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Optimization of Earth Sciences models

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Introduction

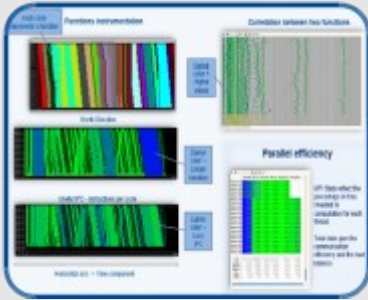
- Created in 2005; more than 400 employees.
- Research, develop and manage information technology.
- Facilitate scientific progress and its application in society.



Earth Science Department

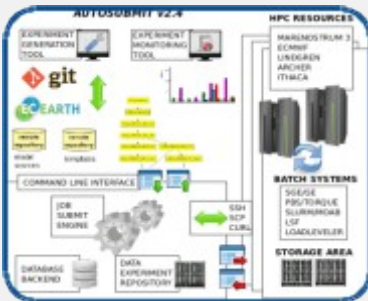
- **Atmospheric composition modelling**
- **Climate prediction modelling**
- **Computational Earth Sciences**
- **Earth Sciences Services**





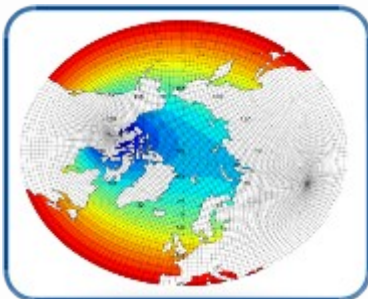
Performance Team

- Provide HPC Services such as performance analysis
- Apply new computational methods



Models and Workflows Team

- Development of HPC user-friendly software framework
- Support the development of atmospheric research software



Data and Diagnostics Team

- Big Data in Earth Sciences
- Provision of data services
- Visualization

- The **necessary refactoring** of numerical codes is receiving lot of attention.
 - Need for computational performance **analysis and optimizations**.
 - Study of **algorithms** suitable for the new generations of HPC platforms.
- Several European **institutions and projects** working together in the same direction (ESiWACE, EsD's, ETP4HPC...)
- **Clock speeds** not increasing further → Supercomputers growing by adding **parallel processing** units.
- **Compilers** doing great work with **low level** optimizations → **Human decisions** in the development are critical to enable optimizations.
- **Overhead** (extra computation and communication) may not be seen as a problem → When demand increase (i.e. higher resolutions), a bad implementation will become a **bottleneck** at some point.
- **High Performance Computing is an essential part of Weather and Climate models nowadays.**

- **Efficient use** of the computational resources
 - Provide **HPC studies** such as performance analysis, identification of bottlenecks and optimization of parallel applications
- **Research** on new computational methods to apply on Earth Sciences models
 - Study of computational and mathematical **algorithms**.
 - Study of novel **architectures** present in new machines.

- Studying the model
 1. Mathematical study
 2. Computational study
 3. Profiling Study
 4. Introducing optimizations
 5. Reproducibility study



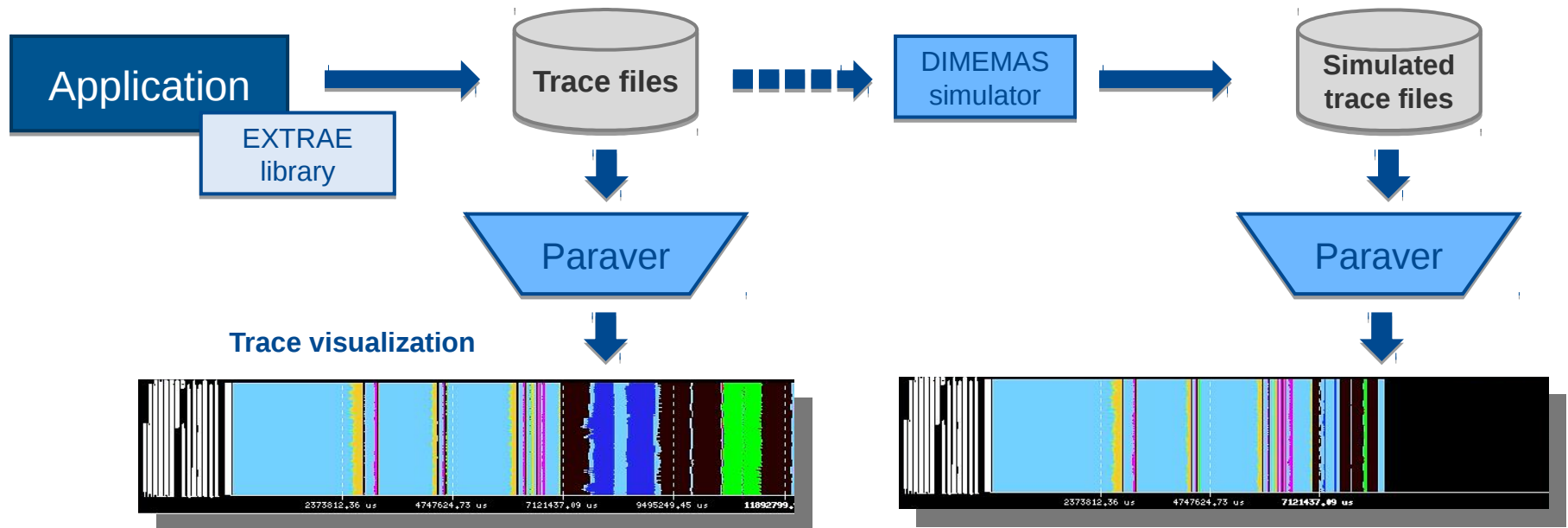
BSC performance tools

- What's **happening** inside a computer during a model execution?
 - This question would be really difficult to answer if we didn't have the proper tools
 - Older approaches, as timing routines fall short to understand what is really happening
- Using the adequate **performance tools** we can try to find an answer

- Having tools able to collect data from every aspect of the application is only part of the equation
- The objective is to **get knowledge** from that data
- Performance tools are intended to use that data to present **useful information**
- It is the expert's job to analyse that information in order to get knowledge and **take conclusions** about the behaviour of the application

- **Trace:**
 - Event & state history of an application run, for a subsequent analysis.

- Since 1991
- Based on traces
- Open Source: <http://www.bsc.es/paraver>
- **Extræe**: Package that generates Paraver trace-files for a post-mortem analysis
- **Paraver**: Trace visualization and analysis browser
 - Includes trace manipulation: Filter, cut traces
- **Dimemas**: Message passing simulator



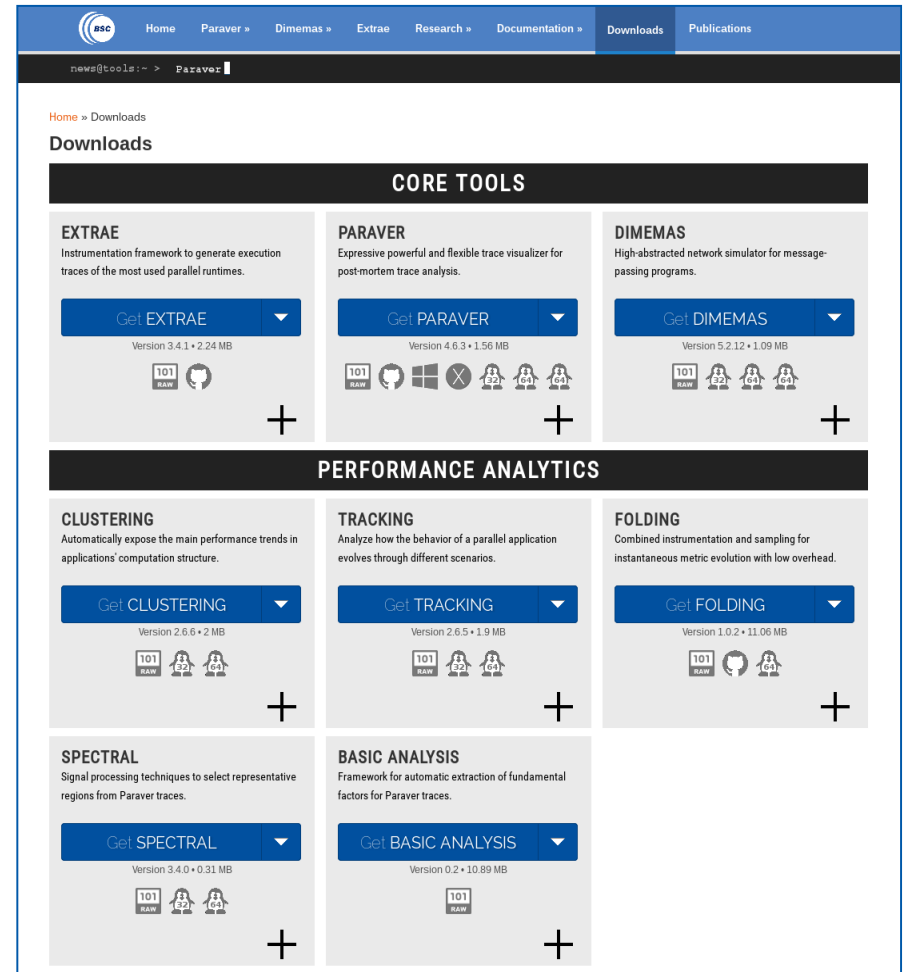
- Download from <http://tools.bsc.es>

- **Extræe**

- Install from sources
 - configure, make, make install
- Main dependencies
 - MPI
 - libxml2
 - libunwind
 - GNU binutils
 - PAPI

- **Paraver & Dimemas**

- Precompiled binaries available



- Flexible parallel program **visualization** tool based on a GUI.
- From **qualitative global** perception to **deep quantitative** analysis.
- Its power lies on its **flexibility** and **expressive power**.
- Expressive power: Separation between visualization (how to display) and semantic module (value to display):
 - Filter.
 - Semantic functions (categorical, logical, numerical).
 - Multiple levels (thread, task, application).
 - Visualization (tables, timelines).

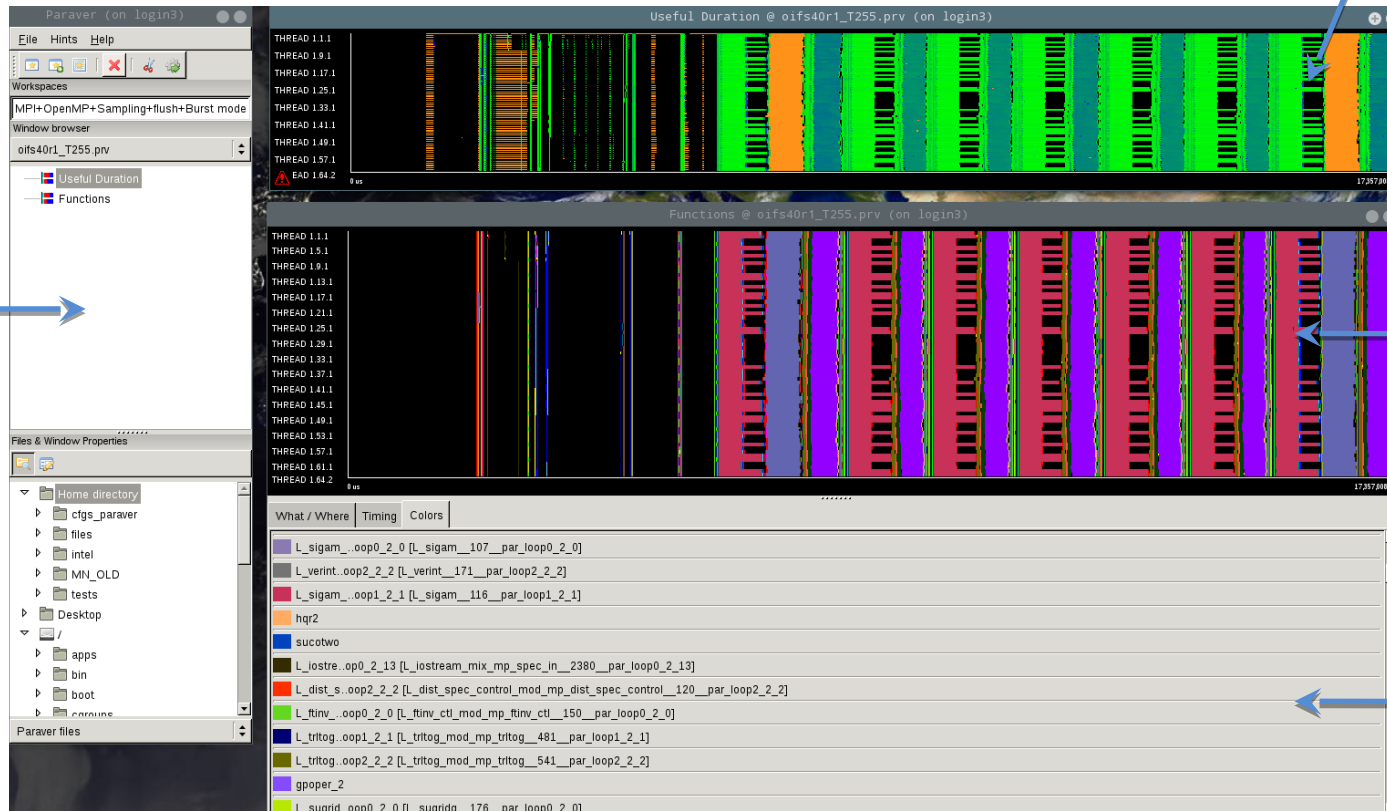
- Paraver is a very flexible data browser for discovering how an application is running in a parallel environment.

