An overview of the application of HPC in CEA codes for simulating nuclear reactors

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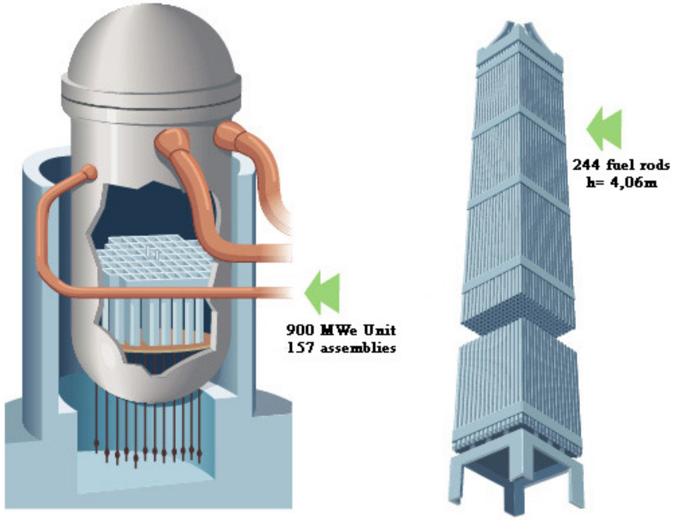
1. Context

Context

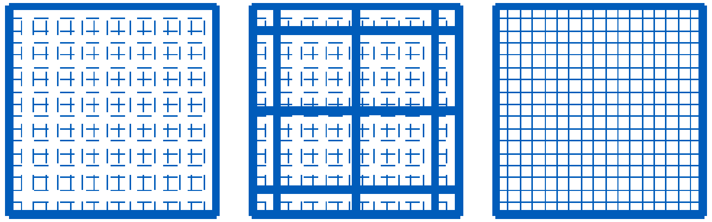
- Reactor physics is a highly multiphysics field involving nuclear physics, neutronics, thermalhydraulics, structural mechanics, material science, ….

- Industries rely on highly verified and validated code systems to perform routine computations based on low-order approximations for optimal precision to computing time ratio.
  - Parametric computations to sweep a very large domain for design and operational studies
  - ex: two-scale (assembly and core) approach in neutronics, 1D simplified thermalhydraulics

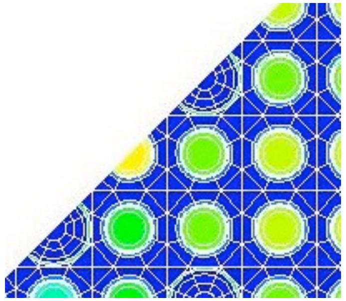


REACTOR PRESSURE VESSEL FUEL ASSEMBLY

- High-fidelity simulations are required to provide sufficient validation on low-order model validity to safety authorities for usual Pressurised Water Reactor from the nuclear fleet or to design new reactors such as Small Modular Reactors, Advanced Modular Reactors, …etc.
  - CFD for mixing grid studies or transport computation in neutronics

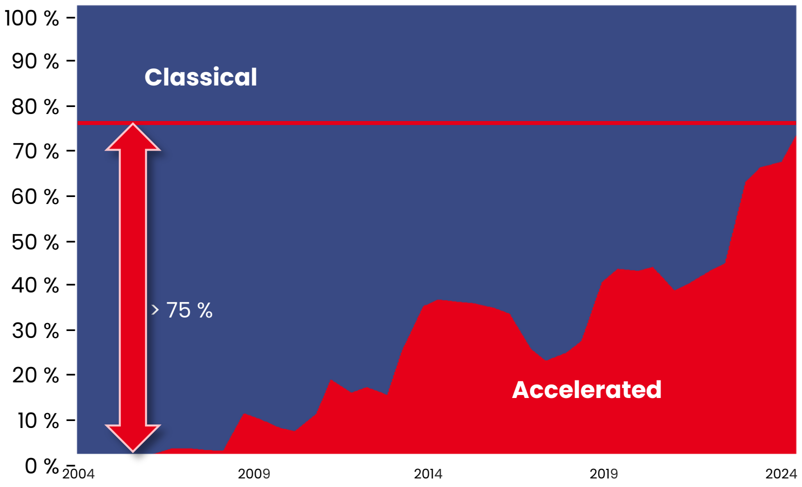


Homogeneous Domain Homogeneous Pin-by-pin

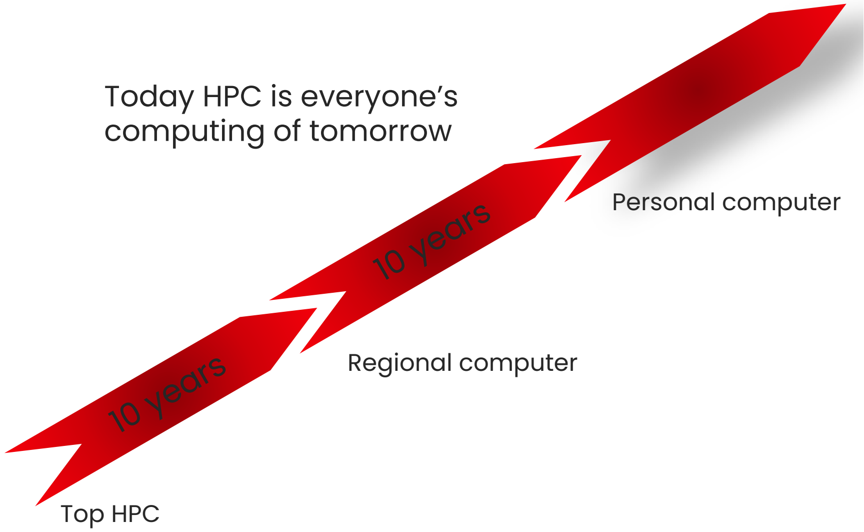


Context

- HPC is a tool in a wide range of domains, **source of competitivity**
  - At CEA, we host machines
  - To take part in the French & European HPC ecosystem
- We just entered the **Exascale** era, that means **GPU**
  - European pre-Exascale systems: Mix of AMD & Nvidia
  - First Exascale machines planned in Europe for 2024/2025
    - Jupiter machine at Jülich (Germany) => Nvidia & Rhea
    - Alice Recoque machine at CEA/TGCC (open call)
  - Need to adapt or re-develop applications with **Performance portability**
- GPU programming models: software catalysts
  - France and Europe had great research but no production tool
- A need for a **long-term sustainable solution**
  - Adapted to **our hardware and software specificities**
  - **Trust** in the roadmap

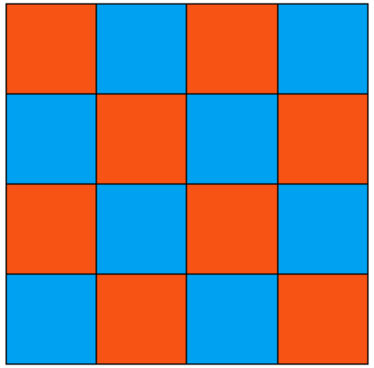


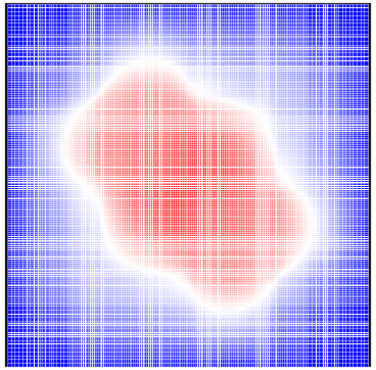
Computing power of the 500 top supercomputers from june 2004 to june 2024 (source Top500)

