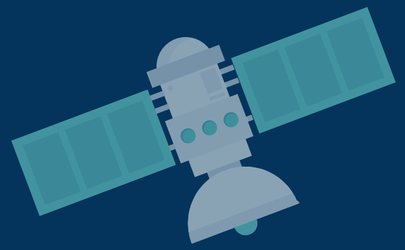
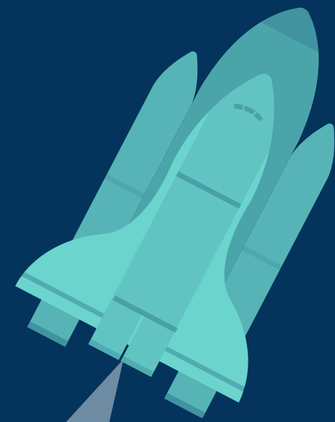
HACC

The Hardware Accelerated Cosmology Code framework



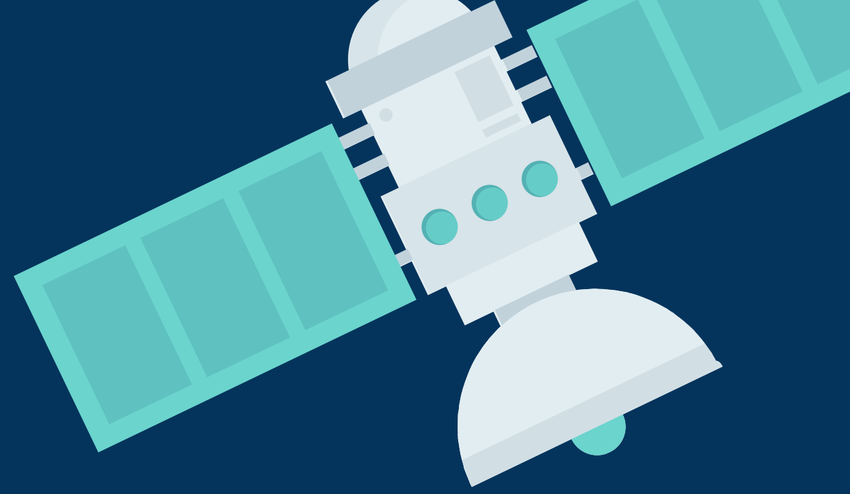


Curated by Roberto Stagi

PARALLEL PROGRAMMING TOOLS AND MODELS - 2020 @ UPC

Presentation Outline

Introduction and set-up
Prepare for the analysis
Analysis Trace
Further Discussion
Conclusions



Part 1

Introduction and set-up

Why HACC?

What is HACC?

The Hardware Accelerated Cosmology Code (HACC) framework uses N-body techniques to **simulate the formation of structure** in collisionless fluids under the influence of gravity in an expanding universe.

The main scientific goal is to **simulate the evolution of the Universe** from its early times to today and to **advance our understanding of dark energy and dark matter**, the two components that make up 95% of our Universe.

The code is a hybrid **MPI-OpenMP** C implementation, and depends on external FFT library.

Steps to build HACC

TAKE THE ENVIRONMENT EXAMPLE FILE

HACC provides some example bash files for environment setup

FILL WITH THE LOCATION OF THE DEPENDENCIES

The environment variables need to point to MPI and FFTW libraries

LAUNCH THE BUILD

Once the environment is set up, just run the build using the Makefile

All the source code is available on my GitHub:
github.com/rstagi/HACC_MareNostrum_analysis/

Part 2

Prepare for the analysis

Input files, job definition, run scripts

Command and options

The executable, called "hacc_tpm", receives some input parameters:

```
hacc_tpm   <INDAT>
           cmbM000.tf
           m000 INIT
           ALL_TO_ALL
           -w -R -N 512
           -a final -f refresh
           -t <GEOMETRY>
```

- INDAT is the path to the input configuration file

- GEOMETRY represents the cartesian decomposition of the MPI processes

Input file and constraints

Inside the INDAT file there are 3 values related to the problem size:

- **np**: number of particles per dimension ("alive" particles)
- **ng**: number of grid points per dimension
- **Physical Box size**: size of the space reference

Constraints:

- **np** must be equal to **ng**
- **np/ng** must be **divisible by any 2D decomposition** of the GEOMETRY (e.g. if 8x4x2, np must be divisible by 8x4, 8x2 and 4x2)

Script to run the jobs

To better design the scaling analysis, the **job** was designed to get the **data from arguments** and **environment variables**:

```
OMP_NUM_THREADS=<OPENMP_THREADS_COUNT> \
sbatch      --job-name=<JOB_NAME> \
            --ntasks=<MPI_TASKS> \
            --chdir=<WORKING_DIRECTORY> \
            --time=<TIME> \
            --qos=<QUEUE_NAME> \
            --get-user-env \
            job_hacc.sh <EXECS_DIRECTORY> <INDAT_FILE> <GEOMETRY>
```

Script to run the jobs (cont.)

- A **script** was designed **for each type of analysis** (strong, weak, openmp, etc.), by just varying environment variables and input arguments
- Each job was running in **its own working directory**
- Each job was instrumented using **Extrae**

All the source code is available on my GitHub:
github.com/rstagi/HACC_MareNostrum_analysis/

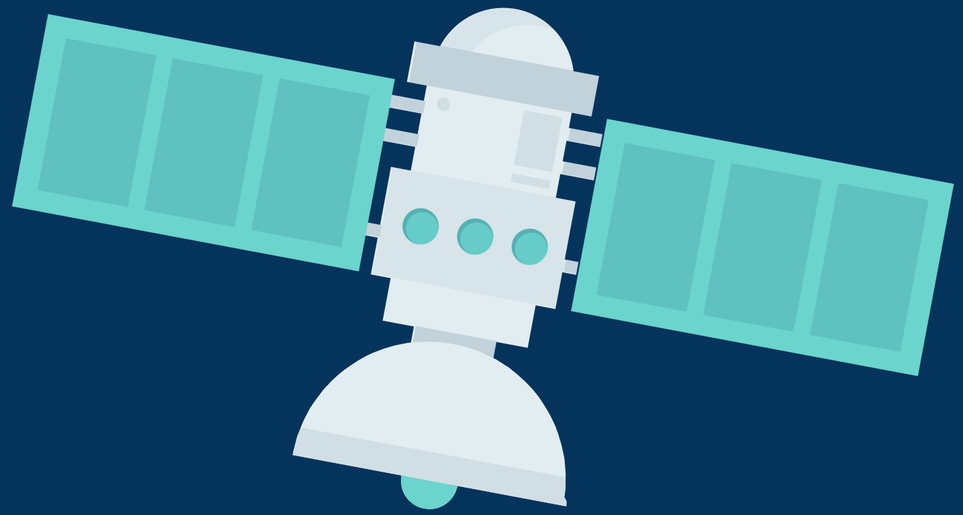
Problem size scaling

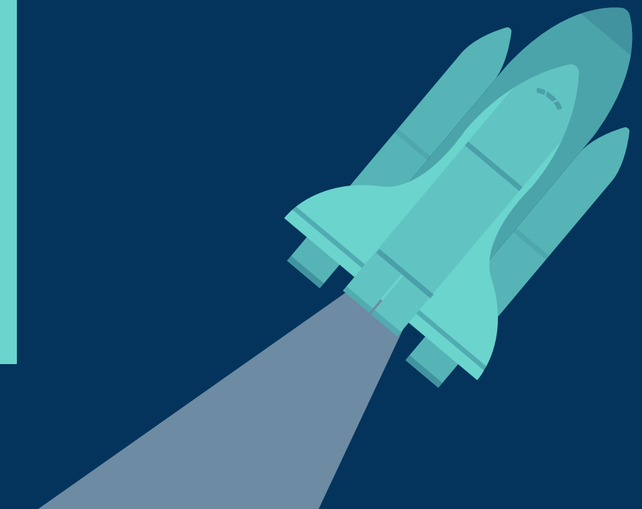
- The size of the example jobs was too large
  - np and ng reduced by at least 13x (problem size 13^3 times smaller)
- Scaling the problem size needed some extra care
- Problem size is defined by the total number of particles
- The space reference was a cube; **np** and **ng** refers to one dimension
- Scaling **X times** the number of particles means scaling **np** and **ng** by the cubic root of X

