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Kokkos: Enabling Performance Portablility

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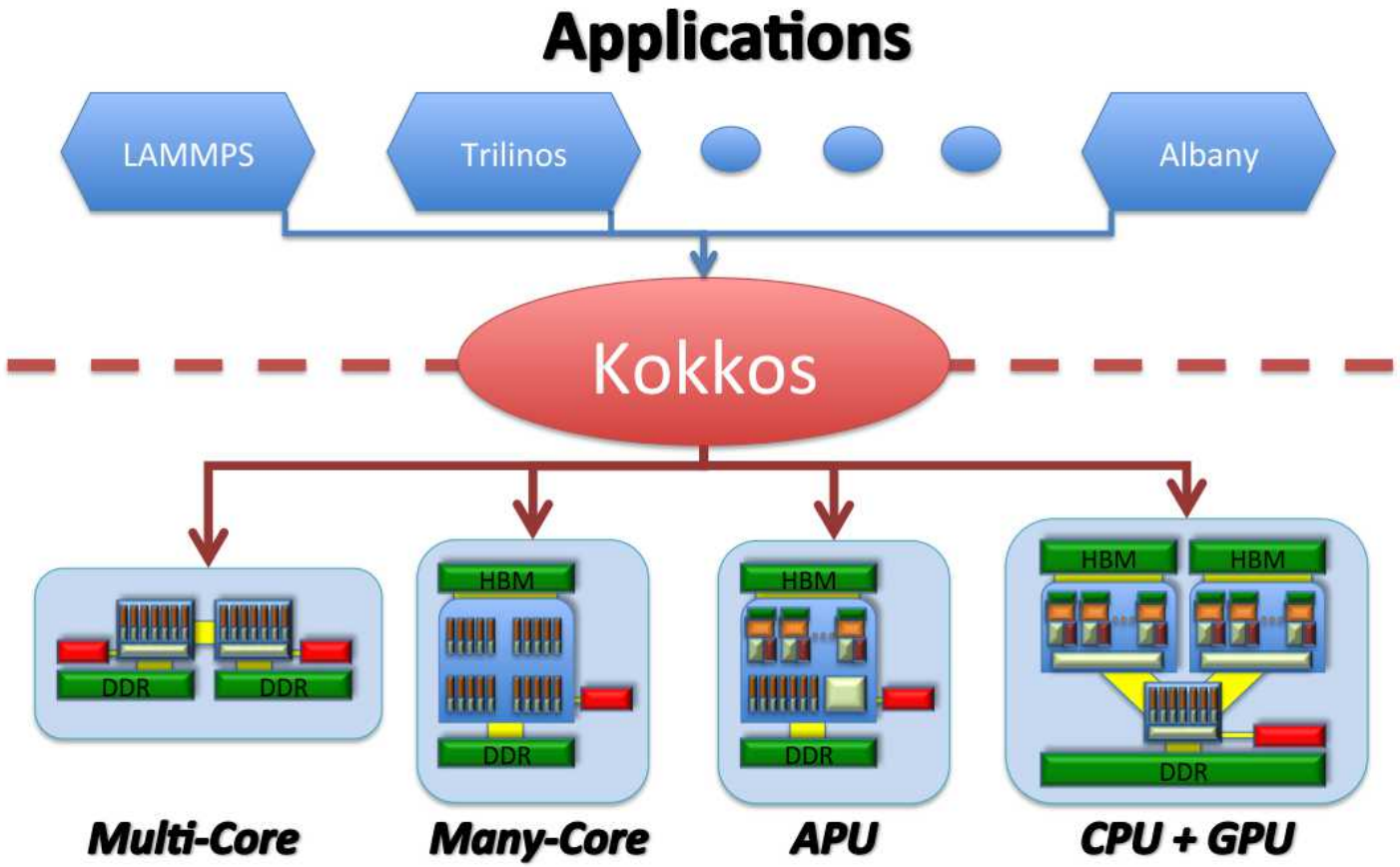
Applications
LAMMPS
Trilinos
Albany
Kokkos
DDR
DDR
HBM
DDR
HBM
DDR
HBM
HBM
DDR
Multi-Core
Many-Core
APU
CPU + GPU
Hardware Architectures

- **Machine model**
  - N execution spaces $\times$ M memory spaces
  - $N \times M$ matrix for memory access performance/possibility
  - Asynchronous execution allowed
- **Implementation Approach**
  - A C++ template library
  - Application focused: each feature is requested by application and used right now
  - Performance focused: very high bar for acceptance if a feature impeders performance
  - C++11 required
  - Target different back-ends for different hardware architectures
- **Distribution**
  - Open Source library
  - Available on Github: github.com/kokkos/kokkos
  - Extensive tutorial: github.com/kokkos/kokkos-tutorials

Execution Pattern: parallel_for, parallel_reduce, parallel_scan, task, ...
Execution Policy: how (and where) a user function is executed

- E.g., data parallel range : concurrently call function(i) for i = [0..N)
- User's function is a C++ functor or C++11 lambda

Execution Space: where functions execute

- Encapsulates hardware resources; e.g., cores, GPU, vector units, ...