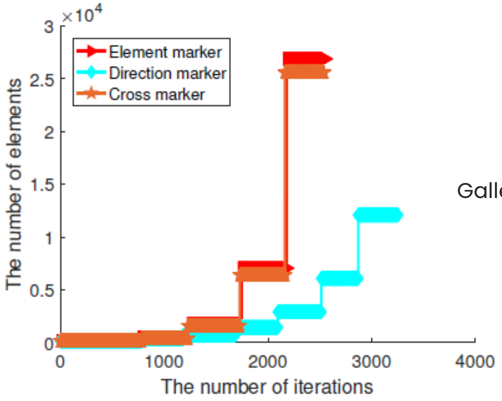


High-fidelity simulations

- Distinguish between particle-based *vs.* mesh-based approaches
  - e.g. Monte Carlo and deterministic methods for neutronics
- For instance, starting point for Monte Carlo is a CAD-like geometry model. This model is meshed for the mesh-class family of methods
- Pre-processing: meshes
- Online stage:
  - Numerical schemes set up for nuclear reactor simulation
    - High-order methods
    - Adaptive methods (AMR)
    - ….
  - Numerical strategies for solving the problem
- Post-processing: Error estimates
- Computer science: algorithms and parallel programming models





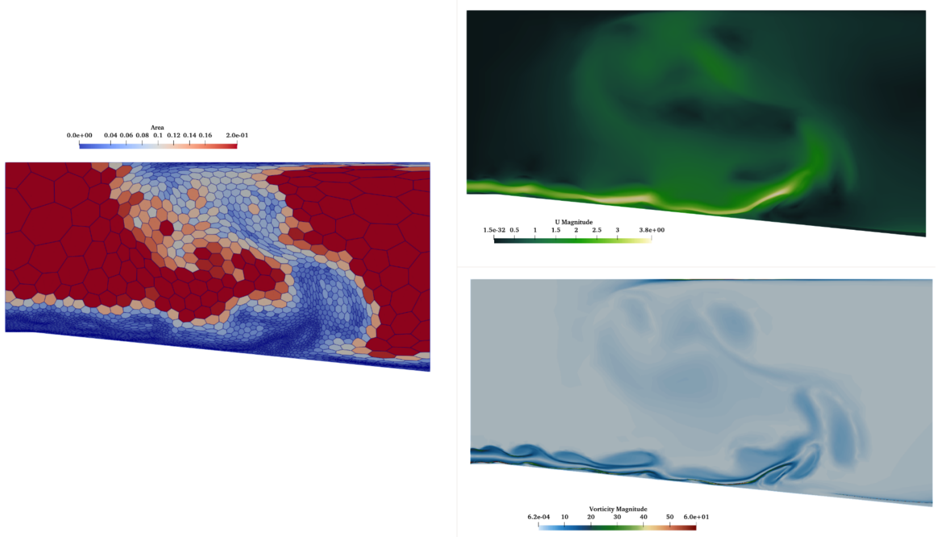


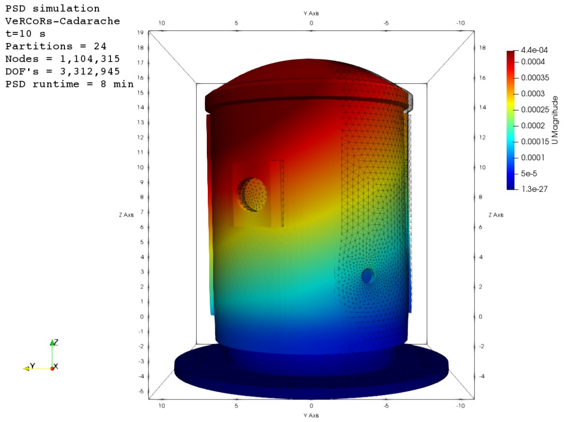
Gallery courtesy: F. Madiot

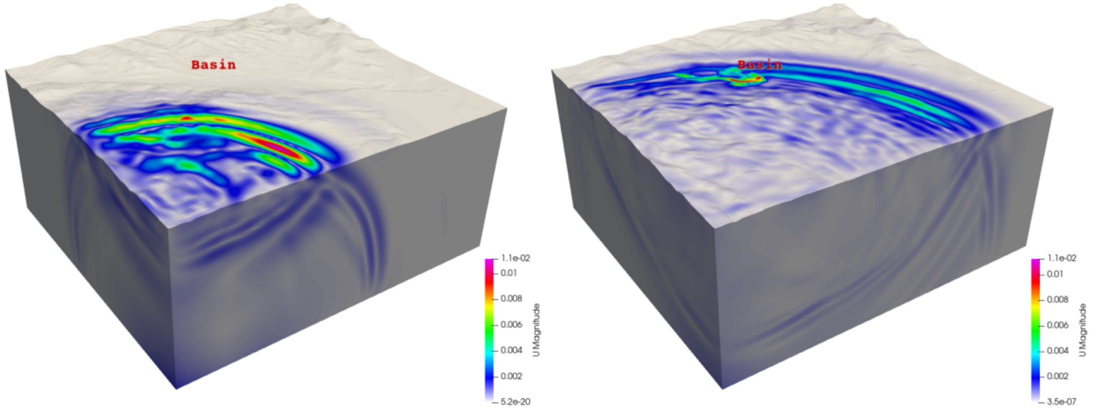
2. Overview of some codes

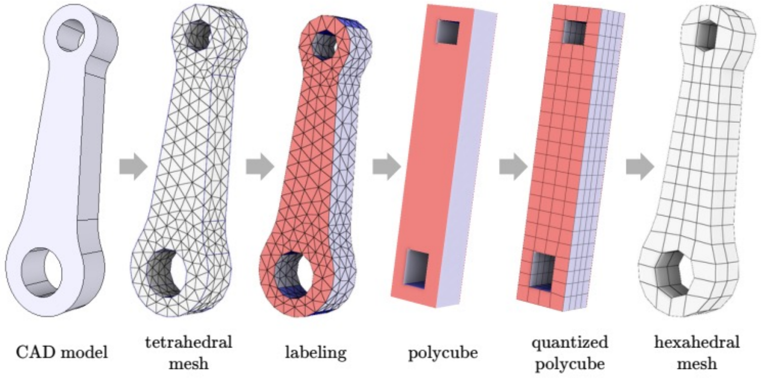
Meshes: towards more complex elements

- Meshes: first part of the model
  (except particle-based methods, *cf*. previous slide)
- Mesh tool within the SALOME environment
  - Co-developed with EDF
  - SMESH: usual simplices
- Polygonal/polyhedral meshes
  - New R&D endeavours
  - Improve accuracy *vs* computational cost ratio
- On-going R&D: Hexahedral meshes using AI algorithms to convert to polycubes
- Recent work: generation of a 6 B-cell mesh with parallel IO management (SNA + MC 2024)





