C++ Best Practices 101: A miniQMC Case Study

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Best Practices

• Generally accepted as superior alternative
  • Easier to reason about
  • Fewer bugs
• Reasonable people can disagree
• Need justification when doing something different
  • If done often, update Best Practices
Resource Acquisition Is Initialization

RAII
Resource Acquisition Is Initialization (RAII)

```cpp
int main(int argc, char** argv)
{
    int error_code=0;
    Kokkos::initialize(argc, argv);
    //Begin kokkos block
    //...
    //end kokkos block
    Kokkos::finalize();
    return error_code;
}
```

```cpp
int main(int argc, char** argv)
{
    int error_code=0;
    //Begin kokkos block
    Kokkos::ScopeGuard _(argc, argv);
    //...
    //end kokkos block
    return error_code;
}
```
Resource Acquisition Is Initialization (RAII)

- Constructor does initialization
- Destructor does finalization
  - Language guarantees destructor is called on scope exit
- Useful as guards or members
Resource Acquisition Is Initialization (RAII)

```c
int main(int argc, char** argv) {
    int error_code=0;
    Kokkos::initialize(argc, argv);
    //Begin kokkos block
    //...
    //end kokkos block
    Kokkos::finalize();
    return error_code;
}
```

- **Guard**
  - Not concerned how the block is exited (early return, exception, etc.)
  - termination functions `abort`, `exit`, `_Exit`, `quick_exit`, `terminate` notwithstanding
Resource Acquisition Is Initialization (RAII)

• Best Practice
  • Use whenever a set of operations has to be paired up
  • Write your own if not provided
    • One class - one responsibility
Smart Pointers

unique_ptr, shared_ptr


struct Mover
{
  // ... 

  /// single particle orbitals
  SPOSet* spo;
  std::unique_ptr<SPOSet> spo;

  // ...

  /// destructor
  ~Mover()
  {
    if (spo != nullptr)
      delete spo;
  }
};
Smart Pointers

- Manage heap allocation
- Use RAII
  - Constructor takes ownership of a heap allocated object/array
  - Does not perform the allocation itself
  - Use `make_smart` to replace raw `new`
Heap Allocations

• Why allocate on the heap in C++?
  • The size cannot be determined at compile time
    • Exact type not known until run time (e.g. polymorphism)
    • Variable length arrays, containers, etc.
    • Degenerate cases: object too large for stack, static space, etc.
  • The lifetime does not fit within a scope {}
  • Move semantics for immovable objects
    • `atomic<int> Alpha() { return atomic<int>(0); }`
    • `unique_ptr<atomic<int>> Alpha() { return unique_ptr(new atomic<int>(0)); }`
Heap Allocations

• Why allocate on the heap in C++17?
  • The size cannot be determined at compile time
    • Exact type not known until run time (e.g. polymorphism)
      • Consider `std::variant` for a bounded set of types
    • Variable length arrays
  • The lifetime may be longer than a scope `{}`
    • Use `std::optional` for lifetimes shorter than a scope
  • Move semantics for immovable objects
    • Mandatory RVO (Return Value Optimization) eliminates some of that need

```cpp
atomic<int> Alpha() { return atomic<int>(0); } 
unique_ptr<atomic<int>> Alpha() { return unique_ptr(new atomic<int>(0)); } 
```
unique_ptr
unique_ptr

- Unique (single) ownership
- Moveable but not copyable
  - Aggregates of `unique_ptr` by default moveable but not copyable
- By default `unique_ptr` destructor destroys held object
  - Calls `~T()`
- Returns space to the heap
unique_ptr

```cpp
struct Mover
{
    // ...

    /// single particle orbitals
    SPOSet* spo;
    std::unique_ptr<SPOSet> spo;

    // ...

    /// destructor
    ~Mover()
    {
        if (spo != nullptr)
            delete spo;
    }
};
```

- Mover aggregates (has as a member) unique_ptr<SPOSet>
- Hand written destructor eliminated
- Decremental development (Kevlin Henney)
RAII

• Best Practice

  • Most classes should not have an explicit (non-defaulted) destructor

    • \(~T() = \texttt{default};\)

      • virtual

      • Visibility (from \texttt{public} to \texttt{protected} or \texttt{private})

      • Non-inlined (in .cpp file)

      • Rule of 5

    • Those that do should be managing a single resource via RAII
Rule of 5 / 3 / 0
Rule of 3

• C++98

• If you declare any of these you should declare all of these

```cpp
struct Alpha
{
    Alpha(Alpha const&); // Copy constructor
    Alpha& operator=(Alpha const&); // Copy assignment operator

    ~Alpha(); // Destructor
};
```

• Compiler will implicitly declare versions of these special member functions if you do not
Rule of 5

• C++11

• If you declare any of these you should declare all of these

```cpp
struct Alpha {
    Alpha(Alpha const&); // Copy constructor
    Alpha& operator=(Alpha const&); // Copy assignment operator
    Alpha& operator=(Alpha&&); // Move assignment operator
    Alpha(Alpha&&); // Move constructor
    ~Alpha(); // Destructor
};
```

