1. GitLab

Présentation du GitLab

https://gitlab.maisondelasimulation.fr/anr-maturation

- Demander à Mathieu Lobet pour créer un compte
- Possibilité de l'utiliser pour tout programme dans le projet Maturation (mini-codes de test, versions alternatives)
- Première version du programme disponible

But du GitLab :

- Travailler en commun au développement des codes via Git
- Outil de reviewing des modifications avant fusion
- Fusion automatique
- Gestion des issues
- Partager le code avec nos collègues
- Mettre en place les bonnes pratiques DevOps
- Mettre en place de l'intégration continue afin de vérifier la conformité des résultats à chaque modification

Contribution de la MdlS

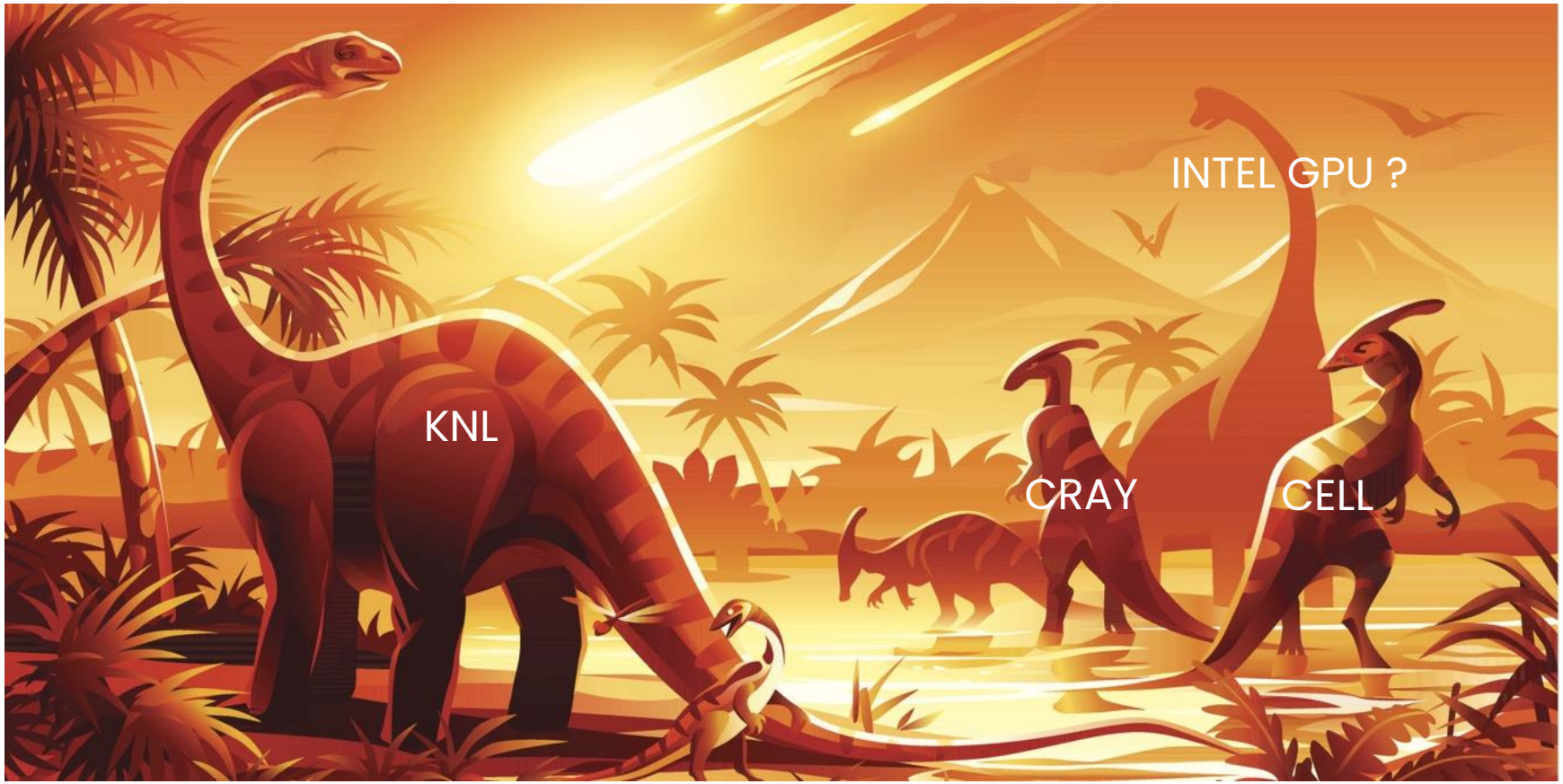
DevOps
- Former l'équipe à Git
- Mettre en place les bonnes pratiques DevOps
- Documentation dev et utilisateur
- Intégration continue et tests automatisés

