

## The reasons of a choice at the CEA

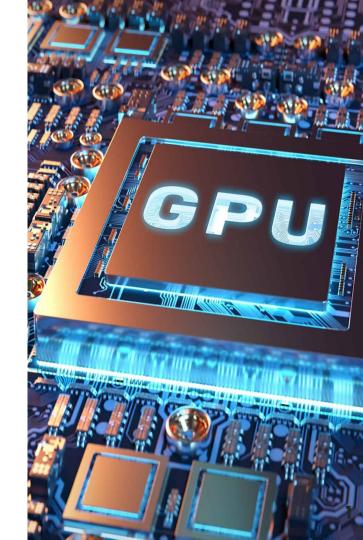


CEA/Riken School Barcelona January 15th 2025



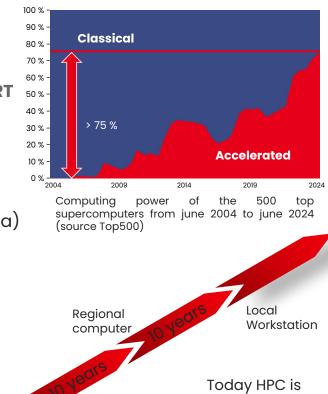
Computing at Exascale with Accelerators at the CEA

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



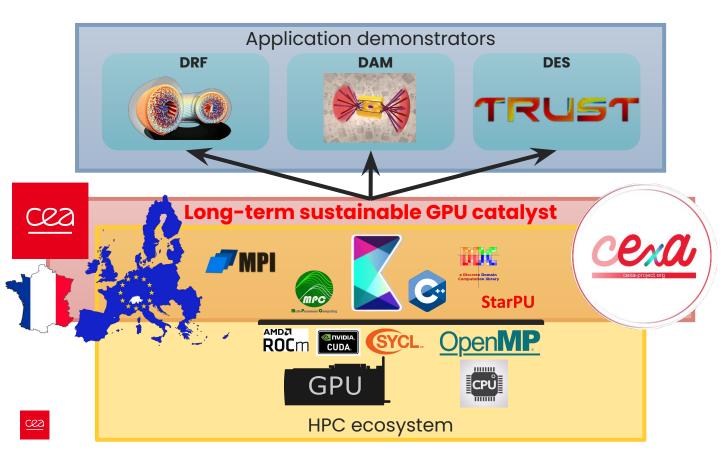
Top HPC

everyone's

tomorrow

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## **CEXA project: goals**



training at large Adapt application demonstrators

Disseminate

and offer

Provide a long-term sustainable software catalyst for GPU computing

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## 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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- OpenACC
- OpenMP (target)
- e Raja
- SYCL
  - OneAPI/DPC++
  - AdaptiveC++/OpenSYCL/hipSYCL

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  - AdaptiveC++ (was OpenSYCL/hipSYCL)

• Production grade, with public support

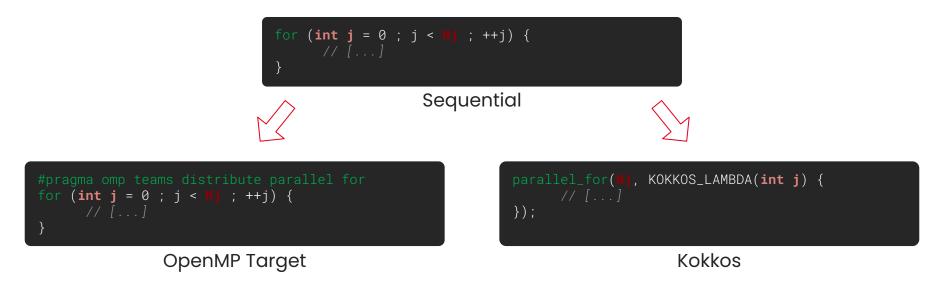
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## **OpenMP & Kokkos : the simplest GPU loop**



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

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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

## 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 ... ۲

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 deviče

Parallel patterns w. asynchronous support

- Independent interactions, Reductions, Scans Iteration strategies
  - Tiled, Hierarchical, ...

