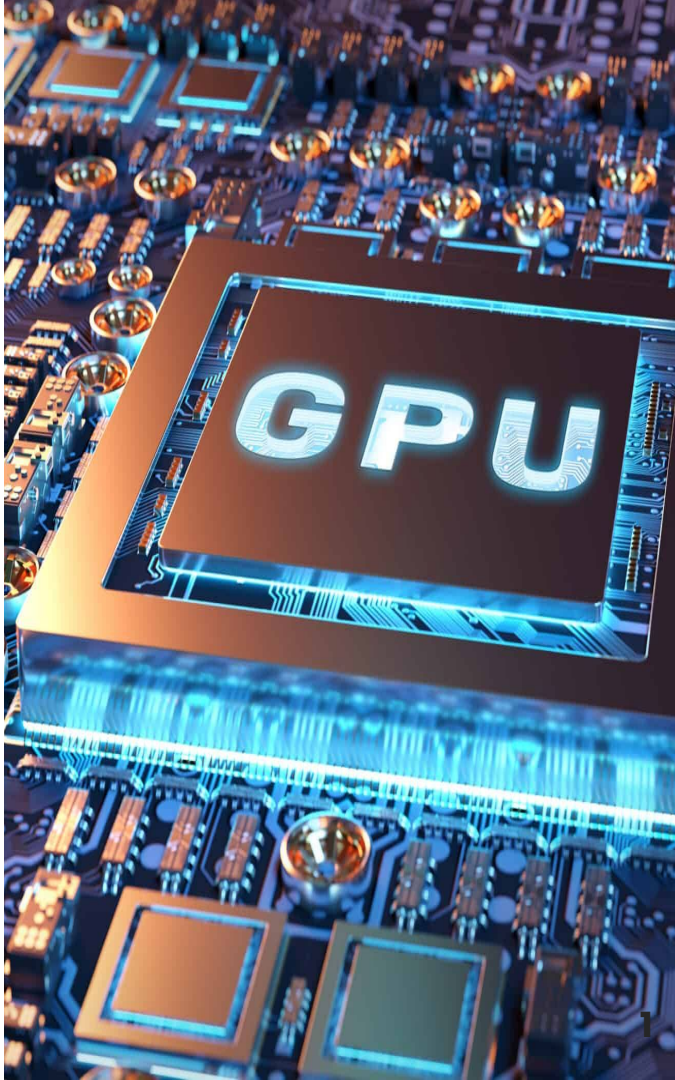
Kokkos at CEA the CExA Project

The reasons of a choice at the CEA



HPSF
HIGH PERFORMANCE SOFTWARE FOUNDATION

cexa-project.org

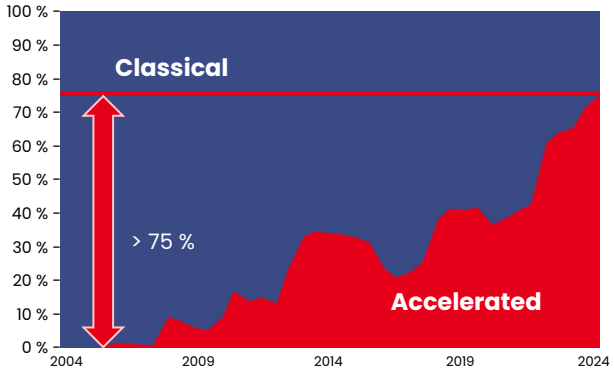
Computing at **Ex**ascale with **A**ccelerators at the **CEA**

GPU usage day
CERFACS
January 23rd 2025

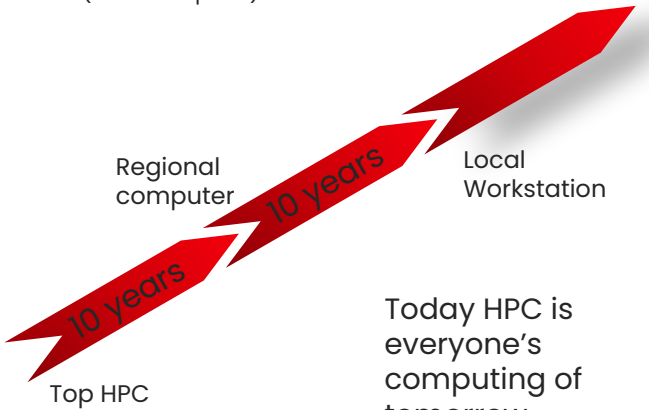
Julien Bigot, the CExA & Kokkos team

Context (2 years ago)

- **CEA**: French Atomic Energy Commissary ("French DoE")
  - Around 20k researchers, 9 research centers all over France
  - Organized in **4** largely independent **divisions**: **DAM**, **DES**, **DRF** & **DRT**
  - **HPC** is a tool largely used **all over CEA**
- We just entered the **Exascale** era, that means **GPU**
  - **US Exascale**: **AMD** & **Intel**, **EU pre-Exascale**: **AMD** & **Nvidia**
  - 2 **Exascale** machines planned in **EU** for 2025
    - Jupiter machine in **Germany**, at Jülich => **Nvidia** + **SiPearl**(Rhea)
    - Jules Vernes machine in **France**, at CEA/TGCC (**open** call)
  - Need to re-develop applications with Performance portability
- GPU middleware: **software catalysts**
  - France and Europe: great research but no production tool
  - App developers are sitting on Buridan's ass
- A **need** for a long-term sustainable solution
  - Adapted to our hardware and software specificities
  - Trust in the roadmap