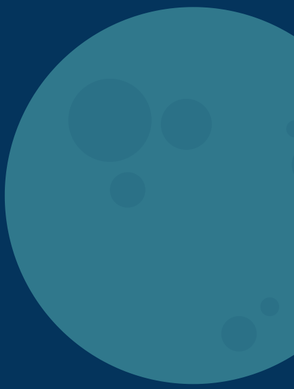
Part 3

Analysis Traces

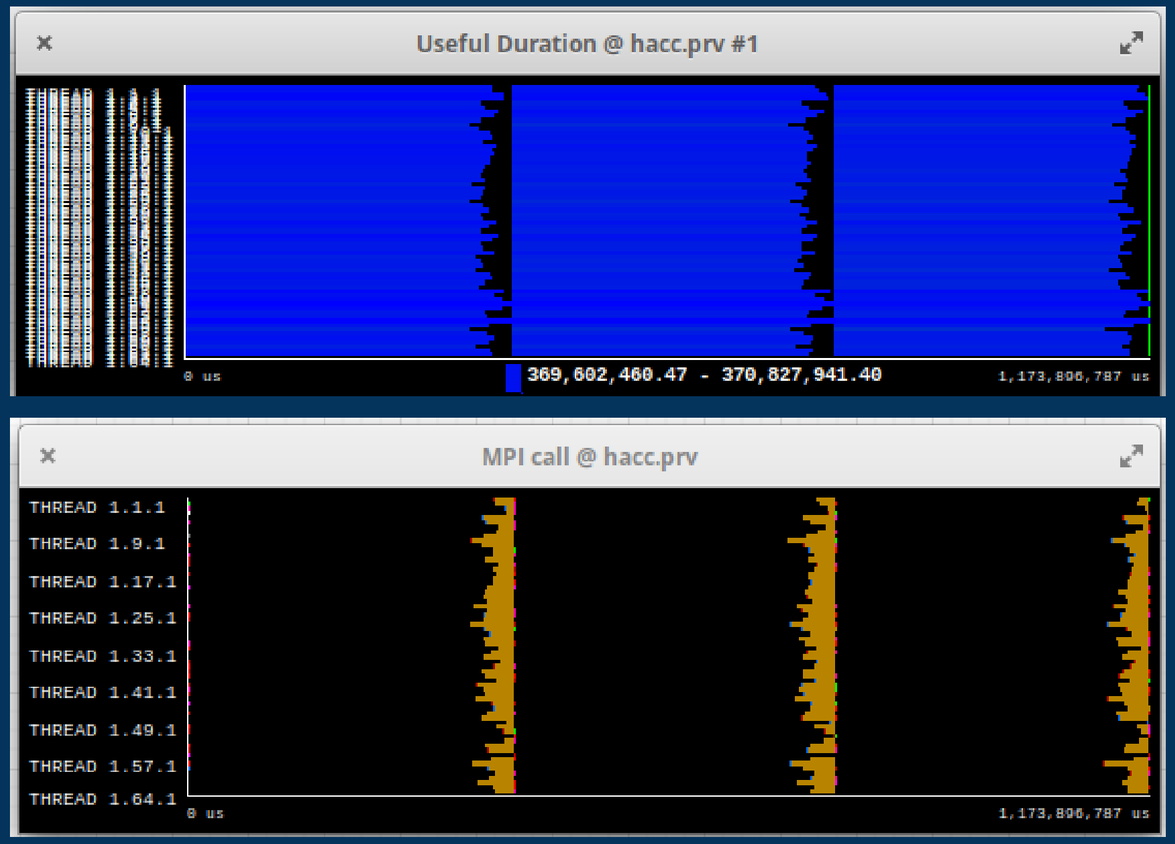
Structure, Scalability, Efficiency Model







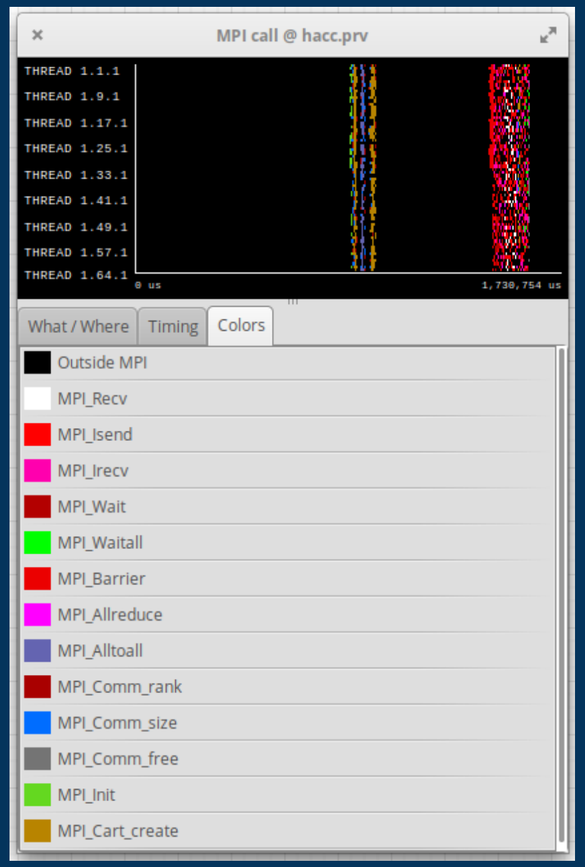
Overall Structure

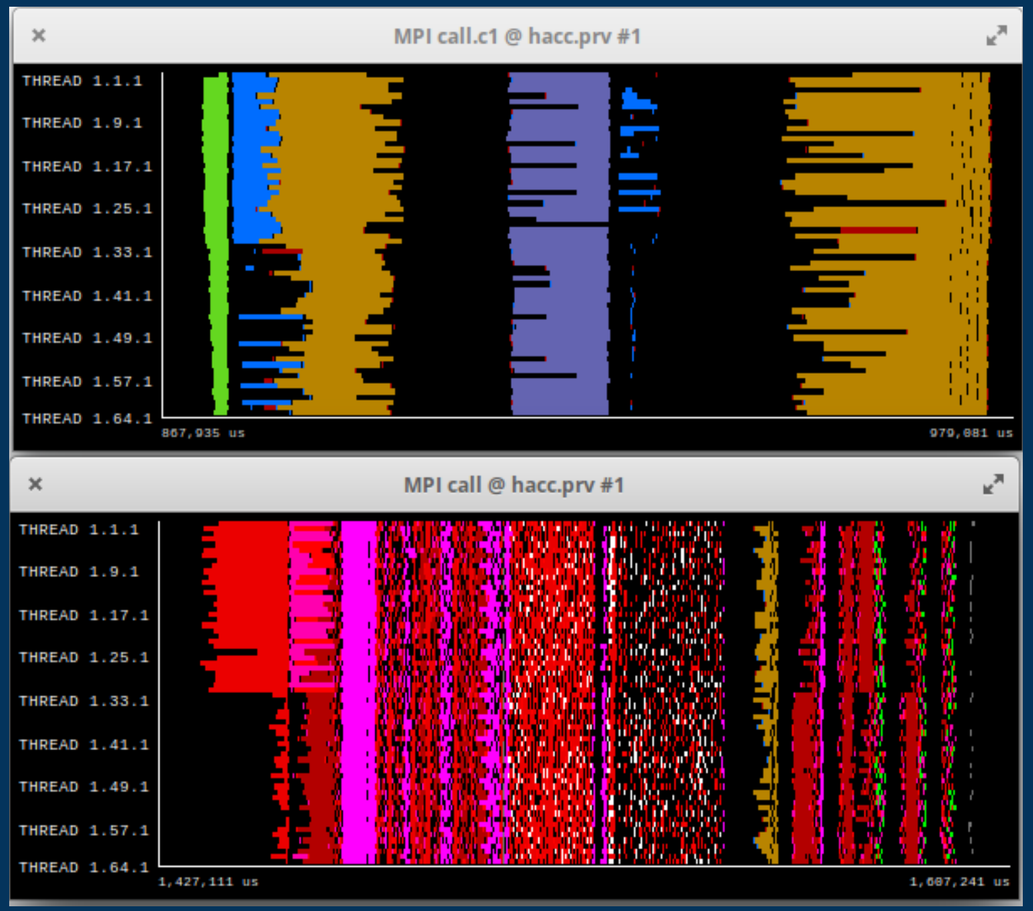


Based on a 64 MPI processes and 1 OpenMP thread execution

- Iterative execution
- Long duration runs for each iteration
- MPI calls at the end of each iteration

