NumPEx
*Exascale computing*

# Exa-MA

*Methods and Algorithms for Exascale*

**Directeurs:** Hélène Barucq (Inria), Christophe Prud'homme (UNISTRA)

# Programme

- Présentation de NumPEx (30min)
- Questions (20min)
- Pause (5min)
- Présentations d'Exa-MA (45min)
- Questions (40min max)

# Exa-MA / Methods and Algorithms for Exascale

## Project : Exa-MA

### Challenges:

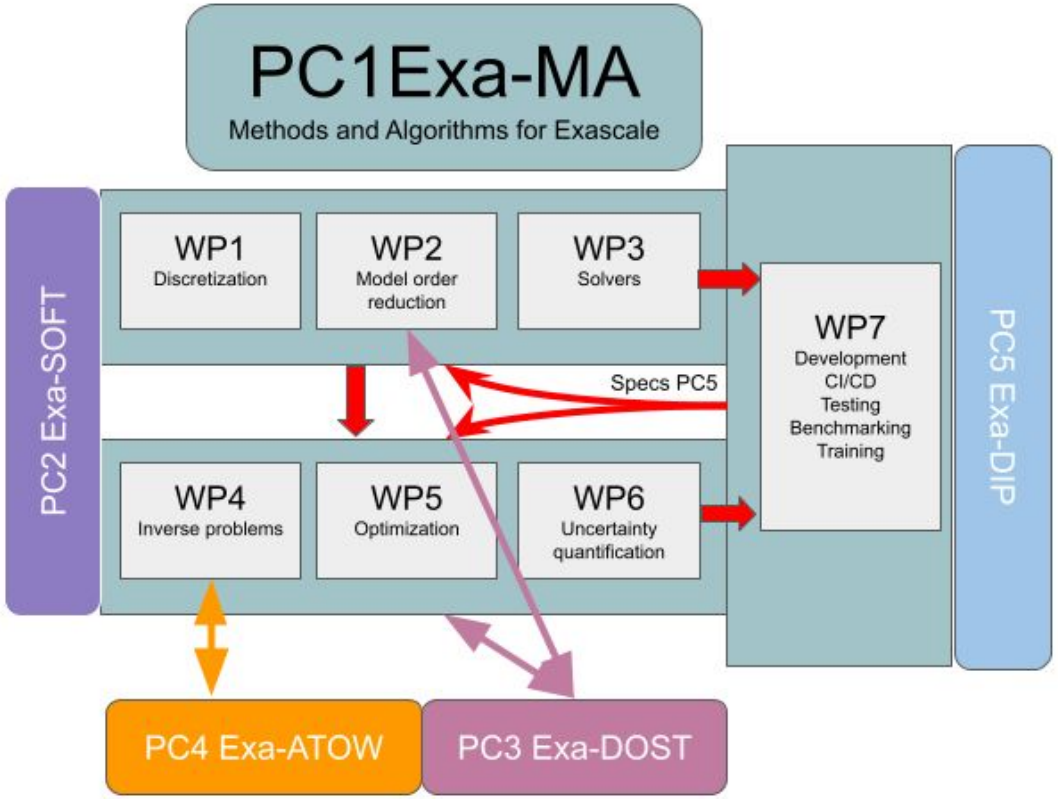
- Enable extreme scale computing for vastly more accurate predictive models
- Create digital copies of physical assets
- Apply to environmental, health, energy, industrial and fundamental knowledge challenges

### Objectives:

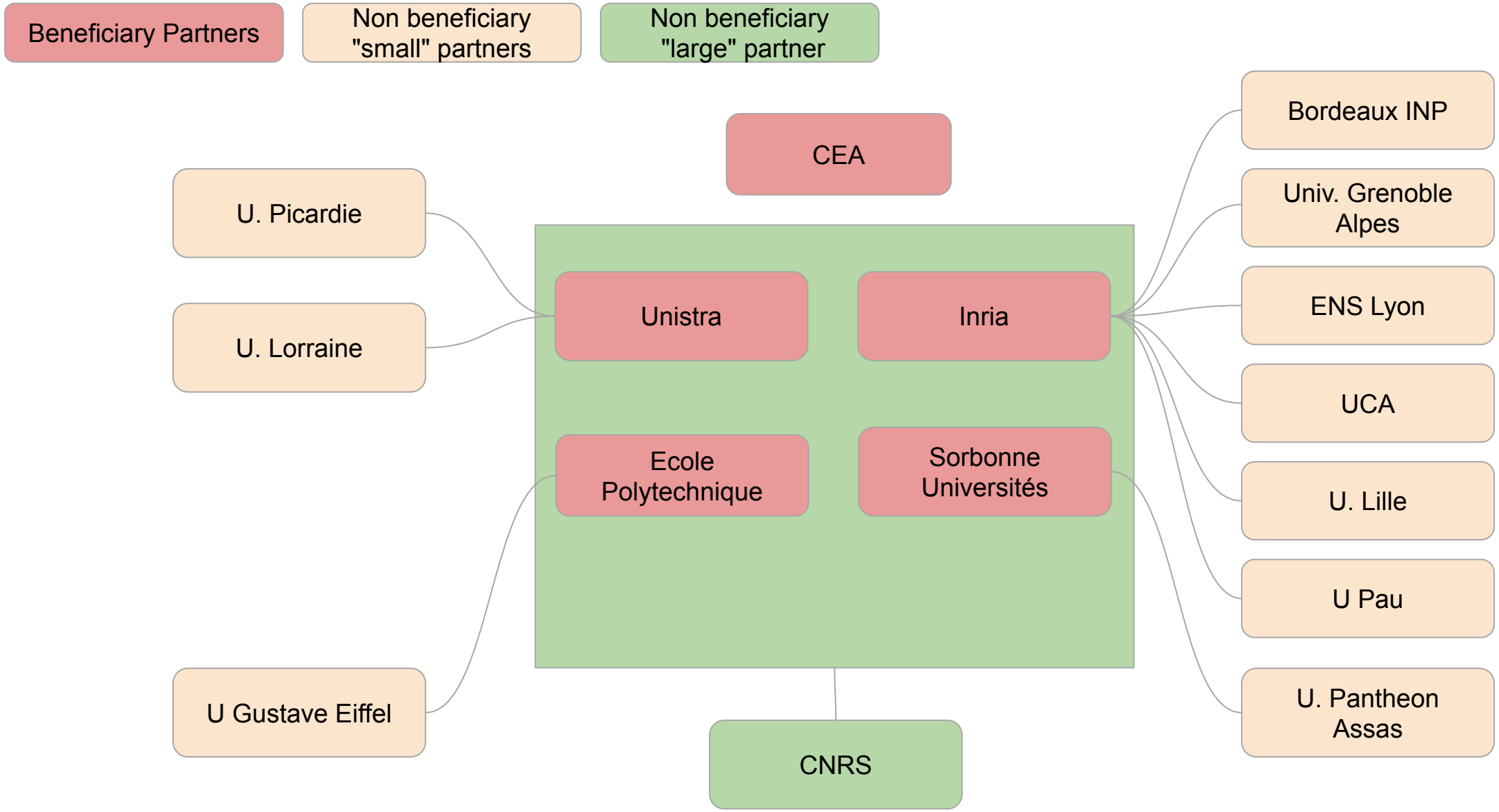
- ***to develop methods, algorithms, and implementations*** *that, taking advantage of the exascale architectures empower modeling, solving, assimilating model and data, optimizing and quantifying uncertainty, at levels that are unreachable at present*
- ***to develop and contribute to software libraries*** *for the exascale software stack*
- ***to identify and co-design Methodological and Algorithmic Patterns*** *at exascale*
- ***to enable AI algorithms*** *to achieve performances at exascale*
- ***to provide demonstrators*** *: mini-apps and proxy-apps openly available*
- ***to create, animate and foster a community*** *around Exascale (and HPC) computing*

### Beneficiary Partners:

*CEA, École Polytechnique, Inria, Sorbonne Université, Université de Strasbourg*
***Requested Budget:*** *6,255 M€* ***Total Budget:*** *24,417 M€*



