Modern C++ in Computational Science

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bit.ly/cpp-siamcse2019

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  - The ability to hire "commodity" developers
- Critically, though, we lose much of this if we do not keep our codebases up to date with modern C++ patterns, features, and idioms.

Disclaimer

There are a ton of things happening on the C++ committee that both directly and indirectly benefit computational science and HPC. (There are a ton of things happening in general—our 2018-10 mailing was larger than the entire works of Shakespeare.) Many of the "big ticket" items have *enormous* implications for HPC, but we will not be talking about them here. Many other small things other people are doing on the committee also have a big impact on HPC, and we don't want to diminish their contributions, but it's our talk and we're going to talk about the stuff we worked on

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  - Networking
  - Reflection
  - Executors

`std::mdspan`

`std::mdspan`: Multidimensional Arrays in C++

ISO-C++ PROPOSAL

P0009
http://wg21.link/P0009r9

```
template <typename T, int I, int J, int K>
void three_loop_gemm(
  std::mdspan<T, I, K> a, std::mdspan<T, K, J> b, std::mdspan<T, I, J> result
)
{
  assert(a.extent(1) == b.extent(0));
  assert(a.extent(0) == result.extent(0));
  assert(b.extent(1) == result.extent(1));
  for(int i = 0; i < a.extent(0); ++i) {
    for(int j = 0; j < b.extent(1); ++j) {
      for(int k = 0; k < a.extent(1); ++k) {
        result(i, j) += a(i, k) * b(k, j);
      }
    }
  }
}
```

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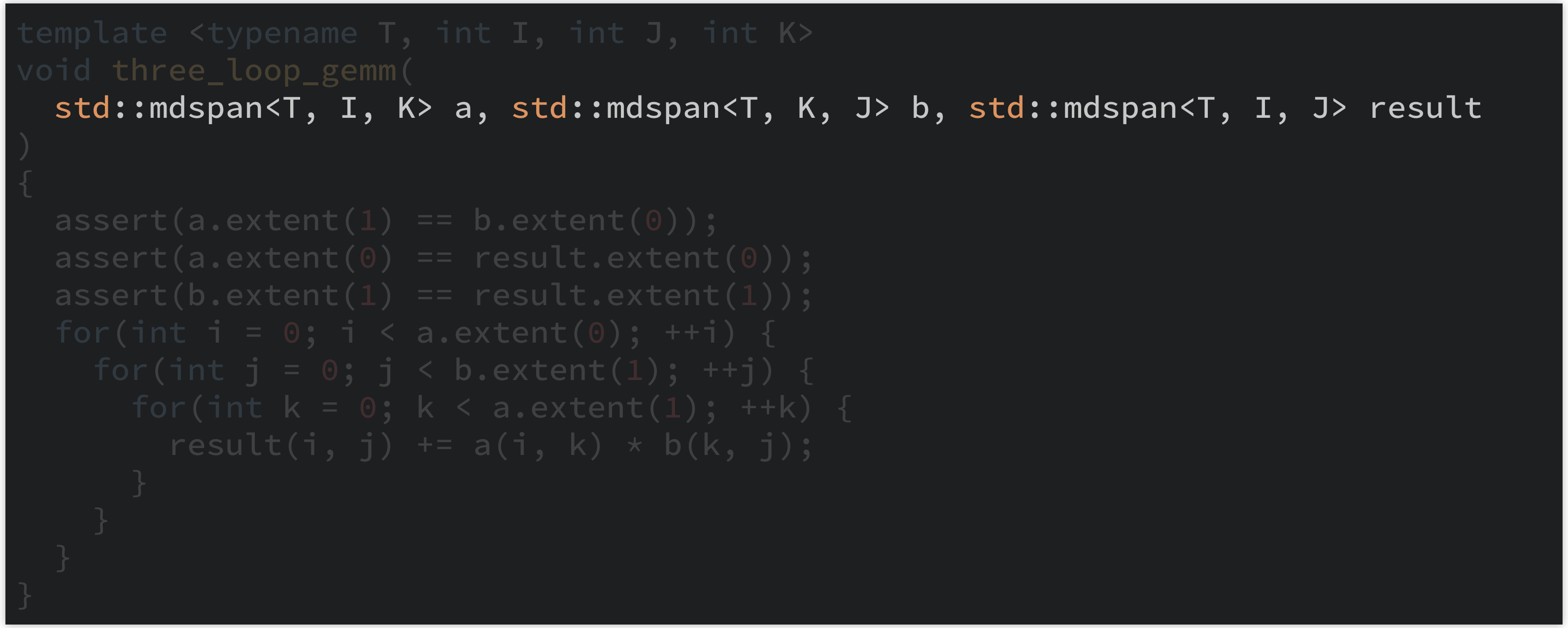

