GPU-accelerated modelling of greenhouse & pollutants gases in ICON-ART with OpenACC

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1 Introduction

Anthropogenic activities have altered air composition by releasing excess greenhouse gases and air pollutants. Numerical modelling of atmospheric transport and chemistry significantly helps with understanding their emissions and impacts. Advanced Graphical Processing Units (GPUs) have improved our ability to develop efficient high-resolution weather and climate models, using, among other tools, compiler directives like OpenACC. In this work, OpenACC directives are used to accelerate the Aerosol and Reactive Transport (ART) module, which is an extension of the new weather and climate model ICON [1], with a first focus on porting the Online Emission Module (OEM) of ART to GPUs. The high-resolution simulations obtained by the GPU-accelerated OEM are used for inverse modeling of greenhouse gas emissions by assimilating concentration measurements from in-situ networks and satellites.

2 Online Emission Module

- Reads in a number of emission fields (crucial inputs for atmospheric chemistry transport models) at the beginning of a simulation.
- Performs essential processing steps, such as temporal scaling of the emissions, during the simulation (hence called **Online**) [2].

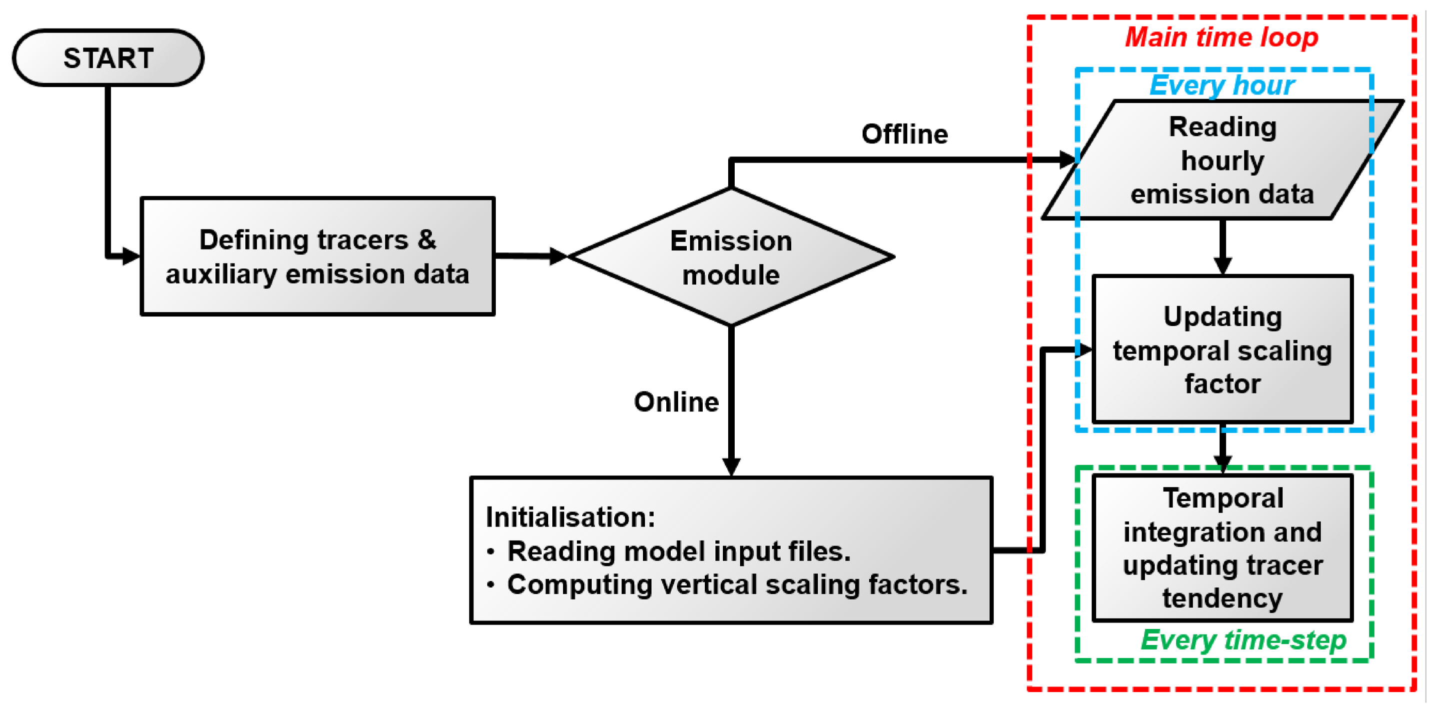

Figure 1. Flowchart of the offline and online emission processing approaches.

3 OpenACC Directives & Parallelism

- **Workers** perform the same instruction using **Vector** operations.
- **Gangs** consist of at least one Worker, which operates on a Vector of data.
- *Collapsing* loops into a single loop increases parallelism.
- The **data** directive facilitates data sharing between multiple parallel regions.

