RÉPUBLIQUE FRANÇAISE
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FRANCE 2030
PROGRAMME DE RECHERCHE
NUMÉRIQUE POUR L'EXASCALE

Exa-MA
Methods and Algorithms for Exascale

Hélène Barucq (INRIA)
Lucas Pernollet (CEA, Project Manager)
Christophe Prud'homme(University of Strasbourg, UNISTRA)

General Assembly Organization

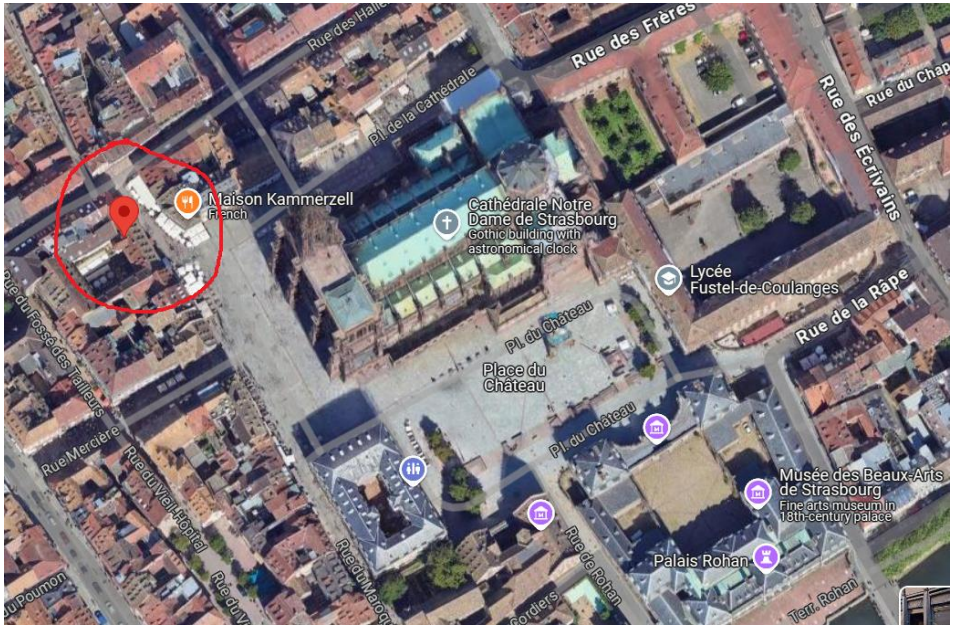
Lucas Pernollet (CEA, Project Manager)

Organization

- **Agenda:**
  - **1st day:**
    - Overall presentation of NumPEx and Exa-MA
    - Our new recruits will introduce themselves
    - Outline of 2 transverse working groups of NumPEx
    - Plenary workshop on interactions between WPs
    - Meeting of the Scientific Board

      ⇒ Let's be careful about time :-)
    - Restaurant
  - **2nd day:**
    - Plenary workshop on collaborations with external partners
    - Breakout sessions to deepen interactions between WPs
- **Locations**
- **Microphones:** DO NOT SWITCH THEM OFF PLEASE

Organization



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NumPEx

Jérôme Bobin (CEA)

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

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

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

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

Exa-DI - Dr J-P. Vilotte, DR CNRS - Valérie Brenner, CEA

The French NumPEx Program
Context and motivations

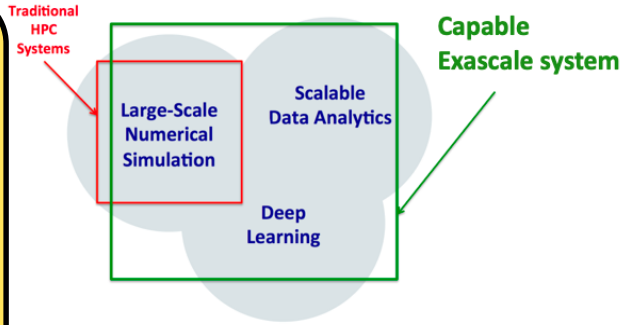
A technological breaktrough

Hybrid scalar/acc.
fewer memory/node
more concurrency

In the digital continuum

Increased flux/volume from the edge to the HPC system

Convergence HPC/HPDA/IA



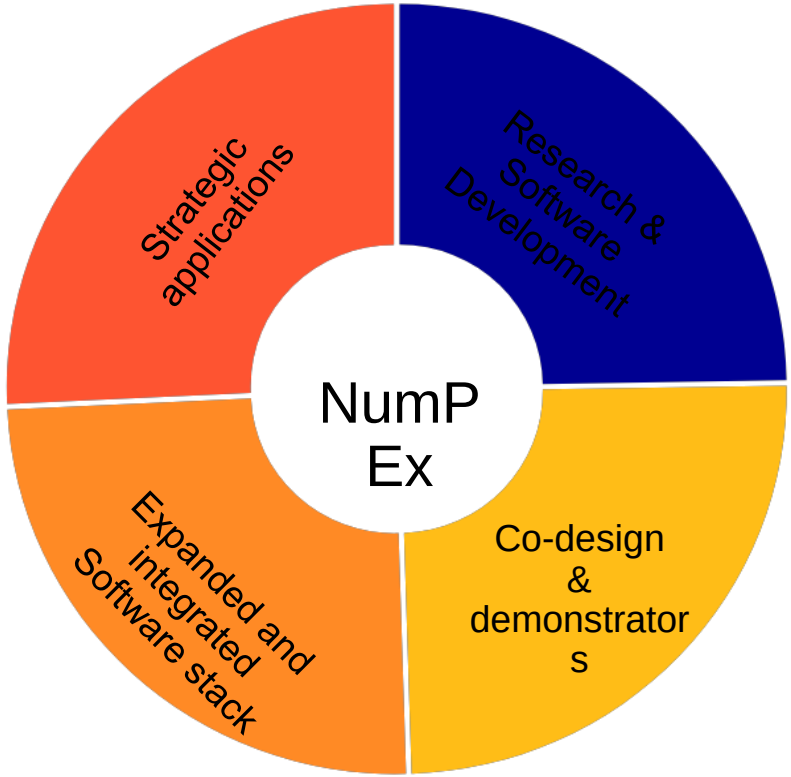
The French NumPEx Program Objectives

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 Exascale and post-Exascale era



