



PEPR NumPEX // Exa-MA

Methods and Algorithms at
ExaScale

Orap49 // 29 November 2022

Christophe Prud'homme & Hélène Barucq

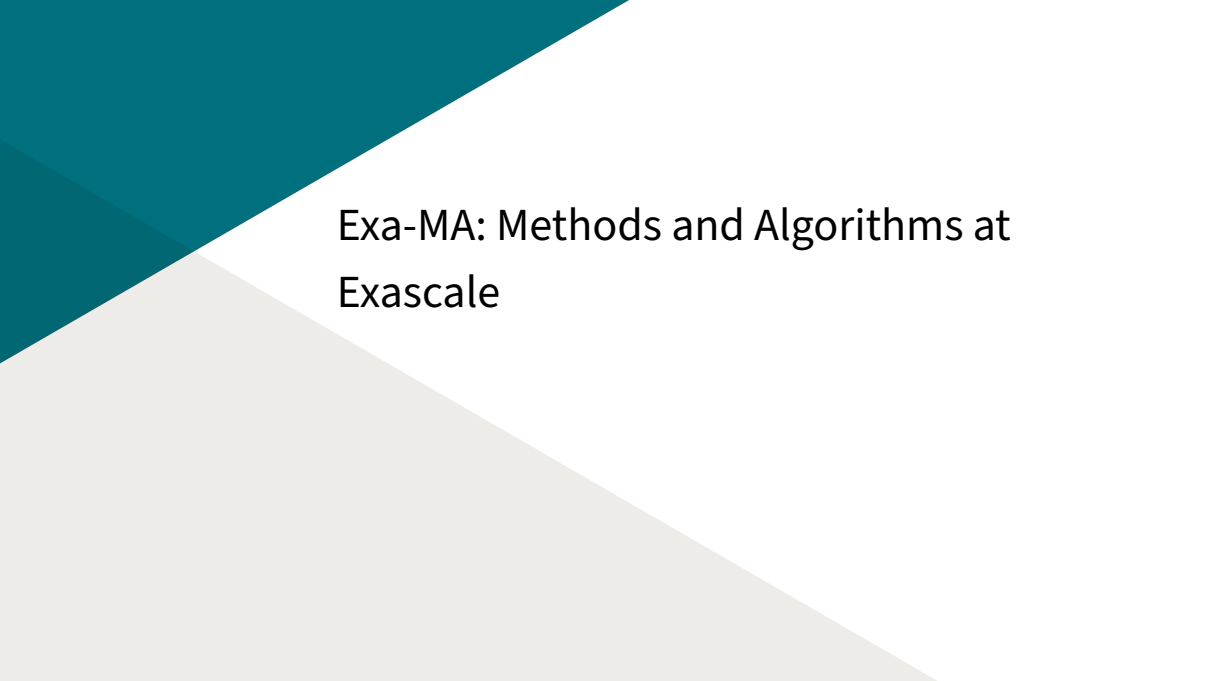
Overview



1. Exa-MA: Methods and Algorithms at Exascale

2. Work Packages

3. Relations

The background of the slide is composed of two large, overlapping geometric shapes. A teal-colored shape occupies the top-left corner, while a light gray shape occupies the bottom-left corner. The rest of the slide is white.

Exa-MA: Methods and Algorithms at Exascale

Objectives



Scale up methods and algorithms in predictive simulation data analysis, up to digital twinning, including uncertainty quantification and inverse problems

- ▶ Produce methods and algorithms
- ▶ Produce patterns
- ▶ Produce software
- ▶ Produce benchmarks

Exa-MA: Methods and Algorithms at Exascale



Challenges

- ▶ (C1) Reduce carbon (GHG) footprint in transportation, buildings, and cities
- ▶ (C2) Design, control, and manufacture of advanced materials
- ▶ (C3) Understand and simulate the human brain
- ▶ (C4) Understand fission and fusion reactions and design advanced experiment facilities for fusion
- ▶ (C5) Monitor the health of our planet: climate prediction, impact assessment of environmental policies, rapid environmental hazards
- ▶ (C6) Monitor and personalize the health of human beings
- ▶ (C7) Design drugs
- ▶ (C8) Design cost-effective renewable energy resources: batteries, biofuels, solar photovoltaics
- ▶ (C9) Understand the Universe

