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Italiadomani PIANO NAZIONALE DI RIPRESA E RESILIENZA
ICSC Centro Nazionale di Ricerca in HPC, Big Data and Quantum Computing

Cosmica a novel CUDA code developed on the Ampere GPU architecture

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Spoke 3 General Meeting, Elba 5-9 / 05, 2024

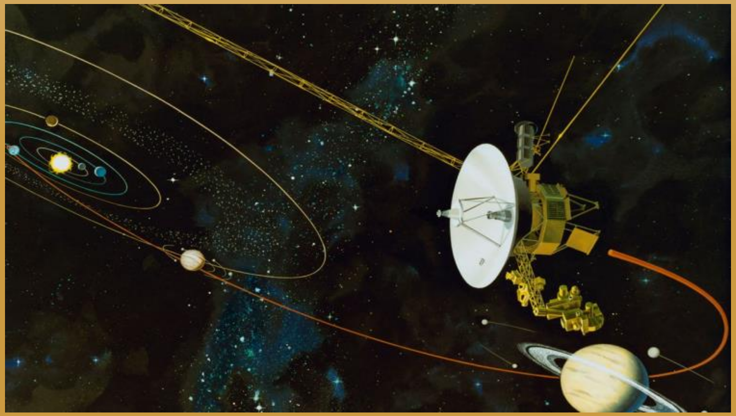
Scientific Rationale

Galactic Cosmic Rays modulation inside the heliosphere (region dominated by solar wind and related phenomena)

- **CR astrophysics (heliospere, propagation & sources modelling)**
- **Space weather (space radiation environment)**
- **Single event effect (device demage)**
- **CR background in space experiments**

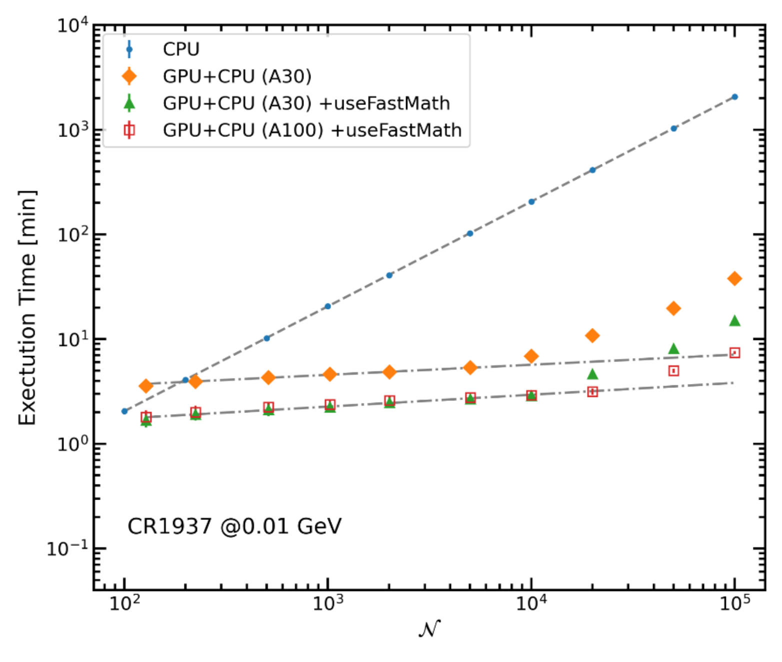
AMS-02 (Earth orbit)

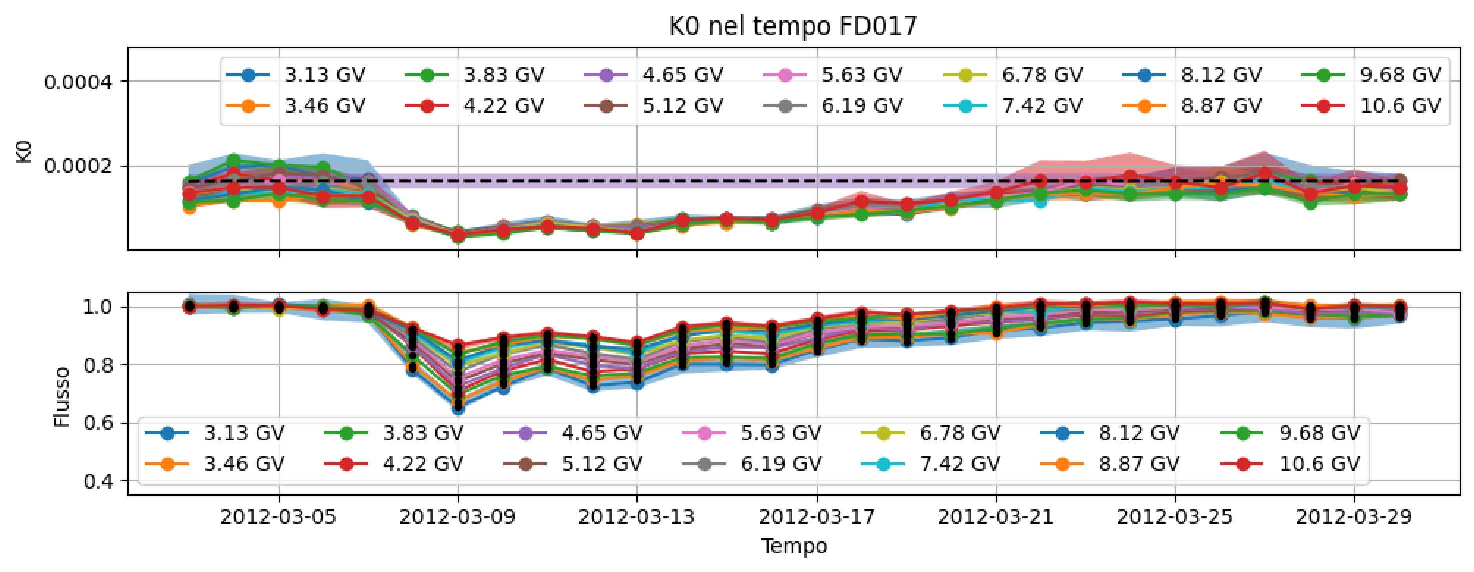
Voyager (Heliosphere boundaries)



Technical Objectives

- **Complete GPU porting of the SDE integration code (Cosmica)**
- **Code optimization based on the NVIDIA Ampere architecture (from hours to few minutes execution time)**
- **Implement different physical models as libraries and test physical parameters**





Methodologies

Diffusion | Advective | Adiabatic loss | Drift

$$\frac{\partial U}{\partial t} = \frac{\partial}{\partial x_i}\left(K^S_{ij}\frac{\partial U}{\partial x_j}\right) + \frac{1}{3}\frac{\partial V_{sw,i}}{\partial x_i}\frac{\partial}{\partial T}\left(\alpha_{rel} TU\right) - \frac{\partial}{\partial x_i}\left[\left(V_{sw,i} + v_{d,i}\right)U\right]$$

