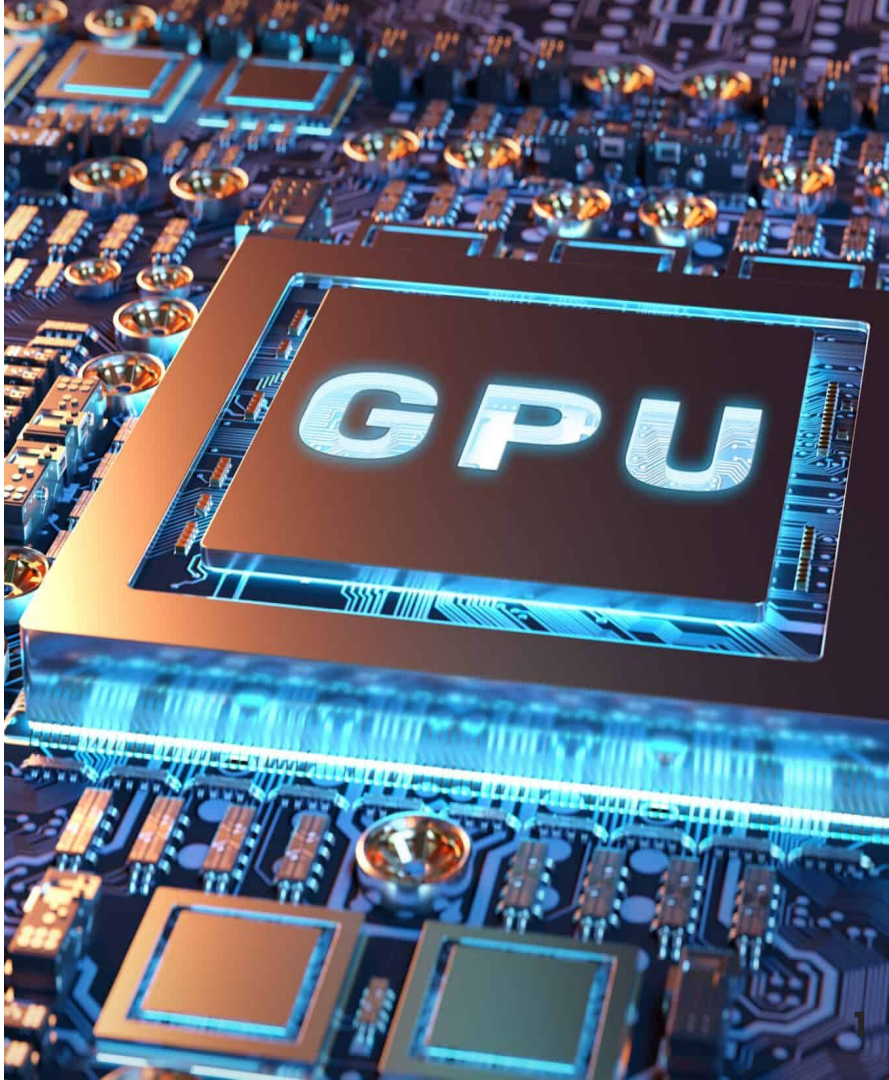
CExA “moonshot” project Computing at Exascale with Accelerators at CEA

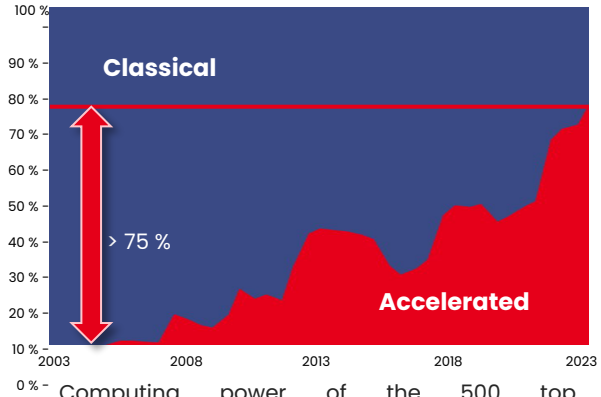
Software catalyst for GPU computing
Latest news



