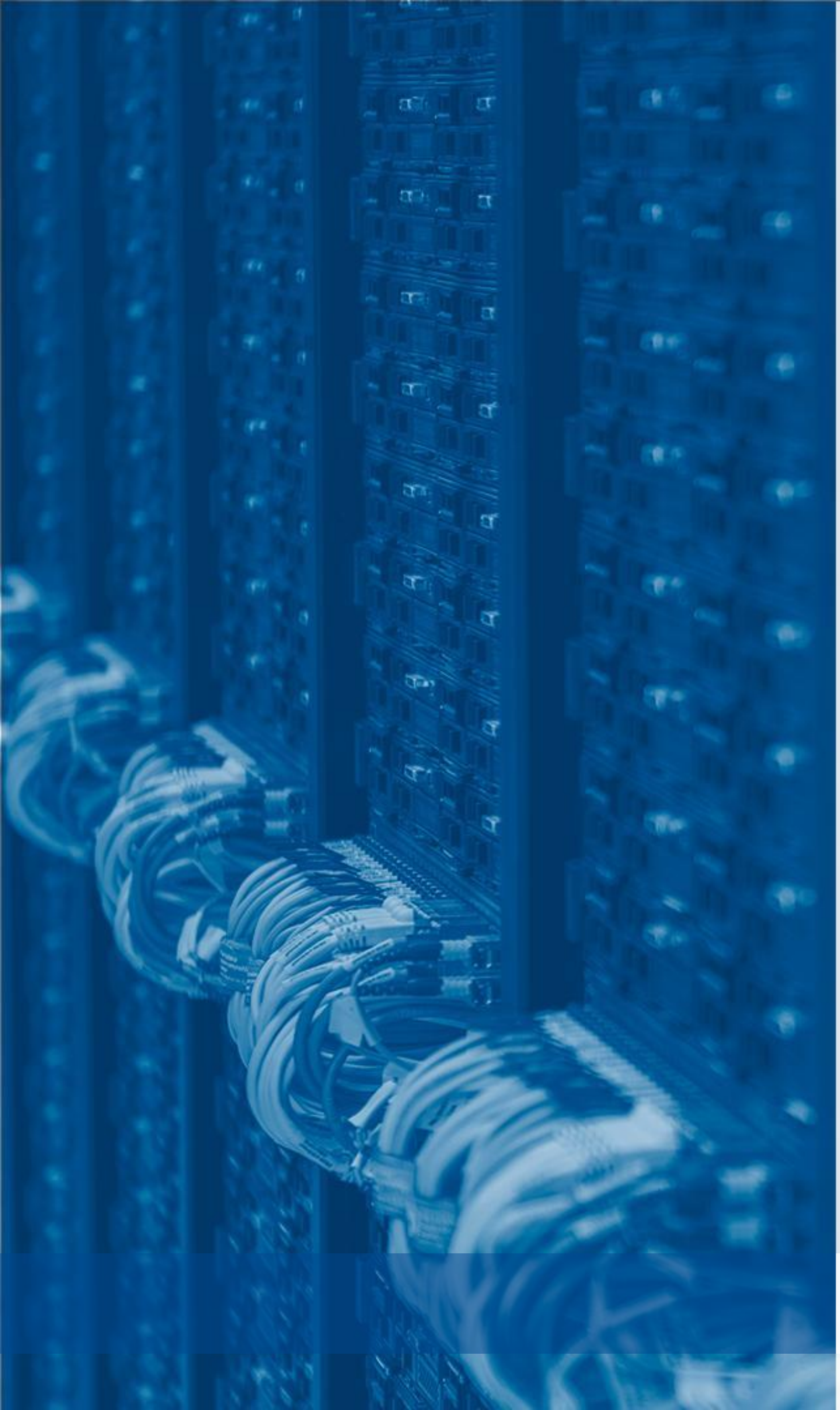

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CAMP First GPU Solver: A Solution to Accelerate Chemistry in Atmospheric Models

Christian Guzman Ruiz, Mario C. Acosta, Matthew Dawson*, Oriol Jorba, Carlos Pérez García-Pando, Kim Serradell

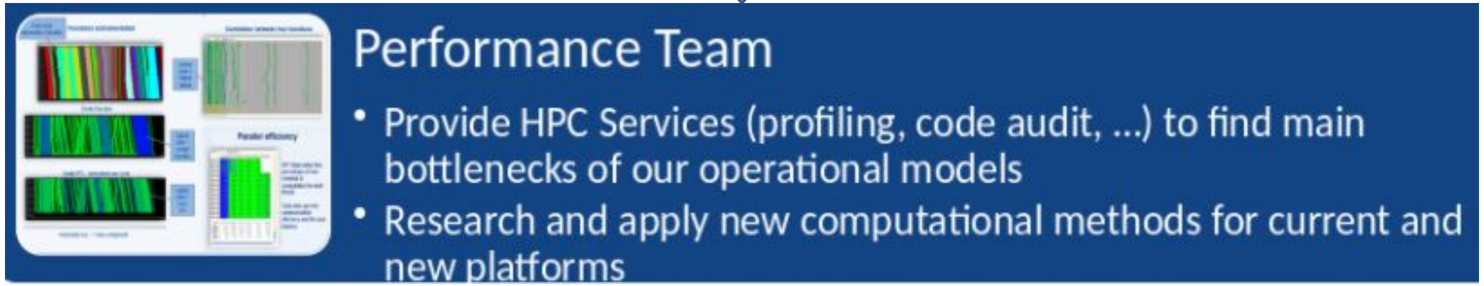
Barcelona SuperComputing Center
***National Center for Atmospheric Research (NCAR)**

7th ENES workshop

BSC Departments

Earth Sciences

To develop and implement global and regional state-of-the-art models for short-term air quality forecast and long-term climate applications



Performance Team

- Provide HPC Services (profiling, code audit, ...) to find main bottlenecks of our operational models
- Research and apply new computational methods for current and new platforms

