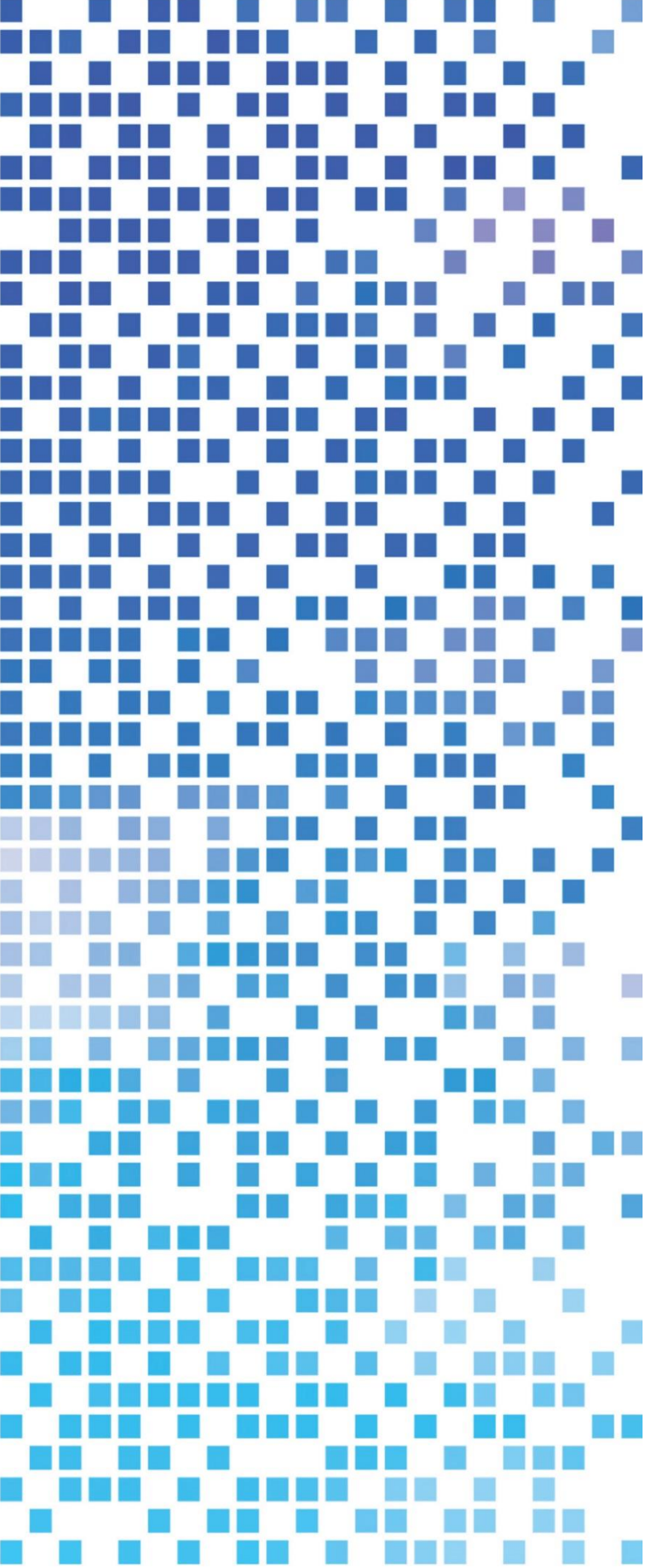

ESCAPE 2

D6.3 Exploitation Plan after closure

Dissemination Level: Confidential

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

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1 Executive Summary

D6.3 Exploitation Plan after closure revisits the planned exploitation activities already defined in D6.2 and identifies both Intellectual Property developed during the project as well as further exploitation activities.

As already mentioned in D6.2, ESCAPE-2 does not lend itself to a consortium-wide exploitation as the output of the project is not a single system but rather concepts and components. As such, apart from the already mentioned aspects such as the HPCW Benchmark and the DSL tool chain, joint exploitation is not further envisaged. However, the already identified activities (see Table 2) remain the focus of the consortium partners, and indeed are already being implemented.

The uptake and maintenance of the HPCW benchmark in ESiWACE2 and the wider scientific community supports the validity of the concept and ensures sustained exploitation of the ESCAPE-2 results after the end of the project.

