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FRANCE 2030 PROGRAMME DE RECHERCHE NUMÉRIQUE POUR L'EXASCALE

ExaMA Work Package 1

Discretization Methods (Geometry/Physics)

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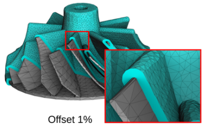
January 19-21, 2026 – ExaMA General Assembly

Overview

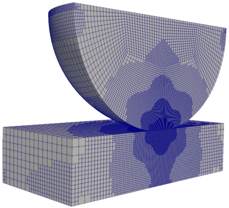
WP1 Objectives

- Objective 1: *Geometric domain representations*

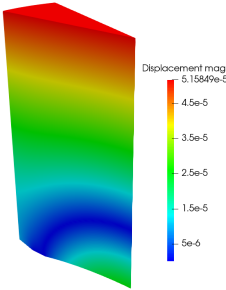


Challenges related to geometric representation robust to defects and resilient to heterogeneous input

- Objective 2: *Mesh adaptivity*



(Un-)structured mesh adaptivity and efficient parallel representations of large-scale models



- Objective 3: *Physics-based models*

Multiple phenomena or process couplings at multiple scales in space and time.

WP1 Tasks

- T1.1 Mesh generation
- T1.2 Adaptive Mesh Refinement for unstructured grids
- T1.3 Adaptive Mesh Refinement for Cartesian or block grids
- T1.4 Finite Element Exascale Framework
- T1.5 Exploit non conforming methods for efficient parallel computations
- T1.6 Time-strategy for evolution equations when the mesh is dynamically adapted
- T1.7 Efficient multimodel/multiphysics coupling

N.B. In Gray, tasks with no WP1 financial support (only engineers assigned to WP7)

Some key achievements (2024-2025)

Toward feature-preserving alpha wrapping

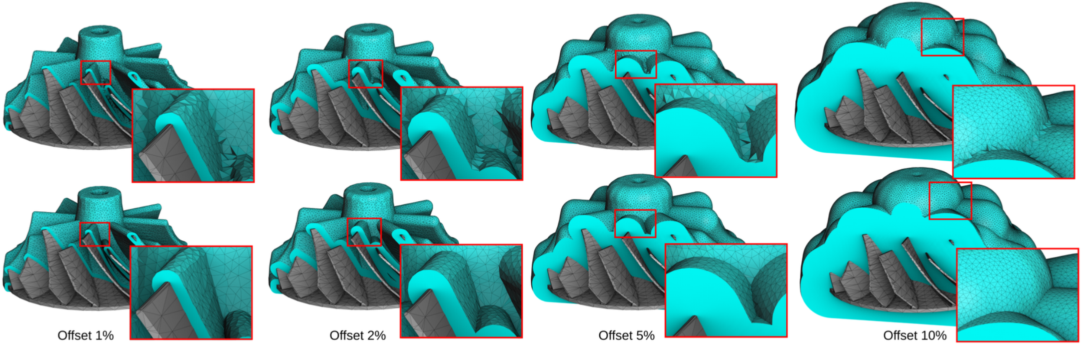
Main achievements

Robust method for generating a watertight, adjustable, and manifold surface mesh that encloses a 3D input.

- Guarantees that the output mesh strictly contains the input geometry.
- Handles triangle soups, polygon soups, and point clouds.
- Feature-preserving variant via so-called *salient* Steiner points.
- Visibility-based criterion for salient point selection.

Christos Georgiadis, postdoctoral fellow (2024).

Toward feature-preserving alpha wrapping

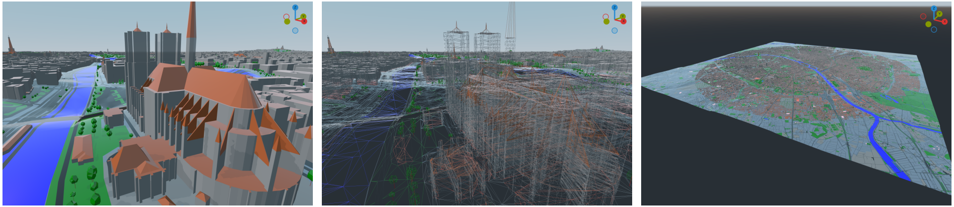


Feature-preserving offsets of a mechanical part, with increasing offset. Top: original alpha wrapping. Bottom: feature-preserving alpha wrapping.