• Compiler will *not necessarily* implicitly declare versions of these special member functions if you do not
Implicitly Declared C++98

• Copy constructor \( T(T \ \text{const} \&) \)
  • Explicitly or implicitly declared

• Copy assignment operator \( T \& \ \text{operator}=(T \ \text{const} \&) \)
  • Explicitly or implicitly declared

• Destructor \(~T()\)
  • Explicitly or implicitly declared
Implicitly Declared C++11

• Copy constructor, copy assignment operator and destructor
  • Explicitly or implicitly declared (C++98 rules still apply)
• Move constructor / assignment operator implicitly declared if
  • Not explicitly declared
  • No user-declared copy constructor
  • No user-declared copy assignment operator
  • No user-declared move assignment operator / constructor
  • No user-declared destructor
• Implicitly declared copy constructor and copy assignment operator are deleted
  • Declared (explicitly or implicitly) move constructor or move assignment operator
Implicitly Declared C++11

• Backwards compatibility with C++98 classes

• C++-utopia rules
  • Rule of 5
    • If you explicitly declare one of the 5, you always have to declare all copy/move constructor/assignment operator
  • C++11 rules have been deprecated since C++11
    • Might be un-deprecated in C++23
Implicitly Declared Deleted

- ...

- Implicitly declared copy / move constructor / assignment operator is deleted

- If any aggregated members have inaccessible or deleted copy / move constructor / assignment operator
Implicitly Declared Deleted

```cpp
class Bravo
{
    std::unique_ptr<Charlie> c;
    //...
};
```

- Because `unique_ptr` has a deleted copy constructor / copy assignment operator

- **Bravo** *implicitly* has a deleted copy constructor / copy assignment operator
Implicitly Declared

• Easier to get correct
• Easier to reason about
• Easier for compilers to optimize
• Less verbose
Rule of 0

• Most classes should not have *any* user-declared *copy / move constructor / assignment operator* or destructor

• Take advantage of implicitly declared special member functions

• Take advantage of implicitly declared deleted special member functions
Rule of 0

- **Best Practice**
  - Strive for Rule of 0
    - No user-declared `copy / move` constructor / assignment operator or destructor
  - Otherwise, Rule of 5 (hopefully rarely)
    - Explicitly declare `copy / move` constructor / assignment operator and destructor
unique_ptr

(Again)
unique_ptr

```cpp
struct einspline_spo : SPOSet {
    /* ... */
};

struct einspline_spo_ref : SPOSet {
    /* ... */
};

SpoSet* build_spo(...) {
    auto my_spo = new einspline_spo(...);
    // ...
    return dynamic_cast<SPOSet*>(my_spo);
}

std::unique_ptr<SpoSet> build_spo(...) {
    std::unique_ptr<einspline_spo> my_spo(new einspline_spo); // C++11
    std::unique_ptr<einspline_spo> my_spo(std::make_unique<einspline_spo>()); // C++14
    // ...
    return my_spo; // Implicit upcasting
}```
unique_ptr

```cpp
struct einspline_spo : SPOSet { /* ... */ };  
struct einspline_spo_ref : SPOSet { /* ... */ };  

std::unique_ptr<SpoSet> build_spo(...)  
{
    std::unique_ptr<einspline_spo> my_spo(new einspline_spo); // C++11  
    std::unique_ptr<einspline_spo> my_spo(std::make_unique<einspline_spo>()); // C++14  
    //...
    return my_spo; // Implicit upcasting  
}

• **Best Practice**

  • Put object into smart pointer as soon as possible
  
  • No raw `new` (or `delete`) whenever possible
  
  • Throw away information (derived type) as late as possible
  
  • No explicit casting whenever possible
```
Casts
struct einspline_spo : SPOSet {
    /* ... */
};
struct einspline_spo_ref : SPOSet {
    /* ... */
};

SpoSet* build_spo(...)
{
    auto spo_main = new einspline_spo(...);
    // ...
    return dynamic_cast<SPOSet*>(spo_main);
}
Casts

- Casting is a many-to-one relationship
- Casting says that you know better than the type system
- Casting can easily lead to bugs
  - Undefined behavior
Undefined Behavior

• Behavior for which C++ imposes no requirements
  • Here be dragons
  • Anything is possible
    • A bool variable can be both true and false
  • Time travel

```cpp
int table[4];
bool exists_in_table(int v)
{
    for (int i = 0; i <= 4; i++) {
        if (table[i] == v) return true;
    }
    return false;
}
```

• Compiler may assume i == 5 never occurs and optimize this to always return true
Undefined Behavior

• Two edged sword
  - Invoking undefined behavior means anything can happen!
  - Compilers may assume undefined behavior cannot happen
    + Can make correct code better (faster and/or smaller)
    + Sanitizers can detect incorrect code at runtime
    + Sometimes defining behavior is more error prone
    + Developers know they can write code which depends on it
Undefined Behavior

• unsigned
  • Addition / subtraction fully defined to wrap
    • Very reasonable and obvious definition
  • Highly error prone
    • Cannot differentiate between accidental wrapping and deliberate wrapping
      • No-false-positive sanitizers cannot differentiate either
Undefined Behavior

• Cannot always detect it
  • `strlen(char const* s)`
    + `s` must not be `nullptr`
    - `s` must be a valid pointer
    - `s` must point to something `'\0'`-terminated
Undefined Behavior

• Best Practice

  • Avoid invoking undefined behavior in your code
  
  • Don’t define behavior just to avoid undefined behavior

    • Defined behavior should be “easy to use correctly and hard to use incorrectly”

  • `assert()` is your friend

    • Remember `assert()` is a macro and should be side-effect free

  • C++23-ish Contracts will also help
Casts

- Casting is a many-to-one relationship
- Casting says that you know better than the type system
- Casting can easily lead to bugs
  - Undefined behavior
static_cast

• Conversion between types
• May have a runtime cost
• Can be used to down cast (Base to Derived) if you know you have an object of the derived type
• “Safest”