Memory Space: where data resides

- AND what execution space can access that data
- Also differentiated by access performance; e.g., latency & bandwidth

Memory Layout: how data structures are ordered in memory

- provide mapping from logical to physical index space

Memory Traits: how data shall be accessed

- allow specialisation for different usage scenarios (read only, random, atomic, ...)

Concepts: Patterns, Policies, and Bodies

Pattern / Policy / Body

```
for (size_t i = 0; i < N; ++i) {
  double y_i = 0;
  for (int j = 0; j < M; ++j) {
    y_i += A[i][j] * x[j];
  }
  y[i] = y_i;
}
```

Terminology:

- **Pattern**: structure of the computations
  for, reduction, scan, task-graph, ...
- **Execution Policy**: how computations are executed
  static scheduling, dynamic scheduling, thread teams, ...
- **Computational Body**: code which performs each unit of work; *e.g.*, the loop body

$\Rightarrow$ The **pattern** and **policy** drive the computational **body**.

Example: $y = Ax$

OpenMP

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

Kokkos

```
parallel_for(N, [=] (const size_t i) {
  double y_i = 0;
  for (int j = 0; j < M; ++j) {
    y_i += A[i][j] * x[j];
  }
  y[i] = y_i;
});
```

Example: $\langle y^T | Ax \rangle$

OpenMP

```
double yAx = 0;
#pragma omp parallel for reduction(+:yAx)
for (int i = 0; i < N; ++i) {
  double Ax_i = 0;
  for (int j = 0; j < M; ++j) {
    Ax_i += A[i][j] * x[j];
  }
  yAx += y[i] * Ax_i;
}
```

Kokkos

```
double yAx = 0;
parallel_reduce(N, [=] (const size_t i, double& yAx_thread) {
  double Ax_i = 0;
  for (int j = 0; j < M; ++j) {
    Ax_i += A[i][j] * x[j];
  }
  yAx_thread += y[i] * Ax_i;
}, yAx);
```

`View` overview:

- **Multi-dimensional array** of 0 or more dimensions
  scalar (0), vector (1), matrix (2), etc.
- **Number of dimensions (rank)** is fixed at compile-time.
- Arrays are **rectangular**, not ragged.
- **Sizes of dimensions** set at compile-time or runtime.
  e.g., 2x20, 50x50, etc.

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Example:

```
View<double***> data("label", N0, N1, N2);  3 run, 0 compile
View<double**[N2]> data("label", N0, N1);   2 run, 1 compile
View<double*[N1][N2]> data("label", N0);    1 run, 2 compile
View<double[N0][N1][N2]> data("label");     0 run, 3 compile
```

Note: runtime-sized dimensions must come first.

`View` life cycle:

- Allocations only happen when *explicitly* specified.
  i.e., there are **no hidden allocations**.
- Copy construction and assignment are **shallow** (like pointers).
  so, you pass `Views` by value, *not* by reference
- Reference counting is used for **automatic deallocation.**

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Example:

```
void assignValueInView(View<double*> data) { data(0) = 3; }

View<double*> a("a", N0), b("b", N0);
a(0) = 1;
b(0) = 2;
a = b;
View<double*> c(b);
assignValueInView(c);
print a(0)
```

What gets printed?

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```

What gets printed?

