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Evaluating the Performance and Energy Efficiency of COSMO-ART, a Fully Online Coupled Model System with Numerical Weather Forecast and Chemical Transport Models

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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 work sets the basis for subsequent studies to tackle challenges related to energy efficient high performance computing in the framework of the Exa2Green project (`http://exa2green.eu/`).

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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 (12), 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 (43). 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 long-wave 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 (24). Although they are not considered a heat-trapping greenhouse gas and have shorter atmospheric lifetimes, they significantly affect the atmospheric radiative fluxes and are acknowledged as one of the most significant and uncertain aspects in anthropogenic forcing over the last 150 years (12, 17). 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 (6, 7, 11, 20, 22, 25). Depending on their size and chemical composition, they can also act as cloud condensation and ice nuclei, and thereby influence the cloud microphysical processes and optical properties (cloud albedo effect, 37) through the contribution to cloud formation. This results in changes in droplet concentrations (2) and precipitation (13, 14, 19, 23, 29, 32, 36), producing a so-called negative indirect radiative forcing (11, 21, 30, 38). Wet scavenging of aerosol particles represents a major removal mechanism for air pollutants from the atmosphere, 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 (12), and remain one of the largest uncertainties in climate modeling and in climate change prediction due to the lack of knowledge in cloud feedbacks (18, 30, 33).

Hence to improve 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 (5, 15, 16). 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. 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. In Sec. 2, we introduce the regional atmospheric model COSMO-ART (41) that accounts for feedbacks between chemistry, aerosols, radiation, and clouds. Sec. 3 and Sec. 4 successively describe the hardware and measurement devices used in evaluation as well as energy-aware techniques employed to determine the energy footprint of the considered application. Sec. 5 shows benchmark results from the Exa2Green project and highlights areas where improvements will be necessary for the baseline optimisation. Finally, we conclude and give directions for further developments of the modeling system in Sec. 6.

2 The COSMO-ART model system

2.1 Model description

COSMO-ART (ART stands for Aerosols and Reactive Trace gases), developed at KIT Karlsruhe (41), is a regional to continental scale model coupled online to the COSMO numerical weather prediction (NWP) and climate model (4). Physical processes like transport, turbulent diffusion, and dry and wet deposition are treated together with photochemistry and aerosol dynamics using the modal approach.

Aerosols dynamics are simulated with the modal aerosol microphysics module MADE (1), expanded in MADEsoot to feature explicit treatment of soot aging through condensation of inorganic (26) and organic substances. MADE describes the aerosol population through five modes representing sub-micron particles consisting of sulphate, ammonium, nitrate, particulate organic matter, water and soot (27) in a range of mixing state. These modes are coupled with the gas phase by condensation and nucleation, and are strongly influenced by anthropogenic emissions of gases and particles. MADEsoot describes the sub-micrometer aerosol population, composed of sea salt (22), mineral dust particles (34, 40), by means of six interacting log-normal modes. For each mode, mass contributions and total number concentration are prognostic quantities, while the standard deviation is fixed.

Specific modules are included to simulate the dispersion of pollen grains (42) and other biological particles. Meteorologically-influenced emissions are also online coupled within the model system. The biogenic VOC (volatile organic compounds) emissions are calculated as functions of the land use type based on the Global Land Cover 2000 dataset and the modeled temperatures and radiative fluxes (39).

The gaseous chemistry in COSMO-ART is solved by a modified version of the Regional Acid Deposition Model, Version 2 (RADM2) mechanism (35), which is extended to describe secondary organic aerosol formation based on a volatile basis set (VBS) approach (3) and hydroxyl radical recycling due to isoprene chemistry (10). The thermodynamic equilibrium between the gas and particulate phases of the inorganic material is achieved through the ISORROPIA II module (9).

COSMO-ART is fully online-coupled, and allows for feedbacks of aerosols on temperature, radiation and cloud condensation nuclei (CCN). Analytical description of modules incorporated for this purpose exists in (5, 41). The radiation scheme used within the model to calculate the vertical profiles of shortwave and longwave radiative fluxes is GRAALS (28). In order to account for the interaction of aerosol particles with the cloud microphysics and radiation, COSMO-ART uses the two-moment cloud microphysics scheme of Seifert and Beheng (31) and comprehensive parameterizations for cloud condensation and ice crystal nucleation (5, 6). The system of stiff ordinary differential equations described by chemical reactions in the aqueous-phase together with the transfer reactions is solved using the Kinetic PreProcessor (KPP, 8).

Detailed model description can be found in the aforementioned publications as well as in (6, 15, 16, 34).

2.2 Model setup

To define a baseline within a code under development, it was necessary to find a run-configuration capable of being recreated in all subsequent versions. The energy-to-solution benchmarking of COSMO-ART concerns one-day long simulations without spin-up stage, using a 222x216x40 discretization of Europe and a time step of 120s. The baseline code incorporates 34 2-d and 45 3-d fields to be written out every hour for a simulation starting on April 13th, which is close to the equinox and thus brings benefits of having approximately half day of night and half day of sun exposure, to ensure a proper activation of the chemistry cycle. Ultimately new input files closer to the equinox (on March 20th) will be created, but the current set of input files is fine for the time being.

This COSMO-ART version is configured to deal with a semi Lagrangian horizontal advection scheme with tricubic interpolation and selective filling diffusion option in combination with the Runge-Kutta dynamical core. Concerning the modelling of wet deposition in aerosols, the baseline has only indirect cloud feedbacks but doesn't include in-cloud scavenging (rainout) and below-cloud scavenging (washout) yet. Amongst physical parameterizations, precipitation formation is performed by a two-moment cloud microphysics scheme instead of a classical bulk microphysics scheme. Another important point is the fact that this version makes use of the Kinetic PreProcessor solver for the resolution of atmospheric chemistry ordinary differential equations.

3 Hardware description

4 Power measurement systems

4.1 Power-Performance measurement framework

To assess the performance and the energy efficiency of COSMO-ART, we employ a version of the integrated framework presented in (**?**) that works in combination with VampirTrace and Vampir, which are profiling/tracing and visualization tools, respectively. To use our approach, COSMO-ART is compiled using the VampirTrace compiler wrappers, which automatically instrument the Fortran code of the model. Next, COSMO-ART is run on the nodes, thus dissipating certain amount of power. The server nodes are connected to power measurement devices that account for the dissipated power/consumed energy and send the power data to the tracing server. The attached VampirTrace `pmlib` plugin employs the client API that sends start/stop primitives in order to gather captured data by the wattmeters onto the tracing server, where an instance of the `pmlib` server is running. Once COSMO-ART run is finished, the VampirTrace `pmlib` plugin receives the power data from the tracing server. The instrumentation post-process generates the performance trace files and the `pmlib` plugin inserts the power data into them.

In addition to the power measurements, we also account for the resource utilization values of the nodes: CPU load, memory usage and storage device utilization.

We run special `pmlib` server instances on the server nodes that retrieve these values from the `proc` file system (leveraging the `psutil` Python library). Thus, `pmlib` plugin instances running with the instrumented application connect with the `pmlib` servers. Finally, using the Vampir visualization tool, the power-performance traces can be easily analyzed through a series of plots and statistics.

5 Benchmark results

6 Conclusion

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