Exploratory PEPR

NumPEx

High Performance Numerics for Exascale

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Pr M. DAYDE CNRS, co-director of NumPEx

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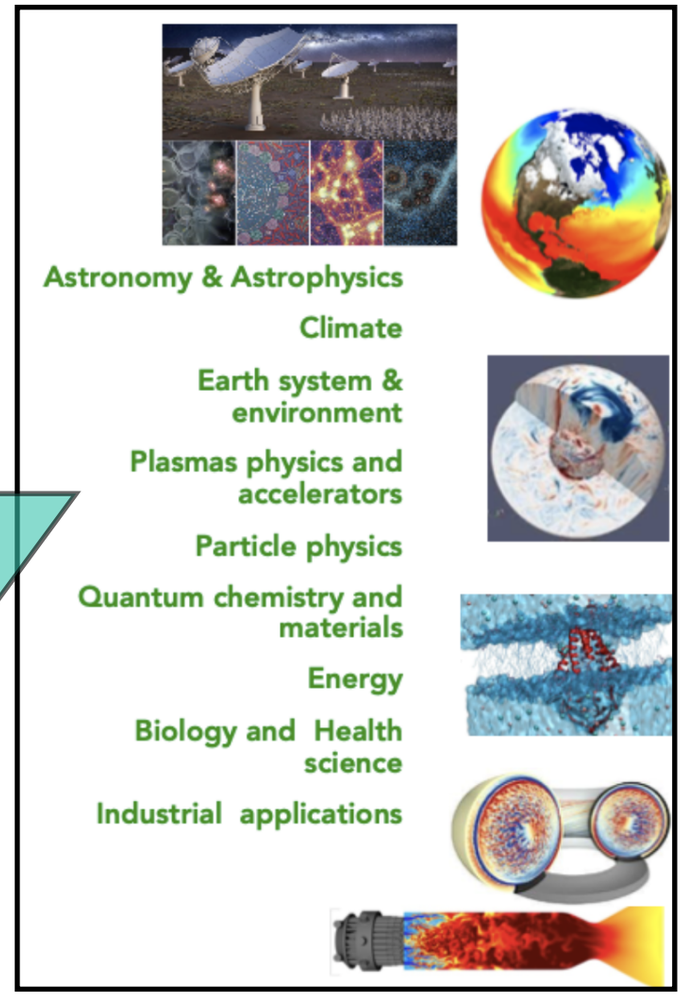
Towards the Exascale: challenges

Exascale system

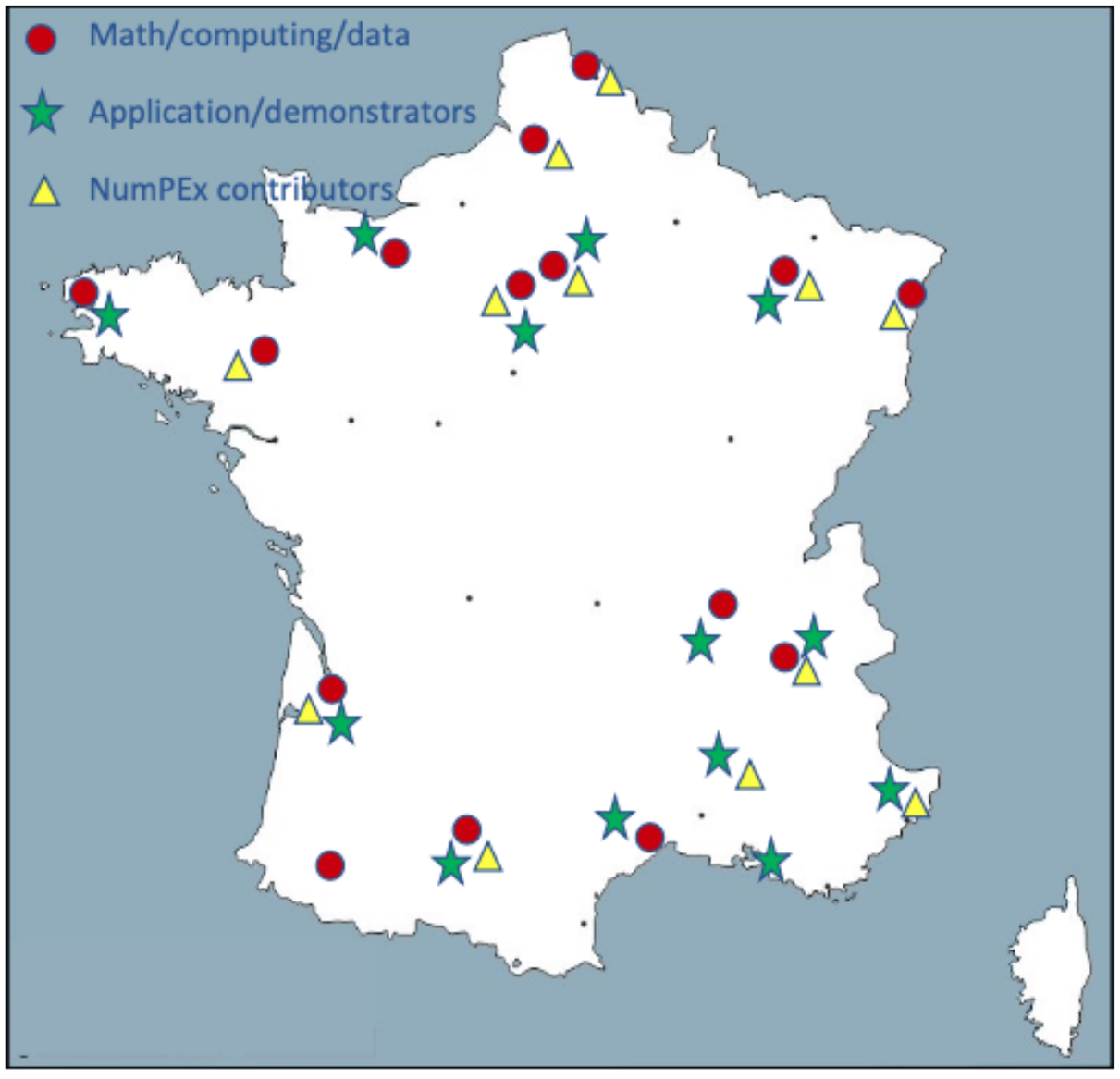
Software stack



Applications

Preparing the applications for the Exascale era requires a major effort to re-design the software stack, by co-design

In the national ecosystem



5 Years 40,8 M€

A five-year effort

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)

