A Tutorial Introduction to RAJA

ATPESC

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With contributions from others on the RAJA Team
Welcome to the RAJA tutorial

- Today, you will learn how to use key RAJA features:
  - Parallel loop execution
    - Simple loops (e.g., non-nested)
    - Complex loop kernels (composition and transformation)
  - Reductions
  - Atomic operations
  - Scan operations

- We will also briefly discuss:
  - RAJA motivation and goals
  - Application considerations for C++ portability solutions like RAJA

See the RAJA User Guide to learn about features not covered today (https://readthedocs.org/projects/raja).
RAJA is an open source project hosted on Github

- The “RAJA/examples” directory contains codes used in this tutorial

https://github.com/LLNL/RAJA
Other materials and related projects are also available...

- **RAJA User Guide**: getting started info and details about today’s topics and more

- **RAJA Performance Suite**: Monitor RAJA performance and assess compilers, used by vendors, used in DOE platform procurements

- **RAJA Proxy Apps**: RAJA versions of DOE proxy apps

- **CHAI**: Array abstraction library that automatically migrates data as needed based on RAJA execution contexts

These are linked on RAJA Github project.
We value your feedback...

- If you have comments, questions, suggestions, etc., please let us know
  - Join our Google Group (linked on RAJA Github project)
  - Or contact us using our project email list: raja-dev@llnl.gov
During today’s presentation...

Please don’t hesitate to ask questions at any time
Let’s start simple...

Simple loop traversal
RAJA encapsulates loop execution details using standard C++ features

Daxpy operation: \( a = a + c \times b; \) \( a, b \) are vectors of length \( N \), \( c \) is a scalar

C-style for-loop

```c
for (int i = 0; i < N; ++i) {
    a[i] += c * b[i];
}
```

The way the loop is expressed is different, but the loop body is the same.

RAJA-style loop

```cpp
RAJA::RangeSegment range(0, N);

RAJA::forall<RAJA::seq_exec>(range, [=] (int i) {
    a[i] += c * b[i];
});
```
There are four core elements to RAJA loop execution

using EXEC_POLICY = RAJA::seq_exec;
RAJA::RangeSegment range(0, N);

RAJA::forall< EXEC_POLICY >( range, [=] (int i) {
    a[i] += c * b[i];
} );

1. Loop execution template (e.g., ‘forall’)
2. Loop execution policy (EXEC_POLICY)
3. Loop iteration space (e.g., ‘RangeSegment’)
4. Loop body (C++ lambda expression)
Elements of RAJA loop execution

```cpp
RAJA::forall< exec_policy >( iteration_space,
    [=] (int i) {
        // loop body
    }
);
```

- RAJA::forall method runs loop iterations based on:
  - Execution policy type (sequential, OpenMP, CUDA, etc.)
Elements of RAJA loop execution

```cpp
RAJA::forall< exec_policy >( iteration_space,
    [=] (int i) {
        // loop body
    }
);```

- **RAJA::forall template runs loop iterations based on:**
  - Execution policy type (sequential, OpenMP, CUDA, etc.)
  - **Iteration space object** (stride-1 range, list of indices, etc.)
Elements of RAJA loop execution

RAJA::forall< exec_policy >( iteration_space,

    [=] (int i) {
        // loop body
    }

);  

- RAJA::forall template runs loop iterations based on:
  - Execution policy type (sequential, OpenMP, CUDA, etc.)
  - Iteration space object (contiguous range, list of indices, etc.)

- Loop body is cast as a C++ lambda expression
  - A closure that stores a function with a data environment
  - Function argument is the loop variable

The programmer must make sure the loop body works with the execution policy.
These core elements will be common threads in our discussion

```
RAJA::forall< exec_policy >( iteration_space, 
    [=] (int i) {
        // loop body
    }
);
```

- **RAJA::forall** template runs loop iterations based on:
  - Execution policy type (sequential, OpenMP, CUDA, etc.)
  - Iteration space object (contiguous range, list of indices, etc.)

- Loop body is cast as a C++ lambda expression
By changing the execution policy, a loop can run in different ways

```cpp
RAJA::forall<exec_policy>( range, [=] (int i) {
    a[i] += c * b[i];
} );
```

- Some execution policy choices...
  - `RAJA::simd_exec`
  - `RAJA::omp_parallel_for_exec`
  - `RAJA::cuda_exec<BLOCKSIZE>`
  - `RAJA::omp_target_parallel_for_exec<NUMTEAMS>`
  - `RAJA::tbb_for_exec`
RAJA provides a variety of execution policy types for simple loops...

- Sequential (strictly)
- “Loop” (let compiler decide which optimizations to apply)
- SIMD (vectorization pragmas applied)
- OpenMP multithreading (CPU)
- TBB (Intel Threading Building Blocks)
- CUDA
- OpenMP target (available target device; e.g., GPU)

Some are works-in-progress:
- OpenMP target (work with IBM)
- TBB (work with Intel)
- ROCm will be available in a future release (work with AMD)
## RAJA support for simple loops

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RAJA
Motivation and Goals
Overarching goals of RAJA:

— *Enable portability* in existing applications with *manageable disruption* to algorithms and programming styles

— Provide a model for new applications to be *portable from the start*

RAJA provides application developers with building blocks that extend the generally-accepted “*parallel for*” idiom.
RAJA design points focus on usability and developer productivity

- Applications should maintain **single-source kernels** (if possible)
- **Easy to grasp** for app developers (most are not CS experts)
- Allow for **incremental and selective** use
- Don’t force **major disruption** to application source code
- Promote implementation flexibility via **clean encapsulation**
- Make it **easy to parameterize execution** via types
- Enable **systematic performance tuning**

Our focus on these points has enabled RAJA adoption.
Reductions
RAJA reduction types hide the complexity of parallel reduction implementations

Dot product: \( \text{dot} = (a, b) \), where \( a \) and \( b \) are vectors and \( \text{dot} \) is a scalar

C-style

```c
double dot = 0.0;
for (int i = 0; i < N; ++i) {
    dot += a[i] * b[i];
}
```

RAJA

```cpp
RAJA::ReduceSum< reduce_policy, double> dot(0.0);

RAJA::forall< exec_policy >( arange, [=] (int i) {
    dot += a[i] * b[i];
} );
```
Elements of RAJA reductions...