# Exa-MA Partners



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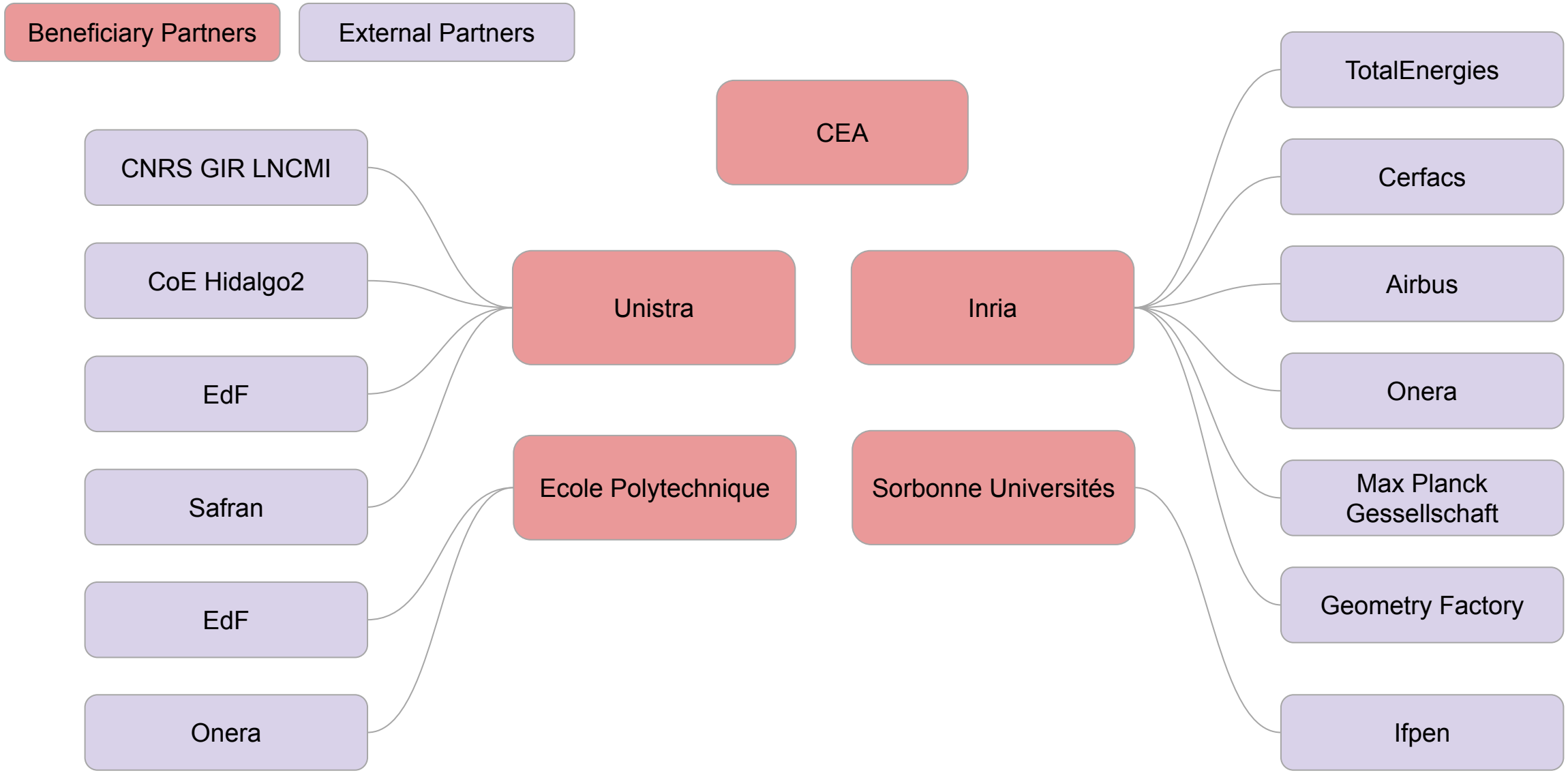

# Somes Numbers and some Dates

## Some Numbers

**Permanent (73)**

- 12 CR
- 12 DR
- 15 IC
- 5 IR
- 13 MDC
- 16 PR

**Non Permanent (22)**

- 2 PY Postdoc
- 10 PY PhD
- 1 PY IR

**Funded**

- 22 PhD
- 12 PY Postdoc
- 29 PY IR

## Some Dates

**PEPR NumPEx**

- Task force, submission
- NumPEx Selected end of August 2022
- 5 PC to create between 09/22 and 04/23

**2022**

**2023**

**NumPEx**

- T0 : April 14
- Workgroups created
- 1st intl workshop on exascale
- Kickoff June 26-28

**Exa-MA**

- Grant Agreements signed by end of june
- Online Onboarding June 14

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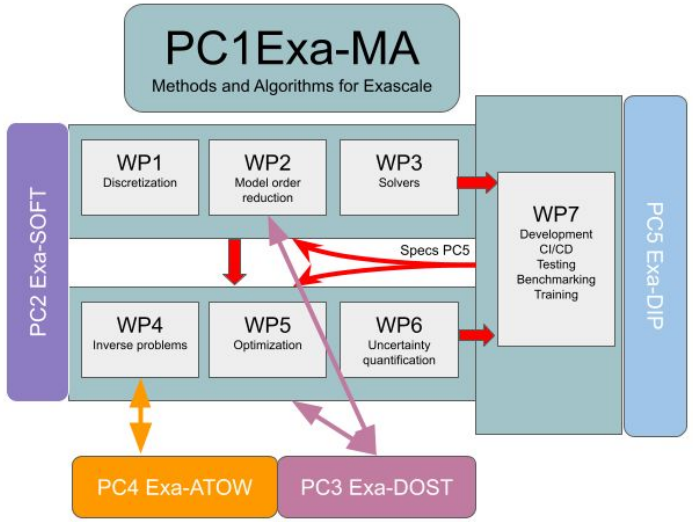



# WP1 - Discretization

Pierre Alliez (Inria), Hélène Barucq (Inria), Isabelle Ramière (CEA)

## WP1: Discretization

### Key Objectives

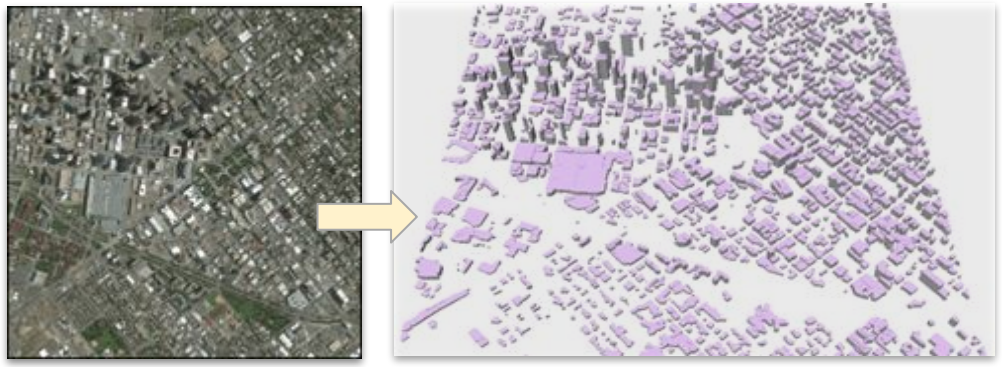
- Geometric and discrete domain representations
- Physics-based models

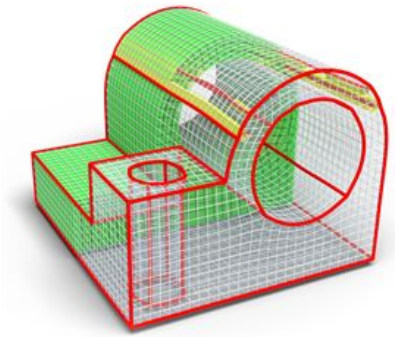
### Tasks

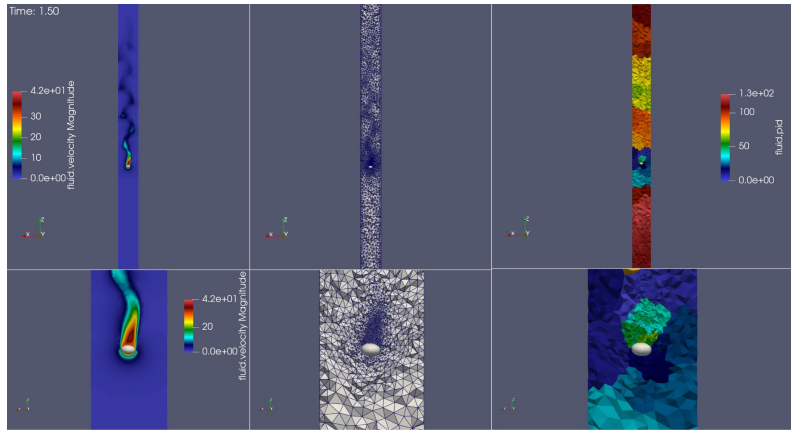
- Mesh generation
  - Large-scale, non-conforming
  - Unconditional robustness
  - Hexahedral block grids
- Adaptive Mesh Refinement
- Non-conforming finite elements
- Parallel and control in time
- Multiphysics partitioned discretization
- Multiscale coupling

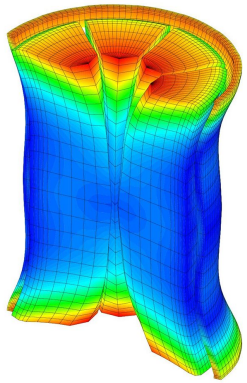
### Stakeholders

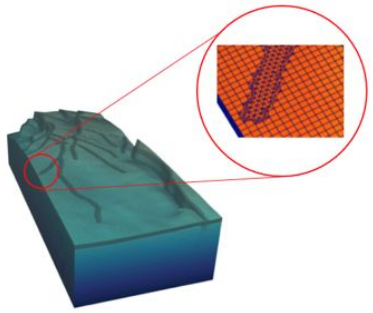
CEA
Inria (Makutu, Titane)
Ecole Polytechnique
Unistra









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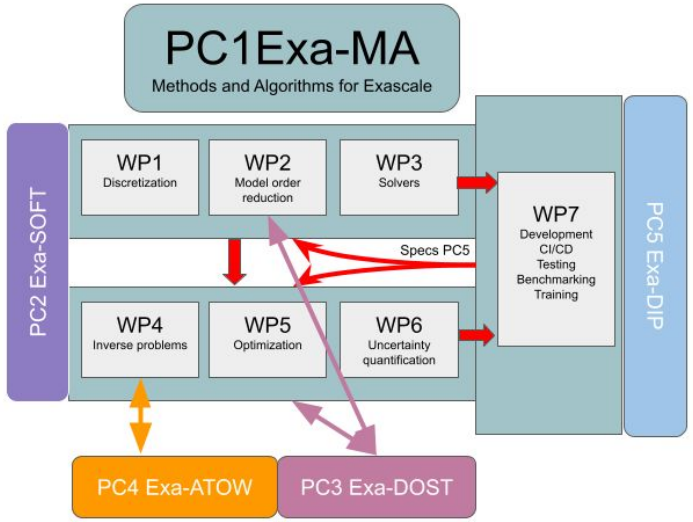



# WP2 - Order reduction and sciML

Emmanuel Franck (Inria, Unistra), Stéphane Lanteri (Inria)