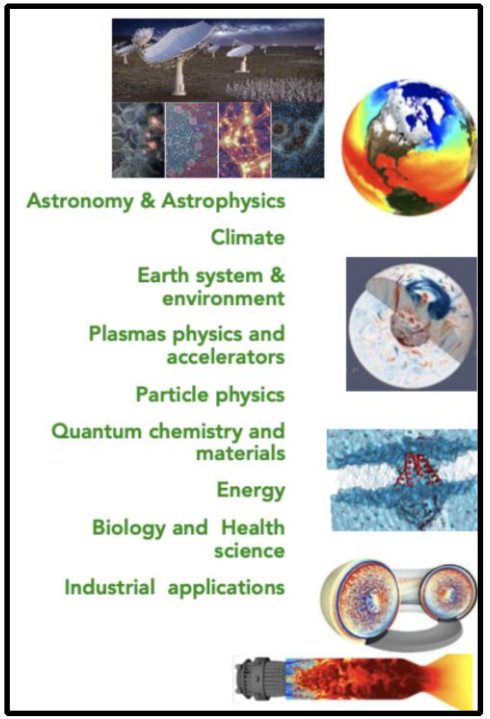
Help aggregate the French HPC/HPDA/IA community

The French NumPEx Program

Objectives

European Pre-Exascale system

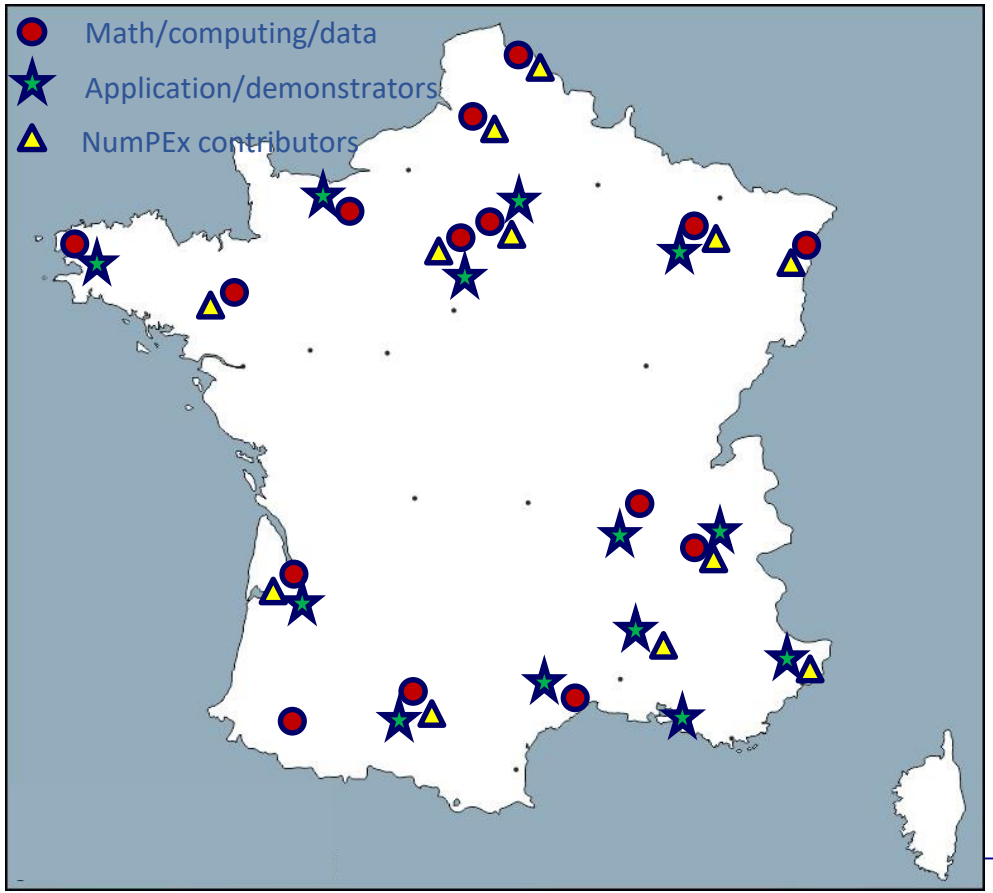
Software stack



Co-develop the exascale software stack

Preparing the applications for the Exascale era

NumPEx by numbers



6 Years
41 M€*

2023-2028
* Funding 41M€=500 man.year non permanent staff
+ 170 man.year permanent staff
Total cost : 81 M€

Core Research Institutions

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

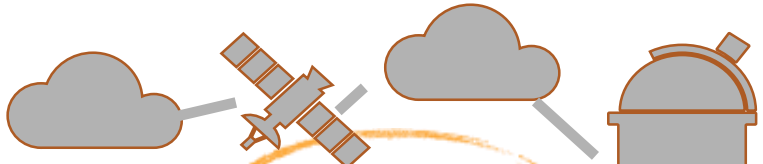
3 Focus Area

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

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

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

Call for Projects

See Later

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

Resilience
L.Morin

Training
M.Krajecki

Software production and integration
B.Raffin

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

International collaborations
J-Y Berthou

The NumPEx call

- **Total budget: 4MEuros/Up to 5 funded 4-years projects**

- **Single call with 3 different topics** :

  1. AI4HPC – HPC4AI
     - SW for the efficient training of large-scale science-driven AI models
     - Open call for AI for HPC
  2. Programming models for accelerated architectures
  3. Efficient workflows for scientific data processing, the case of SKA

- **Details**:

  - Deadline : 1st of April 2025
  - All information and scientific document:

https://anr.fr/PEPR-NumPEx-AAP-2024

More details tomorrow morning in external partners session

Exa-MA

Hélène Barucq (INRIA),
Christophe Prud'homme (University of Strasbourg, UNISTRA)

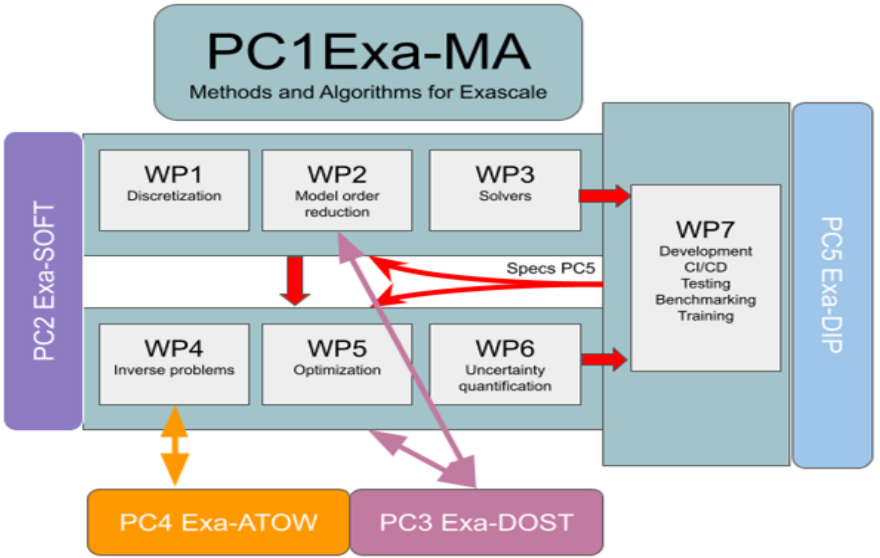
Exa-MA

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:

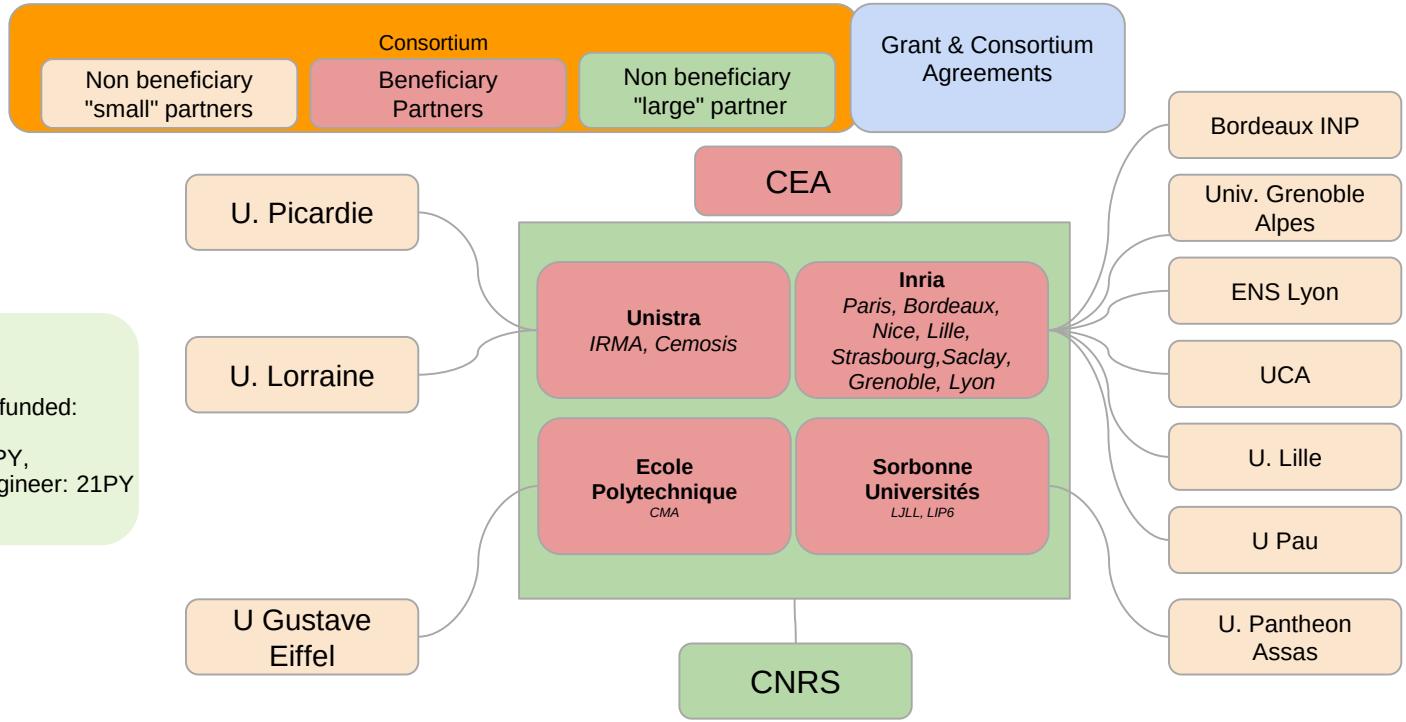
- ***to develop methods, algorithms, and implementations*** *that, taking advantage of the exascale architectures empower modeling, solving, assimilating model and data, optimizing and quantifying uncertainty, at levels that are unreachable at present*
- ***to develop and contribute to software libraries*** *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€*

Consortium

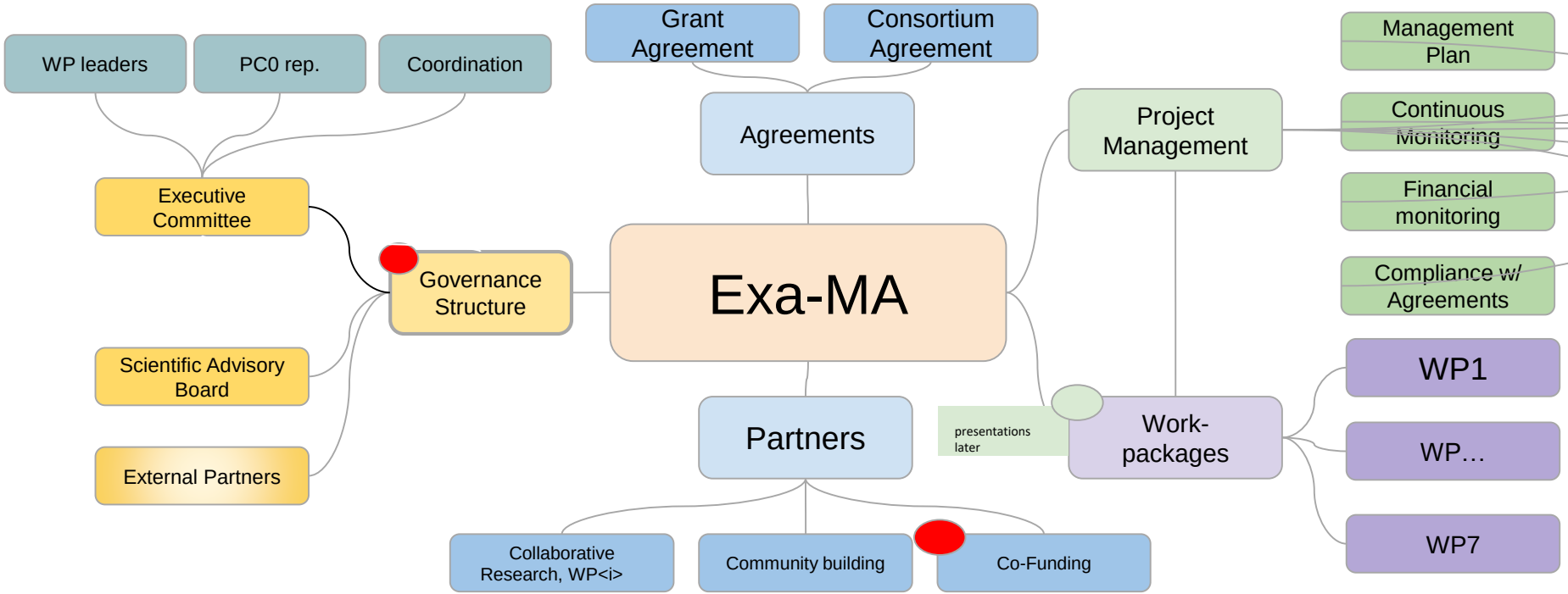


Composition
74 permanent staff
22 Person-years (PY) funded:

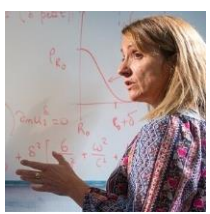
- PhD:22 PY,
- Postdoc: 12 PY,
- Research Engineer: 21PY

