Kokkos, a sustainable performance portability layer

co-developed by CExA, a project for Computing at Exascale on Accelerators at CEA


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ORAP Forum
May 19th 2025
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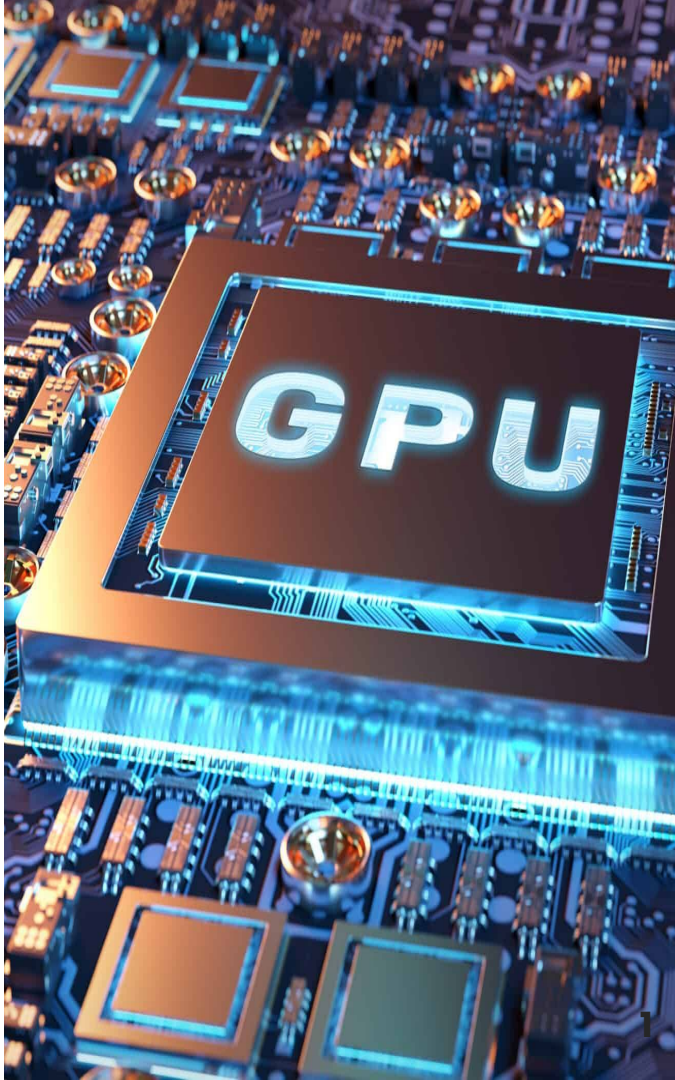
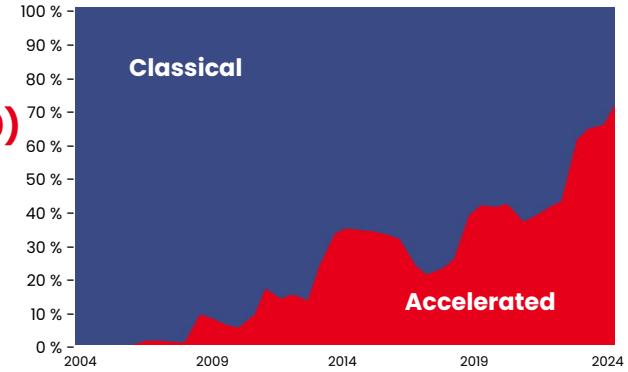
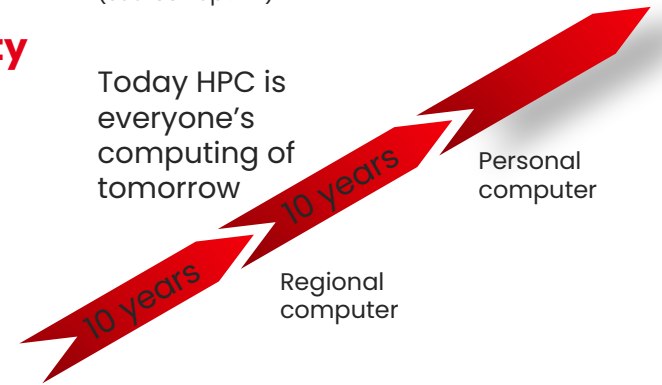


