



ExaMA

Methods and Algorithms at ExaScale

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Overview



1. Introduction

2. Presentation of ExaMA

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Introduction

Introduction



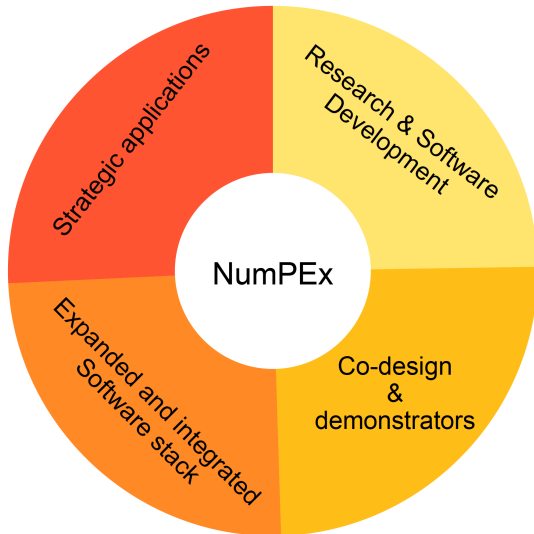
Tour de Table

- ▶ CEA
 - ▶ DAM **Lydie Grospellier** (LG)
 - ▶ DES **Vincent Faucher** (VF) **Isabelle Ramière** (IR)
- ▶ INRIA
 - ▶ Bordeaux **Hélène Barucq** (HB) **Luc Giraud** (LGi)
 - ▶ Grenoble **Arthur Vidard** (AV)
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 - ▶ Sofia **Stephane Lanteri**(INRIA-Sofia) (SL)
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- ▶ UPICARDIE **Mark Asch** (MA)
- ▶ UNISTRA **Christophe Prud'homme**(CP)

Introduction



- ▶ **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**



Introduction

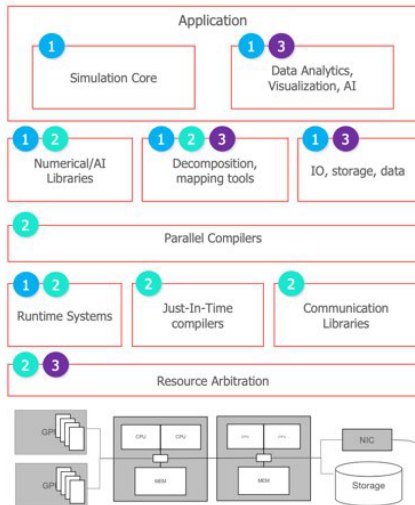
PC123



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

^aPC Projet ciblé \equiv IP Integrated project



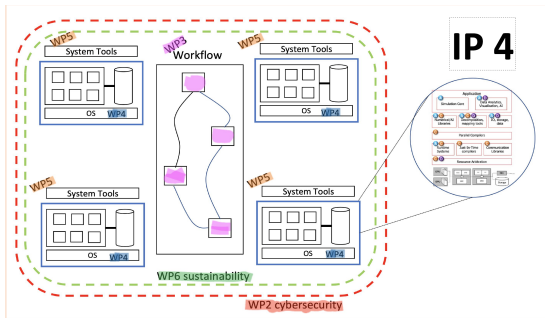
Introduction

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)



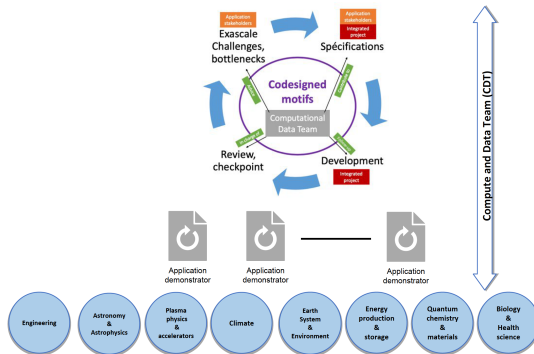
Introduction

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



Introduction

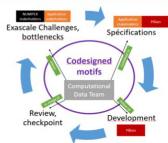
NumPEx Software Integration and Productivity



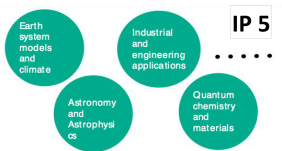
(a) PC1-3



(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

Introduction



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.

Introduction

initial Working Group



- ▶ 10 persons in initial work groups
- ▶ Other teams consulted on various topics
- ▶ Initial Budget: 7 Mio Euros, now a bit more than 6Mio Euros

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Presentation of ExaMA

Presentation of ExaMA



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

Presentation of ExaMA

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]

Persons Involved

VF, MM, SL,

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]

Persons Involved

LG, LGi, IR,...

Proposition

- ▶ need to include computer algebra people

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WP3: Combine data and models at Exascale

[B2, B6, B7, B8, B13]

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

Persons Involved

AV, MA

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

Persons Involved

JG, YP, ET

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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

Persons Involved

LGr + ALL

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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)

Presentation of ExaMA



- ▶ Project proposal by the end of year with inter PC discussion as well as external partners
 - ▶ 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)

Oct 20

Next Global Meeting INRIA Paris

Presentation of ExaMA

Project Management



Project Management

- ▶ Several co-leads per WP
- ▶ Meeting every 2 or 3 weeks to advance the writing

Tools

- ▶ Use of Google Doc and GitHub (repo and project management)
- ▶ Creation of an archived mailing list