Parker Transport Equation

Fokker-Plank (Kolmarov) differential equation

Ito's formula

$$\frac{\partial U}{\partial s} = \sum_i A_{B,i}(s,y)\frac{\partial U}{\partial y_i} + \frac{1}{2}\sum_{i,j} C_{B,ij}(s,y)\frac{\partial^2 U}{\partial y_i \partial y_j} - L_B U + S$$

Stochastic Differential Equations

(MC backward in time numerically integrated)

Particle propagation indipendence

SIMD parallelization on GPU

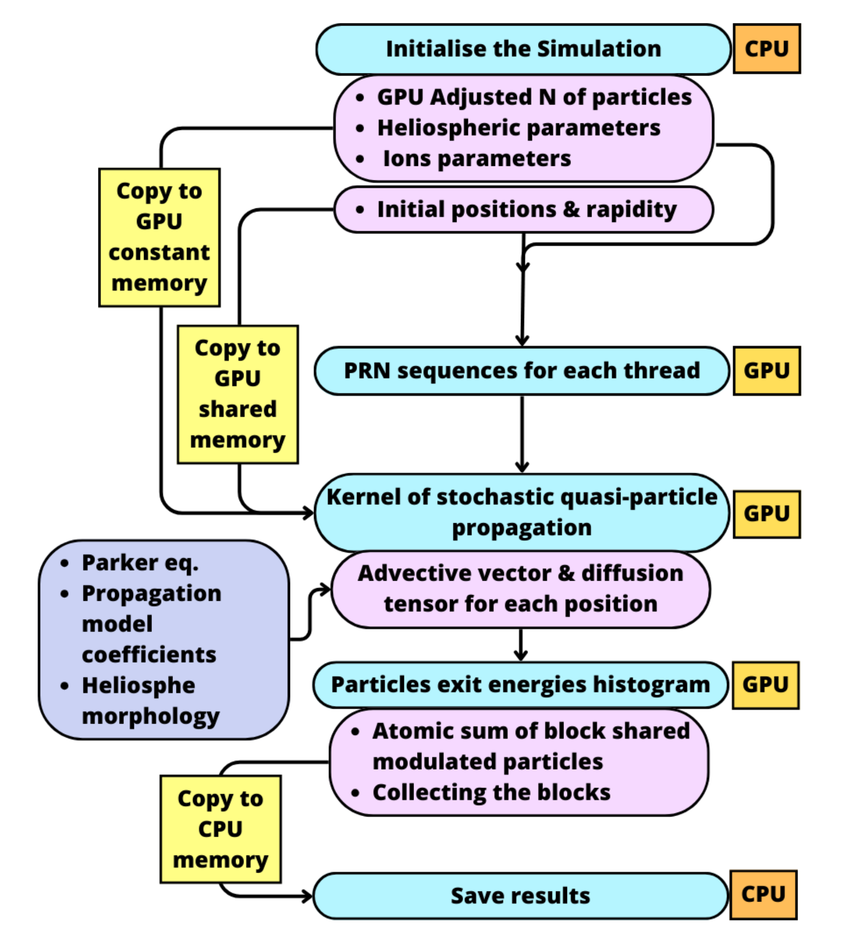
CPU-GPU mixed CUDA code

Everage of N quasi-particles simulated for each input energy

Convolved with Local Interstellar Spectrum

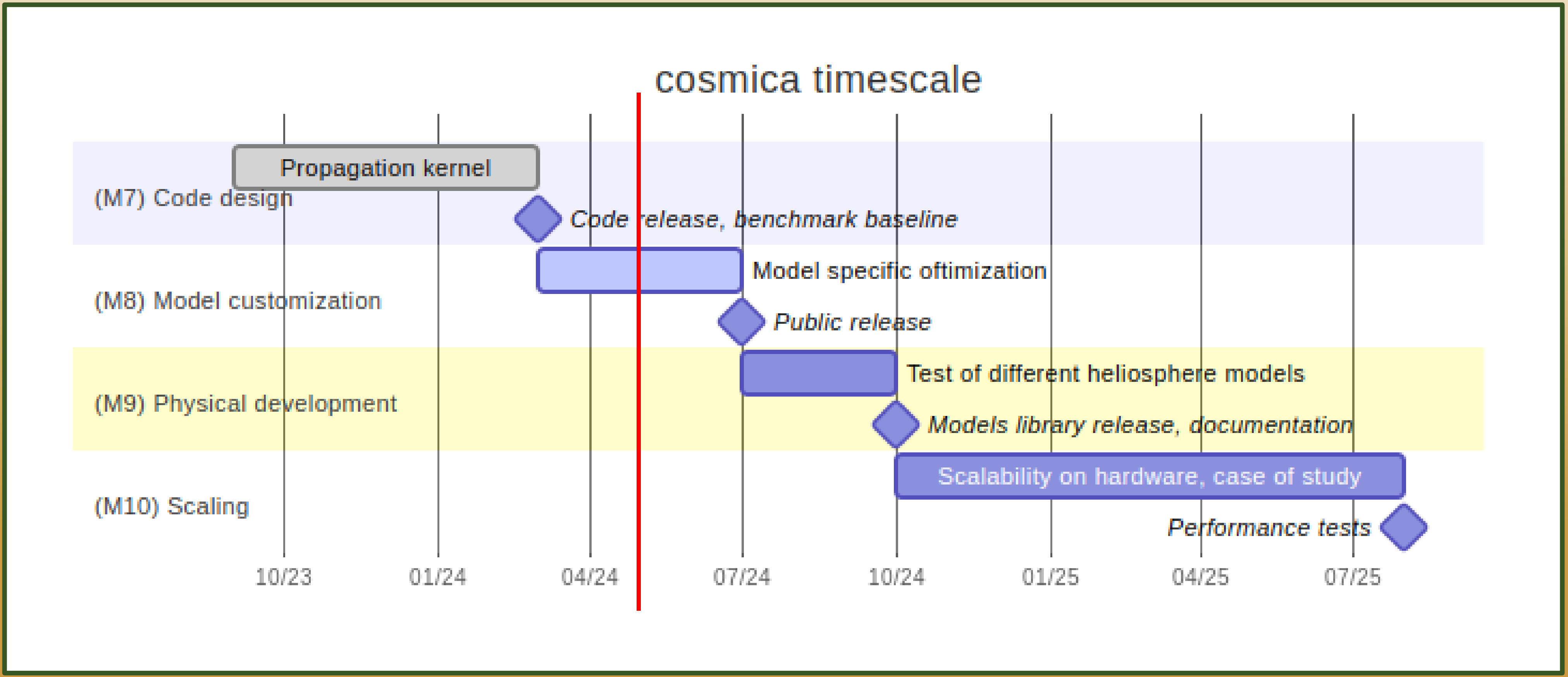
Solutions

Algorithm scheme



- Manage to distribute the simuated energies on all the available GPUs in the cluster
- Profile the code with Nsight Compute and its execution with Nsight System (bottleneck & GPU usage)
- Achieve the algorithm maximum parallelization by reducing register usage, maximising active threads
- Avoid multiple CPU - GPU memory transfer
- Each warp evolves quasi-particles belonging to the same subset of heliospheric variable (maximize the probability of broadcasting)