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Background

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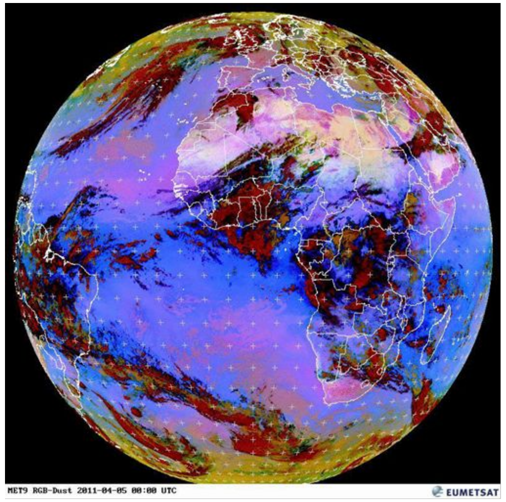
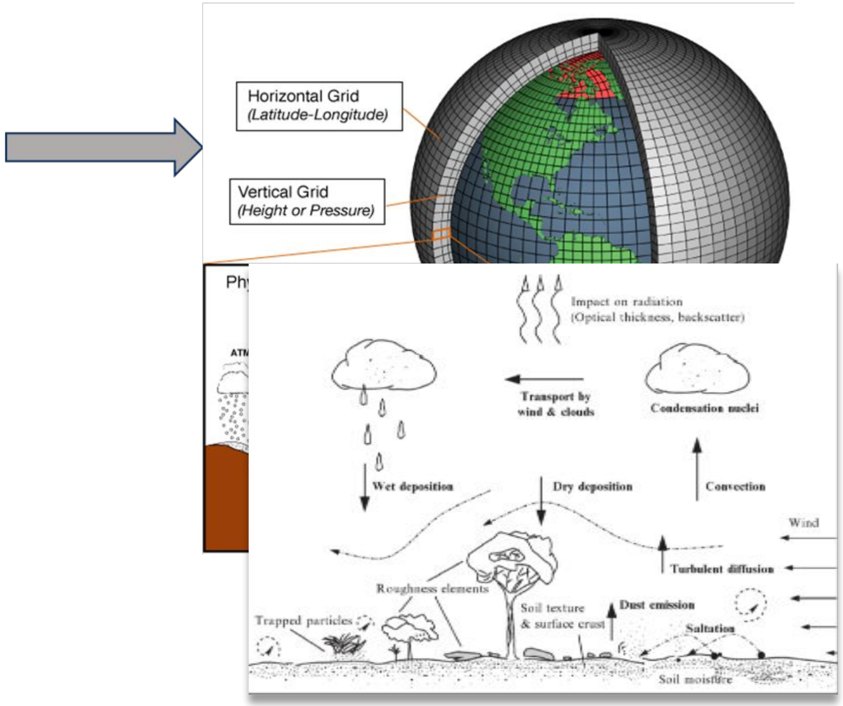
Atmospheric models

Atmospheric models are a **mathematical representation** of atmospheric water, gas, and aerosol cycles.





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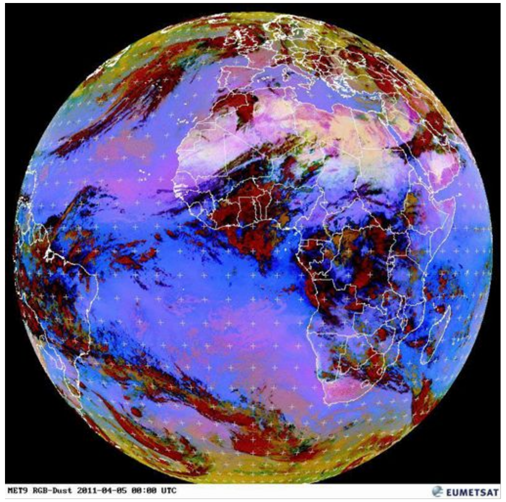
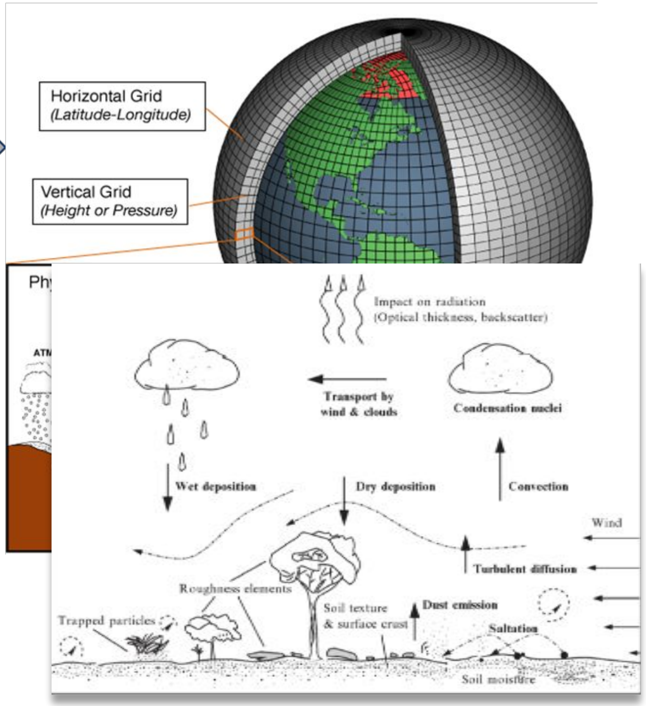
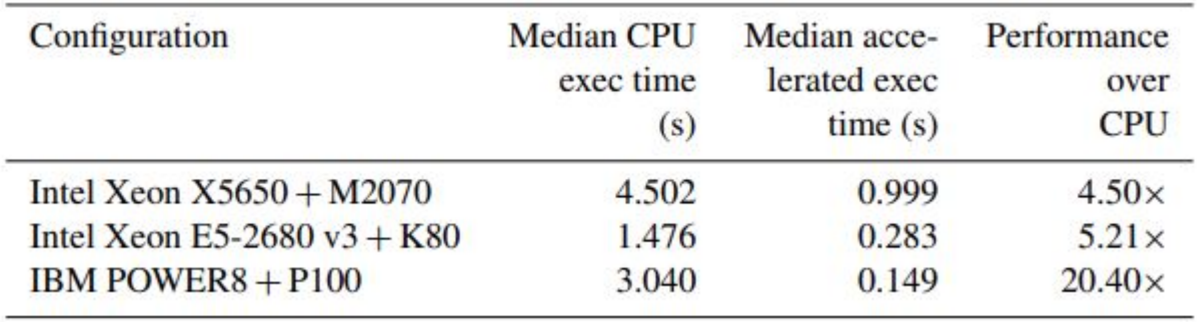




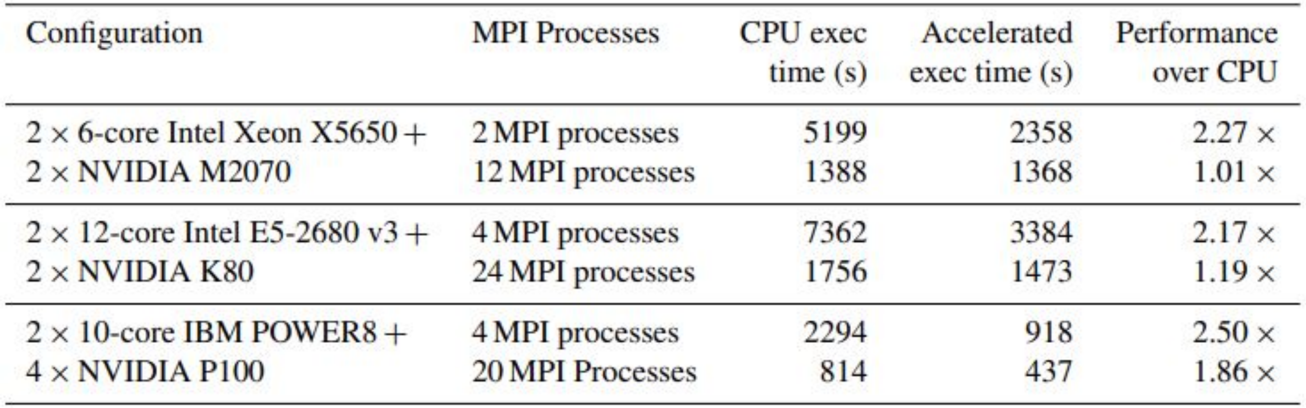
Resolution of chemical processes can take up to 80% of the time execution!