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 prepare 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

2.2.1 Objectives of this deliverable

As per the Description of Action (DoA), D6.3 should capture the IPR and provide measures for exploitation after the project. Therefore, and following on from D6.2 Exploitation Plan, D6.3 should provide an IPR register and identify the exploitation activities of the consortium partners after the end of the project.

2.2.2 Work performed in this deliverable

To produce this deliverable, a final exploitation questionnaire was created and circulated for completion by all consortium partners. Responses were collated and analysed and the findings reported.

2.2.3 Deviations and counter measures

No deviations have been encountered.

3 IPR Register

A questionnaire was developed to help identify the various results produced by the different partners. The responses are summarised in Table 1.

Table 1: IPR Register

Exploitable results/ IP Name	Description/ Functionality	(Joint) Owner(s)	TRL Level	Related deliverable	IP Protection (Patent, Trademark, etc.)	Confidential (if yes, embargo duration)
Panther DG library	Three dimensional p-adaptive discontinuous Galerkin parallel library implementing all the DG operators on the sphere relevant for the semi-Lagrangian (SL) and the semi-implicit (SI) techniques (e.g. gradient, divergence, Laplacian, interpolation) as well as all the related parallel and adaptive data structures.	ECMWF	TRL4	D1.1 D1.2 D1.8	under ECMWF license.	Confidential, 18 months long embargo starting from October 1st 2021
dwarf-D-semi-Lagrangian-DG	Semi-Lagrangian discontinuous Galerkin advection	ECMWF	TRL4	D1.1	Under ECMWF license	Confidential, 18 months long embargo starting from October 1st 2021
Semi-implicit semi-Lagrangian DG prototype dynamical core	Dynamical core prototype based on semi-implicit, semi-Lagrangian time integration combined with discontinuous	ECMWF	TRL4	D1.2	Under ECMWF license	Confidential, 18 months long embargo starting from

Exploitable results/ IP Name	Description/ Functionality	(Joint) Owner(s)	TRL Level	Related deliverable	IP Protection (Patent, Trademark, etc.)	Confidential (if yes, embargo duration)
	Galerkin space dicretization of the rotating Euler equations in spherical geometry					October 1st 2021
First GPU support in RAPS	RAPS model from ECMWF with GPU version of the spectral transform from ESCAPE1 for the benchmark suite HPCW	ECMWF	TRL6	D3.5	RAPS license	None
White paper on resilience	Overview of different methods to achieve fault tolerance	ECMWF / POLIMI/ LU	TRL6	D1.3	None	None
dwarf-D-ellipticSolver-GCR	elliptic solver for a 3D potential flow problem using Generalised Conjugate Residual	ECMWF	TRL7	D1.7	ESCAPE license	None
dwarf-D-advection-SemiLagrangian	semi-Lagrangian time-integration	ECMWF	TRL7	D1.7	ESCAPE license	None
dwarf-D-advection-MPDATA	solid body rotation using the MPDATA advection scheme	ECMWF	TRL7	D1.7	ESCAPE license	None
dwarf-D-cloudMicrophysics-IFSScheme	cloud microphysics parameterisation	ECMWF	TRL7	D1.7	ESCAPE license	None
Finite Volume Module for the IFS	added the Finite Volume for the IFS to the HPCW benchmark suite	ECMWF	TRL6	D3.5	ESCAPE license	None
RAPS version of the IFS	benchmarking version of the IFS for the HPCW benchmarking suite	ECMWF	TRL9	D3.5	RAPS license	None
DSL toolchain	Applicable DSL toolchain (incl. C++ front-end & GPU backend).	DKRZ/ MPI-M	TRL7	D2.2, D2.5	FOSS copyright licenses (BSD, MIT) apply	

