NumPEx
High Performance Numerics for Exascale

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Towards the Exascale: challenges

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

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

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

Math/computing/data
Application/demonstrators
NumPEx contributors

5 Years
40,8 M€
A five-year effort

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

Prepare the applications for the Exascale era

Contribute/accelerate to the emergence of a European Software Stack and strategic applications Exascale capability

Aggregate the French HPC/HPDA/IA Community

Accelerate science/engineering-driven developers training and software productivity

Integrate/validate co-designed methods/libraires with demonstrators and strategic appli.
NumPEx Organisation

- **PC1-ExaMA**: Methods/Algorithms for the Exascale
- **PC2-ExaSoft**: HPC softwares/tools for the Exascale
- **PC3-ExaDost**: Data-oriented softwares/tools for the Exascale
- **PC4-ExaAToW**: Architectures/tools for large-scale workflows
- **PC5-ExaDIP**: Application-driven co-design

Applications:
- Astronomy & Astrophysics
- Climate
- Earth system & environment
- Plasmas physics and accelerators
- Particle physics
- Quantum chemistry and materials
- Energy
- Biology and Health science
- Industrial applications
NumPEx software stack

**PC1-ExaMA**
Methods/Algorithms for the Exascale

**PC2-ExaSoft**
HPC softwares/tools for the Exascale

**PC3-ExaDost**
Data-oriented softwares/tools for the Exascale
NumPEx, ExaMA

Methods/Algorithms for the Exascale

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

Runtime Systems at Exascale

Portable, scalable numerical building blocks and software

Performance analysis and prediction

Energy profiling and control
NumPEx, ExaDost

Data-oriented softwares/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

Large-scale numerical simulations

Scalable Data analytics

IA

Exascale capacity
NumPEx, Exa-AToW
Architectures and tools for large-scale workflows

- Federation of network, data, and compute resources
- Metadata Centric Approach
- 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
Integration and productivity
Training

PC5-ExaDIP
Application-driven co-design

Applications
- Astronomy & Astrophysics
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NumPEx, co-design

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

Identify/develop common/transverse algorithmic/library motifs

Exascale Application Demonstrators

Co-design

Computational Data Team

Integrate & Deliver

Address

Co-develop

Iterative increments

Review-and-Adapt checkpoint

Push application requirements

Pull software developments

Applications

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 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

**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

WP2
Algorithmic motifs

WP3
Software integration & delivery

- 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

Scientific advisory board

Advise

Board of Directors

Steering committee

Management Project office

CDT committee

Targeted Projects (PC)

**PC 1-3:** Exascale software components
18.6 M€

**PC 4:** Exascale workflows
5.3 M€

**PC 5:** Software productivity and demonstrators
9 M€

NumPEx Management Project PCO

**T1:** Structuring, animation and training

**T2:** Dissemination and communication

**T3:** Management

4 M€

3.8 M€

Call for proposal

Participate
NumPEx, sum-up

**PC1-ExaMA**
Methods/Algorithms for the Exascale
6.4M€

**PC2-ExaSoft**
HPC softwares/tools for the Exascale
6.2M€

**PC3-ExaDost**
Data-oriented softwares/tools for the Exascale
5.9M€

**PC4-ExaAToW**
Architectures/tools for large-scale workflows
5.3M€

**PC5-ExaDIP**
Application-driven co-design
9M€

**PC0**
Coordination/Governance
3.8M€

**Call for proposal**
4M€

**Board of directors**
**Steering committee**
**Project office**
**Industrial board**

**Programme management**
**Communication/dissemination**
**Training**

3.8M€
6.4M€
6.2M€
5.9M€
5.3M€
9M€
4M€
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

PC 2: HPC software and tools for the Exascale

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

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**

**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.
Transversal issues/actions

Targeted projects (PC)

PC 1: Methods and algorithms for Exascale

PC 2: HPC software and tools for the Exascale

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

PC 4: Wide-area exascale workflows and architecture

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