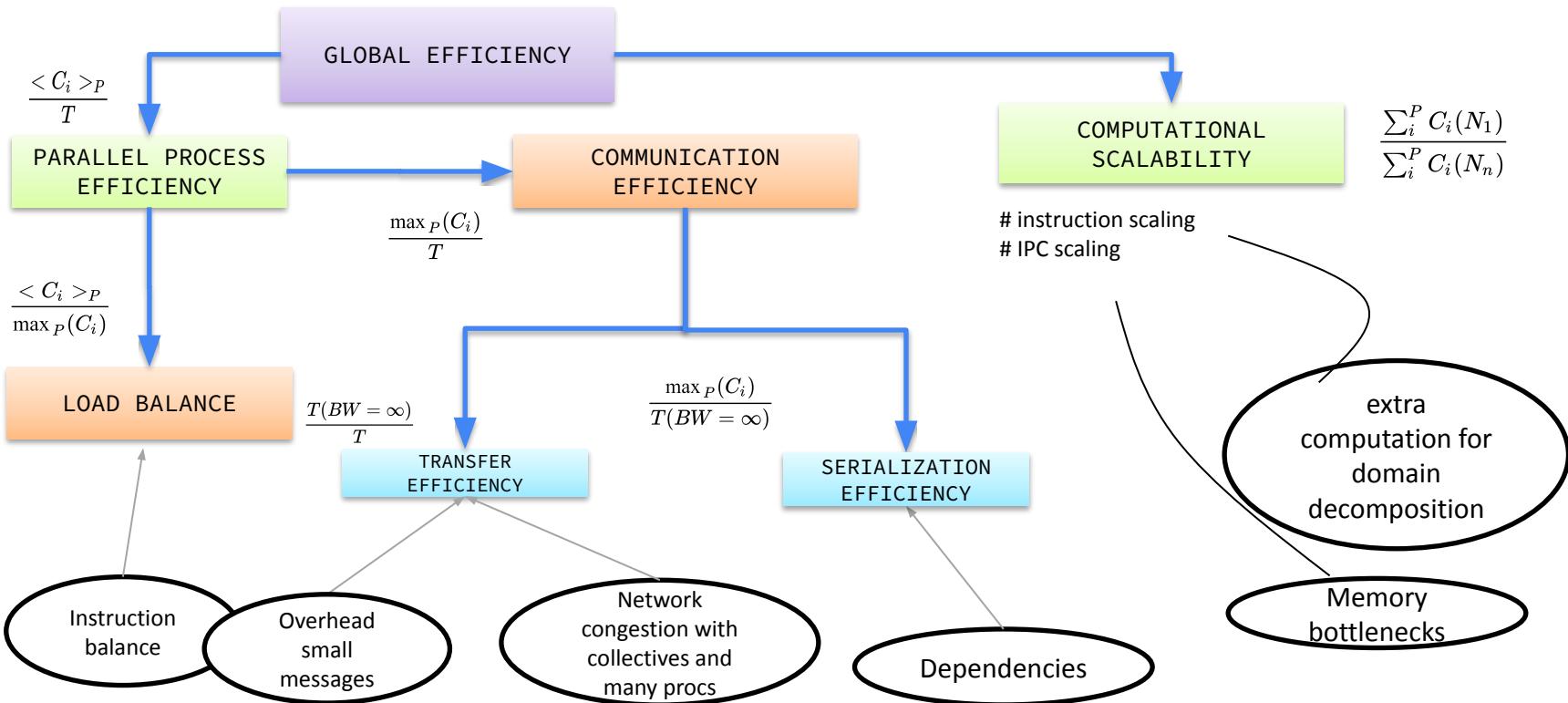






“Collapse” computations





POP metrics AT SCALE

! See how these number change with the number of MPI ranks to identify what limits mostly efficiency in scaling

Number of cores	48	96	192	384	768
Global Efficiency	0.93	0.94	0.93	0.84	0.76
↳ Parallel Efficiency	0.93	0.91	0.87	0.77	0.68
↳ Load balance	0.99	0.98	0.98	0.97	0.95
↳ Communication Efficiency	0.94	0.92	0.89	0.79	0.72
↳ Serialisation	0.95	0.94	0.92	0.85	0.81
↳ Transfer efficiency	0.99	0.99	0.97	0.94	0.89
↳ Computational Scaling	1.00	1.03	1.07	1.09	1.12
↳ Instruction Scaling	1.00	0.99	0.97	0.95	0.92
↳ IPC Scaling	1.00	1.05	1.10	1.18	1.27

! Score-P plugin for this

POP metrics for OpenMP

Which could be the main causes of bottlenecks for an OpenMP application?



POP metrics for OpenMP

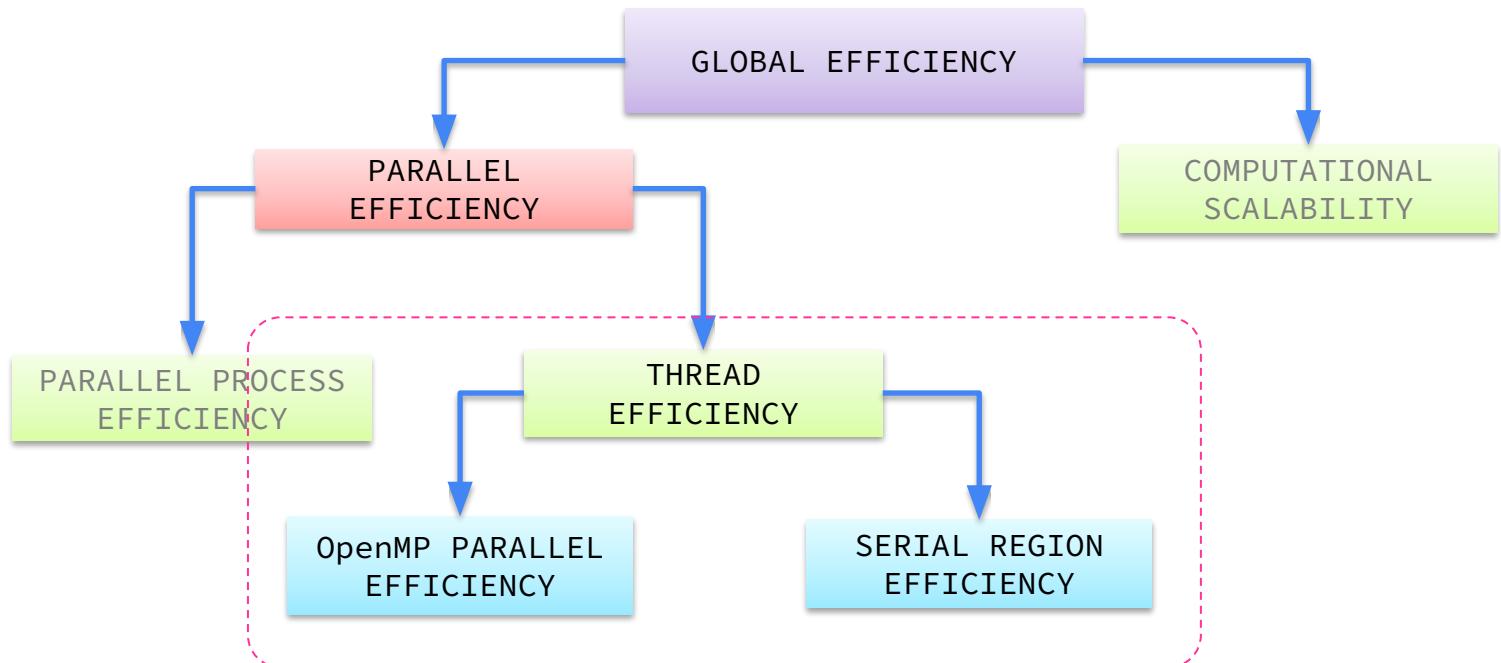
Which could be the main causes of bottlenecks for an OpenMP application?

Serialization:

- time spent in computation outside OpenMP
Are there costly serial region which might exploit OpenMP?

OpenMP parallel efficiency

- Load balance - *Improve scheduling, avoid if*
- Overhead of forking - *Extend parallel regions across multiple loops*
- Synchronizations
- Reduction, Atomic



Profiling softwares Scalasca and Score-P

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Scalasca

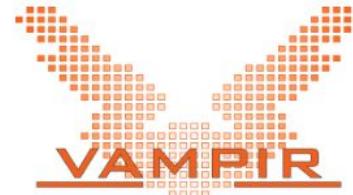
- * Scalable performance analysis of large scale applications, developed at Jülich Supercomputing Centre.
 - * Supports analysis at large scale by exploiting available processors and memory
 - * Ideal tool to investigate synchronization issues and workload imbalance in communication-intensive applications with thousands of cores.
 - * **MPI, OpenMP, user-defined routine** instrumentation
 - * Supports HWC metrics via PAPI.
-
- **Score-P** for source-code instrumentation
 - **CUBE / Vampir** for profile and traces visualization (but ITAC works as well!)

