D5.4 Summer School

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Energy-efficient Scalable Algorithms for Weather and Climate Prediction at Exascale

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1 Executive Summary

The ESCAPE-2 Summer School dissemination activity reported in this deliverable. The School, which had originally been planned for the summer of 2020, was cancelled and finally held online only in July 2021 due to the developments related to the COVID-19 epidemic.

2 Introduction

2.1 Background

ESCAPE-2 will develop world-class, extreme-scale computing capabilities for European operational numerical weather and climate prediction systems. It continues the pioneering work of the ESCAPE project. The project aims to attack all three sources of enhanced computational performance at once, namely (i) developing and testing bespoke numerical methods that optimally trade off accuracy, resilience and performance, (ii) developing generic programming approaches that ensure code portability and performance portability, (iii) testing performance on HPC platforms offering different processor technologies. ESCAPE-2 will combine well-established large-timestep forward-in-time computing with highly scalable, flexible order spatial discretization with minimal data movement.

2.2 Scope of this deliverable

2.2.1 Objectives of this deliverable

Accurate numerical weather prediction relies on massively parallel computing resources and models that can efficiently harness that computational power. As high-performance computing architectures approach the exascale (10^18 floating-point operations per second), forecast models are undergoing significant scientific and technological change in order to run at finer and finer resolution within tight operational constraints.

This deliverable has aimed to introduce students to computational tools currently used in operations and research on weather forecast models, including numerical algorithms, uncertainty quantification models, and high-performance computing tools. Theoretical lectures have been complemented by hands-on training where the students will develop small group projects using the techniques presented in the course.

2.2.2 Work performed in this deliverable

The School organizers arranged a full program of theoretical and practical activities, described in detail below. The School was also granted logistic support from the Fondazione Volta – Lake Como School of Advanced Studies, an Italian no-profit organization which sponsors advanced scientific meetings on a wide range of topics and whose assistance was extremely valuable in increasing the outreach to a larger number of potential participants. Out of 93 applicants, the organizers selected 39 participants (with almost exact gender balance) from different countries, based on their experience and age (preference was given to younger applicants, in order to increase the potential impact of the dissemination activity). Four of the participants however did not attend the School activities in full and did not participate in the proposed group work.

2.2.3 Deviations and counter measures

The Summer School, which had originally been planned for the summer of 2020, was finally held online in July 2021 due to the developments related to the COVID-19 epidemic.

3 Summer School Agenda

The full Summer School timetable is reported below.

	July 19	July 20	July 21	July 22	July 23
9-9.15	Welcome				
9.15-10.00	Perspectives and challenges of exascale NWP (N.Wedi, ECMWF)	Finite volume methods and solvers for NWP (T.Benacchio, POLIMI)	Introduction to Domain Specific Languages (WP2) (M. Röthlin, MeteoSwiss)	Project work	Project work
10.00-11.00	Perspectives and challenges of exascale NWP (N.Wedi, ECMWF)	Exercise session Finite volume methods and solvers for NWP (T.Benacchio, POLIMI)	Exercise session on Domain Specific Languages (WP2) (C. Müller, MeteoSwiss)	Project work	Project work
11.00-11.15	Break	Break	Break	Break	Break
11.15-12.00	Introduction to parallel programming with MPI and OpenACC (I. Epicoco, CMCC)	Uncertainty quantification for NWP (R.Chocat,CEA)	DG methods for NWP (G. Tumolo, ECMWF)	Project work	Project work
12.00-13.00	Introduction to parallel programming with MPI and OpenACC (I. Epicoco, CMCC)	Exercise session Uncertainty quantification for NWP (R.Chocat, CEA)	Exercise session DG methods for NWP (G. Tumolo, ECMWF)	Project work	Project work
13.00-14.15	Lunch break	Lunch break	Lunch break	Lunch break	Lunch break
14.15-15.00	Spectral transform methods for NWP (A. Müller, ECMWF)	Introduction to profiling tools (M.Acosta, BSC)	Presentation of projects by all lecturers	Project work	Presentation of project results
15.00-16.00	Exercise session on Spectral transforms (A. Müller, ECMWF)	Exercise session on profiling tools (M. Acosta, BSC)	Project work	Project work	Presentation of project results
16.00-16.15	Break	Break	Break	Break	Closing
16.15-17.00	Uncertainty quantification for NWP (R.Chocat, CEA)	Introduction to scheduling (P.Karlshöfer, ATOS)	Project work	Project work	
17.00-18.00	Exercise session Uncertainty quantification for NWP (R.Chocat, CEA)	Exercise session on scheduling (P.Karlshöfer, ATOS)	Project work	Project work	