```cpp
RAJA::ReduceSum< reduce_policy, type > sum(init_val);

RAJA::forall< exec_policy >(... { 
    sum += func(i);
});

type reduced_sum = sum.get();
```

- Each reduction type requires:
  - A reduction policy
  - A reduction value type
  - An initial value
Elements of RAJA reductions...

RAJA::ReduceSum< reduce_policy, type > foo(init_val);

RAJA::forall< exec_policy >(... {  
    sum += func(i);
} );

type reduced_sum = sum.get();

- Each reduction type requires:
  - A reduction policy
  - A reduction value type
  - An initial value

- Updating reduction value is what you expect (+=, min, max)
Elements of RAJA reductions...

RAJA::ReduceSum< reduce_policy, type > sum(init_val);

RAJA::forall< exec_policy >(... {
  sum += func(i);
});

type reduced_sum = sum.get();

- Each reduction type requires:
  - A reduction policy
  - A reduction value type
  - An initial value
- Updating reduction value is what you expect (+=, min, max)
- After loop, get reduced value via ‘get’ method or type cast
Elements of RAJA reductions...

RAJA::ReduceSum< reduce_policy, type > sum(init_val);

RAJA::forall< exec_policy >( ... { 
    sum += func(i);
});

type reduced_sum = sum.get();

Reduction policy **must be compatible** with loop execution policy.
RAJA provides reduction policies for all programming model back-ends

RAJA::ReduceSum<reduce_policy, int> sum(0);

- Reduction policies
  
  RAJA::seq_reduce;
  
  RAJA::omp_reduce;
  
  RAJA::cuda_reduce<BLOCK_SIZE>;
  
  RAJA::tbb_reduce;
  
  RAJA::omp_target_reduce<NUMTEAMS>;

Note: SIMD, OpenMP target, and ROCm are works-in-progress.
RAJA supports five common reductions types

RAJA::ReduceSum< reduce_policy, type > r(in_val);

RAJA::ReduceMin< reduce_policy, type > r(in_val);

RAJA::ReduceMax< reduce_policy, type > r(in_val);

RAJA::ReduceMinLoc< reduce_policy, type > r(in_val, in_loc);

RAJA::ReduceMaxLoc< reduce_policy, type > r(in_val, in_loc);

“Loc” reductions give iteration index where reduced value was found.
Multiple RAJA reductions can be used in a kernel

RAJA::ReduceSum< REDUCE_POL, int > sum(0);
RAJA::ReduceMin< REDUCE_POL, int > min(MAX_VAL);
RAJA::ReduceMax< REDUCE_POL, int > max(MIN_VAL);
RAJA::ReduceMinLoc< REDUCE_POL, int > minloc(MAX_VAL, -1);
RAJA::ReduceMaxLoc< REDUCE_POL, int > maxloc(MIN_VAL, -1);

RAJA::forall< EXEC_POL >( a_range, [=](int i) {
    seq_sum += a[i];
    seq_min.min(a[i]);
    seq_max.max(a[i]);
    seq_minloc.minloc(a[i], i);
    seq_maxloc.maxloc(a[i], i);
} );

Remember: Reduction and loop execution policies must be compatible.
Suppose we run the code on the preceding slide with this setup...

‘a’ is an int vector of length ‘N’ (N / 2 is even) initialized as:

```
0  1  2  . . .  N/2  . . .  N-1
a : 1 -1 1 -1 1 . . . 1 -10 10 -10 1 . . . -1 1 -1
```

- This will yield
  - Sum = -9
  - Min = -10
  - Max = 10
  - Max-loc = N / 2
  - Min-loc = N / 2 - 1
    (or N / 2 + 1)*

RAJA provides **reproducible parallel reductions** if you need them.
## RAJA support for reductions

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Iteration spaces:
Segments and IndexSets
A RAJA “Segment” is the basic means to define a loop iteration space

- A “Segment” defines a set of loop indices to run as a unit
  
  Contiguous range [beg, end)
  
  Strided range [beg, end, stride)
  
  List of indices (indirection)

- An “Index Set” is a container of segments

You can run all segments in an IndexSet in one RAJA traversal.
A RangeSegment defines a contiguous sequence of indices (stride-1)

```cpp
RAJA::RangeSegment range( 0, N );

RAJA::forall< RAJA::seq_exec >( range, [=] (int i) {
    // ...
}
);
```

Runs loop indices: \{0, 1, 2, \ldots , N-1\}
A RangeStrideSegment defines a strided sequence of indices

RAJA::RangeStrideSegment srange1( 0, N, 2 );

RAJA::forall< RAJA::seq_exec >( srange1, [=] (int i) {
    // ...
} );

Runs loop indices: {0, 2, 4, ...}

RAJA::RangeStrideSegment srange2( N-1, -1, -1 );

RAJA::forall< RAJA::seq_exec >( srange2, [=] (int i) {
    // ...
} );

Runs loop in reverse: {N-1, N-2, ... , 1, 0}

RAJA supports negative indices and strides.
RAJA::IndexType is a useful parametrization
  — It is an alias to std::ptrdiff_t
  — Appropriate for most compiler optimizations

Use the ‘Typed’ Segment types for other index value types.
A ListSegment defines a set of indices (think “indirection array”)

```cpp
using IdxType = RAJA::Index_type;
using ListSegType = RAJA::TypedListSegment<IdxType>;

// array of indices
IdxType idx[ ] = {10, 11, 14, 20, 22};

// ListSegment object containing indices...
ListSegType idx_list( idx, 5 );

