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Optimizing an Earth Science Atmospheric Application with the OmpSs Programming Model

Workshop on High performance computing in meteorology

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EXCELENCIA SEVERO OCHOA

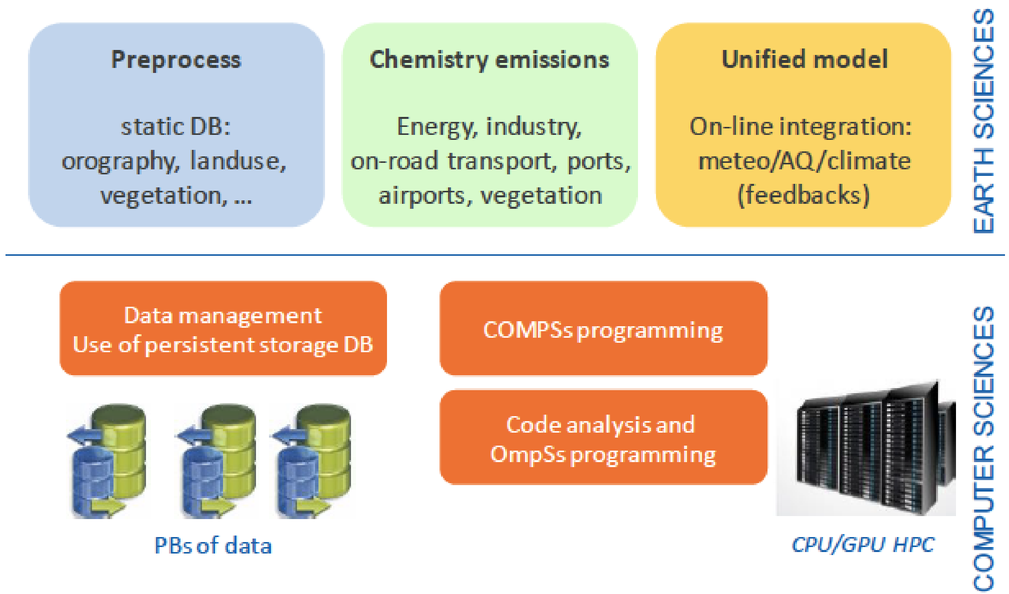
ECMWF, Reading, UK, 31 October 2014

Outline

- Introduction to NMMB/BSC-CTM
- Performance overview of NMMB/BSC-CTM
- Experiences with OmpSs
- Future work

Severo-Ochoa Earth Sciences Application

- Development of a Unified Meteorology/Air Quality/Climate model
  - Towards a global high-resolution system for global to local assessments



- Extending NMMB/BSC-CTM from coarse regional scales to global high-resolution configurations

- Coupling with a Data Assimilation System for Aerosols

- International collaborations:

Meteorology

National Centers for Environmental Predictions

Climate
Global aerosols

Goddard Institute Space Studies

UCIrvine Air Quality

Uni. of California Irvine

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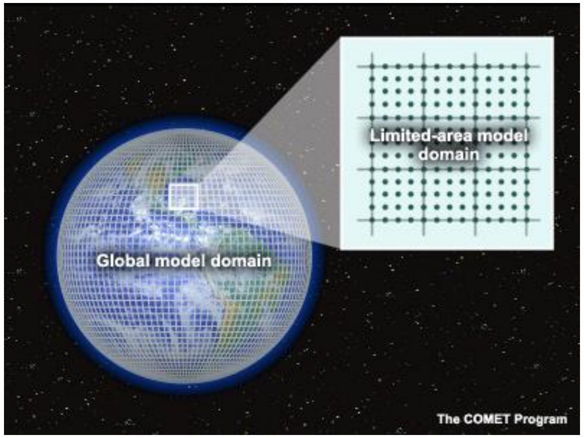
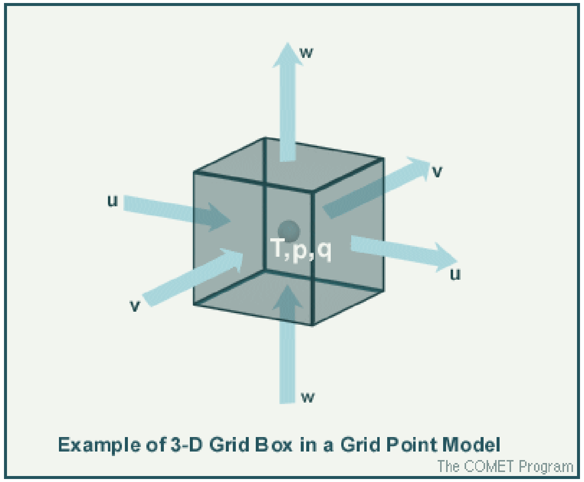
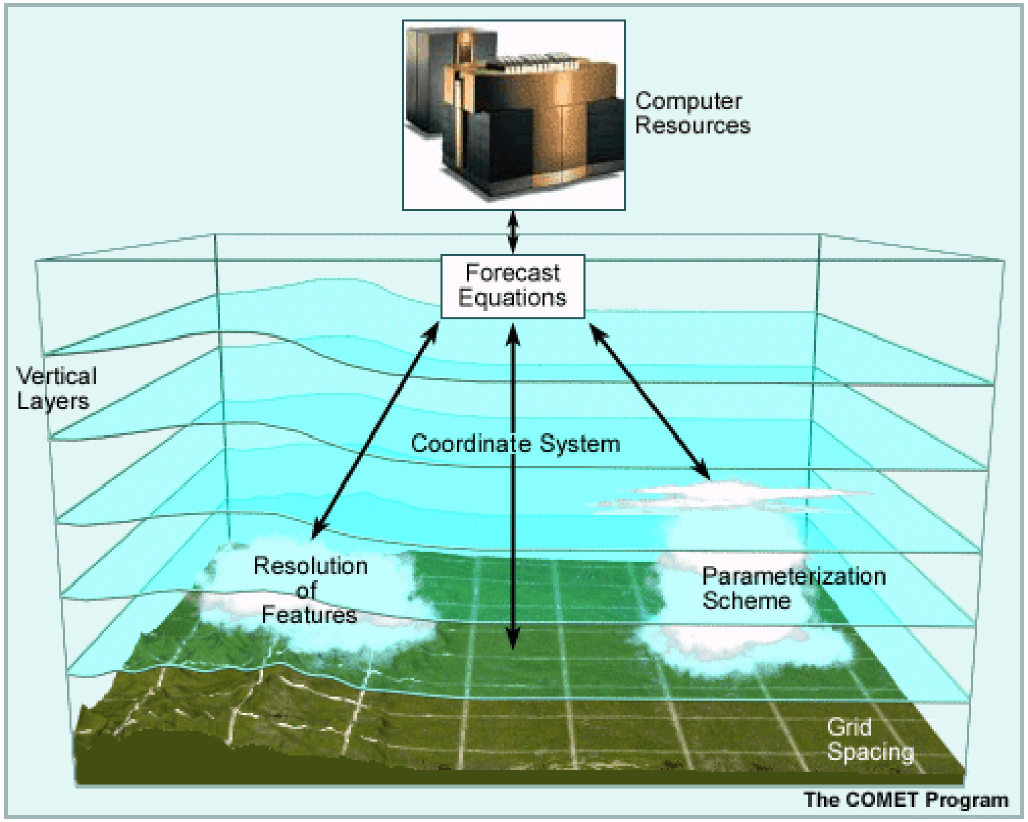
Where do we solve the primitive equations? Grid discretization







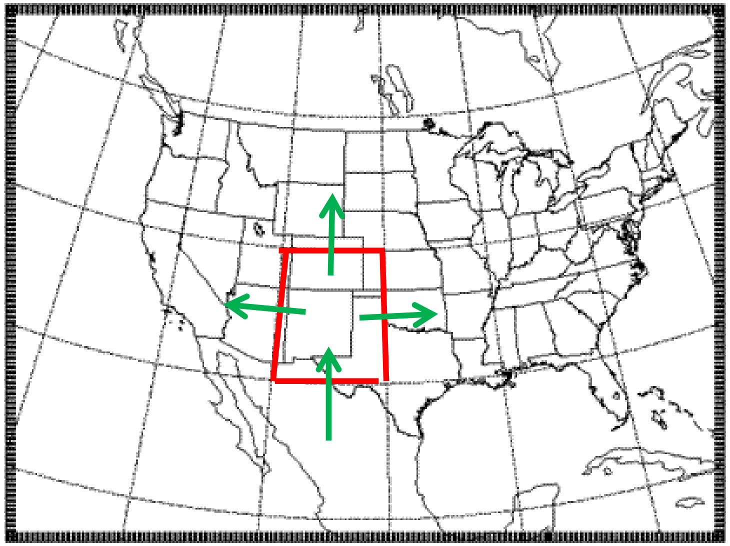
High performance computing resources:
If we plan to solve small scale features we need higher resolution in the mesh and so more HPC resources are required.

Parallelizing Atmospheric Models

- We need to be able to run this models in Multi-core architectures.

- Model domain is decomposed in patches

- Patch: portion of the model domain allocated to a distributed/shared memory node.

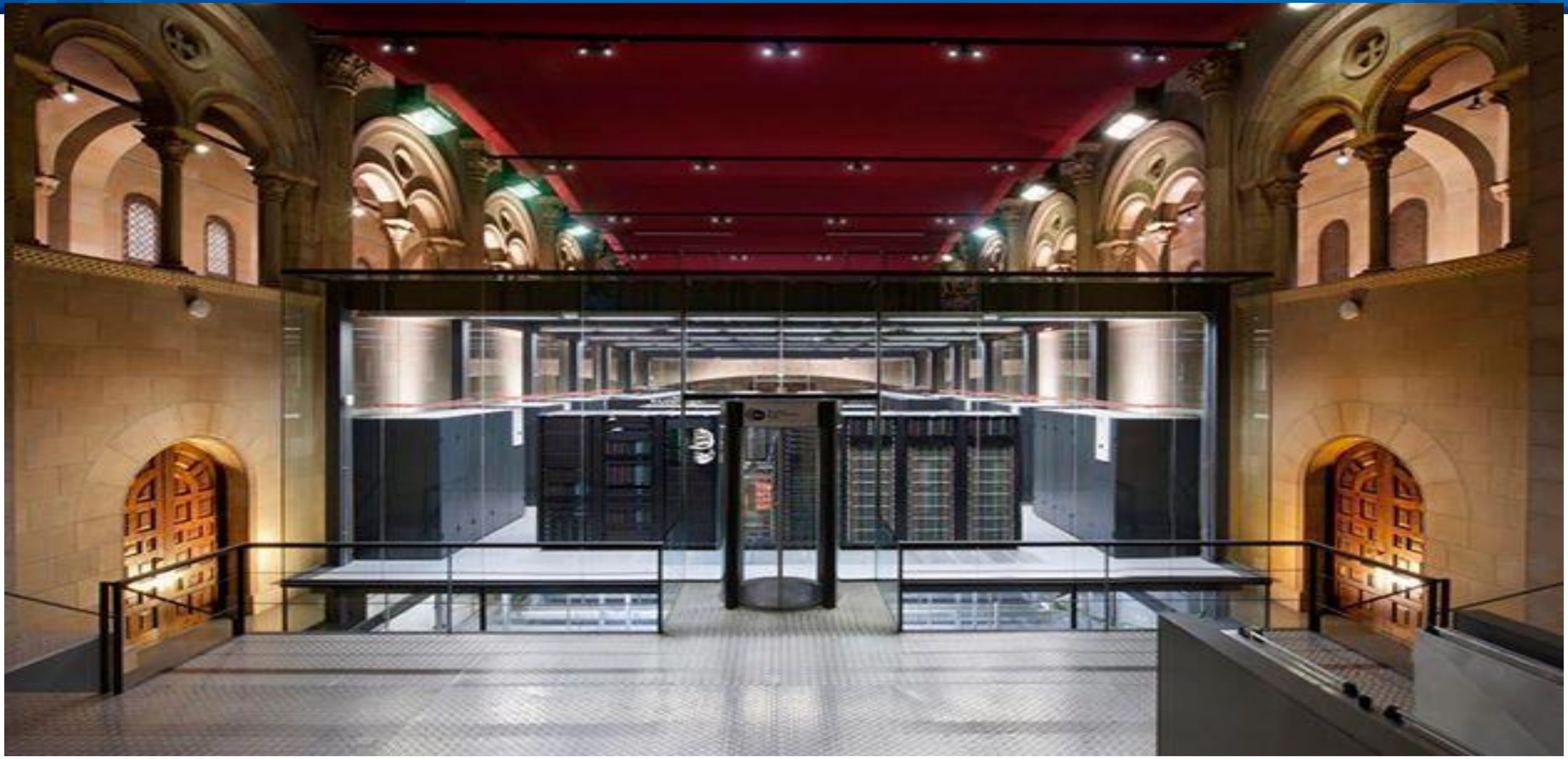


NMMB/BSC-CTM

- NMMB/BSC-CTM is used operationally for the dust forecast center in Barcelona
  - NMMB is the operational model of NCEP

