



ExaMA

Methods and Algorithms at ExaScale

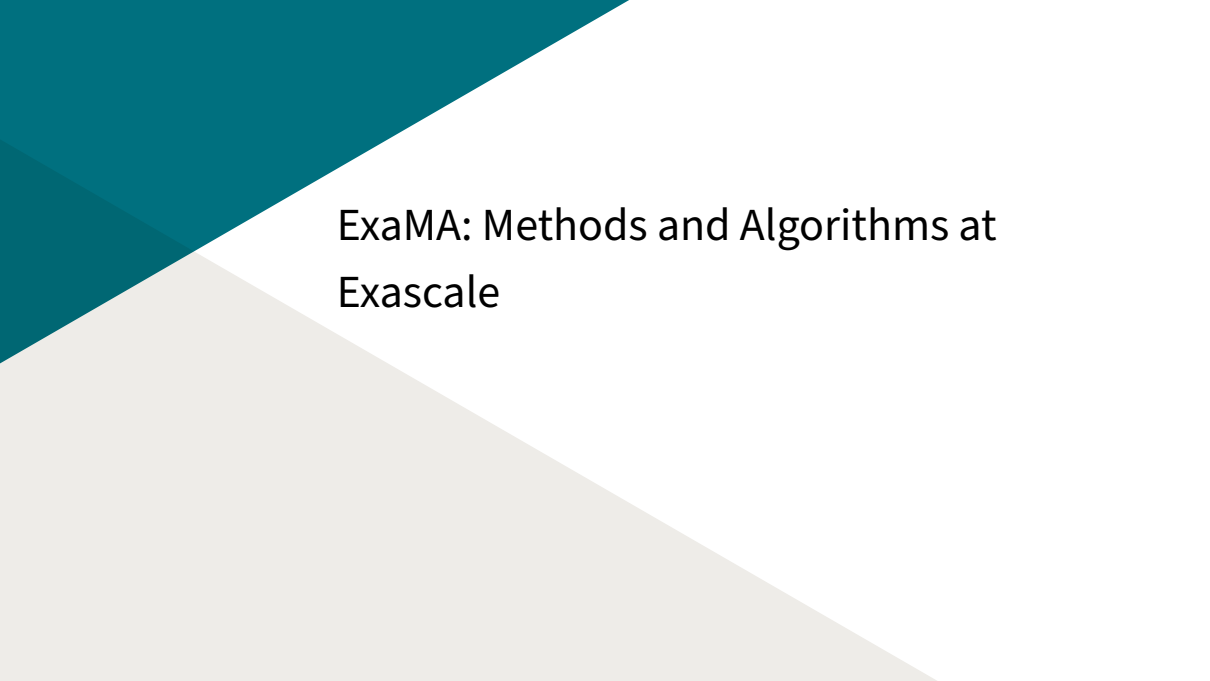
Christophe Prud'homme & Hélène Barucq

October 20, 2022

Overview



1. ExaMA: Methods and Algorithms at Exascale
2. Steering team
3. Identified Bottlenecks/Challenges
4. Work Packages
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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 still in progress)

Organismes financés

- ▶ CEA : DES(1 - 2), DAM (1)
- ▶ INRIA : Bordeaux(2-4), Côte d'Azur (2), Grenoble(1), Lille(1), Paris(1)
- ▶ IPP (CMAP, Inria ASCII, Inria POEMS)
- ▶ UNISTRA (IRMA-MOCO/Cemosis, Inria Tonus)

Other teams

- ▶ Sorbonne Université ? (LJLL: Y Maday, S Labbé; LIP6 Theo Marie, P Jolivet)
- ▶ ENS Lyon ? (Y Robert,)

ExaMA: Methods and Algorithms at Exascale



Budget

- ▶ si un universitaire est dans une equipe inria financée par Numexp, pas de souci
- ▶ Sinon comment collaborer (si necessaire)? Sur les sites, pourra t'on nous appuyer sur les conventions existantes pour mettre en place des collaborations/des co-financements/....co-directions/... ?
 - ▶ Bordeaux:
 - ▶ Cotes d'Azur :
 - ▶ Grenoble :
 - ▶ Lille: :
 - ▶ Paris :
 - ▶ Saclay :
 - ▶ Strasbourg :

Recemment accord cadre inria / cnrs signé



Steering team

Steering team



- ▶ CEA
 - ▶ DAM **Lydie Grospellier** (LGr)
 - ▶ DES **Vincent Faucher** (VF) **Isabelle Ramière** (IR)
- ▶ INRIA
 - ▶ Bordeaux **Hélène Barucq** (HB) **Luc Giraud** (LGi)
 - ▶ Grenoble **Arthur Vidard** (AV)
 - ▶ Lille **El-Ghazali Talbi** (ET)
 - ▶ Paris **Laura Grigori** (LG) **Frédéric Nataf** (FN)
 - ▶ Sofia **Stephane Lanteri**(INRIA-Sofia) (SL)
- ▶ IPP **Josselin Garnier** **Marc Massot** (MM) **Loic Gouarin** (LGo)
- ▶ UPICARDIE **Mark Asch** (MA)
- ▶ UNISTRA **Christophe Prud'homme**(CP) **Emmanuel Franck** (EF) **Yannick Privat** (YP)

to be completed

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Identified Bottlenecks/Challenges

