

Some (Post-)Exascale Challenges

The NumPEX Program and InPEX Project Contributions

KeyNote 2 - Long-term Computing Vision

Feb 13 2024, 2024 ETP4HPC Conference

G. Antoniu (INRIA), JY. Berthou (INRIA), J. Bobin (CEA),

Contributors : M. Krajecki (CNRS), C. Prudhomme (U. de Strasbourg), Hélène Barucq (Inria), R. Namyst (Inria/U. de Bordeaux), A. Buttari (IRIT), J. Bigot (CEA), F. Bodin (U. de Rennes), Mark Asch (U. Picardie), T. Deutsch (CEA), J-P. Vilotte (CNRS), V. Brenner (CEA), B. Raffin (Inria)

15 years ago, Simulating The Future'08 One million core programming workshop



Some international Exascale efforts ...

IESP 2008, ...2012



HOME MEETINGS DOCUMENTS COMMUNITY

 Search

DOCUMENTS

CONTENTS

- 1 Versions of the Roadmap
 - 1.1 Current Version of the IESP Roadmap
 - 1.2 Previous Versions of the IESP Roadmap
- 2 Products of Recent Meetings
 - 2.1 Products of the Cologne Meeting
 - 2.2 Products of the San Francisco Meeting
- 3 Most Recent: Meeting 8 (Kobe, Japan, April 12-13, 2012)
 - 3.1 Day 1: Morning Plenary Presentations
 - 3.2 Day 1: Afternoon Plenary Presentations
 - 3.3 Day 1: Afternoon Breakouts
 - 3.4 Day 2: Morning Plenary Presentations
 - 3.5 Day 2: Reports from afternoon breakouts
 - 3.6 Documents of Interest flowing from this meeting
- 4 Presentations at the IESP exploratory meeting SC08, Austin, TX, 18Nov08
- 5 Meeting 1 (Santa Fe, NM, USA)
 - 5.1 Presentations
 - 5.1.1 Summaries from the meeting breakout groups
 - 5.1.2 Plenary Presentations
 - 5.2 Whitepapers
- 6 Meeting 2 (Paris, France)
 - 6.1 Full Workshop Report

BDEC 2013, 2014 ...2020



The Basis for BDEC

Informed partly by the work of the [International Exascale Software Project](#) (IESP, 2009-2012), in the past five years, the United States, the European Union, Japan, and China have each moved aggressively to develop their own plans for achieving exascale computing in the next decade. Such concerted planning by the traditional high performance computing speaks eloquently about both the substantial rewards that await the success of such efforts, and about the unprecedented technical challenges that apparently block the path upward to get there.

But while these exascale initiatives have understandably focused on the big challenges of exascale for hardware and software architecture, the relatively recent emergence of the phenomena of Big Data in a wide variety of scientific fields represents a tectonic shift that is transforming the entire research landscape on which all plans for exascale computing must play out.

Building on the work of the IESP, the Big Data and Extreme-scale Computing (BDEC) community has staged a series of workshops that have endeavored to map out and account for the ways in which the major issues associated with Big Data intersect with, impinge upon, and potentially change, the national (and international) plans that are now being laid for achieving exascale computing.

Some international Exascale efforts ...

With coordinated European contribution (CSA)

EESI 1&2, EXDCI 1&2 2010, ...2020

e-infrastructure EUROPEAN COMMISSION

EESI

CHALLENGES VISION GUIDANCE RESOURCES ABOUT

European Exascale Software Initiative

Toward Exascale Computing

Our vision
Research for achieving efficient Exascale applications

Big Data and Extreme-scale Computing
Follow EESI around the world

Who's who
contact HPC leaders

EVENTS

CONFERENCE
EESI2 Final Conference
The second European Exascale Software Initiative, EESI2, is organizing its final international conference on May 28 - May 29 (noon till noon), 2015 in Dublin

European HPC strategy

PRACE

ETP 4 HPC EUROPEAN TECHNOLOGY PLATFORM FOR HIGH PERFORMANCE COMPUTING

Search

Newsroom Collaboration Events Activities Results Contact

projects

lises the **European HPC stakeholders**. The project builds upon the achievements of EXDCI and will **Ecosystem** with two main goals:

C Exascale Strategy by supporting the implementation of a common **European HPC strategy**, open to cs (HPDA) and Artificial Intelligence (AI). The expertise of the partners and stakeholders will permit to

HPC at the Exascale through joint community structuring and synchronisation. This entails ensuring ent of the **European HPC eco-system towards Exascale**, such as:

- The development of relationships with other ecosystems including upstream technologies as photonics and electronics, High Performance Embedded Computing (**HiPEAC**) and Big Data (**BDVA**)
- In the context of the upcoming **European Data Infrastructure** (EDI) a road mapping activity toward **future converged HPC, HPDA and AI needs and new services** from PRACE users communities and CoE
- The continuation of **BDEC activities**, for international participation of European stakeholders on the integration from edge computing to HPC, including Data Analytics and AI

The (post)-Exascale race, where are we?

China initiatives:

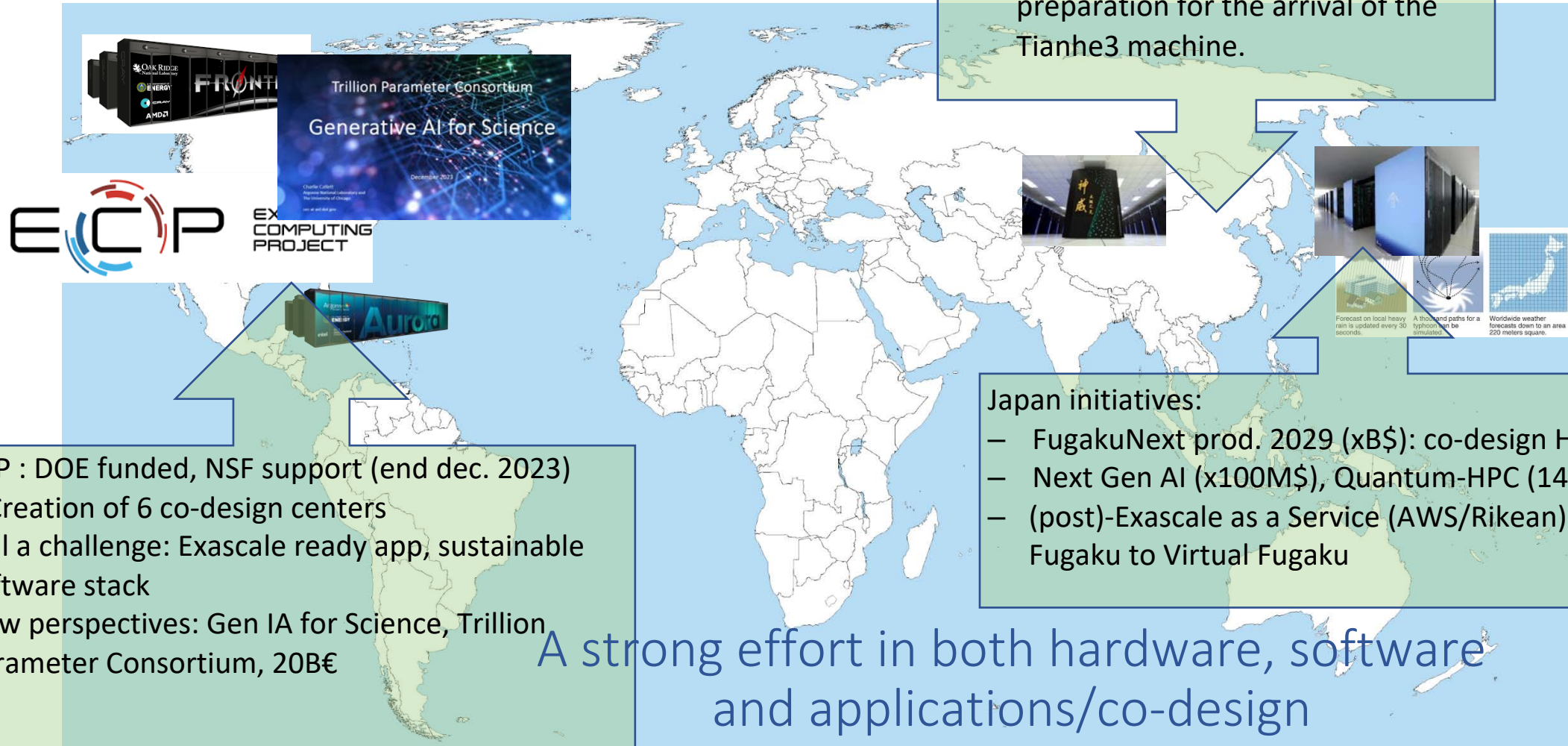
- development of applications in preparation for the arrival of the Tianhe3 machine.