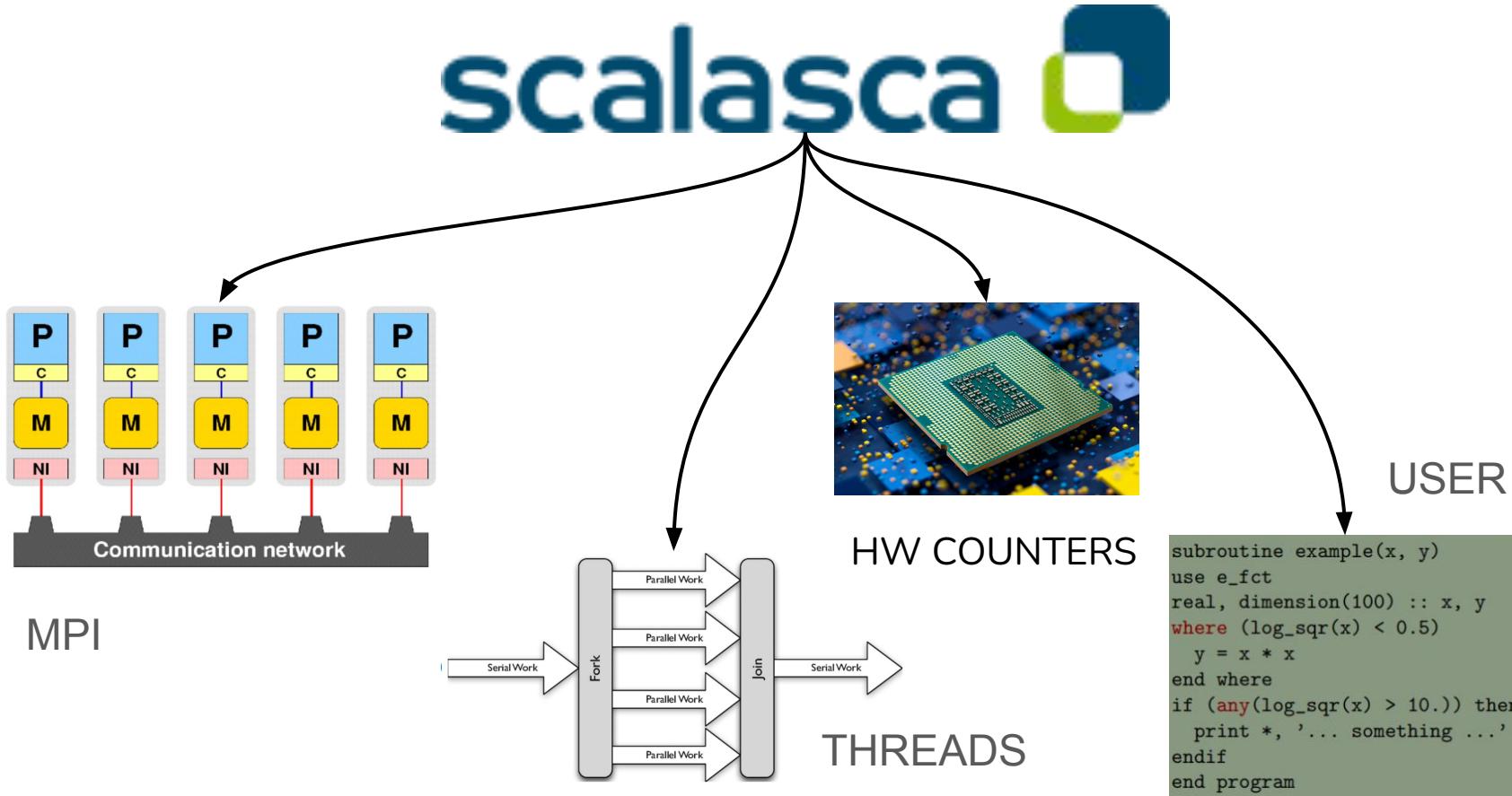


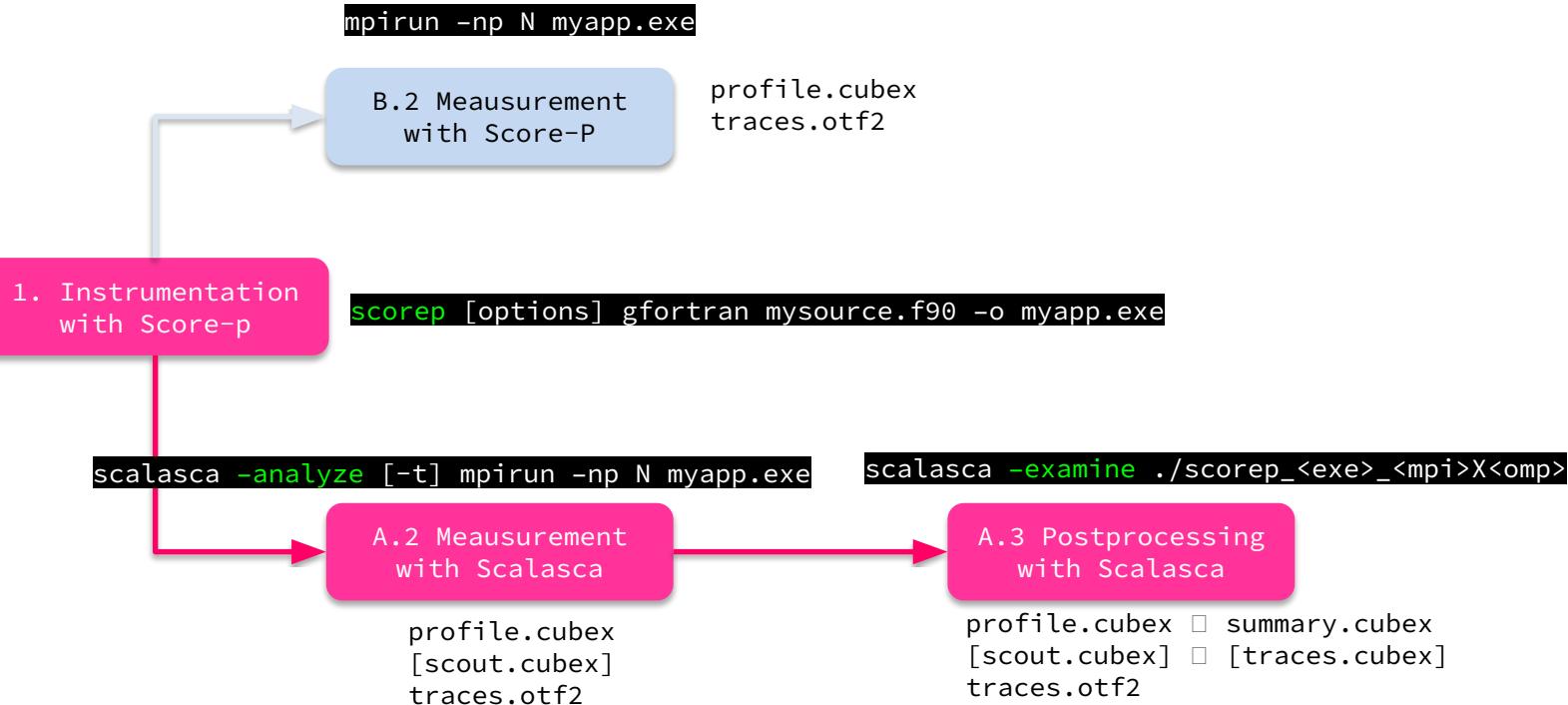
SCALABLE

PERFORMANCE ANALYSIS

OF LARGE SCALE APPLICATIONS





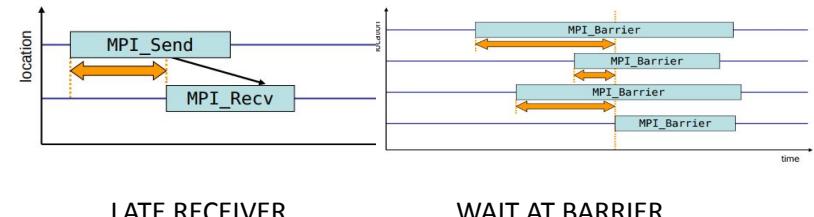


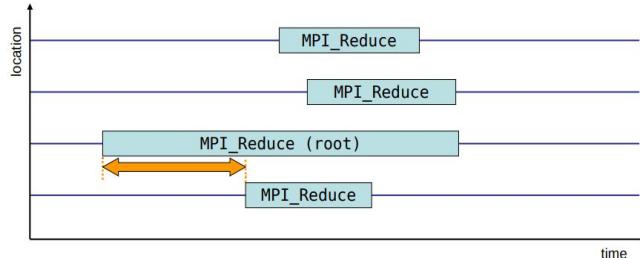
MAIN METRICS

- Time
 - Computation
 - MPI
 - > Synchronization
 - > Management
 - > Communications
 - > MPI I/O
 - OpenMP
- Counts
- Bytes transferred : PtoP vs collective
- MPI io bytes
- + Hardware counters [PAPI]
- + timestamps, locations, communicators (traces)