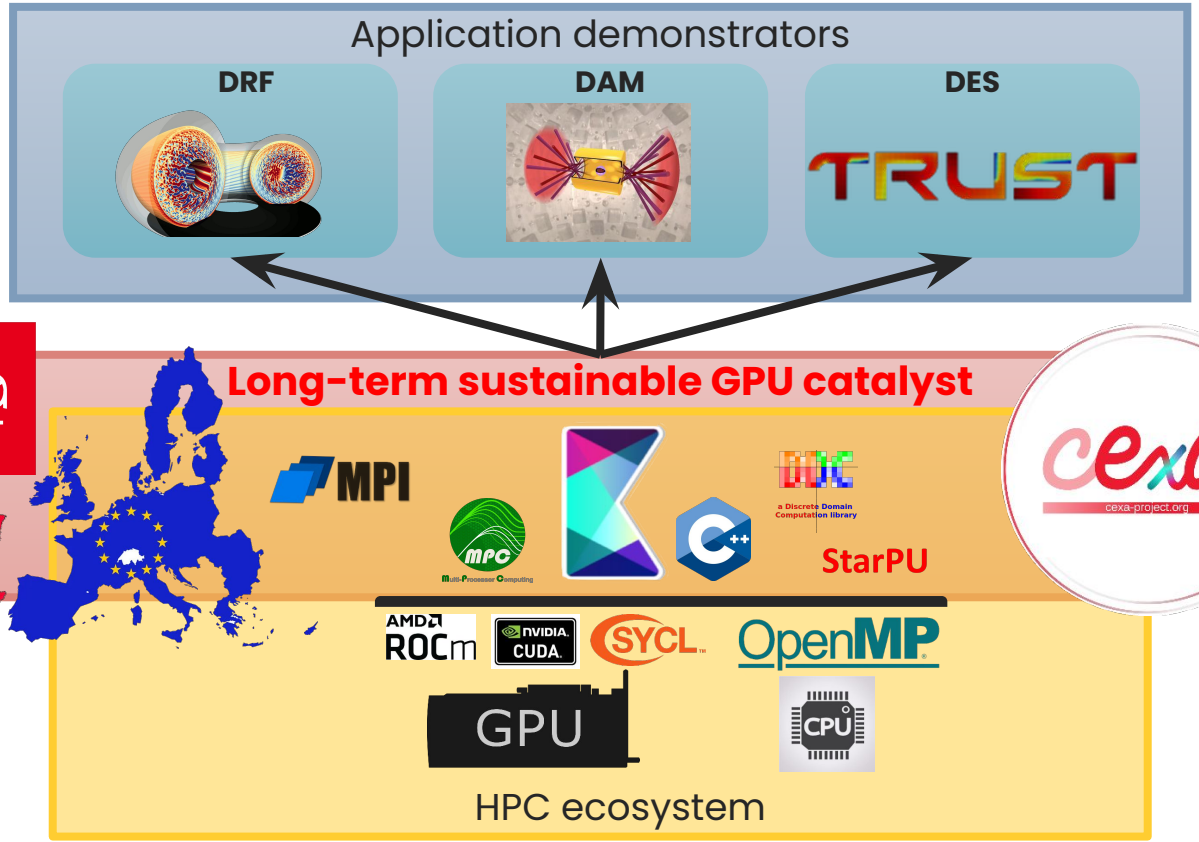


Computing power of the 500 top supercomputers from june 2004 to june 2024 (source Top500)



Today HPC is everyone's computing of tomorrow

CExA project: goals



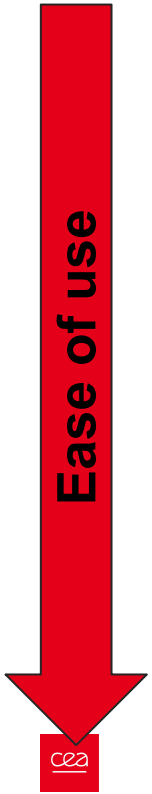
Disseminate and offer training at large

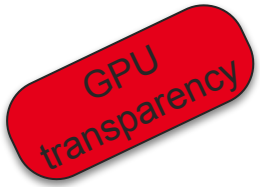
Adapt application demonstrators

Provide a long-term sustainable software catalyst for GPU computing

GPU programming, a vast choice of approaches

- Low-level, assembly-style programming models
  - Nearly manipulate the actual instructions the device understands
  - E.g. HSA, Level Zero, PTX, Spir-V , …
- General-purpose, imperative GPU programming models
  - Manipulate parallel loops, reductions, data transfer to & from device
  - E.g. Cuda, HIP, Kokkos, OpenACC, OpenMP (target), Raja, SYCL
- Combination & assembly of existing GPU kernels
  - Pytorch, StarPU, etc…
- Application framework for specific mesh types, numerical schemes
  - Use domain-specific concepts on GPU
- Pre-written GPU libraries
  - just call them from CPU
  - Neural Networks, Linear Algebra, …





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  - just call them from CPU
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Ease of use

Performance

Performance portability

Domain abstractions

GPU transparency

Generality

Imperative GPU programming, a vast choice of approaches

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

Imperative GPU programming, a vast choice of approaches

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

- **Production grade, with public support**

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- **Vendor neutral**

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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

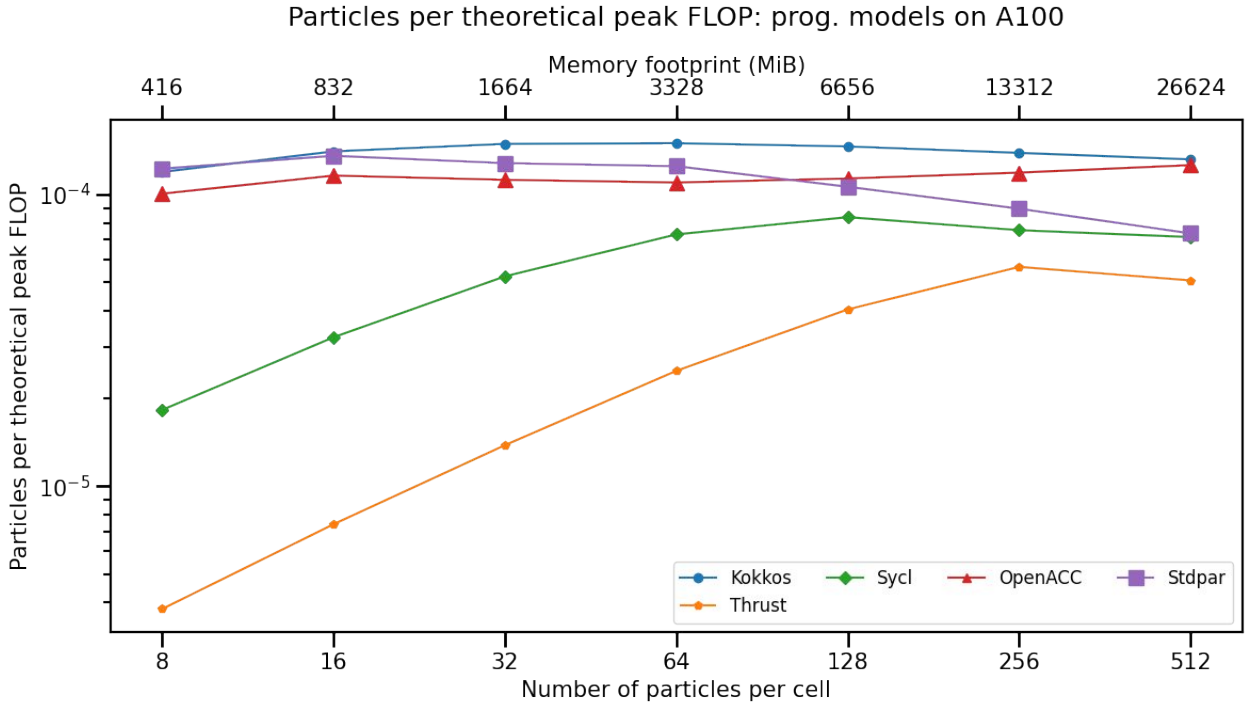
And what about performance?