Japan initiatives:

- FugakuNext prod. 2029 (xB\$): co-design HW/SW/Apps
- Next Gen AI (x100M\$), Quantum-HPC (140M\$)
- (post)-Exascale as a Service (AWS/Rikean): from Fugaku to Virtual Fugaku

ECP : DOE funded, NSF support (end dec. 2023)
+ Creation of 6 co-design centers
Still a challenge: Exascale ready app, sustainable software stack
New perspectives: Gen IA for Science, Trillion Parameter Consortium, 20B€

A strong effort in both hardware, software and applications/co-design



The (post)-Exascale race, where are we?



The International Post-Exascale (InPEX) Project

What to share and coordinate...

- AI for Science, HPC for AI - Datasets for AI training
- Software Exascale stack production, management and sustainability :
 - Packaging, documentation, builds, results, catalogs, continuous integration, Linux builds (E4S, etc.)
- Digital continuum and data management
- Co-design (HW&SW&Apps), benchmarks and evaluation
- Math and algorithm for Exascale
- Energy and environmental impact and sustainability
- Future and disruptive technologies and usage (investment)
- Training



Pre-workshop InPEX, October 2023, Reims, F

The International Post-Exascale (InPEX) Project

InPEX expected outcomes

- Landmark documents largely exploited, worldwide, for supporting future post-exascale science
- Contribute to the implementation of an international, shared, high-quality computing environment based on the principles and practices of co-design
- Formation of a solid network of exascale computing leaders, all around the globe

Actions:

- Dedicated international working groups
- International Post-Exascale (InPEX) workshop series

Participants:

Researchers, engineers, industry, funding bodies



The International Post-Exascale (InPEX) Project

Inpex.science

Date	(10/2023)	11/2023	06/2024	06/2025
Location	Preparatory phase EU (France)	SC'23 - BOF	Workshop1 EU/BSC	Workshop2 Japan
Date	03/2026	09/2026	06/2027	09/2027
Location	Workshop3 US	Workshop4 EU	Workshop5 Japan	Workshop6 US

How to contribute? Send 2 pages white paper to : inpex@inpex.science



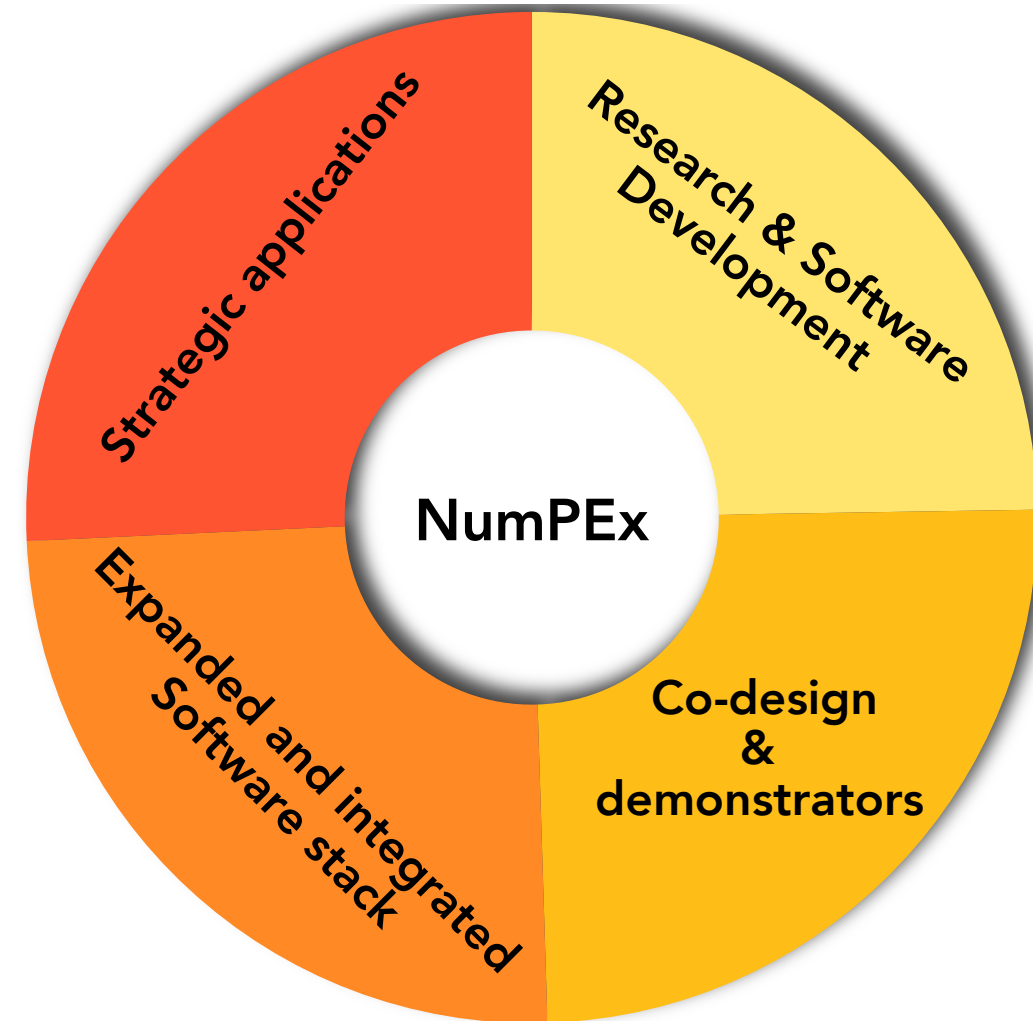
The French NumPEX Program

Consolidating and accelerating the construction of a sovereign European **exascale software stack** and **strategic applications exascale capability** in a **coherent and multi-annual framework**