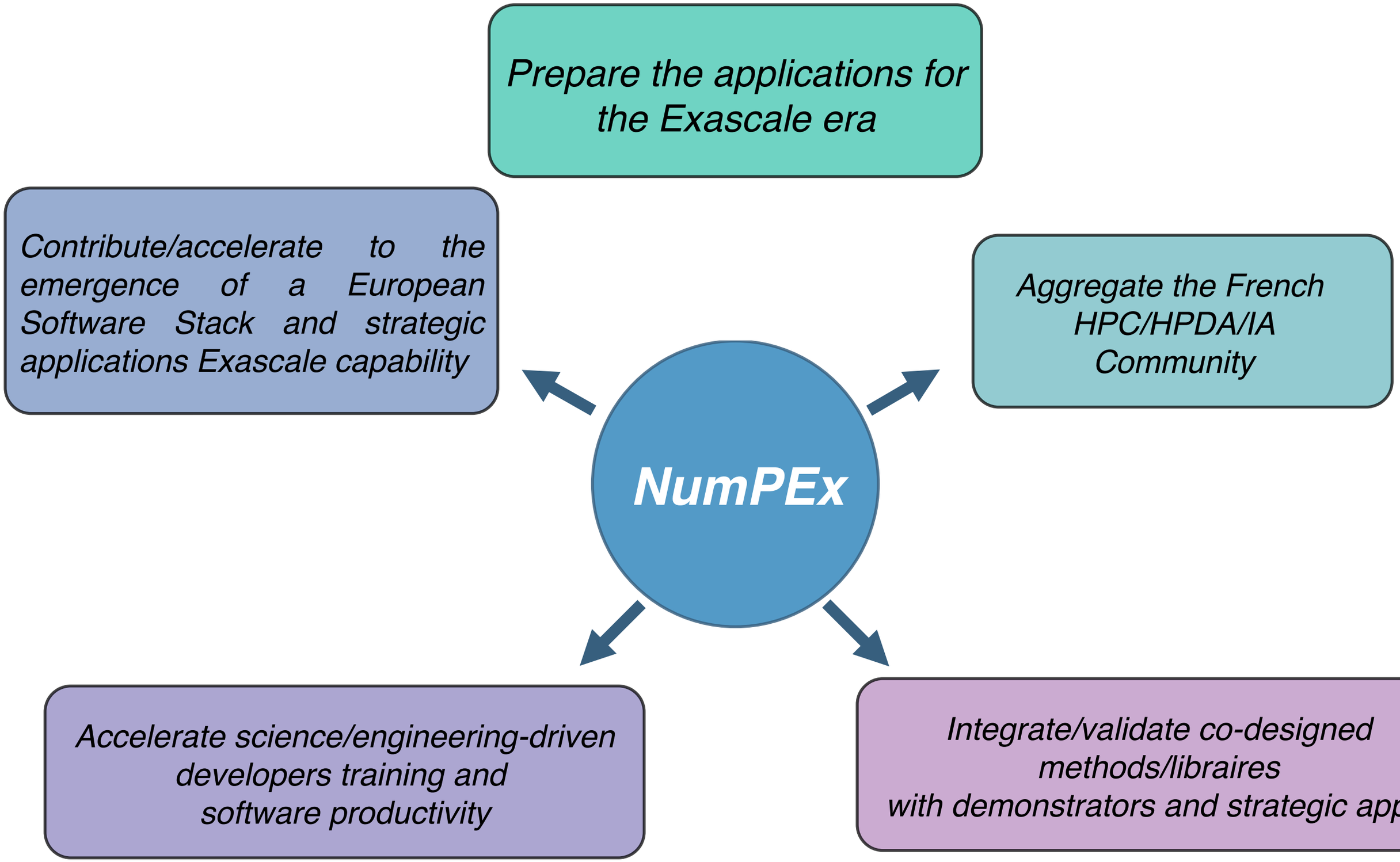
80 R&D teams 500 Researchers

80+top-notch R&D teams
About 500 researchers

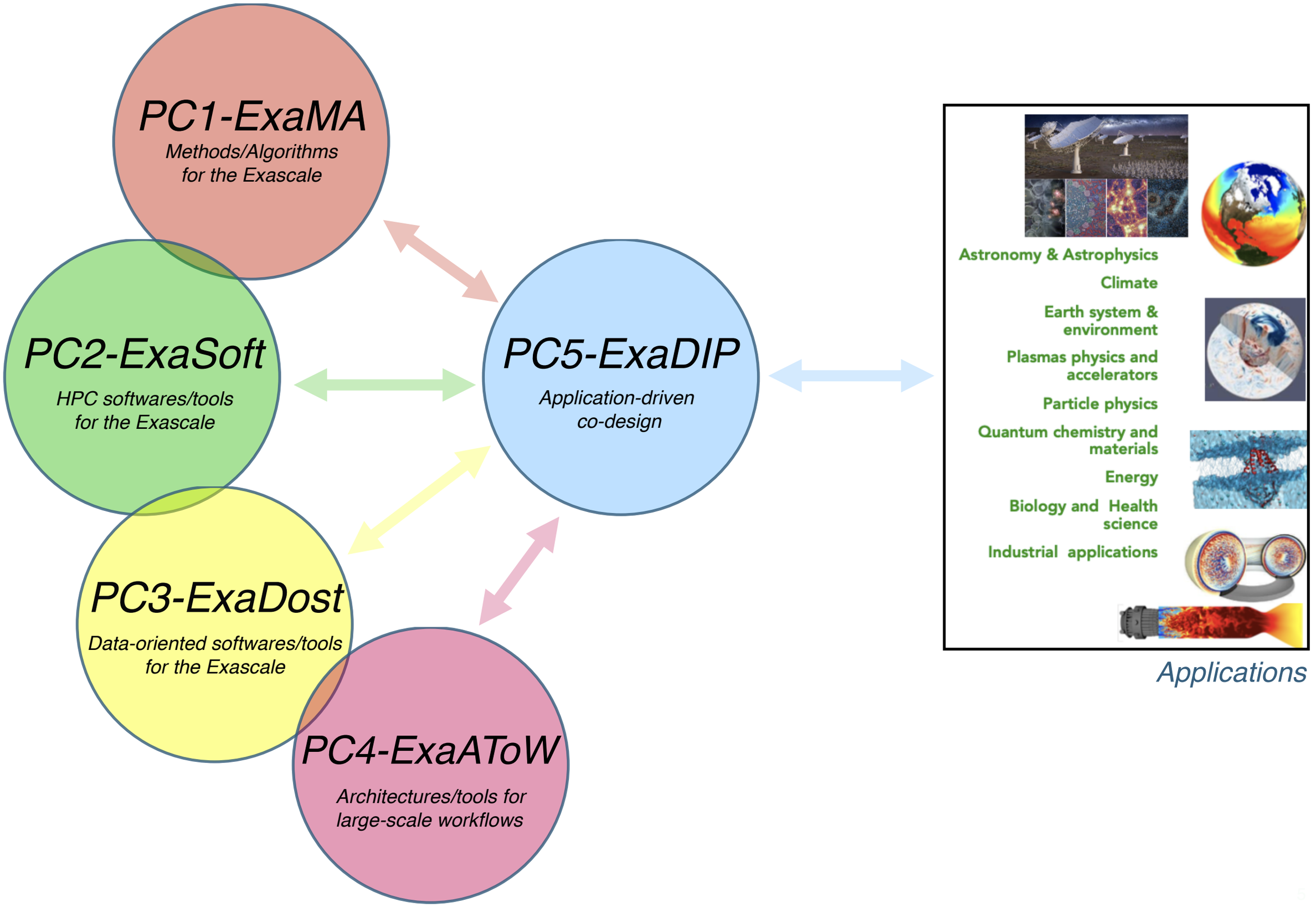
25+to be hired for co-design development