Exploitable results/ IP Name	Description/ Functionality	(Joint) Owner(s)	TRL Level	Related deliverable	IP Protection (Patent, Trademark, etc.)	Confidential (if yes, embargo duration)
HPCW	portable benchmark suite with realistic performance characteristics for our domain.	All Partners	TRL6	D3.5		
HIR	HIR is a formal specification of high-level concepts that define a minimal set of orthogonal elements required for building any DSL or intermediate representation supporting weather and climate models.	MeteoSwiss, MPI, DKRZ, ECMWF, STFC, MetOffice, DWD, CMCC, ETHZ	TRL6	D2.1	Open source	
URANIE	Upgraded workflow management environment for URANIE	CEA /BSC	TRL8	D4.3		
TABC class	Approximation Baysesian Computation Class in URANIE	CEA	TRL6	D4.5	Public LGPL licence (URANIE)	No
TRemoteLauncher class	Based on Libssh library, possibility to run code on different cluster	CEA/ BSC	TRL 6	D4.3	Public LGPL licence (URANIE)	No
Unstructured Jacobi preconditioner	unstructured Jacobi preconditioner for GCR(k) in FVM	LU, ECMWF	TRL7	D1.5	As agreed in ESCAPE-2 IP protection	
Multigrid Toolkit for Atlas/FVM	Multigrid tools for use with FVM utilising Atlas	LU, ECMWF	TRL7	D1.5	As agreed in ESCAPE-2 IP protection	
Multigrid preconditioner for GCR(k)	Multigrid V-cycle preconditioner for GCR(k) with numerous options implemented	LU, ECMWF	TRL7	D1.5	As agreed in ESCAPE-2 IP protection	

Exploitable results/ IP Name	Description/ Functionality	(Joint) Owner(s)	TRL Level	Related deliverable	IP Protection (Patent, Trademark, etc.)	Confidential (if yes, embargo duration)
FT-GCR	Fault tolerant approach to the GCR elliptic solver	LU, POLIMI	TRL4	D1.3, D1.4	As agreed in ESCAPE-2 IP protection	
Dual time stepping for MPDATA	Utilise a dual time stepping approach to MPDATA to allow for FAS multigrid as an accelerator	LU	TRL4	D1.5	As agreed in ESCAPE-2 IP protection	
URANIE HarmonEPS integration	Re-design of the HARMONIE scripting system to accommodate the URANIE tasks	RMI/ACCORD	TRL5	D4.6	NO	NO
HPCWval	Ensemble Consistency Test: Software for verification of model porting and or model changes	RMI	TRL6	D3.2	NO	NO
Fault tolerant implementation of Krylov solvers	Parallel implementation of fault tolerant Krylov solvers in Fortran95	POLIMI LU	TRL5	D1.4		No
Implementation of Krylov solvers in the framework of the Panther Library	Parallel implementation of Krylov solvers in Fortran95, specific for the operators of semi-implicit discretization developed in ESCAPE-2, using Panther data structure and partitioning	POLIMI ECMWF	TRL5	D1.2		Yes- Embargo duration same as Panther
RTE-RRTMGP-NN	Neural network for gas optics computations	DMI/ Robert Pincus (CIRES/NOAA)	TRL6	D1.8	Open source	No

Exploitable results/ IP Name	Description/ Functionality	(Joint) Owner(s)	TRL Level	Related deliverable	IP Protection (Patent, Trademark, etc.)	Confidential (if yes, embargo duration)
RRTMGP / RRTMGP-NN implemented in ecRad	Implementation of code in the IFS radiation scheme	DMI / ECMWF	TRL5	D1.6	Open source	No
Optimizations for ecRad	Node level optimization for CPUs. SPARTACUS a primary focus.	DMI/ ECMWF	TRL5	D1.6	Open source	No
HPCW framework	Framework to ease the compilation, validation and benchmarking of weather and climate models	BULL	TRL6	D3.5	None	No but still internal for ESCAPE-2 and then ESiWACE2 consortiums

4 Exploitable Results and Exploitation Activities

The initial deliverable D6.2 Exploitation Plan already identified mid-way through the ESCAPE-2 project exploitable products and exploitation activities, as presented in Table 2.

Table 2: Exploitation Summary

Exploitable Products	• improved forecasts • improved model performance • HPCW Benchmark • DSL Tool Chain • performance portable NWP models/ codes • improved URANIE • publications • research codes • DG implementation for CFD applications • new/enhanced ocean model with DSL
Exploitation Activities during the Project	• continuous assessment • extend DSL development to other parts of NPW models • benchmarking • road mapping • literature review • benchmark suite analysis

Exploitation Activities after the end of the Project	• operational benchmarking • improve usability and performance • integration into operations • transposition of results to other fields where possible • development of ocean model with DSL • benchmark suite analysis
Consortium-wide/Joint Exploitation	• HPCW benchmark • DSL Tool Chain

4.1 Partner Exploitation

Following on from this, a further questionnaire was circulated that identifies individual use and activities where possible. The results are presented in the following sections.