# WP2: order reduction and SciML

## Key Objectives

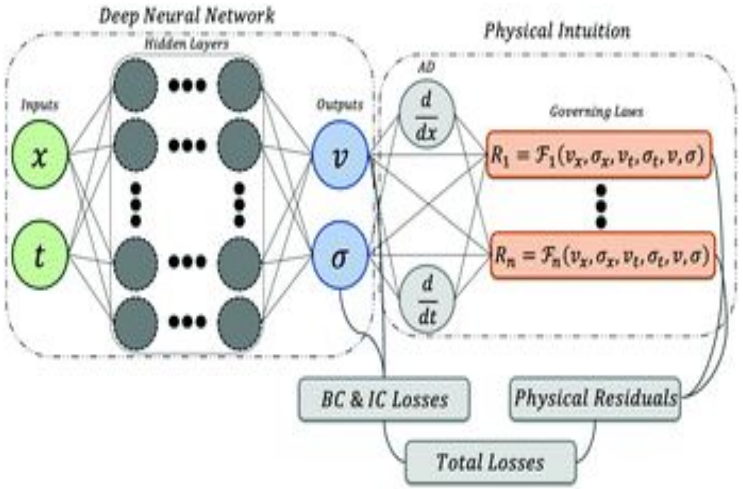
- PINNs for high dimensional parametric PDE
- Neural operator and fast prediction

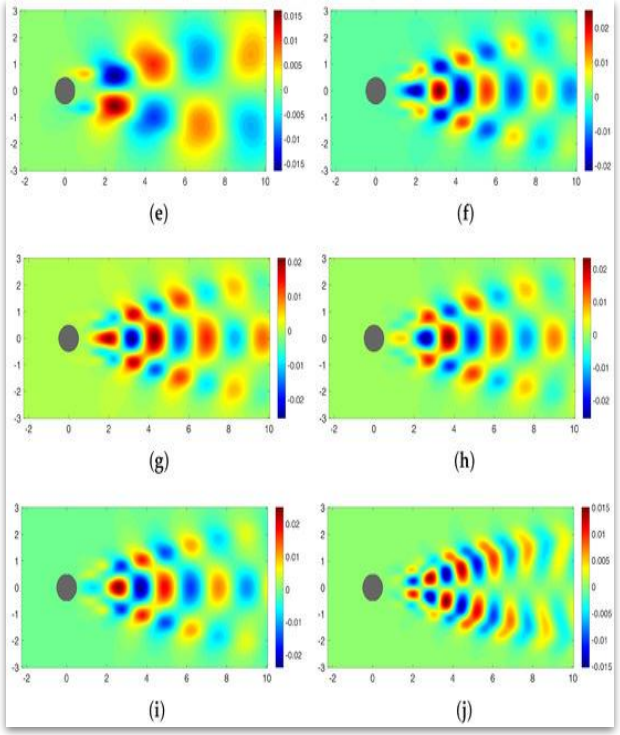
## Tasks

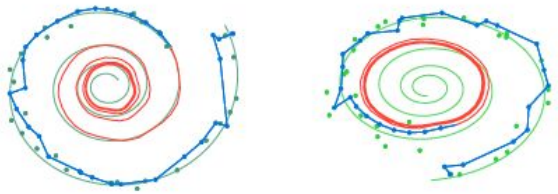
- Physic Informed Neural Networks
  - High dimensional parametric space and sampling
  - Domain decomposition
  - Training methods
- Neural operator
  - General and unstructured meshes
  - Complex and multiscale PDE
  - Coupling with forward and inverse solvers
- Reduce order modeling
  - Auto-encoder/POD + NN hyper-reduction
  - Explicability for learning methods
  - Closure for kinetic equations
- Low/high fidelity models
- Super-resolution

## Stakeholders

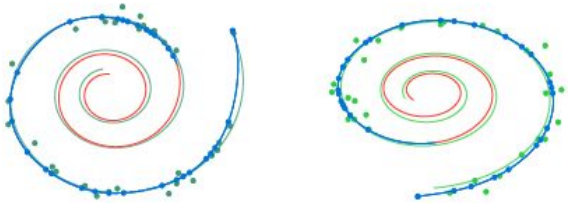
Unista
Inria (Atlantis,Makutu,Tonus)
Ecole Polytechnique



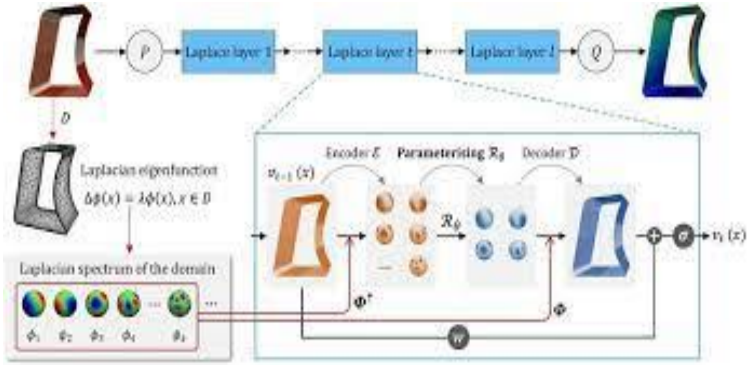



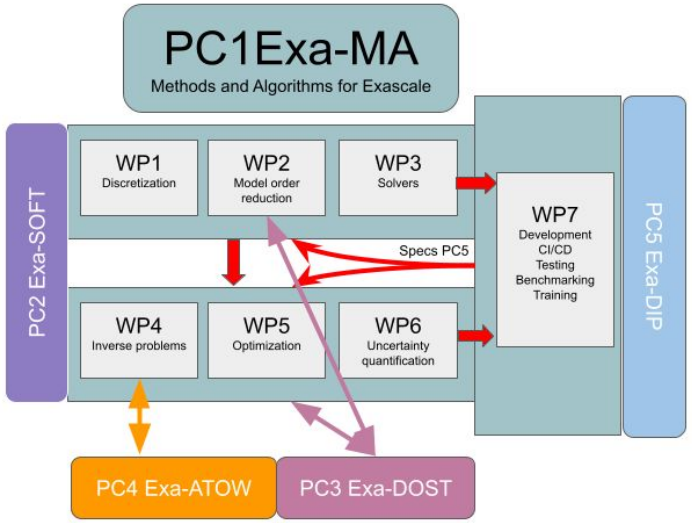



(a) Recurrent Neural Network



(b) Latent Neural Ordinary Differential Equation





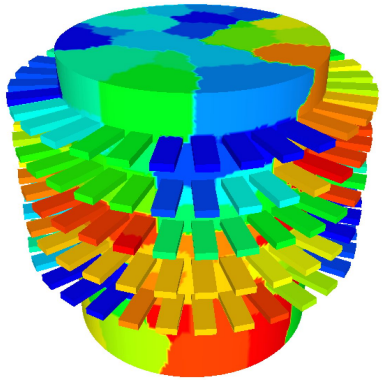

# WP3 - Solvers

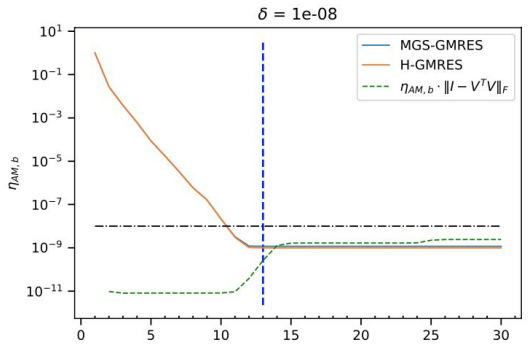
Vincent Faucher (CEA), Luc Giraud (Inria), Frédéric Nataf (CNRS, Inria)

# WP3 : Solvers

## Key Objectives

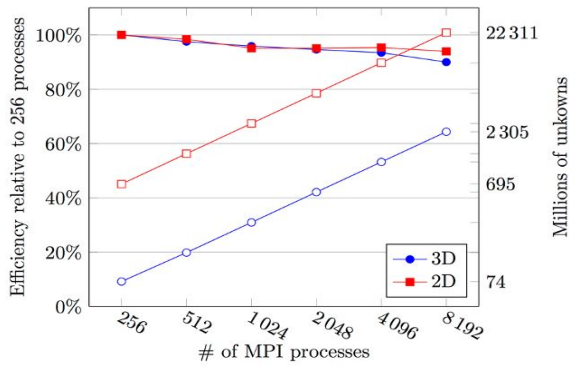
- Design novel generic scalable numerical algorithms
- Enable multi-precision for prescribed accuracy
- Leveraging communication avoiding/hiding, mixed arithmetic and data compression



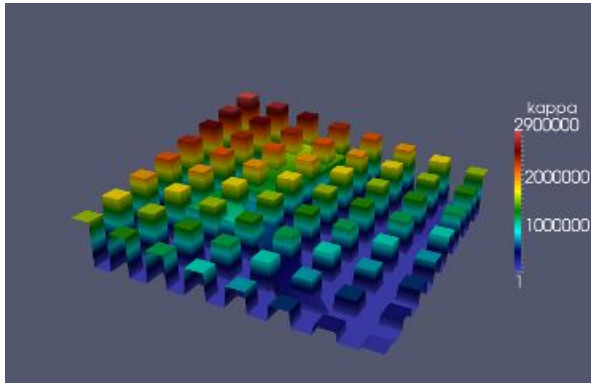



## Tasks

- Robust and scalable solvers
  - Adaptive precision (link with PC2), auto tuning tools
  - Multi level Domain decomposition with provable efficiency
  - Resiliency
- Scalable coupled physics solvers
- Open source libraries: HPDDM, Maphys++, MEDCoupling, PROMISE, use cases via WP7 and interactions with PC2 Exa-Soft