Algorithms

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

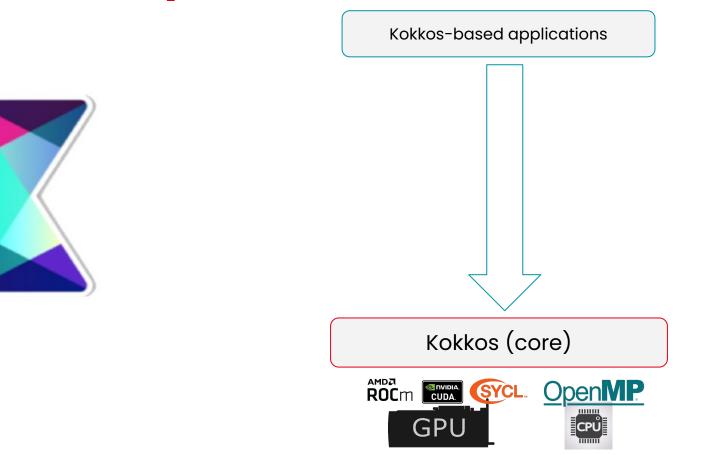
QoL features: portable printf, etc.

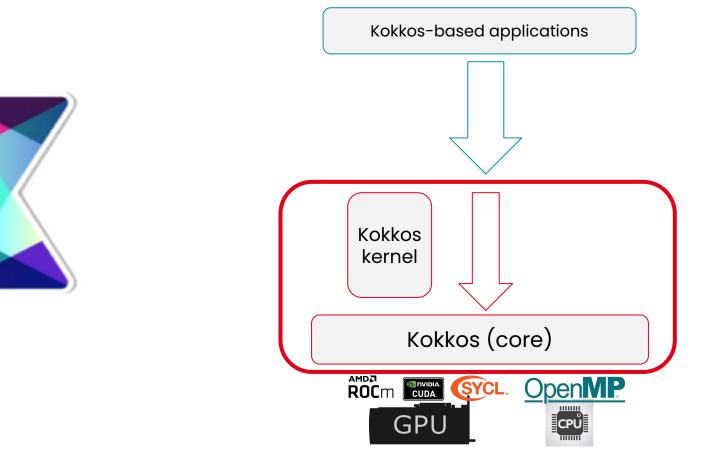
Portable atomic operations

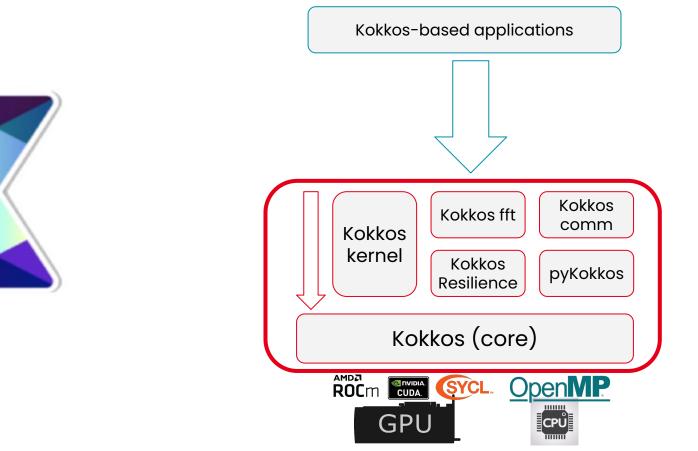
SIMD

Coarse & fine-grain tasks

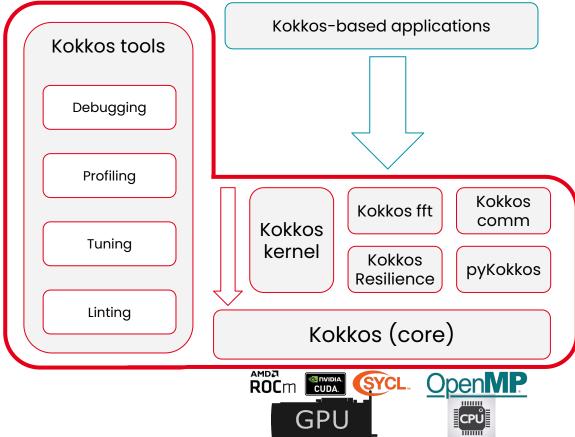
And much more...



