Exa-DI Co-design Motif Workshop

Efficient discretisation for PDEs @ exascale

J-P. Vilotte (CNRS), PI Exa-DI project
NumPEx: 5 years national project (CNRS, CEA, INRIA, Universities) - 40,8 M€

Coordinators: J.Y. Berthoud (INRIA), J. Bobin (CEA), M. Krajecki (CNRS)

Aggregate the French HPC/HPDA/AI community, foster new collaborations and synergies

Co-develop, integrate, validate and deliver an expanded exascale software stack to accelerate Exascale applications productivity and sustainability

Contribute and accelerate the emergence of a European sovereign exascale software stack and performant strategic exascale applications

Build a multidisciplinary national workforce and develop training to improve CSE application development and software integration methodologies
NumPEx work plan

Exascale computing

CSE Applications

ExaMA
algorithmic motifs

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algorithmic motifs

C. Prud’homme (UNISTRA)
H. Barucq (INRIA)

ExaSoft
parallel programming and execution environments

R. Namyst (INRIA)
A; Buttari (CNRS)

ExaDost
in-situ data reduction and analytics, storage, IO

G. Antoniu (INRIA)
J. Bigot (CEA)

ExaAtow
data logistics, workflows across the continuum

J.-P. Vilotte (CNRS)
V. Brenner (CEA)

ExaDIP
software co-design & co-development, integration and delivery

ExaAtow
data logistics, workflows across the continuum

F. Bodin (U. Rennes)
T. Deutsch (INRIA)

Review-and-Adapt
checkpoint

Push application requirements
Pull software developments

Compute Data Team

software co-design & co-development, integration and delivery

Co-design

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Challenges:
- Exascale CS&E applications.
- Expanded Exascale science-driven software stack.
- Exascale software components integration, deployment and reuse.
- Exascale application performance portability and sustainability.

Objectives:
- Co-analyse CSE application demonstrators (ADs) across NumPEx
- Co-identify cross-cutting computational and communication motifs
- Co-develop libraries, frameworks, proxy and mini apps
- Co-develop Community Software Policies and sustainable software foundations
- Integrate and deliver interoperable SDKs as needed by the Exascale ADs
- Exercise, expand and harden sustainable core components for performance portable programming models (e.g. Kokkos, Raja)
- Establish a national computational data team to enable agile co-design projects
- Broaden awareness/use of robust software components in exascale application development methodologies

Team: CNRS, CEA, INRIA
Budget: 9.3 M€ (including CoEs co-funding)
Co-designed software portfolios, proxy-apps & benchmarking

Context:
- Exascale Computing Project (ECP): DOE, NSF
- Fugaku & Fugaku NEXT co-design projects
- Euro-HPC JU initiatives, ETP4HPC

Problematics:
- CSE applications development methodologies, accuracy & performance portability
- Co-designed application-driven software technology and logical software components portfolios
- Proxy-apps / many-apps suites
- Hardware & Integration, Testing & Profiling tools, Benchmarking specifications
High-impact science and engineering exascale challenge problem

Criteria for assessing successful completion of the challenge problem

A figure of merit (FOM) quantifying enhancement of performance and rate of science

Demonstration and assessment of effective Software Development Kits integration

Astronomy & Astrophysics
Earth System Models & environment
Environmental extreme events
Computational biology & Life science
Laboratory laser-plasma physics
High-energy particle physics
Quantum chemistry and materials
Digital health
Environmental & societal risks
Urban systems planning
Magnetically confined fusion plasma (ITER)
Sustainable Transport & mobility
Energy production & transport

Exascale Challenges
• Heterogeneous exascale and post-exascale architectures
• New multi physics and multi-scale capability
• On-line streaming data analysis /reduction
• AI-enabled big data analytics and dimension reduction
• New mathematical approaches and model improvements
• Leveraging robust and accurate logical collection of interoperable software components (libraries, tools and frameworks)
• Improving performance portability by exercising new performance portable programming models
• New scalable task-based programming and execution models
• Foundations for a sustainable exascale scientific software stack
Objectives
• proceed and integrating logical suites of software components and tools with emerging hardware technologies
• Deliver software development kits easily deployable and instantiated into CSE application environments for testing, development acceleration and requirements feedback.
• Facilitate collaboration between software packages, enable integration and/or interoperability with overall NumPEx technologies stack, streamline developer and user workflows, and coordinate releases