CURIE@TGCC, 92k cores, 1.6 Pflops/s,
8-cores Intel Nehalem-EX




## Stakeholders

CEA
Inria (Alpines, Concace, Roma)
Sorbonne University
Unistra

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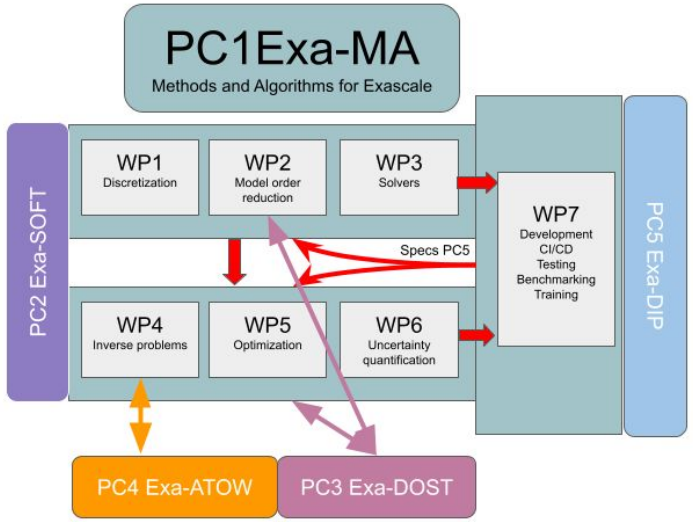



# WP4 - Inverse Problems and Data Assimilation

Mark Asch (U. Amiens, Unistra), Hélène Barucq (Inria), Arthur Vidard (Inria)

# WP4: Inverse Problems and Data Assimilation

## Key Objectives

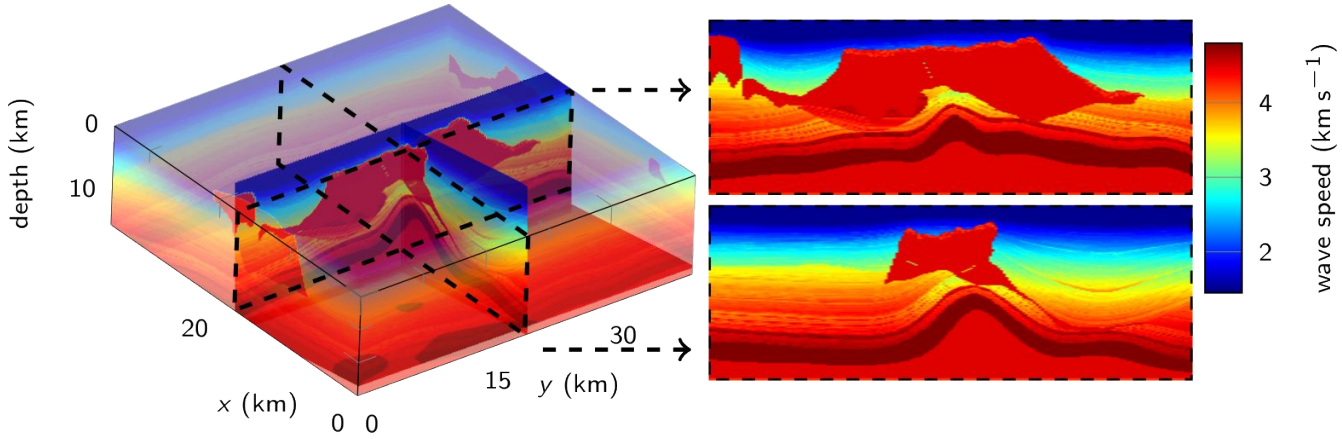
- Improve deterministic inversion methods
- Design new stochastic methods for inverse problems
- Improve observation strategies
- Implement multi-fidelity schedules at exascale

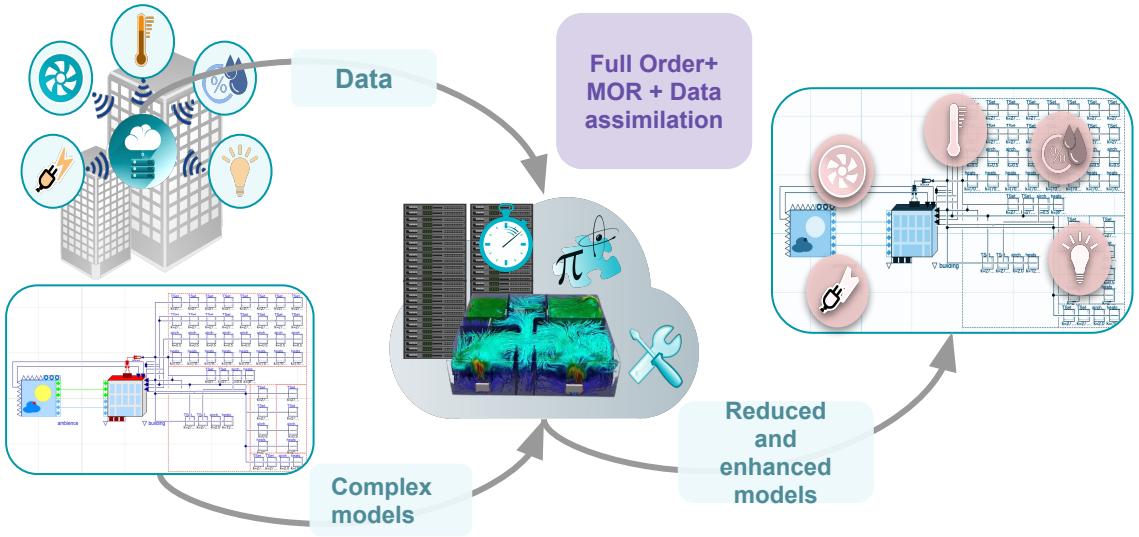
## Tasks

- Deterministic methods
- Stochastic methods
- Observations
- Multifidelity: modelling and inverse problems

## Stakeholders

Ecole Polytechnique
Inria (Airsea, Makutu)
Unistra



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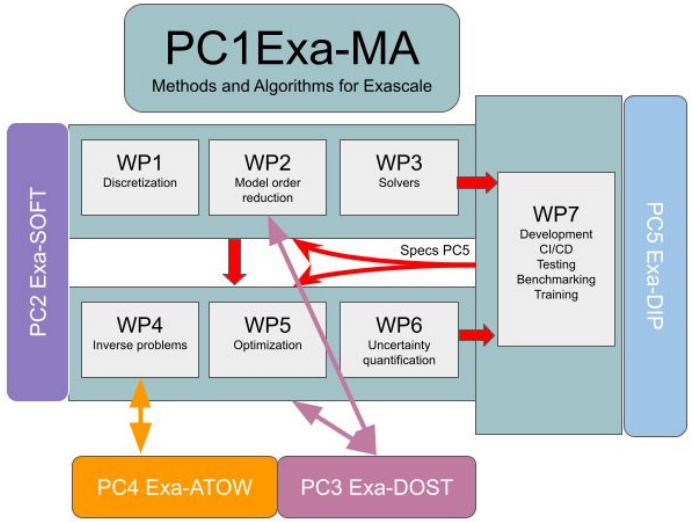


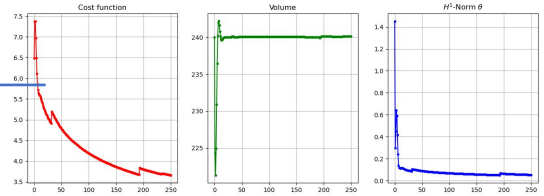

# WP5 - Optimization

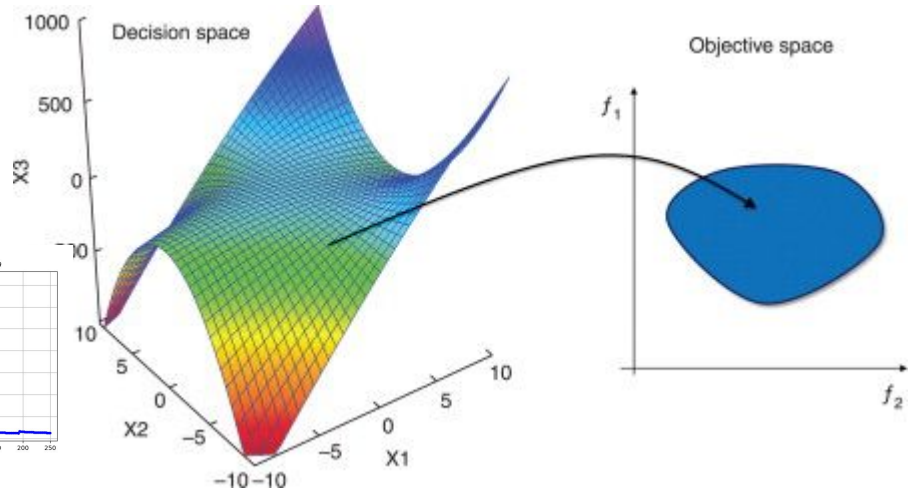
Yannick Privat (Unistra), El-Ghazali Talbi (U. Lille, Inria)

# WP5: Optimization

## Key Objectives

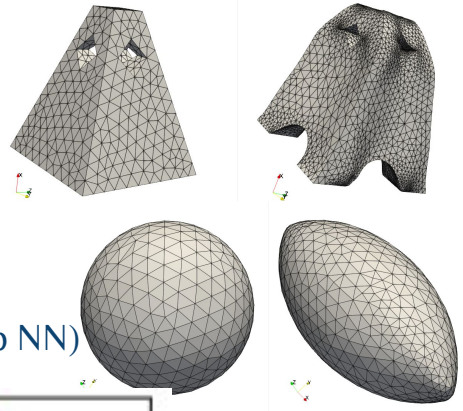
- Solving big optimization problems (decision variables, many-objectives, expensive objectives, big data) using exascale decomposition
- Inverse, continuous, discrete and mixed optimization problems
- Exact, heuristic and data driven optimization algorithms

