

Concepts for designing modern C++ interfaces for MPI

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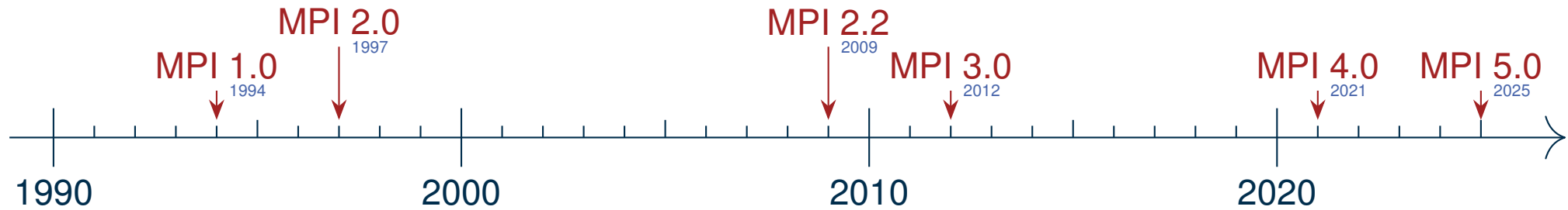
⁵Stony Brook University, Stony Brook, New York, USA

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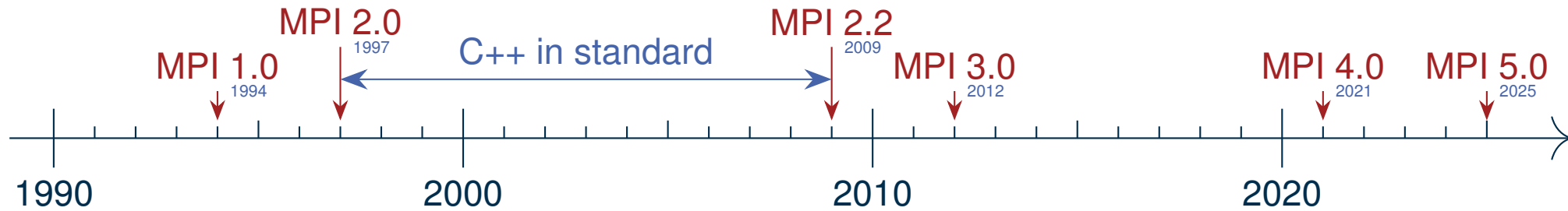
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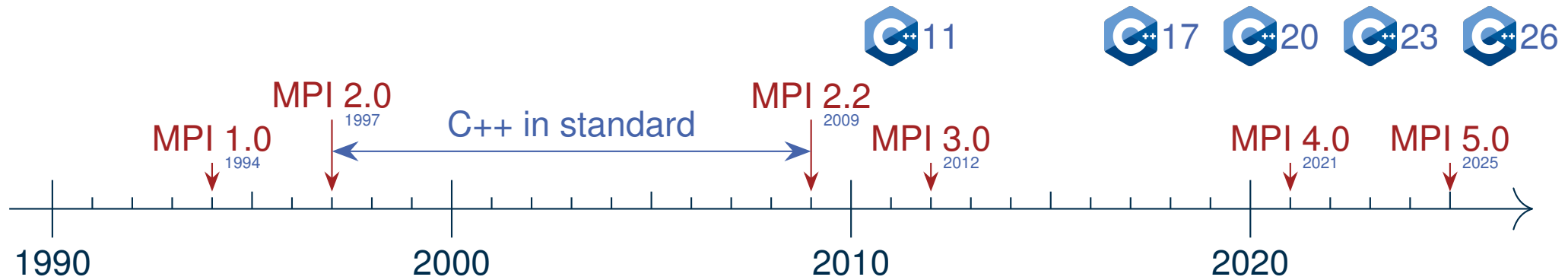
A Brief History of MPI and C++