RAJA::forall< exec_policy >( idx_list, [=] (IdxType i) {
    a[i] += c * b[i];
} );
```

Runs loop indices: {10, 11, 14, 20, 22}

Note: indirection does not appear in loop body.
A RAJA Index Set is a container of Segments

```cpp
RAJA::RangeSegment range1(0, 8);
IdxType idx[] = {10, 11, 14, 20, 22};
ListSegType list2( idx, 5 );
RAJA::RangeSegment range3(24, 28);

RAJA::TypedIndexSet< RAJA::RangeSegment,
                     ListSegType > iset;
iset.push_back( range1 );
iset.push_back( list2 );
iset.push_back( range3 );
```

Iteration space is partitioned into 3 Segments

{ 0, … , 7 } + {10, 11, 14, 20, 22 } + { 24, … , 27 }

range1  list2  range3
An IndexSet can be passed to a RAJA traversal method to run all Segments

using ISET_EXECPOL = RAJA::ExecPolicy< RAJA::omp_parallel_segit, RAJA::seq_exec >;

RAJA::forall<ISET_EXECPOL>(iset, [=] (IdxType i) {
    // loop body
} );

Index sets require a **two-level execution policy:**

- One for iterating over segments ( “..._segit”)
- One for executing segments
RAJA Segment types model C++ iterable interfaces

- A segment type defines three methods:
  - `begin()`
  - `end()`
  - `size()`

- And two types:
  - `iterator` (essentially “random access”)
  - `value_type`

Many **user-defined types** that have these properties can be used as a Segment with RAJA.
Why do we provide Index Sets?

- **Multiphysics codes use indirection arrays** (a lot!) : simplicity & generality – unstructured meshes, material regions on a mesh, etc.
  - Indirection impedes performance: extra instructions, no SIMD, etc.

- **Range Segments are better for performance**
  - When large stride-1 ranges are embedded in iteration patterns...
  - ...you can expose SIMD-izable ranges “in place” to compilers (no gather/scatters)

- **Partitioning and reordering iterations gives flexibility and performance**
  - Avoid fine-grained synchronization (atomics or critical sections) – contention heavy
  - Avoid extra arrays and gather/scatter operations – extra memory traffic
  - Prefer coarse-grained synchronization - light memory contention

With IndexSets, you can change the iteration pattern without changing the way it looks in source code.
IndexSets help enable thread parallelism...

Example: accumulate average element volumes to mesh vertices

```c
for (int j = 0 ; j < N_elem ; ++j) {
    for (int i = 0 ; i < N_elem ; ++i) {
        int ie = i + j * jeoff;
        int* iv = &(elem2vert_map[4*ie]);

        vertvol[ iv[0] ] += elemvol[ie] / 4.0;
    }
}
```

As written, this code will not run correctly in parallel – data races!
Partition elements into independent subsets (colors) to avoid race conditions

using EXEC_POL =

RAJA::ExecPolicy<RAJA::seq_segit,
    RAJA::omp_parallel_for_exec>;

RAJA::forall<EXEC_POL>(colorset, [=](int ie) {

    int* iv = &(elem2vert_map[4*ie]);
    vertexvol[ iv[0] ] += elemvol[ie] / 4.0 ;

});

Important: the loop body looks like the domain expert wrote it!
RAJA Segments and IndexSets work with all back-ends

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Atomic operations
RAJA provides portable atomic operations

```cpp
int* x = ...  
int* y = ...

RAJA::forall< exec_policy >((RAJA::RangeSegment(0, N), [=] (int i) {

  RAJA::atomic::atomicAdd< atomic_policy >(&x[i], 1);
  RAJA::atomic::atomicSub< atomic_policy >(&y[i], 1);

}));
```

Atomic operations perform atomic memory updates (write or read-modify-write).
Atomics may be preferable to reductions

Example: compute a histogram of array values

```cpp
int* a = ... // array length N (a[i] in {0,..,M-1})
int* bins = ... // array length M (M <= N)

using EXEC_POL = RAJA::cuda_exec;
using ATOMIC_POL = RAJA::atomic::cuda_atomic;

RAJA::forall<EXEC_POL>(arange, [=] RAJA_DEVICE (int i) {
    RAJA::atomic::atomicAdd<ATOMIC_POL>(&bins[ a[i] ], 1);
});
```

This is simpler (and may perform better) than using reductions.
The atomic policy determines the atomic implementation

- The RAJA “builtin” atomic policy uses compiler built-in atomics

```cpp
using EXEC_POL = RAJA::omp_parallel_for_exec;

int *sum = ...;

RAJA::forall< EXEC_POL >((arange, [=] (int i) {
    atomic::atomicAdd< RAJA::builtin_atomic >(sum, 1);
} ));
```

The atomic policy must be compatible with loop execution policy.
RAJA also has an “auto” atomic policy

- The RAJA::auto_atomic policy will do the right thing...

```cpp
using EXEC_POL = RAJA::cuda_exec;

int *sum = ...;

RAJA::forall< EXEC_POL >(arange, [=] RAJA_DEVICE(int i) {
    atomic::atomicAdd<RAJA::auto_atomic>(sum, 1);
});
```

Some may prefer this option for easier portability.
RAJA also has an interface modeled after C++ std::atomic

- “AtomicRef” supports:
  - Arbitrary memory locations
  - All RAJA atomic policies

For example:

```c++
double val = 2.0;
RAJA::atomic::AtomicRef<double,
    RAJA::omp_atomic> sum(&val);

sum++;  // Result: sum is 5.
++sum;
sum += 1.0;
```

Atomics
RAJA provides a variety of atomic operations

- Arithmetic: add, sub
- Min, max
- Increment/decrement: inc, dec, including comparisons
- Bitwise-logical: and, or, xor
- Replace: exchange, CAS
- C++ std::atomic style interface

RAJA User Guide describes these atomic operations in detail.
# RAJA support for atomics

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Scan operations
Scan is a basic parallel algorithm building block

- Key primitive to convert serial operations to parallel
  - Based on reduction tree and reverse reduction tree

- Many useful applications:
  - Sorting (radix, quicksort)
  - String comparison
  - Lexical analysis
  - Stream compaction
  - Polynomial evaluation
  - Solving recurrence relations
  - Tree operations
  - Histograms
  - Parallel work assignment

Prefix Sums and Their Applications
Guy E. Blelloch
School of Computer Science
Carnegie Mellon University
Pittsburgh, PA 15213-3890

Blelloch’s Lecture Notes are worth reading.
Parallel prefix sum is the most common scan

```c++
int* in = ...; // arrays of length N
int* out = ...;

RAJA::inclusive_scan< exec_pol >(in, in + N, out);
RAJA::exclusive_scan< exec_pol >(in, in + N, out);
```

Example:

In : 8 -1 2 9 10 3 4 1 6 7  (N=10)

Out (inclusive) : 8 7 9 18 28 31 35 36 42 49

Out (exclusive) : 0 8 7 9 18 28 31 35 36 42

Output array contains partial sums of input array.
RAJA provides “in-place” scan operations

```cpp
int* in  = ...;  // array of length N

RAJA::inclusive_scan_inplace< exec_pol >((in, in + N));

RAJA::exclusive_scan_inplace< exec_pol >((in, in + N));
```

“In-place” scans return result in input array.
RAJA scans work with different operators

RAJA::inclusive_scan< exec_pol >(in, in + N, out,
RAJA::operators::minimum<int>{},
);

In : 8 -1 2 9 10 3 4 1 6 7
Out : 8 -1 -1 -1 -1 -1 -1 -1 -1 -1

RAJA::exclusive_scan< exec_pol >(in, in + N, out,
RAJA::operators::maximum<int>{},
);

In : 8 -1 2 9 10 3 4 1 6 7
Out : -2147483648 8 8 8 9 10 10 10 10 10

If no operator is given, “plus” is the default (prefix-sum).
## RAJA support for scans

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- ☢️ = available
- ☢️ = in progress
- ☢️ = not available
Complex Loops
Let’s look at a nested loop example and apply what we’ve seen so far...

Matrix multiplication: $C = A \times B$, where $A$, $B$, $C$ are $N \times N$ matrices

```c
for (int row = 0; row < N; ++row) {
    for (int col = 0; col < N; ++col) {
        double dot = 0.0;
        for (int k = 0; k < N; ++k) {
            dot += A[k + N*row] * B[col + N*k];
        }
        C[col + N*row] = dot;
    }
}
```
We could nest ‘forall’ statements...

```
RAJA::forall< exec_policy_row >( row_range, [=](int row) {
    RAJA::forall< exec_policy_col >( col_range, [=](int col) {

        double dot = 0.0;
        for (int k = 0; k < N; ++k) {
            dot += A[k + N*row] * B[col + N*k];
        }
        C[col + N*row] = dot;
    }
});
```
...but, this doesn’t work well

- **Each loop level is treated as an independent entity**
  - So parallelizing the row and column loops together is hard

- We can use a parallel execution policy (OpenMP, CUDA, etc.) on the outer row loop
  - Then, each thread executes all code inside it **sequentially**

- Parallelizing the inner column loop introduces potential synchronization for each outer loop iteration
  - Launch a separate parallel computation for each row

- Loop interchange and other transformations **require changing the source code of the kernel (which breaks RAJA encapsulation)**

**We don’t recommend using RAJA::forall for nested loops!!**
The RAJA::kernel API is used to compose and transform complex parallel kernels

```cpp
using KERNEL_POL =
    RAJA::KernelPolicy<
        RAJA::statement::For<1, exec_policy_row>,
        RAJA::statement::For<0, exec_policy_col>,
        RAJA::statement::Lambda<0>
    >;

RAJA::kernel<KERNEL_POL>(RAJA::make_tuple(col_range, row_range),
    [=](int col, int row) {
    double dot = 0.0;
    for (int k = 0; k < N; ++k) {
        dot += A[k + N*row] * B[col + N*k];
    }
    C[col + N*row] = dot;
});
```

Note: lambda expression for inner loop body is same as before.
There are four key elements to the RAJA::kernel interface

- These are analogous to RAJA::forall

1. Loop execution template (‘RAJA::kernel’)
2. Loop execution policies (in ‘KERNEL_POL’)
3. Loop iteration spaces (e.g., ‘RangeSegments’)
4. Loop body (lambda expressions)
Each loop level has an iteration space, and loop variable

using KERNEL_POL =
    RAJA::KernelPolicy<
        RAJA::statement::For<1, exec_policy_row>,
        RAJA::statement::For<0, exec_policy_col>,
        RAJA::statement::Lambda<0>
    >;

RAJA::kernel<KERNEL_POL>(RAJA::make_tuple(col_range, row_range),
                      [=](int col, int row) {
                        // ...
                      });

Order (and types) of tuple items and loop variables must match.
Each loop level has an execution policy...

```
using KERNEL_POL =
  RAJA::KernelPolicy<
    RAJA::statement::For<1, exec_policy_row>,
    RAJA::statement::For<0, exec_policy_col>,
    RAJA::statement::Lambda<0>
  >;

RAJA::kernel<KERNEL_POL>(RAJA::make_tuple(col_range, row_range), [=](int col, int row) {
  // ...
});
```

Integer parameter in ‘For’ statement specifies the tuple item it applies to.

Complex loops

Each loop level has an execution policy...

```
using KERNEL_POL =
  RAJA::KernelPolicy<
    RAJA::statement::For<1, exec_policy_row>,
    RAJA::statement::For<0, exec_policy_col>,
    RAJA::statement::Lambda<0>
  >;

RAJA::kernel<KERNEL_POL>(RAJA::make_tuple(col_range, row_range), [=](int col, int row) {
  // ...
});
```

Complex loops

Each loop level has an execution policy...