NumPEx as the software/middleware component of France Exascale

NumPEx, an overview

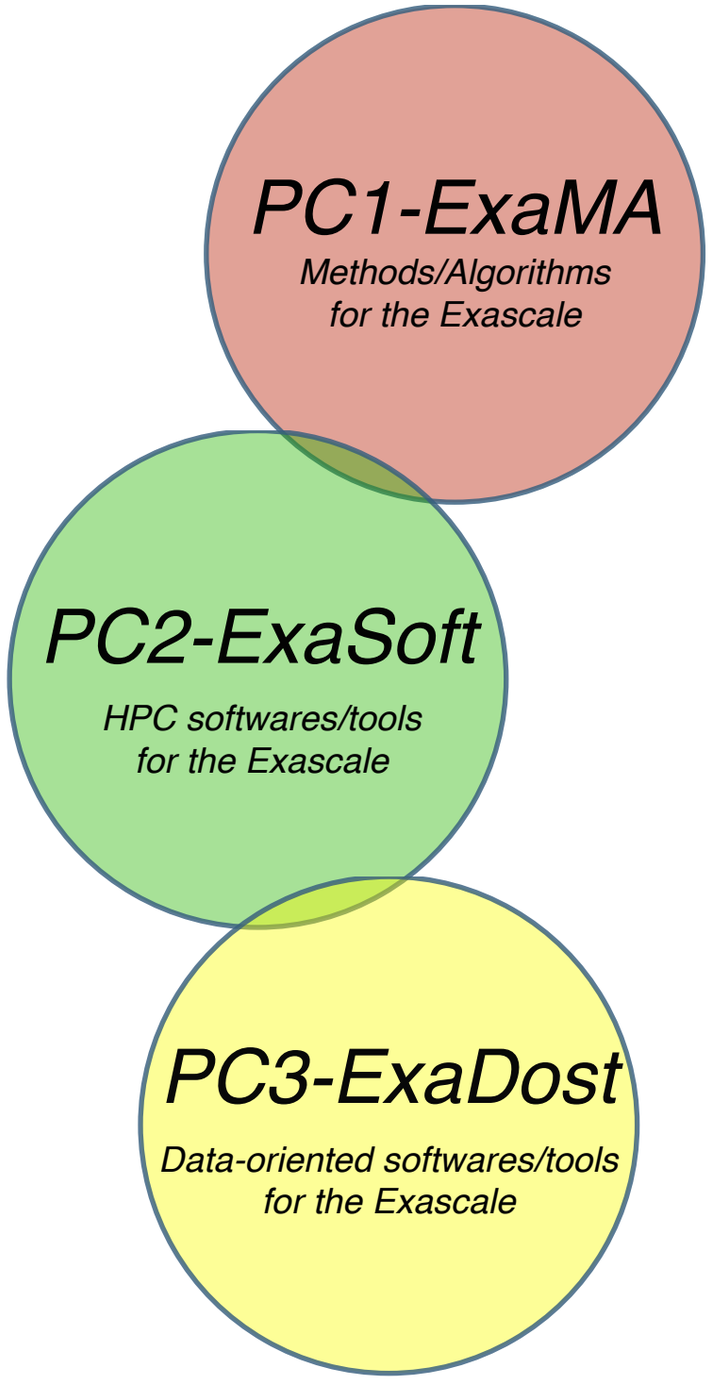


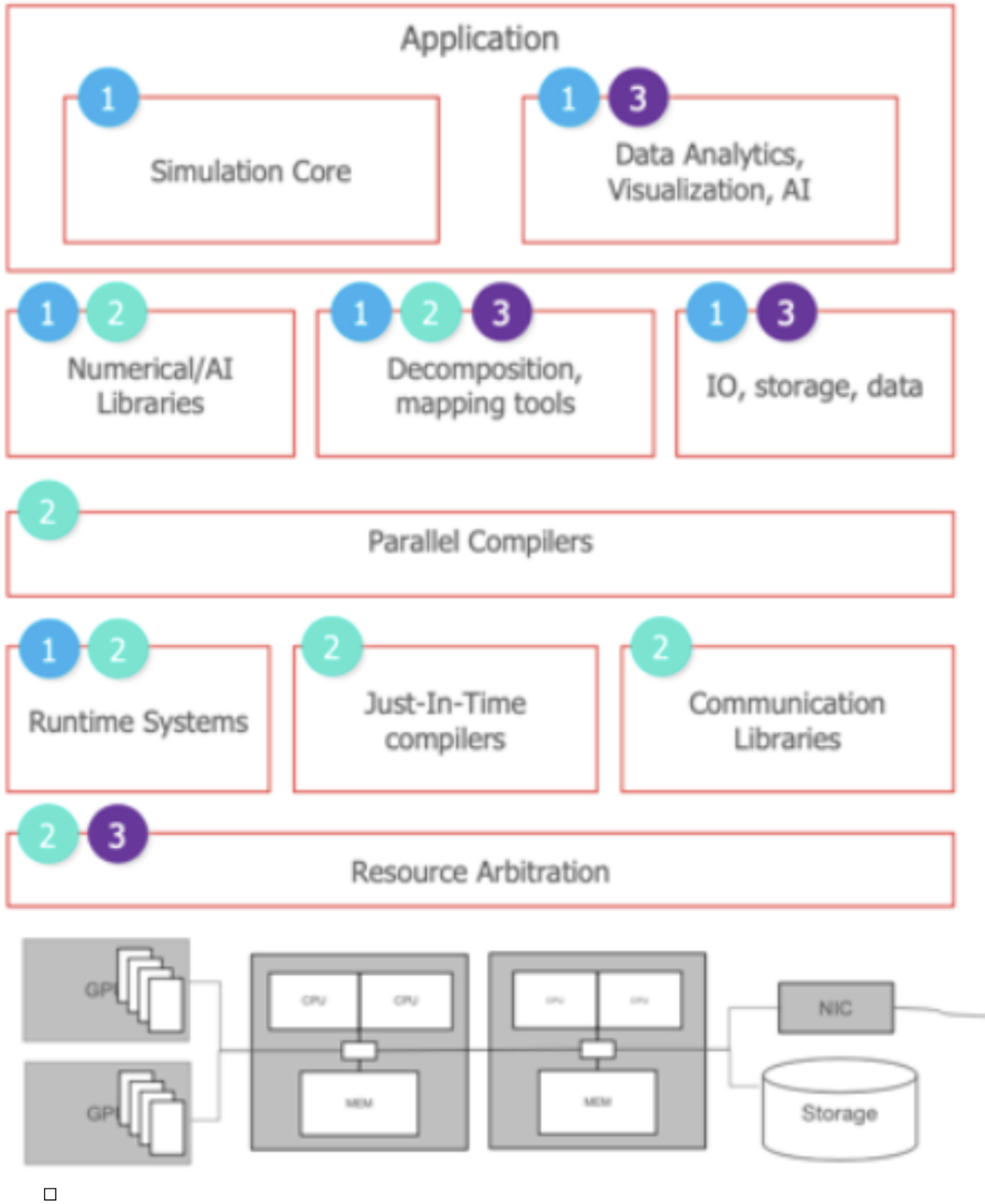
NumPEx Organisation



Applications

NumPEx software stack

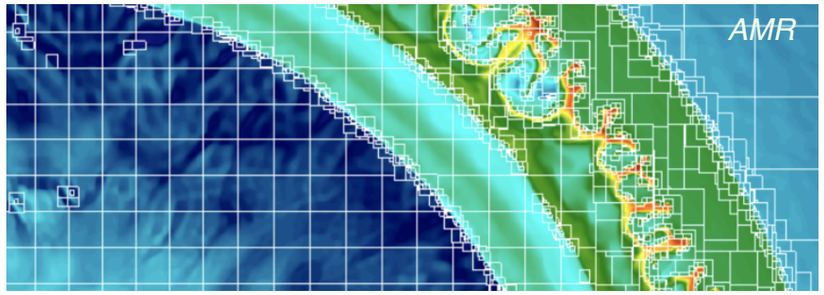




NumPEx, ExaMA

Methods/Algorithms for the Exascale

Discretization



Reduced order and AI-driven methods for multi-fidelity modelling

PC1-ExaMA

Methods/Algorithms for the Exascale

Linear, multi-linear and coupled solvers

Combine data and models, inverse problems

Optimize at Exascale

Quantify uncertainties

NumPEx, ExaSoft

HPC software/tools for the Exascale

High-level approaches for developing efficient and composable parallel software

Just-in-Time code optimization with continuous feedback loop

PC2-ExaSoft

HPC softwares/tools for the Exascale

Runtime Systems at Exascale

Portable, scalable numerical building blocks and software

Performance analysis and prediction

Energy profiling and control

NumPEx, ExaDost

Data-oriented sfotwares/tools for the Exascale

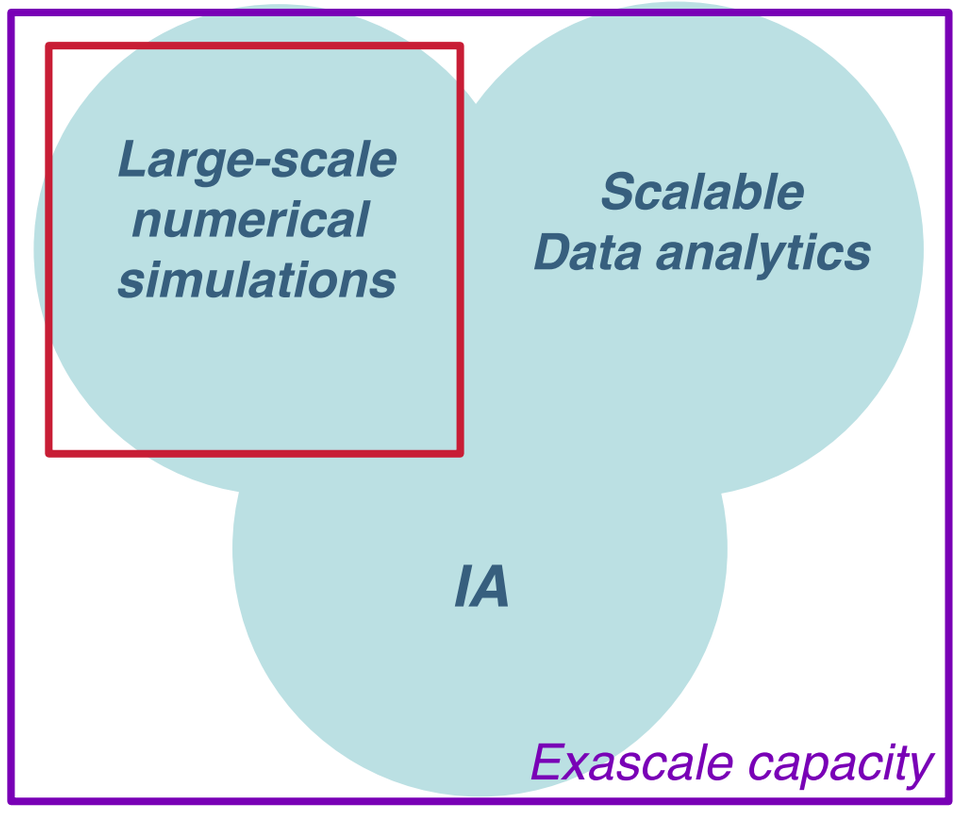
Exascale I/O and storage

Exascale in-situ data processing

Exascale ML-based data analytics

PC3-ExaDost

Data-oriented softwares/tools for the Exascale



NumPEx, Exa-AToW

Architectures and tools for large-scale workflows

Federation of network, data, and compute resources

Metadata Centric Approach

PC4-ExaAToW

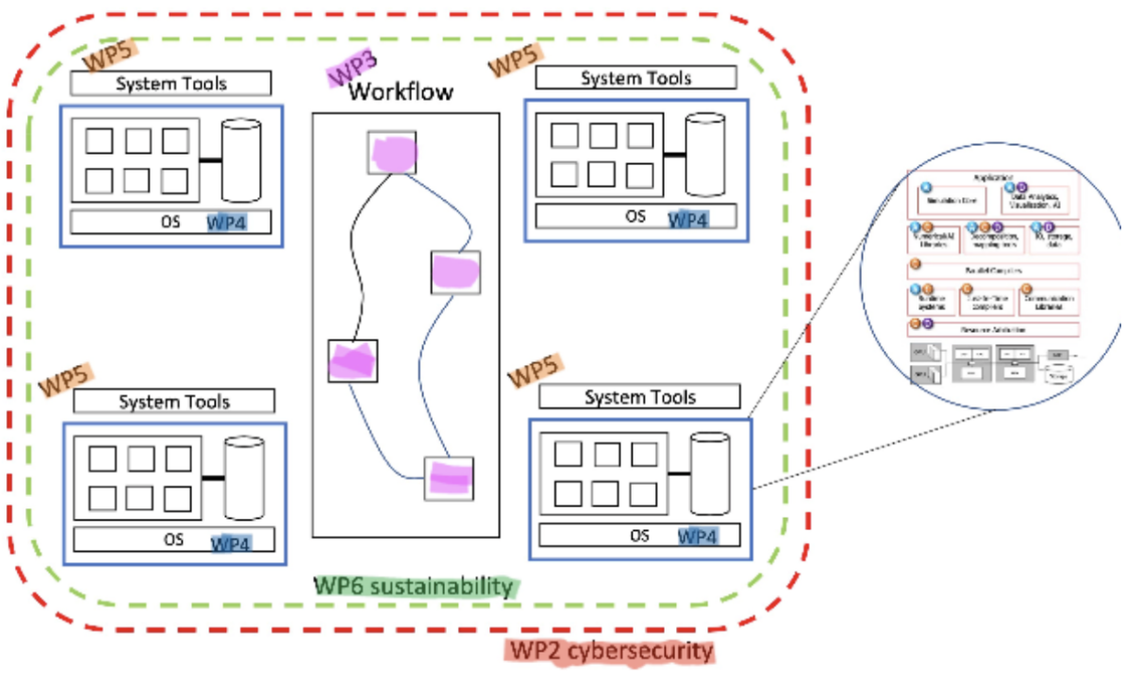
Architectures/tools for large-scale workflows

