D5.6 Dissemination Workshop II

Dissemination Level: Public

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

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1 Executive Summary

On 3rd September 2021, the second of two dissemination workshops sharing the ESCAPE-2 progress with the wider weather, climate and computing community was held. Due to ongoing restrictions surrounding the COVID-10 pandemic, the workshop was help virtually. Over 70 participants attended the workshop.

The first part of the workshop was dedicated to introducing the results of the development work packages:

- WP1: Mathematics and algorithms
- WP2: Programming models and DSL
- WP3: Weather and Climate Benchmarks: HPCW
- WP4: VVUQ

The second part was dedicated to international efforts related to the ESCAPE-2 project:

- Uptake of ESCAPE-2 by ESiWACE-2
- UK Excalibur exascale initiative
- DoE E3SM developments
- WMO Research Board action on Exascalet
- Vulcan developments

2 Introduction

2.1 Background

ESCAPE-2 has developed 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 prepared weather and climate domain benchmarks that will allow a much more realistic assessment of application specific performance on large HPC systems than current generic benchmarks such as HPL and HPCG. These benchmarks are specifically geared towards the pre-exascale and exascale HPC infrastructures that the European Commission and Member States will invest in through the European Commission Joint Undertaking.

ESCAPE-2 also combines generic uncertainty quantification tools for high-performance computing originating from the energy sector with ensemble based weather and climate models to quantify the effect of model and data related uncertainties on forecasting – a capability, which weather and climate prediction has pioneered since the 1960s. This collaboration combines user-friendly tools from one community with scientific expert knowledge from another community to achieve economy of scales beyond the scope of each domain.

2.2 Scope of this deliverable

The second ESCAPE-2 Dissemination Workshop was organised by the European Centre for Medium-Range Weather Forecasts virtually on the 3rd September 2021.

2.2.1 Objectives of this deliverable

D5.6 provides the workshop proceedings including preparatory information.

2.2.2 Work performed in this deliverable

As per the Description of Action (DoA), the work performed for this deliverable included the preparation and execution of the workshop, including workshop announcements, registration processes, as well as organisation of invited talks.

2.2.3 Deviations and counter measures

Erroneously, the Description of Action set the delivery time for the workshop as M26 when it should have been M36. Thus, compared to the DoA there is a delay of 10 months. This has been communicated at the interim periodic review.

In addition, due to ongoing COVID-19 pandemic restrictions, it was decided to hold this workshop online instead of in person.

3 Workshop Announcement

ESCAPE-2 **Final Dissemination Workshop**

Towards Energy-efficient Scalable Algorithms for weather and climate Prediction at Exascale - Status and Prospects

The EU H2020-funded project ESCAPE-2 develops 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.

The Final Dissemination Workshop will present the results of the project together with relevant initiatives from international actors. The workshop agenda is available on the workshop website.

The workshop will be held online, registration is not required.

Workshop Schedule: **3rd September 2021 14:00 - 17:30 BST**

Workshop Location: Online via BlueJeans (Link on Workshop Website)

Workshop website: https://www.hpc-escape2.eu/outreach/events/escape-2-final-dissemination-workshop

4 Workshop Agenda

Time (BST)	Title	Speaker
14:00-14:15	Welcome and Introduction to ESCAPE-2	Peter Bauer & Nils Wedi
14:15-14:30	WP1: Mathematics and algorithms	Luca Bonaventura
14:30-14:45	WP2: Programming models and DSL	Carlos Osuna
14:45-15:00	WP3: Weather and Climate Benchmarks: HPCW	Erwan Raffin, David Guibert, Michiel Van Ginderachter
15:00-15:15	WP4: VVUQ	Adrien Bruneton, Rudy Chocat, Daniel Beltran, Mario Acosta
15:15-15:30	Discussion	All
15:30-15:45	Coffee break	
15:45-16:00	Uptake of ESCAPE-2 by ESiWACE-2	Florian Ziemen, Joachim Biercamp
16:00-16:15	UK Excalibur exascale initiative	Chris Maynard, Bryan Lawrence
16:15-16:30	DoE E3SM developments	Mark Taylor, Peter Caldwell, Gary Geernaert, Xujing Jia Davis
16:30-17:00	WMO Research Board action on Exascale	Kris Rowe, Mark Govett
17:00-17:15	Vulcan developments	Oli Fuhrer
17:15-17:30	Discussion	All
17:30	Adjourn	