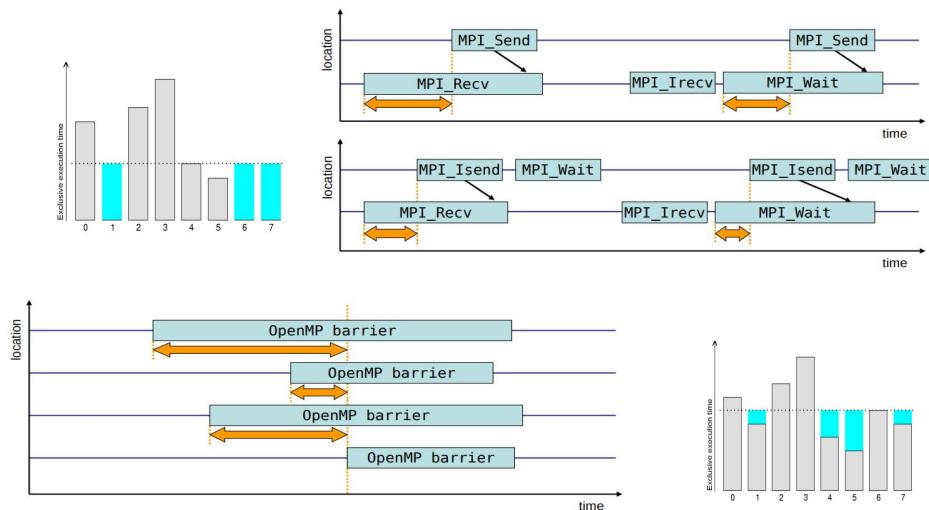
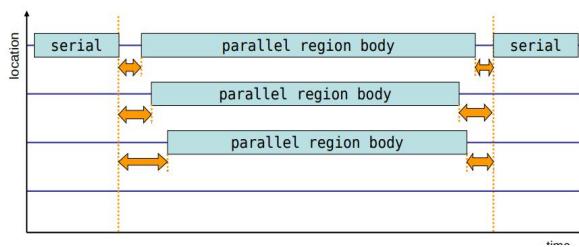
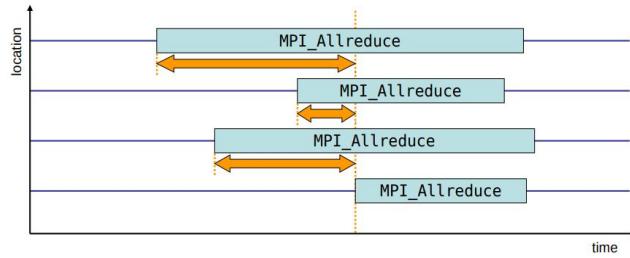
DERIVED METRICS

- MPI and Thread efficiency of POP assessment (plugin)
- Workload balance and synchronization
 - Computational imbalance
 - Idle threads
 - Late receiver, wait at barrier ...

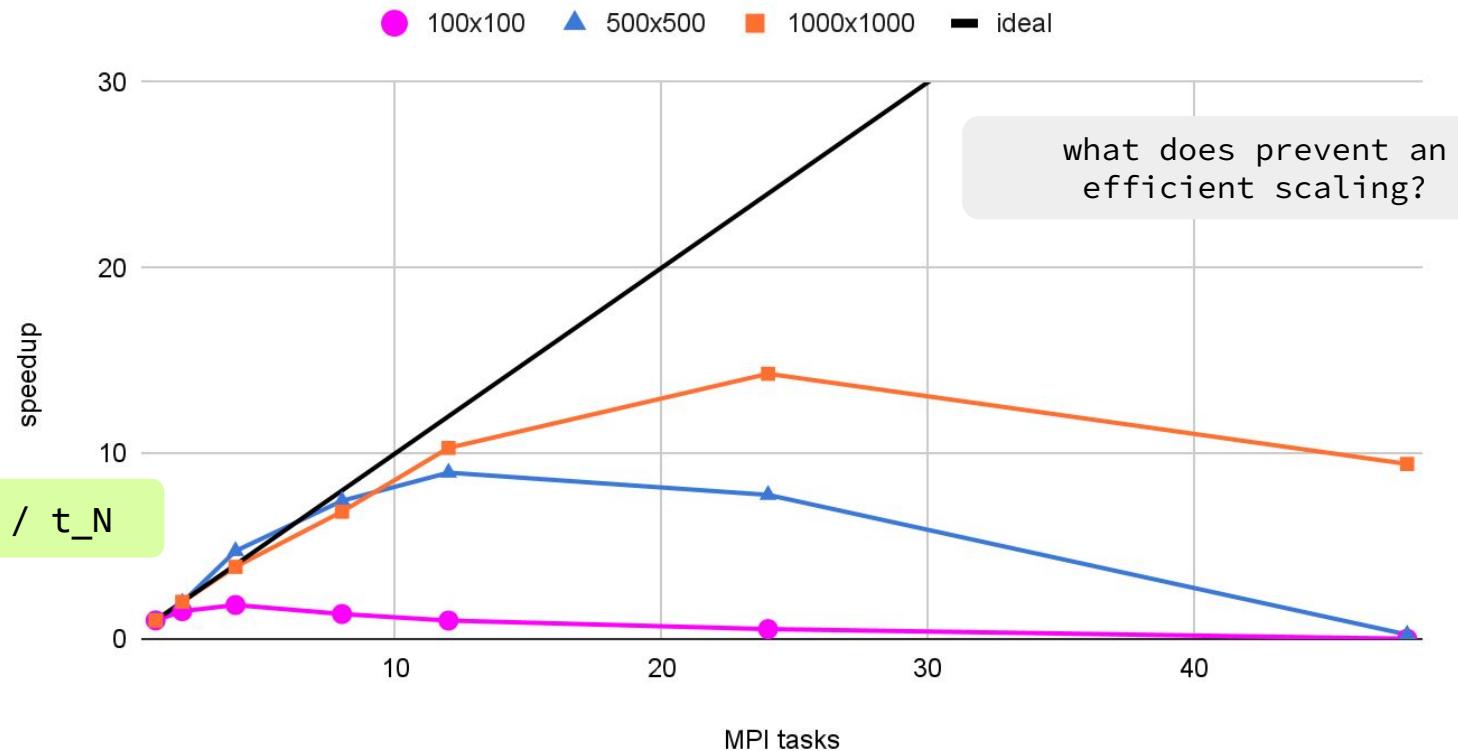




https://www.vi-hps.org/cms/upload/material/tw-original/vi-hps-tw-original-Scalasca_Patterns.pdf



JACOBI EXAMPLE



Scalasca

- * INSTRUMENTATION : add prefix at compile and linking stage

```
scorep [--mpp=mpi --user --openmp --verbose ...] mpif90 source.f90 -o myapp.exe
```

- The options define the events you want to instrument
- If using CMake or autotools the commands differ a bit, check the user guide

- * MEASUREMENT : add prefix to mpirun, -t for traces

```
scalasca -analyze [ -t ] mpirun -np NP ./myapp.exe
```

- Results in folder “scorep_myapp_<NP>X<M>”
- **-t** option for traces
- Never trace at first!

INSTRUMENTATION AND MEASUREMENT

1. Before tracing, check the memory required according to the events traced with

```
scorep-score scorep_cfd_14_trace/profile.cubex
```

Estimated aggregate size of event trace: 1181MB

Estimated requirements for largest trace buffer (max_buf): 85MB

Estimated memory requirements (SCOREP_TOTAL_MEMORY): 87MB

(hint: When tracing set SCOREP_TOTAL_MEMORY=87MB to avoid intermediate flushes or reduce requirements using USR regions filters.)

flt	type	max_buf[B]	visits	time[s]	time[%]	time/visit[us]	region
	ALL	88,407,491	51,464,585	291.42	100.0	5.66	ALL
	USR	88,128,408	51,408,225	59.01	20.2	1.15	USR
	MPI	254,960	42,290	192.44	66.0	4550.40	MPI
	COM	24,096	14,056	39.63	13.6	2819.40	COM
	SCOREP	51	14	0.35	0.1	24757.11	SCOREP

From here you can also infer the amount of time spent in MPI, or USR routines

INSTRUMENTATION AND MEASUREMENT

- With **-r** option you can also get a flat profile of the events traced (MPI, user)

```
scorep-score -r scorep_cfd_14_trace/profile.cubex
```

USR	66,060,288	38,535,168	3.68	1.3	0.10	cfdio_mp_colfunc_
USR	22,020,096	12,845,056	5.09	1.7	0.40	cfdio_mp_hue2rgb_
MPI	188,188	24,024	0.52	0.2	21.47	MPI_Sendrecv
MPI	66,066	14,014	0.81	0.3	57.96	MPI_Allreduce
MPI	60,593	2,028	0.17	0.1	81.59	MPI_Recv
MPI	59,059	2,002	0.02	0.0	8.03	MPI_Send
COM	24,024	14,014	0.07	0.0	5.14	boundary_mp_haloswap_
USR	24,000	14,000	29.97	10.3	2140.95	jacobi_mp_jacobistep_
USR	24,000	14,000	20.26	7.0	1447.21	jacobi_mp_deltasq_

These are ordered according to buffer size, helpful to consider events to filter out.