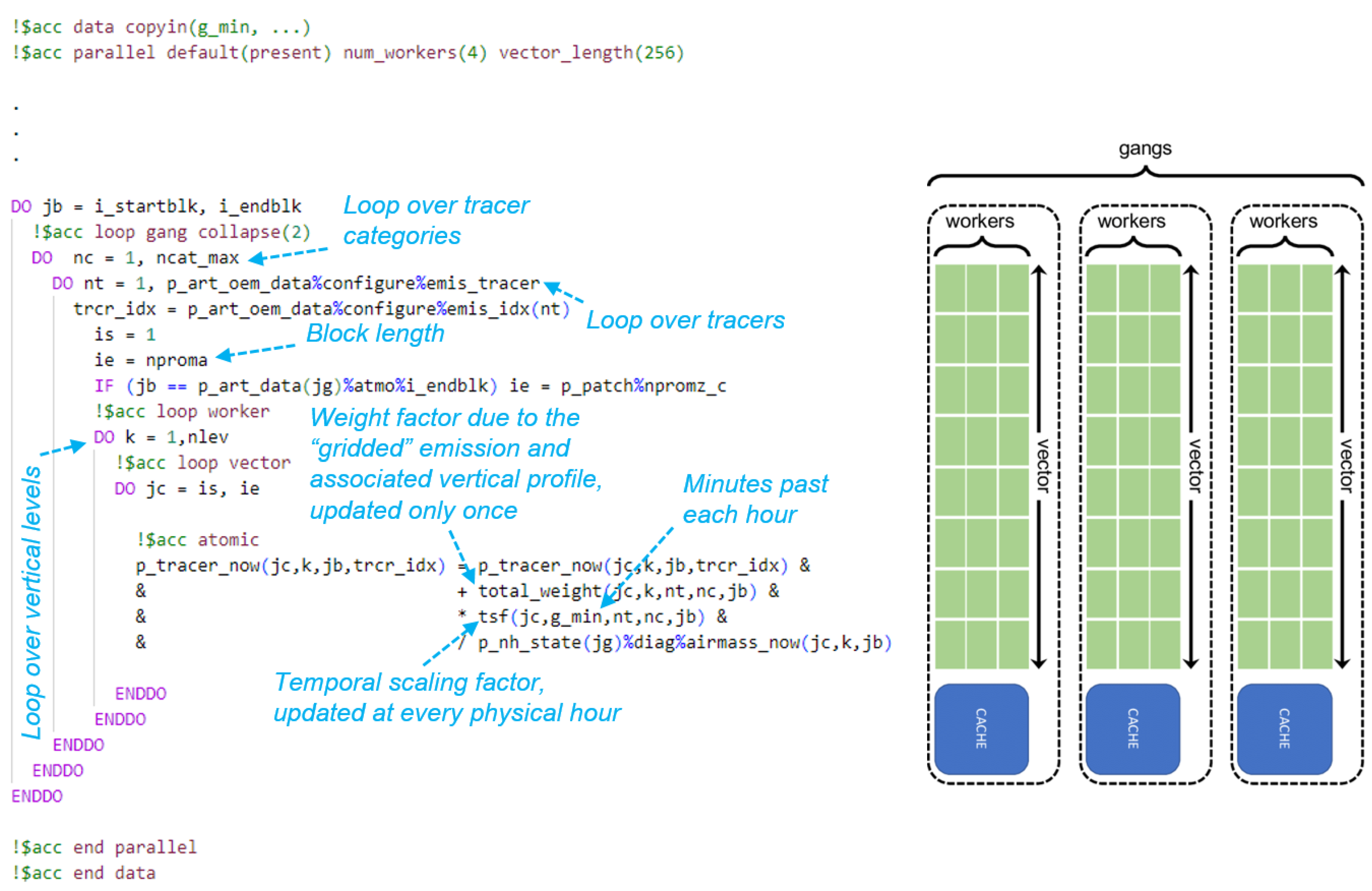

Figure 2. Left: The main loop of the GPU-accelerated OEM called at every time-step. Right: OpenACC levels of parallelism: *Gangs*, *Workers* *Vectors*.

4 Inverse Modelling

- The basic idea of the atmospheric inverse modeling is to work backwards from measurements of gas concentrations to infer their sources.
- The aim is to estimate emissions x in such a way that the simulated concentrations $H(x)$ are as consistent as possible with the observations y^0, taking into account a priori assumptions (x_b).
- For this purpose, the following cost function with two penalty-terms is minimized:

$$J(x) = \frac{1}{2}(y^0 - H(x))^T R^{-1}(y^o - H(x)) + \frac{1}{2}(x - x_b)^T P^{b-1}(x - x_b)$$

- ICON-ART with OEM provides the link between state vector x and $H(x)$ [3].
- **Solution:** Ensemble Kalman filter CarbonTracker Data Assimilation Shell. A low-rank ensemble represents the error covariance matrix P. The Kalman Gain Matrix K is estimated via ensemble correlations:

$$x^a = x^b + K(y^0 - H(x))$$
$$K = (P^b H^t)(R + H P^b H^T)^{-1}$$

- Each ensemble corresponds to a different field perturbed around a reference.