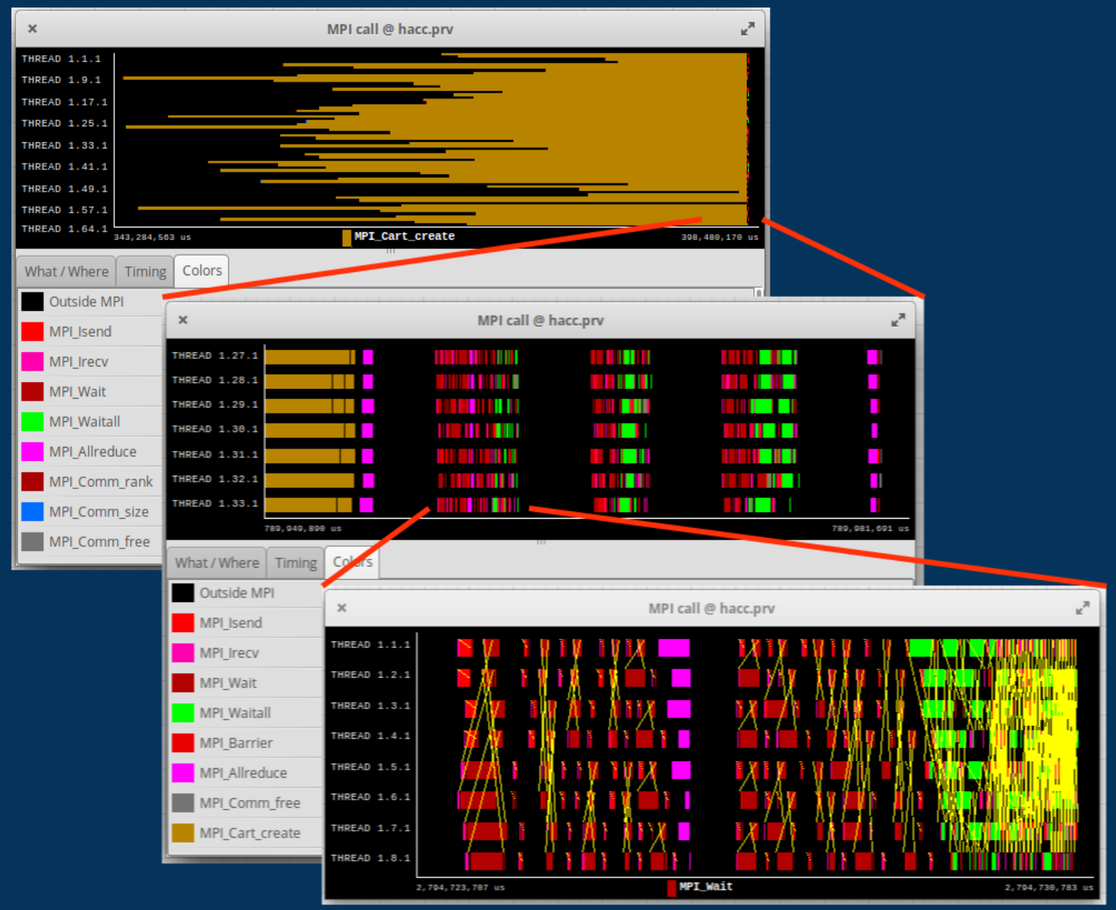
Structure - Initialization





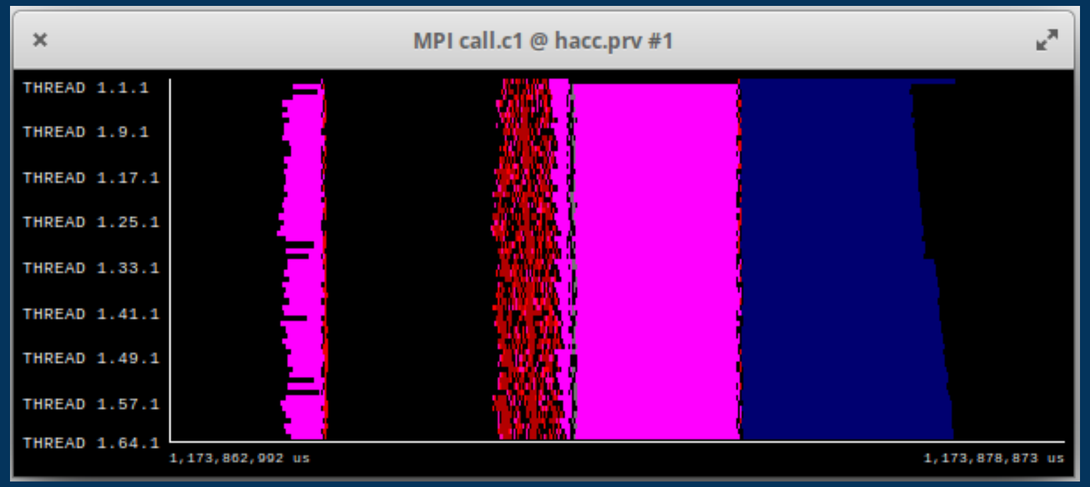
- MPI Cartesian grid init
- MPI All-to-All initialization
- Cartesian 1D, 2D and 3D decomposition init
- Particles load (input data)

Structure - Iteration



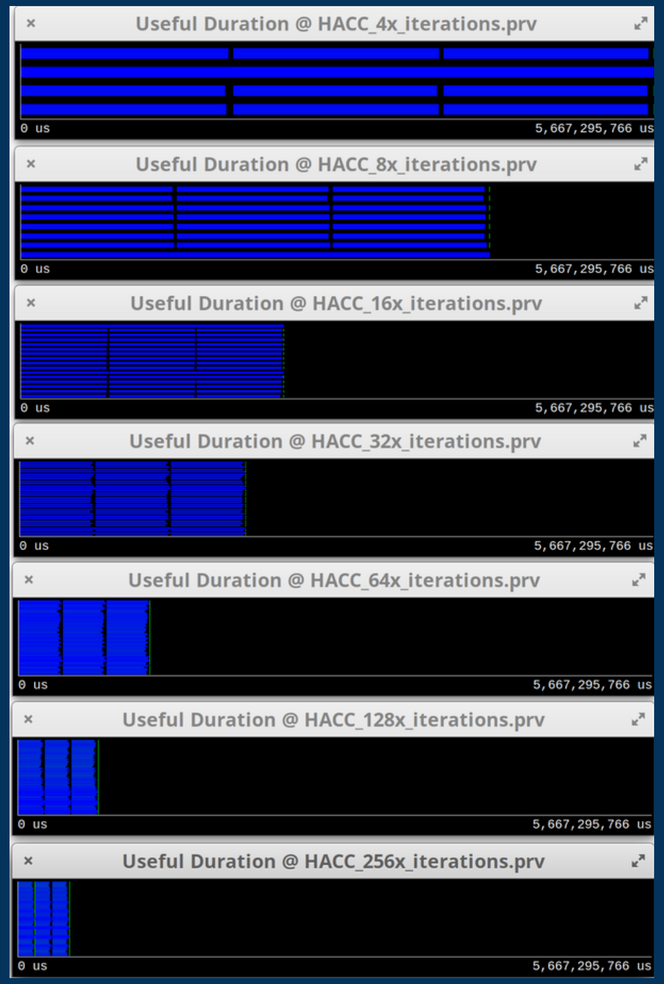
- Long MPI_Cart calls
- Much messaging among all the processes
  - Updating each process on global data
- 3 main data-exchange regions