Useful duration
(communication
vs computation)

Paraver
Control
Window

OpenMP
regions

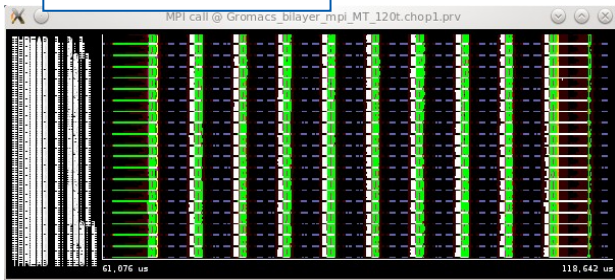
Name of the
OpenMP
regions



General view of an openIFS T255 trace with Paraver

- From timelines to tables

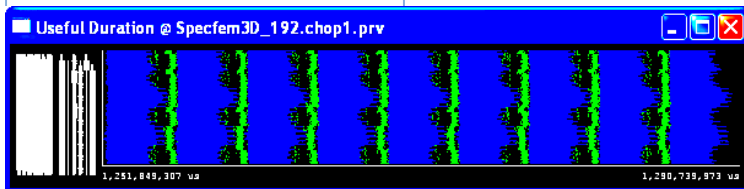
MPI calls



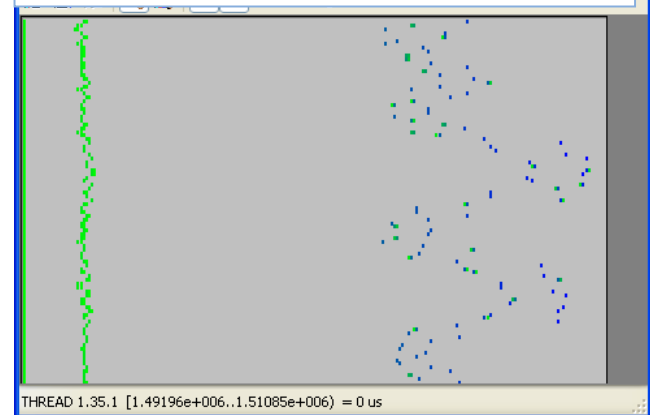
MPI calls profile



Useful Duration

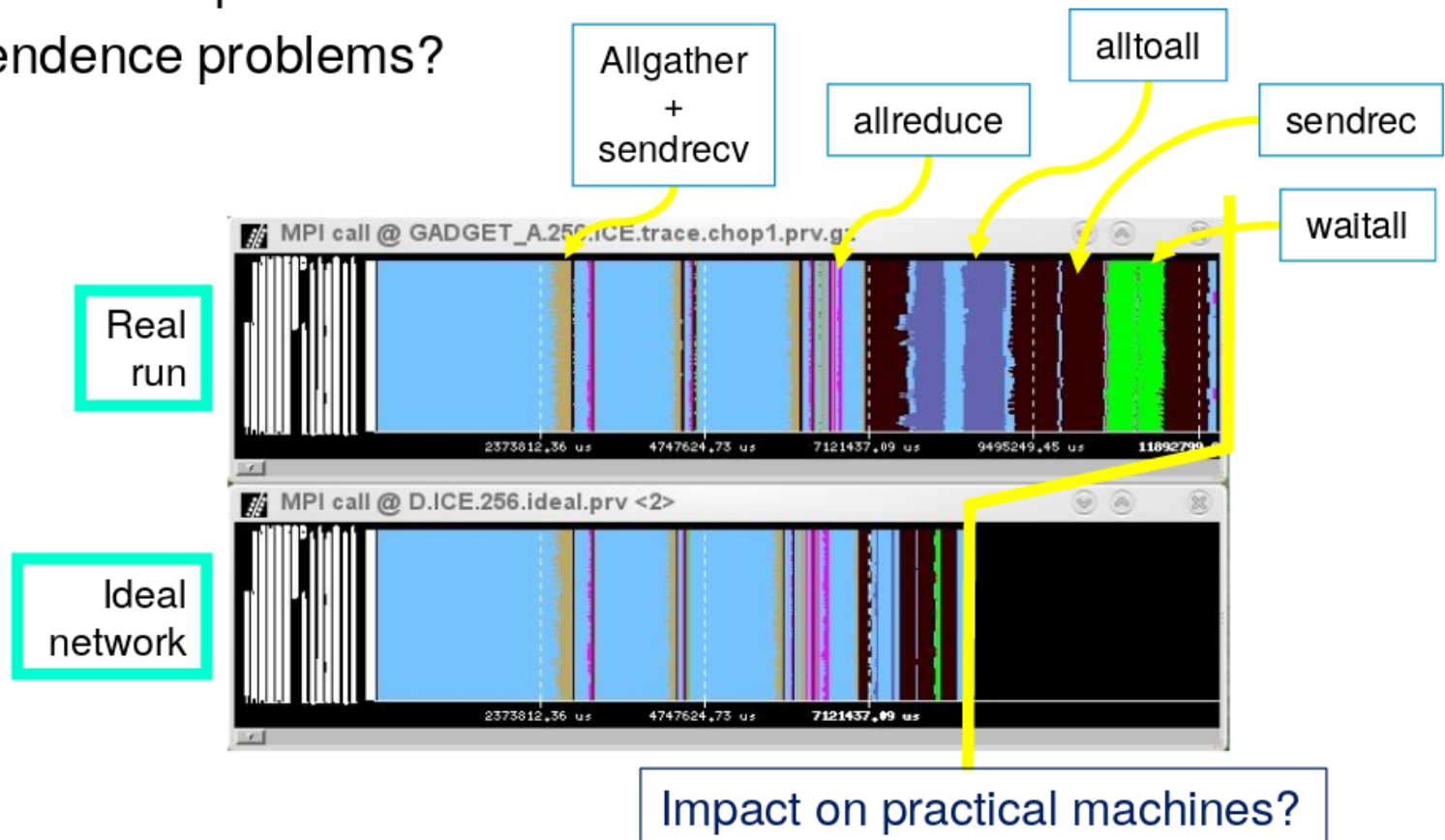


Histogram Useful Duration

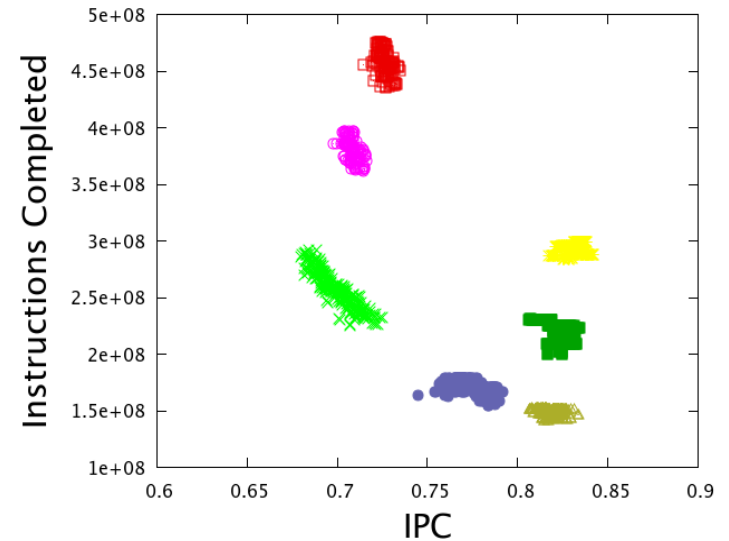
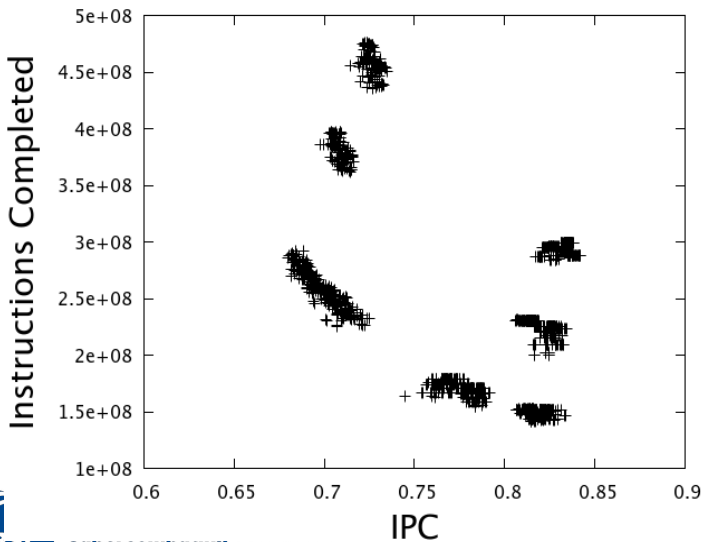
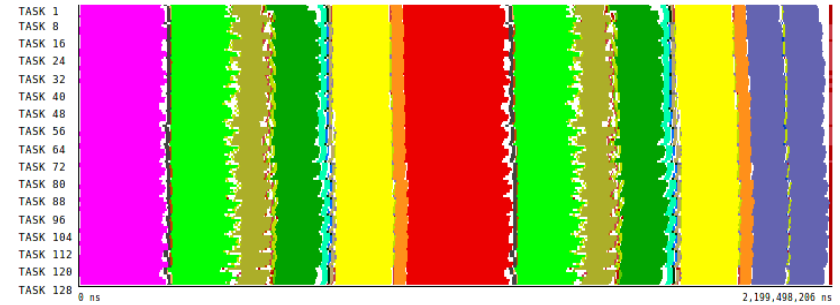
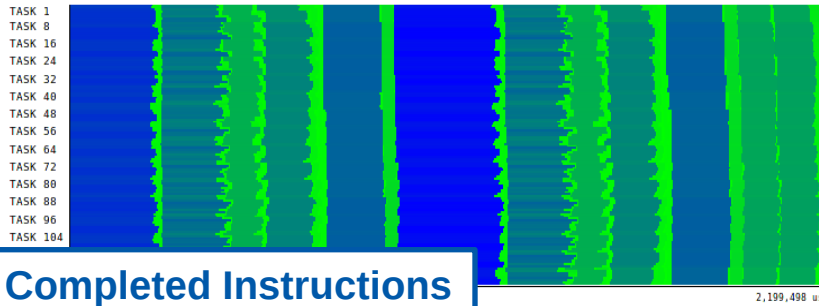


The impossible machine: $BW = \infty$, $L = 0$

- Actually describes/characterizes intrinsic application behavior
 - Load balance problems?
 - Dependence problems?

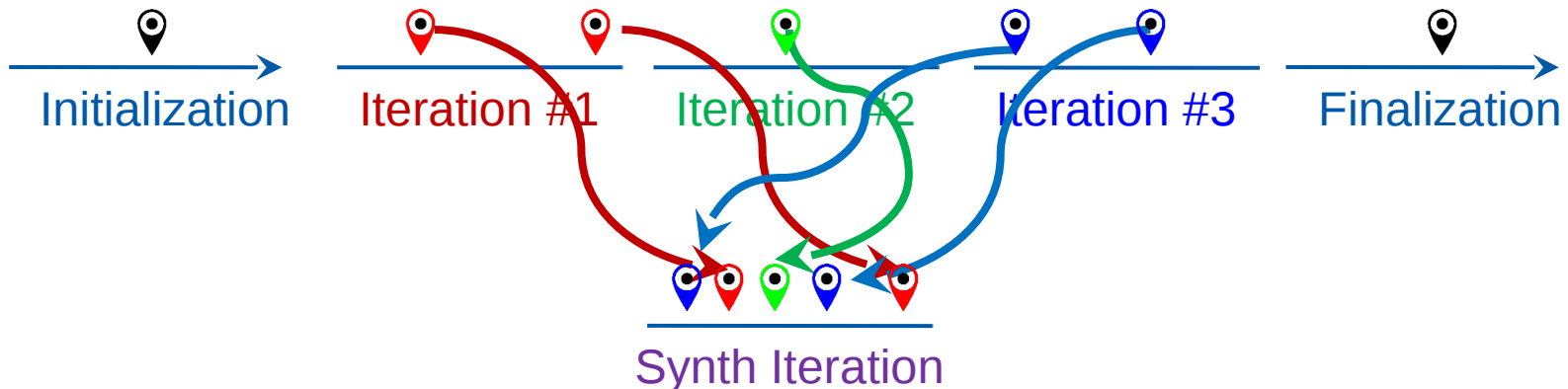
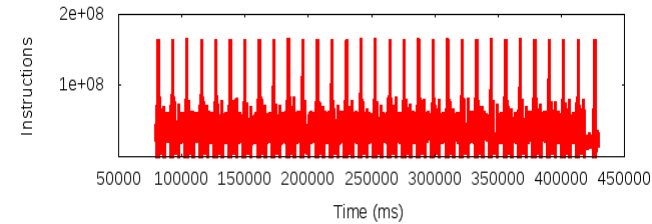


BSC Tools: Clustering



BSC Tools: Folding

- HPC / Scientific applications
 - Repetitive nature
- **Instantaneous metrics with minimum overhead**
 - Combine instrumentation and sampling
 - Instrumentation delimits regions (routines, loops, ...)
 - Sampling exposes progression within a region
 - Captures performance counters and call-stack references

