Exa-DoST:
Exascale Data-oriented Software and Tools

PEPR NumPEx project ANR-23-PECL-0007
1 Jan 2023 – 31 Oct. 2029 (82 months)
PI: Gabriel Antoniu (Inria), Co-PI: Julien Bigot (CEA)

The Exa-DoST "core" team

CEA/DAM - DPTA, SISR, SANL

CEA/DRF - MdlS, IRFM, IRFU

CNRS/INSU, Observatoire de Paris, Observatoire de la Côte d'Azur

Inria - DataMove, KerData, MIND, TADaaM, +SODA, +STATIF, +THOTH

DDN

The NumPEx Program

Co-directors: Dr J. Bobin (CEA), Pr M. Krajecki (CNRS), Dr J-Y. Berthou (INRIA)

Project leaders and co-leaders:

Exa-Ma - C. Prudhomme, U. de Strasbourg– Hélène Barucq, Inria

Exa-Soft - R. Namyst, Inria/U. de Bordeaux - Alfredo Buttari, IRIT

Exa-Dost - G. Antoniu, INRIA - Julien Bigot, CEA

Exa-AtoW - F. Bodin, U. de Rennes - Mark Asch, U. Picardie - Thierry Deutsch, CEA

Exa-DI - J-P. Vilotte, DR CNRS - Valérie Brenner, CEA
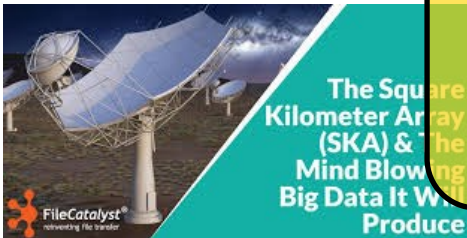
The French NumPEx Program
Context and motivations

A technological breaktrough
Hybrid scalar/acc.
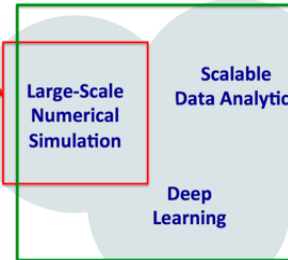fewer memory/node
more concurrency
Mixed precision, …

In the digital continuum
Increased flux/volume from the edge to the HPC system

Convergence
HPC/HPDA/IA

Traditional HPC Systems

Large-Scale Numerical Simulation

Scalable Data Analytics

Deep Learning

Capable Exascale system

The French 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** methods, logic collection of libraries, frameworks and software stack with demonstrators of strategic applications.

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

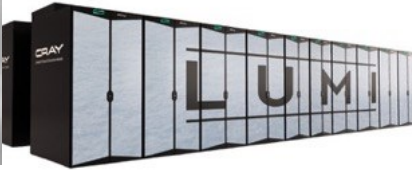**Foster** **national and international collaborations** to prepare for the post-Exascale era

Strategic applications

Research & Software Development

NumP Ex

Expanded and integrated Software stack

Co-design & demonstrators
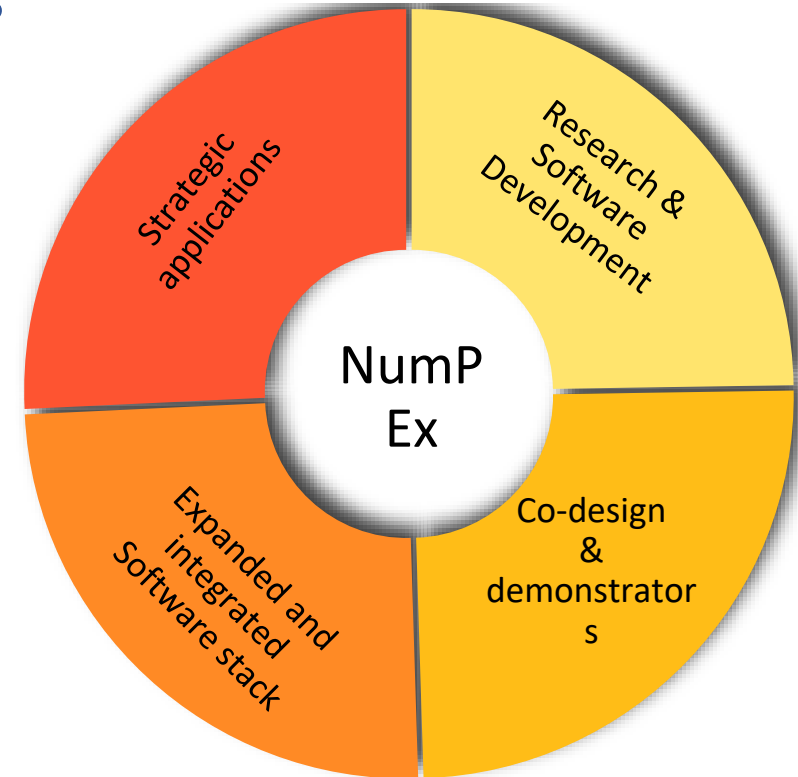
Help aggregate the French HPC/HPDA/IA community

