Exploiting Modern C++ for Portable Parallel Programming in Lattice QCD Applications

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Plan

- C++17 std::par algorithms
- Hierarchy of views in C++20/C++23
- A few notes on accelerator programming:
  - Utilizing C++23 cartesian products for the execution domain
  - C++17 Polymorphic Memory Resources (PMR) for memory buffer management
- Staggered stencil example
- Backup slides: C++20 Concepts
The quintessence of the C++ heterogeneous programming is the standard library algorithms, common programming patterns that can be used as building blocks for solving more complex problems.

- They are provided by `<algorithm>` header
- Most of the algorithms from std library operate only on *iterators*, and not on the *containers*, the feature that makes them truly generic constructions
The standard library algorithms

Examples of SL algorithms:

Iteration and transform:
std::for_each, std::for_each_n, std::transform,
std::transform_inclusive/exclusive_scan,
std::transform_reduce

Reduction:
std::reduce, std::transform_reduce
std::inclusive/exclusive_scan,
std::count, std::count_if,

Searching:
std::search, std::search_n,
std::find, std::find_if/if_not,
std::find_end, std::find_first_of

Memory management:
std::copy, std::copy_n, std::copy_if,
std::move, std::fill, std::fill_n,
std::generate, std::generate_n

Removing and replacing elements:
std::remove, std::remove_if,
std::replace, std::replace_if,
std::unique, std::unique_copy,

Reordering elements:
std::sort, std::stable_sort,
std::partition, std::stable_partition,
std::merge, std::inplace_merge
C++17 std::execution::par

- C++17 introduced higher-level parallelism features that allow to request parallelization of (most) SL algos
- C++17 offers the execution policy parameter that is available for these algos:
  - `std::execution::seq` to execute an algo sequential
  - `std::execution::par` to execute an algo in parallel
  - `std::execution::unseq` to execute an algo with vector instructions
  - `std::execution::par_unseq` to execute an algo in parallel with vector instructions
The iterator-based algo (example)

Evolution of the for loop:

```cpp
#include <algorithm>
#include <execution>
#include <ranges>

std::vector<float> x(N), y(N);

auto l = std::ranges::views::iota(0, N);

std::for_each(std::execution::par,
              std::ranges::begin(l),
              std::ranges::end(l),
              [x_ptr = x.data(), y_ptr = y.data()](const int& i){
                //do something with x_ptr and y_ptr
              });
```
nvc++ uses UVM for automatic CPU-GPU data transfers
only data dynamically allocated in CPU code compiled by nvc++ can be auto-managed.
memory allocated in compute kernels is GPU-exclusive and unmanaged.
CPU and GPU stack memory and global objects can’t be auto-managed.
data allocated outside nvc++-compiled units, even on CPU heap, isn’t managed.
pointers and objects within std::par algo invocations must refer to managed CPU heap data.
dereferencing CPU stack pointers or global objects in GPU code leads to memory violations.
The iterator-based algo (example)

Evolution of the for loop:

```cpp
#include <algorithm>
#include <execution>
#include <ranges>

std::vector<float> x(N), y(N);

auto l = std::ranges::views::iota(0, N);

std::for_each(std::execution::par,
               std::ranges::begin(l),
               std::ranges::end(l),
               [&x = x, &y = y](const int& i){
               //Illegal memory access!
               });
```
The iterator-based algo (example)

Evolution of the for loop:

```cpp
#include <algorithm>
#include <execution>
#include <ranges>
#include <span>

std::vector<float> x(N), y(N);

auto l = std::ranges::views::iota(0, N);

std::for_each(std::execution::par,
               std::ranges::begin(l),
               std::ranges::end(l),
               [x_view = std::span{x}, y_view = std::span{y}](const int& i){
               //Okay, do something x_view, y_view
               });
```
**std::span:**

- is a lightweight, non-owning reference to a contiguous sequence, or a span, of objects of a given type `T` in memory.
- is only a view into a sequence: it does not control the lifetime of the objects it refers to, nor does it allocate or deallocate memory.

```cpp
//Defined in header <span>
template<
    class T,
    std::size_t Extent = std::dynamic_extent
> class span;
```
std::span::subspan:

- creates a std::span that only refers to a portion of the elements of the original std::span, specified by starting index and length