- The general purpose is to improve its scalability and the simulation resolution

MarenoStrum III



- 3,056 compute nodes
- 2x Intel SandyBridge-EP E5-2670 2.6 GHz
- 32 GB memory per node

- Infiniband FDR10
- OpenMPI 1.8.1
- ifort 13.0.1

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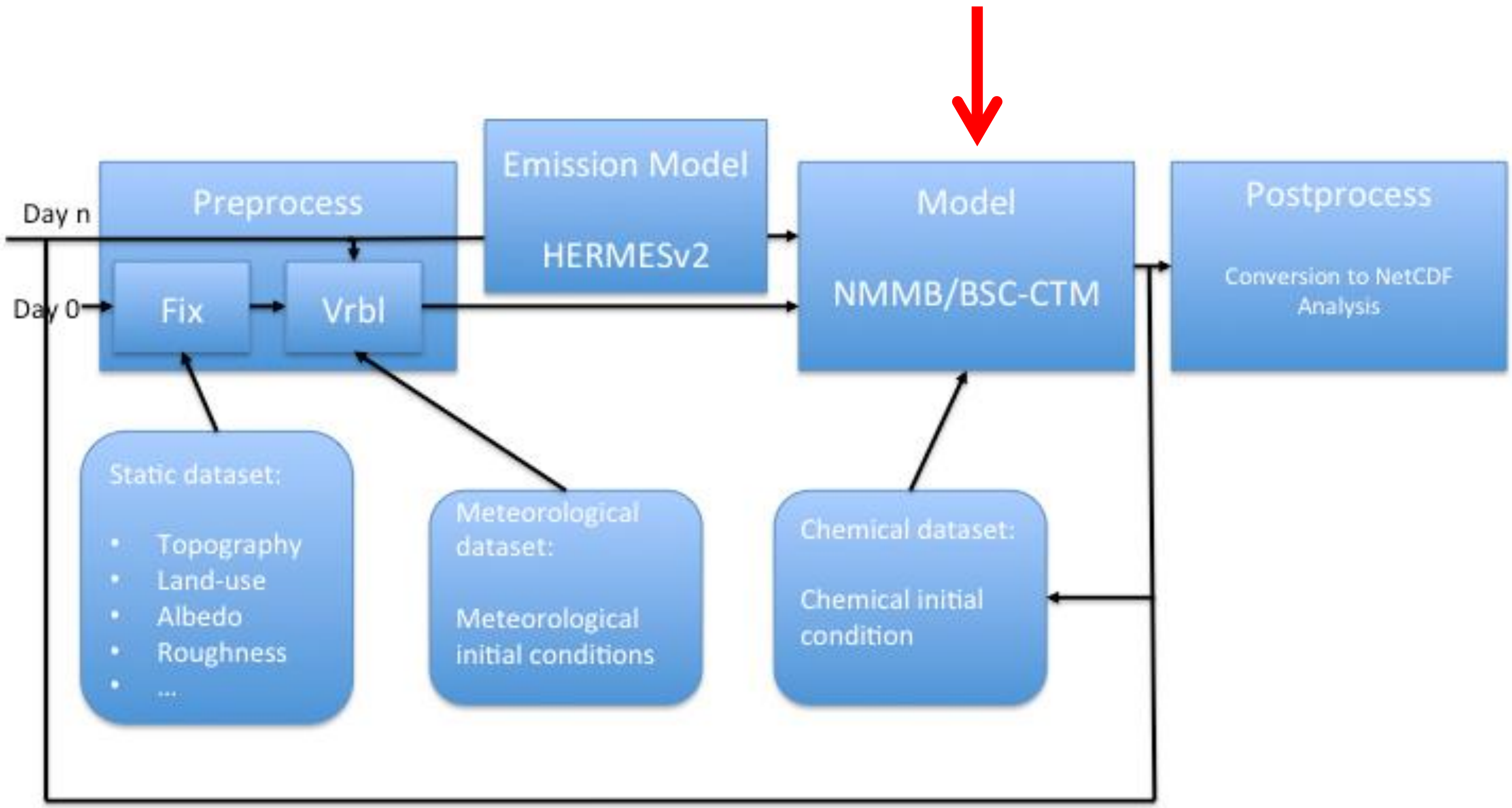
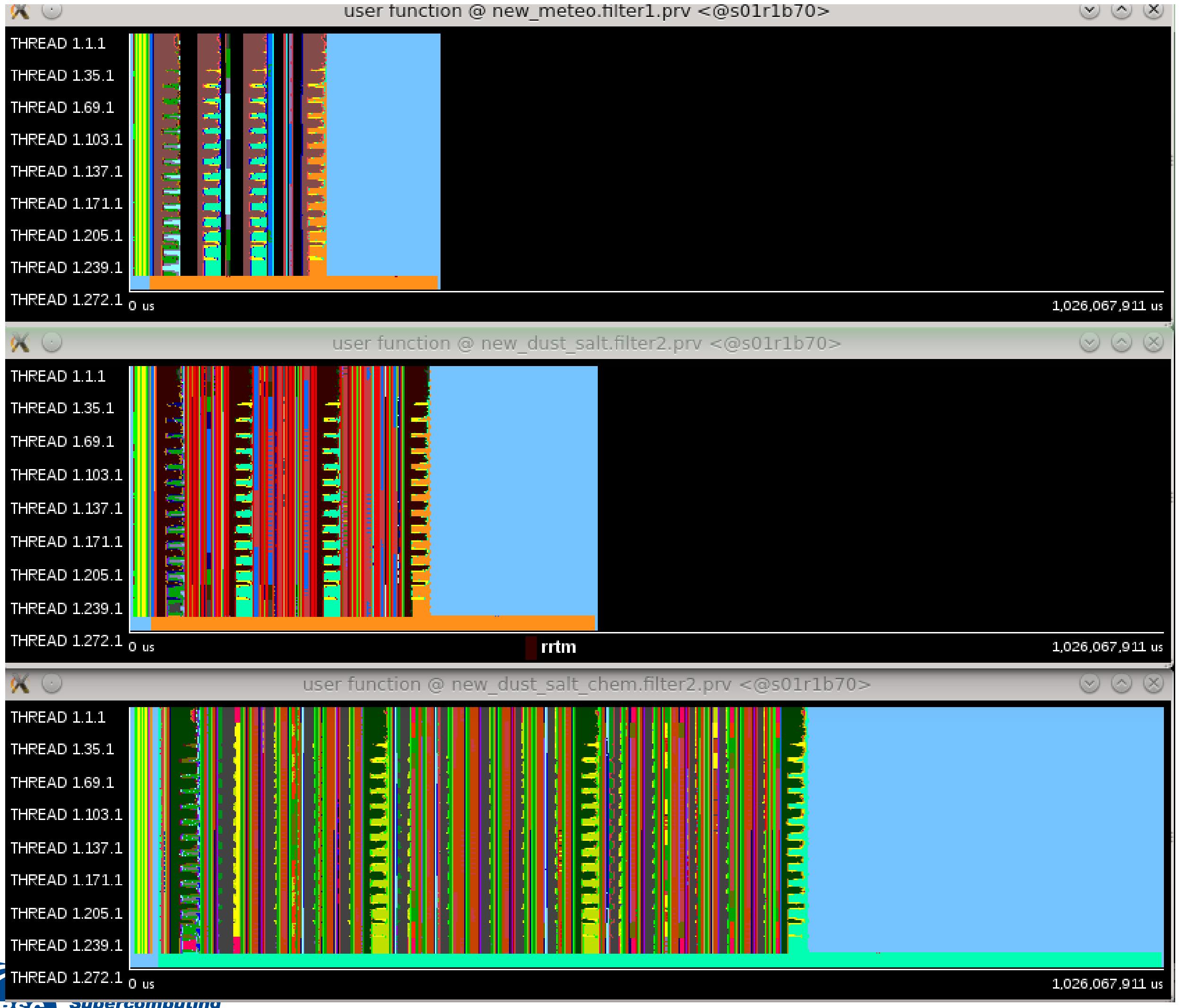
Performance Overview of NMMB/BSC-CTM Model

Execution diagram – Focus on the Model



Paraver

- One hour simulation of NMMB/BSC-CTM, global, 24km, 64 layers



meteo: 9 tracers

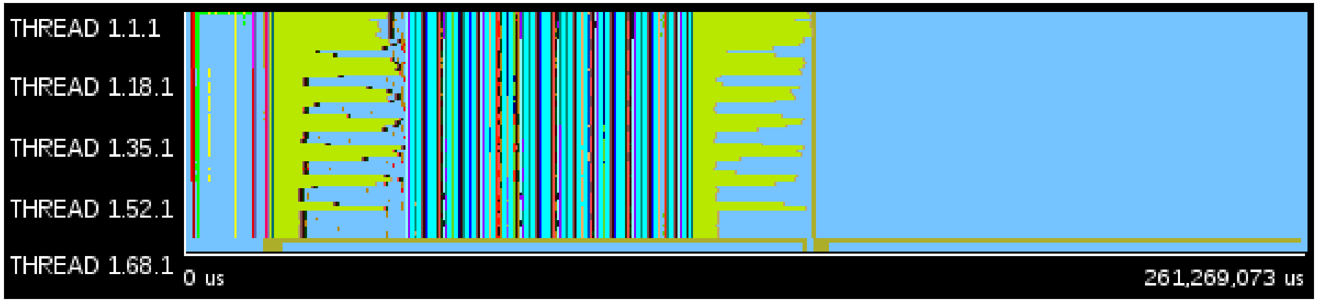
meteo + aerosols:
9 + 16 tracers

meteo + aerosols + gases: 9 + 16 + 53

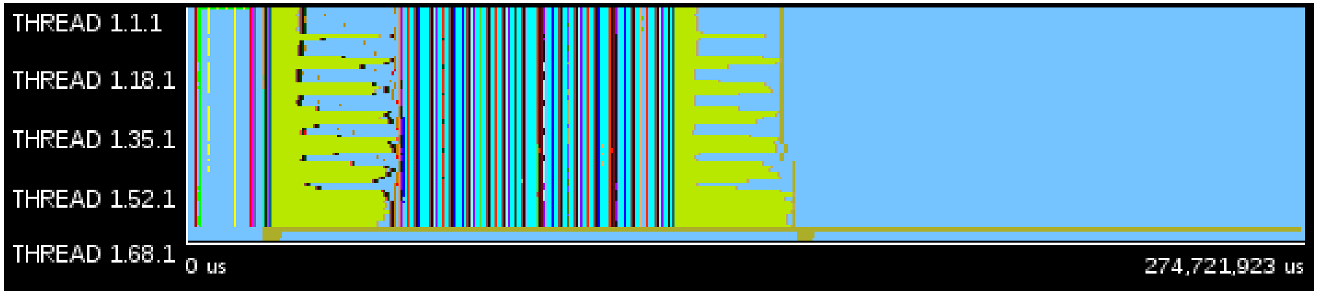
Dynamic load balancing

- Different simulation dates cause different load balance issue (useful functions, global 24km meteo configuration)