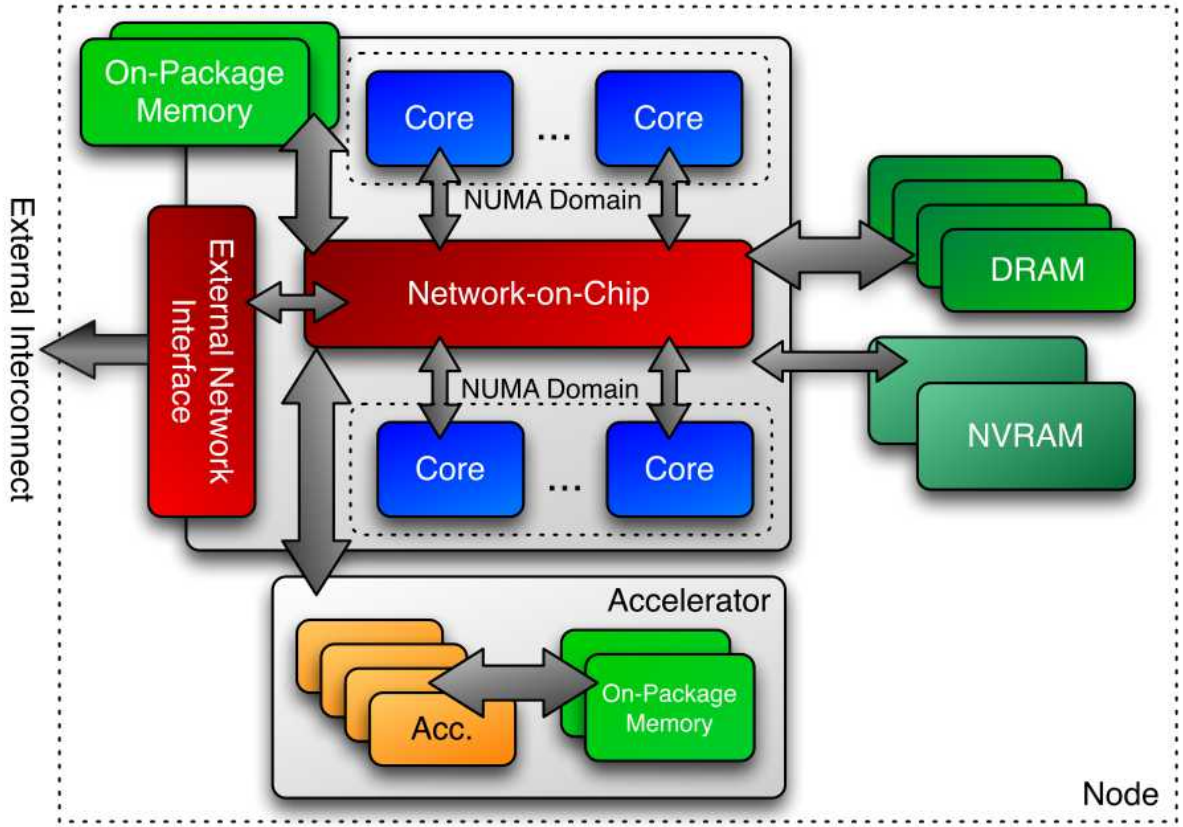
3.0

Example: $\langle y^T | Ax \rangle$

```
#include <Kokkos_Core.hpp>

int main(int argc, char* argv[]) {
  // Initialize Kokkos analogous to MPI_Init()
  Kokkos::initialize(argc, argv);
  ...
  Kokkos::View<double**> A ("A", N,M); // Allocate matrix "A"
  Kokkos::View<double*> x("X",M), y("Y",N); // Allocate vector
  ...
  double yAx = 0;
  Kokkos::parallel_reduce(N, [=] (const size_t i,
                                  double& yAx_thread) {
    double Ax_i = 0;
    for (int j = 0; j < M; ++j) {
      Ax_i += A(i,j) * x(j);
    }
    yAx_thread += y(i) * Ax_i;
  }, yAx);
  ...
  Kokkos::finalize();
}
```

Compute nodes will be **heterogeneous** in cores *and* memory:



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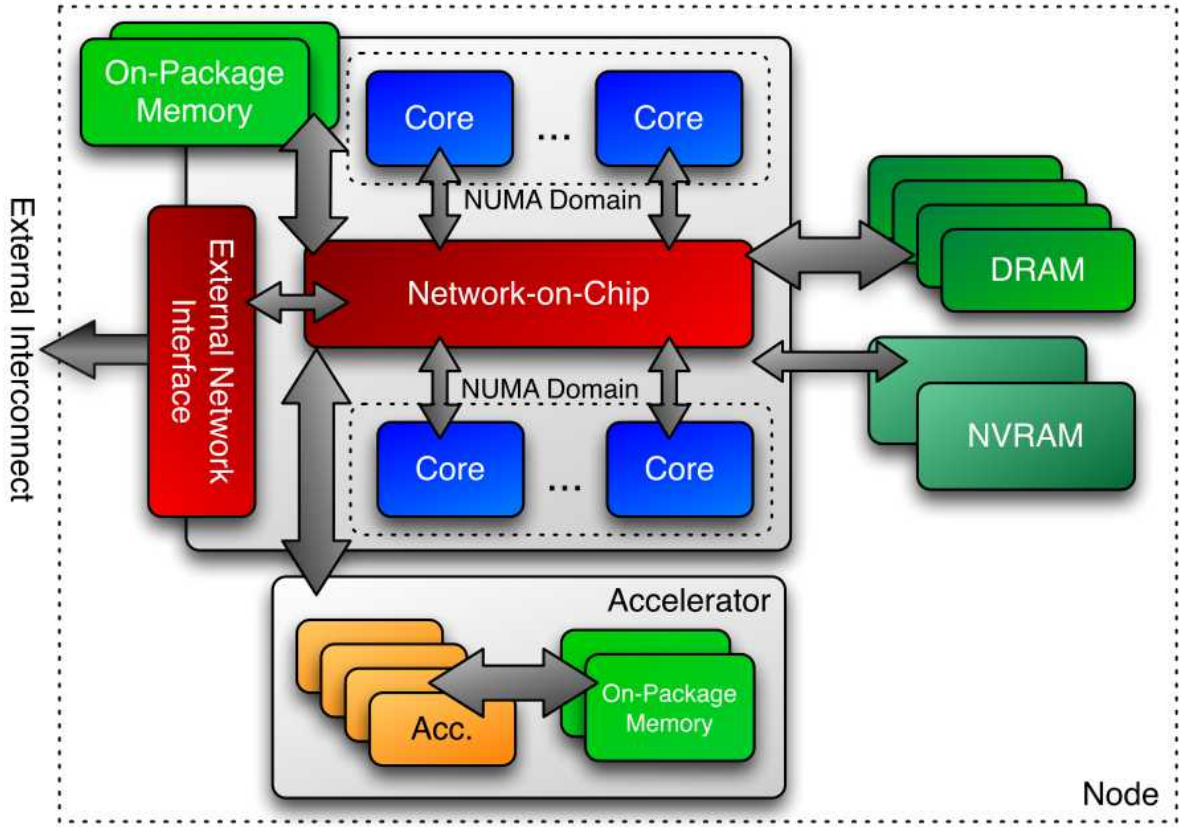