"small" means 1 or 2 persons, "large" means more than 10 persons

Exa-MA Coordination: WP0



Executive committee





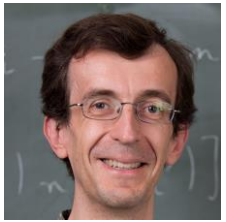













Scientific Advisory Board

WP1 Christophe Geuzaine, University of Liège, Belgium

WP1 Jan Hesthaven Karlsruhe Institute of Technology (KIT), Germany

WP2: Karen Willcox, Oden Institute for Computational Engineering and Sciences, University of Texas at Auston, USA

WP2: Gianluigi Rozza, Scuola Internazionale Superiore di Studi Avazanti, SISSA, Italy

WP3: Jed Brown, Colorado University, Boulder, USA

WP3: Lois Curfman McInnes, Argonne National Laboratory, USA

WP4: Lars Nerger, Alfred Wegener Institute Helmholtz Centre for Polar and Marine Research, Germany

WP5: Albert Zomaya, University of Sydney, Australia

WP5: Pascal Bouvry, University ofLuxembourg, Luxembourg

WP6: Bruno Sudret ETHZ Switzerland

Scientific Advisory Board

- **Strategic Guidance and Expertise**
  - Offer high-level insights and guidance for the research agenda.
  - Suggest innovative ideas and emerging trends in the HPC (High-Performance Computing) field.
- **Evaluation and Feedback**
  - Review project documentation and deliverables; provide constructive feedback.
  - Assess the progress of the project to ensure it remains on track with its objectives.
- **Trend Monitoring**
  - Help the project stay current with recent developments in HPC, numerical methods, AI, and related fields.
  - Advise on cutting-edge techniques and best practices to maintain Exa-MA's competitiveness.
- **Alignment with Broader HPC Objectives**
  - Ensure Exa-MA's research directions are aligned with larger initiatives (e.g., NumPEx, government strategies, international strategies,...).
  - Facilitate synergies with other major HPC projects, software ecosystems, and scientific communities.
- **Participation in Yearly General Meetings**
  - Attend (virtually or in person) the annual general meeting.
  - Engage with Exa-MA project leaders, work package teams, and other SAB members to discuss progress and set objectives.


Christophe Geuzaine, University of Liege, Belgium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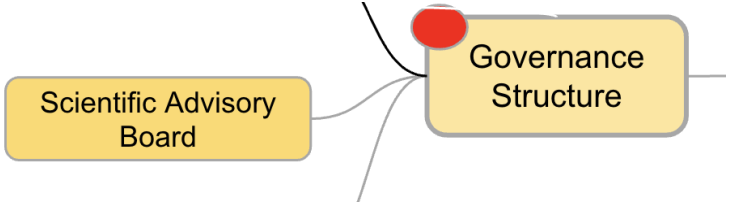
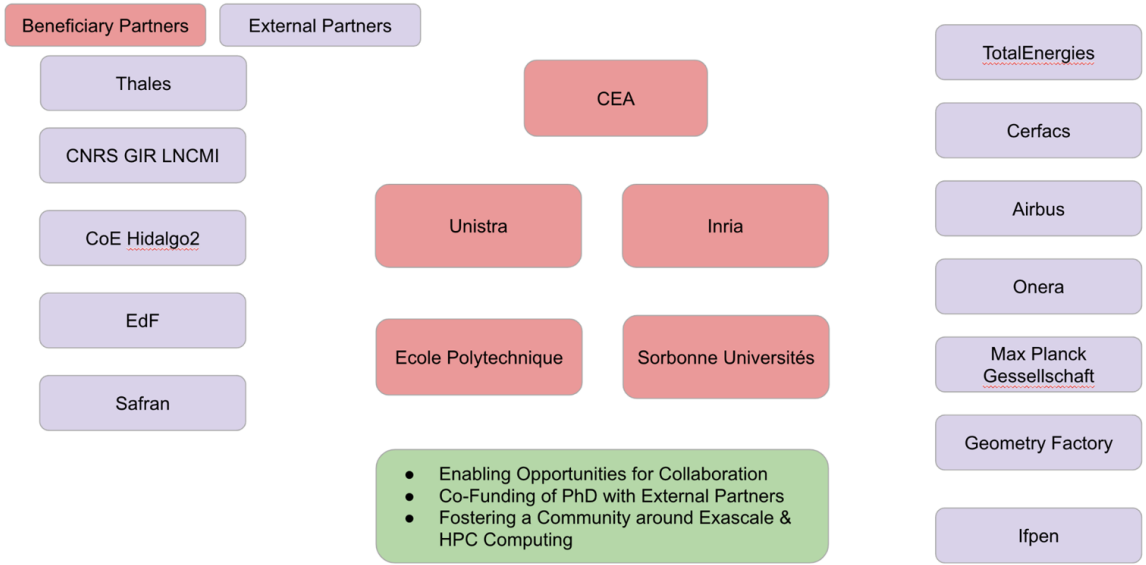
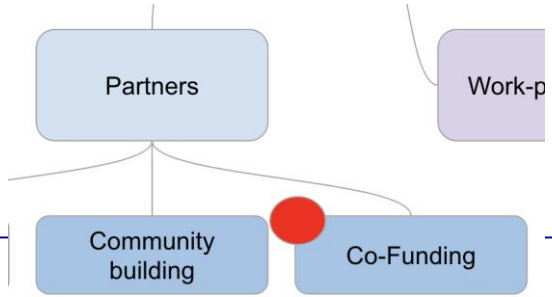


External Partners

Exa-MA co-funds 3 PhD thesis with

- **via 2 calls**
  - **Dec 2023**: 3 projects submitted
    - board composed of people from inside and outside NumPEx.
    - 2 projects co-funded
      - Ecole Polytechnique / ONERA High-order adaptive time coupling for multiphysics simulations
      - INRIA Alpines/ IFPEN+ONERA Neural Linear Solvers and Preconditioners for General Sparse Matrices
    - Specific grant payment agreement
    - Open-source contribution and participation to mini-app/proxy-app activities
    - next call Dec 2024: one position
- **via existing half PhD funding**
  - INRIA Makutu/ TotalEnergies
- **More tomorrow (9:00-10:00)**





Initial Production

- **Deliverables**
  - D0.1 - project management
  - D7.1 - Benchmarking report 2024 (updated yearly)
- **Publications**
  - 13 publications : > HAL
- **Events**
  - Exa-MA meetings : 2023(x2), 2024 (x1)
  - Organization > SciML 2024 > Strasbourg
  - Organization > Symposium @ Coupled 2025
- **Software**
  - > Github NumPEx
- **Data (publications, software archive, datasets)**
  - > Zenodo (EU) NumPEx

