EXASCALE

ExaMA

Methods and Algorithms at ExaScale

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Overview

1. PEPR NumPEX

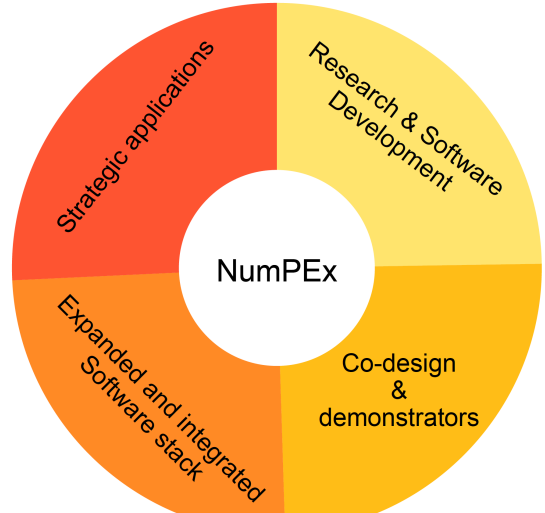
2. ExaMA: Methods and Algorithms at Exascale

PEPR NumPEX

PEPR NumPEX

NumPEX

- **Aggregate the French HPC/HPDA/IA** community
- Contribute and accelerate the emergence of a **European sovereign exascale software stack and strategic applications exascale capability in a coherent and multi-annual framework**
- Integrate and validate **co-designed** innovative methods, libraries and software stack with demonstrators of strategic applications.
- Accelerate science-driven and engineering-driven developers **training and software productivity**



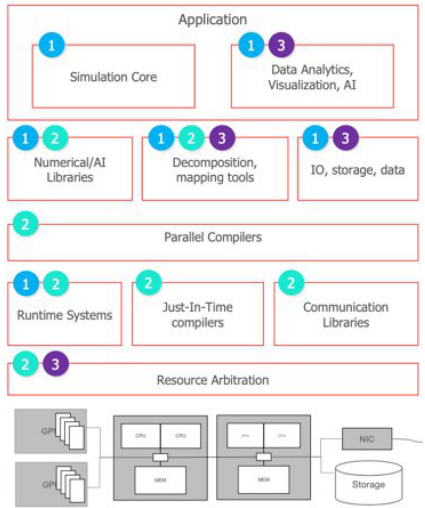
PEPR NumPEX

NumPEx::PC123

PC<n>[a]

1. **PC1 Methods and algorithms for Exascale**
2. **PC2 HPC software and tools for the Exascale**
3. **PC3 Data-oriented software and tools for the Exascale**

[a] PC Projet ciblé ≡ IP Integrated project

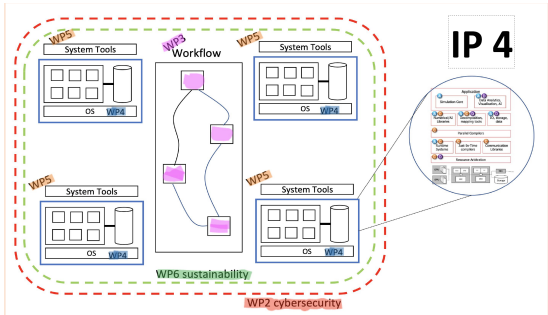


PEPR NumPEX

NumPEx::PC4

Wide-area exascale workflows and architecture

- Data logistic between data sources (e.g. large scientific instruments) and the Exascale system
- Cybersecurity and environmental sustainability focus
- Promoting EU technology (e.g. Atos data node and edge servers)

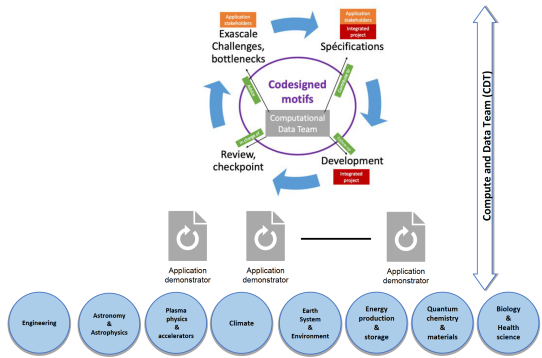


PEPR NumPEX

NumPEx::PC5

IP 5: Co-design development, software productivity, and demonstrators

- Identify and define co-design motifs across domain demonstrators and NumPeX
- Push R&D demonstrators requirements into software R&D (IP 1-4)
- Push integrated software developments into demonstrators