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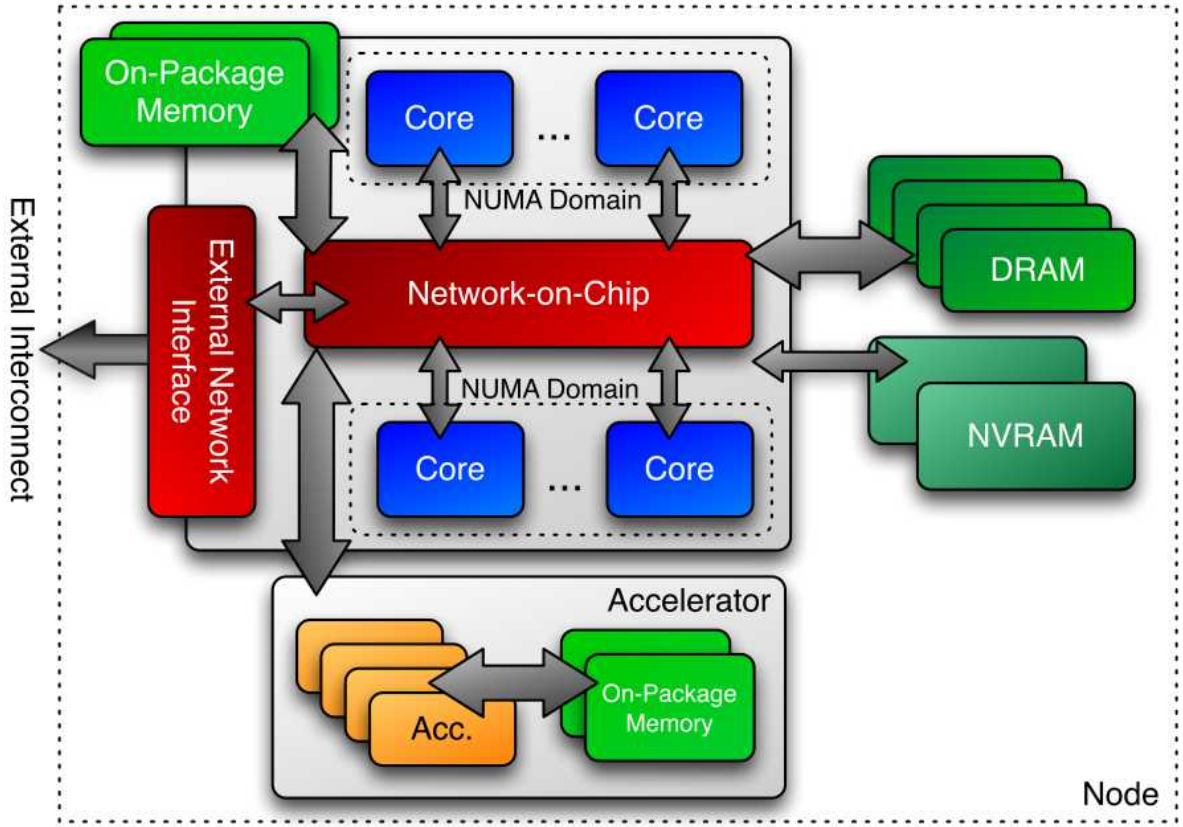
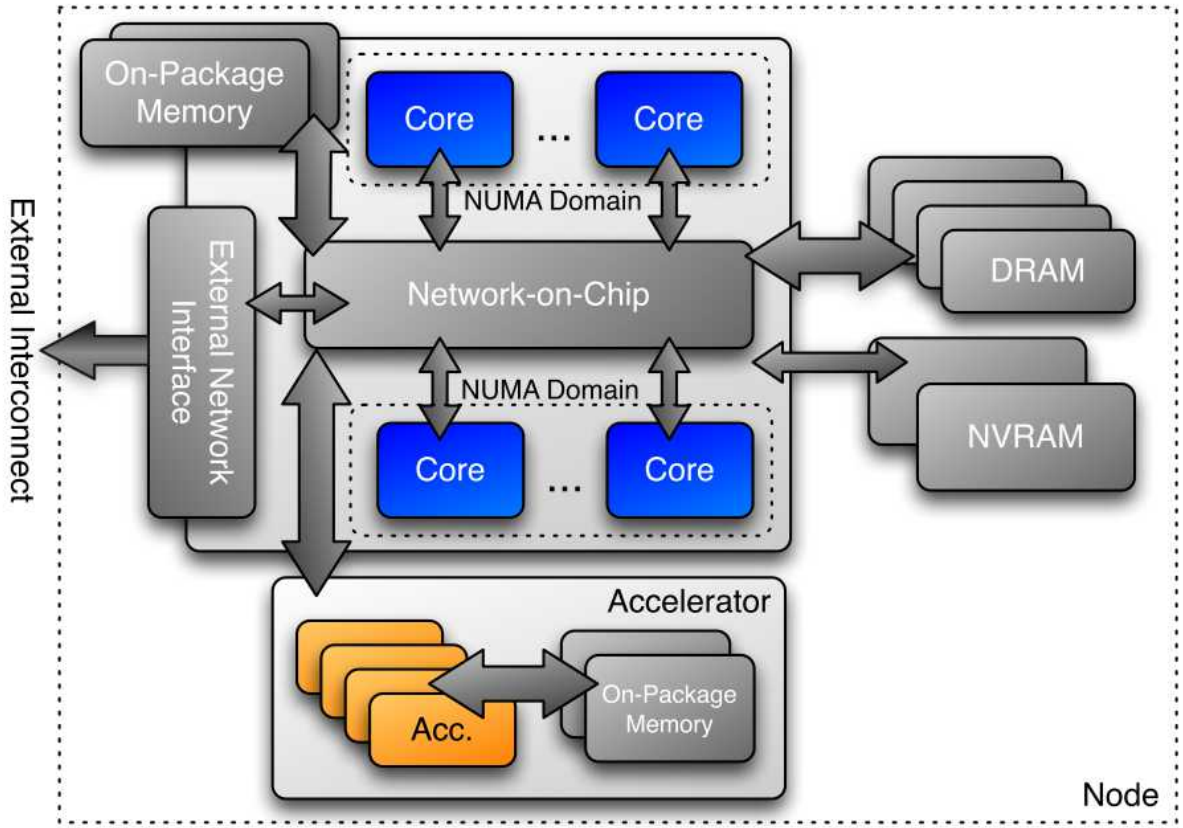