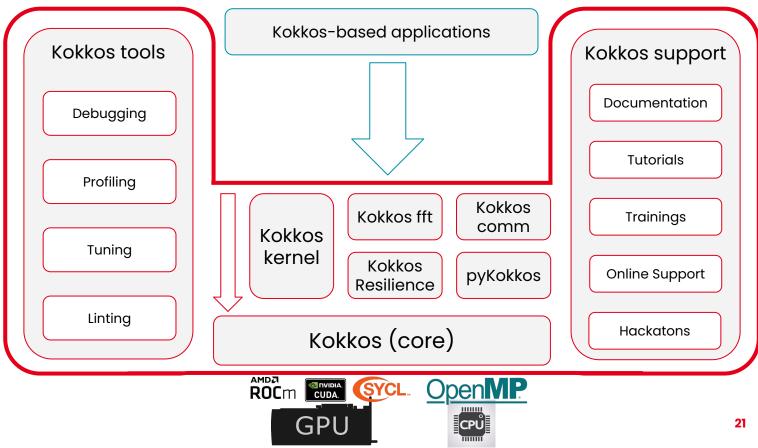






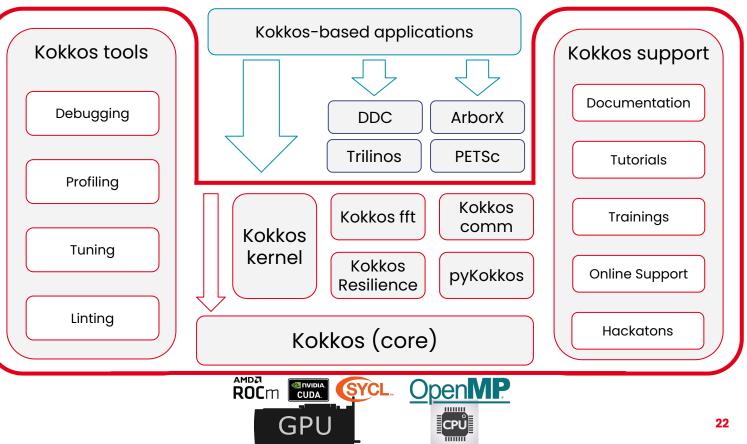




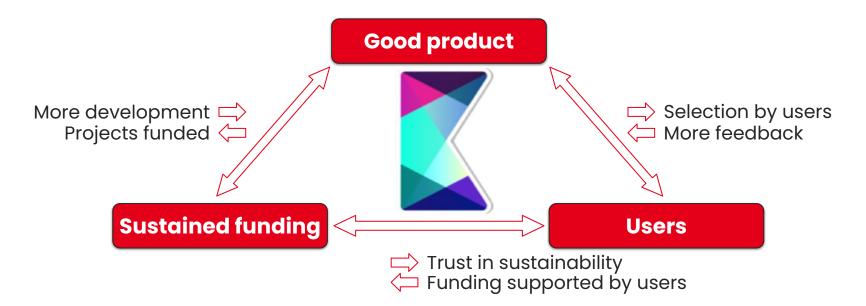


## Kokkos Ecosystem, beyond just the Kokkos project





## Kokkos at the center of a virtuous cycle



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

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## 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)