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

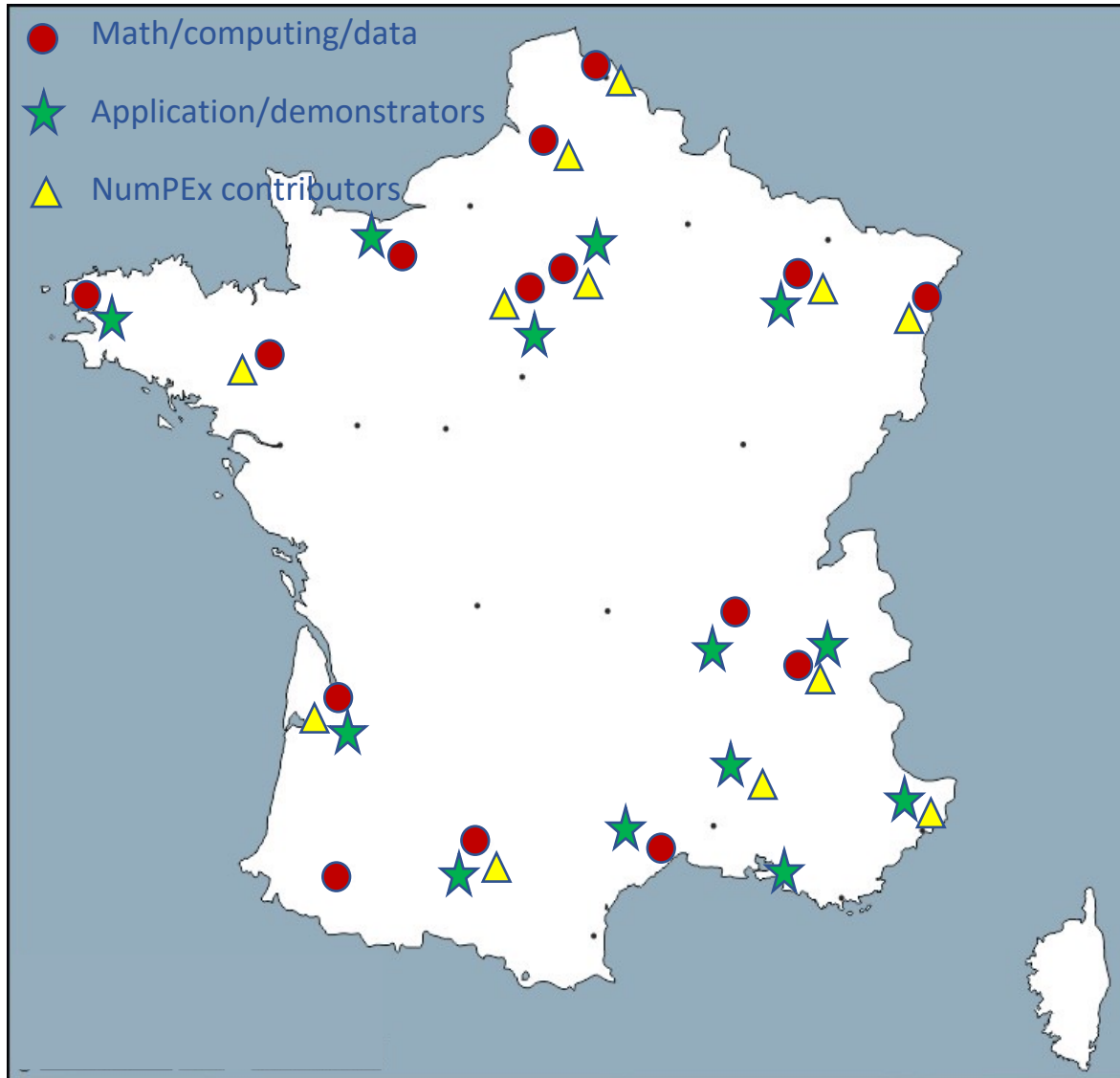
Accelerate science-driven and engineering-driven developers **training and software productivity**

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



Help aggregate the French Edge/Cloud/HPC/HPDA/IA community

NumPEX by numbers



6 Years
41 M€*

2023-2028

* Funding 41M€=500 person.year non permanent staff

+ 170 person.year permanent staff

Total cost : 81 M€

**Core
Research
Institutions**

Core national Research Institutions:
CNRS, CEA, INRIA, Universities,
Engineer schools, Industry

**3
Focus
Area**

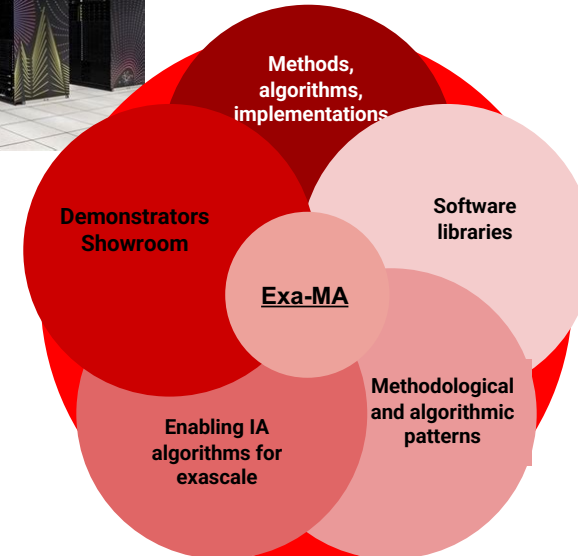
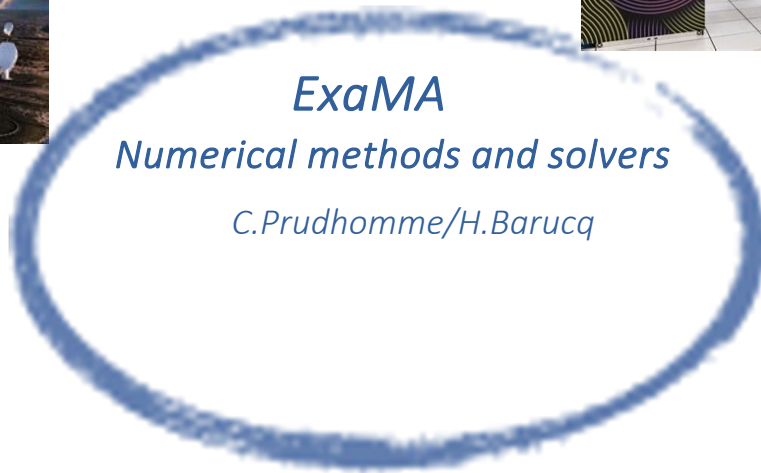
Software stack development (PC 1-3)
Wide-area workflows and architecture (PC 4)
Integration and application development (PC 5)