State of the art - KPP GPU

- Kinetic PreProcessor (KPP) is a analysis tool to solve chemical mechanisms using Rosenbrock methods
- KPP is widely used in the atmospheric community
- The GPU version for the EMAC climate model achieves up to 20x speedup against CPU single-core and 1.86x against 2 CPUs



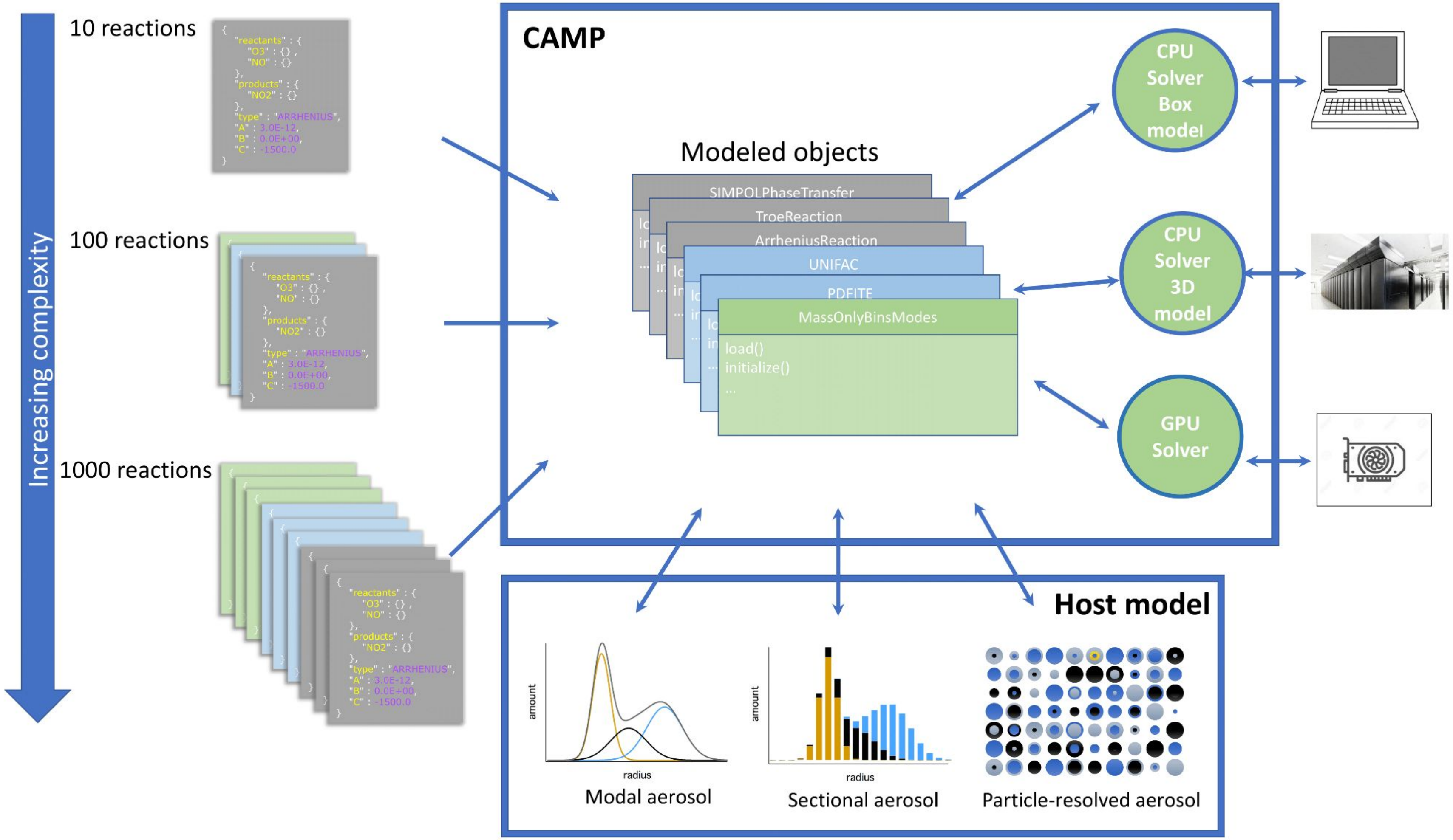
Configuration	Median CPU exec time (s)	Median accelerated exec time (s)	Performance over CPU
Intel Xeon X5650 + M2070	4.502	0.999	4.50×
Intel Xeon E5-2680 v3 + K80	1.476	0.283	5.21×
IBM POWER8 + P100	3.040	0.149	20.40×



Configuration	MPI Processes	CPU exec time (s)	Accelerated exec time (s)	Performance over CPU
2 × 6-core Intel Xeon X5650 +	2 MPI processes	5199	2358	2.27 ×
2 × NVIDIA M2070	12 MPI processes	1388	1368	1.01 ×
2 × 12-core Intel E5-2680 v3 +	4 MPI processes	7362	3384	2.17 ×
2 × NVIDIA K80	24 MPI processes	1756	1473	1.19 ×
2 × 10-core IBM POWER8 +	4 MPI processes	2294	918	2.50 ×
4 × NVIDIA P100	20 MPI Processes	814	437	1.86 ×

Michail Alvanos and Theodoros Christoudia, GPU-accelerated atmospheric chemical kinetics in the ECHAM/MESSy (EMAC) Earth system model , 2017

CAMP: Chemistry Across Multiple Phases



```
{
  "reactants" : {
    "O3" : {} ,
    "NO" : {}
  },
  "products" : {
    "NO2" : {}
  },
  "type" : "ARRHENIUS",
  "A" : 3.0E-12,
  "B" : 0.0E+00,
  "C" : -1500.0
}
```

Dawson, Guzman, Curtis, Acosta, et. al., Chemistry Across Multiple Phases (CAMP) version 1.0, GMD 2022

