EXASCALE

PEPR NumPEX // Exa-MA

Methods and Algorithms at ExaScale

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Overview

Exa-MA: Methods and Algorithms at Exascale

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Objectives

The main objectives are

- O1: 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;
- O2: to develop or contribute to software libraries allowing to assemble specific critical reusable components, hiding the hardware complexity and exposing only the specific methodological interface ;
- O3: to identify and co-design Methodological and Algorithmic Patterns at exascale that can be reused efficiently in large scale applications (eg in weather forecasting);
- O4: to enable AI algorithms to attain performances at exascale, exploiting the methods (O1) and the libraries (O2) developed; and
- O5: to provide demonstrators through mini-apps and proxy-apps that will be openly available and benchmarked.

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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

- T1.1 Geometry and Mesh at Exascale
- T1.2 Adaptive Mesh Refinement for unstructured grids
- T1.3 Adaptive Mesh Refinement for cartesian or block grids
- T1.4 Finite Element Exascale Framework (FEEF)
- T1.5 Exploit non conforming methods for efficient parallel computing
- T1.6 Error control of time discretization for accurate space refinement
- T1.7 Efficient multimodel/multphysics coupling

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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

- T2.1 surrogate models based on physics driven deep learning
- T2.2 PDE operator learning using NN
- T2.3 data driven model order reduction
- T2.4 non-intrusive and weakly intrusive reduced basis methods for parametrized PDEs
- T2.5 mixing low and high fidelity models
- T2.6 real-time models with super resolution methods

Links

PC2-WP2/3/4, PC3-WP3

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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

- T3.1 Acceleration techniques for subspace-based methods;
- T3.2 High dimensional problems ;
- T3.3 Randomization;
- T3.4 Exploiting data-sparsity and multiple precision and enabling resilience;
- T3.5 Adaptive solution strategies for exascale multiphysical and multiscale models;

Links

PC2-WP2/3/4

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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

- T4.1 Deterministic methods
- T4.2 Stochastic methods
- T4.3 Observations
- T4.4 Taking advantage of multi-fidelity modeling
- T4.5 Challenges of multi-fidelity in inverse problems: criteria to update reduced models.

Links

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

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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

- T5.1 Decomposition-based methods
- T5.2 Learning-based methods, e.g. surrogate models and multi-fidelity representation
- T5.3 Reduced order and ML for shape optimization
- T5.4 Auto-tuning for ML

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

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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

- T6.1 Extension of kernel methods to complex inputs/outputs
- T6.2 global sentivitity analysis (GSA)
- T6.3 GSA in the presence of uncontrollable stochastic random input
- T6.4 Multi-scale GSA in code coupling/chaining
- T6.5 GSA with complex input
- T6.6 Links between kernel-based sensitivity indices (HSIC, MMD) and total Sobol indices

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WP7: Demonstrate methods and algorithms at Exascale

- T7.1 Benchmarking on small/mini apps
- T7.2 Co-design with the CDT and PC5
- T7.3 Showroom of methods and algorithms
- T7.4 Training

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

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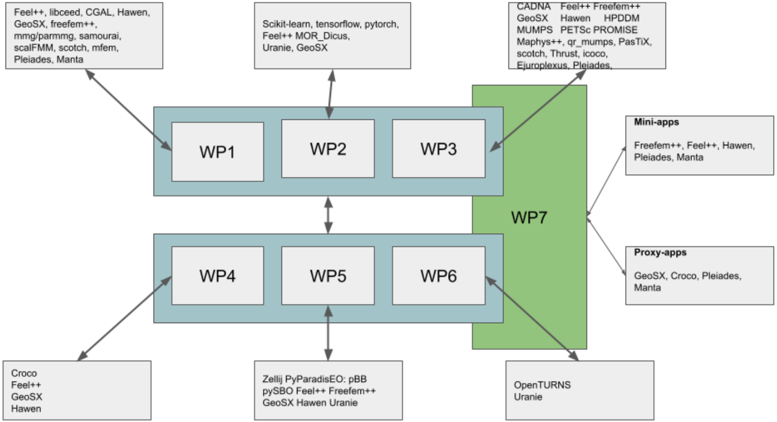
Software - WIP, > Software List



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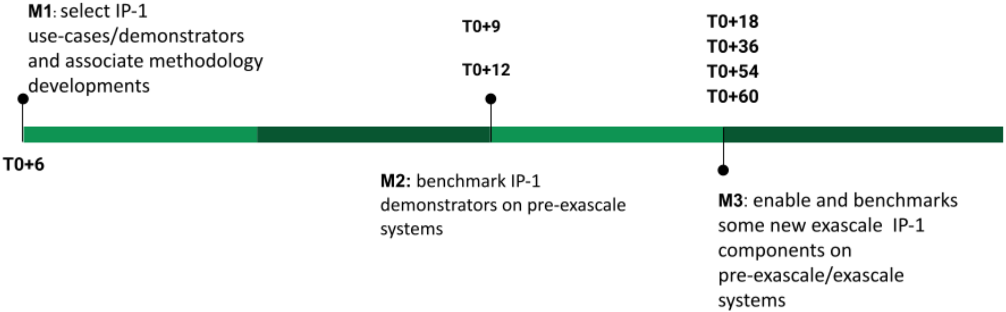
Agenda



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Needs wrt HPC ressources

Software stack

- Enable modern C++ (C++ $\geq$ 17) software, some Fortran and Python software (using wrappoing C++ code)
- Enable conplex software stack and possibly CI/CD pipelines

Runs

- run the benchmarks (mini-apps and proxy-apps) on the HPC platforms, usually "short" runs (minutes to a few hours)
- run on hybrid hardware (not necessarily at scale)

Exa-MA: Methods and Algorithms at Exascale

Status : Teams

Partners

- CEA : DES+DAM
- INRIA : Bordeaux, Côte d'Azur, Grenoble, Lille, Lyon, Paris, Saclay
- IPP : CMAP
- Sorbonne Université : LJLL+LIP6
- UNISTRA : IRMA+Cemosis