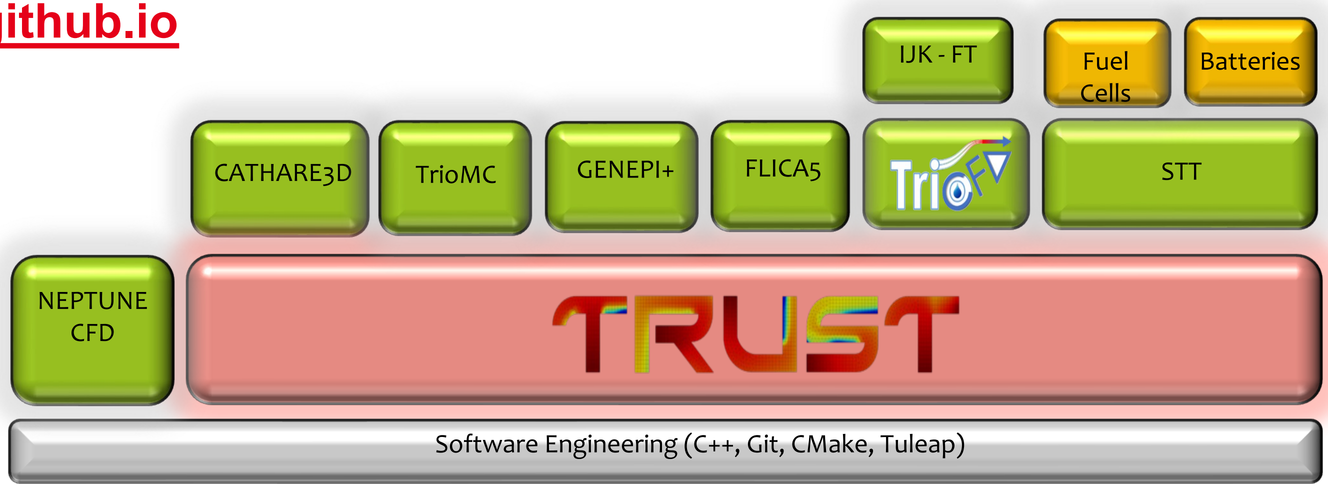




Gallery courtesy: M. A. Badri

TRUST: a brief overview

- TRUST: HPC thermalhydraulic platform for multiphase problems
  - More than 20 years of development
  - Born out of the splitting of Trio_U into TRUST and TrioCFD
  - **Opensource**: https://cea-trust-platform.github.io
  - Initially, incompressible Navier-Stokes
  - Now multiphase and compressible
  - Laminar/Turbulent flow
  - Spatial discretisations: VDF, VEF, MAC, PolyMAC



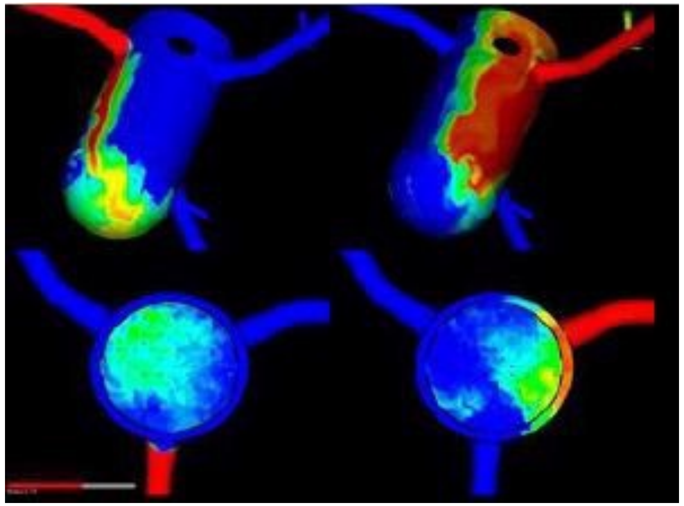
- Several *applications* are developed on the TRUST platform
  - Derived physics application using TRUST as a core building block

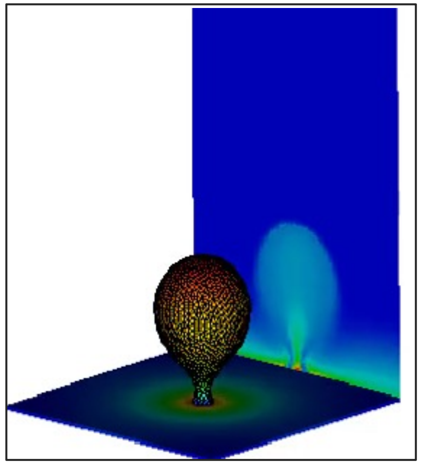
Numerical and physical models of TRUST

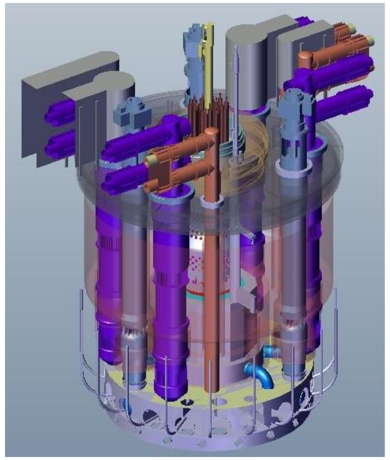
- Front-tracking model:
  - Eulerian mesh where incompressible Navier-Stokes equations are solved
  - Lagrangian moving mesh for the interface location
  - Coalescence or breakup models for bubbles and drops

- Multiphase flow simulation
  - Arbitrary number of phases
  - Source terms and operators for phase coupling
  - Dedicated numerical schemes for resolution

- Examples of performed simulations
  - **Academic case studies**
    - Plane channel with conduction coupling at the wall
    - Flow around an obstacle
    - Pipe flow
    - Isotropic turbulence…
  - **Industrial case studies**
    - Various studies about the core of a reactor
    - Thermal stress in a T-shaped mixing pipe
    - Natural convection in a storage room of waste
    - Atmospheric dispersion (pollution or radio-nuclides) …



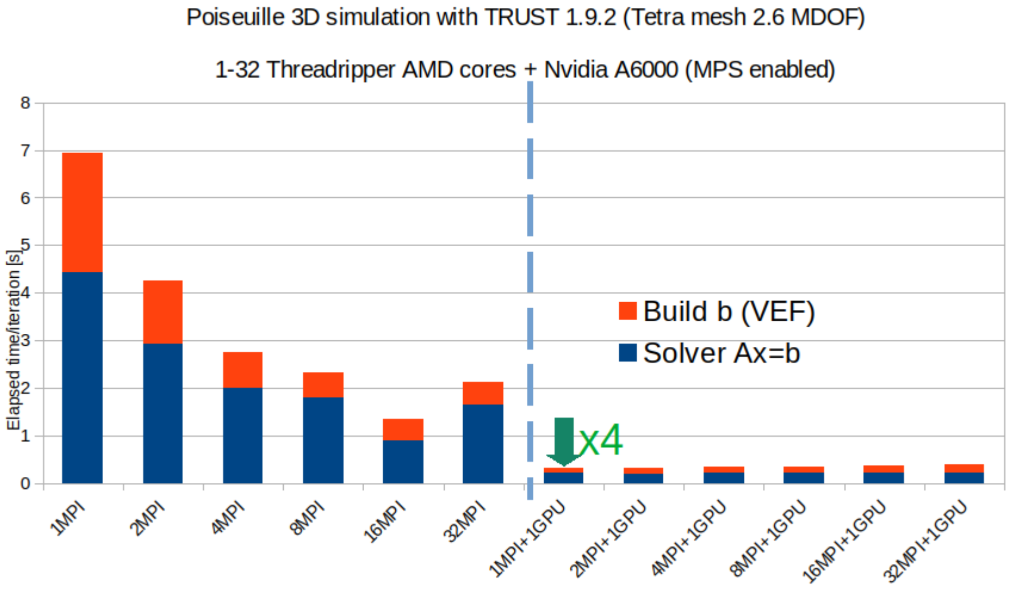




Gallery courtesy: TRUST team

Porting TRUST to GPU

- Computational efforts for models are levelled by HPC cutting-edge technologies (hardware: ex Adastra) and techniques (algorithms, adapted numerical schemes)
    - On-going GPU-porting with OpenMP and Kokkos programming models
    - Promising performance gains from workstation to supercomputer
    - Running a first module (incompressible laminar flow) on a mesh with 1 billion cells, accelerated by 512 Nvidia V100 (JeanZay, IDRIS) or 1024 AMD MI100 (Adastra, CINES)