20/12/2005



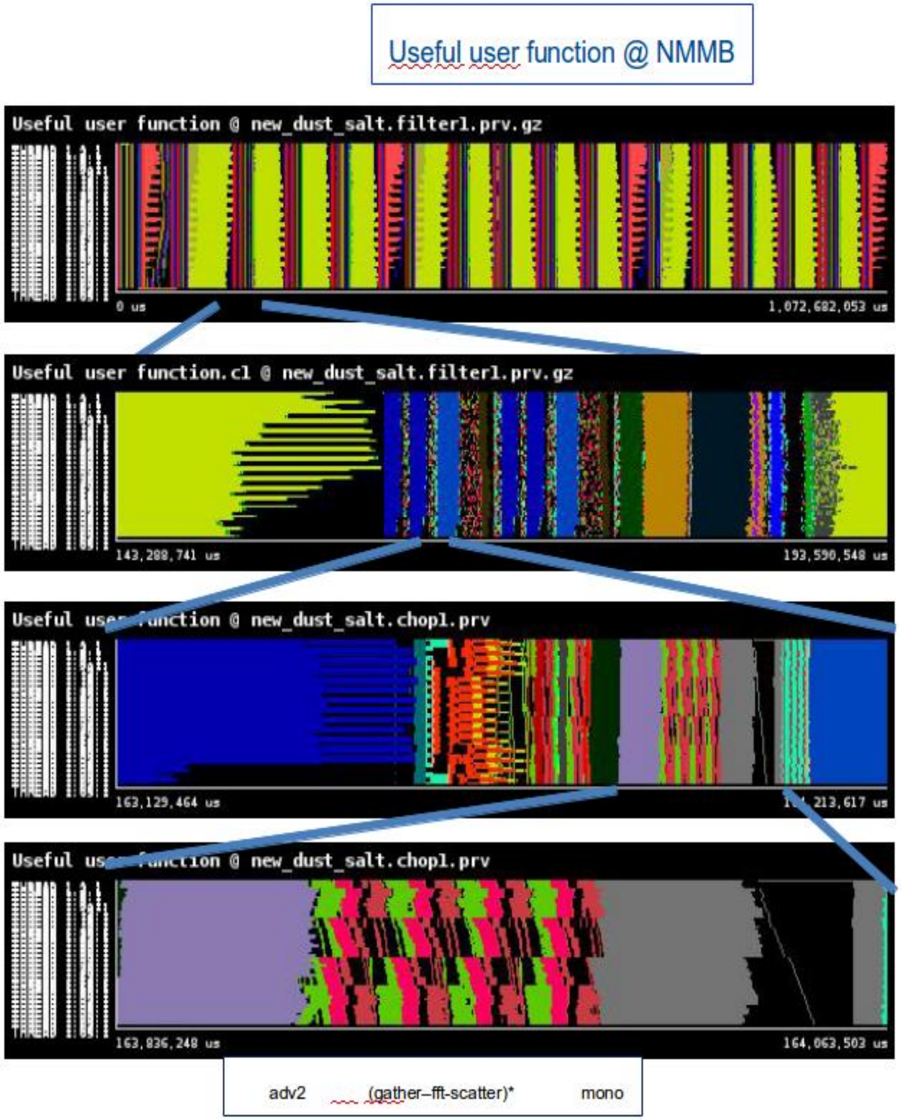
20/07/2005



A "different" view point

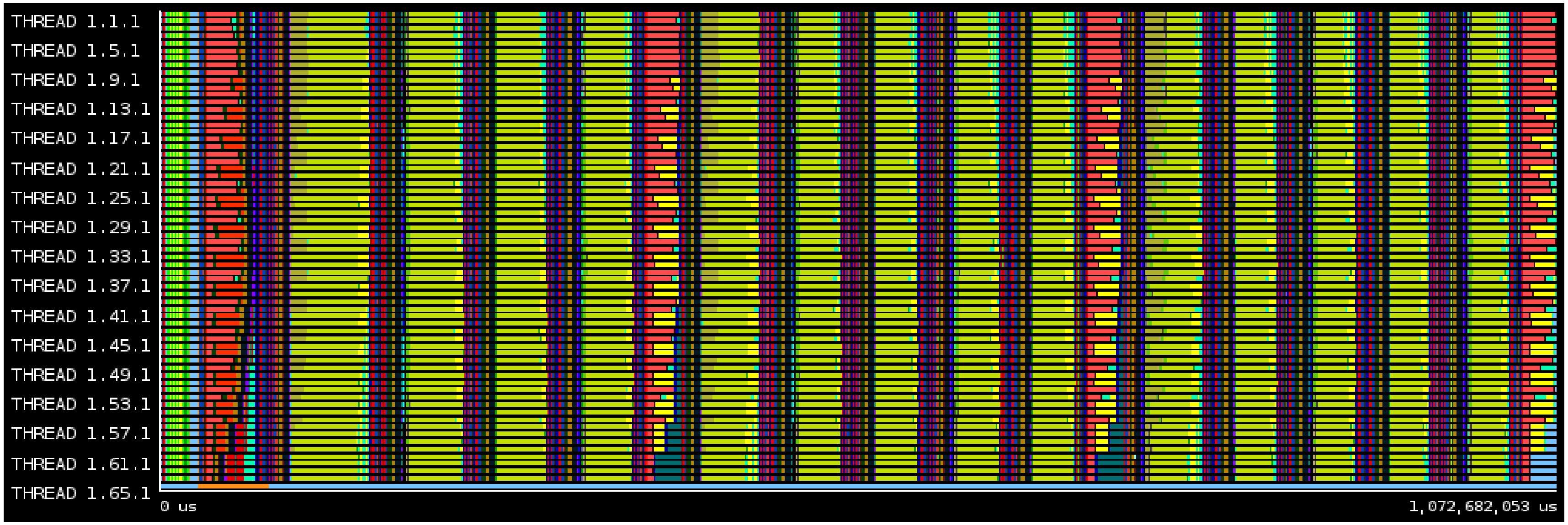
eff.= LB * Ser * Trf

LB	Ser	Trf	Eff
0.83	0.97		0.80
0.87	0.9		0.78
0.88	0.97	0.84	0.73
0.88	0.96	0.75	0.61



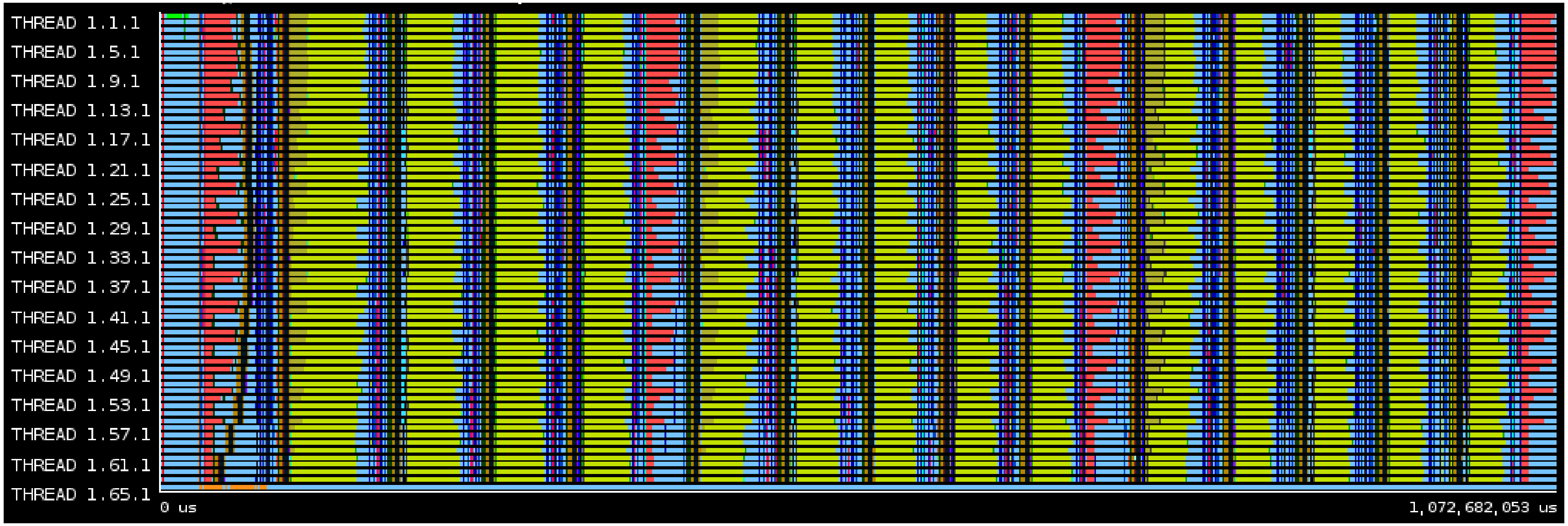
One hour simulation

- One hour simulation, chemistry configuration for global model, 24 km resolution



