

SNIC PRESENTS

SUSTAINABILIT

Destination Earth

Pioneering the Future with Digital Twins

Okke van Eck
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Barcelona Supercomputing Center

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27th of November 2024, Bussum



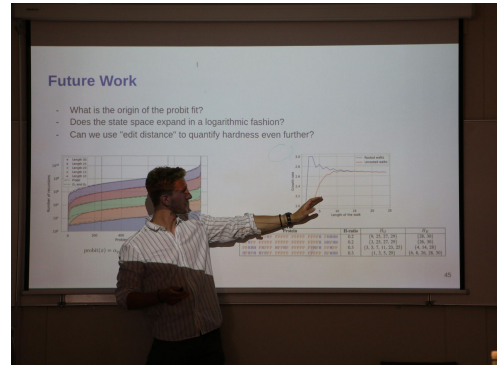
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Who's Okke?



Climate is changing..



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Destination Earth

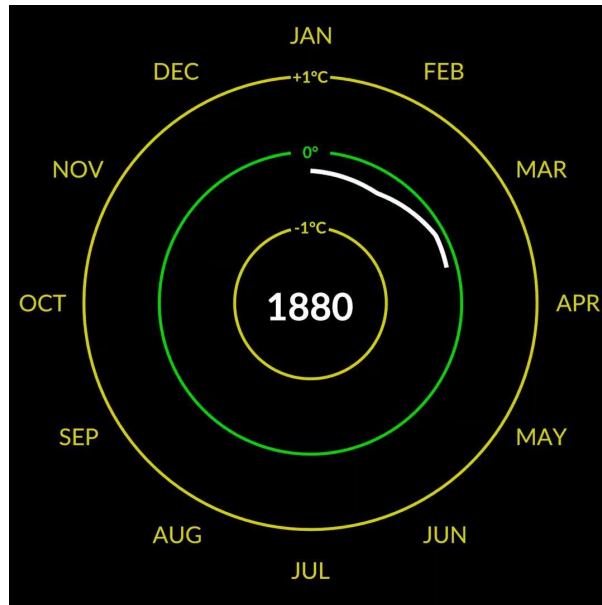
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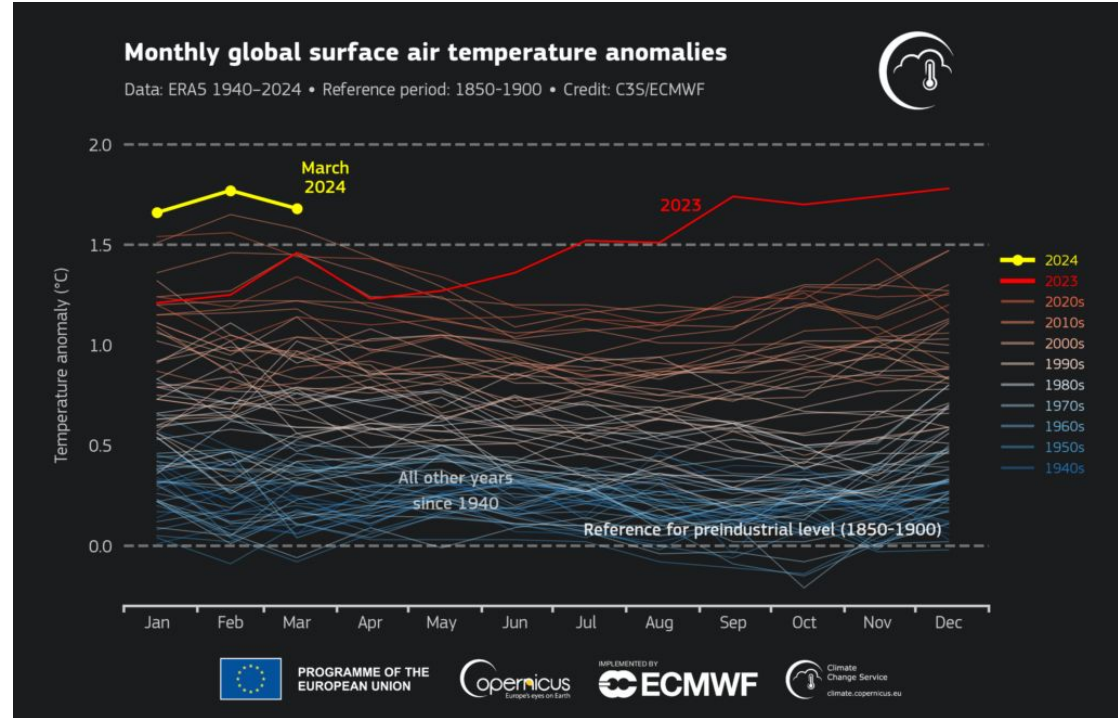
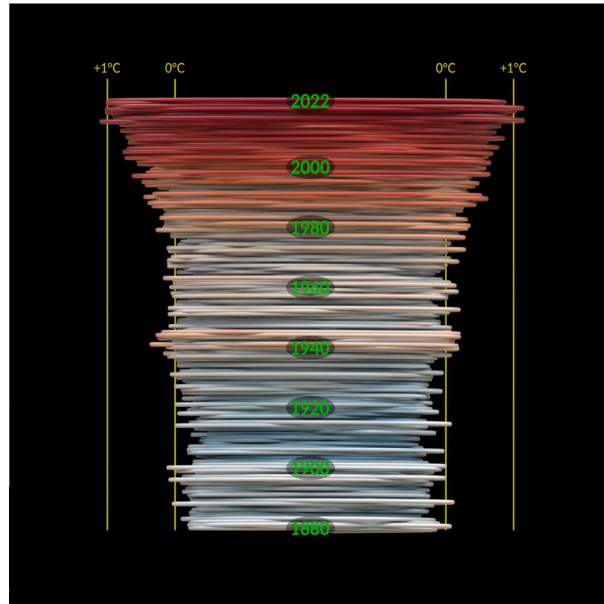
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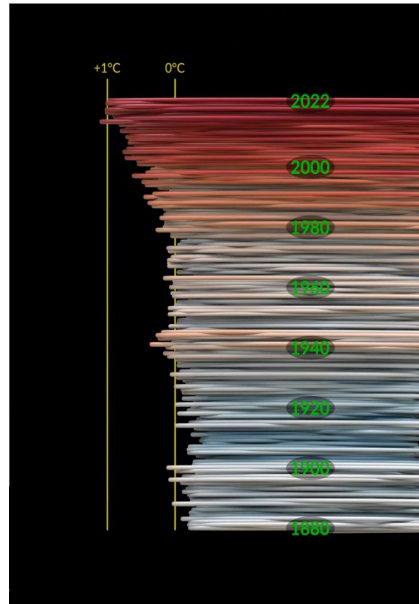
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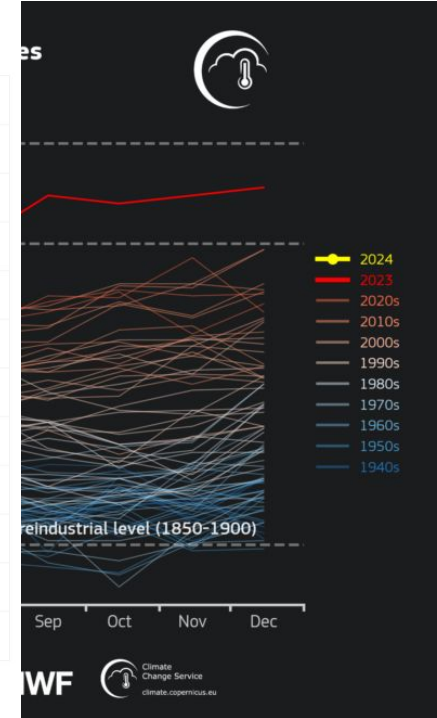
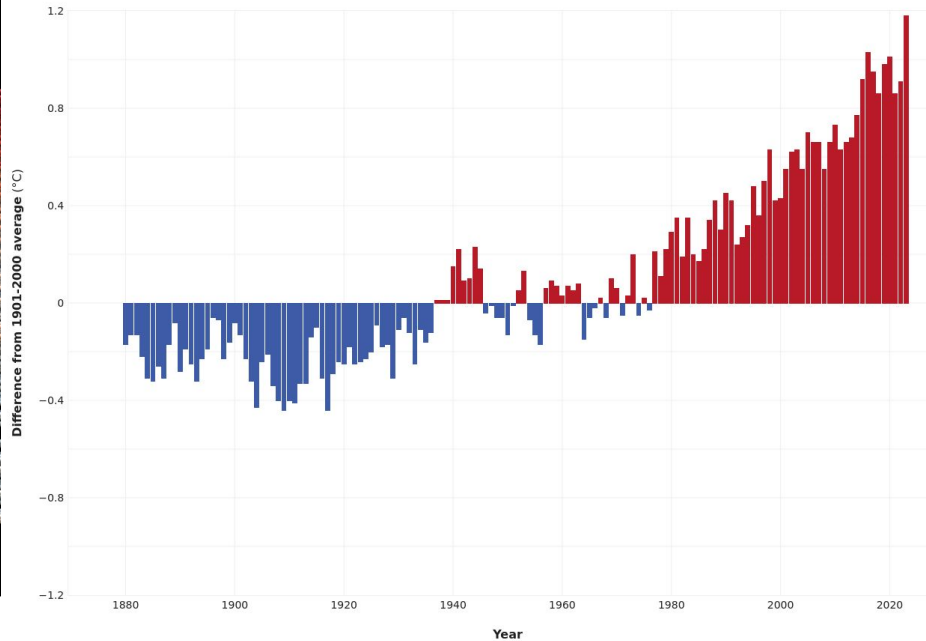
Climate is changing..



Climate is changing..



GLOBAL AVERAGE SURFACE TEMPERATURE



Destination Earth: Digital Twins



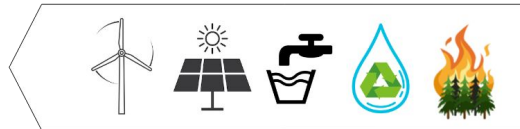
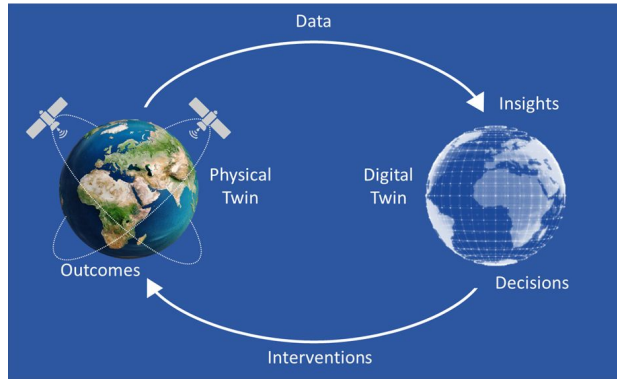
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Destination Earth

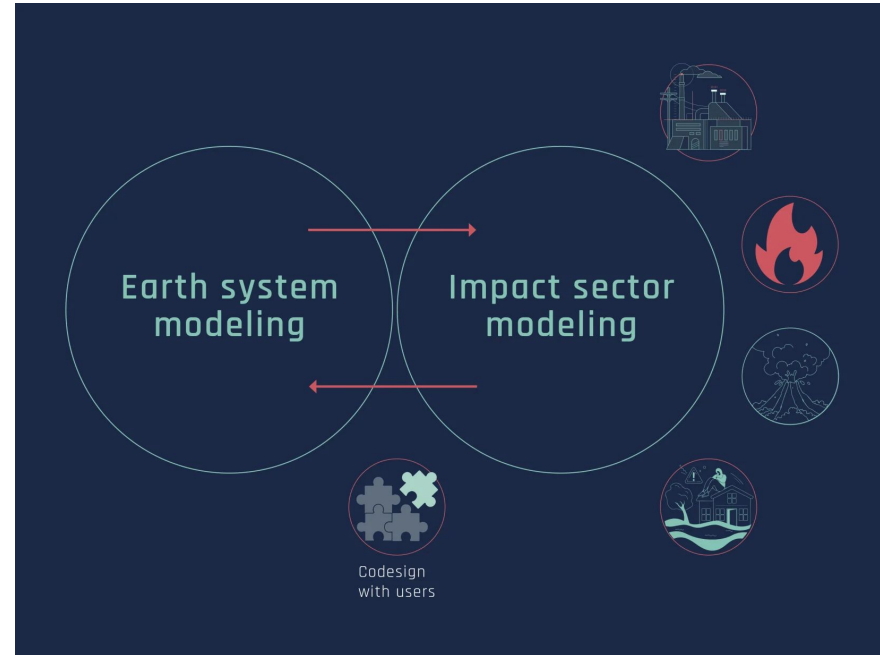
implemented by



Why digital twins?

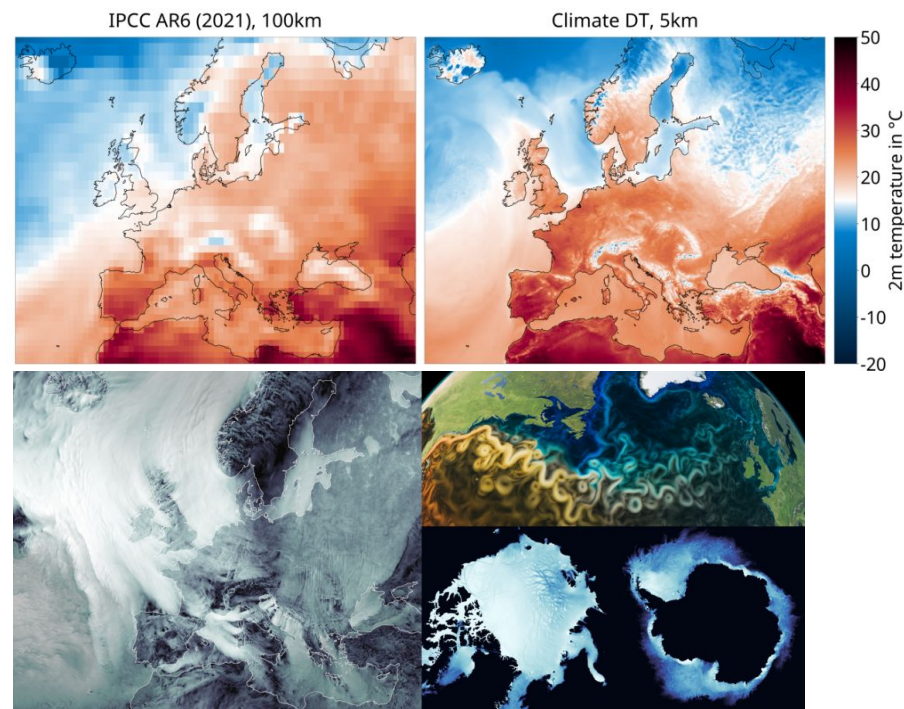
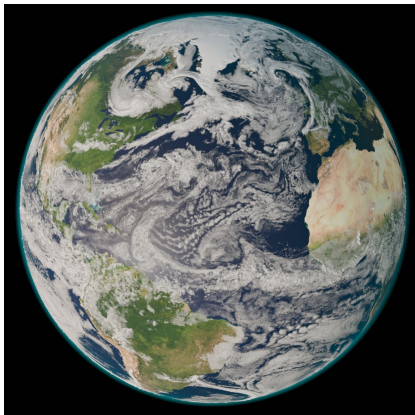


Impact sector applications



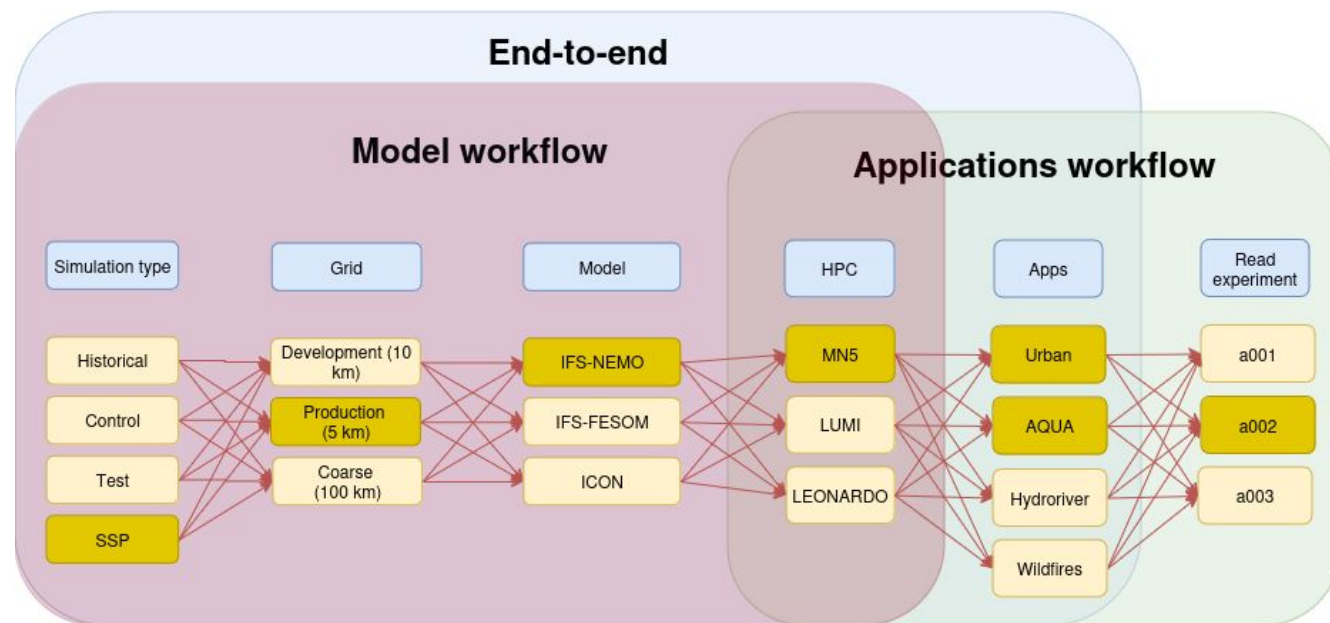
Destination Earth: Digital Twins

- Phase 1 ran from 2022-2024
- 3 different models
- One simulation takes months
- 300+ supercomputer nodes
- Multiple EuroHPC supercomputers



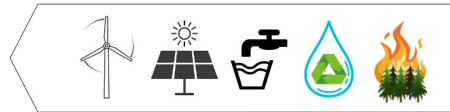
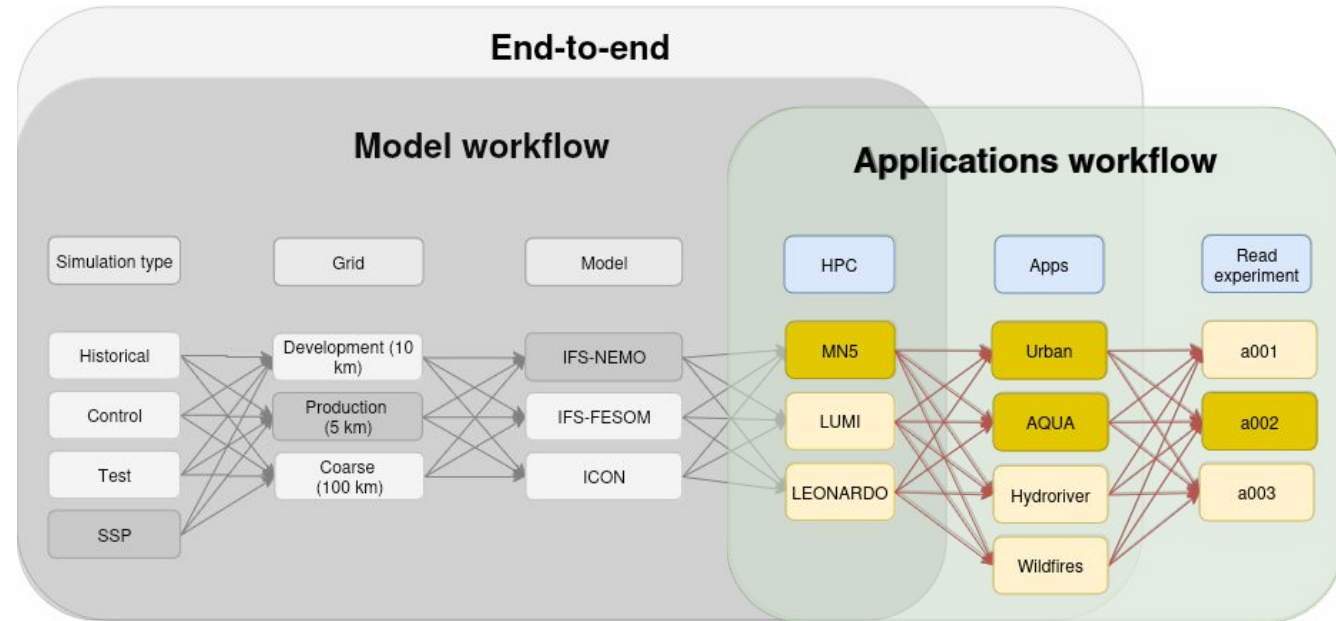
What does it take to run a model?

- AUTOSUBMIT**



What does it take to run a model?

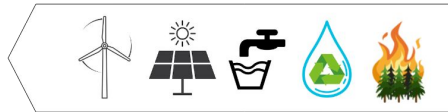
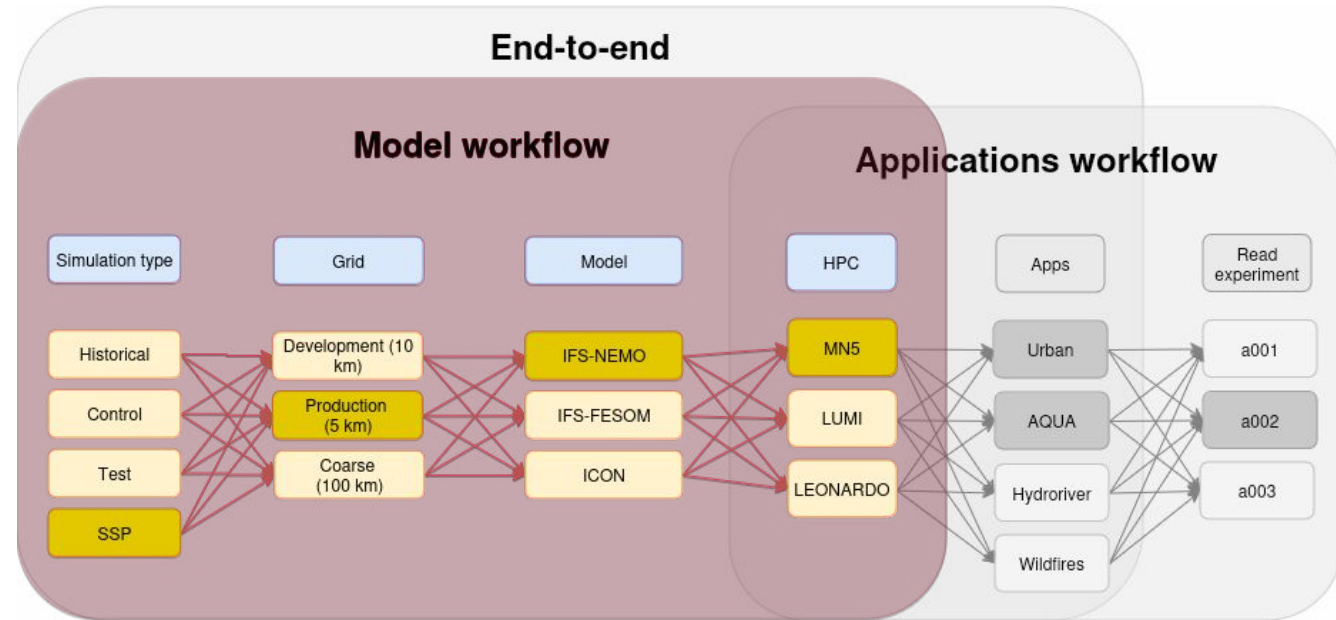
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Impact sector applications

What does it take to run a model?

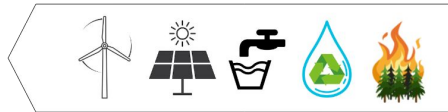
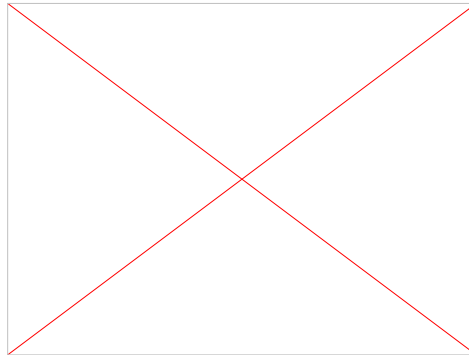
- AUTOSUBMIT**



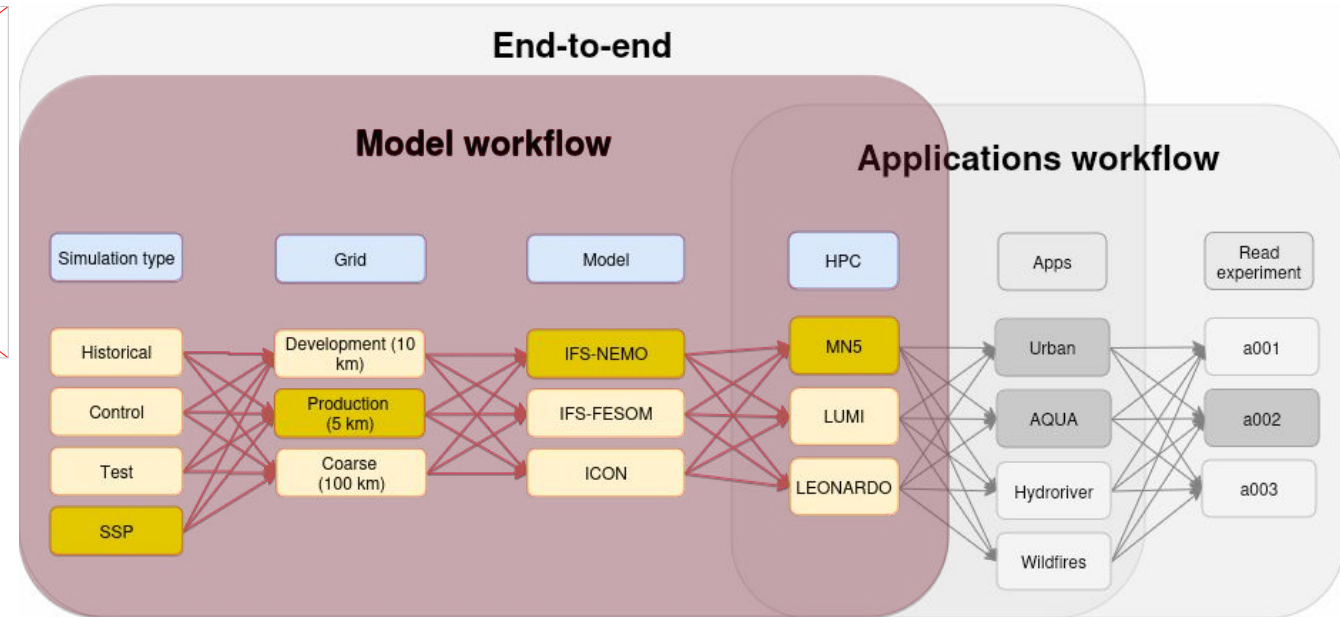
Impact sector applications

What does it take to run a model?

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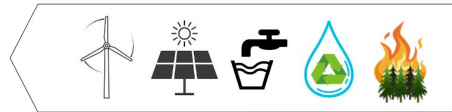
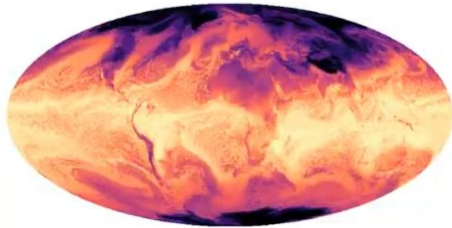


Impact sector applications

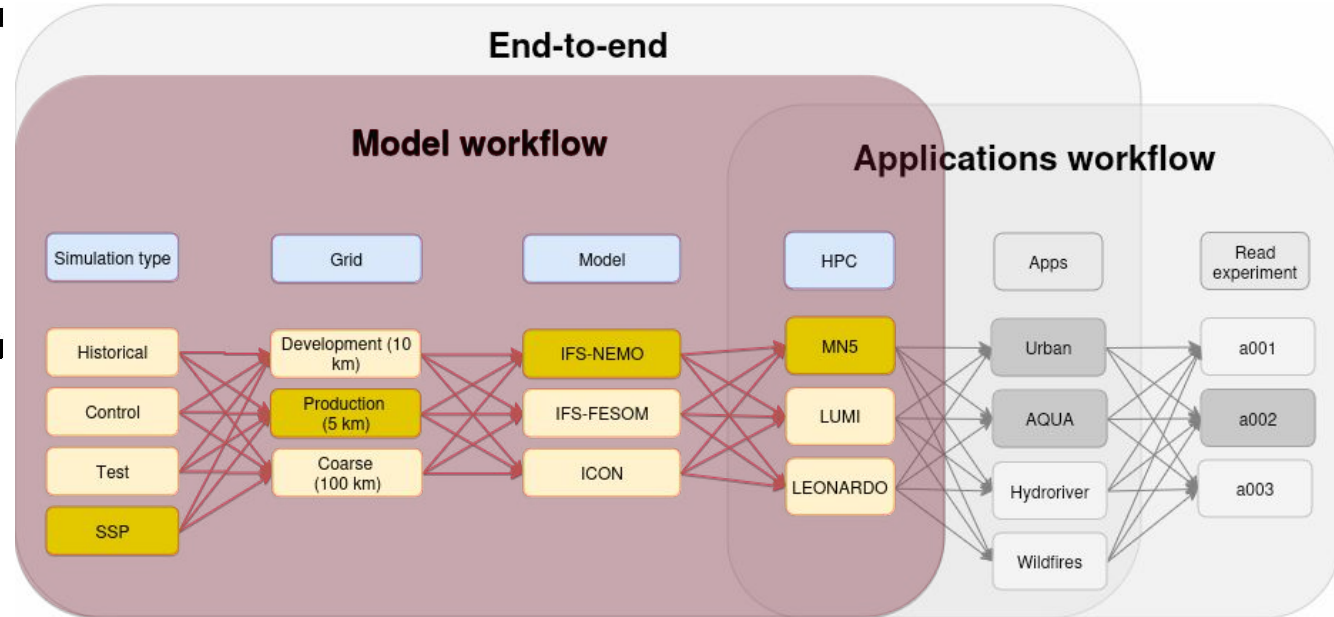


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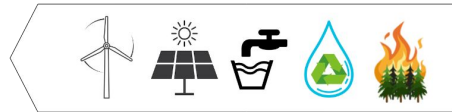
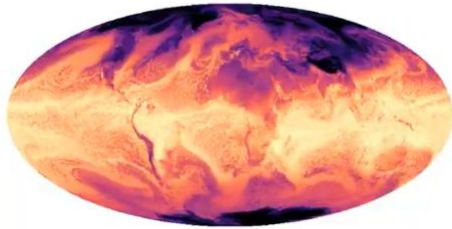


Impact sector applications

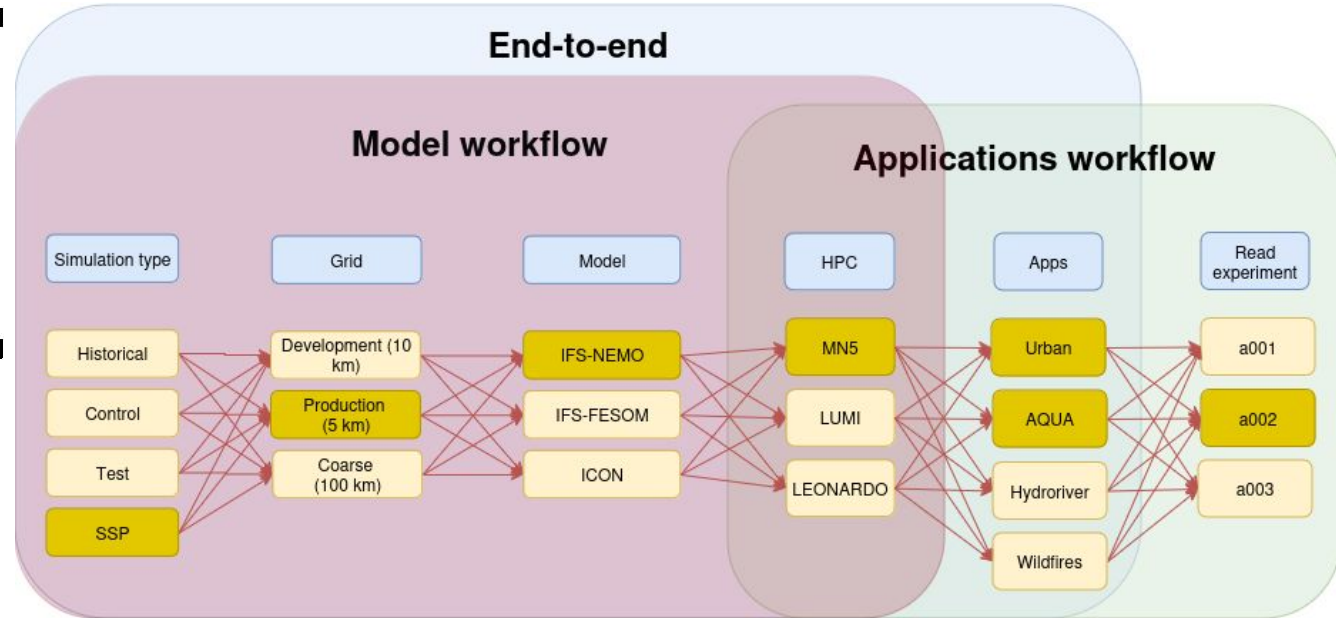


What does it take to run a model?