Exa-MA: Methods and Algorithms at Exascale



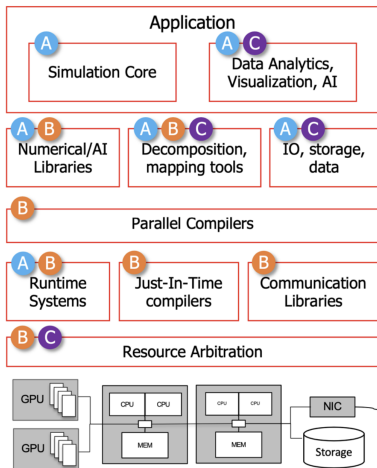
Bottlenecks

- ▶ (B1) Energy efficiency
- ▶ (B2) Interconnect Technology
- ▶ (B3) Memory technology
- ▶ (B4) Scalable systems software
- ▶ (B5) Programming systems
- ▶ (B6) Data Management
- ▶ (B7) Exascale Algorithms
- ▶ (B8) Discovery, design, and decision algorithms
- ▶ (B9) Resilience, robustness and accuracy
- ▶ (B10) Scientific productivity
- ▶ (B11) Reproducibility, replicability of computation
- ▶ (B12) Pre/Post-processing
- ▶ (B13) Integrate Uncertainties

Major Concerns

- ▶ avoidance of communication
- ▶ adaptive parallel grain and more compute-intensive at node level
- ▶ handling of heterogeneous hardware and data representations and
- ▶ self parametrization

Exa-MA is a Part of the NumPEx Software Stack



Enable

- Performance and Scalability
- Productivity
- Reproducibility and reusability
- Efficiency, resilience, robustness

The background of the slide is composed of two large, overlapping geometric shapes. A teal-colored shape occupies the top-left corner, while a light gray shape occupies the bottom-left corner. The rest of the slide is white. The text 'Work Packages' is centered in the white area.

Work Packages

Work Packages



WP1: Discretization

Objectives

- ▶ Geometric domain representations and their discrete counterparts
- ▶ Physics-based models

Specifications

- ▶ Favor high order methods to increase local compute load
- ▶ Favor non-conforming methods to reduce communication

Tasks

- ▶ Geometric representation and their discrete counterparts including valid mesh generation and adaptive mesh refinement (AMR)
- ▶ Space-Time Discretization of PDEs leveraging non-conforming methods and AMR as well as parallel in time methods
- ▶ Multi-Physics and Multiscale coupling

Links

PC2-WP2/3/4, PC3-WP3

Work Packages



WP2: Reduced order and AI driven methods for multi-fidelity modeling

Objectives

- ▶ Develop Reduced order methods
- ▶ Develop methods for multi-fidelity modeling

Specifications

- ▶ Leverage beyond state of the art reduce order, surrogate and machine learning methods
- ▶ Enable Multi-fidelity modeling

Tasks

- ▶ surrogate models based on physics driven deep learning
- ▶ PDE operator learning using NN
- ▶ data driven model order reduction
- ▶ non-intrusive and weakly intrusive reduced basis methods for parametrized PDEs
- ▶ mixing low and high fidelity models
- ▶ real-time models with super resolution methods

Links

PC2-WP2/3/4, PC3-WP3

Work Packages



WP3: Linear, Multi-linear and Coupled Solvers at Exascale

Objectives

- ▶ Focus on generic building blocks(algebraic) for informations
- ▶ Support high dimensional problems

Specifications:

- ▶ Communication avoiding algorithms
- ▶ low-precision computing
- ▶ matrix-free methods
- ▶ operator/data compression

Tasks

- ▶ Acceleration techniques for subspace-based methods;
- ▶ High dimensional problems ;
- ▶ Randomization;
- ▶ Exploiting data-sparsity and multiple precision;
- ▶ Adaptive solution strategies for exascale multiphysical and multiscale models;

Links

PC2-WP2/3/4

Work Packages



WP4: Combine data and models, inverse problems at Exascale

Objectives

- ▶ Improve existing deterministic methods
- ▶ Formulate new stochastic methods.
- ▶ Improve observation strategies.
- ▶ Implement multi-fidelity schedules

Specifications:

- ▶ combine model and data
- ▶ Enable deterministic and stochastic methods

Tasks

- ▶ Deterministic methods
- ▶ Stochastic methods
- ▶ Observations
- ▶ Taking advantage of multi-fidelity modeling
- ▶ Challenges of multi-fidelity in inverse problems: criteria to update reduced models.

