PEPR NumPEX // Exa-MA

Methods and Algorithms at ExaScale

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Overview

1. Exa-MA: Methods and Algorithms at Exascale

2. Work Packages

3. Relations

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

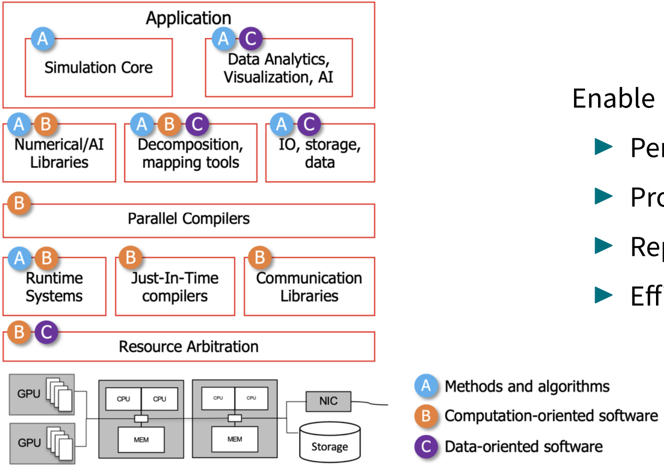
Bottlenecks

- (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

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

Links
PC2-WP2/3/4, PC3-WP3

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

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

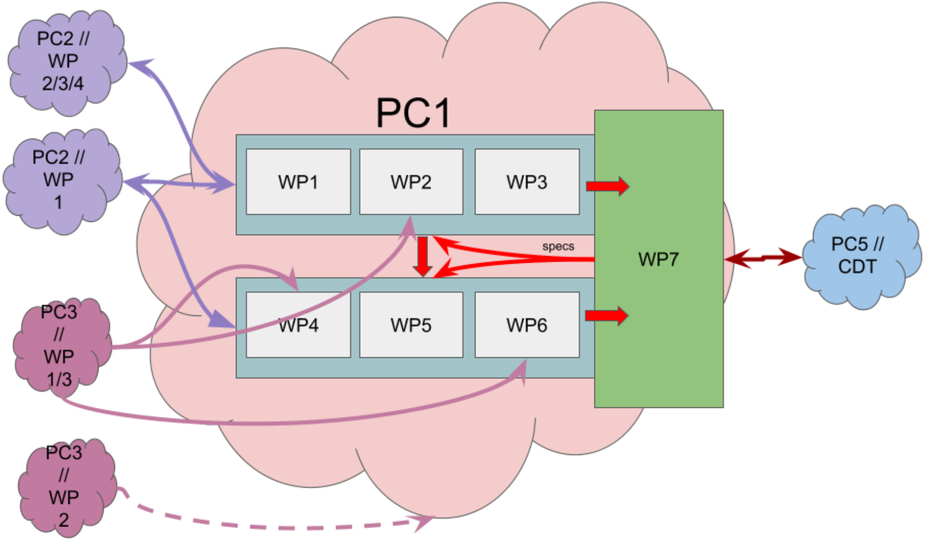
- Extension of kernel methods to complex inputs/outputs
- global sentivitity analysis (GSA)
- GSA in the presence of uncontrollable stochastic random input
- Multi-scale GSA in code coupling/chaining
- GSA with complex input
- Links between kernel-based sensitivity indices (HSIC, MMD) and total Sobol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

Work Packages

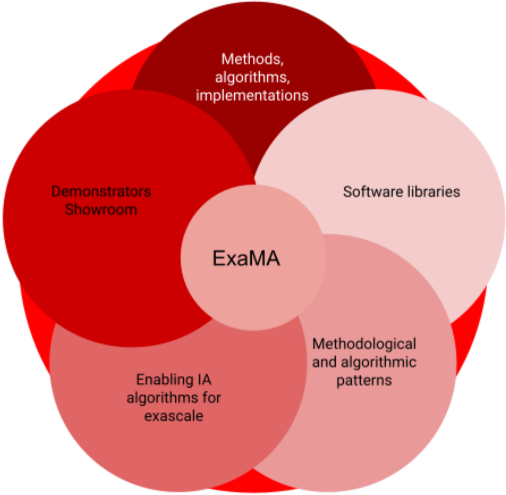
WP7: Demonstrate methods and algorithms at Exascale

