H2020-FETHPC-2014

Coordination of the HPC strategy

EXDCI

European eXtreme Data and Computing Initiative

Grant Agreement Number: FETHPC-671558

D6.5
International Collaboration - Final international identification report

Final

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Table of Contents

List of Figures

List of Tables

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List of Acronyms and Abbreviations

BDEC	Big Data and Extreme-scale Computing
BDV	Big Data Value
BDVA	Big Data Value Association cPPP
BOF	Birds-of-a-Feather Session
CoE	Centres of Excellence for Computing Applications
cPPP	contractual Public-Private Partnership
D	Deliverable
DoW	Description of Work
EC	European Commission
EPCC	Edinburgh Parallel Computing Centre
EsD	Extreme-Scale Demonstrators
ETP4HPC	European HPC Technology Platform
EU	European Union
FET	Future and Emerging Technologies
FP7	Framework Programme 7
H2020	Horizon 2020 – The EC Research and Innovation Programme in Europe
HPC	High Performance Computing
ICT	Innovate, Connect, Transform
IPCEI	Important Project of Common European Interest
ISC	International Supercomputing Conference
LEIT	Leadership in Enabling and Industrial Technologies
M	Month
MoU	Memorandum of Understanding
MPI	Message Passing Interface
NWP	Numerical Weather Prediction
PMO	Project Management Office
PRACE	Partnership for Advanced Computing in Europe,
Q	Quarter
R&D	Research and Development
RIKEN AICS	Advanced Institute for Computational Science, Japan
ROI	Return On Investment
SC	Supercomputing Conference
SKA	The Square Kilometre Array project.
SRA	Strategic Research Agenda
TRL	Technology Readiness Level
US	United States
WG	Working Group
WP	Work Package

Executive Summary

This document reports on the progress of developing international collaborations for the European HPC Projects[1] and analyses the future potential of developing these collaborations, as set up in the objective of Task 6.2 of EXDCI (*Facilitate International Collaboration Opportunities*).

The task has achieved its principal goal according to the Description of Work (DoW): to increase the international collaborations that will be set up between the European projects and actions occurring outside Europe, i.e. it has **established an effective process and tools** for the further development of the international collaborations of the European HPC Ecosystem.

There is an established and recognised presence of all the European HPC projects at the world's largest HPC-related conference (Supercomputing Conference, SC – in the United States). We have developed a template that ensures the delivery of an efficient and effective event. We also maintain a **European HPC Handbook**, which includes up-to-date information on all the Projects – an up-to-date version of this document and other related material (e.g. a summary of European HPC) is available on the ETP4HPC web page dedicated to this task http://www.etp4hpc.eu/euexascale.

We have also approached the most prominent regions in HPC technology development in order to obtain updates on the work taking place in those countries. These actions will help the Projects develop their international collaborations as they mature and produce tangible results. International[2] partners can also access the ETP4HPC networking tool at http://www.etp4hpc.eu/networking in order to contact the members of the association.

The key conclusions of our assessment of the international collaboration opportunities for the European HPC projects are as follows:

- The Projects are open to international collaboration opportunities and willing to engage in activities in order to facilitate this process. Likewise, the international community has demonstrated a high level of interest in the results of the European projects.
- There are a number of areas where cooperation seems possible, and the Projects are able to identify these areas and pinpoint potential partners in both academia and industry. Some projects have already started work involving international partners.
- The European HPC Ecosystem should further facilitate this process by identifying areas of priority where European and overseas projects could jointly contribute to the goals of the international HPC community and organise e.g. common workshops in selected areas and research visits (in particular in the area of Programming Tools), leading to joint calls and other funding mechanisms. Also, a clear dissemination plan is needed in order to help the Projects reach the appropriate partners.

This work is being carried out by ETP4HPC, the European High-Performance Computing Technology Platform, in the context of the EXDCI project. ETP4HPC represents the European

[1] The term 'European Projects' (hereafter referred to as 'Projects') includes all EC-funded European research and development projects (HPC technology, applications, co-design and other), regardless of the EC programme used as their funding instrument.

[2] The term 'international' in this document is used to refer to 'non-European' (i.e. foreign or overseas) projects from outside of Europe.

HPC Technology Value Chain and issues a Strategic Research Agenda (SRA), a multi-annual roadmap for HPC technology development in Europe, the guidelines of which are used to define the contents of the European Commission's HPC Technology R&D Work Programmes. The current European research programme, Horizon 2020, comprises of projects aiming to develop cutting-edge HPC technology. These projects, together with projects funded by previous programmes and other parts of the H2020 programme, present a number of opportunities for international collaboration with similar or complementary initiatives in other regions.

1 Introduction

The objective of Task 6.2 is to facilitate the International Collaboration Opportunities of the European HPC projects. This particular document reports on the work done from the start of the EXDCI project up until February 2018) and it also aims to identify the main directions of the developments of international collaborations in the future (including the EXDCI 2 project – planned to be implemented from 2018 to 2020). This document includes the conclusions of the first EXDCI deliverable in this area – 6.2: 'Analysis of international collaboration opportunities for the European projects'. The work in this task has been carried out by ETP4HPC on behalf of EXDCI and in some of its parts it is a continuation of previous activities of ETP4HPC.

This task aims to facilitate the international collaborations of the European HPC projects. It **federates** the efforts of European HPC in this area by ensuring a single interface for all the projects.

It is important to emphasise that this task initially dealt with HPC technology projects only, but as the European HPC eco-system matured, it has also involved HPC application and co-design projects. Thus, the current 'international collaboration interface' covers the entire European HPC eco-system, as shown in Figure 1.

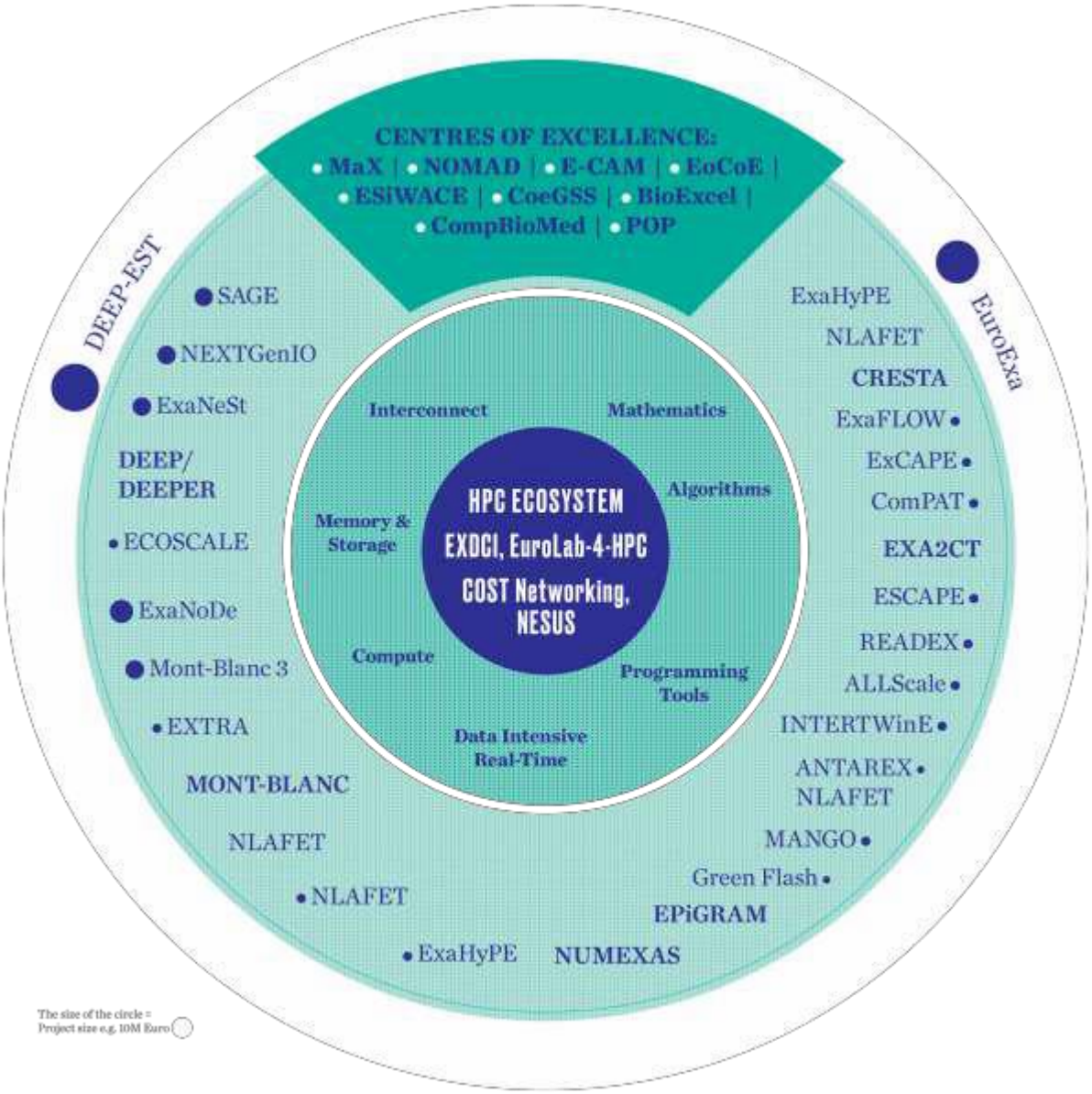

Figure 1 - The European HPC eco-system as of January 2018. The work carried out within this task (and covered by this report) includes all the project types: technology, application (CoEs – Centres of Excellence in Computing Applications) and co-design. /Circles sizes correspond to project funding/.

The objective of this task has been to:

- Help the European HPC Projects connect with other similar or complementary initiatives around the world;
- Present the Projects, with a view to facilitating the initiation of international collaborations;
- Determine what mechanisms could facilitate collaboration between these projects and potential overseas counterparts.

Figure 2 – The proceedings of our SC'17 BOF /Supercomputing Conference Birds-of-a-Feather session/ - the main tool used to date to promote the European HPC projects beyond Europe.

In this document, we first describe the **Background** of the work carried out in this task: the European HPC Ecosystem, the role of ETP4HPC in it, and the Future and Emerging Technologies – HPC research programme. Next, we explain the **Process** selected to deliver the objectives of this task. The following Chapter outlines the **Implementation and Results** of the work carried out. The last Chapter contains the **Conclusions** of this task.

2 Background

2.1 The European HPC Ecosystem and its strategy

The current European HPC Strategy was first defined by the European Commission in a publication titled: 'High Performance Computing: Europe's place in a Global Race' [1] issued in 2012 and adopted by the European Union as an official strategy document in 2013 [2].

Figure 3 - This 2012 document first defined the European HPC Strategy

This document recognises the value of HPC for the European economy and society. The European HPC Ecosystem aims to develop world-class HPC technologies, infrastructures and applications, leading to the eventual production of Exascale systems, and promoting their use for advanced research in science and industry. This will create jobs, enable scientific discoveries, and allow companies to become more efficient. All of this in turn will contribute to the economic competitiveness of the European economy as a whole, and also, to the well-being of the European citizen by equipping our scientists, economists, sociologists, agriculturalists, politicians and engineers to address the Grand Societal Challenges that the continent faces.

The strategy stipulates the need for the balanced development of the European HPC Ecosystem based on three pillars.

- **HPC Infrastructure** (represented by Partnership for Advanced Computing in Europe, PRACE) [3]
- **HPC Technology** (represented by ETP4HPC, the European HPC Technology Platform) [4]
- **Application Expertise** (represented by the Centres of Excellence of Computing Applications, CoEs) [5]

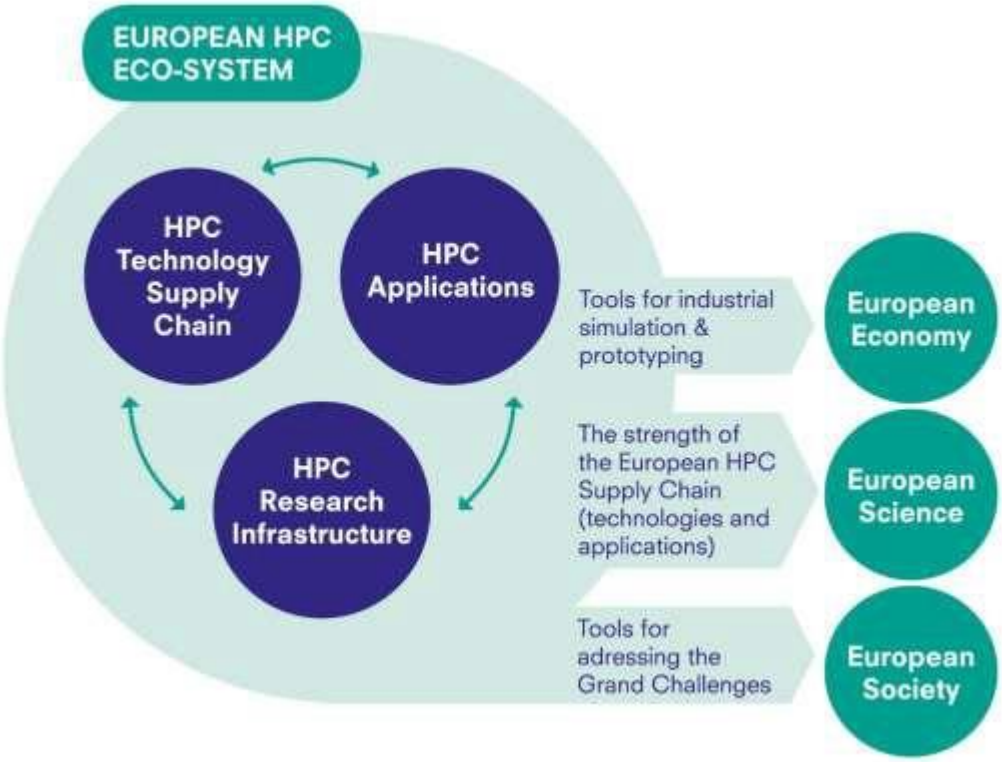

Figure 4 - The interactions between the three pillars of the European HPC Ecosystem and the European economy, science and society.

The strategy above was 'upgraded' in 2016 - Europe now has ambitious plans based on four actions.

(1) The European Cloud Initiative [6] – aimed at building a competitive data and knowledge economy in Europe" to capitalise on the data revolution. Under this initiative, and alongside with a seamless access layer based on Cloud services called EOSC (European Open Science Cloud), a European Data infrastructure (EDI) will federate world-class supercomputing capability with high-speed connectivity and leading-edge data and software services for science, industry and the public sector.

(2) EuroHPC [7] is an initiative signed by thirteen European countries and the EC committing to the joint funding and delivery of European world-class HPC systems. The target is to have at least two pre-exascale computers by 2020 and reach full exascale performance by 2023. The objective is also to develop European HPC technologies able to equip such procured systems and to define test-beds for HPC and big data applications that make use of these supercomputers for scientific, public administration and industrial purposes.

(3) A LEIT call [8] for the development of European low-power processor technology. It is expected that these projects will interact with the other parts of the eco-system and the results of this work will feed into the delivery of the Extreme-scale Demonstrators and also the European pre-exascale and exascale systems.

(4) A special instrument, Important Project of Common European Interest (IPCEI) [9] on HPC and Big Data Enabled Applications, which serves as a financing mechanism for the European exascale ambitions.

2.2 The European HPC Technology Platform – ETP4HPC

Figure 5 - The logo of ETP4HPC - more information on this association is available at www.etp4hpc.eu.

ETP4HPC (European HPC Technology Platform, www.etp4hpc.eu) is an industry-led organisation – an association of companies and research centres involved in HPC technology research in Europe. It aims to build a world-class HPC Supply Chain and increase the global market share of European HPC vendors. It issues **a Strategic Research Agenda** (SRA, www.etp4hpc.eu/sra) to define the EU HPC research priorities in the area of the HPC Technology pillar, and sets out the guidelines which are used by the EU to define its HPC Technology research programme with the Horizon2020 framework.

Figure 6 - The Strategic Research Agenda of ETP4HPC, i.e. the European HPC Technology roadmap that serves as the basis of the EU HPC Technology Calls.

The SRA uses a four-dimensional HPC development model – each of the 'dimensions' represents a building block of HPC technology and has a dedicated chapter within the SRA. Compared to the previous (i.e. pre-2017) versions of the SRA, the current model includes the concept of Extreme-scale Demonstrators [11] – the prototypes of the future European HPC exa-scale level systems.

Figure 7 - The SRA four-dimensional HPC development model, with each area being a separate SRA chapter.

ETP4HPC is managed by a Steering Board of fifteen organisations (European HPC Technology vendors, SMEs, international companies and European research centres) elected by its General Assembly, i.e. all active members who are able to demonstrate research activities in Europe. Any organisation with an interest in the development of HPC technology can become an Associated Member.

ETP4HPC is also one of the two partners in the EXDCI (European Extreme Data and Computing Initiative) project led by PRACE. The objective of EXDCI is to coordinate the European HPC strategy. In this project, ETP4HPC leads the delivery of the SRA, the development of international collaboration opportunities for the European HPC Technology Projects and a work package on the measurement of the European HPC ecosystem.

The majority of the participants of the European HPC projects are also ETP4HPC members [11]. As one of its objectives, ETP4HPC represents the HPC technology Ecosystem in dealings with e.g. the European Commission, the European member states and the international HPC community. ETP4HPC is also the EC's partners in the contractual Public-Private Partnership for HPC, which also includes the CoEs.

ETP4HPC acts as a single point of contact for European HPC technology, and had already represented European HPC technology prior to the EXDCI project through e.g. participation in events, organising information sessions and direct contact with overseas companies, government bodies and vendors.

ETP4HPC has also developed working relationships with the European Big Data Community (BDVA, [12]) with an objective to synchronise the technology roadmaps of the two areas.

2.3 The current European HPC Landscape

The current European HPC Landscape includes three types of projects: HPC technology projects, Centres of Excellence in Computing Applications (CoEs – i.e. the European HPC applications expertise) and HPC co-design projects.

Table 1 - The FETHPC-1-2014 HPC Technology Projects - the currently running European HPC technology projects [13].