Timescale, Milestones, KPIs



From Trieste meeting (October 2023): Expected Results

Identified optimization points:

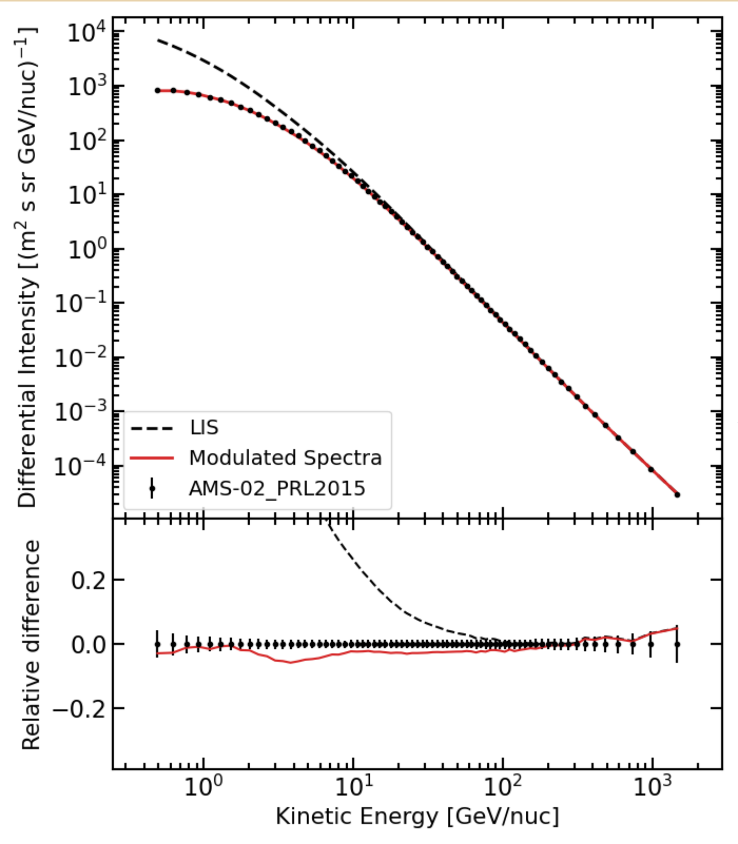
- Passing from particle energy to rigidity (one SDE becomes trivial)
- Optimazing the registers and shared memory usage (avoid memory saturation)
- Occupancy optimization managing threads and blocks number
- Remove the code bottleneck: branch diverging, infinity loops, stucked particle propagation
- Configure the heliosphere morphology model

Expected results:

- Produce consistent simulations with same CPU precision
- Simulation speedup ≥ 50 times CPU code

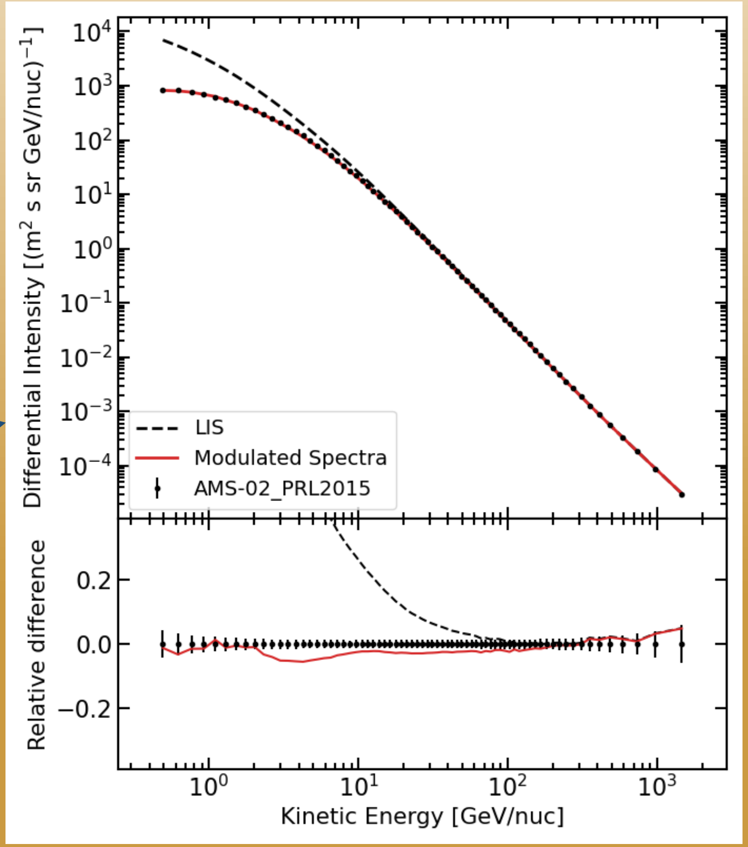
Accomplished Work, Results

- Stable version 1 of Cosmica (within 2% of statistical simulation error)