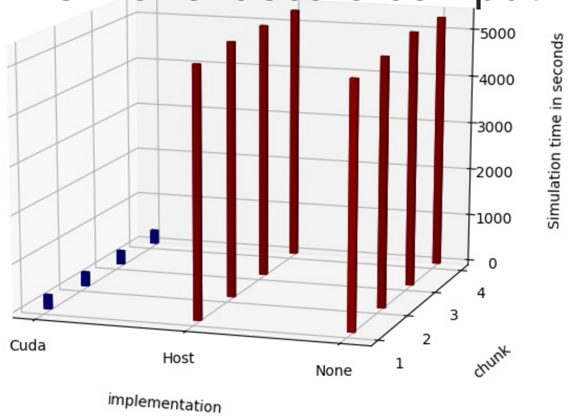
Gallery courtesy: P. Ledac

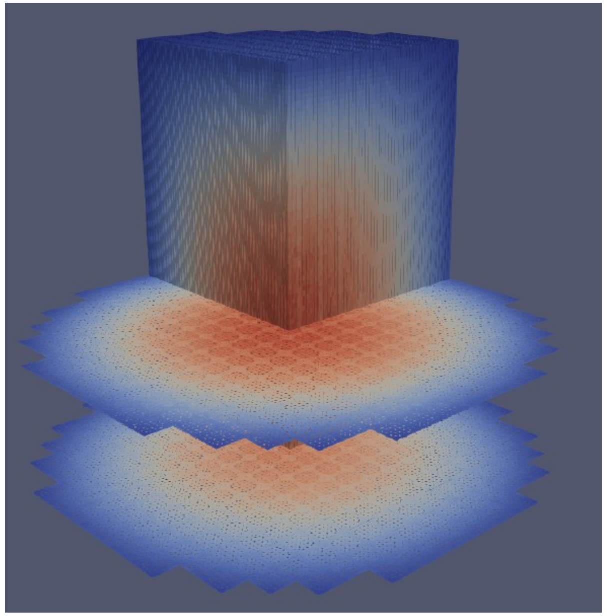
Advanced neutron transport (Monte Carlo)

- Monte Carlo: embarrasingly parallel
  - TRIPOLI-4 developed at CEA

- PATMOS
  - Prototype for testing new programming paradigms for Monte Carlo in particle
  - Developed at SERMA
  - Led to the seeding of the Tripoli-5 project supported by EDF and co-developed with IRSN
  - Very efficient scaling on the Hoogenboom-Martin (PWR) benchmark
  - On-the-fly Doppler broadening (to account for feedback with thermalhydraulics)

- On-going GPU-porting of Monte Carlo algorithm in view of exascale computing
  - Testing of several programming models: Cuda, OpenACC, OpenMP offloading, Kokkos





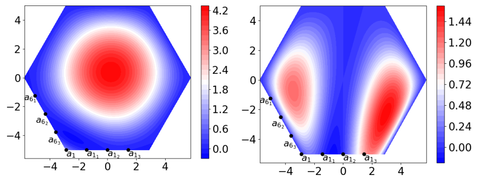
Coupling of PATMOS and THEDI (1D thermalhydraulics): power distribution

Gallery courtesy: TRIPOLI-5 team

Advanced neutron transport (deterministic)

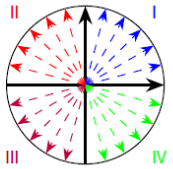
- Deterministic neutron transport: APOLLO3® code for industrial schemes

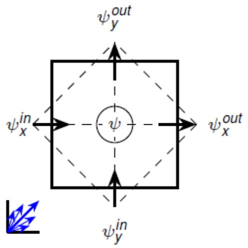
- HPC
  - Vectorisation of sweep kernel with Kokkos
  - Porting to GPU: not just simple rewriting but re-conceiving the sweep algorithm

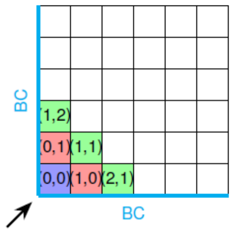


- Numerical schemes
  - High-order DGFEM* on structured meshes (improvement of *dofs* vs time)
  - Towards one-step: PhD works on dynamic homogenisation and coupled IDT-TH computation

DGFEM*: Discontinuous Galerkin Finite Element Method

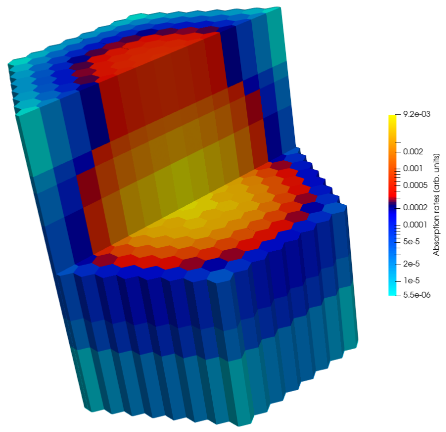






Sweep algorithm for source iteration

Power distribution Takeda 4 benchmark



Performance tests and results: AVX

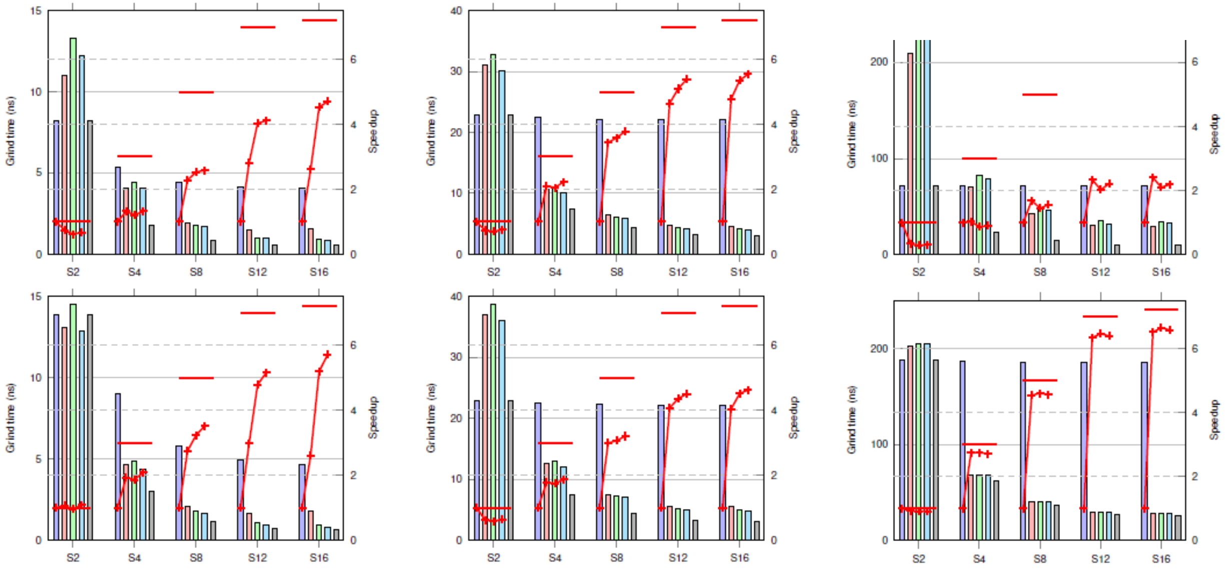


Figure 3 – GCC (up) and Clang (down) using AVX. Left to right: $\mathcal{DD}0, \mathcal{DD}1, \mathcal{DD}2$. Bars: grind-time (left to right: Scalar, A, B, C, Ideal). "+": measured speedup. "–": ideal speedup.