5 Abstracts

5.1 WP1: Mathematics and algorithms

Speaker: Luca Bonaventura (POLIMI)

WP1 develops mathematical methods and implement advanced and disruptive algorithms suitable for extreme-scale parallelism that achieve major improvements in

the accuracy, efficiency, fault-tolerance, and scalability of dynamical cores and of physical parametrizations for next-generation weather and climate prediction models. Moreover, WP1 extracts and provides a range of relevant algorithmic motifs (weather and climate dwarfs) as a prerequisite for other work packages. These include key algorithms of advection, time-stepping methodologies, and of physical parametrizations, representative for leading European weather and climate models.

5.2 WP2: Programming models and DSL

Speaker: Carlos Osuna (MSWISS)

WP2 defines, develops, and applies a DSL toolchain applicable to a comprehensive list of weather and climate dwarfs. The code adaptation and code generation via the DSL toolchain are demonstrated for a number of representative and fundamentally different mathematical algorithms and horizontal discretizations. Moreover, WP2 develops and promotes APIs and generic interfaces across the DSL toolchain in order to improve reusability and inter-operability, and leverage code adaptation to emerging HPC architectures.

5.3 WP3: Weather and Climate Benchmarks: HPCW

Speaker: Erwan Raffin (ATOS BULL), et al.

WP3 develops a hierarchy of benchmarking components representing the key elements in the workflow of weather and climate prediction systems and re-integrate and test code adaptations generated from the DSL toolchain. This work establishes a representative High Performance Climate and Weather benchmark (HPCW). HPCW serves as a benchmark for (pre)-exascale applications of climate and weather codes and will facilitate communication with HPC hardware developers and vendors. The value of HPCW is demonstrated using the range of available hardware architectures.

5.4 WP4: VVUQ

Speaker: Rudy Chocat (CEA)

WP4 develops a generic European VVUQ package for weather and climate simulations that is deployable on supercomputers and that prepares workloads of pre-exascale computations on many-core configurations. The VVUQ package is being demonstrated for both dwarf and full forecasting system workloads, and scenarios are explored with optimized case performance based on the available VVUQ methodologies. WP4 confronts ensemble-based and other methodologies to improve VVUQ practices and to produce a generic VVUQ framework for climate simulation at the European level.

5.5 Uptake of ESCAPE-2 by ESiWACE-2

Speaker: Florian Ziemen (DKRZ)

An important component of the ESCAPE-2 dissemination activities is the coordination with the centre of excellence for weather and climate (ESiWACE-2). Several research tasks that have been initiated and demonstrated in the ESCAPE and ESCAPE-2 projects will be handed over and continued by ESiWACE-2 such that a larger user group can benefit from the sustainable support and usability platform created by this centre of excellence. In particular, the ESCAPE approach to domain specific programming languages and the weather and climate benchmarks form parts of this

platform and will be further evolved and combined with similar solutions delivered by other ESiWACE-2 partners. Ultimately, interoperable toolkits and benchmarks will be developed within ESiWACE-2 including their performance assessment at scale.