The French NumPEx Program
Objectives

A.recoque supercomputer

European Pre-Exascale system

Software stack

Astronomy & Astrophysics

Climate

Earth system & environment

Plasmas physics and accelerators

Particle physics

Quantum chemistry and materials

Energy

Biology and Health science

Industrial applications

**Co-develop the exascale software stack
Preparing the applications for the Exascale era**

NumPEx by numbers
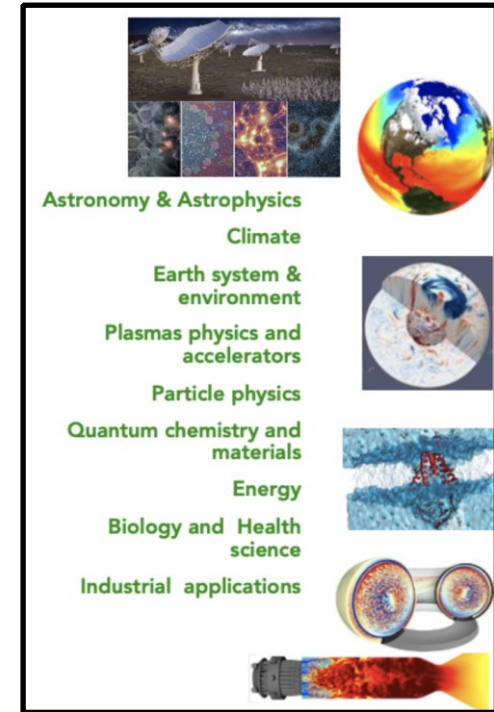
Legend:
- 🔴 Math/computing/data
- ⭐ Application/demonstrators
- 🔺 NumPEx contributors
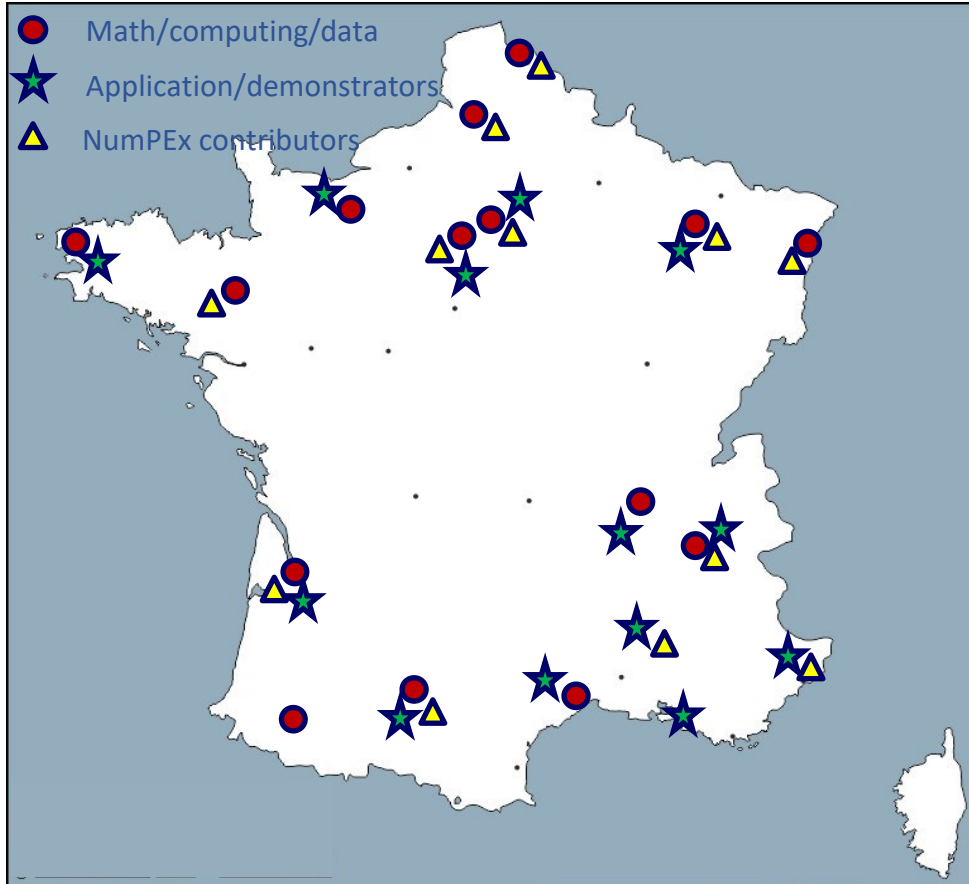
6 Years 41 M€*