```cpp
enum class E { Five = 5, };
E e = E::Five;
std::cout << static_cast<std::underlying_type_t<E>>(e) << \n'; // 5
```
const_cast

• Remove const/volatile
  • No run time cost
  • Only legal if the original object is non-\texttt{const}
  • Usually to interface with legacy code or C code

• C: Array of pointers to non-\texttt{const} cannot be promoted to an array of pointers to \texttt{const}

```c
// Warning in C++; invalid in C (see execv for details)
int A(int argc, char const* const argv[]) { return !!argv[argc]; }
int main(int argc, char* argv[]) { return A(argc, argv); }
```
int i = 2;
int const& ci = i;
++const_cast<int&>(ci);
std::cout << i << 'n'; // 3
reinterpret_cast

- “Pretend” the bits are really for the new type
  - No run time cost
  - Tends to be at the lowest abstraction levels
  - Dereferencing only legal for “similar” types according to type aliasing
  - See CppReference.com for details
dynamic_cast

• Checked down / cross casting
  • Uses RTTI (Run Time Type Information)
    • Source type has to have at least one virtual function
  • Expensive
    • May be O(n) (n is the hierarchy depth)
    • strcmp of mangled names (gcc)
dynamic_cast

- `dynamic_cast<T*>(p)` returns `nullptr` if `p` is not convertible to a pointer to `T`

- `dynamic_cast<T&>(u)` throws `std::bad_cast` if `u` is not convertible to a reference to `T`

- Down cast asks an object “Are you really type T?”
  - Not good OO design

- Cross cast (multiple inheritance) asks an object “Do you have capability C?”
C style cast

• In the beginning…

• (type)variable
  • Combination of static_cast, reinterpret_cast & const_cast

• Actually worse…

```cpp
struct Base { virtual ~Base() = default; };
struct Derived : private Base {};

Derived d;
Base* b = (Base*)((Derived*)&d);
```

• Functional cast (C++)
  • type(variable)

• And many, many more…
Casts

• Rarely a need to up cast

• `unique_ptr` does not define the equivalent of explicit casting operations

• **Best Practice**
  
  • Rarely cast
```cpp
struct einspline_spo : SPOSet { /* ... */ };  
struct einspline_spo_ref : SPOSet { /* ... */ };  