```
using KERNEL_POL =
  RAJA::KernelPolicy<
    RAJA::statement::For<1, exec_policy_row>,
    RAJA::statement::For<0, exec_policy_col>,
    RAJA::statement::Lambda<0>
  >;

RAJA::kernel<KERNEL_POL>(RAJA::make_tuple(col_range, row_range), [=](int col, int row) {
  // ...
});
```

Complex loops

Each loop level has an execution policy...

```
using KERNEL_POL =
  RAJA::KernelPolicy<
    RAJA::statement::For<1, exec_policy_row>,
    RAJA::statement::For<0, exec_policy_col>,
    RAJA::statement::Lambda<0>
  >;

RAJA::kernel<KERNEL_POL>(RAJA::make_tuple(col_range, row_range), [=](int col, int row) {
  // ...
});
```

Complex loops

Each loop level has an execution policy...

```
using KERNEL POL =
  RAJA::KernelPolicy<
    RAJA::statement::For<1, exec_policy_row>,
    RAJA::statement::For<0, exec_policy_col>,
    RAJA::statement::Lambda<0>
  >;

RAJA::kernel<KERNEL POL>(RAJA::make_tuple(col_range, row_range), [=](int col, int row) {
  // ...
});
```

Complex loops

Each loop level has an execution policy...

```
using KERNEL POL =
  RAJA::KernelPolicy<
    RAJA::statement::For<1, exec_policy_row>,
    RAJA::statement::For<0, exec_policy_col>,
    RAJA::statement::Lambda<0>
  >;

RAJA::kernel<KERNEL POL>(RAJA::make_tuple(col_range, row_range), [=](int col, int row) {
  // ...
});
```

Complex loops

Each loop level has an execution policy...

```
using KERNEL POL =
  RAJA::KernelPolicy<
    RAJA::statement::For<1, exec_policy_row>,
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  >;

RAJA::kernel<KERNEL POL>(RAJA::make_tuple(col_range, row_range), [=](int col, int row) {
  // ...
});
```

Complex loops

Each loop level has an execution policy...

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using KERNEL POL =
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    RAJA::statement::For<1, exec_policy_row>,
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    RAJA::statement::Lambda<0>
  >;

RAJA::kernel<KERNEL POL>(RAJA::make_tuple(col_range, row_range), [=](int col, int row) {
  // ...
});
```

Complex loops

Each loop level has an execution policy...

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using KERNEL POL =
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    RAJA::statement::Lambda<0>
  >;

RAJA::kernel<KERNEL POL>(RAJA::make_tuple(col_range, row_range), [=](int col, int row) {
  // ...
});
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Complex loops

Each loop level has an execution policy...

```
using KERNEL POL =
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  >;

RAJA::kernel<KERNEL POL>(RAJA::make_tuple(col_range, row_range), [=](int col, int row) {
  // ...
});
```

Complex loops

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RAJA::kernel<KERNEL POL>(RAJA::make_tuple(col_range, row_range), [=](int col, int row) {
  // ...
});
```

Complex loops

Each loop level has an execution policy...

```
using KERNEL POL =
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    RAJA::statement::For<0, exec_policy_col>,
    RAJA::statement::Lambda<0>
  >;

RAJA::kernel<KERNEL POL>(RAJA::make_tuple(col_range, row_range), [=](int col, int row) {
  // ...
});
```

Complex loops

Each loop level has an execution policy...

```
using KERNEL POL =
  RAJA::KernelPolicy<
    RAJA::statement::For<1, exec_policy_row>,
    RAJA::statement::For<0, exec_policy_col>,
    RAJA::statement::Lambda<0>
  >;

RAJA::kernel<KERNEL POL>(RAJA::make_tuple(col_range, row_range), [=](int col, int row) {
  // ...
});
```

Complex loops

Each loop level has an execution policy...

```
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RAJA::kernel<KERNEL POL>(RAJA::make_tuple(col_range, row_range), [=](int col, int row) {
  // ...
});
```

Complex loops

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    RAJA::statement::Lambda<0>
  >;

RAJA::kernel<KERNEL POL>(RAJA::make_tuple(col_range, row_range), [=](int col, int row) {
  // ...
});
```

Complex loops

Each loop level has an execution policy...

```
using KERNEL POL =
  RAJA::KernelPolicy<
    RAJA::statement::For<1, exec_policy_row>,
    RAJA::statement::For<0, exec_policy_col>,
    RAJA::statement::Lambda<0>
  >;

RAJA::kernel<KERNEL POL>(RAJA::make_tuple(col_range, row_range), [=](int col, int row) {
  // ...
});
```

Complex loops
Complex loops

Loop interchange done by changing the execution policy, not algorithm code

```
using KERNEL_POL =
    RAJA::KernelPolicy<
        RAJA::statement::For<1, exec_policy_row>,
        RAJA::statement::For<0, exec_policy_col>,
        RAJA::statement::Lambda<0>
    >;

using KERNEL_POL =
    RAJA::KernelPolicy<
        RAJA::statement::For<0, exec_policy_col>,
        RAJA::statement::For<1, exec_policy_row>,
        RAJA::statement::Lambda<0>
    >;
```

'For' statements are swapped.