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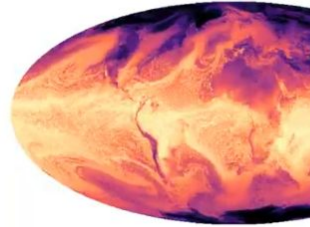


Impact sector applications

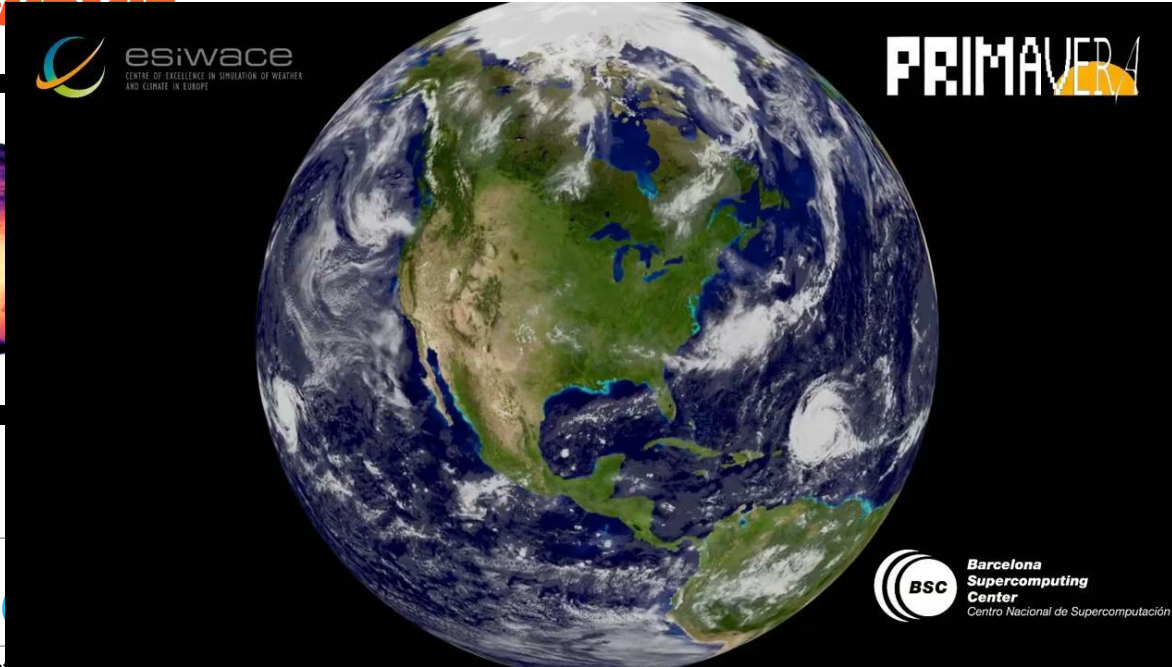


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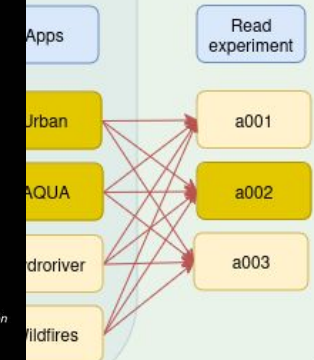
• **AUTOS** 



Impact sector applications



ns workflow



Performance Engineering



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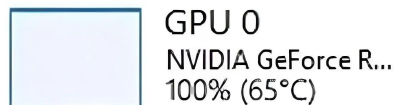
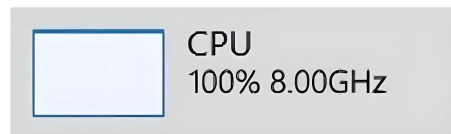
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Performance Engineering

“I paid for the whole PC, I gonna use the whole PC”



Devices and drives (4)



Local Disk (C:)

5.69 GB free of 222 GB



Single Dump 7 (E:)

4.44 GB free of 1.81 TB



Local Disk (D:)

2.85 GB free of 931 GB



Media (F:)

5.27 GB free of 238 GB

Network locations (3)



public (\\192.168.1.201) (R:)

5.14 GB free of 7.21 TB



Public (\\192.168.1.200) (S:)

4.07 GB free of 5.43 TB



Media (\\192.168.1.250) (Z:)

86.6 TB free of 86.6 TB

Performance Engineering

“I paid for the whole PC, I gonna use the whole PC”



Performance Engineering

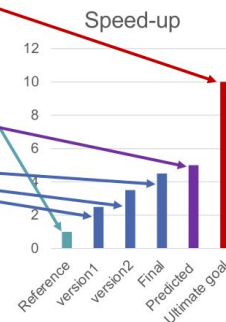
Follow these simple steps:

Systematic approach



Given an application ...

1. Understand (user) **requirements**
2. Understand **current performance**
3. **Can** it be done?
4. **How** can it be done?
5. **Tuning**
Not there yet? => back to 2
6. Analyze & document the result



Performance Engineering

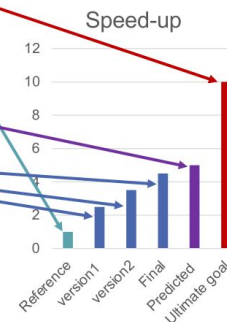
Follow these simple steps:

Systematic approach



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Thank you Ana Varbanescu!



Performance Engineering

Always optimize your application for a specific system!



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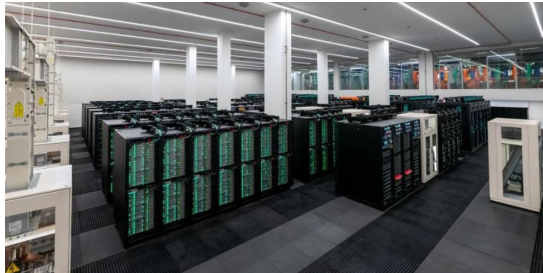
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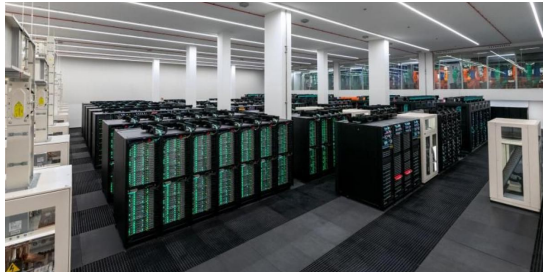
Performance Engineering

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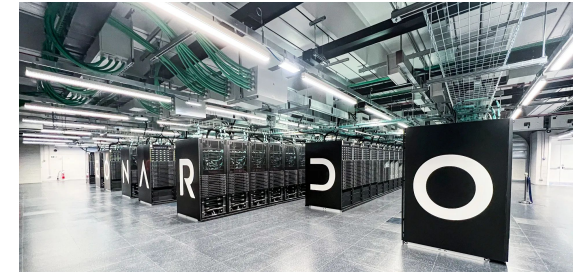
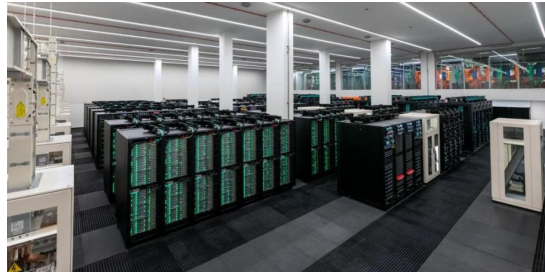
Performance Engineering

Always optimize your application for a specific system!



Performance Engineering

Always optimize your application for a specific system!



Performance Engineering



Rank	TOP500 Rank	System	Cores	Rmax (PFlop/s)	Power (kW)	Energy Efficiency (GFlops/watts)
12	5	LUMI - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE EuroHPC/CSC Finland	2,752,704	379.70	7,107	53.428
15	8	MareNostrum 5 ACC - BullSequana XH3000, Xeon Platinum 8460Y+ 32C 2.3GHz, NVIDIA H100 64GB, Infiniband NDR, EVIDEN EuroHPC/BSC Spain	663,040	175.30	4,159	48.320
28	7	Leonardo - BullSequana XH2000, Xeon Platinum 8358 32C 2.6GHz, NVIDIA A100 SXM4 64 GB, Quad-rail NVIDIA HDR100 Infiniband, EVIDEN EuroHPC/CINECA Italy	1,824,768	241.20	7,494	32.187

Performance Engineering

Performed optimizations:

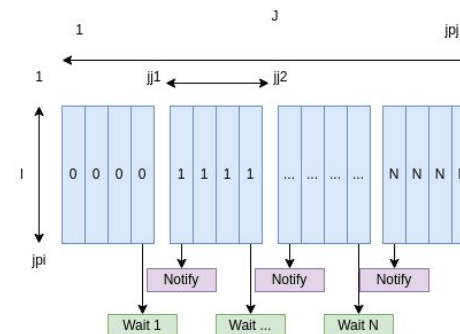
- CPU 

- GPU 

Performance Engineering

Performed optimizations:

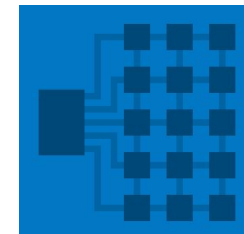
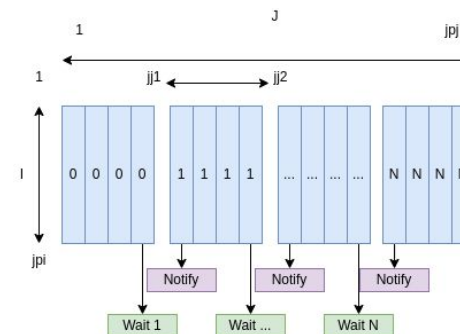
- CPU 
 - OpenMP regions (1.2x - 2.8x depending on the region)
- GPU 



Performance Engineering

Performed optimizations:

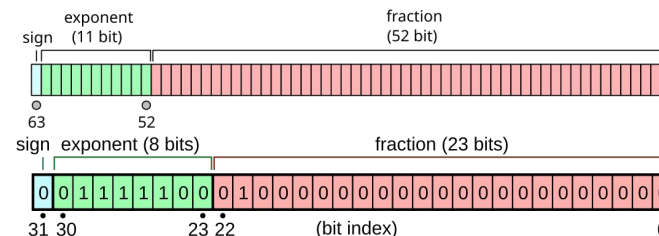
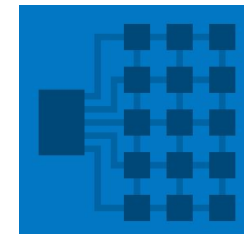
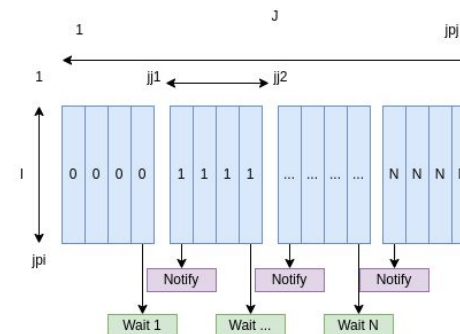
- CPU 
 - OpenMP regions (1.2x - 2.8x depending on the region)
 - MultIO improvement (1.03x)
- GPU 



Performance Engineering

Performed optimizations:

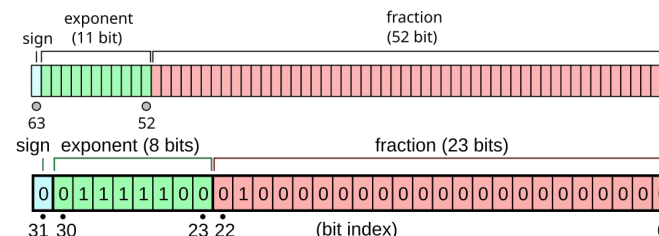
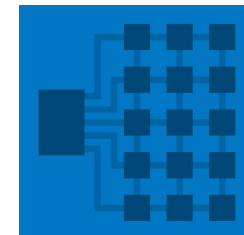
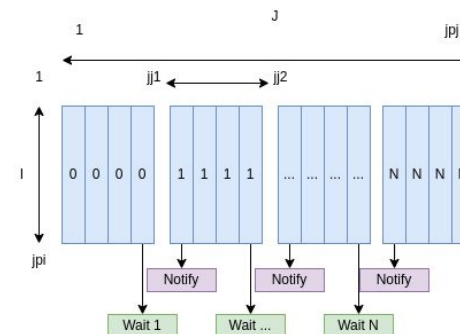
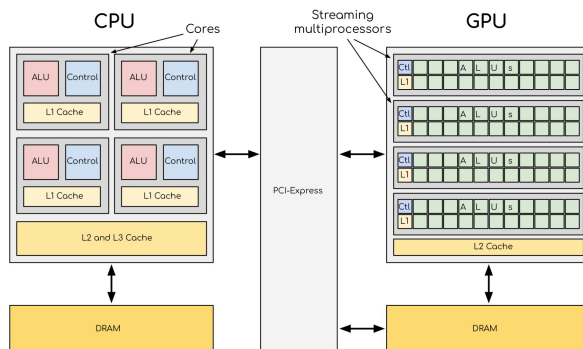
- CPU 
 - OpenMP regions (1.2x - 2.8x depending on the region)
 - MultIO improvement (1.03x)
 - Mixed Precision (1.2x)
- GPU 



Performance Engineering

Performed optimizations:

- CPU 
 - OpenMP regions (1.2x - 2.8x depending on the region)
 - MultIO improvement (1.03x)
 - Mixed Precision (1.2x)
- GPU 
 - Porting pilot-regions of Sea-Ice module to GPUs (5.9x)



Performance Profiling



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HPC 101



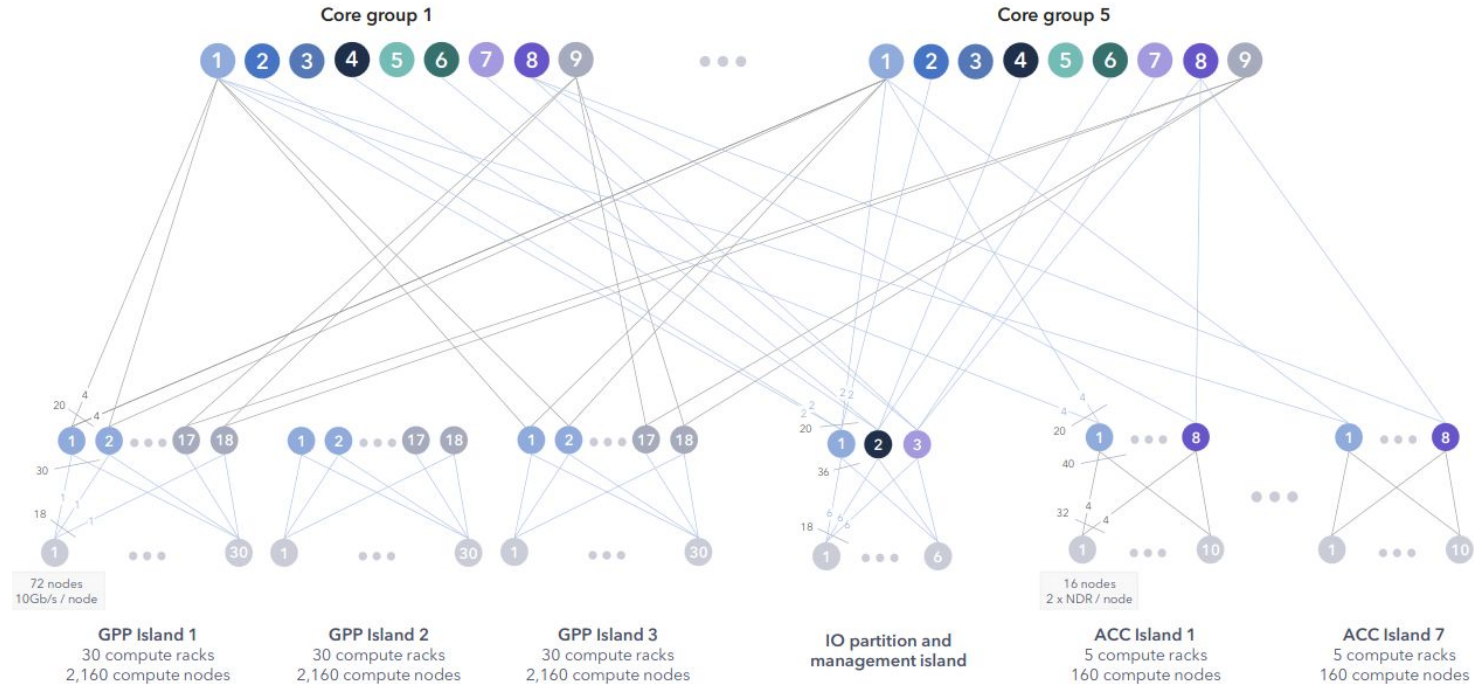
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Destination Earth