Ktirio-geom - A CGAL based library for Urban Geometry Modeling

Main achievements: Generate watertight meshes from heterogeneous data.

- Seamless integration of elevation, buildings, roads, rivers and vegetation.
- Large-scale tile based processing for entire cities, integrated to a GUI. (e.g. Paris with 150K Buildings - 200M triangles - 10GB mesh)
- Optimized terrain generation. From 250K (naive) to 300 triangles per tile.
- Dual Licensing (GPL + Commercial) is under discussion.



Watertight mesh visualization of Paris (6km radius) generated with Ktirio-geom.

Javier Cladellas, Engineer-WP7 (2025-2026)

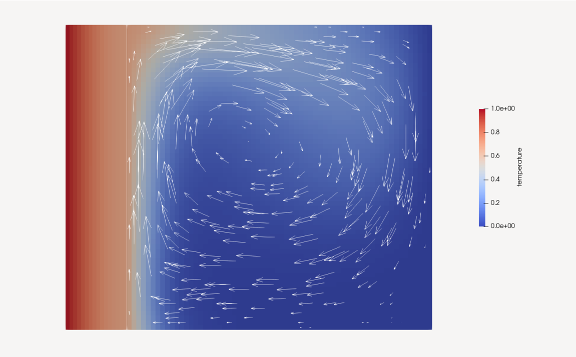
High-order Space-Time Coupling HPC Library

Main achievements

- Context: Multiphysics simulations with partitioned approach
- Numerical analysis of the multi-step coupling scheme in terms of precision and stability
- High-order polynomials in time to predict the evolution of the coupling conditions during a coupling time step
- Error estimates to dynamically drive the coupling time step
- Development of a C++ high-order space-time coupling HPC library for multiphysics applications CWIPI
- Integrated in Samurai library

A. Simon, PhD thesis (2024-2027); A. Simon *et al.*, Comptes Rendus. Mécanique 2025.

High-order Space-Time Coupling HPC Library



Key Achievements

- Dynamic time step adaptation capability
- High-order explicit and implicit coupling
- Demonstrated on conjugate heat transfer test case (solid-fluid)

Towards exascale thermoelastic partitioned coupling

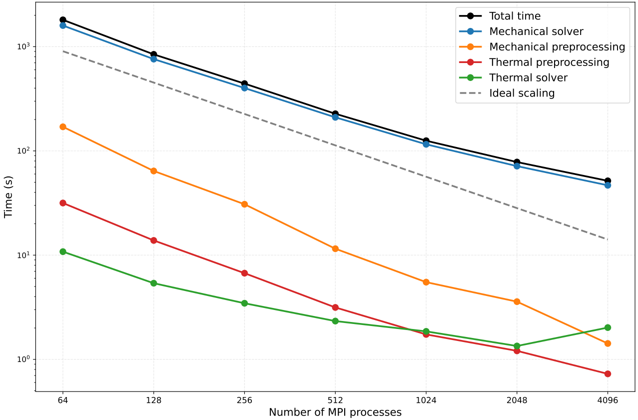
Main achievements

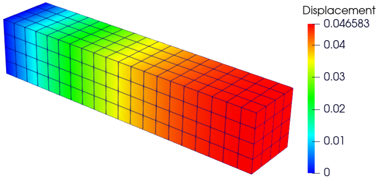
- Thermomechanical analytical formulation on undeformed geometry (initial configuration) via an (Piola-Kirchhoff) effective conductivity;
- Partitioned (block Gauss-Seidel fixed-point) coupling for flexibility, improving memory management and efficient solvers reuse;
- Numerical equivalence between the deformed and initial geometry approaches is verified in a reference thermomechanical solver (Cast3M);
- Porting to MFEM (HPC library) : Strong scalability tests on a CEA Topaze cluster (AMD EPYC Milan CPUs) demonstrate near-ideal speedup on to **several thousand MPI processes** on **meshes with hundreds of millions of degrees of freedom.**

→ Large-scale HPC thermomechanical simulations while preserving mesh quality.

P. Dubois, PhD thesis (2024-2027); P. Dubois *et al.*, proc. CSMA 2026.

Towards exascale thermoelastic partitioned coupling





Bar test case – Effective conductivity thermoelastic coupling. MFEM calculations on Topaze, iterative solver, 83×10^6 node mesh, one computing core per MPI process.