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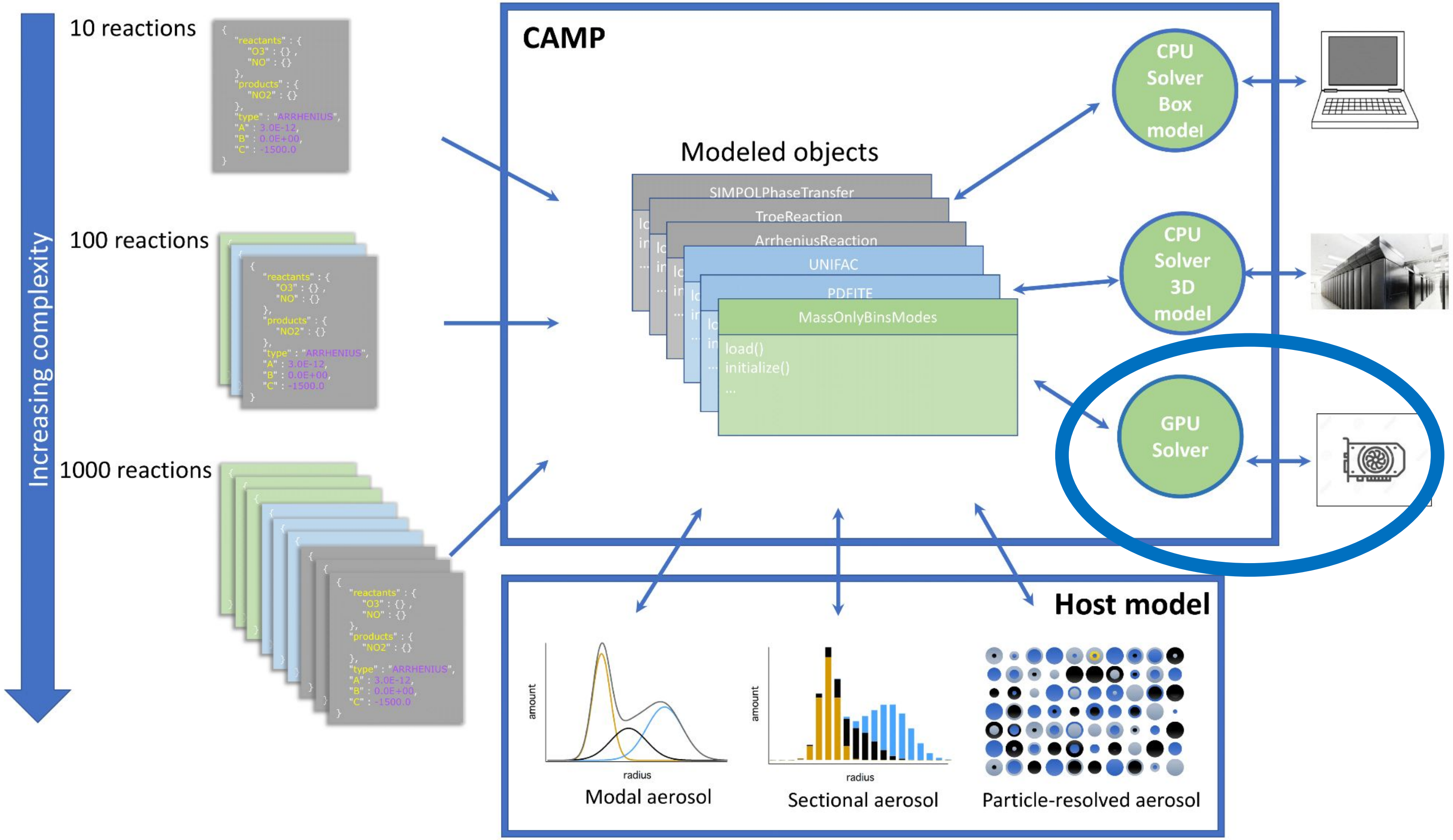
CAMP: Chemistry Across Multiple Phases