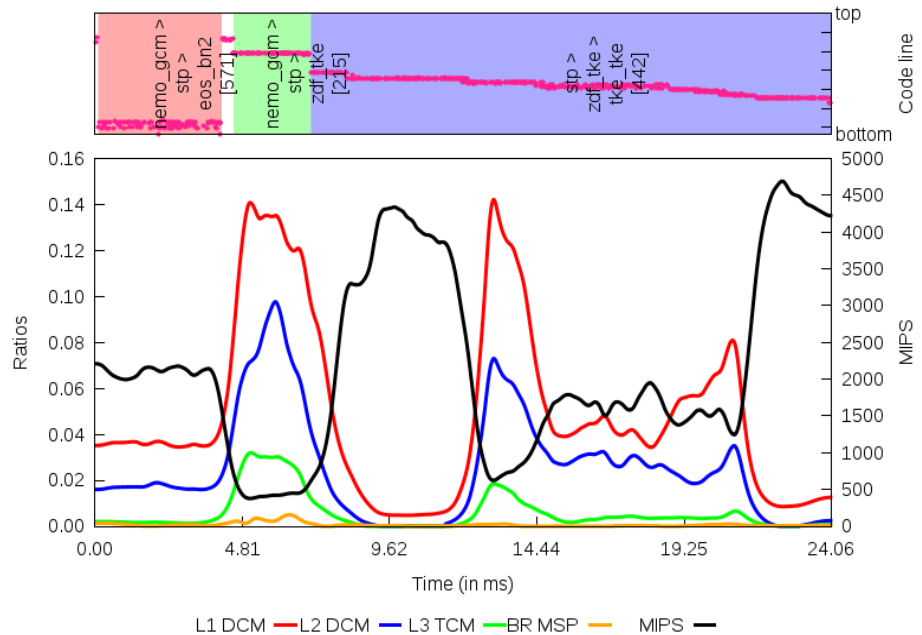
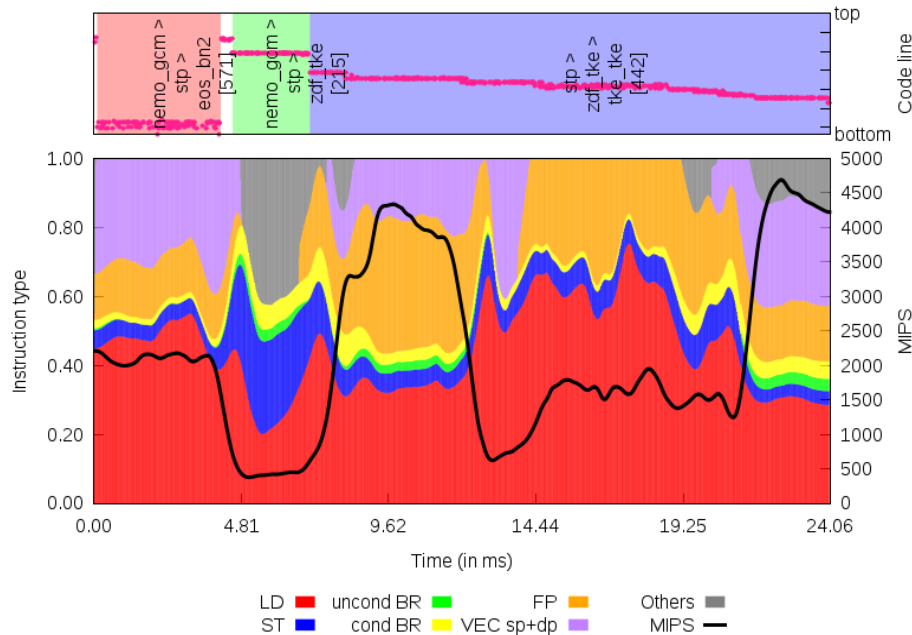


BSC Tools: Folding

- The first performance decrease coincides with a lot of store instructions but also other not categorized instructions, and the second with an increase of load and vector operations.
- The minimum value in the MIPS plot line coincides with a peak of the data cache misses ratio.

Evolution for Instruction mix model
Appl * Task * Thread * - Group_0 - Cluster_3

Evolution for Architecture impact model
Appl * Task * Thread * - Group_0 - Cluster_3





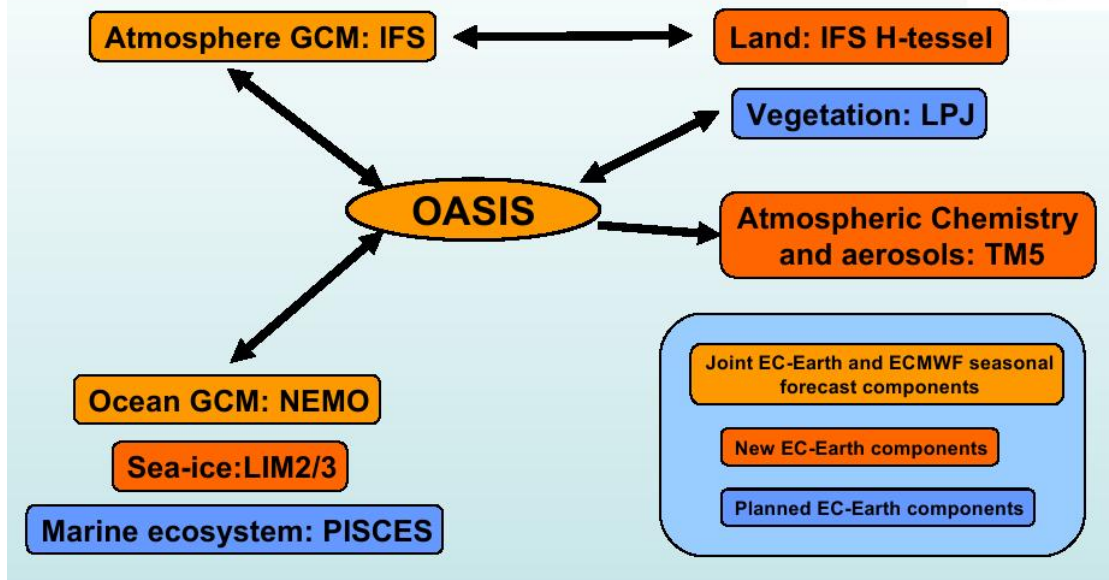
The EC-Earth model

- Earth System Model
- Reliable in-house predictions of global climate change
- Part of a Europe-wide consortium
- Being used in large European projects
 - EMBRACE
 - EUPORIAS
 - IS-ENES
 - SPECS
 - EsiWACE
 - PRIMAVERA
- 3.1 version → IFS + NEMO-LIM + OASIS



- EC-Earth 3.2
 - Integrated Forecasting System (IFS 36r4) as atmosphere model
 - Nucleus for European Modelling of the Ocean (NEMO 3.6) as ocean model
 - OASIS3-MCT coupler
 - Louvain-la-Neuve sea-Ice Model 3 (LIM3) as sea ice model

EC-EARTH components

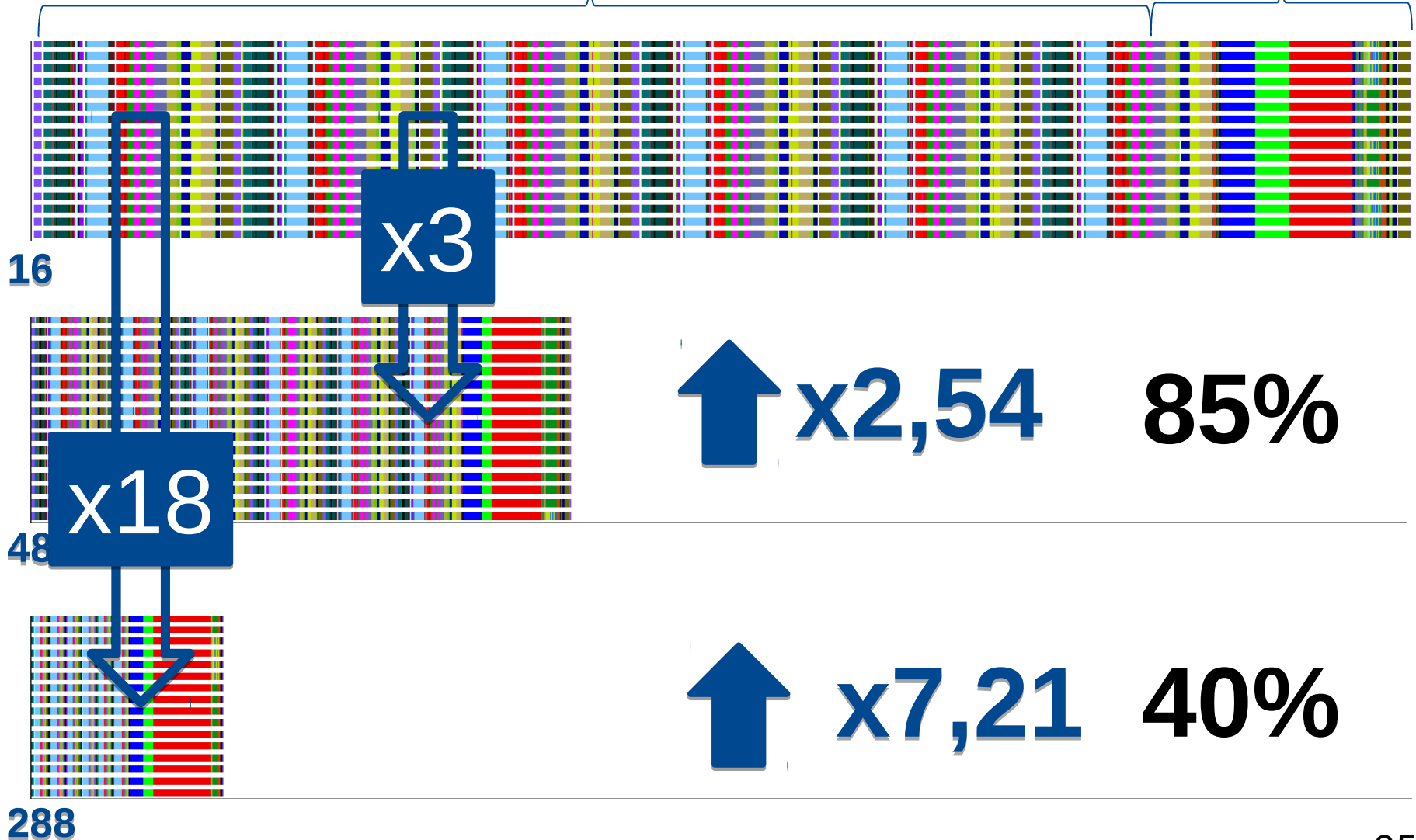




NEMO model optimization

OPA

LIM

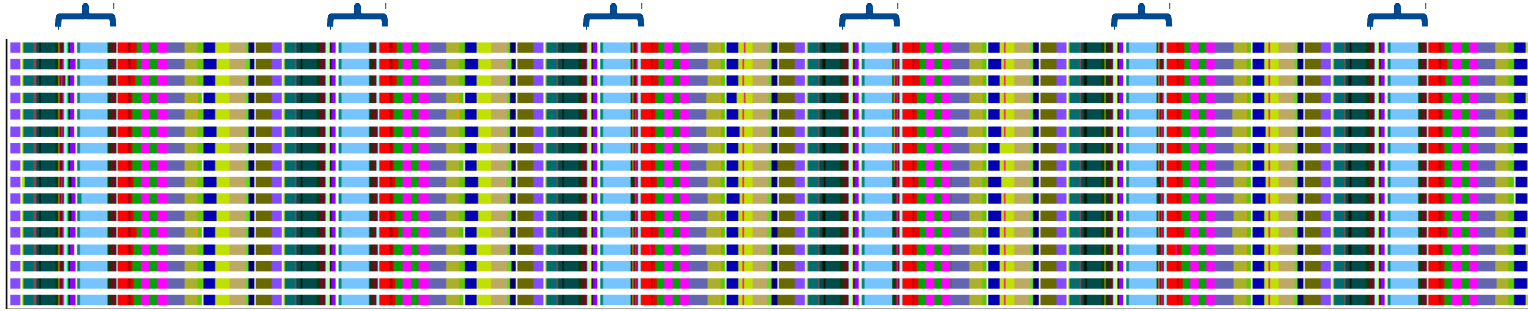


*Timelines have the same duration

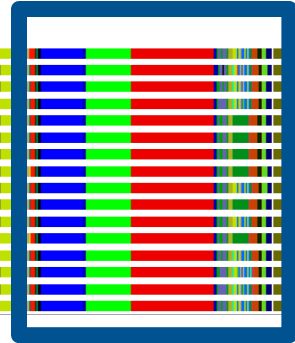
LIM and dynspg as bottlenecks



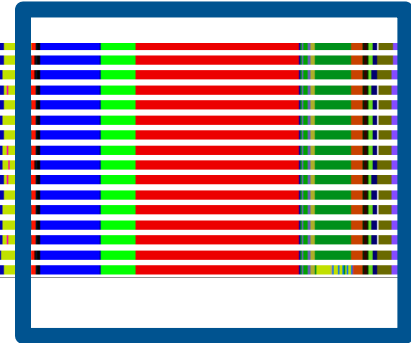
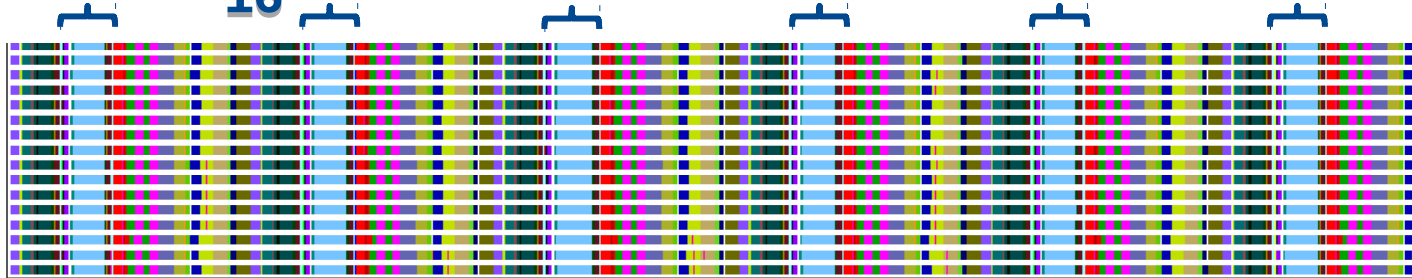
dynspg