4 Abstracts and Lectures

We report here the detailed abstracts of all the lectures.

4.1 Perspectives and challenges of exascale NWP

Nils P. Wedi

ECMWF, (European Centre for Medium Range Weather Forecasts), Reading (UK), Bologna (Italy), Bonn (Germany)

Using the 40-year history of ECMWF's Integrated Forecasting System (IFS) as an example, the lecture is an introduction to the development and current state-of-the-art of global numerical weather prediction (NWP), as well as to the challenges faced in the future. It is intended to provide an overview and context for the algorithmic and technological developments covered in more detail during the summer school. The first part will start with some examples of meteorological phenomena and associated forecasting challenges, leading in part two towards mapping these in a series of technological challenges onto the emerging and diverse high-performance computing (HPC) architectures.

4.2 Introduction to parallel programming with MPI and OpenACC

Italo Epicoco

CMCC, (Euro-Mediterranean Centre for Climate Change), Lecce, Italy

The lecture proposes a basic introduction to the parallel programming paradigms addressing the distributed memory approach, through the Message Passing Interface (MPI), and the shared memory approach with OpenACC that allows the use of compiler directives and supports the execution on heterogeneous parallel architectures. The lecture will also provide an overview of the evaluation of the parallel efficiency and scalability. During the hands-on session, the students will be guided in the implementation of a simple example of parallel code.

4.3 Spectral transform methods for NWP

Andreas Müller

ECMWF, (European Centre for Medium Range Weather Forecasts), Reading (UK), Bologna (Italy), Bonn (Germany)

Many global atmospheric models are based on the spectral transform method with spherical harmonics. Transforming the fields from physical space to spectral space converts spatial derivatives into algebraic expressions. This makes the spectral transform method a very efficient approach for solving differential equations. One of the atmospheric models based on the spectral transform method with spherical harmonics is the Integrated Forecasting System (IFS). IFS is used very successfully by the European Centre for Medium-range Weather Forecasts (ECMWF) for operational weather prediction. This lecture explains together with the hands-on exercises the basic idea behind the spectral transform method, presents the issue of aliasing and different approaches to solve it and discusses the performance of the spectral transform and how it compares to other commonly used numerical methods used for weather prediction.

4.4 Uncertainty quantification for NWP

Rudy Chocat

CÉA, (Alternative Energies and Atomic Energy Commission), France

Verification, Validation and Uncertainty Quantification (VVUQ) is a common topic for all fields based on the simulation to model phenomenon such as Numerical Weather Prediction (NWP). This lecture will define each term based on the open-source URANIE platform, initially designed for UQ, adapted for verification, which focuses on numerical aspects, and validation, which compares the reality with the model. Different modules of the URANIE platform will be introduced:

- The sampler to generate a design of experiments;
- The modeler to build a surrogate model;
- The sensitivity to quantify the impact of inputs;
- The calibration to identify the tuned parameters according to experiments.

4.5 Finite volume methods and linear solvers for NWP

Tommaso Benacchio

Politecnico di Milano, Italy

Finite volume methods are used worldwide for operational weather and climate prediction. The lecture will cover the basics of finite volume methods, starting from the one-dimensional scalar case, then moving on to the discretization of the three-dimensional compressible fluid flow equations in conservation form using the next-generation Finite Volume Module (FVM) of the ECMWF Integrated Forecast System as an example. The second part of the lecture will discuss iterative methods for the solution of linear systems as found in semi-implicit time discretization used in FVM. In the interactive practical session, we will study the accuracy and performance of an iterative solver with different parameter values (solver tolerance,horizontal and vertical resolution, orography height) in a simplified setting.