Application
- Optimisation CPU
- Portage et optimisation GPU
- Tests de performance
- Tests de compilateurs
- Tests de différentes architectures (ARM, x86, etc)

2. Kokkos

Life in our HPC world

Evolution in HPC : exotic and disruptive hardware are permanently appearing (and disappearing) in super-computers history



A lot of work for HPC developers

New technologies are exciting for researchers but may be stressful for application developers and users :

- May require vendor specific programming models
- May require new programming paradigms
- Algorithms may have to be rewritten

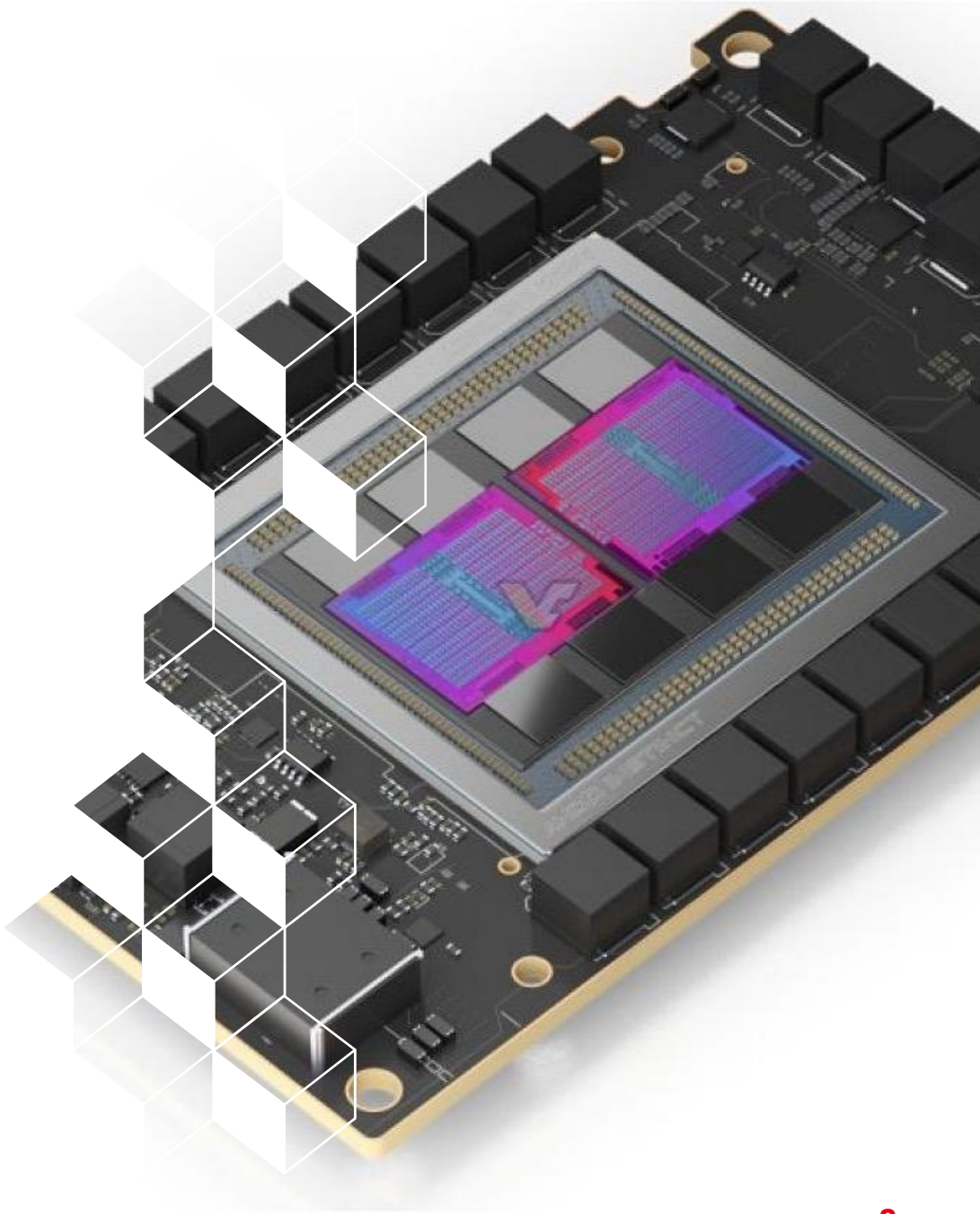
Developers must :