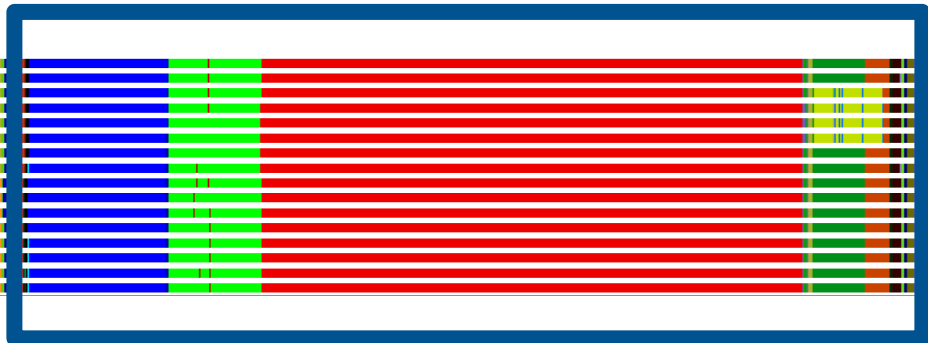
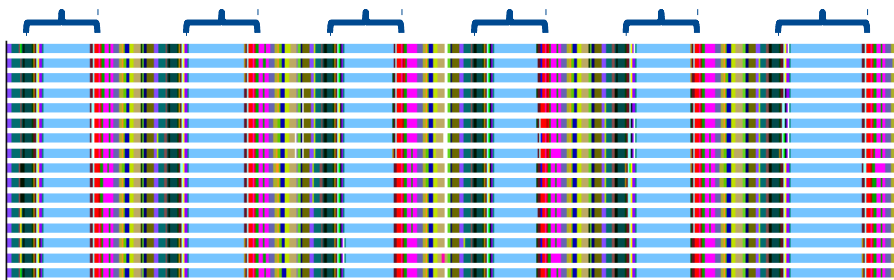
LIM



16

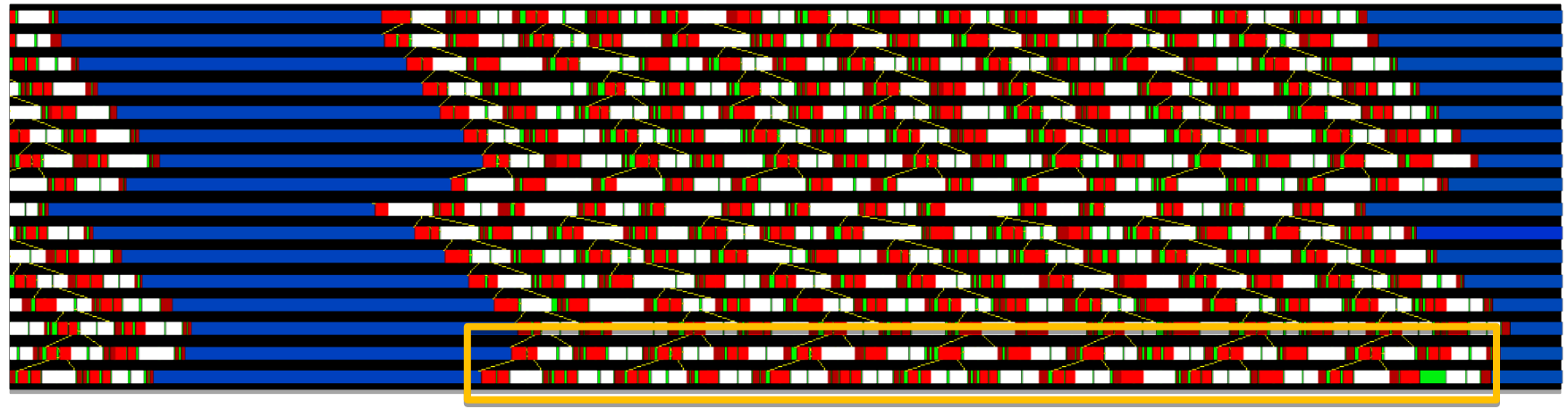
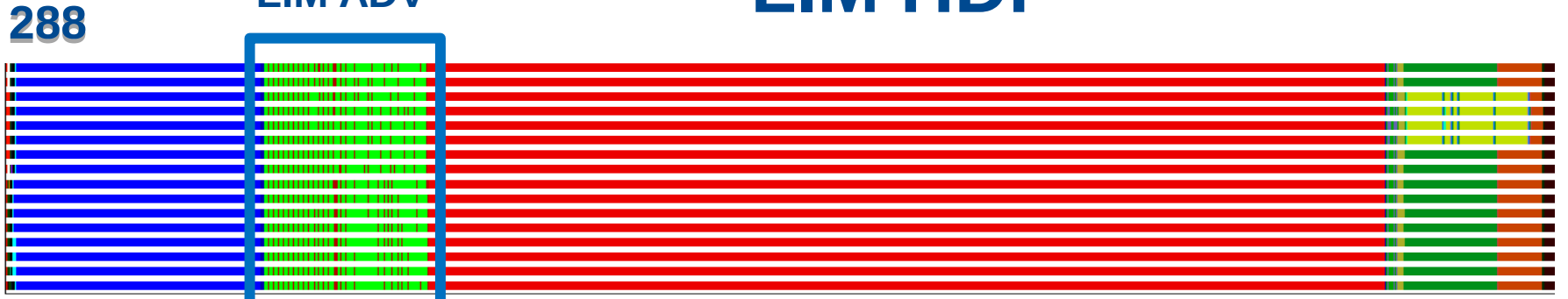


48



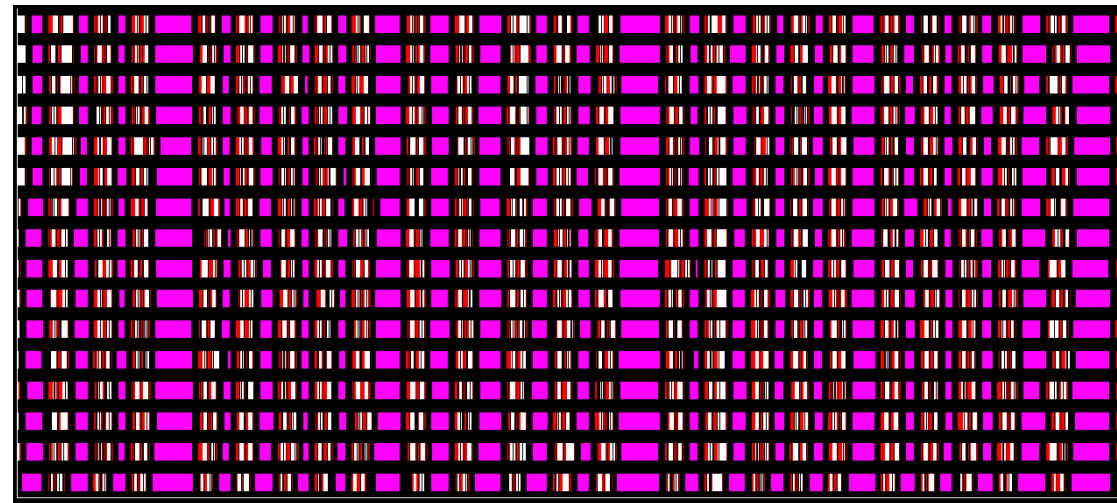
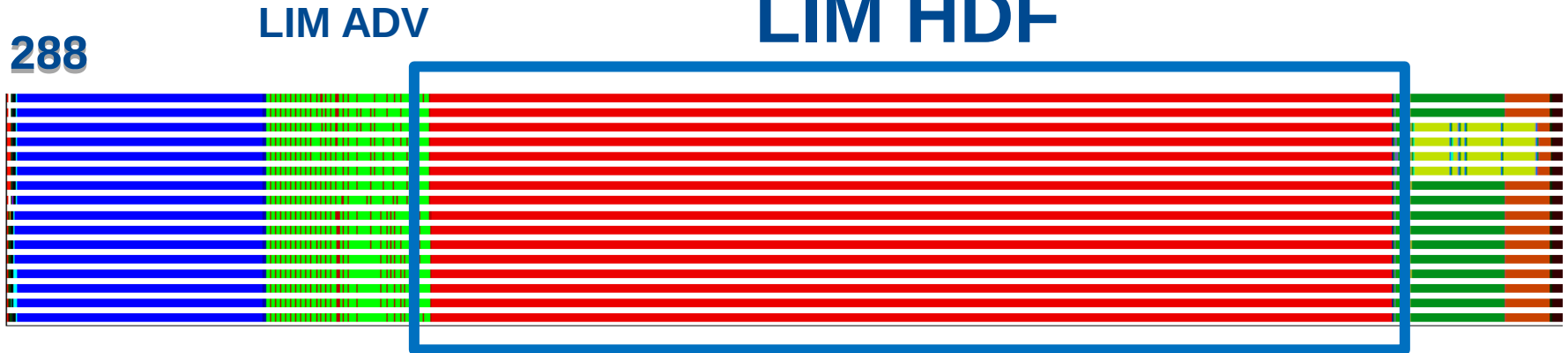
288

LIM HDF



- Outside MPI
- MPI Isend
- MPI Recv
- MPI Wait

7 border interchanges

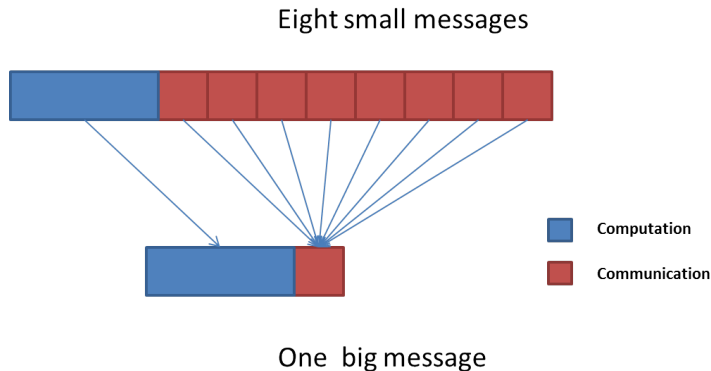


Only **20%** of the time invested on
computation

Global Communication at **every**
loop iteration → **60%** of the time

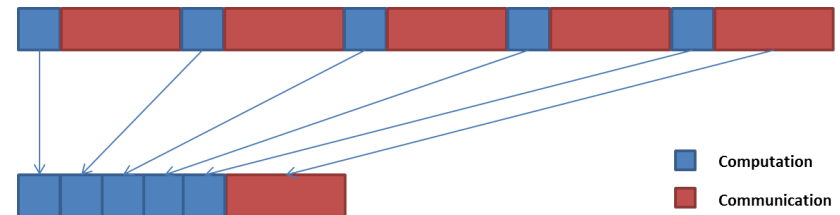
MPI message packing

Taking in account that NEMO is really sensitive to latency, messages aggregation is the best way to reduce the time invested in communications. Therefore, consecutive messages have been packed wherever the computational dependencies allow to do so.



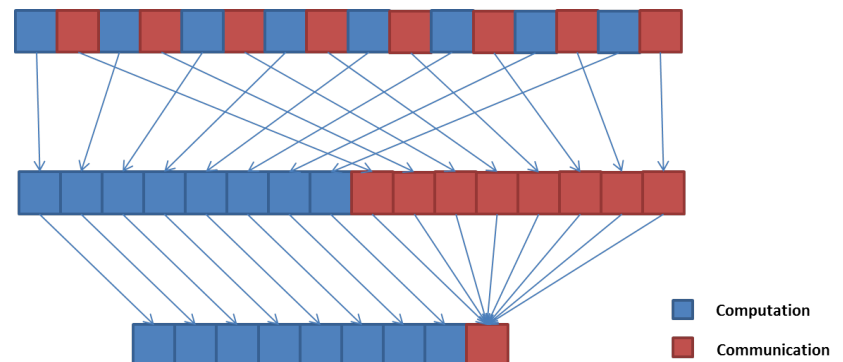
Convergence check reduction

Some routines use collective communications to perform a convergence check in iterative solvers. The cost of this verifications is really high, reaching a 66% of the time. Wherever the model allowed it, we reduced the frequency of this verifications in order to increase parallel efficiency.

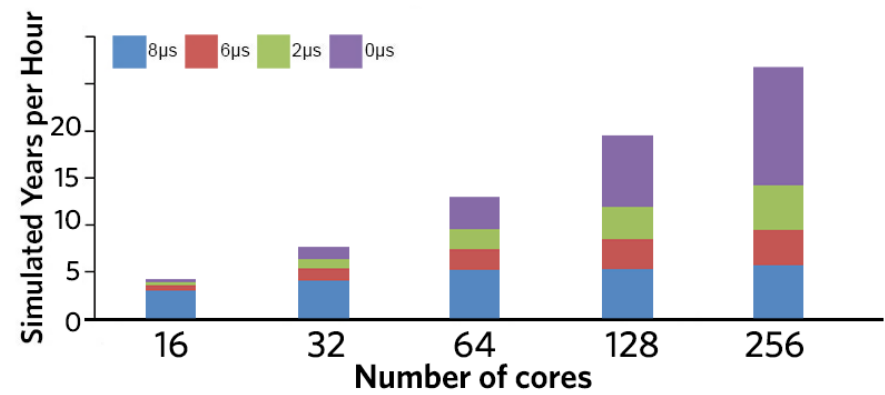
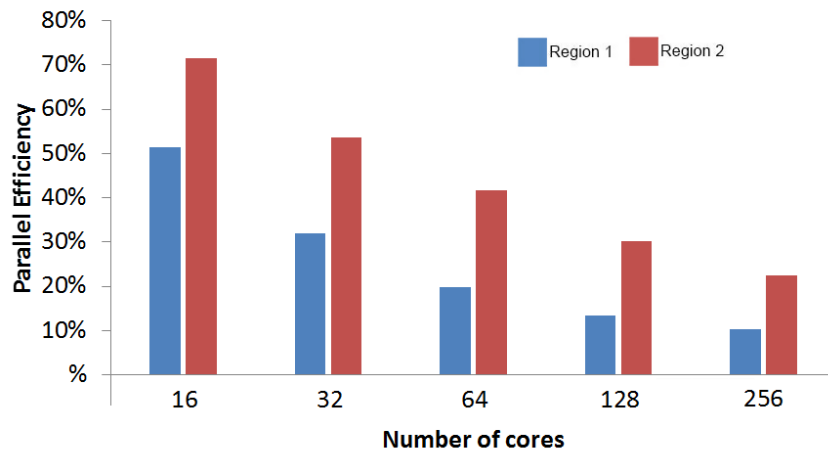


Reordering

In order to apply the message packing optimization to as many routines as it was possible, it was necessary to rearrange some computation and communication regions, taking into account the dependencies between them, to reduce the number of messages. This way it was possible to compute (and communicate) up to 41 variables at the same time, resulting in a dramatic reduction of the granularity.