Acronym	Title
ALLScale	An Exascale Programming, Multi-objective Optimisation and Resilience Management Environment Based on Nested Recursive Parallelism – http://www.allscale.eu
ANTAREX	AutoTuning and Adaptivity appRoach for Energy efficient eXascale HPC systems – http://www.antarex-project.eu/
ComPat	Computing Patterns for High Performance Multiscale Computing – http://www.compat-project.eu/
ECOSCALE	Energy-efficient Heterogeneous COmputing at exaSCALE – http://www.ecoscale.eu/
ESCAPE	Energy-efficient SCalable Algorithms for weather Prediction at Exascale – http://www.ecmwf.int/en/research/projects/escape
ExaFLOW	Enabling Exascale Fluid Dynamics Simulations – http://exaflow-project.eu/
ExaHyPE	An Exascale Hyperbolic PDE Engine – http://exahype.eu/
ExaNeSt	European Exascale System Interconnect and Storage – http://www.exanest.eu/
ExaNoDe	European Exascale Processor Memory Node Design – http://exanode.eu/
ExCAPE	Exascale Compound Activity Prediction Engine – https://www.ecmwf.int/escape
EXTRA	Exploiting eXascale Technology with Reconfigurable Architectures – https://www.extrahpc.eu/
greenFLASH	Green Flash, energy efficient high performance computing for real-time science (no website available)
INTERTWINE	Programming Model INTERoperability ToWards Exascale (INTERTWinE) – http://www.intertwine-project.eu/partners
MANGO	MANGO: exploring Manycore Architectures for Next-GeneratiOn HPC systems – http://www.mango-project.eu/
Mont-Blanc 3	Mont-Blanc 3, European scalable and power efficient HPC platform based on low-power embedded technology – https://www.montblanc-project.eu/montblanc-3

NEXTGenIO	Next Generation I/O for Exascale – http://www.nextgenio.eu/
NLAFET	Parallel Numerical Linear Algebra for Future Extreme-Scale Systems – http://www.nlafet.eu/
READEX	Runtime Exploitation of Application Dynamism for Energy-efficient eXascale computing – http://www.readex.eu/
SAGE	Percipient StorAGE for Exascale Data Centric Computing – http://www.sagestorage.eu/

Table 2 - The current European Centres of Excellence in Computing Applications [14].

Acronym	Title
BioExcel	Centre of Excellence for Biomolecular Research - https://bioexcel.eu/
COEGSS	Center of Excellence for Global Systems Science - http://coegss.eu/
CompBioMed	A Centre of Excellence in Computational Biomedicine – http://www.compbiomed.eu/
E-CAM	An e-infrastructure for software, training and consultancy in simulation and modelling - http://www.compbiomed.eu/
EoCoE	Energy oriented Centre of Excellence for computer applications - http://www.eocoe.eu/
ESiWACE	Excellence in SImulation of Weather and Climate in Europe - https://www.esiwace.eu/
MaX	Materials design at the eXascale - www.max-center.eu
NoMaD	The Novel Materials Discovery Laboratory - https://nomad-coe.eu/
POP	Performance Optimisation and Productivity - https://pop-coe.eu/

Table 3 - The current European HPC co-design projects [15].

Acronym	Title
DEEP-EST	Dynamical Exascale Entry Platform (and DEEP-ER and DEEP-EST) - http://www.deep-projects.eu/
EuroExa	https://twitter.com/euroexa, https://ec.europa.eu/digital-single-market/en/news/euroexa-european-co-design-exascale-applications

2.4 EXDCI's Position on International Collaboration

In 2015, prior to the start of the EXDCI project, ETP4HPC defined its position on international collaboration [16]. To achieve HPC leadership, Europe must engage in international cooperation. This cooperation should target two objectives:

- Develop synergies with the most active areas in HPC technologies research and their optimal usage. Priority should be given to developing links with Japan and the US, which demonstrate the longest experience in HPC and the most structured and mature related programmes;
- Collaborate with some of the countries which are in the early stages of developing their HPC strategies (e.g. Australia, South Africa, Brazil), in order to encourage them to utilise the expertise and capabilities of the European HPC ecosystem. This cooperation should not only focus on HPC technologies but also on policies to develop wider use of HPC within the scientific and industrial communities.

PRACE has undertaken similar activities by signing MoU agreements with other regions [e.g. 17].

3 The Process

The process[3] selected is based on two types of activities:

- **Increasing Visibility** – Enabling platforms that would allow the Project to advertise their achievements and initiate contacts with other regions. This part of the process includes: 1/ Supercomputing Conference Birds-of-a-Feather (SC BoF) events, 2/ the European HPC Handbook and 3/ the European Exa-scale Effort website (www.etp4hpc.eu/euexascale).
- **Direct Contact** – Interactions with the representatives of other regions in order to share updates on HPC-related developments.

We also approached all the projects and offered them an opportunity to participate in the preparation and delivery of these elements. The final result reflects the opinion of the projects involved.

4 Implementation and Results

4.1 SC BoFs (Supercomputing Conference Birds-of-a-Feather events)

The Supercomputing Conference (SC, http://www.supercomp.org/), held annually in the U.S., has been selected as the main vehicle to increase the visibility of the European HPC Projects. It is the largest event of this type in the world and it attracts all the main stakeholders from all parts of the world. We decided to use the Birds-of-a-Feather (BOF) sessions organised within the SC as the optimal tool for presenting such work. In addition, ETP4HPC had previously held successful BOFs at SC'12, '13, '14 and '15, hence some accumulated experience was available within the project.

Within this project, we have organised a BoF at SC'16 and 17. SC'16 BoF is described in D6.2. The main success of SC'17 BoF (14 Nov 2017, Denver, Colorado) is an established process

[3] We chose to present all of the European HPC projects together, regardless of their programme origin (i.e. FP7 or Horizon 2020).

that can be used to organise future events, SC BoFs and other types of event alike, for which the programme of this BoF provides a template. It includes:

- An update on the European HPC eco-system and its strategy
- A presentation of three European HPC projects (three projects have been selected by the leaders of EXDCI WP2, 3, 4 and 6 (Technology, Applications, Cross-cutting issues and International Collaboration) based on descriptions submitted by the projects – a call for presentations had been opened prior to the BoF).
- A Holistic View of European HPC – a high-level summary of European HPC in the light of current HPC trends (a map representing this summary is available at: http://www.etp4hpc.eu/map-of-european-hpc-eco-system.html)
- Updates and comments from other regions (US and Japan)
- A panel discussion (involving all the speakers).

This ‘template’ delivers an efficient BoF with a stable audience of 120-140 attendees.

Figure 8 - The programme of the European SC'17 BoF - as presented on the flyer distributed prior to and at the event (below).

Figure 9 - The front page of the SC'17 BoF Flyer.

Europe will present a holistic view of its HPC development and showcase those of its projects that contribute to the global Exa-scale R&D effort.

The European HPC Technology and Application programme covers the entire HPC system stack and application expertise; including HPC system prototypes (see http://www.etp4hpc.eu/en/euexascale.html for a full description).

We will summarise our ambitions, the global contribution of our projects and discuss how they can fit into the global HPC technology effort. The European EXDCI project (www.exdci.eu) SC17 booth and professional publications (European HPC Handbook) on the ETP4HPC website, will facilitate the networking prior to and after the BoF.

Figure 10 - The abstract of the SC'17 BoF submission - it received a top score (3 = 'Accept' out of 3).

A post-BoF report is available the the BoF webpage at www.etp4hpc.eu/euexascale. The main conclusion of the event is that Europe and other regions should get involved in joint co-design projects.

4.2 The European HPC Handbook

The SC'17 BoF saw the publication of the European HPC Handbook in professional format – designed by a graphic designer and printed by a printing company. All the projects contributed their descriptions to this publication. It was distributed at the BoF and is also available in PDF at www.etp4hpc.eu/euexascale. It will be updated with additional projects (as they start operating) on the occasion of future BoFs.

Figure 11 - The front cover of the 2017 European HPC Handbook - a professional publication issued by task 6.2 of EXDCI, distributed at the European SC'17 BoF and available at www.etp4hpc.eu/euexascale.

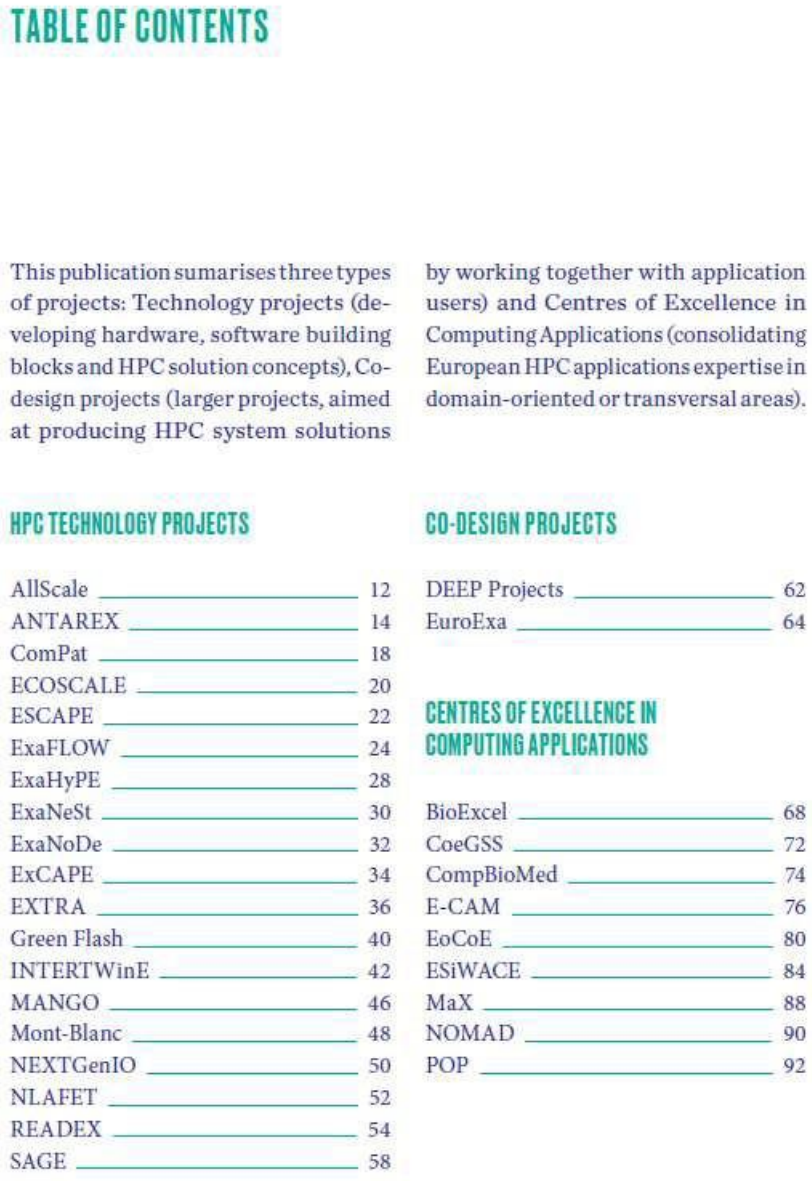

TABLE OF CONTENTS

This publication sumarises three types of projects: Technology projects (developing hardware, software building blocks and HPC solution concepts), Co-design projects (larger projects, aimed at producing HPC system solutions by working together with application users) and Centres of Excellence in Computing Applications (consolidating European HPC applications expertise in domain-oriented or transversal areas).

HPC TECHNOLOGY PROJECTS

CO-DESIGN PROJECTS

CENTRES OF EXCELLENCE IN COMPUTING APPLICATIONS

Figure 12 - The Table of Contents of the 2017 European HPC Handbook.

4.3 European Exascale Effort webpage

ETP4HPC maintains a web page – http://www.etp4hpc.eu/euexascale – on which updated information on the EXDCI international collaboration activities is stored. This includes the material of the BoF sessions, the current (downloadable) European HPC Handbook and a Summary of European HPC – a downloadable document including a high-level description of European HPC.

Figure 13 - The European Exascale Effort website run by ETP4HPC.

Figure 14 - A short summary of the development of European HPC available at www.etp4hpc.eu/euexascale.

4.4 Direct Contact

ETP4HPC has also begun the process of interacting directly with other regions by identifying the main contacts and organising meetings with them. It has a focus on Japan – as relations with the US are already sufficiently mature they have been advanced through a number of events and organisations (e.g. SC and BDEC). The scope of this work is included in D6.2.

5 Conclusions

As the European HPC projects mature and the European HPC Eco-system enters the phase of validating the results of its work (e.g. by using the technologies developed to build supercomputer prototypes – such as the concept of European Extreme-Scale Demonstrators [17] developed by ETP4HPC), some of the projects will require assistance, in order to take

advantage of their increased international visibility and the contacts that have been initiated. The BoF process and related material developed by this project is an excellent tool to increase the visibility and continue promoting European HPC projects at international level. EXDCI will focus on maintaining this effort.

The EXDCI survey (analysed in D6.2) indicates that 31% of all the Projects expressed a need for a tool that would help implement this process. These Projects work mainly in the Programming Tools area (67% - followed by Algorithms and Memory/Storage). All of these Projects identify **joint workshops as an appropriate mechanism,** followed by research visits. **EXDCI should help by facilitating such workshops and visits and securing appropriate funding.**

The project will continue developing relations with the US and Japan with the objective to obtain more detailed information on the development of their ecosystems.

6 Annex

6.1 Annex 1 – The 2017 European HPC Handbook

Available at www.etp4hpc.eu/euexascale

EuropEan HigH-pErformancE computing

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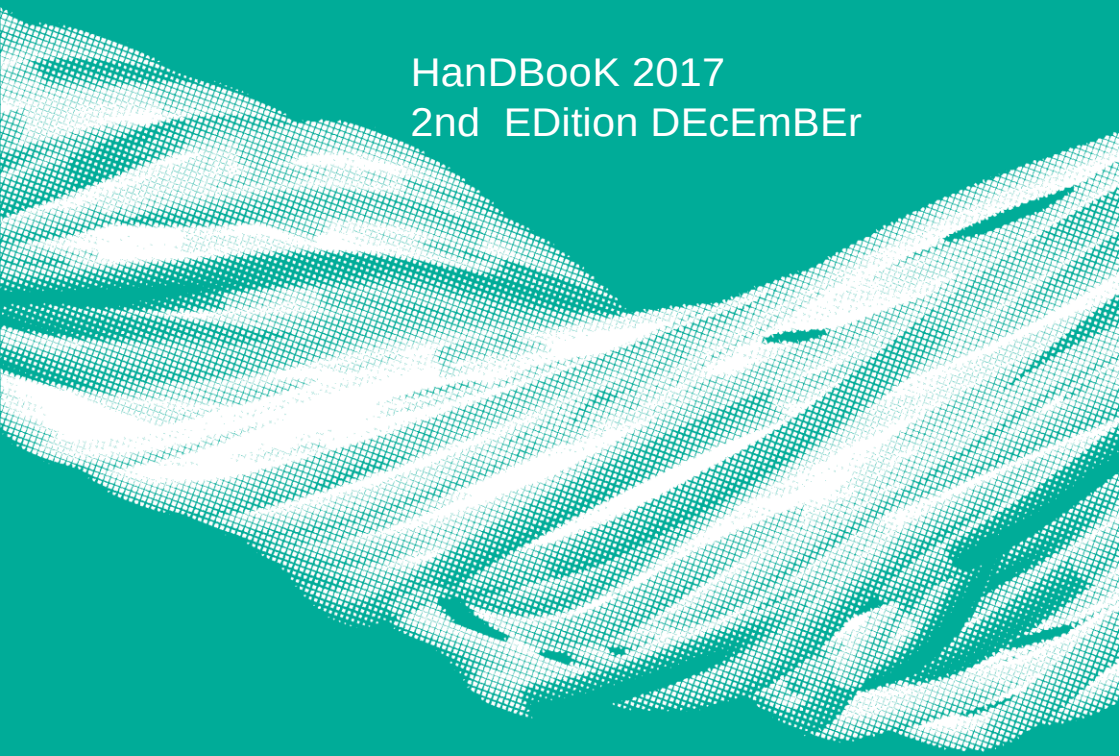

ETP 4 HPC

EUROPEAN TECHNOLOGY PLATFORM FOR HIGH PERFORMANCE COMPUTING

e-dci
European Extreme Data & Computing Initiative

EUROPEAN TECHNOLOGY
PLATFORM FOR HIGH
PERFORMANCE COMPUTING

www.Etp4
Hpc.Eu
www.Etp4Hpc.Eu/
EuExascalE
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Hpc.Eu

mEssagE

Dear Partners,

The European Union's Horizon 2020 Research Programme is now in full swing and significant investments in HPC R&D are taking place. European project consortia are delivering results in the area of HPC technology provision and application expertise. Whilst these results are expected to serve the greater objective of building a globally compet- itive HPC ecosystem in Europe, they might also contribute to the progress of the worldwide HPC community in its reaching of Exascale and other targets. This opens opportunities worldwide for synergies and collaborations with projects from other regions.

We encourage the members of the global HPC Community to familiarise themselves with the outcomes of the European HPC technology and applica- tion projects. We hope that successful collaborations will materialise through them in order to accelerate and optimise our global efforts.

EXDCI Project Coordinator
sergi girona

ETP4HPC Chairman
Jean-pierre panziera

taBlE of contEnts

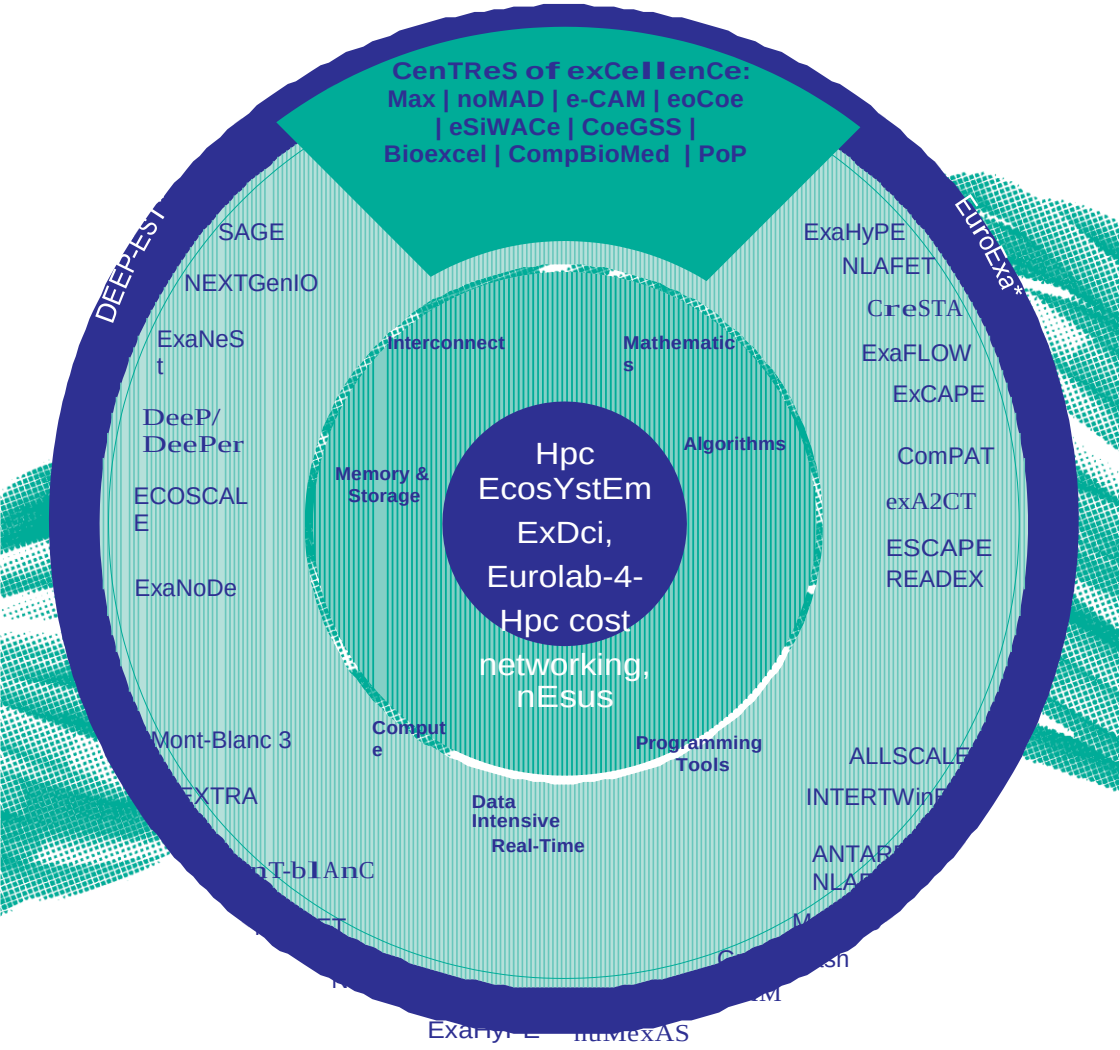
This publication sumarises three types of projects: Technology projects (de- veloping hardware, software building blocks and HPC solution concepts), Co- design projects (larger projects, aimed at producing HPC system solutions by working together with application users) and Centres of Excellence in Computing Applications (consolidating European HPC applications expertise in domain-oriented or transversal areas).