- Update their knowledge to handle new hardware specificity and programming models
- Rewrite or duplicate part of their applications
- Bet on a technology without long-term vision

- A conservative estimate from the Kokkos team : An application of 200 000 lines need a full-time engineer during a year to switch programming models
- We have been working for more than 4 years to port the SMILEI application and we are still on it
- Easier for large application teams with dedicated HPC engineers
- Impossible for applications maintained by a single physicist, PhDs or Postdocs

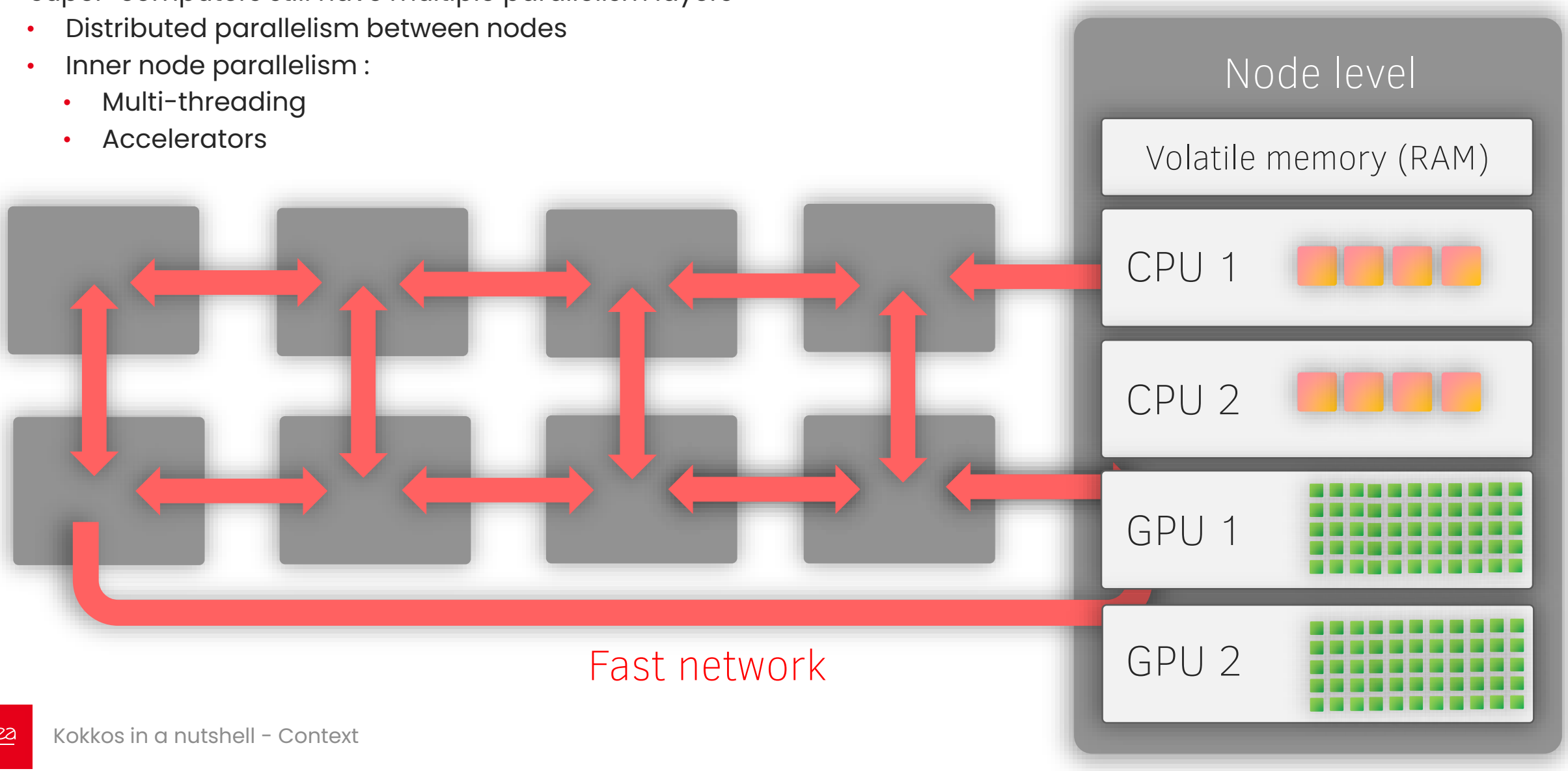
Current state of HPC hardware

- Super-computers tend to be more and more heterogeneous : The CPU is coupled with one or multiple accelerator cards, most often GPUs
- The pure computational power is not balanced, mostly dominated by the GPU side
- NVIDIA used to dominate the HPC GPU market (as Intel used to be for CPUs)
  - Good for technology stability (programming models, optimization, etc)
  - Bad for market price and innovation
- Today's landscape is composed of many vendors with emergent actors :
  - AMD CPUs and GPUs
  - ARM based processors and accelerators
  - Intel GPUs



How to program heterogeneous systems

- Super-computers still have multiple parallelism layers
  - Distributed parallelism between nodes
  - Inner node parallelism :
    - Multi-threading
    - Accelerators