Context 1+ year ago

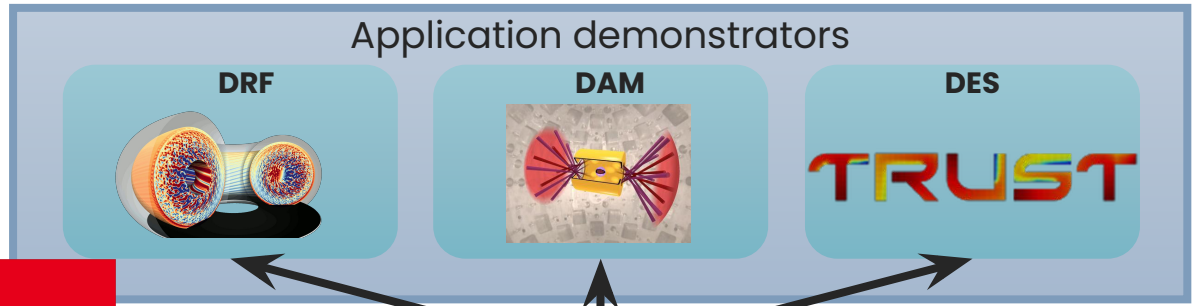
- HPC is a tool in a wide range of domains at CEA
- We just entered the **Exascale** era, that means **GPU (>82% Top500)**
  - European pre-Exascale systems: Mix of AMD & Nvidia
  - US Exascale systems: AMD & Intel
  - First European Exascale machines are coming
    - *Jupiter* at Jülich (Germany) => Nvidia & Rhea
    - *Alice Recoque* at **CEA/TGCC** (call still open)
  - Need to re-develop applications with **Performance portability**
- GPU programming models: **software catalysts**
  - France and Europe: great research but no production tool
- A **need** for a long-term sustainable solution
  - **Adapted** to our hardware and software specificities
  - Where we can have **trust** in the roadmap

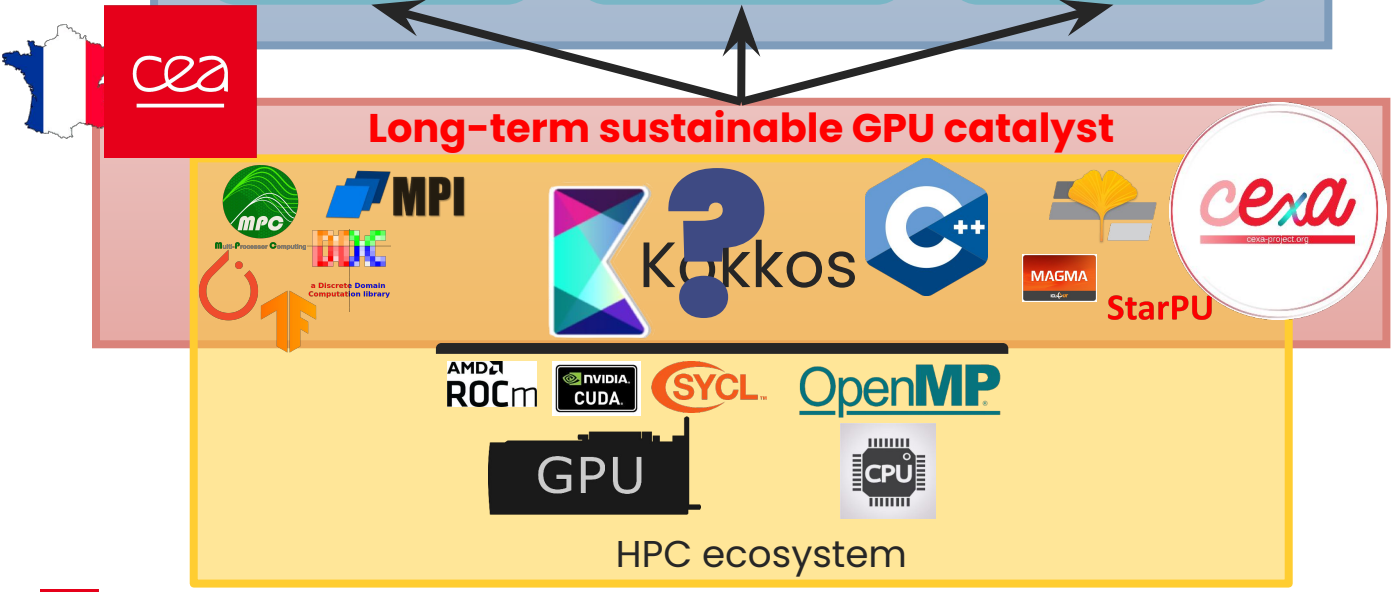


Computing power of the 500 top supercomputers from june 2004 to june 2024 (source Top500)