Cosmica

Preliminary code



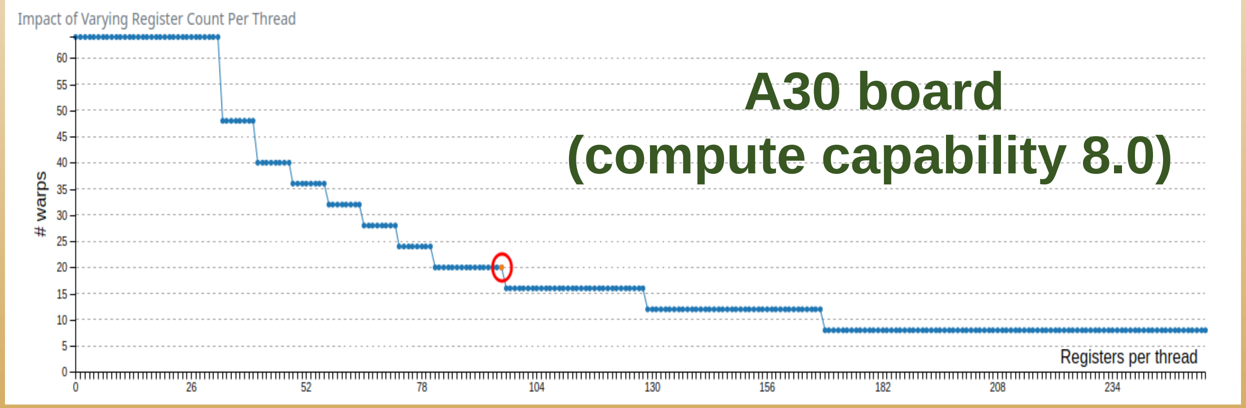
Accomplished Work, Results

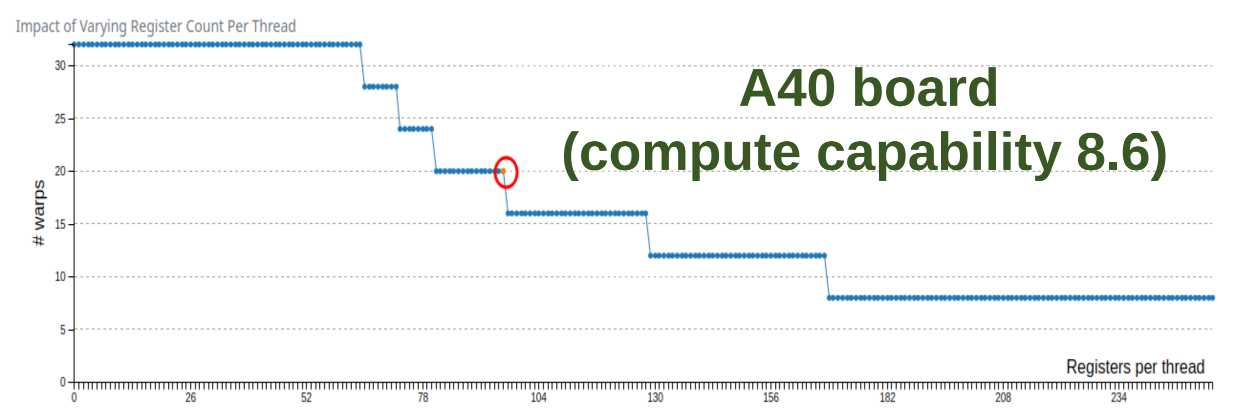
➢ **Profiling of the execution bottleneck of single GPU kernel functions**

96 registers used for the heliospheric propagation kernel function (maximum registers per thread = 32)

⬇

Registers from other warps are allocated and the number of active warps is sub-optimal





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Accomplished Work, Results

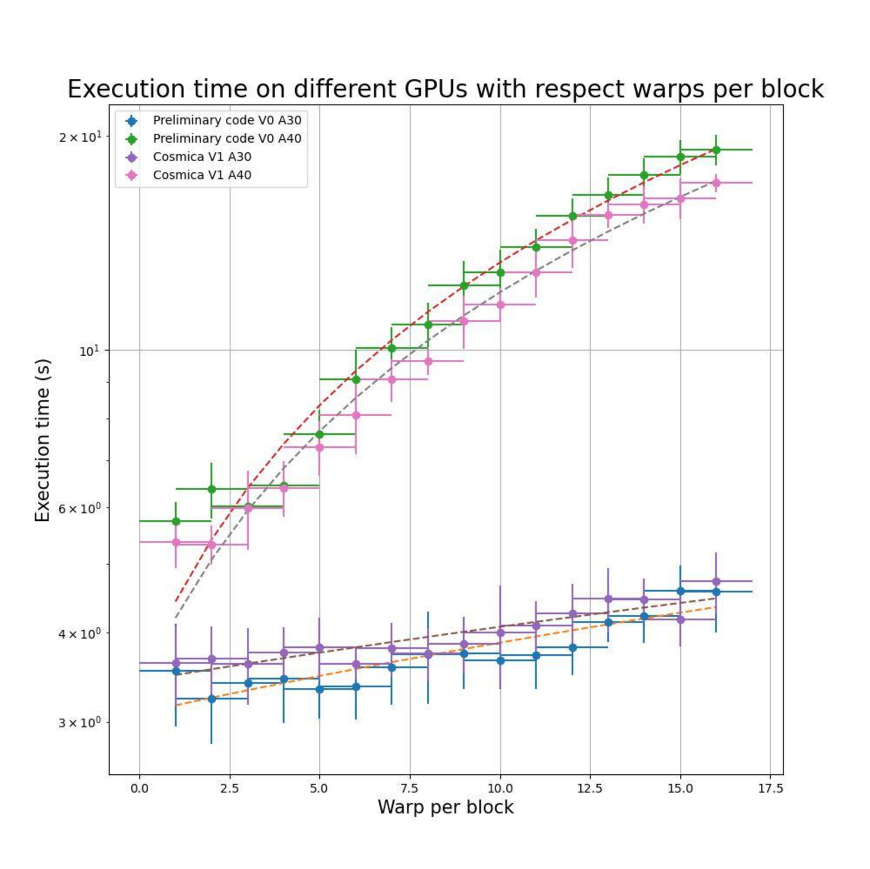
➢ Profiling of the execution bottleneck of single GPU kernel functions

Time	Total Time	Instances	Avg	Med	Min	Max	StdDev	Category	Operation
100.0%	429.333 s	14	30.667 s	27.342 s	15.777 s	57.753 s	12.226 s	CUDA_KERNEL	HeliosphericPropagation(curandStatePhilox4_32_10 *, PropagationParameters_t, particle_t *, i
0.0%	64.642 µs	18	3.591 µs	4.144 µs	608 ns	4.513 µs	1.319 µs	MEMORY_OPER	[CUDA memcpy Host-to-Device]
0.0%	55.904 µs	42	1.331 µs	1.280 µs	1.216 µs	1.792 µs	150 ns	MEMORY_OPER	[CUDA memcpy Device-to-Host]
0.0%	39.616 µs	14	2.829 µs	2.816 µs	2.816 µs	2.848 µs	16 ns	CUDA_KERNEL	kernel_max(particle_t *, float *, unsigned long)
0.0%	28.127 µs	14	2.009 µs	2.016 µs	1.984 µs	2.048 µs	22 ns	CUDA_KERNEL	histogram_atomic(const particle_t *, float, float, int, unsigned long, float *, int *)
0.0%	21.408 µs	14	1.529 µs	1.536 µs	1.504 µs	1.536 µs	13 ns	CUDA_KERNEL	histogram_accum(const float *, int, int, float *)
0.0%	6.560 µs	14	468 ns	480 ns	448 ns	480 ns	15 ns	MEMORY_OPER	[CUDA memset]
0.0%	3.008 µs	1	3.008 µs	3.008 µs	3.008 µs	3.008 µs	0 ns	CUDA_KERNEL	init_rdmgenerator(curandStatePhilox4_32_10 *, unsigned long long)

- Execution time strongly dominated by the heliospheric propagation computation
- Max exit energy search and histogram building are negligible in the execution time
- Even memory set and transfer between host and device occupy less than 0.1%

Accomplished Work, Results

- **Performance test on the local farm and different GPUs comparison**



Comparable performance for A30 board

Small improvement for A40 board

NVIDIA A30

- Compute capability: 8.0
- Clock rate: 1 440 000
- Multiprocessor count: 56
- Warps per Multiprocessor: 64