For example here the first routines related to IO at the end of the run require large buffers, and are not interesting for our analysis.

INSTRUMENTATION AND MEASUREMENT

3. Filter events

```
cat filter.file
SCOREP_REGION_NAMES_BEGIN
    EXCLUDE
        cfdio_mp_colfunc_
        cfdio_mp_hue2rgb_
SCOREP_REGION_NAMES_END
```

And check the estimated buffer with filter applied

```
scorep-score -f filter.file scorep_cfd_14_trace/profile.cubex
```

Estimated aggregate size of event trace: 5MB

Estimated requirements for largest trace buffer (max_buf): 320kB

Estimated memory requirements (SCOREP_TOTAL_MEMORY): 4097kB

If satisfied, repeat the measurement with **scalasca analyse -f filter.file**

POSTPROCESSING AND VISUALIZATION

- * POSTPROCESSING : derive metrics with Scalasca

```
scalasca -examine [options] scorep_myapp_NPXM
```

- derives metrics from the fundamental ones
- opens the profile in CUBE

- * VISUALIZATION : open *.cubex with cubegui

```
cube scorep_myapp_NPXM/summary.cubex
```

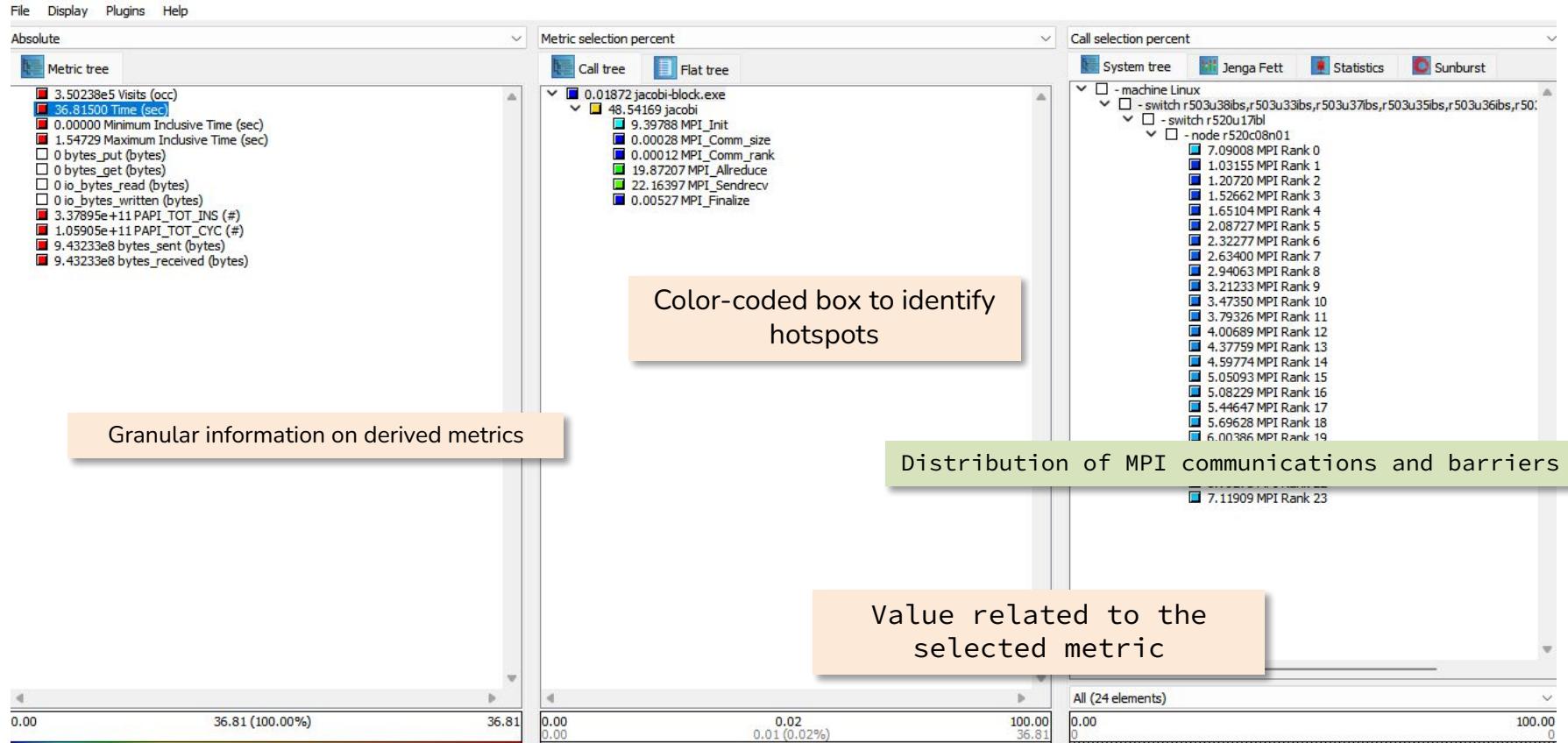
There are a number of environment variable to customize your measurement

<https://scorepci.pages.jsc.fz-juelich.de/scorep-pipelines/docs/scorep-6.0/html/scorepmeasurementconfig.html>

export SCOREP_PAPI_METRIC → PAPI_TOT_INS, PAPI_TOT_CYC, ...

export SCOREP_TOTAL_MEMORY → to increase the buffer memory against buffer flushes

GUI



MANUAL INSTRUMENTATION

- * Score-P automatically instruments the user-defined routines in the source code
 - * Additional instrumentation is possible to label source code regions as with a name
1. Include the scorep file with definitions after “implicit none”

```
#include "scorep/SCOREP_User.inc"
```

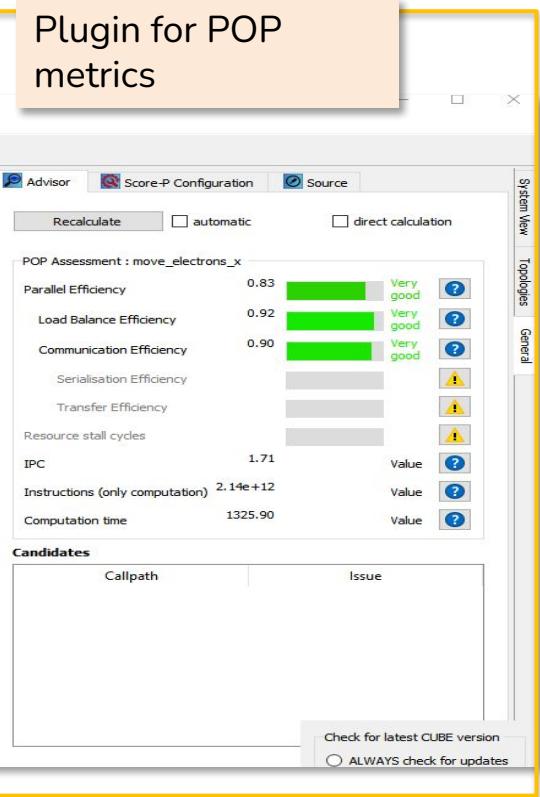
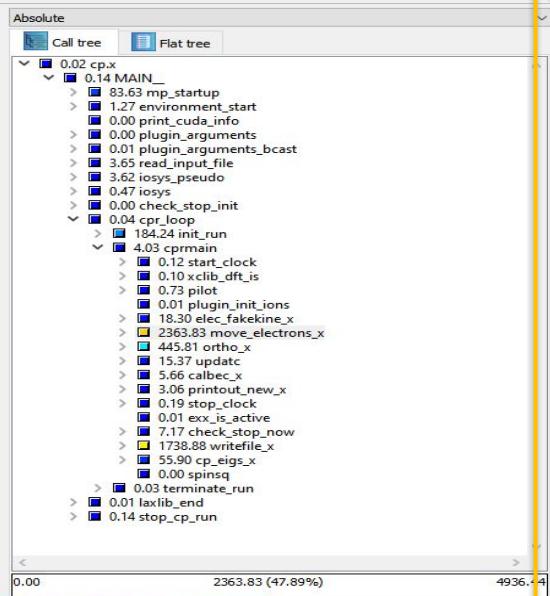
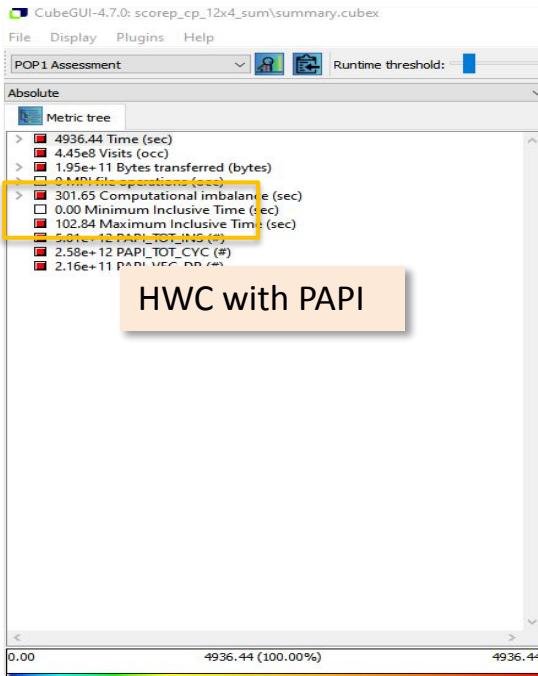
2. Initialize an handle

```
SCOREP_USER_REGION_DEFINE( myhandle1 )
```