CExA project: goals





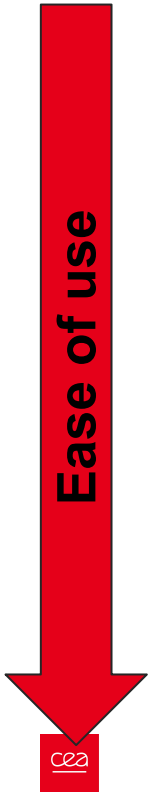
Disseminate and offer training

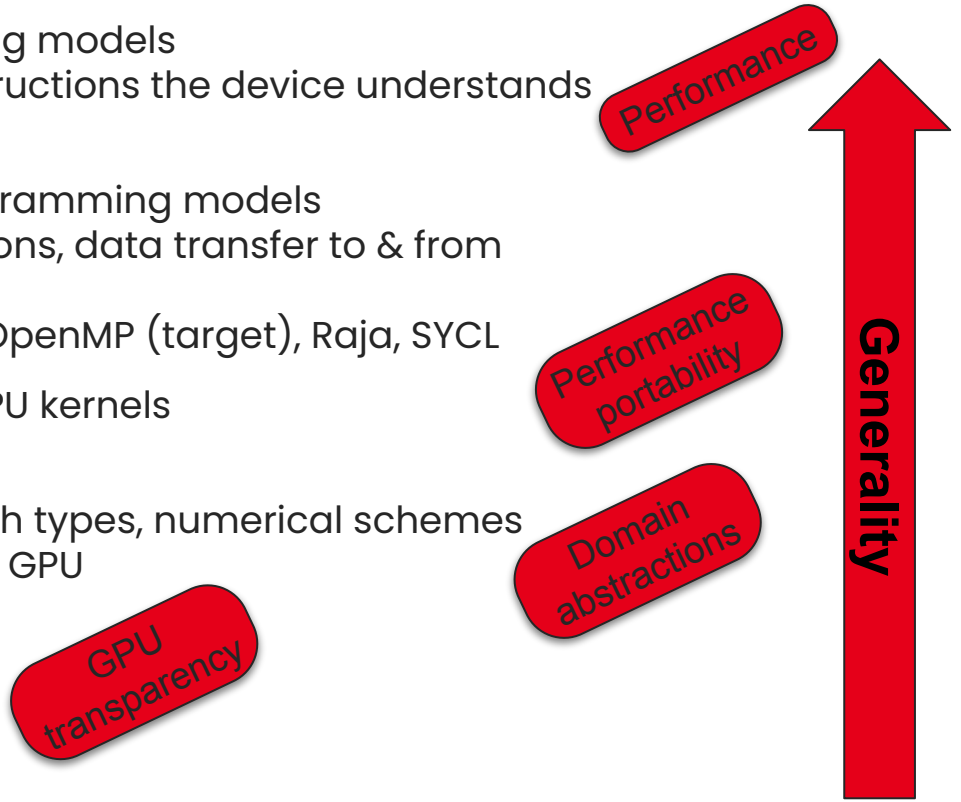
Adapt application demonstrators

Provide a long-term sustainable software catalyst for GPU computing

How to write code for GPU?

- 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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Ease of use

Performance

Performance portability

Domain abstractions

GPU transparency

Generality

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Available solutions

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

Available solutions

- Cuda
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- **Raja**
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- **Production grade, with public support**

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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

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
  - With variable performance

Kokkos

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

Available solutions

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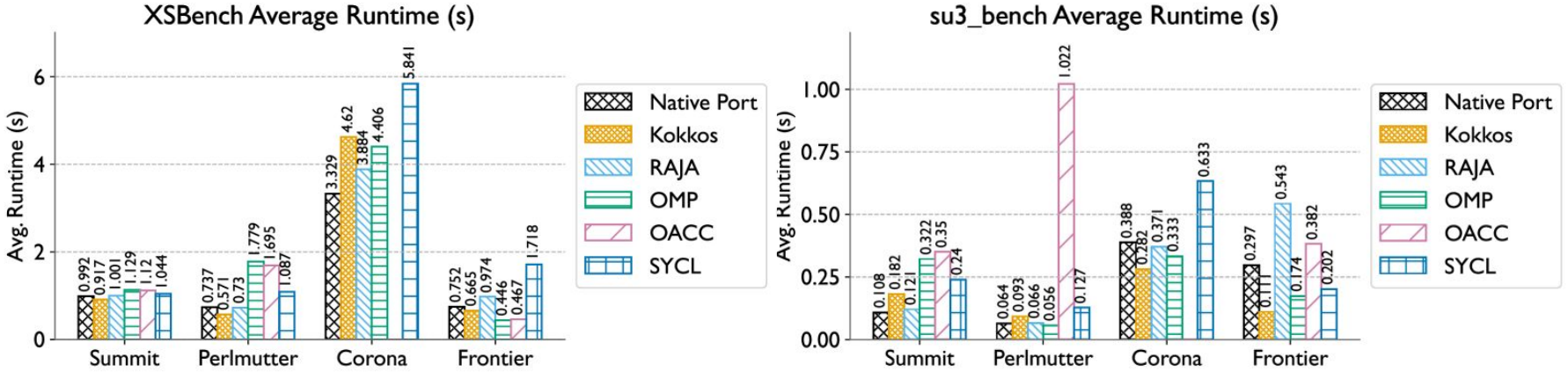
- Production grade, with public support
- Vendor neutral
- Annotations
  - Works best with imperative languages: C, Fortran, …
  - Compiler integration: potential for additional optimizations
  - Seq. first, requires to re-design applications for GPU
- Library
  - Suited to language with deep encapsulation: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