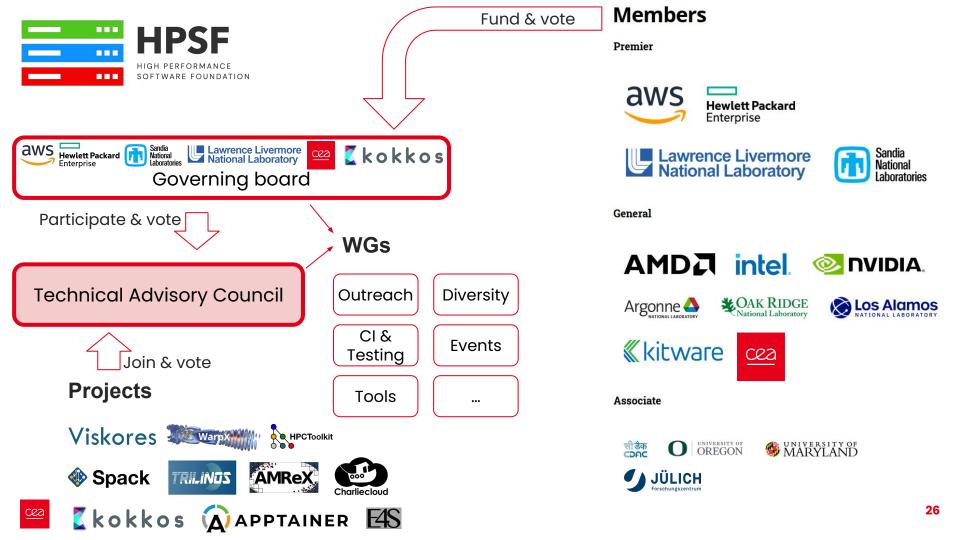






- 1. A neutral hub for open source, high performance software.
- 2. HPSF supports projects that advance portable software for diverse hardware by:
  - Increasing adoption
  - Aiding community growth
  - Enabling development efforts
- **3**. Lowering barriers to productive use of today's and future high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

## **Under the Linux Foundation**



## **HPSF Software life-cycle**

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- **Core** projects have a **reliable** & **sustainable development** process
  - The developer base is strong and diverse The funding sources are multiple 0
  - 0
  - 0
- The governance is well specified No single institution has a majority in the project lead
  - The project also fulfils all Established requirements 0

### **Established** projects are **open to new developers** with a **wide base of users**

- The user base is wide and diverse 0
  - 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 0
  - And an aim to widen developer and user-base beyond a single 0 institution

Core

Established

Sandbox

# 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

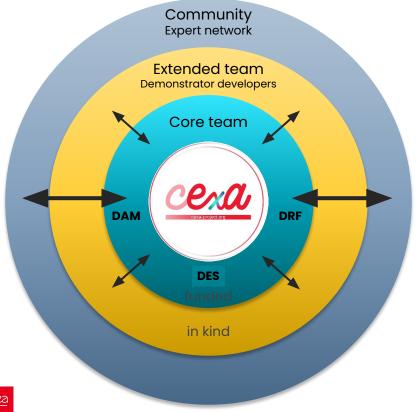


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International Organization for Standardization

## **CEXA project in practice**



#### Core team

- Management, implementation and dissemination
- Fully integrated in the Kokkos team
- 13 researchers from all over CFA
- 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 CExA:
  - Identification of needs
  - Usage of CExA 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 => Cf. Asahi-san pres
  - Kokkos-comm
    - Message passing integrated with Kokkos => Cf. Taboada-san pres

## **CEXA: what's next?** Can we collaborate?

### Kokkos-python interface

- Can we use **pytorch** inference in applications?
  - Pytorch -> MLIR -> Kokkos
  - w. Sandia & IFPEN
- Can we interface **python** calling **Kokkos**?
  - pykokkos-base
  - Or even generate Kokkos from Python
    - pykokkos
  - Integrate Kokkos optimized kernels in JAX?
  - w. MDFT application
  - => Asahi-san

### Can we help Fortran codes with Kokkos?

- Progressively translate kernel to Kokkos
  - Call them from Fortran
  - Kokkos-Fortran-interop
- Auto-generate Kokkos layout & glue code
  - Using fparser python-based Fortran parser
  - w. BigDFT application
- Can we create Kokkos annotations for Fortran?
  - Would Riken be interested to explore?

How can we help with optimization

- Can we use Auto-tuning ?
- w. Dyablo application & Lilia Zahouar

And of course, application porting, w. BigDFT, Dyablo, Gysela, MDFT, Triclade, Trust/TrioCFD, ...