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
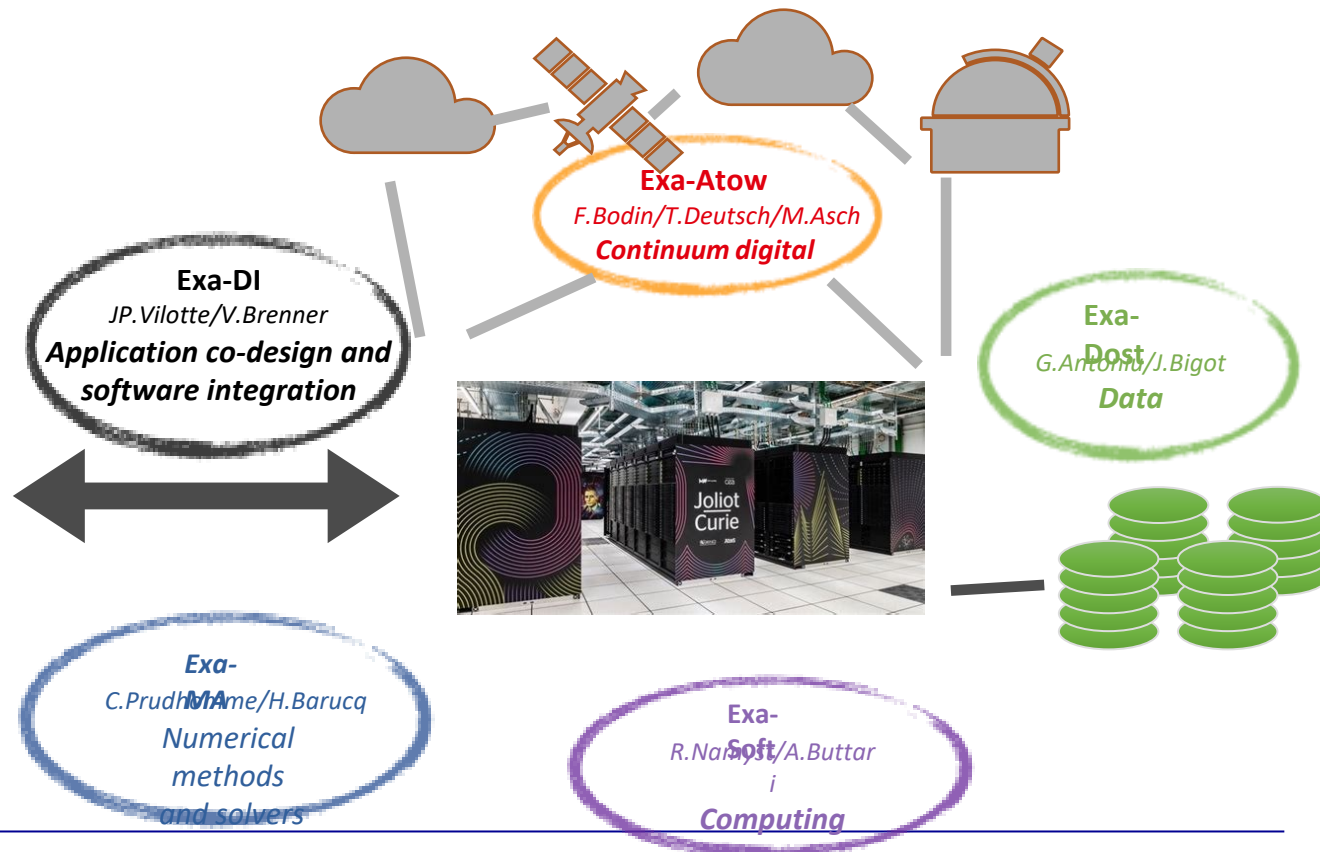
3 Focus Area