Smilei code

- Particle per peak FLOP
- On A100
- Strong scaling
- Higher is better

Ester El Khoury, Mathieu Lobet, Kevin Peyen, Juan-Jose Silva Cuevas

Maison de la Simulation



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

Kokkos parallel patterns

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

Kokkos parallel patterns

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

```
parallel_reduce(Nj, KOKKOS_LAMBDA(int j, double& accumulator) {
      // [...]
      accumulator += /* [...] */ ;
}, result);
```

```
parallel_scan(Nj, KOKKOS_LAMBDA(int j, double& result, bool isfinal)
{
      // [...]
      accumulator += /* [...] */ ;
      if(is_final) {
            // [...]
      }
}, result);
```

- For
  - independent iterations
- Reduce
  - Accumulate into a single value
- Scan
  - N independent prefix reduction

Kokkos parallel patterns: easy debug

```
parallel_for("loop1", Nj, KOKKOS_LAMBDA(int j) {
      // [...]
});
```

- Naming loops ease debugging & profiling
- Integrated with kokkos-specific tools
- Get a trace with names includes
- Get a name in debug messages
- Omitted in the presentation, but a good practice overall

Kokkos parallel patterns: Policies

```
parallel_for(RangePolicy(1, Nj, chunk_size), KOKKOS_LAMBDA(int j) {
      // [...]
});
```

Beyond simple 1D execution

- RangePolicy for 1D iteration
  - Begin / end iteration boundaries
  - Chunk_size hint for improved performance
- MDRange policy for multi-dimensional iterations
  - Multi-D begin / end iteration boundaries
  - Tiling hint hint for improved performance

Kokkos parallel patterns: ExecutionSpace

```
parallel_for(RangePolicy(DefaultExecutionSpace(), 0, Nj), KOKKOS_LAMBDA(int j) {
      // [...]
});
```

- ExecutionSpace defines where to run
  - `Cuda`, `HIP`, `SYCL`, `HPX`, `OpenMP`, `OpenMPTarget`, `Threads`, `Serial`
  - 3 exec spaces per execution max: Serial + parallel Host + parallel Device
- Choose where to run at compile time with a `#define`
  - Usually set from CMake
- 2 predefined aliases are often enough
  - DefaultExecutionSpace: parallel Device, or parallel Host, or Serial
    - Most of the time, this is the default
  - DefaultHostExecutionSpace: parallel Host, or Serial
    - When using host-only code

Kokkos parallel patterns: hierarchical parallelism

```
parallel_for(TeamPolicy(Nj, team_size), KOKKOS_LAMBDA(const team_handle& team) {
      // [...]
      parallel_for(TeamThreadRange(team, Ni, chunk_size), KOKKOS_LAMBDA(int i) {
            // [...]
      });
      // [...]
});
```

- Default loops can not be nested
- 2-level nesting is supported by teams of threads
  - Matches groups / threads support in GPU
  - But also available on CPU
  - Intermediate (scratch) memory allocation available

Kokkos parallel patterns are asynchronous

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

- Asynchronous execution
- Result visibility is only assured after a fence
- Or between kernels running on the same execution space

Kokkos views: multi-dimensional arrays

```
View<int**, MemorySpace> my_matrix("matrix", Nx, Ny);
```

- Multi-dimensional arrays
  - Type & dimensionality specified: `int**` => 2D integer array
  - Dynamic sizes are parameters: `Nx, Ny`
  - Static sizes are also possible: `int*[4]` => 2D array, 4 × dynamic
- Behaves like a C++ `shared_ptr`
  - Shared ownership with reference counting (like in python)
- With a name for debugging/profiling
- MemorySpace is part of the type, defaults should be used
  - `CudaSpace, CudaHostPinnedSpace, CudaUVMSpace, HIPSpace, HIPHostPinnedSpace, HIPManagedSpace, SYCLDeviceUSMSpace, SYCLHostUSMSpace, SYCLSharedUSMSpace,` **`HostSpace`**`,` **`SharedSpace`**`, SharedHostPinnedSpace`
  - Check of accessibility between MemorySpace & ExecutionSpace

Kokkos views copies & co.

```
auto dview = subview(oview, pair(start, end), ALL, slice_idx);
```

- Make a new reference to a subset of an existing view
  - Modifying the result modifies the source
  - pair: select a subrange, ALL: keep the dimension, integer: slice the dimension

```
void deep_copy(const ExecSpace &exec_space, const ViewDest &dest, const ViewSrc &src);
```

- Copy data between 2 views
  - Potentially on distinct memory spaces
  - An asynchronous operation

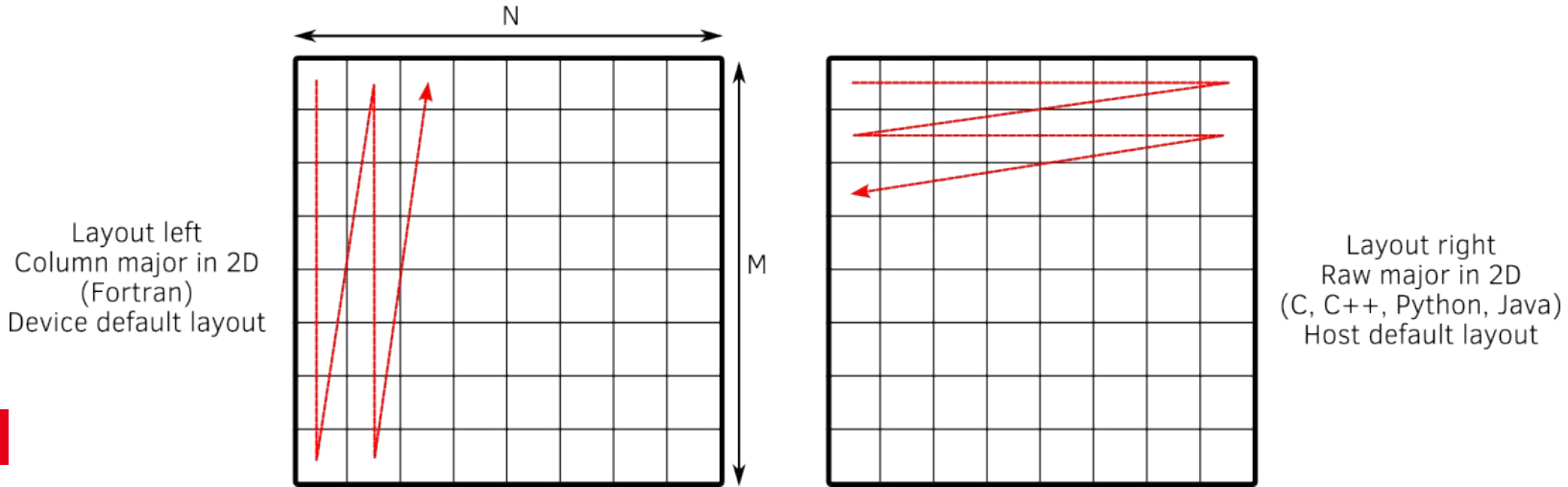
```
auto dview = create_mirror(mspace, a_view); // allocates & copy a new view of same size
auto dview = create_mirror_view_and_copy(mspace, a_view); // allocates & copy if necessary
```

- Allocates & copy to a new memory space

Kokkos views layout

```
View<double**, LayoutLeft> A("A", M, N);
```

- Layout specifies the linearization of multi-D indices into memory
  - `LayoutLeft` (a.k.a Fortran, default on GPU)
  - `LayoutRight` (a.k.a C, default on Host)
  - `LayoutStride` (generic, useful for subviews)



What's in Kokkos (core library)?