Structure - Ending



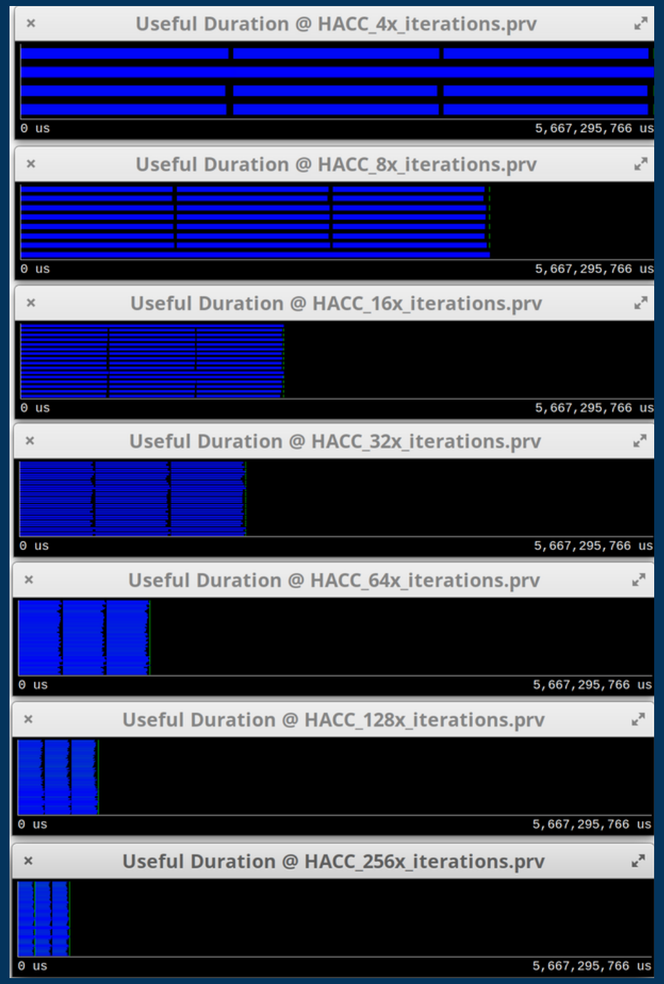
- Final additional MPI_Allreduce
- MPI Finalize

Strong Scaling analysis

4x		2x2x1
8x		2x2x2
16x		4x2x2
32x		4x4x2
64x		4x4x4
128x		8x4x4
256x		8x8x4

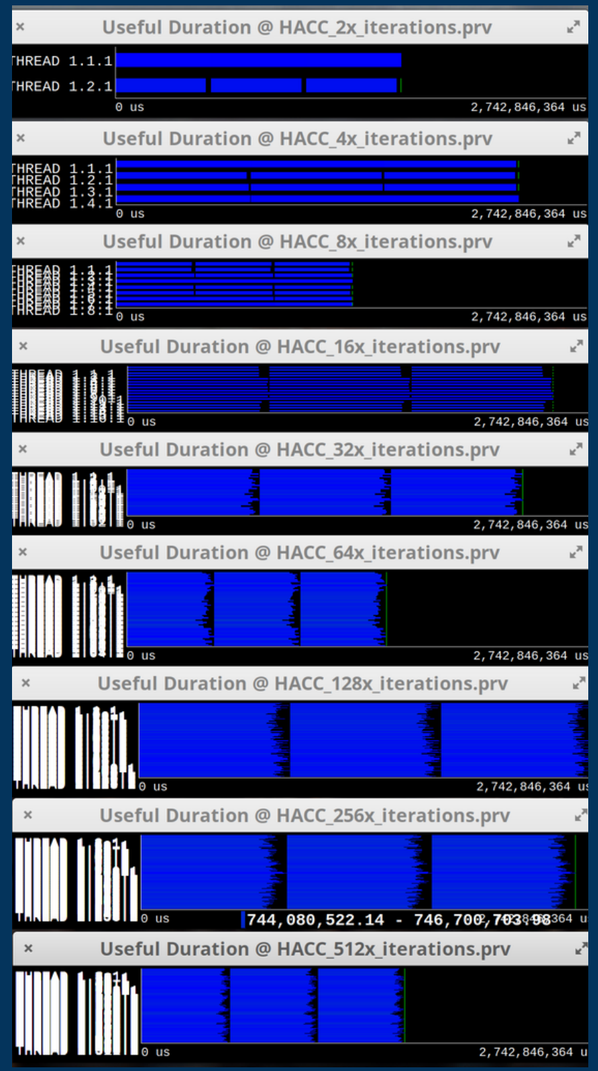
- Could not find an input good for each number of processes
- The one used in the end covered most executions, but it was
  - too large for 1x and 2x
  - too small for 512x
- Input file has:
  - np = ng = 64
  - Physical Box = 40

Strong Scaling - model factors



Number of processes	4	8	16	32	64	128	256
Parallel efficiency	97.76	97.54	97.82	95.69	92.26	88.86	85.60
Load balance	97.76	97.54	97.89	95.69	92.27	89.17	85.90
Communication efficiency	100.00	100.00	99.92	100.00	100.00	99.66	99.64
Serialization efficiency	NaN	NaN	NaN	100.00	100.00	99.67	99.66
Transfer efficiency	NaN	NaN	NaN	100.00	100.00	99.99	99.99
Computation scalability	100.00	67.73	60.23	35.78	32.01	27.23	22.05
Global efficiency	97.76	66.07	58.91	34.23	29.54	24.20	18.88
IPC scalability	100.00	102.42	102.06	103.10	102.19	102.48	102.67
Instruction scalability	100.00	65.88	59.16	34.67	33.47	27.75	22.08
Frequency scalability	100.00	100.39	99.74	100.08	93.60	95.74	97.26
Speedup	1.00	1.35	2.41	2.80	4.83	7.92	12.36
Average IPC	1.43	1.46	1.46	1.47	1.46	1.46	1.47
Average frequency (GHz)	2.07	2.08	2.06	2.07	1.94	1.98	2.01
#							
#Runtime (us)	6E+09	4.2E+09	2.35E+09	2E+09	1.17E+09	715515178	458606311
#Runtime (ideal)	NaN	NaN	NaN	2E+09	1.17E+09	715459614	458549405
#Useful duration (average)	6E+09	4.1E+09	2.3E+09	2E+09	1.08E+09	635812539	392549075
#Useful duration (maximum)	6E+09	4.2E+09	2.35E+09	2E+09	1.17E+09	713071963	456967525
#Useful duration (total)	2E+10	3.3E+10	3.68E+10	6E+10	6.92E+10	8.1384E+10	1.0049E+11
#Useful duration (ideal max)	NaN	NaN	NaN	2E+09	1.17E+09	713071963	456967525
#Useful instructions (total)	7E+13	9.9E+13	1.11E+14	2E+14	2E+14	2.3611E+14	2.9672E+14
#Useful cycles (total)	5E+13	6.8E+13	7.59E+13	1E+14	1.34E+14	1.6124E+14	2.0225E+14