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      }
    }
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```

`std::mdspan<T, I, K>` is a multidimensional view with extents `I` and `K` (both of which can be runtime-sized, using `std::dynamic_extent`)

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These assertions can be evaluated at compile time if the extents `I`, `J`, and `K` are static sizes

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}
```

Indexing uses the call operator for now.
(Work is in progress to also use the subscript operator `[]`, see https://wg21.link/p1161r2)

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std::mdspan Does Much More…

- mdspan is just an alias for basic_mdspan (just like string is an alias for basic_string):

```
template<class T, ptrdiff_t... Extents>
   using mdspan = basic_mdspan<T, extents<Extents...>>;
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ElementType is the element data type

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`Extents` is an instance of a template `std::extents<...>` that contains the shape information.

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`LayoutPolicy` is a customization point that lets you control how multi-indices are translated into memory offsets.

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`AccessorPolicy` is a customization point that lets you control how memory offsets are translated into values, references, and pointers.

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  - compressed layouts (with the help of an `AccessorPolicy`)

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  - Access data atomically (using P0019, `atomic_ref`!)

std::atomic_ref

Atomic Operations on Non-Atomic Memory

ISO-C++ PROPOSAL

P0019 http://wg21.link/P0019

```
std::vector<double> my_data;
/* ... */
// Before:
atomic_fetch_add(&my_data[i], 5.0);
// After:
auto a = atomic_ref{my_data[i]};
a += 5.0;
```

Atomic Operations on Non-Atomic Memory

```
template <class T>
void my_function(std::vector<T>& my_data, T value) {
  /* ... */
  // Before:
  ????????
  // After:
  auto a = atomic_ref{my_data[i]};
  a += value;
}
```

Executors

Executors: A Generic Abstraction for Execution

ISO-C++ Proposal

P0443:
https://wg21.link/p0443r10

(and many more…)

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ISO-C++ PROPOSAL

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ISO-C++ PROPOSAL

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- One of the most ambitious generic programming exercises ISO-C++ has ever undertaken
- Provides a generic abstraction for the execution model in the presence of a restricted programming model

Executor Example

```
template <class DataContainer>
DataContainer my_algorithm(DataContainer& data) {
  apply_transformation(data);
  DataContainer result = allocate_result_container_for(data);
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  auto data = get_neighbor_info(network_executor);
  // if it's large enough, put it on the GPU
  if(data.size() > THRESHOLD) {
    auto gpu_executor = get_nearest_gpu_executor(network_executor);
    auto gpu_data = migrate_data(std::move(data), network_executor, gpu_executor);
    auto gpu_result = my_algorithm(gpu_executor, gpu_data);
    auto result = migrate_data(std::move(gpu_result), gpu_executor, network_executor);
    return result;
  }
  else {
    // Otherwise, do it in place
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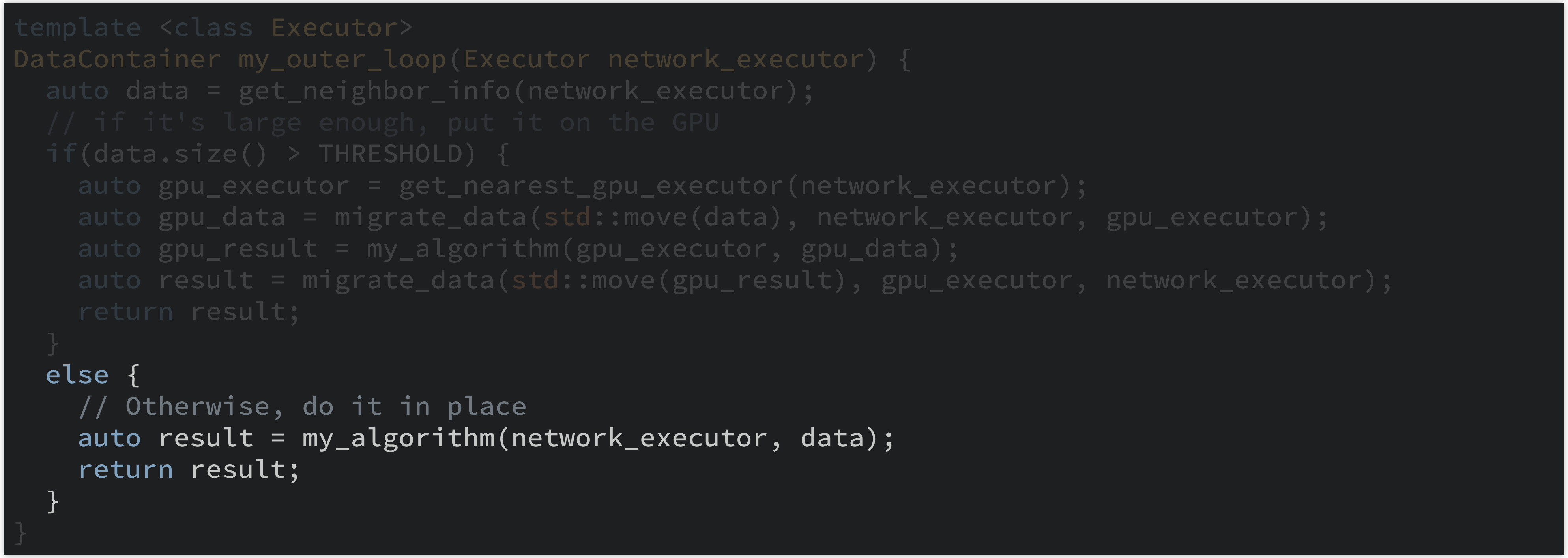

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    return result;
  }
  else {
    // Otherwise, do it in place
    auto result = my_algorithm(network_executor, data);
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}
```