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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

Identified Bottlenecks/Challenges



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

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Work Packages

Work Packages

WP1: Modeling and Discretization



- ▶ Geometric representation and their discrete counterparts [B2, B6, B7, B9, B11-B13]
- ▶ physics-based models[B7, B10]

Data

Contributors VF, MM, PA, CP, PH Links with
PC2-WP2/3, PC3-WP3

Work Packages



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

- ▶ AI-driven, data-driven, reduced-order, and more generally surrogate models[B2, B7, B8, B10-B13]
- ▶ Multi-fidelity models [B2, B7, B8]

Data

Contributors: SL, EF, HB, CP, JG

Links with PC2-WP2/3, PC3-WP3

Work Packages



WP3: 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]

Data

Contributors: LG, LGi, VF, FN, PJ, ... Links with PC2-WP2/3

Work Packages



WP4: Combine data and models, inverse problems at Exascale

[B2, B6, B7, B8, B13]

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

Data

Contributors: AV, MA, HB, CP, JG
Links with PC2-WP2/3, PC3-WP3

Work Packages

WP5: Optimize at Exascale



[B6-B8, B10, B13]

► Optimization

- shape, dynamic shape optimization
- combinatorial optimization
- policy based optimization
- automated learning/AI for advanced design

data

Contributors: ET, YP, CP

Links with PC2-WP2/3, PC3-WP2

Work Packages



WP6: Quantify uncertainty at Exascale - Links with P2-WP2/3,P3-WP2/3

[B6-B8, B10, B13]

- ▶ Uncertainty quantification including
 - ▶ uncertainty propagation
 - ▶ sensitivity analysis
 - ▶ robust inversion
 - ▶ UQ at different scales
 - ▶ weak vs strong UQ

data

Contributors: JG, (JMM,) MA

Links with PC2-WP2/3,PC3-WP2/3

Work Packages



WP7: Demonstrate methods and algorithms at Exascale

[B1-B13]

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

Data

Contributors: LGr et ALL

Links with PC2-WP2/3, PC3-WP2/3 and PC5

Work Packages



Deliverables

- ▶ 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.
- ▶ Software libraries allowing to assemble specific critical reusable components, hiding the hardware complexity and exposing only the specific methodological interface
- ▶ Methodological and Algorithmic Patterns at exascale that can be reused efficiently in large scale applications (eg in weather forecasting)
- ▶ Enabling AI algorithms to attain performances at exascale, exploiting the methods (point 1) and the libraries (point 2) developed.
- ▶ Demonstrators

Work Packages

Milestones



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

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 word "Relations" is centered in the white area.

Relations

Relations

Entreprises



Entreprises

- ▶ Will depend on final team, will be discussed in next coordination meeting
- ▶ Expected: EDF, Safran, Total, Atos
- ▶ Others: PlasticOmnium, Arkema, Entreprise consortium MOR_DICUS...

Relations



EPIC & PEPR

EPIC

- ▶ Will depend on final team, will be discussed in next coordination meeting
- ▶ Expected: Onera (discussions also next week)

PEPR

- ▶ Expected: IA
- ▶ Others: Diadem, TRACCS-Météo...

Relations



Europe

CoE

- ▶ Will depend on final team, will be discussed in next coordination meeting
- ▶ Expected: Hidalgo2, Cheese
- ▶ Others: CoE EoCoE-3

Europe

- ▶ Will depend on final team, will be discussed in next coordination meeting
- ▶ Others: ERC-Synergy EMC2, EuroHPC Microcard, H2020 RIA Digital Twin Bim2Twin, EuroHPC European Master for HPC - EUMaster4HPC

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Project Management

Project Management

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)

Project Management

Work plan



Project Management

- ▶ Several co-leads per WP
- ▶ Meeting almost every week to advance the writing

Tools

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



Budget

Budget



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Questions

Questions



- ▶ Quid des thématiques transverses ? eg résilience, energie
- ▶ Quelle est la stratégie logicielle ? Open-Source ? Closed Source ? Probablement 80/90% open source, le reste fermé
- ▶ doit-on déclarer en partenaire un établissement parce qu'un de ces membres participe au projet? C'est plutôt oui même si la personne n'intervient pas avec un financement de NumpeX. A voir donc avec le consortium.
- ▶ doit-on prévoir les possibles co-financements externes dans le montage du projet? autrement dit, les accords existant déjà entre les différents établissements sont-ils suffisants pour mettre en place des co-financements? Il existe des ED qui refusent qu'il y ait deux financeurs de thèse différents, besoin de conventions de reversement donc.