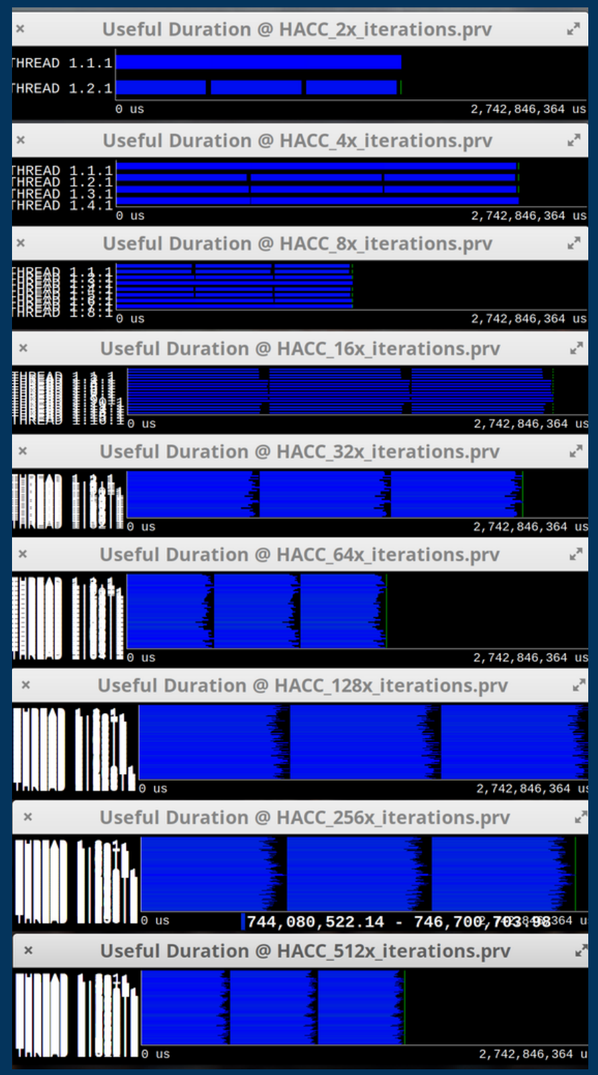
Weak Scaling analysis

2x		2x1x1
4x		2x2x1
8x		2x2x2
16x		4x2x2
32x		4x4x2
64x		4x4x4
128x		8x4x4
256x		8x8x4
512x		8x8x8

- Could not generate first trace
  - Extrae indefinitely waiting for processes to end(?)
  - Time taken from SLURM job data

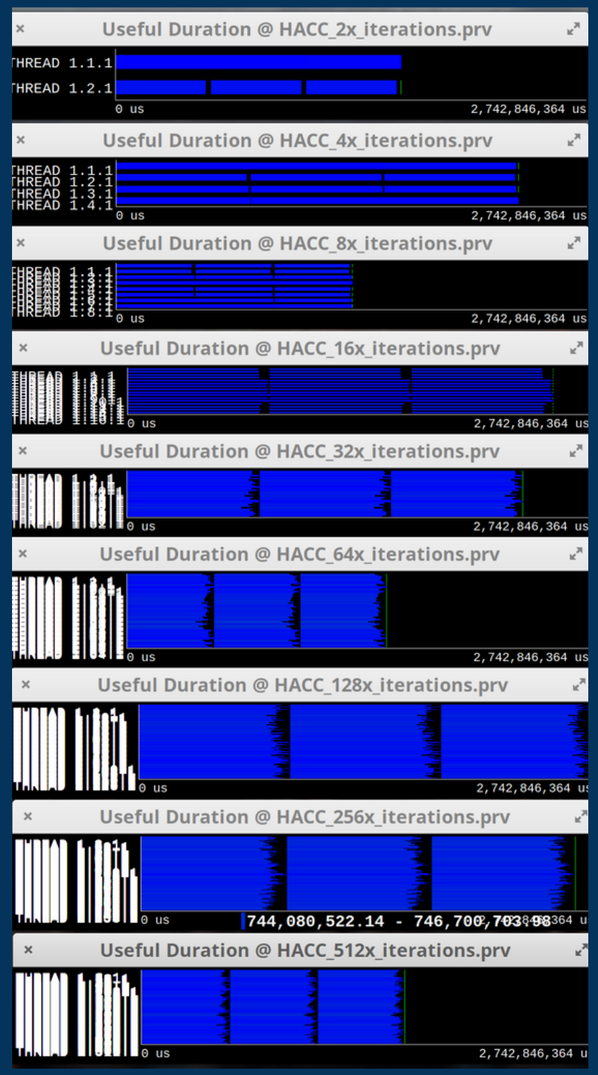
- Input files sizes started from:
  - np = ng = **24**
  - Physical Box = **20**
- ...arriving to:
  - np = ng = **192**
  - Physical Box = **160**

Weak Scaling - model factors



Number of processes	2	4	8	16	32	64	128	256	512
Parallel efficiency	97.26	98.61	97.43	95.75	94.48	91.18	92.09	87.91	89.87
Load balance	97.26	98.82	97.64	95.77	94.74	91.19	92.10	87.92	90.14
Communication efficiency	100.00	99.78	99.78	99.98	99.72	100.00	100.00	99.99	99.69
Serialization efficiency	NaN	NaN	NaN	NaN	99.72	100.00	100.00	100.00	99.70
Transfer efficiency	NaN	NaN	NaN	NaN	100.00	100.00	100.00	100.00	99.99
Computation scalability	100.00	69.94	120.50	66.78	72.87	114.94	63.97	69.95	112.96
Global efficiency	97.26	68.96	117.40	63.95	68.85	104.81	58.91	61.49	101.52
IPC scalability	100.00	101.65	100.58	101.15	101.29	100.71	101.28	101.38	100.79
Instruction scalability	100.00	68.51	119.85	65.59	71.69	120.18	65.41	71.65	120.49
Frequency scalability	100.00	100.43	99.96	100.66	100.36	94.97	96.57	96.29	93.02
Speedup	1.00	1.42	4.83	5.26	11.33	34.48	38.77	80.93	267.20
Average IPC	1.46	1.48	1.46	1.47	1.47	1.47	1.47	1.48	1.47
Average frequency (GHz)	2.07	2.08	2.07	2.08	2.07	1.96	2.00	1.99	1.92
#									
#Runtime (us)	1.66E+09	2E+09	1E+09	3E+09	2E+09	2E+09	2.7E+09	3E+09	1.6E+09
#Runtime (ideal)	NaN	NaN	NaN	NaN	2E+09	2E+09	2.7E+09	3E+09	1.6E+09
#Useful duration (average)	1.62E+09	2E+09	1E+09	2E+09	2E+09	1E+09	2.5E+09	2E+09	1.4E+09
#Useful duration (maximum)	1.66E+09	2E+09	1E+09	3E+09	2E+09	2E+09	2.7E+09	3E+09	1.6E+09
#Useful duration (total)	3.23E+09	9E+09	1E+10	4E+10	7E+10	9E+10	3.2E+11	6E+11	7.3E+11
#Useful duration (ideal max)	NaN	NaN	NaN	NaN	2E+09	2E+09	2.7E+09	3E+09	1.6E+09
#Useful instructions (total)	9.72E+12	3E+13	3E+13	1E+14	2E+14	3E+14	9.5E+14	2E+15	2.1E+15
#Useful cycles (total)	6.68E+12	2E+13	2E+13	8E+13	1E+14	2E+14	6.5E+14	1E+15	1.4E+15

Weak Scaling - efficiency



2x	2x1x1	0.82
4x	2x2x1	0.58
8x	**2x2x2**	**0.99**
16x	4x2x2	0.54
32x	4x4x2	0.58
64x	**4x4x4**	**0.88**
128x	8x4x4	0.49
256x	8x8x4	0.52
512x	**8x8x8**	**0.85**

Perfect cubic decomposition!