3. Add APIs to start and stop the regions

```
#start the region to name as “block”
SCOREP_USER_REGION_BEGIN( myhandle, "block", SCOREP_USER_REGION_TYPE_COMMON )
...
#stop the region to name as “block”
SCOREP_USER_REGION_END( myhandle )
```

GUI



POP ASSESSMENT PLUGIN

try different algorithm?

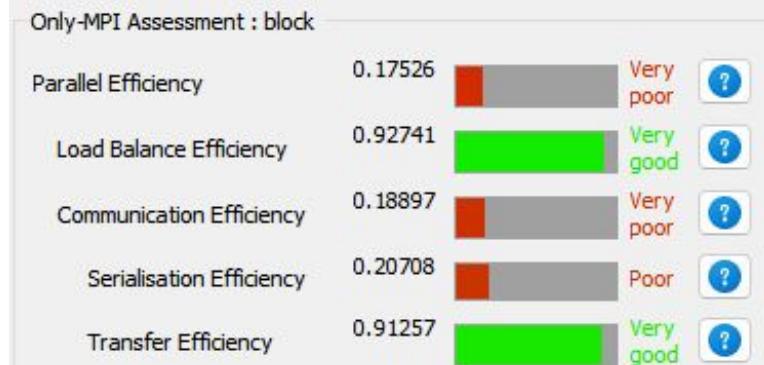
4



12



24



48

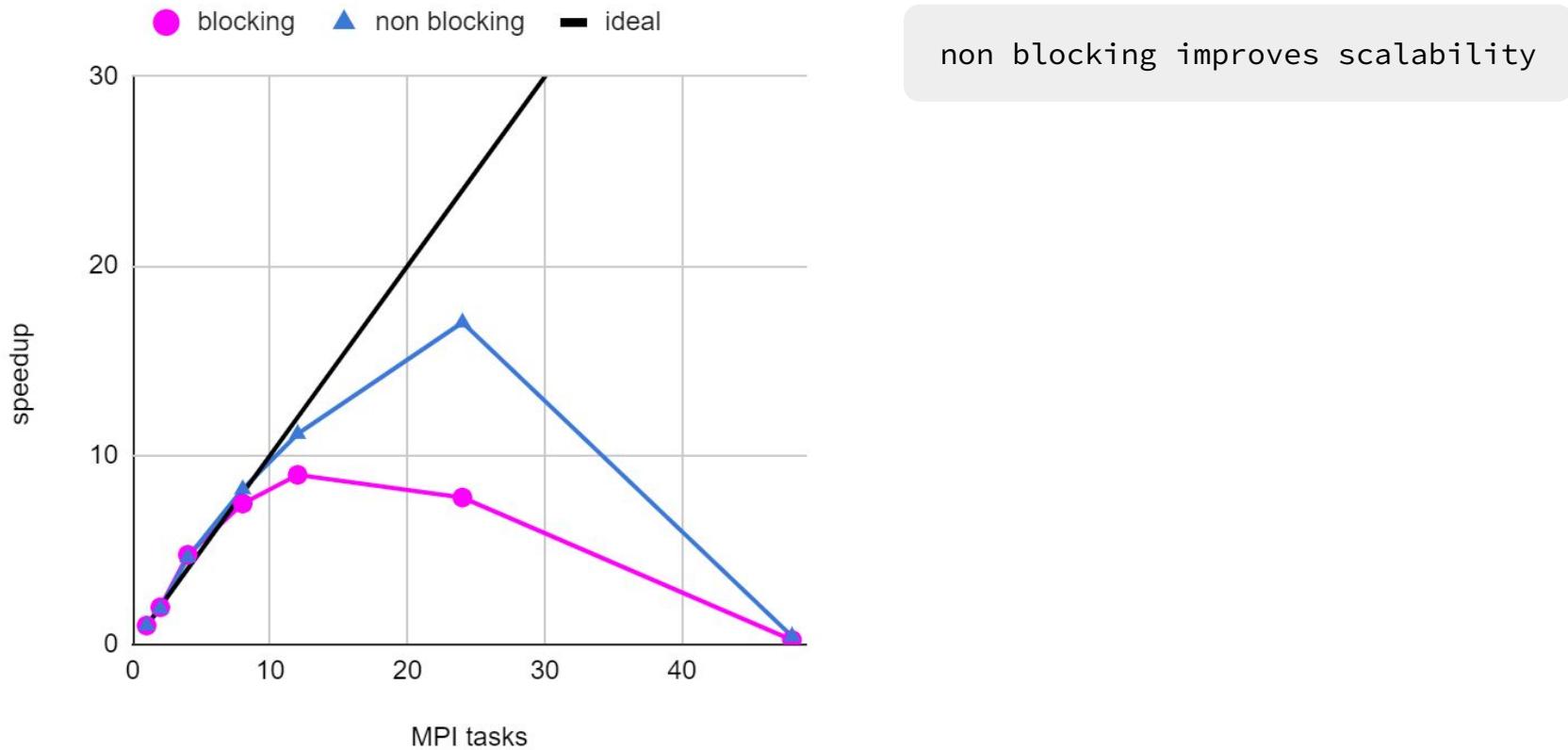


JACOBI EXAMPLE

try a non-blocking communication

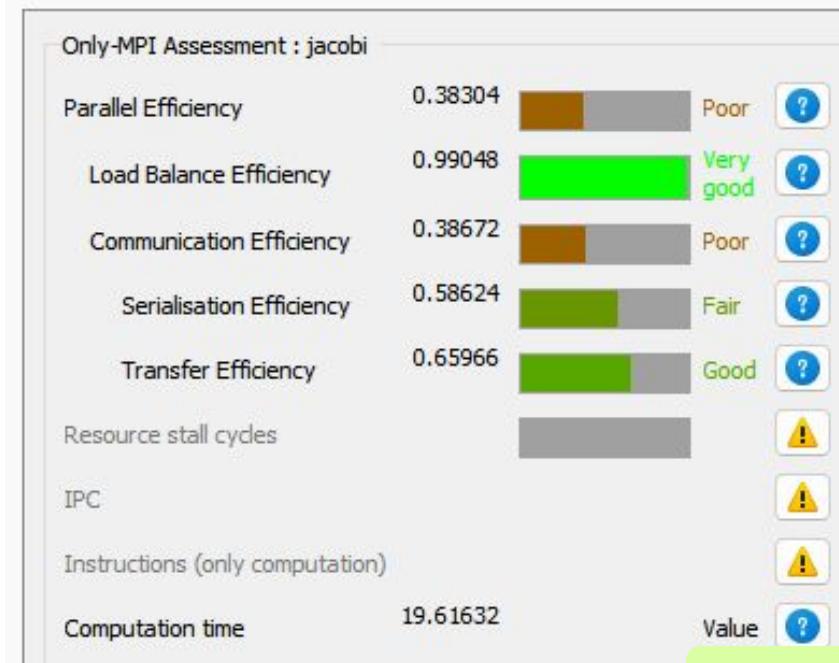
```
[lbellen1@login02 2-itac]$ diff isendirecv/Fortran/jacobi-mpi-sendrecv.f90 sendrecv/Fortran/jacobi-mpi-sendrecv.f90
101,104c101,104
<     call mpi_isend(grid(1,1), ny, MPI_DOUBLE, myrank-1, 0, MPI_COMM_WORLD,requests(1), ierr)
<     call mpi_irecv(grid(1,0), ny, MPI_DOUBLE, myrank-1, 0, MPI_COMM_WORLD, requests(2), ierr)
<     !call mpi_sendrecv(grid(1,1),ny,MPI_DOUBLE,myrank-1,0,grid(1,0),ny,&
<           MPI_DOUBLE,myrank-1,0,MPI_COMM_WORLD,status,ierr)
---
>     !call mpi_isend(grid(1,1), ny, MPI_DOUBLE, myrank-1, 0, MPI_COMM_WORLD,requests(1), ierr)
>     !call mpi_irecv(grid(1,0), ny, MPI_DOUBLE, myrank-1, 0, MPI_COMM_WORLD, requests(2), ierr)
>     call mpi_sendrecv(grid(1,1),ny,MPI_DOUBLE,myrank-1,0,grid(1,0),ny,&
>                       MPI_DOUBLE,myrank-1,0,MPI_COMM_WORLD,status,ierr)
111,114c111,114
<     call mpi_isend(grid(1,local_nx), ny, MPI_DOUBLE, myrank+1, 0, MPI_COMM_WORLD, requests(3), ierr)
<     call mpi_irecv(grid(1,local_nx+1), ny, MPI_DOUBLE, myrank+1, 0, MPI_COMM_WORLD,requests(4), ierr)
<     !call mpi_sendrecv(grid(1,local_nx), ny, MPI_DOUBLE, myrank+1, 0,grid(1,local_nx+1),&
<           ny, MPI_DOUBLE, myrank+1, 0, MPI_COMM_WORLD, status,ierr)
---
>     !call mpi_isend(grid(1,local_nx), ny, MPI_DOUBLE, myrank+1, 0, MPI_COMM_WORLD, requests(3), ierr)
>     !call mpi_irecv(grid(1,local_nx+1), ny, MPI_DOUBLE, myrank+1, 0, MPI_COMM_WORLD,requests(4), ierr)
>     call mpi_sendrecv(grid(1,local_nx), ny, MPI_DOUBLE, myrank+1, 0,grid(1,local_nx+1),&
>                       ny, MPI_DOUBLE, myrank+1, 0, MPI_COMM_WORLD, status,ierr)