From Europlexus/CAST3M to MANTA

- Europlexus: *Explicit* dynamics for structures and compressible fluids
- Fluid / structure interactions
- Industrial applications
- Finite-elements, finite-volumes, sph, discrete element method
- ~40 years of development

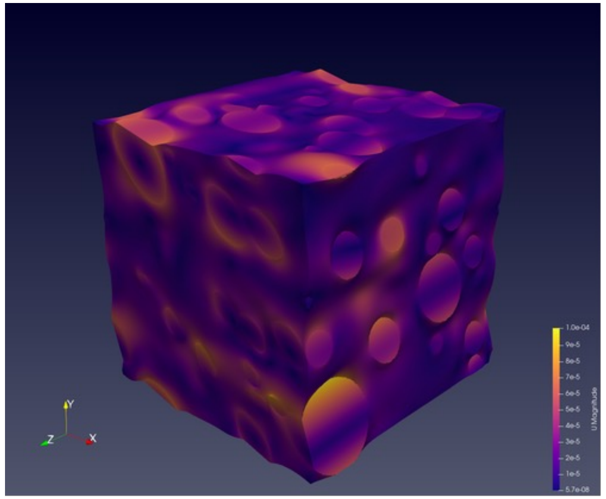
- CAST3M: Generic tool for “*implicit* problems”
- Mainly geared for (non-linear) mechanics
- … but also applied to incompressible fluids, electromagnetism, metallurgy, …
- Industrial applications
- Finite-elements
- ~40 years of development

- **M**echanical **A**nalysis **N**umerical **T**oolbox for advanced **A**pplications
- Next gen., **HPC** oriented
- *Both implicit and explicit problems*
- Structure / compressible fluids / … , interactions
- Industrial applications
- Every mesh-based method (FE, FV, HDG, …)
- C++
- “automatic parallelism”
- Easy to maintain and evolve on the long term
- Open-source

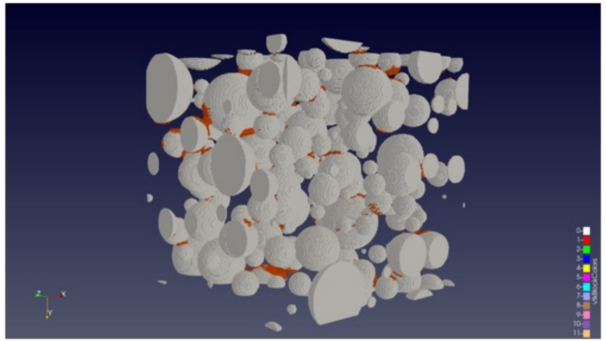
MANTA: current status

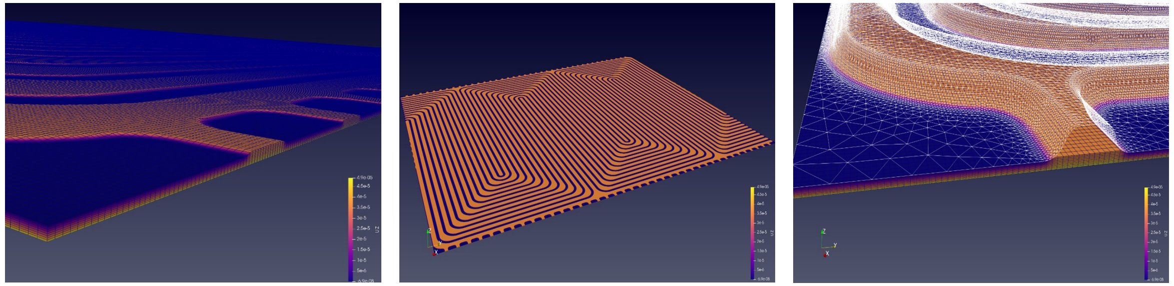
- **On-going development at CEA with contribution from EDF**

- **Collaboration between software and mechanical research engineers**
  - Support: I/O med, mesh partitioning, parallel solvers, …
  - Management for checkpoint/restart
  - Performance portability: hybrid parallelisation techniques (MPI+X) CPU, then GPU



- REV simulation
- 2-phase: elastic inclusions and elasto-plastic matrix
- Contrast: 100
- Periodic boundary conditions
- 400x10e6 dofs
- 16384 MPI subdomains
- Implicit calculation



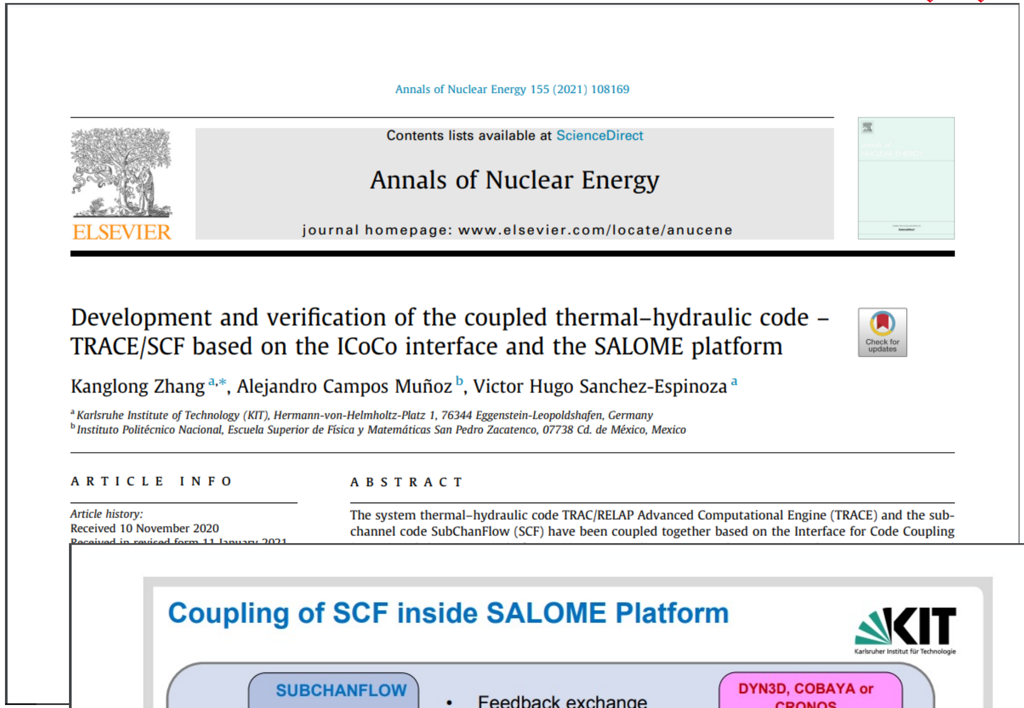


Shaping test for a fuel cell plate

Gallery courtesy: O. Jamond

One to bind them all

- Physical systems require multiphysics modelling
- Partitioned coupling approach
  - Few monolithic code with intricate coupling of all physics (*e.g.* SIMMER)
  - Simpler maintainance
- Code coupling: ICoCo + MEDCoupling (SALOME)
  - ICoCo = Interface for Code Coupling
  - MEDCoupling = Library with remapping options for quantities defined as fields (scalars/vectors on a mesh)
  - C3PO open-source python library (https://github.com/code-coupling/c3po)
    - Provides algorithms and accelerations for coupling
- NumPEx (ExaMA WP3) project on code coupling for exascale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Development and verification of the coupled thermal–hydraulic code – TRACE/SCF based on the ICoCo interface and the SALOME platform