Machine Actionable Data/Project Plan

Data Logistic

Application & Workflow Support

Federation Governance



NumPEx ExaDIP

Application-driven co-design software development, integration and productivity

Co-design management

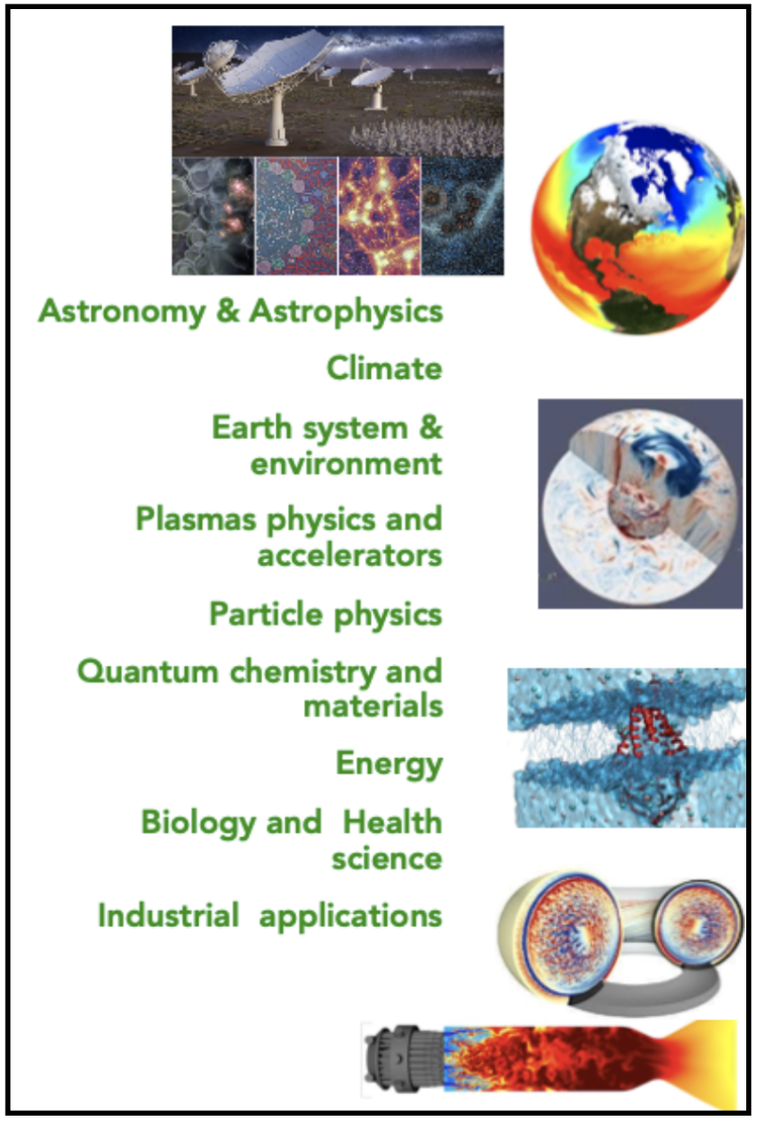
Co-design

PC5-ExaDIP

Application-driven co-design

Integration and productivity

Training

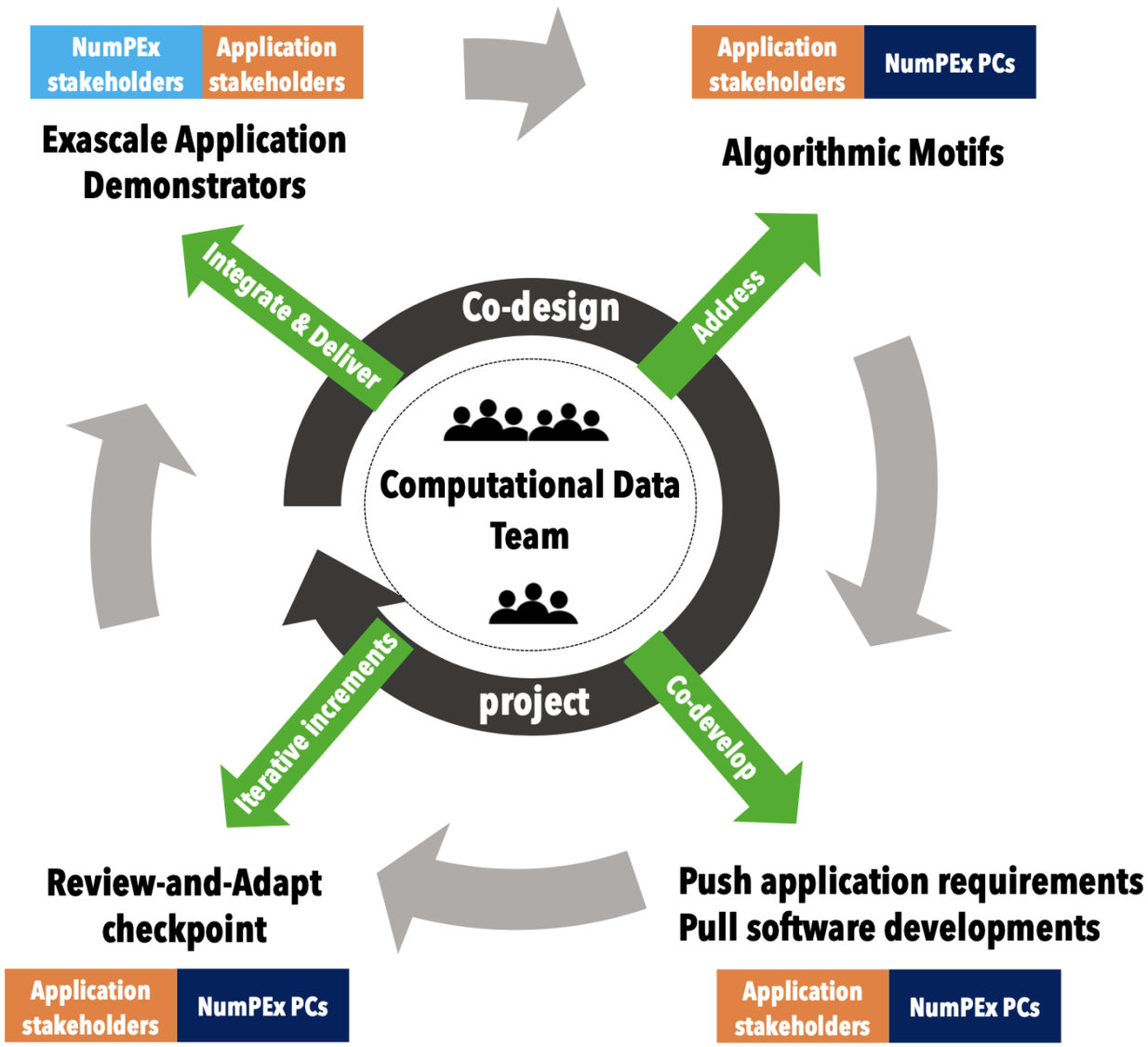


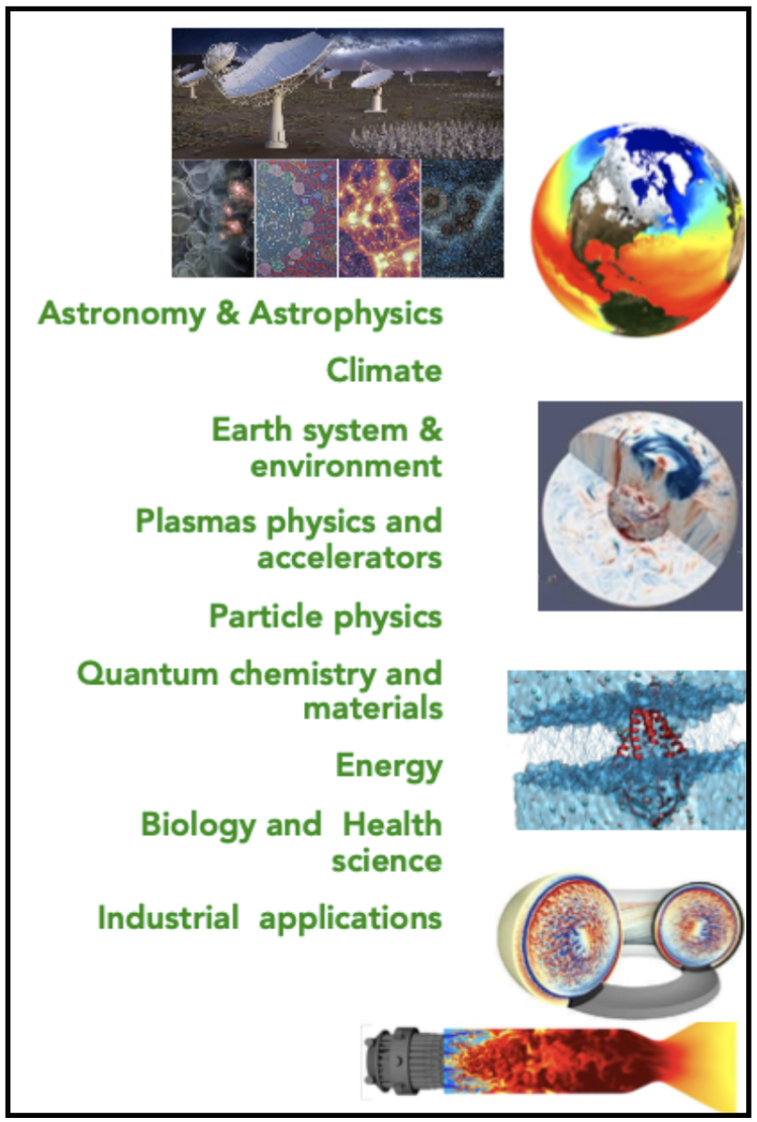
Applications

NumPEx, co-design

Application-driven co-design software development, integration and productivity

Identify/develop common/transverse algorithmic/library motifs





Applications

NumPEx, co-design demonstrators

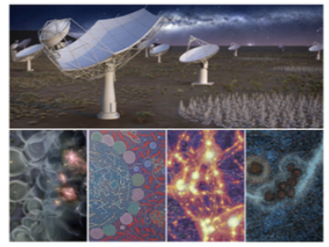
Application Demonstrator

What is an Application Demonstrator

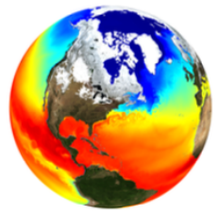
Objective:

Accelerate the development and enhance the capability and the performance of strategic CSE applications

- High-impact science and engineering exascale *challenge problem*
- Detailed criteria for assessing successful completion of challenge problem
- A *figure of merit* (FOM) formula quantifying performance or capability enhancement of challenge
- Demonstration and assessment of effective software integration with demonstrators