- Near-perfect scalability up to 1024 MPI processes, after gains are still noticeable.
- Mechanical problem-solving phase largely dominates the total computation time.
- Easy implementation of the Gauss-Seidel fixed-point strategy

Other activities related to WP1 (2024-2025)

Activities related to the WP1 'ecosystem'

GPU acceleration of CGAL AABB tree component (distance and intersection computations)

- Binary radix trees (stackless traversal) and non-branching intersection tests
- Speedups up to 2-3 orders of magnitude relative to single-core CPU baseline
- INRIA Titane team

Modified equation analysis for finite volume schemes on adaptive meshes

- Quantify the influence of AMR on the accuracy and order of the FV schemes
  $\rightarrow$ High-order schemes require precise flux reconstruction to maintain accuracy
  $\rightarrow$ Optimal convergence rate recovered.
- HPC@Maths/Ecole Polytechnique

Activities related to the WP1 'ecosystem'

Development & Benchmarking of Discretisation Applications using Feel++

- Development
  - Low to High order FE library (Kokkos with backend and C++23)
  - Link with Exa-DI GT High-Order Discretization library
- Benchmarking
  - Low to high order FEM for elliptic problem using previous library (see D7.1)
  - Distance function (Ray tracing and Levelset)
  - bench.feelpp.org
- UNISTRA (cf. Thomas Saigre - Engineer WP7)

Activities related to the WP1 'ecosystem'

Discontinuous finite elements towards exascale computing

- Numerical investigation of stabilization in the Hybridizable Discontinuous Galerkin (HDG) method for linear anisotropic elastic equation
  → Find the optimal stabilization parameters in HDG discretization (Exascale-friendly) for elastic wave equation.
  → paper in CMAME, 2024; Collaboration with Mumps tech (joint paper submitted 2025)
- Domain decomposition based upon Trefftz formulation for solving anisotropic acoustic wave equation in the time-harmonic regime
  → PhD thesis defended in March 2025 by Ibrahima Djiba
- INRIA Makutu team

Collaboration

Inter-WP Collaborations

- **Collaboration with WP2**: *Collaboration on new generation of numerical methods* mixing classical discretizations with neural networks *(paper in M2AN accepted) ; next step: build a computational framework based upon uniform discretization grids complemented with local adaptation technique, internship*
- **Collaboration with WP3**: *Technical meeting on* fixed-point acceleration methods *(April 2025), Invitation to technical seminar.*
- **Collaboration with WP4**: *Bayesian inverse problems is one target of WP4; collaboration with WP1 in which* efficient deterministic inversion techniques *are proposed; application: seismic*
- **Collaboration with WP7**: T1.1-T1.2 (J. Cladellas), T1.4 (T. Saigre), T1.3 (S. Dubois, A. Hoffmann)

External Collaborations

- **Collaboration with other PCs**:
  - **Exa-DI interaction - GT Block-structured AMR, GT High-Order Discretization**
  - **Exa-DoST interaction - AMR I/O** (Sylvain Joube, postdoctoral fellow, CEA/Ecole polytechnique - 24 months - started Nov. 2025)
- **International collaborations**: *NASA Summer Program 2025 - 1 month*
  Scientific Context: Advanced numerical methods for multiphysics simulations in aerospace applications

  Methodological Objectives
  - High-order, scalable algorithms for coupled PDE systems
  - Validation through test cases (conjugate heat transfer, 2D jets)
  - Integration into open-source C++ libraries (`samurai`, `ponio`)
  - Emphasis on modularity and performance

  Applications: two-phase flows, rarefied gases, reactive flows, plasma physics, etc.
  Teams: HPC@Maths/Ecole Polytechnique, ONERA, NASA.

Next Steps

Plans for 2026

- T1.1:
  - Scalable (distributed) CGAL Mesh generation (Inria innovation lab with Geometry Factory)
  - Release of Ktirio-geom library for urban geometry modeling
- T1.2: Development and Benchmarking of ParMMG
- T1.3 *PhD thesis : Parallel simulation and adaptive mesh refinement for 3D solids mechanics problems (2026-2029)*
- T1.4: Release and improvements of Kokkos low to high order FE C++23 lib
- T1.5 *PhD thesis : (2026-2029)*
- T1.6 *PhD thesis : Development of high-resolution, error-controlled methods for scalable, multiscale EDP simulation in time and space (2026-2029)*
- T1.7: Continuation of both PhD theses (P. Dubois & A. Simon)

Questions?