↓

According to HACC documentation

Decomposition analysis

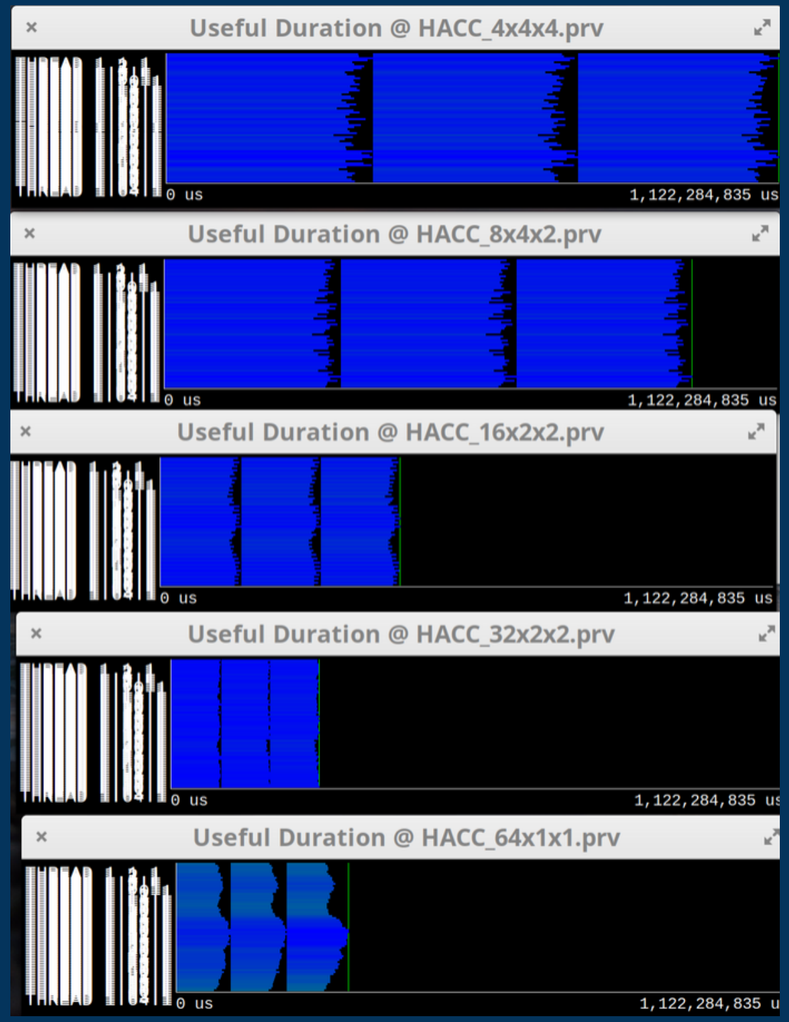
4x4x4

8x4x2

16x2x2

32x2x1

64x1x1



Decomposition	4x4x4	8x4x2	16x2x2	32x2x1	64x1x1
Parallel efficiency	90.26	92.04	91.39	95.99	80.97
Load balance	90.56	92.05	91.40	96.98	81.07
Communication efficiency	99.67	99.99	99.99	98.98	99.88
Serialization efficiency	99.67	100.00	100.00	99.02	99.92
Transfer efficiency	100.00	100.00	99.99	99.96	99.96
Computation scalability	100.00	113.92	252.78	389.46	397.05
Global efficiency	100.00	116.17	255.95	414.19	356.17
IPC scalability	100.00	98.79	98.45	99.21	100.62
Instruction scalability	100.00	115.79	264.14	403.29	404.33
Frequency scalability	100.00	99.60	97.21	97.34	97.59
Speedup	1.00	1.15	2.56	4.15	3.56
Average IPC	1.48	1.46	1.45	1.46	1.48
Average frequency (GHz)	2.05	2.04	1.99	1.99	2.00
#					
#Runtime (us)	1.12E+09	9.66E+08	4.4E+08	2.7E+08	3.15E+08
#Runtime (ideal)	1.12E+09	9.66E+08	4.4E+08	2.7E+08	3.15E+08
#Useful duration (average)	1E+09	8.89E+08	4E+08	2.6E+08	2.55E+08
#Useful duration (maximum	1.12E+09	9.66E+08	4.4E+08	2.7E+08	3.15E+08
#Useful duration (total)	6.48E+10	5.69E+10	2.6E+10	1.7E+10	1.63E+10
#Useful duration (ideal max	1.12E+09	9.66E+08	4.4E+08	2.7E+08	3.15E+08
#Useful instructions (total)	2E+14	1.69E+14	7.4E+13	4.9E+13	4.84E+13
#Useful cycles (total)	1.33E+14	1.16E+14	5.1E+13	3.3E+13	3.26E+13

Decomposition analysis (cont.)

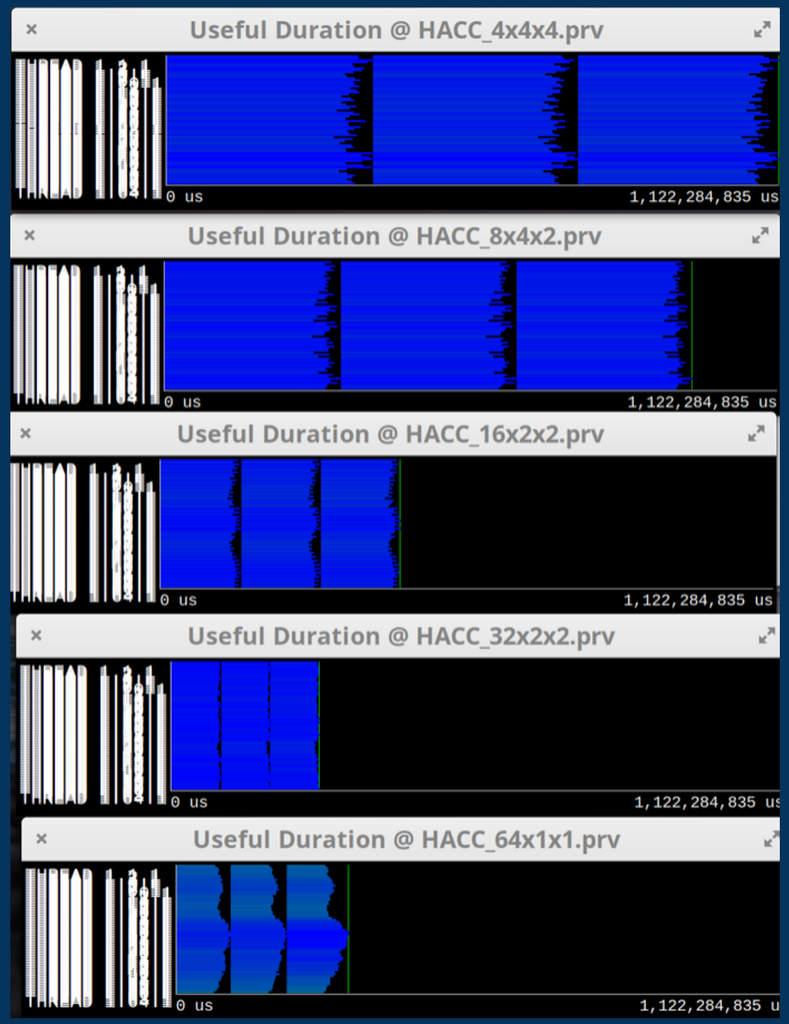
4x4x4

8x4x2

16x2x2

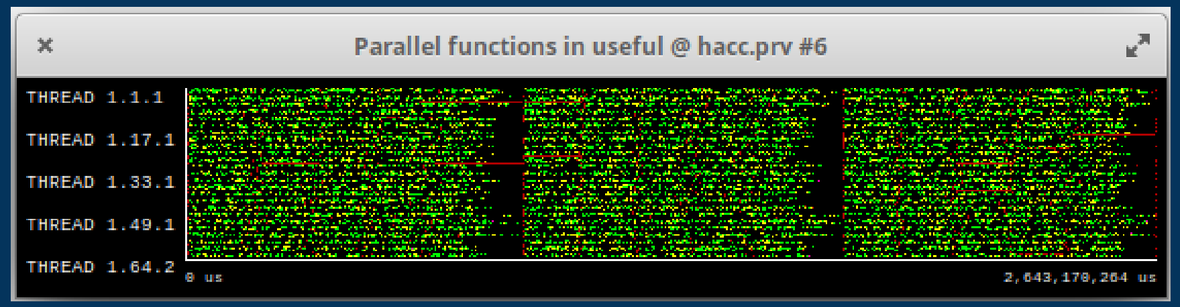
32x2x1

64x1x1



- Input file was:
  - np = ng = **64**
  - Physical Box = **50**
- Maybe because of a better distribution on a single dimension?
- ...or maybe on 2D (32x2x1)?