4.6 Introduction to profiling tools and performance analysis

Mario Acosta, Daniel Beltran

BSC, (Barcelona Supercomputing Centre), Barcelona, Spain

Most applications targeting exascale machines require some degree of rewriting to expose more parallelism, and many face severe strong-scaling challenges if they are effectively to progress to exascale, as it is demanded by their science goals. The community needs different approaches to figure out how to increase the computational performance of the climate and weather models and how to adapt them for the new generation of supercomputers, when the increase of computer power will be mandatory to reduce the uncertainties of climate simulations and the massive paralellization could be a problem in terms of exploiting the computational efficiency adequately.

4.7 Managing workload on clusters - SLURM

Paul Karlshöfer

Atos, France

Modern supercomputers have to deal with a very diverse workload from a multitude of user communities. To ensure that jobs are distributed efficiently across the machine, and that execution order is fair, workload managers handle the scheduling on most large-scale machines. SLURM, being the most popular in Europe, is a prominent example. In this lecture, students will get to know the general architecture and topology of supercomputers, as well as the main features of SLURM. We will also discuss some common pitfalls and best practices to use the available resources most efficiently.

4.8 The dusk & dawn Toolchain for unstructured Weather and Climate Codes on the Extreme Scale

Matthias Röthlin, Christoph Mueller

MeteoSwiss, Zurich, Switzerland

How to write climate and weather codes that guarantee portability, performance and (developer) productivity at the same time is still an open question. Our lecture will propose the approach of Domain Specific Languages (DSLs) as a possible solution. It will be explained how DSLs can truly decouple model developer concerns from performance and parallelization matters by virtue of special purpose compilers. We will use the dusk & dawn toolchain as a worked example to illustrate the learnings. The toolchain has reached maturity for Finite Difference Codes and is being enhanced to also accept Finite Volume computations on icosahedral triangle meshes at MeteoSwiss. An exercise will be proposed, starting with some simple "hello world" code in dusk and proceeding to implement FVM differential operators (gradient, curl, divergence).

4.9 Discontinuous Galerkin methods for NWP

Giovanni Tumolo

ECMWF, (European Centre for Medium Range Weather Forecasts), Reading (UK), Bologna (Italy), Bonn (Germany)

In this lecture discontinuous Galerkin (DG) methods for numerical weather prediction (NWP) will be described. Both strengths and limitations of such methods applied to atmospheric modeling will be discussed and possible ways to improve their efficiency reviewed. A particular strategy based on combining a high order DG discretization with p-adaptivity techniques and efficient semi-Lagrangian and semi-implicit time integrators will be presented in the context of simplified NWP model equations. An outlook towards the parallel implementation of such numerical formulation in the case of a dynamical core prototype will also be discussed.

5 Student Projects

A number of hands-on practical project activities based on contents of the previously listed lectures were offered during the School. Participants were evenly distributed among the different activities, in order to promote group work and interaction with the teacher. The results of each activity were briefly presented at the end of the School. A full list of the proposed activities is reported below.

5.1 Uncertainty quantification for NWP

Teacher: Rudy Chocat

CÉA, (Alternative Energies and Atomic Energy Commission), France

The focus of the student project will be to perform a complete VVUQ analysis on the shallow water code with different level of complexity. The goal is to identify the meaning of each inputs.

5.1.1 Main goals

Improvement of VVUQ knowledge and performing analysis using the URANIE platform.

5.1.2 Specific objectives/tasks

- Chain the Shallow water model with the URANIE platform using the python API;
- Perform Graphics uncertainty analysis;
- Sensitivity indicators to understand the code;
- Identify the unknown Inputs;
- If needed, use machine learning to speed up the code;
- Run parallel computation;
- Understand the URANIE documentation.