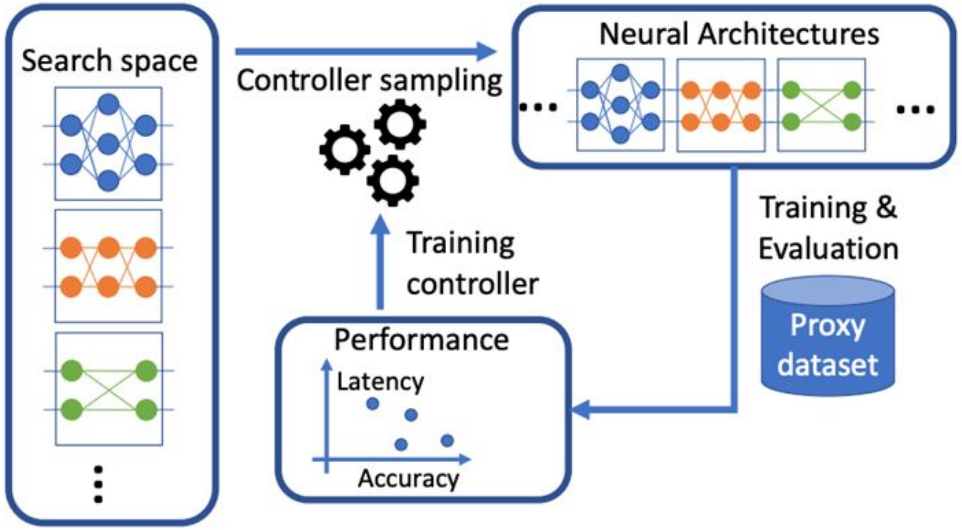



## Tasks

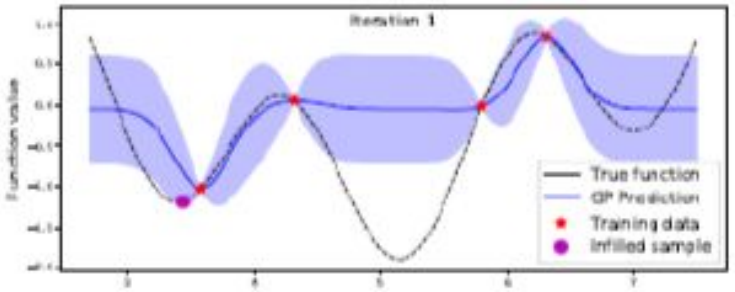
- Exascale combinatorial and continuous optimization
  - Exact optimization (Branch and bound, tree search)
  - Heuristic optimization (Computational intelligence)
- Exascale surrogate-based optimization
  - Multi-fidelity models
  - Coupling of surrogates, optimization and sampling
- Exascale shape optimization
  - Involving multiphysics models
- Exascale optimization for AutoML (Automated design of deep NN)






## Stakeholders

CEA
Ecole Polytechnique
Inria (Bonus)
Sorbonne Université
Unistra



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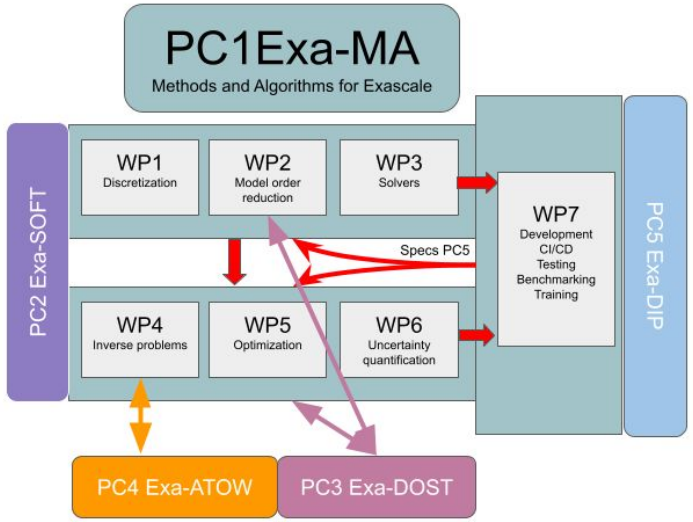



# WP6
# Uncertainty Quantification

Josselin Garnier (Ecole Polytechnique), Amandine Marrel (CEA)

# WP6: Uncertainty Quantification

## Key Objectives

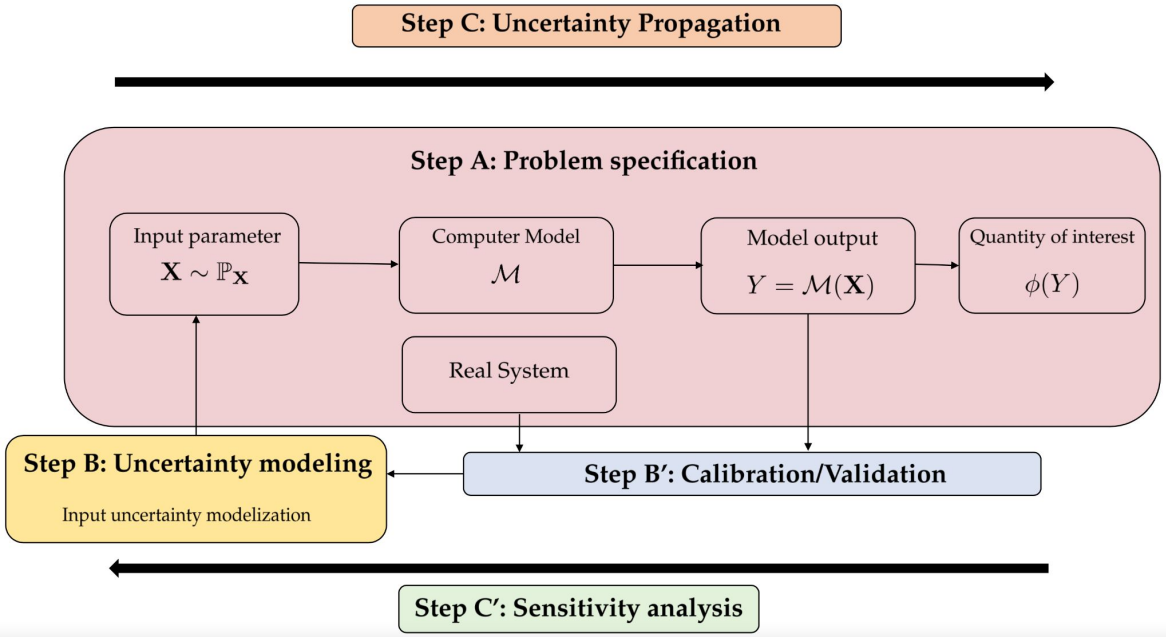
- Uncertainty Quantification for multi-physics and/or multi-scale problems
- Uncertainty propagation, sensitivity analysis, robust inversion

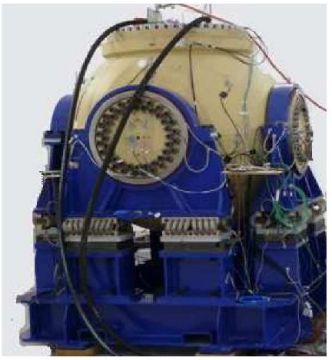
## Tasks

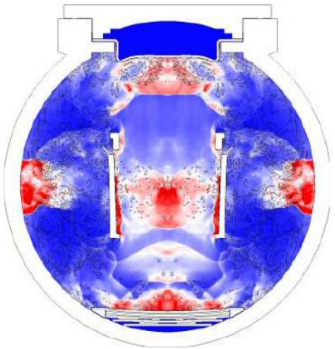
- Kernel-based sensitivity analysis for high-dimensional data
- UQ in a PDE solving framework
  - Propagation of uncertainties on the initial conditions
  - UQ on meshes for exascale applications
  - Stochastic spectral methods
- Surrogate modeling for UQ
  - UQ for surrogate models under physical constraints
  - Tractability of Bayesian approaches for Gaussian Process Regression with high-dimensional inputs
  - Metamodels for nested, chained and coupled codes
- Acceleration of the bricks of the UQ process steps by leveraging exascale calculations

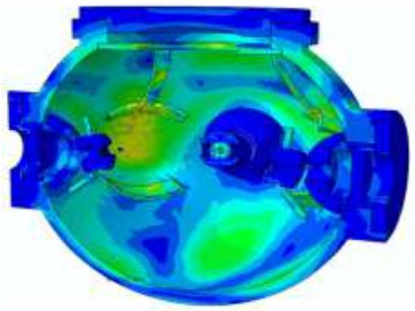
## Stakeholders

CEA
Ecole Polytechnique







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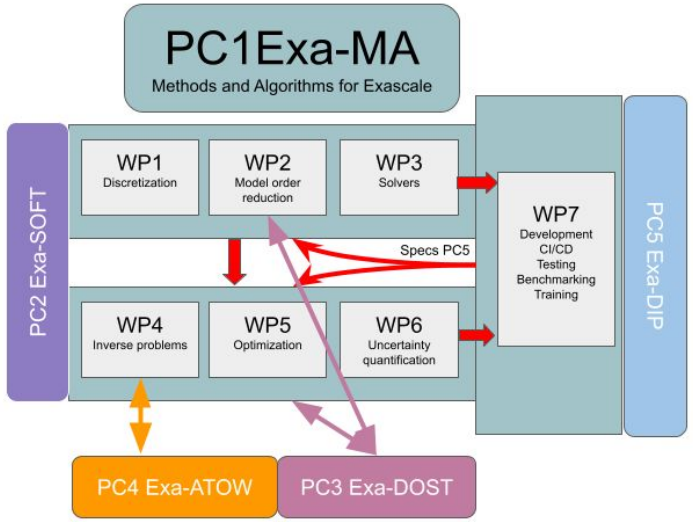