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

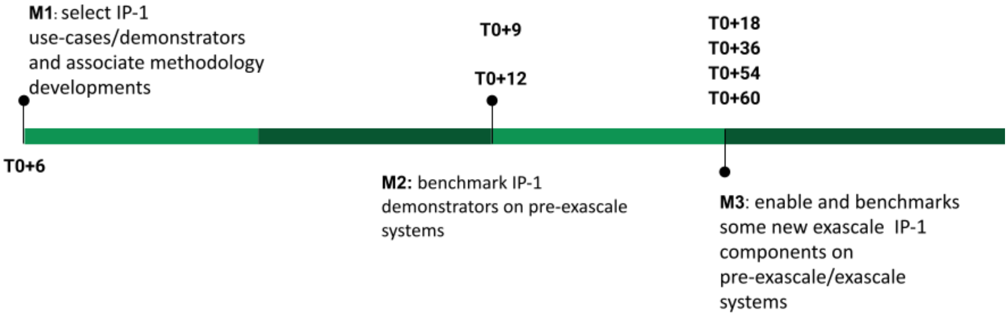
Links
PC2-WP1/2/3/4,PC3-WP2/3 and PC5


PC2 // WP 2/3/4
PC2 // WP 1
PC3 // WP 1/3
PC3 // WP 2
PC1
WP1
WP2
WP3
WP4
WP5
WP6
WP7
specs
PC5 // CDT

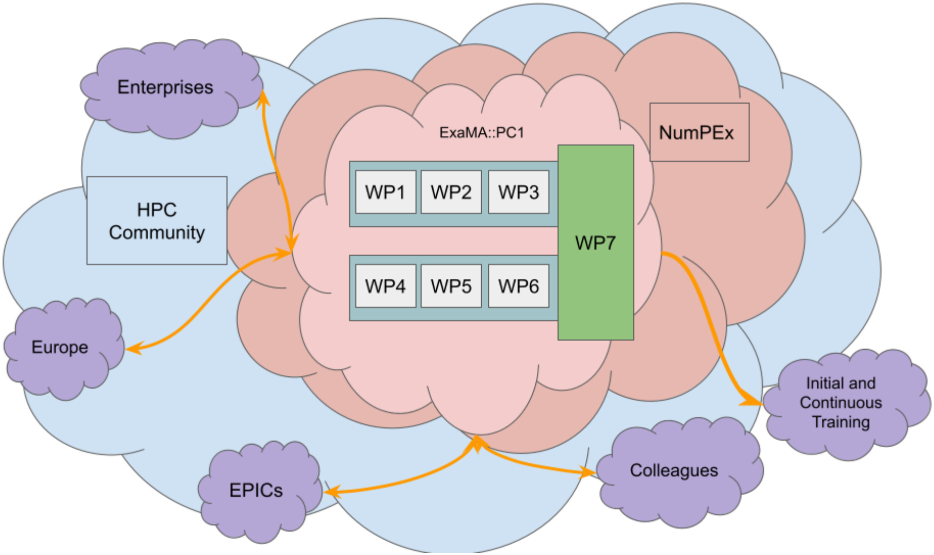
Deliverables



Milestones


M1: select IP-1 use-cases/demonstrators and associate methodology developments
T0+6
T0+9
T0+12
M2: benchmark IP-1 demonstrators on pre-exascale systems
T0+18
T0+36
T0+54
T0+60
M3: enable and benchmarks some new exascale IP-1 components on pre-exascale/exascale systems

Relations


Enterprises
ExaMA::PC1
NumPEx
HPC
Community
WP1
WP2
WP3
WP7
WP4
WP5
WP6
Europe
Initial and
Continuous
Training
EPICs
Colleagues

Relations

External Partners

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
- better structuring our community to respond effectively to European and international calls for projects.

Relations

External Partners

- Entreprises
- EPIC
- Academia
- European projects (CoE,...)
- International collaborations

Tools

External partners will not receive direct funding, BUT the following tools are at our disposal

- Co-funding activities (PhD, post-doc, engineers, etc.)
- Collaboration through co-supervision of PhD students and post-docs
- Collaboration through software developments
- Collaboration through Use Cases
- Co-organization of events
- Consortium creation for European and international projects
- Regular communication on the project and its advances
- Participation to ExaMA and NumPEx events

External Partners

We would like to propose a specific statute and representation of external partners.

Statute

Gouvernance of ExaMA:

- Steering committee : PC1 pilots, PC1 WP leaders and representants of NumPEx
- Scientific advisory committee (european and international)
- **External partners board with both institutional and scientific representatives**

We are building the Exa-MA community

Thank you for your attention!

Appendix

Appendix

NumPEx::Exa-MA

Partners

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