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

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

Exa-Atow
F.Bodin/T.Deutsch/M.Asch
Continuum digital

Exa-Dost
G.Antoniu/J.Bigot
Data

Exa-MA
C.Prudhomme/H.Barucq
Numerical methods and solvers

Exa-Soft
R.Namyst/A.Buttari
Computing

The French NumPEx Tranversal groups

Accelerated architectures and programming models

S.Thibault/M.Pérache

AI

T.Moreau/E.Franck/J.Bobin

Computing centers

F.Bodin/N.Lardjanne

Energy management and optimization

A.Guermouche/G Da Costa

Gender/Equity/Diversity
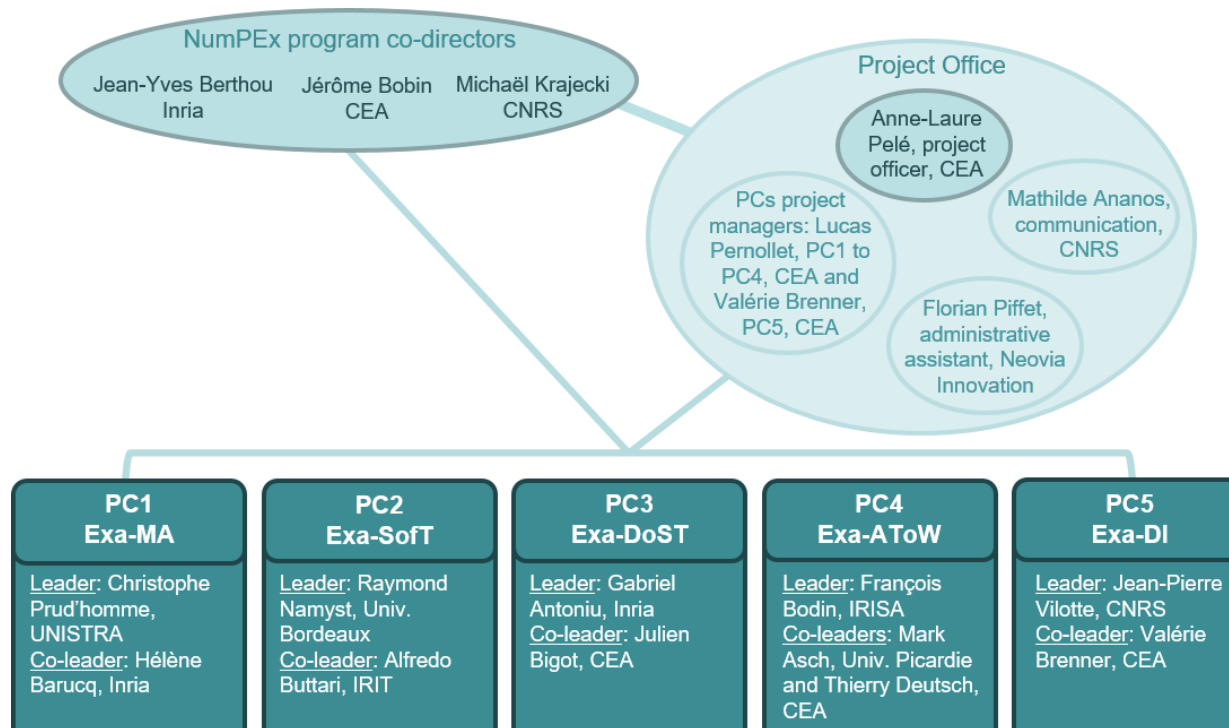
A-L Pelé/V. Grandgirard

Training

M.Krajecki

Software production and integration

B.Raffin

International collaborations

J-Y Berthou

Organisation

NumPEx program co-directors
- Jean-Yves Berthou, Inria
- Jérôme Bobin, CEA
- Michaël Krajecki, CNRS

Project Office
- Anne-Laure Pelé, project officer, CEA
- PCs project managers: Lucas Pernollet, PC1 to PC4, CEA and Valérie Brenner, PC5, CEA
- Mathilde Ananos, communication, CNRS
- Florian Piffet, administrative assistant, Neovia Innovation

PC1 Exa-MA
Leader: Christophe Prud'homme, UNISTRA
Co-leader: Hélène Barucq, Inria

PC2 Exa-SofT
Leader: Raymond Namyst, Univ. Bordeaux
Co-leader: Alfredo Buttari, IRIT

PC3 Exa-DoST
Leader: Gabriel Antoniu, Inria
Co-leader: Julien Bigot, CEA

PC4 Exa-AToW
Leader: François Bodin, IRISA
Co-leaders: Mark Asch, Univ. Picardie and Thierry Deutsch, CEA

PC5 Exa-DI
Leader: Jean-Pierre Vilotte, CNRS
Co-leader: Valérie Brenner, CEA

YoungPEx

Create a network of young recruits in NumPEx (internships, theses, postdocs on fixed-term contracts, and permanent young employees).

Develop a cross-disciplinary community through PCs, thereby enriching exchanges and even fostering collaborations.

Propose original initiatives to the NumPEx management, such as:

• Actions during General Assemblies (AGs)

• Seminars

• Actions for the integration of young recruits into NumPEx

• Communication, training, careers

• …

Don't miss the YoungPEx workshop !

The International Post-Exascale (InPEx) Project

InPEx expected outcomes

- Identify future trends/disruptions, missing software components
- Contribute to the share/development of software components: @deployable, @maintenable, @robust, @sustainable => **partnership factory**
- Landmark documents largely exploited, worldwide, for supporting future post-exascale science
- Develop an international network of exascale computing experts and leaders

Actions:

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

Participants:

Researchers, engineers, industry, funding bodies

Pre-workshop InPEx, October 2023, Reims

The International Post-Exascale (InPEx) Project
Inpex.science

| Date	(10/2023)	11/2023	06/2024	04/2025
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

Latest InPEx meeting, Kanagawa /Japan, 14-17 April 2025

Four parallel sessions:

- AI and HPC
  - Sharing AI-centric benchmarks of hybrid workflows
  - Generative AI for Science
- Software production and management
- Digital Continuum and Data management

Data at Exascale: Challenge at Hardware Level

- Increasing **gap between compute and I/O** performance on large-scale systems
  - Ratio of I/O to computing power divided by ~10 over the last 10 years on the top 3 supercomputers

- … and data deluge!
  - At NERSC, **data volume x41** in 10 years

- New storage tiers and advanced architectures to try to mitigate this increasing bottleneck
  - More complex on-node memory layout
 - Emerging complex applications and workflows have to adapt