**80
R&D teams
500
Researchers**

The French NumPEX Program - workplan



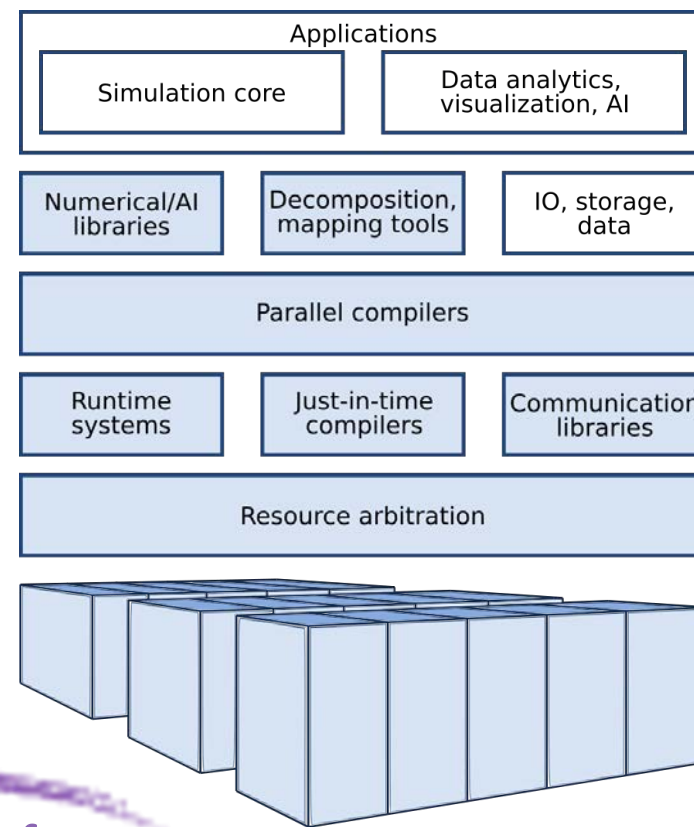
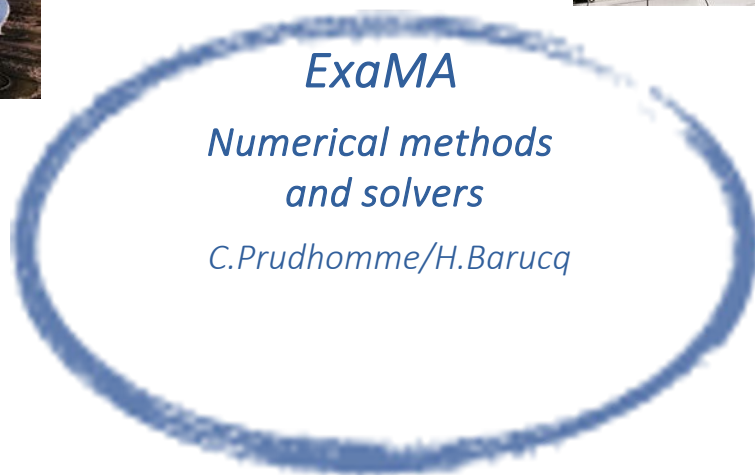
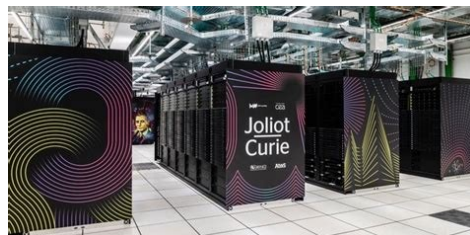
Applications



The French NumPEX Program - workplan



Applications



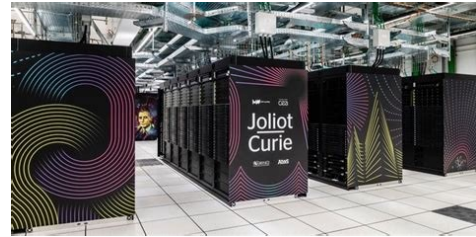
The French NumPEX Program - workplan



Applications



ExaMA
Numerical methods and solvers
C.Prudhomme/H.Barucq



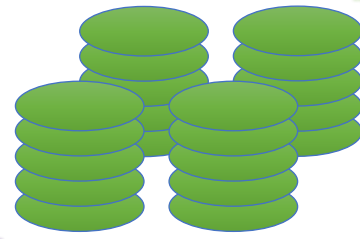
WP1: Exascale I/O and storage

WP2: Exascale in-situ data processing

WP3: Exascale ML-based data analytics

WP4: Shared building blocks & integrated illustrators

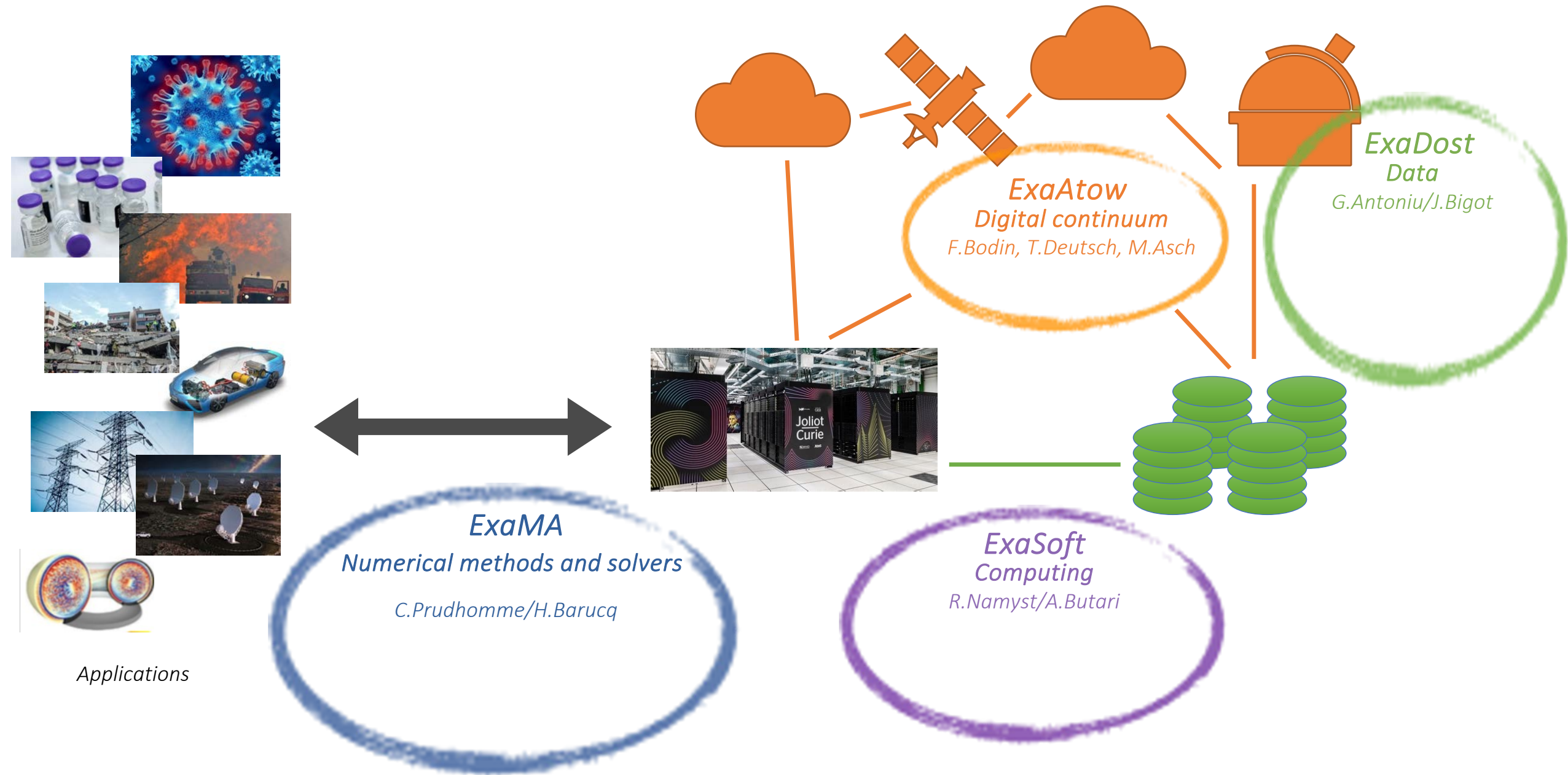
WP5: Management, dissemination and training