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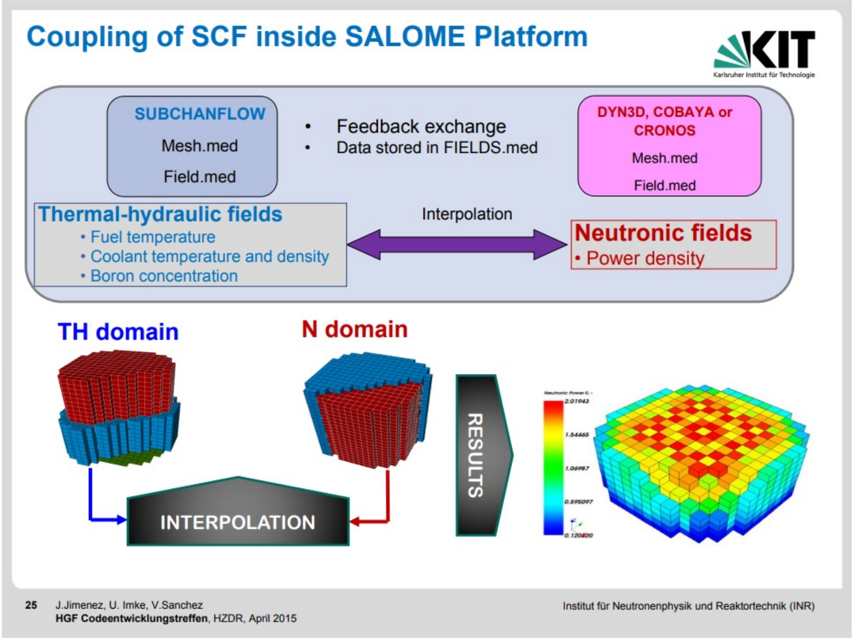
ABSTRACT

The system thermal–hydraulic code TRAC/RELAP Advanced Computational Engine (TRACE) and the sub-channel code SubChanFlow (SCF) have been coupled together based on the Interface for Code Coupling



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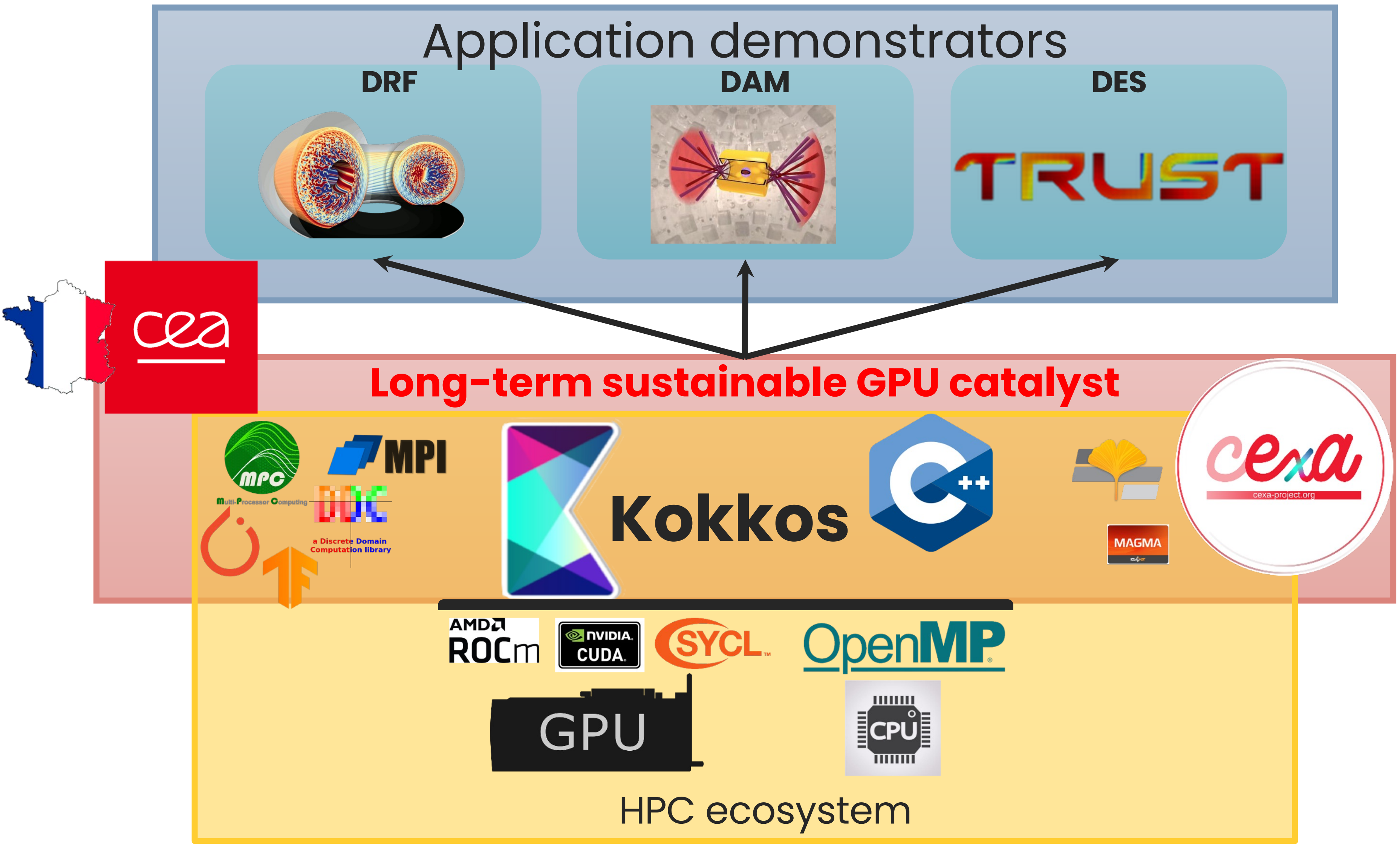
3. Performance portability

The CExA project



Disseminate and offer training in CEA and at large

Adapt application demonstrators

Provide a long-term sustainable software catalyst for GPU computing

Available solutions

- Cuda
- HIP
- **Kokkos**
- OpenACC
- **OpenMP (target)**
- Raja
- SYCL
  - OneAPI/DPC++
  - AdaptiveC++/OpenSYCL/hipSYCL

- Production grade, with public support
- Vendor neutral
- Annotations
  - Works best with imperative languages: C, Fortran, …
  - Compiler integration: potential for additional optimizations
  - Requires to re-design applications for GPU
- Library
  - Suited to language with deep encapsulation: C++, …
  - On top of vendor backends: easier to port to new hardware
  - Requires to re-write applications for GPU