5.1.3 Required knowledge

Basic knowledge of programming and statistics is necessary for this exercise.

5.1.4 Recommended readings

Blanchard, J.-B. Damblin, G., Martinez, J.-M., Arnaud, G., Gaudier, F. The Uranie platform: an Open-source software for optimisation, meta-modelling and uncertainty analysis. EPJ Nuclear Sciences & Technologies, 2018. Pdf available at https://arxiv.org/pdf/1803.10656.pdf

5.2 5.2 Spectral transform methods for NWP

Teacher: Andreas Müller

ECMWF, (European Centre for Medium Range Weather Forecasts), Reading (UK), Bologna (Italy), Bonn (Germany)

The focus of the student project will be on writing a simple spectral transform code in Python to get a better understanding of the spectral transform method. This will allow the students to understand the basic functionality of the method. The code written by the students will also serve as an example for improving the performance of scientific code in general. We will consider different strategies to analyse and optimise the efficiency of code. This makes this project not only well suited for students who are interested in understanding the fundamental idea behind the spectral transform method but also for students who want to learn how to improve the computational performance of their own code. The focus will be on general principles for improving the performance of scientific codes and not on specific features of the Python language which we will use.

5.2.1 Main goals

Implement a simple spectral transform method and optimise its computational performance.

5.2.2 Specific objectives/tasks

- Create a latitude-longitude mesh;
- Write Python function to compute Legendre transformation;
- Write Python function to compute (slow) Fourier transformation;
- Use the previously written functions to write a spectral transform code in Python;
- Test the code;
- Analyse the performance of the code;
- Discuss ideas on how to parallelise the spectral method;
- Implement a basic parallelization in Python.

5.2.3 Required knowledge

Basic knowledge of programming is necessary for this exercise.

5.2.4 Recommended readings

Boyd, J. P. Chebyshev and Fourier Spectral Methods. Dover Publishers, New York, 2000. Chapter 1 and 18.

Eijkhout, V., van de Geijn, R., and Chow, E. Introduction to High Performance Scientific Computing. Zenodo. 2016. Available (pdf and html version) at http://doi.org/10.5281/zenodo.49897 Especially Chapter 1-3.

5.2.5 Additional readings

Severance, C. and Dowd, K. High Performance Computing. Connexions, 2012. Available (pdf and html) at http://cnx.org/content/col11136/1.5

Durran, D. R. Numerical Methods for Fluid Dynamics. Springer, 2010. Chapter 6.1–6.4

5.3 5.3 Introduction to parallel programming with MPI and OpenACC

Teacher: Italo Epicoco

CMCC, (Euro-Mediterranean Centre for Climate Change), Lecce, Italy

During the project work, the students will be provided with a teaching code that implements a shallow water model based on the finite volume numerical approach. The students shall identify those parts of the code that can be executed in parallel and implement the MPI data exchange. Advanced students can proceed further with parallelization embedding the OpenACC directives to get a hybrid parallelization MPI+OpenACC.

5.3.1 Specific objectives/tasks

- Knowledge of distributed memory and shared memory parallel programing
- Basic knowledge of MPI library
- Basic knowledge of OpenACC directives
- Analysis of the code to identify source of parallelization
- Analysis of the loops to identify data dependency and potential race conditions
- Theoretical evaluation of parallel scalability
- Knowledge of distributed memory and shared memory parallel programing
- Basic knowledge of MPI library
- Basic knowledge of OpenACC directives
- Analysis of the code to identify source of parallelization
- Analysis of the loops to identify data dependency and potential race conditions
- Theoretical evaluation of parallel scalability

5.3.2 Required knowledge

Basic knowledge of C or Fortran programming languages is necessary for this project.

5.4 5.4 Introduction to profiling tools and performance analysis

Teacher: Mario Acosta, Daniel Beltran

BSC, (Barcelona Supercomputing Centre), Barcelona, Spain

The objective of this course for the student is to learn how *Paraver* and *Dimemas* tools can be used to analyze the computational performance of parallel applications and to familiarize with the tools usage as well as instrumenting applications with *Extrae*. This guide will provide a more practical introduction about these tools and how to apply them on climate and weather models, as well as a complete walk-through step by step.