WP1: Discretization

P. Alliez (Inria, Nice), H. Barucq (Inria, Pau), I. Ramière (CEA, Cadarache),

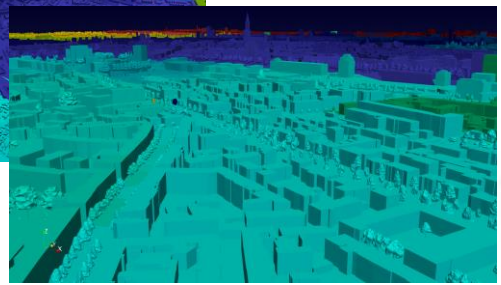
WP1

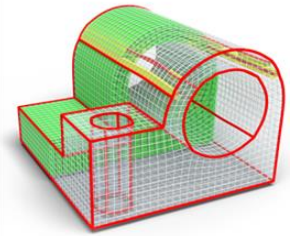
Key Objectives

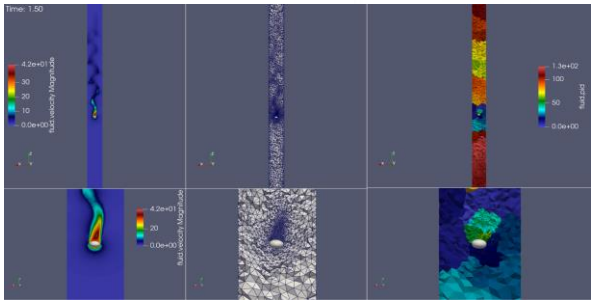
- Geometric and discrete domain representations
- Advanced numerical methods dedicated to physics-based simulation and parallel computing

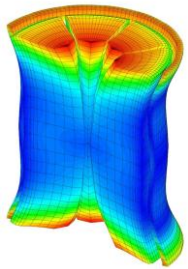
Tasks

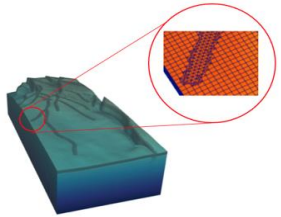
- Mesh generation
  - Large-scale, non-conforming
  - Unconditional robustness
  - Hexahedral block grids
- Adaptive Mesh Refinement
  - Unstructured grids
  - Cartesian or block grids
- Non-conforming finite elements
  - Treffz and HDG methods
- Error control in time and space
- Multiphysics coupling
  - Efficient and generic partitioned coupling
  - High-order time adaptive coupling
- Multiscale coupling











WP2: Model order, Surrogate, Scientific Machine Learning methods

E. Franck (Inria, Strasbourg), S. Lanteri (Inria,Nice)

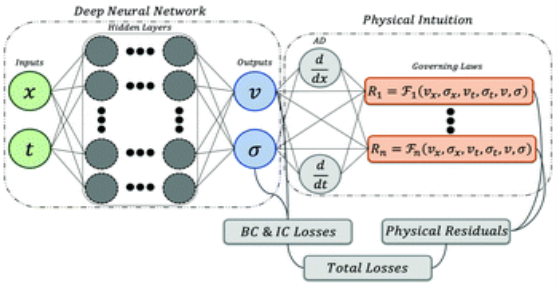
WP2: order reduction and SciML

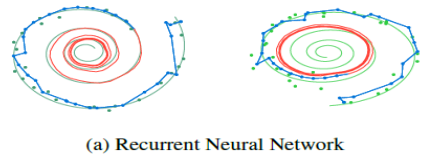
Key Objectives

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

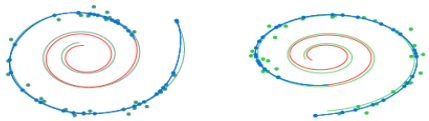
Tasks

- 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
- Reduced order modeling
  - (Non intrusive) Reduced Basis/Non linear compressive reduced basis
  - Auto-encoder/POD + NN hyper-reduction
  - Explicability for learning methods
  - Closure for kinetic equations
- Low/high fidelity models

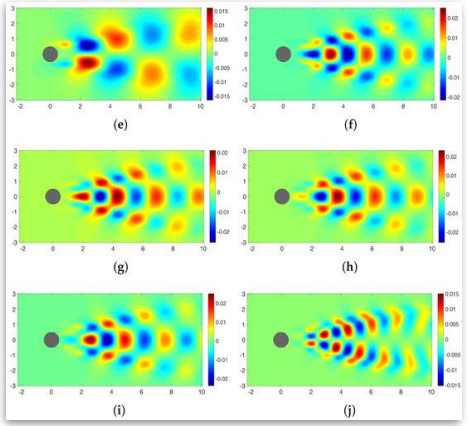


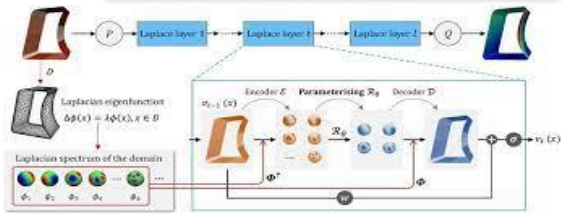


(a) Recurrent Neural Network



(b) Latent Neural Ordinary Differential Equation





WP3: Solvers

V. Faucher (CEA, Cadarache), L. Giraud (Inria, Bordeaux),
F. Nataf (Inria, Paris)

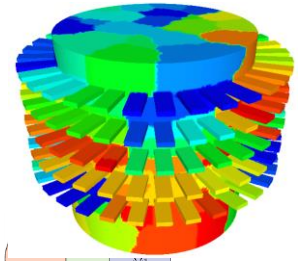
WP3: Solvers

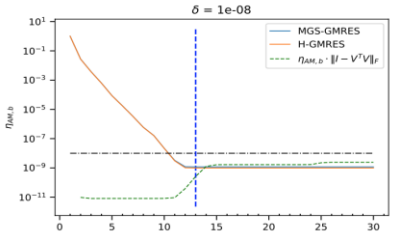
Key Objectives

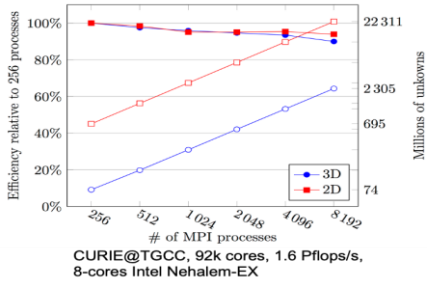
- Design novel generic scalable numerical algorithms
- Enable multi-precision for prescribed accuracy
- Leveraging communication avoiding/hiding, mixed arithmetic and data compression