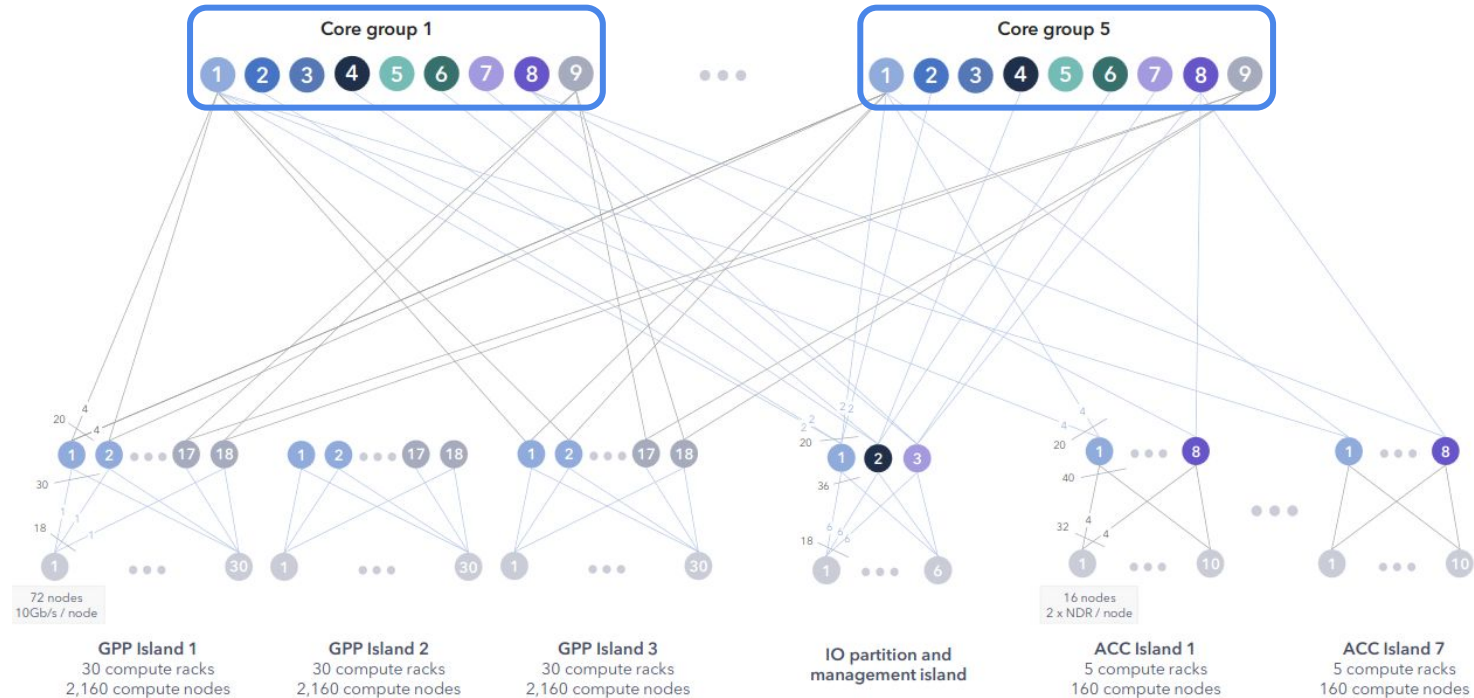
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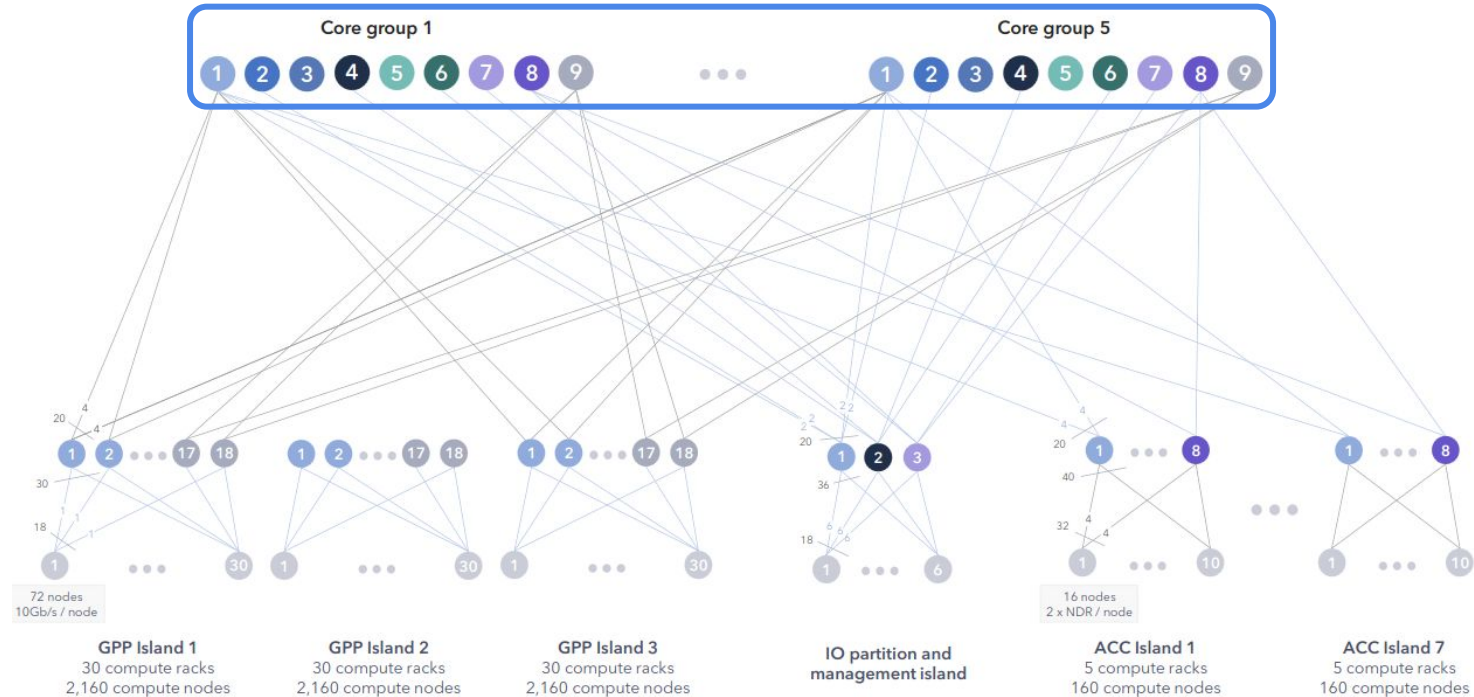
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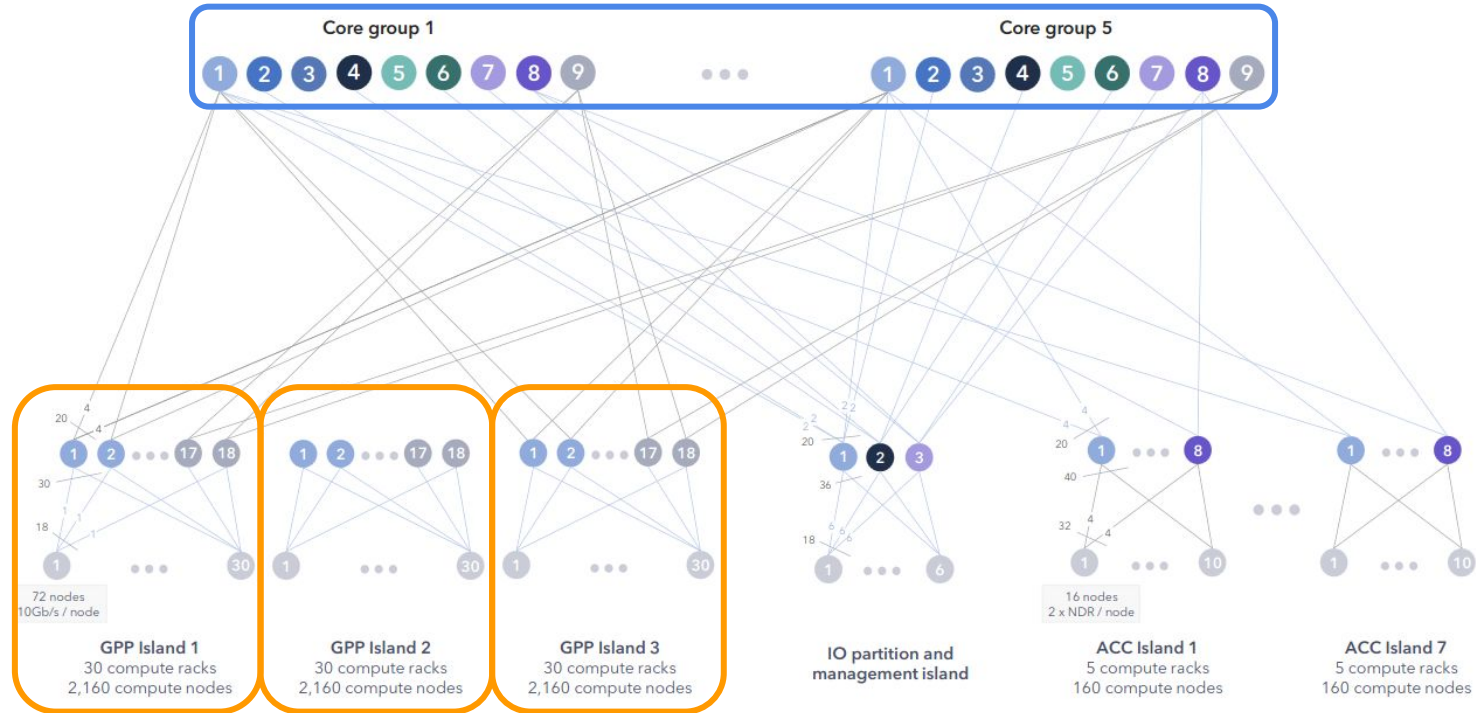
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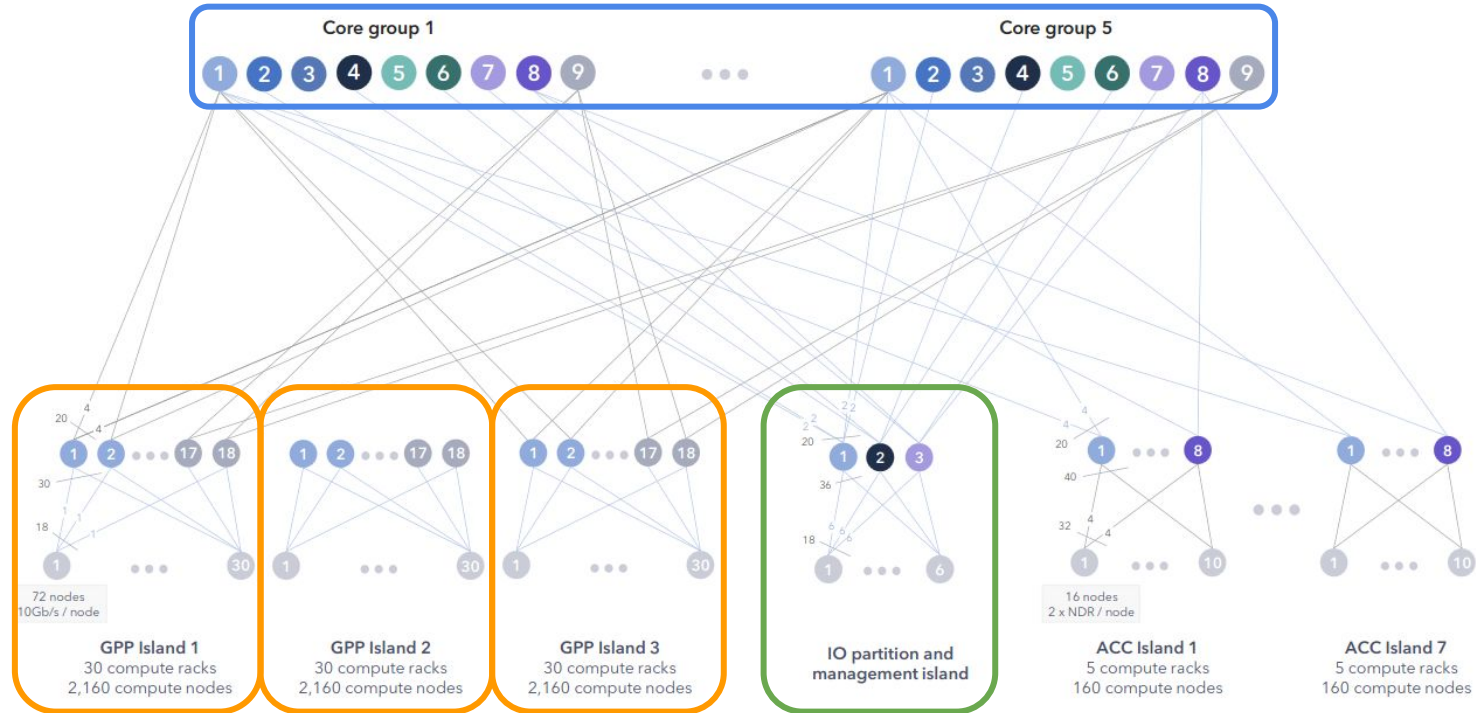
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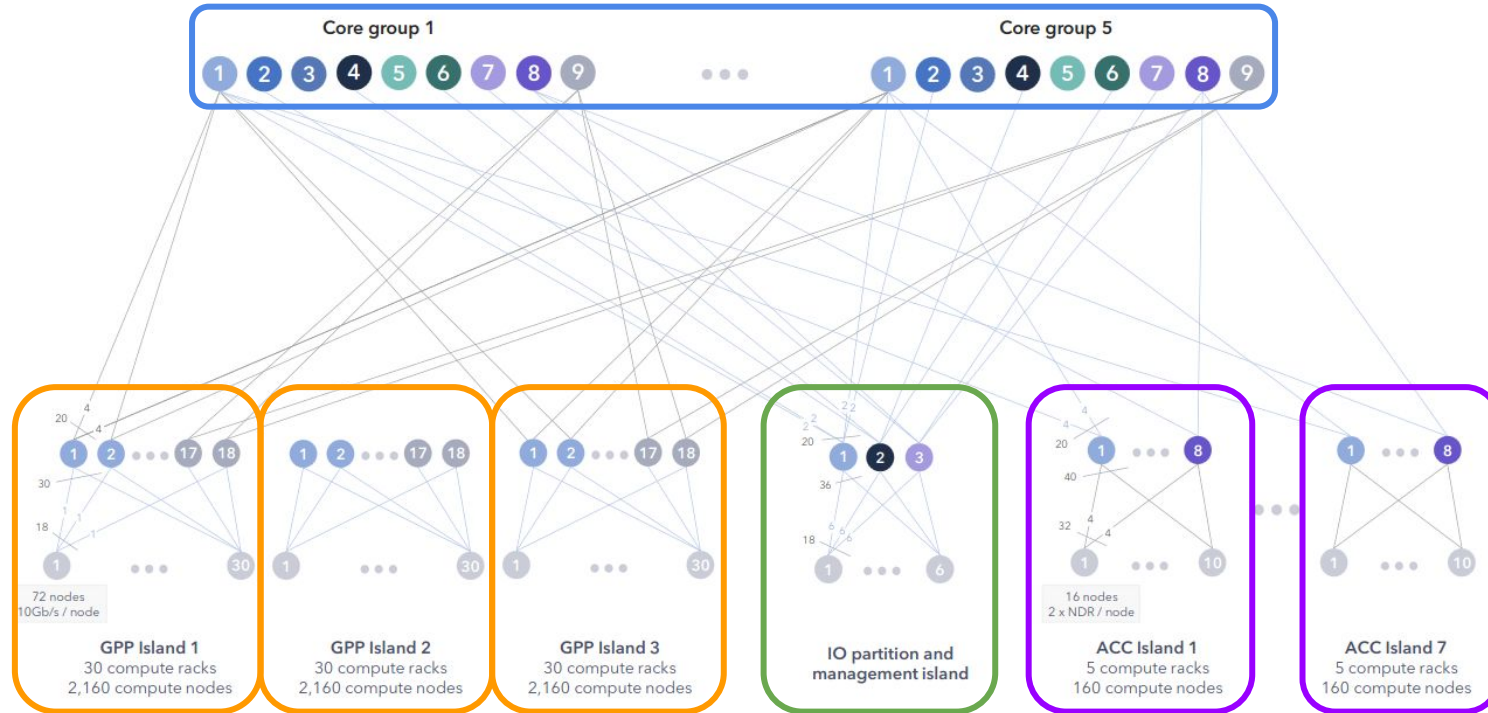
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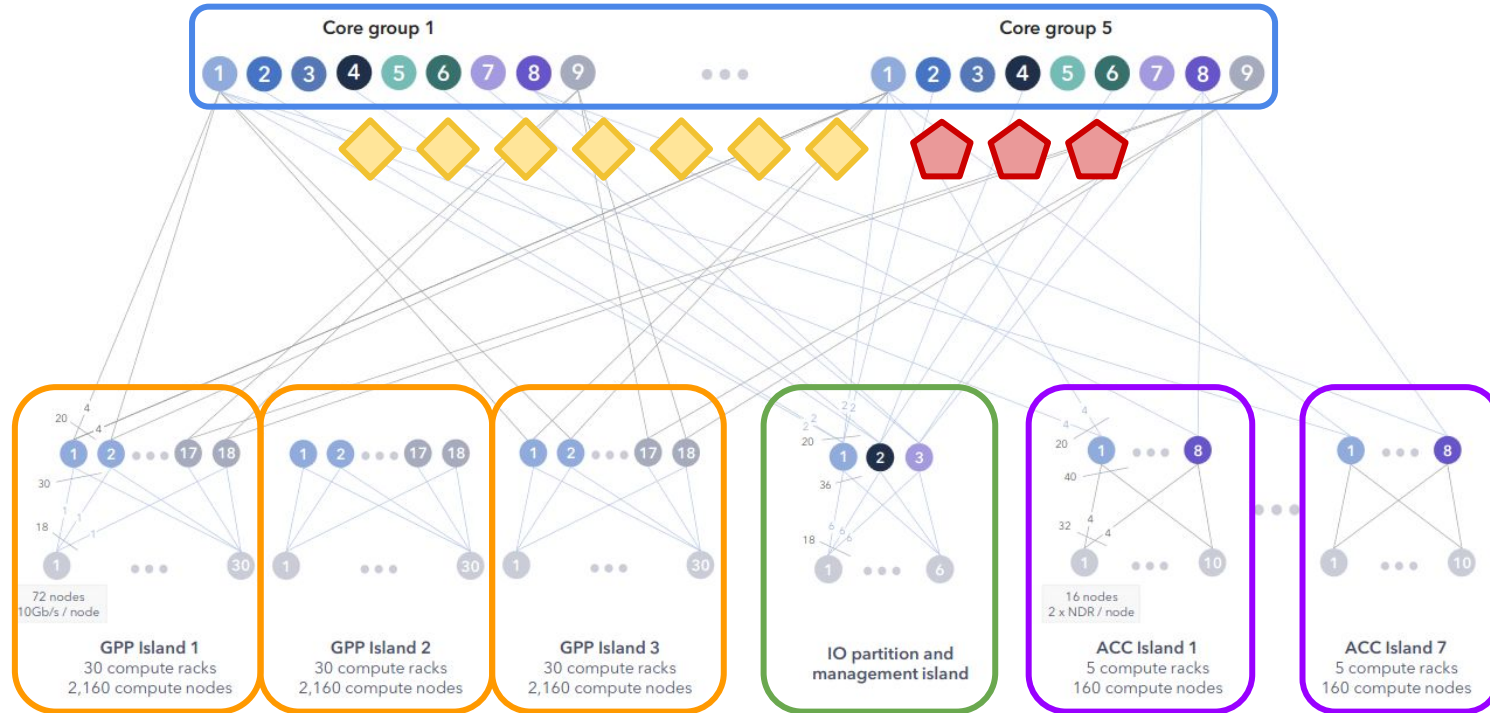
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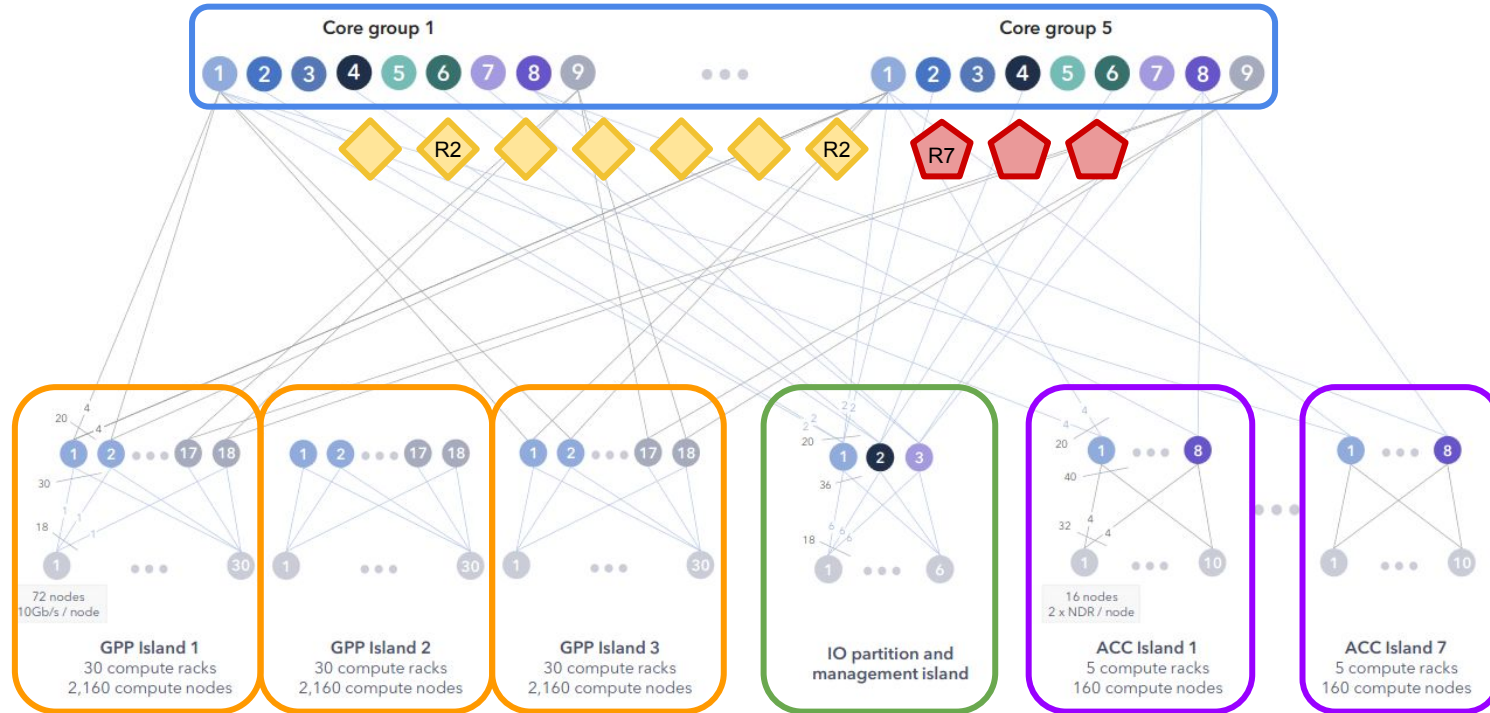
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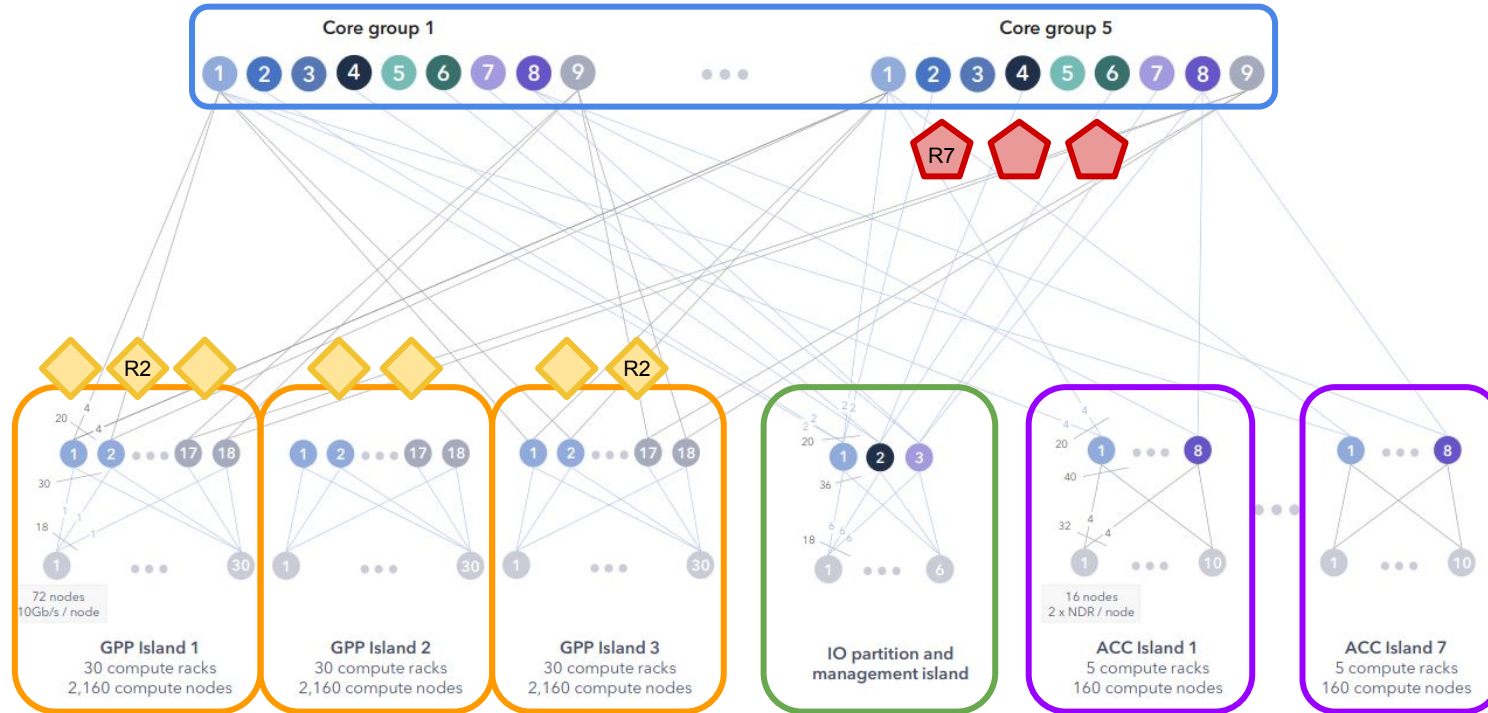
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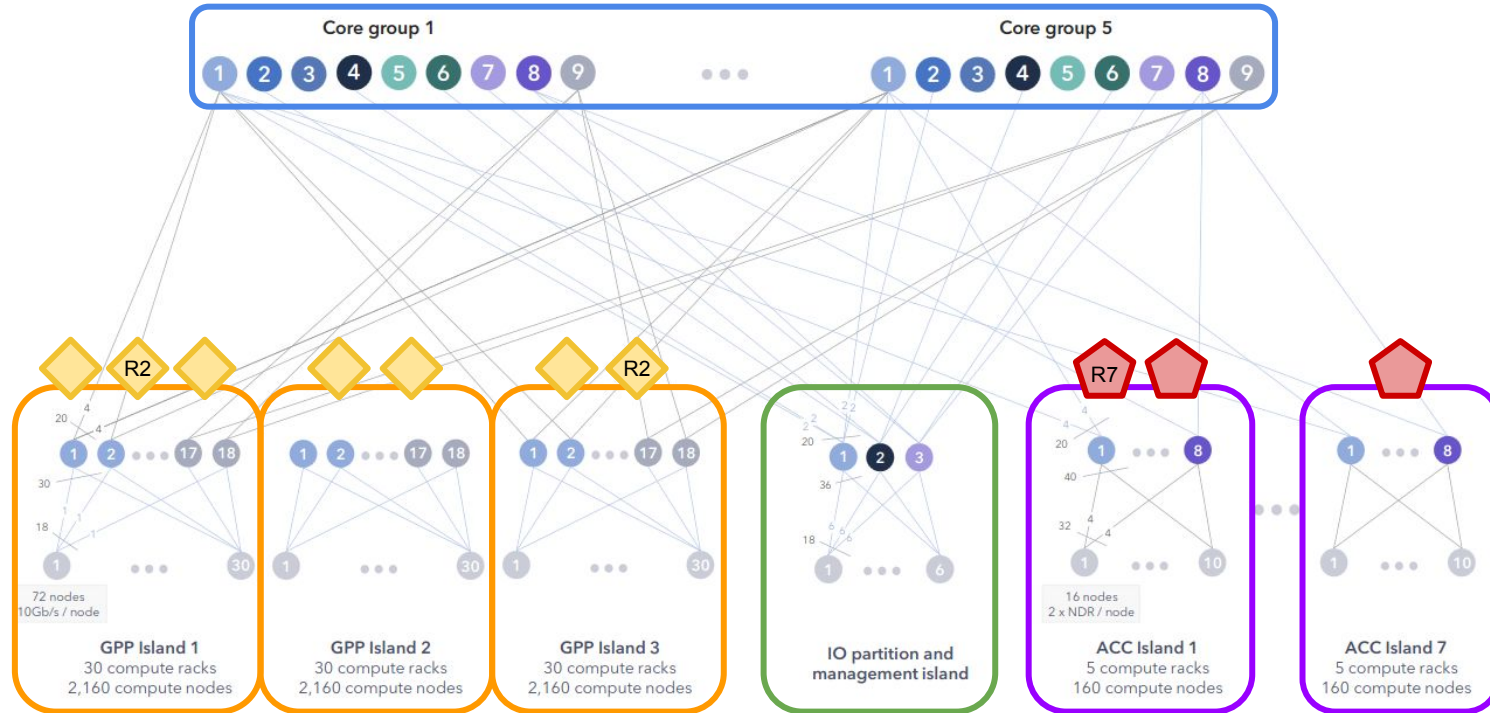
HPC 101



HPC 101

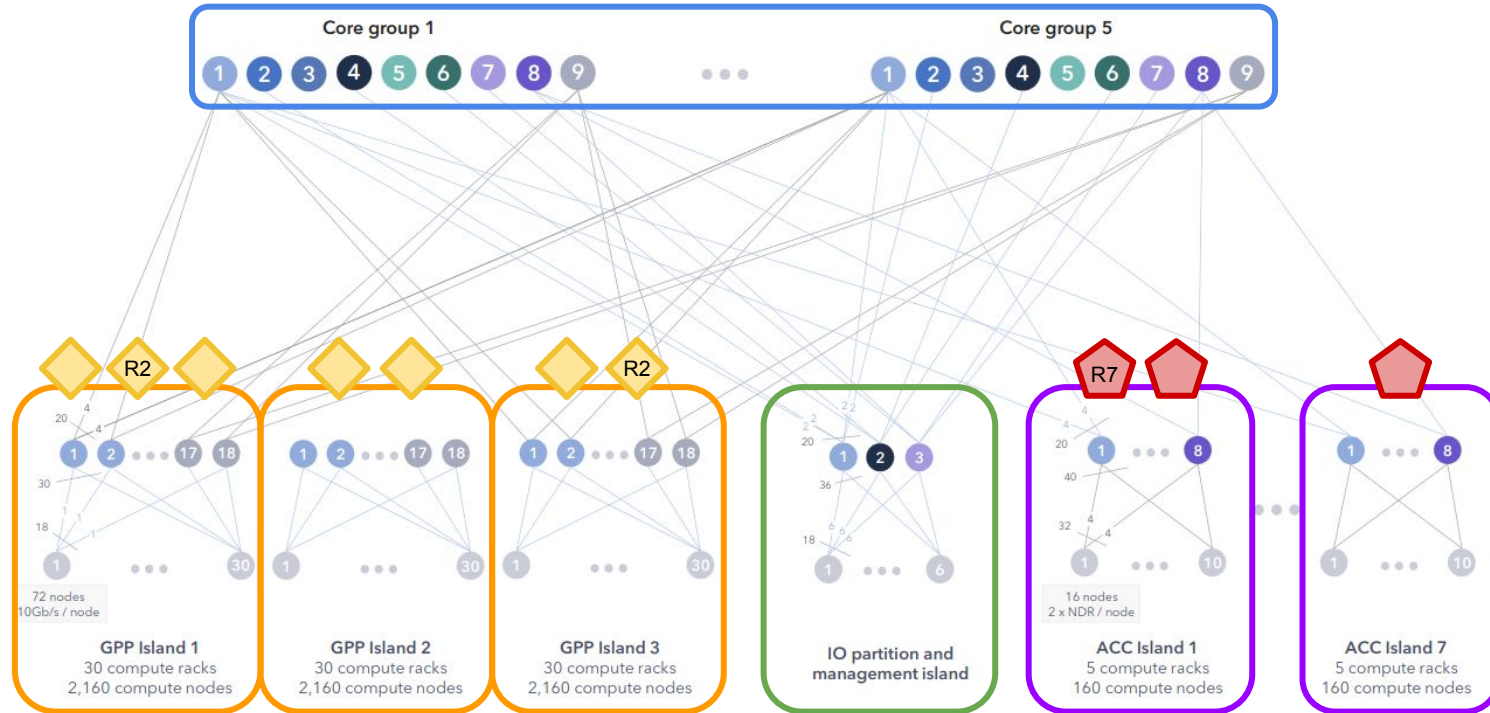


HPC 101



HPC 101

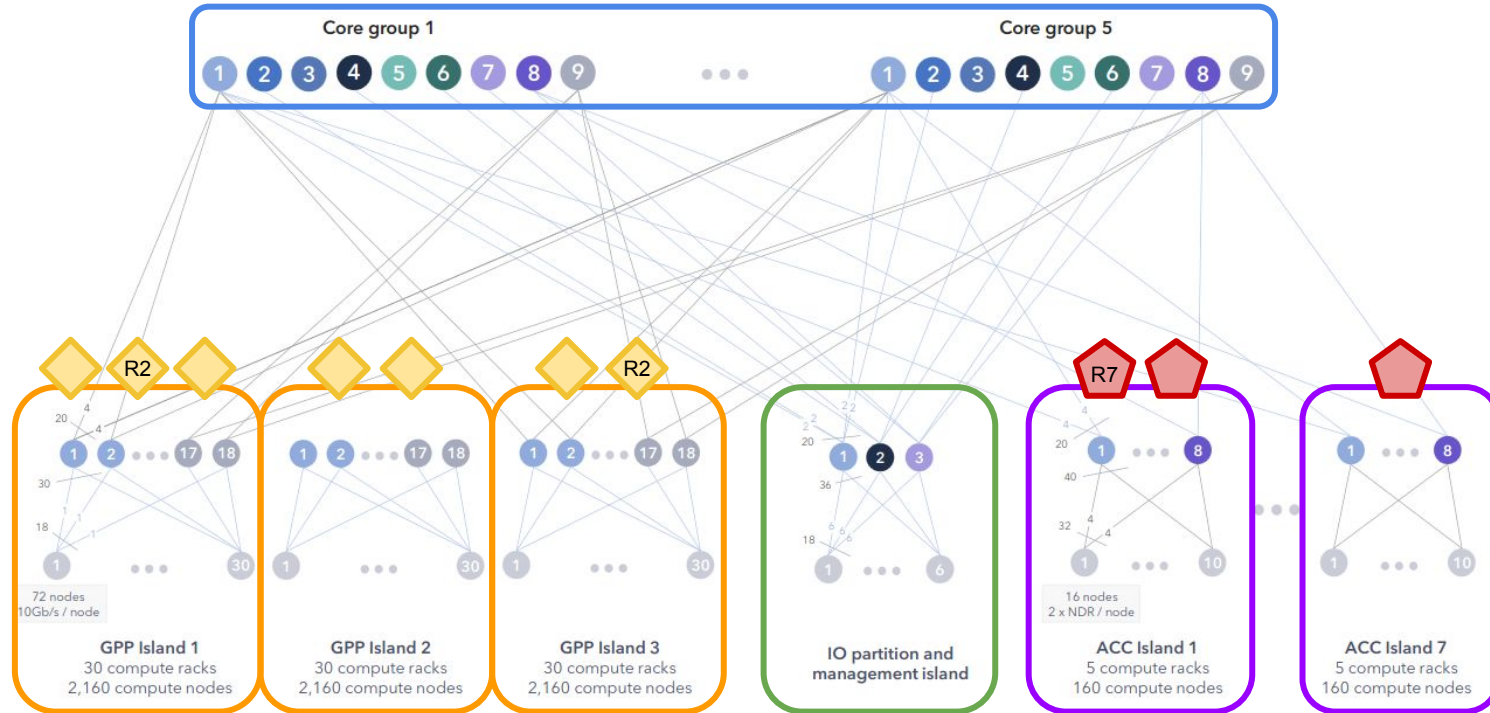
Operations:   



HPC 101

Operations:   

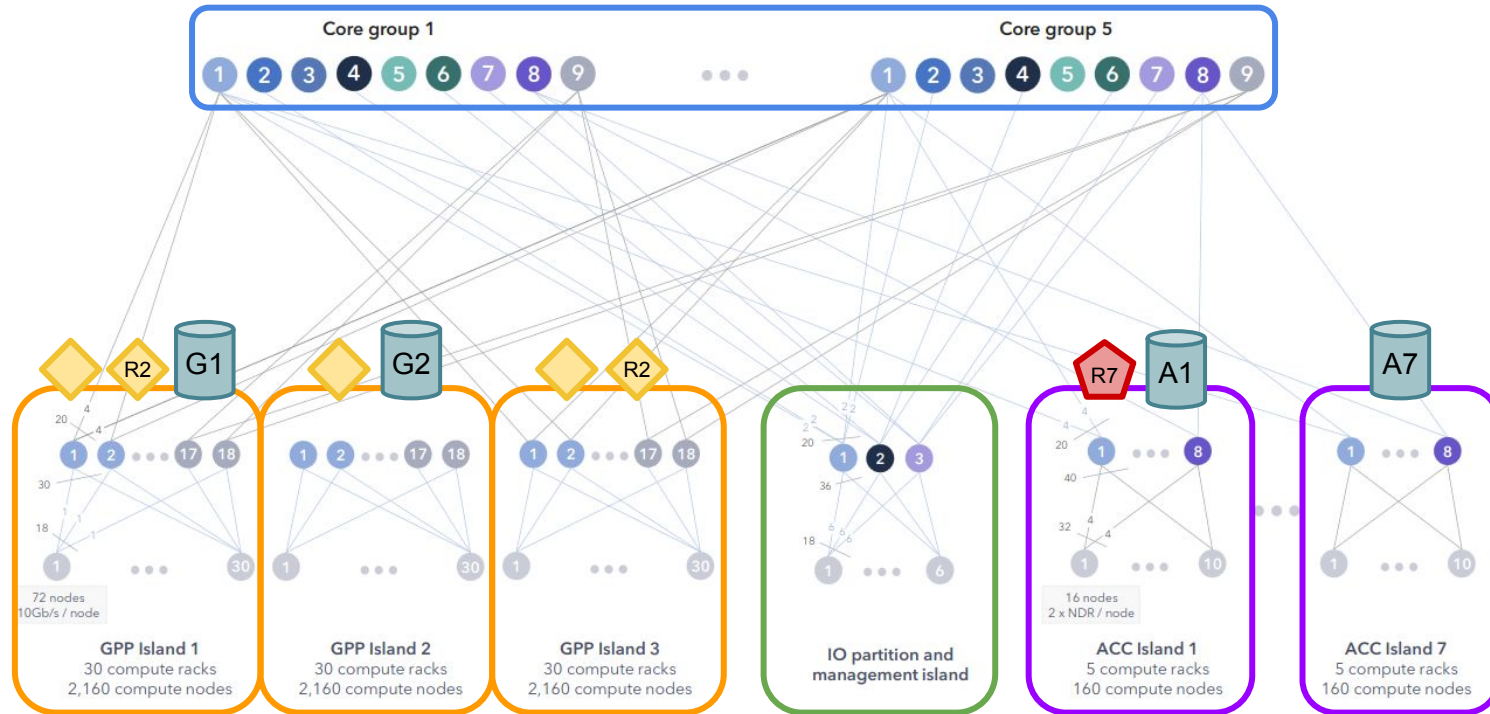
Cycle 0



HPC 101

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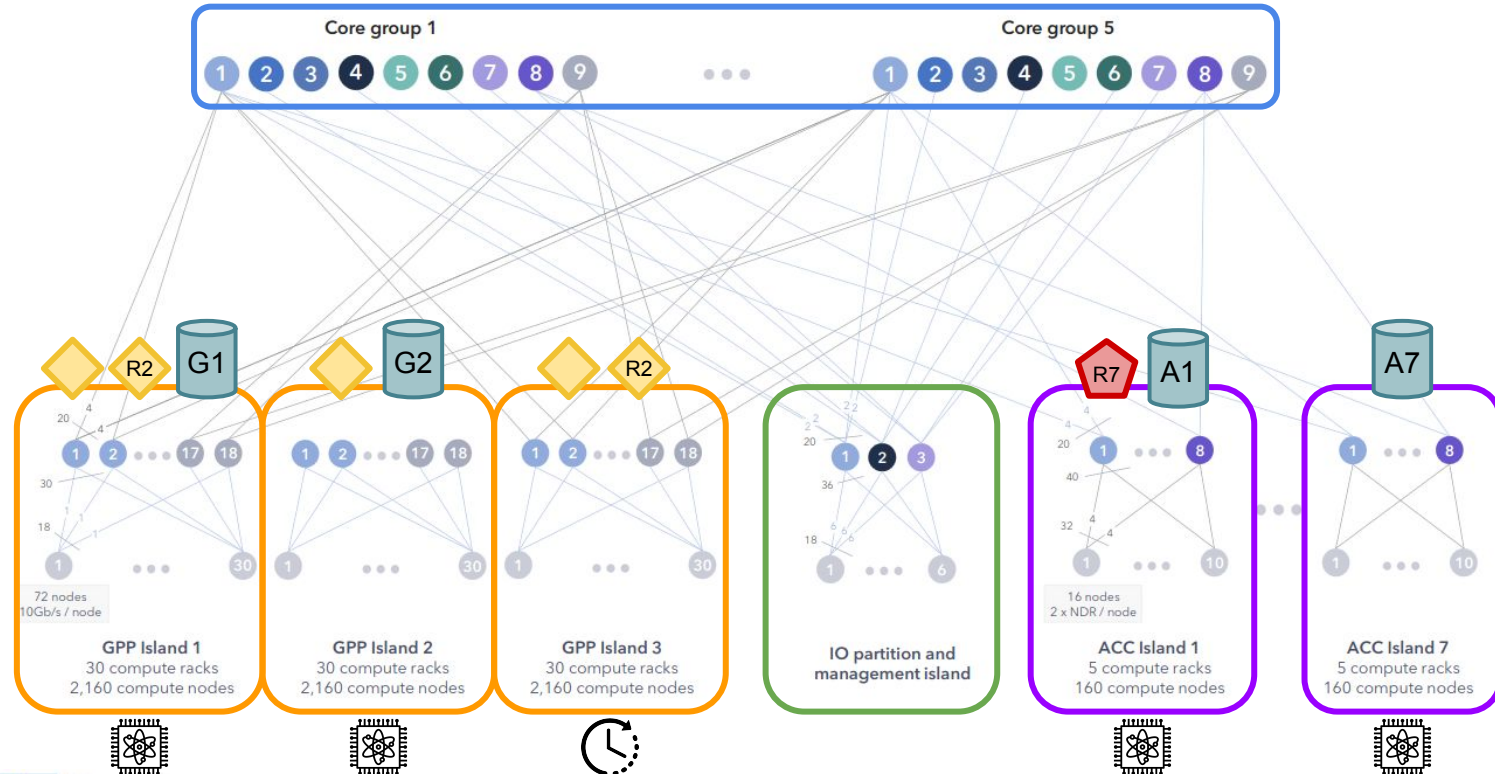
Cycle 1