Multi-dimensional arrays

- Layout auto change for performance

Parallel patterns w. asynchronous support

- Independent interactions, Reductions, Scans

Iteration strategies

- Tiled, Hierarchical, ...

What's in Kokkos (core library)?

Multi-dimensional arrays

- Layout auto change for performance

Other containers

- Key-value maps, ScatterView …

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 "team-local" fast memory on the device

Parallel patterns w. asynchronous support

- Independent interactions, Reductions, Scans

Iteration strategies

- Tiled, Hierarchical, …

Algorithms

- Sorting
- Random number generation
- Many of STL parallel algorithms
- …

QoL features: portable printf, etc.

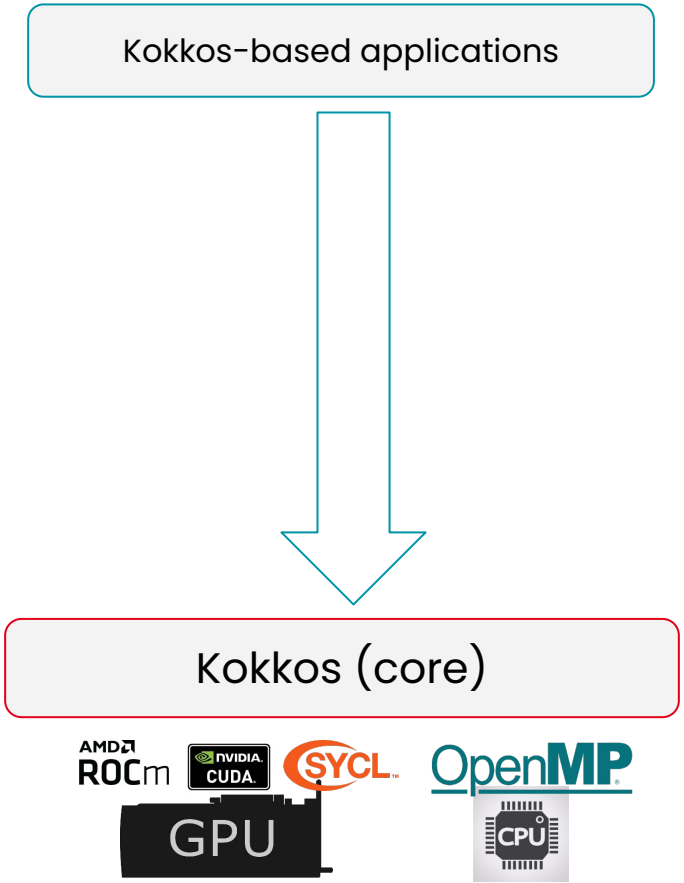
Portable atomic operations

SIMD

Coarse & fine-grain tasks

And much more…

Kokkos Ecosystem



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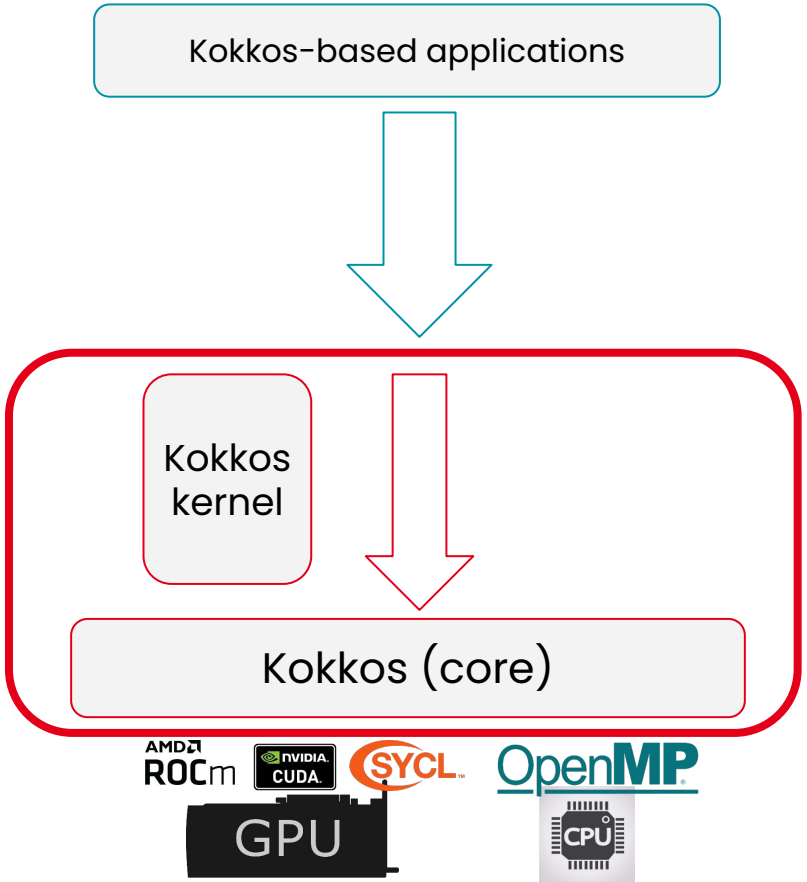

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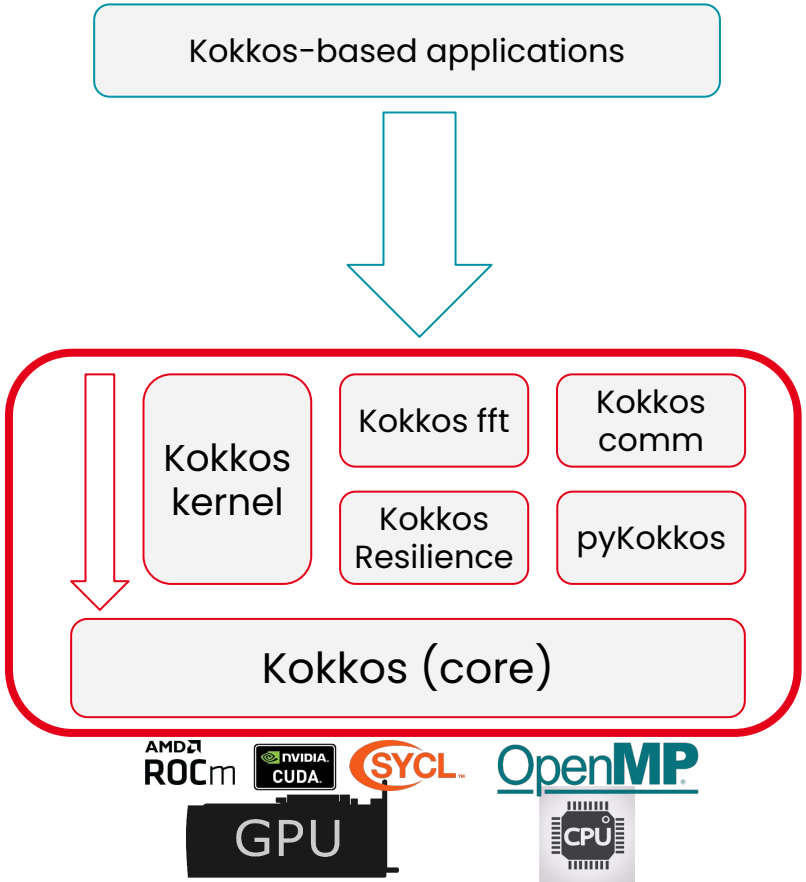