One hour simulation

- Useful functions



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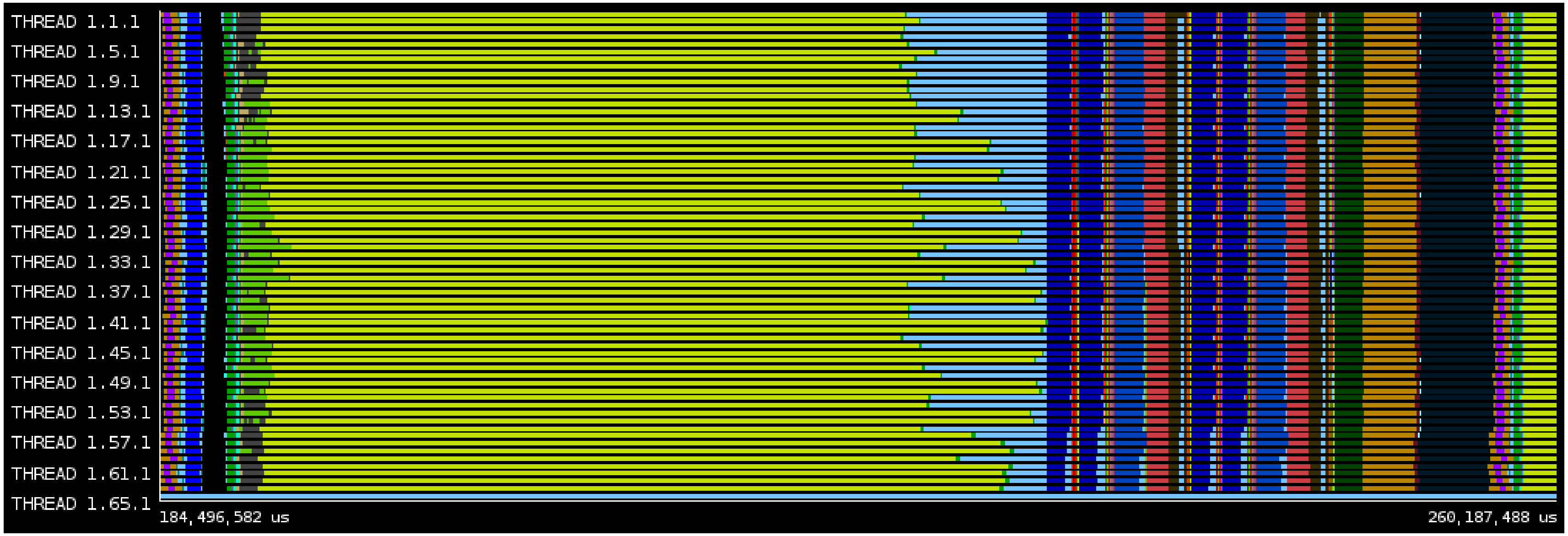
Zoom on EBI solver and next calls

- EBI solver (run_ebi) and the calls till the next call to the solver



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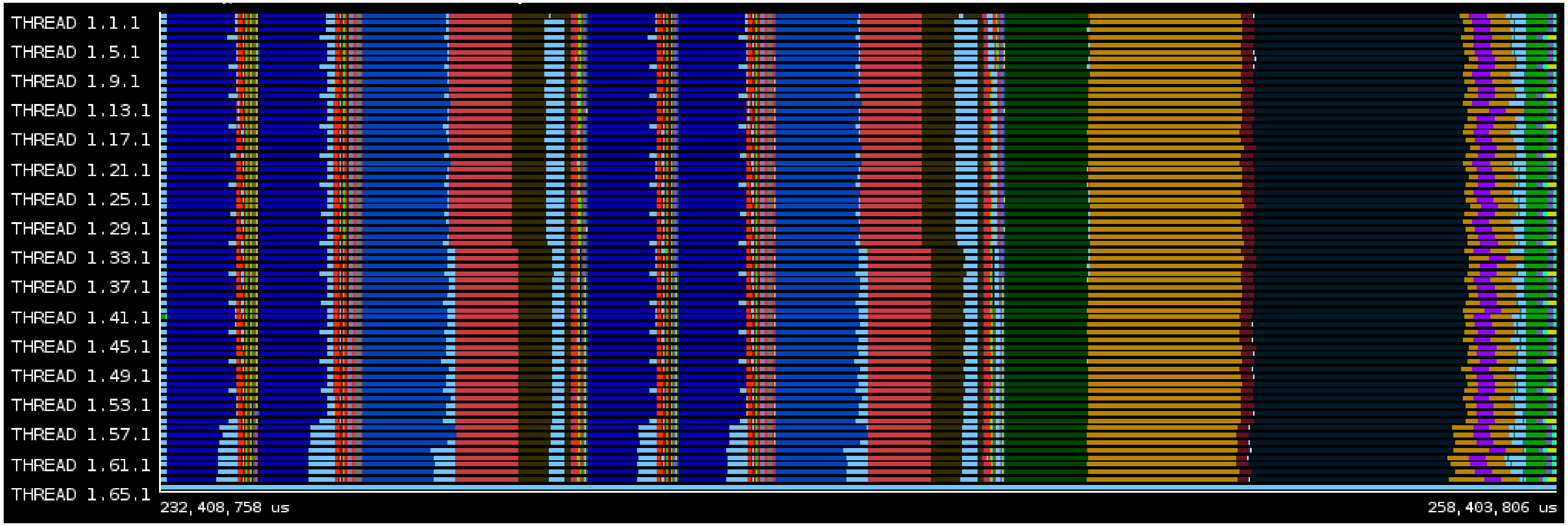
Zoom between EBI solvers

- The useful functions call between two EBI solvers
- The first two dark blue areas are horizontal diffusion calls and the light dark is advection chemistry.



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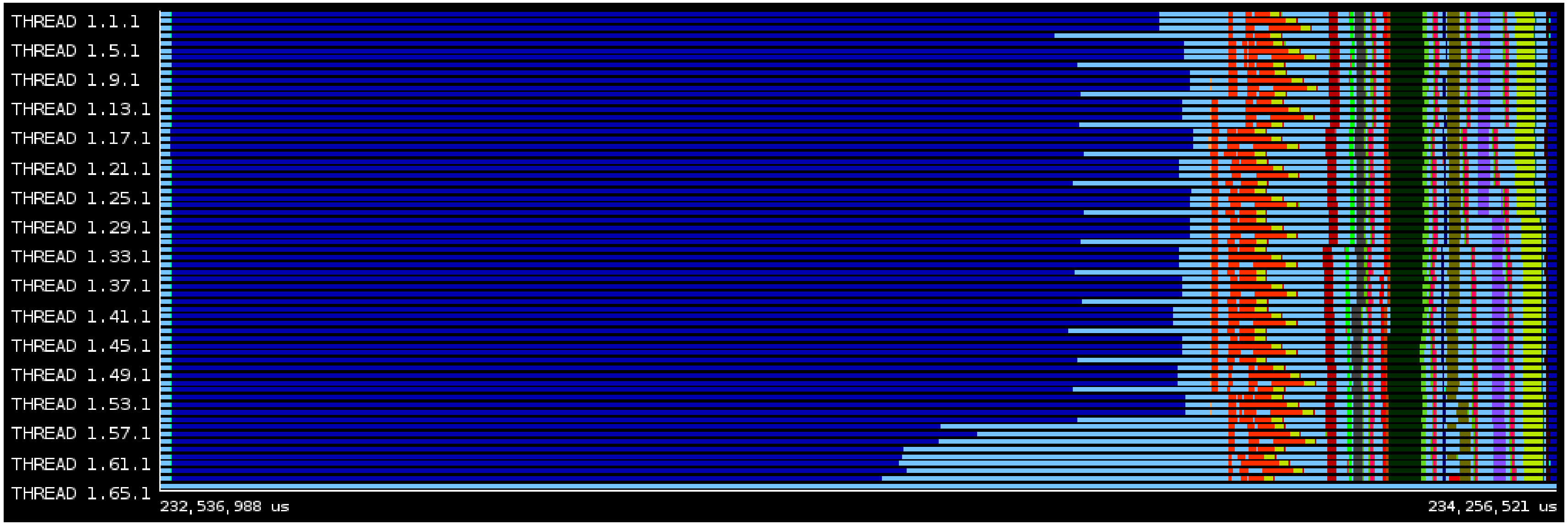
Horizontal diffusion

- We zoom on horizontal diffusion and the calls that follow
- Horizontal diffusion (blue colour) has load imbalance



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Experiences with OmpSs

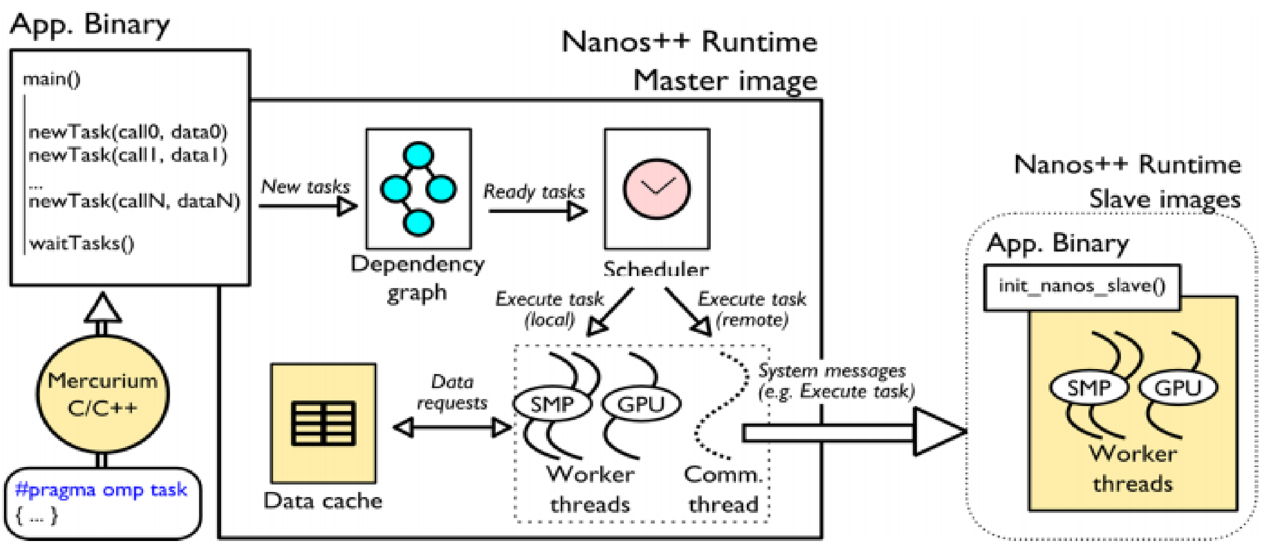
Objectives

- Trying to apply OmpSs on a real application
- Applying incremental methodology
- Identify opportunities
- Exploring difficulties

OmpSs introduction

- Parallel Programming Model
  - Build on existing standard: OpenMP
  - Directive based to keep a serial version
  - Targeting: SMP, clusters, and accelerator devices
  - Developed in Barcelona Supercomputing Center (BSC)
    - Mercurium source-to-source compiler
    - Nanos++ runtime system

https://pm.bsc.es/ompss



Studying cases

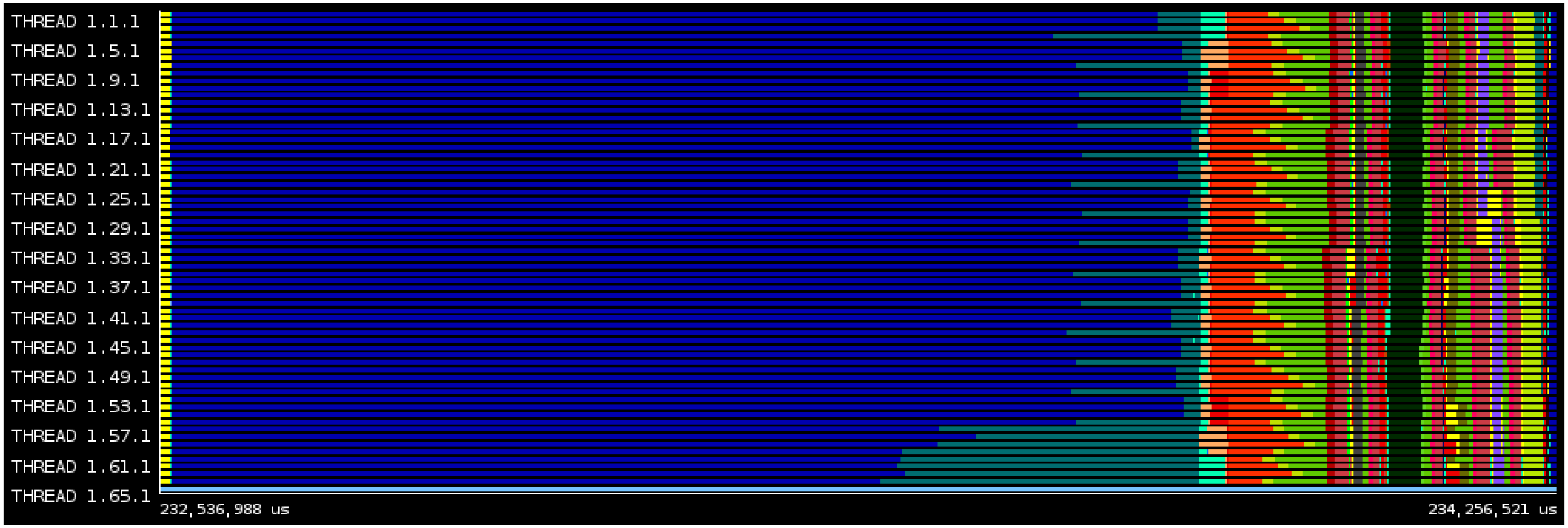
- Taskify a computation routine and investigate potential improvements and overlap between computations of different granularities