HPC 101

Operations:   

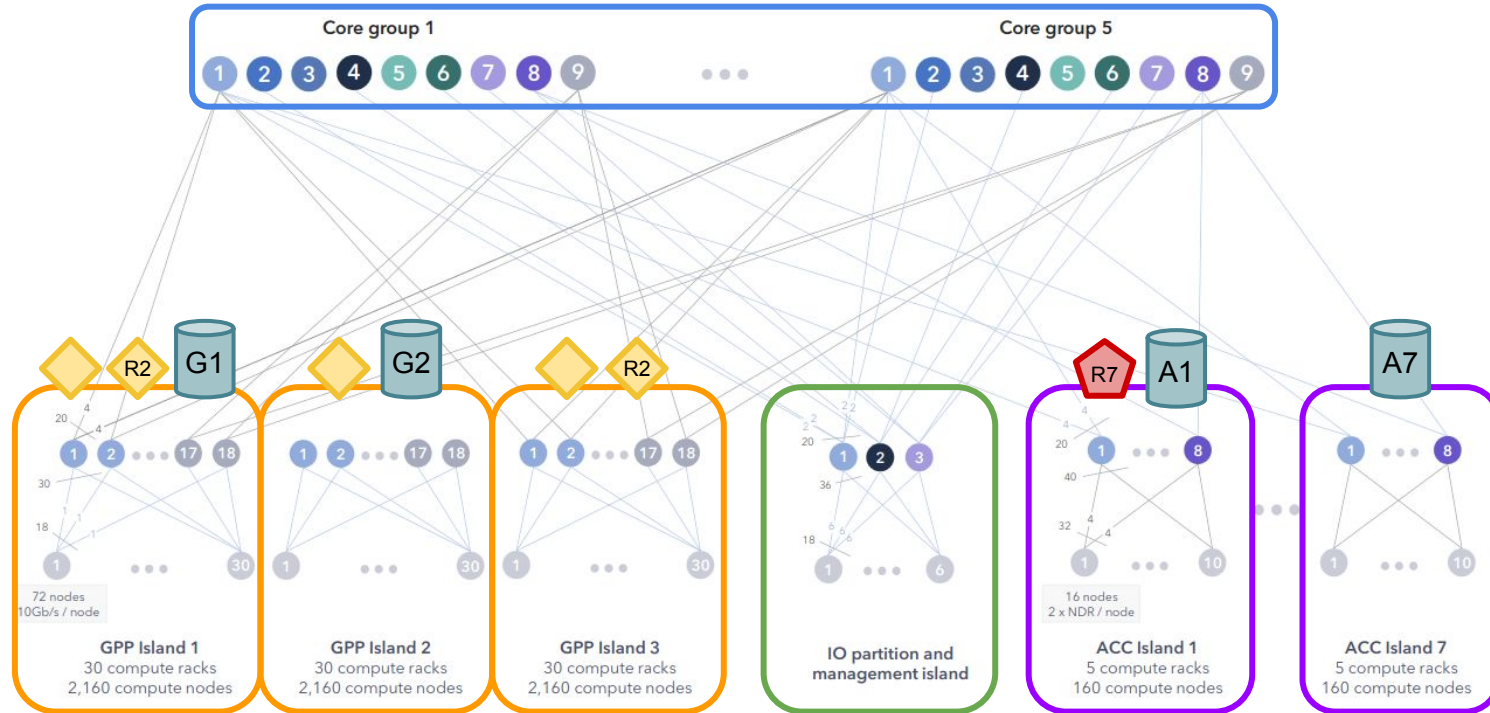
Cycle 1



HPC 101

Operations:   

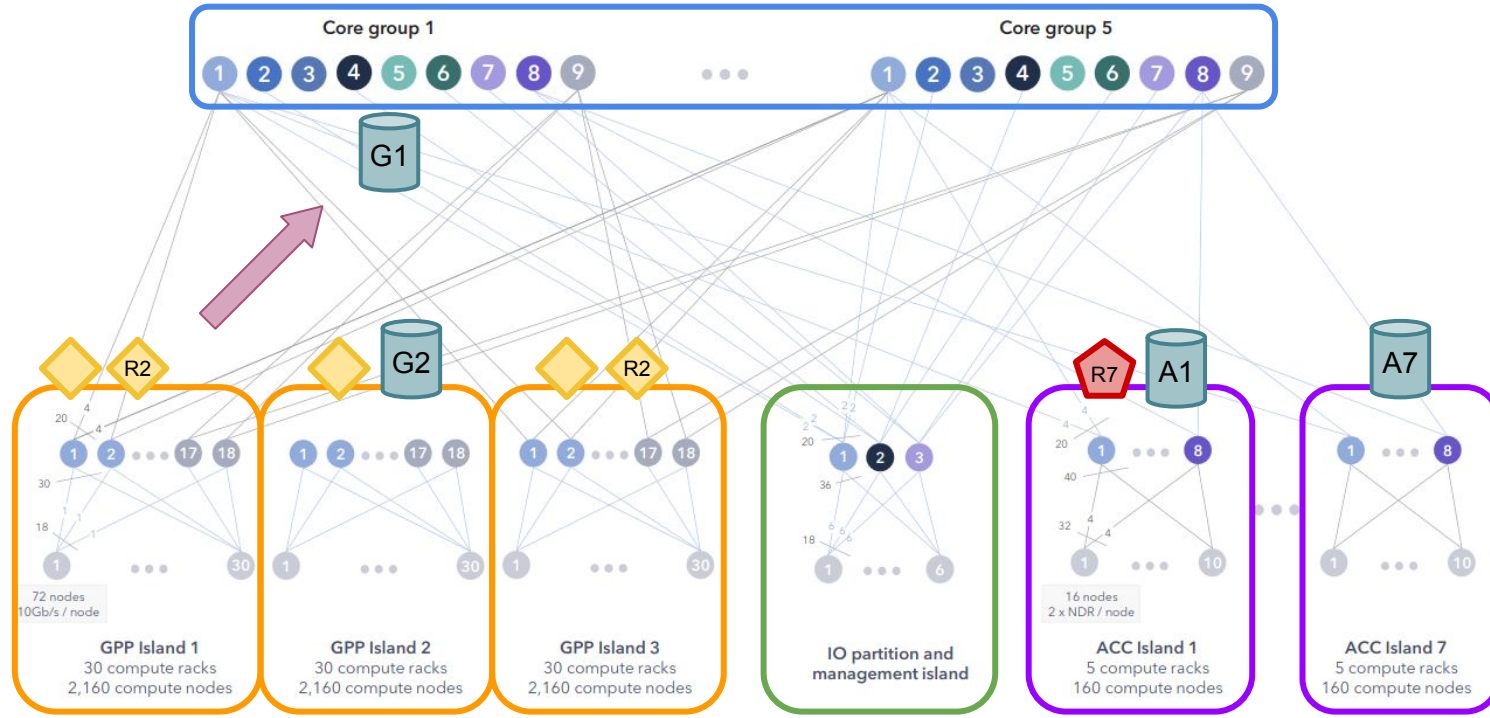
Cycle 2



HPC 101

Operations:   

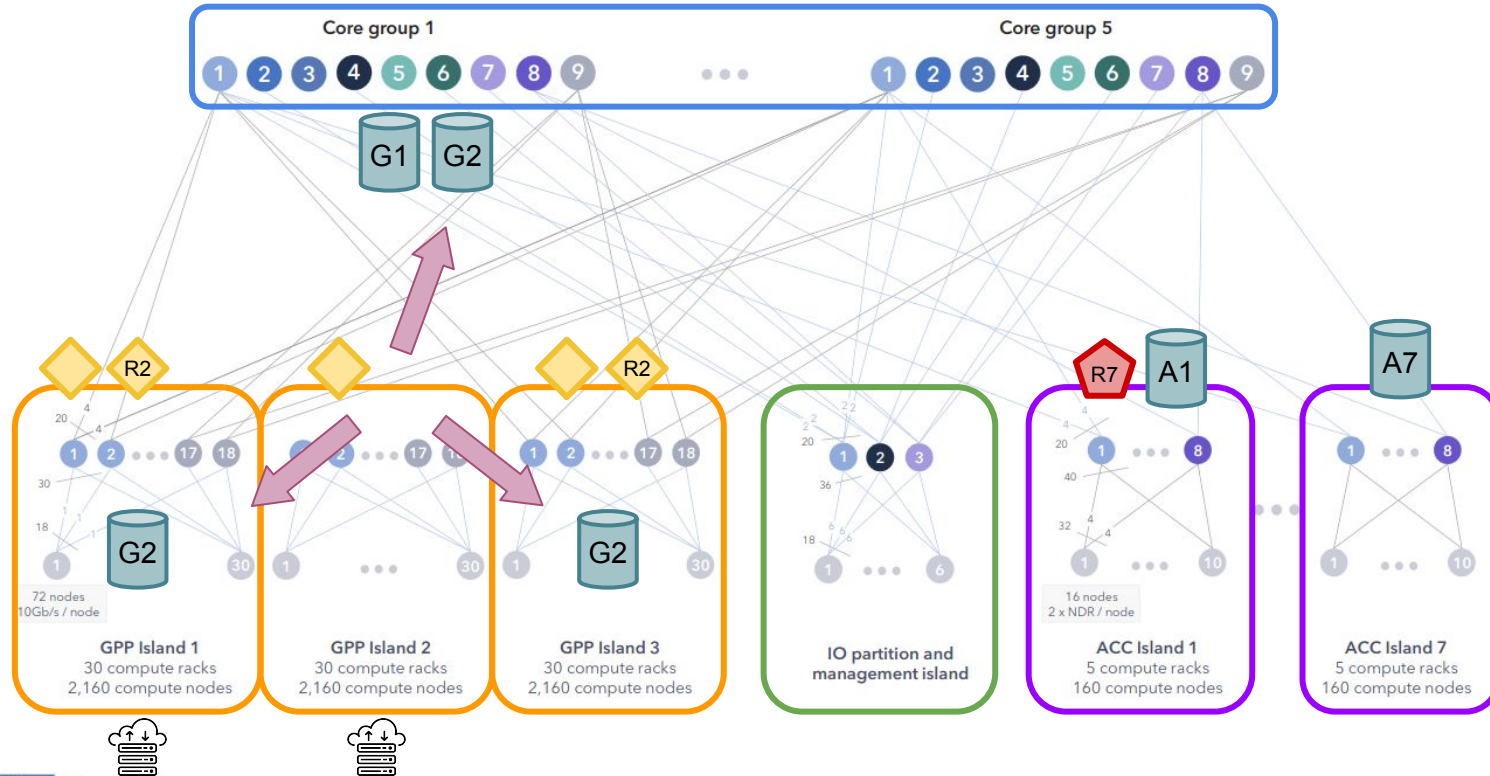
Cycle 2



HPC 101

Operations:   

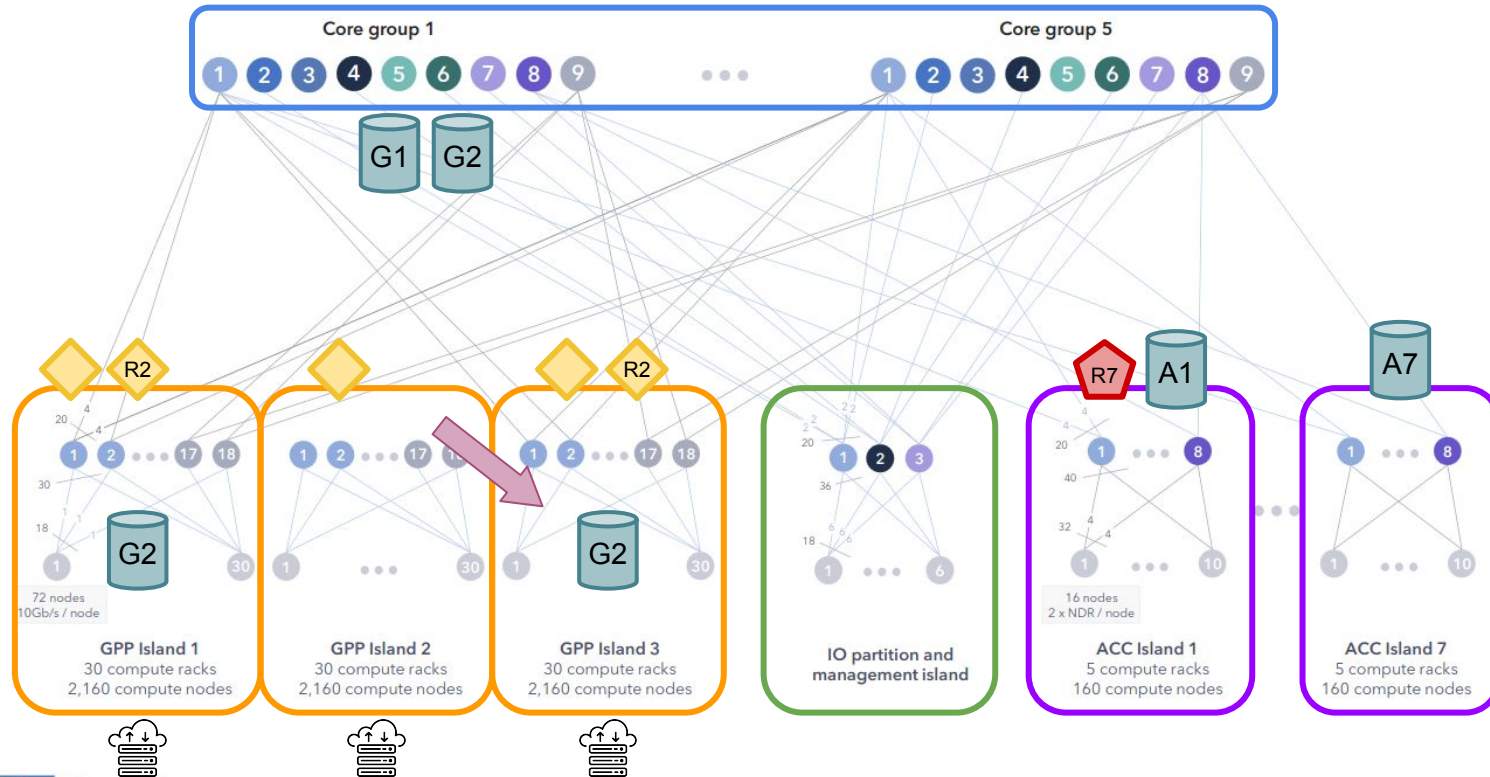
Cycle 2



HPC 101

Operations:   

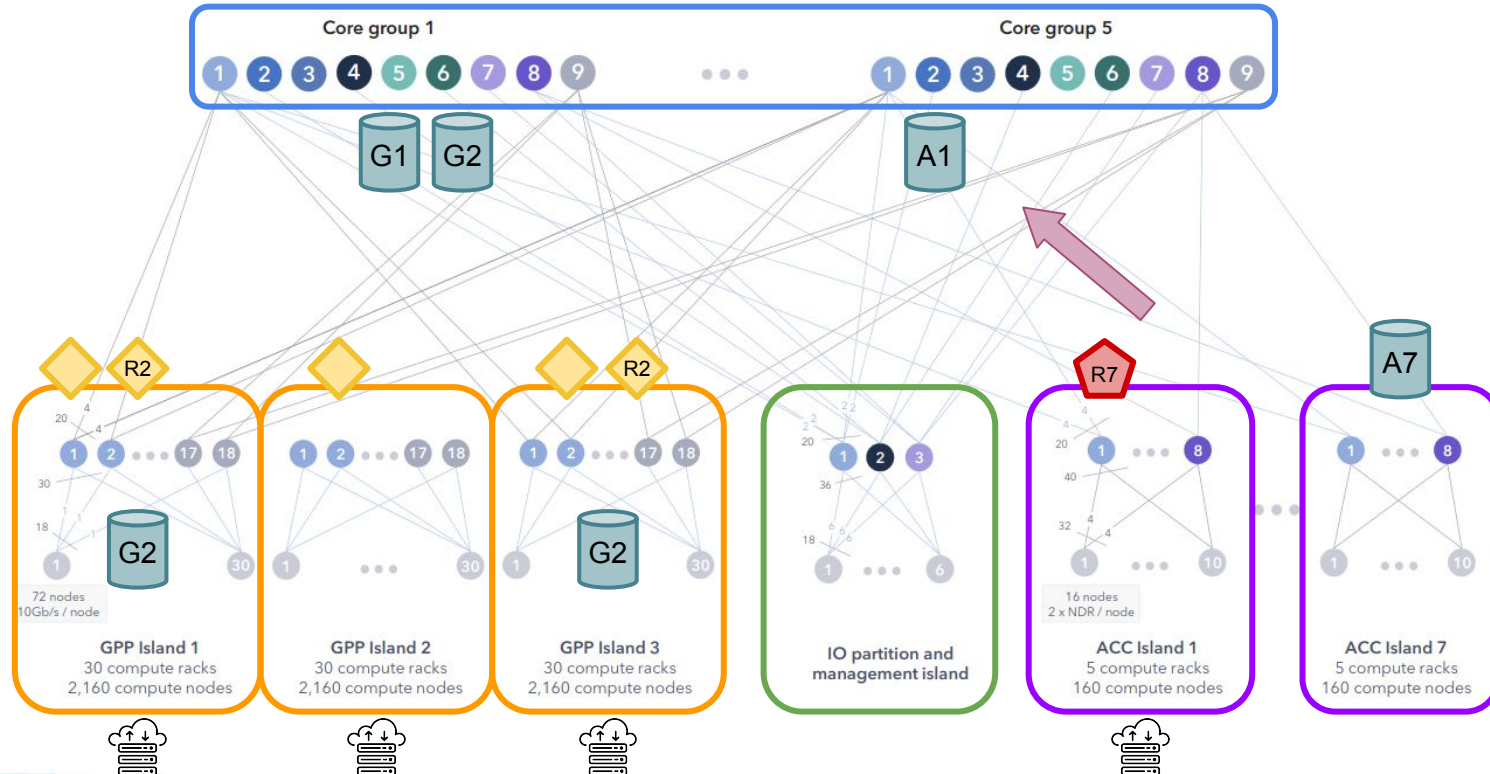
Cycle 2



HPC 101

Operations:   

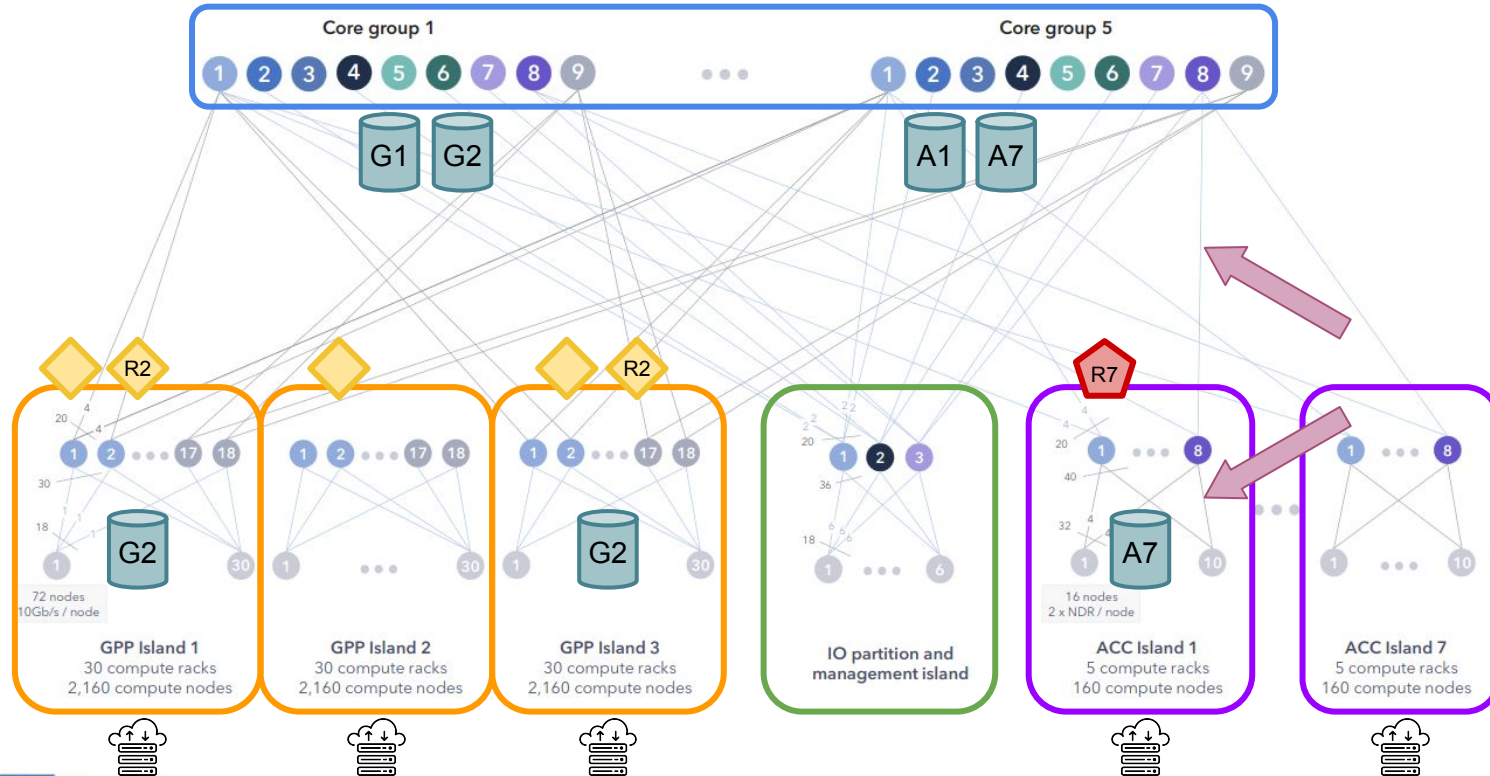
Cycle 2



HPC 101

Operations:   

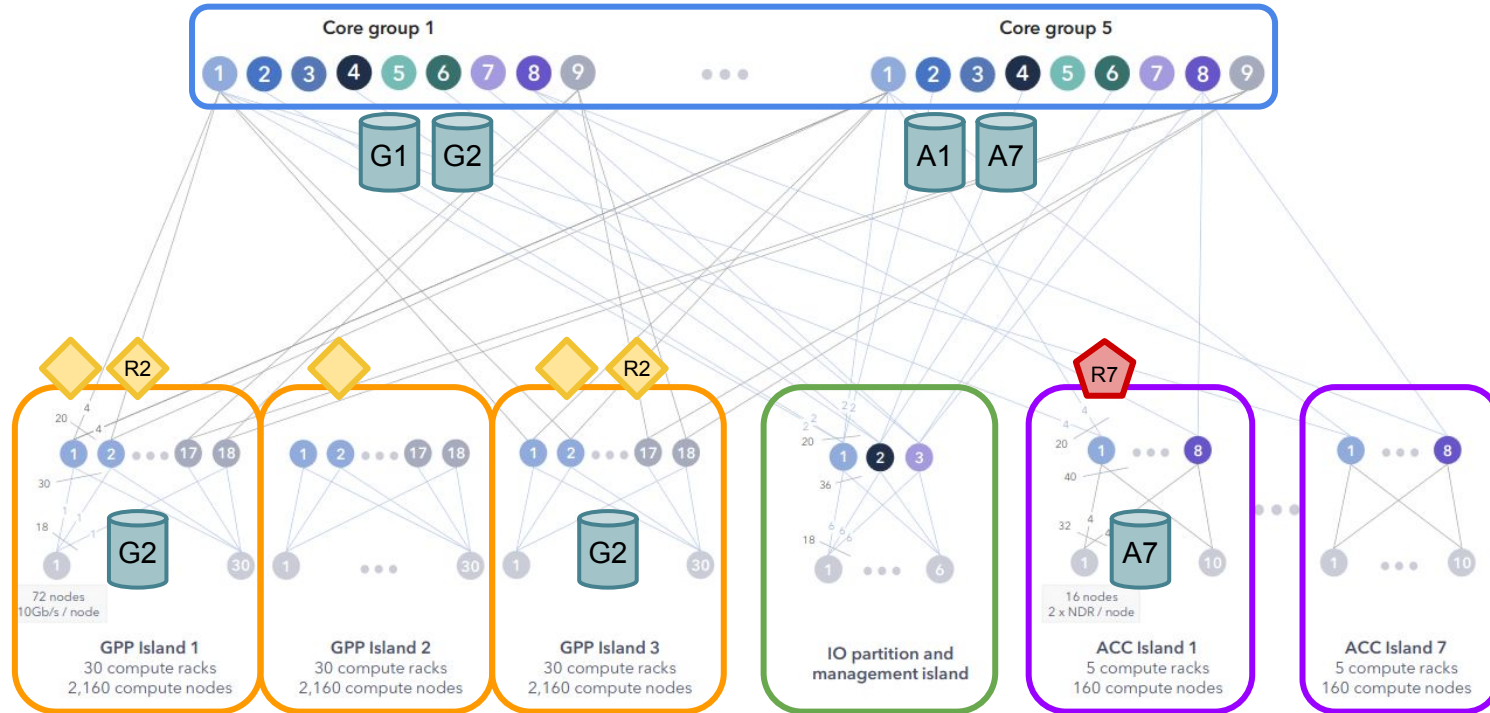
Cycle 2



HPC 101

Operations:   

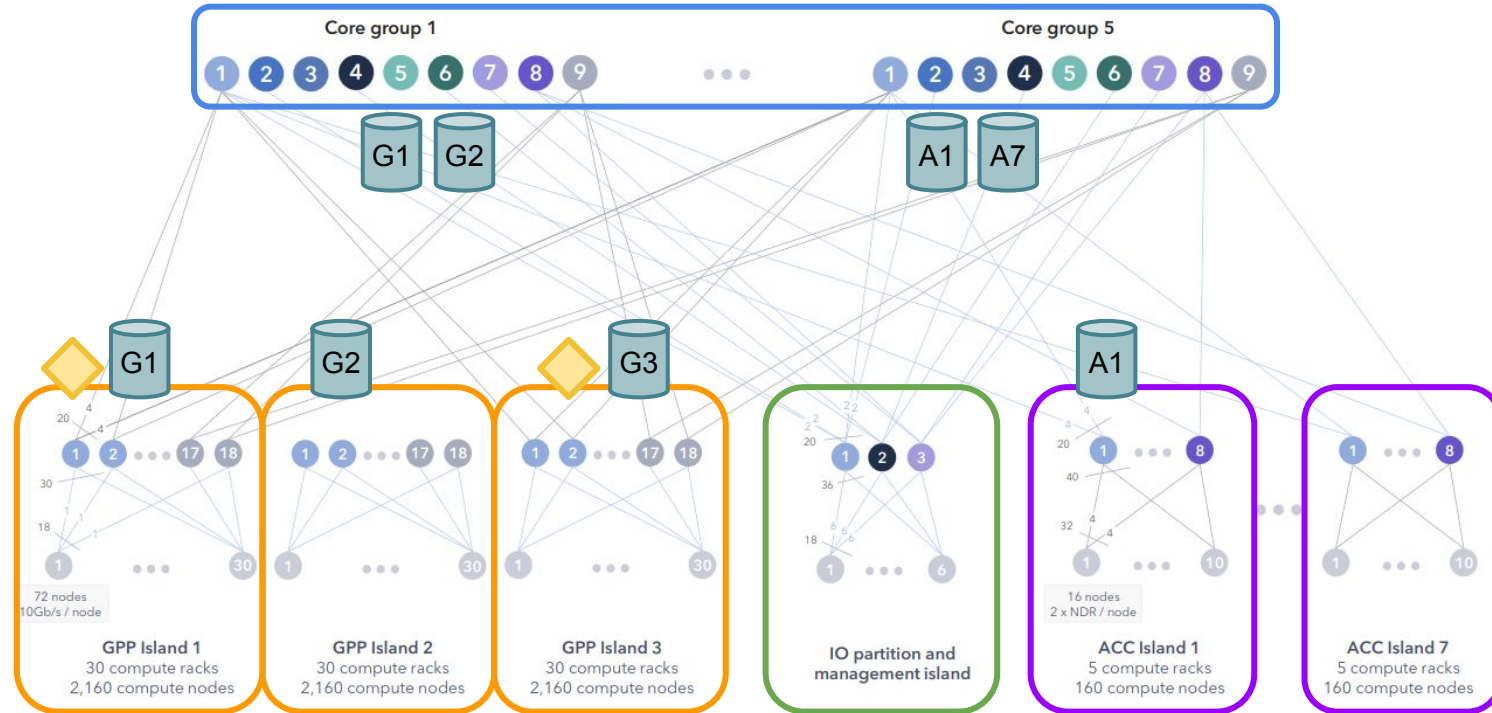
Cycle 3



HPC 101

Operations:   

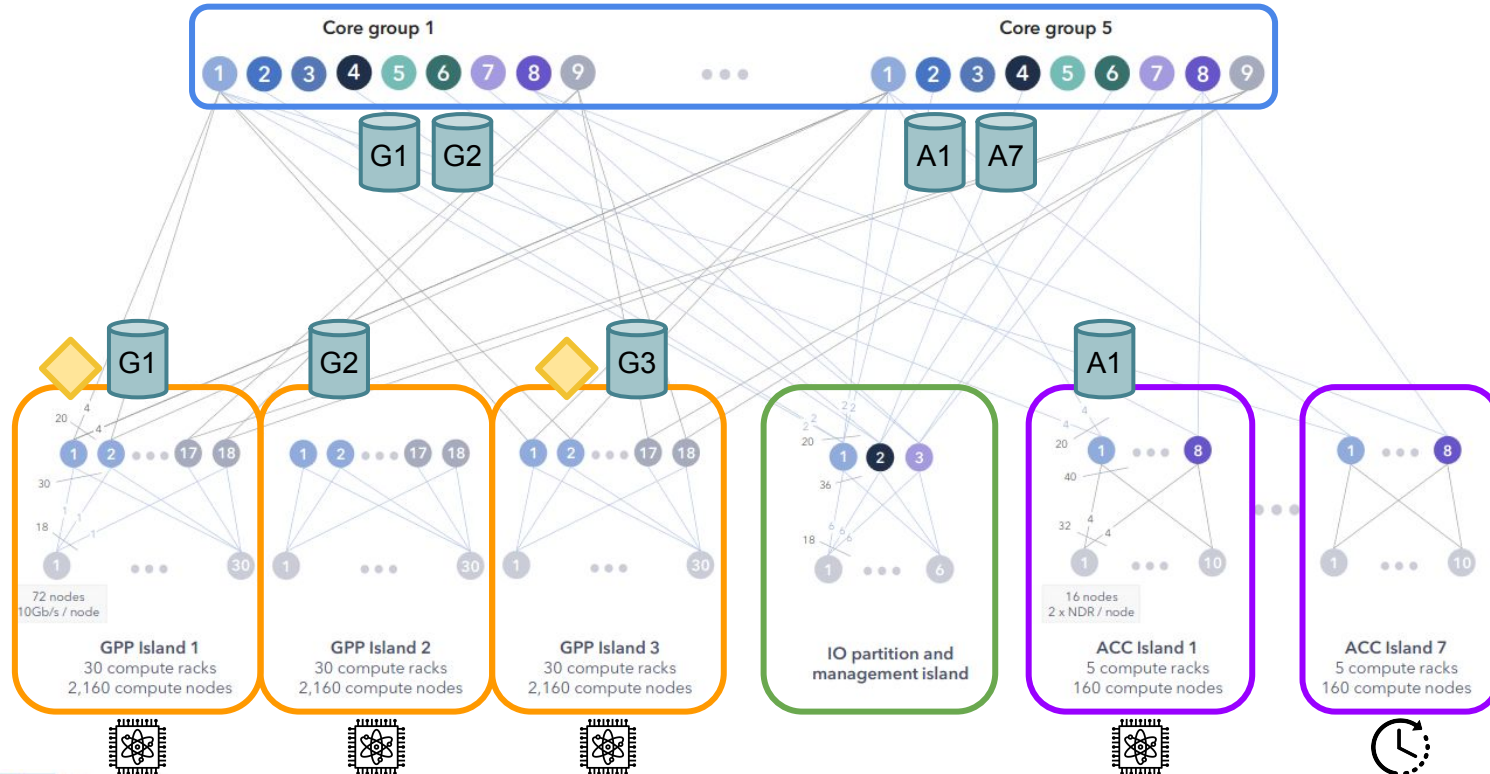
Cycle 3



HPC 101

Operations:   