Astronomy & Astrophysics

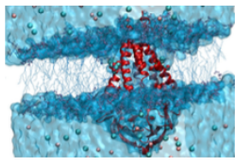


Climate

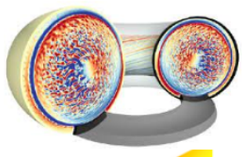
Earth system & environment

Plasmas physics and accelerators

Particle physics



Quantum chemistry and materials

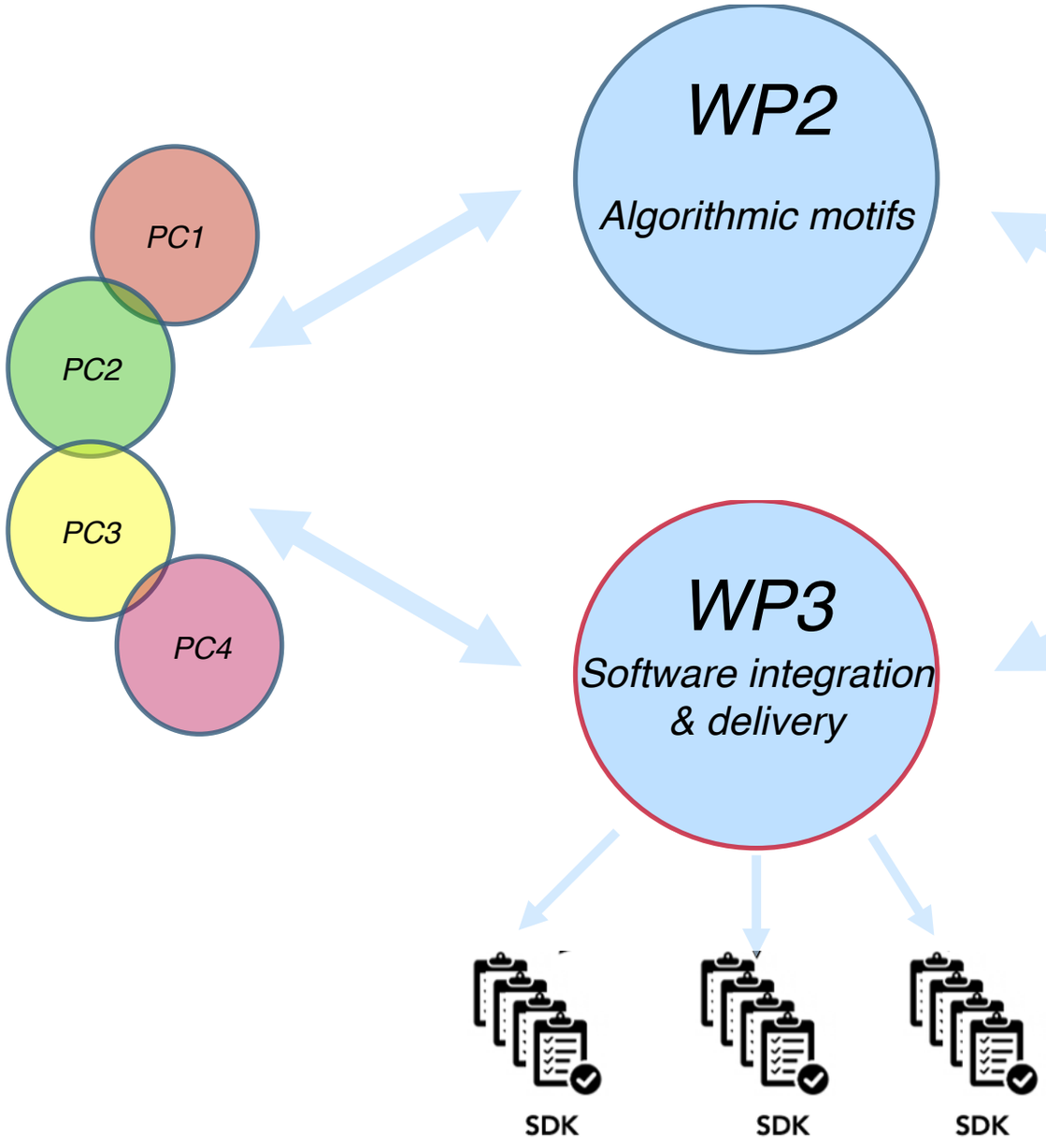


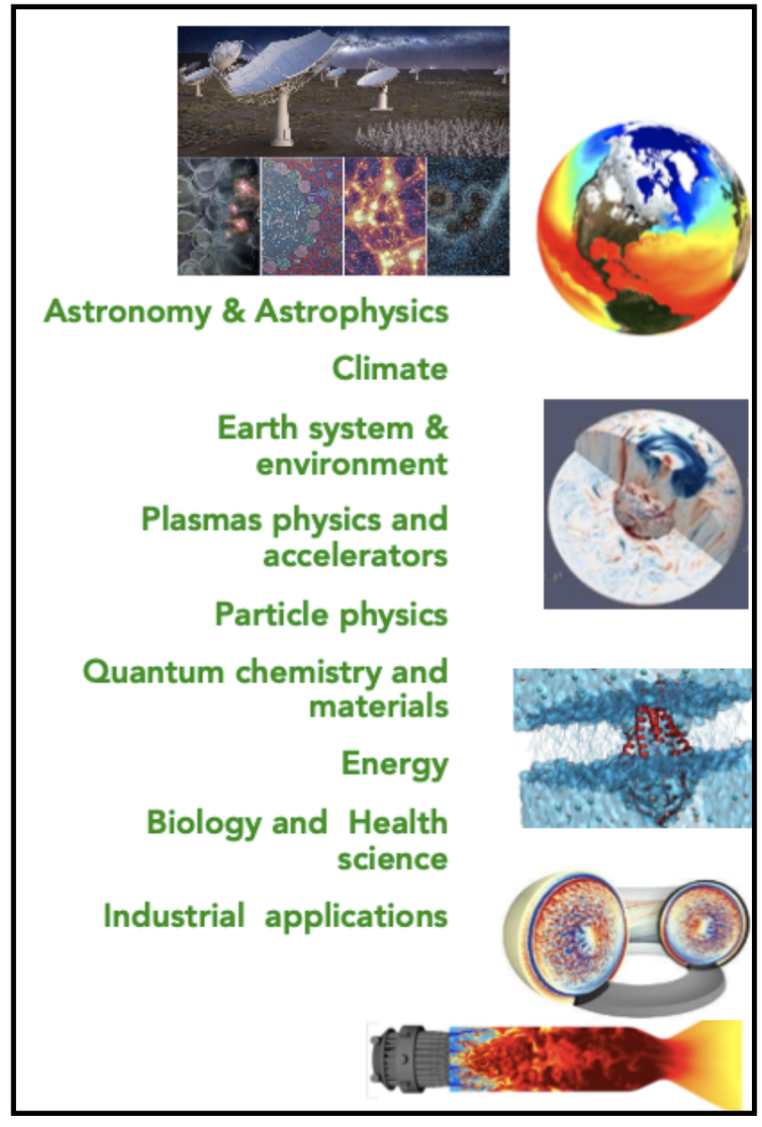
NumPeX Application Demonstrators

- Addressing on a science and engineering Exascale challenge problem
- Enabled by combined deployment and use of interoperable models, software components and technologies (*crossing* different NumPeX PCs
- Driven by community practices and CSE application development methodologies
- Assessed by measuring ***rate of science work*** enabled by successful and possibly inter-dependent developments.

NumPEx, co-design integration/productivity

Application-driven co-design software development, integration and productivity





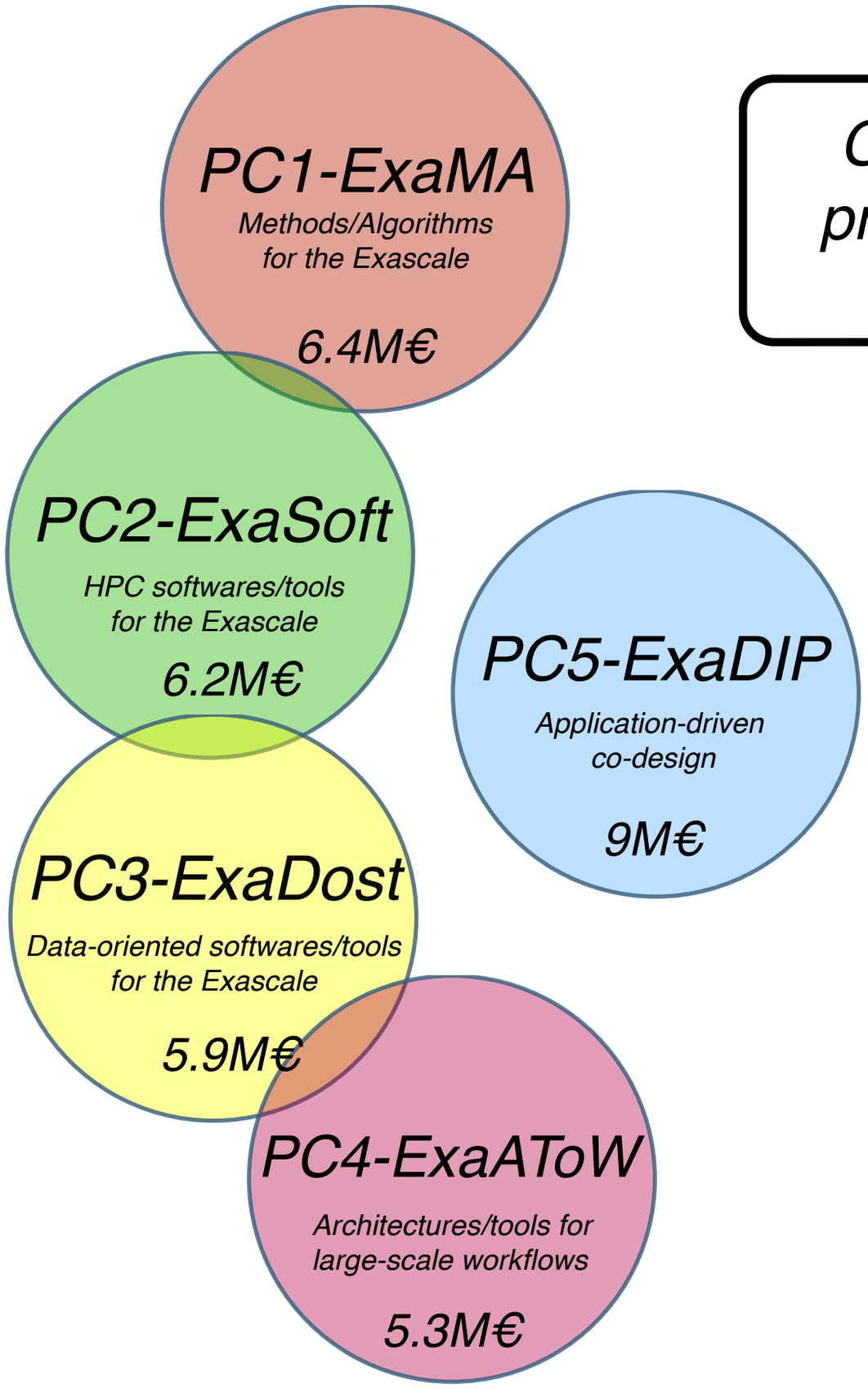
Applications

- **Logical application-driven collections of value-added interoperable software components**
- **Integrated and packaged using common meta-builder systems enabling combined deployment of software components as needed by CSE applications**

NumPEx, sum-up

NumPEx : organisation

NumPEx, sum-up



Call for proposal
4M€

PC0
Coordination/Governance
3.8M€

Board of directors

Steering committee

Project office

Industrial board

Programme management

Communication/dissemination

Training

NumPEx, take-away messages

NumPEx is an ambitious program to:

- prepare the scientific/engineering applications for the forthcoming HPC syst.