- However, communications are the main performance problem. Even in the 16-core case parallel efficiency is really bad.
- The figure at the right shows how sensitive the model is to network latency.
- Communications efficiency drops much more faster than computational.



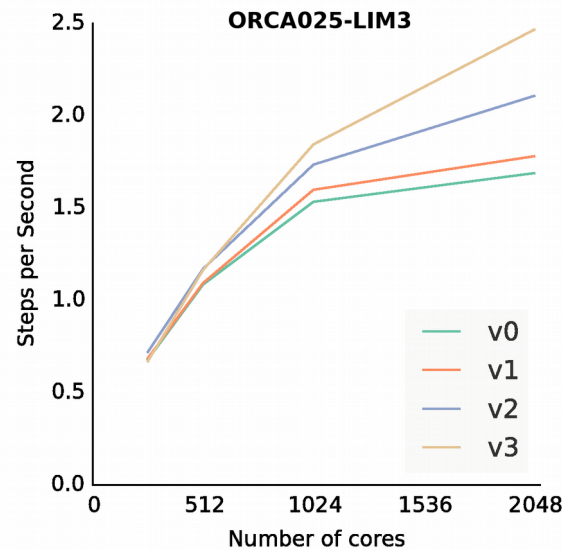
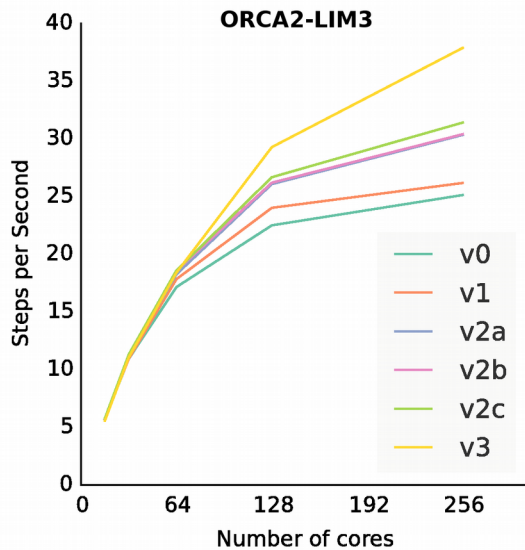
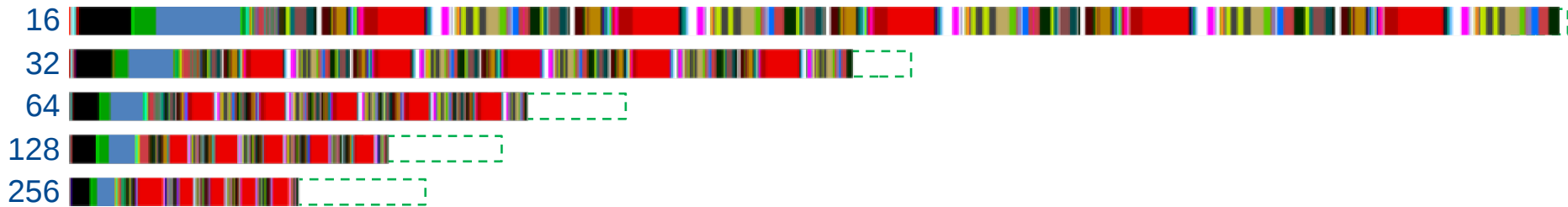
NEMO 3.6 optimization: Results



Original code

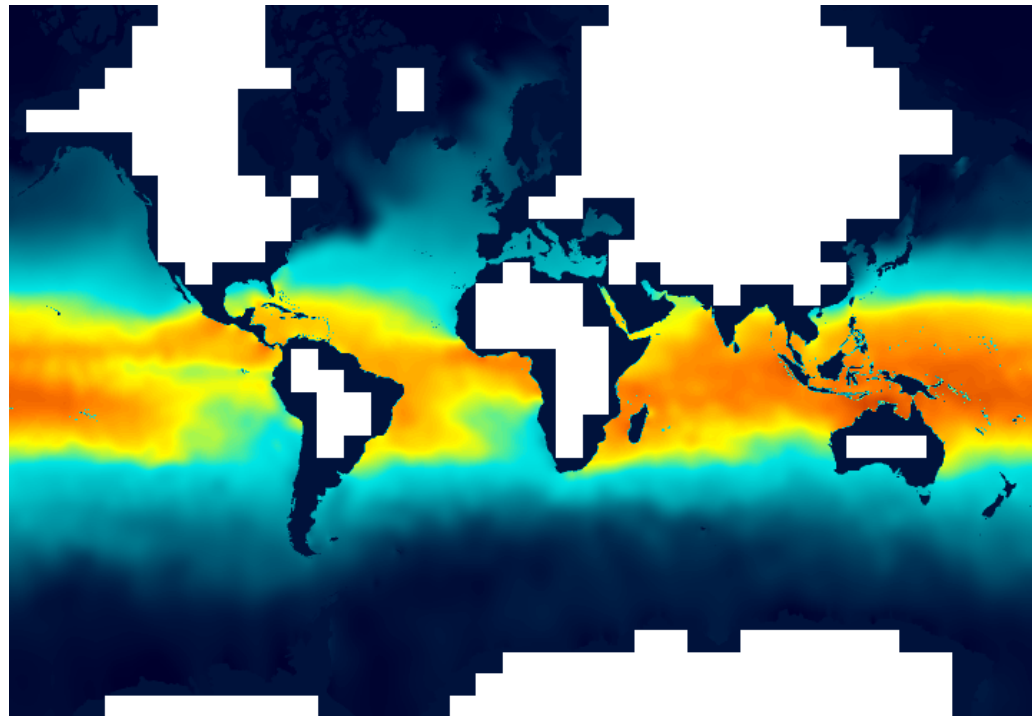


Optimized code

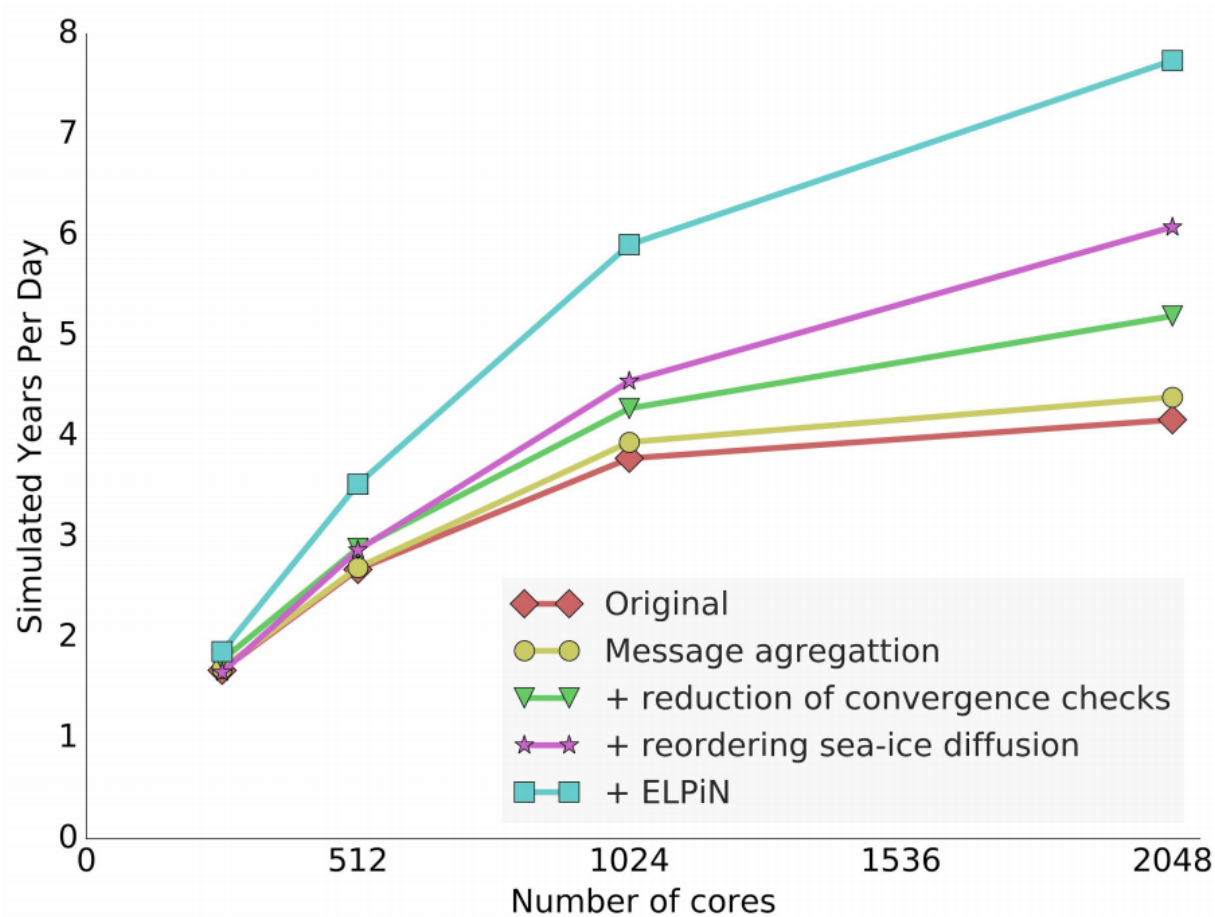


- V0 → Original
- V1 → Message packing
- V2 → Conv. Check reduction
- V3 → Reordering

- A tool that allows to find proper namelist parameters to exclude land-only processes in NEMO simulations
- NEMO decomposes automatically the domain:
 - Computes and communicates in land-only processes and then discards the result → waste of resources



- ORCA025 domain decomposed in 1287 sub-domains
- 312 are land-only and therefore removed (24% of the total grid)



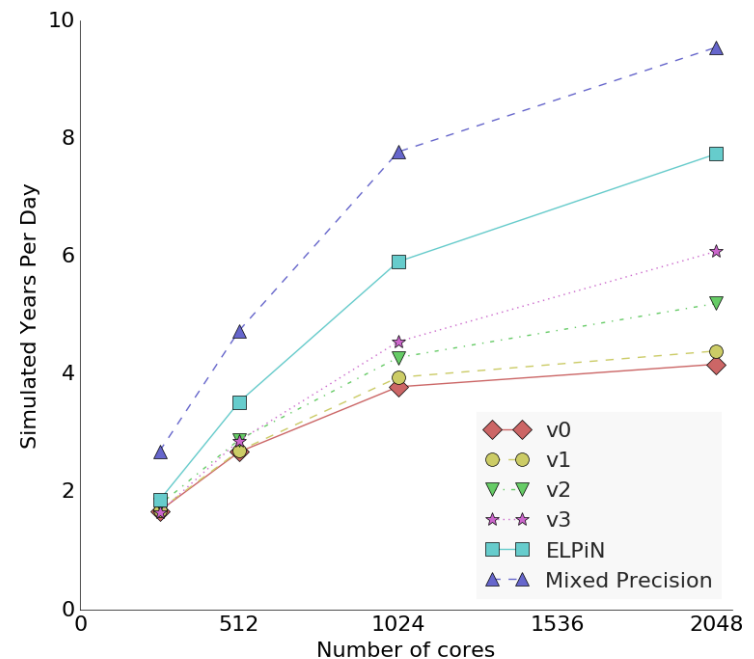
Impact of optimizations done on the NEMO model for an ORCA025-LIM3 simulation

Use of single precision in NEMO



- BSC began an exploratory study to know which impact in computational performance may have a reduction of the precision in NEMO.
- First results show a 40% improvement on ORCA025-LIM3, by only introducing mixed precision in the ocean side.
- Further studies may determine which parts of the code are tolerant to a reduction in precision.

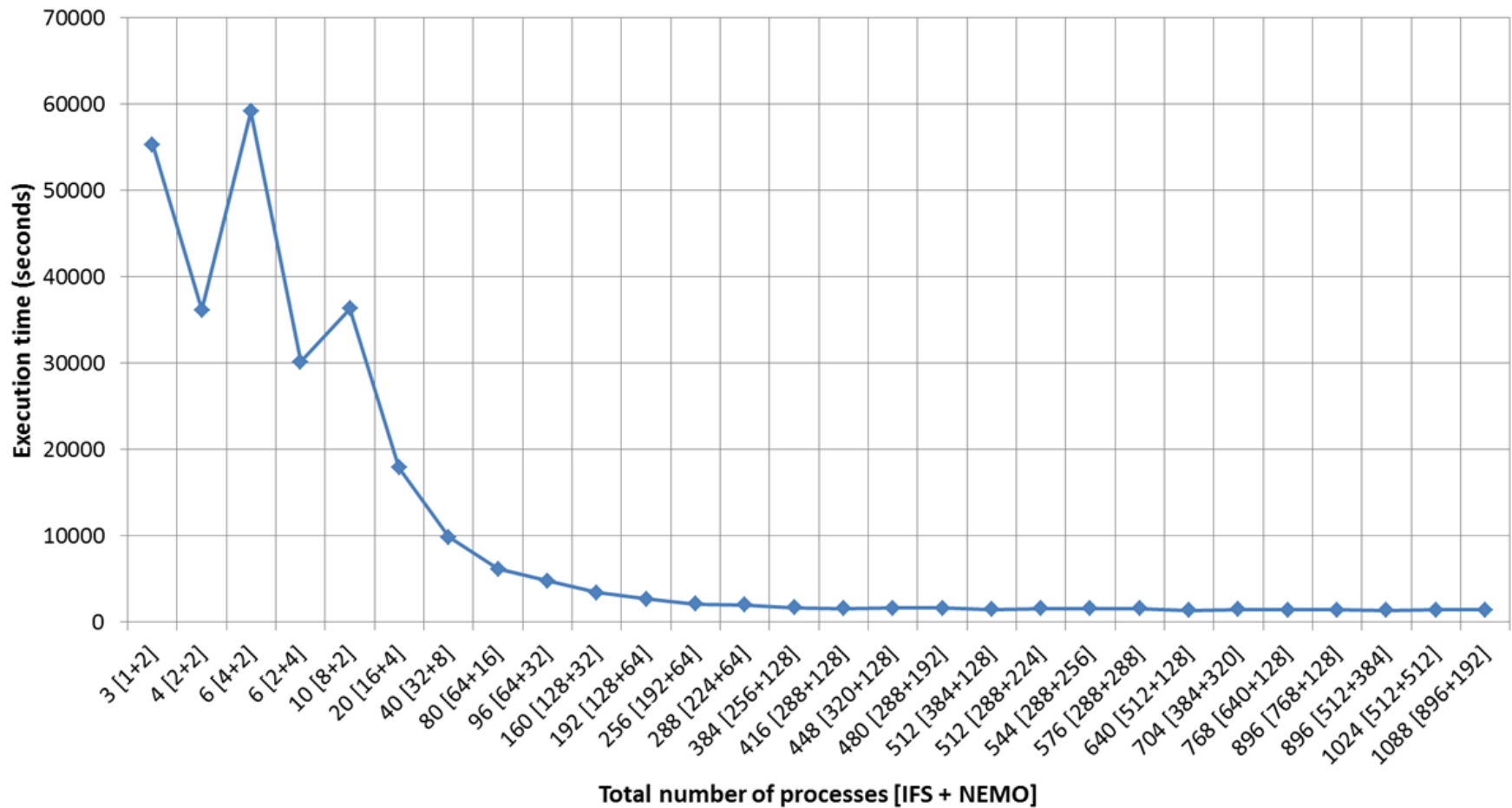
“At present, there is no other measure within our reach that could have a greater impact on performance.”