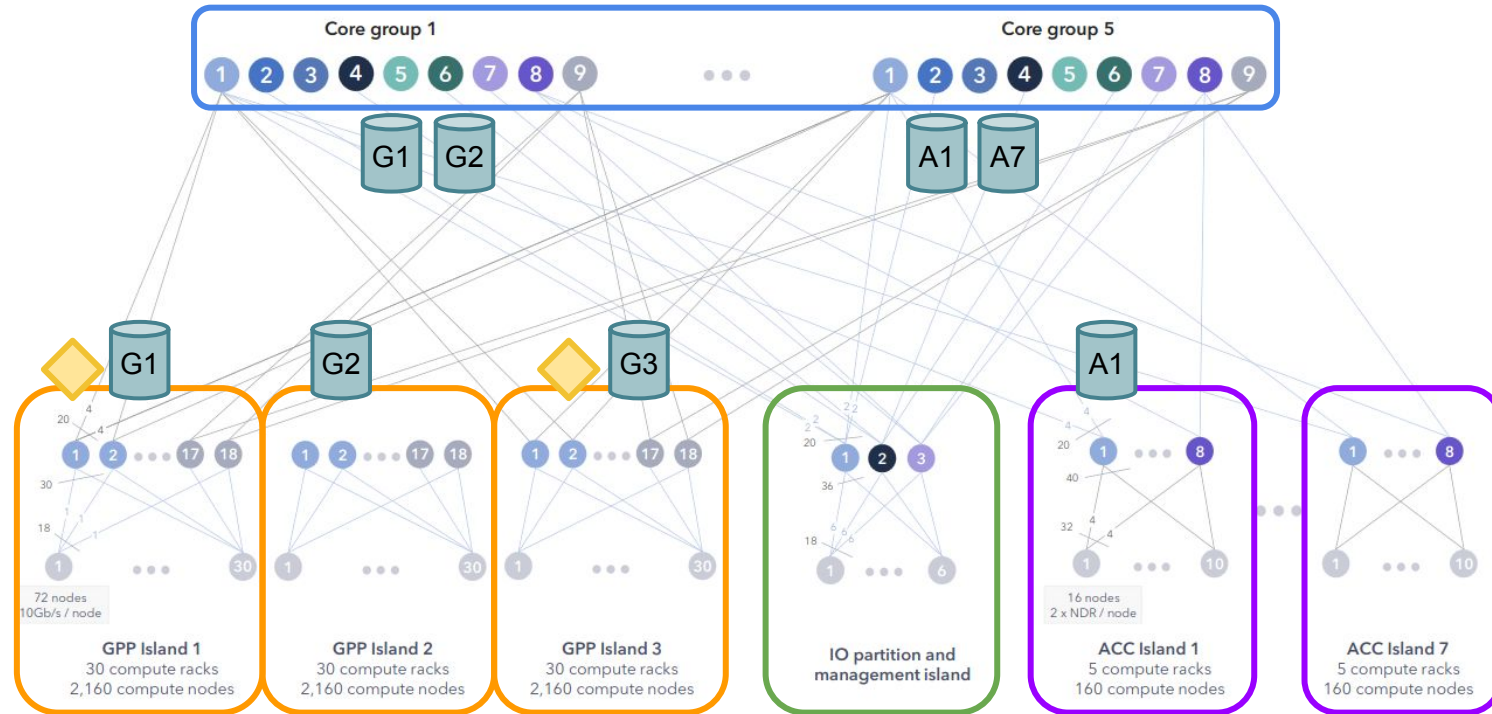
Cycle 3



HPC 101

Operations:   

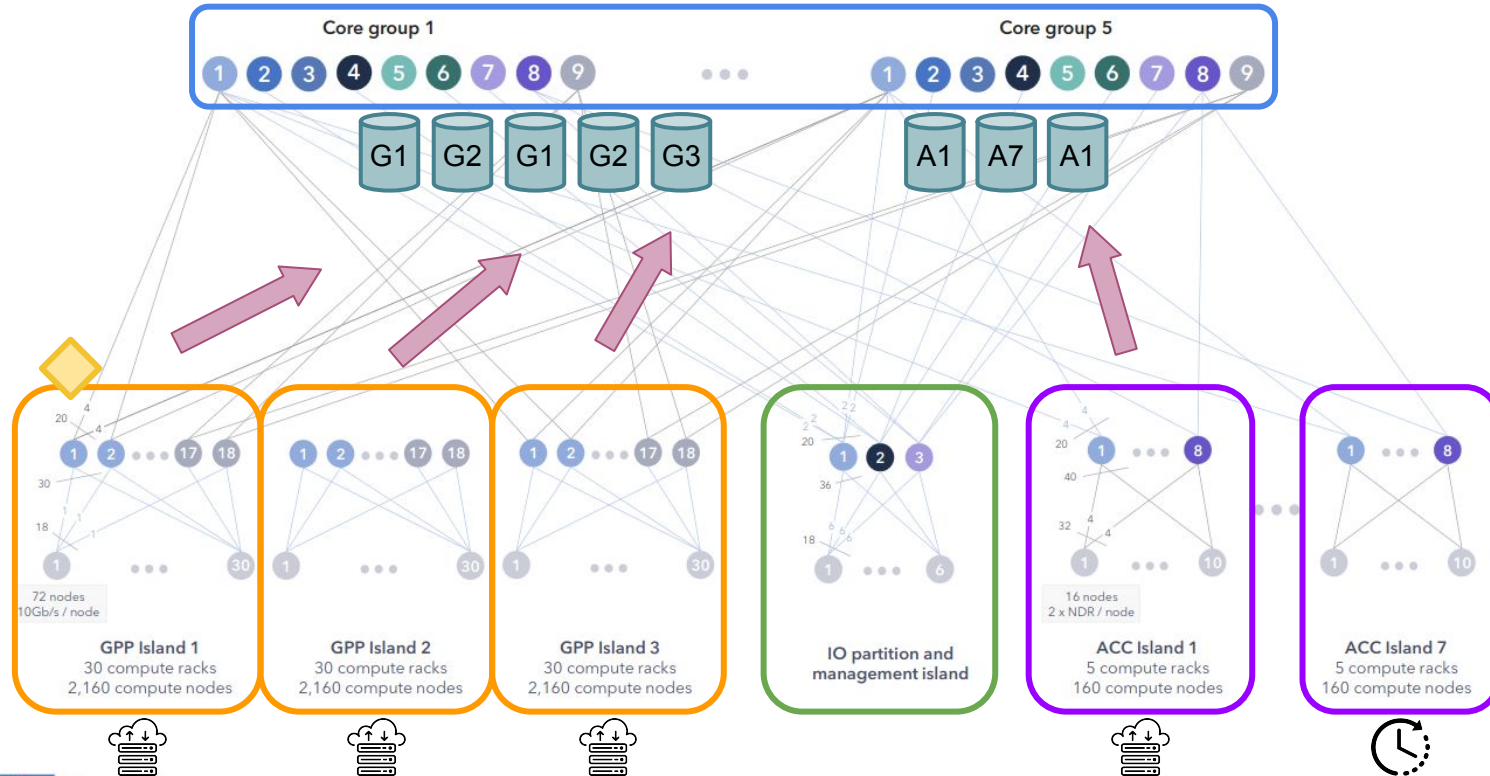
Cycle 4



HPC 101

Operations:   

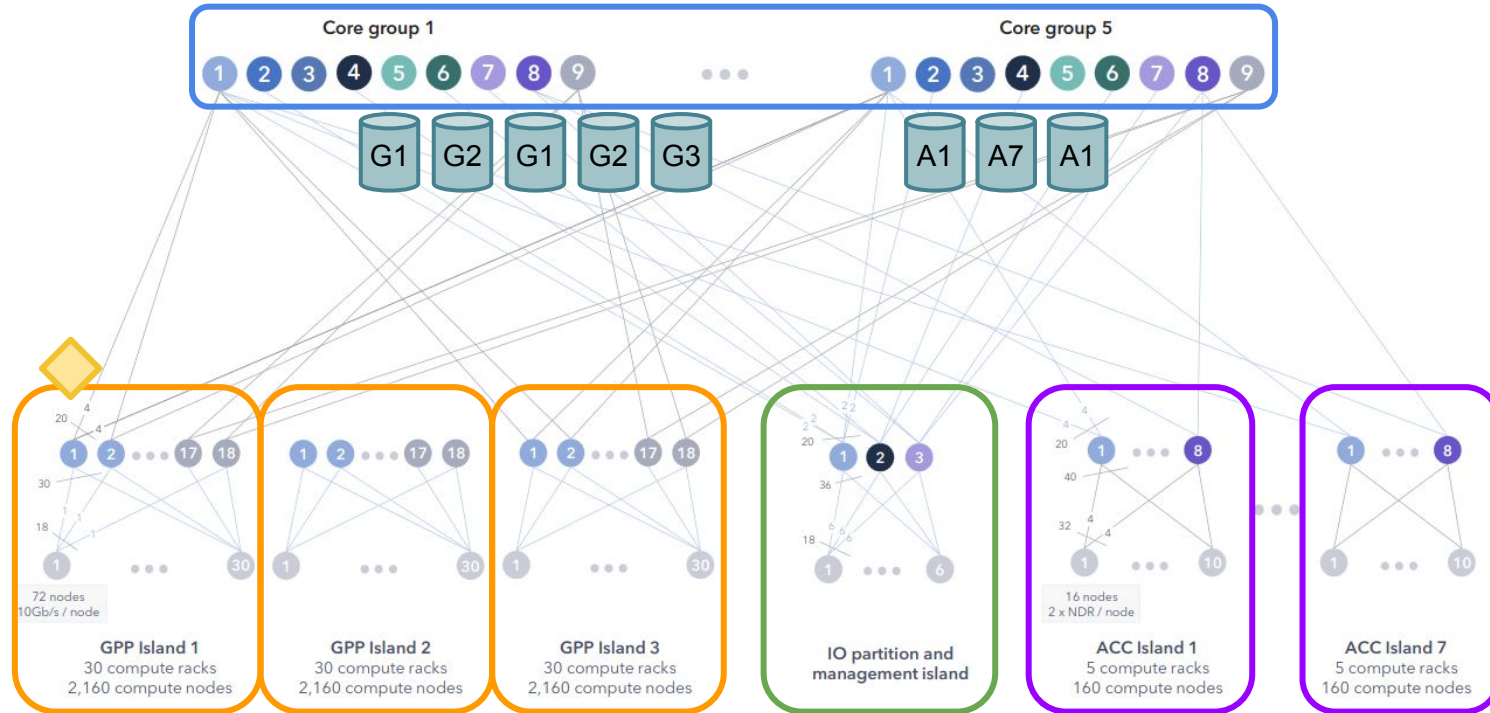
Cycle 4



HPC 101

Operations:   

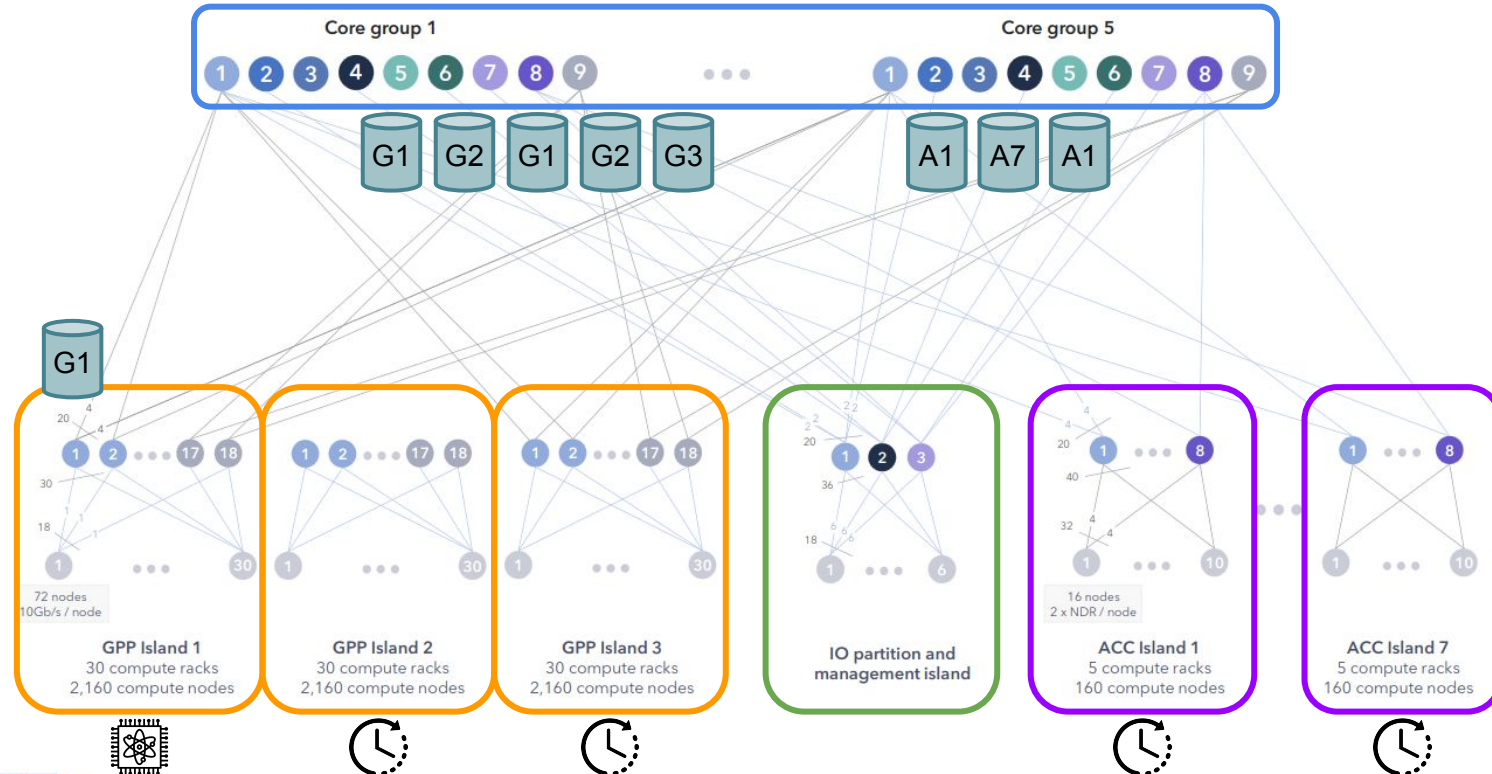
Cycle 5



HPC 101

Operations:   

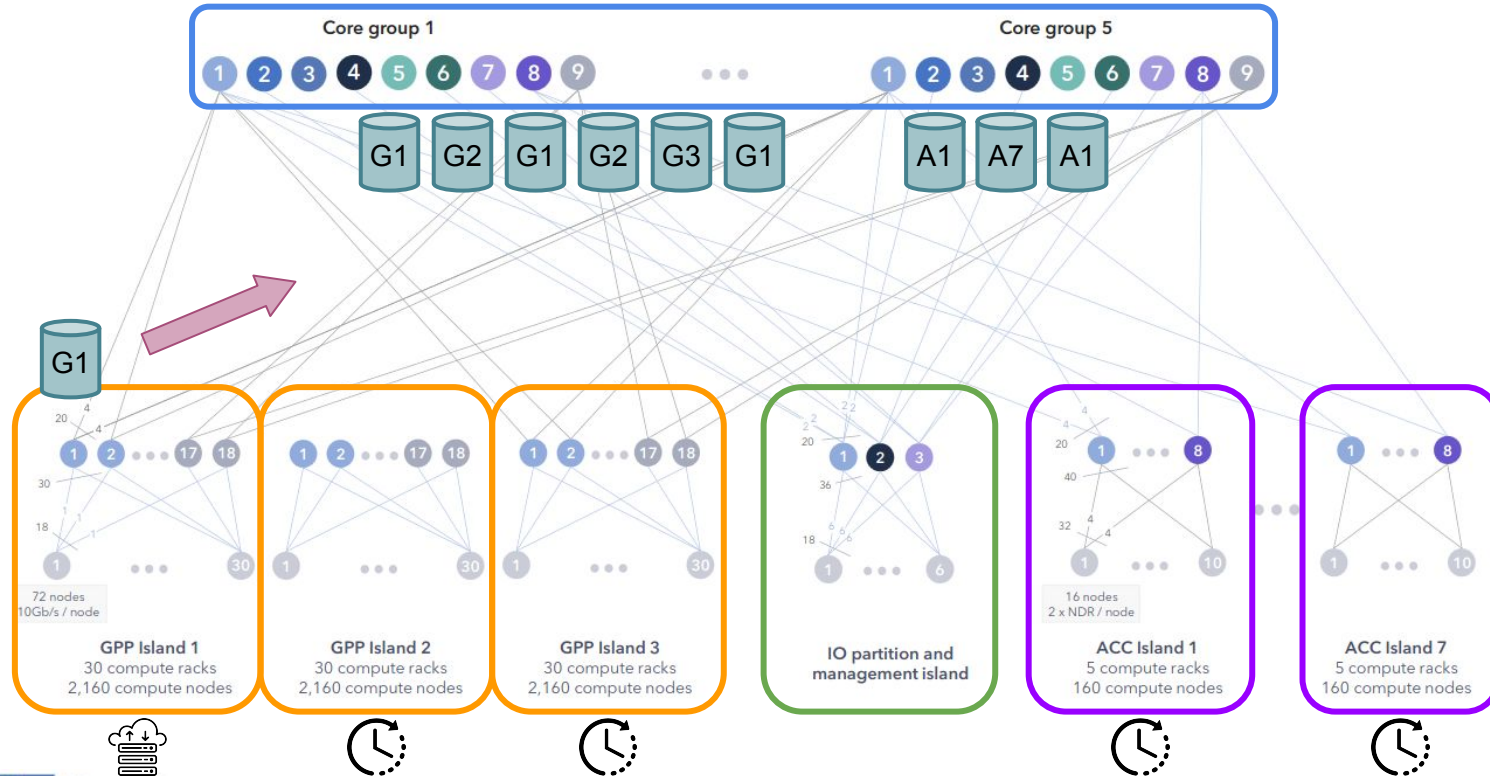
Cycle 5



HPC 101

Operations:   

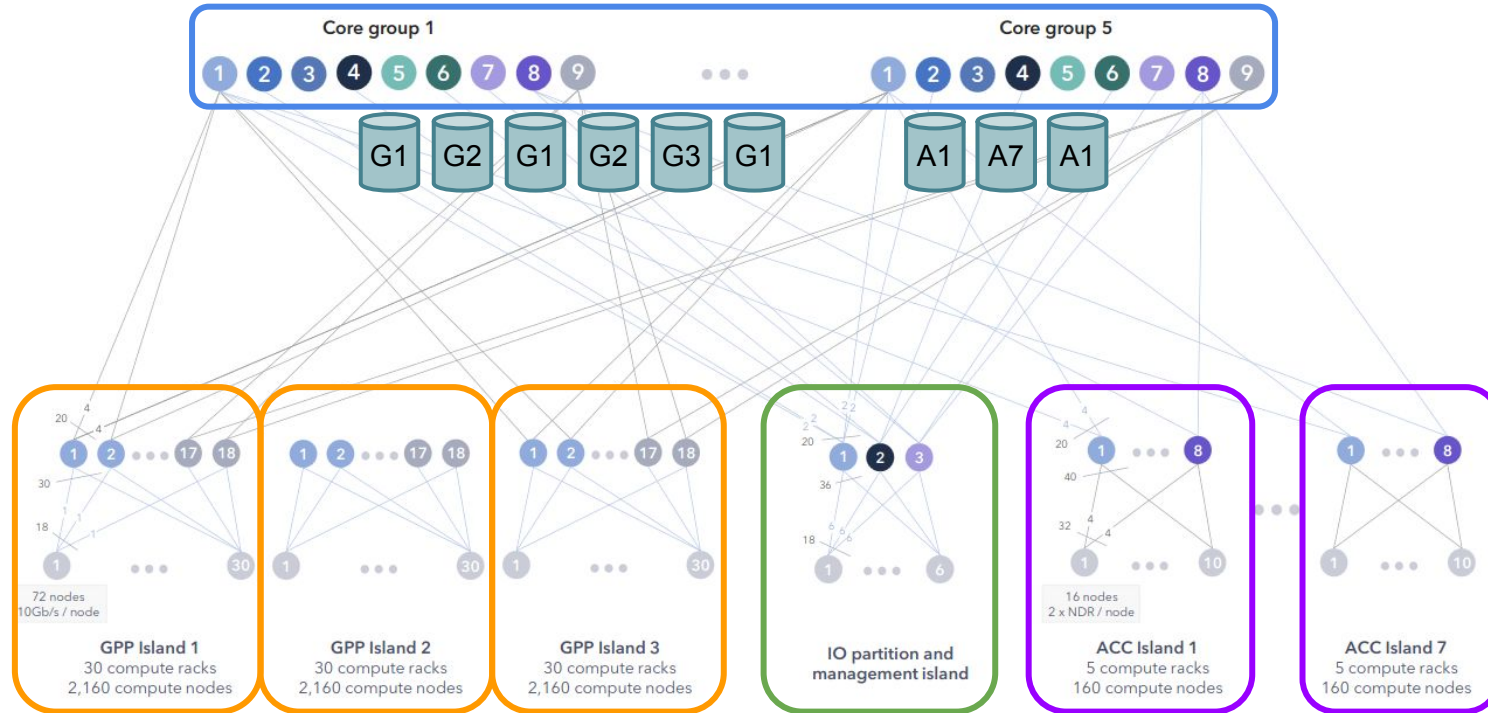
Cycle 6



HPC 101

Operations:   

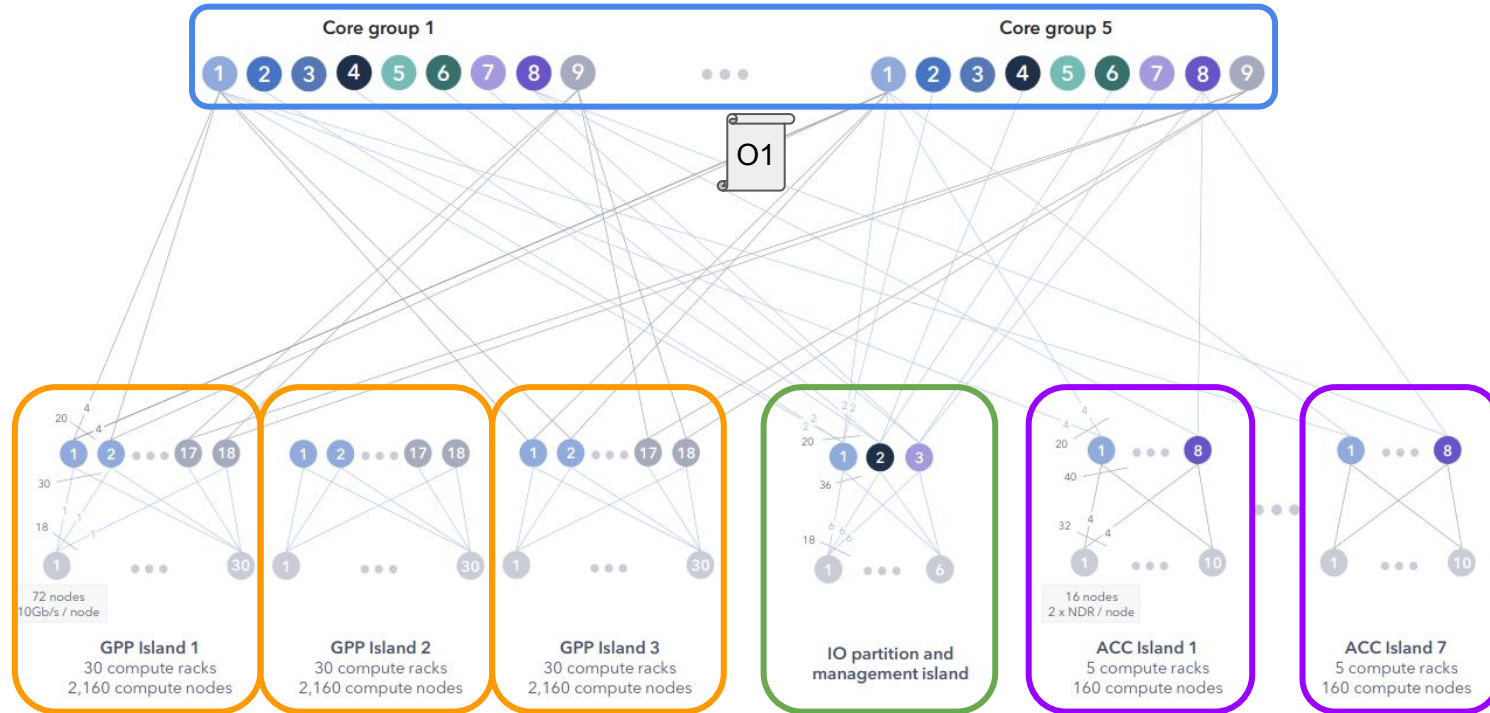
Cycle 6



HPC 101

Operations:   

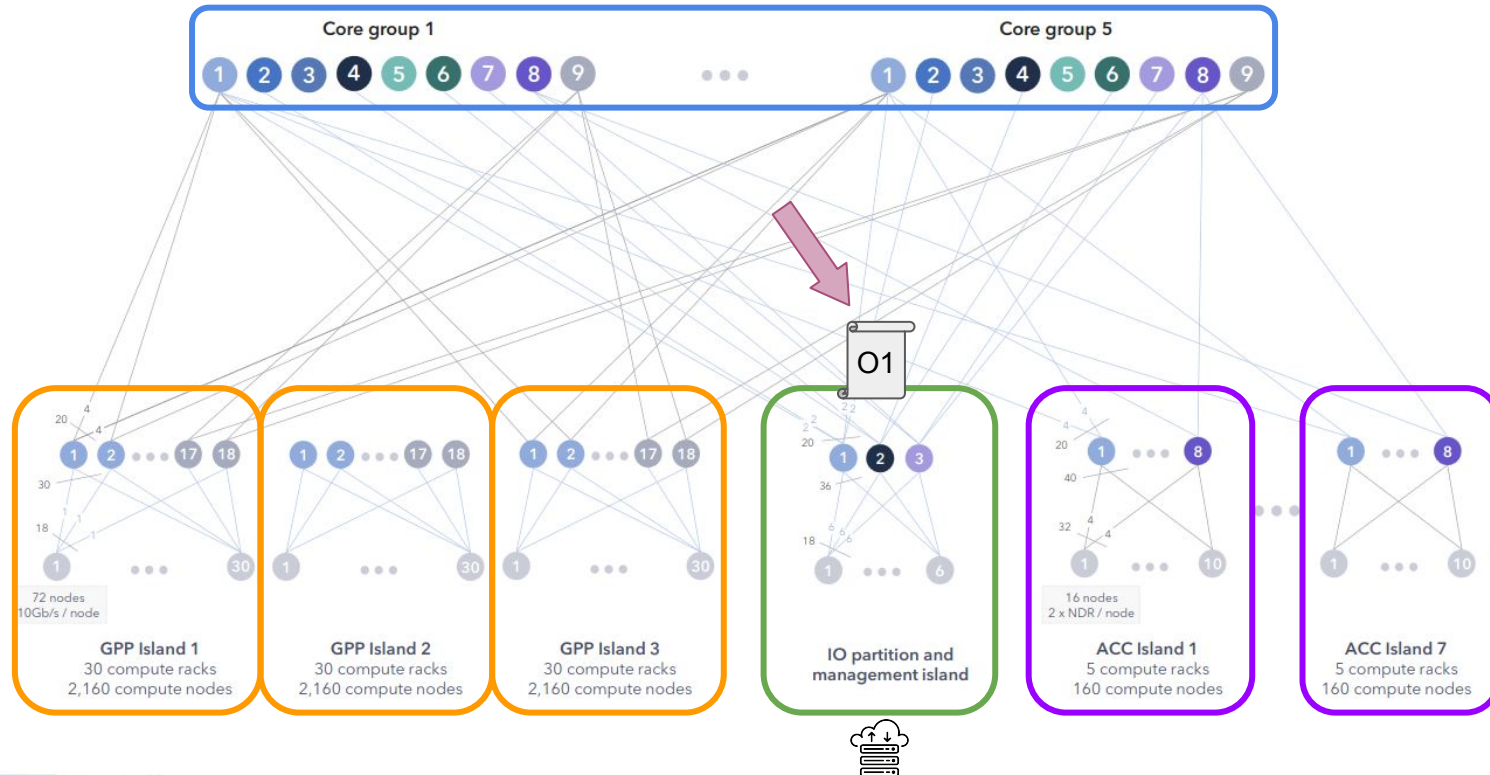
Cycle 7



HPC 101

Operations:   