- contribute to the French/European software stack for future Exascale systems

- bridge the gap between the computer science/application communities

- help building a community for advanced scientific software development

Open to propositions of applicative demonstrators !
Many job openings too!

www.numpex.fr

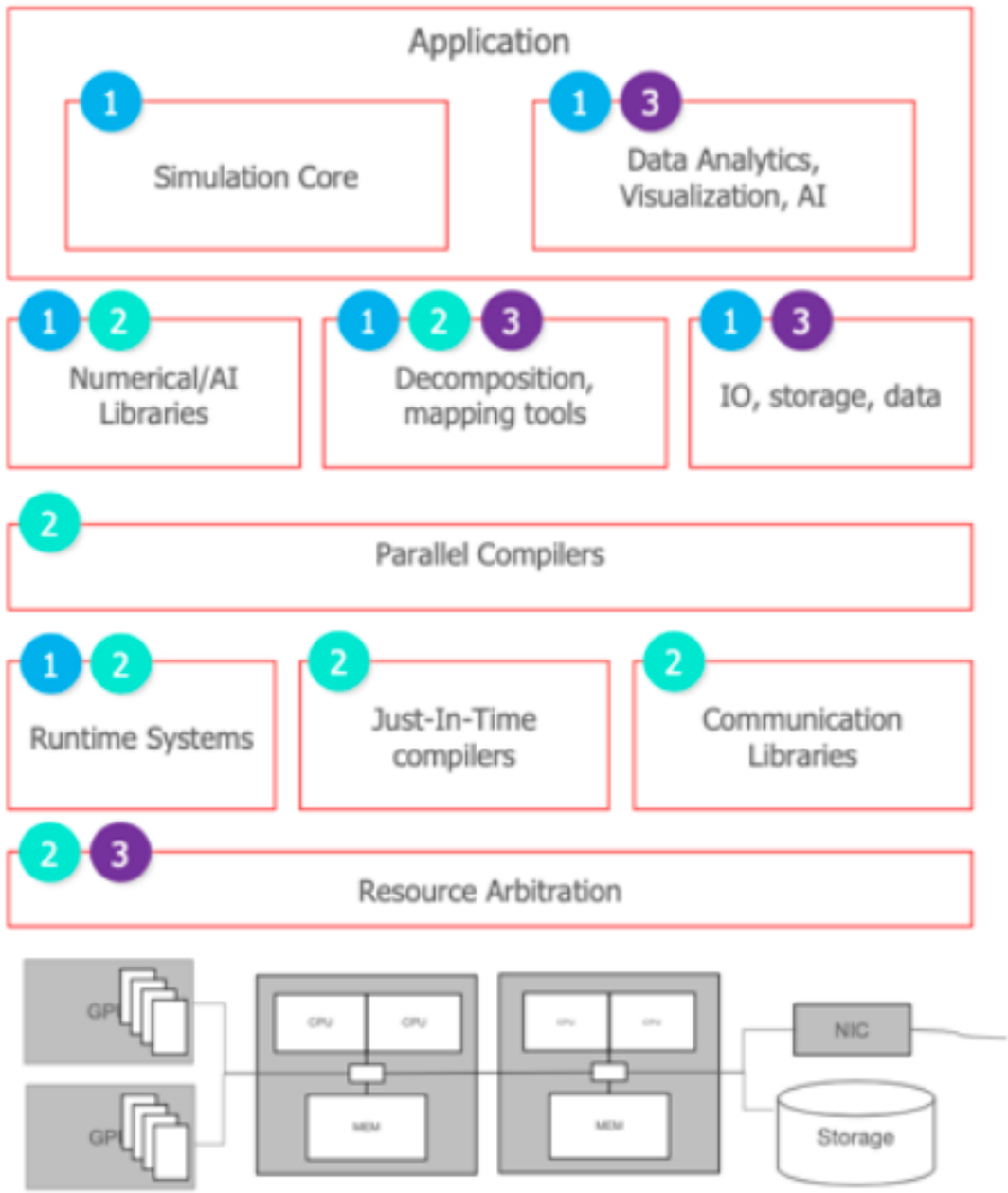
NumPEx: towards a consistent software stack

Integrated Projects (PC)

PC 1 : Methods and algorithms for Exascale 1

PC 2: HPC software and tools for the Exascale 2

PC 3: Data-oriented software and tools for the Exascale 3



PC1-ExaMA-Methods and algorithms

WP1-Discretization

WP2-Reduced order and AI-driven methods for multi-fidelity modelling

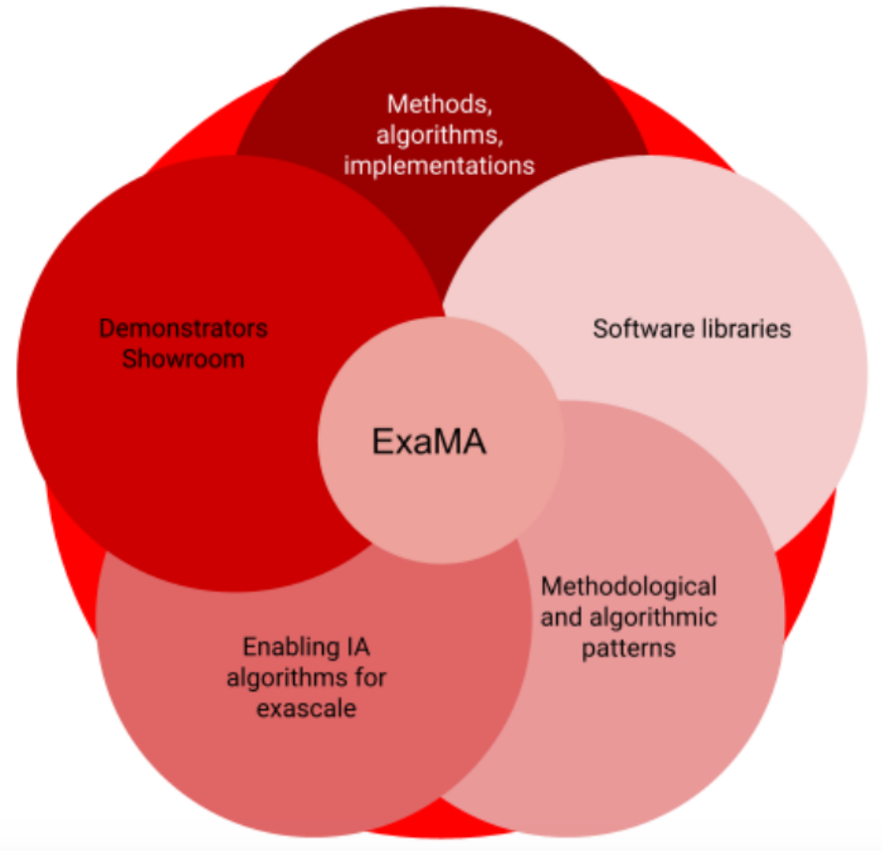
WP3-Linear, multi-linear and coupled solvers at Exascale

WP4-Combine data and models, inverse problems at Exascale

WP5-Optimize at Exascale

WP6-Quantify uncertainties

WP7-Demonstrators



PC2-ExaSOFT-HPC softwares and tools

WP1-High-level approaches for developing efficient and composable parallel software