NVIDIA A40

- Compute capability: 8.0
- Clock rate: 1 740 000
- Multiprocessor count: 84
- Warps per Multiprocessor: 48

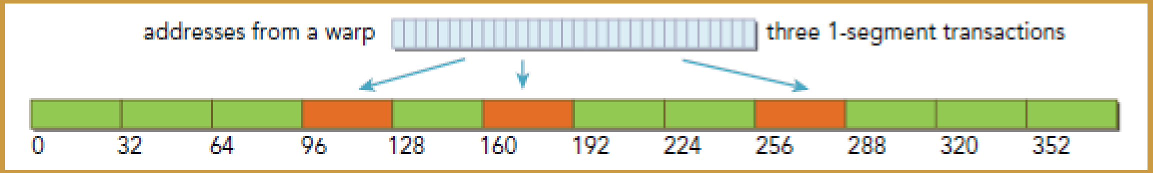
Accomplished Work, Results

- **Preliminary reduction of register usage** → Quasi-particle coordinate and energy are stored in shared memory

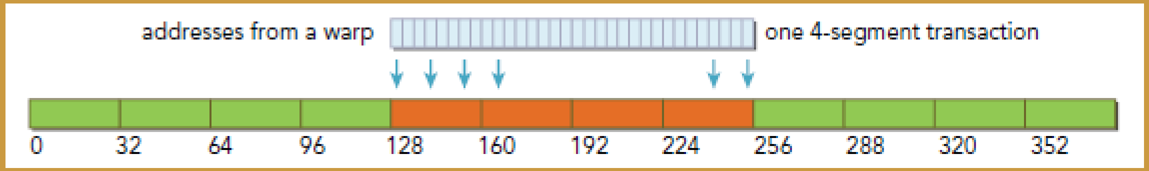
- **N threads allocated and warps per block optimization** → Best WpB for each GPU; N quasi-particle rounded; Full filling the first warps

- **Synchronous memeory access to particle evolving variable**

Array of struct



Struct of array



Accomplished Work, Results

Computational resources used:

- Local cluster: 10 GPUs (6 A30, 4 A40), Condor job submission system
- From Trieste meeting 10 k GPU hours used:
  - Test
  - Benchmark
  - Forbush calibration test

Expected computational resources comsuption:

- Study of K_0 diffusion parameter during Forbush (application for PICA resource)
  - At least other 10 k GPU hours
  - Memory (negligible order of GB)

Next Steps and Expected Results

NEXT STEPS:

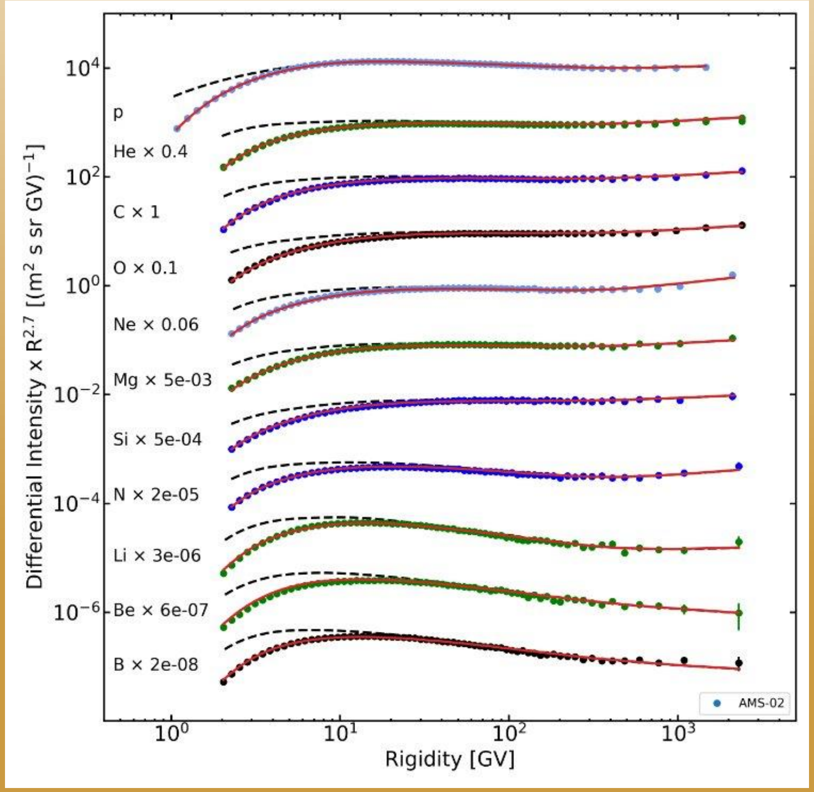
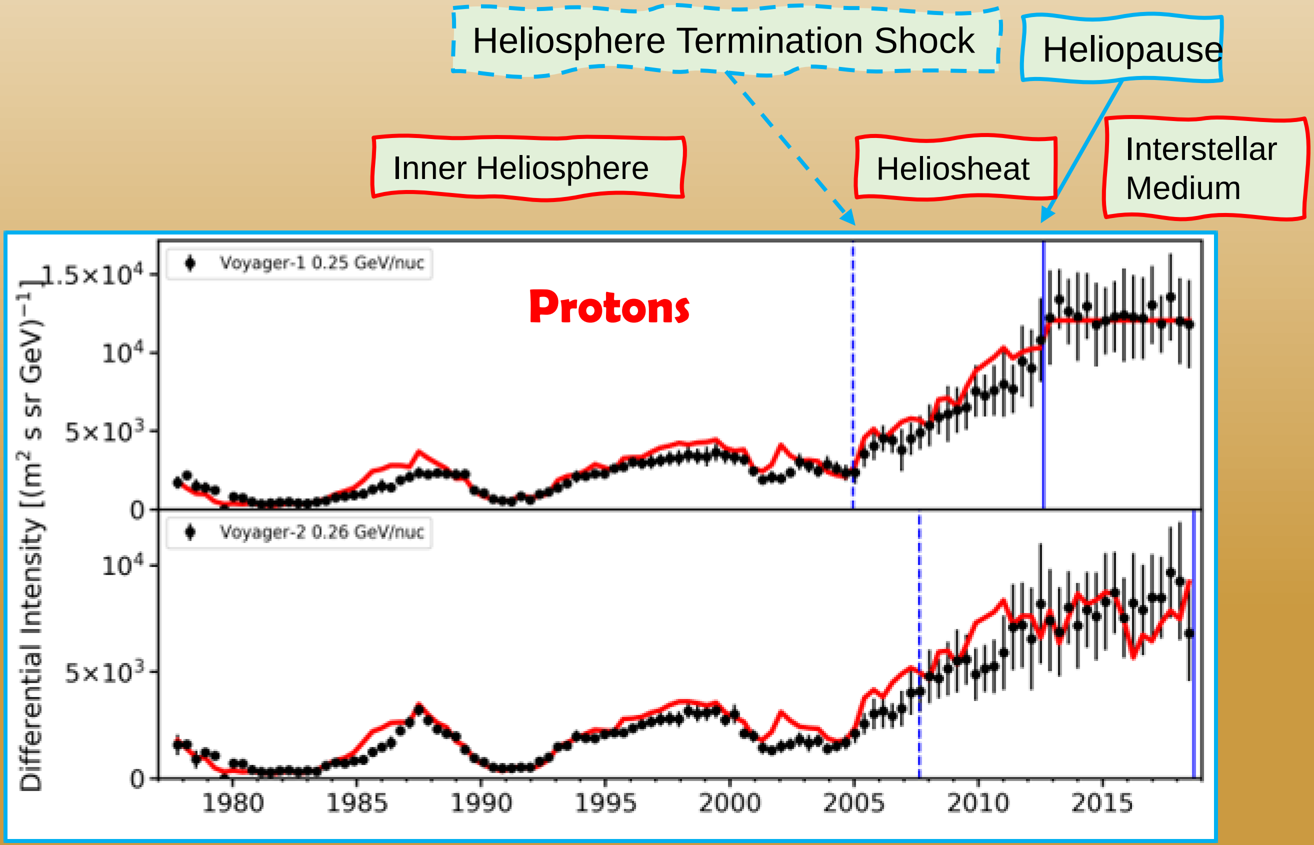
- Passing from particle energy to rigidity (one SDE becomes trivial)
- Customization based on physical model
- Finalize computational resource request (throught PICA)