- Overlap communication with packing and unpacking costs

- Overlap independent coarse grain operations composed of communication and computation phases

Horizontal diffusion + communication

- The horizontal diffusion has some load imbalance(blue code)
- There is some computation about packing/unpacking data for the communication buffers (red area)
- Gather (green colour) and scatter for the FFTs



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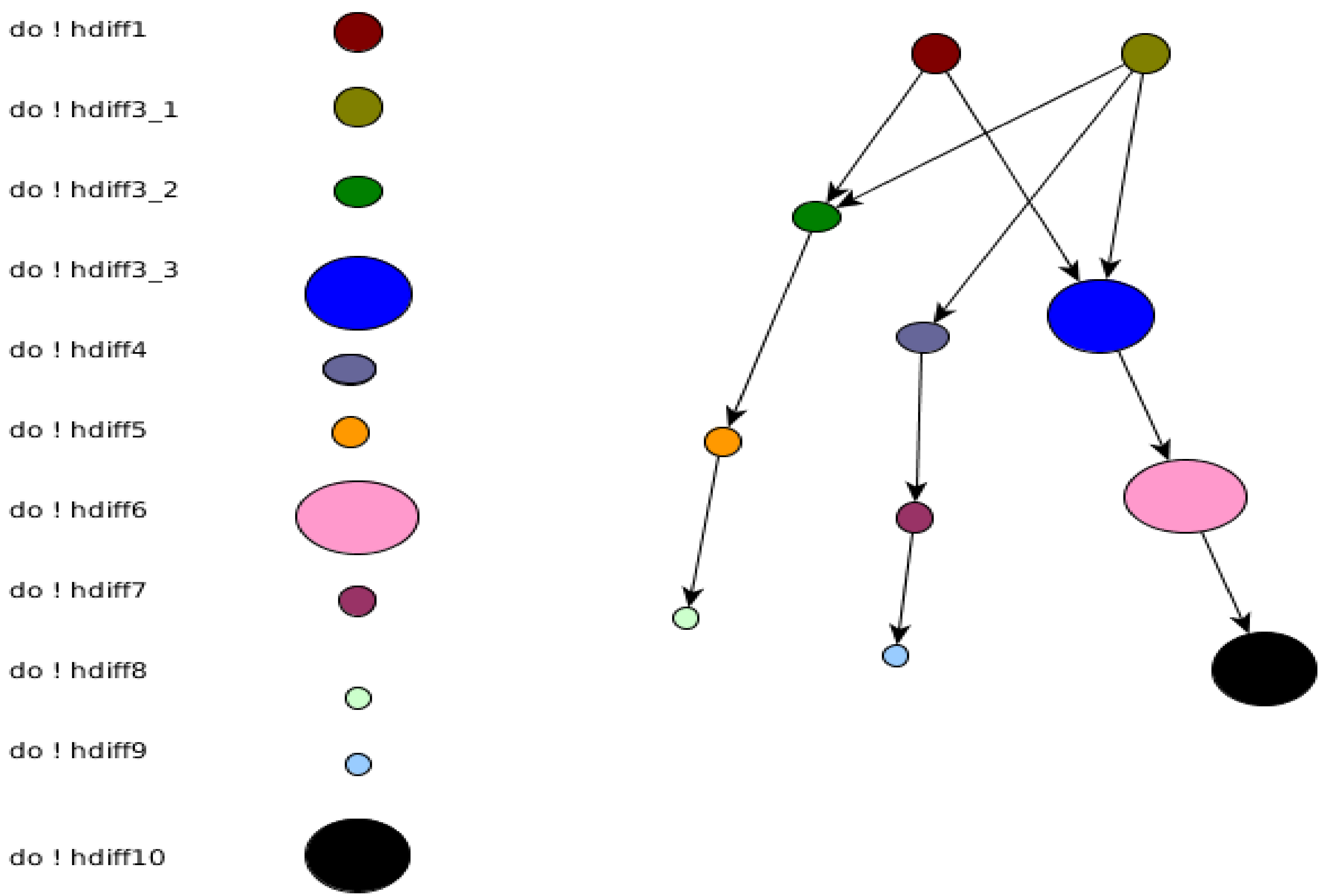
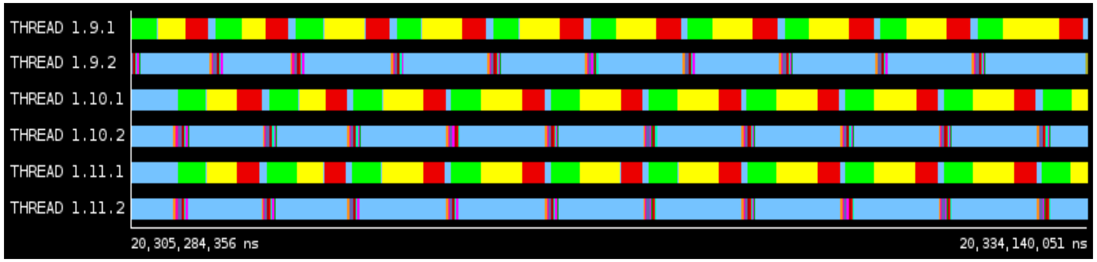
Horizontal diffusion skeleton code

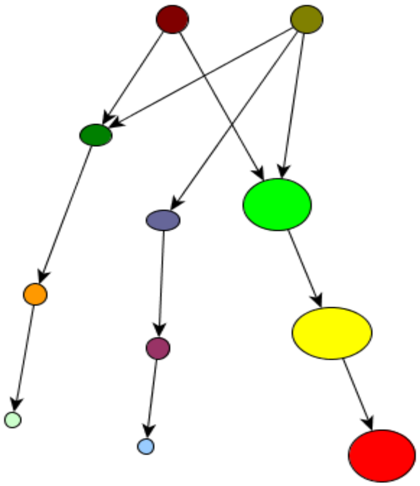
- The hdiff subroutine has the following loops and dependencies



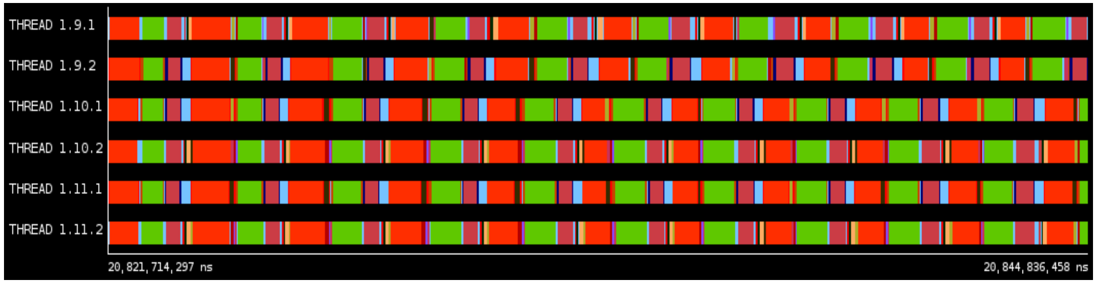
Parallelizing loops

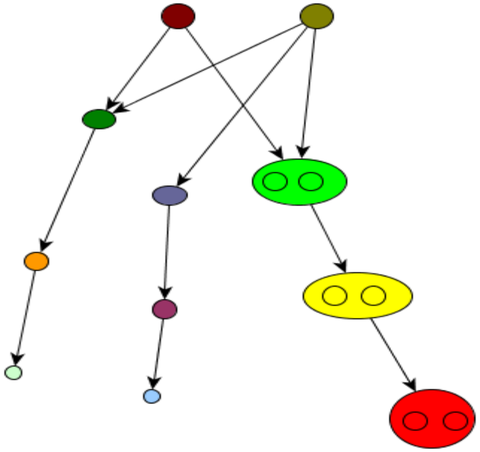
- Part of hdiff with 2 threads





- Parallelizing the most important loops

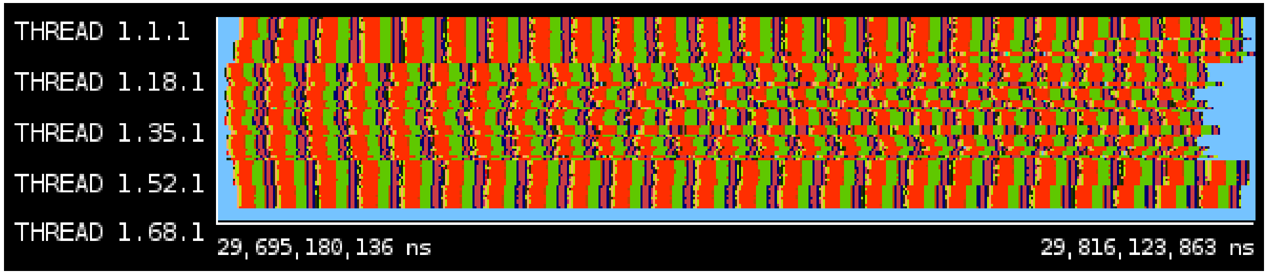




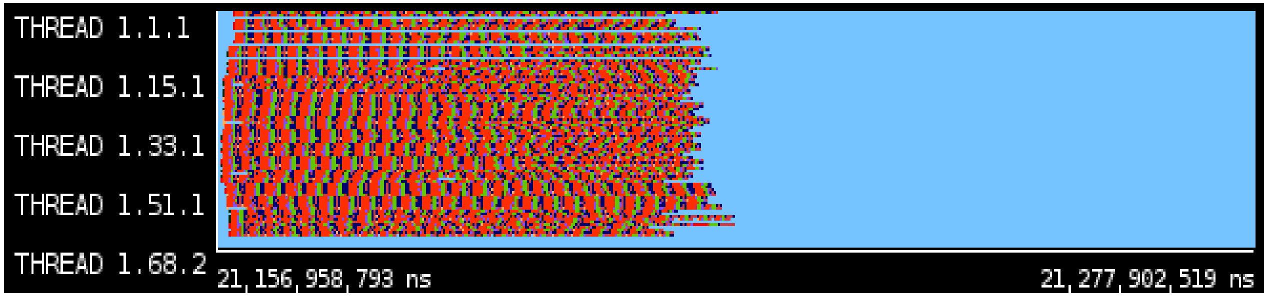
- We have a speedup of 1.3 by using worksharing

Comparison

- The execution of hdiff subroutine with 1 thread takes 120 ms



- The execution of hdiff subroutine with 2 threads takes 56 ms, the speedup is 2.14