Many-core revolution: 20-year "just recompile" **free ride is over**.

How much do I have to **learn and change** to use these nodes?

Execution Space

a homogeneous set of cores and an execution mechanism
(i.e., "place to run code")



Execution spaces: `Serial`, `Threads`, `OpenMP`, `Cuda`, ...

Important concept: Execution spaces

Every parallel operation is executed in an **execution space** set at compile time as part of an **execution policy**.

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- `ExecutionPolicy<ExecutionSpace>(...)`
- Available **execution spaces**:

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- If no `ExecutionSpace` is provided to an execution policy the **default execution space** is used.
- Giving an integer N as policy is equivalent to `RangePolicy<>(N)`

Kokkos function and lambda portability annotation macros:

Function annotation with `KOKKOS_INLINE_FUNCTION` macro

```
struct ParallelFunctor {
  KOKKOS_INLINE_FUNCTION
  double helperFunction(const size_t s) const {...}
  KOKKOS_INLINE_FUNCTION
  void operator()(const size_t index) const {
    helperFunction(index);
  }
}
// Where kokkos defines:
#define KOKKOS_INLINE_FUNCTION inline                              /* #if CPU-only */
#define KOKKOS_INLINE_FUNCTION inline __device__ __host__ /* #if CPU+Cuda */
```