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}
```

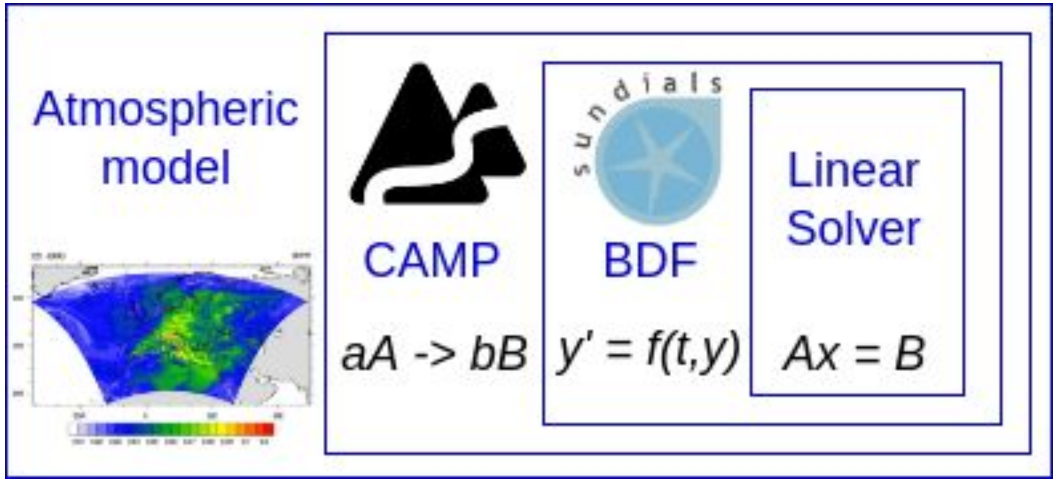
Our objective!

Dawson, Guzman, Curtis, Acosta, et. al., Chemistry Across Multiple Phases (CAMP) version 1.0, GMD 2022

CAMP CPU Solver

- CAMP uses the Backward Differentiation Formula (BDF) from CVODE, which is a solver for ordinary differential equation (ODE) systems.

- BDF requires a linear solver package. The default option is the KLU algorithm for the CPU execution, while it also has a CUDA version of the Biconjugate Gradient (BCG) algorithm.



Implementation

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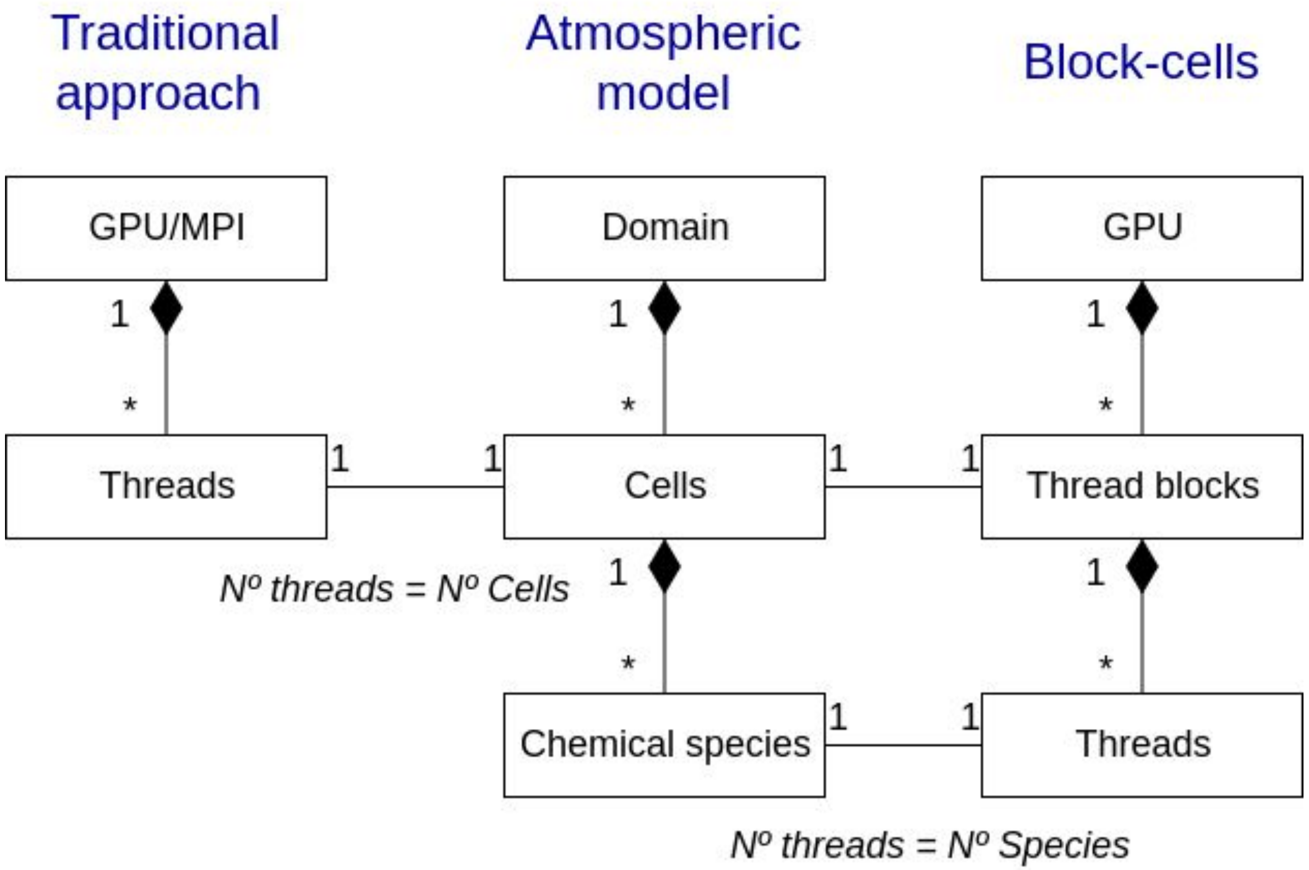
Block-cells (GPU parallelization strategy)

- Block-cells assigns each atmospheric cell to a GPU thread block
- Uses as many threads as chemical species

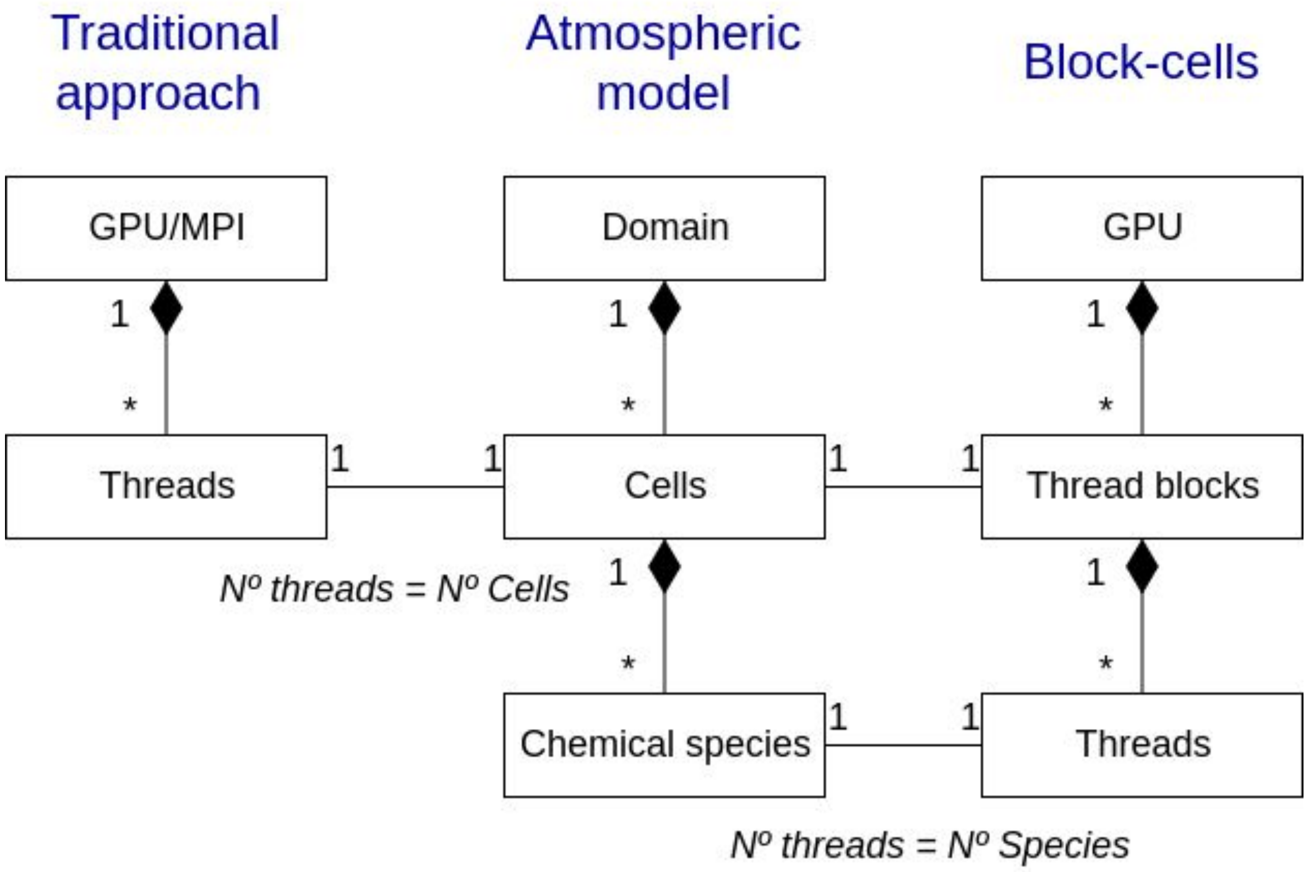


Guzman et. al. Studying a new GPU treatment for chemical modules inside CAMP, 19th ECMWF Workshop

Block-cells (GPU parallelization strategy)

- Higher occupancy than traditional approaches (more threads computing data)

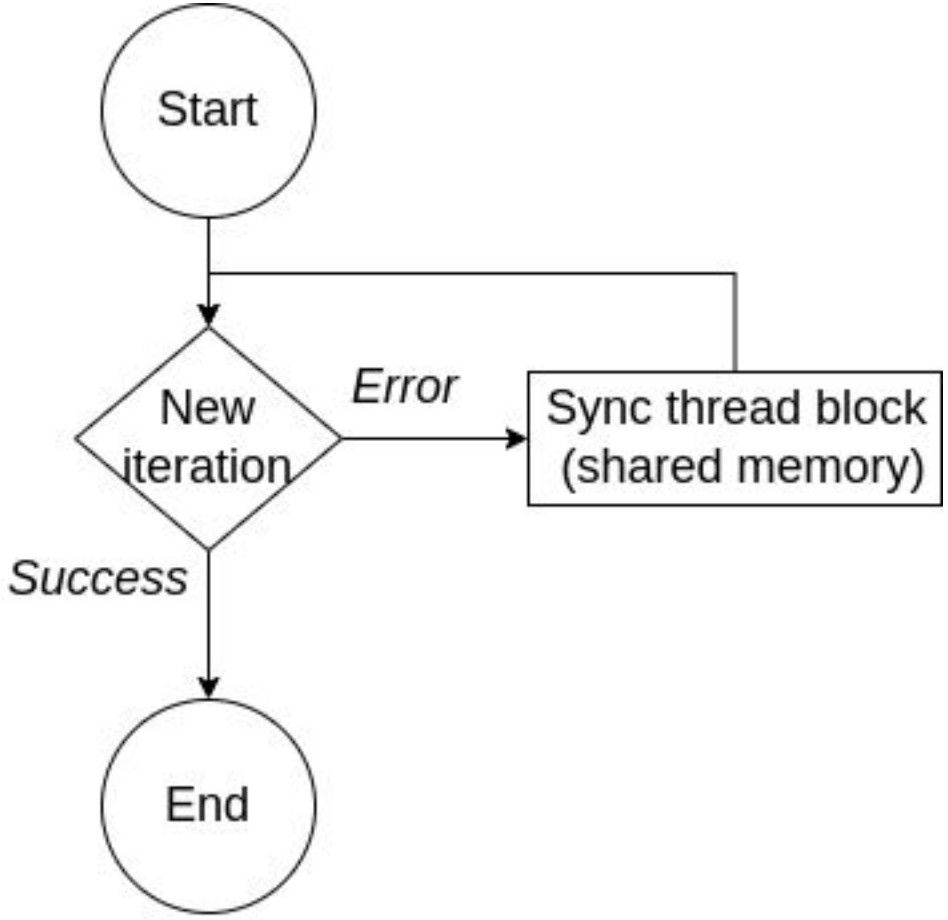
- 34x speedup against CPU single-thread for the CAMP BCG linear solver