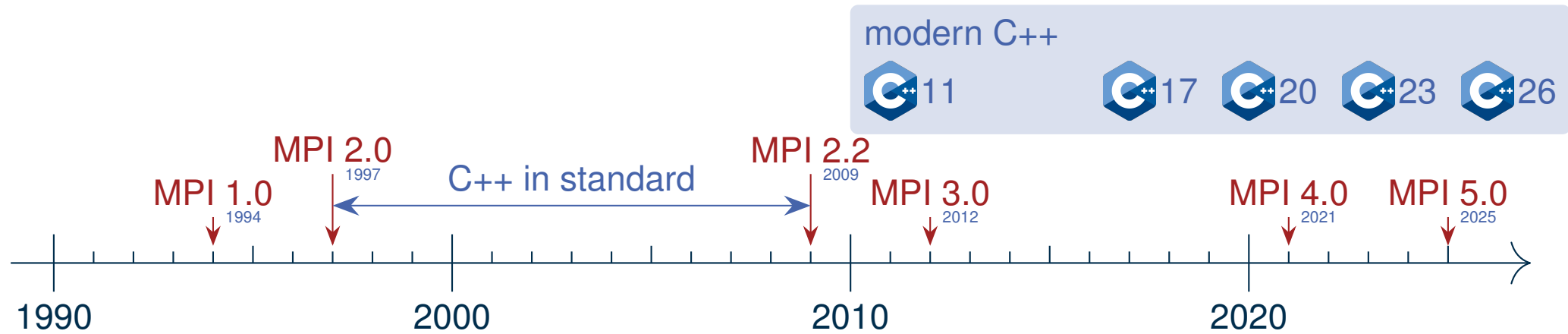
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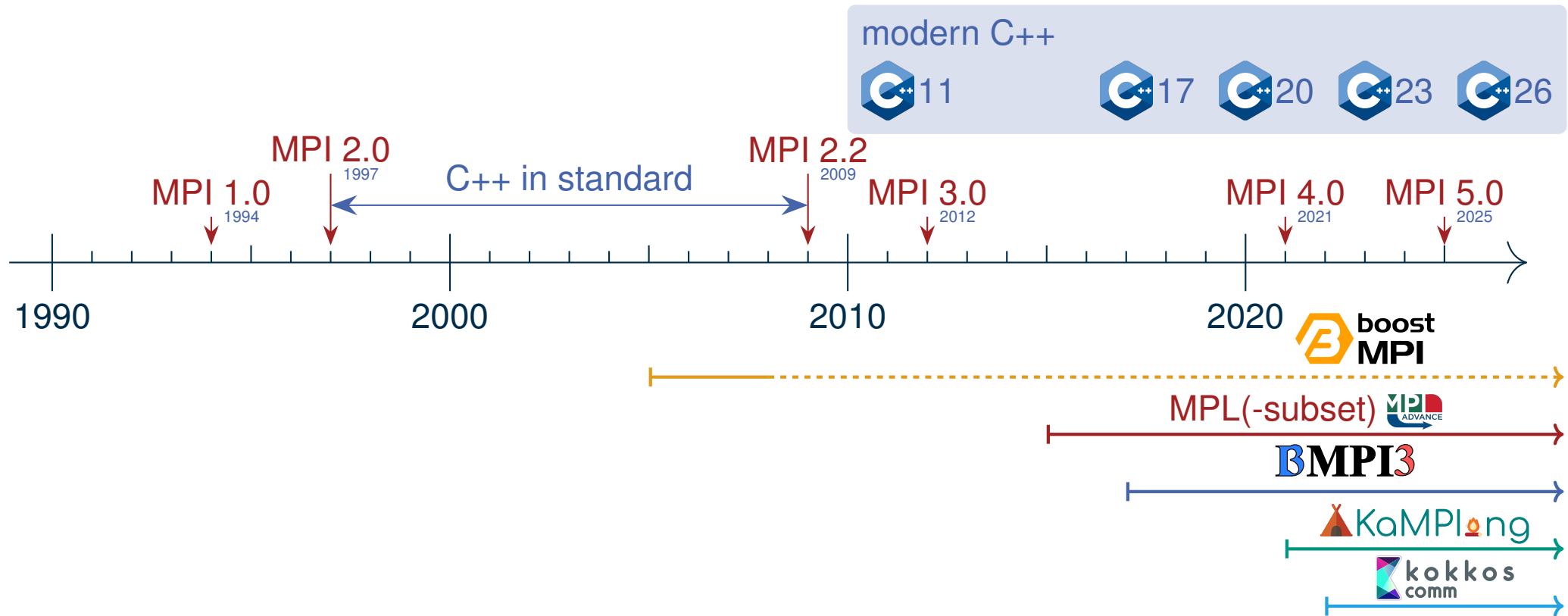
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