4.1.1 ECMWF

Products	Results to be incorporated
Panther library (including RK-DG and SL-DG advection diffusion equation for tracers and SISL-DG dycore)	Polynomial order flexibility, high order accuracy and parallel efficiency for efficient high resolution modelling.
Panther library	Paper: Tumolo G., Deconinck. W., and Paronuzzi S.V., Panther: a p-adaptive discontinuous Galerkin parallel library for efficient high order computations, in preparation.
SL-DG advection	Efficient and scalable tracers transport scheme that can be useful e.g. in atmospheric chemistry applications.
SL-DG advection	Paper: Tumolo G., Parallel p-adaptive semi-Lagrangian discontinuous Galerkin advection, in preparation.
SL-DG advection	Paper: Tumolo G, departure point approximations for high order Lagrange-Galerkin methods: accuracy and efficiency assessment in a parallel framework, in preparation.
SISL-DG dynamical core prototype	Unconditional stability hence long time step capability together with locality and high order accuracy will allow to exploit the novel emerging parallel architecture towards exascale NWP.
SISL-DG dynamical core prototype	Paper: Tumolo G., a semi-implicit semi-Lagrangian p-adaptive discontinuous Galerkin dynamical core prototype, in preparation.
Panther library + SL-DG advection + SISL-DG dycore	Lecture given at the ECMWF 2020 Annual seminar on Numerical Methods
Panther library + SL-DG advection + SISL-DG dycore	Lecture given at the ESCAPE2 Summer School on Exascale HPC for NWP.

GPU support in IFS	first GPU support in RAPS
HPCW benchmark suite	benchmarking dwarfs and models created for WP3
Activities	
SL-DG advection: Accurate, efficient and scalable tracer transport scheme that can be used by current and future ECMWF dynamical core for the EU Copernicus atmospheric composition modelling and forecast system. SL-DG advection: further developments including terrain following vertical coordinate option and flux form formulations for better integration in the ECMWF forecast system. SISL-DG dynamical core prototype: further development including flux form formulation of continuity equation for better integration in the ECMWF forecast system. Combining GPU efforts for RAPS with GPU efforts from other parts of the model	

4.1.2 DKRZ

Products	**Results to be incorporated**
Performance portable ICON model	D2.2, D2.5
Hardware procurements + evaluations	D3.5
Activities	
Extend the application of the DSL approach; maintain toolchain: optimize backend, improve usability of front end. Establish HPCW as a reference benchmark suite for our domain. The framework for maintaining and promoting HPCW in the long term will be set up in collaboration with the EU funded Centre of Excellence ESiWACE.	

4.1.3 MPI-M

Products	**Results to be incorporated**
Performance portable ICON model	D2.5, D2.6
Activities	
Further research and development of the DSL approach in different projects; assist in maintaining and optimization mainly of the front end, but also the toolchain at large; help organize community driven effort in this.	

4.1.4 MSWISS

Products	**Results to be incorporated**
Dawn DSL toolchain compiler (https://github.com/MeteoSwiss-APN/dawn)	Software implementation of a DSL incorporating an HIR, compiler optimizations and code generation for accelerators. Open source with MIT license
Activities	
Activities will continue within other projects: ESiWACE2: establish the DSL developed in ESCAPE-2 by implementing a full dynamical core of ICON as a production ready product	

EXCLAIM: further development of general python based DSL toolchain ICON-22: Internal MeteoSwiss project to bring in production the results of DSL developments.

4.1.5 BSC

Products	**Results to be incorporated**
n/a	
Activities	
To develop the PANTHER dwarf mixed-precision version, BSC used a methodology already tested and used in the context of other projects (NEMO ocean model, ESIWACE2, IS-ENES3, …). Nevertheless, this specific exercise has contributed to increase the portability and flexibility of the tool, improving the support of the mixed-precision workflow to other Fortran codes.	