Guzman et. al. Studying a new GPU treatment for chemical modules inside CAMP, 19th ECMWF Workshop

Communicating data between threads

- All **communications** are performed at **thread block level**
- An example: A thread triggers an error due to a negative concentration
- The error is shared between the other threads in the block by using shared memory



GPU BDF convergence loop

Test environment

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Hardware

- **CTE-POWER cluster:**
  - **2 x IBM Power9** 8335-GTH @ 2.4GHz (3.0GHz on turbo, 20 cores and 4 threads/core, total **40 cores per node)**
  - **4 x GPU NVIDIA V100 (Volta)** with 16GB HBM2**.**
  - Compilers: GCC version 6.4.0 and NVCC version 10.2

Software configuration

Architecture	Parallel resources	Parallelization language
CPU	1, 40	MPI
GPU	Nº of different chemical concentrations (species x cells)	CUDA

- The evaluation is performed over the code included in the most external loop in BDF. The code related to previous initializations is excluded.

- Chemical mechanism: Gas phase chemistry from Carbon bond 2005 (CB05) | Chemical species: 156 | Cells (ODE systems): 100-10,000 | GPU Shared memory size per block: 256 | CVODE absolute tolerance: 0.01% | BCG tolerance: 1.0e-30

Results

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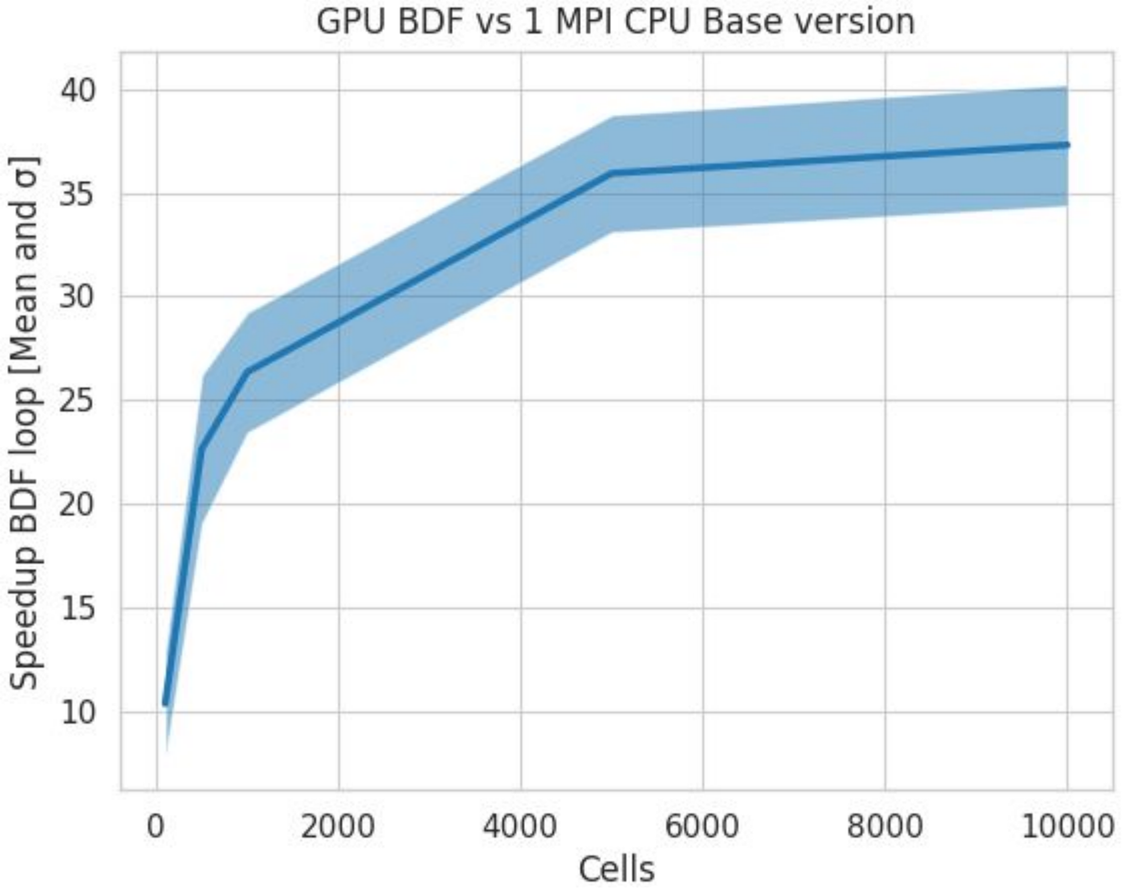
Speed-up

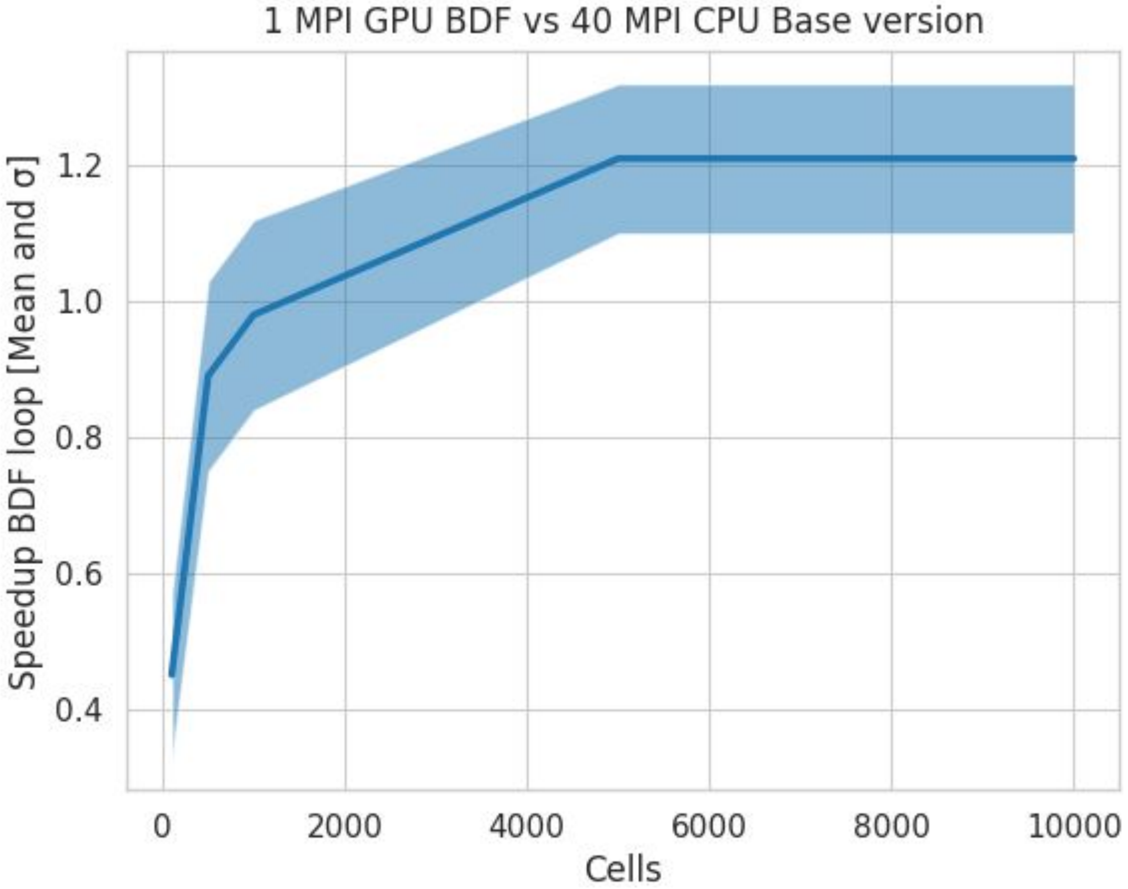
- Up to 35x speedup in average vs single-thread
- Standard deviation around 2



Speed-up against 40 processes

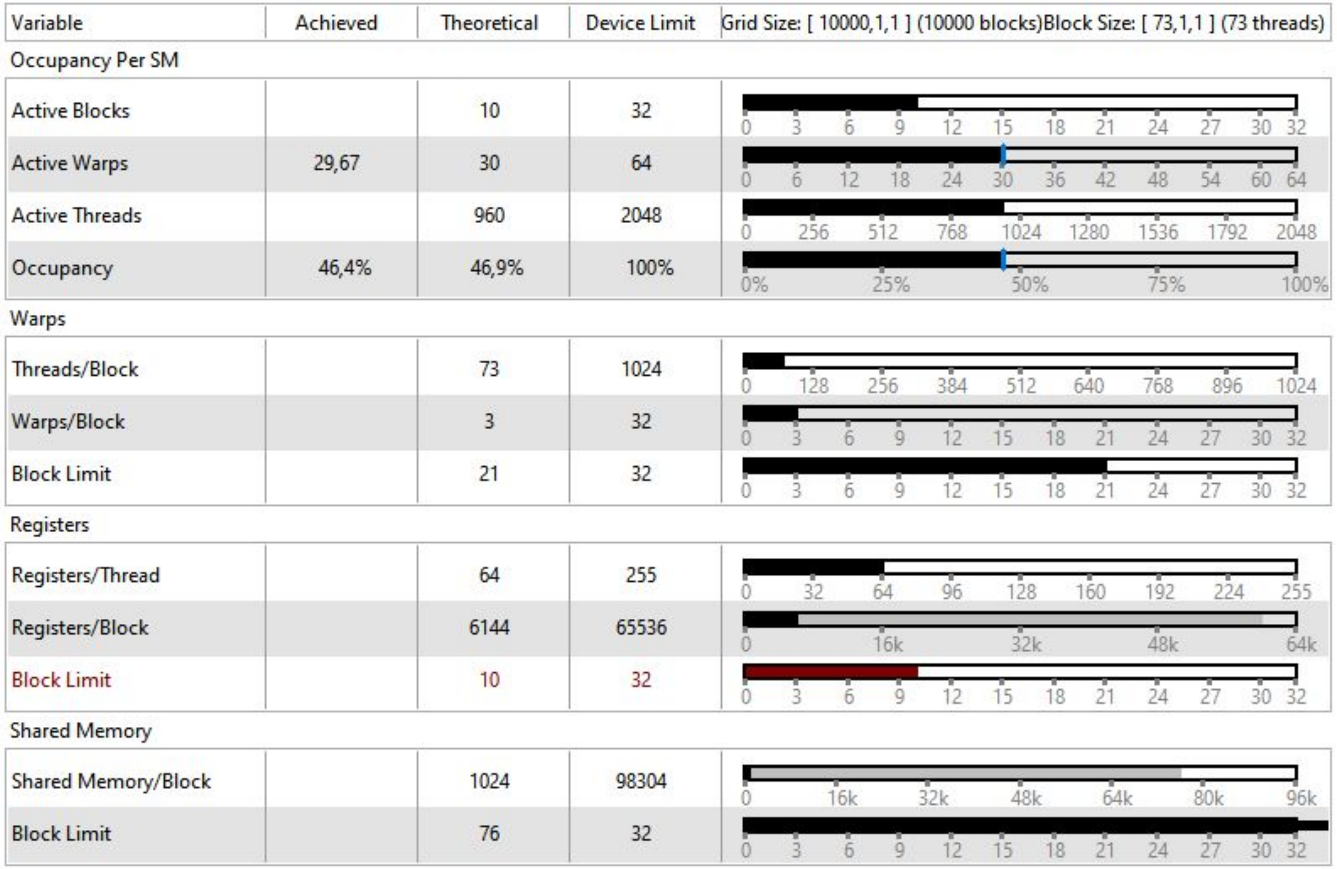
- 1.2x speed-up against a fully CPU node (40 MPI processes)

- Since there’s no communication between threads, we estimate 4.8x speed-up using the full GPU resources in a node (4 GPUs)   - *Ongoing work*



Kernel profiling

- Some optimizations already performed (like adjusting the number of registers per thread)
- The register usage is likely preventing the kernel from fully utilizing the GPU
- This usage is mostly produced by the algorithm definition, which computes big data like the Jacobian matrix



Variable	Achieved	Theoretical	Device Limit	Grid Size: [10000,1,1] (10000 blocks)Block Size: [73,1,1] (73 threads)
Occupancy Per SM				
Active Blocks		10	32	
Active Warps	29,67	30	64	
Active Threads		960	2048	
Occupancy	46,4%	46,9%	100%	
Warps				
Threads/Block		73	1024	