Executor Example

```
template <class Executor>
DataContainer my_outer_loop(Executor network_executor) {
  auto data = get_neighbor_info(network_executor);
  // if it's large enough, put it on the GPU
  if(data.size() > THRESHOLD) {
    auto gpu_executor = get_nearest_gpu_executor(network_executor);
    auto gpu_data = migrate_data(std::move(data), network_executor, gpu_executor);
    auto gpu_result = my_algorithm(gpu_executor, gpu_data);
    auto result = migrate_data(std::move(gpu_result), gpu_executor, network_executor);
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But this isn't very generic...

Executor Example

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Executor Example

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template <class Executor>
DataContainer my_outer_loop(Executor network_executor) {
  auto data = get_neighbor_info(network_executor);
  // if it's large enough, put it on the GPU
  auto gpu_executor = get_nearest_gpu_executor(network_executor);
  auto threshold = std::query(gpu_executor, transfer_threshold(data, network_executor));
  if(data.size() > threshold) {
    auto gpu_data = migrate_data(std::move(data), network_executor, gpu_executor);
    auto gpu_result = my_algorithm(gpu_executor, gpu_data);
    auto result = migrate_data(std::move(gpu_result), gpu_executor, network_executor);
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Solution: Put the customization on the executor!

Executor Example

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DataContainer my_outer_loop(Executor network_executor) {
  auto data = get_neighbor_info(network_executor);
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Executor Example

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template <class Executor>
DataContainer my_outer_loop(Executor network_executor) {
  auto data = get_neighbor_info(network_executor);
  // if it's large enough, put it on the GPU
  auto gpu_executor = get_nearest_gpu_executor(network_executor);
  auto cost_model = std::query(my_algorithm, cost_model(network_executor, gpu_executor));
  auto should_transfer = std::query(cost_model, transfer_recommendation(data));
  if(should_transfer) {
    auto gpu_data = migrate_data(std::move(data), network_executor, gpu_executor);
    auto gpu_result = my_algorithm(gpu_executor, gpu_data);
    auto result = migrate_data(std::move(gpu_result), gpu_executor, network_executor);
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Even better: ask the algorithm!

Executor Example

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DataContainer my_outer_loop(Executor network_executor) {
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}
```

Executor Example

What happens if I have a network-capable GPU direct executor?

```
void my_program() {
  auto gpu_direct_executor = /*...*/;
  // ...
  for(auto iter : my_iterations) {
    // ...
    auto result = my_outer_loop(gpu_direct_executor);
    // ...
  }
}
```

Executor Example

What happens if I have a network-capable GPU direct executor?

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void my_program() {
  auto gpu_direct_executor = /*...*/;
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Executor Example

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  auto gpu_direct_executor = /*...*/;
  // ...
  for(auto iter : my_iterations) {
    // ...
    auto result = my_outer_loop(gpu_direct_executor);
    // ...
  }
}
```

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- Use algorithms, not loops
- Write to the most restricted programming model you can
- Use Kokkos (or something similar that is tracking standards for you)

Questions?