

The NumPEx Program

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Exascale, what's at stake ?



Exascale for scientific breakthrough, environmental sustainability, resilient society, and industrial competitiveness

Answering key scientific questions

Supporting the development of COVID-19 treatments



Weather and climate models



Leading to engineering breakthough

Earthquake simulation

Renewables can power the world



Materials simulation



Al for wind farm layout optimization



Astrophysics









Transportation



Exascale, a new paradigm





International initiatives





The European context





The NumPEx program - objectives



Contribute and accelerate the emergence of a European sovereign exascale software stack and strategic applications exascale capability in a coherent and multi-annuel framework

Integrate and validate **co-designed** innovative methods, libraries and software stack with demonstrators of strategic applications.

Accelerate science-driven and engineering-driven developers training and software productivity

Foster **national and international collaborations** to prepare for the Exascale and post-Exascale era



The NumPEx program - objectives



Applications





Energy

Biology and Health science

Industrial applications



Co-design the exascale software stack Preparing the applications for the Exascale era

NumPEx by numbers







Software stack development (PC 1-3) Wide-area workflows and architecture (PC 4) Integration and application development (PC 5)

80 **R&D** teams 500 **Researchers**









Work Packages in ExaDoST













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NumPEx transversal actions





Applications

NumPEx transversal actions





Sustainability - a 4-stages strategy



- NumPEx is a production project, with a focus on the upcoming European Exascale systems ...
- Prepare for the post-Exascale challenges, with trends towards more heterogeneous HW (FPGA, chiplets, etc)
- « Exascale" challenges will also will be widespread at all levels of the computing ecosystem from small-size clusters to supercomputers
- Common challenges in Tier0, Tier1 ... and future non-HPC systems as well.



- CSE application teams cannot craft codes for each hardware/system architectures
- Need for architecture-agnostic software stack, co-designed libraries
- Change CSE applications codes development methodologies to building on portable/ maintained SW/libraries with minimum performance portability.

> Separation of concern between application-dependent/HW-dependent components

- An illustrative example WarpX (Gordon Bell prize 2022)
 - PIC-based code for matter/laser interaction simulations
 - Based on AMRex (ECP project), highly portable AMR library



- Highly portable code, run a wide range of HPC systems : Frontier (OLCF), LUMI (CSC), Adastra (CINES), Fugal (Riken) to only name a few

- Application codes build upon a collection of software components, multi-year development roadmaps
- generation algorithmic - NumPEx will build and deliver Software Development Kits exascale capabilities Toward productive and sustainable exascale algorithmic motifs - composed of a framework of interoperable **CSE** applications Libraries Domain softwares and libraries Advanced data components Extreme strong structures and scalability and logistics for capability - domain-specific/application-specific components exascale architectures System **SDK** components - key to build trust with the CSE application teams Increasing performance Performance on portability exascale for long-term development roadmaps architectures Improving Frameworks libraries quality, su Interoperability interoperability Complementarity

PROGRAMME DE RECHERCH

NumPEx

FRANCE

Next

Goal: push forward software development and deployment practices

- Support NumPEx software packaging effort (Spack, Guix, Nix)
- Contribute to package managers (HPC-centric specificities)
- Collaborate with to FR computing centers to deploy PM on their machines
- Develop EU/International collaborations
- GitHub/CI to open to anyone complying with the community policy

Within NumPEx, a workforce of 3 FTE in addition to in-kind contribution





Guix



- With the increased complexity of the CSE applications codes, HW and HPC/HPDA/AI usages, code development requires a radical change, relying on common tools
- Long-term visibility on library development/maintenance for CSE application teams is mandatory
- Sustainable codes not only need long-term maintenance but also development/evolution



Building a large user community (e.g. co-design activity, training, etc)

What business model for a sustainable SW stack, especially in Europe ?



NumPEx is an ambitious programme to:

- contribute to the European Exascale software stack
- help preparing scientific and industrial applications to the Exascale
- Long-term sustainability with portable/interoperable/deployable SW stack
- Help building an Exascale community with application teams, computing centers
- Fostering international collaborations, pushing new dev./deploy. methods