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```
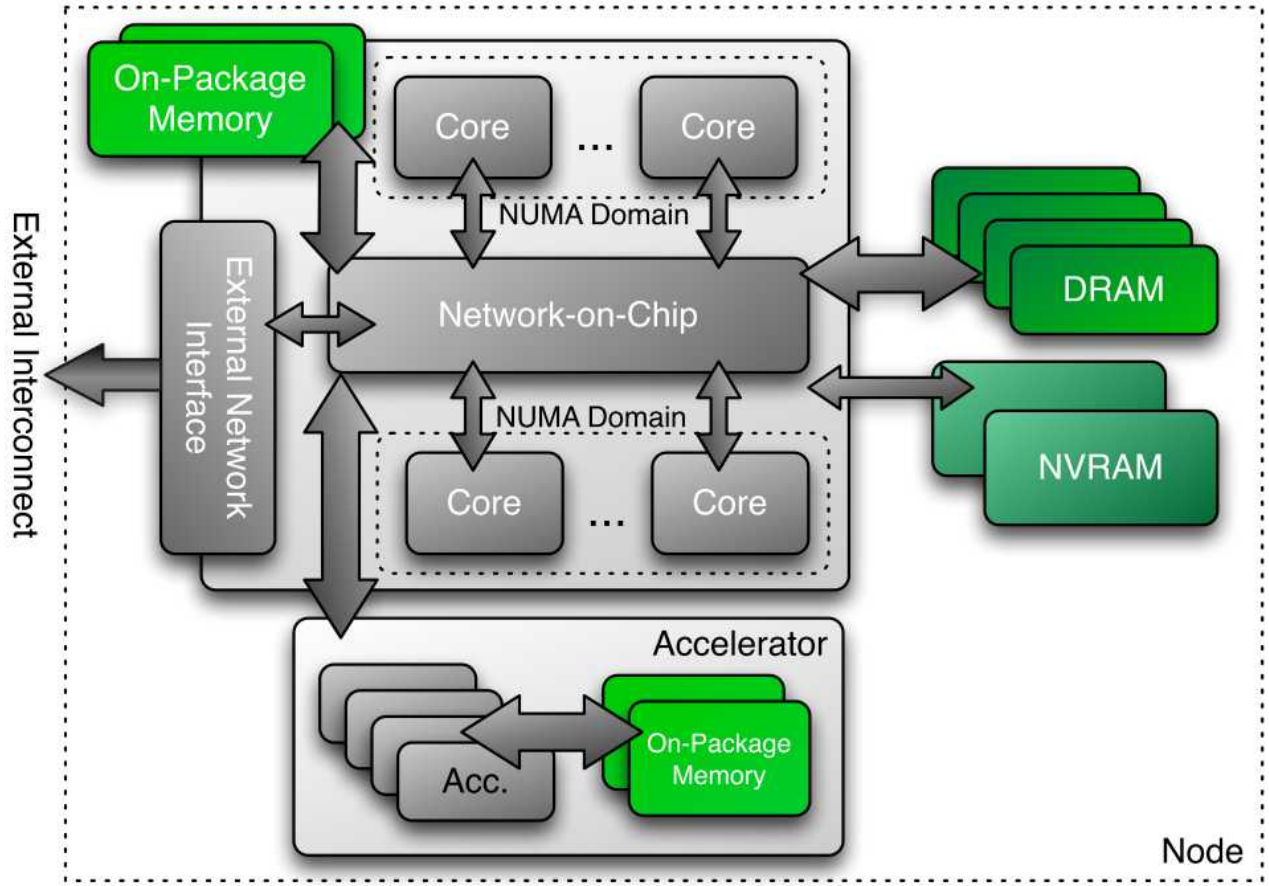

Lambda annotation with `KOKKOS_LAMBDA` macro (CUDA requires v 7.5)

```
Kokkos::parallel_for(numberOfIterations,
  KOKKOS_LAMBDA (const size_t index) {...});

// Where kokkos defines:
#define KOKKOS_LAMBDA [=]              /* #if CPU-only */
#define KOKKOS_LAMBDA [=] __device__ /* #if CPU+Cuda */
```

Memory space:
explicitly-manageable memory resource
(i.e., "place to put data")



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- Each **execution space** has a default memory space, which is used if **Space** provided is actually an execution space
- If no `Space` is provided, the view's data resides in the **default memory space** of the **default execution space**.

Example: $\langle y^T | Ax \rangle$

```
...
// Allocate explicitly in CudaSpace
Kokkos::View<double**, Kokkos::CudaSpace> A ("A", N,M);
Kokkos::View<double*, Kokkos::CudaSpace> x("X",M), y("Y",N);
...
double yAx = 0;
// Run explicitly in the Cuda execution space
Kokkos::parallel_reduce(Kokkos::RangePolicy<Kokkos::Cuda>(N),
  KOKKOS_LAMBDA (const size_t i, double& yAx_thread) {
  double Ax_i = 0;
  for (int j = 0; j < M; ++j) {
    Ax_i += A(i,j) * x(j);
  }
  yAx_thread += y(i) * Ax_i;
}, yAx);
...
```

Important concept: Layouts

Every `View` has a `Layout` set at compile-time.