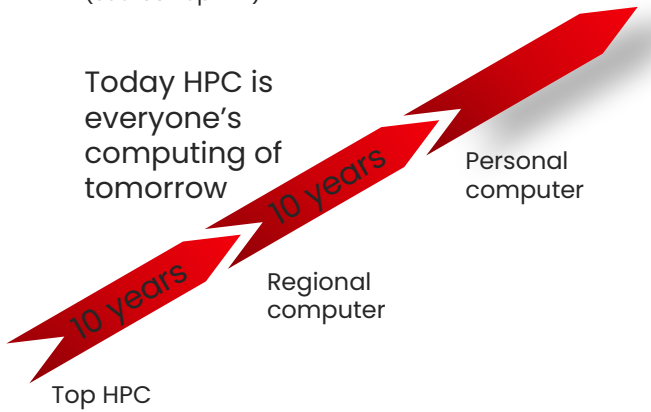
CEA-Riken meeting – 22 May 2024
Julien Bigot & CExA team

Context

- **CEA** is organized in 4 divisions (DAM, DES, DRF & DRT)
  - HPC is a tool used all over CEA, source of competitivity
  - CEA relies on self hosted machines, but is also included in the French & European 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
    - Jules Vernes, French machine at **CEA/TGCC** (open)
  - Need to re-develop applications with **Performance portability**
- GPU middleware: 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
  - Trust in the roadmap



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



Available solutions

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

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

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OpenMP versus Kokkos for a simple GPU loop

```
double* x;
double* y;
double* A;

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

```
View<double*, Kokkos::HostSpace> x;
View<double*, Kokkos::HostSpace> y;
View<double*> A;