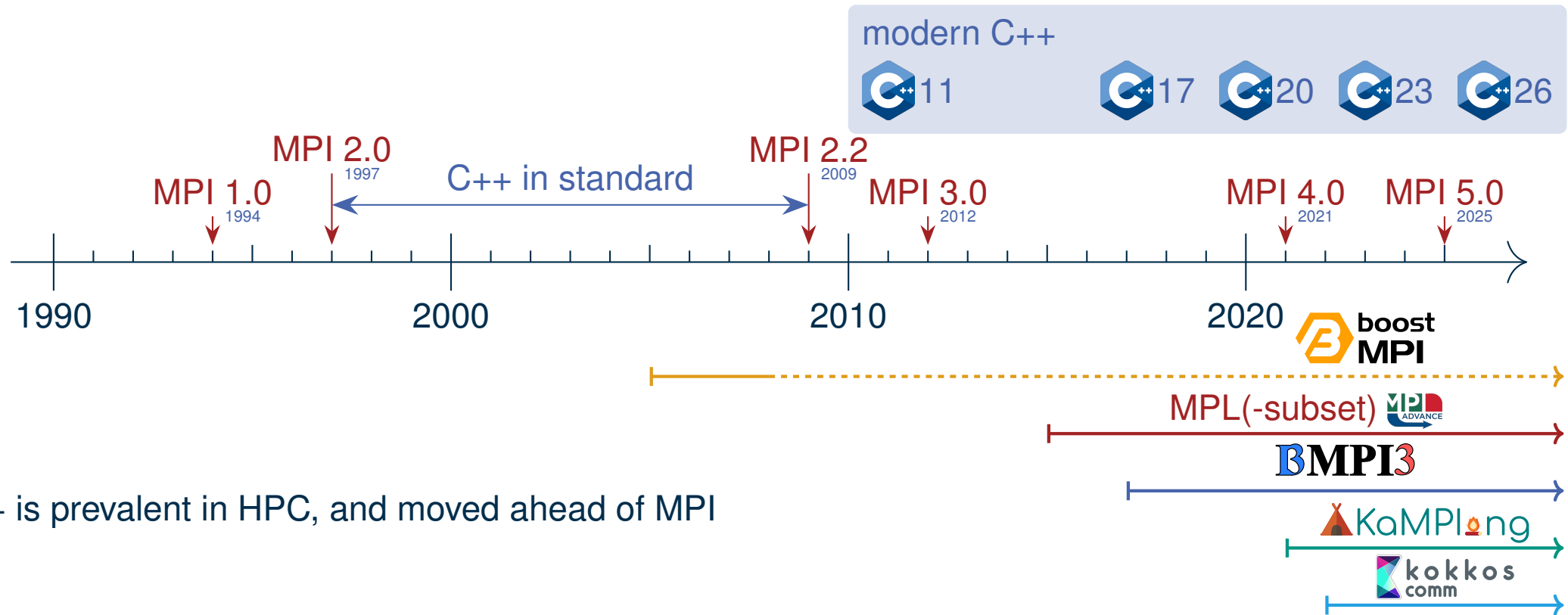
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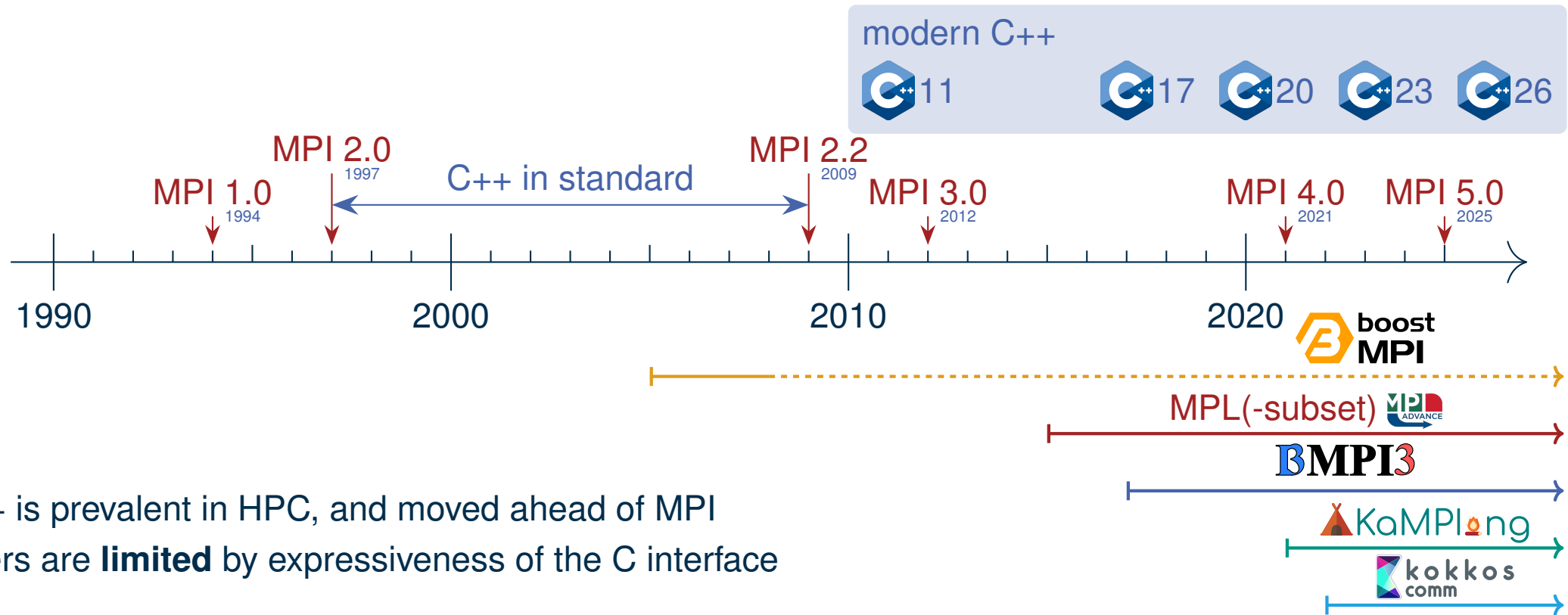
A Brief History of MPI and C++