Outer row loop (1), inner col loop (0)

Outer col loop (0), inner row loop (1)
A kernel can be composed from any number of lambdas

RAJA::kernel_param<KERNEL_POL>(
  RAJA::make_tuple(col_range, row_range, dot_range),

  RAJA::tuple<double>{0.0}, // thread local variable for 'dot'

  [=] (int col, int row, int k, double& dot) { // lambda 0
    dot = 0.0;
  },

  [=] (int col, int row, int k, double& dot) { // lambda 1
    dot += A[k + N*row] * B[col + N*k];
  },

  [=] (int col, int row, int k, double& dot) { // lambda 2
    C[col + N*row] = dot;
  }
);
The execution policy composes ‘statements’ into a kernel

using KERNEL_POL =
  RAJA::KernelPolicy<
    RAJA::statement::For<1, exec_policy_row,
    RAJA::statement::For<0, exec_policy_col,

      RAJA::statement::Lambda<0>, // init: dot = 0.0
      RAJA::statement::For<2, RAJA::seq_exec,
        RAJA::statement::Lambda<1> // inner loop: dot += ...
      >,
      RAJA::statement::Lambda<2> // C[col + N*row] = dot;

    >
  >
>;

Nesting ‘RAJA::statement’ types is analogous to nesting for-loops and other statements in a C-style loop nest.
Complex loops

You can collapse loops in an OpenMP parallel region...

```cpp
using KERNEL_POL =
  RAJA::KernelPolicy<
    RAJA::statement::Collapse<RAJA::omp_parallelCollapse_exec,
      RAJA::ArgList<1, 0>, // row, col

      RAJA::statement::Lambda<0>, // dot = 0.0
      RAJA::statement::For<2, RAJA::seq_exec,
        RAJA::statement::Lambda<1> // inner loop: dot += ...
        >,
      RAJA::statement::Lambda<2> // set C[col + N*row] = dot;

    >;

RAJA::kernel_param<KERNEL_POL>(
  RAJA::make_tuple(col_range, row_range, dot_range),
  // lambdas used to compose kernel body...
);
```

This policy distributes iterations in loops ‘1’ and ‘0’ across CPU threads.
You can launch loops as a CUDA kernel...

```cpp
using KERNEL_POL =
    RAJA::KernelPolicy<
        RAJA::statement::CudaKernel<
            RAJA::statement::For<1, RAJA::cuda_block_exec, // row
            RAJA::statement::For<0, RAJA::cuda_thread_exec, // col
                RAJA::statement::Lambda<0>, // dot = 0.0
                RAJA::statement::For<2, RAJA::seq_exec,
                    RAJA::statement::Lambda<1> // dot += ...
                >,
                RAJA::statement::Lambda<2> // set C = ...
            >,
            RAJA::statement::Lambda<2> // set C = ...
        >;
```

This policy distributes ‘row’ indices over CUDA thread blocks and ‘col’ indices over threads in each block; i.e., same as defining indices inside the kernel as:

```cpp
int row = blockIdx.x;
int col = threadIdx.x;
```
Another CUDA kernel variant...

```
using KERNEL_POL =
    RAJA::KernelPolicy<
        RAJA::statement::CudaKernel<
            RAJA::statement::For<1, RAJA::cuda_threadblock_exec<BS>>,
            RAJA::statement::For<0, RAJA::cuda_threadblock_exec<BS>>,
            RAJA::statement::Lambda<0>, // dot = 0.0
            RAJA::statement::For<2, RAJA::seq_exec,
                RAJA::statement::Lambda<1> // dot += ...
            >,
            RAJA::statement::Lambda<2> // set C = ...
        >
    >;
```

This policy distributes ‘row’ and ‘col’ indices over 2-dimensional BS X BS CUDA thread blocks.
RAJA kernel policies combine ‘Statements’ and ‘StatementLists’

- **A Statement is an action**: execute a loop, invoke a lambda, set a thread barrier, etc. For example,

```
Lambda<0>
```

- **A StatementList is an ordered list of Statements** processed as a sequence; e.g.,

```
For<0, exec_policy0, Lambda<0>,
   For<2, exec_policy2, Lambda<1>
   >
>
```

- These policy constructs form a simple domain specific language (DSL) that relies only on standard C++11 support

**A RAJA::KernelPolicy type is a StatementList.**
The current list of RAJA::statement types...

- `For< Id, ExecPolicy, EnclStmts >` – abstracts a for-loop
- `Lambda< Id >` – invoke a lambda expression
- `Collapse< ExecPolicy, ArgList<...>, EnclStmts >` – collapse multiple, perfectly nested loops
- `If< Conditional >` – select parts of a policy to use at runtime
- `CudaKernel< EnclStmts >` – launch a CUDA kernel
- `CudaSyncThreads` – CUDA sync threads barrier (similar for OpenMP will be added)
The current list of RAJA::statement types...

- **SetShmemWindow< EnclStmts >** – set window into a shared memory buffer
- **Tile< Id, TilePolicy, ExecPolicy, EnclStmts >** – tile (or cache blocking) of an outer loop
- **Hyperplane< Id, HpExecPolicy, ArgList<...>, ExecPolicy, EnclStmts >** – hyperplane iteration over multiple indices

Other statement types will appear in RAJA as new use cases arise.
## RAJA support for complex loops

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- **Green** = available  
- **Yellow** = in progress  
- **Red** = not available
Views and Layouts
Matrices and tensors are ubiquitous in scientific computing applications

- They are expressed most naturally as multi-dimensional arrays
- For efficiency in C/C++, they are usually allocated as 1-d arrays.

```c
double* A = new double[ N * N ];
// ...
```

Recall matrix multiplication example

```c
double dot = 0.0;
for (int k = 0; k < N; ++k) {
    dot += A[k + N*row] * B[col + N*k];
}
C[col + N*row] = dot;
```

- Here, we manually convert 2-d indices (row-col) to a pointer offset
- We could also use a macro...

```c
#define A(r, c) A[c + N*r]
```

- Or...
RAJA Views and Layouts enable a variety of multi-dimensional indexing patterns

- A RAJA View enables multi-dimensional indexing into an array based on a RAJA Layout type

```cpp
double* A = new double[ N * N ];

const int DIM = 2;
RAJA::View< double, RAJA::Layout<DIM> > Aview(A, N, N);
```

- This leads to a natural indexing method

```cpp
double dot = 0.0;
for (int k = 0; k < N; ++k) {
    dot += Aview(row, k) * Bview(k, col);
}
Cview(row, col) = dot;
```
RAJA Views and Layouts support any number of dimensions

double* A = new double[ N0 * ... * Nn ];

const int DIM = n + 1;
View< double, Layout<DIM> > Aview(A, N0, ..., Nn);