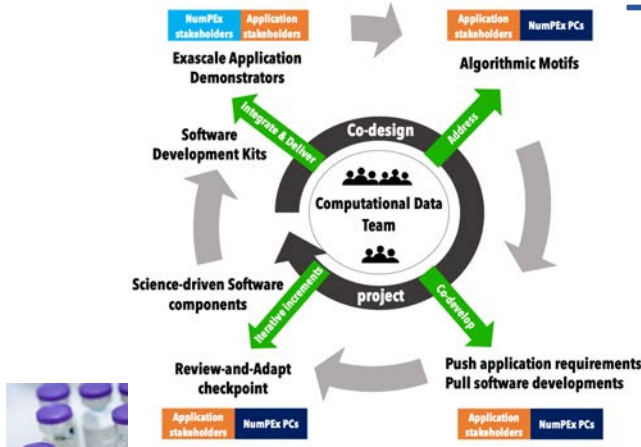
ExaSoft
Computing
R.Namyst/A.Butari

ExaDost
Data
G.Antoniou/J.Bigot

The French NumPEX Program - workplan



The French NumPEX Program - workplan



Applications

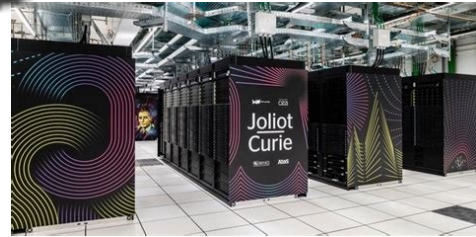
ExaDI
Application co-design and software integration
 JP.Vilotte/V.Brenner

ExaAtow
Digital continuum
 F.Bodin, T.Deutsch, M.Asch

ExaDost
Data
 G.Antoniu/J.Bigot

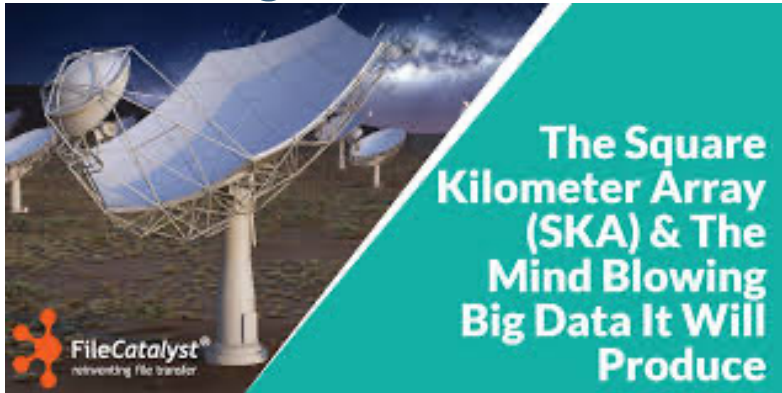
ExaMA
Numerical methods and solvers
 C.Prudhomme/H.Barucq