{
      View<double*> dx;
      deep_copy(dx, x);
      View<double*> dy;
      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);
}
```

Ease of use does not offer a clear selection criterion

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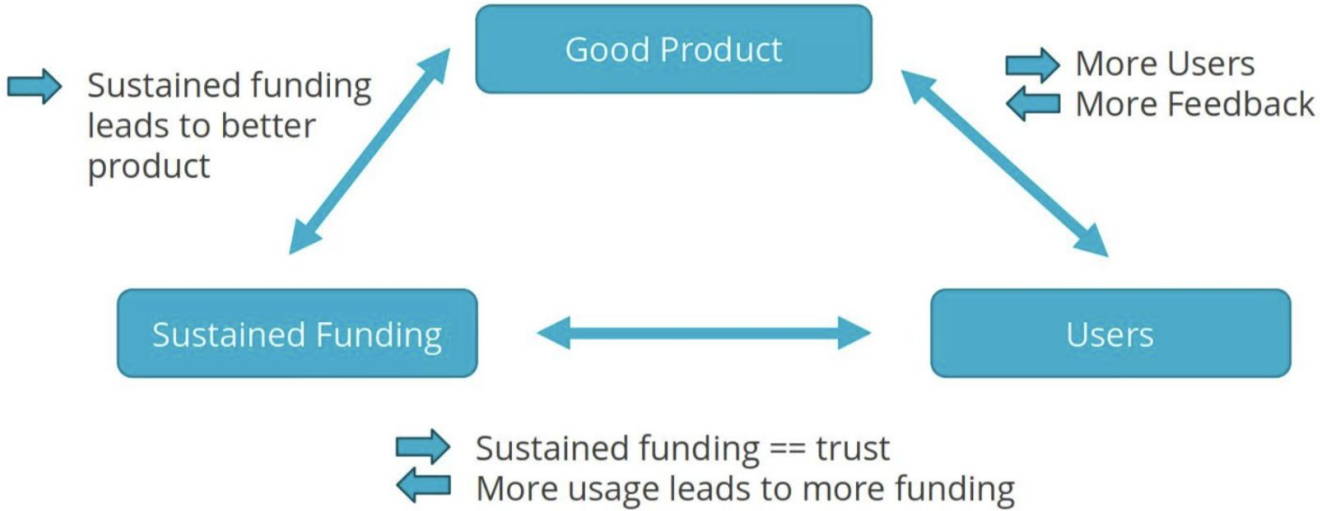
- Production grade, with public support
- Vendor neutral
- Annotations
  - Works best with imperative languages: C, Fortran, …
  - Compiler integration: potential for additional optimizations
  - Requires to re-design applications for GPU
- Library
  - Suited to language with deep encapsulation: C++,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

With CExA, CEA chooses Kokkos



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

© Christian Trott &
Damien Lebrun Grandie

The

Launched in September 2023,
Publicly announced last week

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ng in CEA
at large

computing

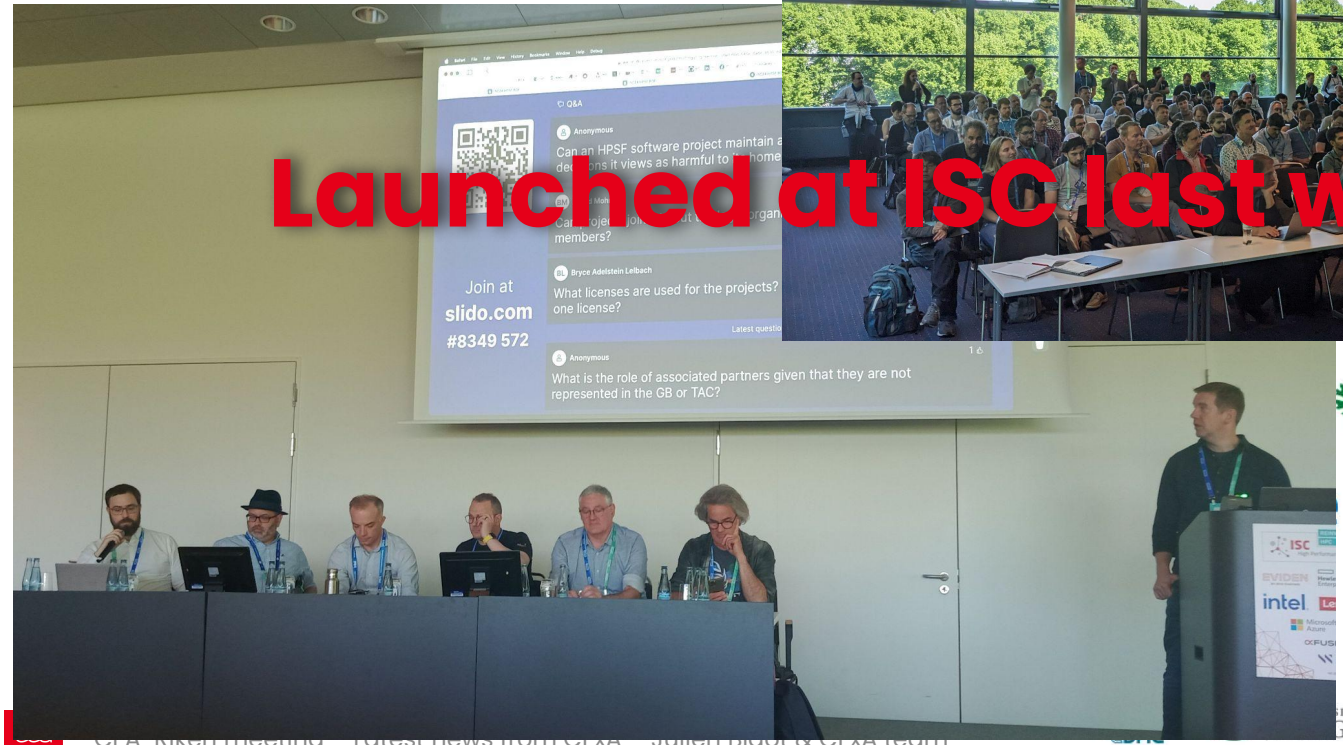
CExA in short

"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

HIGH PERFORMANCE SOFTWARE FOUN Members

HPSF Goals



Launched at ISC last week

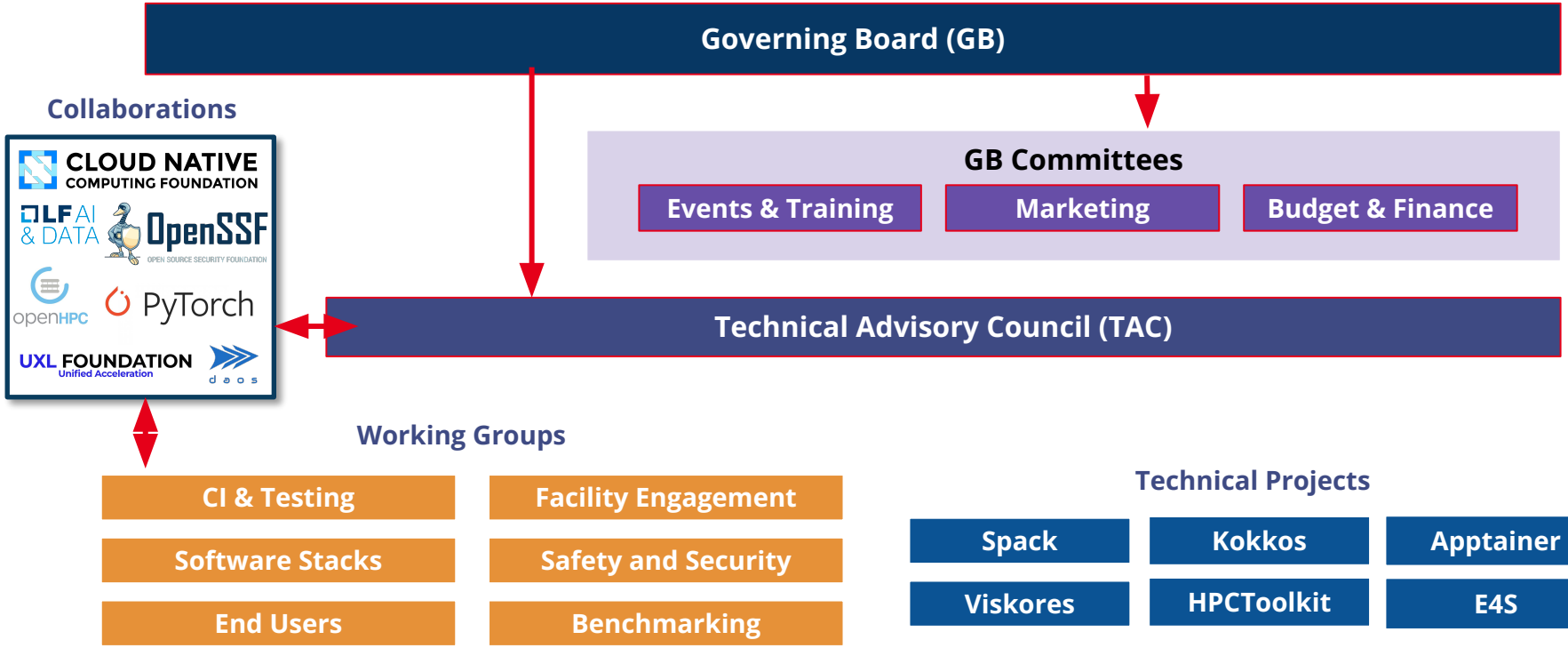
OAK RIDGE National Laboratory

Los Alamos NATIONAL LABORATORY

cea

UNIVERSITY OF MARYLAND

Two ways to participate

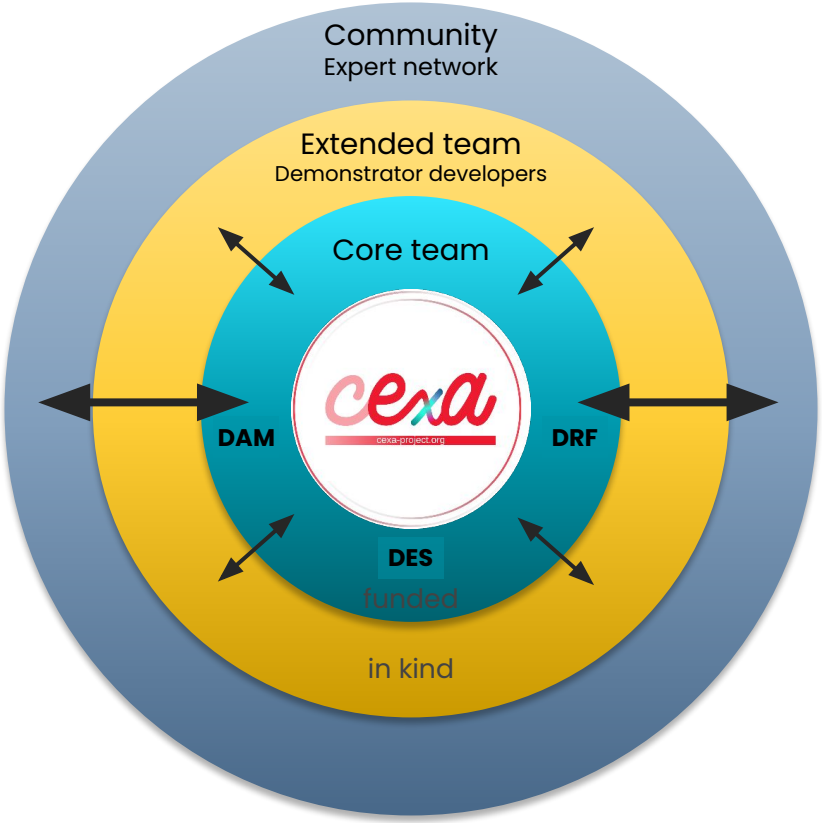


Two (independant) ways to participate

- Joining as a member
  - You need to join the Linux Foundation (Non-profit/academic, as associate for $0)