Hpc tEcHnologY proJEcts

co-DEsign proJEcts

cEntrEs of ExcEllEncE in computing applications

EuropEan Exa-scalE proJEcts


CenTReS of exCellenCe:
Max | noMAD | e-CAM | eoCoe
| eSiWACe | CoeGSS |
Bioexcel | CompBioMed | PoP
DEEP-EST
EuroExa*
SAGE
NEXTGenIO
ExaNeSt
DeeP/
DeePer
ECOSCALE
ExaNoDe
ExaHyPE
NLAFET
CreSTA
ExaFLOW
ExCAPE
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INTERTWinE
ANTAREX
NLAFET
ExaHyPE
MaMExAS

Hpc tEcHnologY proJEcts

allscale

AllScale enables developers to be productive and to port applications to any scale of system

The AllScale project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 671603

www.allscale.eu

Leading organisation
Universitaet Innsbruck

Partners Involved
Queen's University Belfast (QUB)
IBM Research (IBM)
NUMECA International (NUM) Royal Institute of Technology (KTH)
Friedrich-Alexander-Universität (FAU)

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+ 43 512 507 53204

objectives

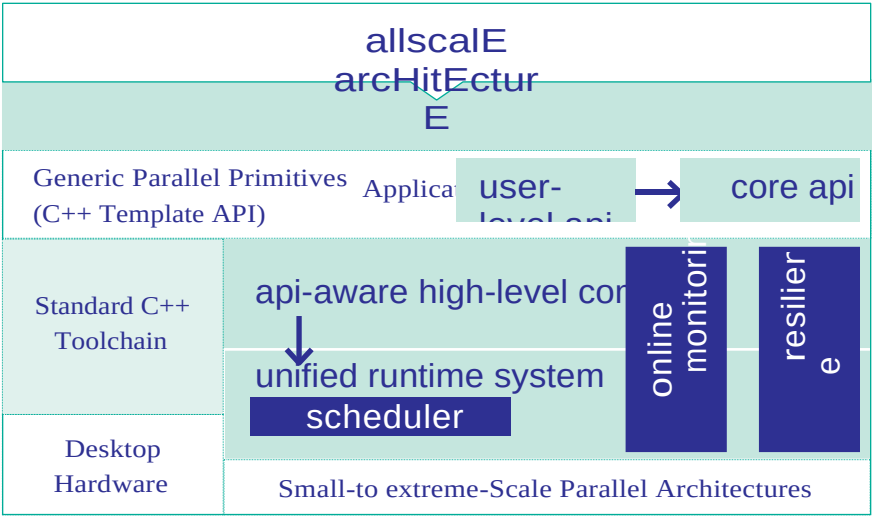
AllScale is an innovative programming approach for ExaScale, decoupling pro- gram specification of parallelism by the programmer from management tasks automatized by the underlying runtime system. The programmer is exposed to a single, generic parallel model that provides a global view of parallelism and locality which is automatically mapped by exploiting recursive parallelism to a variety of parallel resources with the help of the AllScale toolchain that supports:

- Automated applications port- ing from small- to extreme scale architectures
- Flexible tuning of program execu- tion to fulfil trade-offs among execu- tion time, energy and resource usage
- Efficient management of hardware resources and associated parame- ters (e.g. clock speed)
- Seamless integration of resilience management measures to compen- sate for isolated hardware failures,
- Online performance monitoring and analysis.

The key-enablers of this approach are the utilization of nested recursive parallel primitives, the empowerment of the runtime system to actively man- age the distribution of work and data throughout the system, and the utili- zation of

advanced compiler analysis

12



to aid the runtime system in steering program executions.

AllScale is expected to boost the parallel applications development pro- ductivity, their performance portability, and runtime efficiency. It will reduce energy consumption, thus improving the resource efficiency utilization of small to extreme scale parallel systems. The achieved outcomes are validated with applications from fluid dynamics, environment hazard and space weather simulations provided from SME, indus- try and academic institutions.

allscale api based on c++ templates

user-level api:

- High-level abstractions (e.g. grids, meshes, stencils, channels)
- Familiar interfaces (e.g. parallel for loops, map-reduce)

core-level api:

- Generic function template for re- cursive parallelism
- Set of recursive data structure templates
- Synchronization, control- and da- ta-flow primitives

anta
rEx

www.antarex-project.eu

Highlights of your project

Energy-efficient heterogeneous super- computing architectures need to be coupled with a radically new software stack capable of exploiting the benefits offered by the heterogeneity at all the different levels (supercomputer, job, node) to meet the scalability and energy efficiency required by Exascale super- computers. ANTAREX will solve these challenging problems by providing a breakthrough approach to express ap- plication self-adaptivity at design-time and to runtime manage and autotune applications for green and heterogenous High Performance Computing (HPC) systems up to the Exascale level.

what are anticipated technology (hw/sw/ methodology) suggested for inclusion in an EsD project and describe the current maturity?

The compiler technology being devel- oped consists of a separation of con- cerns (where self-adaptivity and energy efficient strategies are specified aside to application functionalities) promoted by the use of LARA, a Domain Specific Language (DSL) inspired by aspect-ori- ented programming (AOP) concepts for heterogeneous systems. The project

includes the development of standalone libraries, methodologies and tools fo- cused on code analysis and optimiza- tion, runtime application autotuning, and resource and power management. We have different maturity levels among the tools and libraries. The tech- nology behind the DSL has several years of development, the libraries and tools have different levels of maturity (some have started in this project, others started in previous projects and have been extended), and the integration of all the tools and libraries in a single framework is still in development.

The framework is based on the fol- lowing technologies (www.antarex-pro- ject.eu/dissemination#tools):

- The mARGOt autotuner (autotuning framework which enhances the application with an adaptation layer): gitlab.com/margot_project/core
- The Examoon framework (A highly scalable framework for performance and energy monitoring of super- computing machine in production): github.com/fbeneventi/examon
- The Lib Versioning Compiler (easy dynamic compilation with versioning support): github.com/skeru/libVersioningCompiler

- The PowerManager (Power capper that selects the best performance point for each core in order to main- tain a power constraint while adapt- ing at the workload parallelization strategy): data-archive.ethz.ch/deliv- ery/DeliveryManagerServlet?dps_ pid=IE5768287
- The CLAVA + LARA compiler frame- work (C/C++ source-to-source tool for code instrumentation and trans- formations controlled by the LARA language): demo available at specs. fe.up.pt/tools/clava (the tool will be publically deployed during the ANTAREX project)

How should this technology be used / inte- grated (i/f, apis)

The DSL is being used to control the integration between the several librar- ies/tools and target applications. Other third party tools and libraries can be used to output information (e.g., re- sultant from analysis and profiling) to LARA strategies. These LARA strat- egies can then take into account the input information to decide about some code transformations, instrumentation, and autotuning knobs and calls. In ad- dition, with the ANTAREX approach other instrumentation and monitoring libraries and/or autotuning schemes can be holistically integrated by the use of LARA strategies to transform and inject extra code in the application source code.

are there any pre- or co-requisite items

The approach aims at avoiding manual modifications on source code, so requi- sites would mostly be writing strategies in the LARA DSL or adapting existing ones. Besides that, the DSL framework (CLAVA) needs a Java runtime, and each tool/library has its own specific dependences.

any extra work/interaction (on top of current project roadmap) needed to make them ready?

Some of the technologies in develop- ment are already deployed in HPC sys- tems in production, however to have a production-ready framework that inte- grates all the tools, we consider that it will need extra work beyond the project.

what information / actions are needed to best prepare for EsD projects?

Ensure that each individual component has a clear interface and is well docu- mented, start the integration in order to have a proof-of-concept and assess the current state, in order to prepare a plan of what would be necessary to have a fully-fledged product ready for HPC systems.

compat

Computing Patterns for High Performance Multiscale Computing

www.compat-project.eu

Leading organisation

University of Amsterdam

Partners Involved

University of Amsterdam
University College London
Institute of Bioorganic Chemistry – Poznan Supercomputing and Networking Centre
Bayerische Akademie der Wissenschaften – Leibniz-Rechenzentrum
Max-Planck-Gesellschaft zur Förderung der Wissenschaften e.V
University Leiden
The Hartree Centre/STFC
Allinea Software
CBK Sci Con
National Research University ITMO
Brunel University

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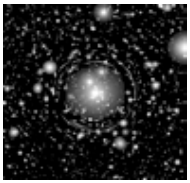
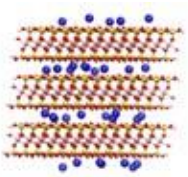
The CoMPAT project is a major com- ponent of the Horizon 2020 “Towards Exascale Computing” research theme. We have assembled a Pan-European team combining leading players from Academia and commercial entities active in real world applications. Multiscale phenomena are ubiquitous and they are the key to understanding the complexity of our world. our Main objective is to develop generic and re- usable High Performance Multiscale Computing algorithms to address the exascale challenges of heterogeneous architectures and will enable us to run multiscale applications with extreme data requirements while achieving scalability, robustness, resiliency, and energy efficiency.

nine grand challenge applica- tions demonstrate the viability of our approach, these applications are ex- ascale-ready and pave the road to un- precedented scientific discoveries. The grand challenge applications have been selected from four different science do- mains. nuclear fusion: the interactions between turbulence at very small scales and the large scale plasma behaviour holds the key to control its magnetic confinement in order to produce clean and carbon free energy for the indefinite future. Astrophysics: the formation processes of stars in their clustered environment, as well as the origin and propagation of structure in the stellar disk of the Milky Way Galaxy. Materials science: prediction of the materials properties of macroscopic samples of matter based on the specification of the atoms and molecules comprising it. biomedicine: pathophysiology of vascular disease, as well as to provide personalised models of the vasculature in near to or real time for the purpose of supporting of clinical decision-making. The approach is to identify three multiscale computing patterns, realise generic algorithms for all three, im- plement the selected grand challenge applications as tailor-made instantia- tions of the computing patterns, which will serve to demonstrate the efficacy of the new algorithms. The insight we gain en-route will be used to develop performance prediction models in order to anticipate the efficiency of the appli- cations on future exascale machines.

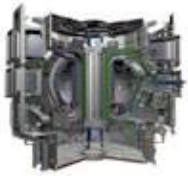
granD cHallEngE application



Astrophysics



Materials



Fusion

biomedicine

Multiscale Coupling libraries (MuSCle, AMuSe, MPWide)

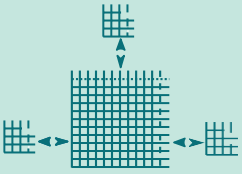
Parallel execution libraries (ADIoS, MPI, openMP)

multiscalE

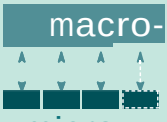
MM1

HigH pErformancE multiscalE

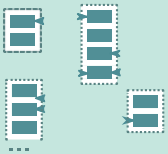
extreme Scaling

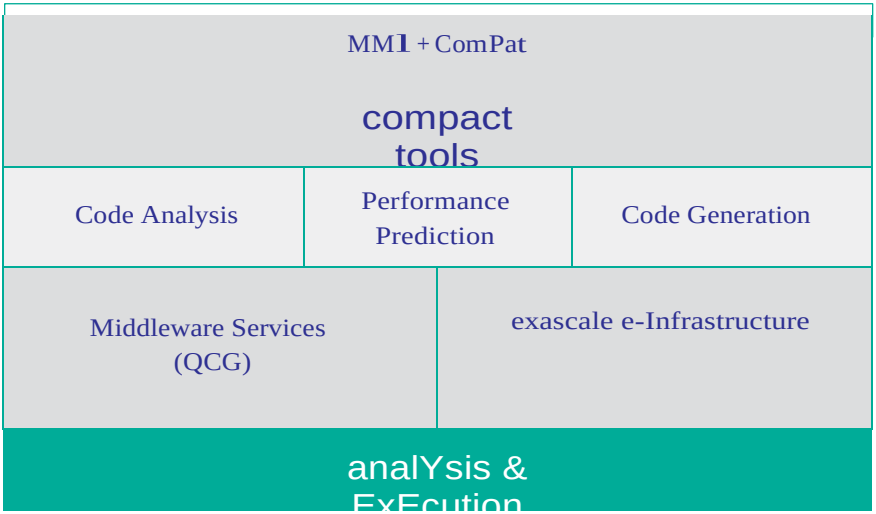


Heterogeneous
Multi-scale Computing



replica Computing





The Multiscale Modelling and Simulation Framework (MMSF) is a theoretical and practical way to model, characterise and simulate multiscale phenomena. MMSF currently compris- es a 4-stage pipeline, going from devel- oping a multiscale model to executing a multiscale simulation.

Our approach is based on Generic Multiscale Computing Patterns that allow us to implement customized al- gorithms to optimise under generic exascale application scenarios. The extreme Scaling computing pattern where one (or a few) of the single scale models in the overall multiscale model dominates all others by far, in terms of required computing power. In the Heterogeneous Multiscale Computing pattern, we couple a macroscopic model to a large and dynamic number of micro- scopic models. replica Computing is a multiscale computing pattern that combines a potentially very large number of terascale and petascale simulations (also known as 'replicas') to produce robust outcomes

The multiscale computing patterns determine the ordering and composi- tion of models that are coupled within a multiscale application. In order to orchestrate the execution of the applica- tion on HPC resources and specifically exascale systems, we require a compre- hensive technology stack.

EcoscalE

Energy-efficient Heterogeneous COmputing at exaSCALE

www.ecoscale.eu

Leading organisation

Telecommunication Systems Institute (TSI)

Partners Involved

Telecommunication Systems Institute
Queen's University Belfast
STMicroelectrnics
Acciona
University of Manchester
Politecnico di Torino
Chalmers University of Technology
Synelixis Solutions

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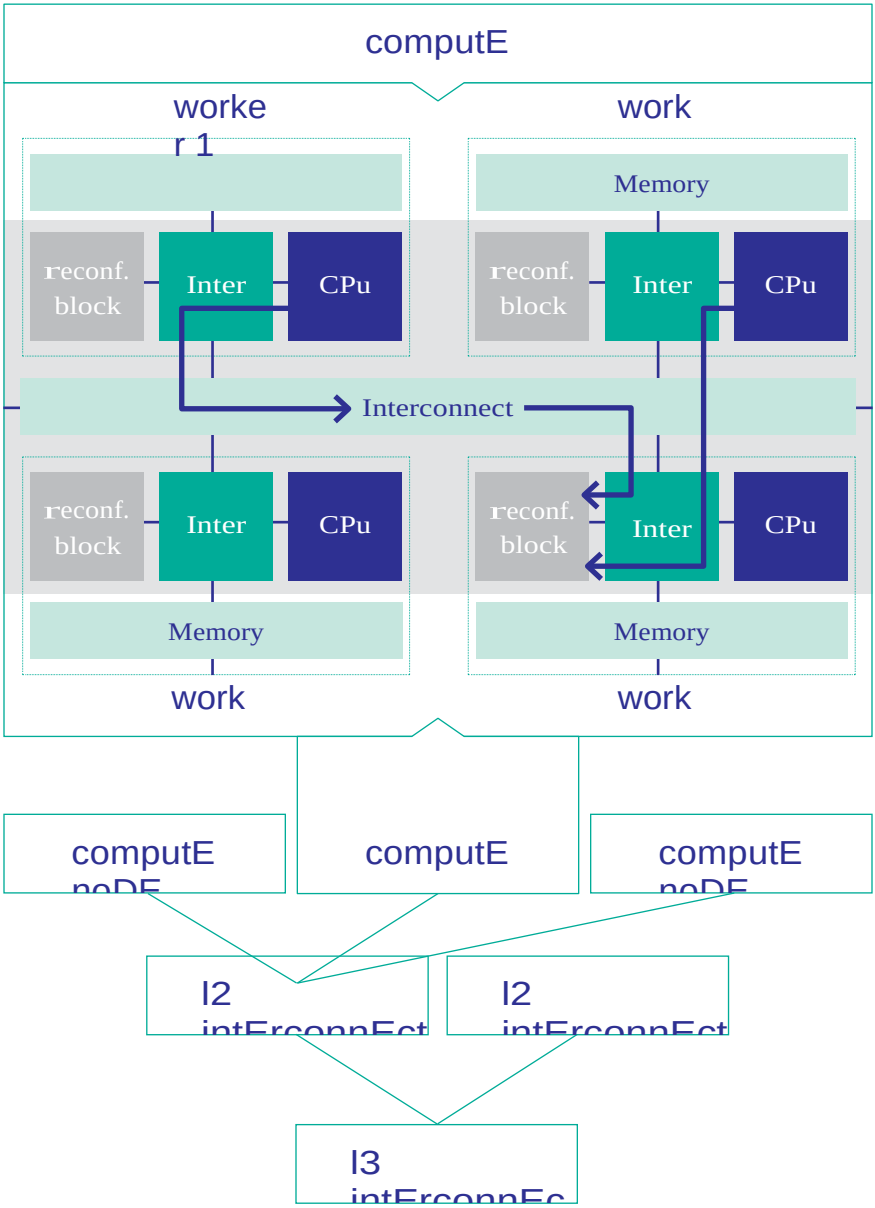
+30 694427772

ECOSCALE tackles the exascale chal- lenge by providing a novel heterogene- ous energy-efficient hierarchical archi- tecture, a hybrid distributed OpenCL programming environment and a runt- ime system. The ECOSCALE architec- ture, programming model and runtime system follows a hierarchical approach where the system is partitioned into multiple autonomous Workers (i.e. compute nodes). Workers are inter- connected in a tree-like structure in order to form larger Partitioned Global Address Space (PGAS) partitions. To further increase the energy efficiency of the system, the Workers employ re- configurable accelerators that perform coherent memory accesses in the virtual address space while being programmed by OpenCL.