A Brief History of MPI and C++

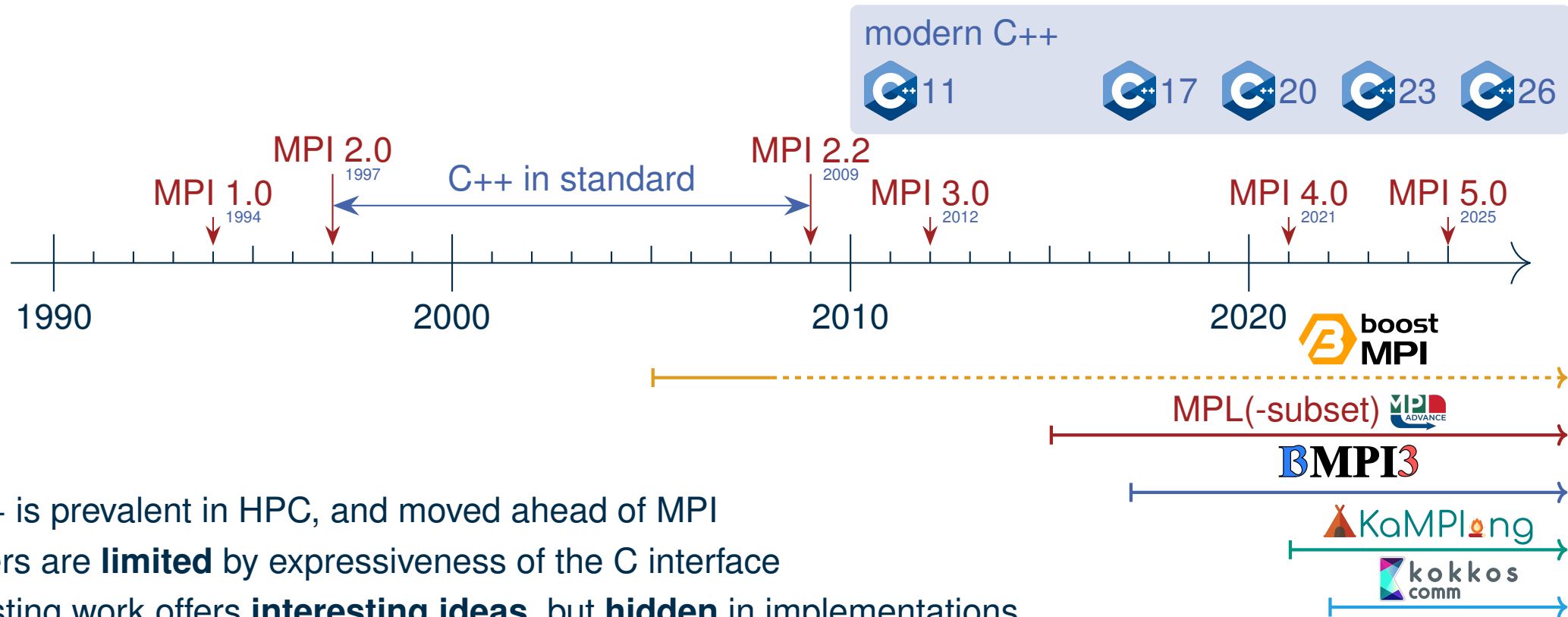


A Brief History of MPI and C++

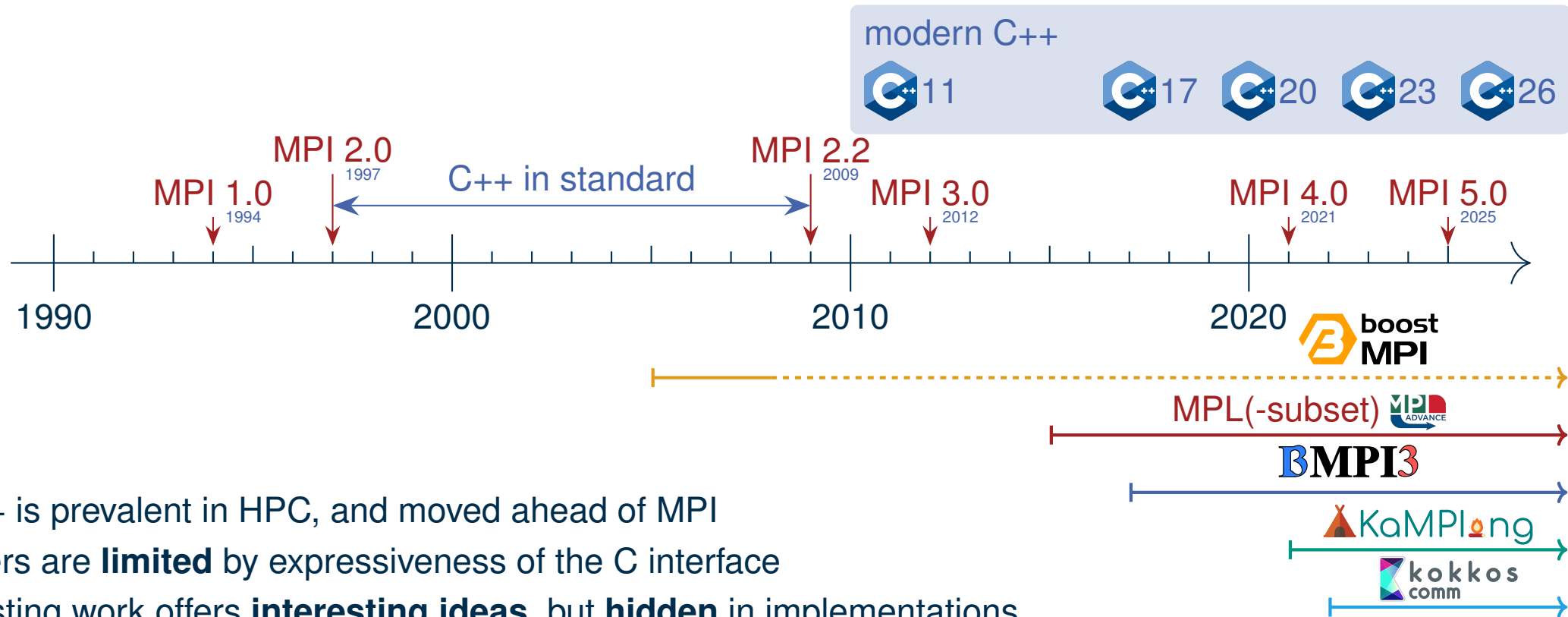


- C++ is prevalent in HPC, and moved ahead of MPI
- Users are **limited** by expressiveness of the C interface

A Brief History of MPI and C++

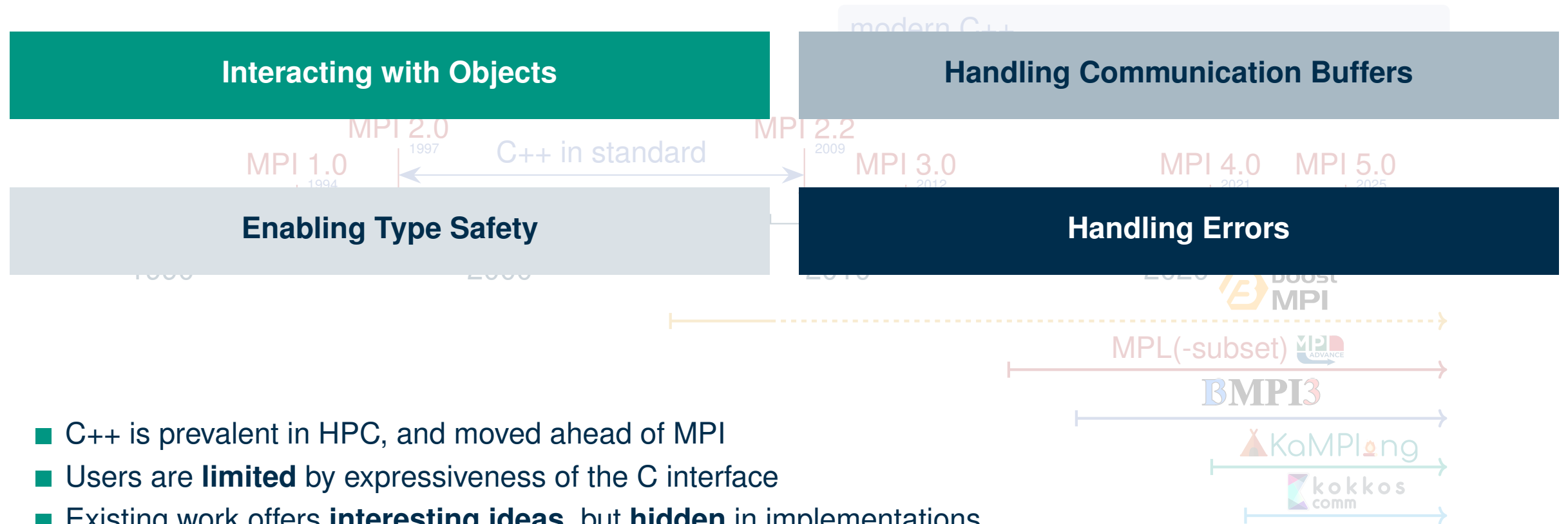


A Brief History of MPI and C++



- C++ is prevalent in HPC, and moved ahead of MPI
- Users are **limited** by expressiveness of the C interface
- Existing work offers **interesting ideas**, but **hidden** in implementations
- **Our goal:** define **semantic concepts** to **bridge** MPI and idiomatic C++

A Brief History of MPI and C++



- C++ is prevalent in HPC, and moved ahead of MPI
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Modeling Objects