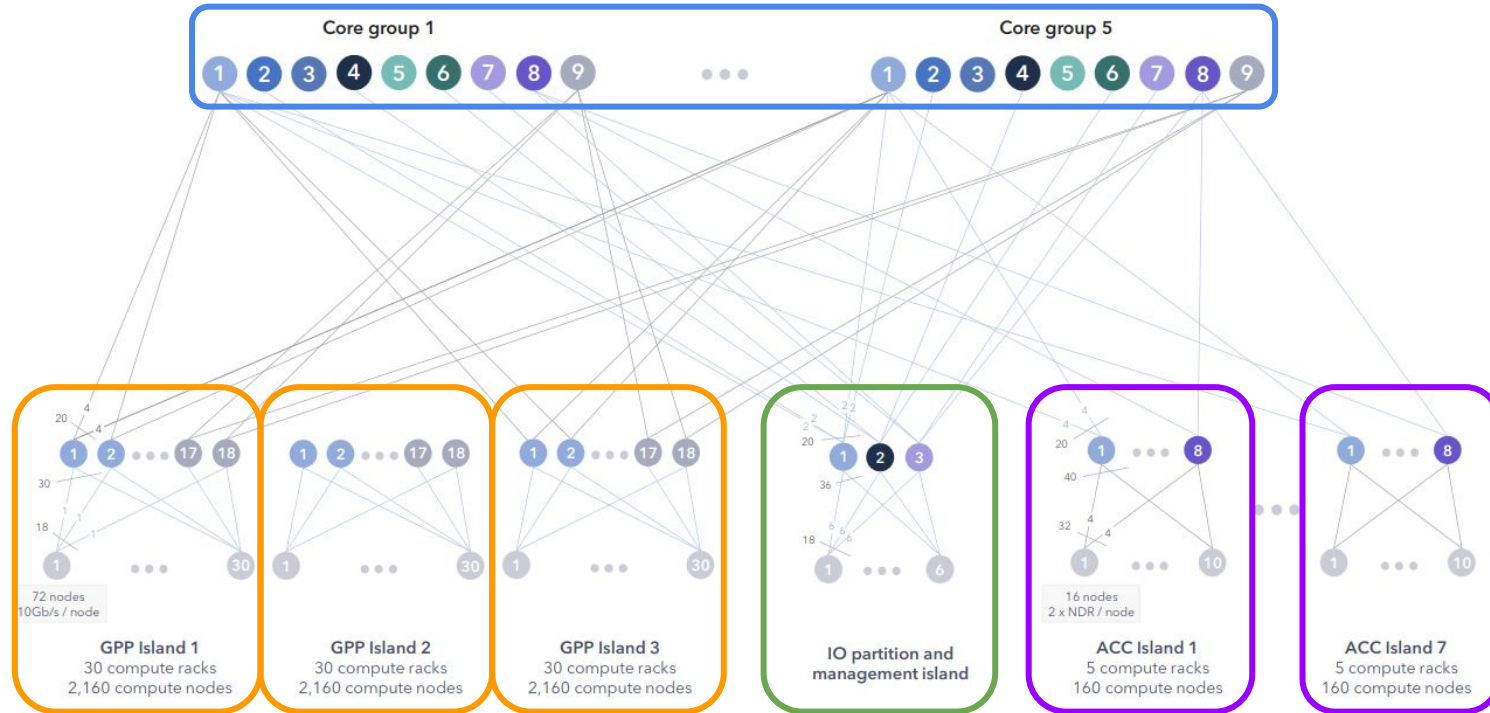
Cycle 8



HPC 101

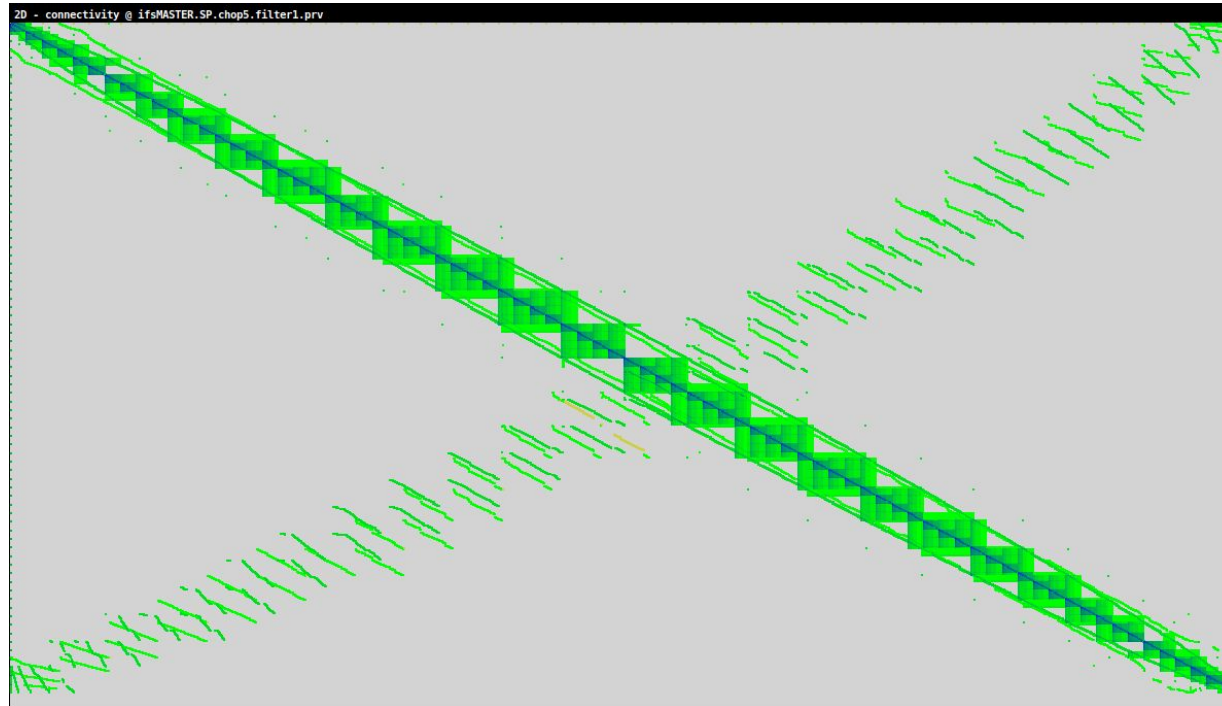
Operations:   

Cycle 9



Performance Profiling

Performance profiling



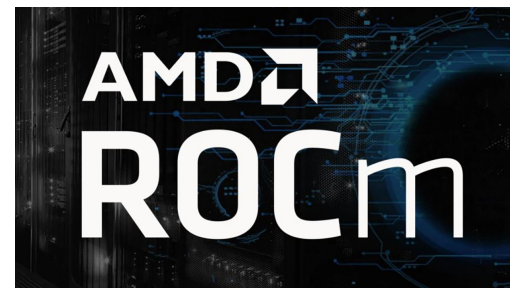
Performance profiling

Tools to use:

Performance profiling

Tools to use:

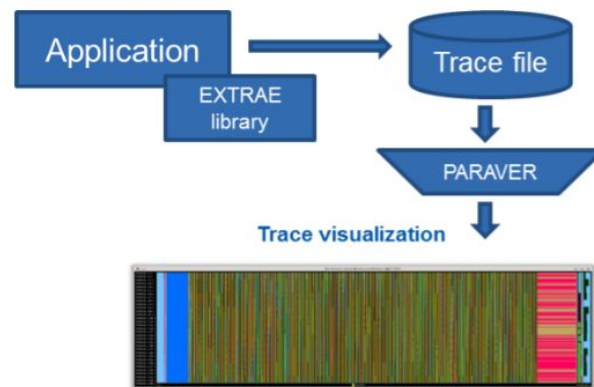
- GPU → Depends on platform!



Performance profiling

Tools to use:

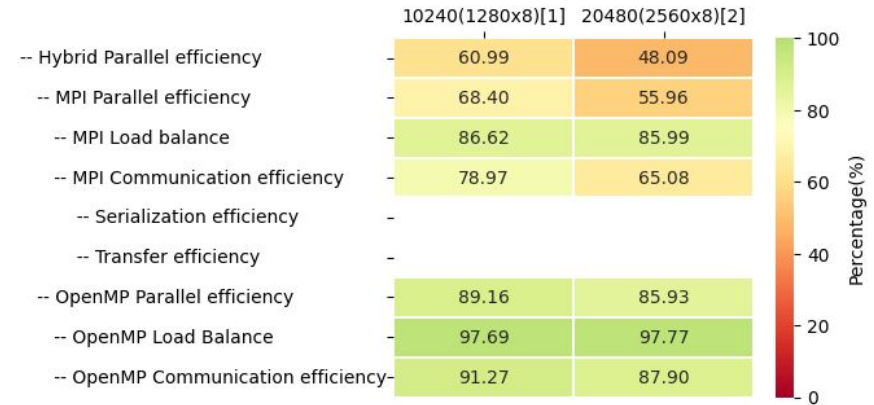
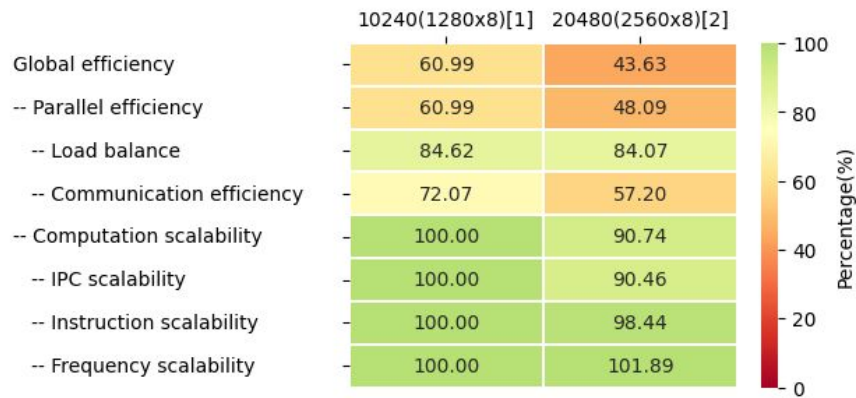
- GPU → Depends on platform!
- CPU → Extrae & Paraver



CPU Profiling



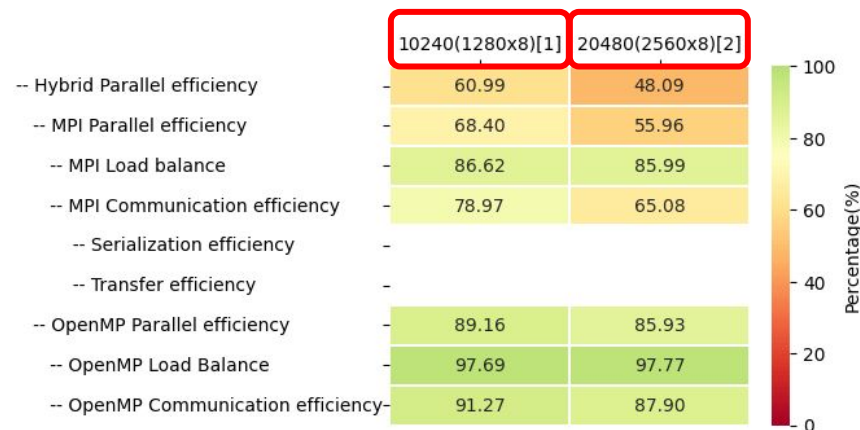
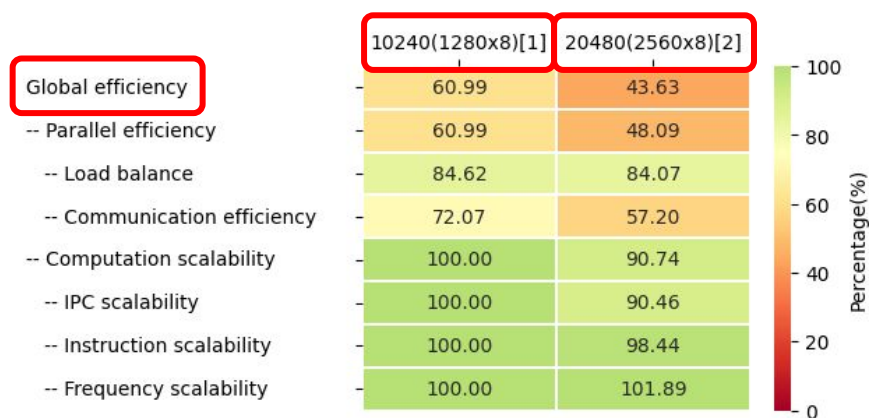
- CPU Model factors



CPU Profiling



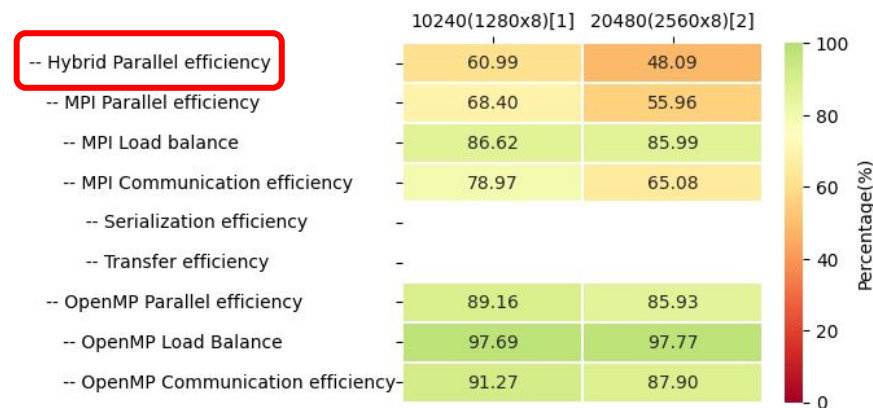
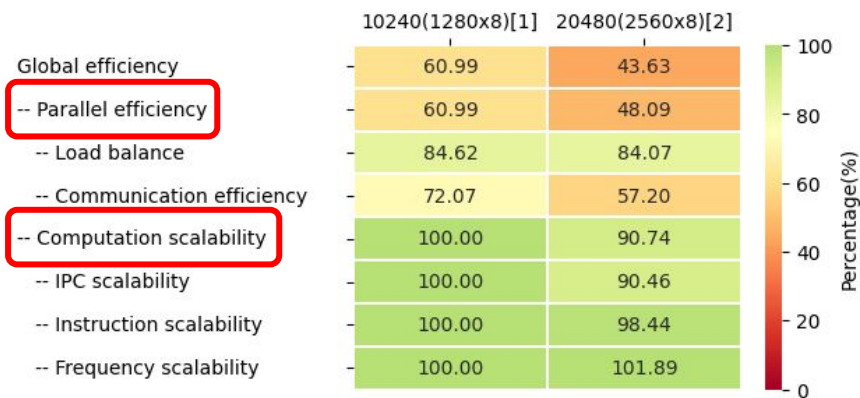
- CPU Model factors



CPU Profiling



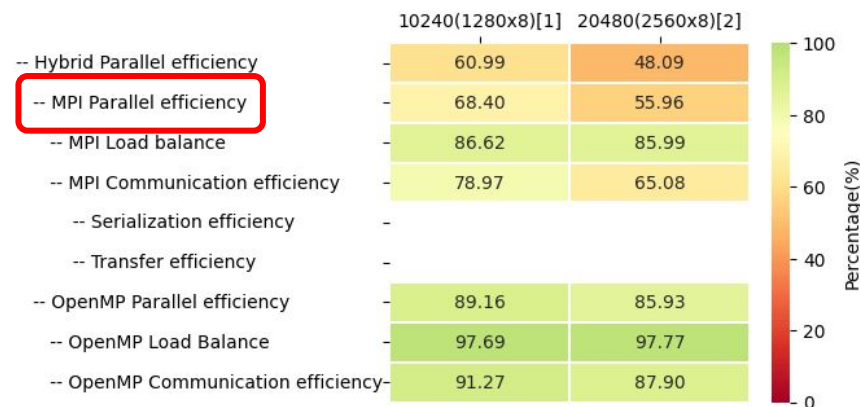
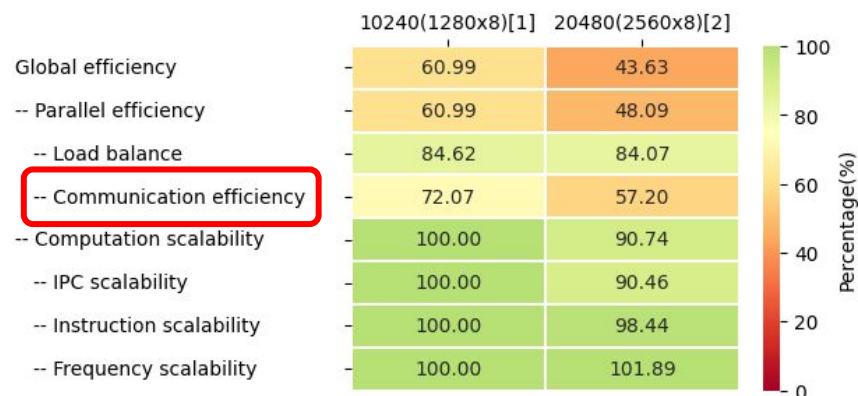
- CPU Model factors