// iterate over nth index and hold others fixed
for (int i = 0; i < Nn; ++i) {
  Aview(i0, i1, ..., i) = ;
}

// iterate over jth index and hold others fixed
for (int j = 0; j < Nj; ++j) {
  Aview(i0, i1, ..., j, ..., iN) = ;
}

The right-most index is stride-1 by default.
RAJA provides methods to make layouts for other indexing patterns

- **Permuted layout**

```cpp
RAJA::Layout< 3 > perm_layout =
    RAJA::make_permuted_layout( 
        {{5, 7, 11}},
        RAJA::as_array< RAJA::Perm<1, 2, 0> >::get() );
```

A 3-d layout with indices permuted:
- Index ‘0’ has extent 5 and stride 1
- Index ‘1’ has extent 7 and stride 55 (= 5 * 11)
- Index ‘2’ has extent 11 and stride 5

The “identity” permutation (e.g., RAJA::Perm<0, 1, 2>) gives a layout the same as if no permutation is used.
A RAJA permuted layout example...

const int s0 = 5;  // extent of dim 0
const int s1 = 7;  // extent of dim 1
const int s2 = 11; // extent of dim 2

double* B = new double[s0 * s1 * s2];

RAJA::Layout<3> perm_layout =
RAJA::make_permuted_layout( {{s0, s1, s2}},
   RAJA::as_array< RAJA::Perm<1, 2, 0> >::get() );

RAJA::View< double,
   RAJA::Layout<3, int, 0> > Bview(B,
   perm_layout);

// Equivalent to indexing as: B[i + j*s0*s2 + k*s0]
Bview(i, j, k) = ...;
A RAJA offset layout applies offsets to indices

```c
double* C = new double[11];

RAJA::Layout<1> off_layout =
    RAJA::make_offset_layout<1>({ {-5} }, {{5}});  

RAJA::View< double, RAJA::Layout<1> > Cview(C, off_layout);

for (int i = -5; i < 6; ++i) {
    CView(i) = ...;
}
```

Offset layouts are useful for index space subsetting operations such as halo regions.
RAJA offset layouts support permutations too

RAJA::Layout<2> offset_layout2 =
    RAJA::make_offset_layout<2>( {{-1, -5}}, {{2, 5}} );

A layout for 2-d index space [-1, 2] X [-5, 5].
Index ‘1’ (right-most) has stride 1 and index ‘0’ has stride 11.

RAJA::Layout<2> permoffset_layout2 =
    RAJA::make_offset_layout<2>( {{-1, -5}}, {{2, 5}});
    RAJA::as_array< RAJA::Perm<1, 0> >::get() );

A layout for 2-d index space [-1, 2] X [-5, 5] (same as above. But, now index ‘0’ has stride 1 and index ‘1’ has stride 4.

As before, when no permutation is given, the convention is that the right-most View index has stride-1.
RAJA layout methods can convert between multi-dimensional and linear indices

RAJA::Layout<3> layout(5, 7, 11);

A 3-d layout with extents 5, 7, 11.

// Convert i=2, j=3, k=1 to 1-dim index:
// lin = 188 (= 1 + 3 * 11 + 2 * 11 * 7)
int lin = layout(2, 3, 1);

// Convert linear index to 3d indices:
// i, j, k = {2, 3, 1}
layout.toIndices(lin, i, j, k);
RAJA layout also support “projections”

- When a dimension has **zero extent**, the linear index space is invariant in that dimension

```cpp
// 3-d layout with second dimension extent is zero
RAJA::Layout<3> layout(3, 0, 5);

// The second (j) index is projected out
int lin1 = layout(0, 10, 0); // lin1 = 0
int lin2 = layout(0, 5, 1);  // lin2 = 1

// The inverse mapping always produces a 0 for j
int i, j, k;
layout.toIndices(lin2, i, j, k); // i,j,k = {0, 0, 1}
```
Application considerations
RAJA is motivated by constraints of large, production, multi-physics applications

- **Large code bases**
  - O(100K) – O(1M) SLOC and many numerical kernels (O10K)

- **Platform diversity**
  - Codes run on laptops, commodity clusters, advanced technology systems
  - ASC program procures large commodity and advanced technology systems in 3-5 year cycles

- **Long service lives**
  - Codes used in production daily for decades – must be viable over several platform generations

- **Continual development**
  - New modeling capabilities added to codes throughout their lifetimes
  - Adopting new technologies (h/w & s/w) cannot disrupt users
RAJA design emphasizes usability and developer productivity

- **Single-source kernels** (no platform-specific variants if possible)
- **Easy to grasp** for (non-CS) application developers
- Allows for **incremental and selective** adoption
- Provides necessary **features not found in other models**
- **Doesn’t force major disruption** to application algorithm patterns or data structures
  - Loop bodies are unchanged in most cases
  - Works with existing code constructs
  - Allows application-specific customizations

Application developers typically wrap RAJA in a layer to match their code’s style.
RAJA promotes flexibility via type parameterization

- Define **type aliases in header files**
  - Easy to explore implementation choices in a large code base
  - Reduce source code disruption
RAJA promotes flexibility and tuning via type parameterization

- Define **type aliases in header files**
  - Easy to explore implementation choices in a large code base
  - Reduces source code disruption

- Assign execution policies to “**loop classes**”
  - Easier to search execution policy parameter space

```cpp
using ELEM_LOOP_POLICY = ...; // in header file
RAJA::forall<ELEM_LOOP_POLICY>( /* do elem stuff */ );
```

Application developers must determine the appropriate “loop taxonomy” and policy selection for their code.
“Bring your own” memory management

- RAJA does not provide a memory model (by design)
  - Users must manage memory space allocations and transfers

```cpp
RAJA::forall<RAJA::cuda_exec>(range, [=] __device__ (int i) {
    a[i] = b[i];
});
```