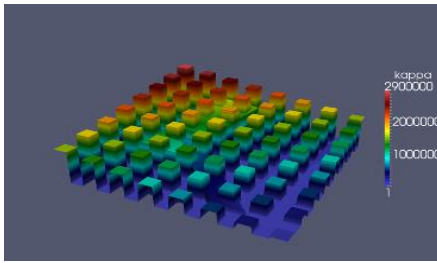
Tasks

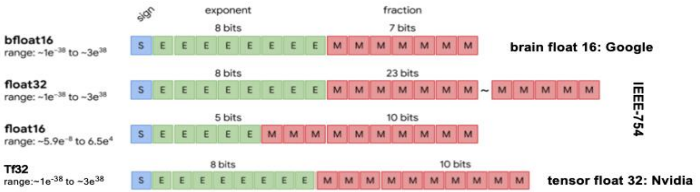
- Robust and scalable solvers
  - Adaptive precision (link with PC2), auto tuning tools
  - Multi-level Domain decomposition with provable efficiency
  - Resiliency
- Scalable coupled physics solvers
- Open source libraries: HPDDM, Composyx, MEDCoupling, PROMISE, use cases via WP7 and interactions with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











WP4: Inverse Problems and Data Assimilation

M. Asch (UNISTRA,Amiens), H. Barucq (Inria,Pau), A. Vidard (Inria,Grenoble)

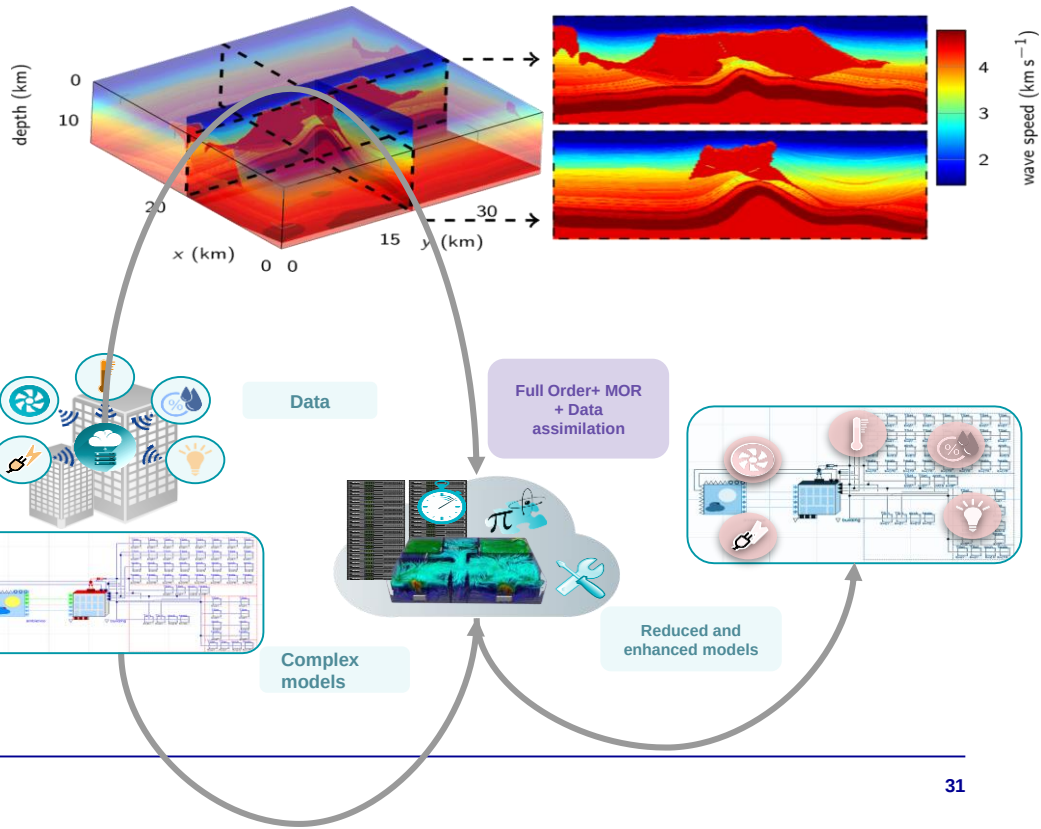
WP4: Inverse Problems and Data Assimilation

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



WP5: Optimization

El-Ghazali Talbi (Inria,Lille)

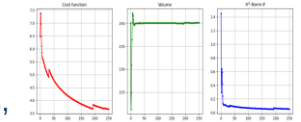
WP5: Optimization

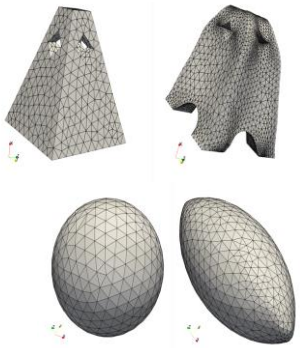
Key Objectives

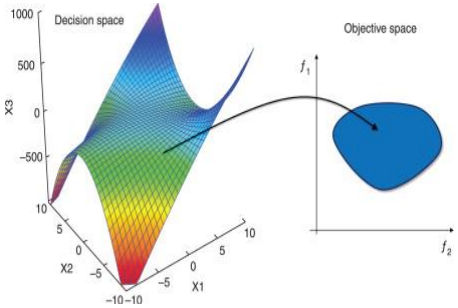
- Solving big optimization problems (decision variables, many-objectives, expensive objectives, big data) using exascale decomposition
- Inverse, continuous, discrete and mixed optimization problems
- Exact, heuristic and data driven optimization algorithms

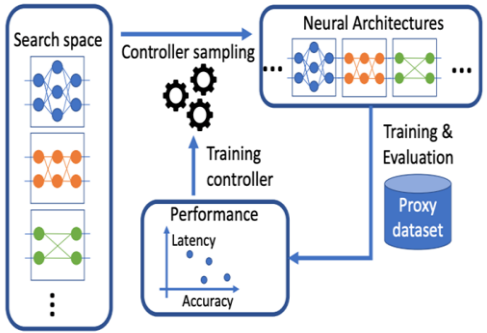
Tasks

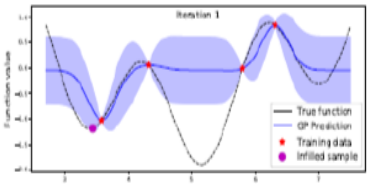
- Exascale combinatorial and continuous optimization
  - Exact optimization (Branch and bound, tree search)
  - Heuristic optimization (Computational intelligence)
- Exascale surrogate-based optimization
  - Multi-fidelity models
  - Coupling of surrogates, optimization and sampling
- Exascale shape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