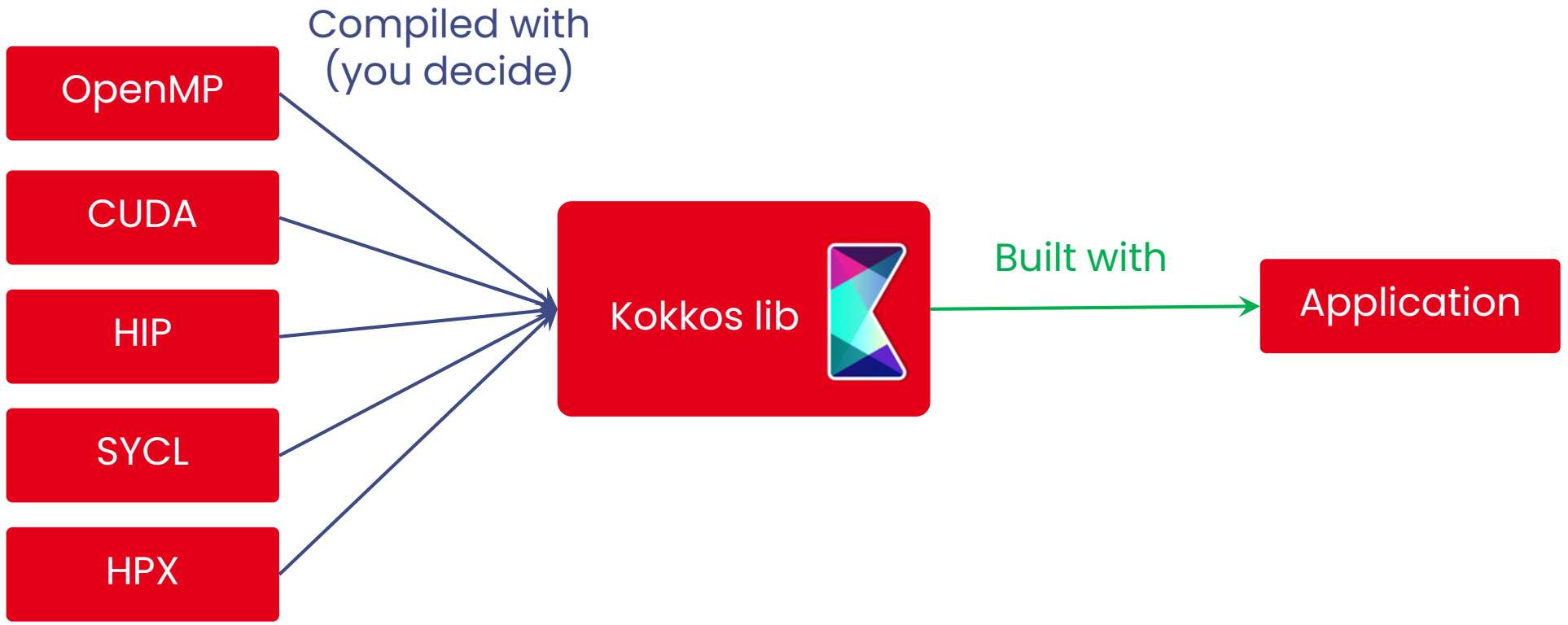


Need for performance portable programming models

- Developers still need a model MPI + X so far, may change in the future
- A performance portable programming model offers decent performance across a wide range of architectures using a single source code
- The choice depends on the value of the cursor between many parameters :
  - Performance
  - Portability
  - Maturity (bugs, features)
  - Long-term support
  - Code maintainability
  - Programing complexity (required programming skilled)
  - Ecosystem and interoperability

Kokkos, what is it ?

Kokkos is performance portability parallel programming model build upon the C++-17 standard designed to abstract already-existing parallel programming models



Kokkos, what is it ?

Kokkos is a good trade-off:

- Portable: compile for all CPU and GPU of the market and have access to experimental hardware thanks to close contact with vendors
- Performance: build on top of vendor-specific back-ends (i.e. CUDA, HIP, SYCL)
- Maturity: well established project since 2012 adopted by more than 100 projects
- Long-term support: used and developed by many DOE labs, part of the ECP project
- Maintainability: descriptive single source code
- Complexity: build upon advanced C++ without the need to master it, common objects and functions used in numerical science, extensive documentation, tutorial materials, chat room for questions
- Ecosystem and interoperability: expanding solution for common needs of modern science and engineering codes (math libs, debuggers, performance analysis)

Kokkos main capability

Basic features:

- Parallel loop: one-dimension, multi-dimensions, reduction patterns and more like OpenMP
- Multidimensional arrays like Fortran or Python
- Memory and execution policy to decide where data is located and where kernels are run
- Implicit data layout and data access management for performance

More advanced features:

- Thread safety, thread scalability and atomic operation
- Hierarchical parallelism (threading, vectorization, SIMT, etc.)
- Optimization capability

Tools:

- Compatibility with classical debuggers and profilers
- Build-in algorithm (sorting) like Thrust and mathematic features (linear algebra)
- Interoperability with Python, Fortran and other programming models

However, be careful, Kokkos is not magic

Portability and performance portability are not the same

- Hardware optimized algorithms may not scale
- Best performance with a single source implementation is not always possible, especially targeting both CPU and GPU, due to hardware differences
  - May need specific algorithm or parallelism hierarchies to leverage the maximum performance of a specific architecture
  - Kokkos will not do that for you
  - Trade-off between best performance and other goals (portability, etc)