Ratio of I/O bandwidth (GBps) / TFlops of the top 3 of the Top500
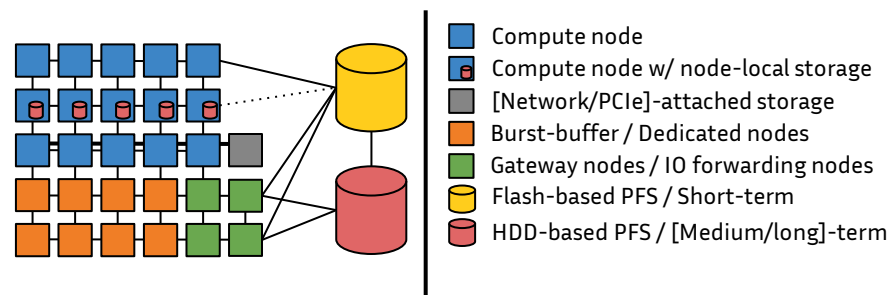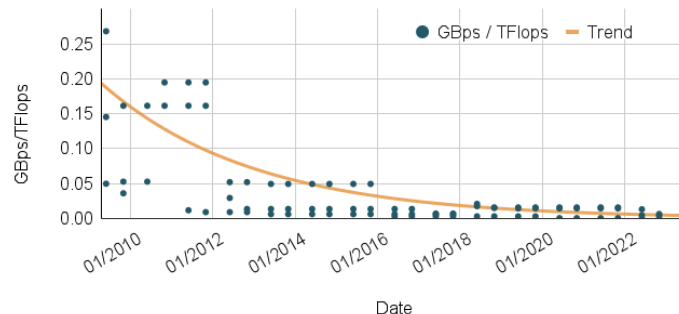
Trend in storage technologies available on extreme-scale systems

Data at Exascale: Challenge at Usage level

- HPC centers do not live in isolation anymore
  - Edge - Cloud - HPC continuum

- Emerging workloads are hybrid
  - High-performance simulation
  - High-performance data analytics
  - Machine learning and artificial intelligence

- Interaction with data from the outside world sensors
  - Large scientific instruments
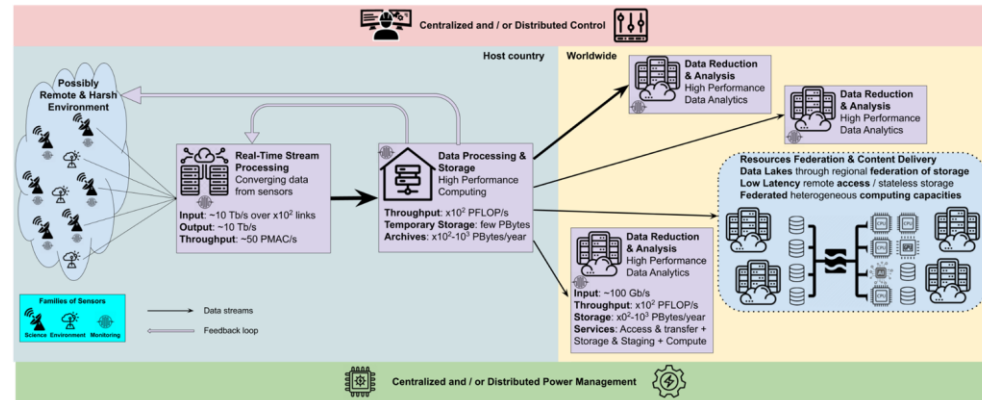
SKA data workflow from sensors to HPC centers
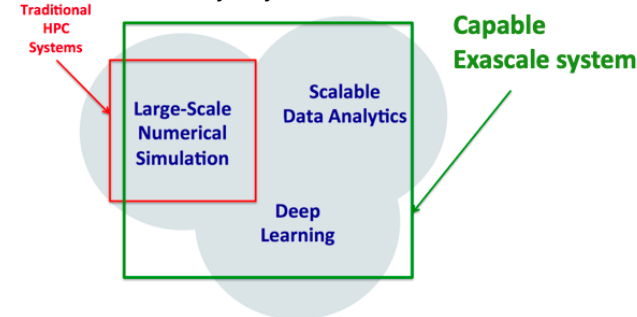
Exa-DoST: Expected Outcomes

Approach:

- **Research** on data-oriented tools for HPC
- Transverse, **re-usable tools**
- Usable **in production** at exascale

⇒ ExaDoST will produce:

- **New approaches** to handle the data challenge at exascale
- Transverse **libraries & tools** that implement these approaches

Validated in illustrators at full scale

Fill the gaps in the existing software stack designed by previous projects (e.g. ECP)