WP6: Uncertainty Quantification

C. Gauchy (CEA,Saclay), J. Garnier (EP)

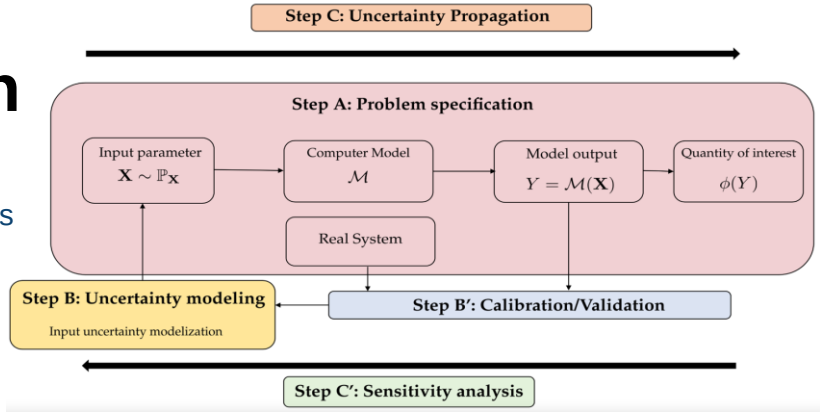
WP6: Uncertainty Quantification

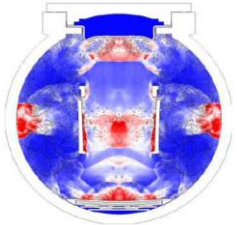
Key Objectives

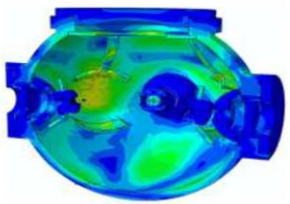
- Uncertainty Quantification for multi-physics and/or multi-scale problems
- Uncertainty propagation, sensitivity analysis, robust inversion

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







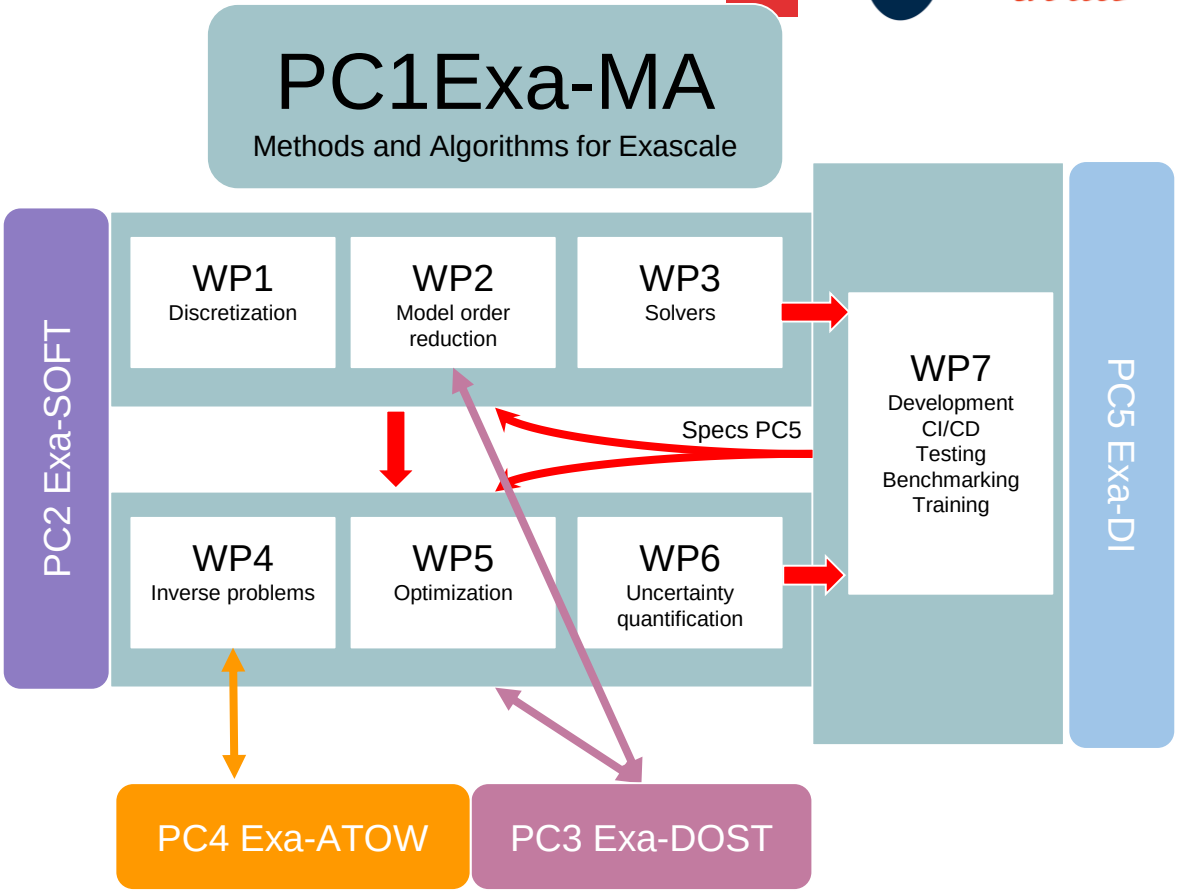
WP7: Software

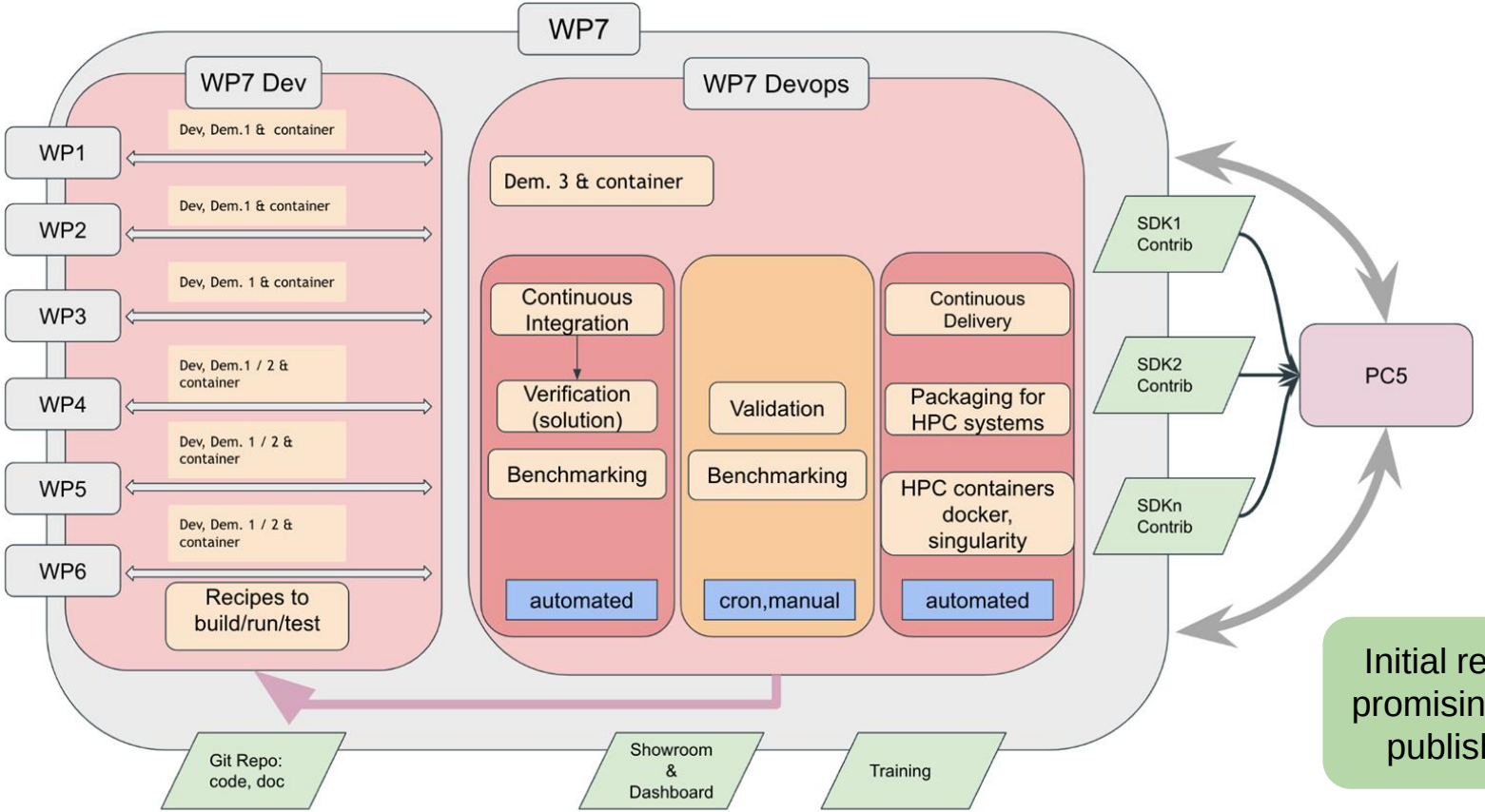
L. Grospellier(CEA, Bruyères le Chatel), C. Prud'homme(UNISTRA)