Flexibility/Interoperability
• support a wide range of CSE application algorithmic requirements
• enable exploration of new algorithms and frameworks as need by the CSE applications.
• avoid unnecessary restrictions on programming models and how application developers construct their algorithms
• allow application developers to interact with software components at different levels of abstraction
• exercise and harden abstraction layers (e.g. Kokkos, Raja) for hardware-aware technologies

Proxy and mini app suites
• represent algorithms, data structures and layouts, optimisation and other computational characteristics
• allow to measure performance gain, scalability, performance portability, and software quality
• enable continuous integration, testing and benchmarking experiments with standardised performance tools to guide optimisations, understand bottlenecks and trade-off between software components
Efficient discretisation for PDEs @ Exascale
- PDE-based multi-physics multi-scale simulations (FV, FEM, SEM, HDG), unstructured hexahedral and tetrahedral meshes, AMR

Block-structured AMR @ Exascale
- Multi-physics CFD, transport and particle-based simulations

Particle-based methods @ Exascale
- MD, QMD, AIMD, gravitational N-body, SPH, PIC simulations

On-line analysis @ Exascale
- Online analysis, reduction, aggregation, AI-based multi physics and multi-scale coupling

Big data analytics @ Exascale
- AI-based data analytics, scattering transform, detection, classification, reinforcement learning, manifold learning, DML training

Artificial Intelligence @ Exascale
- Physics-based machine learning, PINNs, surrogate models, DML learning, AI-based inverse, inference, control and design problems

Combinatorial methods @ Exascale
- Static and dynamic combinatorial (graph) kernels at scale

Cross-cutting co-design algorithmic motifs
- Accelerate the development and improve performance portability of exascale ADs
- Address common patterns of communication and computation
- Improve scientific software development methodologies balancing trade-off between fine-grained control and modularity based on integrated/interoperable libraries

Agile co-development projects
- Co-analyse existing software components, e.g. from ECP co-design centres
- Co-identify gaps and missing functionalities as needed by the ADS
- Co-develop logical software components (libraries, programming and execution models, frameworks) with different interoperability levels and abstraction layers
- Integrate into re-usable SDKs that can be easily managed, deployed and instantiated as needed by ADs
- Co-develop meaningful proxy-apps and mini-apps to integrate, test and benchmark the developed software components (performance, trade-offs)
**Exa-DI flow of product delivery and deployment**

**Exa-DI Program Forum**
Program Manager (CDT), Release Train Engineer (CDT), NumPEx PCs’ representatives, ADs leaders

**Co-design project: algorithm motif 1**
Product owner (CDT), Scrum Master (CDT), Agile team: CDT experts, NumPeX PCs’ experts, ADs experts

**Co-design project: algorithm motif 2**
Product owner (CDT), Scrum Master (CDT), Agile team: CDT experts, NumPeX PCs’ experts, ADs experts

**Co-design project: SDK 1**
Product owner (CDT), Scrum Master (CDT), Agile team: CDT experts, NumPeX PCs’ experts, ADs experts

**Co-design project: SDK 2**
Product owner (CDT), Scrum Master (CDT), Agile team: CDT experts, NumPeX PCs’ experts, ADs experts

**Enabling team**
Transactional Software packaging technologies
Spack, OpenHPC, GUIX-HC
Singularity...
CDT experts

**Communications and release**
GitLab, OpenHPC, workshops, conferences, publications

**HPC and CSE broader community**

**Co-design / Co-development agile software projects**
Algorithmic Motifs

**Software Development Kits (SDKs)**
Integration of software components (libraries, frameworks)

**Application Demonstrators**
Integration of NumPEx ST products via SDKs

**EuroHPC/GENCI Systems**
Exascale, Pre-exascale
National (TGCC, IDRIS, CINES)

Contributions complies with SDK specifications and NumPEx Software Community Policies