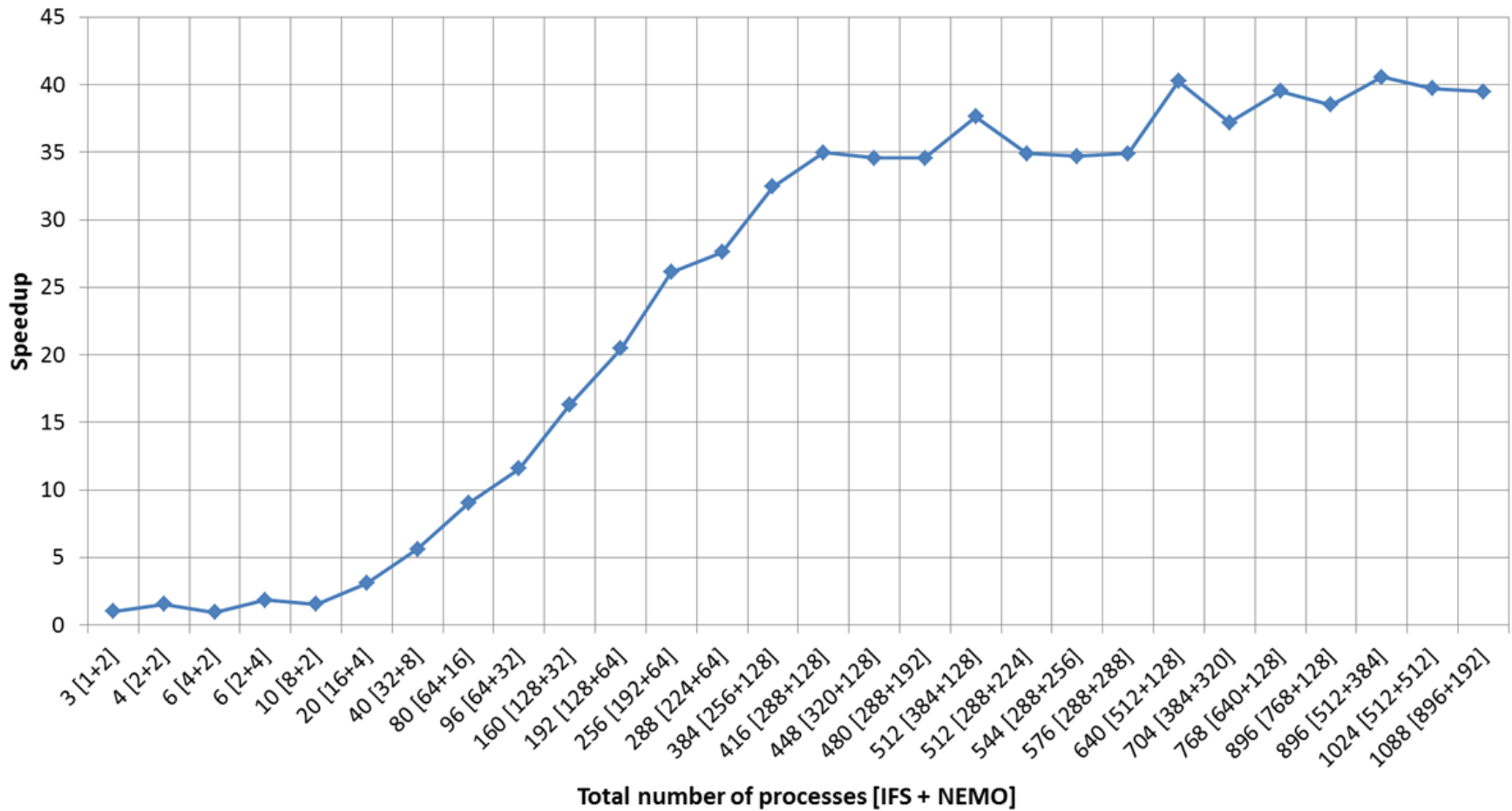


Optimization of the EC-Earth coupled model

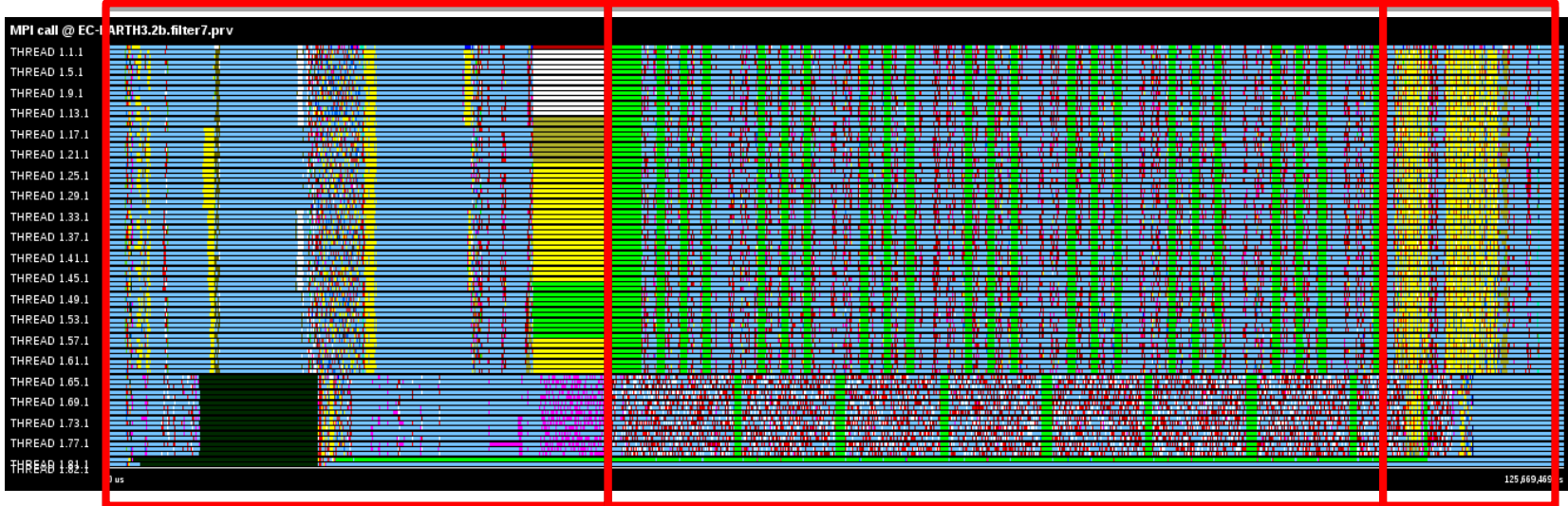
Execution time of EC-Earth 3.2beta coupled
T255L91-ORCA1L75, 3 months