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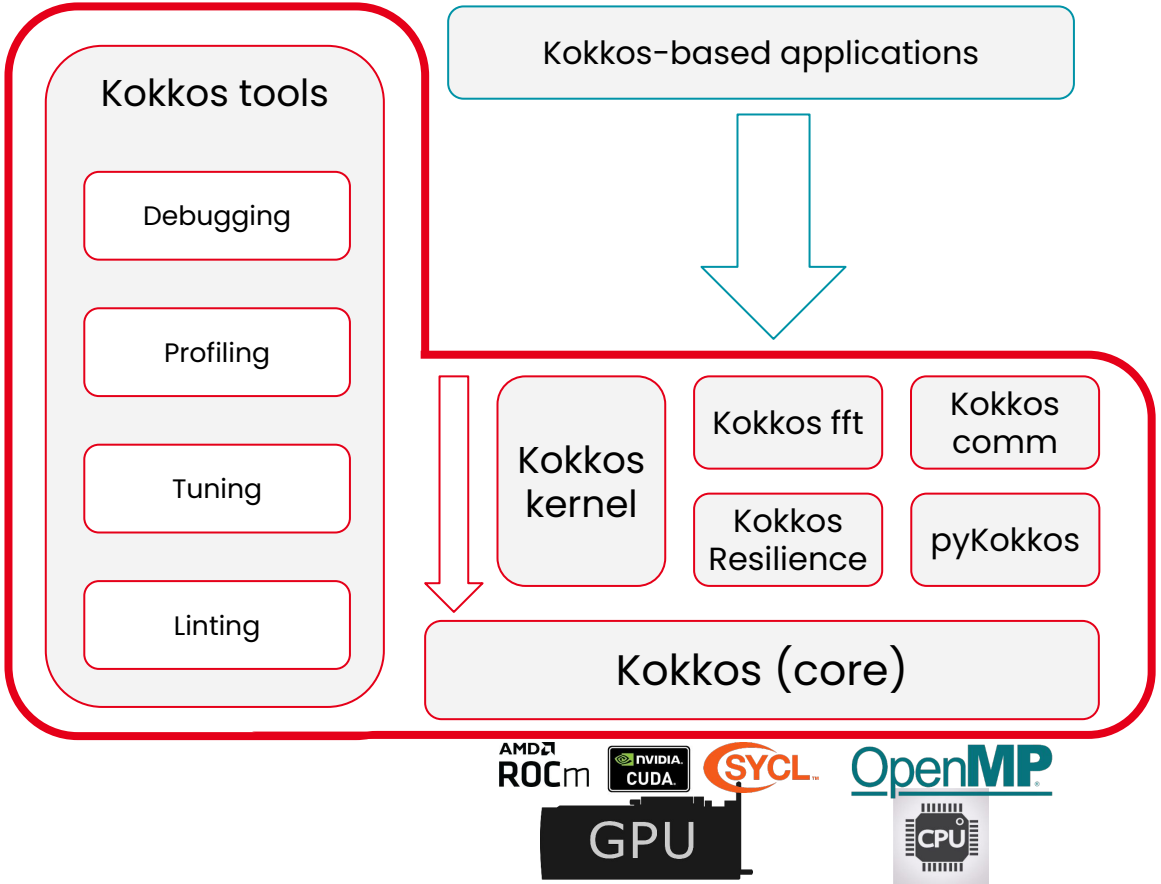

Kokkos Ecosystem

Kokkos tools

- Debugging
- Profiling
- Tuning
- Linting

Kokkos-based applications

Kokkos kernel

Kokkos fft

Kokkos comm

Kokkos Fortran

pyKokkos

Kokkos (core)

Kokkos support

- Documentation
- Tutorials
- Trainings
- Online Support
- Hackatons

AMD ROCm NVIDIA CUDA SYCL OpenMP

GPU

CPU

Kokkos Ecosystem, beyond just the Kokkos project

Kokkos tools

- Debugging
- Profiling
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Kokkos-based applications

- DDC
- ArborX
- Trilinos
- PETSc

Kokkos kernel

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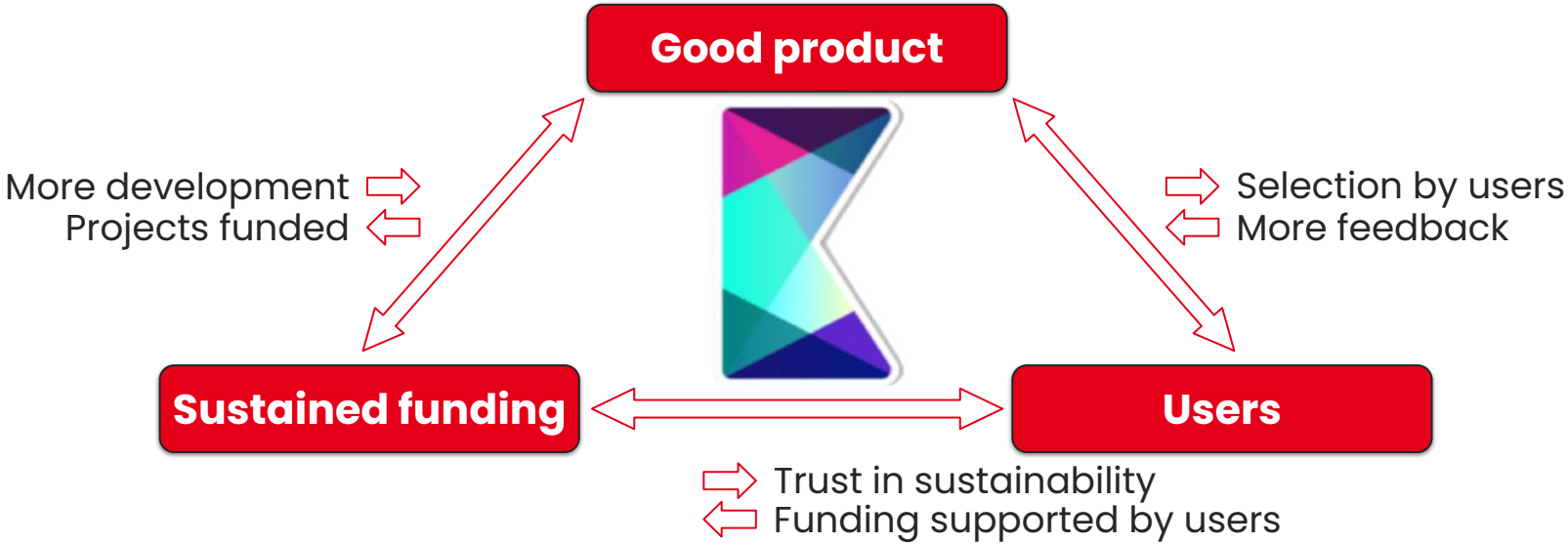
AMD ROCm · NVIDIA CUDA · SYCL · OpenMP