Warps/Block		3	32	
Block Limit		21	32	
Registers				
Registers/Thread		64	255	
Registers/Block		6144	65536	
Block Limit		10	32	
Shared Memory				
Shared Memory/Block		1024	98304	
Block Limit		76	32	

Conclusions

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Conclusions

- Our Block-cells strategy increase the GPU parallel threads against traditional implementations (Nº Threads = Nº Cells)

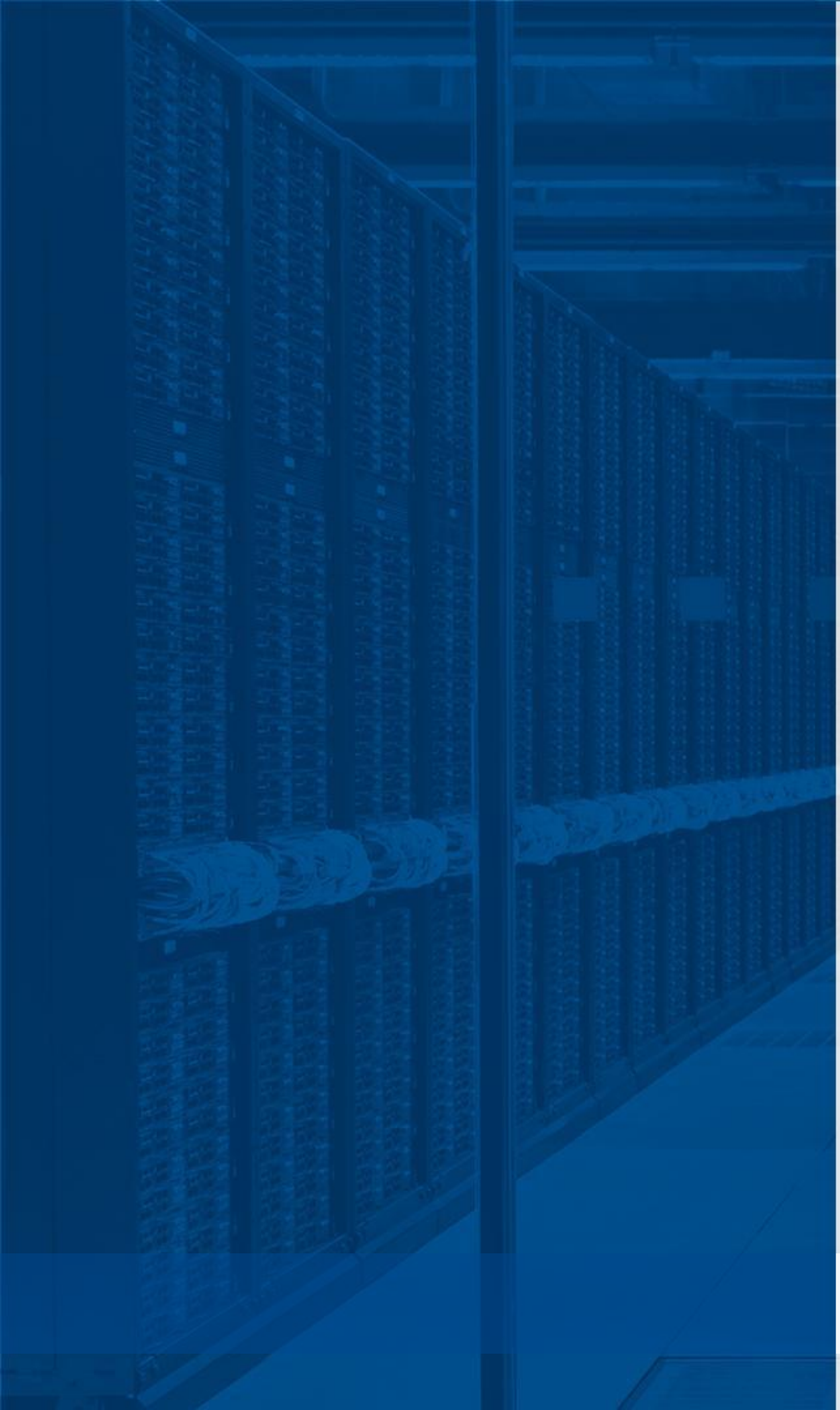
- The CUDA BDF loop performs up to 35x times faster than CPU single-thread
  - 1.2x speed-up against CPU using the fully resources node.
  - Since the load is independent between threads, we estimate up to 4.8x speedup using 4 GPUs per node.

- The kernel profiling suggests a limitation on the performance by memory

- Our approach can be used in more chemical applications thanks to the versatility of the CAMP module.

Future work

- Add multi-device functionality to compute up to 4 GPus per node.
- Balance load between CPU and GPU architectures.
- Integrate our implementation inside an atmospheric model.



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Thank you

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