WP2-Just-in-Time code optimization with continuous feedback loop

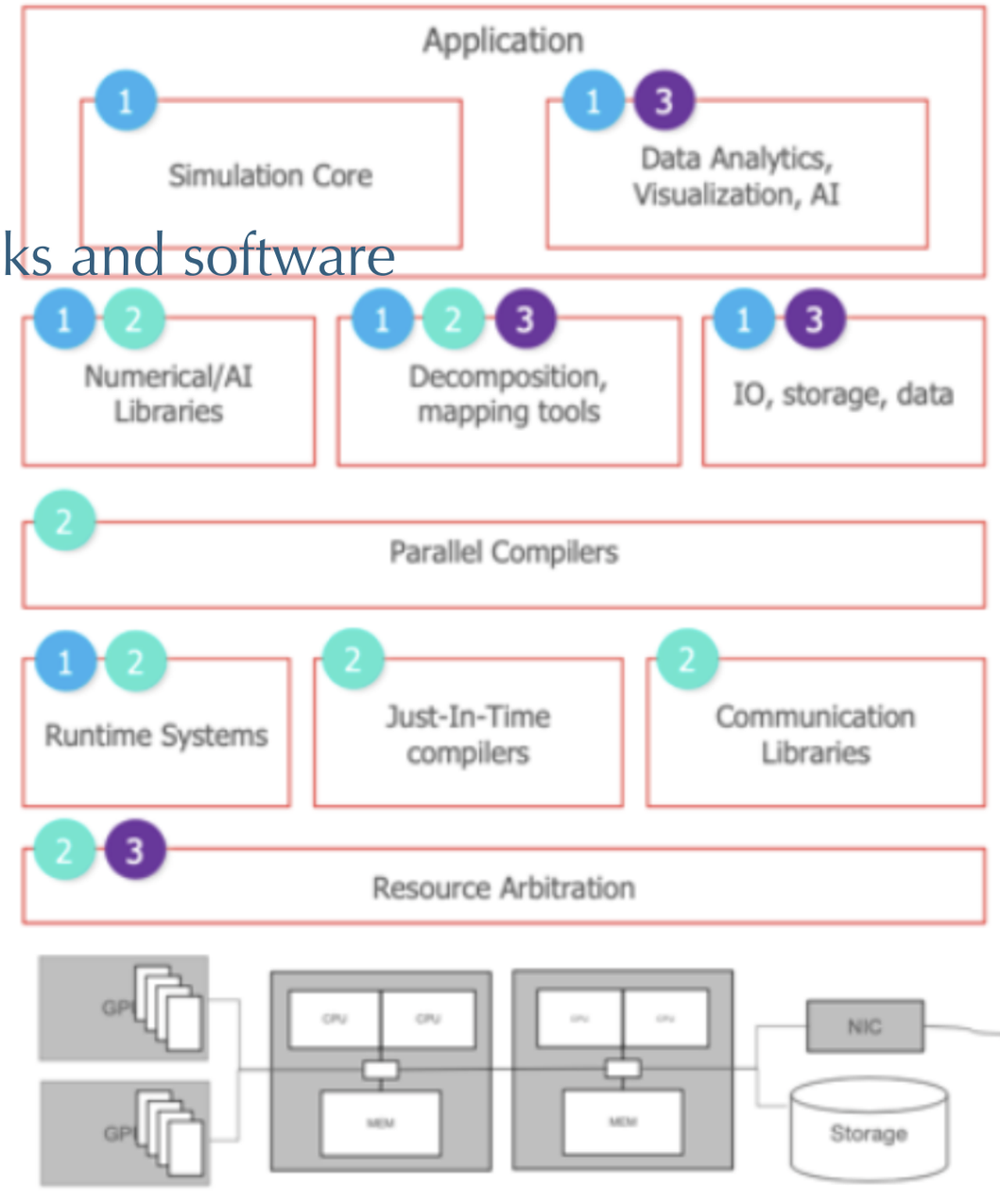
WP3-Runtime Systems at Exascale

WP4-Portable, scalable numerical building blocks and software

WP5-Performance analysis and prediction

WP6-Energy profiling and control

WP7-Demonstrators



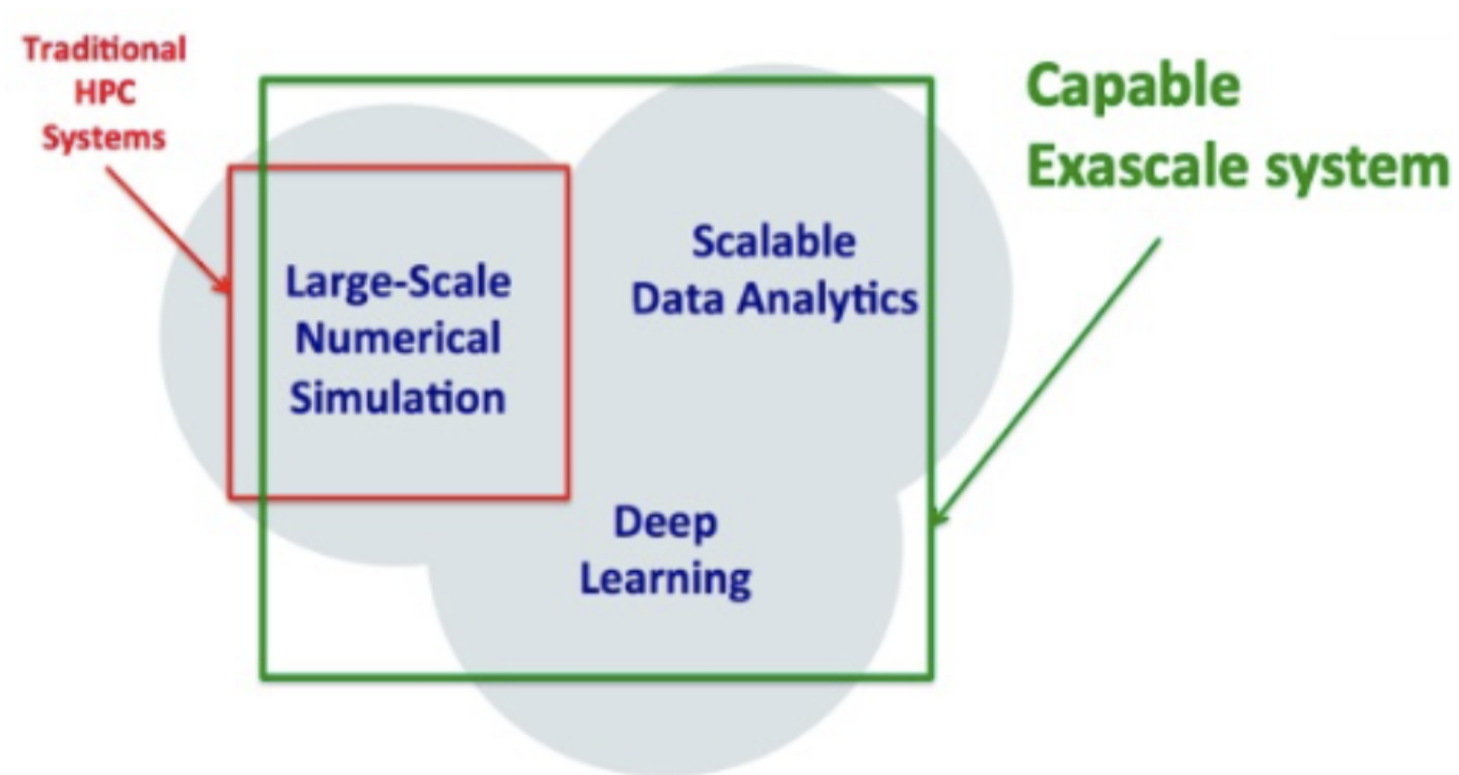
PC3-ExaDOST-Data-oriented softwares and tools

WP1-Exascale I/O and storage

WP2-Exascale in-situ data processing

WP3-Exascale ML-based data analytics

WP4-Demonstrators



NumPEx: Exascale in the data continuum

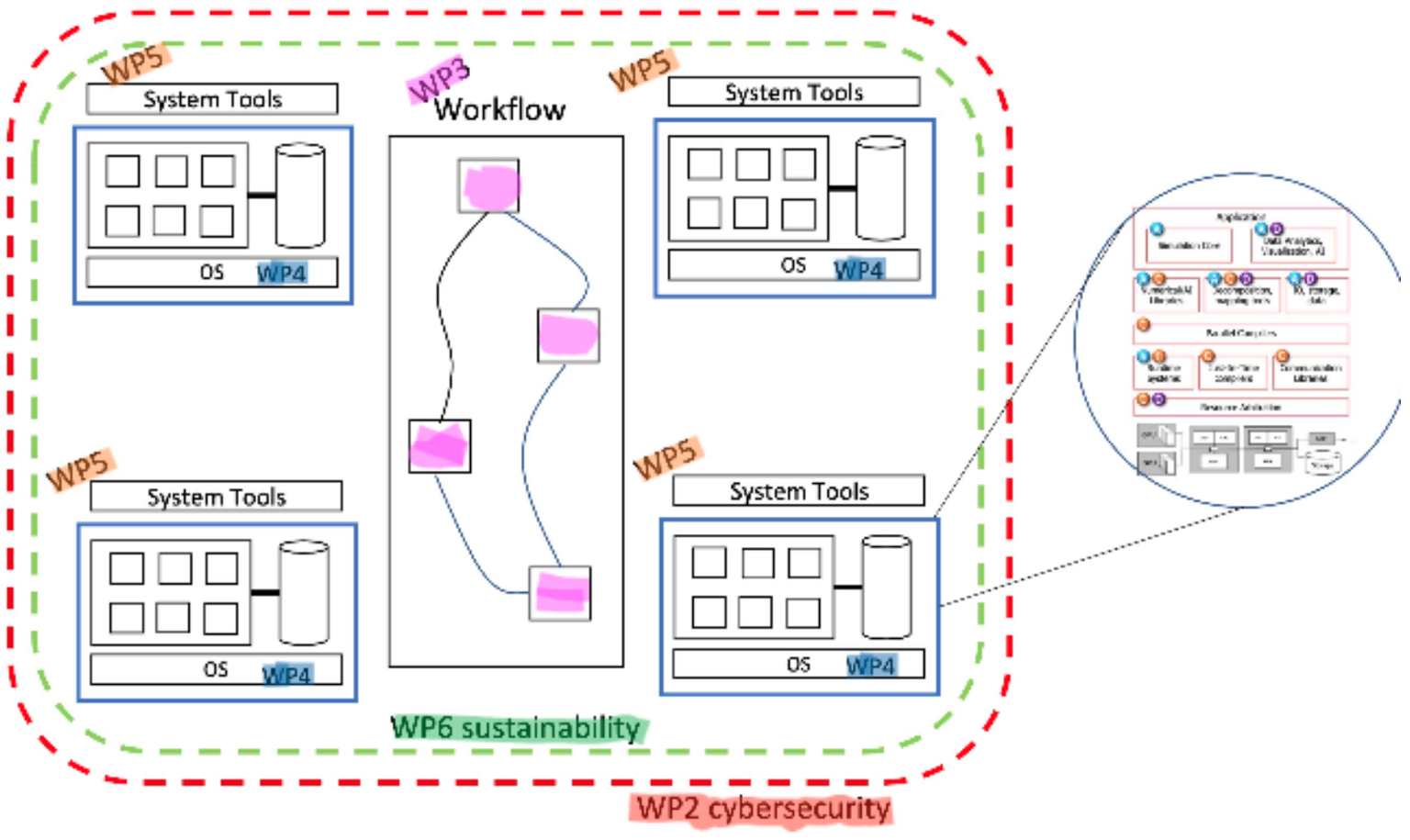
Integrated Projects (IP)

PC 4: Wide-area exascale workflows and architecture

- Data logistic between data sources (e.g. large scientific instruments) and the Exascale system

- Cybersecurity and environmental sustainability focus

- Promoting EU technology (e.g. Atos data node and edge servers)