And what about performance?



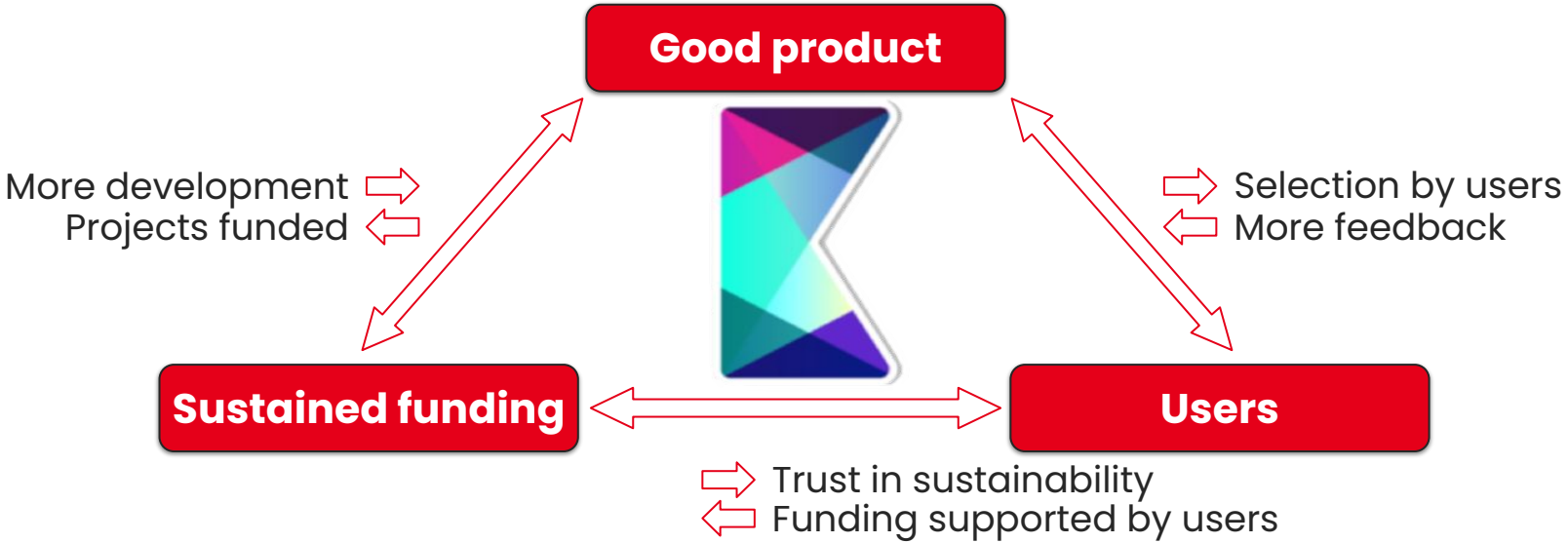
Average runtime of the XSBench (left) and su3_bench (right) proxy apps across all platforms and programming models.
Lower is better.

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

Kokkos at the center of a virtuous cycle

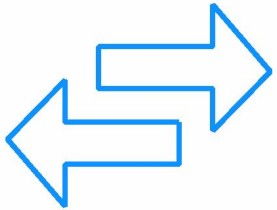


There is strength in numbers:
collaboration on core products is good for everyone

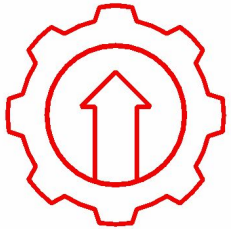
Kokkos, a HPSF project

HPSF
HIGH PERFORMANCE SOFTWARE FOUNDATION

Performance



Portability



Productivity

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

HPSF
HIGH PERFORMANCE SOFTWARE FOUNDATION

Fund & vote

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Los Alamos NATIONAL LABORATORY EST.1943
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UNIVERSITY OF MARYLAND
UNIVERSITY OF OREGON
UTokyo
Universität der Bundeswehr München