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View<double***, Layout, Space> name(...);
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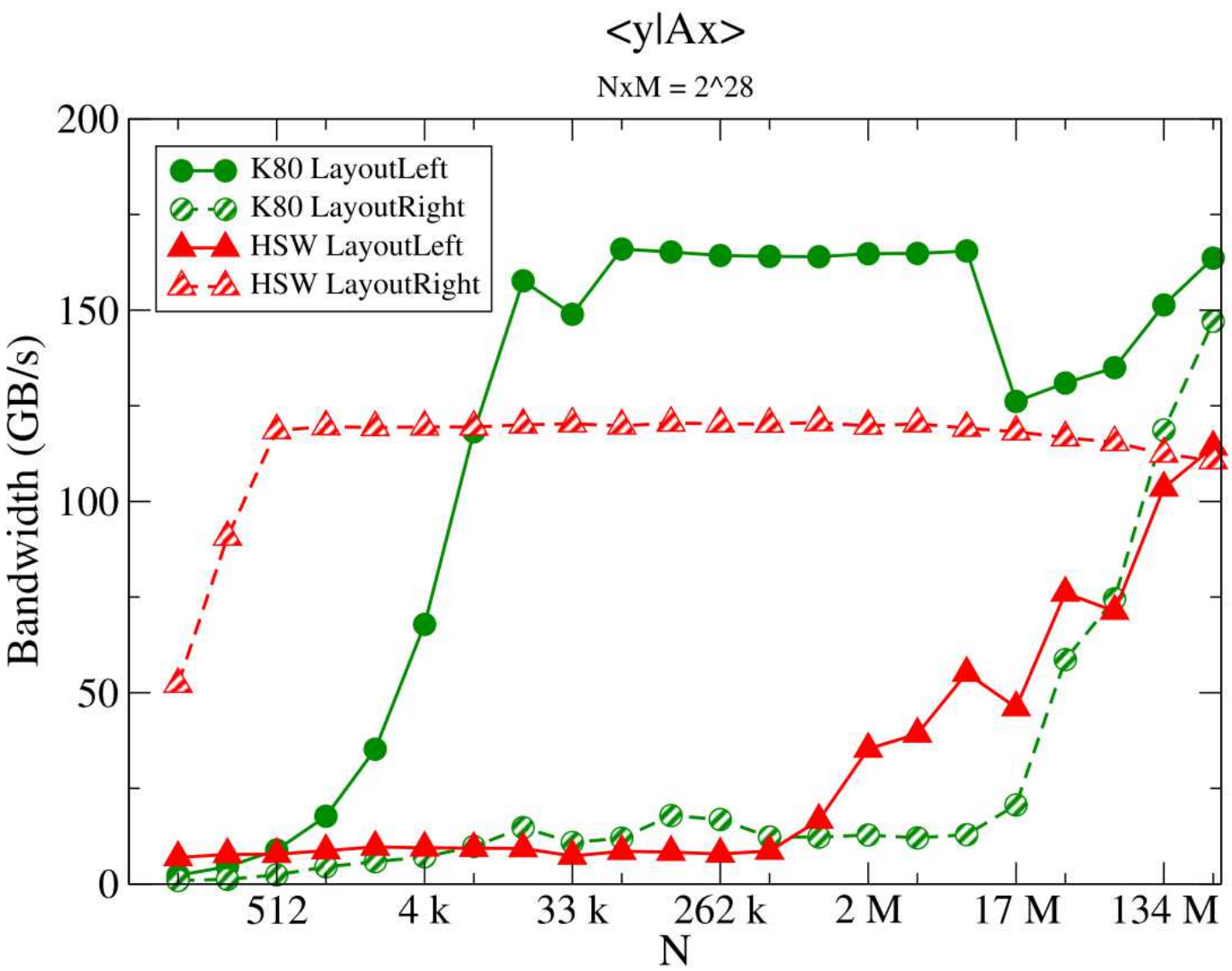
```

- Most-common layouts are `LayoutLeft` and `LayoutRight`.
  `LayoutLeft`: left-most index is stride 1.
  `LayoutRight`: right-most index is stride 1.
- If no layout specified, default for that memory space is used.
  `LayoutLeft` for `CudaSpace`, `LayoutRight` for `HostSpace`.
- Layouts are extensible: ~50 lines
- Advanced layouts: `LayoutStride`, `LayoutTiled`, ... extensible

Example: $\langle y^T | Ax \rangle$

```
...
// Allocate explicitly with LayoutRight
Kokkos::View<double**, Kokkos::LayoutRight> A ("A", N,M);
Kokkos::View<double*> x("X",M), y("Y",N);
...
double yAx = 0;
// Run explicitly in the Cuda execution space
Kokkos::parallel_reduce(N,
  KOKKOS_LAMBDA (const size_t i, double& yAx_thread) {
  double Ax_i = 0;
  for (int j = 0; j < M; ++j) {
    Ax_i += A(i,j) * x(j);
  }
  yAx_thread += y(i) * Ax_i;
}, yAx);
...
```


<y|Ax>
NxM = 2^28
K80 LayoutLeft
K80 LayoutRight
HSW LayoutLeft
HSW LayoutRight
Bandwidth (GB/s)
200
150
100
50
0
512
4 k
33 k
262 k
2 M
17 M
134 M
N

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Parallel execution patterns can be **nested** by using a **TeamPolicy**.

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- Team:

```
parallel_xx(TeamPolicy<>(WorkSets,TeamSize[,VectorLength]), ... );
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- Thread: `parallel_xx(TeamThreadRange(team_handle,Begin,End),...);`

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- Vector: `parallel_xx(ThreadVectorRange(team_handle,Begin,End),...);`