5.4.1 Main Goals

Analyze the computational performance of a numerical model and understand the main bottlenecks

5.4.2 Specific objectives/tasks

- Define performance analysis fundamentals (objectives, methods, metrics, hardware counters, etc.);
- Describe the BSC performance analysis tools suite (Extrae, Paraver, Dimemas);
- Interpret uses cases from Climate and/or weather models that illustrate how to identify and solve performance issues;
- Apply profiling techniques to identify performance bottlenecks in your code;
- Summarise typical performance problems;
- Discuss specific knowledge about performance analysis applied to earth system modelling;

5.4.3 Required knowledge

Basic knowledge of programming and paralellization is necessary for this exercise

5.4.4 Recommended readings

Performance tools. https://www.bsc.es/discover-bsc/organisation/scientific-structure/performance-tools

5.5 5.5 Discontinuous Galerkin methods for NWP

Teacher: Giovanni Tumolo

ECMWF, Reading (UK), Bologna (Italy), Bonn (Germany)

The hands-on project work will provide students with a teaching code in Python implementing a semi-Lagrangian discontinuous Galerkin method for the advection equation in one dimension in space, as well as a standard Runge-Kutta DG scheme for the same equation. Both DG schemes will be based on the nodal DG approach.Students will be asked to parallelize the codes provided via proper MPI data exchanges. They will also be guided into the comparison between the two approaches (standard Eulerian RK-DG vs. SL-DG). More proficient students can further explore the SL-DG approach by modifying the code to obtain a version based on modal bases. The choice of focusing on 1-D problems in space comes from pedagogical reasons but a tensor product approach can easily help moving towards higher dimensional implementations.

5.5.1 Specific objectives/tasks

- To learn the fundamental building blocks of a DG code in Python for the advection equation in the two main approaches available, i.e. RK-DG and SL-DG;

- To identify the data required to be exchanged between different processes in order to run the code in parallel;
- To introduce appropriate MPI communication calls;
- To compare the fully Eulerian RK-DG approach and the SL-DG one.

5.5.2 Required knowledge

Basic coding knowledge is required, as well as basic knowledge about numerical methods, including local Galerkin methods and numerical quadratures.

5.6 5.6 The dusk&dawn Toolchain for unstructured Weather and Climate Codes on the Extreme Scale

Teachers: Matthias Röthlin, Christoph Mueller

MeteoSwiss, Zurich, Switzerland

Two small projects will be offered where students write a simple but complete model code, either for a diffusion problem and/or a shallow water solver, in dusk.The projects are suited for students that wish to gain hands-on experience using DSLs. This is especially interesting for students that already have experience writing code in a general purpose programming language and will be able to appreciate the contrast. On the other hand, the two projects come with quite verbose explanations, starting out from the continuous equations and present the discretization using the FVM. This allows students that are new to numerical methods a motivating and complete experience in implementing a simple PDE solver.

5.6.1 Required knowledge

Some basic programming knowledge is necessary.

6 Conclusion

The School was quite successful in allowing students and young researchers from a large number of countries and with very different backgrounds to get acquainted with crucial issues in exascale computing, NWP and advanced numerical methods. The School also allowed the participants to develop a firs- hand knowledge of some of the main results of the ESCAPE-2 project, getting them involved in practical sessions strictly related to the main project research areas. The feedback from the participants was extremely positive, as documented in an anonymous poll carried out at the end of the school. Out of 35 participants who effectively took part to the School, 18 gave their feedback in this poll. 83% of the respondents rated the School's general organization excellent and 17% rated it as very good. 44% of the respondents considered that the School was extremely helpful and relevant for their research and 44% considered it very helpful and relevant. 72% of the respondents rated the interaction with the lecturers excellent and 28% very good.

Document History

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