The novel UNILOGIC (Unified Logic) architecture, introduced with- in ECOSCALE, is an extension of the UNIMEM architecture. UNIMEM provides shared partitioned global ad- dress space while UNILOGIC provides shared partitioned reconfigurable re- sources. The UNIMEM architecture gives the user the option to move tasks and processes close to data instead of moving data around and thus it reduces significantly the data traffic and related energy consumption and delays. The proposed UNILOGIC+UNIMEM ar- chitecture partitions the design into several Worker nodes that communi- cate through a fat-tree communication infrastructure.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I2
I3

EscapE

Energy efficient Scalable Algorithms for weather Prediction at Exascale (ESCAPE)

www.hpc-escape.eu

Leading organisation

European Centre for Medium-Range Weather Forecasts (ECMWF), UK

Partners Involved

Météo-France (MF), FR
Royal Météorologique de Belgique (RMI), BE Danmarks Meteorologiske Institut (DMI), DK Federal Officeof Meteorologyand Climatology (MSwiss), CH
Deutscher Wetterdienst (DWD), DE
Loughbourough University (LU), UK
Irish Centre for High-End Computing (ICHEC), IR
Poznan Supercomputing and Networking Centre (PSNC), PL
Atos/Bull (Bull), FR
NVIDIA (NVIDIA), CH
Optalysys (OSYS), UK

Contact name(s)

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ESCAPE stands for Energy-efficient Scalable Algorithms for Weather Prediction at Exascale. The project will develop world-class, extreme-scale computing capabilities for European operational numerical weather predic- tion (NWP) and future climate mod- els. The biggest challenge for state-of- the-art NWP arises from the need to simulate complex physical phenome- na within tight production schedules. Existing extreme-scale application soft- ware of weather and climate services is ill-equipped to adapt to the rapidly evolving hardware. This is exacerbated by other drivers for hardware devel- opment, with processor arrangements not necessarily optimal for weather and climate simulations. ESCAPE will redress this imbalance through innova- tion actions that fundamentally reform Earth system modelling.

ESCAPE addresses the ETP4HPC Strategic Research Agenda 'Energy and resiliency' priority topic, developing a holistic understanding of energy-effi- ciency for extreme-scale applications using heterogeneous architectures, ac-celerators and special compute units. The three key reasons why this project will provide the necessary means to take a huge step forward in weather and climate modelling as well as interdis- ciplinary research on energy-efficient high-performance computing are:

- Defining and encapsulating the fundamental algorithmic building blocks ('Weather & Climate Dwarfs') underlying weather and climate ser- vices. This is the prerequisite for any subsequent co-design, optimization, and adaptation efforts.
- Combining ground-breaking fron-tier research on algorithm devel- opment for use in extreme-scale, high-performance computing ap-plications, minimizing time- and cost-to-solution.
- Synthesizing the complementary skills of all project partners. ECMWF and leading European regional fore- casting consortia are teaming up with excellent university research and experienced high-performance computing centres, two world-lead- ing hardware companies, and one European start-up SME, providing entirely new knowledge and technol- ogy to the field.

ESCAPE is funded by the European Commission under the Future and Emerging Technologies — High- Performance Computing call for re- search and innovation actions, grant agreement 671627.

Exaflow

www.exaflow-project.eu

Leading organisation

Royal Institute of Technology - KTH, Sweden

Partners Involved

University of Stuttgart, USTUTT, DE (Institute of Aerodynamics and Gas Dynamics, IAG, High Performance Computing Center Stuttgart, HLRS)
Ecole Polytechnique Federale de Lausanne, EPFL, CH
Imperial College London, IC,UK
University of Southampton, SOTON, UK
The University of Edinburgh, UEDIN, UK
McLaren Racing Ltd, McLaren, UK
Automotive Simulation Center Stuttgart, ASCS, DE

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intro

ExaFLOW stands for “Enabling Exascale Fluid Dynamics Simulations”. Computational Fluid Dynamics (CFD) is a prime contender for reaching exas- cale performance: In fluid dynamics there is virtually no limit to the size of the systems to be studied via numerical simulations, which can be exploited for extreme parallel scaling. Moreover, fluid flows are an essential element of many industrial and academic prob- lems: A crude estimate shows that 10% of the energy use in the world is spent overcoming turbulent friction. As such, collaboration between software crea- tors and European industries within automotive, manufacturing, aerospace, energy and health care is crucial.

The goals of ExaFLOW comprise four key innovation areas, including aspects of - mesh adaptivity,

- resilience,
- strong scaling at exascale through novel CG-HDG discretisations, and,
- I/O efficiency improvements.

progress so far

In all these areas, significant progress has been made since the project start. For instance, we have developed fault tolerance mechanisms, such that the new algorithm “survives” >90% of the errors that would otherwise have resulted in an execution failure; this all with very little overhead both in fault-free execution and in recovery. We are currently putting that capa- bility into Nektar++, which will also include a multi-layer checkpoint ap- proach, supplementing classic to- disk checkpoints with inexpensive “diskless checksum checkpoints” that may be sampled more frequently. Similar de- velopments are also added to Nek5000 using an innovative checkpoint/revolve algorithm. For the improvement of IO strategies we implemented a new tool called FieldIOBenchmarker which is in- tegrated in our applications, and allows to use XML, HDF5 and SIONlib. Finally, we have considered a number of differ- ent pre- conditioners (including Hypre based on PETSc), which are ready to be used in the forthcoming h- and p- type refinements in Nek5000 and Nektar++. Moreover, during first 18 months of the project we have managed to make four new releases/updates of the codes used in the project:

OpenSBLI, has been released un- der the GNU General Public License on GitHub. See opensbli.github.io This is an open-source release which features automated code generation capabilities.

- ExaGS, a new low latency commu- nication kernel for Nek5000, will be released under an open-source license soon.
- Nek5000 v16 has been released in and moved to GitHub. See github. com/Nek5000.
- Nektar++ versions 4.3 and 4.4 have been released.

use cases

The two industrial partners who work on two different automotive use cases are McLaren Racing and the Automotive Simulation Center of Stuttgart which represents Opel in this project. The “McLaren Front Wing” use case is run by Imperial College London and McLaren Racing and it is representative of one of the major points of interest in Formula 1, i.e. the interaction of vortical structures generated by the front wing endplate with the front wheel wake. The Opel use case focuses on the sim- ulation of an unsteady turbulent flow, which originates from the separation of the flow on the rear part of the Opel Astra GTC.

The other two use cases are academ- ic. The “Wing profile NACA4412” is run by KTH Stockholm and the University of Southampton, and the “Jet in cross-flow” is run by KTH Stockholm and the University of Stuttgart.

All ExaFLOW innovations are clear- ly targeted to enhance the efficiency and exploitability of a number of ex- isting and heavily used open-source codes on today’s largest-scale (and in the future exascale) systems. More precisely, the spectral codes Nek5000 and Nektar++, and the finite difference codes OpenSBLI and NS3D.

project details

Start date: 01/10/2015
End date: 30/09/2018
Duration: 36 months
Budget: euro 3,3 million Reference: GA no 671571
Call: H2020-FeTHPC-2014

Simulation using Nektar++ using ARCHER on the RP1 Elemental Track Car

ExaHypE

An Exascale Hyperbolic PDE Engine

www.exahype.eu

Leading organisation
Technical University of Munich

Partners Involved
Technical University of Munich
Universita degli Studi di Trento
Durham University
Frankfurt Institute for Advanced Studies
Ludwig-Maximilians-Universität München
RSC Technologies
Bavarian Research Alliance

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ExaHypE Vision

Hyperbolic systems of PDE resulting from conservation laws are the basis to simulate a wide range of problems, ranging from weather forecast, complex earthquake physics, hematic flows in patients up to the most catastrophic events in the universe. In this project, we develop an exascale-ready “engine” that shall enable teams of computational scientists to more quickly realize grand challenge simulations based on hyperbolic PDE models.

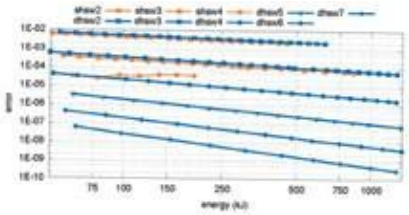
ExaHypE algorithms

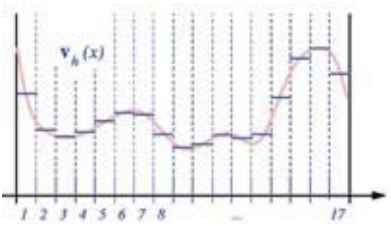
The developed engine implements a high-order discontinuous Galerkin ap- proach with ADER time stepping and a-posteriori finite-volume limiting, which promises to combine high-order accuracy and excellent robustness of solutions. Problems are discretised on tree-structured fully adaptive Cartesian meshes, for which advanced paralleli- sation approaches and load-balancing algorithms are developed in the project.

ExaHypE Engine

The hyperbolic PDE engine developed in the ExaHyPE project is available as open source source software, hosted at www.exahype.org.

The consortium provides a guide-book coming along with the released code which contains, besides documen- tation, rationale and further documen- tation links.



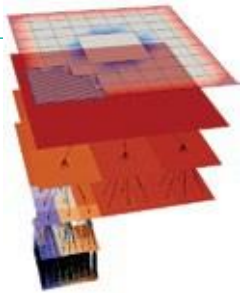


High order

finite Volume

code

tree



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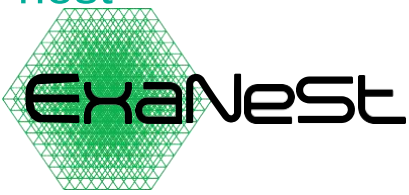
nest



www.exanest.eu

Leading organisation
FORTH

Partners Involved
Iceotope
Allinea
EnginSoft
eXact lab
MonetDB
Virtual Open Systems
Istituto Nazionale di Astrofisica (INAF)
National Institutefor Nuclear Physics(INFN)
The University of Manchester
Universitat Politècnica de València
Fraunhofe

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project Highlights

- ARMv8 with *UNIMEM* (global sharable coherent memory scheme)
  1. Supporting MPI and Partitioned Global Address Space (PGAS)
  2. low energy compute, low over- head communications
  3. UNILOGIC FPGA acceleration
- Networking – *unified* compute & storage, low latency
- Storage – converged offering local- ity while distributed, non-volatile memories
- Real Applications – Scientific, Engineering, Data Analytics
- Data Centre Infrastructure – Power, Cooling, Mechanicals, Total Liquid Cooling

Exanest Block Diagram

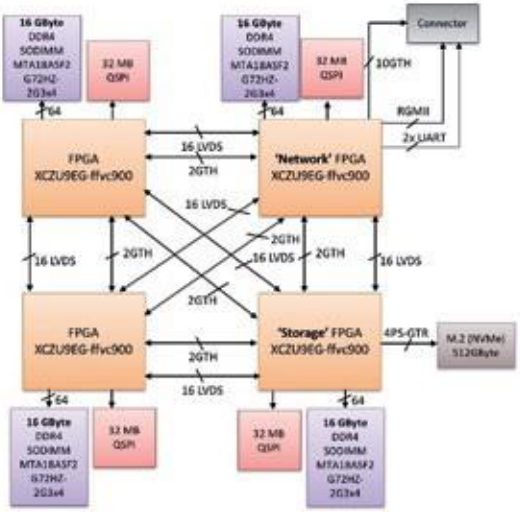

Fig. 1: 120mm x 130mm Quad FPGA/ARM Node with NVRAM and DRAM

Fig. 2: Initial Total Liquid Cooled Prototype

prototype outcomes

- Networking, Storage and Application Developments – Ready to support the Nest, Nodes and the Ecosystem,
  1. The Nest – Ready to power, connect and liquid cool differ- ent distributed compute nodes (@3.2kW/u, 762mmx600mm cabinets)
  2. FPGA/ARM Nodes – Initial Nodes for the Nest with 4 FPGAs
- Commercialization outlook, in co-operation with external partners, including KALEAO

ExanoDe

European Exascale Processor & Memory Node Design

www.exanode.eu

Leading organisation

CEA

Partners Involved

CEA
ARM Limited
ETH Zürich
FORTH
Fraunhofer ITWM
Scapos AG
University of Manchester
Atos Bull
Virtual Open Systems
Barcelona Supercomputing Center Forschungszentrum Jülich
Kalray SA
CNRS (University of Sherbrooke)

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The ExaNoDe research project is supported by the European Commision under the “Horizon 2020 Framework Programme” with grant number 671578

project Highlights

ExaNoDe designs core technologies for a high energy efficient and highly inte- grated heterogeneous compute node towards Exascale computing.
Key technologies:

- low-power ARMv8 computing architecture
- 3-D integration (interposer) of System-on-Chips (SoC) for higher compute density combined with high-bandwith, low-latency data communication interfaces
- UNIMEM-based advanced memory architecture for high scalability

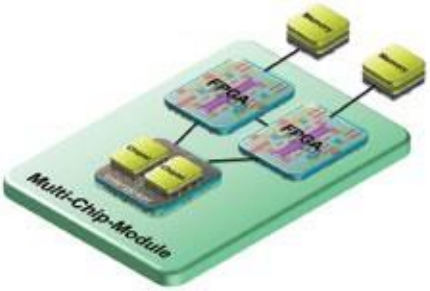
project’s contribution to Exascale computing

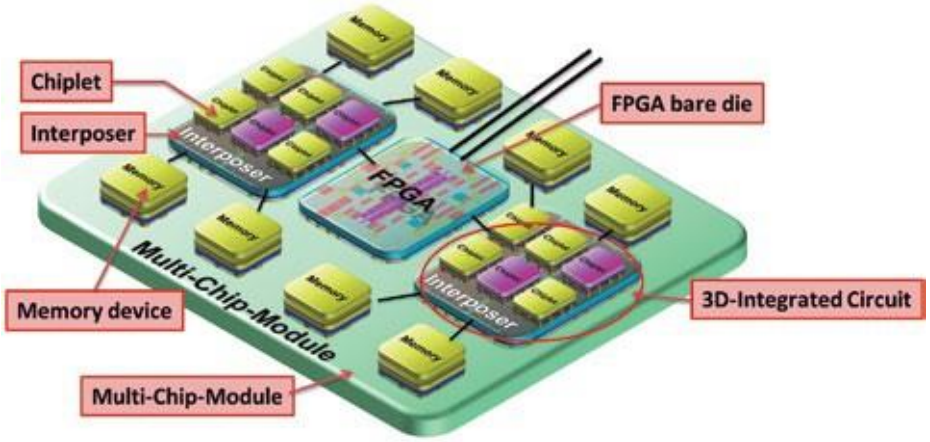
ExaNoDe will deliver an HW/SW inte- grated prototype available for collabo- ration including:

- Technology and design solutions for interposer based computing device for HPC applications,

- Integration of devices in a Multi-Chip-Module (MCM) to improve compute density,
- Operating system and library sup- port for resource sharing.

The ExaNoDe prototype will be for pro- totype-level use by system integrators, software teams and subsequent evalu- ation through industrial deployment.





ExaNoDe as part of a global strategy

EUROSERVER
redesigns the enterprise server:
Lower cost through system integration
Energy efficiency: low-power 64 bit processor and more efficient software
Mutualization (sharing) of I/O resources
www.euroserver-project.eu

ECOSCALE
focuses on acceleration
Energy-Efficient Heterogeneous COmputing at exaSCALE
www.ecoscale.eu

EXANEST
Storage, Interconnect, Cooling
Packaging
Apps
European Exascale System Interconnect and Storage
www.exanest.eu

Exc
apE

www.excape-h2020.eu

Leading organisation
Imec

Partners Involved
Imec
IT4I Czech National Supercomputing Centre
AstraZeneca
Janssen
Pharmaceutica
IDEAConsult
Intel JKU
Linz
University of Aalto
Royal Holloway
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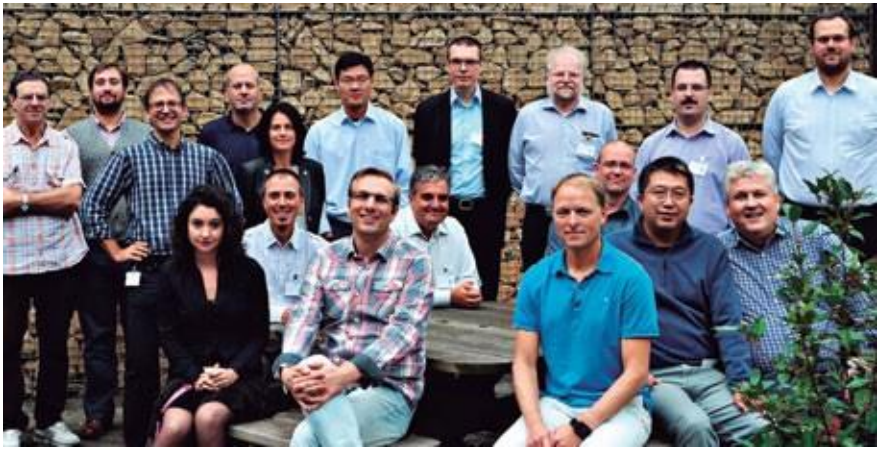

project Executive summary

The ExCAPE project is scaling up ma- chine learning techniques to solve chal- lenging problems on HPC machines. Our driving application is compound-activi- ty prediction for drug discovery. We are preparing data, developing the state of the art for machine learning algorithms, and researching programming models to implement them.

project Description

Our main achievements so far include:

- Public release of an data set that resembles industry data in terms of size and distribution of hits and misses, and experiments showing the potential of novel compound descriptors for doing multi-target predictions at scale
- Open source release of HyperLoom, a programming model and task ex- ecution system that runs on HPC systems and is designed to cope with machine learning
- Open source release of SMURFF, a matrix factorization package allow- ing sophisticated combinations of techniques such as GFA and Macau
- Exploration of the use of and hard- ware implications of sparse matrix techniques to deal with large sparse feature vectors, and the impact on deep learning
- Benchmarking of ML techniques on large scale data sets using HyperLoom
- Novel algorithms to improve scal- ability of matrix factorisation on large machines
- Demonstrating the computation- al requirements of conformal prediction
- Novel clustering implementations for pre-processing compound data

project areas of international collaboration

- Experts in scheduling machine learning tasks on HPC systems
- Pharma companies to compare scal- ability of learning approaches
- Machine learning experts to explore scalability of different classes of algorithms
- Other users and developers of large scale multi-target learning

Extra

Exploiting eXascale Technology with Reconfigurable Architectures

www.extrahpc.eu

Leading organisation
Ghent University, Belgium

Partners Involved
Imperial College London,
UK University of Cambridge,
UK University of
Amsterdam, NL Politecnico
di Milano, IT Ruhr University
Bochum, DE
Telecommunication Systems Institute,
GR Synelixis, GR
Maxeler, UK

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Our objective is to create a *flexible explo- ration platform for the development and optimization of architectures, tools, and applications targeting Exascale systems using reconfigurable technology*. We aim to provide an open-source research platform to enable sustainable research on reconfigurable architectures and tools, and prepare all stakeholders (applica- tion, systems, and tool developers) for the emergence of efficient reconfigur- able accelerators for Exascale systems. Our work revolves around 5 activities:

understand the requirements

We use three different case-studies - Asian option pricing, retinal image seg- mentation, and Diffusion Monte-Carlo
- to investigate the performance, scala- bility, and energy efficiency challenges that emerge in HPC-like applications at Exascale level. We aim to provide mech- anisms to cope with these challenges in both hardware and software.