4.1.6 CEA

Products	**Results to be incorporated**
ABC class	New ABC methods
D4.1 to define the terms VVUQ	/
Activities	
Improvement of the ABC class adding new methods Complete analysis of the ACRANEB2 dwarf in D4.4 including the original use of UQ methods for numerical precision, an article is considered jointly with ECMWF, BSC and RMI.	

4.1.7 LU

Products	**Results to be incorporated**
Principles of preconditioning, dual time stepping FAS for MPDATA and multigrid techniques developed during ESCAPE-2 to be applied to LU research codes for use in engineering applications	Publications for engineering applications such as low speed aerodynamics and flows past isolated structures, as well as limited area atmospheric flows. UK's EPSRC funding proposal extending these developments to simulations of CO_2 trapping methodologies is being developed.
Activities	
Continued development of dual time stepping MPDATA using FAS multigrid Unstructured Jacobi and Multigrid preconditioner for GCR(k) incorporated into FVM for use at high resolution Multigrid Toolkit and existing architecture added to FVM Developed Multigrid techniques to be applied to engineering applications using LU developed codes Extending testing of FT-GCR in more relevant NWP codes	

4.1.8 RMI

Products	**Results to be incorporated**
Publication: Precision analysis using the Ensemble based Consitency Test	Deliverable 4.3: Section 4.3 Precision analysis Deliverable 3.2

Activities
Use of the Ensemble Bases Consistency test algorithms when porting the operational model to new machines Use of URANIE for VVUQ in both operational and research activities

4.1.9 POLIMI

Products	Results to be incorporated
Publication	Benacchio, T., Bonaventura, L., Altenbernd, M., Cantwell, C.D., Düben, P. D.,Gillard, M., Giraud, L., Göddeke, D., Raffin, E., Teranishi, K., Wedi, N. (2021), Resilience and fault-tolerance in high-performance computing for numerical weather and climate prediction, The International Journal of High Performance Computing Applications, Vol. 35, pp. 285-311.
Publication	L. Bonaventura, J. Garres Diaz, Flexible and efficient discretizations of multilayer models with variable density, Applied Mathematics and Computation, Vol. 402, 126097, 2021
Activities	
Further (upcoming) publications: Agullo, E., Altenbernd, M., Anzt, H., Bautista-Gomez, L., Benacchio, T., et al. (2021), Resiliency in Numerical Algorithm Design for Extreme Scale Simulations, submitted to The International Journal of High Performance Computing Applications, preprint: https://arxiv.org/abs/2010.13342. Vismara, F., Benacchio, T., and Bonaventura, L. (2021), A seamless, extended DG approach for advection-diffusion problems on unbounded domains, submitted to Journal of Scientific Computing, preprint: https://arxiv.org/abs/2012.05954 M. Gillard, Benacchio, T. (2021), FT-GCR: a fault-tolerant generalized conjugate residual elliptic solver, submitted to Journal of Computational Physics, preprint: https://arxiv.org/abs/2103.07210 Chew, R., Benacchio, T., Hastermann, G., and Klein, R. (2021), A one-step blended soundproof-compressible model with balanced data assimilation: theory and idealised tests, submitted to Monthly Weather Review, preprint: https://arxiv.org/abs/2103.11861	

4.1.10 DMI

Products	Results to be incorporated
https://github.com/peterukk/rte-rrtmgp-nn Contributions by user “peterukk“ to: https://github.com/ecmwf/ecrad/tree/develop	RRTMGP and RRTMGP-NN implementation in ecRad in IFS, and in ecRad in HARMONIE-AROME.
Activities	
The code products will be fully implemented and tested in weather modelling codes – mainly in HARMONIE-AROME.	

4.1.11 CMCC

Products	Results to be incorporated

New course for summer schools in HPC and algorithms for weather and climate applications	Dwarf suite DSL toolchain
Activities	
Integration of the NEMO dwarf into the NEMO oceanic model Evaluation the DSL toolchain as tool to optimize part of the NEMO code Exploitation of the HPCW to assess the performance of the computational infrastructure at CMCC	

4.1.12 BULL

Products	**Results to be incorporated**
HPCW framework	First version of the HPCW framework
Publication of HPCW benchmark results	Publication on HPCW framework and results obtained by BULL
Projects	Extension and benchmarking of HPCW for the ESiWACE CoE
Activities	
HPCW benchmark analysis and extension.	