ExaSoft
Computing
 R.Namyst/A.Butari

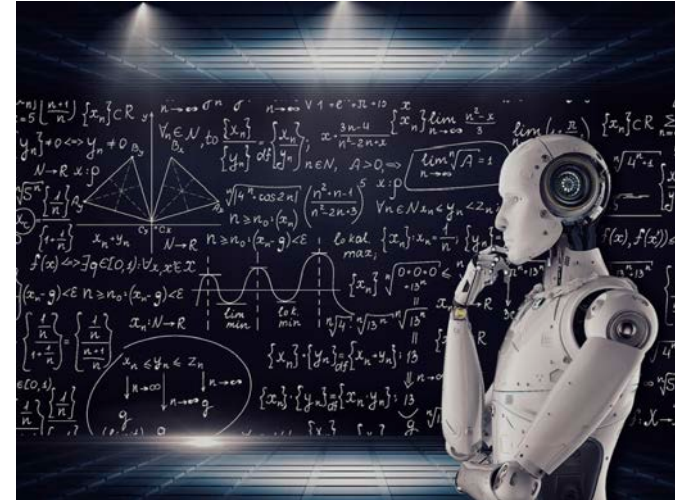


Focus on some post-exascale challenges

From edge to HPC systems The digital continuum



AI4Science – Science4AI



Software/application co-design



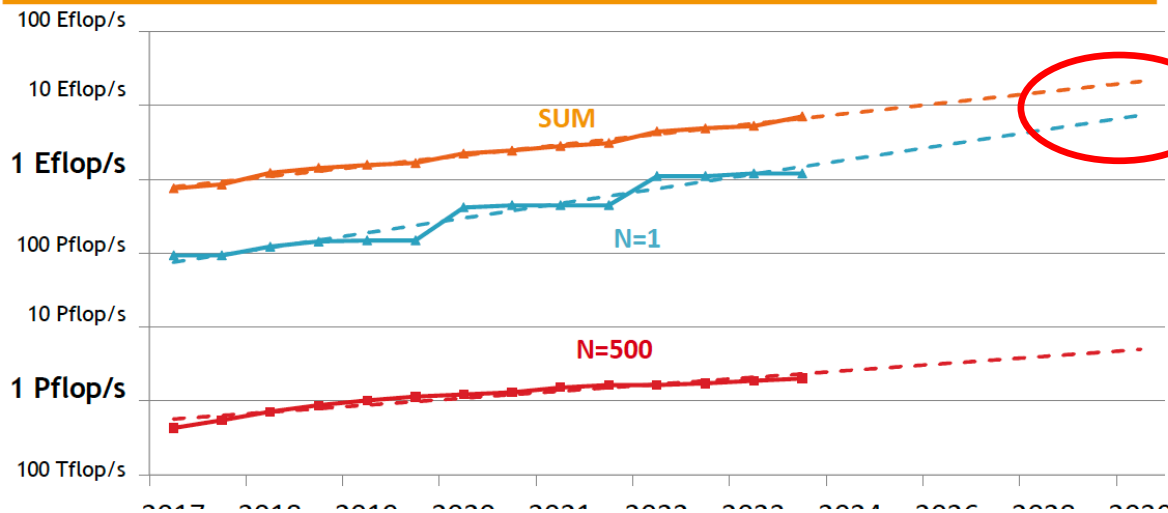
Software, the new frontier



Software, the new frontier



PROJECTED PERFORMANCE DEVELOPMENT

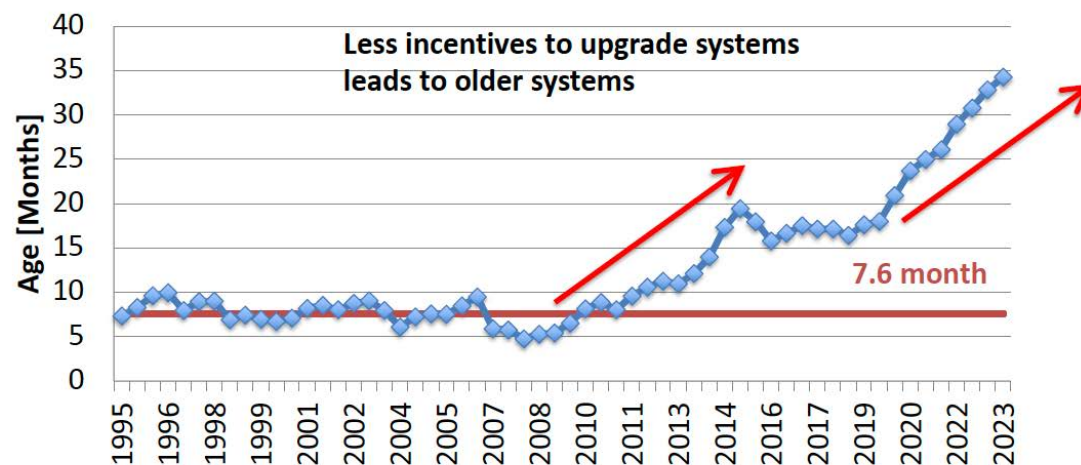


SC23 TOP500 HIGHLIGHTS



- Frontier is #1 and remains only ExaScale system in the TOP500 - for now
 - 4 new systems in TOP10! + one upgrade
 - And 9 additional new systems in TOP50
- First Intel Sapphire CPUs (25) and GPUs (4) on the list
- HPC systems are used longer and replaced less often
 - Due to an increasing number of technological limits
 - Leads to strong concentration at the top (research as well as commercial)
- TOP500 shows new reduced growth-rates since 2017!
 - End of original Moore's Law scaling
 - Unlikely to achieve 10 Exascale by the end of the decade unless we fundamentally change "business"!

AVERAGE SYSTEM AGE



Software, the new frontier



Software is the new power

- The race for power is slowing down: we're aiming for 10 Exaflops in 2030, not 1000
- => Importance of **Math&software development to gain effective power**: new digital schema, precision mix, innovative discretization methods, energy aware algorithms, ...
- Capitalize on and consolidate software production in Europe and worldwide
- Importance of software sustainability
- Offer an "industrial" production environment converging towards "As a Service".
- Broaden the potential user base towards new AI/HPC/HPDA/Cloud/Edge uses
- Enable and facilitate, or even make possible, what was not possible before, through the coupling of components produced in different contexts (e.g. Kokkos/StarPU/HWLOC) and thus enable the emergence of new services, uses and capacities to move towards exascale

At stake: consolidating and accelerating the construction of a **sovereign European exascale software stack**

Software, the new frontier



Software Integration challenge

Context:

- **HPC applications and machines are gaining in complexity** (think compute continuum, HPC/HPDA/DL hybridization), leading to high costs to build and deploy applications on supercomputers, **impairing portability and reproducibility**.
- The standard software installation process on supercomputers is reaching its limits
module load + cmake/make install

At Stake:

- Need for a HPC dev-ops methodology for fast deployment while ensuring performance and supporting reproducibility efforts

NUMPEX Strategy: Modern Software Packaging (SPACK and GUIX)

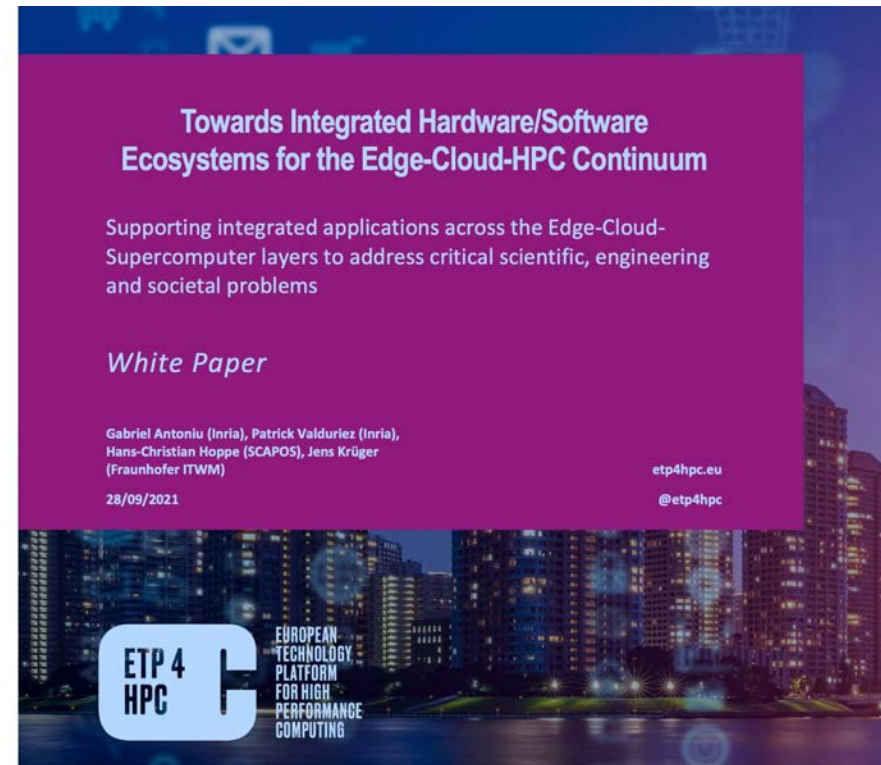
- Have users work with package managers to capture software dependencies with compilation process to automate deployment.
 - Can generate containers or be used directly if installed on supercomputer.
`guix pack -f docker mysoft`
`guix install mysoft`
 - Can also be used by system admin to generate modules