Design, Develop, and Deploy the open research platform

We focus on the design and implemen- tation of the Open Research Platform, covering its reconfigurability-specific features and design tools. This work includes, for example, research on Virtual Coarse Grained Reconfigurable Arrays (VCGRAs), static and dynamic workload partitioning, efficient data of- floading, and parallel memory systems. Furthermore, the CAOS toolchain is developed to support the design and deployment of reconfigurable acceler- ators, and will integrate the main anal- ysis and optimization tools developed in EXTRA, with support for community extensions in the future.

research novel tools

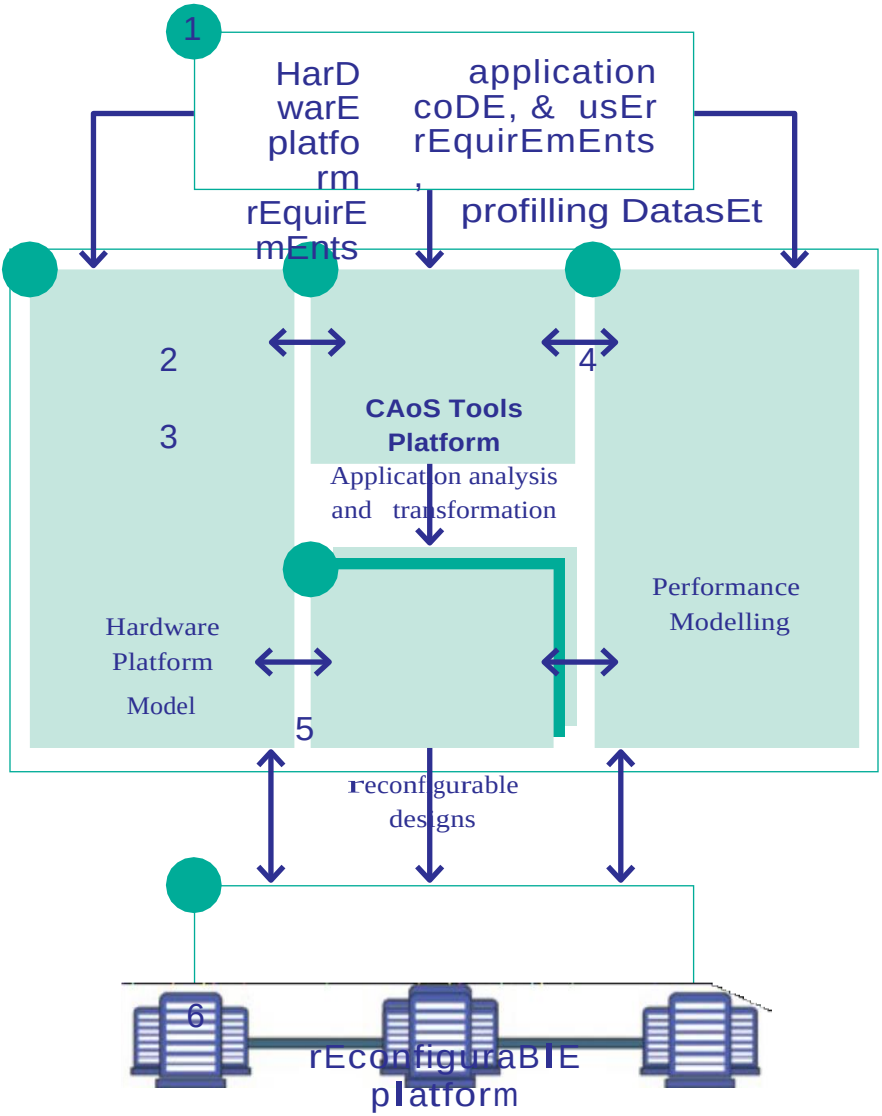
We strive to advance the state-of-art compilation tools for reconfigurable hardware, covering just-in-time synthe- sis, hardware monitoring, emergency management, and hardware debugging.

investigate reconfigurable applications

We search for generalizable optimi- zation opportunities in HPC appli- cations, to leverage reconfiguration, as well as implement, integrate and evaluate their impact on HPC systems.

propose new ideas for reconfigurable technology

Based on the combined analysis of ap- plications, programming technologies and tools, and hardware platforms, we aim to propose technological improve- ments that will increase the efficiency of future reconfigurable systems. The main aspects of this activity include the improvement of the reconfiguration process and finding efficient interface solutions for coupling the FPGA fabric and the processing units.


1
HarD warE platfo rm rEquirE mEnts
application coDE, & usEr rEquirEmEnts ,
profilling DatasEt
2
3
4
CAoS Tools Platform
Application analysis and transformation
Hardware Platform Model
Performance Modelling
5
reconfigurable designs
6
rEconfiguraBlE platform

platform orverview

The Open Research Platform has six main components to support the optimization of applications for the next-generation reconfigurable HPC systems. For this purpose, the platform provides an integrated system that com- bines models for various reconfigurable architectures, tools and applications, allowing researchers to focus on any of these aspects separately or together.

The *platform input* includes information about the application (e.g., source-code, performance requirements, profiling information) and the specification of the target platform (e.g., size, resources, simulated/hardware). The *Hardware Platform Model* guides the design and optimization process for a specific target platform. The *Tools Platform* (e.g., CAOS) generates a re- configurable design through a set of analysis and transformations steps on the application code. The *Performance Modeling* component checks the fit of the expected performance with the user requirements at every stage of the devel- opment process. One or more *candidate reconfigurable design* versions is gener- ated to support design-space exploration and select the most suitable implemen- tation to execute on the *Reconfigurable Platform*, which in turn combines the hardware architecture and runtime of the reconfigurable HPC system.

green flash

www.greenflash-h2020.eu

Leading organisation
Observatoire de Paris

Partners Involved
University of Durham
Microgate
PLDA

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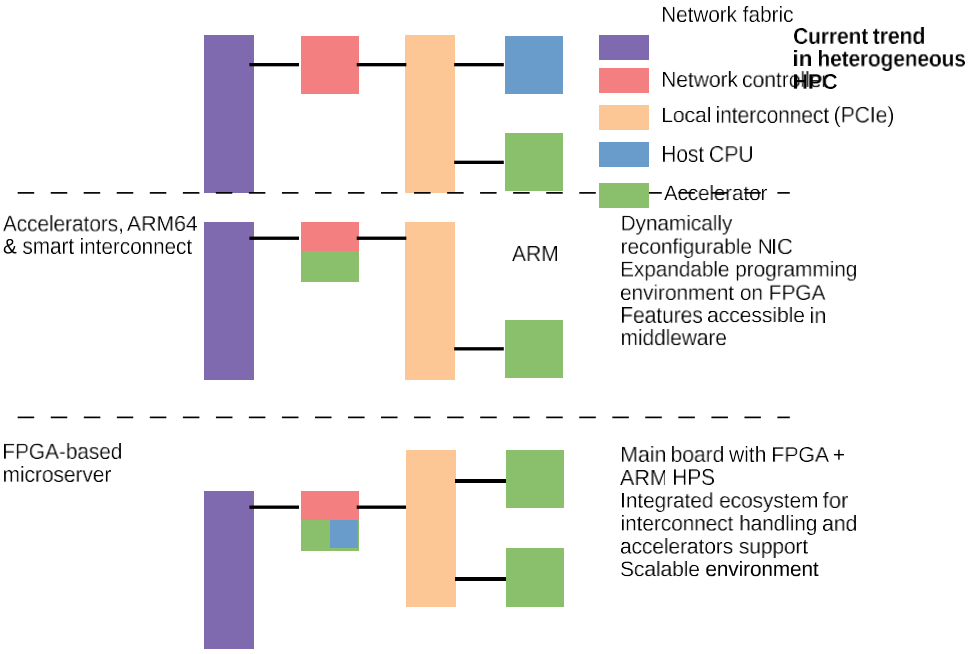
project Executive summary

The main goal of Green Flash is to de- sign and build a prototype for a Real- Time Controller targeting the European Extremely Large Telescope (E-ELT) adaptive optics instrumentation.

On one hand, we propose to demon- strate the scalability of accelerator based solutions for real-time HPC da- ta-intensive applications. On the other hand, an alternative to the commodity accelerator solution for real-time con- trol is to build tailored processor boards, based on high cell density FPGAs. The emergence of new FPGA products, inte- grating an ARM-based Hard Processor System (HPS) with the FPGA fabric, could enable a new approach, merging the concept of compute node in a HPC cluster and specialized processor board in an application specific facility. Our strategy is based on a strong interaction between academic and industrial part- ners. A prototype harboring all the fea- tures is used to assess the performance. It also provides the proof of concept for a resilient modular solution to equip a large scale European scientific facility, while containing the development cost by providing opportunities for return on investment.


Network fabric
Current trend in heterogeneous HPC
Network controller
Local interconnect (PCIe)
Host CPU
Accelerator
Accelerators, ARM64 & smart interconnect
ARM
Dynamically reconfigurable NIC
Expandable programming environment on FPGA
Features accessible in middleware
FPGA-based microserver
Main board with FPGA + ARM HPS
Integrated ecosystem for interconnect handling and accelerators support
Scalable environment

intErtwinE

Programming Model Interoperability towards Exascale

www.intertwine-project.eu

Leading organisation

EPCC, University of Edinburgh

Partners Involved

EPCC (University of Edinburgh),
UK BSC, SP
KTH, SE
Fraunhofer ITWM, DE
DLR, DE
T-Systems SfR, DE
Universitat Jaume I, Sp
Inria, FR
University of Manchester, UK

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project Executive summary

The first Exascale computers will be very highly parallel systems, consisting of a hierarchy of architectural levels. To program such systems effectively and portably, application programming interface (APIs) with efficient and ro- bust implementations must be ready in the appropriate timescale. A single, “silver bullet” API which addresses all the architectural levels does not exist and seems very unlikely to emerge soon enough. We must therefore expect that using combinations of different APIs at different system levels will be the only practical solution in the short to medium term. INTERTWinE is focused on the challenges that lie in interoperability between APIs, both at the specification level and at the implementation level.

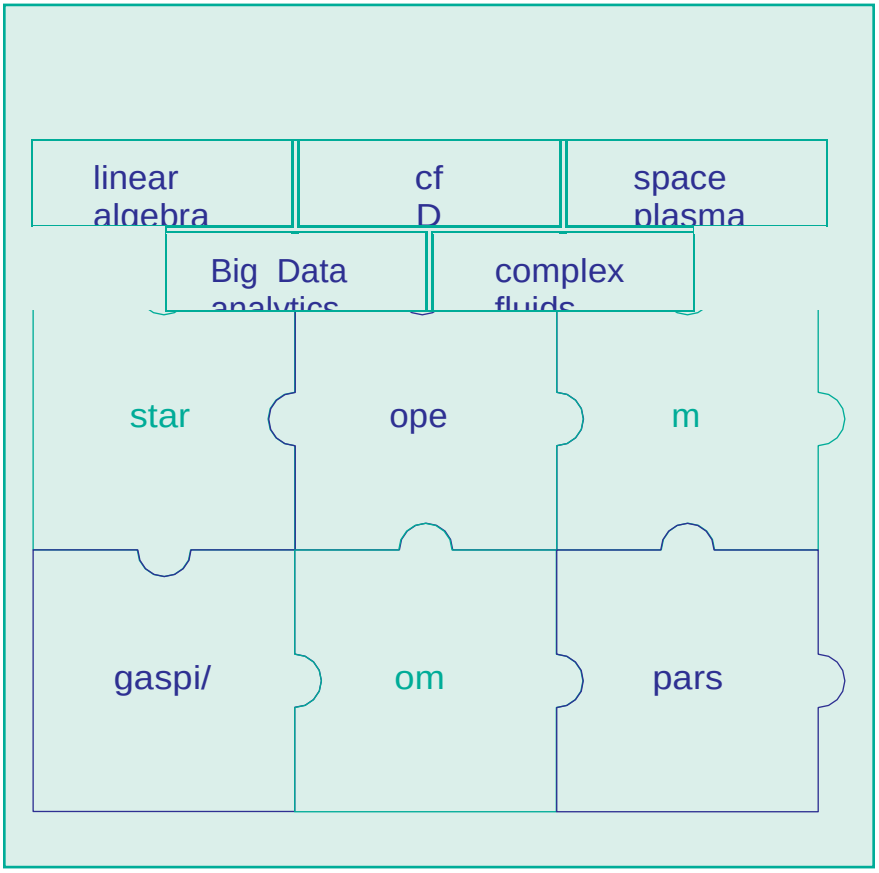
project Description

INTERTWinE brings together the principal European organisations driving the evolution of programming models and their implementations. Our focus is on six key programming APIs: MPI, GASPI, OpenMP, OmpSs, StarPU, and PaRSEC, each of which has a project partner with extensive experience in API design and implementation. The project is working closely with the rele- vant standards bodies and development teams for these APIs, to solve interop- erability problems.

Interoperability requirements, and evaluation of implementations, are be- ing driven by porting a set of kernels and applications to various different API combinations. These codes will be publicly released later in the project.

Driven by these application require- ments, INTERTWinE is designing and implementing two new runtime APIs: a Resource Manager to allow multiple runtimes to negotiate resource sharing within a node, and a Directory/Cache to support execution of task-based programming models on distributed systems by abstracting the communi- cation layer.

The project is also helping devel- opers combine multiple APIs in their applications, by running a programme of training courses and producing a se- ries of Best Practice Guides.



INTERTWinE's target APIs and applications areas.

areas of international collaboration

INTERTWinE partners are very active in pursuing interoperability issues and new API developments in three interna- tional standards bodies: the MPI Forum, the GASPI Forum, and the OpenMP ARB. Project partners are participating in the relevant working groups to pro- pose and test modifications and exten- sions to these important APIs.

INTERTWinE also has collabora- tions with runtime development teams in the US: we are closely connected to the PaRSEC team at the University of Tennessee, and also to the Center for Computing Research at Sandia National Laboratories, working on the OpenMPI library.

mango

Exploring Manycore Architectures for Next-GeneratiOn HPC systems

www.mango-project.eu

leading organisation

Universitat Politècnica de València, Spain

Partners Involved

Universitat Politècnica de València, SP
Centro Regionale Information Communication Technology, IT
Faculty of Electrical Engineering and Computing, University of Zagreb, HR
Politecnico di Milano / Dipartimento di Elettronica, Informazione e Bioingegneria, IT
École polytechnique fédérale de Lausanne, CH Pro Design Electronic GmbH, DE
Eaton Corporation, FR
Thales Group, FR
Philips, NL

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MANGO project is building a large-sys- tem prototype for proper exploration of future HPC architectures including CPUs, GPUs, Manycores, and FPGA- based accelerators. The prototype em-beds highly heterogeneous accelerators in a common infrastructure (a network) which provides guarantees of perfor-mance and QoS to the applications. MANGO is deploying all the software stack (at server side and at accelera- tor side) to let users easily adapt and port their applications to new emerg- ing scenarios with multitude of highly heterogeneous accelerators. For this, specific components such as an API and the resource manager is provided. MANGO delivers all the hardware com- plements plus innovative cooling tech- niques using termoshypons. MANGO is in search of interested users to use and test the system for their applica- tions and integration into larger scale systems.

mont-
Blanc

www.montblanc-project.eu

Leading organisation
Bull (Atos Group)

Partners Involved
ARM
AVL
BSC
Bull/Atos
CRNS (Centre National de la Recherche Scientifique) / LIRMM
ETH Zurich
HLRS
Universidad de Cantabria (Santander)
University of Graz
Université de Versailles Saint Quentin

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TW @MontBlanc_EU
FB @MontBlancEU

Project Mont-Blanc is now in its third phase. All phases of the Mont-Blanc project share the vision of developing a European Exascale approach leveraging commodity power-and cost-efficient embedded technologies.

The key outcome of the project is the deployment of ARM-based computing platforms enabling ARM architecture in HPC, which boost system software development and allow to test real sci- entific applications at scale.

Based on the experience gained from the development of various platforms since 2011 and implementing a co-de- sign approach, the Mont-Blanc project now aims to define the architecture of an Exascale-class compute node based on the ARM architecture, and capable of being manufactured at industrial scale.

our top achievements

1. Demonstrating that it is possible to run HPC workloads with European embedded technology
2. Contributing to the design of a next-generation exascale-class machine with a co-design approach
3. Testing and scaling REAL scientific applications on a non-conventional HPC architecture

nExtgenio

Next Generation I/O for the Exascale

www.nextgenio.eu

Leading organisation
EPCC – The University of Edinburgh

Partners Involved
Intel Deutschland GmbH
Fujitsu
Barcelona Supercomputing Center
Technische Universität Dresden
Allinea, now part of ARM
European Centre for Medium Range Weather Forecasts
ARCTUR

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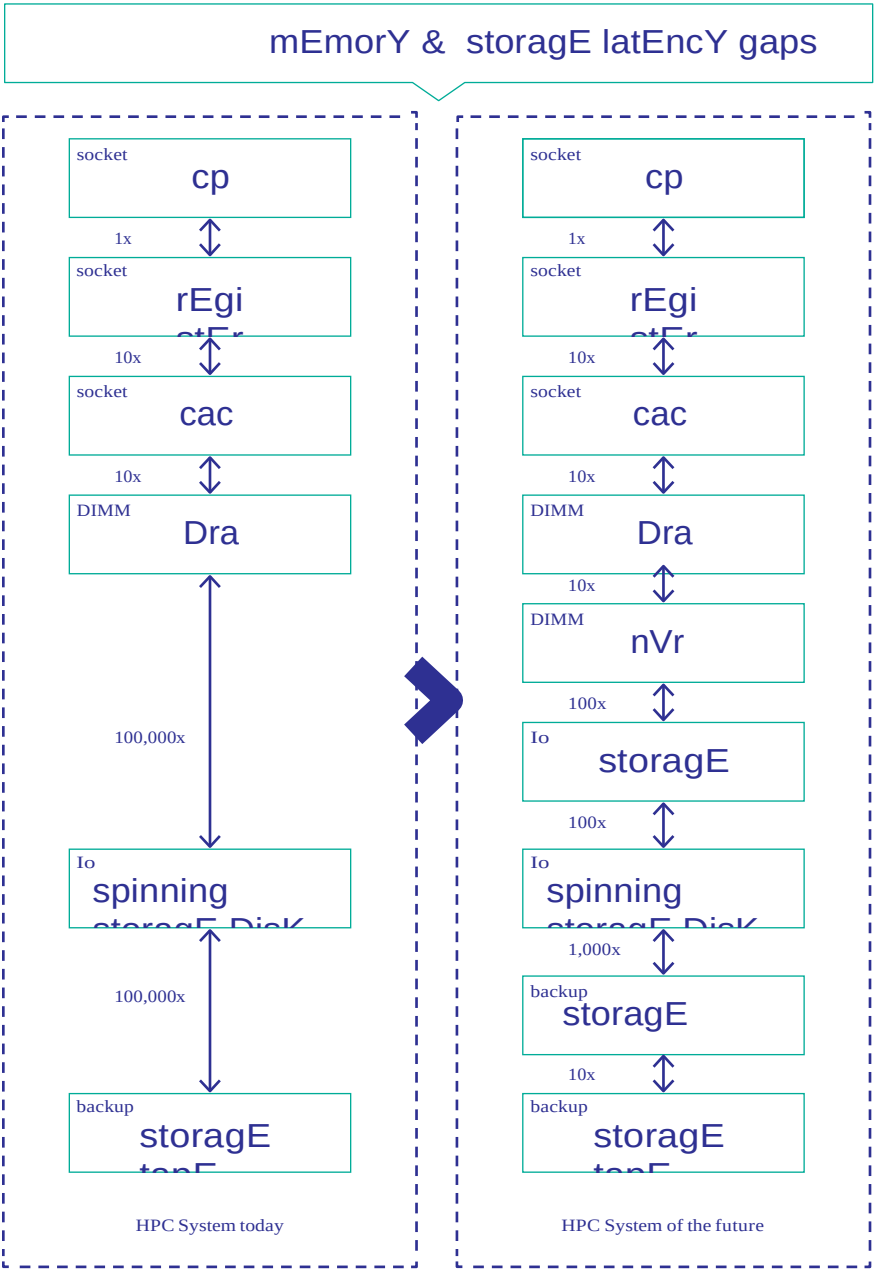
The NEXTGenIO project addresses the I/o performance challenge not only for Exascale, but also for HPC and data intensive computing in general. NEXTGenIO is developing a prototype computing platform that uses on-node non-volatile memory, bridging the latency gap between DRAM and disk. In addition to the hardware that will be built as part of the project, NEXTGenIO is developing the software stack that goes hand-in-hand with this new hard- ware architecture, and is testing the developments using a set of applications that include both traditional HPC (e.g. CFD and weather) and novel workloads (e.g. machine learning and genomics). In addition to a detailed understand- ing of the wide range of use cases for non-volatile memory, key outcomes of NEXTGenIO are:

- Prototype compute nodes with non-volatile memory
- Profiling and debugging tools
- Data and power/energy aware job scheduling system
- Filesystem and object store
- Library for persistent data structures
- Workload benchmark generator & I/O workflow simulator


mEmorY & storagE latEncY gaps
socket
cp
1x
socket
rEgi
10x
socket
cac
10x
DIMM
Dra
100,000x
Io
spinning
100,000x
backup
storagE
HPC System today
socket
cp
1x
socket
rEgi
10x
socket
cac
10x
DIMM
Dra
10x
DIMM
nVr
100x
Io
storagE
100x
Io
spinning
1,000x
backup
storagE
10x
backup
storagE
HPC System of the future

nlafEt

Parallel Numerical Linear Algebra for Future Extreme Scale Systems

www.nlafet.eu

Leading organisation
Umeå University, Sweden

Partners Involved
Umeå University, SE
University of Manchester, UK
Institue National de Recherche en Informatique et an Automatique, Inria, FR
Science and Technology Facilities Council, UK

Contact name(s)
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nlafEt mission

Today's largest HPC systems have a se- rious gap between the peak capabilities of the hardware and the performance realized by high-performance comput- ing applications. NLAFET is a direct response to this challenge. NLAFET will enable a radical improvement in the performance and scalability of a wide range of real-world applications, by developing novel architecture-aware algorithms, and the supporting runtime capabilities to achieve scalable perfor- mance and resilience on heterogeneous architectures.

The validation and dissemination of results will be done by integrating new software solutions into challeng- ing scientific applications in materi- als science, power systems, study of energy solutions, and data analysis in astrophysics. The software will be pack- aged into open-source library modules.

nlafEt sample results

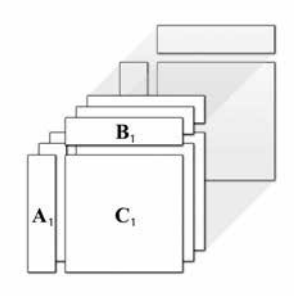
Developments so far have mainly fo- cused on small-scale homogeneous sys- tems. In the final project period, more emphasis will be put on heterogeneous systems including accelerator hardware and large-scale architectures.

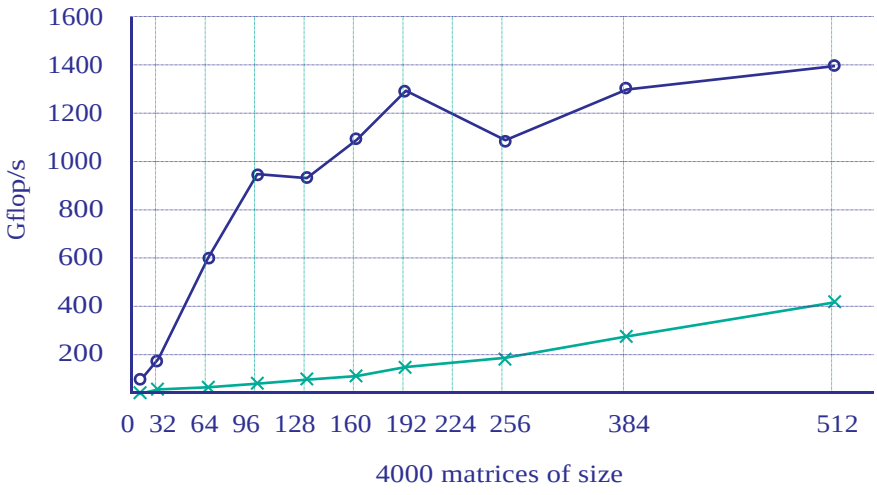
The main scientific and technologi- cal achievements during the first period include advances in the development of Parallel Numerical Linear Algebra algorithms for dense and sparse linear systems and eigenvalue problems, the development of communication avoid- ing algorithms, an initial assessment of application use cases, and an evaluation of different runtime systems and au- to-tuning infrastructures.

nlafEt impact

The main impact is to develop, deploy and make software available to the sci- entific community and industry, and thereby providing novel tools for their computational challenges. The work on the batched BLAS specification has already achieved considerable impact with industry in reaching a community standard. The idea is to group multiple independent BLAS operations on small matrices as a single routine (see Figure). The Graph shows performance on a 68 cores Intel Xeon Phi KNL for 4000 GEMM operations on matrices of size 16-by-16 up to 512-by-512. For example, for 4000 matrices of size 64-by-64 around 100 times speedup is obtained. Sample applications for batched BLAS can be found in Structural me- chanics, Astrophysics, Direct sparse solvers, High-order FEM simulations, and Machine learning.

Batched Blas





rEaDEx

Runtime Exploitationof Application Dynamism for Energy-efficient eXascale computing

www.readex.eu

Leading organisation

Technische Universität Dresden
Center for Information Services and High Performance Computing

Partners Involved

Gesellschaft für Numerische Simulation mbH
Intel Exascale Labs Paris
IT4Innovations, VSB - Technical University of Ostrava
National University of Ireland Galway
Norwegian University of Science and Technology
Technische Universität München

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Prof. Dr. Wolfgang E. Nagel

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overview

The importance of energy efficiency is constantly increasing in High Performance Computing (HPC). While systems can be adapted to individual applications in order to reduce energy consumption, manual tuning of plat- form parameters is a tedious and often neglected task.

The READEX project automates this by developing a tools-aided meth- odology for dynamic auto-tuning that combines technologies from two ends of the computing spectrum: system sce- nario methodology from the embedded world and auto-tuning from the field of HPC.

rEaDEx tools-aided methodology

The READEX methodology has been designed for exploiting the dynamic behaviour of software. At design time different runtime situations (RTS) are detected and optimized system config- urations are determined. RTSs with the same configuration are grouped into scenarios, forming the tuning mod- el. At runtime, the tuning model is used to switch system configurations dynamically.

impact and Validation

In order to validate the impact of the READEX project, several real-world applications are employed. In a co- de- sign approach, selected applications are being hand-tuned and both the im- provements in energy efficiency and the effort spent will be compared with the automatic tuning approach.

Design time analysis

Design time analysis (DTA) is car- ried out with the Periscope Tuning Framework (PTF). It uses a multi- agent based approach to identify RTSs and to determine optimized system config- urations. These are settings for tun- ing parameters, e.g., core and uncore frequencies. It also provides means for the specification of domain knowl- edge (DK) to improve the automatic tuning results. Part of the DK is the specification of application tuning pa- rameters, which allows users to offload computation to accelerated devices. The result of DTA is a tuning model that guides runtime tuning.

runtime-tuning

During production runs of the user's application, the READEX Runtime Library takes control. It is designed to apply the different configuration in a lightweight manor.

Moreover the READEX Runtime Library will be able to adapt to chang- ing application behaviour. The latter is to be implemented by state-of-the-art machine learning mechanisms, which are currently under development.

funding

Funded by the European Union's Horizon 2020 research and innovation programme „FET-Proactive – towards exascale high performance computing" under grant agreement No 671657.

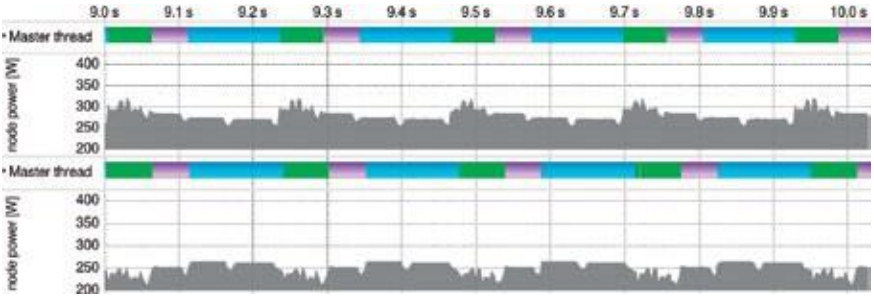

Fig 1. A comparison of a program executed with default settings (top) and with an optimized tuning model that applies power saving strategies (bottom). The power saving strategies are core frequency scaling (in regions that are green, savings of approx. 40 Watt) and uncore frequency scaling (in regions that are purple, savings of approx. 20 Watt). Vampir [www.vampir.eu] is used to compare the different program runs. The power consumption is measured using HDEEM [https://doi.org/10.1109/E2SC.2014.13].

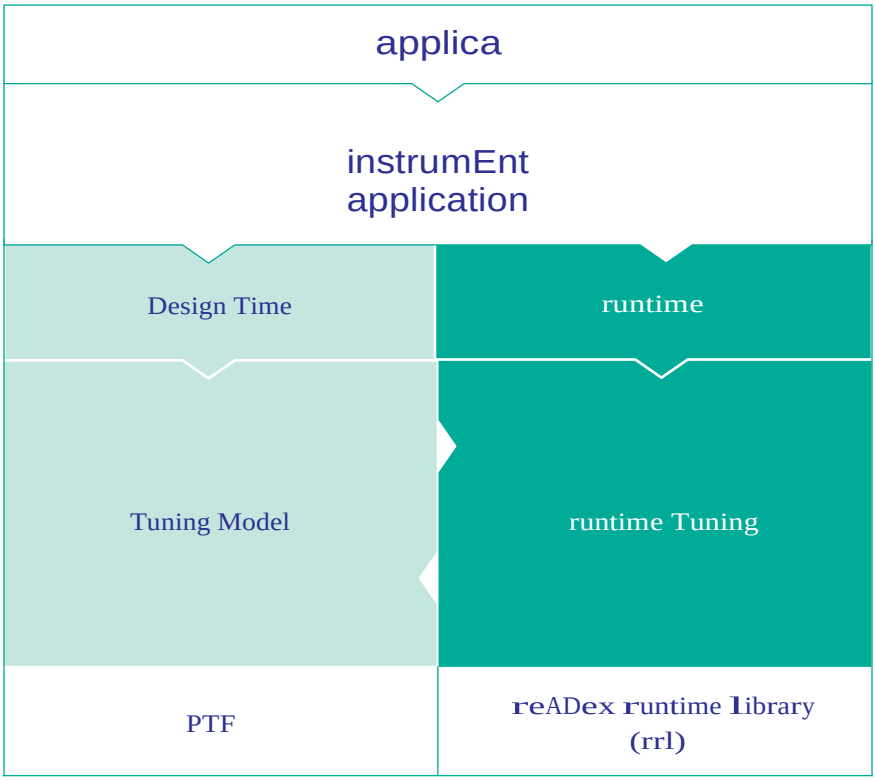

Fig 2. An overview of the READEX architecture.

sagE

Percipient StorAGe for Exascale Data Centric Computing

www.sagestorage.eu

Leading organisation
Seagate

Partners Involved
Seagate Systems, UK
Allinea Software [ARM], UK
Bull [ATOS], FR
United Kingdom Atomic Energy Authority, UK
Commissariat à l énergie atomique et aux énergies alternatives (CEA), FR
Deutsche Forschungszentrum für Künstliche Intelligenz GmbH (DFKI), DE
Diamond Light Source, UK
Forschungszentrum Juelich, DE
The Royal Institute of Technology, KTH
Science and Technology Facilities Council, UK

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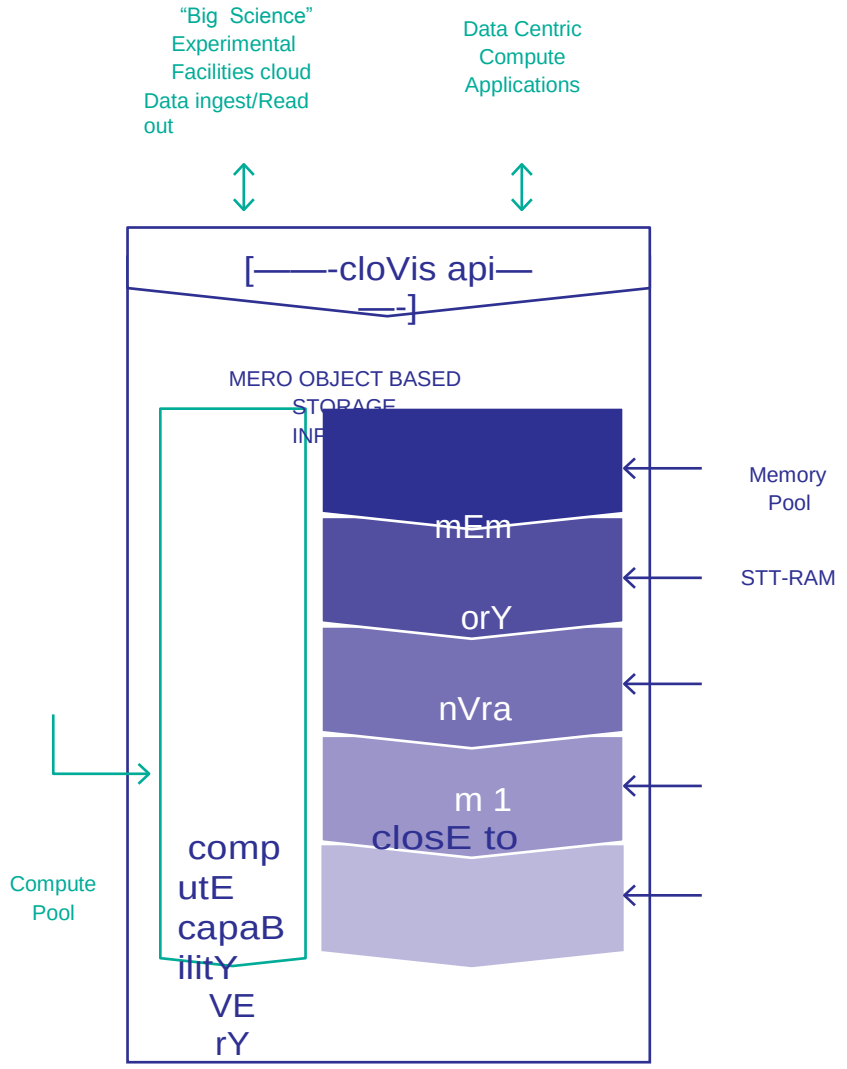
The StorAGe for Exascale Data Centric Computing (SAGE) system, researched and built as part of the SAGE pro- ject, aims to implement a Big Data/ Extreme Computing (BDEC) and High Performance Data Analytics (HPDA) capable infrastructure suit- able for Extreme scales - Exascale and beyond. Increasingly, overlaps occur between Big Data Analysis and High Performance Computing (HPC), caused by the proliferation of massive data sources, such as large, dispersed scientific instruments, sensors, and so- cial media data, whose data needs to be processed, analyzed and integrated into computational simulations to derive scientific and innovative insights. The SAGE storage system, will be capable of efficiently storing and retrieving immense volumes of data at Extreme scales, with the added functionality of “Percipience” or the ability to accept and perform user defined computations in- tegral to the storage system. The SAGE system is built around the Mero object storage software platform, and its API Clovis, and its supporting ecosystem of tools and techniques, that will work to- gether to provide the required function- alities and scaling desired by Extreme scale workflows. The SAGE system will seamlessly integrate a new generation of storage device technologies, including

non-volatile memories as they become available. The SAGE system will also offer a very flexible API and a powerful software framework suitable for easy extensibility by third parties.

The two racks of the SAGE system is now integrated into the Juelich Supercomputing Centre and undergoing software integration and application testing. Any communities interested in testing the SAGE prototype are advised to write to: info@sagestorage.eu.



Pool

RRAM
Pool

tiEr

Scratch
Storage Pool

Archival
Pool

Programming
Models/Workflows

co-DEsign proJEcts

DEEp projects

Dynamical Exascale Entry Platform

www.deep-projects.eu

Leading organisation

Forschungszentrum Jülich (Jülich Supercomputing Centre)

Partners Involved

Current partners in DeeP-eST:

Forschungszentrum Jülich
Intel
Leibniz Supercomputing Centre
Barcelona Supercomputing Center
Megware Computer Vertrieb und Service GmbH
Heidelberg University
EXTOLL
The University of Edinburgh
Fraunhofer ITWM
Astron
KU Leuven
National Center For Supercomputing Applications (Bulgaria)
Norges Miljo-Og Biovitenskaplige Universitet
Haskoli Islands
European Organisationfor Nuclear Research (CERN)
ParTec

Partners in DeeP and DeeP-er:

CERFAC
S CGG
CINECA
Eurotech
EPFL
Seagate
INRIA
Mellanox
The Cyprus Institute
Universität Regensburg

Contact name(s)

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Highlights of your project

The DEEP projects (DEEP, DEEP-ER and DEEP-EST) present an innovative solution for next generation super- computers, aiming at most efficiently organising heterogeneous resources. This is achieved by addressing the main Exascale challenges – including scal- ability, programmability, end-to-end performance, resiliency, and energy efficiency – through a stringent co-de- sign approach.

The DEEP projects developed the Cluster-Booster architecture – which combines a standard HPC Cluster with the Booster, a unique cluster of high-throughput many-core processors
–, and extended it by including a mul- ti-level hierarchy based on innovative memory technologies. Additionally, a full software stack has been created by extending MPI – the de-facto standard programming model in HPC –, and com- plementing it with task-based I/O, and resiliency functionalities. The next step in the DEEP project's roadmap is the generalisation of the Cluster-Booster concept towards the so-called *"Modular Supercomputing Architecture"*, in which the Cluster and the Booster are com- plemented by further computing mod- ules with characteristics tailored to the needs of new workloads, such as the ones present in high-performance data analytics (HPDA).