  - Joining HPSF at one of three levels:
    - Premier: $175k per year
    - General: $2.5k - $50k 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 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

Project organization



- **Core team**
  - Management, implementation and dissemination
  - 8 permanent researchers from all over CEA
  - 3 recrutements done, 3 more candidates selected
    - 1 as a permanent researcher !
  - Funding for 2 or 3 more hire expected next year
- **Extended team**
  - Demonstrator developers
    - Not funded
    - Find their interest in the participation
  - 3 new demonstrators to be selected next 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 improvement
  - Cheat-sheets creation
- Support our applications
  - Test UVM viability & performance
  - Add required solvers to Kokkos-kernels
- Improve software quality
  - Setup GPU CI for CEA libraries
  - Maintaining Kokkos Spack recipes
  - Huge refactor & redesign of `create_mirror[_view][_and_copy]`
- 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
    - Find out more in programming model session

Taking part in Kokkos weekly developers meetings

Kokkos training & community animation

- First training with Christian Trott & Damien Lebrun last september in Saclay
  - >80 participants
- Kokkos slack now has a `#general-fr` channel (~10% of the whole community)
- CExA virtual café once a month
  - Informal presentations & discussions, in French about Kokkos, its ecosystem & GPU at large

- Kokkos virtual tea-time once a month
  - Informal presentations & discussions, in English about Kokkos, its ecosystem & GPU at large
  - With our US partners

- Next Kokkos training on 17-19 June @ Saclay
  - with Damien Lebrun & Luc Berger-Vergiat
  - Registrations still open
- CEA / EDF / Inria summer school in summer 2025

https://indico.math.cnrs.fr/e/kokkos_days

The core team

Julien Bigot
Principal investigator

Ansar Calloo
Group leader

Cedric Chevalier
Group leader

Mathieu Lobet
Group leader

Yuuichi Asahi
Senior developer

Thierry Antoun
Developer

Rémi Baron
Senior developer

Thomas Padioleau
Senior developer

Thomas Padioleau
Developer

The extended team

Pierre Ledac

Trust/TrioCFD lead

Virginie Grandgirard

GyselaX++ lead

François Letierce

Triclade lead

Julien Jaeger

DAM link

Édouard Audit

Network animator

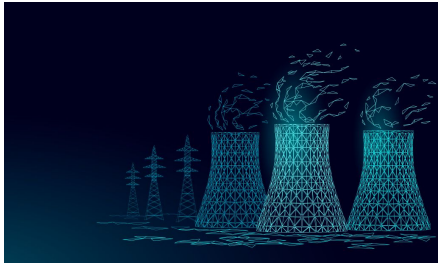
Samuel Kokh

DES link

Patrick Carribault

DAM link

To conclude



- A sovereignty tool to exploit French & EU Exascale supercomputers
- Fill the value chain of high performance computing and ensure sustainability of application developments
- A strong dynamic all over the CEA and beyond
- A knock-on effect with new synergies identified every weeks with code developers
- A strong impact on the programs of CEA as well as on many societal challenges

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