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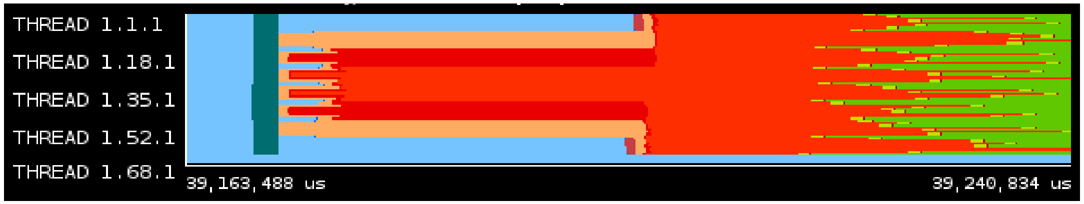
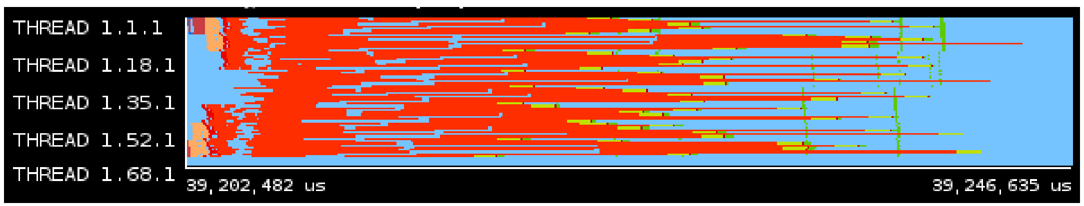
Issues related to communication

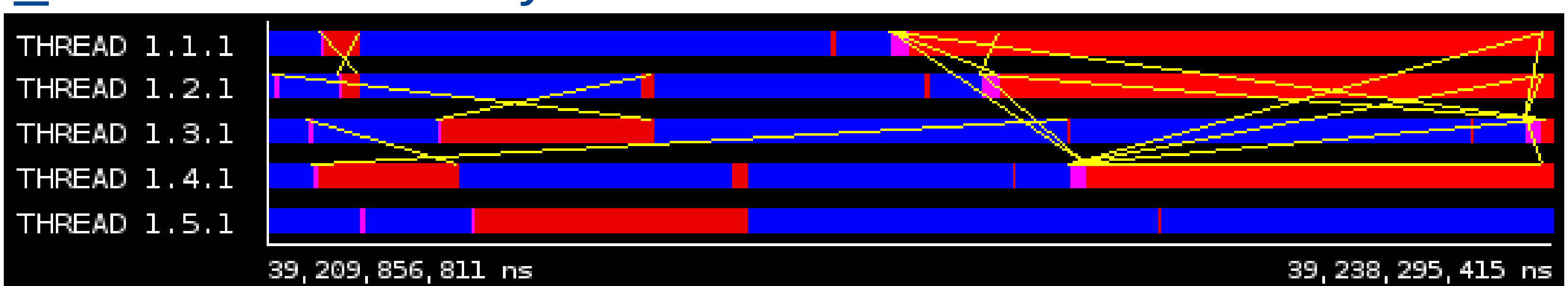
- We study the exch4 subroutine (red colour)



- The useful function of exch4 has some computation

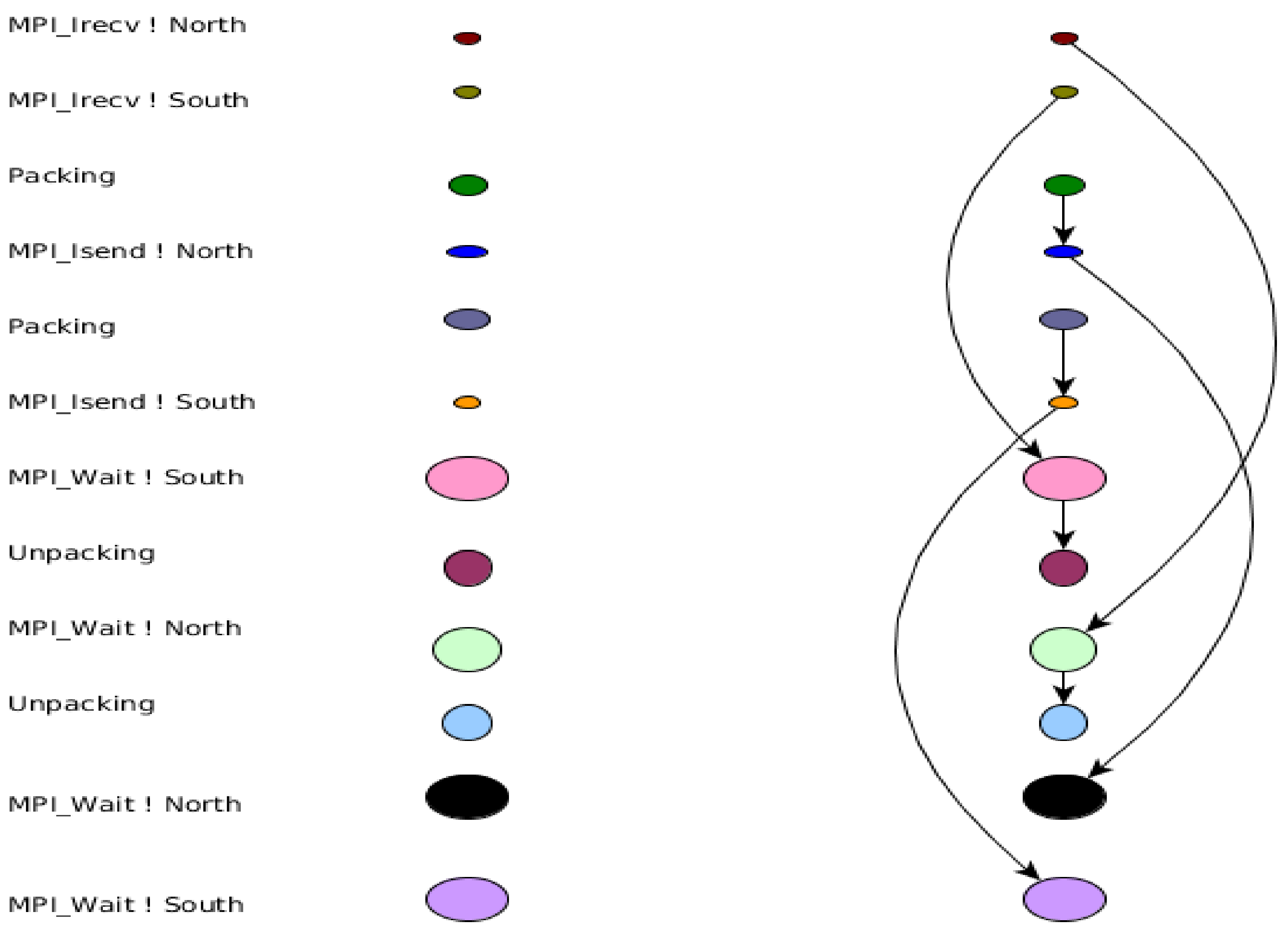


- The communication creates a pattern and the duration of the MPI_Wait calls can vary



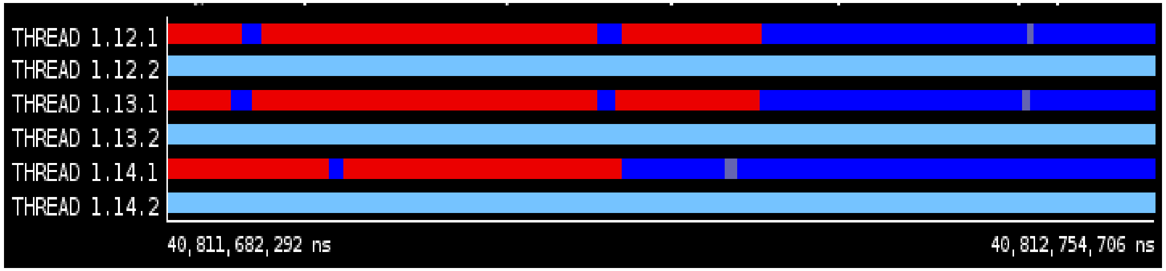
Issues related to communication

- Big load imbalance because message order
- There is also some computation

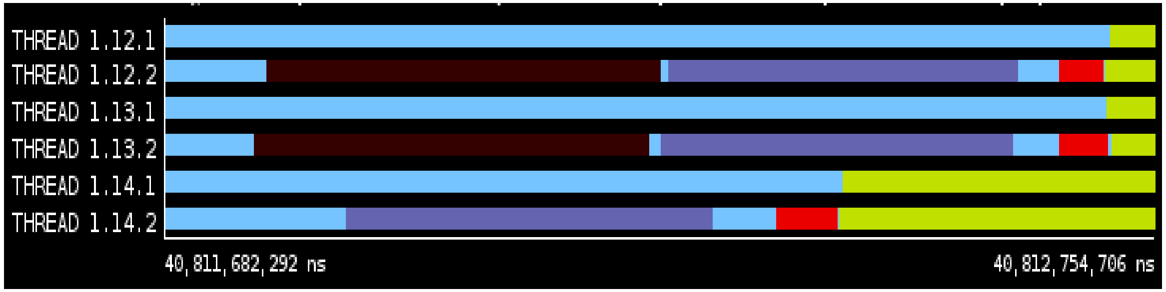


Taskify subroutine exch4

- We observe the MPI_Wait calls in the first thread

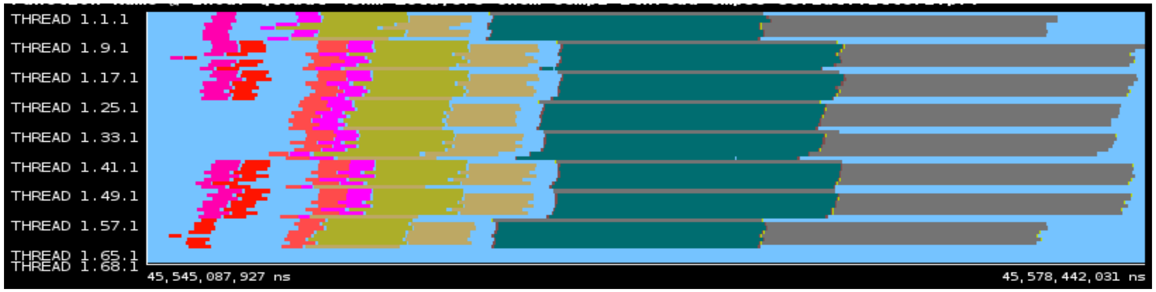


- In the same moment the second thread does the necessary computation and overlaps the communication