CPU Profiling



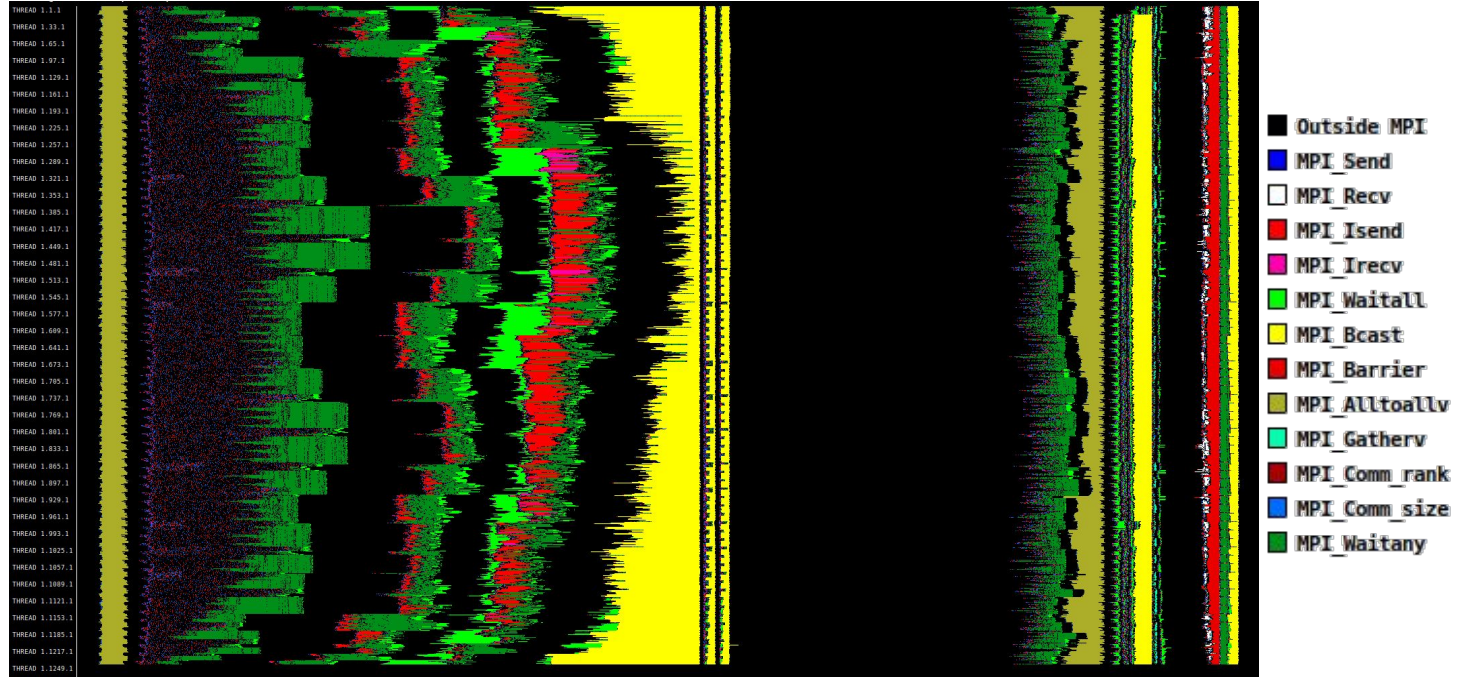
- CPU Model factors



CPU Profiling



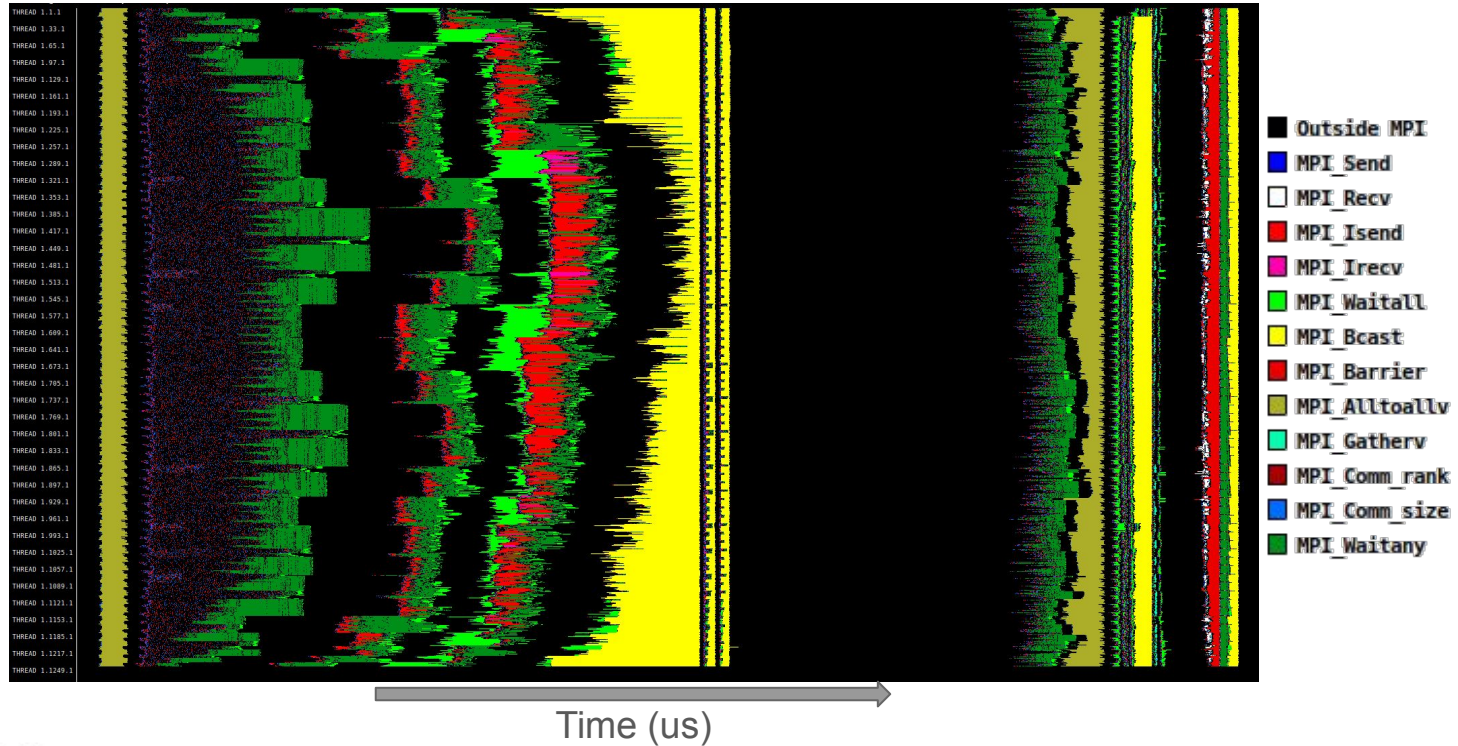
- Extrae
- Paraver



CPU Profiling



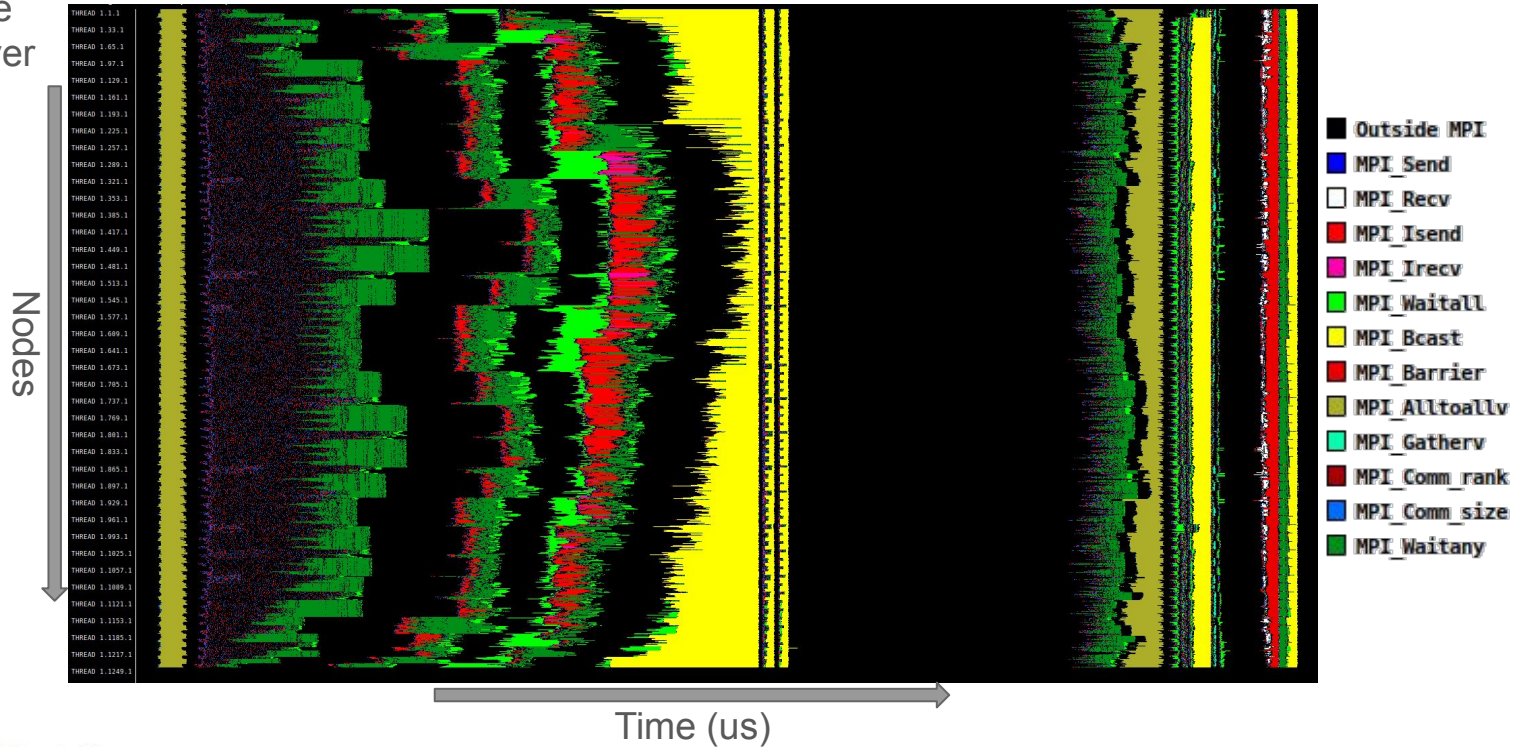
- Extrae
- Paraver



CPU Profiling



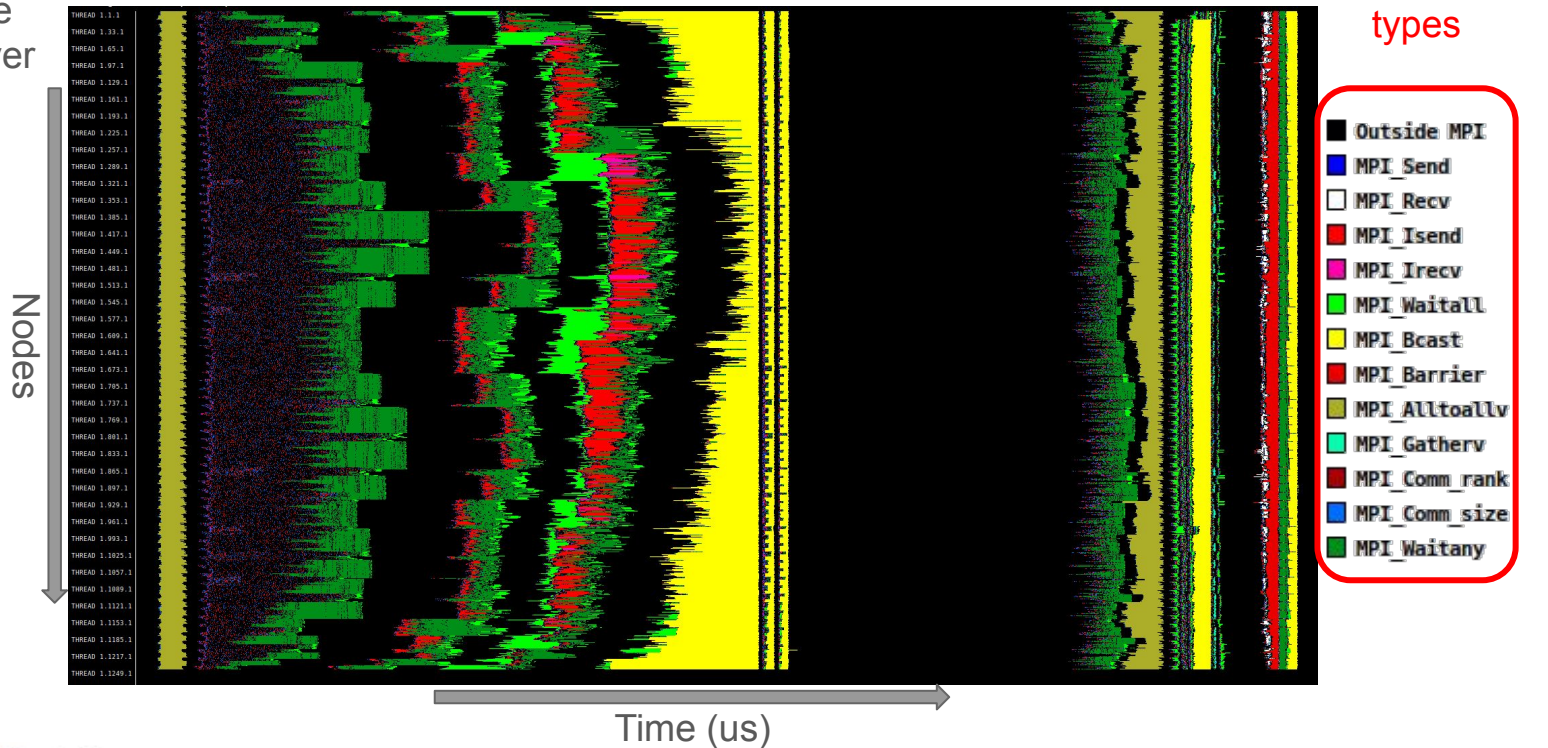
- Extrae
- Paraver



CPU Profiling



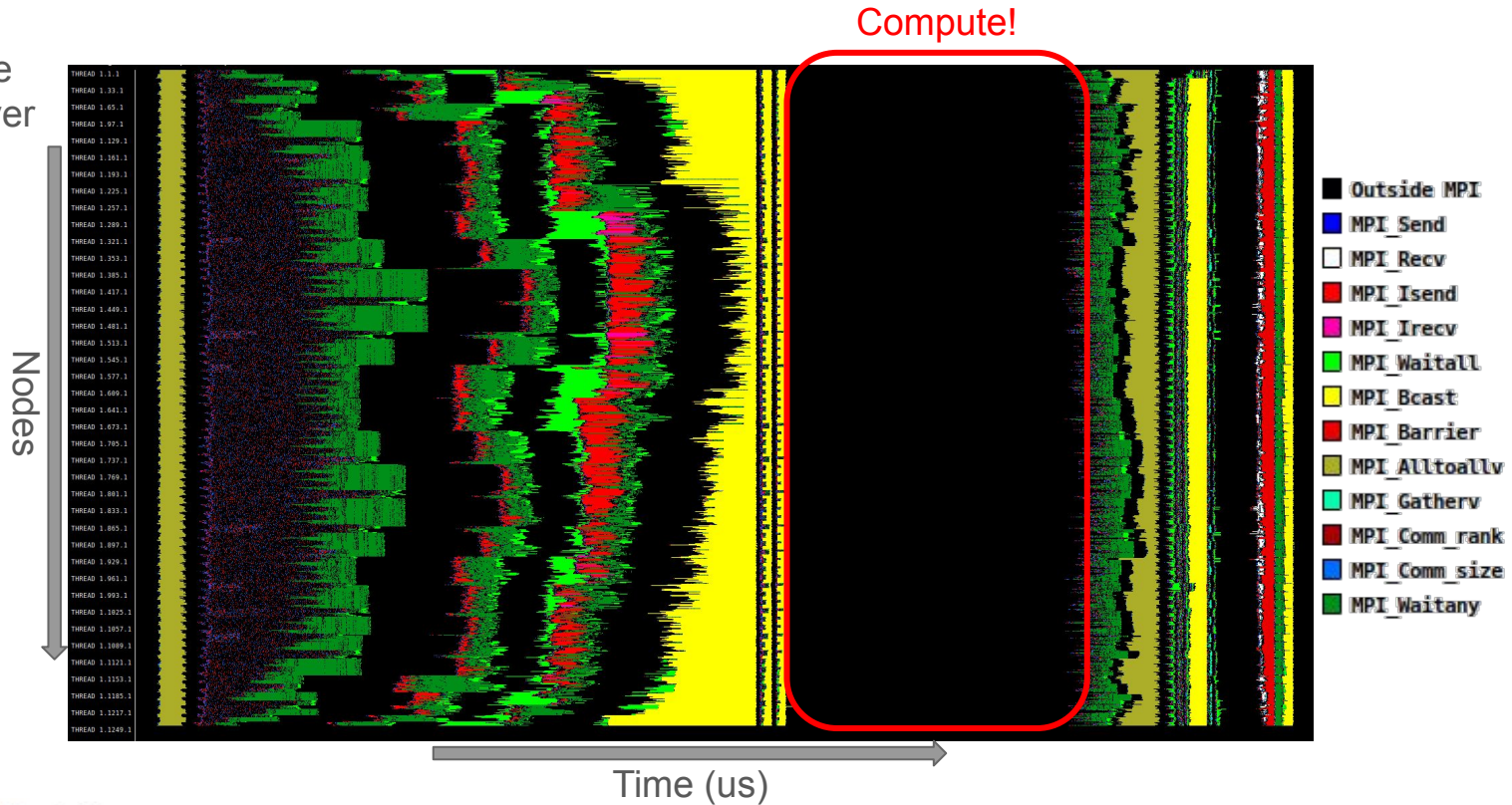
- Extrae
- Paraver



CPU Profiling



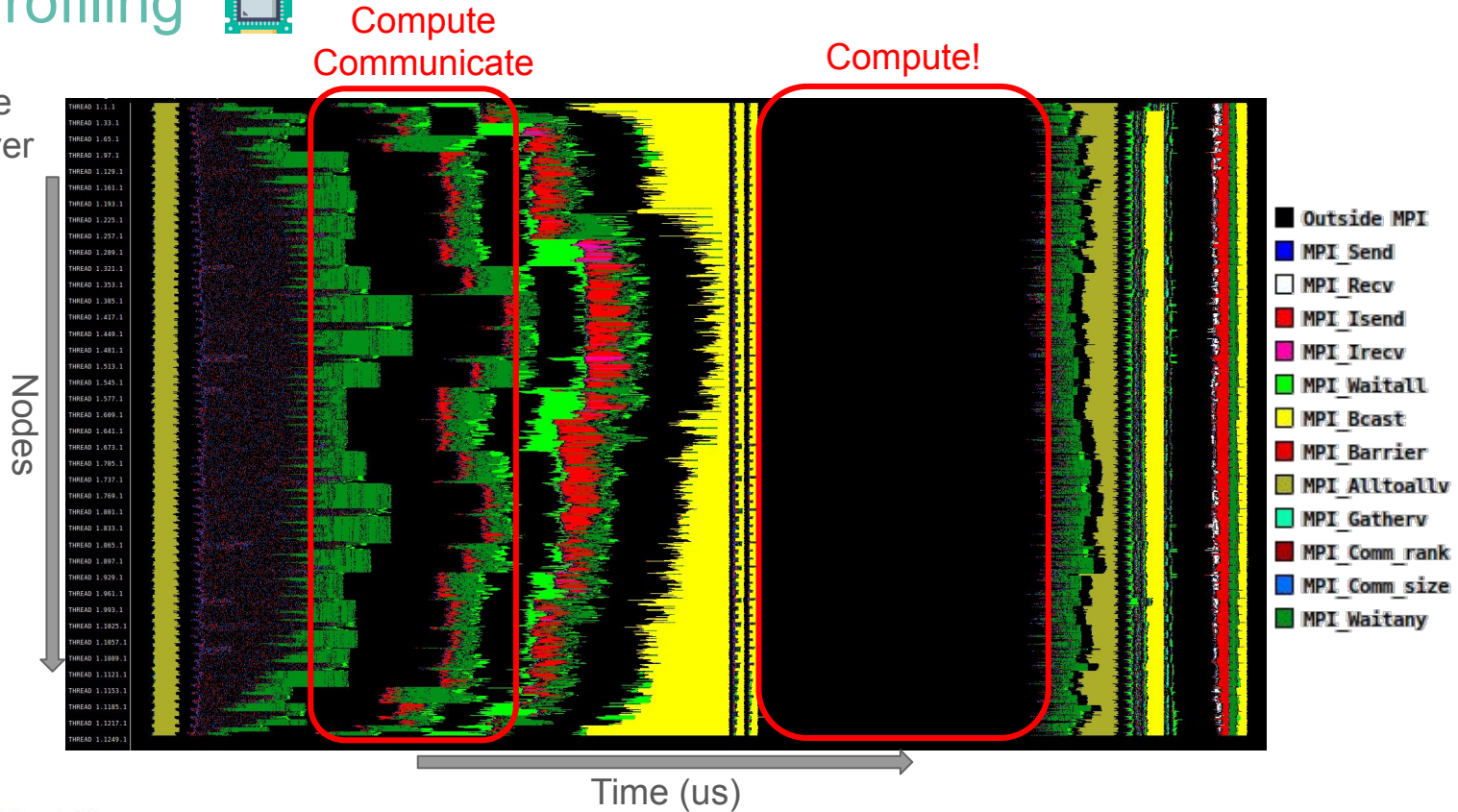
- Extrae
- Paraver



CPU Profiling



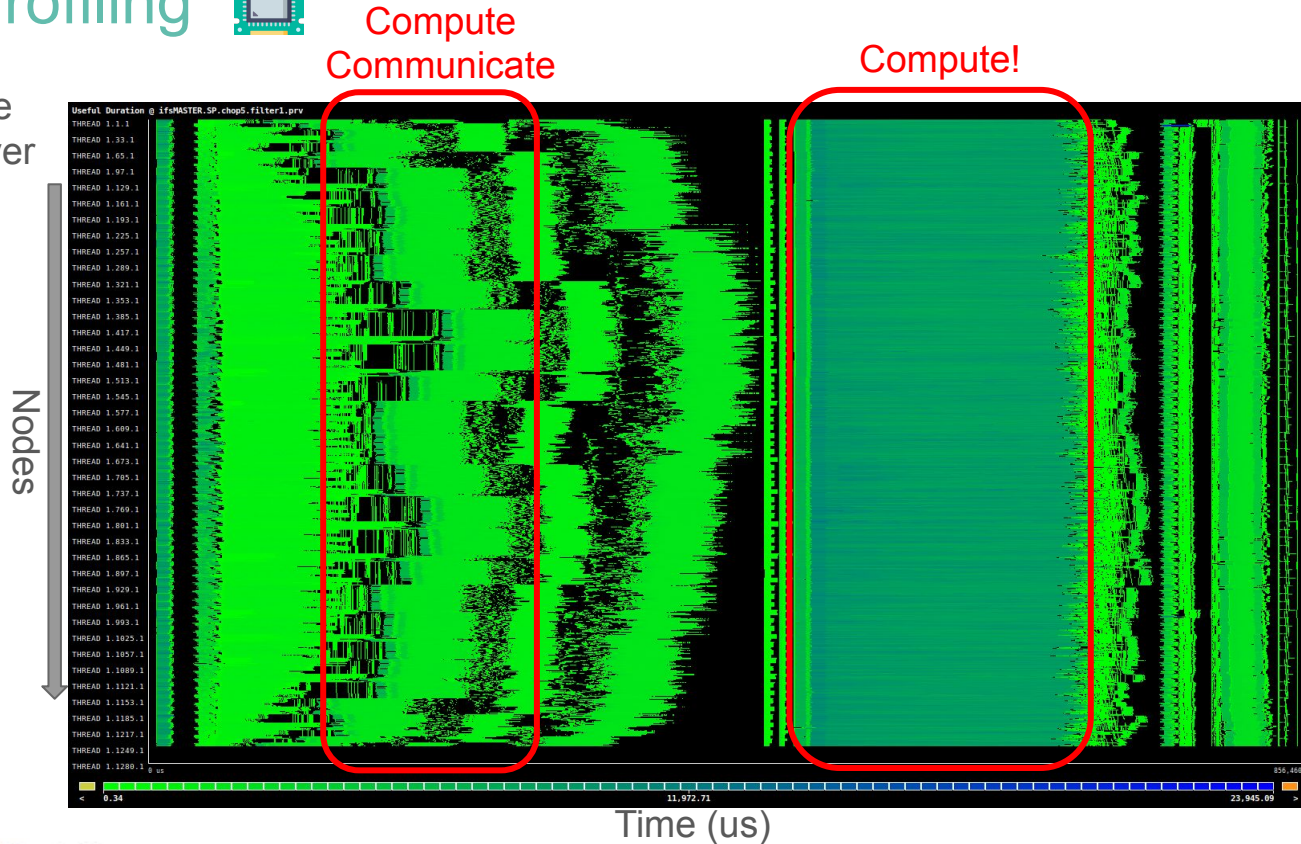
- Extrae
- Paraver



CPU Profiling



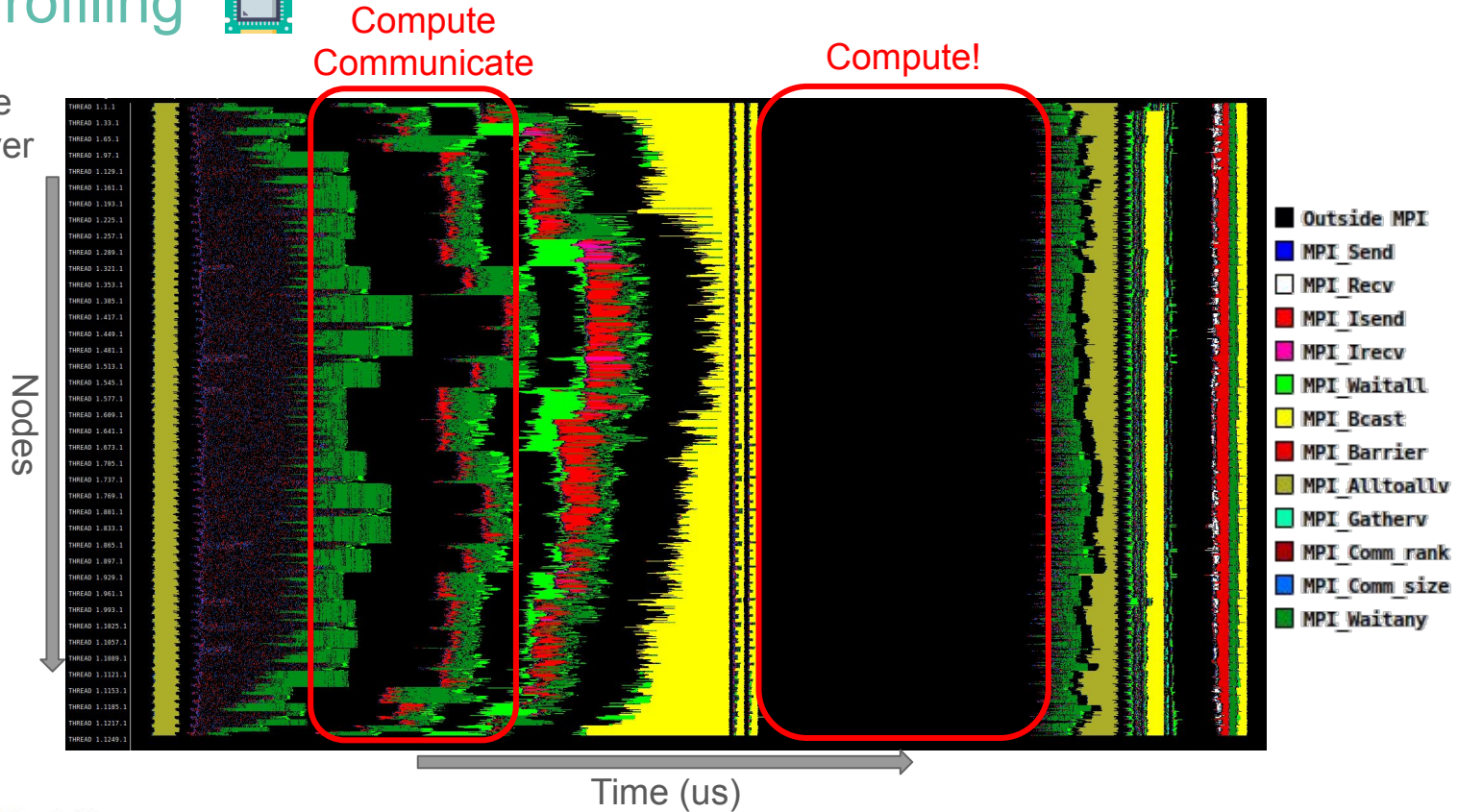
- Extrae
- Paraver



CPU Profiling



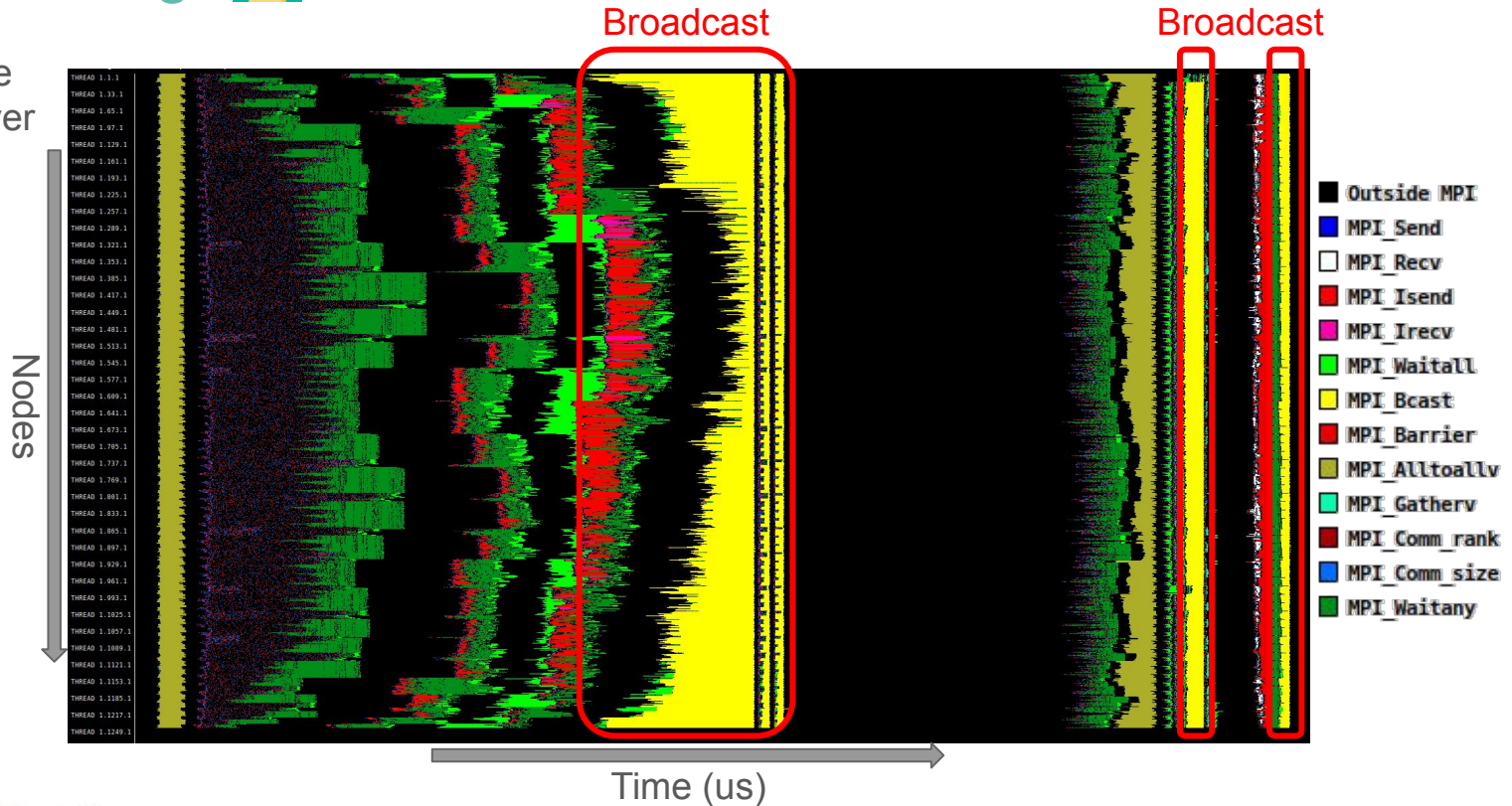
- Extrae
- Paraver



CPU Profiling



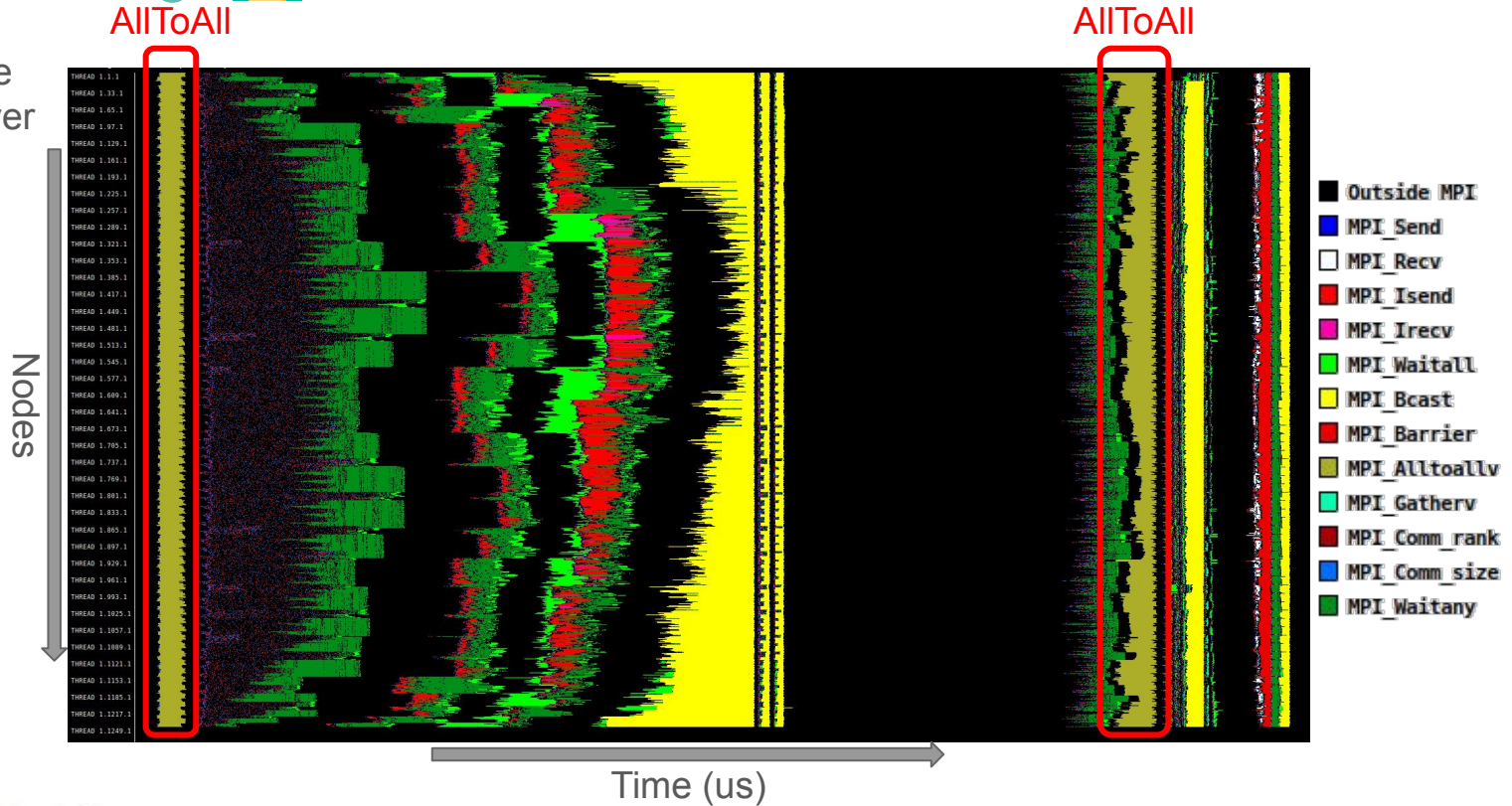
- Extrae
- Paraver



CPU Profiling



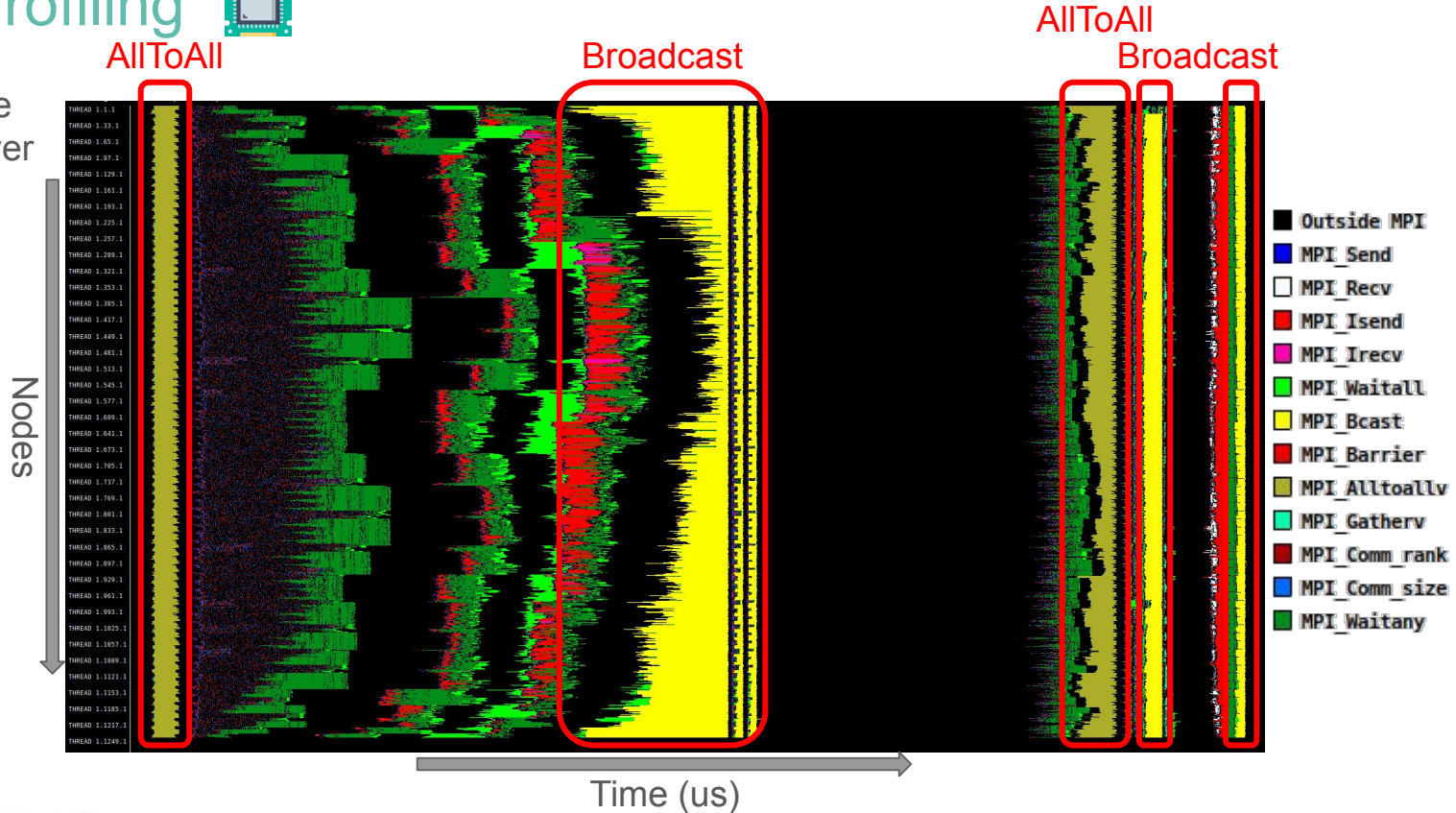
- Extrae
- Paraver



CPU Profiling



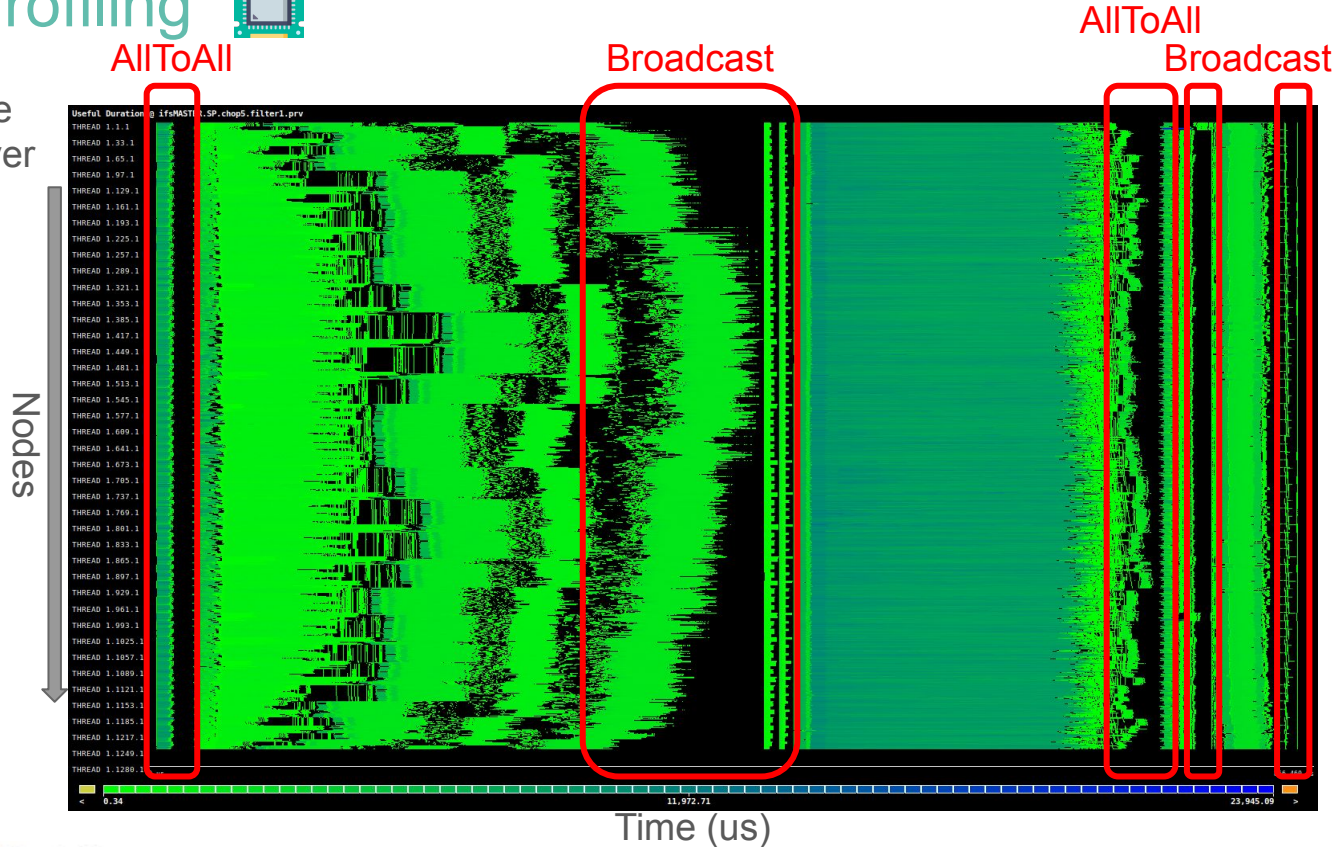
- Extrae
- Paraver



CPU Profiling



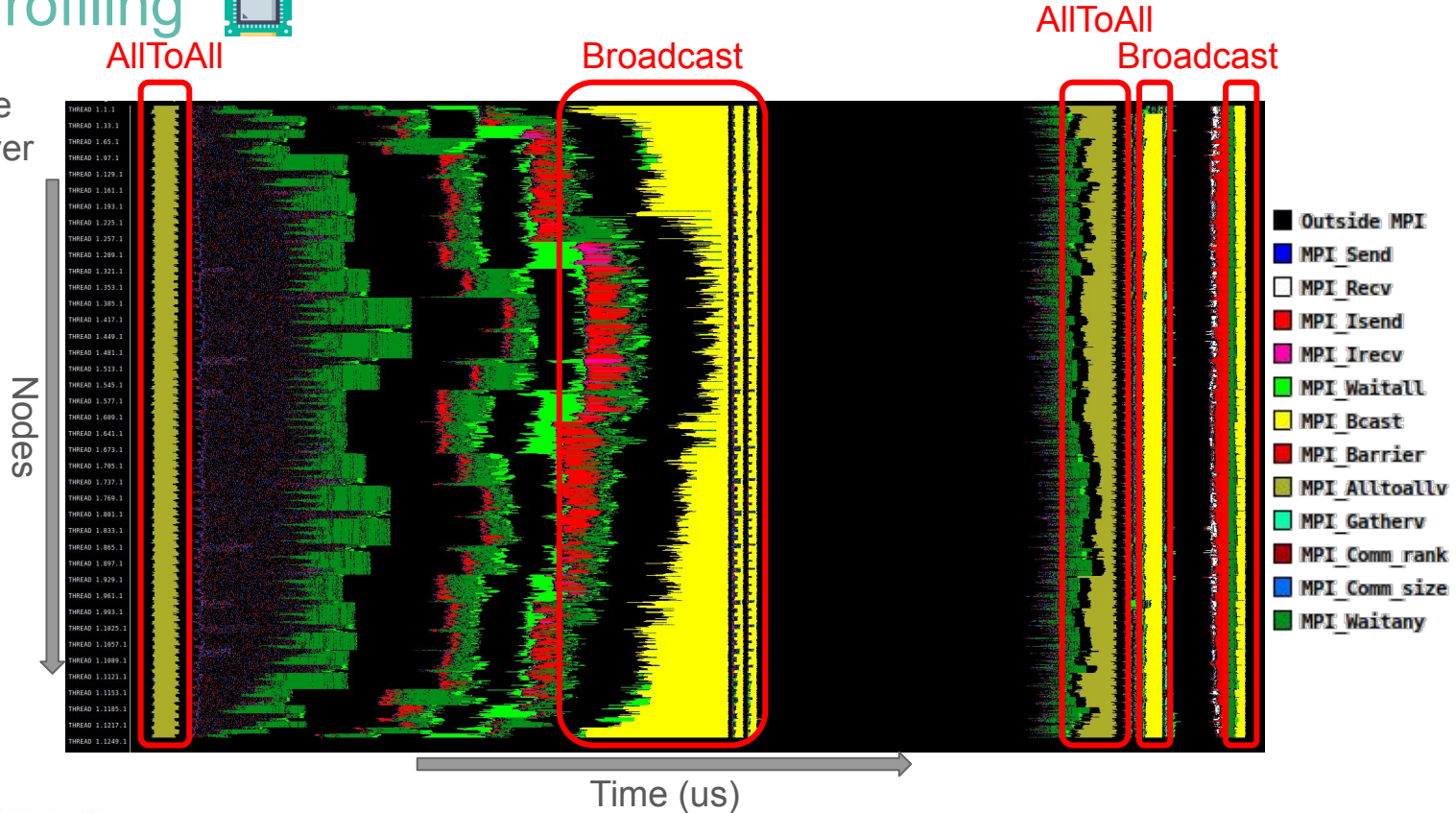
- Extrae
- Paraver



CPU Profiling



- Extrae
- Paraver

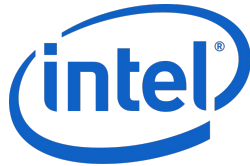


GPU Profiling

Platform matters!