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Governing board

Participate & vote

Technical Advisory Council

Join & vote

WGs & committees

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

Projects

Spack
Charliecloud
AMReX
HPCToolkit
APPTAINER
E4S
TRILINOS
kokkos
OpenCHAMI
VISKORES
HPX
WarpX
ENVIRONMENT MODULES
CHAPEL

The TAC has established a project lifecycle as a path to sustainability

Emerging

- Committed to open governance
- Working towards best practices
- Important projects for the HPC ecosystem

Established

- Wide usage by at least 3 orgs of sufficient size and scope
- Steady commits from at least one organization
- Robust development practices

Core

- Used commonly in production environments
- Steady commits from *more* than one organization
- Large, well-established project communities
- Sustainable cycle of development and maintenance

HPSF
HIGH PERFORMANCE SOFTWARE FOUNDATION

Neutrality through HPSF

1. Sustaining OSS projects requires a community
2. Building a community requires trust
    - Projects will continue to be available
    - Projects are usable by anyone
    - No one organization can control the direction of the project
    - Projects are open to new contributors and new ideas
3. Trust gets us users; some users become contributors
4. Neutral, open governance ensures that we can build the broadest possible communities

The CExA project

“adopt and adapt” strategy based on Kokkos

Kokkos : **a strong technical basis**

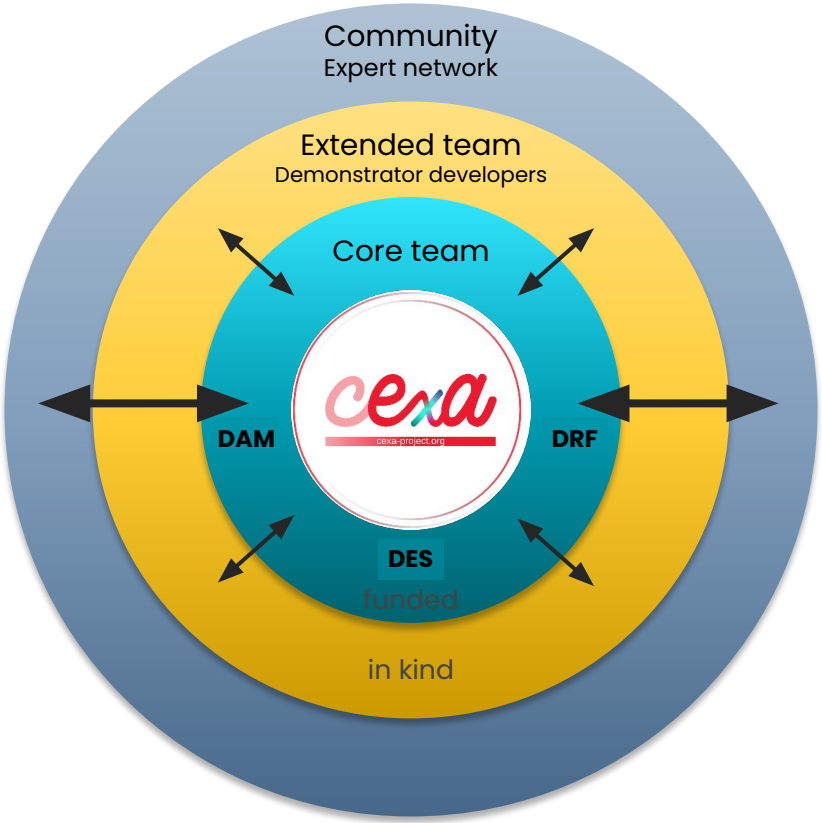
- A software architecture ready for the future
- Mature, free, libre, and open-source
- An **independent foundation** to own the product
  - HPSF under the Linux Foundation

- A standardisation effort in ISO C++
  - A **stepping stone** one step ahead toward **parallel 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

CExA project in practice



- **Core team**
  - Management, implementation and dissemination
  - 12 researchers from all over CEA
  - 6 dedicated recrutements
    - 1 as a permanent researcher !
  - Funding for 2 or 3 hires expected every 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

Kokkos development today

Primary teams

Contributions & support

- Number of commits by institution
- In the last 6 month

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: ExecutionSpace

```
parallel_for<ExecutionSpace>(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
  - DefaultHostExecutionSpace: parallel Host, or Serial
    - When using host-only code

Kokkos parallel patterns: Policies

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

Beyond simple 1D execution

- Give an instance of ExecutionSpace for multi-GPU or multi-Stream support
- 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: 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
```