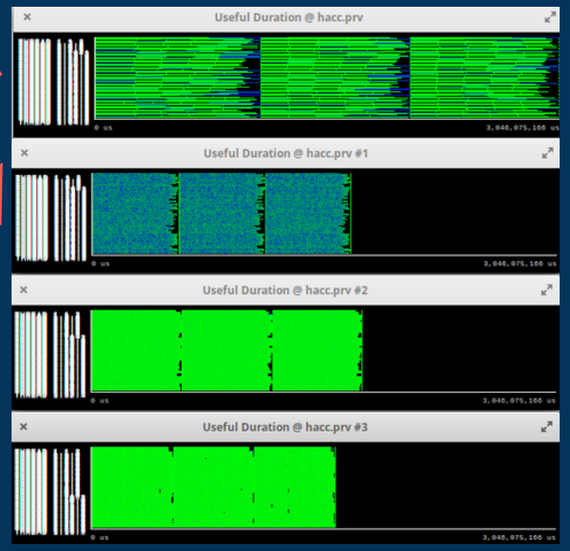
OpenMP Scaling Analysis



→ Iterations' inner computations benefit of OpenMP parallelization

Strong Scaling

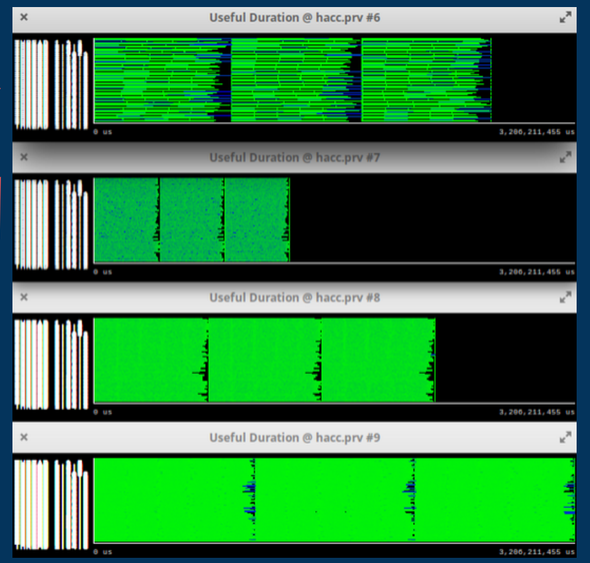
1x
2x
4x
8x



2.14x speedup!

Weak Scaling

1x
2x
4x
8x



1.93 of efficiency!

Part 4

Further Discussions

Where is it improvable?

Poor instruction scalability

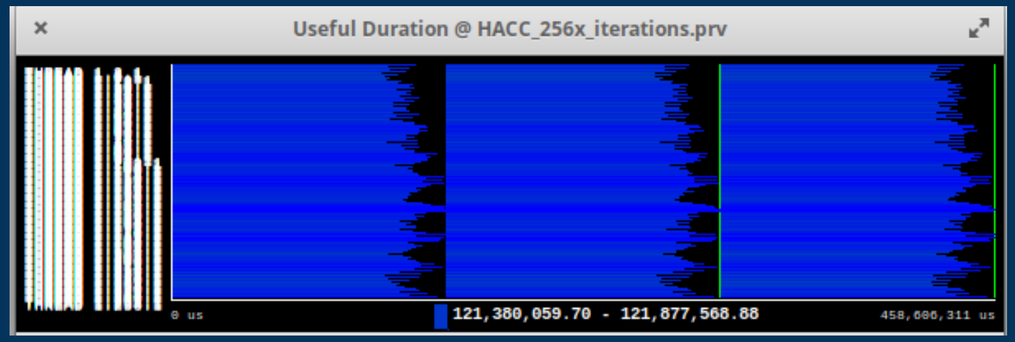
Recalling the strong scaling analysis...

IPC scalability	100.00	102.42	102.06	103.10	102.19	102.48	102.67
Instruction scalability	100.00	65.88	59.16	34.67	33.47	27.75	22.08
Frequency scalability	100.00	100.39	99.74	100.08	93.60	95.74	97.26
Speedup	1.00	1.35	2.41	2.80	4.83	7.92	12.36
Average IPC	1.43	1.46	1.46	1.47	1.46	1.46	1.47
Average frequency (GHz)	2.07	2.08	2.06	2.07	1.94	1.98	2.01
#							
#Runtime (us)	6E+09	4.2E+09	2.35E+09	2E+09	1.17E+09	715515178	458606311
#Runtime (ideal)	NaN	NaN	NaN	2E+09	1.17E+09	715459614	458549405
#Useful duration (average)	6E+09	4.1E+09	2.3E+09	2E+09	1.08E+09	635812539	392549075
#Useful duration (maximum)	6E+09	4.2E+09	2.35E+09	2E+09	1.17E+09	713071963	456967525
#Useful duration (total)	2E+10	3.3E+10	3.68E+10	6E+10	6.92E+10	8.1384E+10	1.0049E+11
#Useful duration (ideal max)	NaN	NaN	NaN	2E+09	1.17E+09	713071963	456967525
#Useful instructions (total)	7E+13	9.9E+13	1.11E+14	2E+14	2E+14	2.3611E+14	2.9672E+14

- There might be instructions somehow related to the number of processes
  - e.g. distribute particles on more processes?
- Code might be replicated

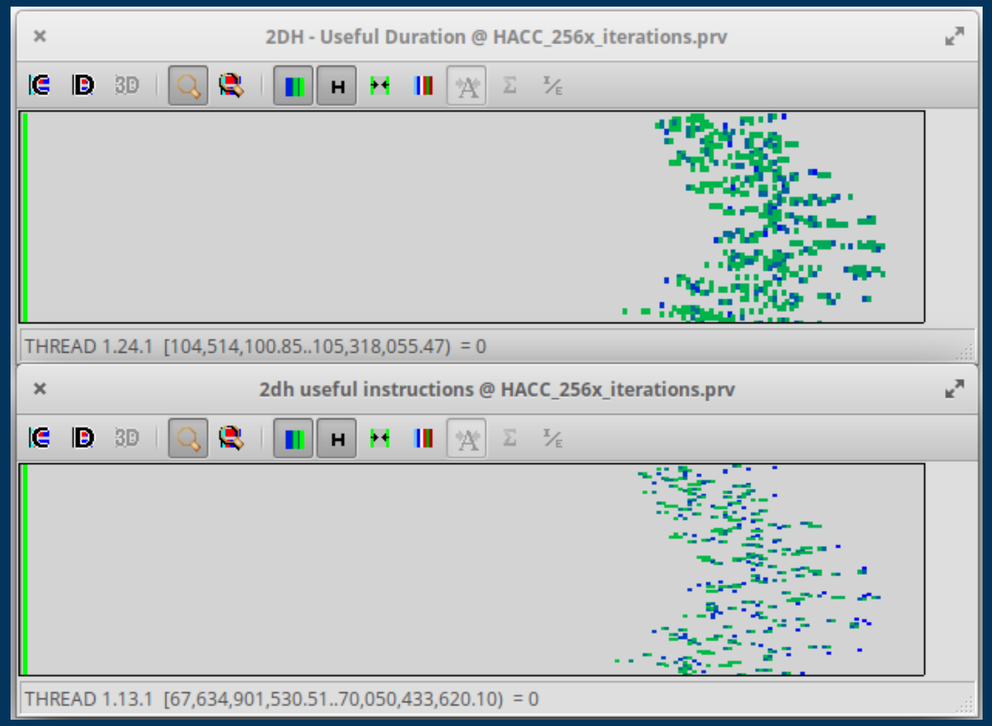
Load imbalance

Recalling the strong scaling analysis...