- MPI users interact with **objects**
 - communicators, data types, requests, groups, info objects,
...
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 - ... and move semantics

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```
class Comm {  
public:  
    Comm(Comm const &other, Group const &group) {  
        MPI_Comm_create(other.handle(), group.handle(), &comm_);  
    }  
    Comm(Comm &&other) { ... }  
    operator=(Comm && other) { ... }  
    ~Comm() { MPI_Comm_free(&comm_); }  
private:  
    MPI_Comm comm_;  
};
```

Modeling Objects

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class Comm {...};
```

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 - via RAII (Resource Acquisition Is Initialization) ...
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```
class Comm {...};

auto construct() {
    mpi::Comm comm{parent_comm, group};
    return comm;
}

void foobar(mpi::Comm comm) {
    // ...
    // comm gets freed at
    // end of scope
}

auto comm = construct();
foobar(std::move(comm));
```


Modeling Objects

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 - but that sometimes conflicts with MPI's implicit global state

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 - ... and move semantics
 - but that sometimes conflicts with MPI's implicit global state
- **session model** aligns well with object oriented design

```
MPI_Session session = MPI_SESSION_NULL;
MPI_Session_init(MPI_INFO_NULL,
                 MPI_ERRORS_RETURN, &session);
MPI_Group group = MPI_GROUP_NULL;
MPI_Group_from_session_pset(session,
                             "mpi://WORLD", &group);
MPI_Comm comm = MPI_COMM_NULL;
MPI_Comm_create_from_group(group,
                            "org.example",
                            MPI_INFO_NULL,
                            MPI_ERRORS_RETURN, &comm);
MPI_Group_free(&group);
// ...
MPI_Comm_free(&comm);
MPI_Session_finalize(&session);
```

Modeling Objects

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 - via **opaque handles** in C
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```
MPI_Session session = MPI_SESSION_NULL;
MPI_Session_init(MPI_INFO_NULL,
                 MPI_ERRORS_RETURN, &session);
MPI_Group group = MPI_GROUP_NULL;
MPI_Group_from_session_pset(session,
                             "mpi://WORLD", &group);
MPI_Comm comm = MPI_COMM_NULL;
MPI_Comm_create_from_group(group,
                           "org.example",
                           MPI_INFO_NULL,
                           MPI_ERRORS_RETURN, &comm);

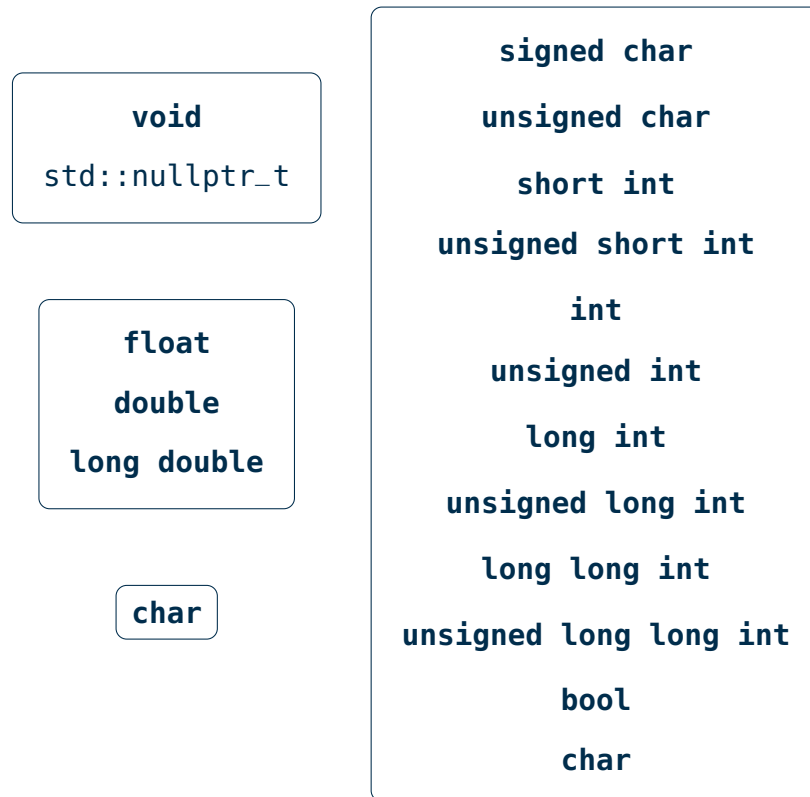
MPI_Group_free(&group);
// ...
MPI_Comm_free(&comm);
MPI_Session_finalize(&session);
```



```
mpi::Session session;
mpi::Comm comm = session.group_from_pset("mpi://WORLD")
                    .create_comm("org.example");
```

Modeling Data

Safe Type Mapping



Modeling Data

Safe Type Mapping

fundamental types

void
`std::nullptr_t`

float
double
long double

char

signed char
unsigned char
short int
unsigned short int
int
unsigned int
long int
unsigned long int
long long int
unsigned long long int
bool
char