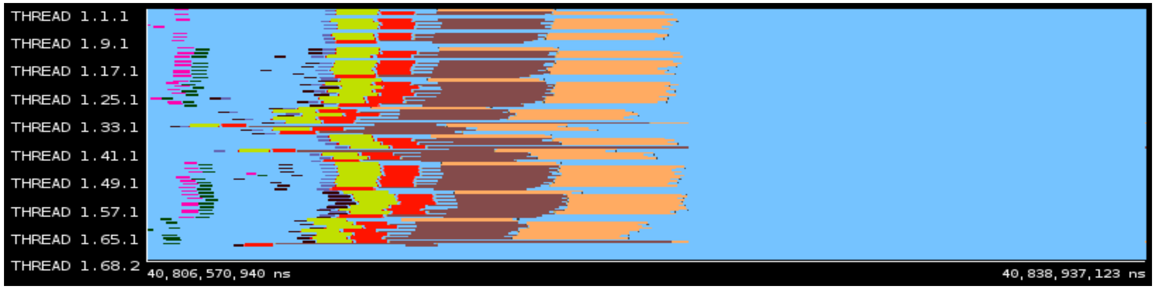


Taskify subroutine exch4

- The total execution of exch4 subrouting with 1 thread



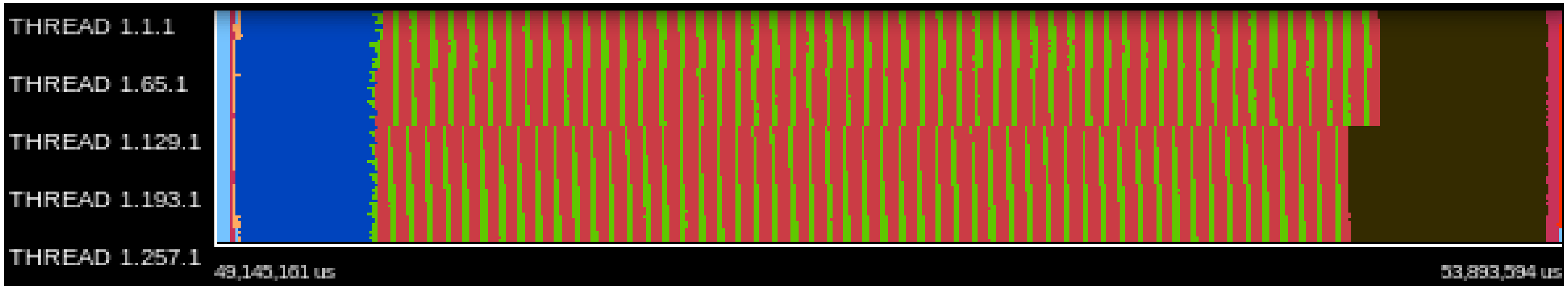
- The total execution of exch4 subroutine with 2 threads



- With 2 threads the speedup is 1.76 (more improvements have been identified)

Advection chemistry and FFT

- Advection chemistry (blue color) and 54 calls to gather/FFT/scatter till monotonization chemistry (brown color)



- Initial study to test the improvements of the execution with the OmpSs programming model

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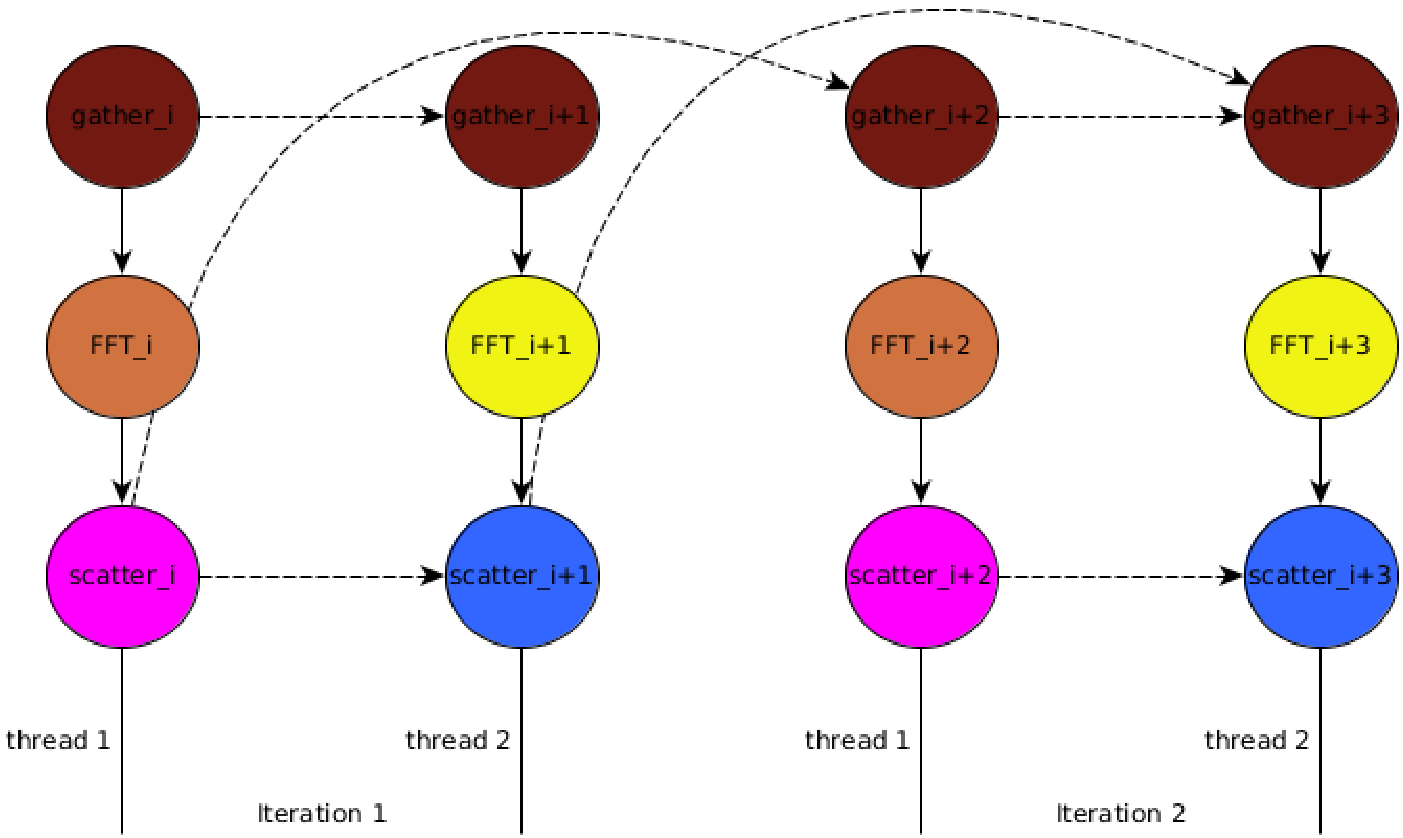
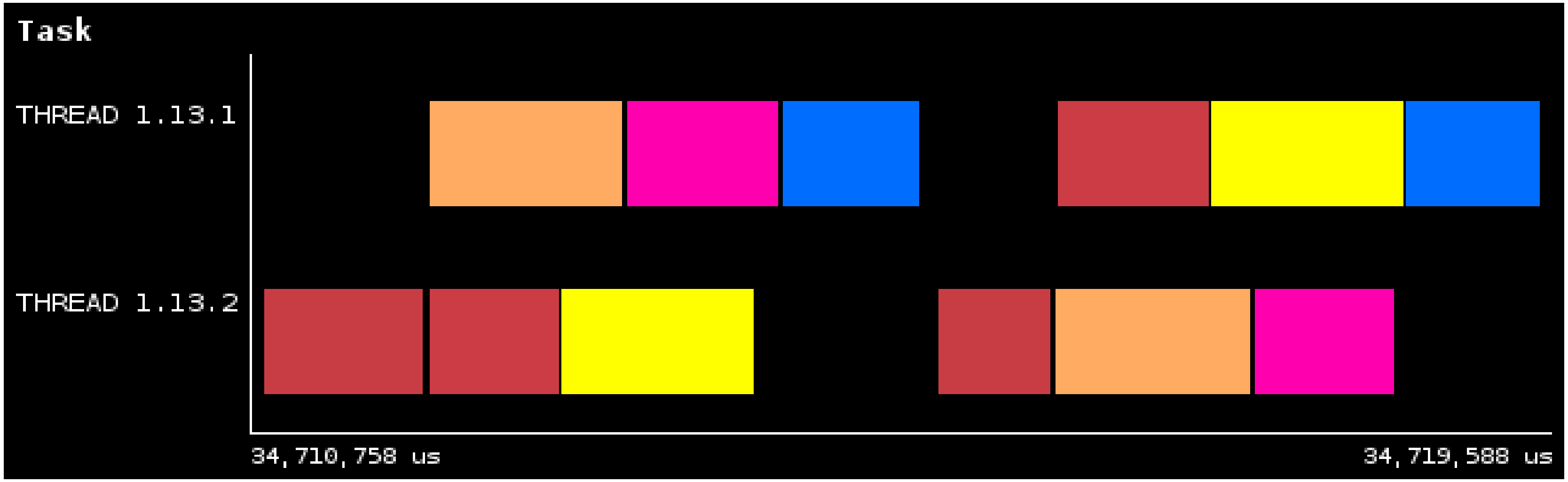
Study case: gather/FFT/scatter

- Workflow, two iterations, using two threads, declaring dependencies



Study case: gather/FFT/scatter

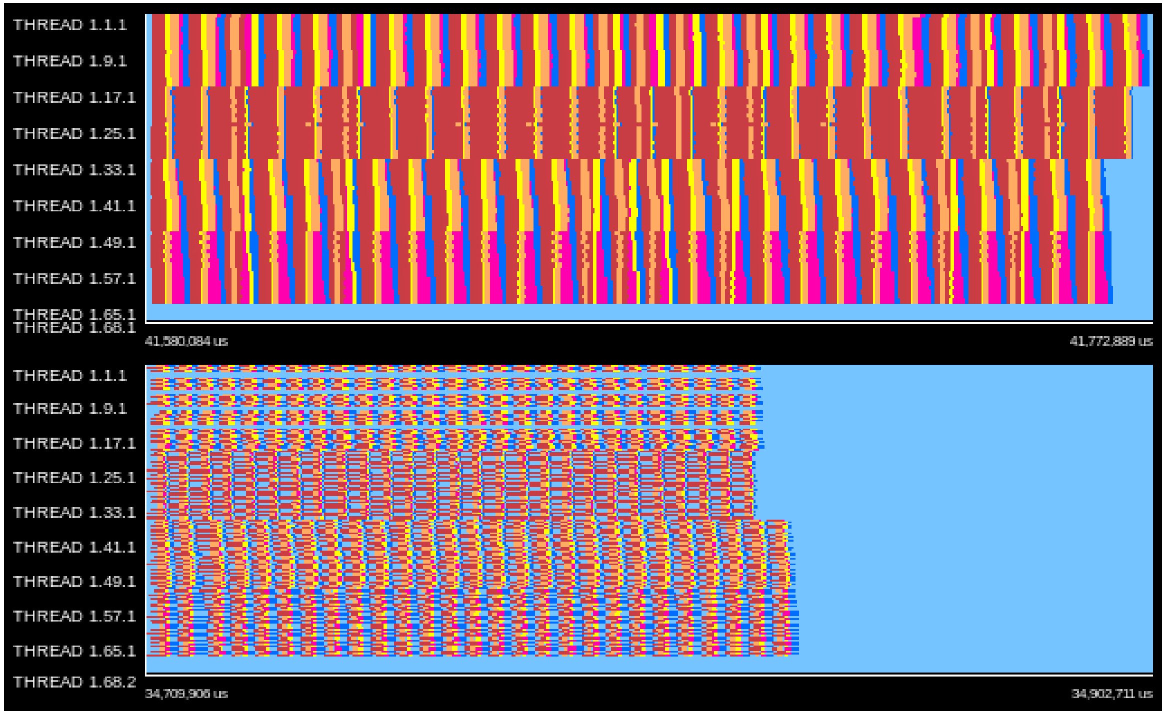
- Paraver view, two iterations, four tracers totally