Questions?

Appendix

GPU acceleration of CGAL AABB tree component (distance and intersection computations)

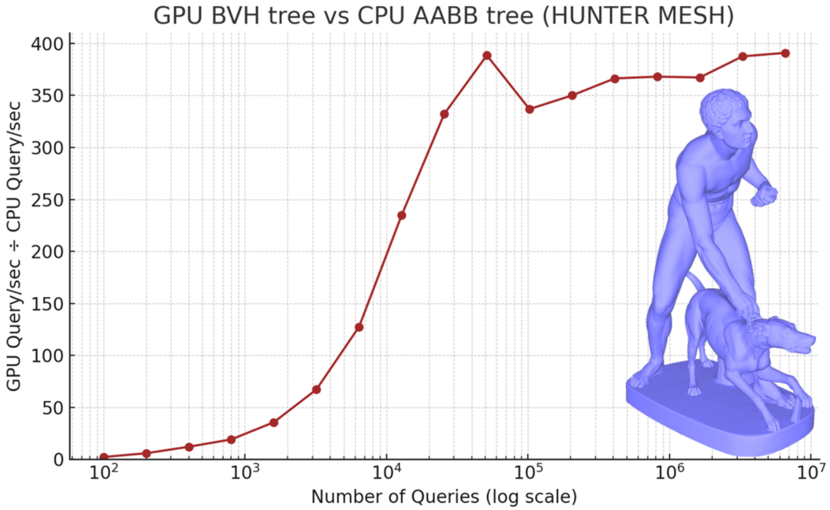
Main achievements

Large reductions in pairwise detection costs, with speedups up to 2-3 orders of magnitude relative to the single-core CPU baseline.

- Binary radix trees (stackless traversal)
- Non-branching ray-box intersection test
- Separate static hierarchy construction from real-time query passes
- Query grouping and work ordering to preserve memory access coherence
- CUDA implementation

Ketevan Peranidze, undergraduate intern from MIT (2025).

GPU acceleration of CGAL AABB tree component



Modified equation analysis for finite volume schemes on adaptive meshes

Objective

Quantify perturbations in modified equations of FV schemes on adaptive meshes

Methodology

- Modified equation analysis
- Flux approximation impact
- Symbolic computations

Key Results

- AMR enhances efficiency for multiscale PDEs
- Inadequate flux reconstruction degrades accuracy
- Loss quantified in high-order methods
- Rigorous symbolic framework

Authors: T. Bellotti, L. Gouarin, J. Massot, M. Massot, P. Matalon, L. Séries, C. Tenaud

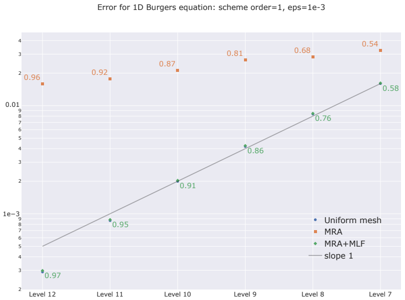
Modified equation analysis for finite volume schemes on adaptive meshes

Main Finding

High-order schemes require precise flux reconstruction to maintain accuracy in smooth regions.

Scientific Implications

- Accuracy vs. efficiency trade-off in high-order methods
- Need for robust flux reconstruction
- Adaptive mesh optimization



Exa-DI interaction - GT High-Order Discretization

Project Overview

- Modern C++23 high-order FE framework in Feel++
- Low to high order ($k = 0$ to $k = 10+$), Kokkos backend
- Runtime *and* compile-time polynomial order
- Simplices, hypercubes, prisms, pyramids
- Geometry order $\neq$ basis order (super/iso-parametric)

Code Example

```
// P2 triangle (compile-time order)
Lagrange<Simplex<2,1>, 2> p2_tri;
auto phi = p2_tri.evaluate(0.25, 0.25);
// Q3 quad (runtime order)
Lagrange<Hypercube<2,1>, Dynamic> qk(3);
// P4 on P1 geometry (superparametric)
Lagrange<Simplex<3,1>, 4> p4_tet;
```

Key Achievements

- **C++20 Concepts**: Type-safe interfaces, clear error messages
- **Exascale-ready**: No virtual functions, compile-time sizes, Kokkos-compatible
- ***p*-adaptivity**: Variable polynomial order per element
- **Orthonormal bases**: Dubiner (simplices), tensor Legendre (hypercubes)