The Edge-Cloud-HPC continuum



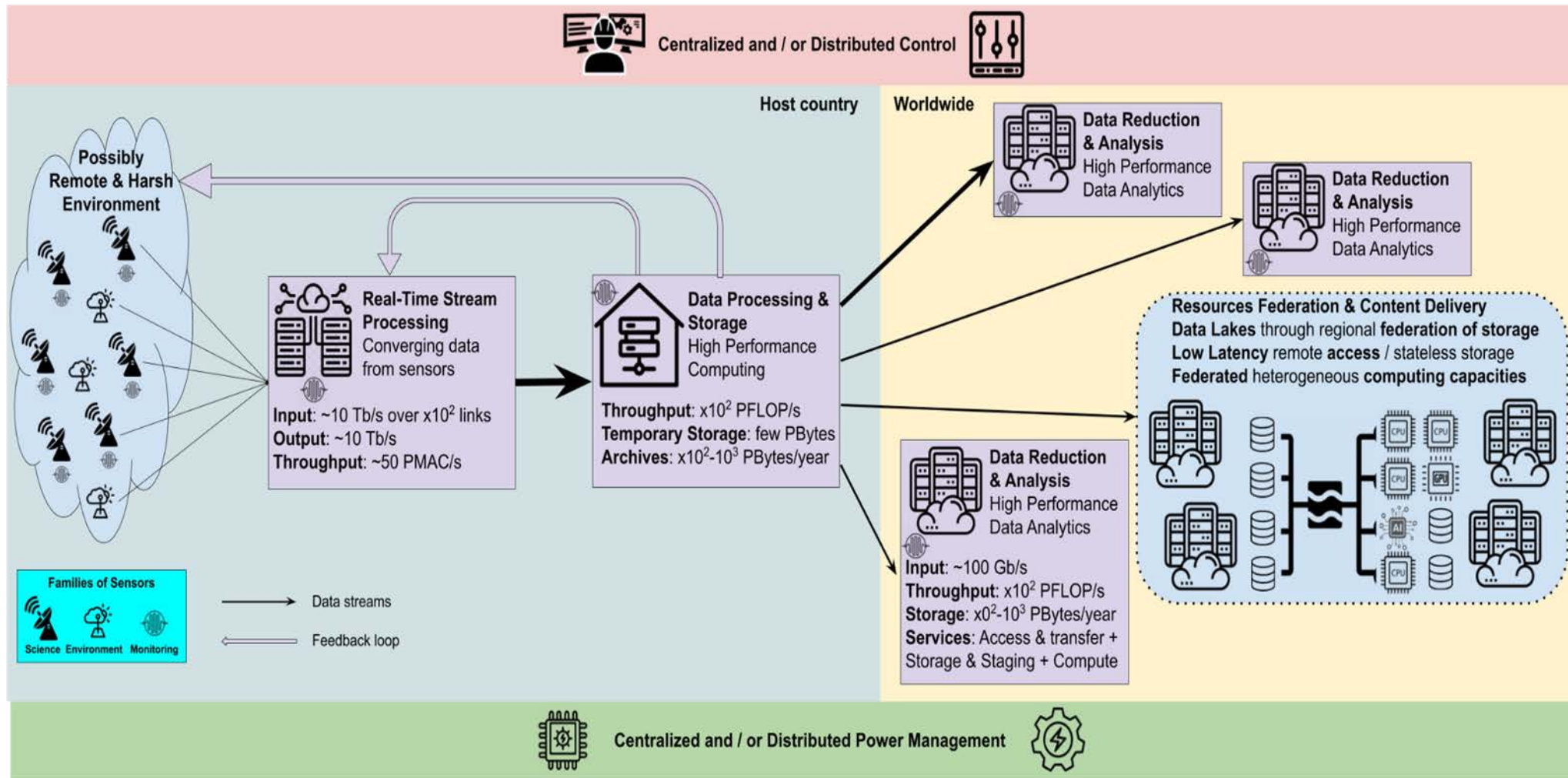
Distributed workflows
across edge, cloud and HPC systems



- The Exascale machine is part of a “datasphere”
 - Data from large scientific instruments
 - Data from sensors (IoT)
 - Data from simulations
- The primary challenge: developing integrated software ecosystems across this continuum
 - At an extreme scale with stringent cybersecurity constraints



The SKA data workflow from sensors to HPC centers



Observation data product delivery

- Data streaming reduction and processing,
- Edge computing and content delivery network

Data Science analysis: R&D component & software development

- Emerging technologies compute, I/O, storage, wide area workflows
- Distributed & heterogeneous architecture, content delivery network
- Power management

The digital continuum: open challenges

Unification of HPC Simulations/Big Data/AI towards a data-centric view

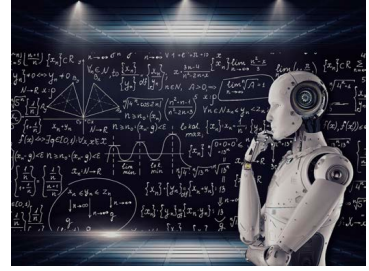
Moving, storing and processing data across the continuum: **how to deal with the 3 Vs of Big Data?**

- **Extreme Volume across the continuum**
 - Support the access and processing of “cold”, historical data and “hot”, real-time data + (virtually infinite) simulated data
- **Extreme Velocity across the continuum**
 - Unified real-time data processing (in situ/in transit, stream-based) in a common software ecosystem
 - Need disruptive reduction in data movement cost with new devices, packaging
 - All real-time data may not be storable in archives => real time training (bandwidth-oriented)
- **Extreme Variety across the continuum**
 - Unified data storage abstractions to enable distributed processing and analytics across the continuum
 - Interoperable data formats, "Semantic interoperability" through shared ontologies
- Digital Continuum is a **multi-tenant** and **multi-owner** environment.
 - Collected data used with multiple purposes
 - Computing Infrastructure is also **shared**

The Post-Exascale digital continuum: action plan

- Coordinate efforts to share workflows solutions and services for the convergence of AI/HPC/HPDA/Cloud/Edge
- Develop the concept of EaaS, Exascale as a Service, for Tier-0 European systems
- Contribute to the development of a data-everywhere, FAIR, ecosystem in Europe
- Identifying new emerging usages including urgent computing and digital twins

AI4Science / Science4AI



AI everywhere, a game-changer at the post-Exascale era

- AI at all stages from numerical methods to workflows, etc.
- **Trend towards AI-centric HW, which also puts huge constraints on the HPC SW stack**

