Exa-DI Co-design Motif Workshop

Block-structured AMR @ exascale

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PI and co-PI Exa-DI project

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NumPEx: Capable Exascale

**NumPEx**: 6 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 to and accelerate the emergence of a European sovereign exascale software stack and productive strategic exascale applications

- Establish a multidisciplinary national workforce and develop training to improve CSE application development and software integration methodologies

**NumPEx**

- Co-design & demonstrator applications
- Expanded and integrated software stack
- Strategic applications
- Research & Software Development

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NumPEx work plan

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

ExaDIP
software co-design & co-development, integration and delivery
J.-P. Vilotte (CNRS)
V. Brenner (CEA)

CSE Applications
**Exa-DI project**

**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 Software Development Kits (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 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)
CSE application demonstrators

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

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
Identified cross-cutting algorithmic motifs

Efficient discretisation for PDEs @ Exascale
- PDE-based multi-physics multi-scale simulations (FV, FEM, SEM, HDG), unstructured hexahedral and tetrahedral meshes, isotrope & anisotrope 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 physic 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

Goals
- proceed and integrate logical suites of software components and tools addressing cross-cutting computation and communication patterns with emerging hardware technologies
- Deliver them as software development kits easily deployable and instantiable within CSE application environments for testing, accelerating exascale development and feedback.
- Improve scientific software development methodologies balancing trade-off between fine-grained control and modularity based on integrated/interoperable libraries

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

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
- support collaborative and coordinated continuous integration/benchmarking experiments with standardised performance tools to guide optimisations
**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

**Timeline:**

- SDK release 1
- SDK release 2
- .............
- SDK release n
Multi-scale and particle-based multi-physics and multi-scale simulations
• Separating data structures and basic operations from algorithms that use them

Algorithms
- Block-structured mesh representation
- Data abstractions and containers (mesh, particles, embedded boundaries)
- Operation stubs and operator formats
- AMR time stepping (sub-cycling) approaches
- Linear Multigrid solvers
- ODE solvers
- Memory management and I/O optimisation
- Communications (particle-particle, particle-mesh)
- Task-based parallelism and dynamic execution model
- Load balancing
- Abstraction layers (portable programming model)

Application Demonstrators
- Cosmology/astrophysics
  - Dyablo-GINEA, Dyablo-WholeSUN, PHARE
- Ocean Modelling
  - Croco/NEMO
- Magnetically confined fusion plasma
  - Gisela-X
- Earth & environment
  - GEOXIM-IFPEN, GEOSX-Total
- Aeronautics/CFD Combustion
  - Sonics/Onera, Safran, Yales2
- Industrial Risk & Safety evaluation
  - Manta

Software components, standards
- **ECP AMReX**: AMReX, ALPINE/ZFP, PETSc, Hypre, SUNDIALS, CodeGen MxUI/MUI, AMRVis, SENSEI, VisIt, ParaView, Exa I/O/HDF5, Kokkos, RAJA
- **NumPEx**: Dyablo, SAMURAI, ArcaneFramework, GEOS, MGRIT/Parareal, PyMGRIT, MCGSolver, MUMPS, Scotch, LvArray, DDC, AGIOS, Damaris, METIS, HDF5

ECP AMReX SDK: https://amrex-codes.github.io/amrex/

http://cucis.ece.northwestern.edu/projects/DAMSELF/

ATPESC 2022, July 31 – August 12, 2022
**Exa-DI flow of product integration and delivery**

**Enabling team**
- Transactional Software packaging technologies
  - Spack, OpenHPC, GUIX-HPC, NIX
  - CDT experts

**Exa-DI strategic Committee**:
- WP leads & co-leads, PCs representatives
- ADs leaders

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

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

**Co-design project: algorithmic 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

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

**HPC and CSE broader community**

**Workshops on co-design Motifs**
- Application Demonstrators R&D PCs teams

**Mini-apps and proxy-apps**
- Application Demonstrators R&D PCs teams

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

**APIs**

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

**EuroHPC/GENCI Systems**
- Exascale & Pre-exascale National (TGCC, IDRIS, CINES)
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 logical software components portfolios
- Co-develop well-specified proxy-apps / many-apps suites
- Software integration, testing & profiling tools, benchmarking specifications
Workshop objectives and return

Develop and share a common understanding of:
- Exa-DI agile co-design and co-development process driving collaboration between software packages development and integration with overall NumPEx technologies, streamline developer and user workflows, maintaining testing and benchmarking, and coordinate SDK releases
- role and responsibility 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 block-structured AMR @ exascale

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

Co-analyse the software stack developed in the ECP AMReX project:
- what software components can be leveraged,
- what gaps and missing functionalities need to be addressed
- what new and/or alternative components need to be co-developed by agile teams (objectives, deliverables)
- what mini-apps and proxy-apps can 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 a follow-up with a mini-apps / proxy-apps GT