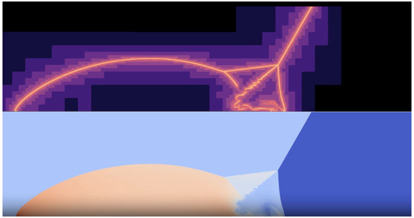
Future Work

- Polygon/polyhedron support (in development)
- Matrix-free operator integration
- Performance benchmarking on EuroHPC systems

Exa-DI interaction - GT Block-structured AMR

Project Overview

- Identify open source software to compare
- Define physical problem suitable for AMR benchmarking
- Numerical scheme selection
- Establish performance metrics



Key Achievements

- First tests with Euler equations
- 4 selected software
  - Dyablo
  - samurai
  - Kalypsso
  - Astro

Future Work

- Define reference solutions (double mach reflection, Riemann problems,...)
- Compare accuracy and performance of the different AMR methods and codes

Exa-DoST interaction - AMR I/O

Objective

- Identify I/O requirements for AMR libraries
- Define a common I/O strategy for both AMR libraries
- Allow data compression without or with loss

Methodology

- Bibliography on wavelet compression
- Analysis of various formats for AMR data
- Work with Kitware team on HyperTreeGrid format and its improvements

Involved Persons

- Sylvain Joube (Post-doc CEA/Ecole polytechnique - 24 months - started Nov. 2025)
- Maxime Delorme (CEA)
- Arnaud Durocher (CEA)
- Julien Bigot (CEA)
- Loïc Gouarin (CNRS/Ecole polytechnique)

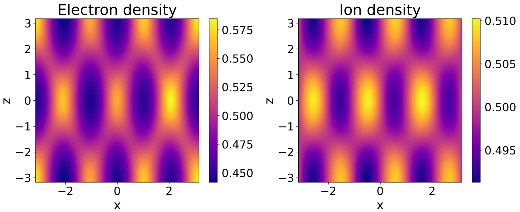
Numerical Study of Magnetized Multi-Species Plasmas

Project Overview

- Magnetized multi-species plasma simulation with multiscale challenges
- Gyromoment approach filtering fast cyclotron frequencies
- Electron-ion coupling through Poisson equation and Lorentz force
- 2D simplified configuration representative of Hall thrusters

Key Achievements

- Multiscale treatment: Larmor radius, cyclotron frequency, and inertia handled
- Asymptotic-preserving scheme for stiff electron-Poisson system
- Dual timescales captured: Fast electron vs. slow ion dynamics
- Stable numerical results with small parameters ($\varepsilon = \chi = 10^{-2}$)



Participants: Z. Tazakkati, T. Pichard, J. Massot, M. Massot

Unified Two-Scale Two-Phase Flow Model

Project Overview

- Two-scale two-phase flow model for separated-to-disperse transitions
- Full thermodynamics extension from isothermal formulation
- Scale separation approach: disperse phase via sub-scale model
- Atomization modeling through interface regularization process

Participants

W. Haegeman, G. Orlando, S. Kokh, M. Massot, L. Gouarin, P. Matalon, S. Dubois

Key Achievements

- Thermodynamic consistency across scales enforced
- Parasitic terms eliminated from inter-scale mass transfer
- Interface regularization validated via numerical proof of concept

(a) without inter-scale mass transfer

(b) with inter-scale mass transfer

Modeling Hybrid Dense-Rarefied Flows

Project Overview

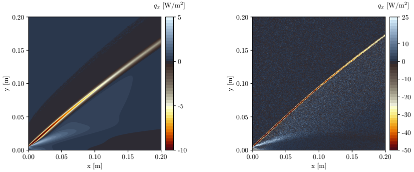
- Multi-regime flow simulation via moment methods
- Relaxation scheme coupling systems without interfaces
- Adaptive resolution based on local rarefaction
- Rocket plume expansion demonstration case

Participants

P. Bernigaud, A. Clout, D. Biasone, S. Dubois, A. Hoffmann, M. Massot

Key Achievements

- 40% cost reduction vs. full-order simulation
- DSMC validation (8M cells reference)
- Accurate heat flux and expansion capture
- Stable mathematical framework proven



(a) Relaxed method of moments

(b) Reference DSMC