Expected results:

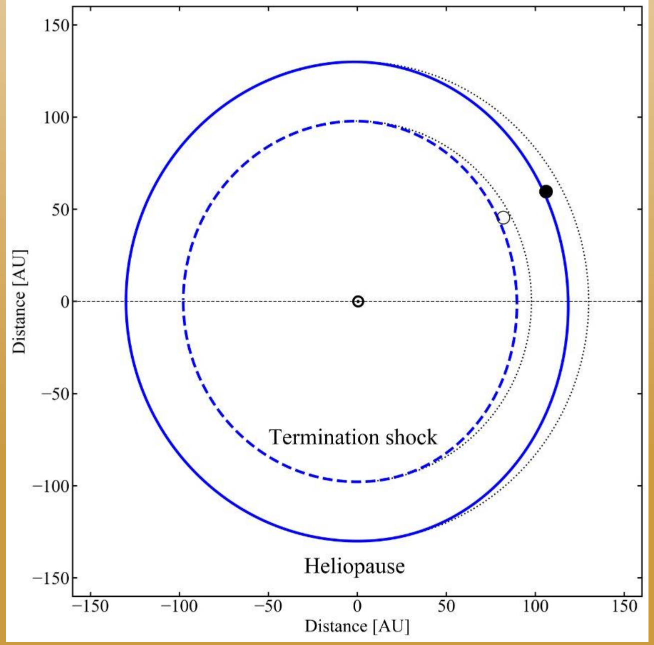
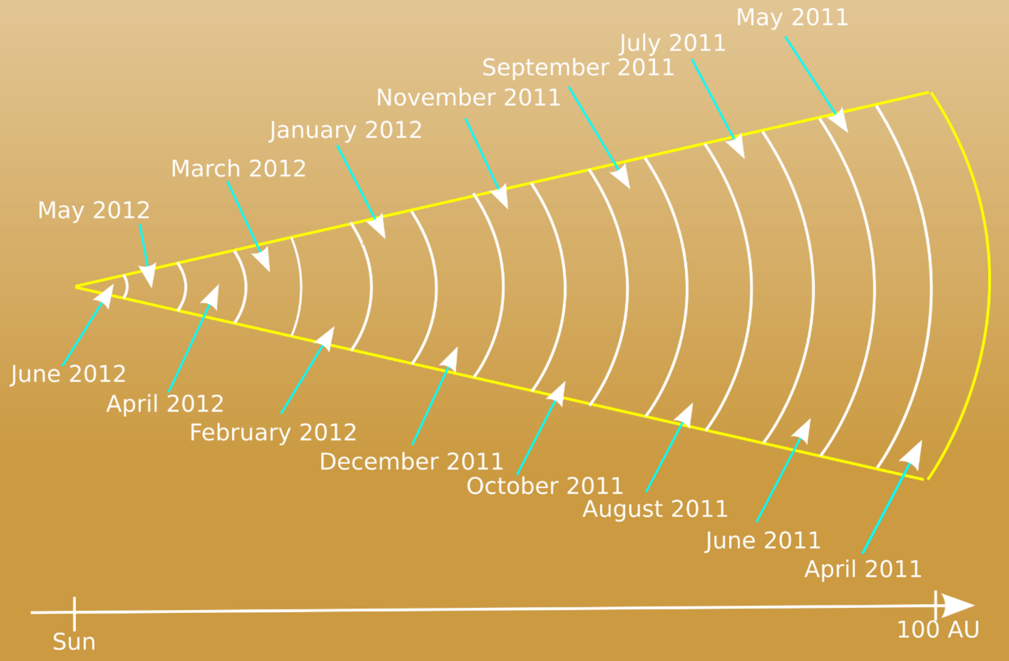
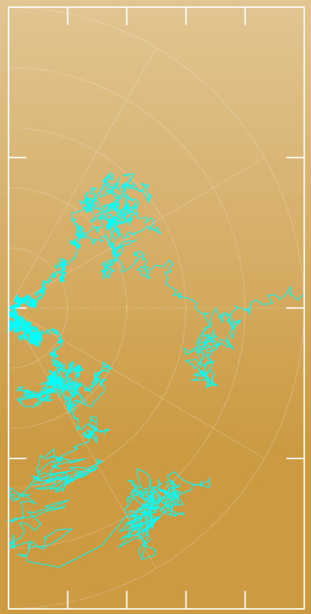
- First results relevant for physical application (scale use case)