//Defined in header <span>
constexpr std::span<element_type, std::dynamic_extent>
subspan( size_type Offset,
    size_type Count = std::dynamic_extent ) const;
Field class with views:

```cpp
template <GenericContainerTp container_tp, typename Arg>
class Field{
    private:
        const Arg arg; // copy of the arguments

        container_tp v; // could be std::vector, std::span (or subspan)

    public:

        decltype(auto) View() {
            // ...
            return Field(std::span{v}, arg);
        }

        decltype(auto) ParityView(const FieldParity parity) {
            // define parity args etc...
            return Field(std::span{v}.subspan(parity_offset, parity_length), parity_arg);
        }
};
```

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std::mdspan:

- is a non-owning view into a contiguous sequence of objects that reinterprets it as a multidimensional array
- (accepted) proposal can be found https://www.open-std.org/jtc1/sc22/wg21/docs/papers/2022/p0009r18.html
- the reference implementation is due to Kokkos dev team https://github.com/kokkos/mdspan

//Defined in header <mdspan>

```cpp
template<
    class T,
    class Extents,
    class LayoutPolicy = std::layout_right,
    class AccessorPolicy = std::default_accessor<T>
>
class mdspan;
```
Fine-grained accessors:

```cpp
template<bool is_constant, size_t... dofs>
inline decltype(auto) mdaccessor(const std::array<size_t, (Ndim + sizeof...(dofs))>& strides) const {

    using dext = stdex::dynamic_extent;

    using Map = stdex::layout_stride::mapping<stdex::extents<size_t, dext, dext, dext, dext, dofs...>>;

    using Extents= stdex::extents<size_t, dext, dext, dext, dext, dofs...>;

    if constexpr(is_constant){
        return stdex::mdspan<
            const data_tp, Extents, stdex::layout_stride>{
            v.data(), Map{Extents{X[0], X[1], X[2], X[3]}, strides}} ;
    }
}

template<bool is_constant> auto Accessor() const {
    if constexpr(Arg::type == FieldType::VectorFieldType) {
        if constexpr(nParity == 2) {
            return mdaccessor<is_constant, nColor, nColor, nDir, nParity>(strides);
        }
    }
}
```
std::ranges::ref_view:

- is a view of the elements of some other range
- wraps a reference to that range

std::ranges::reverse_view:

- represents a view of underlying sequence with reversed order.

```cpp
#include <ranges>

std::array<int, N> x{0,1,2,3};

std::ranges::ref_view y{x}; // y=(0,1,2,3)

std::ranges::reverse_view z{x}; // z=(3,2,1,0)
```
Example 3

Stencil computing with views:

```cpp
void apply(SpinorView auto &out, const SpinorView auto &in, const auto idx, const Parity p) {

    std::array X = convert_coords(idx);
    //
    std::ranges::ref_view X_view{X};
    // or
    //auto X_view = X | std::views::all;

    auto out = FieldAccessor{out};
    const auto in = FieldAccessor<is_constant>{in};
    //
    auto res = compute_stencil(in, parity, X_view);

    #pragma unroll
    for (int c = 0; c < Ncolor; c++){
        out(X_view,c) = res(c);
    }
}
```

C++23 cartesian product

- `std::view::cartesian_product`:
  - is a range adaptor that produces a view of tuples calculated by the n-ary cartesian product of the provided ranges
  - proposal can be found https://www.open-std.org/jtc1/sc22/wg21/docs/papers/2022/p2374r4.html

```cpp
//Defined in header <cartesian_product.hpp>
auto X = std::views::iota(0, Nx);
auto Y = std::views::iota(0, Ny);
auto Z = std::views::iota(0, Nz);
auto T = std::views::iota(0, Nt);

//T is the slowest index, X is the fastest
auto ids = std::views::cartesian_product(T, Z, Y, X);
```
Example 4

Kernel launcher:

```cpp
void launch(SpinorView auto &o, const SpinorView auto &i, const FieldParity p, const auto &idx) {
    //...
    std::for_each(std::execution::par_unseq,
                  ids.begin(),
                  ids.end(),
                  DslashKernel);
}

void operator()(Spinor auto &o, const Spinor auto &i, const FieldParity p) {
    using spinor_tp = typename std::remove_cvref_t<decltype(i)>;
    using container_tp = spinor_tp::container_tp;
    //Setup exe domain
    const auto [Nx, Ny, Nz, Nt] = o.GetCBDims(); //Get CB dimensions

    auto X = std::views::iota(0, Nx);
    //...
    auto T = std::views::iota(0, Nt);

    auto idx = std::views::cartesian_product(T, Z, Y, X);

    if constexpr (is_allocator_aware_type<container_tp>) {
        auto&& o_view = o.View();
        const auto&& i_view = i.View();

        launch(o_view, i_view, p, idx);
    }
}
```
C++17 PMR provided a "polymorphic" interface to memory management:

- allow you to allocate memory in a way that is independent of the underlying allocator
- useful for applications that need to control how memory is allocated, or need to be able to run on multiple platforms with different allocators
- includes polymorphic allocator-aware versions of several SL containers, e.g.,
  ```
  std::pmr::vector, std::pmr::string, and std::pmr::unordered_map
  ```
When is it useful?

▶ Performance improvement
  - can reduce allocation overhead and improve cache utilization

▶ Memory usage control
  - has more control over how memory is allocated (deallocated).

▶ Memory tracking and debugging
  - can be used to implement custom memory resources that track memory usage for debugging

▶ Custom memory pools
  - allows the creation of memory pools with specific allocation strategies, which can be useful for cases where one has objects of the same size being frequently created (destroyed), i.e., can help reduce fragmentation and the overhead of frequent allocations.
Memory resources:

- `std::pmr::memory_resource`  
  - the base class for all memory resources in the PMR library.

- `std::pmr::monotonic_buffer_resource`  
  - a memory resource that allocates memory from a single buffer

- `std::pmr::unsynchronized_pool_resource`  
  - a memory resource that allocates memory from a pool of pre-allocated blocks

- `std::pmr::synchronized_pool_resource`  
  - same as above but with synchronization for concurrent access.
Example 5

PMR in action:

```cpp
#include <memory_resource>

// ptr is a pre-allocated memory pool
// bytes = 2*N*sizeof(float);

std::pmr::monotonic_buffer_resource pmr_buff(ptr, bytes);

std::pmr::vector<float> x(N, &pmr_buff); // populate N*sizeof(float) bytes
std::pmr::vector<float> y(N, &pmr_buff); // populate next N*sizeof(float) bytes

auto l = std::ranges::views::iota(0, N);

std::for_each(std::execution::par,
               std::ranges::begin(l),
               std::ranges::end(l),
               [x_view = std::span{x}, y_view = std::span{y}](const int& i){
                 // Okay, do something x_view, y_view
               });
```
Example 5

PMR in action (allocation in stack):

```
#include <memory_resource>

std::array<std::bytes, 2*N> stack_buff;

std::pmr::monotonic_buffer_resource pmr_buff(stack_buff.data(), stack_buff.size(),
                                           std::pmr::null_memory_resource());

std::pmr::vector<float> x(N, &pmr_buff); // populate N*sizeof(float) bytes
std::pmr::vector<float> y(N, &pmr_buff); // populate next N*sizeof(float) bytes
```
PMR in action:

```cpp
std::pmr::vector<float> x(N, &pmr_buff); // populate N*sizeof(float) bytes
std::pmr::vector<float> y(N, &pmr_buff); // populate next N*sizeof(float) bytes

// ... do something with x, y
x.resize(0); // destroy x container
y.resize(0); // destroy y container

// reset pmr buffer:
pmr_buff.release();

// now create new containers:
std::pmr::vector<float> u(N, &pmr_buff); // populate N*sizeof(float) bytes
std::pmr::vector<float> v(N, &pmr_buff); // populate next N*sizeof(float) bytes
```
C++17 Polymorphic Memory Resource

Caveat:

- C++ standard requires that any (allocator-aware) container must be initialized

Possible solution:

- create a custom container with a given initialization pattern (e.g., target specific)
Example 6