PC4-ExaATOW-Architectures and tools for large-scale workflows

WP1-Federation of network, data, and compute resources

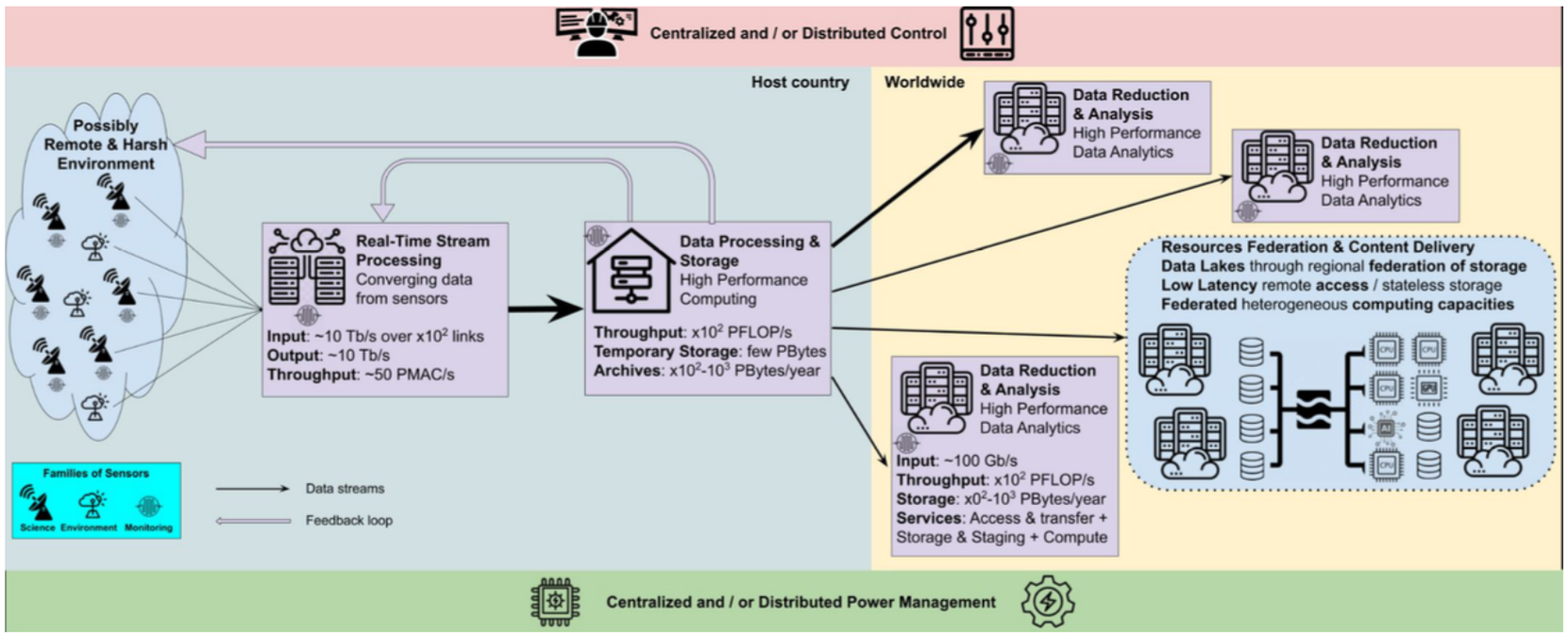
WP2-Metadata Centric Approach

WP3-Machine Actionable Data/Project Plan

WP4-Data Logistic

WP5-Application & Workflow Support

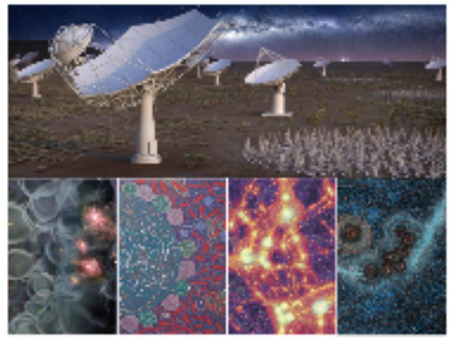
WP6-Federation Governance

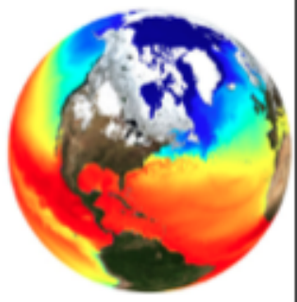


NumPEx: co-design

PC 5: Co-design development, motifs and demonstrators, software productivity

Motifs and demonstrators
Identify and define co-design motifs across domain demonstrators and NumPeX PC 1-4
Push R&D demonstrators requirements into software R&D (PC 1-4)
Push integrated software developments into demonstrators





Astronomy & Astrophysics

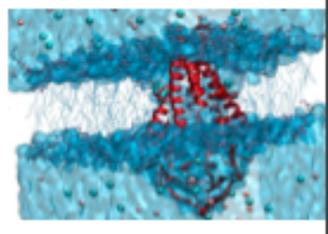
Climate

Earth system & environment

Plasmas physics and accelerators

Particle physics

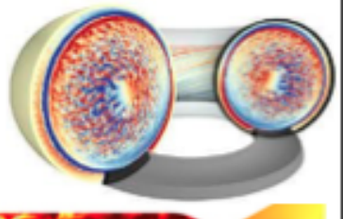
Quantum chemistry and materials

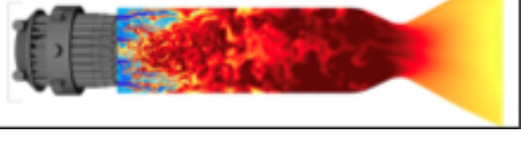


Energy

Biology and Health science

Industrial applications

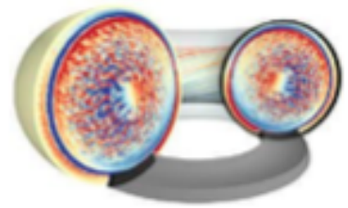


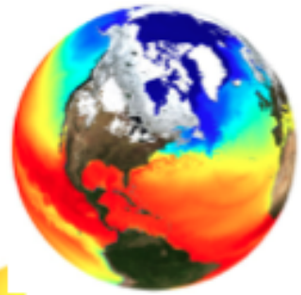


NumPEx: co-design

PC 5: Co-design development, software productivity, and demonstrators

Motifs and demonstrators





NumPEx Exascale Scientific Software Stack (NE3S)

Robust (tested, CI)

Packaged and deployable

Interoperable

Documented, open source, bug tracking, user forums

Hardware portable (processors, accelerators)

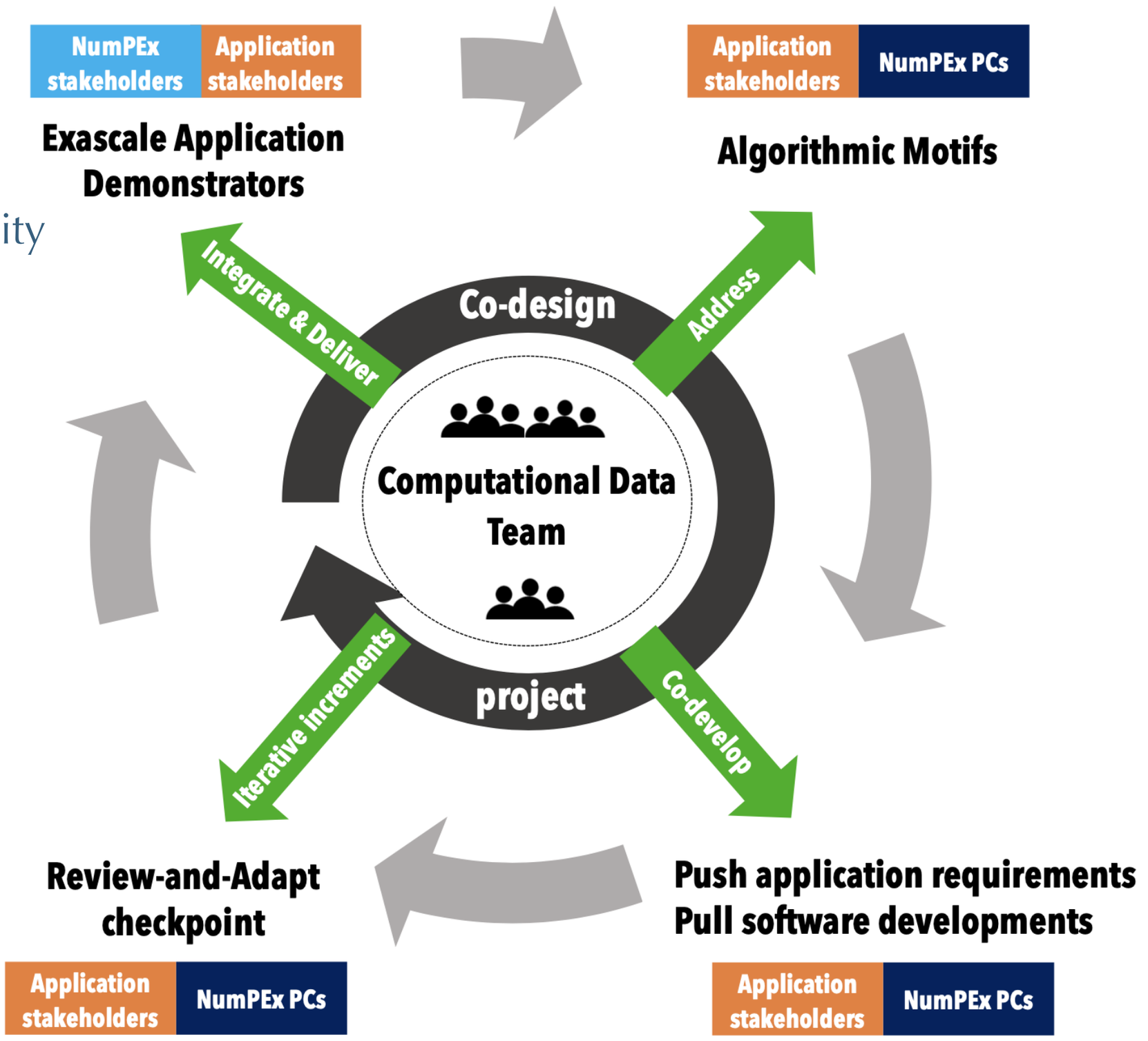
PC5-ExaDIP-Application-driven co-design software development, integration and productivity

WP1-Co-design management

WP2-Co-design

WP3-Integration and productivity

WP4-Training



Application demonstrator

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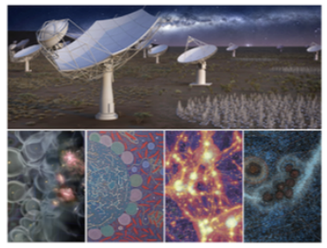

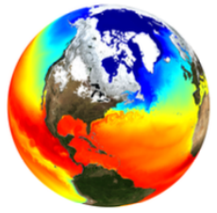

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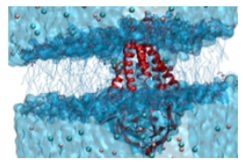
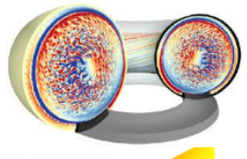


Particle physics

Quantum chemistry and materials



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- Driven by community practices and CSE application development methodologies
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Transversal issues/actions