117c117
<     call mpi_waitall(4, requests, MPI_STATUSES_IGNORE, ierr)
---
> !     call mpi_waitall(4, requests, MPI_STATUSES_IGNORE, ierr)
```

JACOBI EXAMPLE



POP ASSESSMENT PLUGIN

blocking



non blocking



non blocking reduces dependencies

ITAC

Source-code instrumentation providing summary and **Trace** Collector and Analyzer for communication hotspots

- * **MPI** and **OpenMP** time and imbalance
- * **USR routines** instrumentation
- * **Ideal traces** to measure interconnect vs waiting time

```
module load intel-oneapi-mpi intel-oneapi-compilers intel-oneapi-itac
mpiifort -trace [-tcollect] mycode.f90
srun ./mycode → *.stf
traceanalyzer *.stf
```

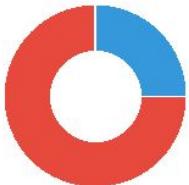
Summary: jacobi-mpi-instr.exe.stf

Total time: 8 sec. Resources: 24 processes, 1 node.

[Continue >](#)

Ratio

This section represents a ratio of all MPI calls to the rest of your code in the application.



Serial Code - 2.01 sec 25.1 %

OpenMP - 0 sec 0 %

MPI calls - 5.99 sec 74.8 %

Exclude from total time

Where to start with analysis

For deep analysis of the MPI-bound application click "Continue >" to open the tracefile View and leverage the **Intel® Trace Analyzer** functionality:

- *Performance Assistant* - to identify possible performance problems
- *Imbalance Diagram* - for detailed imbalance overview
- *Tagging/Filtering* - for thorough customizable analysis

Top MPI functions

This section lists the most active MPI functions from all MPI calls in the application.

MPI_Sendrecv	3.03 sec (37.5 %)
MPI_Allreduce	2.94 sec (36.4 %)
MPI_Finalize	0.013 sec (0.161 %)
MPI_Comm_size	0.000271 sec (0.00335 %)
MPI_Comm_rank	0.000165 sec (0.00204 %)

MOST TIME-CONSUMING MPI CALLS

To optimize node-level performance use:

Intel® VTune™ Profiler for:

- algorithmic level tuning with hpc-performance and threading efficiency analysis;
- microarchitecture level tuning with general exploration and bandwidth analysis;

Intel® Advisor for:

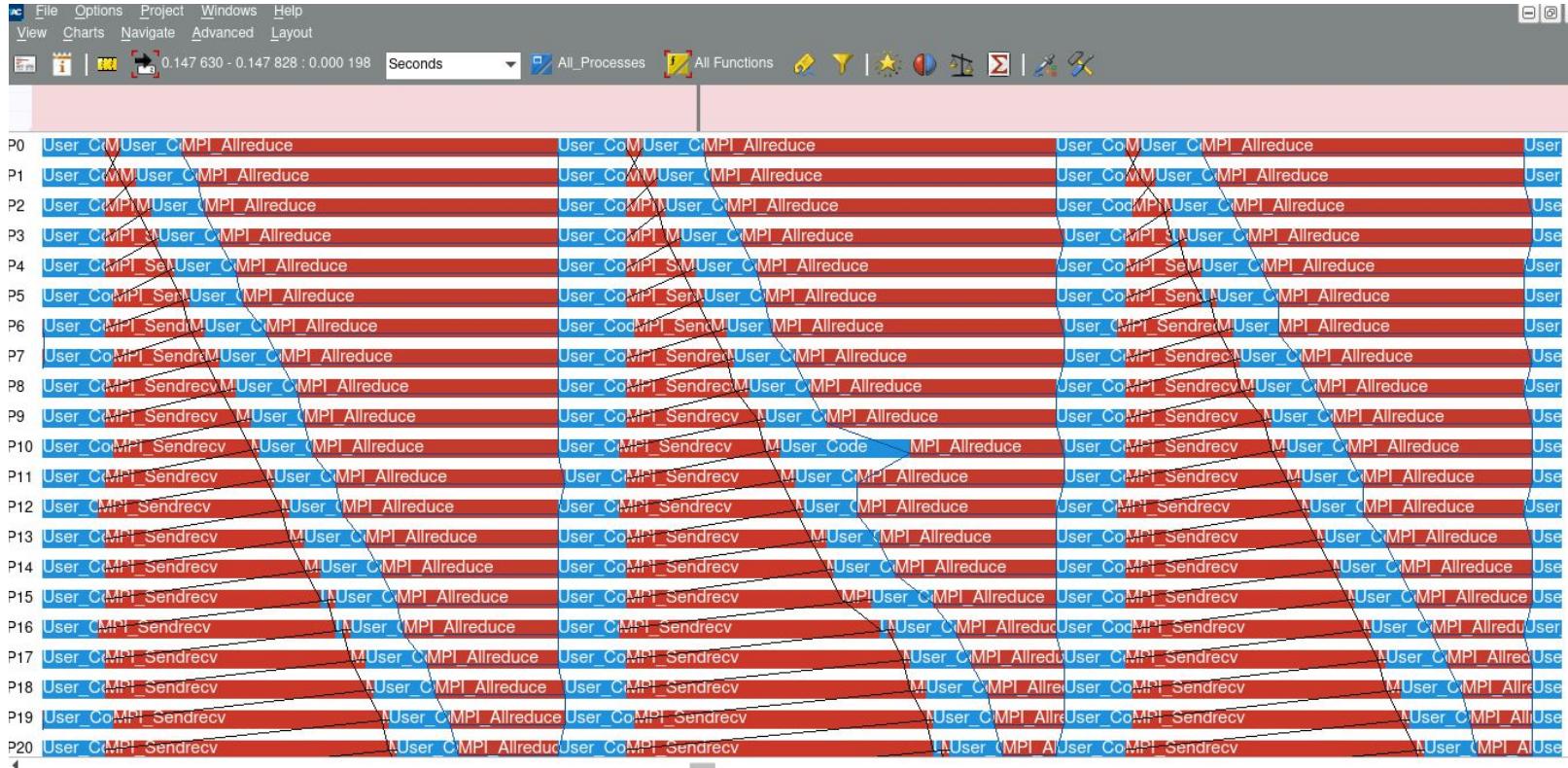
- vectorization optimization and thread prototyping.