SpoSet* build_spo(...)  
{  
    auto my_spo = new einspline_spo(...);  
    // ...  
    return dynamic_cast<SPOSet*>(my_spo);  
}  
```
unique_ptr<T[]>
unique_ptr<T[]>

- `std::unique_ptr<char[]> up(new char[size]);`
  - Moveable
  - Size not queryable
  - Default initializes (doesn’t zero) array

- `std::vector<char> v(size);`
  - Copyable, resizable, etc.
  - Size queryable
  - Value initializes (zeros) the array
unique_ptr<T[]>

• C++11
std::unique_ptr<char[]> up(new char[size]);

• C++14
std::unique_ptr<char[]> up(std::make_unique<char[]>(size));
std::unique_ptr<char[]> up(new char[size]);

• make_unique
• No raw new
• Value initializes (zeros) the array

• C++20
std::unique_ptr<char[]> up(std::make_unique_default_init<char[]>(size));
shared_ptr
shared_ptr

- Reference counted
  - increment/decrement happen atomically
- Copyable
  - Copying increments the reference count
- Trackable / breaking cycles
  - weak_ptr
    - Separate control block (deleter, strong/weak refCounts, etc.)
  - make_shared combine object and control block into one allocation
shared_ptr

- Useful when you do not know the last user of the data structure
  - Across threads
- Hard to reason about
  - Essentially a hidden global variable
InfoStream
(miniQMC)
InfoStream

- Wrapper around output streams
  - Turning on/off, redirecting to cout, cerr, file
- Hard to reason about
  - May or may not own a stream
  - Copy/move semantics incorrect
- Streams are non-trivial to wrap
class InfoStream
{
public:
    InfoStream(std::ostream* output_stream)
    : prevStream(NULL), nullStream(new std::ostream(NULL)), ownStream(false)
    {
        currStream = output_stream;
    }

    InfoStream(InfoStream& in)
    : prevStream(NULL), nullStream(new std::ostream(NULL)), ownStream(false)
    {
        redirectToSameStream(in);
    }

    ~InfoStream();

    std::ostream& getStream(const std::string& tag = "") {
        return *currStream;
    }

    void flush() { currStream->flush(); }

private:
    // Keep track of whether we should delete the stream or not
    bool ownStream;

    std::ostream* currStream;

    // save stream during pause
    std::ostream* prevStream;

    // Created at construction. Used during pause
    std::ostream* nullStream;
};

template<class T>
inline InfoStream& operator<<(InfoStream& o, const T& val)
{
    o.getStream() << val;
    return o;
}

class InfoStream
{
    public:
        explicit InfoStream(std::ostream* output_stream)
        : currStream(output_stream)
        {} 

        explicit InfoStream(InfoStream& in)
        {
            redirectToSameStream(in);
        }

        std::ostream& getStream() const {
            return *currStream;
        }

        void flush() const {
            currStream->flush();
        }

private:
    // Keep track of whether we should delete the stream or not
    std::unique_ptr<std::ofstream> ownStream;

    std::ostream* currStream = nullptr;

    // save stream during pause
    std::ostream* prevStream = nullptr;

    // Used during pause
    static std::ostream nullStream;

    template<typename T>
    friend InfoStream& operator<<(InfoStream& o, const T& val)
    {
        return o.getStream() << val;
    }
};
class InfoStream
{
public:
  InfoStream(std::ostream* output_stream)
    : prevStream(NULL), nullStream(new std::ostream(NULL)), ownStream(false)
  {
    currStream = output_stream;
  }
  InfoStream(InfoStream& in)
    : prevStream(NULL), nullStream(new std::ostream(NULL)), ownStream(false)
  {
    redirectToSameStream(in);
  }
  ~InfoStream();
  std::ostream& getStream(const std::string& tag = "") { return *currStream; }
  void flush() { currStream->flush(); }
private:
  // Keep track of whether we should delete the stream or not
  bool ownStream;
  std::ostream* currStream;
  // save stream during pause
  std::ostream* prevStream;
  // Created at construction. Used during pause
  std::ostream* nullStream;
};

template <class T>
inline InfoStream& operator<<(InfoStream& o, const T& val)
{
  o.getStream() << val;
  return o;
}
InfoStream

• Single parameter constructors should be explicit
class InfoStream
{
public:
-infoStream(std::ostream* output_stream)
  : prevStream(NULL), nullStream(new std::ostream(NULL)), ownStream(false)
  { currStream = output_stream; }
InfoStream(InfoStream& in)
  : prevStream(NULL), nullStream(new std::ostream(NULL)), ownStream(false)
  { redirectToSameStream(in); }
~InfoStream();
std::ostream& getStream(const std::string& tag = "") { return *currStream; }
void flush() { currStream->flush(); }
private:
// Keep track of whether we should delete the stream or not
bool ownStream;
std::ostream* currStream;
// save stream during pause
std::ostream* prevStream;
// Created at construction. Used during pause
std::ostream* nullStream;
};

template<class T>
inline InfoStream& operator<<(InfoStream& o, const T& val)
{ o.getStream() << val;
  return o; }

• Share a common sentinel
```cpp
class InfoStream
{
public:
    InfoStream(std::ostream* output_stream)
        : prevStream(NULL), nullStream(new std::ostream(NULL)), ownStream(false)
    {
        currStream = output_stream;
    }
    InfoStream(InfoStream& in)
        : prevStream(NULL), nullStream(new std::ostream(NULL)), ownStream(false)
    {
        redirectToSameStream(in);
    }
    ~InfoStream();
    std::ostream& getStream(const std::string& tag = "") {
        return *currStream;
    }
    void flush() { currStream->flush(); }
private:
    // Keep track of whether we should delete the stream or not
    bool ownStream;
    std::ostream* currStream;
    // save stream during pause
    std::ostream* prevStream;
    // Created at construction. Used during pause
    std::ostream* nullStream;
};