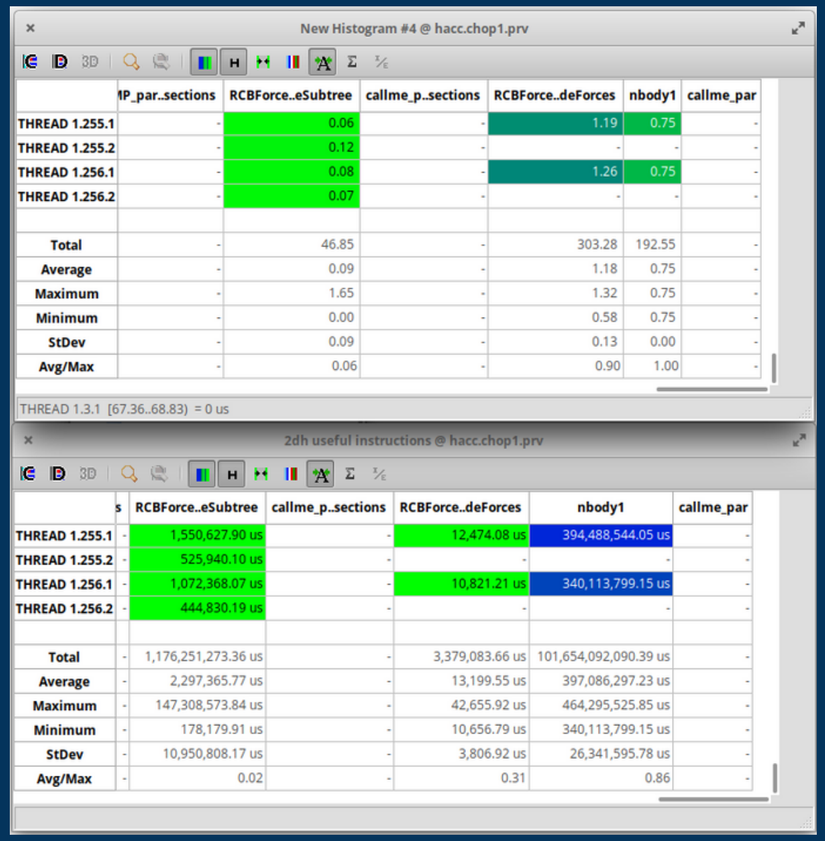
Number of processes	4	8	16	32	64	128	256
Parallel efficiency	97.76	97.54	97.82	95.69	92.26	88.86	85.60
Load balance	97.76	97.54	97.89	95.69	92.27	89.17	85.90
Communication efficiency	100.00	100.00	99.92	100.00	100.00	99.66	99.64

Load imbalance (cont.)



- Useful duration correlated to useful instructions
- Dynamic load balance could be a possible improvement

Low IPC

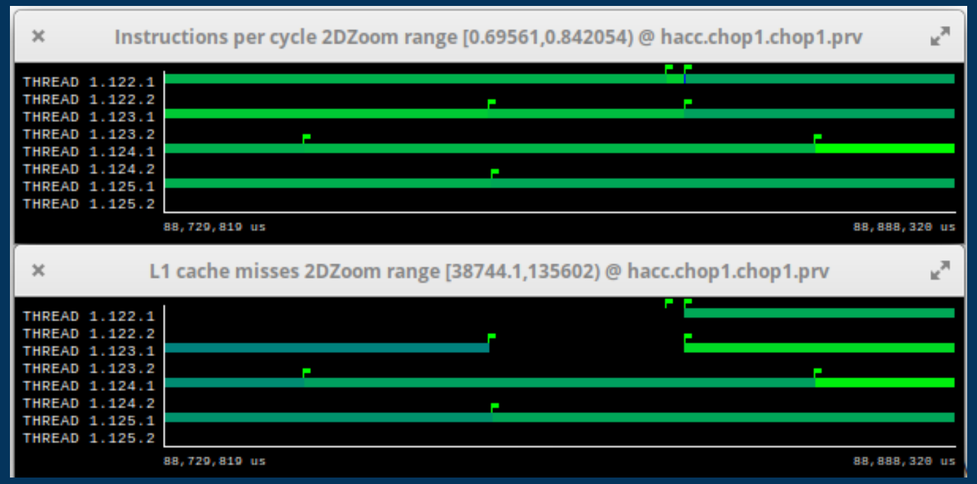


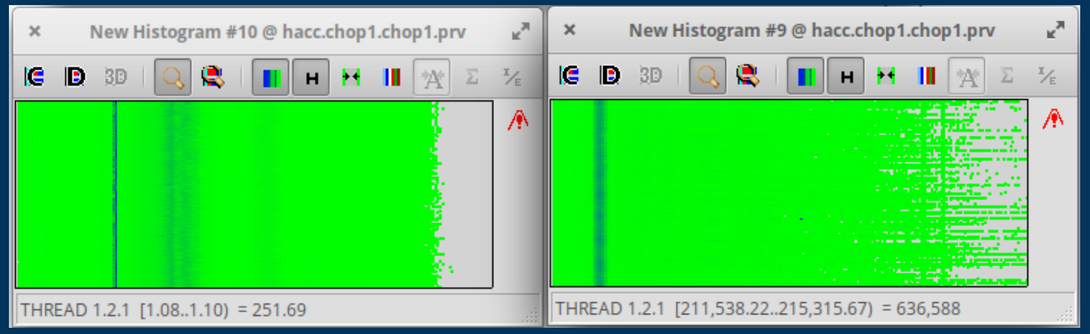
	MP_par..sections	RCBForce..eSubtree	callme_p..sections	RCBForce..deForces	nbody1	callme_par
THREAD 1.255.1	-	0.06	-	1.19	0.75	-
THREAD 1.255.2	-	0.12	-	-	-	-
THREAD 1.256.1	-	0.08	-	1.26	0.75	-
THREAD 1.256.2	-	0.07	-	-	-	-
Total	-	46.85	-	303.28	192.55	-
Average	-	0.09	-	1.18	0.75	-
Maximum	-	1.65	-	1.32	0.75	-
Minimum	-	0.00	-	0.58	0.75	-
StDev	-	0.09	-	0.13	0.00	-
Avg/Max	-	0.06	-	0.90	1.00	-

	s	RCBForce..eSubtree	callme_p..sections	RCBForce..deForces	nbody1	callme_par
THREAD 1.255.1	-	1,550,627.90 us	-	12,474.08 us	394,488,544.05 us	-
THREAD 1.255.2	-	525,940.10 us	-	-	-	-
THREAD 1.256.1	-	1,072,368.07 us	-	10,821.21 us	340,113,799.15 us	-
THREAD 1.256.2	-	444,830.19 us	-	-	-	-
Total	-	1,176,251,273.36 us	-	3,379,083.66 us	101,654,092,090.39 us	-
Average	-	2,297,365.77 us	-	13,199.55 us	397,086,297.23 us	-
Maximum	-	147,308,573.84 us	-	42,655.92 us	464,295,525.85 us	-
Minimum	-	178,179.91 us	-	10,656.79 us	340,113,799.15 us	-
StDev	-	10,950,808.17 us	-	3,806.92 us	26,341,595.78 us	-
Avg/Max	-	0.02	-	0.31	0.86	-

- Looked at the call stack and related hardware counters
- The most used function, has a very low IPC (0.75)

Low IPC - cache misses





- Despite of low IPC, cache misses and IPC look uncorrelated
- As a consequence, the low IPC is probably due to long instructions
  - Unfortunately, Extrae was not able to trace the line number
- Long instructions might be divisions or square roots
  - Could not verify, related PAPI counters not available

Part 5

Conclusions

Small wrap-up

Conclusions

- HACC has an iterative structure, based on multiple steps of the same computation, whose scaling capability is not bad (neither outstanding)
- It uses MPI Cartesian decomposition, whose geometry affects application performance (even if not in a clearly defined way)
- OpenMP offers a very important aid to computation efficiency
- Presents some load imbalance and poor instruction scalability
- The most used function has a low IPC, probably due to long instructions (e.g. divisions or square roots)

Thank you!

Any questions?