Kokkos Uses the concept of data parallelism as OpenMP does

```
for (int j = 0 ; j < column_size ; ++j) {
        for (int i = 0 ; i < line_size ; ++i) {
                y[j] += x[i] * A[j][i];
        }
}
```

Pattern: structure of the computation (for, reduction, scan, graph)

Execution policy: how computations are executed (static, dynamic, task)

Body: code which performs each unit of work

OpenMP versus Kokkos for a simple loop

```
#pragma omp parallel for
for (int j = 0 ; j < column_size ; ++j) {
    for (int i = 0 ; i < line_size ; ++i) {
        y[j] += x[i] * A[j][i];
    }
}
```

```
parallel_for( column_size,
    KOKKOS_LAMBDA(const int j) {
        for (int i = 0 ; i < line_size ; ++i) {
          y(j) += x(i) * A(j,i);
        }
    }
)
```

- Kokkos syntax is different but still understandable as OpenMP
- Kokkos uses the notion of lambda function in C++: small structure that describes a function

Execution pattern

What basic pattern to execute:

- Kokkos::parallel_for -
- Kokkos::parallel_reduce
- Kokkos::parallel_scan
- etc

```
#pragma omp parallel for reduction(+:sum)
for (int i = 0 ; i < N ; ++i) {
    sum += x[i];
}
```

```
parallel_reduce( N,
    KOKKOS_LAMBDA(const int i, double& sum) {
        sum += x[i];
    },
sum)
```

Execution space

Where computation is executed:
- Kokkos::serial – Serial execution on CPU
- Kokkos::DefaultHostExecutionSpace – Host execution
- Kokkos::DefaultExecutionSpace - Device if compiled for GPU, else Host

Execution space can also make the back-end explicit:
- Kokkos::Cuda
- Kokkos::OpenMP
- Kokkos::HIP

The selection depends on:
- Compile-time options
- Default choices
- Run-time choices

Warning: Kokkos only sees a single device per process. Therefore, multi-device requires MPI.

Execution policy

How computation is executed:

- Kokkos::RangePolicy – 1D loop
- Kokkos::MDRangePolicy – multi-D loop
- Kokkos::TeamPolicy – for hierarchical parallelism

- Adapt the parallel execution to the hardware and to the characteristics of the algorithm

```
parallel_for( N,
    KOKKOS_LAMBDA (int n) { /* ... */ }
);
```

```
parallel_for(
    RangePolicy<DefaultExecutionSpace>(0, N),
    KOKKOS_LAMBDA(int n) { /* ... */ }
);
```

OpenMP vs Kokkos

Case 1:

- I only want to use the CPU (ignore the GPU if exists)
- I want to use OpenMP backend
- I compile Kokkos only with the OpenMP backend

```
// OpenMP
#pragma omp parallel for
for (int i = 0 ; i < N ; ++i) {
    /* ... */
}
```

```
// Kokkos
Kokkos::parallel_for( N,
    KOKKOS_LAMBDA (int i) { /* ... */ }
);
```

```
// Kokkos explicit execution policy
Kokkos::parallel_for(
    Kokkos::RangePolicy<Kokkos::DefaultExecutionSpace
>(  0, N ),
    KOKKOS_LAMBDA(int n) {
        /* ... */
    }
);
```

```
// Kokkos explicited execution policy
Kokkos::parallel_for(
    Kokkos::RangePolicy<Kokkos::OpenMP>( 0, N ),
    KOKKOS_LAMBDA(int n) {
        /* ... */
    }
);
```

OpenMP vs Kokkos

Case 2:

- I use a hybrid node with a CPU and a GPU
- I compile Kokkos with OpenMP for the CPU and with CUDA for the GPU

```
// OpenMP CPU code
#pragma omp parallel for
for (int i = 0 ; i < N ; ++i) {
    /* ... */
}
```

```
// Kokkos CPU code
parallel_for(
    RangePolicy<DefaultHostExecutionSpace>(0, N ),
    KOKKOS_LAMBDA(int n) {
        /* ... */
    }
);
```

```
// OpenMP GPU code
#pragma omp target teams distribute parallel for
for (int i = 0 ; i < N ; ++i) {
    /* ... */
}
```

```
// Kokkos GPU code
parallel_for(
    RangePolicy<DefaultExecutionSpace>( 0, N ),
    KOKKOS_LAMBDA(int n) {
        /* ... */
    }
);
```

Loops and debugging

- Each loop can be assigned a name to facilitate the debugging part

```
// Kokkos
Kokkos::parallel_for( N,
    KOKKOS_LAMBDA (int i) { /* ... */ }
);
```

```
// Kokkos
Kokkos::parallel_for("my loop", N,
    KOKKOS_LAMBDA (int i) { /* ... */ }
);
```

Multi-D Arrays equivalent = Kokkos::view

- Kokkos::view is a class designed to represent a multi-dimensional array with additional capabilities:
  - Simple accessor (i, j ,k …)
  - Abstracted or explicit memory layout (row major, column major, etc.)
  - Static or dynamic dimensions
  - Resize capacity like std::vector
  - Memory space – where the array is stored
  - Memory Traits – additional properties (atomic operation, shared memory, etc.)
  - Can be assigned a name for debugging
  - Shallow copy by default like Python (reference counting)

Kokkos::view simple examples

```
// simple 1d array
View <int*> A ("A",N);

// 3d dynamic array
View <double***> A ("A",Nx, Ny, Nz);

// simple 1d array with static dimension
View<char[4]> A ("A");

// partly static/dynamic 2d array
View<float*[4]> A ("A",N);
```

Memory Space

- On heterogeneous systems, devices have a separate memory from the RAM
- Memory space enables to decide where the view data is located:
  - Kokkos::HostSpace
  - Kokkos::CudaSpace
  - Kokkos::HIPSpace
  - Kokkos::SharedSpace – for unified memory between host and device

- By default, the memory space is the one of the default Execution Space (should be the device if using it)

- Contratry to OpenMP or OpenACC, no need to map a host and device view

Kokkos::view examples with Memory Space

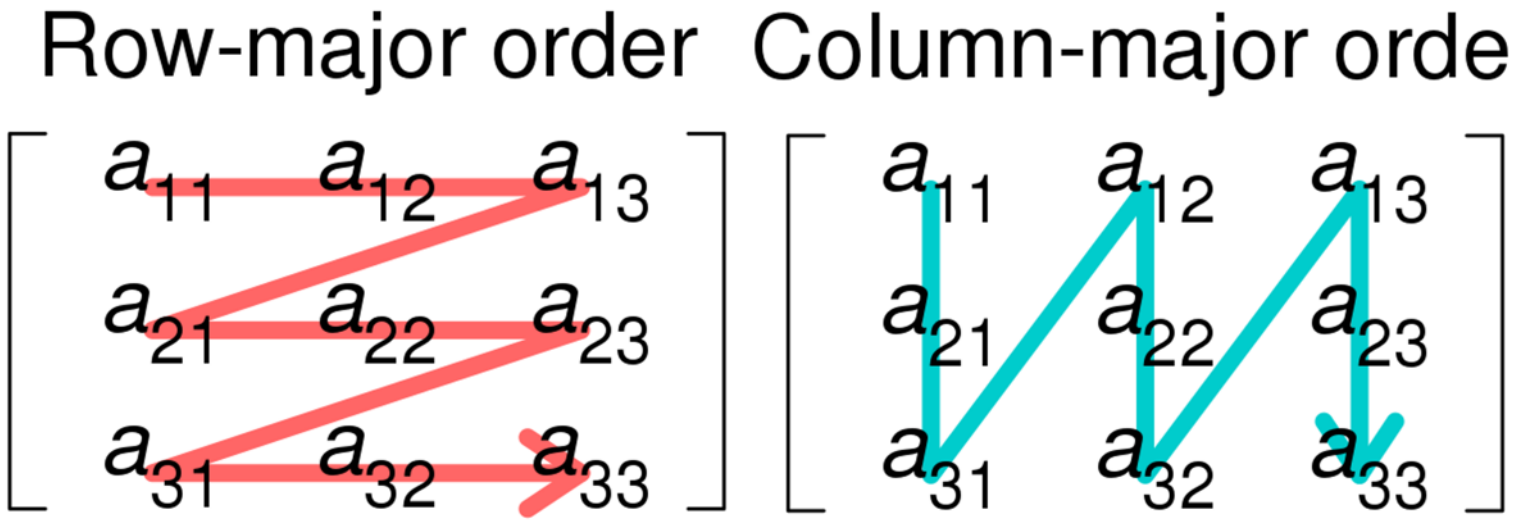
```
// simple 1d dynamic array
View <int*, HostSpace> A ("A",N);

// simple 1d dynamic array
View <int*, DefaultExecutionSpace::memory_space> A ("A",N);


// 3d dynamic array allocated in the device memory using CUDA
View <double***, CudaSpace> A ("A",Nx, Ny, Nz);
```