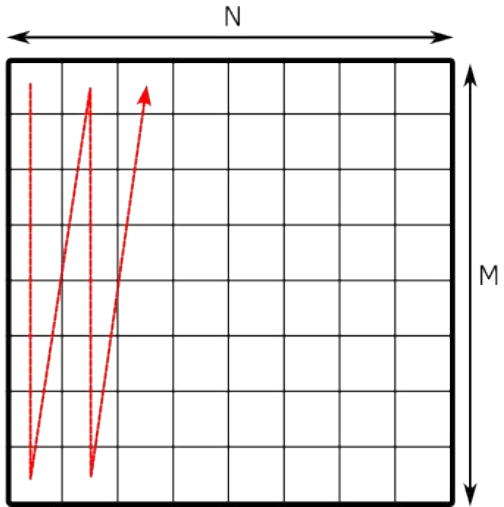
- Allocates & copy to a new memory space

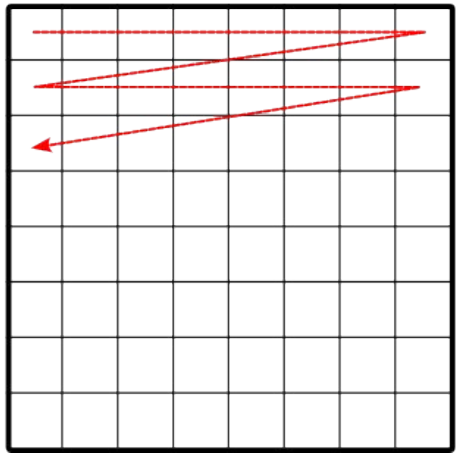
Kokkos views layout

```
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)

Layout left
Column major in 2D
(Fortran)
Device default layout





Layout right
Raw major in 2D
(C, C++, Python, Java)
Host default layout

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

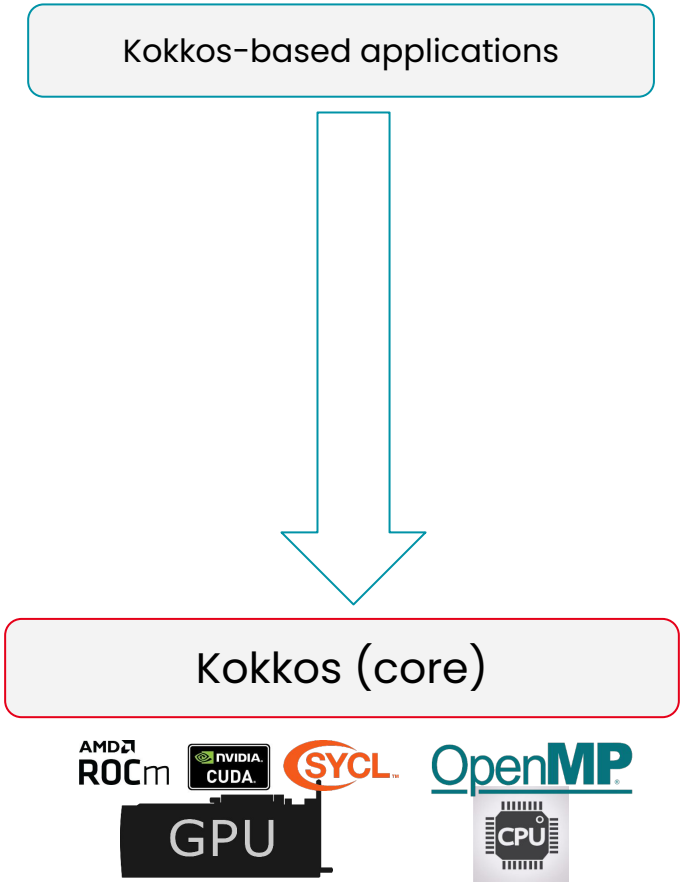
Coarse & fine-grain tasks

And much more…

What's new in Kokkos (core library)?

- Multi-GPU support for CUDA, HIP, and SYCL
  - Launch kernels on multiple devices from a single host process
- Many Team-Level Algorithms
  - Extended API with a new overload for team-level support
- Build systems update
  - support linking against build tree & building with hidden visibility