Custom pmr container:

```cpp
namespace impl {
    namespace pmr {
        template <typename T>
        class vector {
            public:
                using allocator_type = std::pmr::polymorphic_allocator<T>;
                using value_type = typename std::allocator_traits<allocator_type>::value_type;
                using size_type = typename std::allocator_traits<allocator_type>::size_type;
            ...
            private:
                pointer data_;  
                size_type size_;  
                allocator_type alloc_;  
            ...
        }
    }
}
} // end of impl
```
Custom pmr container (cont.):

```cpp
namespace impl {
    namespace pmr {
        template <typename T>
        class vector {
        public:

            explicit vector(size_type n, std::pmr::memory_resource* mr) : data_(nullptr),
                size_(n),
                alloc_(mr) {

                data_ = alloc_.allocate(n);
                //
                if (init_pmr_space == TargetMemorySpace::Device) {
                    std::fill(std::execution::par_unseq,
                        this->begin(),
                        this->end(),
                        zero_);
                }
```
Container Zoo:

```cpp
std::vector<float> x(N);
std::pmr::vector<float> y(N, &pmr_buff);
impl::pmr::vector<float> z(N, &pmr_buff);

static_assert( std::is_same_v<decltype(x), decltype(y)> == false);
static_assert( std::is_same_v<decltype(x), decltype(z)> == false);
static_assert( std::is_same_v<decltype(y), decltype(z)> == false);

auto u = std::span{x};
auto v = std::span{y};
auto w = std::span{z};

static_assert( std::is_same_v<decltype(v), decltype(u)> == true);
static_assert( std::is_same_v<decltype(v), decltype(w)> == true);
static_assert( std::is_same_v<decltype(u), decltype(w)> == true);
```
Stencil tests (WIP)

Platform:

- nvc++ compiler ver 23.5
- NVIDIA A100 node
- link: https://github.com/alexstrel/dataparallel-lqft-cpp2x

2d Schwinger model stencil (2048 x 2048):

- init launch: 0.022sec.
- pmr buffer reuse: 0.002sec.
- msrc init launch (N = 8): 0.15sec.
- msrc pmr buffer reuse (N = 8): 0.019sec.

4d staggered stencil (L = 16, T = 16):

- init launch: 0.0011sec.
- pmr buffer reuse: 0.0005sec.
Conclusion

- `std::execution::par`:
  - express parallel algorithm with standard language
  - plain C++ code
  - memory operation via UVM

- limitations:
  - does not specify launch parameters
  - no async versions

- beyond C++20:
  - range-based parallel algos
  - support for async. execution (sender/receiver)
Beyond C++20

- nvc++ experimental features (require `--experimental-stdpar` flag)

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| Multi-dimensional spans (mdspan) | C++23       | C++17           | P0009             | https://github.com/NVIDIA/libcuda /
|                                |             |                 |                   | xx                                |
|                                |             |                 |                   | xx                                |
| Multi-dimensional arrays (mdarray) | C++23       | C++17           | P1684             | https://github.com/kokkos/mdspan  |
| Senders and receivers          | C++23       | C++20           | P2300             | https://github.com/NVIDIA/stdexec |
| Linear algebra                 | C++23       | C++17           | P1673             | https://github.com/kokkos/stdlibas |
C++20 concepts

- allow to specify constraints on template arguments at *compile* time
- can be used to select the most appropriate function overloads and template specializations
- (a lot of) built-in concepts defined in the `<concepts>` header (e.g. `std::copy_constructible`, `std::destructorible` etc.)

```cpp
template <typename T>
class Complex = std::is_floating_point_v<typename T::value_type>
and requires {
    { std::declval<T>().real() } -> std::convertible_to<typename T::value_type>;
    { std::declval<T>().imag() } -> std::convertible_to<typename T::value_type>;
};

//
decltype(auto) foo(const auto x, auto y) { /*do something*/ }
// same as above but now restricted to complex floating point
decltype(auto) foo(const Complex auto x, Complex auto y) { /*do something*/ }
```
```cpp
template <typename T>
concept GenericContainer = requires{
    typename T::value_type;
    typename T::size_type;
    typename T::iterator;

    { std::declval<T>().data() } -> std::same_as<typename T::value_type*>;
    { std::declval<T>().size() } -> std::same_as<typename T::size_type >;
    //
    { std::declval<T>().begin() } -> std::convertible_to<typename T::iterator>;
    { std::declval<T>().end() } -> std::convertible_to<typename T::iterator>;
};

template <typename T>
concept GenericSpinorField = requires{
    // here container_tp stands for std::vector<>, std::span<> or std::subspan<>
    requires GenericContainer<typename T::container_tp>;

    requires (T::Nspin() == 1ul or T::Nspin() == 4ul);
    requires (T::Ncolor() == 3ul);
};
```