GPU · CPU

Kokkos at the center of a virtuous cycle



There is strength in numbers:
collaboration on core products is good for everyone

Kokkos an anteroom for standard C++

ISO C++ is **standardizing** base tools for **HPC**

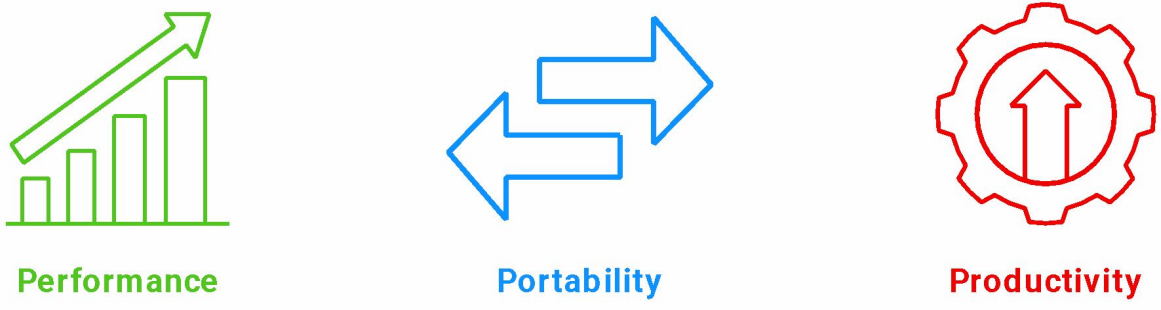
- Parallel programming is entering the **ISO C++ language**
  - Parallel algorithms, sender/receivers, etc.
- The Kokkos team spearheads the standardization of many **features**
  - Multi-D arrays (`std::mdspan`)
  - Vectorization (`std::simd`)
  - Linear algebra (`std::linalg`)
  - And much more to 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 keeps maintaining a **stable 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`)

Here comes HPSF

HPSF
HIGH PERFORMANCE SOFTWARE FOUNDATION



1. A neutral hub for open source, high performance software.
2. HPSF supports projects that advance portable software for diverse hardware by:
   - Increasing adoption
   - Aiding community growth
   - Enabling development efforts
3. Lowering barriers to productive use of today's and future high performance computing systems.

Under the Linux Foundation

Fund & vote

Governing board

Participate & vote

Technical Advisory Council

Join & vote

WGs

- Outreach
- Diversity
- CI & Testing
- Events
- Tools
- ...

Projects

Viskores, WarpX, HPCToolkit, Spack, TRILINOS, AMReX, Charliecloud, kokkos, APPTAINER, E4S

Members

Premier

aws, Hewlett Packard Enterprise, Lawrence Livermore National Laboratory, Sandia National Laboratories

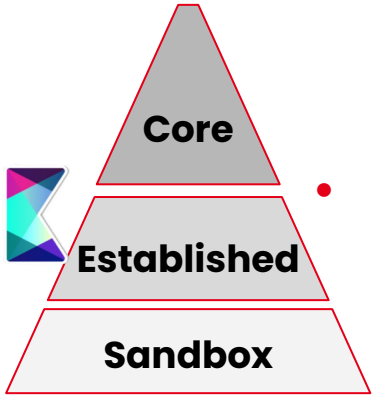
General

AMD, intel, NVIDIA, Argonne National Laboratory, Oak Ridge National Laboratory, Los Alamos National Laboratory, kitware, cea

Associate

CDAC, University of Oregon, University of Maryland, Jülich Forschungszentrum

HPSF Software life-cycle



- **Core** projects have a **reliable** & **sustainable development** process
  - The developer base is strong and diverse
  - The funding sources are multiple
  - The governance is well specified
    - No single institution has a majority in the project lead
  - The project also fulfils all Established requirements
- **Established** projects are **open to new developers** with a **wide base of users**
  - The user base is wide and diverse
  - The development process is well documented and newcomers-friendly
  - The development is strong and steady
  - The project also fulfils all Sandbox requirements
- **Sandbox** projects are **free**, **open**, **neutral**, and **aim for the above**
  - Are free, libre, open-source HPC-related LF projects
  - With a code of conduct
  - And an aim to widen developer and user-base beyond a single institution

Two (independant) ways to participate

- Joining as a **member** (for institutions)
  - You need to join the Linux Foundation (Non-profit/academic, as associate for $0)
  - Joining HPSF at one of **three levels**:
    - Premier: $175k / year
    - General: $2.5k - $50k / year depending on size of organization
    - Associate: $0 for non-profit / academic
  - **Take a stand**, fund it & **get a say** on where the funding goes to

- Joining as a **project** (for software project)
  - For the High Performance Computing ecosystem
  - That need a **neutral home** to facilitate multi-institutional collaborations
  - Providing **vendor neutral** solutions to engineering and science computational needs
  - Committed to building an **open developer and user community**

With CExA, CEA goes for Kokkos!

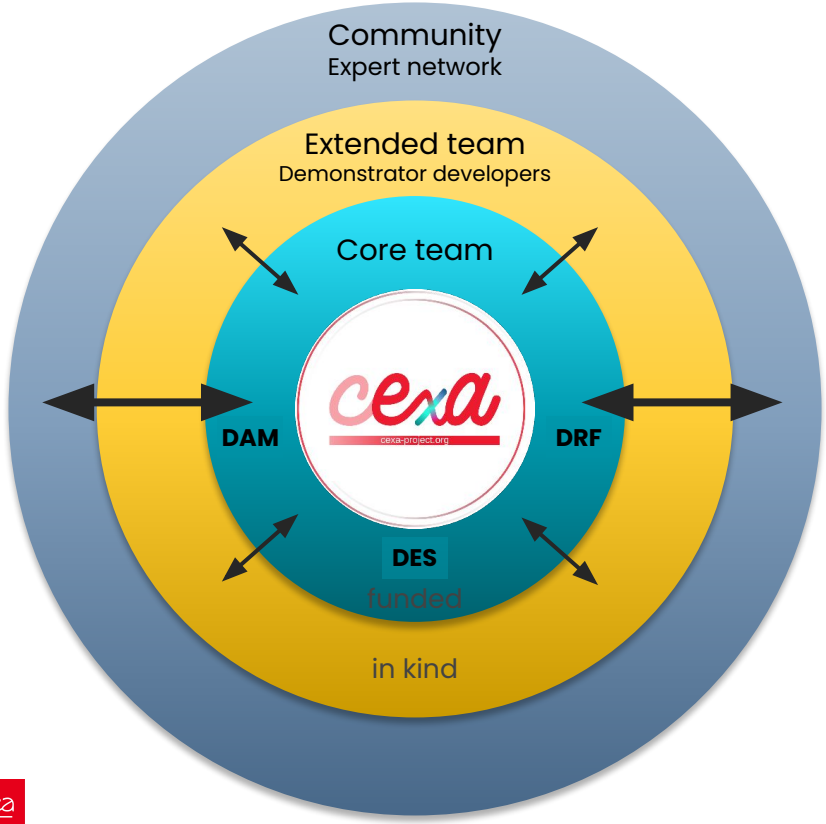
“adopt and adapt” strategy based on Kokkos