Thanks for your attention
NOT ICSC RESOURCES

Scientific Rationale

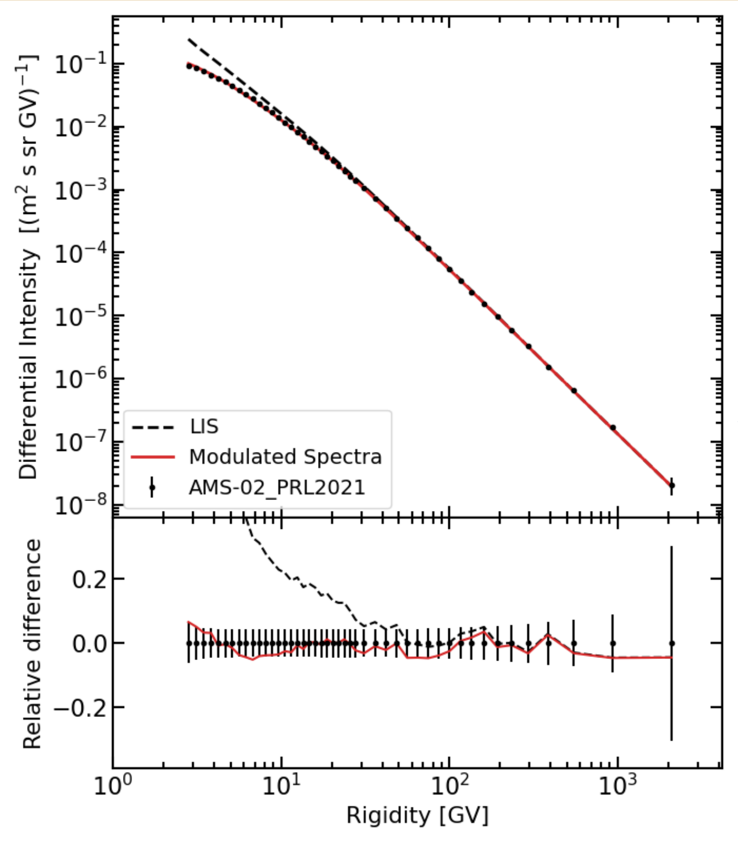
Local CR modulation	Time evolution along an orbit
	

Methodologies

Heliosphere & Heliosheat	Carrington regions	Particle propagation path
		

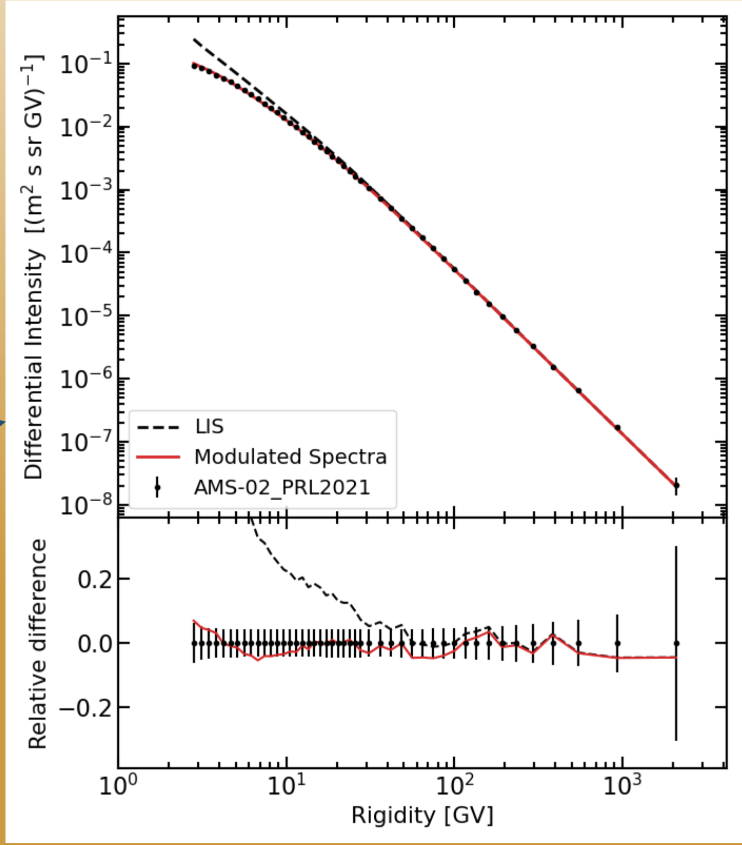
Accomplished Work, Results

- **Stable version 1 of Cosmica (within 2% of statistical simulation error)**



Cosmica

Preliminary code



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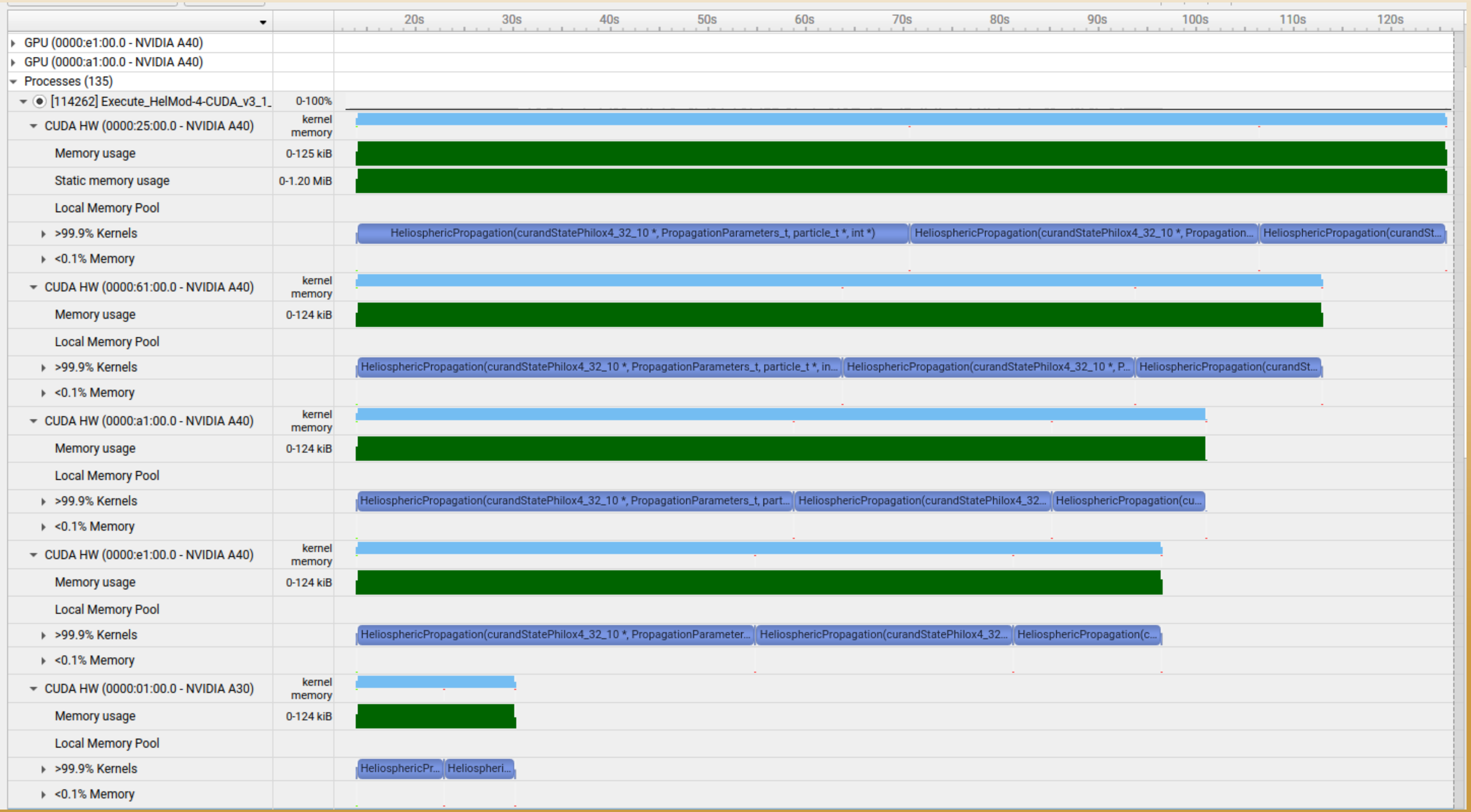
Nsight analysis (multi energy)