- Thread 1:
  - Iteration 1: FFT_1, scatter_1, scatter_2
  - Iteration 2: gather_4, FFT_4, scatter_4
- Thread 2:
  - Iteration 1: gather_1, gather_2, fft_2
  - Iteration 2: gather_3, FFT_3, scatter_3

Study case: gather/FFT/scatter - Performance

- Comparing the execution time of 54 calls to gather/FFT/scatter with one and two threads



- The speedup with two threads is 1.56 and we have identified potential improvements

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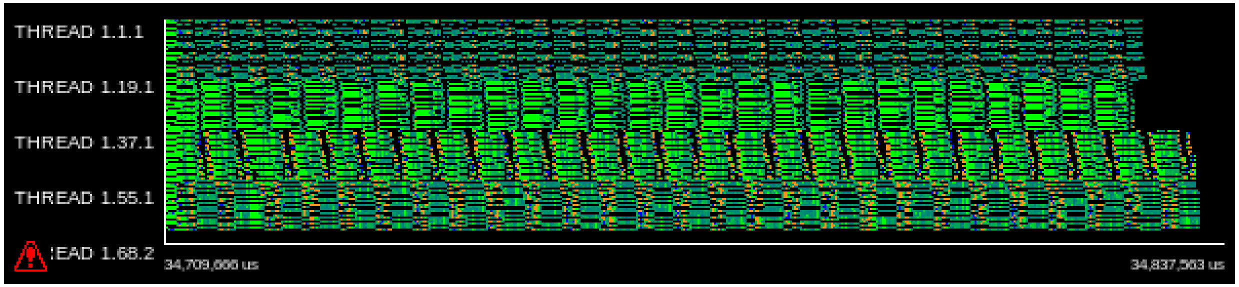
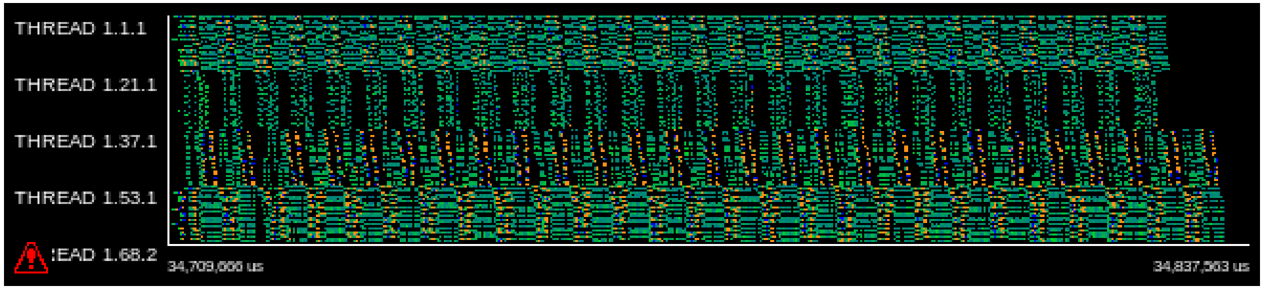
MPI Bandwidth

- MPI bandwidth for gather/scatter

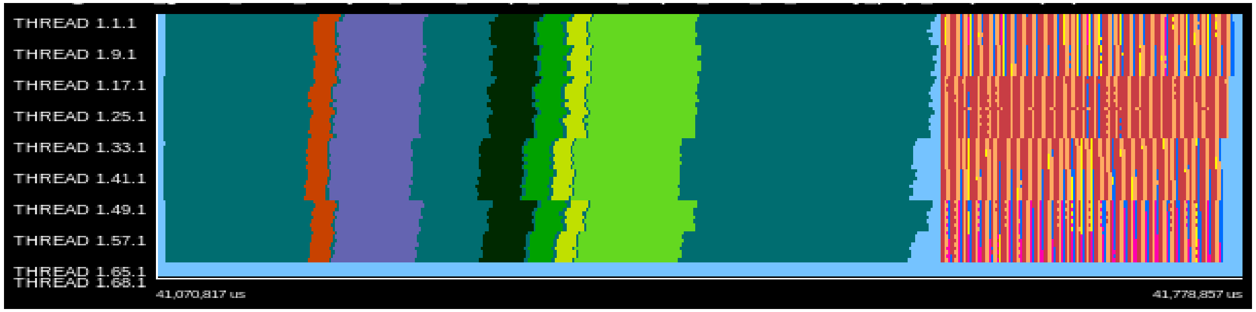


- MPI bandwidth over 1GB/s for gather/scatter

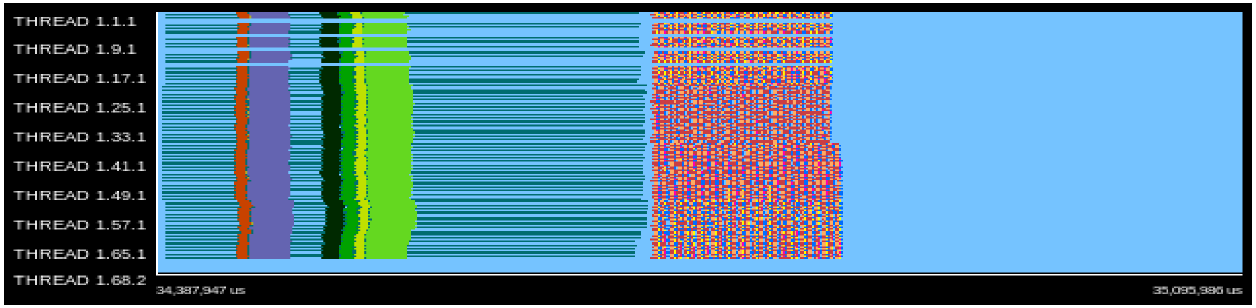


Combination of advection chemistry and FFT

- Advection chemistry with worksharing (not for all the loops), FFTs for one thread



- Similar but with two threads



- The speedup for the advection chemistry routine is 1.6 and overall is 1.58

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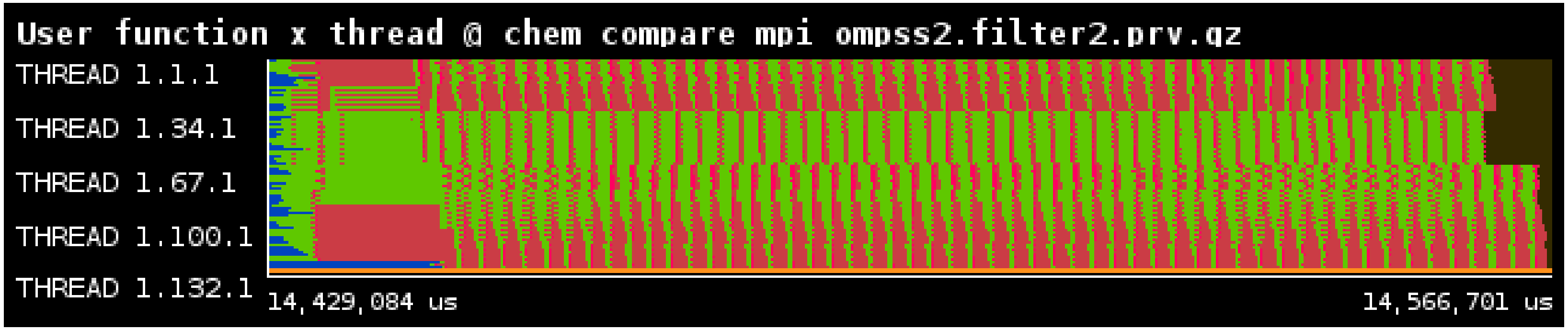
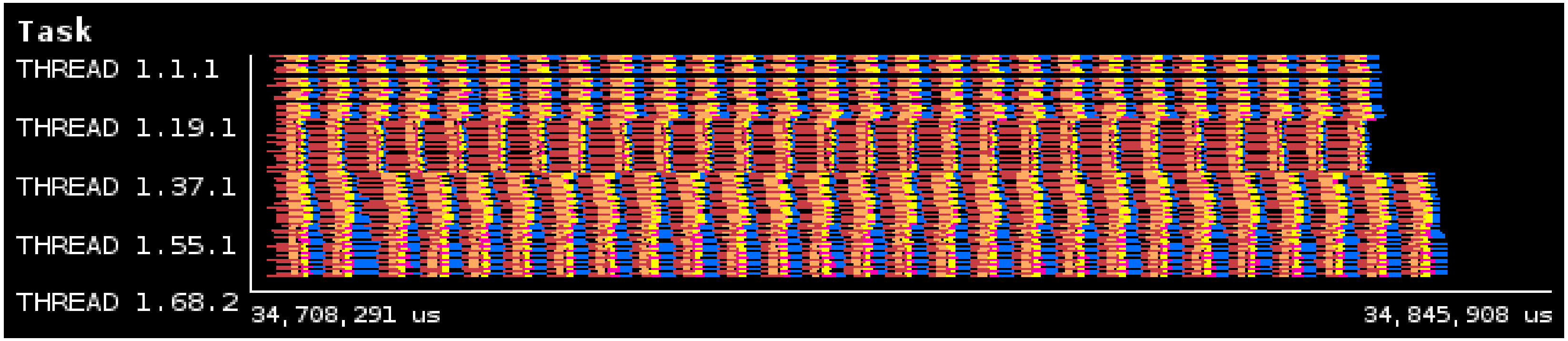
Comparison between MPI and MPI+OmpSs

- Pure MPI, 128 computation processes and 4 I/O



- MPI + OmpSs: 64 MPI processes + 64 threads + 4 I/O



- The load imbalance for the FFT with pure MPI is 28% while with MPI+OmpSs is 54%

Incremental methodology with OmpSs

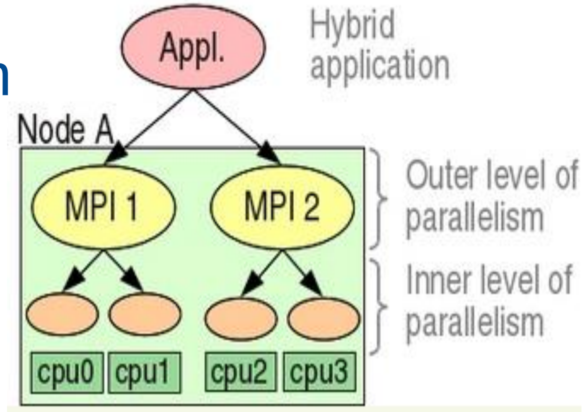
- Taskify the loops
- Start with 1 thread, use if(0) for serializing tasks
- Test that dependencies are correct (usually trial and error)
- Imagine an application crashing after adding 20+ new pragmas (true story)
- Do not parallelize loops that do not contain significant computation

Conclusions

- The incremental methodology is important for less overhead in the application
- OmpSs can be applied on a real application but is not straightforward
- It can achieve pretty good speedup, depending on the case
- Overlapping communication with computation is a really interesting topic
- We are still in the beginning but OmpSs seems promising

Future improvements

- Investigate the usage of multithreaded MPI
- One of the main functions of the application is the EBI solver (run_ebi). There is a problem with global variables that make the function not reentrant. Refactoring of the code is needed.
- Porting more code to OmpSs and investigate MPI calls as tasks
- Some computation is independent to the model's layers or to tracers. OpenCL kernels are going to be developed to test the performance on accelerators
- Testing versioning scheduler
- The dynamic load balancing library should be studied further (http://pm.bsc.es/dlb)
- Apply OmpSs for a data assimilation simulation



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Thank you!

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