- Kokkos : a **strong technical basis**
  - A software architecture ready for the future
  - Mature, free, libre, and open-source
  - An **independent foundation** to own the product
    - HPSF under the Linux Foundation
  - A standardisation effort in ISO C++
    - A **stepping stone** one step ahead toward **HPC C++**
- Some **adaptations required**
  - For European **hardware**
    - There is no real hardware sovereignty without software sovereignty
  - For **applications** from CEA, France and Europe
    - Take our specificities into account

HPSF
HIGH PERFORMANCE SOFTWARE FOUNDATION

ISO International Organization for Standardization

CExA project in practice



- **Core team**
  - Management, implementation and dissemination
  - Fully integrated in the Kokkos team
  - 13 researchers from all over CEA
  - 3 recrutements done, 5 more funded
  - Funding for 3 more hires expected next year
- **Extended team**
  - Demonstrator developers
    - Not funded
    - Find their own interest in the participation
  - 2-3 new demonstrators every year
- **Community**
  - Federation of an expert network
  - Co-design of C**ExA**:
    - Identification of needs
    - Usage of C**ExA** in applications
  - Priority target for dissemination
  - Sustainability of the work

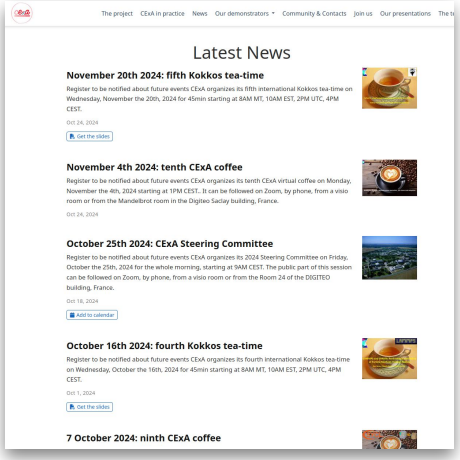
CExA: what's going on?

- Help with **documentation**
  - Website, Cheat-sheets, …
- **Trainings**, lots of training!
- **Support** our applications
  - Test **unified memory** viability & performance
  - Add required solvers to **Kokkos-kernels**
- Improve software **quality**
  - Work on **GPU CI**
  - Co-maintaining Kokkos **Spack recipes**
- Ease **code migration**
  - From **Fortran**
  - From **C (with classes)**
  - From **OpenMP (CPU)**

- Test **hardware** & improve kokkos for it
  - **Intel PVC** backend improvement
  - **Nvidia Grace Hopper** memory management handling
- Add **our contributions** to Kokkos ecosystem
  - **DDC**
    - Discrete data & computation
  - **kokkos-fft**
    - Performance portable FFT with a Kokkos API
  - **Kokkos-comm**
    - Message passing integrated with Kokkos

Kokkos training & community animation

- Many Kokkos trainings
  - September 2023 with C. Trott & D. Lebrun Grandié in Saclay
  - March 2025 Hackathon at IDRIS
  - September 2024 w. D. Lebrun Grandié & L. Berger-Vergiat
  - November 2024 Mission Numérique CEA in Grenoble
  - January 2025 CEA/Riken winter school in Barcelona
  - January 2025 Hackathon w. Intel
  - January 2025 ED 127 training
  - April 2025 Mission numérique in Cadarache
  - Summer school 2025 w. EDF & Inria
- Kokkos virtual tea-time once a month
  - Informal presentations & discussions, in English
    - about Kokkos, its ecosystem & GPU at large



https://anr.fr/fr/detail/call/pepr-numpex-appel-a-projets-numerique-pour-lexascale-2024/

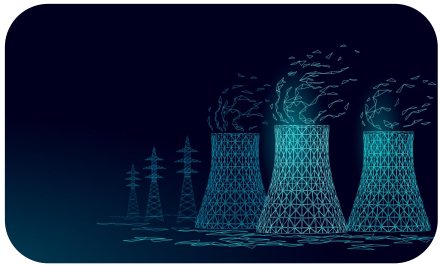
What's next? ANR GPU call (NumPEx)

- Part of NumPEx call: 2nd thematic axis
  - 1.8 M€ total on GPU for 1 or 2 projects between 500k€ & 1.8M€ each
- 3 sub-axes
  - Modern C++ programming models to **generate GPU executables** (Kernels)
    - Guidelines for application development
    - **Improvement of programming models for low & higher level**
    - Compile-time memory safety checking
    - Auto tuning, tooling & integration with dynamic kernel scheduling runtimes
  - Exploration of **programming models coming from other communities** (AI, etc.) for numerical simulation
  - Tools & programming models extensions to help **porting large code bases to GPU**
- Evaluation criteria
  - Collaboration with existing application demonstrators & pre-existing technical choices & research in NumPEx
  - Integration & usage of proposed tools & libraries in everyday production of large French & European codes
  - Roadmap for an integration in sustainable libraries (such as Kokkos) ensuring high TRL, long-term support & vendor neutrality and independence

To conclude

- Kokkos is a strong vendor-neutral, performance portable Exascale programming model with GPU support

- CExA & **HPSF** ensure it is a sovereign and sustainable approach that can be relied on for the foreseeable future



- A strong dynamic all over the CEA and beyond
- A knock-on effect with new synergies identified every weeks with code developers

The core team

Julien Bigot
Principal investigator

Ansar Calloo
Senior developer

Cedric Chevalier
Senior developer

Mathieu Lobet
Senior developer

Paul Gannay
Developer

Yuuichi Asahi
Senior developer

Rémi Baron
Senior developer

Thomas Padioleau
Senior developer

Paul Zehner
Developer

Hariprasad Kannan
Developer

The extended team

Pierre Ledac

Trust/TrioCFD lead

Virginie Grandgirard

GyselaX++ lead

François Letierce

Triclade lead

Julien Jaeger

TGCC link

Édouard Audit

Network animator

Samuel Kokh

DES link

Patrick Carribault

TGCC link

Join us & join the fun!