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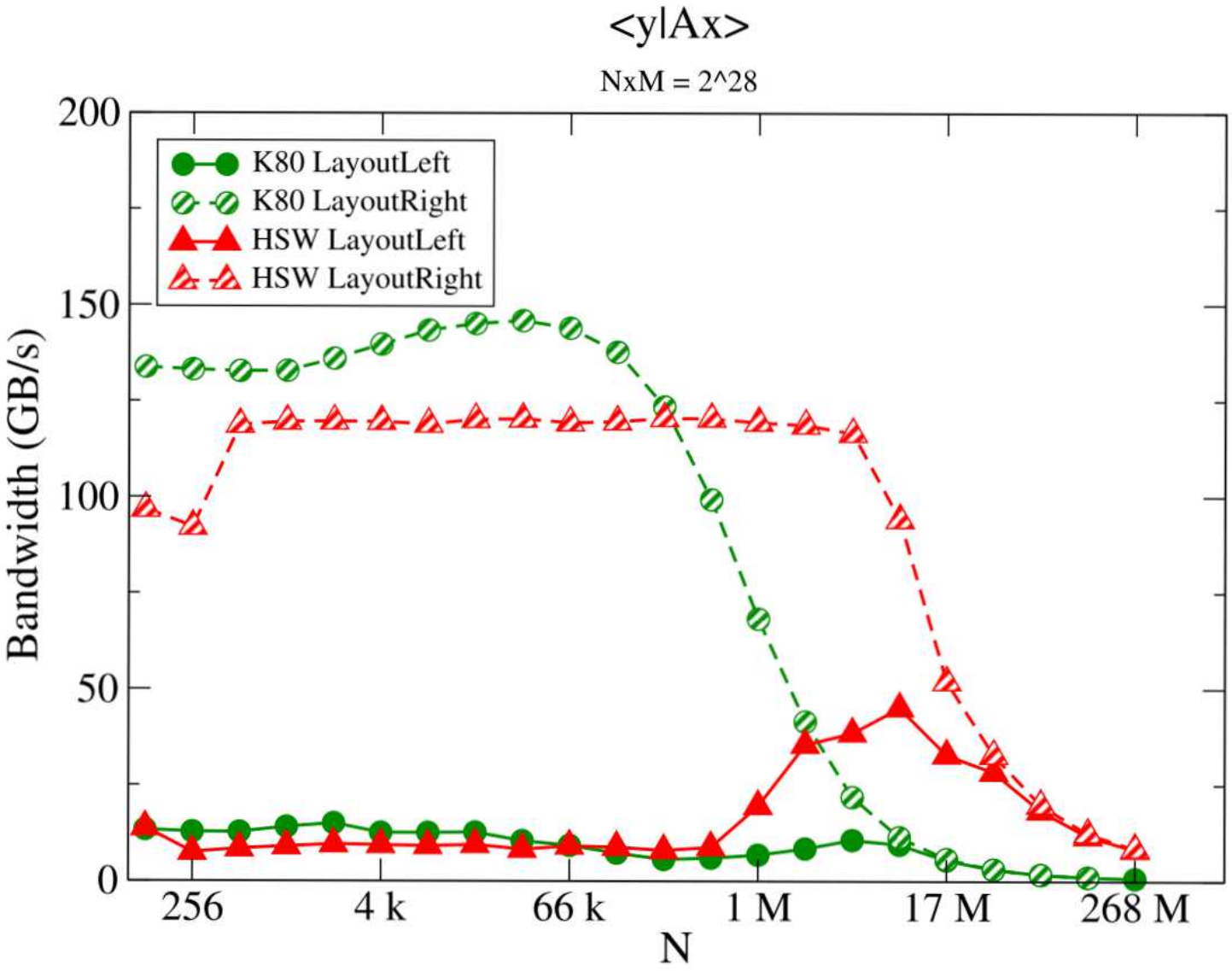
- The **Vector Level** is optional, and the provided vector length has not on all platforms meaning.
- The **body** of a **TeamPolicy** kernel is executed as a **parallel region** with respect to each team.
- Threads within a team are guaranteed to run concurrent, teams are not.

Example: Hierarchical Parallelism

```
...
// Execution policies use a 'member type' as argument
typedef Kokkos::TeamPolicy<>::member_type team_type;
double yAx = 0;
// Split rows over teams, with Kokkos choosing team size
Kokkos::parallel_reduce(Kokkos::TeamPolicy<>(N, Kokkos::AUTO),
  KOKKOS_LAMBDA (const team_type& team, double& yAx_team) {
  double Ax_i = 0;
  // Do nested dot product with the team
  Kokkos::parallel_reduce(Kokkos::TeamThreadRange(team, M),
    [&] (const int& j) {
    Ax_i += A(i,j) * x(j);
  },Ax_i);
  // Only one thread per team adds to the result
  Kokkos::single(Kokkos::PerTeam(team), [&] () {
    yAx_team += y(i) * Ax_i;
  });
}, yAx);
...
```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256
4 k
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1 M
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268 M
N

Features which were not discussed:

- Atomics: Support of arbitrary sized atomics
- Team Scratch Pads: Exposes Cuda shared memory functionality
- Algorithms: Sort and Random Numbers
- Containers: DualView, std::vector replacement, unordered map
- ExecutionTags: have classes act as functors with multiple tagged operators
- Custom Reductions/Scans: use functors with join, init and final functions
- Profiling support: simple inbuild capabilities + hooks for third party tools

Whats next (next couple of years and subject to finding people):

- Kernels package in Trilinos: BLAS, Sparse LA, Graph algorithms
- Task support: under development, prototype on CPUs
- Remote memory spaces: incorporate shmem like capabilities
- More debugging features: e.g. runtime identification of potential write conflicts