4.2 Uptake in other Research

As can be seen in Figure 1, ESCAPE-2 feeds into a number of other HPC and weather and climate related projects.

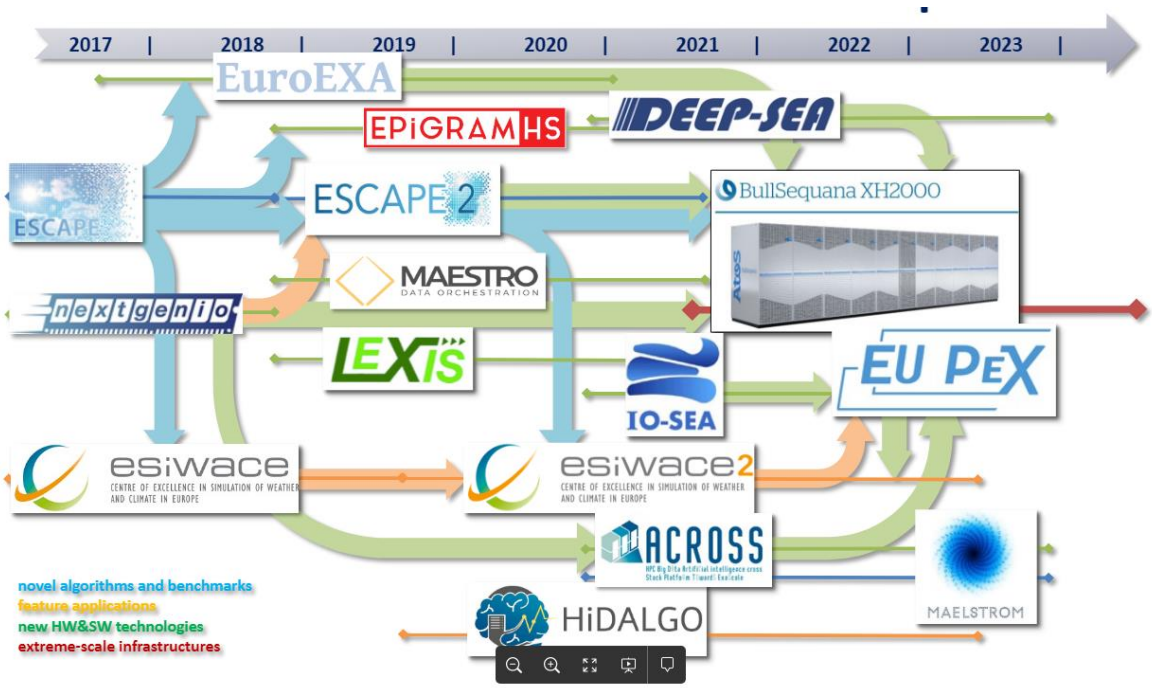


Figure 1: ECMWF Weather and Climate Projects Roadmap

The most important uptake will be through ESiWACE2[1]. ESCAPE-2 feeds into ESiWACE2 that disseminates the future evolution of weather and climate models to an operational community. This concept is rapidly emerging as an accepted development template for the entire weather and climate prediction community in the future. The fundamental technical developments in ESCAPE-2 will be propagated into ESiWAC2 for further dissemination and maintenance. This includes the HPCW benchmarks which will serve as application demonstrators in the ESiWACE2 Centre of Excellence for quantifying the computability of the exascale science challenge.

Other projects as well as research centres will also benefit from the developments within ESCAPE-2, e.g. through the release of new dwarfs.

5 Conclusion

As already mentioned in D6.2, ESCAPE-2 does not lend itself to a consortium-wide exploitation as the output of the project is not a single system but rather concepts and components. As such, apart from the already mentioned aspects such as the HPCW Benchmark and the DSL tool chain, joint exploitation is not further envisaged. However, the already identified activities (see Table 2) remain the focus of the consortium partners, and indeed are already being implemented.

The uptake and maintenance of the HPCW benchmark in ESiWACE2 and the wider scientific community supports the validity of the concept and ensures sustained exploitation of the ESCAPE-2 results after the end of the project.