Links

PC2-WP1/2/3/4, PC3-WP3

Work Packages

WP5: Optimize at Exascale



Objective: Design and implement of large scale optimization problems

- ▶ combinatorial continuous and mixed optimization
- ▶ surrogate-based optimization
- ▶ shape optimization

Specifications / Tasks

- ▶ Decomposition-based methods
- ▶ Learning-based methods, e.g. surrogate models and multi-fidelity representation
- ▶ Auto-tuning for ML
- ▶ Reduced order and ML for shape optimization

Links

PC2-WP1/2/3/4, PC3-WP2

Work Packages



WP6: Quantify uncertainty at Exascale

Objectives

- ▶ Sensitivity analysis for dimension reduction, ranking and more generally understanding the influence of uncertain input parameters.
- ▶ Propagation of uncertainties
- ▶ Surrogate modeling for UQ
- ▶ Acceleration of the bricks of UQ process steps by leveraging exascale calculations

Links

PC2-WP1/2/3/4, PC3-WP2/3

Specifications / Tasks

- ▶ Extension of kernel methods to complex inputs/outputs
- ▶ global sensitivity analysis (GSA)
- ▶ GSA in the presence of uncontrollable stochastic random input
- ▶ Multi-scale GSA in code coupling/chaining
- ▶ GSA with complex input
- ▶ Links between kernel-based sensitivity indices (HSIC, MMD) and total Sobol indices

Work Packages

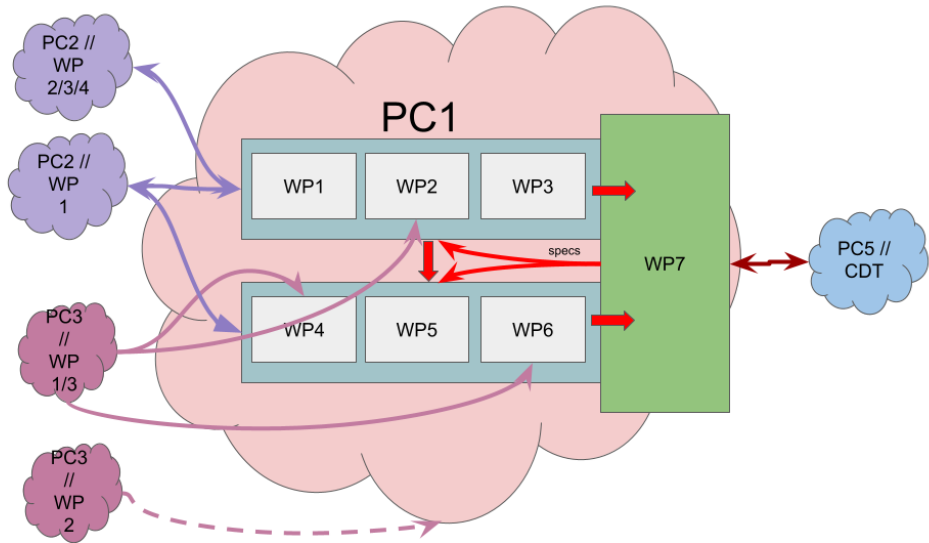


WP7: Demonstrate methods and algorithms at Exascale

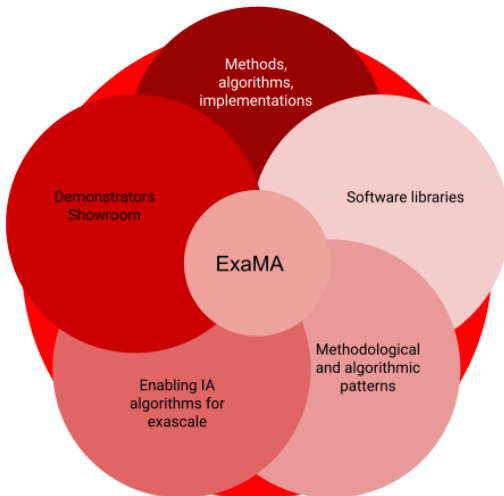
- ▶ Benchmarking on small/mini apps
- ▶ Showroom of methods and algorithms
- ▶ Co-design with the CDT and PC5