5.6 UK Excalibur exascale initiative

Speaker: Bryan Lawrence (University of Reading/ NCAS)

The 5-year UK Exascale Computing ALgorithms & Infrastructures for the Benefit of UK Research (Excalibur) initiative supports code development, data science and career development towards exascale capabilities for use cases of national relevance such as weather and climate prediction or fusion. The programme aims to address these topics across disciplines and through common software, to co-design solutions but also to identify points where radical design changes need to happen in order to achieve progress. Regarding code development for example, the separation of concerns between scientist friendly code layers and performance-portability optimized layers is a prominent task in Excalibur. The intimate connection between computing and data is clearly recognized and focused actions on I/O servers, I/O middleware and efficient data handling across the entire memory hierarchy and within federated infrastructures are in place. The Excalibur tasks align with other international work programmes and contribute to ESiWACE and ESCAPE through additional UK national funding.

5.7 DoE E3SM developments

Speaker: Mark Taylor (Sandia National Labs), et al.

The US Department of Exascale Energy's Earth-system Model (E3SM) represents an important international counterpart to the European efforts promoted in ESCAPE-2 and ESiWACE-2. The US efforts are backed up by substantial investments in computing infrastructure towards exascale systems like Frontier in 2022 and Aurora in 2023. E3SM's approach relies partly on the original Fortran programming models that are enhanced exploiting enhanced parallelism on GPU type processors and partly on code rewrites in C++ using the Kokkos abstraction toolchain. Initial benchmarks show enhanced performance on GPU type platforms when workloads (i.e. model complexity and resolution) are sufficiently large such that the individual parallel performance of GPU processors can be fully exploited.

5.8 WMO Research Board action on Exascale

Speaker: Kris Rowe (WMO)

The UN's World Meteorological Organization (WMO) is presently undergoing a reorganisation and has reviewed its approach to research. This offers an opportunity to include strategic projects on exascale computing, data handling and machine learning as key topics alongside atmospheric physics research, numerical modelling, observation programmes and many regionally focused activities. This results in concept notes currently being prepared for the WMO Research Board on exascale computing and on machine learning that aim to identify the main computing and data handling challenges that the weather and climate computing community faces and to define the effective use of machine learning tools for accelerating computing and enhancing information extraction from vast amounts of diverse data. It also presents options for addressing such challenges. The presented solutions align well with ESCAPE and ESiWACE activities towards open and free, across-platform tools and

benchmarks, the support of less developed countries and the investment in shared centres which drive the main technology developments to become accessible by the entire community.

5.9 Vulcan developments

Speaker: Oli Fuhrer (Vulcan & AI2)

Through its private Vulcan branch the Paul Allen foundation created an activity dedicated to climate science and advancing climate model computing through new programming models suitable for exploiting accelerator-based architectures. The developments are based on NOAA's new operational weather prediction dynamical core (FV3) and Python-wrapping to produce a scientist friendly front-end and a domain specific language toolchain to drive back-ends that achieve portability and performance on a variety of processor types. Choosing Python has the advantage of a quickly growing software ecosystem that facilitates development, numerical library support and machine learning. The toolchain is based on GT4Py that is also used in ESCAPE-2 and other European prediction system adaptation efforts. The Vulcan developments show the potential for achieving better code usability, which will clearly accelerate scientific code development, but also demonstrate how good HPC performance at scale can be achieved given the complex algorithmic basis of our codes.

6 Availability of Resources

All presentations will be made available on the workshop page. In addition, it is planned that the recording will also be made available on the page.

7 Conclusion

With over 70 participants, the second ESCAPE-2 Dissemination Workshop was to be successful.