[1] https://esiwace.eu/

Document History

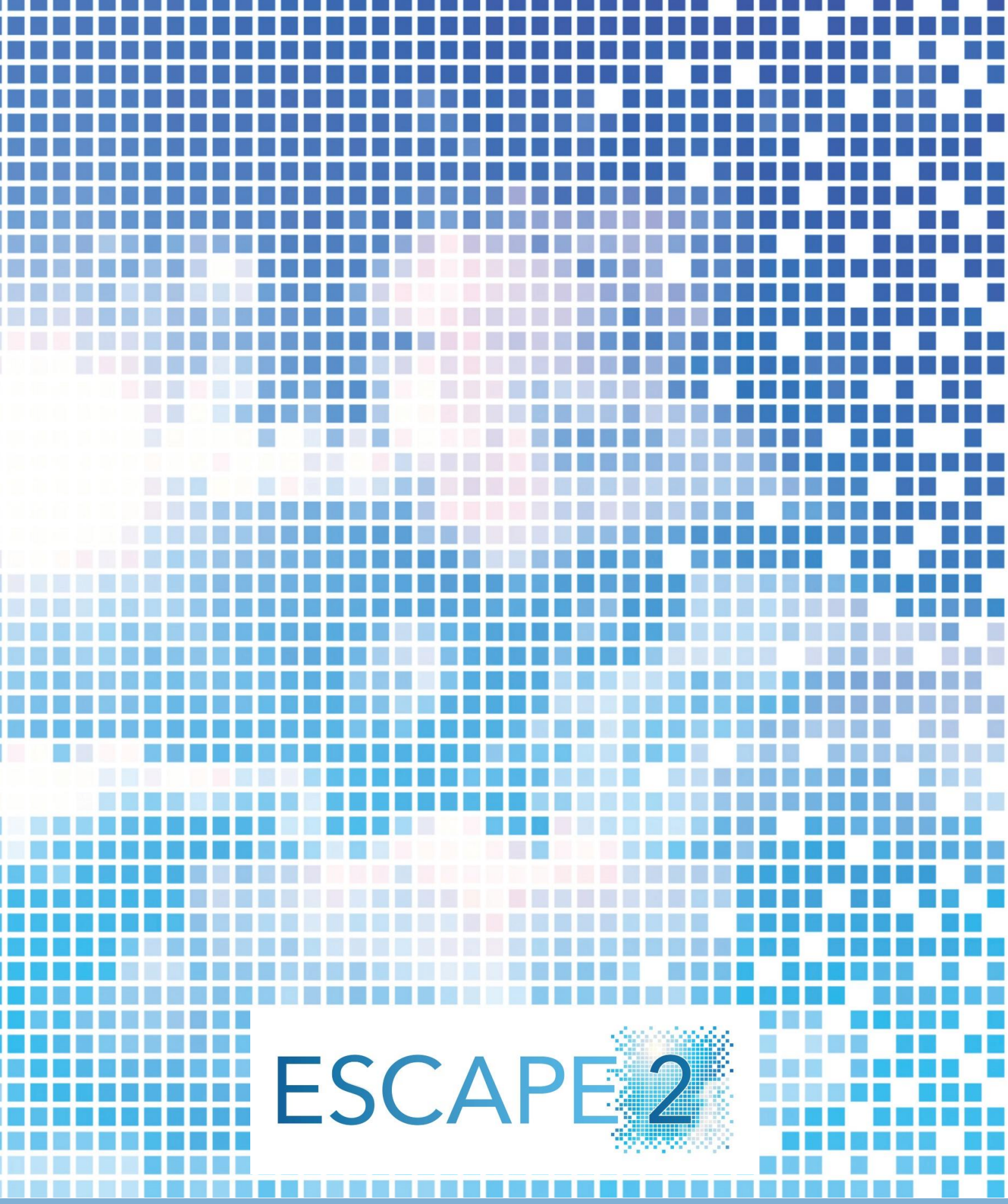
Version	Author(s)	Date	Changes
0.1	Daniel Thiemert (ECMWF)	10/09/2021	Initial version with Partner inputs
1.0	Daniel Thiemert (ECMWF)	16/09/2021	Final version

Internal Review History

Internal Reviewers	Date	Comments
Erwan Raffin	15/09/2021	Accepted with minor modification requests

Effort Contributions per Partner

Partner	Efforts
ECMWF	0.5
Total	**0.5**



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