## **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 extended team



## 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
  - 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
  - International

<b></b>	The project CExA in practice News Our demonstrators * Community & Contacts Join us Our presentation	ns The t
	Latest News	
	November 20th 2024: fifth Kokkos tea-time Registre for notifier about hunse week: CDA opigarios as this international Kokkos tas dress on Montangia, November 10:20: 2024 for denin stateming at IAM MT, IAM IST, 27M UTC. 401 0:13: 2017	
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	October 25th 2024: CEXA Steering Committee Register to exolified and hume events: CEA suggests to B 3028 benering Committee on Pride, and the tradition of the andreal memory, accurately and MCIST. The public and the the suggest of the andreal memory, accurately and the streng balance of the source and the data of the andreal memory accurate public the bottlets and accurate the andreal memory accurate public the bottlets and accurate the source of the source of the source of the bottlets and accurate the source of the source of the bottlets of the bottlets and accurate of the source of the source of the bottlets of the bottlets and accurate of the source of the source of the bottlets of the bottlets and accurate of the bottlets of the bottlets of the bottlets of the bottlets and accurate of the bottlets of the bottlets of the bottlets of the bottlets and accurate of the bottlets of the bottlets of the bottlets of the bottlets and accurate of the bottlets of the bottlets of the bottlets of the bottlets and accurate of the bottlets of the bottlets of the bottlets of the bottlets and accurate of the bottlets of the bottlets of the bottlets of the bottlets and accurate of the bottlets of the bottlets of the bottlets of the bottlets and accurate of the bottlets of	
	October 16th 2024: fourth Kokkos tea-time Repair to be notified abox (thate events CDA organizes is fourin international Kokkas tea drin on Winebacki), October the time, 32/4 for Genes scaring at DAM MT, 19AM IST, 2/44 UTC, 4/44 CT. In 1, 258 M. Carterian	
	7 October 2024: ninth CExA coffee	





## 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

### Thank you, and please accept a little gift from the project

## 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



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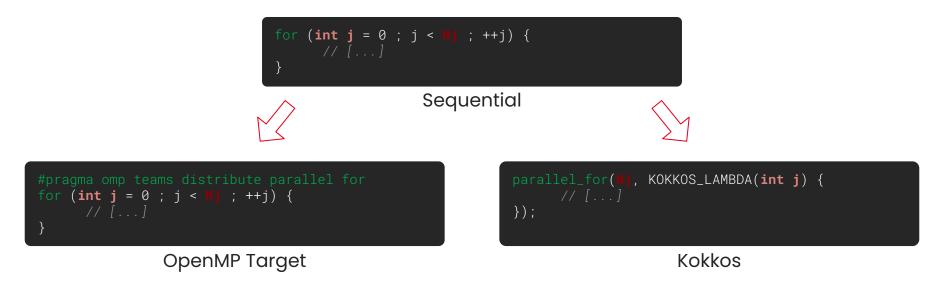
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    parallel_for(Nj, KOKKOS_LAMBDA(int j) {
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        }
});
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```

Kokkos

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## Compilation

#### 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)

#### **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

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### Kokkos parallel patterns

## parallel\_for(Nj, KOKKOS\_LAMBDA(int j) { // [...] });

## Kokkos parallel patterns

parallel\_for(Nj, KOKKOS\_LAMBDA(int j) {
 // [...]
});

parallel\_reduce(N), KOKKOS\_LAMBDA(int j, double& accumulator) {
 // [...]
 accumulator += /\* [...] \*/ ;
}, result);

For

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

## Kokkos parallel patterns: easy debug

- 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**

- 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

- 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

- 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

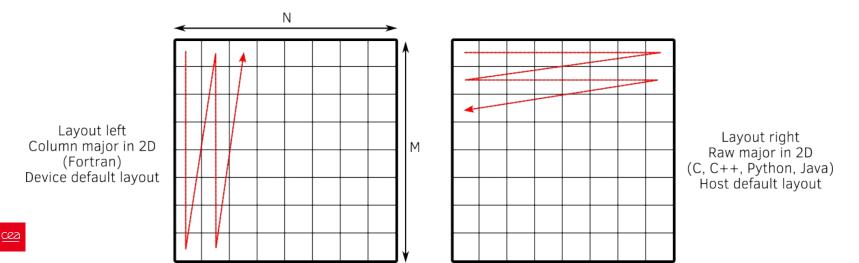
auto dview = create\_mirror(mspace, a\_view); // allocates & copy a new view of same size auto dview = create\_mirror\_view\_and\_copy(mspace, a\_view); // allocates & copy if necessary

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)



## Kokkos: a library with a history