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MPI data types

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Safe Type Mapping

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MPI data types

MPI_Type_contiguous
MPI_Type_vector
MPI_Type_create_hvector
MPI_Type_indexed
MPI_Type_create_hindexed
MPI_Type_create_struct
MPI_Type_create_subarray

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`bool`
`char`

`std::array<int, 3>`

`double[5]`

`enum class MyEnum {...};`

```
struct MyType {  
    int a;  
    std::array<int, 3> b;  
    double c;  
    char d;  
};
```

MPI data types

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`MPI_Type_create_subarray`

Modeling Data

Safe Type Mapping

fundamental types

float
double
long double

char

```
template<typename T, size_t N>
struct type_traits<std::array<T, N>> {
    static MPI_Datatype type() {
        MPI_Datatype type;
        MPI_Type_contiguous(N,
            type_traits<T>::type(),
            &type);
        return type;
    }
};
```

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unsigned int
long int
unsigned long int
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bool
char

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Modeling Data

Safe Type Mapping

fundamental types

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double
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```
template<typename T, size_t N>  
struct type_traits<std::array<T, N>> {  
    static MPI_Datatype type() {  
        MPI_Datatype type;  
        MPI_Type_contiguous(N,  
            type_traits<T>::type(),  
            &type);  
        return type;  
    }  
};
```

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MPI data types

MPI_Type_contiguous

MPI_Type_vector

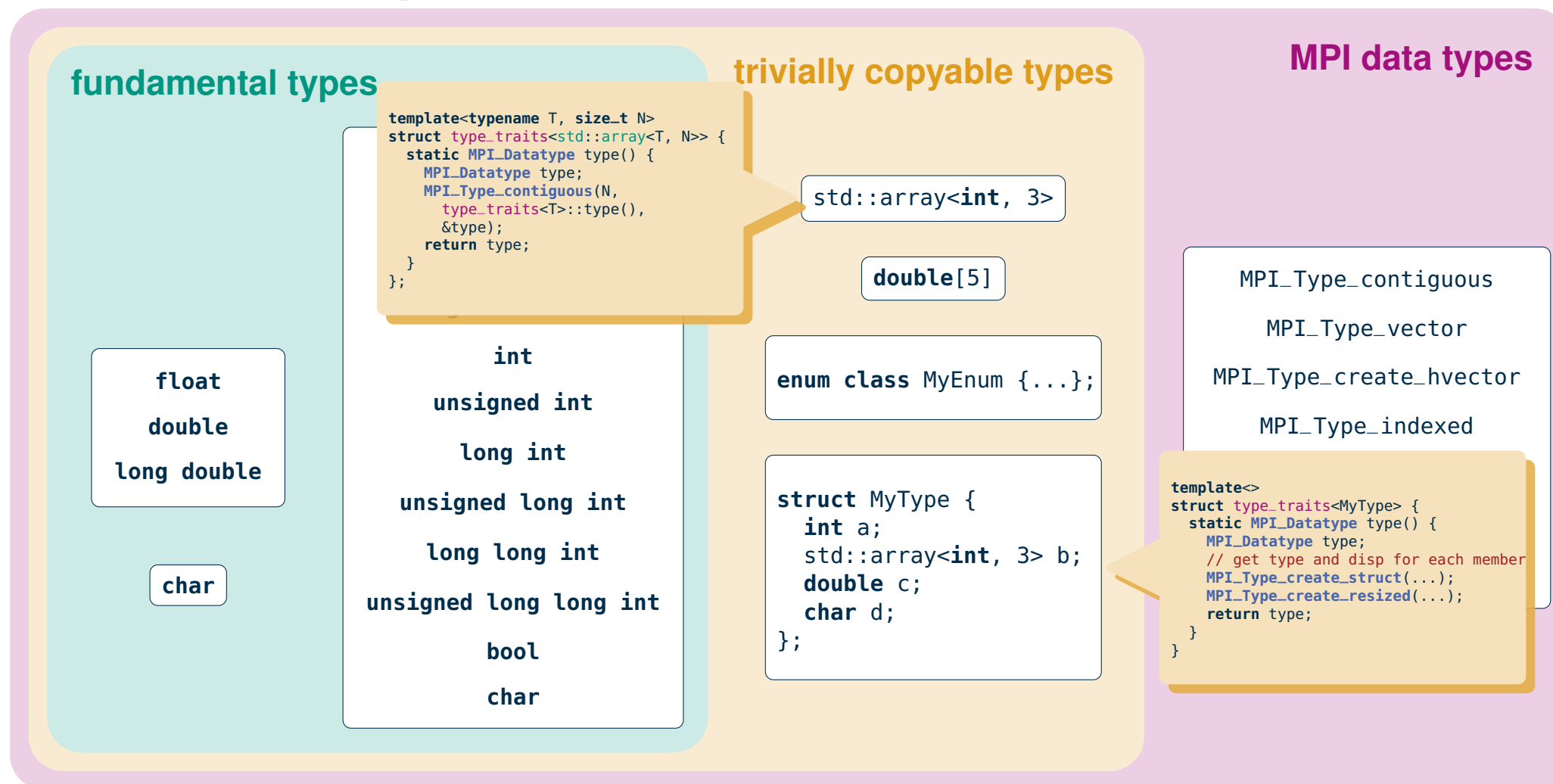
MPI_Type_create_hvector

MPI_Type_indexed