For more information, see documentation for the respective tool:

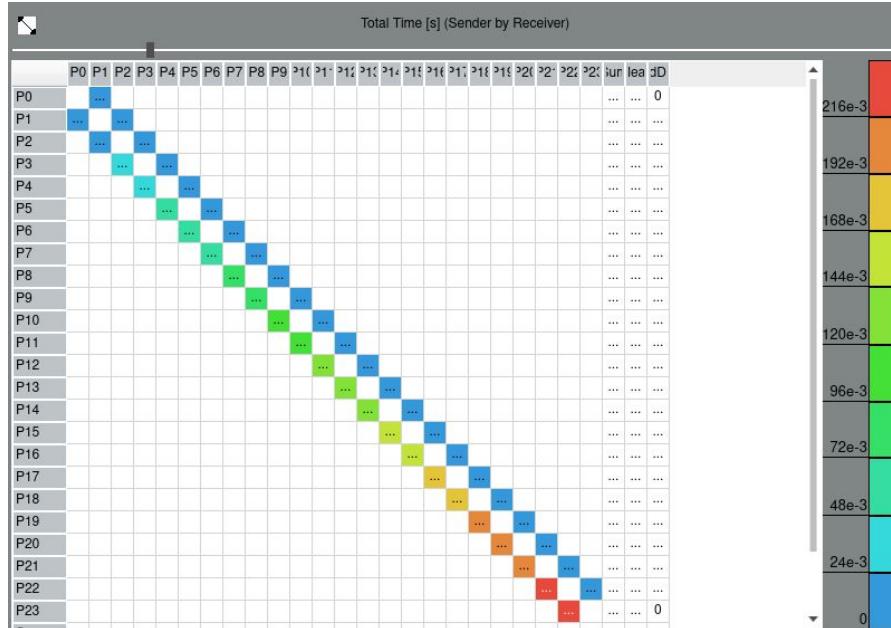
[Analyzing MPI applications with Intel® VTune™ Profiler](#)

[Analyzing MPI applications with Intel® Advisor](#)

ITAC - TRACE VISUALIZATION



ITAC - MESSAGE PROFILE

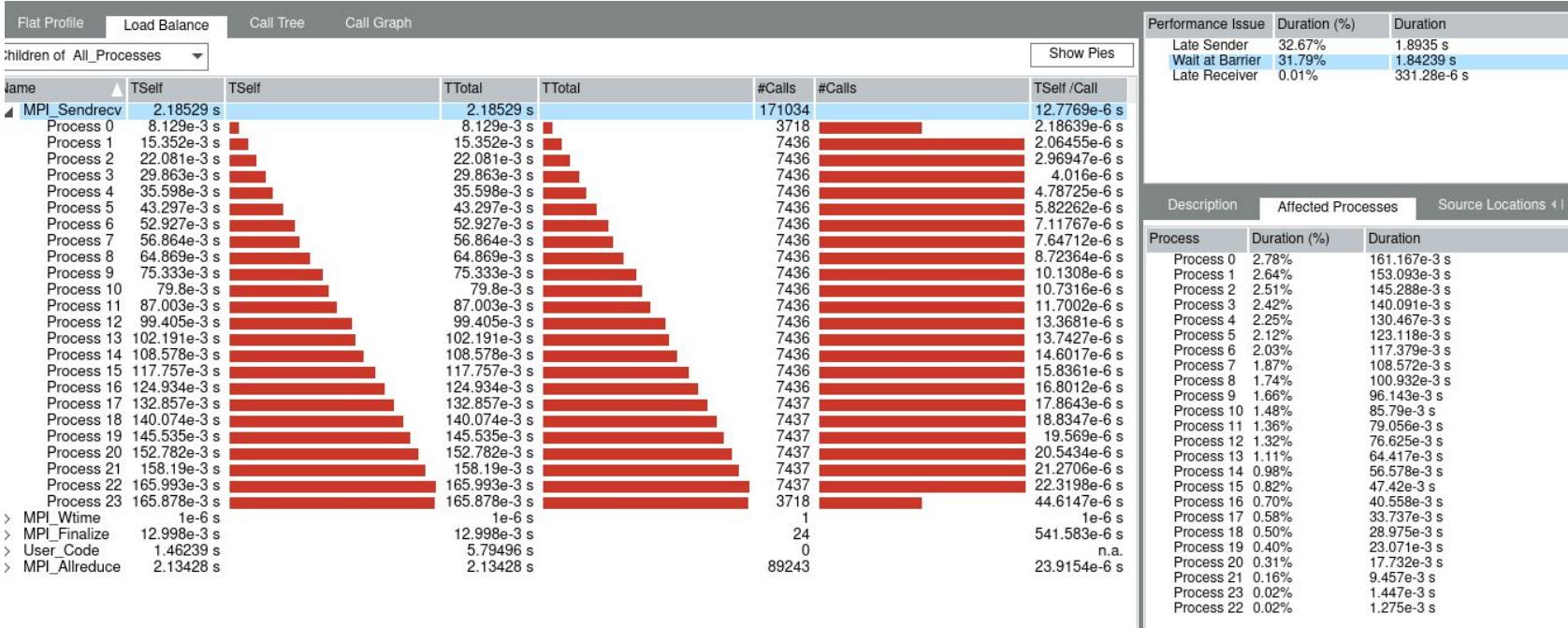


TIME

MESSAGE VOLUME

AVERAGE TRANSFER TIME

ITAC - FUNCTION PROFILE

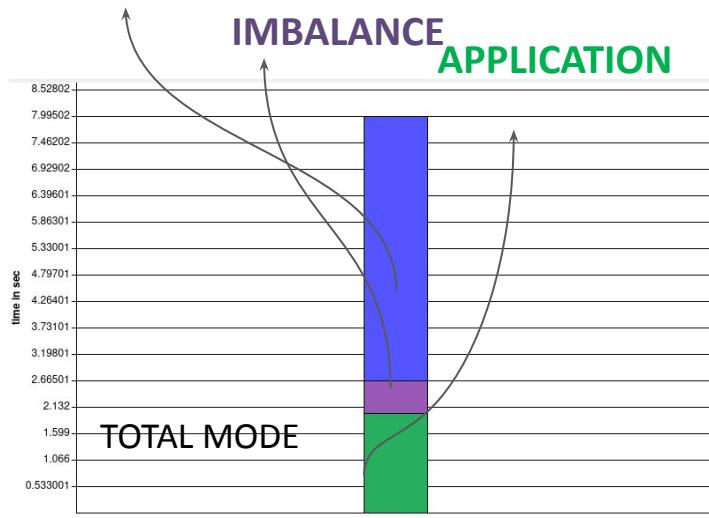


ITAC - IDEAL TRACES

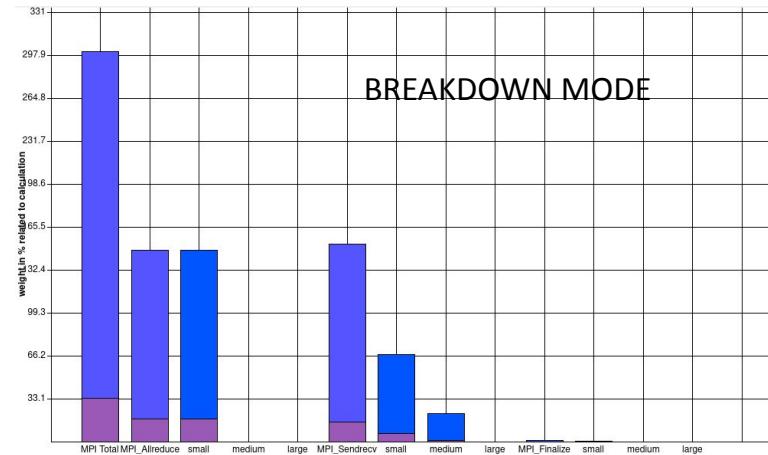


ITAC - IMBALANCE DIAGRAM

INTERCONNECT



Advanced > Event timeline
Advanced > Imbalance Diagram



Interconnect → time spent waiting

Imbalance → load balance

time transfer → $T_{real} - T_{ideal}$

APPLICATION PERFORMANCE SNAPSHOT

- * Does not require source code instrumentation
- * Provides summaries about MPI, OpenMP and memory
- * Provides hints on the bottleneck, suggest analysis with VTUNE

```
mpirun <options> aps <my-app>
```

```
aps --report aps_result_<date>
```

APPLICATION PERFORMANCE SNAPSHOT



Application Performance Snapshot

Application: `cfd`
Report creation date: 2024-06-20 16:49:45
Number of ranks: 56
Ranks per node: 56
HW Platform: Intel(R) Xeon(R) Processor code named Sapphirerapids
Frequency: 2.00 GHz
Logical Core Count per node: 112
Collector type: Driverless Perf system-wide counting

69.13 s 0.88 F 0 130.01

Elapsed Time IPC Rate SP GFLOPS DP GFLOPS

2.79 GHz

Average CPU Frequency

MPI Time

22.24 s 32.17% of Elapsed Time
MPI Imbalance
8.99 s
13.01% of Elapsed Time

TOP 5 MPI Functions % of Elapsed Time

MPI Function	% of Elapsed Time
MPI_Finalize	10.2%
MPI_Ssend	9%
MPI_Allreduce	7.92%
MPI_Init	2.99%
MPI_Sendrecv	1.97%

Disk I/O Bound

0.01% of Elapsed Time
Disk read
0.4 KB
Disk write
0.0 KB

CPU Utilization

99.6%
Average CPU Utilization
111.56 out of 112 logical CPUs

Memory Footprint

Resident
125.46 MB

Resident per Node
7026 MB

Virtual
843.12 MB

Virtual Per Node
47215 MB

Your application is MPI bound.