Take into account French & European specificities

Ensure French & European needs are taken into account in roadmaps

Fully application agnostic

Fully open-source

Work Packages in Exa-DoST

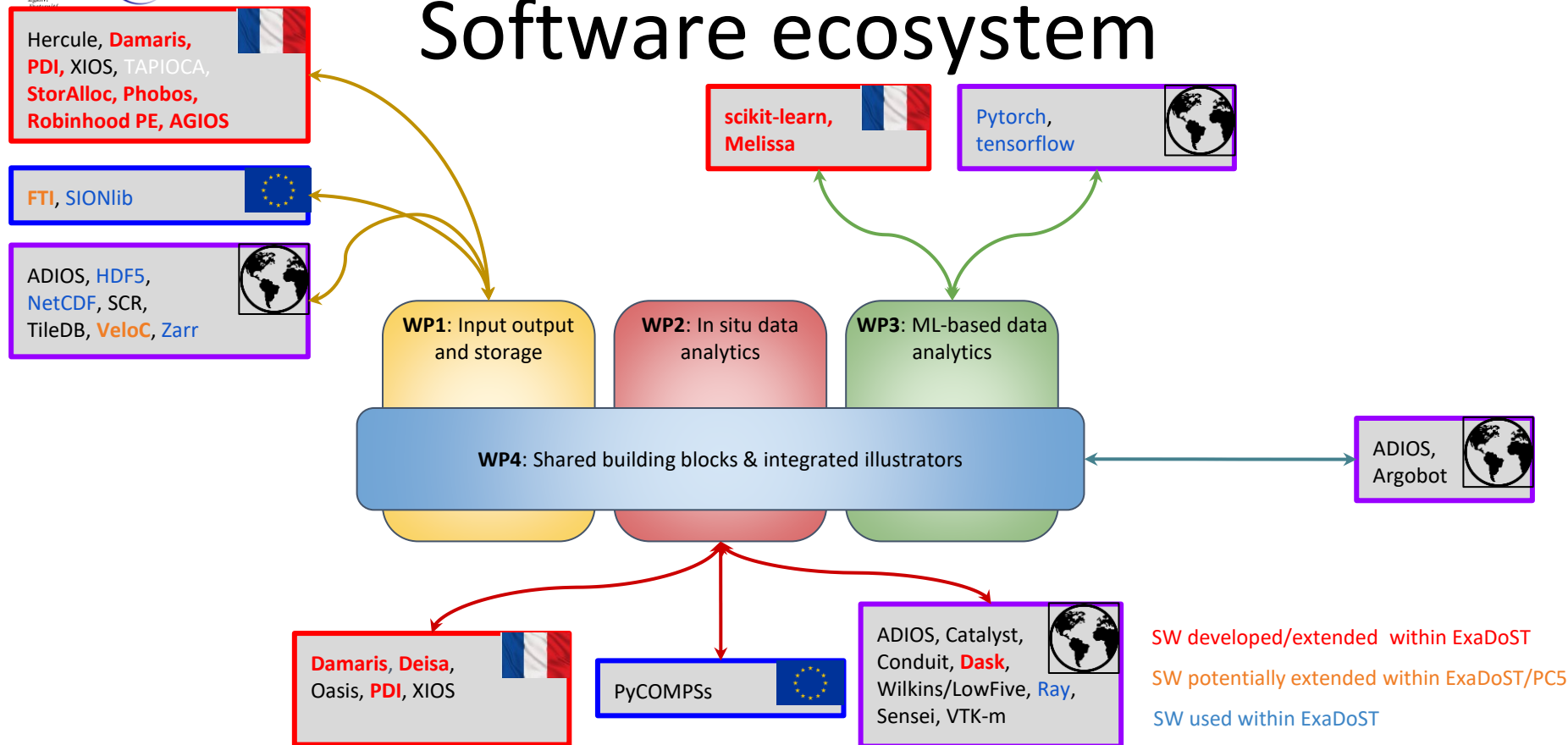**WP1**: Exascale I/O and storage

WP2: Exascale In-situ data processing

WP3: Exascale ML-based data analytics

WP4: Shared building blocks & integrated illustrators

WP5: Management, dissemination and training

Software ecosystem

Hercule, **Damaris,**
PDI, XIOS, TAPIOCA,
StorAlloc, Phobos,
Robinhood PE, AGIOS

FTI, SIONlib

ADIOS, HDF5,
NetCDF, SCR,
TileDB, **VeloC**, Zarr

scikit-learn,
Melissa

Pytorch,
tensorflow

WP1: Input output
and storage

WP2: In situ data
analytics

WP3: ML-based data
analytics

WP4: Shared building blocks & integrated illustrators

ADIOS,
Argobot

Damaris, **Deisa**,
Oasis, **PDI**, XIOS

PyCOMPSs

ADIOS, Catalyst,
Conduit, **Dask**,
Wilkins/LowFive, Ray,
Sensei, VTK-m

SW developed/extended within ExaDoST

SW potentially extended within ExaDoST/PC5

SW used within ExaDoST

Illustrator 1: GYSELA towards exascale

Main challenge : optimized management of huge amount of data with in-Situ AI-based diagnostics

- GYSELA a non-linear 5D gyrokinetic code developed for 25 years at CEA/IRFM to simulate plasma turbulence in tokamaks.
- Optimized up to 730k CPU -> Intensive use of petascale resources (~150 millions of CPU h / year)