2-years HPC DevOps Engineer position

Deployment and CI on supercomputers for the C++ Kokkos library within the "Moonshot" CExA project

CEA is recruiting DevOps engineers for a 2-year period to join the CExA "Moonshot" project team, which is setting up CEA's GPU computing software stack around the Kokkos C++ library, to contribute to innovative packaging, deployment and continuous integration approaches for supercomputers, based in particular on Spack. A team of more than 10 people is currently being set up. The positions will be based at the CEA Saclay site near Paris.

2-years C++ expert engineer position

Contribution to the development of the Kokkos GPU computing library within the CExA "Moonshot" project

Join the CEA's ambitious "Moonshot" project, CExA, and contribute to the development of the Kokkos GPU computing library. We are recruiting six talented and enthusiastic C++ development engineers for a period of 2 years to work at our CEA Saclay site near Paris.

https://cexa-project.org

And what about performance?

An Evaluative Comparison of Performance Portability across GPU Programming Models

Joshua H. Davis[2], Pranav Sivaraman[2], Isaac Minn[2], Konstantinos Parasyris[1], Harshitha Menon[1], Giorgis Georgakoudis[1], Abhinav Bhatele[2]

[2]Department of Computer Science, University of Maryland
[1]Center for Applied Scientific Computing, Lawrence Livermore National Laboratory

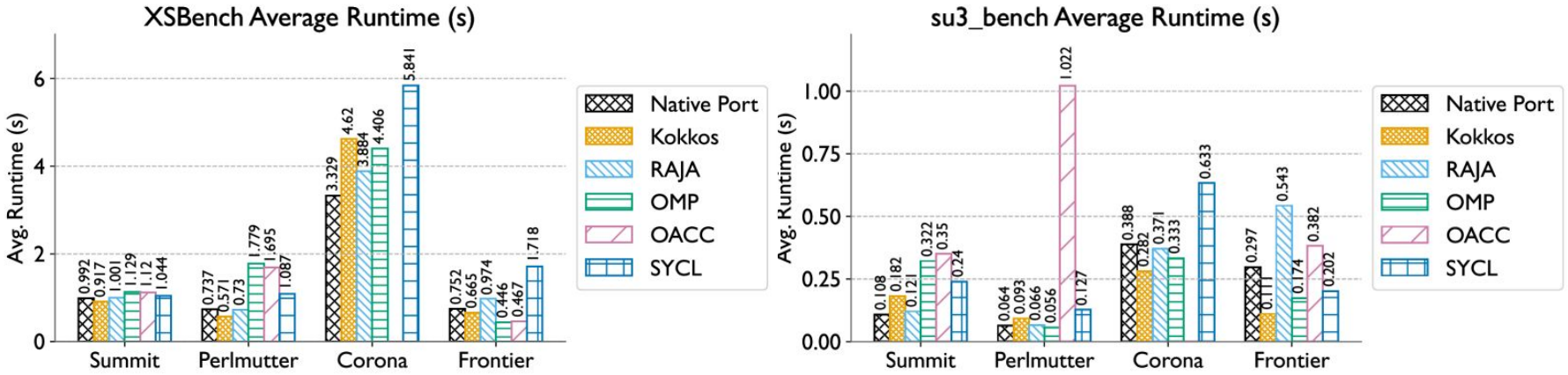
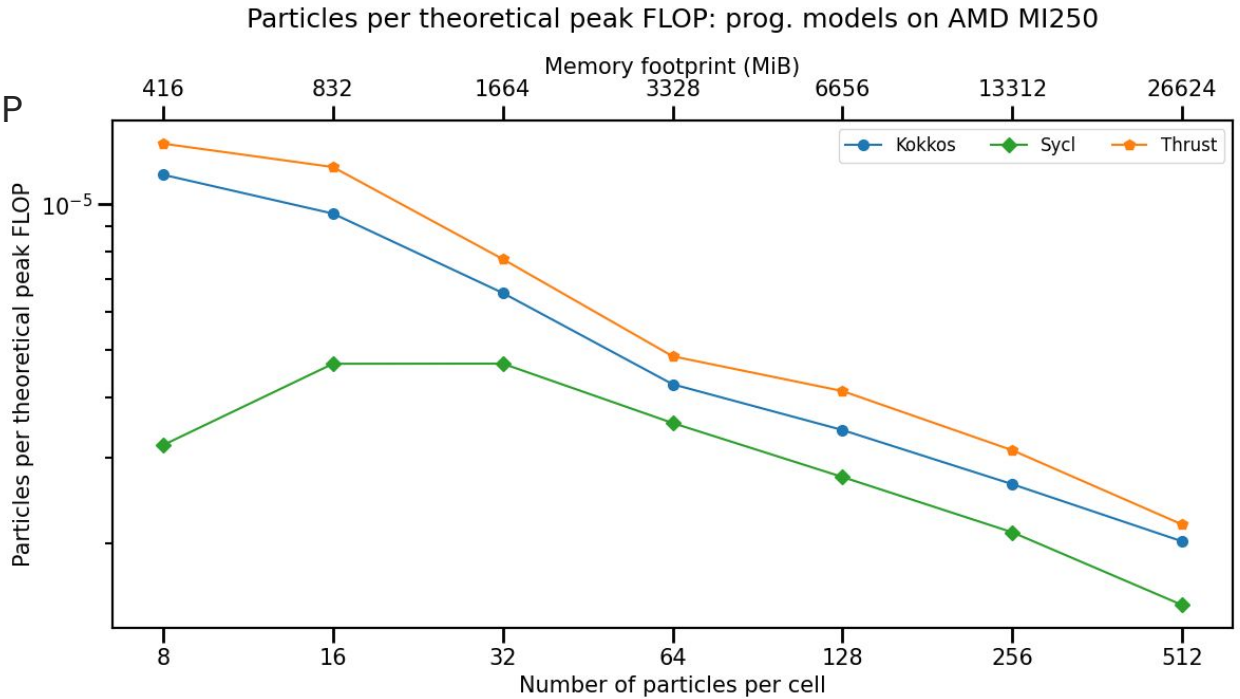


Figure 1: Average runtime of the XSBench (left) and su3_bench (right) proxy apps across all platforms and programming models. Lower is better.

And what about performance?

Smilei code

- Particle per peak FLOP
- On MI250
- Strong scaling
- Higher is better



Ester El Khoury, Mathieu Lobet, Kevin Peyen, Juan-Jose Silva Cuevas

Maison de la Simulation

What kind of software is in HPSF so far?

Build & Deploy

- Build your software with tools that support all major computing architectures
- Deploy with cloud-ready packaging and container technologies on everything from your laptop to the largest exascale supercomputers

Develop & Sustain

- Leverage performance-portable software technologies
- Reuse high-quality scientific computing libraries including programming models, solvers, and visualization
- Foster community development for modeling and simulation applications

Analyze & Tune

- Profile your software with tools targeted at HPC environment
- Tune your software using information that connects performance data to how your software leverages HPSF projects

Spack

E4S

APPTAINER

kokkos

Charliecloud

TRILINOS

Viskores

HPCToolkit