Speedup of EC-Earth 3.2beta coupled T255L91-ORCA1L75



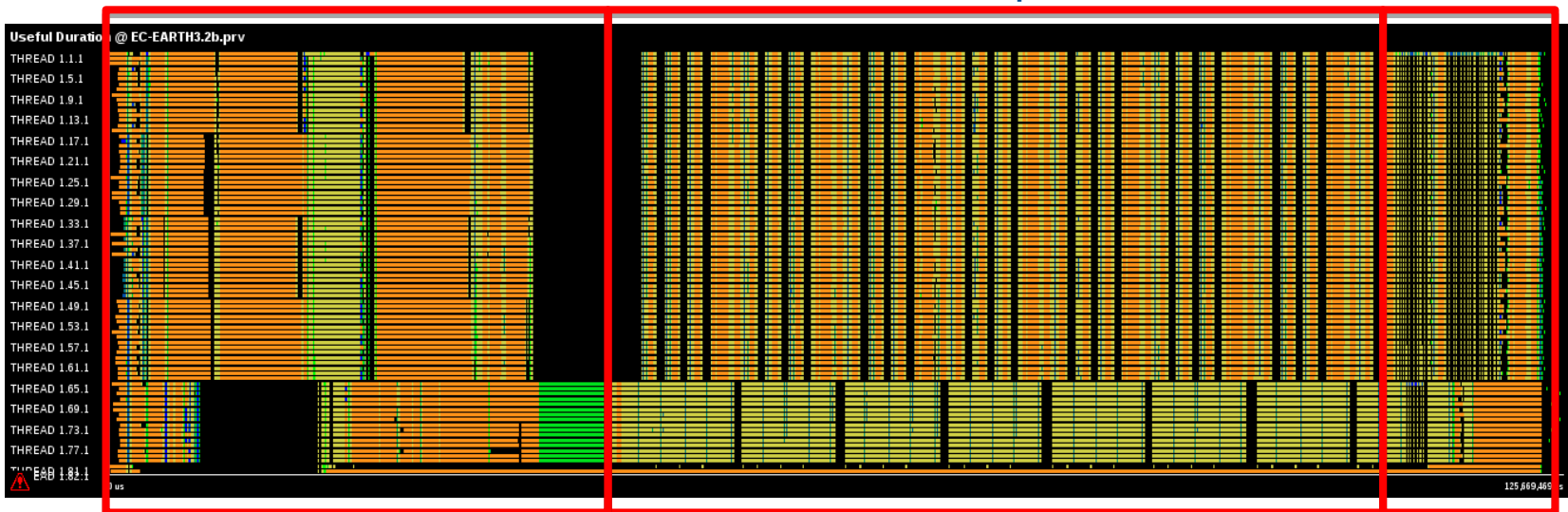
EC-Earth trace analysis



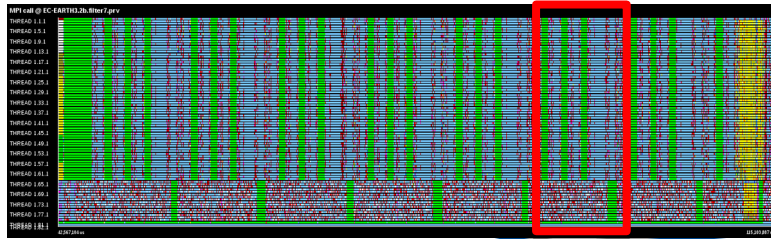
Initialization

Time steps

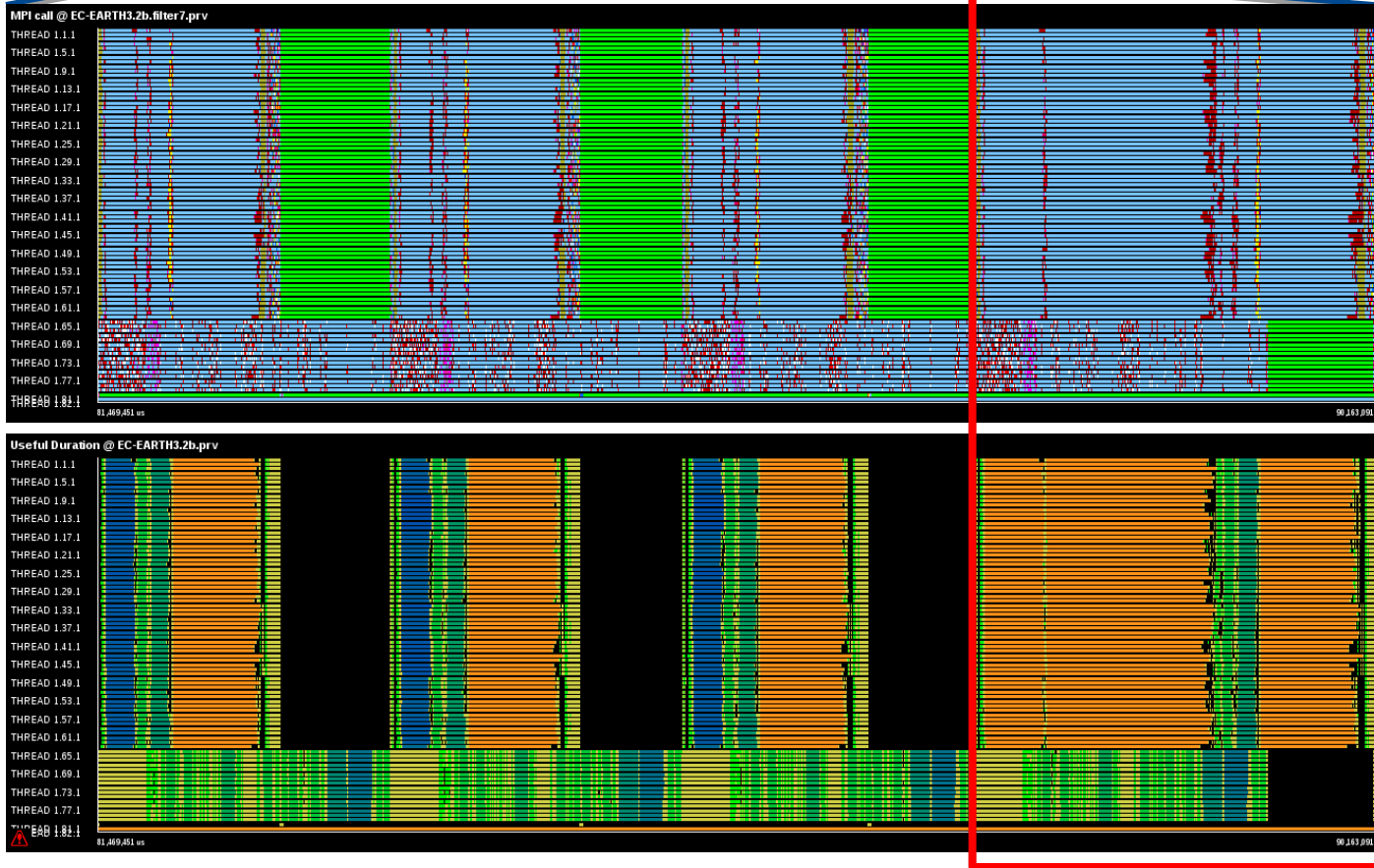
Finalization



EC-Earth trace analysis



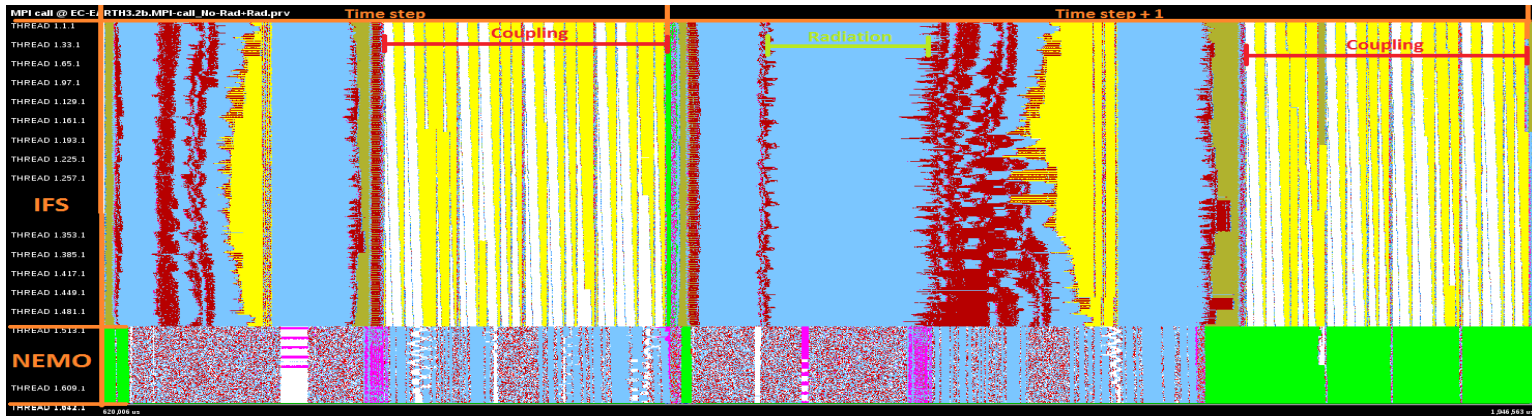
1 of every 4 time steps, IFS executes radiation routines, where NEMO has to wait



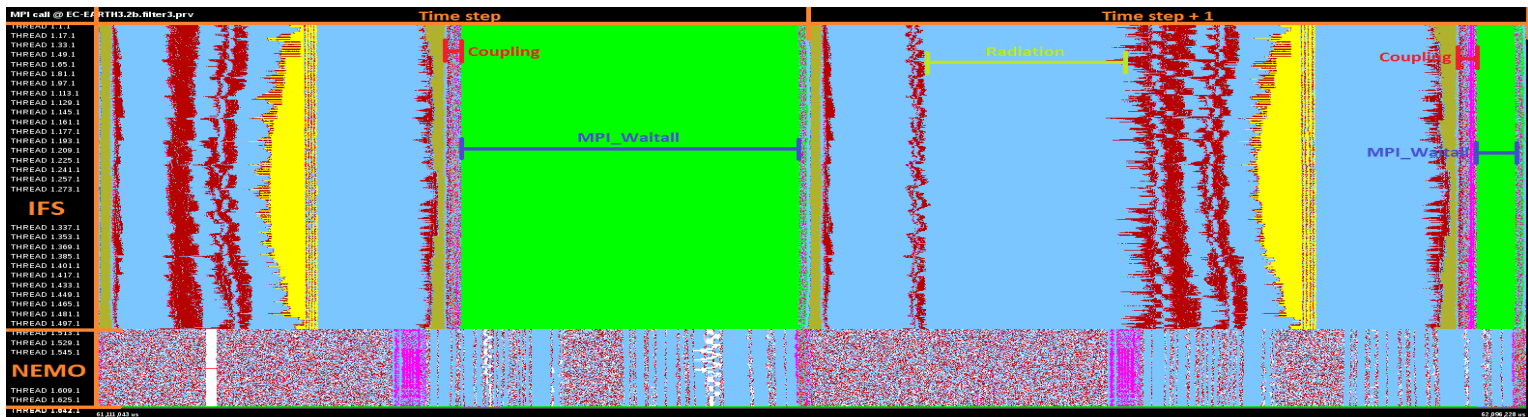
EC-Earth coupling optimizations



Collaboration with the EC-Earth Technical Working Group to improve the model execution



Success case: coupling field gathering and OPT option of OASIS coupler for global conservative transformations

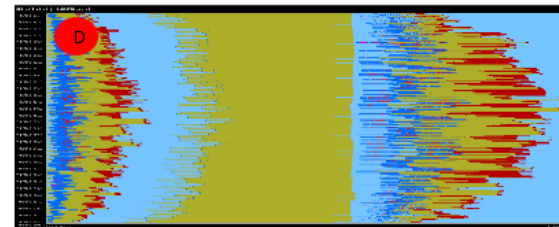
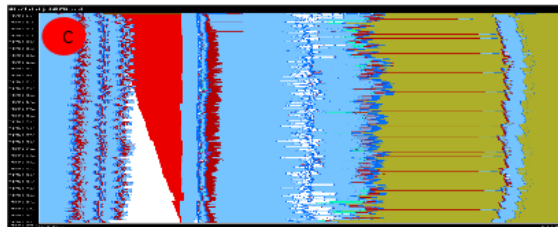
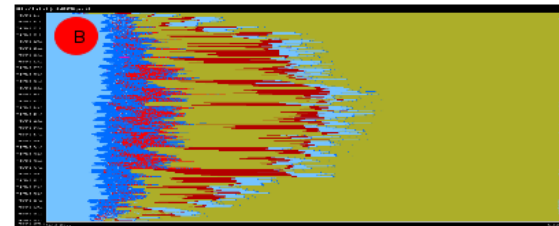
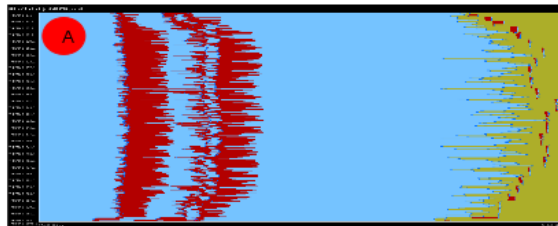
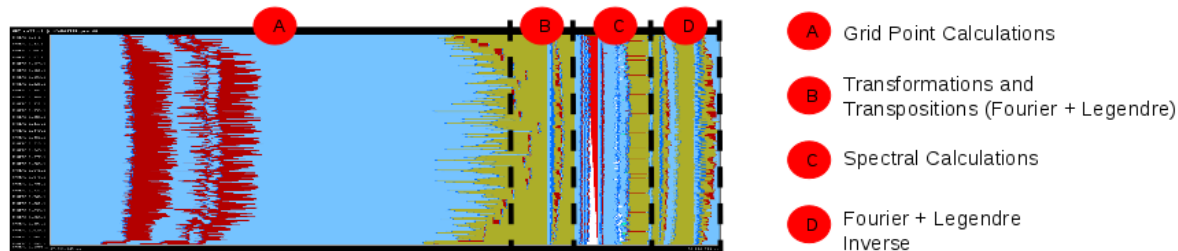


Coupling process improved up to 90%

Optimizations included in trunk EC-Earth 3.2.2, substantially benefiting CMIP6 simulations⁴⁰

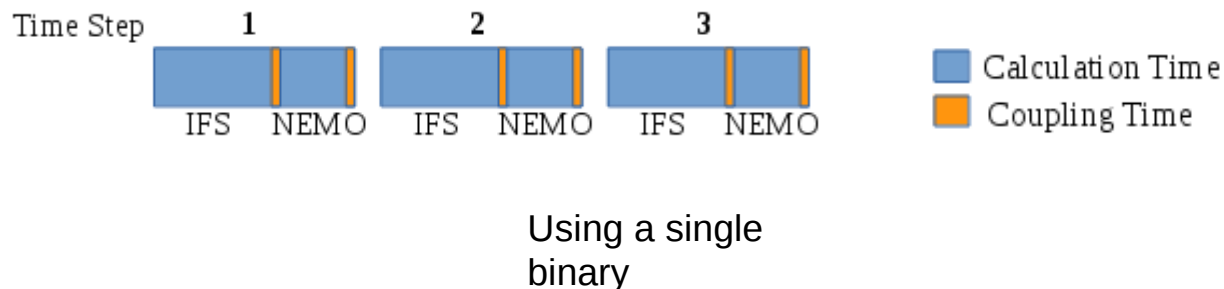
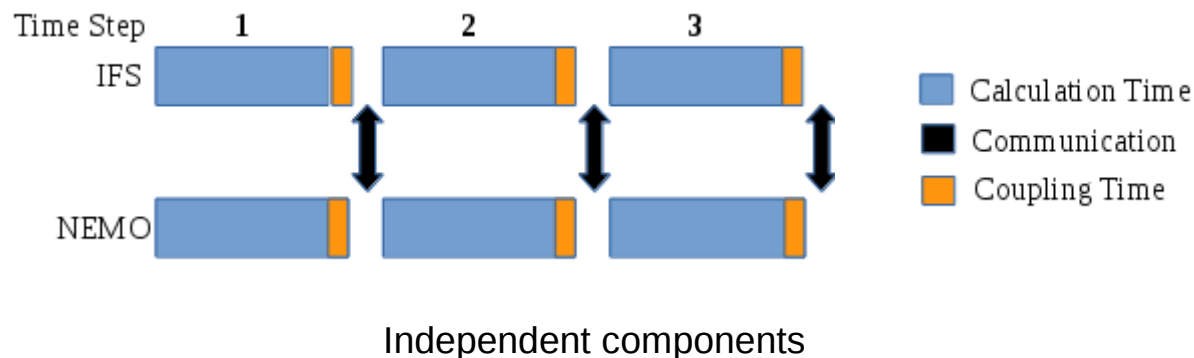
- BSC is collaborating with the Research department at ECMWF to improve the computational performance of IFS/OpenIFS models.
- Key activities:
 - Contribution for the next official release of IFS to use the BSC tools (Extrac, Paraver...).
 - IFS/OpenIFS performance analysis and optimization.
 - IFS-NEMO coupling comparison:
 - Independent components (via OASIS) vs single binary.

A profiling analysis of IFS43r1 and OpenIFS40r1 was done using BSC Tools. These analysis can be useful to highlight which parts of the code could be improved in the future.