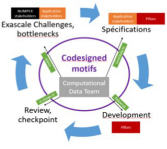


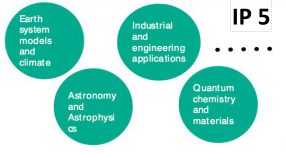
PEPR NumPEX

NumPEx::Software Integration and Productivity

(a) PC1-3

(b) PC4





(c) PC5

NumPEx Exascale Scientific Software Stack (NE3S)

- Robust (tested, CI)
- Packaged and deployable
- Documented, open source, bug tracking, user forums
- Hardware portable (processors, accelerators)
- Interoperable

ExaMA: Methods and Algorithms at Exascale

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ExaMA $\equiv$ PC1 $\equiv$ IP1

NUMPEX/ExaMa concentrates on the exascale aspects of the numerical methods, ensuring their scalability to existing and forthcoming hardware.

Leaders: C Prud'homme & H Barucq

- 5 Work packages
- wide range of topics:
  - Modeling and discretize
  - Linear, multi-linear and coupled solvers at Exascale
  - Combine data and models at Exascale
  - Optimize and quantify uncertainties at Exascale
- Demonstrators through mini-apps will be used to verify the properties of the methods and algorithms developed.

ExaMA: Methods and Algorithms at Exascale

NumPEx::PC1 Team (a work in progress)

- CEA
- INRIA
- IPP
- UNISTRA

Various discussions are occuring on which university to integrate.

ExaMA: Methods and Algorithms at Exascale

Identified Bottlenecks/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

ExaMA: Methods and Algorithms at Exascale

Identified Bottlenecks/Challenges

- (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

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WP1: Modeling and Discretization

- Geometric representation and their discrete counterparts [B2, B6, B7, B9, B11-B13]
- physics-based models[B7, B10]
- AI-driven, data-driven, reduced-order, and more generally surrogate models[B2, B7, B8, B10-B13]
- Multi-fidelity models [B2, B7, B8]

Proposition

- Extract AI-driven, data-driven, reduced-order, and more generally surrogate models
- need to discuss multifidelity

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WP2: Linear, Multi-linear and Coupled Solvers at Exascale

- Acceleration techniques for subspace-based methods [B1, B2, B5, B7, B9-B10].
- High dimensional problems [B1, B2, B5, B7, B10]
- Randomization [B1, B2, B7, B10]
- Exploiting data-sparsity and multiple precision [B1, B2, B5, B7, B10]
- Adaptive solution strategies for exascale multiphysical and multiscale models [B7, B9-B11]

Propositions

- need to include computer algebra people ?
- need to include resilience experts ?

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WP3: Combine data and models, inverse problems at Exascale

[B2, B6, B7, B8, B13]

- Deterministic methods
- Stochastic methods
- Observations
- Taking advantage of multi-fidelity modeling

proposition

- add Inverse Problem to WP 3 (currently in WP 4)

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WP4: Optimize and quantify uncertainty at Exascale

[B6-B8, B10, B13]

- Optimization
  - shape, dynamic shape optimization
  - combinatorial optimization
  - policy based optimization
  - automated learning/AI for advanced design
- Uncertainty quantification including
  - uncertainty propagation
  - sensitivity analysis
  - robust inversion
  - UQ at different scales
  - weak vs strong UQ

Proposition

Split WP5 into two parts: Optimization and UQ

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WP5: Demonstrate methods and algorithms at Exascale

[B1-B13]

- Properties Verification on small/mini apps within PC1
- Co-design with the CDT and PC5

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Principles

- **Openness** and **transparency** of the project
- **Collaboration** with other projects :
  - co-design with PC5, collaboration with PC2,3,4
  - collaboration with other projects e.g. EuroHPC projects(Coe) and other PEPR (IA, Diademe,TRACCS-Météo...
- **Inclusiveness** of the community
  - use the project as leverage for co-funding or, also, collaborating outside the project eg phd co-advisors
  - training : initial(train future PhD students) and continuous (broader community)

ExaMA: Methods and Algorithms at Exascale

- Project proposal by the end of year with inter PC discussion as well as external partners
  - UNISTRA is the lead partner for PC1
  - budget is a bit more than 6Mio, we expect roughly a bit less than 1Mio: PhD, Engineers, Post-Docs
  - find synergies with ITI IRMIA++: research and funding wise
  - 20 pages including images
  - a detailed financial annex
  - **Note**: The context and the general principles are already there, we need to focus on the research and the details within the given framework
- End of year/March 2023 discussion with ANR, Contracting,...
- Project start in March/April 2023 (in sync with other PCs)
- Total duration : 5 years (+18 months)