Weak scaling of GYSELA on CEA-HF
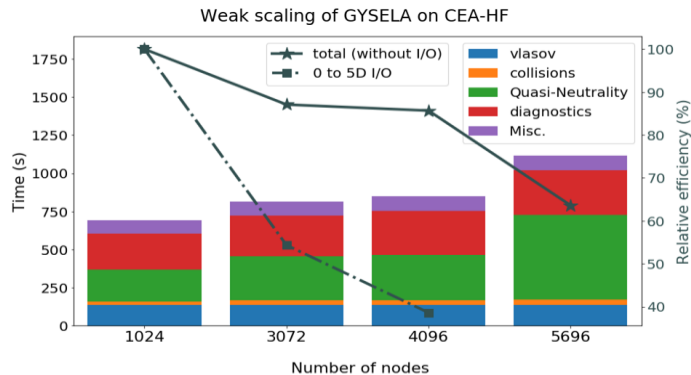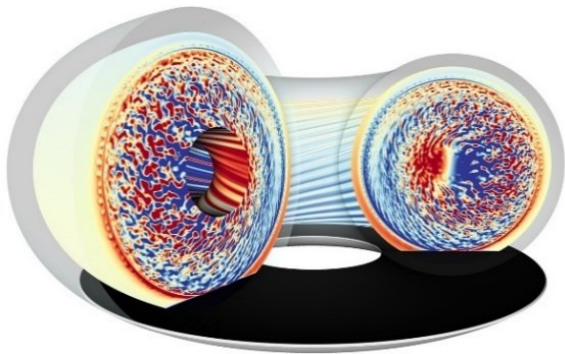
Relative efficiency of 85% on more than 500k cores

[V. Grandgirard et al., PASC 2022]

Typical simulation:
- **100 billion points** (5D mesh: 3D space + 2D velocity)
- **~7 million of CPU hours** (3.5 days / 65k cores)

- **I/O scalability** is **an issue**: ~50% for 3072 nodes and ~38% for 4096 nodes. Crash on 5696 nodes
- **Need to be solved for exascale** ITER-like **simulations**

Illustrator 2: Square Kilometer Array (SKA)

Based on SotA software used to process large surveys (DDFacet)