template<class T>
inline InfoStream& operator<<(InfoStream& o, const T& val)
{
    o.getStream() << val;
    return o;
}
```

- Use member initializers
- Otherwise, does construct then assign
- Requires default constructibility
InfoStream

• Declare member functions which do not modify state as const
class InfoStream
{
public:
    InfoStream(std::ostream* output_stream)
        : prevStream(NULL), nullStream(new std::ostream(NULL)), ownStream(false)
    {
        currStream = output_stream;
    }
    InfoStream(InfoStream& in)
        : prevStream(NULL), nullStream(new std::ostream(NULL)), ownStream(false)
    {
        redirectToSameStream(in);
    }
~InfoStream();

    std::ostream& getStream(const std::string& tag = "") { return *currStream; }
    void flush() { currStream->flush(); }

private:
    // Keep track of whether we should delete the stream or not
    bool ownStream;
    std::ostream* currStream;
    // save stream during pause
    std::ostream* prevStream;
    // Created at construction. Used during pause
    std::ostream* nullStream;
};

template<class T>
inline InfoStream& operator<<(InfoStream& o, const T& val)
{
    o.getStream() << val;
    return o;
}

• Use unique_ptr<ofstream> for ownStream
• Automatically deletes the stream on destruction if we own it
• No explicit destructor needed for InfoStream
• Makes InfoStream non-copyable
class InfoStream
{
public:
InfoStream(std::ostream* output_stream)
: prevStream(NULL), nullStream(new std::ostream(NULL)), ownStream(false)
{
    currStream = output_stream;
}

InfoStream(InfoStream& in)
: prevStream(NULL), nullStream(new std::ostream(NULL)), ownStream(false)
{
    redirectToSameStream(in);
}

~InfoStream();

std::ostream& getStream(const std::string& tag = "") { return *currStream; }
void flush() { currStream->flush(); }

private:
    // Keep track of whether we should delete the stream or not
    bool ownStream;
    std::ostream* currStream;
    // save stream during pause
    std::ostream* prevStream;
    // Created at construction. Used during pause
    std::ostream* nullStream;
};

template<typename T>
inline InfoStream& operator<<(InfoStream& o, const T& val)
{
    o.getStream() << val;
    return o;
}

• Are move semantics correct?
  • No
  • Moving fundamental data types (ints, pointers, etc.) is the same as copying them
  • currStream may have multiple InfoStream owners
  • All deleting them in their destructors
class InfoStream {
public:
    InfoStream(ostream* output_stream)
        : prevStream(NULL), nullStream(new ostream(NULL)), ownStream(false)
    {
        currStream = output_stream;
    }
    InfoStream(InfoStream& in)
        : prevStream(NULL), nullStream(new ostream(NULL)), ownStream(false)
    {
        redirectToSameStream(in);
    }
    ~InfoStream();
    std::ostream& getStream(const string& tag = "") { return *currStream; }
    void flush() { currStream->flush(); }
}

private:
    // Keep track of whether we should delete the stream or not
    bool ownStream;
    std::ostream* currStream;
    // save stream during pause
    std::ostream* prevStream;
    // Created at construction. Used during pause
    std::ostream* nullStream;

    template<class T>
    inline InfoStream& operator<<(InfoStream& o, const T& val) {
        o.getStream() << val;
        return o;
    }
class InfoStream
{
public:
    InfoStream(std::ostream* output_stream)
        : prevStream(NULL), nullStream(new std::ostream(NULL)), ownStream(false)
    {
        currStream = output_stream;
    }
    InfoStream(InfoStream& in)
        : prevStream(NULL), nullStream(new std::ostream(NULL)), ownStream(false)
    {
        redirectToSameStream(in);
    }
    ~InfoStream();
    std::ostream& getStream(const std::string& tag = "") { return *currStream; }
    void flush() { currStream->flush(); }
private:
    // Keep track of whether we should delete the stream or not
    bool ownStream;
    std::ostream* currStream;
    // save stream during pause
    std::ostream* prevStream;
    // Created at construction. Used during pause
    std::ostream* nullStream;
};

template<class T>
inline InfoStream& operator<<(InfoStream& o, const T& val)
{
    o.getStream() << val;
    return o;
}

• Cannot insert manipulators into InfoStream

InfoStream out(&std::cout);
out << "Hello, world";
out << std::endl;  // fails to compile

• \texttt{endl} is really a function \texttt{template}

template<class charT, class traits>
basic_ostream<charT, traits>& endl(basic_ostream<charT, traits>& os);

• Cannot infer \(T\) in

operator<<(InfoStream& o, const T&)

• This is \textit{subtle}
class InfoStream
{
public:
    InfoStream(std::ostream* output_stream)
        : prevStream(NULL), nullStream(new std::ostream(NULL)), ownStream(false)
        { currStream = output_stream; }
    InfoStream(InfoStream& in)
        : prevStream(NULL), nullStream(new std::ostream(NULL)), ownStream(false)
        { redirectToSameStream(in); }
    ~InfoStream();
    std::ostream& getStream(const std::string& tag = "") { return *currStream; }
    void flush() { currStream->flush(); }
private:
    // Keep track of whether we should delete the stream or not
    bool ownStream;
    std::ostream* currStream;
    // save stream during pause
    std::ostream* prevStream;
    // Created at construction. Used during pause
    std::ostream* nullStream;
};

template<class T>
inline InfoStream& operator<<(InfoStream& o, const T& val)
{ o.getStream() << val;
  return o; }
class InfoStream
{
public:
    InfoStream(std::ostream* output_stream)
    : prevStream(NULL), nullStream(new std::ostream(NULL)), ownStream(false)
    { currStream = output_stream; }

    InfoStream(InfoStream& in)
    : prevStream(NULL), nullStream(new std::ostream(NULL)), ownStream(false)
    { redirectToSameStream(in); }

    ~InfoStream();

    std::ostream& getStream(const std::string& tag = "") { return *currStream; }

    void flush() { currStream->flush(); }

private:
    // Keep track of whether we should delete the stream or not
    bool ownStream;

    std::ostream* currStream;

    // save stream during pause
    std::ostream* prevStream;

    // Created at construction. Used during pause
    std::ostream* nullStream;
};

template<class T>
InfoStream& operator<<(InfoStream& o, const T& val)
{ o.getStream() << val; return o; }

class InfoStream
{
public:
    explicit InfoStream(std::ostream* output_stream)
    : currStream(output_stream)
    {}

    explicit InfoStream(InfoStream& in)
    { redirectToSameStream(in); }

    std::ostream& getStream() const { return *currStream; }

    void flush() const { currStream->flush(); }

private:
    // Keep track of whether we should delete the stream or not
    std::unique_ptr<std::ofstream> ownStream;

    std::ostream* currStream = nullptr;

    // save stream during pause
    std::ostream* prevStream = nullptr;

    // Used during pause
    static std::ostream nullStream;

    template<typename T>
    friend InfoStream& operator<<(InfoStream& o, const T& val)
    { return o.getStream() << val; }
};
class InfoStream
{
public:
explicit InfoStream(std::ostream* output_stream)
: currStream(output_stream)
{} 
explicit InfoStream(InfoStream& in)
{ redirectToSameStream(in); }
std::ostream& getStream() const { return *currStream; }
void flush() const { currStream->flush(); }
private:
// Keep track of whether we should delete the stream or not 
std::unique_ptr<std::ofstream> ownStream;
std::ostream* currStream = nullptr;
// save stream during pause
std::ostream* prevStream = nullptr;
// Used during pause
static std::ostream nullStream;

//template<typename T>
friend InfoStream& operator<<(InfoStream& o, const T& val)
{ return o.getStream() << val; }
};
InfoStream

- Constructors are `explicit`
- Share a common `nullStream`
- Uses member initializers
- `const` member functions
- All variables initialized
- `ownStream` is stored in a `unique_ptr`
- No explicit destructor
- `InfoStream` inserter is hidden friend