- New Kokkos::View implementation
  - Now mdspan-based
- Improved sorting performance
- Updated SIMD support to align with C++26
- Improved Thread-Safety
  - Kernels can be submitted from multiple threads to the same execution space
- Clarified support for View of Views
  - Introduced a new `SequentialHostInit` view allocation property
- Improved clang-tidy Conformity

Kokkos Ecosystem



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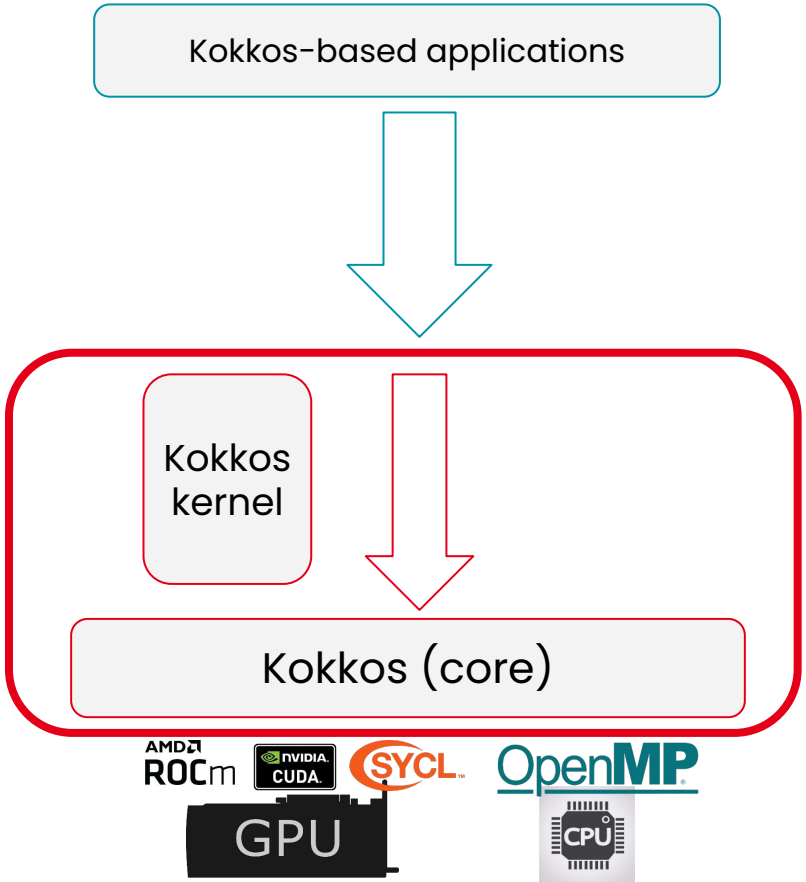

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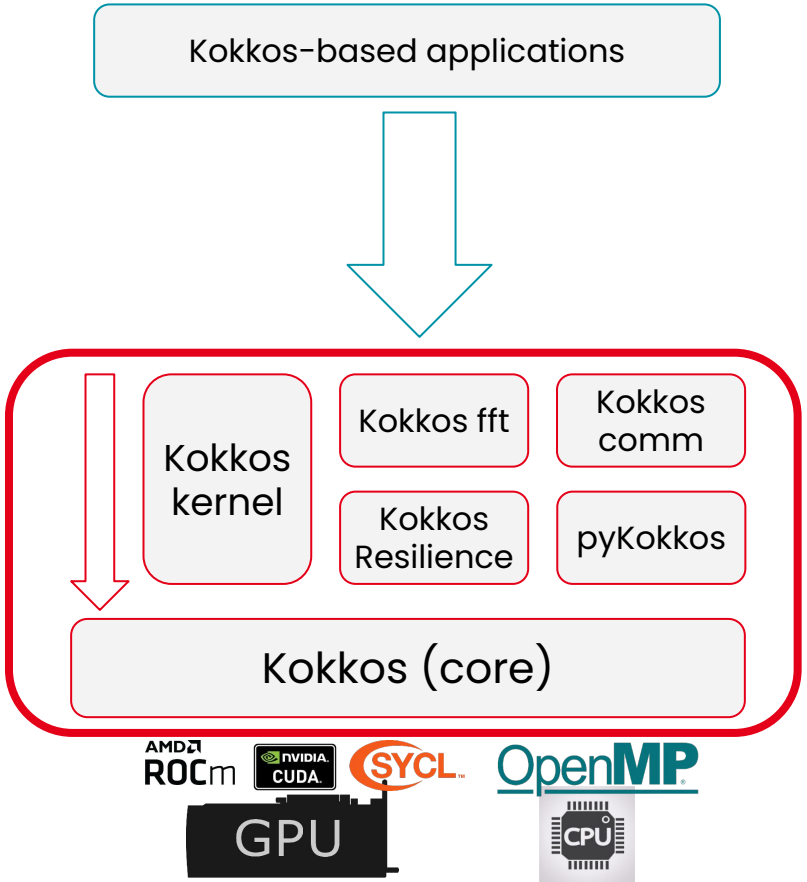
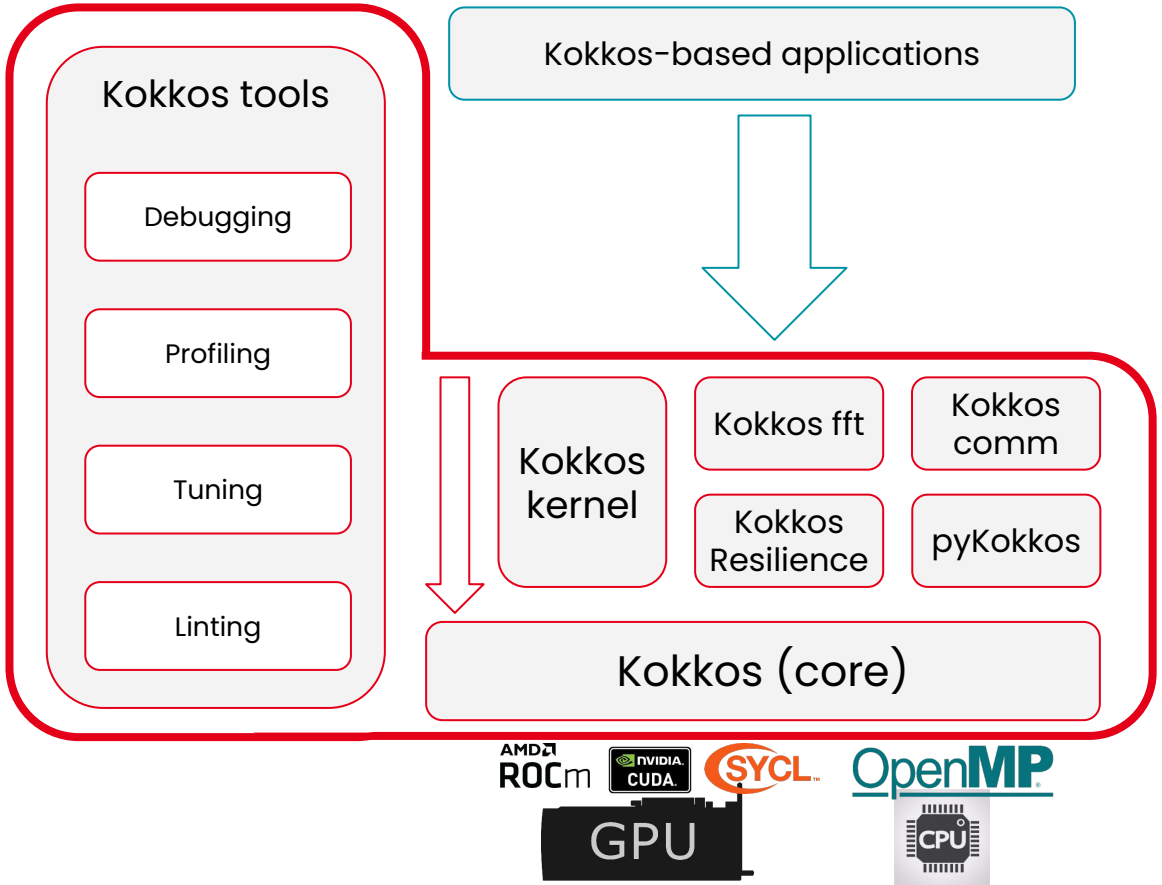


Kokkos Ecosystem



Kokkos Ecosystem

Kokkos tools

- Debugging
- Profiling
- Tuning
- Linting

Kokkos-based applications

Kokkos kernel

Kokkos fft

Kokkos comm

Kokkos Resilience

pyKokkos

Kokkos (core)

Kokkos support

- Documentation
- Tutorials
- Trainings
- Online Support
- Hackatons

AMD ROCm NVIDIA CUDA SYCL OpenMP GPU CPU

Kokkos Ecosystem

Kokkos tools

- Debugging
- Profiling
- Tuning
- Linting

Kokkos-based applications

- DDC
- ArborX
- Trilinos
- PETSc

Kokkos kernel

- Kokkos fft
- Kokkos comm
- Kokkos Resilience
- pyKokkos

Kokkos (core)

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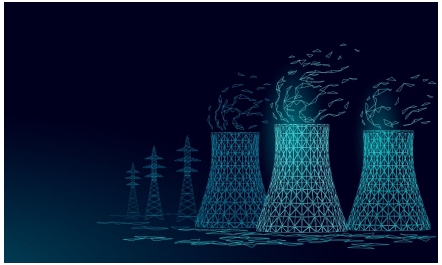
AMD ROCm · NVIDIA CUDA · SYCL · OpenMP

GPU · CPU

To conclude



- Kokkos is a strong vendor-neutral, performance portable Exascale programming model with GPU support
- A worldwide collaborative effort for an application first strategy
- 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