OpenMP & Kokkos : the simplest GPU loop

```
for (int j = 0 ; j < Nj ; ++j) {
        // [...]
}
```

Sequential

```
#pragma omp teams distribute parallel for
for (int j = 0 ; j < Nj ; ++j) {
        // [...]
}
```

OpenMP Target

```
parallel_for(Nj, KOKKOS_LAMBDA(int j) {
        // [...]
});
```

Kokkos

Execute in parallel, on a separate GPU thread each,

the same workload *[...]*

identified by a unique identifier `j`

`Nj` times between `0` and `Nj-1`

OpenMP & Kokkos : memory transfer

```
double* x = malloc(Ni*sizeof(double));
double* y = malloc(Nj*sizeof(double));
double* A = omp_target_alloc(
     Ni*Nj*sizeof(double),
     omp_get_initial_device());

#pragma omp target data \
     map(to: x[0:Ni]) \
     map(from: y[0:Nj])
{
#pragma omp teams distribute parallel for
for (int j = 0 ; j < Nj ; ++j) {
          for (int i = 0 ; i < Ni ; ++i) {
                    y[j] += x[i] * A[j*Ni+i];
          }
}
```

OpenMP Target

```
View<double*, Kokkos::HostSpace> x(Ni);
View<double*, Kokkos::HostSpace> y(Nj);
View<double*> A(Nj, Ni);

{
auto dx = create_mirror_view_and_copy(dev, x);
auto dy = create_mirror_view(dev, y);
parallel_for(Nj, KOKKOS_LAMBDA(int j) {
          for (int i = 0 ; i < Ni ; ++i) {
          dy(j) += dx(i) * A(j,i);
          }
});
deep_copy(y, dy);
}
```

Kokkos

Copy x to GPU from device before kernel
and y from GPU to device after kernel
Keep A on the device

What's in Kokkos

- Multi-dimensional arrays
  - Layout auto change for performance
- Other containers
  - Key-value maps, …
- Automatic ref-counted Host/Device memory allocation & management
- Host/device memory transfers
- Support of "dual" arrays with one version on each side
  - Up-to-date tracking & automatic transfers when required
- Scratch memory
  - Using "core-local" fast memory on the device

- Parallel patterns w. asynchronous support
  - Independent interactions, Reductions, Scans
- Iteration strategies
  - Tiled, Hierarchical, …
- Algorithms
  - Sorting
  - Random number generation
  - Most of STL parallel algorithms
  - …
- QoL features: portable printf, etc.
- Portable atomic operations
- SIMD
- Coarse & fine-grain tasks
- And much more…

Kokkos an anteroom for standard C++

C++ is (at last) standardizing base tools for HPC

- **Parallel programming** is slowly entering the **ISO C++ language**
  - Parallel algorithms, sender/receivers, etc.
- **The Kokkos team** leads the **standardization** of many required features
  - Multi-D arrays (`std::mdspan`)
  - Vectorization (`std::simd`)
  - Linear algebra (`std::linalg`)
  - And much more to come (mixed precision, etc.)

Kokkos offers a **stable API** today for the features of the **C++ of tomorrow**

- Standardization is slow (9 years for mdspan)
  - Consensus with all communities
- Kokkos offers the **features today**
  - And will **keep maintaining the API** on top of standardized ISO C++
    - With added interoperability layers (Cf. `kokkos::view` / `std::mdspan`)
  - And in a **GPU-compatible** implementation (Cf. `kokkos::array`)

HIGH PERFORMANCE SOFTWARE FOUNDATION

HPSF Goals

- Provide neutral home for key HPC projects to enable collaboration between government, industry and academia
- Promote use of HPSF projects
- Ensure that HPC software is accessible and reliable by providing CI and turn-key builds
- Ensure that HPC software is secure and ready for cloud through collaborations with CNCF and OpenSSF
- Sponsor events and training to grow a diverse, skilled workforce for software in the HPSF ecosystem.

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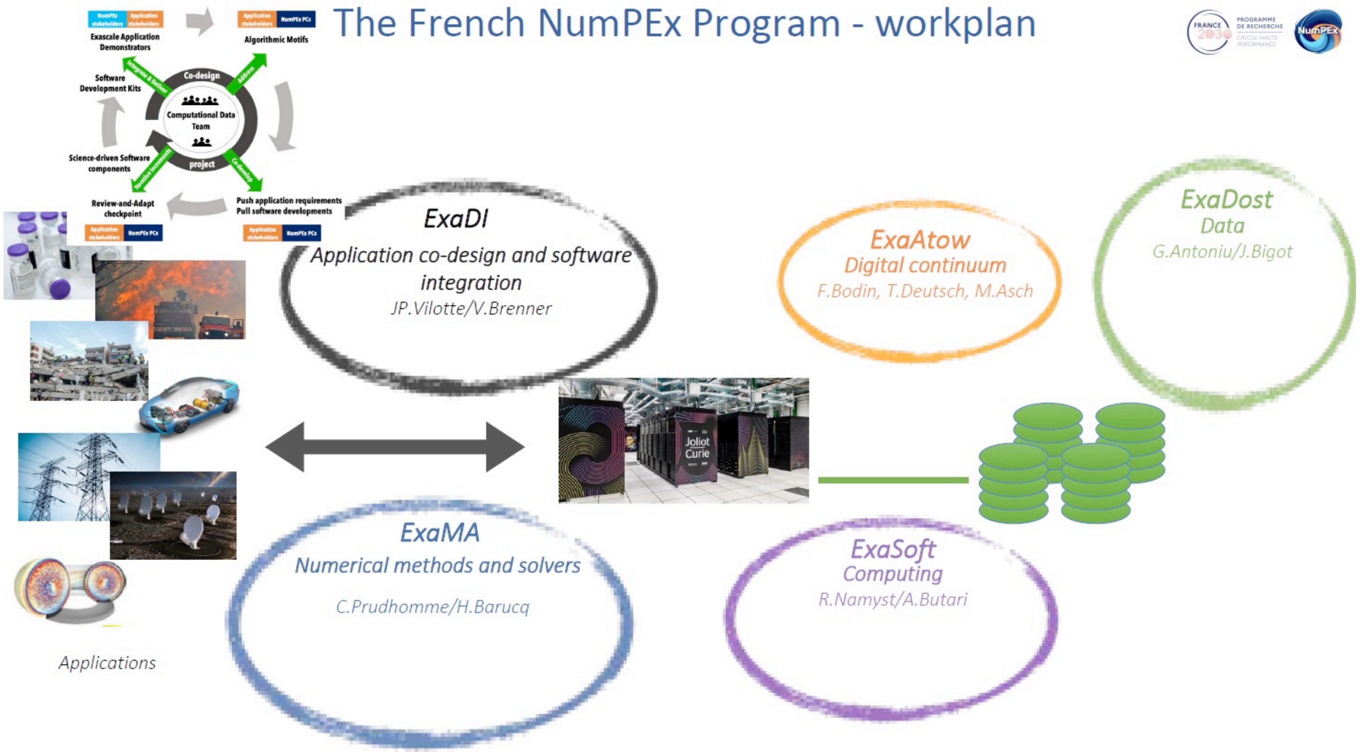
University of Maryland