Example of the IFS profiling study using Paraver for each phase of IFS43r1

- BSC and ECMWF will work together to evaluate the advantages and disadvantages of coupling the ocean component (NEMO) to IFS as:



- Open version of the ECMWF model
 - Integrated Forecasting System (IFS)
 - Single column model (SCM)
 - Offline-surface model (OSM)
- Currently working with v-1 operational version (40r1)
- Hybrid parallelization (MPI+OpenMP)
- Next plans
 - Run a 1km global configuration (T7999) in ESIWACE CoE
 - Port to OmpSs
 - Apply Dynamic Load Balancing library (DLB)
 - Adding XIOS support





Conclusions

- **Trace analysis** can guide the users in **understanding** their code's behaviour and efficiency
- **Performance tools** help in finding specific code parts that should be improved and which is the cause of the performance degradation
- A precise analysis and prediction can generate ideas that direct the **restructuring** of the application in the most productive way
- **Little changes** in the configuration can significantly **improve the performance**
- These tools provide the information but its **user's task** to get conclusions from the different metrics



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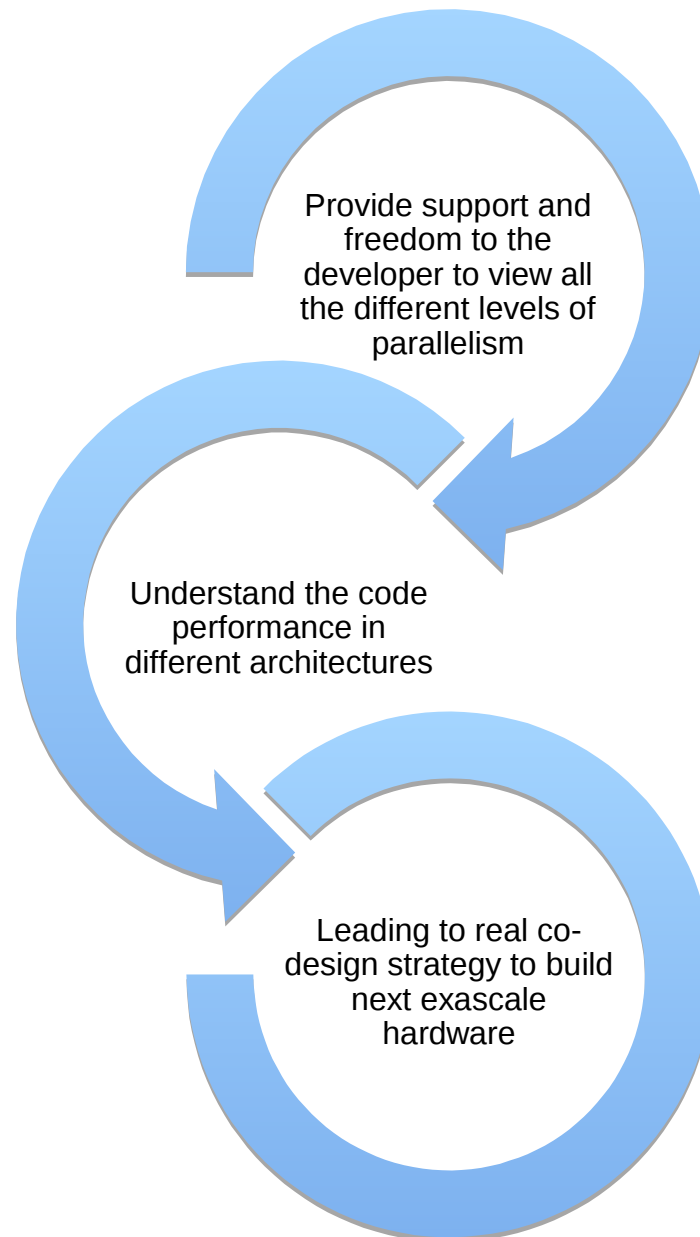
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EXCELENCIA
SEVERO
OCHOA

Thank you!

For further information please contact
miguel.castrillo@bsc.es



1. Mathematical study

- Some methods could be better than others
 - Discretization used (explicit, implicit, semi-implicit...)
 - Parallel adaptation (solvers, preconditioners...)
- How to implement new algorithms for new architectures

2. Computational study

- Achieve load balance among components
- Reduce overhead introduced by parallel applications
- Ensure the computational algorithm takes advantage of the architecture

3. Profiling Study

- General profiling
- Profiling applied to Earth System Models

1. Introducing optimizations

- Improvement of the mathematical and/or computational algorithm
 - Apply scientific methods which are found in the literature
 - Improve the method using a new approach
- Revolution: Create a new (and better) algorithm taking into account the research line followed

2. Reproducibility study

- Evaluate if the accuracy and reproducibility of the model is similar using or not the optimizations proposed
- Take into account the nature of climate models
 - How to evaluate, in parallel executions, if the differences between runs are significant or not.

Extrae configuration: extrae.xml



```
<!-- Configuration of some MPI dependant values -->
<mpi enabled="yes">
  <!-- Gather counters in the MPI routines? -->
  <counters enabled="yes" />
</mpi>

<!-- Emit information of the callstack -->
<callers enabled="yes">
  <!-- At MPI calls, select depth level -->
  <mpi enabled="yes">1-3</mpi>
  <!-- At sampling points, select depth level -->
  <sampling enabled="yes">1-5</sampling>
</callers>

<!-- Configuration of some OpenMP dependant values -->
<openmp enabled="yes">

-----

<!-- Configuration of some pthread dependant values -->
<pthread enabled="no">

-----

<!-- Configuration of User Functions -->
<user-functions enabled="yes" list="/home/bsc41/bsc41273/user-functions.dat" exclude-automatic-functions="no">
  <!-- Gather counters on the UF routines? -->
  <counters enabled="yes" />
</user-functions>
```

Trace MPI calls

Trace call-stack events
@ MPI calls

Trace user functions (from list)

Extrae configuration: extrae.xml



```
<!-- Configure which software/hardware counters must be collected -->
<counters enabled="yes">
  <!-- Configure the CPU hardware counters. You can define here as many sets
  as you want. You can also define if MPI/OpenMP calls must report such
  counters.
  Starting-set property defines which set is chosen from every task.
  Possible values are:
  - cyclic : The sets are distributed in a cyclic fashion among all
  tasks. So Task 0 takes set 1, Task 1 takes set 2,...
  - block  : The sets are distributed in block fashion among all tas
  Task [0..i-1] takes set 1, Task [i..2*i-1] takes set 2, ...
  - Number : All the tasks will start with the given set
  (from 1..N).
  -->
  <cpu enabled="yes" starting-set-distribution="1">
    <!-- In this example, we configure two sets of counters. The first will
    be changed into the second after 5 calls to some collective
    operation on MPI_COMM_WORLD. Once the second is activated, it will
    turn to the first after 5seconds (aprox. depending on the MPI call
    granularity)
    If you want that any set be counting forever, just don't set
    changeat-globalops, or, changeat-time.

    Each set has it's own properties.
    domain -> in which domain must PAPI obtain the information (see
    PAPI info)
    changeat-globalops=num -> choose the next set after num
    MPI_COMM_WORLD operations
    changeat-time=numTime -> choose the next set after num Time
    (for example 5s, 15m (for ms), 10M (for minutes),..)
    -->
    <set enabled="yes" domain="all" changeat-time="0">
      PAPI_TOT_INS,PAPI_TOT_CYC,PAPI_L1_DCM,PAPI_L2_DCM,PAPI_L3_TCM,PAPI_FP_INS,PAPI_BR_MSP
    </set>
    <set enabled="yes" domain="all" changeat-time="0">
      PAPI_TOT_INS,PAPI_TOT_CYC,PAPI_LD_INS,PAPI_SR_INS,PAPI_BR_UCN,PAPI_BR_CN,PAPI_VEC_SP,RESOURCE_STALLS
    <sampling enabled="no" period="1000000000">PAPI_TOT_CYC</sampling>
    </set>
  </cpu>

  <!-- Do we want to gather information of the network counters?
  Nowadays we can gather information about MX/GM cards.
  -->
  <network enabled="no" />

  <!-- Obtain resource usage information -->
  <resource-usage enabled="no" />

  <!-- Obtain malloc statistics -->
  <memory-usage enabled="no" />
</counters>
```

./papi_avail

Name	Code	Avail	Deriv	Description (Note)
PAPI_L1_DCM	0x80000000	Yes	No	Level 1 data cache misses
PAPI_L1_ICM	0x80000001	Yes	No	Level 1 instruction cache misses
PAPI_L2_DCM	0x80000002	Yes	Yes	Level 2 data cache misses
PAPI_L2_ICM	0x80000003	Yes	No	Level 2 instruction cache misses
PAPI_L3_DCM	0x80000004	No	No	Level 3 data cache misses
PAPI_L3_ICM	0x80000005	No	No	Level 3 instruction cache misses
PAPI_L1_TCM	0x80000006	Yes	Yes	Level 1 cache misses
PAPI_L2_TCM	0x80000007	Yes	No	Level 2 cache misses
PAPI_L3_TCM	0x80000008	Yes	No	Level 3 cache misses
PAPI_CA_SNP	0x80000009	No	No	Requests for a snoop
PAPI_CA_SHR	0x8000000a	No	No	Requests for exclusive access to shared cache line
PAPI_CA_CLN	0x8000000b	No	No	Requests for exclusive access to clean cache line
PAPI_CA_INV	0x8000000c	No	No	Requests for cache line invalidation
PAPI_CA_ITV	0x8000000d	No	No	Requests for cache line intervention
PAPI_L3_LDM	0x8000000e	Yes	No	Level 3 load misses
PAPI_L3_STM	0x8000000f	No	No	Level 3 store misses
PAPI_BRU_IDL	0x80000010	No	No	Cycles branch units are idle
PAPI_FXU_IDL	0x80000011	No	No	Cycles integer units are idle
PAPI_FPU_IDL	0x80000012	No	No	Cycles floating point units are idle
PAPI_LSU_IDL	0x80000013	No	No	Cycles load/store units are idle
PAPI_TLB_DM	0x80000014	Yes	No	Data translation lookaside buffer misses
PAPI_TLB_IM	0x80000015	Yes	No	Instruction translation lookaside buffer misses
PAPI_TLB_TL	0x80000016	Yes	Yes	Total translation lookaside buffer misses
PAPI_L1_LDM	0x80000017	Yes	No	Level 1 load misses
PAPI_L1_STM	0x80000018	Yes	No	Level 1 store misses
PAPI_L2_LDM	0x80000019	Yes	No	Level 2 load misses
PAPI_L2_STM	0x8000001a	Yes	No	Level 2 store misses

PAPI counters

HW counters to capture

Extrac configuration: extrac.xml



```
<!-- Bursts library enabled? This requires an special library! -->
<bursts enabled="no">
  <!-- Specify the threshold. This is mandatory! In this example, the
  threshold is limited to 500 microseconds
  -->
  <threshold enabled="yes">500u</threshold>
  <!-- Report MPI statistics? -->
  <mpi-statistics enabled="yes" />
</bursts>

<!-- Enable sampling capabilities using system clock.
Type may refer to: default, real, prof and virtual.
Period stands for the sampling period (50ms here)
plus a variability of 10ms, which means periods from
45 to 55ms.
-->
<sampling enabled="no" type="default" period="50m" variability="10m" />

<!-- Enable dynamic memory instrumentation (experimental) -->
<dynamic-memory enabled="no" />

<!-- Enable I/O (read, write) instrumentation (experimental) -->
<input-output enabled="no" />

<!-- Do merge the intermediate tracefiles into the final tracefile?
Named according to the binary name
options:
synchronization = { default, task, node, no } (default is node)
max-memory = Number (in Mbytes) max memory used in merge step
joint-states = { yes, no } generate joint states?
keep-mpits = { yes, no } keep mpit files after merge?
-->
<merge enabled="yes"
  synchronization="default"
  tree-fan-out="16"
  max-memory="512"
  joint-states="yes"
  keep-mpits="yes"
  sort-addresses="yes"
  overwrite="yes"
/>
```

} Enable sampling

Extrac wrapper: sets environment and loads required library

```
#!/bin/bash

export EXTRAE_HOME=/apps/CEPBAT00LS/extrae/3.3.0/mpi+libgomp4.2/64
export EXTRAE_CONFIG_FILE=./extrae.xml
#export LD_PRELOAD=${EXTRAE_HOME}/lib/libmpitrace.so # For C apps
export LD_PRELOAD=${EXTRAE_HOME}/lib/libmpitracef.so # For Fortran apps

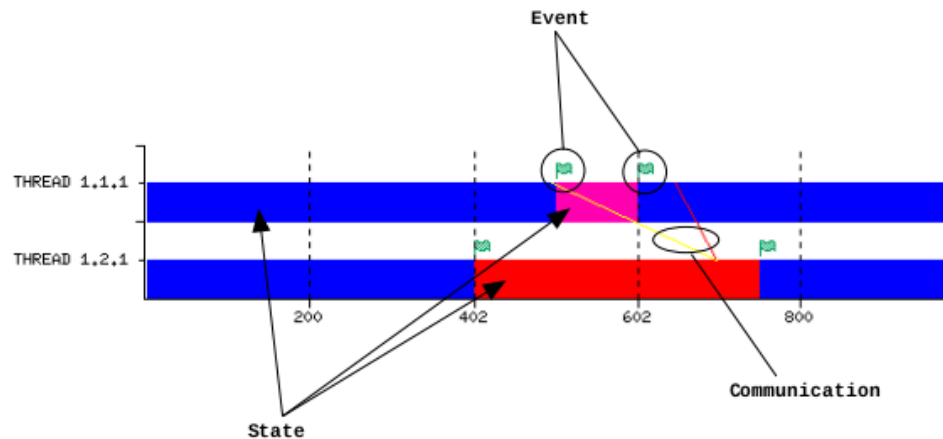
## Run the desired program
$*
```

Add the wrapper to your batch script

```
#!/bin/sh
# @ initialdir = .
# @ output = trace.out
# @ error = trace.err
# @ total_tasks = 128
# @ cpus_per_task = 1
# @ tasks_per_node = 16
# @ wall_clock_limit = 00:10:00

srun -n 128 ./trace.sh ./opa
```

- **Paraver traces:** made up from records (timestamp + event or activity) of three different kind:
 - **State records:** intervals of thread status, i.e, waiting in a barrier (either MPI or OpenMP), waiting for a message, computing...
 - **Event records:** punctual event occurred in a given timestamp, as entry & exit points of user functions, MPI routines, OpenMP parallel regions...
 - **Communication records:** relationship between two objects, as communication between two processes (MPI), task movement among threads (OpenMP/OmpSs) or memory transfers (CUDA/OpenCL).



- Paraver traces are composed by **three files** (one ASCII trace file + two metadata optional files):
 - ASCII trace file (**.prv**): defines the objects structure and contains **a list of all the trace records**.
 - Paraver configuration file (**.pcf**): defines **labels and colors associated to states and events**.
 - Names configuration file (**.row**): defines the **row labels** that will be displayed in the application.

```
#Paraver (22/05/01 at  
16:20):1021312:2(16,16):1:2(1:1,1:2)  
1:1:1:1:1:0:100:4  
1:2:1:2:1:0:200:4  
1:1:1:1:1:100:300:1  
1:1:1:1:1:200:500:4  
3:1:1:1:1:300:325:2:1:2:1:200:330:10:3000  
2:1:1:1:1:300:60000000:1  
.  
.  
.  
.  
.
```

Trace file (.prv)

	Average values	CLAIX
Event	150-200 ns	140 ns
Event + PAPI	750 ns – 1 us	600 ns
Event + callstack (1 level)	600 ns	690 ns
Event + callstack (6 levels)	1.9 us	2.6 us