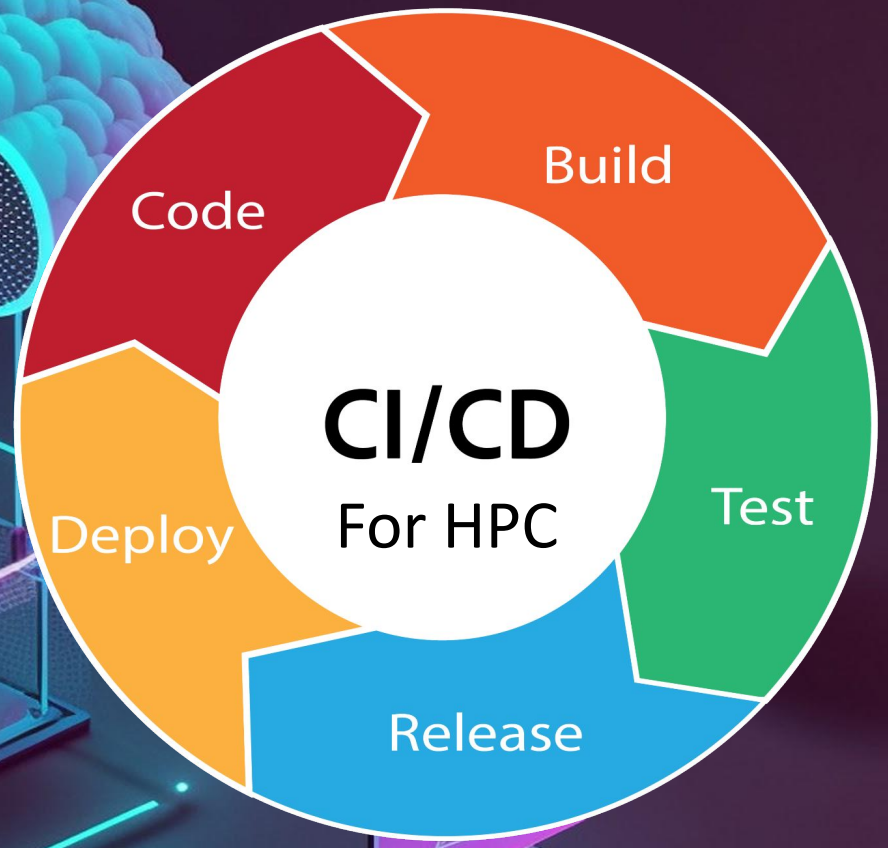

# WP7 Development, Testing Benchmarking, Co-design, Showroom, Training

Lydies Grospellier (CEA), Christophe Prud'homme (UNISTRA)

# WP7 - Dev, DevOps, Benchmark, ...

## Key Objectives

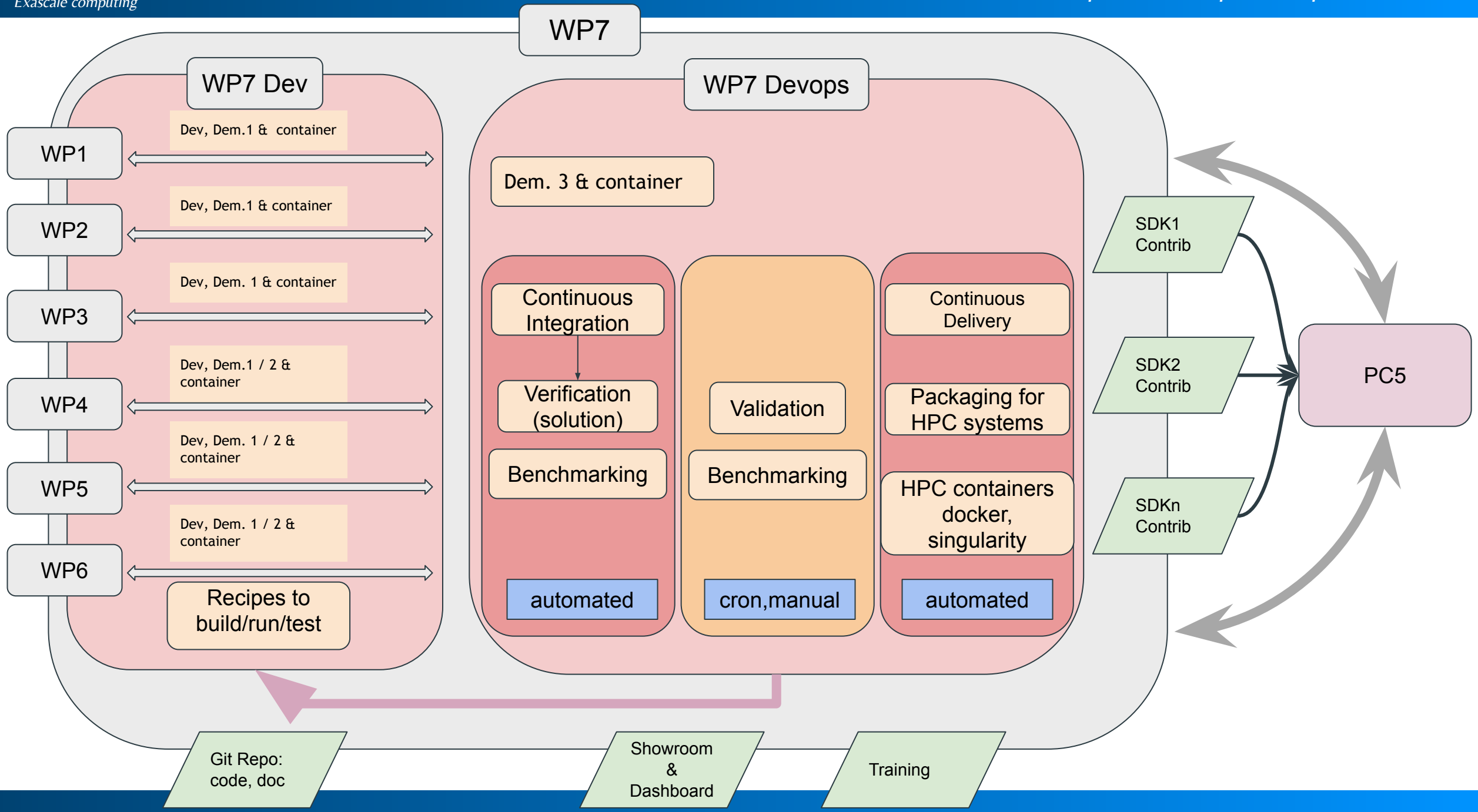
- **Developing Software**
  - Testing including benchmarking to verify exascale capabilities and handling of identified challenges from simple to advanced software
  - Delivering of software packages in the framework proposed by ExaDIP in terms of CI/CD;
- **Coordinating co-design** activities within Exa-MA with ExaDIP;
- **Enabling a showroom** of Exa-MA results
- **Building training material** from the results of Exa-MA



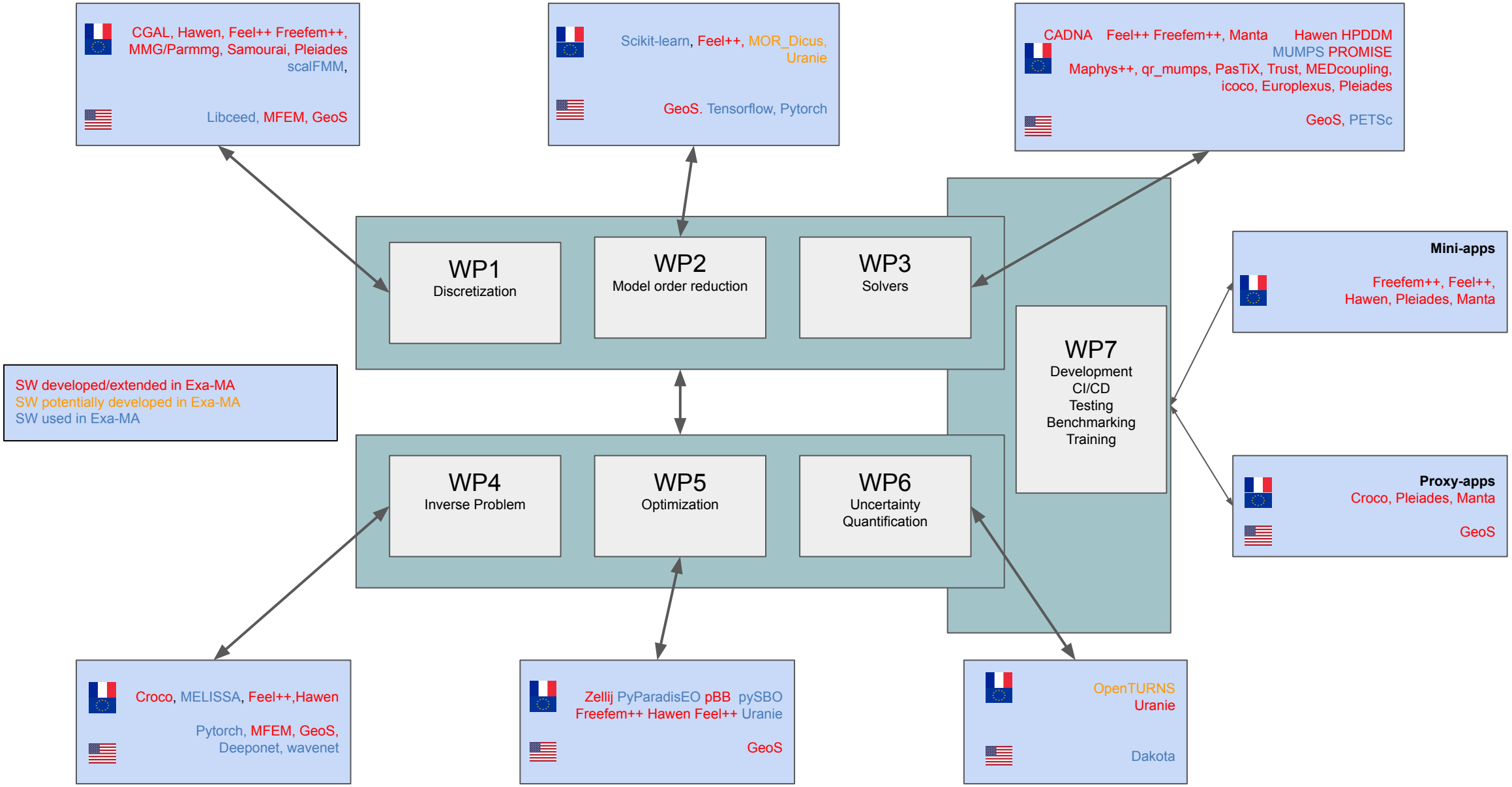

## Stakeholders

ALL

# WP7 - Workflow, Operations, Inputs, outputs



# *WP7 - Software*



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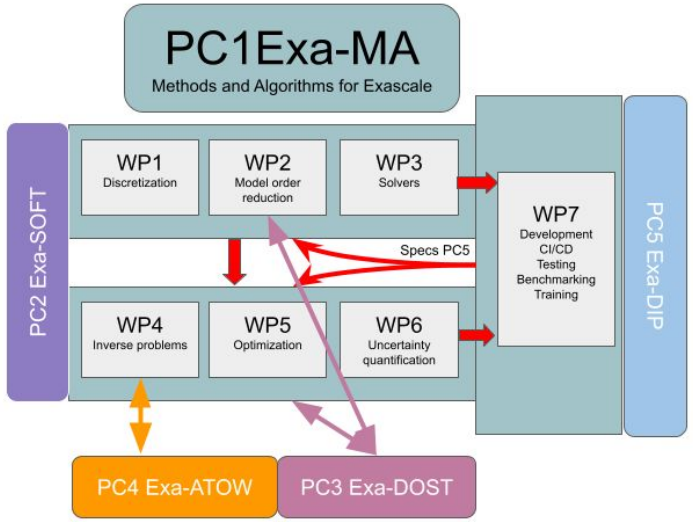