```cpp
class InfoStream {
public:
    explicit InfoStream(std::ostream* output_stream)
    : currStream(output_stream)
    {}
    explicit InfoStream(InfoStream& in)
    { redirectToSameStream(in); }
    std::ostream& getStream() const { return *currStream; }
    void flush() const { currStream->flush(); }
private:
    // Keep track of whether we should delete the stream or not
    std::unique_ptr<std::ofstream> ownStream;
    std::ostream* currStream = nullptr;
    std::ostream* prevStream = nullptr;
    // Used during pause
    static std::ostream nullStream;
    // Template
    template<typename T>
    friend InfoStream& operator<<(InfoStream& o, const T& val)
    { return o.getStream() << val; }
};
```
Are move semantics correct

Still no

currStream can point to ownStream

Fix

Explicitly delete copy / move operations and declare destructor (Rule of 5)
InfoStream

- Best Practice
  - No maybe or maybe not ownership semantics
  - InfoStream should either never own a stream or always own a stream
  - Get copy/move semantics correct
    - Rule of 0
    - Much easier to do when first writing class
  - Explicitly = delete otherwise (rarely)
class InfoStream
{
public:
    InfoStream(std::ostream* output_stream)
        : prevStream(NULL), nullStream(new std::ostream(NULL)), ownStream(false)
    {
        currStream = output_stream;
    }
    InfoStream(InfoStream& in)
        : prevStream(NULL), nullStream(new std::ostream(NULL)), ownStream(false)
    {
        redirectToSameStream(in);
    }
    ~InfoStream();
    std::ostream& getStream(const std::string& tag = "") { return *currStream; }
    void flush() { currStream->flush(); }
private:
    // Keep track of whether we should delete the stream or not
    bool ownStream;
    std::ostream* currStream;
    // save stream during pause
    std::ostream* prevStream;
    // Created at construction. Used during pause
    std::ostream* nullStream;
};

template<class T>
inline InfoStream& operator<<(InfoStream& o, const T& val)
{
    o.getStream() << val;
    return o;
}
Refactoring
Refactoring

```
const std::vector<WaveFunction*> extract_wf_list(const std::vector<Mover*>& mover_list)
{
    std::vector<WaveFunction*> wf_list;
    wf_list.reserve(mover_list.size());
    for (auto it = mover_list.begin(); it != mover_list.end(); it++)
        wf_list.push_back(&(*it)->wavefunction);

    return wf_list;
}
```

• Non-controversial stuff

• `reserve()` space if amount is known

• `const` on return type has no effect
Refactoring

```cpp
std::vector<WaveFunction*> extract_wf_list(const std::vector<Mover*>& mover_list)
{
    std::vector<WaveFunction*> wf_list;
    wf_list.reserve(mover_list.size());
    for (auto it = mover_list.begin(); it != mover_list.end(); it++)
        for (auto it = std::begin(mover_list); it != std::end(mover_list); it++)
            wf_list.push_back(&(*it)->wavefunction);
    return wf_list;
}
```

- `.begin()`
  - Less general
  + Less characters

- `std::begin(c)`
  + More general
    - Generic (template) code
  + More characters
std::vector<WaveFunction*> extract_wf_list(const std::vector<Mover*>& mover_list) {
    std::vector<WaveFunction*> wf_list;
    wf_list.reserve(mover_list.size());
    for (auto it = mover_list.begin(); it != mover_list.end(); it++)
    for (std::vector<Mover*>::const_iterator it = mover_list.begin(); it != mover_list.end(); it++)
        wf_list.push_back(&(*it)->wavefunction);
    return wf_list;
}

- auto
  - Terse
  - Exact match
  + Writers over Readers

- std::vector<Mover*>::const_iterator
  - Verbose
  - Possible implicit conversion
  + Readers over Writers
Loops & Algorithms
(more refactoring)
Evolution of loops

