Noname manuscript No.
(will be inserted by the editor)

Evaluating the performance and energy efficiency of COSMO-ART, a fully online coupled model system composed of a numerical weather forecast model and a chemical transport model.

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Received: date / Accepted: date

Abstract In this paper we present COSMO-ART, an extension of the operational weather forecast model of the German Weather Service (DWD), developed for the evaluation of the interactions of reactive gases and aerosol particles with the state of atmosphere at the regional scale. It includes secondary aerosols, directly emitted components like soot, mineral dust, sea salt and biological material as pollen. Processes such as emissions, coagulation, condensation, dry deposition, wet removal, and sedimentation of aerosols are taken into account. The overall performance of this application on HPC systems is analysed by a profiling and tracing study to determine hotspots and identify critical paths. Moreover, we describe measurement devices and energy-aware techniques employed to evaluate the energy footprint of the considered application and to get detailed insights about power bottlenecks. Our motivation is to improve corresponding code sections to sustain high performance while minimizing energy-to-solution. This preliminary study sets the basis of broader considerations to tackle challenges related to energy efficient high performance computing in the framework of the Exa2Green project (`http://exa2green.eu/`).

Keywords High performance computing · Energy-aware computing · Green computing · Numerical weather prediction · Atmospheric chemistry · Aerosols modelling · Profiling methods · Benchmark analysis · COSMO-ART coupled model

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1 Introduction

Comprehensive scientific assessments of climate-warming trends over the past 50 years have shown that the state and dynamics of the Earth's climate system have undergone unprecedented major changes, as evidenced by increases in global average atmosphere and ocean temperatures, widespread melting of snow and ice, and rising sea levels. The last report of the Intergovernmental Panel on Climate Change, released in September 2013 (6), concluded that most of the observed temperature increases since the mid 20th Century have been caused by increasing concentrations of greenhouse gases resulting from anthropogenic activities such as fossil fuel burning and deforestation. Long-lived greenhouse gases, for example carbon dioxide, methane and nitrous oxide, are chemically stable and linger homogeneously well-mixed and over time scales of a decade to thousands of years in the atmosphere; whereas short-lived gases such as water, suphur dioxide and carbon monoxide which respond physically or chemically to changes

in temperature, act primarily as a feedback mechanism. Some extremly powerful greenhouse gases, such as fluorinated gases can even have a warming effect on the atmosphere up to 23000 times greater than carbon dioxide (26). Fortunately the European Parliament, which has gained worldwide recognition as a leader in climate policy, has passed legislation in March 2014 to phase out fluorinated gas emissions by two-thirds by 2030, towards the internationally agreed goal of keeping global warming below 2 degrees Celsius compared to the temperature in pre-industrial times.

Current cumulative releases of human-induced gas emissions enhances the greenhouse effect to the Earth's atmosphere and thus creates a large imbalance between incoming solar absorbed radiation and outgoing longwave radiation emitted back to space, through radiative trapping. While the Earth's temperature is dependent upon the greenhouse-like action of the atmosphere, the Earth's radiation balance is strongly influenced by several other factors such as the type of surface that sunlight first encounters. Forests, grasslands, ocean surfaces, ice caps, deserts, and cities all absorb, reflect, and radiate radiation differently. Sunlight falling on a white glacier surface strongly reflects back into space, resulting in minimal heating of the surface and lower atmosphere. Sunlight falling on a dark desert soil is strongly absorbed, on the other hand, and contributes to significant heating of the surface and lower atmosphere. Cloud cover also affects greenhouse warming by both reducing the amount of solar radiation reaching the earth's surface and by reducing the amount of radiation energy emitted into space.

Aerosols are suspensions of liquid, solid or mixed particles in the air (including sea salt, mineral dust, sulphate, nitrate, organic carbon and black carbon), with highly variable chemical composition and size distribution (17). Although they are not considered a heat-trapping greenhouse gas and have shorter atmospheric lifetimes, they significantly affect the Earth's radiation budget and are acknowledged as one of the most significant and uncertain aspects in anthropogenic forcing over the last 150 years (6, 10). Enhanced aerosols concentrations can impact the climate system by reflecting (e.g. pure sulfates and nitrates) or absorbing (e.g. black carbon) solar radiation and thereby exert a cooling or warming effect on the Earth-atmosphere system, causing a so-called direct radiative forcing (3–5, 13, 15, 18). Depending on their size and chemical composition, they can also act as cloud condensation and ice nuclei and profoundly impact the cloud microphysical processes and optical properties (cloud albedo effect, 24), leading to changes in droplet concentrations (1) and precipitation (7, 12, 16, 19, 21, 23), and therefore producing a negative indirect radiative forcing (5, 14, 20, 25). However, the effects of anthropogenic aerosols on clouds and the hydrological cycle as well as the cloud lifetime effect are especially hard to assess and quantify (6), and remain one of the largest uncertainties in climate modeling and in climate change prediction due to the lack of understanding of cloud feedbacks (11, 20, 22).

Hence to enhance our understanding of aerosol-cloud interactions and reduce uncertainties of aerosol effects in climate, the research community is making a concerted international effort to represent the underlying chemical processes through models. These models, such as ART (Aerosols and Reactive Trace gases) extension, developed at the Karlsruhe Institute of Technology (KIT), offer a key opportunity to reduce the climate uncertainty, particularly on the regional scale (2, 8, 9). These models can be coupled with climate models, such as the regional weather forecast model COSMO (Consortium for Small-scale Modelling), jointly developed by a consortium of European weather centers including the German weather service DWD and MeteoSwiss, and used in the climate version COSMO-CLM by a wide research community. The extended COSMO-ART model provides a detailed description of air pollution chemistry and aerosol processes, and is mainly designed to study air quality and aerosol meteorology feedbacks on short, episodic to annual time scales. It is capable of simulating aerosol distributions as well as their interactions over Europe as well as other regional domains.

COSMO-ART is computationally much more demanding than the COSMO core since a large number of additional tracers and processes have to be considered. Thus this model is currently severely-limited in terms of applicability and expensive in terms of energy consumption. COSMO has recently been ported to GPUs within the framework of the High Performance and High Productivity Computing (HP2C) Initiative to optimize it for computational and energy efficiency. Although these developments will facilitate the application of COSMO for numerical weather prediction and climate simulations, they do little to address the coupling with the ART model extension, for which significant investments are still required to take it to a similar level. The efficiency of ART is being addressed in the EU Exa2Green project. In Sec. 2, we introduce the aerosol model and its its integration into COSMO. Sec. 3 presents the hardware considerations. In Sec. 4 we describe measurement devices and energy-aware techniques employed to evaluate the energy footprint of the considered appli-

cation. Finally, Sec. 5 presents a benchmark analysis of COSMO-ART from the Exa2Green project to highlight the critical components and an outline of the next steps for model optimization. The ultimate goal of the project is to deliver a prototype code, which provides an energy efficiency of at least five times of the baseline value. Such an implementation would allow the community to investigate critical questions at higher resolution and over longer periods, at reduced cost to the environment.

2 COSMO coupled with ART extension

2.1 Model description and set-up

3 Hardware description

4 Power measurement systems

5 Benchmark results

Acknowledgements This research was supported by the Exa2Green research project co-funded under the EU 7th Framework Program Future and Emerging Technologies (FET) Proactive Initiative: Minimising Energy Consumption of Computing to the Limit (MINECC). The authors would like to thank the High Performance and High Productivity Computing Initiative (`www.hp2c.ch`).)

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