WP7 Software

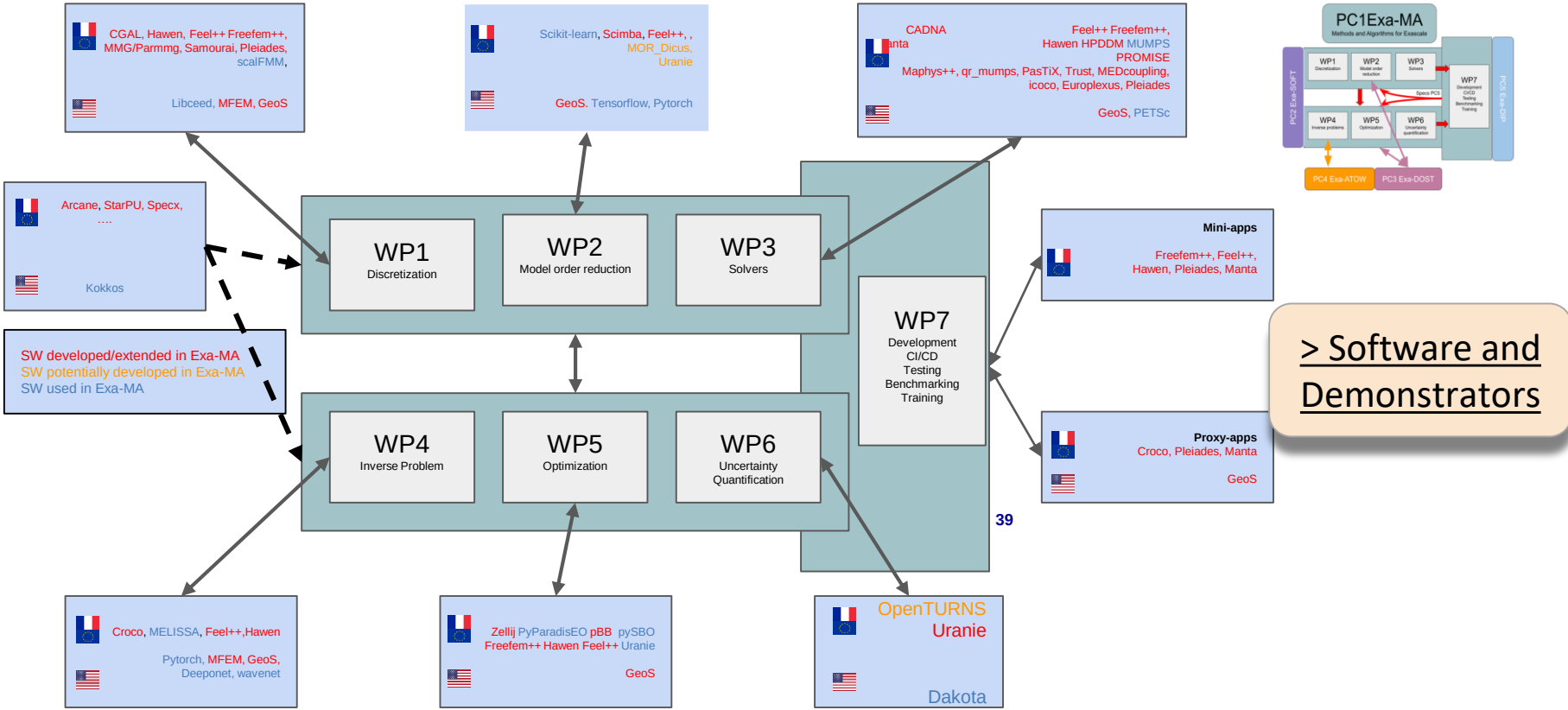
A transverse workpackage

- **Developing Software**
  - **Contribute to development** locally or on WP topics
  - **Port** to pre-exascale/exascale supercomputers
  - **Test including benchmarking** to verify exascale capabilities and handling of identified challenges from simple to advanced software
  - **Deliver software packages** in the framework proposed by ExaDIP in terms of CI/CD;
- **Coordinating and contributing co-design** activities within Exa-MA with Exa-DI, Contribute Software Develop Kit
- **Enabling a showroom** of Exa-MA results
- **Building training material** from the results of Exa-MAa
- **Interaction with all other WPs** + PC2, PC3, PC4, PC5





Initial results promising and published



> Software and Demonstrators

Some Last Words Before it Begins

What We Hope to Achieve at the General Assembly?

- **Showcase Our Team**
  - Introduce the junior researchers funded (or closely affiliated) with Exa-MA and highlight their contributions.
- **Share Early Achievements**
  - Present initial results and progress across all work packages.
- **Engage With External Partners**
  - Foster discussions and exchange ideas on potential collaborations and co-funded research.
- **Build Connections**
  - Strengthen relationships among all participants through networking opportunities and breaks.
- **Gather Feedback From the SAB**
  - Obtain early input and strategic guidance from the Scientific Advisory Board to shape upcoming project activities.

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