```cpp
const std::vector<WaveFunction*> extract_wf_list(const std::vector<Mover*>& mover_list) {
    std::vector<WaveFunction*> wf_list;
    wf_list.reserve(mover_list.size());
    for (auto it = mover_list.begin(); it != mover_list.end(); it++)
        wf_list.push_back(&(*it)->wavefunction);
    return wf_list;
}
```
Evolution of loops

```cpp
for (auto it = mover_list.begin(); it != mover_list.end(); it++)
    wf_list.push_back(&(*it)->wavefunction);

for (auto& m : mover_list)
    wf_list.push_back(&m->wavefunction);

std::for_each(std::begin(mover_list), std::end(mover_list),
               [](Mover& mover){ wf_list.push_back(&m->waveFunction); });

std::transform(std::begin(mover_list), std::end(mover_list), std::back_inserter(wf_list),
               [](Mover* m){ return &m->wavefunction; });
```
Evolution of loops

- Most flexible
- Hardest to reason about
  - Have to reason about init, condition, expression & body
    - Modify it
    - Control flow (break / continue)

```cpp
for (auto it = mover_list.begin(); it != mover_list.end(); it++)
    wf_list.push_back(&(*it)->wavefunction);

for (auto& m : mover_list)
    wf_list.push_back(&m->wavefunction);

std::for_each(std::begin(mover_list), std::end(mover_list),
               [&] (Mover& mover) { wf_list.push_back(&m->waveFunction); });

std::transform(std::begin(mover_list), std::end(mover_list), std::back_inserter(wf_list),
               [] (Mover* m) { return &m->wavefunction; });
```
Evolution of loops

- Somewhat easier to reason about
  - No access to iterators
    - No `it` to modify
  - Only have to reason about the body
    - Control flow (`break` / `continue`)

```cpp
for (auto it = mover_list.begin(); it != mover_list.end(); it++)
    wf_list.push_back(&(*it)->wavefunction);

for (auto& m : mover_list)
    wf_list.push_back(&m->wavefunction);

std::for_each(std::begin(mover_list), std::end(mover_list),
              [&](Mover& mover){
                  wf_list.push_back(&m->waveFunction);
              });

std::transform(std::begin(mover_list), std::end(mover_list), std::back_inserter(wf_list),
               [](Mover* m){ return &m->wavefunction; });
```
Evolution of loops

for (auto it = mover_list.begin(); it != mover_list.end(); it++)
   wf_list.push_back((*it)->wavefunction);

for (auto& m : mover_list)
   wf_list.push_back(&m->wavefunction);

std::for_each(std::begin(mover_list), std::end(mover_list),
   [&](Mover& mover){ wf_list.push_back(&m->waveFunction); });

std::transform(std::begin(mover_list), std::end(mover_list), std::back_inserter(wf_list),
   [](Mover* m){ return &m->wavefunction; });

• Algorithm
  • Even easier to reason about
  • Benefits of range-based for
  • No need to reason about control flow
    • well, except for exceptions
  • Every element is accessed

• More verbose
Evolution of loops

- Algorithm
- Self-documenting
- Most declarative
- More verbose
- Requires knowledge of conversion (`back_inserter`) and algorithms (`transform`) out there.

```cpp
for (auto it = mover_list.begin(); it != mover_list.end(); it++)
    wf_list.push_back((&(*it)->wavefunction);

for (auto& m : mover_list)
    wf_list.push_back(&m->wavefunction);

std::for_each(std::begin(mover_list), std::end(mover_list),
              [&](Mover& mover){ wf_list.push_back(&m->waveFunction); });