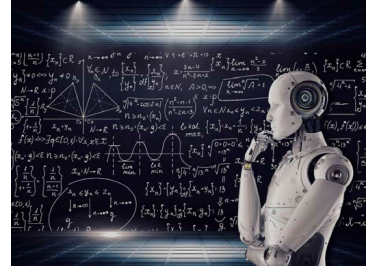
International initiatives have started, Europe must stay in the race

- US AI program, Trillion Parameter Initiative (www.tpc.dev).
- Initiatives to produce extreme scale LLMs, AuroraGPT, FugakuGPT, ...
- **Pushing for European initiatives, with a strong focus on Science**

Challenges of HPC/AI convergence

- How to develop **validated/robust/trustworthy AI models** for Science
- In the post-Exascale era, data-centric era, should **benefit from AI-centric software**
- **HPC/AI software stack convergence ?**

AI4Science / Science4AI



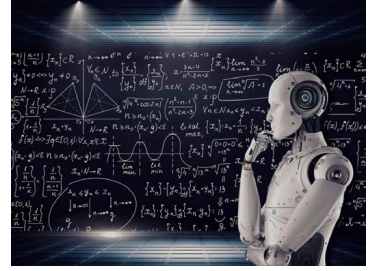
AI for science – towards HPC/AI hybridization

- End of Moore's law, **develop hybrid approaches based on AI** to accelerate parts of scientific computing applications

=> 10 Exascale performance with x25 EDP+Data science pp and x42 HW improvements, some AI-based solvers can be sped up by 6 orders of magnitude, etc., weather forecast with Graphcast

- **Hybridization of HPC SW with AI** : physics-informed AI models for simulation codes, observational data reduction, digital twins.
- **Push forward a post-Exascale-ready SW stack embedding AI solutions** that answer the needs of the application communities

AI4Science / Science4AI

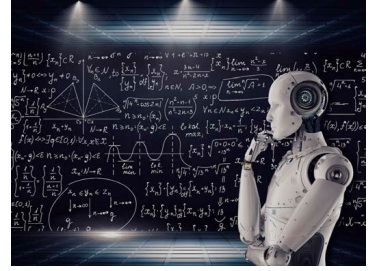


AI at scale at the post-Exascale era

- **Rapid emergence of extremely large AI models** (*e.g. LLM, multimodal GPT, diffusion models, etc*), which require huge compute capacity, massive storage.
- **Challenges in data management and computing** on Exascale/post-Exascale grade systems, with massive use of heterogeneous accelerated architecture.
- **Push a post-Exascale SW stack** that further covers AI-based libraries, with **interfaces between traditional HPC** libraries and standard **AI/Machine Learning framework**.

AI4Science / Science4AI

Accelerate AI for Science



- **Accelerate the diffusion and application of AI at all stages**, with a very strong focus on AI for scientific and engineering applications.
- Build upon an AI-centric co-design activity, focusing on **shared flexible open AI-centric application use-cases/mini-apps**, with curated data and well-defined application dependent metrics.

Fostering international initiatives and collaborations

- **Foster AI-centric European initiatives**, with a specific focus on **enabling the development of AI at scale for Science, not only focused on large foundation models**.

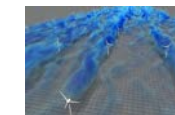
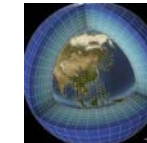
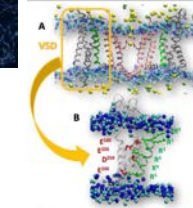
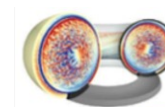
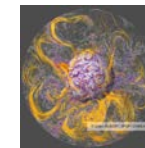
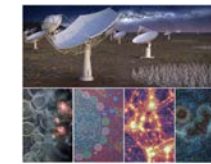
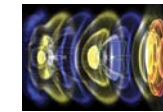
Software/application co-design

Key challenges

- How to get post-Exascale ready applications ?
- How to expand an application-driven SW stack ?
- How to make applications portable and sustainable at the post-Exascale era ?

International context

- Early-binding HW/SW/application co-design approach at Rikken (Japan)
- In the USA, DOE co-design centers were a key component of the Exascale Computing project (ECP)
- Inspired by ECP, co-design is central in the NumPEX project (FR)



Astronomy & Astrophysics

Earth System Models & Climate

Earth sciences & environment

Computational biology & Life science

Laboratory laser-plasma physics

High-energy particle physics

Quantum chemistry and materials

Digital health

Environmental & societal risks

Urban systems planing

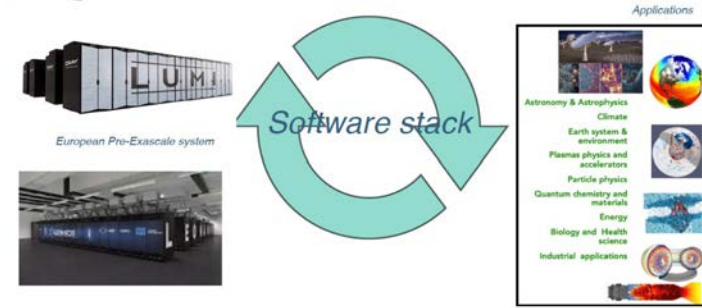
Magnetically confined fusion plasma

Sustainable Transport & mobility

Energy production & transport

Software/application co-design

Help the applications get prepared for post-Exascale challenges



- Towards **shared and common mini-apps/proxy-apps**, centered about technical functionalities/bottlenecks (AMR, I/O, AI, etc.)
- **Shared benchmarks** are central to test/evaluate portability/performance/deployability on different HW.

Towards a post-Exascale application-driven software stack

- Application code development is a long and costly journey, greater **reuse** of **composable/interoperable SW components**
- **Long-term visibility/sustainable development for applications is key.**

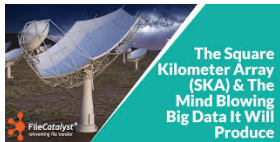
Take away messages



Software, the new frontier

Consolidating and accelerating the construction of a sovereign European **exascale software stack** (portable, interoperable, reproducible, sustainable)

Support and foster the development of disruptive Math & models

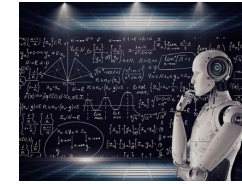


From edge to HPC system: the digital continuum

Coordinate efforts to share workflows, solutions and services for the convergence of HPC/Cloud/Edge

EaaS: **Exascale as a Service**, for Tier-0 European systems

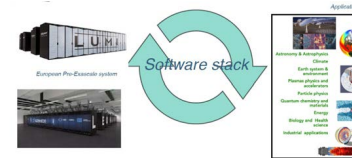
Develop a data-everywhere, FAIR, ecosystem in Europe



AI4Science – Science4AI

Push an **hybrid AI/HPC software stack**, to accelerate HPC and provide AI at scale

Support AI for Science, foster fully open AI use-cases/benchmarks, **not restricted to GenAI**



Software/application co-design

HW/SW/application co-design to help the communities get prepared for post-Exascale

Foster the use/reuse of modular/interoperable and portable SW components

Push sustainable SW development model