GPU Profiling

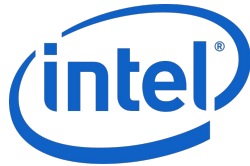
Platform matters!



GPU

GPU Profiling

Platform matters!



GPU

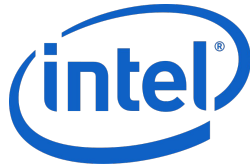


CRAY

Compiler

GPU Profiling

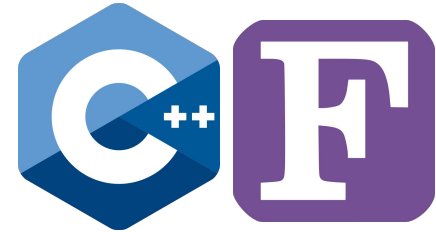
Platform matters!



GPU



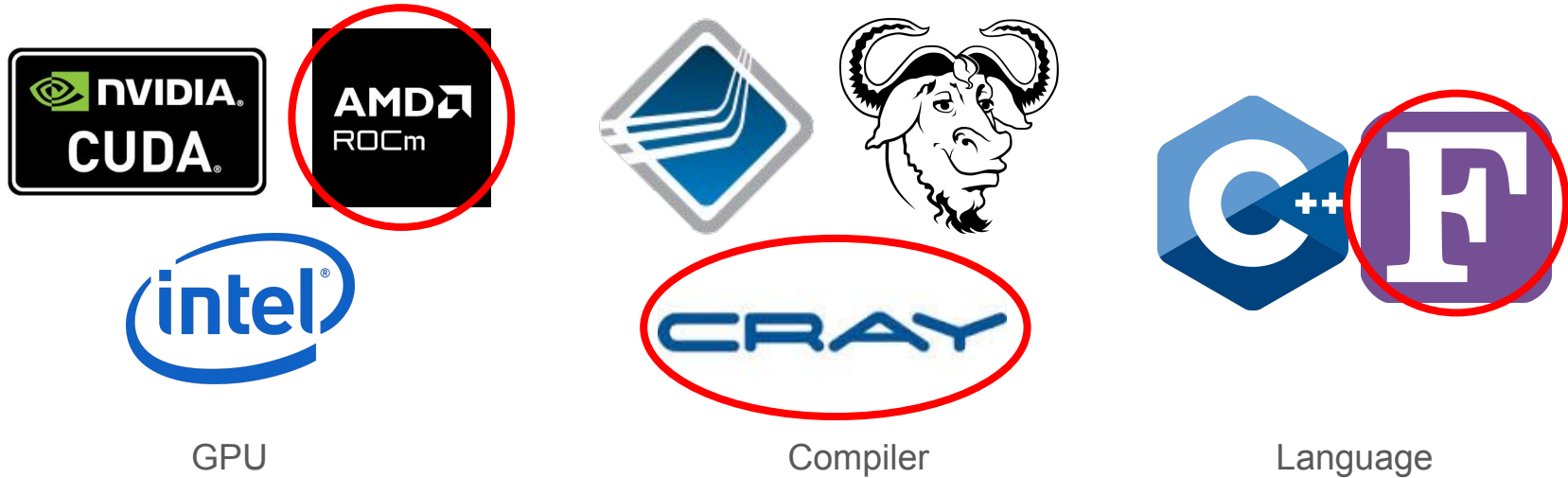
Compiler



Language

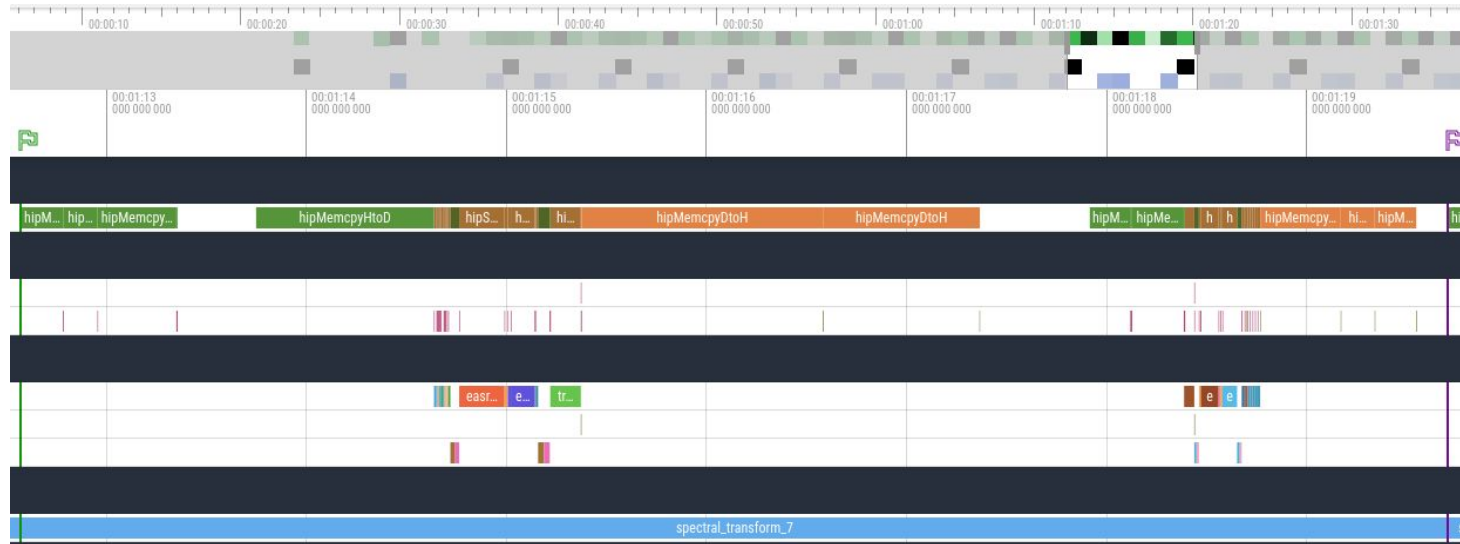
GPU Profiling

Platform matters!



GPU Profiling

```
rocprow --hip-trace --roctx-trace -o ./rocprow/rocprow.csv $BIN
```

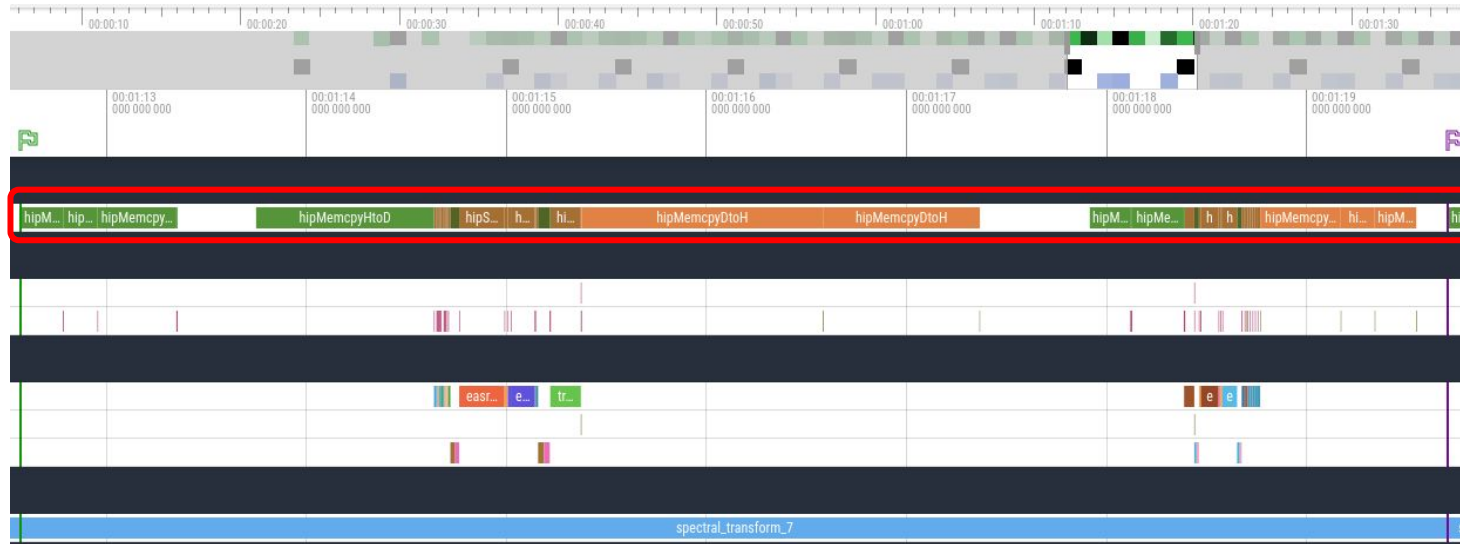


Perfetto visualization

GPU Profiling



```
rocprow --hip-trace --roctx-trace -o ./rocprow/rocprow.csv $BIN
```

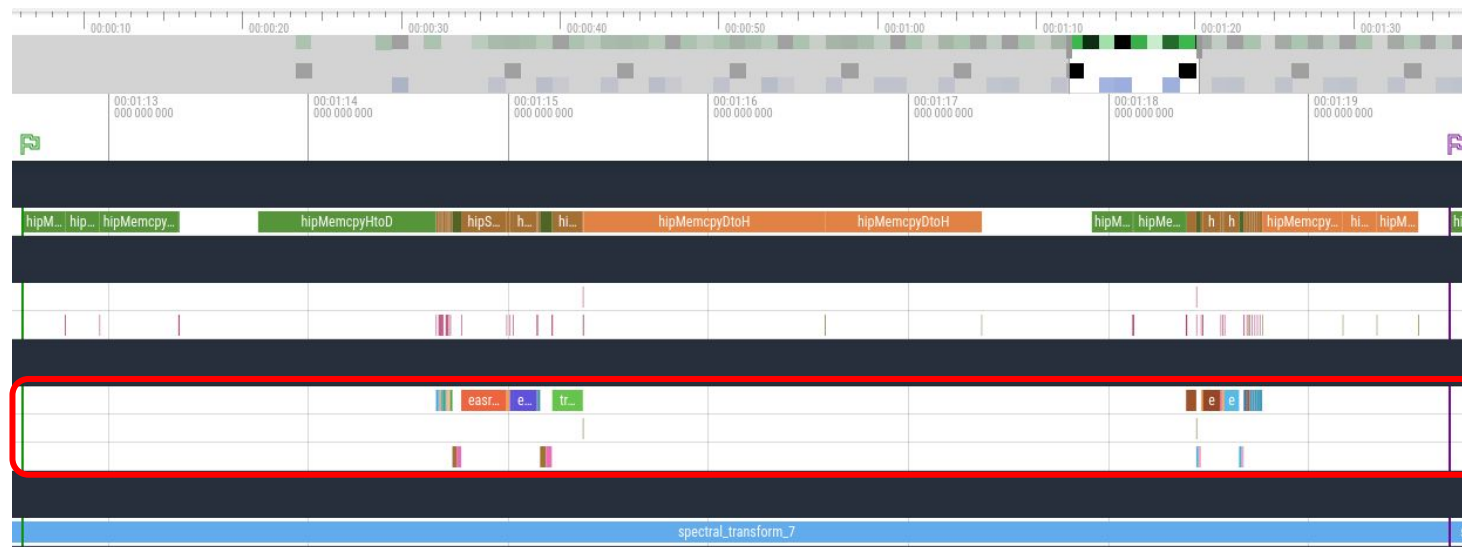


Perfetto visualization

GPU Profiling



```
rocprow --hip-trace --roctx-trace -o ./rocprow/rocprow.csv $BIN
```

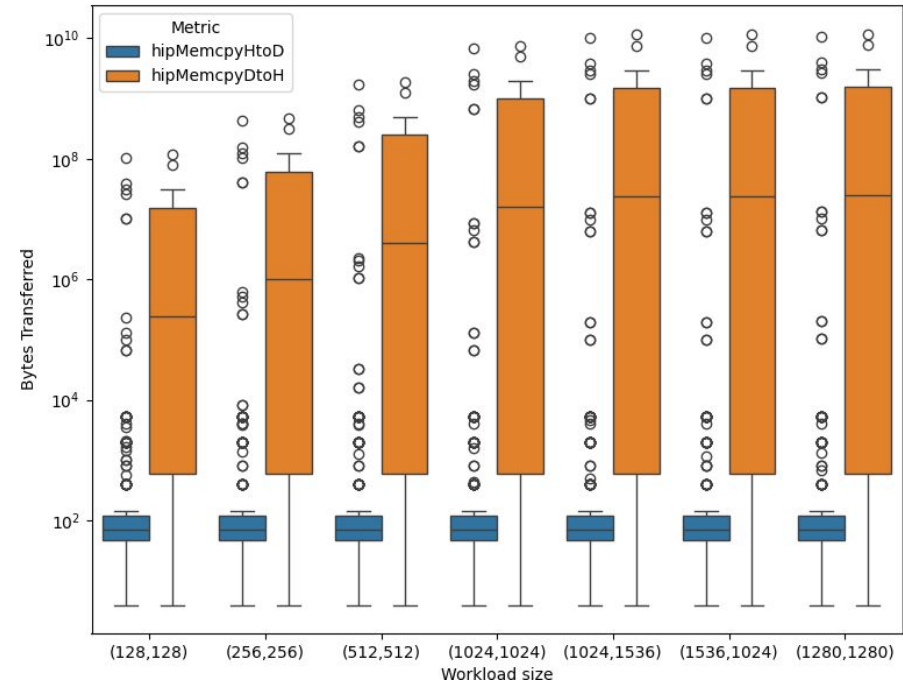


Perfetto visualization

GPU Profiling



GPU Profiling



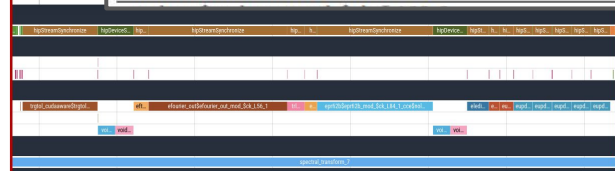
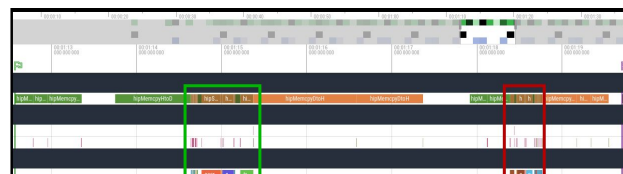
GPU Profiling



Kernel name	Calls	TotalDurationNs	AverageNs	Percentage
casres1b\$casres1b_mod.\$sk.L75.1	10	2 164 195 747	216 419 574	19,8255
trltol_cudaaware\$trltol_mod.\$sk.L559.4	10	1 531 345 585	153 134 558	14,0282
efourier_in\$efourier_in_mod.\$sk.L61.2.cce\$noloop\$form	10	1 198 170 052	119 817 005	10,9760
efourier_out\$efourier_out_mod.\$sk.L56.1	10	875 120 791	87 512 079	8,0167
epfr1b\$epfr1b_mod.\$sk.L84.1.cce\$noloop\$form	10	740 841 358	74 084 135	6,7866
eupdspb\$eupdspb_mod.\$sk.L86.1	60	612 827 387	10 213 789	5,6139
void real_pre_process_kernel<...>(...)	20	513 296 858	25 664 842	4,7021
trgtol_cudaaware\$trgtol_mod.\$sk.L563.3	10	479 085 073	47 908 507	4,3887
epfr1b\$epfr1b_mod.\$sk.L90.2	60	299 659 753	4 994 329	2,7451
void ip_inverse_length768_SBRR<...>(...)	10	282 009 617	28 200 961	2,5834
void real_post_process_kernel.interleaved_1D<...>(...)	20	226 225 138	11 311 256	2,0724
void ip_inverse_length512_SBRR<...>(...)	10	216 095 188	21 609 518	1,9796
trmtol_cudaaware\$trmtol_mod.\$sk.L205.1	10	178 045 797	17 804 579	1,6310
evdtuv\$evdtuv_mod.\$sk.L132.2	10	149 741 079	14 974 107	1,3717
efourier_in\$efourier_in_mod.\$sk.L58.3.cce\$noloop\$form	10	148 382 992	14 838 299	1,3593
eledir\$eledir_mod.\$sk.L98.1	10	139 369 528	13 936 952	1,2767
espsnde\$espsnde_mod.\$sk.L87.1	10	115 237 936	11 523 793	1,0557
eltinv\$eltinv_mod.\$sk.L136.2.cce\$noloop\$form	10	113 872 491	11 387 249	1,0431
trltom_cudaaware\$trltom_mod.\$sk.L218.1	10	110 770 720	11 077 072	1,0147
void ip_forward_length768_SBRR<...>(...)	10	110 712 645	11 071 264	1,0142
void ip_forward_length512_SBRR<...>(...)	10	110 086 079	11 008 607	1,0085
efdir\$efdir_mod.\$sk.L89.2.cce\$noloop\$form	10	94 305 395	9 430 539	0,8639
efsc\$efsc_mod.\$sk.L97.2	10	89 873 545	8 987 354	0,8233
evutvd\$evutvd_mod.\$sk.L108.2	10	85 680 570	8 568 057	0,7849
evutvd\$evutvd_mod.\$sk.L89.1	10	68 517 640	6 851 764	0,6277
evdtuv\$evdtuv_mod.\$sk.L113.1	10	66 336 511	6 633 651	0,6077
efsc\$efsc_mod.\$sk.L75.1	10	58 245 610	5 824 561	0,5336
epfr1b\$epfr1b_mod.\$sk.L85.3.cce\$noloop\$form	60	57 399 205	956 653	0,5258
eltdir\$eltdir_mod.\$sk.L157.3.cce\$noloop\$form	10	57 060 646	5 706 064	0,5227
eltdir\$eltdir_mod.\$sk.L156.2.cce\$noloop\$form	10	22 749 187	2 274 918	0,2084
<barrier packet>	20	753 461	37 673	0,0070
evdtuv\$evdtuv_mod.\$sk.L170.4	10	97 760	9 776	0,009
evutvd\$comm\$evutvd\$comm_mod.\$sk.L106.2.cce\$noloop\$form	10	63 681	6 368	0,0006
trgtol_cudaaware\$trgtol_mod.\$sk.L456.8	10	32 960	3 296	0,0003
trgtol_cudaaware\$trgtol_mod.\$sk.L457.9	10	23 040	2 304	0,0002

Table 8: Global overview of the eTrans kernels for 10 iterations. The blue highlighted rows are the 6 user kernels which are analysed. The green highlighted rows have a smaller kernel granularity. The yellow highlighted rows are library calls.

GPU Profiling



Kernel name	Calls	TotalDurationNs	AverageNs	Percentage
casre1b\$casre1b_mod.\$ck.L75.1	10	2 164 195 747	216 419 574	19,8255
trltog.cudaaware\$trltog_mod.\$ck.L559.4	10	1 531 345 585	153 134 558	14,0282
efourier_in\$efourier_in_mod.\$ck.L61.2.cce\$noloop\$form	10	1 198 170 052	119 817 005	10,9760
efourier_out\$efourier_out_mod.\$ck.L56.1	10	875 120 791	87 512 079	8,0167
epfrf2b\$epfrf2b_mod.\$ck.L84.1.cce\$noloop\$form	10	740 841 358	74 084 135	6,7866
eupdspb\$eupdspb_mod.\$ck.L86.1	60	612 827 387	10 213 789	5,6139
void real_pre_process_kernel<...>(...)	20	513 296 858	25 664 842	4,7021
trgtol.cudaaware\$trgtol_mod.\$ck.L563.3	10	479 085 073	47 908 507	4,3887
			1 994 329	2,7451
			8 200 961	2,5834
			1 311 256	2,0724
			1 609 518	1,9796
			7 804 579	1,6310
			4 974 107	1,3717
			4 838 299	1,3593
			3 936 952	1,2767
			1 523 793	1,0557
			1 387 249	1,0431
			1 077 072	1,0147
			1 071 264	1,0142
			1 008 607	1,0085
			9 430 539	0,8639
			9 987 354	0,8233
			5 568 057	0,7849
			6 851 764	0,6277
			6 633 651	0,6077
			6 824 561	0,5336
			956 653	0,5258
			7 606 064	0,5227
			2 274 918	0,2084
				0,0070
				0,009
				0,0006
				0,0003
				0,0002

Table 8: Global overview of the ecTrans kernels for 10 iterations. The blue highlighted rows are the 6 user kernels which are analysed. The green highlighted rows have a smaller kernel granularity. The yellow highlighted rows are library calls.

GPU Profiling



```
rocprof -i rocprof_counters.txt -o ./rocprof/rocprof.csv $BIN
```

Index,KernelName,gpu-id,queue-id,queue-index,pid,tid,grd,wgr,lds,scr,vgpr,sgpr,fbar,sig,obj,GPUBusy,Wavefronts,VALUInsts,VFetchInsts,VWriteInsts,VALUUtilization,VALUBusy,WriteSize,L2CacheHit,MemUnitBusy,MemUnitStalled,LDSBankConflict

```
0,"eltinv$eltinv_mod_$ck_L136_2_cce$no-loop$form.kd"0,0,0,26071,26071,1579087872,256,0,0,4,48,33664,0x0,0x14b05013c040,100.0000000000,24673248.0000000000,17.0000000000,0.0000000000,0.0000000000,100.0000000000,20.7725185968,12332528.0000000000,49.9978626693,77.1977044758,55.9370012636,0.0000000000
1,"eprfilb$eprfilb_mod_$ck_L85_3_cce$no-loop$form.kd"0,0,2,26071,26071,157593600,256,0,0,4,72,38592,0x0,0x14b05013c100,100.0000000000,2462400.0000000000,20.0000000000,0.0000000000,0.0000000000,100.0000000000,24.2834884261,1227104.0000000000,49.9996649935,71.7003018579,49.2693704348,0.0000000000
2,"eprfilb$eprfilb_mod_$ck_L90_2.kd"0,0,4,26071,26071,56320,256,0,0,24,80,37696,0x0,0x14b05013c080,100.0000000000,0,880.0000000000,111907.6136363636,0.0000000000,0.0000000000,96.8019501699,9.6155911525,1008455.6562500000,81.3899031130,60.5181117611,43.6472872603,0.0000000000
3,"eprfilb$eprfilb_mod_$ck_L85_3_cce$no-loop$form.kd"0,0,6,26071,26071,157593600,256,0,0,4,72,38592,0x0,0x14b0...
```

GPU Profiling



```
rocprof -i rocprof_counters.txt -o ./rocprof/rocprof.csv $BIN
```

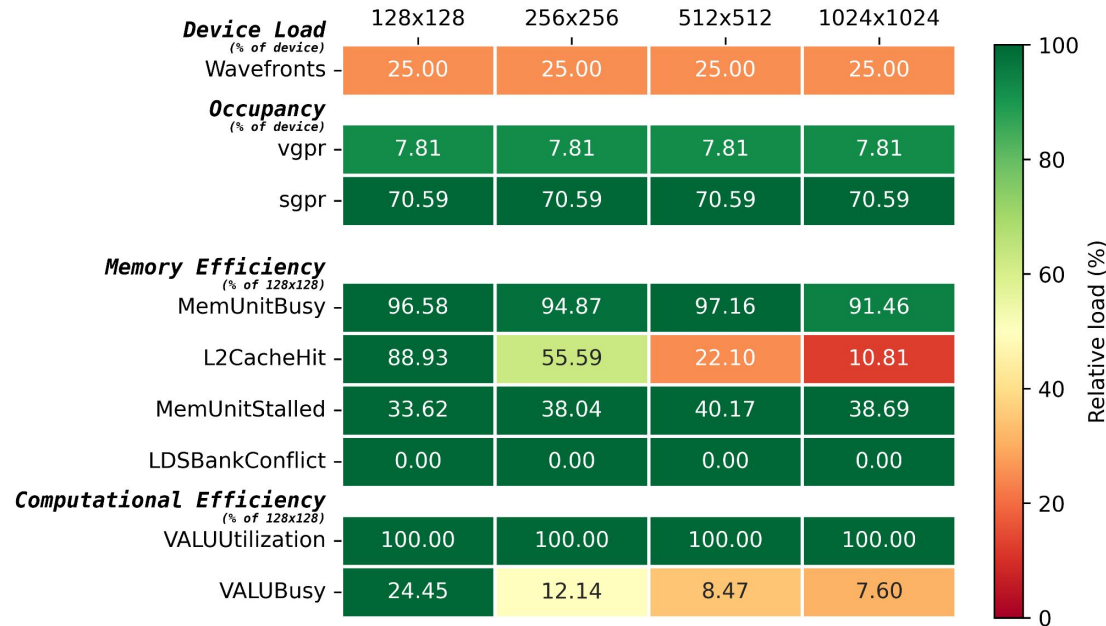
```
Index,KernelName,gpu-id,queue-id,queue-index,pid,tid,grd,wgr,lds,scr,vgpr,sgpr,fbar,sig,obj,GPUBusy,Wavefronts,VA  
LUInsts,VFetchInsts,VWriteInsts,VALUUtilization,VALUBusy,WriteSize,L2CacheHit,MemUnitBusy,MemUnitStalled,LDSBankC  
onflict
```

```
0,"eltinv$eltinv_mod_$ck_L136_2_cce$no-loop$form.kd"0,0,0,26071,26071,1579087872,256,0,0,4,48,33664,0x0,0x14b0501  
3c040,100.0000000000,24673248.0000000000,17.0000000000,0.0000000000,0.0000000000,100.0000000000,20.7725185968,123  
32528.0000000000,49.9978626693,77.1977044758,55.9370012636,0.0000000000  
1,"eprfilb$eprfilb_mod_$ck_L85_3_cce$no-loop$form.kd"0,0,2,26071,26071,157593600,256,0,0,4,72,38592,0x0,0x14b0501  
3c100,100.0000000000,2462400.0000000000,20.0000000000,0.0000000000,0.0000000000,100.0000000000,24.2834884261,1227  
104.0000000000,49.9996649935,71.7003018579,49.2693704348,0.0000000000  
2,"eprfilb$eprfilb_mod_$ck_L90_2.kd"0,0,4,26071,26071,56320,256,0,0,24,80,37696,0x0,0x14b05013c080,100.0000000000  
0,880.0000000000,111907.6136363636,0.0000000000,0.0000000000,96.8019501699,9.6155911525,1008455.6562500000,81.38  
99031130,60.5181117611,43.6472872603,0.0000000000  
3,"eprfilb$eprfilb_mod_$ck_L85_3_cce$no-loop$form.kd"0,0,6,26071,26071,157593600,256,0,0,4,72,38592,0x0,0x14b0  
...
```

GPU Profiling



GPU Model factors for easre1b\$easre1b_mod_\$ck_L75_1.kd.



The earth is still alive..

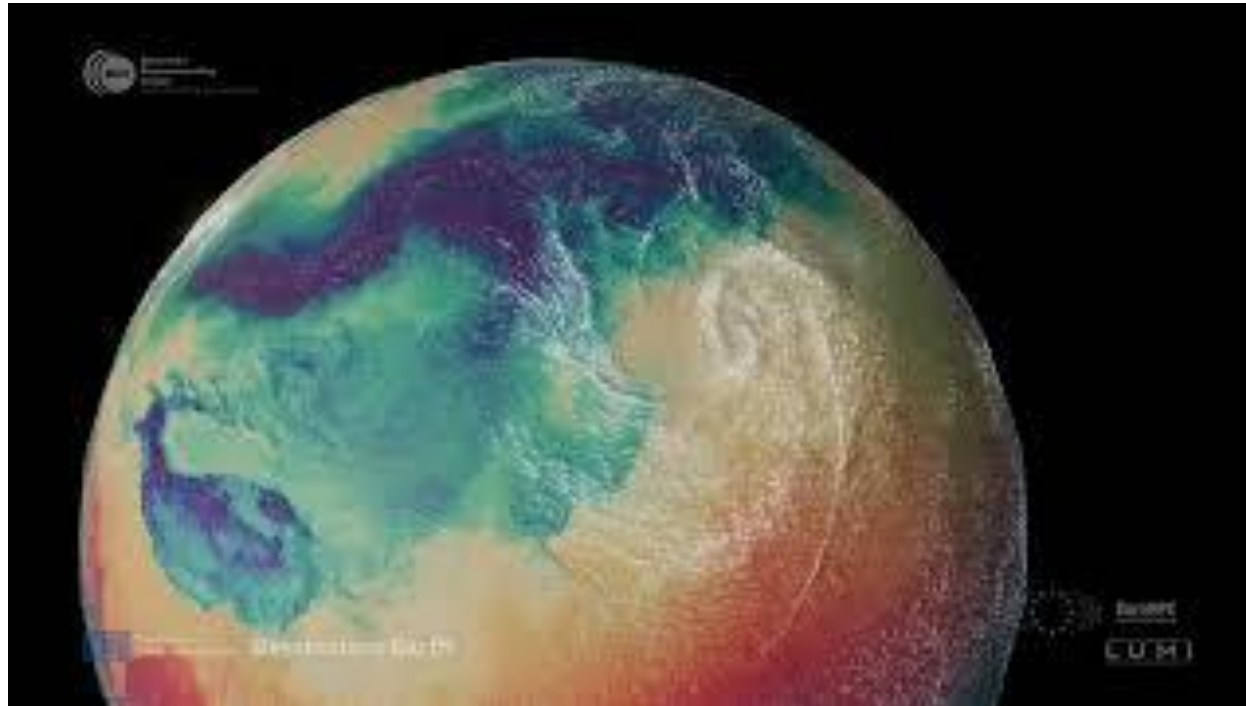


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Destination Earth implemented by



The earth is still alive..



SNIC PRESENTS

SUSTAINABILIT

Destination Earth

Pioneering the Future with Digital Twins

Okke van Eck
GPU Research Engineer
Barcelona Supercomputing Center

okke.vaneck@bsc.es



27th of November 2024, Bussum



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implemented by