std::transform(std::begin(mover_list), std::end(mover_list), std::back_inserter(wf_list),
               [](Mover* m){ return &m->wavefunction; });
```
Evolution of loops

for (auto it = mover_list.begin(); it != mover_list.end(); it++)
    wf_list.push_back(&(*it)->wavefunction);

for (auto& m : mover_list)
    wf_list.push_back(&m->wavefunction);

std::for_each(std::begin(mover_list), std::end(mover_list),
    [](Mover& mover){ wf_list.push_back(&m->waveFunction); });

std::transform(std::begin(mover_list), std::end(mover_list), std::back_inserter(wf_list),
    [](Mover* m){ return &m->wavefunction; });

- Still on the fence about Best Practice
  - Prefer algorithms to hand-coded loops
    - If there isn’t one, write one
  - Prefer range-based for to hand-coded loops
    - Less verbosity matters
    - Especially for small bodies
template<class T, typename TBOOL>
const std::vector<T*> filtered_list(const std::vector<T*>& input_list, const std::vector<TBOOL>& chosen)
{
        using filtered_type = std::vector<T*>;
        using size_type = typename filtered_type::size_type;

        std::vector<T*> final_list;
        final_list.reserve(input_list.size());
        for (int size_type iw = 0; iw < input_list.size(); iw++)
                if (chosen[iw])
                        final_list.push_back(input_list[iw]);
        final_list.shrink_to_fit();
        return final_list;
}

- Only use all-uppercase for macros
  - “Stop the CONSTANT SHOUTING” - Jonathan Wakely

- Don’t implicitly mix types

- Consider making this an algorithm

- != vs. <, ++iw vs. iw++

- Tension between C++ way and OpenMP way
Templates for common code

(Refactoring)
SPOSet* build_SPOSet(bool useRef,...)
{
    if (useRef)
    {
        auto* spo_main = new miniqmcreference::einspline_spo_ref<...>;
        spo_main->set(nx, ny, nz, num_splines, nblocks);
        spo_main->Lattice.set(lattice_b);
        return dynamic_cast<SPOSet*>(spo_main);
    }
    else
    {
        auto* spo_main = new einspline_spo<OHMMS_PRECISION>;
        spo_main->set(nx, ny, nz, num_splines, nblocks);
        spo_main->Lattice.set(lattice_b);
        return dynamic_cast<SPOSet*>(spo_main);
    }
}

namespace
{
    // Helper for public build_SPOSet which builds it independent of the
dervied SPOSetType
    template<typename SPOSetType>
    std::unique_ptr<SPOSet>
    build_SPOSet(...)
    {
        std::unique_ptr<SPOSetType> spo_main(new SPOSetType);
        spo_main->set(nx, ny, nz, num_splines, nblocks);
        spo_main->Lattice.set(lattice_b);
        return spo_main;
    }
} // namespace

std::unique_ptr<SPOSet> build_SPOSet(bool useRef,...)
{
    return useRef ?
        build_SPOSet<miniqmcreference::einspline_spo_ref<...>>((nx, ny, nz, num_splines, nblocks, lattice_b, init_random)) :
        build_SPOSet<miniqmcreference::einspline_spo<...>>((nx, ny, nz, num_splines, nblocks, lattice_b, init_random));
}
• Refactor common code into function template

• Anonymous namespace

• Consider \texttt{variant<einspline\_spo<...>, einspline\_spo\_ref<...>>}

• C++17

```cpp
namespace 
{
  // Helper for public build\_SPOSet which builds it independent of the
  // derived SPOSetType
  template<typename SPOSetType>
  std::unique\_ptr<SPOSet>
  build\_SPOSet(...) 
  { 
    std::unique\_ptr<SPOSetType> spo\_main(new SPOSetType);
    spo\_main->set(nx, ny, nz, num\_splines, nblocks);
    spo\_main->Lattice.set(lattice\_b);
    return spo\_main;
  }
} // namespace

std::unique\_ptr<SPOSet> build\_SPOSet(bool useRef,...) 
{ 
  return useRef ?
    build\_SPOSet<miniqmcreference::einspline\_spo\_ref<...>>(nx, ny, nz, num\_splines, nblocks, lattice\_b, init\_random) :
    build\_SPOSet<miniqmcreference::einspline\_spo<...>>(nx, ny, nz, num\_splines, nblocks, lattice\_b, init\_random);
}
```
Placement new
new

- new T(…)
  - Needed for lifetimes different than a scope
  - Performs two operations
    - Acquire space from heap
    - Construct an object into that space
Placement new

- `new (address) T(...)`
  - Needed for lifetimes different than a scope
  - Performs one operation
    - Acquire space from heap
  - Construct an object into that space
Placement new

- **Fraught with peril!**
  - User responsibility
    - Space is uninitialized
    - \(~T()\) is eventually called exactly once
  - Otherwise, undefined behavior
    - Rules about uninitialized space, lifetime of objects, pointers & references, type punning, etc. are expert-level complicated
void resize()
{
    psi.resize(nBlocks);
    grad.resize(nBlocks);
    hess.resize(nBlocks);

    psi = Kokkos::View<vContainer_type>("Psi", nBlocks);
    grad = Kokkos::View<gContainer_type>("Grad", nBlocks);
    hess = Kokkos::View<hContainer_type>("Hess", nBlocks);

    for (int i = 0; i < nBlocks; ++i)
    {
        //psi[i].resize(nSplinesPerBlock);
        //grad[i].resize(nSplinesPerBlock);
        //hess[i].resize(nSplinesPerBlock);

        //Using the "view-of-views" placement-new construct.
        new (&psi(i)) vContainer_type("psi_i", nSplinesPerBlock);
        new (&grad(i)) gContainer_type("grad_i", nSplinesPerBlock);
        new (&hess(i)) hContainer_type("hess_i", nSplinesPerBlock);
    }
}

Kokkos View of Views

• Placement new should not be over existing objects
• Existing object destructor never called
• In a loop
• Recommendation
• Avoid placement new
Best Practices
Best Practices

- C++ Core Guidelines

- Collaborative Collection of C++ Best Practices - Jason Turner
  - https://github.com/lefticus/cppbestpractices

- C++ Coding Standards
  - Andrei Alexandrescu & Herb Sutter

  Preface: Think.

  0. Don’t sweat the small stuff