- Complex iterative pipeline: optimize I/O footprint and upscale
- Ongoing work: definition of benchmarks and motifs identification
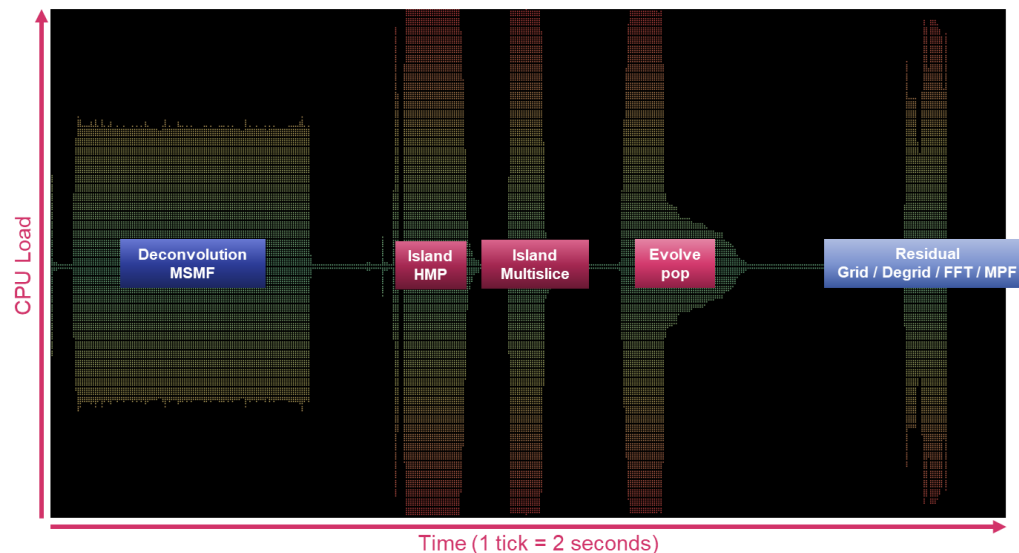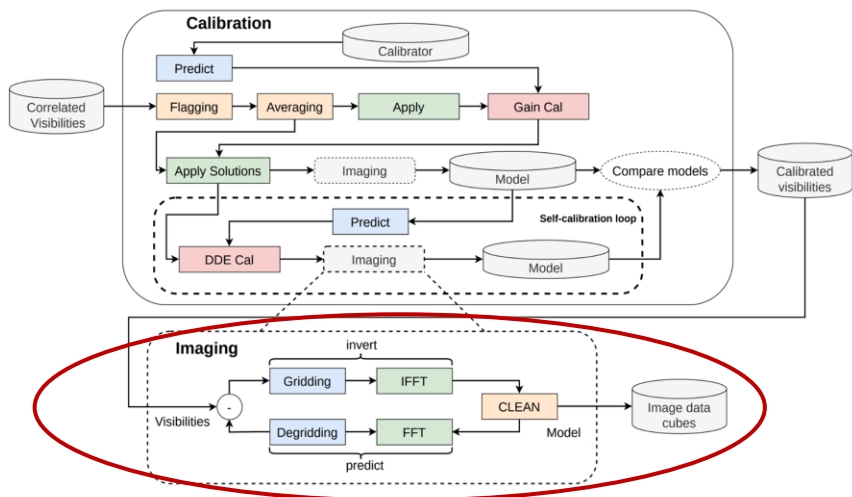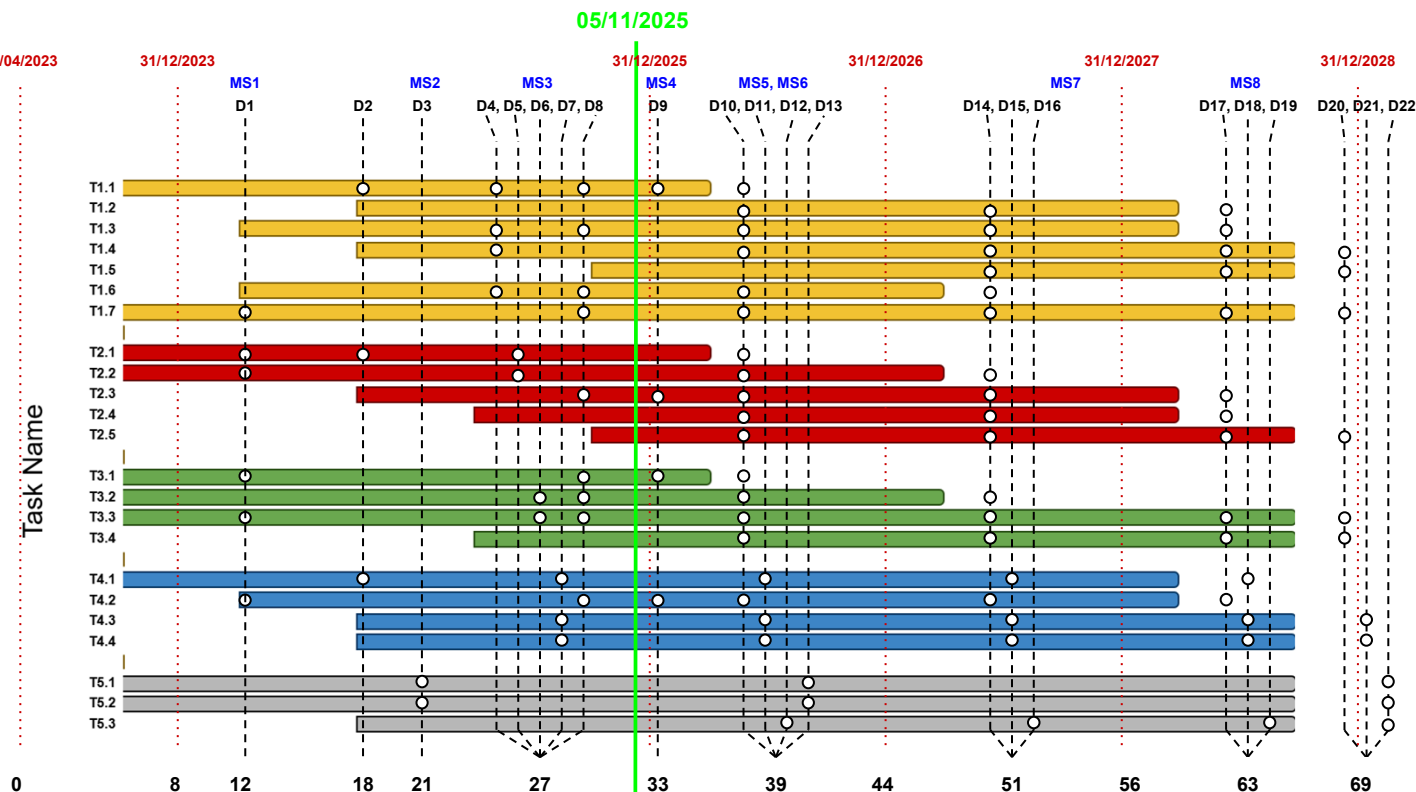
Illustrators overview

Integrated cross-WP illustrators

- Gysela (CEA/DRF/IRFM)
- SKA (CNRS + …)

Motif-specific motivators

- Coddex (CEA/DAM)
- CROCO (CNRS + Inria + …)
- Dyablo (CEA/IRFU)

Updated Gantt Chart

Hiring: Status

WP	PhD students	Engineers	Post-doc	Total
WP1	1	2	0	**3**
WP2	1	4	0	**5**
WP3	1	1	1	**3**
WP4	0	2	0	**2**
WP5	0	0	0	**0**
Total	**3** (6 prévus)	**9** (12 prévus)	**1** (2 prévus)	**13** (19 prévus)

Collaborations with Other Projects

Within NumPEx

- Exa-AtoW: collaboration within the ECLAT joint lab on SKA (WP1, WP4), InPEx (WP1-WP5)
- Exa-DI: deployment of tools (particularly from WP2) for SKA, GYSELA), joint meetings
- Exa-MA: joint ANR project with the team of Emmanuel Franck on turbulence models (WP4)

With other PEPR programs (France 2030)

- PEPR TRACCS: HPC/IA coupling (WP3)
- PEPR Cloud : scalable storage (WP1), SKA demonstrator (WP1, WP4)

At European level

- EoCoE-III Gysela-X++ exascale demonstrator (https://www.eocoe.eu/)

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in NumPEx