



EXDCI-2 – WP3

“Foreseen activities on applications side”

M. Bode (RWTH Aachen) and [S. Requena \(GENCI\)](#)

- WP3 “Excellence in HPC applications and usages”
 - Objectives
 - Develop a roadmap of HPC applications and usages
 - Foster engagement with users communities and CoEs
 - Prepare industrial codes to exascale
 - 3 main tasks (Bode, Requena)
 - T3.1 : Roadmap of HPC applications and usage (Lambert, André)
 - T3.2 : Engagement with HPC users communities and CoEs (Aloisio, Krieg)
 - T3.3 : Preparation of industrial codes to exascale (Margetts, Fournier)
 - 5 deliverables
- 
- D3.1 : Report updated roadmap of HPC applications & usages (M24)
 - D3.2 and D3.3 : Reports on joint brainstorming activities (M15 & M27)
 - D3.4 and D3.5 : Reports on organization of WP3 workshops during HPC Summit Week 2019 and 2020 (M15 & M27)
- 

- Deliverable D3.1 due *M24*
- Context
 - Vision documents *very recently* available (PRACE SSC Sci. Case, ETP4HPC SRA3 [soon SRA4], BDEC2, ...)
 - Involvement of experts into BDEC2 and SRA4 task forces
 - *Rapid* changes in HW and SW: convergence of (new)architectures, hybrid approaches for HPC and Big data (HPDA, IA/MD); coupling large scale instruments, urgent computing, ...
 - Need some caution and time before *consolidated* roadmaps can be prepared
- New sources of information [many contacts already established]
 - "CoEs", "EuroHPC Application pillar", HPC "FET"
 - Other fields related to AI and DL: Nuclear fusion, Turbulent combustion, climate, ...
 - Social sciences (Humanities)
- Proposed timetable
 - Summer 2019: draft of the deliverable using available information (see above)
 - Fall 2019: draft review by contacts from the above sources of information
 - Dec. 2019: revised draft send for review by other stakeholders
 - Feb. 2020: finalization of the deliverable



EXDCI2 WP3-T3.1 Roadmap of HPC applications and usages – Outline of the document (1/2)

1. Introduction

- Gap analysis since last EXDCI WP3 roadmap document in terms of HW, new architectures, new usages (fast development of AI/DL), coupling with large scale instruments, end-to-end workflows...
- Reports issues : 3rd PRACE SC, ETP4HPC SRAs, BDEC2 reports, EuroHPC RIAG and INFRAG reports, DoE ECP, ...

2. « Physical simulation vs/with ML », « HPC vs/with BD »

- ↗ Needs of compute power for simulation based pb based on physical laws
AND ↗ of apps using DL → **rise of hybrids methods**

3. Number of examples in many scientific fields

- Sciences of the universe (Sacha Brun)
- Climate (based on Extreme Earth)
- Combustion (also based on EXCELERAT)

3. Number of examples in many scientific fields (cont.)

- Material sciences (also based on Max1 and 2)
- Biosciences (also based on CompBioMed and BioExcel, with additional input from Rossen Apostolov)
- Social sciences (based on documents provided by Melissa Terras, and based also on HIDALGO)
- Engineering and industrial applications
- Other fields ?

4. Conclusions

- Application based Hybrid approaches and convergence of infrastructures...
- Better validation, verification, uncertainties quantification, ...
- Need of train, retrain skills

- Initial analysis and discussion about the main topics to address
 - HPDA was identified as a key topic for 2019.
 - AI, ML and DL were suggested as potential topics for 2020.
- Organization activity of the EXDCI2 Workshop
 - “*1st European Communities Workshop on Exascale Computing*” with a focus on “*High Performance Data Analytics*”
 - during the EuroHPC Summit Week 2019 (Poznan, Poland) on May 16, 2019,
 - organized in two sessions one dedicated to the Centre of Excellences (chaired by G. Lonsdale) and another one to the FETHPC projects (led by G. Aloisio).
 - presentations covered various aspects of HPDA from big data processing and parallel data analysis, heterogeneous infrastructure to deal with different aspects of HPDA, to provenance and reproducibility of simulation results.

EXDCI2 WP3-T3.2 Engagement with HPC users communities and CoEs

- Workshop on converged HPC / AI HW/SW infrastructures and usages
- 1/2 to 1 day workshop organised with CoE and ETP4HPC
- Concrete deployments of converged architectures
- Concrete use of »HPC for AI « and »AI for HPC «
- Work in progress for the organisation but ???
 - D3.4 « Reports on organization of WP3 workshops during EuroHPC Summit Week 2019” ???

A promotional banner for EuroHPC Summit Week. The background is dark blue with a wireframe hand pointing towards server racks and vertical light streaks. The text is white and yellow. The EuroHPC logo (a circle of stars) is in the top right. The text "EuroHPC Summit Week" is in the middle right. The date and location "From 23 to 27 March 2020 | Porto, Portugal" and the hashtag "#EHPCSW" are at the bottom. The DCI logo is in the bottom right corner.

 EuroHPC
Joint Undertaking

**EuroHPC
Summit Week**

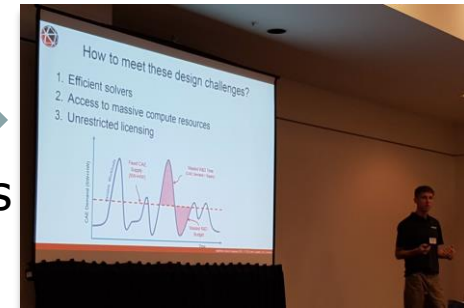
From **23 to 27 March 2020** | Porto, Portugal **#EHPCSW**

 dci
European
Extreme Data
& Computing
Initiative

Two strategies: (i) High level view of an industrial community and (ii) more detailed case studies

Strategy (i) Industrial Community

- Engineering applications
 - Sectors - Manufacturing, Energy, Transport, Construction
- Key event - NAFEMS World Congress 2019
 - 17-20 June 2019, Quebec, Canada
 - Consult **>600 firms attending** who use industrial codes
- Data Collection Methods
 - Birds of a Feather brainstorming activity
 - Industrial users questionnaire
 - ISVs roadmap questionnaire
- Deliverables
 - Contributions to future WP3 reports



Strategy (ii) Case Studies

- Select a list of candidate or relevant industrial codes
 - Codes should already be well-adapted to HPC
 - List issues that should be solved or improve on for each code to allow usage in exascale context
 - List possible workarounds or variants
 - Identify common issues
- Use outcome of recent works : Teratec meeting Dec 2th, INFRAG reports, BDEC2 meetings, ...
 - Participation of EDF, Renault, CGG, Michelin, Naval Group, SAP, Dompé, ...
- Beyond Exascale : Quantum computing in industry (TOTAL, Airbus, ...)

WP3 plans for second year

- 2 first deliverables submitted on time in June 2019

- D3.2 « Reports on joint brainstorming sessions among scientific and industrial users communities"»

- Task 3.1 :

- D3.1 in preparation "updated roadmap of HPC applications"
- Involvement in BDEC2 and SRA4 task forces



- Task 3.2 :

- Organisation of new workshops during EuroHPC Summit Week 2020



- Task 3.3 :

- Surveys amongst ISV and industrial communities, industrial uses cases
- Results will feed WP3 deliverables