# WP0 - Coordination

Hélène Barucq (Inria), Michel Dayde (CNRS, PC0), Lucas Pernollet (CEA), Christophe Prud'homme(Unistra) and the WP leaders

# Key Objectives

- **Project Management**: Focuses on communication, goal-oriented work, and daily management.
- **Technical and Scientific Management:** Oversees the technical direction of the project and integrates results.

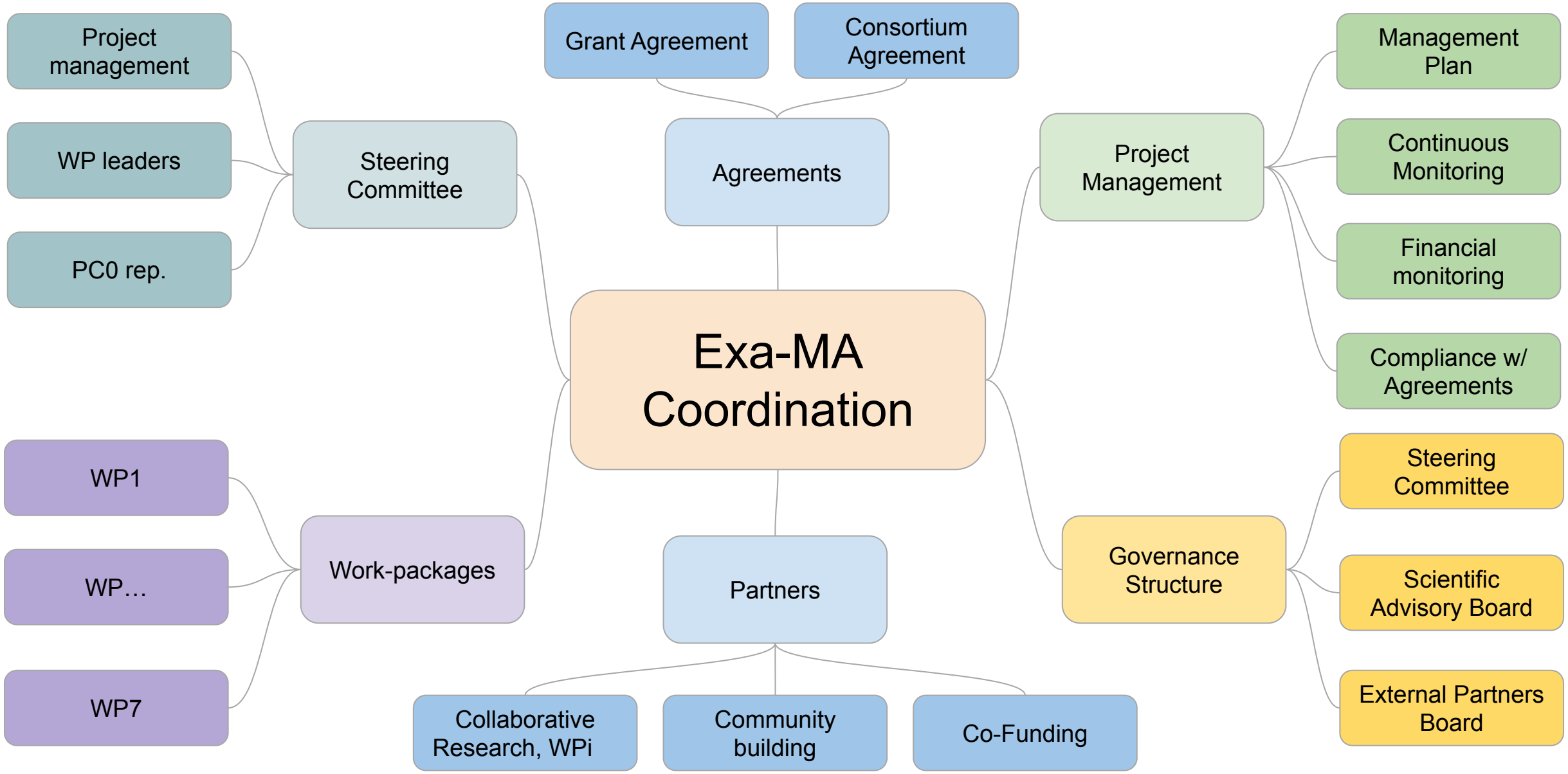
# Tasks

- **Administrative Management**: Handles reporting including finances reports.
- **Establishing Governance Bodies**: WP0 will establish governance bodies to ensure effective action governance and management procedures.
- **Project Management Handbook**: Aims to create a Project Management Handbook that defines responsibilities and tools for efficient management.
- **Scientific and Technical Report:** aims to report on the advancements of the project, annual frequency
- **Grant Agreement (GA)** : Settles the fundings of the project, currently under signature
- **Consortium Agreement (CA)**: Settles intellectual property matters, with a focus on open-source software and a publication retention time policy if possible patents are identified.

# StakeHolders

ALL; WP leaders + PC0 rep

# WP0 - Organization



# *WP0 - Timeline*

**2022**

**PEPR NumPEx**

- Task force, submission
- NumPEx Selected
- 5 PC to create between 0922 and 0423

**2023**

**Exa-MA**

- T0: 14/04/2023
- Management plan
- Online on boarding, 06/23
- **Grant Agreement signed by end of june 2023**
- Consortium Agreement 1y
- 1st Recruiting
- **1st GA in presence, fall 2023**
- 1st int'l workshop

**2024**

**Exa-MA**

- Recruiting cont.
- **Consortium Agreement signed by Apr 2024**
- Reference benchmarks on existing software
- 1st EU exascale computer (jupiter) by end 2024
- 1st release of software stack
- 2nd GA
- 2nd Int'l workshop

**2025**

**Exa-MA**

- All recruiting should be done
- 2nd EU exascale computer (Jules Vernes) by end of 2025
- 2nd release of software stack
- Benchmarking reports
- 1st training
- 3rd GA
- 3rd Int'l workshop

**2026**

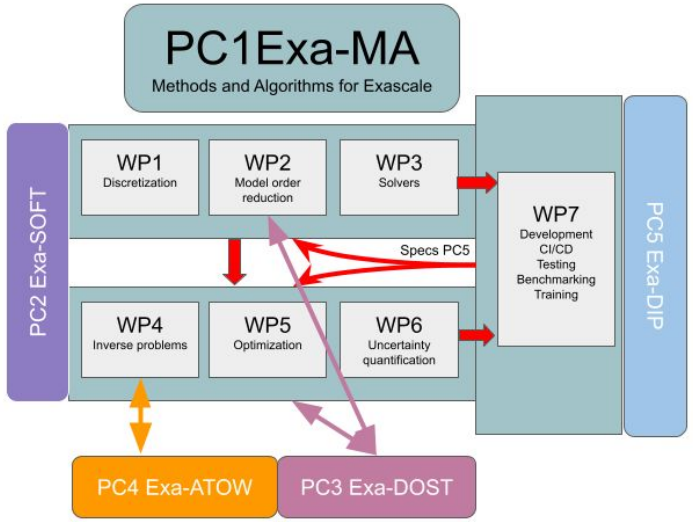
**Exa-MA**

- 1st PhD defenses
- 3rd release of software stack
- Benchmarking reports
- 1st Benchmarking reports on exascale systems
- Training
- 4th GA
- 4th Int'l workshop