Are ‘a’ and ‘b’ accessible on GPU?
“Bring your own” memory management

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    a[i] = b[i];
});
```

- Some possibilities:
  - **Manual** – use `cudaMalloc()` , `cudaMemcpy()` to allocate, copy to/from device
  - **Unified Memory (UM)** – use `cudaMallocManaged()` , paging on demand
  - **CHAI** ([github.com/llnl/chai](https://github.com/llnl/chai)) – automatic copies as needed

Are ‘a’ and ‘b’ accessible on GPU?

CHAI was developed to complement to RAJA.
CHAI provides array abstractions for transparent, automatic data copies

```cpp
// CPU memory
chai::ManagedArray<int> a...;
chai::ManagedArray<const int> b...;

// GPU memory

RAJA::forall<RAJA::cuda_exec>(range,
    [=] __device__ (int i) {
        a[i] = b[i];
    } );

RAJA::forall<RAJA::seq>(range,
    [=] (int i) {
        printf("%d, %d \n", a[i], b[i]);
    } );
```
CHAI provides array abstractions for transparent, automatic data copies

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chai::ManagedArray<const int> b...;

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    });
```

CHAI supports UM too, so you can assess its performance.
C++ lambda usage requires care

- Capture by-value or by-reference (\([=]\) vs. \([&]\))?
  - Value capture is required for GPU execution and when using RAJA reductions, when using CHAI, ...
C++ lambda usage requires care

- Capture by-value or by-reference ( \([=]\) vs. \([&]\) )?
  - **Value capture is required** for GPU execution, when using RAJA reductions, when using CHAI, ...

- You **cannot** use ‘break’ or ‘continue’ statements in a lambda
C++ lambda usage requires care

- **Issue**: global variables aren’t captured (C++ standard):
  ```cpp
  extern double global_var;
  RAJA::forall<RAJA::cuda_exec>(range, [=] (int i) {
      a[i] += global_var;
  });
  ```

- **Solution**: make a local reference:
  ```cpp
  double& ref_to_global_var = global_var;
  RAJA::forall<RAJA::cuda_exec>(range, [=] (int i) {
      a[i] += ref_to_global_var;
  });
  ```

For CPU code, you get lucky (maybe).
C++ lambda usage requires care

- Issue: local stack arrays aren’t captured for CUDA device code (nvcc compilation error):

```cpp
int[4] bounds = { 0, 1, 8, 9};

RAJA::forall<RAJA::cuda_exec>(range, [=] __device__ (int i) {
    for (int bound = 0; bound < 4; bound++) {
        my_bound = bounds[bound];
    }
});
```
C++ lambda usage requires care

- Solution: wrap the array in a struct:

```cpp
struct array_wrapper {
    int[4] array;
} bounds;

bounds.array = { 0, 1, 8, 9};

RAJA::forall<RAJA::cuda_exec>(range, [=] __device__ (int i) {
    for (int bound = 0; bound < 4; bound++) {
        my_bound = bounds.array[bound];
    }
});
```
CUDA device lambdas need annotations

- A lambda passed to a CUDA device function must have the "__device__" decoration
  - e.g., when using RAJA CUDA execution policies

- A lambda can also be marked "__host__ __device__"

- Beware of using a "__host__ __device__" lambda in host code
  - The CPU code will be much slower than if you use an undecorated lambda

RAJA provides macros to help with this.
RAJA (like other similar approaches) is an enabling technology – not a panacea

— Loop characterization and performance tuning are manual processes
  • Good tools are essential...

— Memory motion is critical. Pay attention to it!
Performance portability takes effort

- Application **coding styles may need to change** regardless of programming model (e.g., GPU execution)
  - Change algorithms to ensure correct parallel execution
  - Recast some patterns as reductions, scans, etc.
  - Move variable declarations to innermost scope to avoid threading issues
  - Virtual functions and C++ STL are problematic for GPU execution

Simpler is almost always better — use simple types and arrays.
RAJA features are supported for a variety of programming model back-ends

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- **Green** = available
- **Yellow** = in progress
- **Red** = not available
Supplemental materials to this tutorial are available online

- Complete working example codes are available in the RAJA source repository
  - [https://github.com/LLNL/RAJA](https://github.com/LLNL/RAJA)
  - Many similar to the examples we presented today
  - After cloning the repo (instructions on GitHub), look in the “RAJA/examples” directory

- The RAJA User Guide provides more details
  - Topics we discussed today, configuring & building RAJA, etc.
  - Available online: [http://raja.readthedocs.org/projects/raja](http://raja.readthedocs.org/projects/raja)
    (also linked on the RAJA GitHub project)
Related software is available

- The RAJA Proxy App Suite
  - RAJA versions of some important HPC proxies (more in the works)
  - [https://github.com/LLNL/RAJAProxies](https://github.com/LLNL/RAJAProxies)

- The RAJA Performance Suite
  - Algorithm kernels in RAJA and baseline (non-RAJA) forms
  - Sequential, OpenMP (CPU), OpenMP target, CUDA variants
  - We use it to monitor RAJA performance and assess compilers
  - Essential for our interactions with vendors
  - Benchmark for CORAL and CORAL-2 systems
  - [https://github.com/LLNL/RAJAPerf](https://github.com/LLNL/RAJAPerf)
Related software is available

- **CHAI**
  - Provides automatic data copies to different memory spaces behind an array-style interface
  - Designed to work with RAJA
  - Could be used with other lambda-based C++ abstractions
  - [https://github.com/LLNL/CHAI](https://github.com/LLNL/CHAI)

Wrap up
Again, we would appreciate your feedback...

- If you have comments, questions, suggestions, etc., please talk to one of us at the hands-on session

- You are welcome to join our Google Group: https://groups.google.com/forum/#!forum/raja-users

- Or contact us via email: raja-dev@llnl.gov
Thank you for your attention and participation

Questions?
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