The first part of the workshop was dedicated to introducing the results of the development work packages:

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Document History

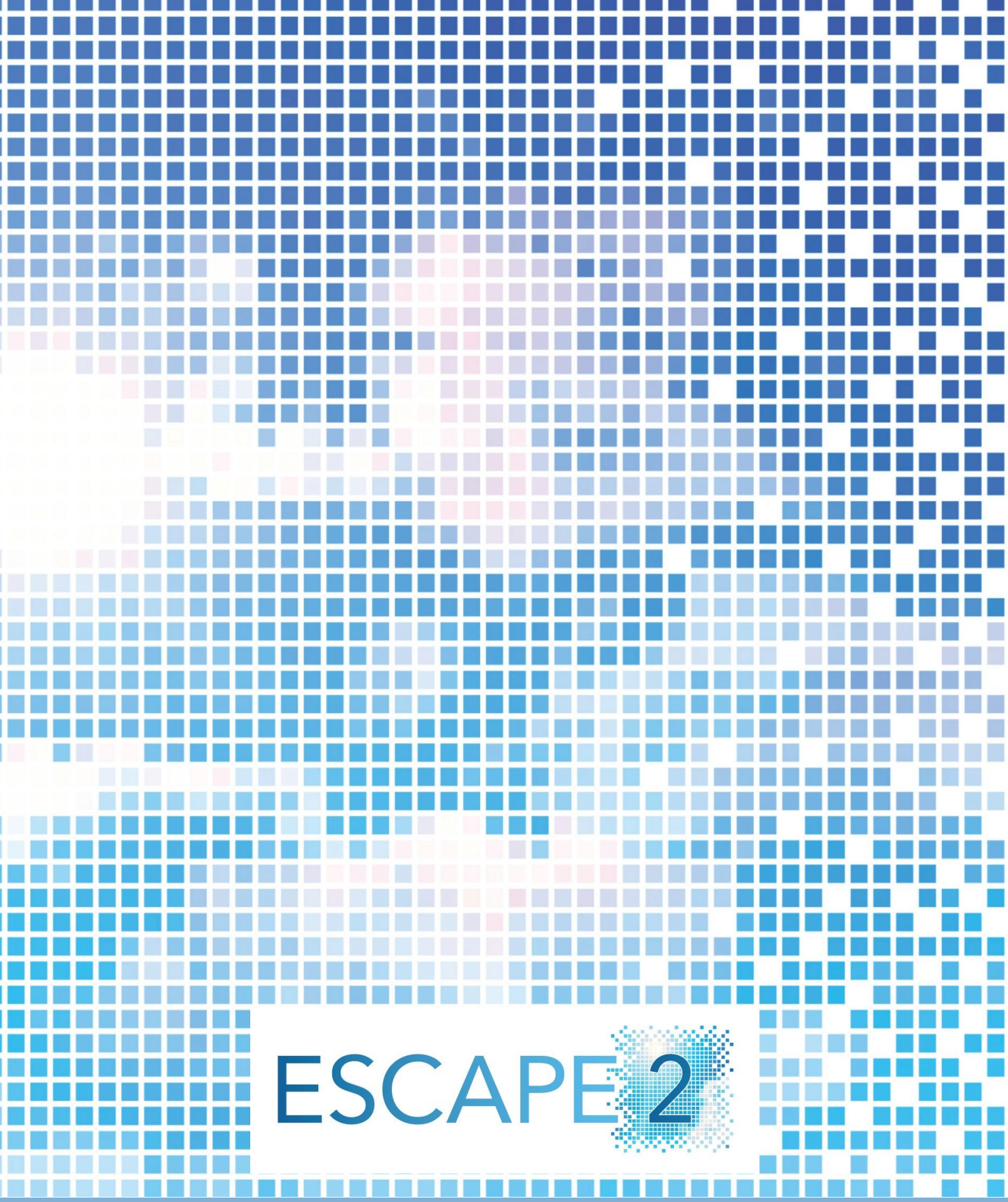
Version	Author(s)	Date	Changes
0.1	Daniel Thiemert (ECMWF)	07/09/2021	Initial structure
1.0	Daniel Thiemert (ECMWF)	22/09/2021	Final version

Internal Review History

Internal Reviewers	Date	Comments
Peter Bauer (ECMWF)	20/09/2021	Approved with comments

Effort Contributions per Partner

Partner	Efforts
ECMWF	0.5
Total	**0.5**



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