NumPEx

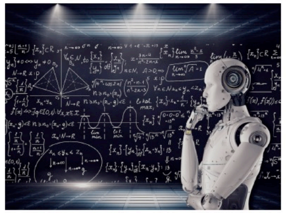
- French project to co-design the exascale software stack and prepare applications to exascale era
- Funded by PEPR (Programme et Equipements Prioritaires de Recherche)
  - Exascale Computing Project (USA): co-design centres, software stack
- Partners: CEA, CNRS, INRIA, Universities,…



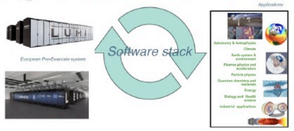
Some Exascale/post-Exascale challenges

From edge to HPC systems
The digital continuum

AI4Science – Science4AI



Software/application co-design



Software, the new frontier

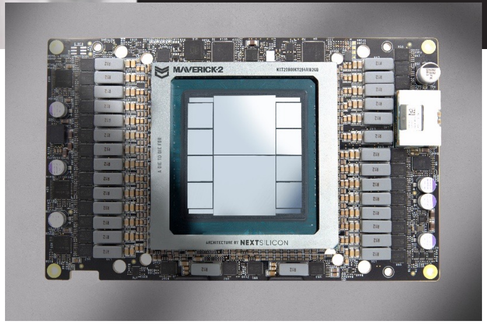
4. Concluding remarks

Concluding remarks

- Code development/maintainance is a tedious and everlasting process
  - Essential as numerical and physical models are safeguarded within code systems (decades)
  - Accounting for all constraints to deliver industrial-grade material (results, software and methods)

- GPU porting: still a challenge but necessary for exascale computation, requires the design and implementation of new algorithms

- Forthcoming short-term challenges
  - Floating-point arithmetics to explore intensive verification and numerical quality of codes and improve algorithms with mixed precision
  - More AI/ML to explore: promising to bridge the gaps on models



- How to adapt the codes to forthcoming hardware? Is it possible to win the rat race?
  - Quantum Computing: 2nd quantum revolution on the march, assess the relevance for our problems (linear algebra, iterative solvers), theoretical transition from the usual algorithms

Thanks for listening

Figures/Plots/Graphs – courtesy of DM2S and CExA team

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Compilation

OpenMP Target

- Use an OpenMP compiler
  - Compatible with the target construct
  - Compatible with the hardware you target
- Each vendor provides its own OpenMP compiler
  - Usually based on LLVM infra
- Default Clang/LLVM & GCC also try to support this
  - For some hardware

Kokkos

- A C++ template library
  - No direct code generation, rely on vendors C++-like languages
- Multiple “backends”, selection at compile time
  - OpenMP, Cuda, OneAPI, HIP, …
- Maximum 3 backends enabled at once
  - Serial backend
  - 1 Host parallel backend (openmp)
  - 1 Device parallel backend (cuda, HIP, Sycl)

References

[1] "Numerical modeling of a moderate hydrogen leakage in a typical two-vented fuel cell configuration", E. Saikali, P. Ledac *et. al.*, International Conference on Hydrogen Safety, September 2021

[2] SALOME: https://www.salome-platform.org/?lang=en

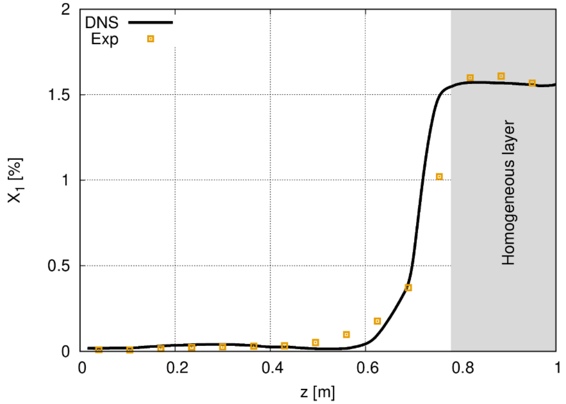
[3] TRUST: code https://github.com/cea-trust-platform; website https://cea-trust-platform.github.io/

[4] "PATMOS: A prototype Monte Carlo transport code to test high performance architectures", E. Brun, S. Chauveau, F. Malvagi , M&C 2017, April 2017

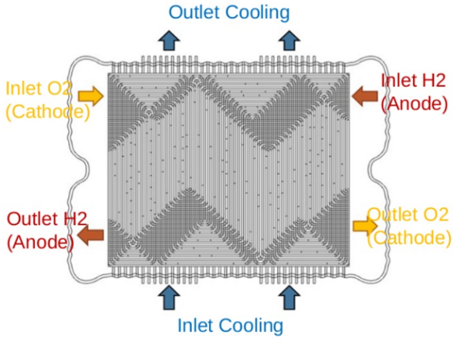
[5] "High-order Wachspress functions on convex polygons through computer algebra", D. Labeurthre, A. Calloo, R. Le Tellier, Journal of Computational Physics, 2022

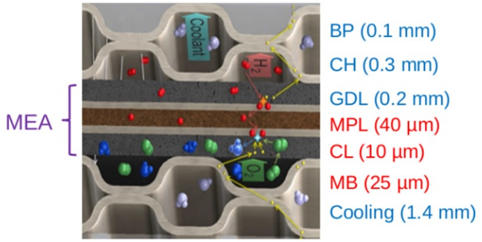
High-fidelity simulations for new systems

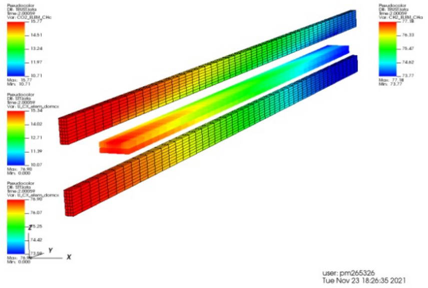
- GAMELAN (moderate hydrogen leakage) – 2 billion mesh cells, 50 000 cores [1]
- PEMFC and batteries – complex geometries



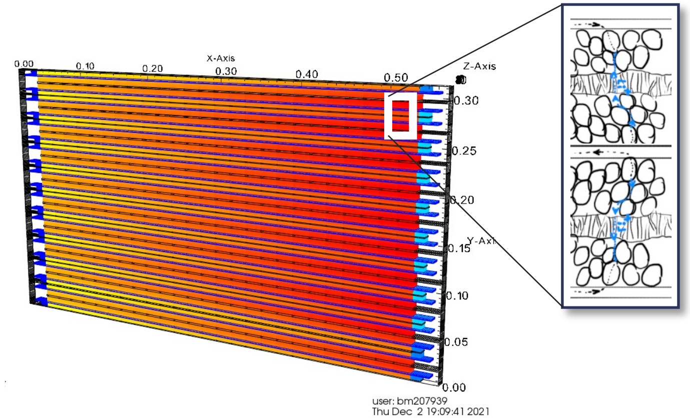
GAMELAN: reference results by CEA

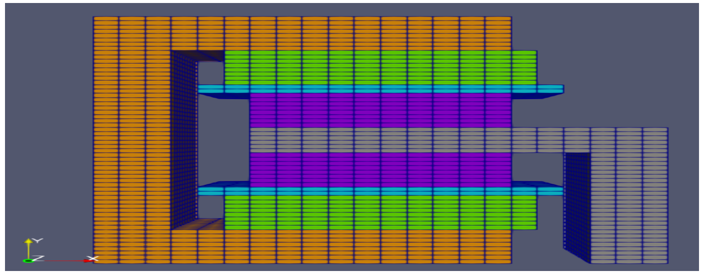






Battery simulation





MEDCoupling representation of PEMFC