The developments cut across the complete HPC stack and amount to a fully integrated system prototype combining hardware with system soft- ware, programming environments and highly tuned applications. The latter are a total of 15 ambitious and highly relevant applications from HPC and HPDA domains, which drive co-design and serve to evaluate the projects' ideas and demonstrate their benefits.

project areas of international collaboration

- Prototype development: exchange of lessons learned
- Application porting: Exchange of experience in code modernisation, especially KNL optimisation
- Domain scientists / application de- velopers: invited to test the project developments with their codes

EuroExa

The Largest Group of ExaScale Projects and Biggest Co-Design Effort

www.euroexa.eu

Leading organisation

ICCS (Institute Of Communication And Computer Systems), GR

Partners Involved

ARM - UK, ICCS (Institute Of Communication And Computer Systems), GR
The University Of Manchester, UK
BSC (Barcelona Supercomputing Center), SP
FORTH (Foundation For Research And Technology Hellas), GR
The Hartree Centre of STFC, UK
IMEC, BE
ZeroPoint Technologies, SE
Iceotope, UK
SynelixisSolutionsLtd.MaxelerTechnologies,GR
Neurasmus, NL
INFN(Istituto Nazionale Di Fisica Nucleare), IT
INAF (Istituto Nazionale Di Astrofisica, IT
ECMWF (European Centre For Medium-Range Weather Forecasts), International And Fraunhofer, DE

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EuroEXA is a program that represents a significant EU investment to innovate across a new ground-breaking platform for computing in its support to deliver Exa-Scale computing. Originally the informal name for a group of H2020 re- search projects, ExaNeSt, EcoScale and ExaNoDe, EuroEXA now has it's own EU investment as a co-design project to further develop technologies from the project group and support the EU in its bid to deliver EU based ExaScale supercomputers.

This project has a €20m investment over a 42-month period and is part of a total €50m investment made by the EC across the EuroEXA group of projects supporting research, innovation and action across applications, system soft- ware, hardware, networking, storage,

liquid cooling and data centre technologies. Together bringing the technologies required to enable the digital economy, the future of computers, and the drive towards Exa-Scale capability. The project is also supported by a high value donation of IP from ARM and Synopsys.

Funded under H2020-EU.1.2.2. FET Proactive (FETHPC-2016-01) as a result of a competitive selection pro- cess, the consortium partners bring a rich mix of key applications from across climate/weather, physics/energy and life-science/bioinformatics. The project objectives include to develop and deploy an ARM Cortex technology processing system with FPGA acceleration at pe- ta-flop level by 2020, it is hoped that this will enable an Exa-Scale procurement for deployment in 2022/23.

"*To deliver the demands of next gen- eration computing and Exa-Scale HPC, it is not possible to simply optimize the components of the existing platform. In EuroEXA, we have taken a holistic ap- proach to break-down the inefficiencies of the historic abstractions and bring signif- icant innovation and co-design across the entire computingstack."* John Goodacre, Professor of Computer Architectures at the University of Manchester

"This is a world class program that aims to increase EU computingcapabil- ities by 100 times, the EuroEXA project is truly an exceptional collection of EU engineering excellence in this field. We have all set our ultimate goal – to enable the power-efficient delivery of the world's biggest supercomputer" Peter Hopton, Founder of Iceotope and Dissemination Lead for EuroEXA

As part of the H2020 competitive process, the 16 organisations of EuroEXA (above) have been selected for their technologies and capabilities from across 8 Countries.

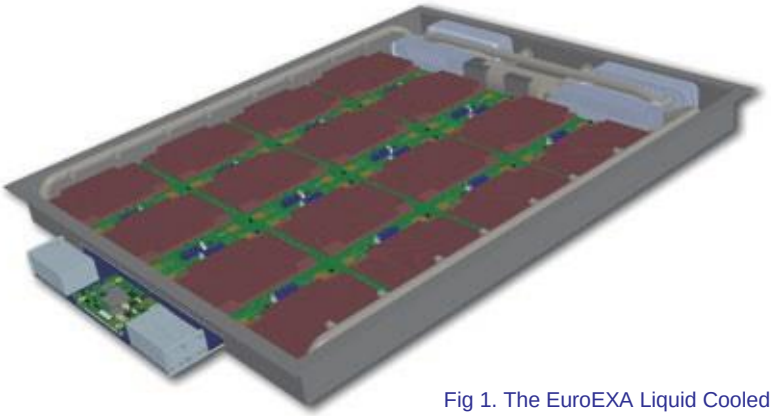

Fig 1. The EuroEXA Liquid Cooled Blade, 16 x Quad Processor Nodes in 1u Short Depth

cEntr Es o f ExcEll EncE in comp uting

BioExcel

Centre of Excellence for Computational Biomolecular Research

www.bioexcel.eu
Twitter: @BioExcelCoE
Youtube: https://goo.gl/5dBzmw

Leading organisation

KTH Royal Institute of Technology, SE

Partners Involved

The University of Manchester, UK
University of Utrecht, NL
Institute of Research in Biomedicine (IRB), SP European Molecular Biology Laboratory (EMBL-EBI), UK
Forschungszentrum Jülich, DE
The University of Edinburgh, UK
Max Planck Gesellschaft, DE
Forward Technologies, SE
Barcelona Supercomputing Center,
SP Ian Harrow Consulting, UK

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project Executive summary

BioExcel is the European Centre of Excellence (CoE) for provision of support to academic and industrial researchers in the use of high-end computing in biomolecular research. The center works on enabling better science by improving the most popular biomolecular software and spreading best practices and expertise among the communities through consultancy and training. The long-term vision of the center is to be a central hub for biomo- lecular modelling and simulations.

project Description

Much of the current Life Sciences research relies on intensive biomolecular modelling and simulation. As a result of this, both academic and industrial researchers are facing significant chal- lenges when it comes to applying best practices for optimal resource usage and workflow productivity, and to finding a faster path to achieve results.

High-performance computing (HPC) and *high-throughput computing* (HTC) techniques have now reached a level of maturity in widely used codes and platforms, but taking full advantage of these requires training and guidance by experts. The services ecosystem re- quired for that is presently inadequate, so a suitable infrastructure needs to be set up in a sustainable way.

BioExcel CoE was thus established to provide the necessary solutions for long-term support of the biomolecular research communities: fast and scala- ble software, user-friendly automation workflows and a support base of expert core developers. The main services offered by the center include hands-on training, tailored customization of code and personalized consultancy support. The BioExcel CoE actively engages with a number of interest groups, formed by members of academic and industrial communities, which lay the foundation of the long-term basis for user-driven governance of the center:

- academic and non-profit end users,
- industrial end users,
- software vendors and academic code providers,
- non-profit and commercial resource providers, and
- related international projects and initiatives.

The establishment of the centre is funded by the EC Horizon 2020 pro- gram (H2020-EU.1.4.1.3 675728).

project areas of international collaboration

The center engages with a number of international organizations and initia- tives which have complementary efforts in the area of computational biomo- lecular research. Some of them include:

- ELIXIR (www.elixir-europe.org)
- Molecular Science Software Institute (www.molssi.org)
- Software Sustainability Institute (SSI) (www.software.ac.uk)
- Open PHACTS foundation (www.openphacts.org)
- PRACE (www.prace-ri.eu)
- Common Workflow Language (www.commonwl.org)
- HPC-Europa3 (www.hpc-europa.eu)

solutions

softwarE

Widely used, fast and scalable codes for integrative modelling and molecular simulations

corE DEVElopErs

The scientists who wrote the code and know it best work with us!

worKflows

User-friendly and efficient systems for workflow executions and data cessing

sErVicEs

traini ng

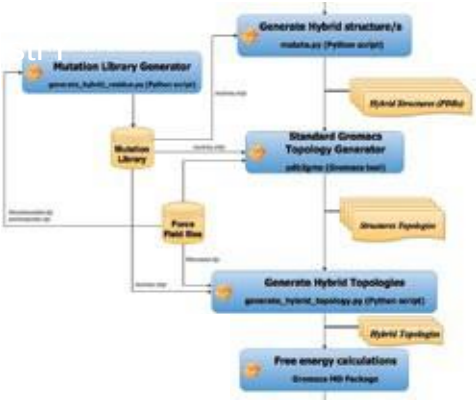
Webinars, “ask-me-anything” sessions, hands-on workshops for everyone from newbies to advanced users

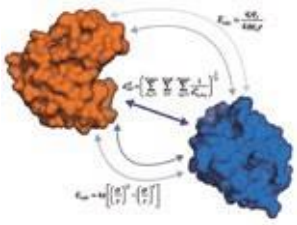
customisati on

Tailored solutions adapted to your needs

consultancY

Personalized support with software usage, tuning and scientific as rese





coegss

Centre of excellence for Global Systems Science

CoeGSS
Centre of excellence for
GLOBAL SYSTEMS SCIENCE

www.coegss-project.eu

Leading organisation

Coordinator: University of Potsdam
Technical Coordinator: High Performance Computing Center Stuttgart, University of Stuttgart

Partners Involved

ATOS, ATOS Spain SA
CHALMERS, Chalmers Tekniska Hoegskola AB
COSMO, The CoSMo Company CSP, CSP s.c.a r.l.
DIALOGIK, Non-profit Institute for Communication and Cooperation Research
GCF, Global Climate Forum EV
IMT, IMT School for Advanced Studies Lucca ISI, Institute for Scientific Interchange
PSNC, Poznań Supercomputing and Networking Center
TOP-IX, TOP-IX Consortium
UP, University of Potsdam
USTUTT, High Performance Computing Center Stuttgart, University of Stuttgart

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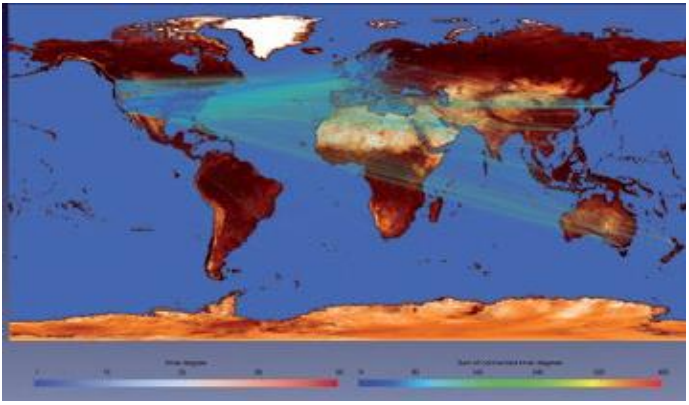

The globalisation of humanity's social and industrial activities, as observed over the past decades, has caused a growing need to address the global risks and opportunities involved. Some of these prominent challenges include:

- The global health risks – from dia- betes to pandemics – involved in the spread of unhealthy social habits as well as the opportunity to achieve major global health improvements through healthy behaviour.
- The global diffusion of green growth initiatives, including policy initia- tives, business strategies and life- style changes for successful as well as inefficient pathways.
- The challenges of global urban- isation, with special focus on the impact of infrastructure decisions regarding indicators like congestion, real estate prices and greenhouse gas emissions.

Approaches that address the above-mentioned challenges are inves- tigated by a newly-emerging research area: the Global Systems Science (GSS). However, with these transdisciplinary problems the demand for compute per- formance due to data and time con- straints increases drastically so that the assistance of High Performance Computing (HPC) is necessary. With re- spect to the problem statements above, the main topics within the CoeGSS pro- ject are the development of the technol- ogy and the environment for successful collaboration between the stakeholders

dealing with global challenges on the one hand and the High Performance Computing institutions that provide the mandatory capabilities to address those complex challenges at the required scale on the other.

So far, the use of HPC in GSS studies for processing, simulating, analysing, and visualizing large and complex data is very limited due to a lack of tailored HPC-enabled tools and technologies. Whereas typical GSS applications are data-bound, the traditional HPC tools and libraries are optimized to solve the computationally bound problems and thus, are of limited use in this area. The main difference between typical HPC applications and the envisioned GSS ones lies in the data sources and outputs as well as the used algorithms. Whereas lots of traditional high performance application codes, like those of compu- tational fluid dynamics, require massive parallelism and high computational power, GSS applications demand ad- ditional capabilities, for instance huge and varying data or in a generic manner, data-centric computation.

Looking for a trade-off between the data-centric programming models of the Cloud infrastructures and the highly efficient and scalable HPC technologies is therefore one of the key challenges for the success of the CoeGSS project.

compBiomed

Computational BioMedicine

www.compbiomed.eu

Partners Involved

University College London (UCL)
University of Amsterdam (UvA)
University of Edinburgh (UEDIN)
SURFsara (SARA)
Barcelona Supercomputing Centre (BSC)
University of Oxford (UOXF)
University of Geneva (UNIGE)
University of Sheffield (USFD)
CBK SCICON (CBK
Universitat Pompeu Fabra (UPF)
LifeTec Group (LTG)
Acellera (ACE)
Evotec (EVO)
Bull Atos (BULL)
Janssen (JAN)

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Contact Details

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project Executive summary

CompBioMed is a user driven CoE de- signed to nurture and promote the up- take and exploitation of HPC within the biomedical modeling community. Three distinct exemplar research areas will be pursued: cardiovascular, molecu- larly-based and neuro-musculoskeletal medicine. This will feed directly back to the clinic enabling healthcare providers to understand the mass of available data and provide clinical decision support

project Description

CompBioMed is comprised of 15 Core Partners from across Europe and with- in academic, industrial and clinical research institutions. We have suple- mented this with a growing number of Associate Partners, with whom we can work to provide HPC-solutions and draw on their knowledge to grow our own resources.

The research in the project inves- tigates three main pipelines: cardio- vascular, molecular-based medicine

and neuro-musculoskeletal medicine. Functional codes are currently being produced from these pipelines that are being shared and tested. The Centre of Excellence has so far employed 50 codes, of which 1/3 are open source and a sim- ilar number can be classified as HPC.

Through a symbiotic relationship with clinical partners, we will use the imaging and medical data provided by them to feed into our codes and establish programs that wil enable healthcare pro- viders to find the most applicable solu- tion for time-limited medical decisions.

project areas of international collaboration

The number of academic and industrial Associate Partners is constantly grow- ing. However, we would be keen to en- gage further with healthcare providers and clinical practitioners. We are also looking to involve further countries classified as having fewer HPC resourc- es through the Innovation Exchange Program.

E-

cam www.e-cam2020.eu

Leading organisation

Ecole Polytechnique Fédérale de Lausanne

Partners Involved

École Polytechnique Fédérale de Lausanne, CH (Coordinator)
University College Dublin, IR
Freie Universität Berlin, DE
Universita degli Studi di Roma La Sapienza, IT Centrenationaldelarecherchescientifique, FR Technische Universität Wien, AT
University of Cambridge, UK
Max-Planck-Institutfür Polymerforschung, DE
École Normale Supérieure de Lyon, FR
Forschungszentrum Jülich, DE
Universitat de Barcelona, SP
Daresbury Laboratory, Scientific and Technology Facilities Council, UK
Scuola Internazionale Superiore Di Trieste, IT Universiteit van Amsterdam, NL
Scuola Normale Superiore Pisa, IT
Aalto University, FI
CSC-IT Centre for Science Ltd, Fi
Irish Centre for High-End Computing, IR

Contact name(s)

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Ana Catarina Mendonça(Project Coordinator)

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project Description

The E-CAM Centre of Excellence is an e-infrastructure for software devel- opment, training and industrial dis- cussion in simulation and modelling. E-CAM is based around the experi- ence and scientific community of the extended CeCAM family, established over more than four decades and central in promoting fundamental research on advanced computational methods, as well as the computational and hard- ware expertise of the European part- nership PRACE. We are a partnership of 16 CeCAM nodes, 3 PrACe centres, 13 industrial partners and one Centre for Industrial Computing (the Hartree Centre at Daresbury). Our training and software development activities are spread across Europe at the different Node locations.

The goals of E-CAM are pursued via a set of coordinated actions and net- working. Its main tasks are as follows:

- software development targeted at specific end-users needs, and includ- ing testing of scaling and portability;
- development of the E-CAM repos- itory, an open source repository of software modules and packages for simulations in academy, mate- rial and life science, engineering. Modules include up to date docu- mentation and benchmarks;
- training and dissemination in the field of computational science via

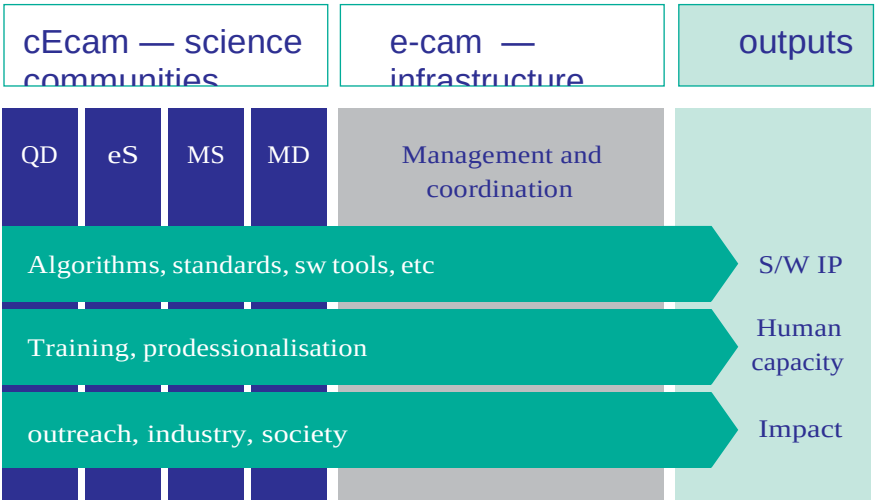
a series of workshops and online training modules;

- extended software development workshops for production of modules for the repository based on in- put from the community and the industrial partners;
- scoping workshops for discussion and problem definition with indus- trial end-users;
- state-of-the-art workshops for monitoring developments, identifying new directions and transferring knowledge to industry;
- support for academic and industrial research via a set of pilot projects supervised by scientists in the team and sustained by E-CAM funded post-doctoral fellows;
- keeping application developers up- to-date in software developments for current and future HPC systems;
- service-on-demand model to support industry community towards extreme scale HPC applications.

Our approach is focused on four scientific areas, critical for high-per- formance simulations relevant to key societal and industrial challenges. These areas are classical molecular dynamics, electronic structure calcu- lations, quantum dynamics and meso- and multi-scale modelling. E-CAM develops new scientific ideas and trans- fers them to algorithm development, optimisation, and parallelization in these four respective areas, and deliv- ers the related training. Postdoctoral researchers are employed under each scientific area, working closely with the scientific programmers to create, oversee and implement the different software codes, in collaboration with our industrial partners.

project areas of international collaboration

E-CAM envisages international coop- eration through the participation at our events (www.e-cam2020.eu/events), by getting involved in the discussions, and by proposing training content for future workshops. Our disposition for international collaboration comes through CECAM, which explicitly sup- ports the attendance of international visitors at its workshops and schools, and welcomes applications to organise events from everybody interested in computational science.



E-CAM structure: the four scientific pillars are quantum dynamics, electronic structure, molecular dynamics and meso- and multiscale modelling. The transversal activities are software development training and discussion with industry.