**2027**

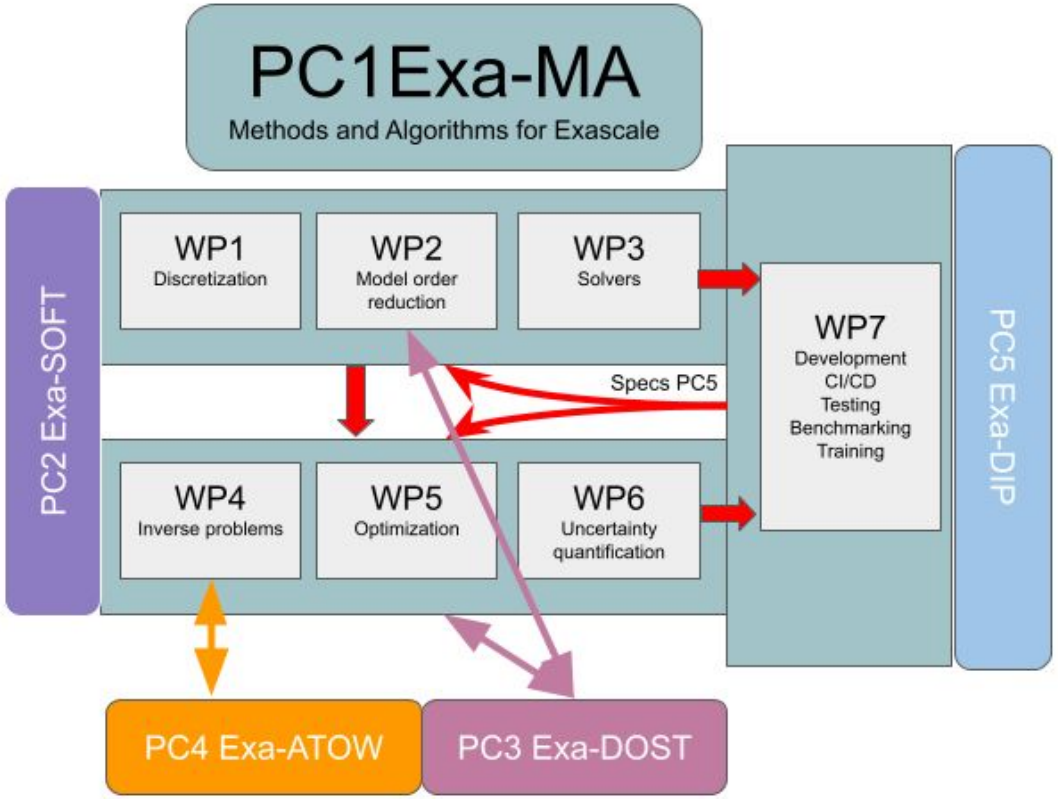
**Exa-MA**

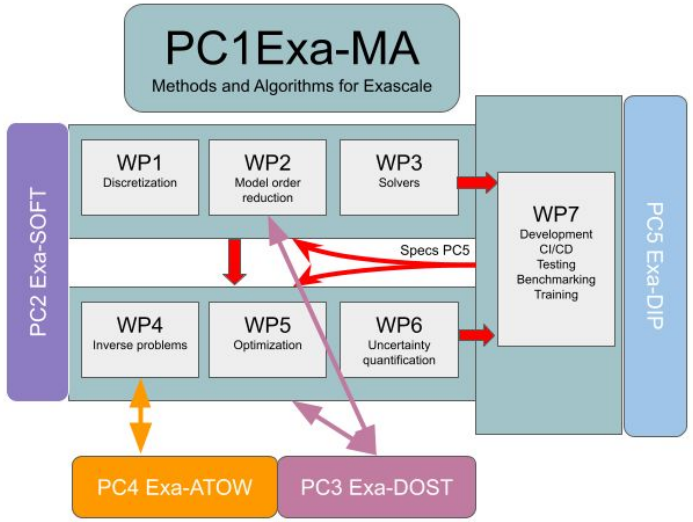
- last PhD defenses
- 4th release of software stack
- Benchmarking reports
- Benchmarking reports on exascale systems
- Training
- 5th GA
- 5th Int'l workshop




# Exa-MA Questions

- Collaborations with Other PC
  - PC2 runtime systems and software stack
- Collaborations with External Partners
- Benchmarking? WP7 will provide(develop?) tools for non regression
- Connections
  - Project Time-X https://time-x.eu/ (parallelization in time)
  - Quantum computing ? NumPEx is not focused on quantum computing, future calls will address the link. Already some EU projects are funded
- Computing resources access at french and european level
  - WP7 will coordinate at french and eu level






# Exa-MA DOE Software Stack Analysis

The point of view of Exa-MA (19 votes)

No vote is allowed if software is unknown or not used.

June 13 version

| Solver Libraries (19 responses) Exa-MA | | Impact of not having software product/tool/library available | | | |
|---|---|---|---|---|---|
| | | Very High | High | Medium | Low |
| Likelihood of Risk | Very High | | | | |
| | High | | Hypre, Scipy, MFEM Solvers, Sundials, Zoltan/Zoltan2, ARPACK | | |
| | Medium | | PETSc, SuperLU, Eigen | KokkosKernels, PARDISO, Trilinos, SuperLU-Dist, STRUMPACK, SPARSKIT, SparsePACK | |
| | Low | BLAS, LAPACK | | PyMatLib | Krino |

| Math, Meshing, Discretization (19 responses) Exa-MA | | Impact of not having software product/tool/library available | | | |
|---|---|---|---|---|---|
| | | Very High | High | Medium | Low |
| Likelihood of Risk | Very High | | | | |
| | High | | MFEM | | |
| | Medium | | METIS, ParMETIS | Sculpt, libigl | Overlink |
| | Low | | | SAMRAI, Portage, Tangram | STK, UMR, Axom |

| Compilers, Runtimes, Languages (19 responses) Exa-MA | | Impact of not having software product/tool/library available | | | |
|---|---|---|---|---|---|
| | | Very High | High | Medium | Low |
| Likelihood of Risk | Very High | | | | |
| | High | | C | PyKokkos, KokkosRemoteMemorySpaces | Legion |
| | Medium | C++, GCC | MPICH, OpenMPI, Fortran, HIP, CUDA, Python, OpenMP, LLVM, PyTorch, TensorFlow, Boost | Kokkos, MPI, Intel Compiler Suite, Intel MPI | |
| | Low | | RAJA Suite, Flang | FleCSI | Perl |

| System Imaging, Monitoring (19 responses) Exa-MA | | Impact of not having software product/tool/library available | | | |
|---|---|---|---|---|---|
| | | Very High | High | Medium | Low |
| Likelihood of Risk | Very High | | | | |
| | High | | | | |
| | Medium | | SLURM | CharlieCloud, VmWare, LSF | LDMS, Flux, SICM, AppSysFusion, GMI, Maestro/Merlin, Splunk |
| | Low | | | | |

| Visualisation And Analysis (19 responses) Exa-MA | | Impact of not having software product/tool/library available | | | |
|---|---|---|---|---|---|
| | | Very High | High | Medium | Low |
| Likelihood of Risk | Very High | | | | |
| | High | | | | |
| | Medium | | VTK/VTKm, Paraview | Visit, Catalyst, Conduit | Cinema, Ascent |
| | Low | | | | |

| Build, Development, Software (19 responses) Exa-MA | | Impact of not having software product/tool/library available | | | |
|---|---|---|---|---|---|
| | | Very High | High | Medium | Low |
| Likelihood of Risk | Very High | | | | |
| | High | | Spack | | |
| | Medium | CMake | Ninja, gdb, git, Gitlab, git-lfs, Valgrind, AllineaForge, TotalView | Caliper, PAPI, KokkosTools | Archer, CDash, STAT |
| | Low | | Autoconf/Automake | BLT | |

| IO Storage, Data Management (19 responses) Exa-MA | | Impact of not having software product/tool/library available | | | |
|---|---|---|---|---|---|
| | | Very High | High | Medium | Low |
| Likelihood of Risk | Very High | | | | |
| | High | HDF5/Parallel-HDF5 | | | |
| | Medium | | NetCDF, pNetCDF, SEACAS | UnifyFS, HPSS, MarFS, SILO, Exodus, yamlcpp, CGNS, libz, ADIOS, szip/AEC | ZFP, GUFI, HIO, SCR, Sina/Kosh, DB2, Matio |
| | Low | | | | |

# DOE Software Stack Analysis

The point of view of Exa-MA (18 votes)

No vote is allowed if software is unknown or not used.

June 6 version

| Solver Libraries | | Impact of not having software product/tool/library available | | | |
|---|---|---|---|---|---|
| | | Very High | High | Medium | Low |
| Likelihood of Risk | Very High | | | | |
| | High | Eigen, Sundials | Hypre, Scipy, MFEM Solvers, Zoltan/Zoltan2, ARPACK | KokkosKernels | |
| | Medium | | PETSc, SuperLU | PARDISO, Trilinos, SuperLU-Dist, STRUMPACK, SPARSKIT, SparsePACK | |
| | Low | BLAS | LAPACK | | Krino, PyMatLib |

| Math, Meshing, Discretization | | Impact of not having software product/tool/library available | | | |
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| | Medium | | METIS, ParMETIS | libigl | Overlink |
| | Low | | | SAMRAI, Sculpt | STK, UMR, Portage, Tangram, Axom |

| Compilers, Runtimes, Languages | | Impact of not having software product/tool/library available | | | |
|---|---|---|---|---|---|
| | | Very High | High | Medium | Low |
| Likelihood of Risk | Very High | | | | |
| | High | | C, TensorFlow | PyKokkos, KokkosRemoteMemory Spaces | Legion |
| | Medium | C++, GCC | MPICH, OpenMPI, HIP, CUDA, Python, OpenMP, LLVM, PyTorch, Boost | MPI, Intel Compiler Suite, Intel MPI | Kokkos |
| | Low | | RAJA Suite, Flang, Fortran | FleCSI, Perl | |

| System Imaging, Monitoring | | Impact of not having software product/tool/library available | | | |
|---|---|---|---|---|---|
| | | Very High | High | Medium | Low |
| Likelihood of Risk | Very High | | | | |
| | High | | | | |
| | Medium | | SLURM | CharlieCloud, VmWare, LSF | LDMS, Flux, SICM, AppSysFusion, GMI, Maestro/Merlin, Splunk |
| | Low | | | | |

| Visualisation And Analysis | | Impact of not having software product/tool/library available | | | |
|---|---|---|---|---|---|
| | | Very High | High | Medium | Low |
| Likelihood of Risk | Very High | | | | |
| | High | | | Catalyst | |
| | Medium | | VTK/VTKm, Paraview | Visit, Conduit | Cinema, Ascent |
| | Low | | | | |

| Build, Development, Software | | Impact of not having software product/tool/library available | | | |
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| | Low | | Autoconf/Automake | BLT | |

| IO Storage, Data Management | | Impact of not having software product/tool/library available | | | |
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| | | Very High | High | Medium | Low |
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| | High | HDF5/Parallel-HDF5 | | | |
| | Medium | | NetCDF, pNetCDF, SEACAS | UnifyFS, HPSS, MarFS, SILO, Exodus, yamlcpp, ADIOS, szip/AEC | ZFP, GUFI, HIO, SCR, Sina/Kosh, CGNS, libz, DB2, Matio |
| | Low | | | | |