Links

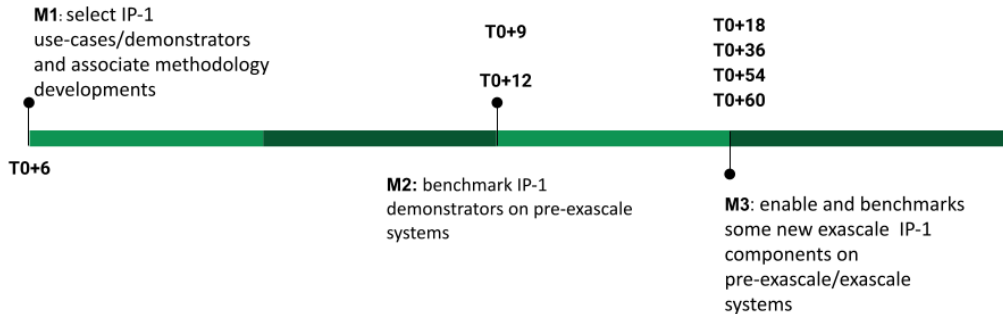
PC2-WP1/2/3/4, PC3-WP2/3 and PC5



Deliverables



Milestones





Relations

Relations



External Partner Status

Setting up this network and creating a group of external partners, we will succeed in

- ▶ bringing together our community to solve scientific challenges to move to the Exascale
- ▶ jointly develop software bricks to scale up to exascale
- ▶ creating/strengthening collaborations between external partners and Exa-MA partners via project co-leads, co-funding and/or use cases
- ▶ better structuring our community to respond effectively to European and international calls for projects.

Relations

Entreprises



Entreprises

- ▶ Expected: EDF, Safran, TotalEnergies, Atos, Airbus
- ▶ Positive contact: Roche

Relations

EPIC & PEPR



EPIC

- ▶ Expected: Onera
- ▶ Positive contact: Ifpen

PEPR

- ▶ Expected: IA
- ▶ Others: Diadem, TRACCS-Météo (in particular PC1-WP4)

Relations

Europe

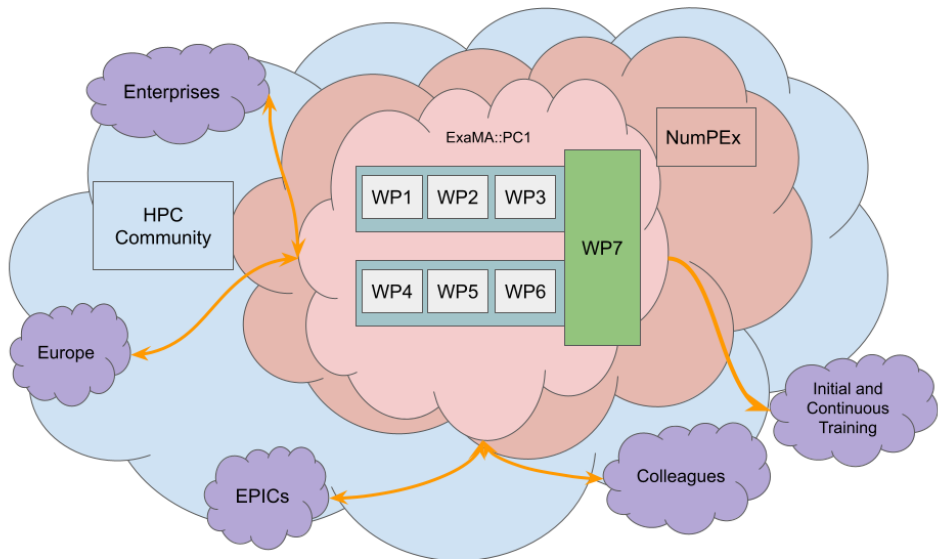


CoE

- ▶ Expected: Hidalgo2, Cheese-2P
- ▶ Others: CoE EoCoE-3

Europe

- ▶ Expected: ERC-Synergy WholeSun, ERC-Synergy EMC2, EuroHPC Microcard, EuroHPC European Master for HPC - EUMaster4HPC
- ▶ Others ?



We are building the Exa-MA community

Thank you for your attention!

The background of the slide is composed of two large, overlapping geometric shapes. A teal-colored shape occupies the top-left corner, while a light beige shape occupies the bottom-left corner. The rest of the slide is white. The word "Appendix" is centered in the white area.

Appendix

Appendix

NumPEx::Exa-MA



Partners

- ▶ CEA
- ▶ INRIA : Bordeaux, Côte d'Azur, Grenoble, Lille, Paris, Saclay
- ▶ IPP
- ▶ Sorbonne Université
- ▶ UNISTRA