EocoE

Energy Oriented Centre Of Excellence

www.eocoe.eu

Leading organisation

CEA — Maison de la Simulation

Partners Involved

BATH University
BSC
CEA
CERFAC
S CNR
CNRS
CYI
EDF R&D
ENEA
Fraunhauffer / IWES
FZJ
INRIA
MPG
PSNC
RWTH
AACHEN
ULB
UNITN
UNITOV
UPSud
UVSQ
SUN

Contact name(s)

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project Executive summary

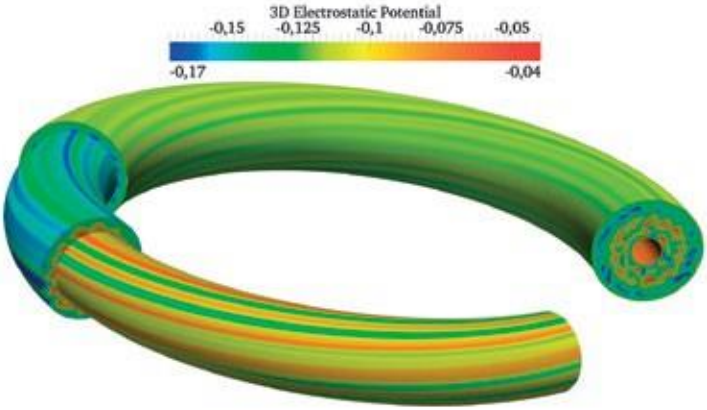
The Energyoriented Centreof Excellence incomputingapplications(EoCoE: read as “Echo”) is focusing on simulation for renewable energy production, storage and delivery and on related transversal high-end expertise in applied mathe- matics and HPC.

EoCoE leverages HPC to foster and accelerate the European transition to a reliable and low carbon energy sup- ply, harnessing the coming revolution in hardware and HPC architectures, calling for a similar paradigm change in the way application codes are designed. EoCoE assists the energy transition via targeted support to four numeri- cal-modelling-hungry areas related to renewable energy:

- Meteorology: making real time weather “nowcasting” possible in order to efficiently couple solar and wind farm energy production to the grid
- Materials: enabling high-through- put computing to discover novel ma- terials for batteries, photo- voltaic cells or supercapacitors.
- Water: geothermal and hydro- pow- er – using HPC for the management of resources, strategy of usage and estimating the influence of climate change
- Fusion: code coupling and mesh generation at the Exascale for fu- sion for energy simulation.

These four pillars are anchored within a strong transversal multidis- ciplinary basis providing high-end expertise in applied mathematics and HPC. This basis is using and develop- ing new programming tools, models and algorithms in order to prepare the applications to the next generation of hardware.

EoCoE is structured around a cen- tral Franco-German hub coordinating a pan-European network, gathering a total of 8 countries and 23 teams. Its partners are strongly engaged in both the HPC and energy fields. The primary goal of EoCoE is to create a new, long lasting and sustainable community around computational energy science. EoCoE resolves current bottlenecks in application codes; it develops cut- ting-edge mathematical and numerical methods, and tools to foster the usage of Exascale computing. Dedicated ser- vices for laboratories and industries are established to leverage this expertise and to develop an ecosystem around HPC for energy.



success stories

FUSION — Tokamak Physicsat IRFM, Cadarache: "Without the help of the EoCoEnetwork, engagingin thesenew paths toward exascale would be much more difficult."

GYSELA code describes a set of major phenomena that take place in- side Tokamaks: instabilities, turbulent transport, plasma-wall interaction, and heating. EoCoE project and the system- atic code auditing procedure it enabled has largely contributed to the improve- ment of GYSELA performance.

"EoCoE: Makingrealtimeweather nowcastingpossiblein post-Mooreera"

SolarNowcast aims to forecast the solar irradiation from fisheye lens from webcam images.

A full performance evaluation on the Forecast code allowed to identify a big optimization potential, both on serial and parallel levels. Optimization efforts improved the execution time by 2 to 5, getting closer to real time effective use.

project areas of international collaboration:

We are interested in collaborations in the area of HPC (e.g. programming models, exascale architectures, linear solvers, I/O) and also with people work- ing in the energy domain and needing expertise for carrying out ambitious simulation. See our service page for more details: www.eocoe.eu/services

EsiwacE

Centre of Excellence in Simulation of Weather and Climate in Europe (ESiWACE)

project Executive summary

Sciencedriverfor ESiWACEistheestablishment of global weather and climate modelsthatallowsimulatingconvective clouds and small-scale ocean eddies to enablereliablesimulationofhigh-impact

www.esiwace.eu

Partners Involved

Deutsches Klimarechenzentrum, Germany (Coordinator)
European Centre for Medium-Range Weather Forecasts, UK (Co-Coordinator) Centre Nationaldela Recherche Scientifique- Institut Pierre Simon Laplace, FR
Max-Planck-Institut für Meteorologie, DE
CentreEuropéendeRechercheetdeFormation Avancée en Calcul Scientifique, FR
Barcelona Supercomputing Center, Spain
Science and Technology Council, UK
Met Office, UK
University of Reading, UK
Sveriges Meteorologiska och Hydrologiska Institut, SE
National University of Ireland Galway - Centre for High End Computing, IR
Fondazione Centro Euro-Mediterraneo sui Cambiamenti Climatici, IT
Deutscher Wetterdienst, DE
Seagate Systems UK Limited,
UK Bull / Atos, FR
Allinea / ARM, UK

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regional events. This is not possible to- day but needs exascale. We address and quantify the computational challenges in achieving the science case.

project Description

ESiWACE leverages two European net- works: ENES (European Network for Earth System Modelling) and ECMWF (European Centre for Medium-Range Weather Forecasts).

The project is pushing weather and climate models towards global 1-2.5 km resolution, cf. Figures 1 and 2. This work will yield predictions on the scal- ability and computability in weather and climate modelling at exascale. Future work in the scope of ESiWACE comprises very high-resolution runs of coupled atmosphere-ocean models based on ICON and EC-Earth, as well as the associated workflow and data management considerations.

Other contributions of ESiWACE are handbooks on system and software stacks that are required for installation and operation of the various complex models on HPC platforms. This will substantially improve usability and portability of the weather and climate models.

Finally, ESiWACE develops strate- gies and software to improve exploit- ability of the high volume of Earth System data that will be produced by ex- ascale weather and climate simulations.

project areas of international collaboration

ESiWACE has links to both HPC industry and many other European initiatives. International collabora- tion and exchange has been initiated with the Geophysical Fluid Dynamics Laboratory and the National Center for Atmospheric Research (USA), the Computational Climate Research Team at RIKEN (Japan) and groups in China.

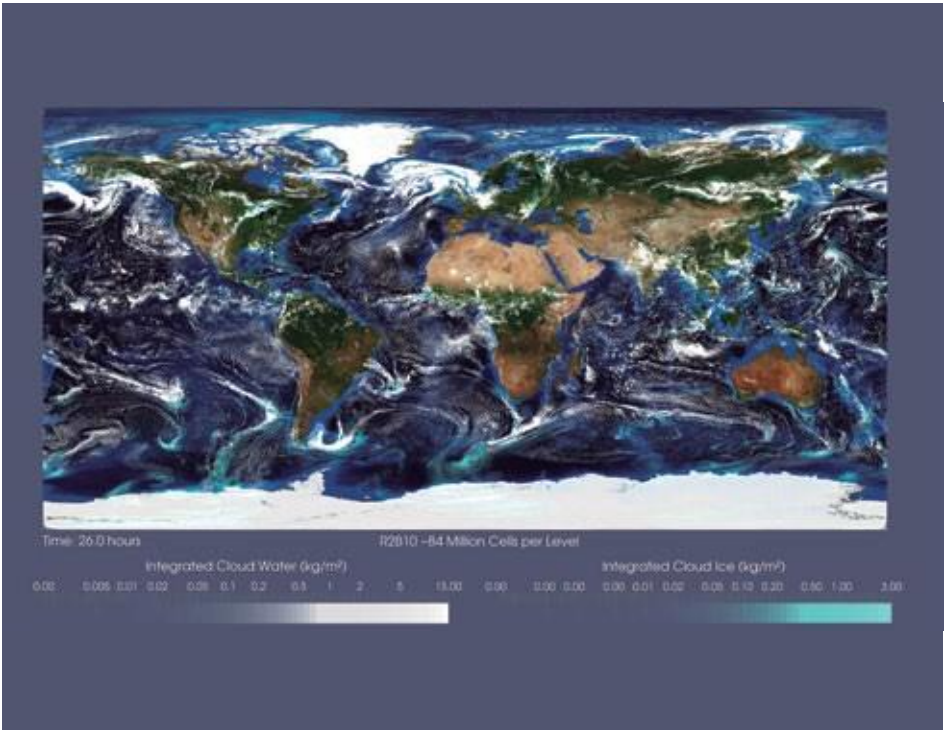

Fig. 1: 26hr weather forecast at 2.5km global resolution using the ICON model.

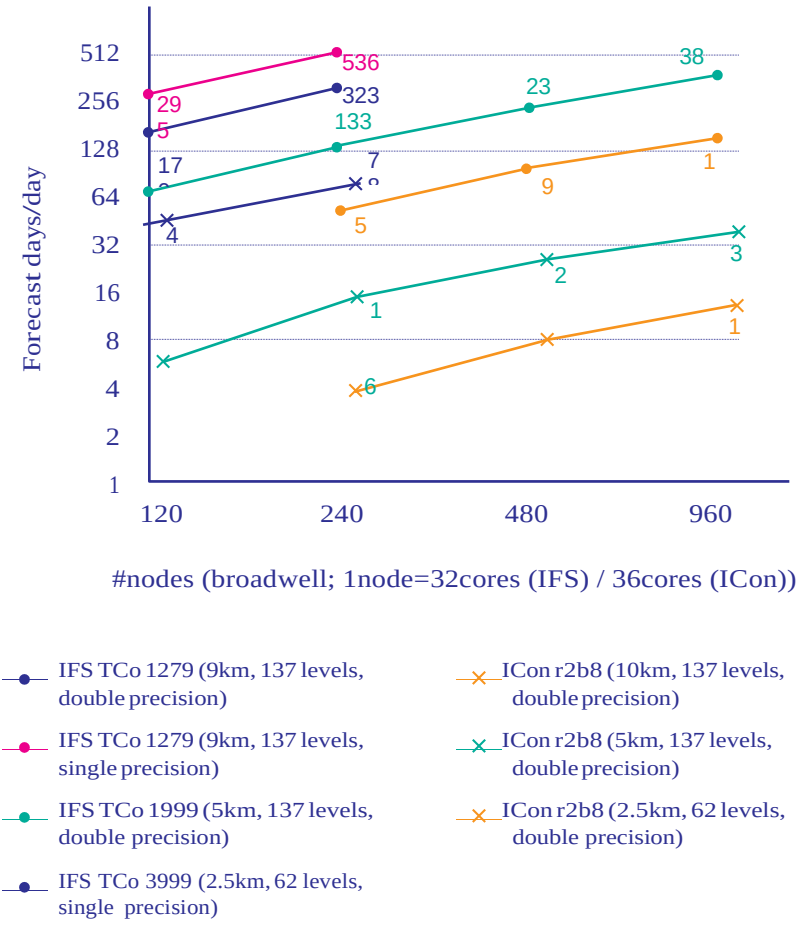

Fig. 2: Strong scalability of the models IFS and ICON in atmosphere-only simulations.

max

Materials design at the eXascale

www.max-centre.eu

Partners Involved

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ICN2 Barcelona, E (Pablo Ordejón)
FZJ Jülich, D (Stefan Blügel, Dirk Pleiter) EPFL Lausanne, CH (Nicola Marzari) CINECA Bologna, I (Carlo Cavazzoni) BSC Barcelona, E (José Cela)
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project Executive summary

MaX - Materials design at the eXascale is a Center of Excellence with focus on: driving the evolution and exascale tran- sition of materials science codes; creat- ing an integrated ecosystem of codes, data, workflows and analysis tools for HPC and high-throughput computing; supporting and training developers and end-users in academia and industry.

project Description

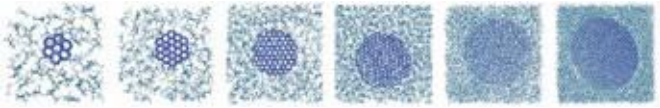
The starting point of *MaX* is the rec- ognized strength of Europe in first prin- ciples materials science applications, i.e. codes that allow predictive simulations of materials and their properties from the laws of quantum physics and chem- istry, without resorting to empirical parameters. The exascale perspective is expected to boost the massive use of these codes in designing materials structures and functionalities for re- search and manufacturing. The effort

to prepare such codes for the exascale transition is beyond the possibilities of individual research teams.

MaX addresses this challenge by focusing on five complementary open-source codes (Siesta, Quantum Espresso, Yambo, Fleur, and the Aiida materials informatics infrastructure). Five developing teams of such codes work with experts from five HPC cen- tres, in addition to three partners fo- cused on business/dissemination. With them, MaX has undertaken major code refactoring, released new versions with enhanced performance, modularity and inter-operability as well as new capabilities, developed workflows and turn-key solutions for properties cal- culations and curated data sharing, organized major training events. It has produced first kernel and domain specific libraries, progressed towards green computing ('energy to solution' measures), and in hardware-software codesign. *MaX* Users Portal offers ba- sic and advanced services supporting science and industry.

project areas of international collaboration

MaX is collaborating with many Materials simulations and design centers and projects worldwide, and is interested in strengthening and fur- ther expanding these collaborations on frontiers of current applications and on exascale oriented efforts. We are also interested in collaborating with new-ly established teams and initiatives in Europe and worldwide, including those in the developing countries in collabo- ration with our partner ICTP.



nomaD

The Novel Materials Discovery (NOMAD) Laboratory - a European Centre of Excellence (CoE)

www.nomad-coe.eu

Leading organisation

Fritz Haber Instituteofthe Max Planck Society

Partners Involved

Leibniz Supercomputing Centre, Garching
Barcelona Supercomputing Centre
Max Planck Computing and Data Facility
CSC — IT Center for Science
Aaalto University
University of Barcelona
University of Cambridge
Humboldt-Universität zu Berlin
King's College London
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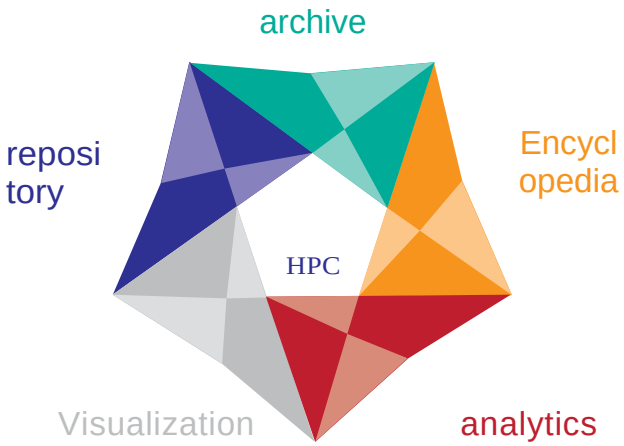
project Executive summary

The *NOMAD Laboratory CoE* maintains the largest *Repository* of open access data derived from the most impor- tant materials science codes available today and provides these data also in code-independent formats. big-Data tools and data mining services are developed for the discovery of novel information to advance materials sci- ence and engineering.



project Description

As data in the *NOMAD Repository* is generated from different codes, it is heterogeneous and difficult to use for analytics. To overcome this obstacle, the NOMAD team has developed meth- ods to convert heterogeneous data from over 30 major computational materi- als science codes to a homogeneous, code-independent format. In parallel, a number of tools have been developed to intuitively access, query and visualize this data. The *NOMAD Encyclopedia* is a user-friendly, public access point to NOMAD's code-independent data that allows users to explore the data in order to understand the structural, mechan- ical, and thermal behaviours of a large variety of materials, their electronic properties, and more. The team has also developed tools (>10) for the *NOMAD Big-Data Analytics Toolkit*. These tools will help scientists and engineers to select materials that will be most useful for specific applications or predict and identify promising new materials worth further exploration. In order to allow interactive data exploration, as well as enhanced training and dissemination, prototypes for *Advanced Visualization* (remote visualization and virtual reali- ty) have also been developed. Delivery of these tools and services is made possible by our High-Performance Computing expertise and hardware.

project areas of international collaboration

The *NOMAD Laboratory* CoE is well placedtocollaboratewithotherinterna- tionalinitiatives incomputational mate- rials science, alsofromothercontinents, including those led by members of the *NOMAD* Scientific Advisory Committee in the US (MICCoM) and Japan (CMI^2).

project Executive summary

The POP objective is to help improve the performance obtained by applica- tions on current systems, help identify the really important issues in a quan- titative way and help the community maximize the productivity of their development efforts when addressing very large scales.

Leading organisation
Barcelona Supercomputing Center

Partners Involved
Barcelona Supercomputing Center (BSC)
Universitaet Stuttgart (USTUTT(HLRS))
Forschungszentrum Julich GMBH (JSC)
Numerical algorithms Group Ltd (NAG)
Rheinisch-Westfaelische Technische Hochschule Aachen (RWTH-AACHEN)
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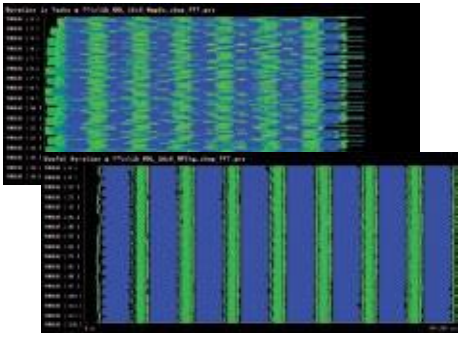
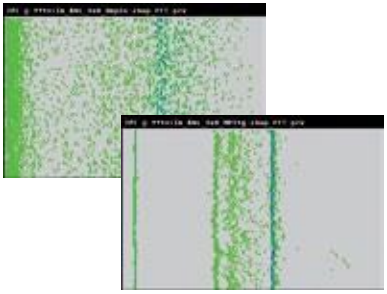
POP is providing a service to cus- tomers from all application domains (engineering, sciences, data analytics, climate, medical, media, deep learning, …). Customers apply by filling a small request service form in the project web page (www.pop-coe.eu). The main ser- vice is an "assessment" report where an external view is given to the customer on the performance issues experience by the application and recommenda- tions on what would be the most pro- ductive code refactoring directions. A unified set of metrics and methodolo- gy have been set up to homogenize the

reports across partners. In some cases a “proof of concept (POC)”follow up service is performed where POP experts help customers to apply the proposed techniques and demonstrate the actual performance gains.

The customer gets an assessment report between 5 and 15 pages with a description of the identified issues and recommendations on how to address them. Performance gains from just 10% up to 10x have already been ob- served on different POC services. Close to 100 assessments have already been performed. UK, Germany and Spain. are the countries with more services received, but almost 25% of the services are to countries outside the consortium. The POP CoE is actually a hub estab- lishing links and sharing experiences among a very large community.

One of the activities of the project is to gather feedback from customers on the quality of the service provided so that we can improve our operation. Overall, the customers are very happy and value very positively the assess- ments and recommendations received. Under their permission, reports are made available in the project web page. We also include there summarized suc- cess stories and customer testimonials.





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