This may be caused by high busy wait time inside the library (imbalance), non-optimal communication schema or MPI library settings. Use [MPI profiling tools](#) like [Intel® Trace Analyzer](#) and [Collector](#) to explore performance bottlenecks.

	Current run	Target	Tuning Potential
MPI Time	32.17%	<10%	<div style="width: 100%; background-color: #800000; height: 10px;"></div>
CPU Utilization	99.6%	>90%	<div style="width: 99.6%; background-color: #800000; height: 10px;"></div>
Memory Stalls	29.7%	<20%	<div style="width: 29.7%; background-color: #800000; height: 10px;"></div>
Vectorization	99.5%	>70%	<div style="width: 99.5%; background-color: #800000; height: 10px;"></div>
Disk I/O Bound	0.01%	<10%	<div style="width: 0.01%; background-color: #800000; height: 10px;"></div>

Memory Stalls

29.7% of Pipeline Slots
Cache Stalls
29.3% of Cycles
DRAM Stalls
0.2% of Cycles
DRAM Bandwidth
Average
4.92 GB/s
Peak
218.29 GB/s
Bound
0.2%

NUMA
2.6% of Remote Accesses

Vectorization

99.5%
Instruction Mix
SP FLOPs
0% of uOps
DP FLOPs
21.2% of uOps
Packed: 99.5% from DP FP
128-bit: 99.5%
256-bit: 0%
512-bit: 0%
Scalar: 0.5% from DP FP
Non-FP
78.8% of uOps
FP Arith/Mem Rd Instr. Ratio
0.63
FP Arith/Mem Wr Instr. Ratio
1.98

VTUNE

- * Does not require source code instrumentation
- * Analyze **CPU** and **(Intel) GPU** performances
- * Supports **MPI**, **OpenMP** and **OpenMP target** codes
- * Provides **traces** with for CPU and GPU utilization, memory access and cache BW

```
vtune -collect <collection-name> ./matrix
```

- performance-summary
- hotspot
- memory-access
- **hpc-performance**

VTUNE hpc-performance collection

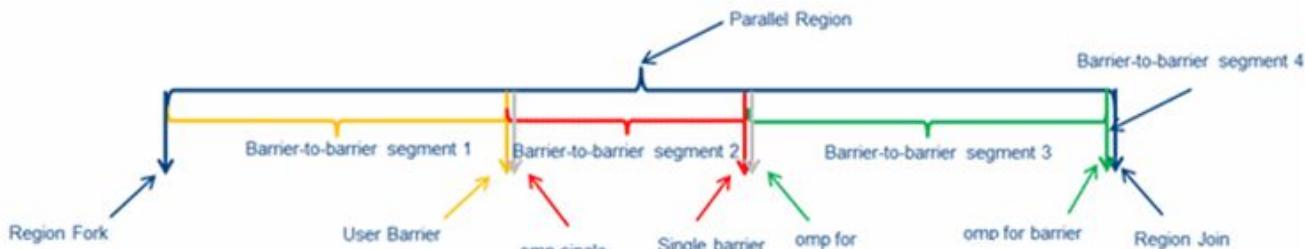
```
!$omp parallel shared ( n ) private ( i, j, prime )
!$omp do reduction ( + : total )
do i = 2, n
    prime = 1
    do j = 2, i - 1
        if ( mod ( i, j ) == 0 ) then
            prime = 0
            exit
        end if
    end do
    total = total + prime
end do
!$omp end do
!$omp end parallel
```

```
ifort -g -qopenmp -O2 -parallel-source-info=2 prime_openmp.f90 -o prime_openmp.exe
vtune -collect hpc-performance ./prime_openmp.exe
```

VTUNE hpc-performance collection

Provides the time spent in the implicit barriers

```
#pragma omp parallel
{
    ....
#pragma omp barrier
#pragma omp single
{
    ...
}
#pragma omp for
{
    ...
}
}
```



VTUNE hpc-performance collection

HPC Performance Characterization ⓘ

Analysis Configuration Collection Log Summary Bottom-up

INTEL VTUNE PROFILER

Elapsed Time ⓘ: 15.247s

SP GFLOPS ⓘ: 0.000
DP GFLOPS ⓘ: 0.000
x87 GFLOPS ⓘ: 4.988
CPI Rate ⓘ: 0.899
Average CPU Frequency ⓘ: 3.1 GHz
Total Thread Count: 12

Effective CPU Utilization ⓘ: 13.4%

Average Effective CPU Utilization ⓘ: 6.436 out of 48

Serial Time (outside parallel regions) ⓘ: 0.101s (0.7%)

Parallel Region Time ⓘ: 15.146s (99.3%)

Estimated Ideal Time ⓘ: 8.229s (54.0%)

OpenMP Potential Gain ⓘ: 6.917s (45.4%)

Top OpenMP Regions by Potential Gain

This section lists OpenMP regions with the highest potential for performance improvement. The Potential Gain metric shows the elapsed time that could be saved if the region was optimized to have no load imbalance assuming no runtime overhead.

OpenMP Region	OpenMP Potential Gain (%) ⓘ	OpenMP Region Time ⓘ
MAIN__\$omp\$parallel:12@g100_work/cin_staff/bellen1/courses_genrepos/debugging-and-code-optimization/profilin g/2023/4-vtune/prime_openmp.f90:174:195	6.917s 45.4%	15.146s

*N/A is applied to non-summable metrics.

VTUNE hpc-performance collection

HPC Performance Characterization ② 📈

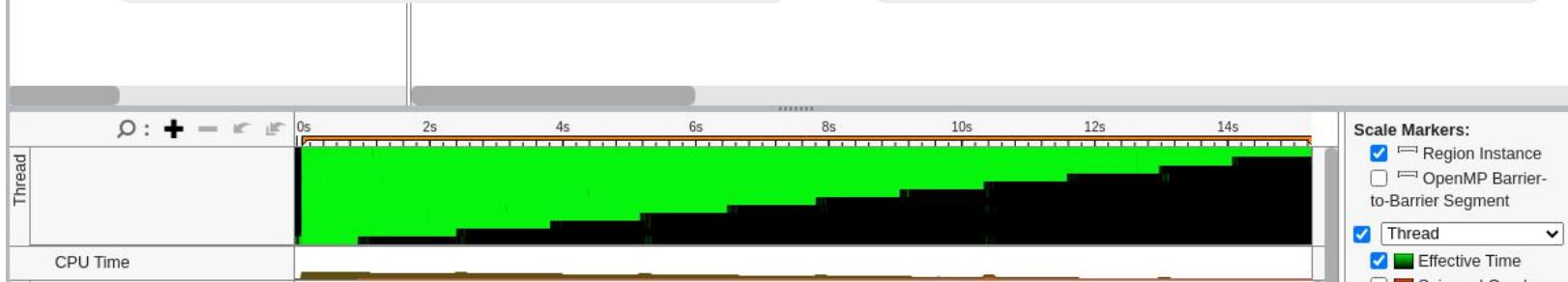
Analysis Configuration Collection Log Summary Bottom-up

Grouping: OpenMP Region / OpenMP Barrier-to-Barrier Segment

STATIC SCHEDULE

OpenMP Region / OpenMP Barrier-to-Barrier Segment	Elapsed Time	SP GFLOPS	OpenMP Potential Gain						CPU Time ▾	S
			Imbalance	Lock Contention	Creation	Scheduling	Reduction	Atomics		
MAIN__\$omp\$parallel:12@g100_work/cin_st	15.146s	5.022	6.917s	0s	0s	0s	0s	101.207s		
MAIN__\$omp\$loop_barrier_segment@/g100_wor	15.146s	5.022	6.917s	0s	0s	0s	0s	101.207s		
▶ MAIN__\$omp\$barrier_segment@/g100_wor	0.000s	0.000	0.000s	0s	0s	0s	0s	0s		
▶ [Serial - outside parallel regions]	0.101s	0.000						0.074s		

IDENTIFY SOURCE OF POTENTIAL GAIN → WORKLOAD IS NOT BALANCED



Scale Markers:

- Region Instance
- OpenMP Barrier-to-Barrier Segment
- Thread
- Effective Time
- Spin and Quiesce

VTUNE hpc-performance collection