Memory layout

- The layout is how the memory is stored and organized
- The data layout can impact the performance and depends on the computing architecture
- Kokkos determines the suitable layout by default for the memory space



- Kokkos::LayoutRight – Row-major order
- Kokkos::LayoutLeft – Column-major order
- Kokkos::LayoutStride – custom ordering

Kokkos::view examples with Layout

```
// simple 2d array (default layout)
View <int**, HostSpace> A ("A",N, M);

// simple 2d array
View <int**, HostSpace, LayoutRight> A ("A",N, M);
View <int**, HostSpace, LayoutLeft> A ("A",N, M);
```

Memory traits

- Memory traits are additional properties given to the view on how the data is accessed
  - Kokkos::Unmanaged – allocation is not managed by Kokkos, can be useful to map a view with an already existing array (via std::vector or cudaMalloc for instance)
  - Kokkos::Atomics – atomics operations on the array elements
  - Kokkos::RandomAccess – optimize for random access. If the view is also const this will trigger special load operations on GPUs (i.e. texture fetches).
  - Kokkos::restrict - There is no aliasing of the view by other data structures in the current scope

Building applications with Kokkos

- Kokkos primary build system is CMAKE
- Makefile can be designed for simple projects

- Kokkos can be built and installed easily from sources as a library (recommended for large applications)
- It can be built as well inline
- It can be pulled via Spack

- The back-end to use is provided at compile time, for instance
  - -Dkokkos_ENABLE_CUDA=ON
  - -Dkokkos_ENABLE_OPENMP=ON

- One CPU, one GPU and one serial backend at a time
- Device architecture can as well be provided if not detected by default

Kokkos::view examples with Layout

```
int main(int argc, char* argv[])
{


  constexpr int nvar = 2;   // compile time size
  int nx = 100;                          // run time
size
  double* array = new double[nx*nvar];

  for (int ix=0; ix<nx; ++ix)
  {
    array[ix*2 + 0] = 1.0*ix;
    array[ix*2 + 1] = 2.0*ix;
  }

  return 0;
}
```

```
int main(int argc, char* argv[])
{
  Kokkos::ScopeGuard    scope(argc,    argv);    //
initialize & finalize

  constexpr int nvar = 2;   // compile time size
  int nx = 100;                          //   run   time
size
  Kokkos::View<double*[nvar]> array("Array", nx);

  Kokkos::parallel_for(nx, KOKKOS_LAMBDA (int ix)
  {
    array(ix, 0) = 1.0*ix;
    array(ix, 1) = 2.0*ix;
  });

  return 0;
}
```