Multi GPu

- Energy bins with different avarage propagation time are not equally distributed between the GPU in the cluster
- Evident faster execution of the propagation computation in the A30 boards



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- The number of warps per block was varied from 2 to 32 for each GPU board (only the avilable values of warps per block are taken into account)

Register allocation unit size	256
Register allocation granularity	warp
Max registers per Block	65536
Warp allocation granularity (for register allocation)	4
Registers used by the kernel	106

Registers allocated =

$$\text{int\_round}\left(\frac{NRegPerKernel * WarpSize}{RegAllocUnit * WarpGranularity}\right) * RegAllocUnit * WarpGranularity * NWarps$$

We use 106 registers for the heliospheric propagation kernel function (maximum registers per thread = 32)

↓

Registers from other warps are allocated and the number of active warps is sub-optimal

↓

With more that 16 warps we exceed the GPU resources

↓

Nregisters = 73 728 for 18 Warps

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Accomplished Work, Results

➢ Profiling of the execution bottleneck of single GPU kernel functions

ID	Estimated Speedup	Function Name	De	Duration	Runtime Improvement (1.88419e+11)	Compute Throughput	Memory Throughput	# Registers	Grid Size	Blc	Cycles
0	77.38	init_rdmgenerator	i...	0.00	0.00	0.22	4.75	20	19, 1, 1		5078
1	77.38	init_rdmgenerator	i...	0.00	0.00	0.19	3.97	20	19, 1, 1		6069
2	77.38	init_rdmgenerator	i...	0.00	0.00	0.28	6.07	20	19, 1, 1		3985
3	66.07	init_rdmgenerator	i...	0.00	0.00	0.35	5.30	19	19, 1, 1		4362
4	77.38	init_rdmgenerator	i...	0.00	0.00	0.29	6.27	20	19, 1, 1		388[illegible]
5	77.38	HeliosphericPropag...	...	22.33	17.28	8.70	1.87	106	19, 1, 1		29148005356
6	77.38	HeliosphericPropag...	...	25.74	19.92	8.38	1.82	106	19, 1, 1		33595308941
7	66.07	HeliosphericPropag...	...	18.35	12.12	1.61	2.6[illegible]	108	19, 1, 1		17053851356
8	77.38	HeliosphericPropag...	...	27.41	21.21	7.95	1.7[illegible]	106	19, 1, 1		35775477854
9	77.38	HeliosphericPropag...	...	33.64	26.03	7.71	1.67	106	19, 1, 1		43896109450
10	97.62	kernel_max	...	0.00	0.00	0.30	1.33	16	2, 1, 1		6114
11	97.62	kernel_max	...	0.00	0.00	0.30	1.34	16	2, 1, 1		6139
12	97.62	kernel_max	...	0.00	0.00	0.30	1.34	16	2, 1, 1		6135
13	97.62	kernel_max	...	0.00	0.00	0.30	1.34	16	2, 1, 1		6083
14	97.62	histogram_atomic	...	0.00	0.00	0.10	2.00	16	2, 1, 1		4902

- The grid for this launch is configured to execute only 19 blocks, which is less than the GPU's 56 multiprocessors, underutilizing some multiprocessors
- Between 66 - 77% improvement of the most time comsuming function

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Nsight compute analysis

A40 multi energy

- E

ID	Estimated Speedup	Function Name	De	Duration	Runtime Improvement (5.04838e+11)	Compute Throughput	Memory Throughput	# Registers	Grid Size	Blc	Cycles
0	92.86	init_rdmgenerator	i...	0.00	0.00	0.29	4.21	19	4, 1, ...		5703
1	95.24	init_rdmgenerator	i...	0.00	0.00	0.21	4.34	20	4, 1, ...		5805
2	95.24	init_rdmgenerator	i...	0.00	0.00	0.20	4.32	20	4, 1, ...		5838
3	95.24	init_rdmgenerator	i...	0.00	0.00	0.20	4.28	20	4, 1, ...		5879
4	95.24	init_rdmgenerator	i...	0.00	0.00	0.20	4.14	20	4, 1, ...		6087
5	92.86	HeliosphericPropag...	...	17.33	16.09	1.62	2.58	108	4, 1, ...		16115947797
6	95.24	HeliosphericPropag...	...	66.38	63.22	3.79	0.82	106	4, 1, ...		86615042692
7	96.43	kernel_max	...	0.00	0.00	0.49	0.7[illegible]	16	2, 1, ...		5565
8	95.24	HeliosphericPropag...	...	70.58	67.22	3.71	0.8[illegible]	106	4, 1, ...		92057442068
9	95.24	HeliosphericPropag...	...	52.01	49.53	3.61	0.79	106	4, 1, ...		67881794652
10	95.24	HeliosphericPropag...	...	61.59	58.66	3.56	0.77	106	4, 1, ...		80385971314
11	97.62	kernel_max	...	0.00	0.00	0.30	1.35	16	2, 1, ...		6085
12	97.62	kernel_max	...	0.00	0.00	0.30	1.34	16	2, 1, ...		6126
13	97.62	kernel_max	...	0.00	0.00	0.30	1.32	16	2, 1, ...		6128
14	97.62	kernel_max	...	0.00	0.00	0.30	1.35	16	2, 1, ...		6122

- The grid for this launch is configured to execute only 4 blocks, which is less than the GPU's 84 multiprocessors, underutilizing some multiprocessors
- Number of threads per block not a multiple of the warp dimension (rounded in the next version)
- Between 92 – 95% improvement of the most time comsuming function

Stronger effect of the warp per block on the A40 boards

Accomplished Work, Results

- **Stable version 1 of Cosmica**
- **Profiling of the execution bottleneck of single GPU kernel functions**
- **Performance test on the local farm and different GPUs comparison**
- **Preliminary reduction of register usage**
- **N threads allocated and warps per block optimization**
- **Synchronous memeory access to particle evolving variable**

Next Steps and Expected Results

Customization based on physical model:

- **Insert the student thesis work (reduction of 1 model parameter)**
- **Heliosheat new analysis (paper just accepted)**
- **Finalize computational resource request (throught PICA)**