5 GPU Performance

- Up to 2X overall ICON-ART and 7X OEM speed-ups on GPUs.
- Nearly identical results between CPUs and GPUs after 720 time-steps.
- Simulations are now possible on a much finer spatial resolution.

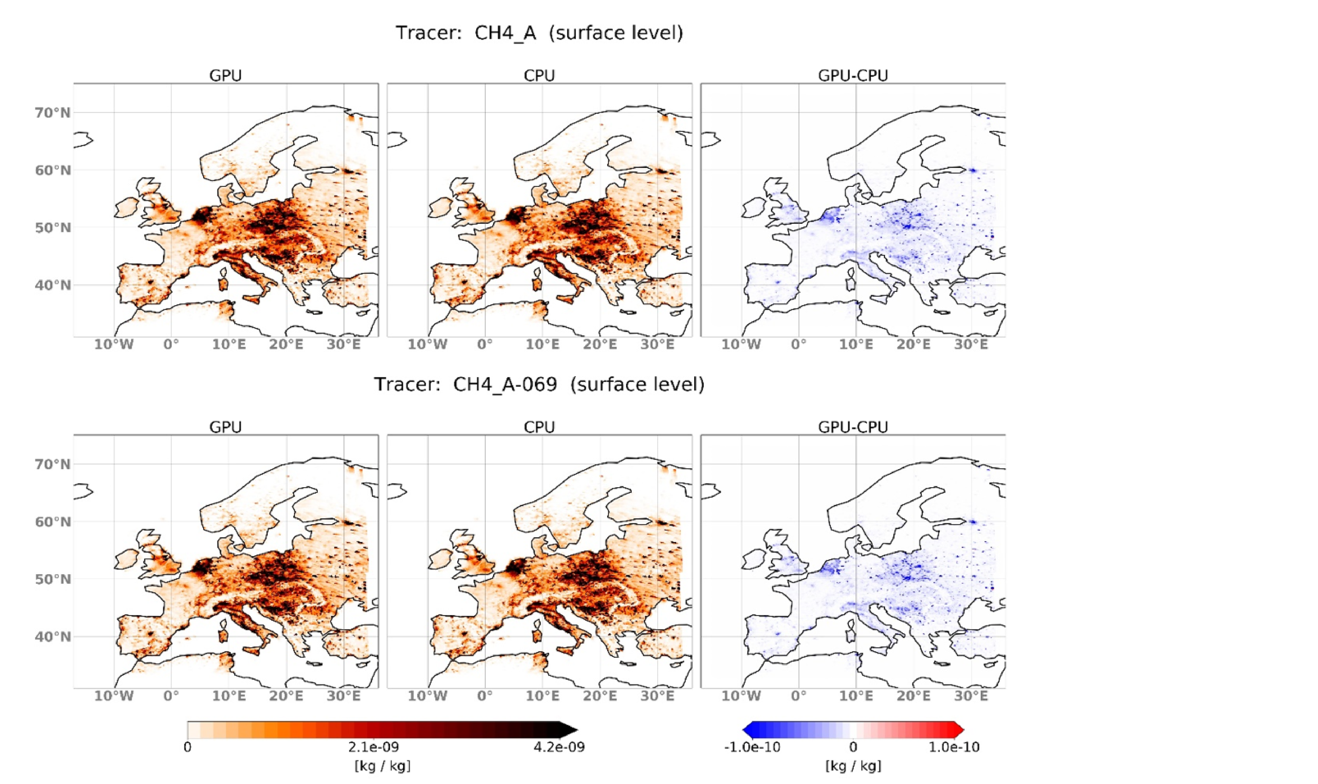

Figure 3: CPU vs. GPU: Methane distribution over Europe for a case with 192 ensemble tracers on a grid with a total of $\sim$ 5 million cells (60 vertical levels). Top: Concentration field for the baseline scenario. Bottom: Its 69^{th} ensemble.

6 Conclusion

- Ported OEM of the ICON-ART framework to GPUs.
- Achieved good agreement between CPU and GPU results, demonstrating accuracy and reliability.
- Faster computation times on GPUs enabled high-resolution inverse modelling.
- Currently, implementing a Vegetation Photosynthesis and Respiration Model (VPRM) in the GPU code, further enhancing capabilities.

Acknowledgement

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References

[1] M. A. Giorgetta *et al.*, *Journal of Advances in Modeling Earth Systems* **10**(7), 1613 (2018).
[2] M. Jähn *et al.*, *Geoscientific Model Development* **13**(5), 2379 (2020).
[3] J. Schröter *et al.*, *Geoscientific Model Development* **11**(10), 4043 (2018).