**APIs**
Software Development Kits

- Logical collections of value-added interoperable software components as needed by ADs,
- Integrated and delivered using meta-builder and container systems enabling a combined deployment on exascale systems and combination as needed by CSE applications

Community Software Policies

- Improve software quality, usability, access and sustainability;
- Provide foundation for deeper levels of interoperability
- Establish a certification process to label software (maturity, portability, compliance)

Software packaging and deployment technologies

- Promote common Meta-builder systems (e.g. SPACK, GUIX, NIX) and container technologies (e.g. Singularity)
- Extend/harden new capabilities enabling deployment on exascale systems and regression testing

Software Integration hub

- Enable access to externally managed software integration and testing platforms
- Synergetic collaborations with national computing facilities, vendors and other initiatives

ExaDI Software Development Kits (SDKs)

Timeline:

SDK release 1  SDK release 2  ................ SDK release n
Ecosystem

- Unstructured PDE discretisation libraries
- High-order meshes libraries
- Unstructured adaptive mesh refinement
- Dynamic unstructured anisotropic meshing
- Efficient high-order operator format / Representation
- Batched dense tensor contractions
- Distributed linear algebra operations
- Scalable matrix-free solvers
- General interpolation
- Visualisation of high-order meshes and functions

NumPEx Application Demonstrators

- **Climate/Ocean**
  - Croco, PEPR TRACCS
- **Aeronautics/CFD, Combustion**
  - Sonics/Onera, Safran/INRIA, Yales2
- **Magnetically confined fusion plasma**
  - Gisela-X
- **Earth & environment**
  - GEOXIM-IFPEN, GEOSX-Total
  - Coe ChEese-2P: xSHELLS, SPECfem3D
- **Coupled Urban systems**
  - Coe Hidalgo2, OpenFOAM
- **Industrial Risk & Safety evaluation**
  - Manta

Software components, standards

- **ECP CEED**: MFEM, LibCEED, LibParanumal, PUMI, Omega_h, MAGMA, PETSc, SUNDIALS, Hypre, SLEPC, SuiteSparse, Gingko, METIS, GLVis, VisIt, ParaView, Umpire, OCCA, RAJA, HDF5/ADIOS, PyPi
- **NumPEx**: Feel++, Freefem++, GEOSX, MANTA, Mathphys++, Gyselalibx, PetSc, Hypre, MUMPS, PaStiX, Chameleon, HPDDM, Alien, Scotch, PARADIGM/CWPI, METIS, GAMMA's mesh, Mmg/ParMmg, DDC, CGGAL, MED/Coupling, AGIOS, HDF5, StarPU, Dask, Deisa, Kokkos-Kernels, PyPi

Efficient Discretisation for PDEs @ Exascale
Workshop objectives and return

**Develop and share a common understanding of:**
- Exa-DI co-design and co-development agile process driving collaboration between software packages, integration and/or interoperability with overall NumPEx technologies, streamline developer and user workflows, maintaining testing and benchmarking, and coordinate SDK releases
- role and responsibility in this process between the R&D teams in the different NumPEx PCs, the ADs’ development teams, and the Exa-DI Computational and Data Team
- CDT application liaisons and one-to-many interactions based on the development of efficient discretisation for PDEs @ exascale

**Co-identify across several ADs:**
- existing exascale software issues and barriers,
- software components (libraries, frameworks, abstraction layers, programming and execution environments) to be developed and integrated for accelerating exascale ADs development and improving their performance portability

**Co-analyse the software stack developed in the ECP CEED project:**
- what software components can be leveraged,
- what gaps and missing functionalities need to be addressed
- what new complementary and/or alternative components need to be co-developed by agile teams (objectives, deliverables)
- what mini-apps and proxy-apps need to be co-developed with the ADs and shared with specifications for testing and benchmarking methodologies

**Co-define agile co-development teams**
- identified contributions of different R&D teams in-and-across the NumPEx PCs, and of the ADs,
- necessary resources and expertises to be gathered in the CDT to drive the agile co-development process

**Organise follow-up with series of identified deep-dive sessions**