```
template<>  
struct type_traits<MyType> {  
    static MPI_Datatype type() {  
        MPI_Datatype type;  
        // get type and disp for each member  
        MPI_Type_create_struct(...);  
        MPI_Type_create_resized(...);  
        return type;  
    }  
};
```

Modeling Data

Safe Type Mapping



Modeling Data

Safe Type Mapping

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trivially copyable types

`std::array<int, 3>`

`double[5]`

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MPI data types

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`MPI_Type_indexed`
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`MPI_Type_create_struct`
`MPI_Type_create_subarray`

Modeling Data

Handling Memory Buffers

```
std::vector<int> v = {...};  
MPI_Sendrecv(v.data(), v.size(), MPI_INT, dest, ...);
```

Modeling Data

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template<typename T>
int sendrecv(std::vector<T> const& s, int dest, ...) {
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Problem: ad-hoc, limited to a fixed set of containers → **Solution:** define general concepts

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int MPI_Sendrecv(const void *sendbuf,
                 int sendcount,
                 MPI_Datatype sendtype,
                 int dest,
                 int sendtag,
                 void *recvbuf,
                 int recvcount,
                 MPI_Datatype recvtype,
                 int source,
                 int recvtag,
                 MPI_Comm comm,
                 MPI_Status *status)
```

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send buffer

recv buffer

Modeling Data

Handling Memory Buffers

```
template<DataBuffer SendBuf>
int sendrecv(SendBuf&& s, int dest, ...) {
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```

send buffer

recv buffer

```
template <typename T>
concept DataBuffer =
```

Modeling Data

Handling Memory Buffers

```
template<DataBuffer SendBuf>
int sendrecv(SendBuf&& s, int dest, ...) {
    return MPI_Sendrecv(std::ranges::data(s), s.size(), MPI_INT, dest, ...);
}
```

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int MPI_Sendrecv(const void *sendbuf,
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```

send buffer

recv buffer

```
template <typename T>
concept DataBuffer =
    std::ranges::contiguous_range<T>;
```

Modeling Data

Handling Memory Buffers

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template <typename T>
concept DataBuffer =
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```

Modeling Data

Handling Memory Buffers

```
template<DataBuffer SendBuf>
int sendrecv(SendBuf&& s, int dest, ...) {
    return MPI_Sendrecv(std::ranges::data(s), std::ranges::size(s), mpi::type(s), dest, ...);
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send buffer

recv buffer

```
template <typename T>
concept DataBuffer =
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    std::ranges::sized_range<T> && mpi::Typed<T>;
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Handling Memory Buffers

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template<SendBuffer SendBuf>
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template <typename T>
concept SendBuffer =
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    std::ranges::input_range<T>;
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Handling Memory Buffers

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template <typename T>
concept SendBuffer =
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    std::ranges::input_range<T>;

template <typename T>
concept RecvBuffer =
    DataBuffer<T> &&
    std::ranges::output_range<T,
        std::ranges::range_value_t<T>>;
```


Modeling Data

Handling Memory Buffers

```
template<SendBuffer SendBuf>
int sendrecv(SendBuf&& s, int dest, ...) {
    return MPI_Sendrecv(std::ranges::data(s), std::ranges::size(s), mpi::type(s), dest, ...);
}
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```
template <typename Buf>
concept Typed = requires(Buf buf) {
    { mpi::type(buf) } -> std::same_as<MPI_Datatype>;
};
```

```
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Modeling Data

Handling Memory Buffers

```
template<SendBuffer SendBuf>
int sendrecv(SendBuf&& s, int dest, ...) {
    return MPI_Sendrecv(std::ranges::data(s), std::ranges::size(s), mpi::type(s), dest, ...);
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template <typename Buf>
concept Typed = requires(Buf buf) {
    { mpi::type(buf) } -> std::same_as<MPI_Datatype>;
};
```

```
template <typename Buf>
requires mpi::has_static_type<
    std::ranges::range_value_t<Buf>> ||
    has_type_member<Buf>
MPI_Datatype type(Buf &buf) {
    if constexpr (has_type_member<Buf>) {
        return buf.type();
    } else {
        type_traits<std::ranges::range_value_t<Buf>>();
    }
}
```

```
template <typename T>
concept DataBuffer =
    std::ranges::contiguous_range<T> &&
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```

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template <typename T>
concept SendBuffer =
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```

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Modeling Data

Handling Memory Buffers

```
template<SendBuffer SendBuf>
int sendrecv(SendBuf&& s, int dest, ...) {
    return MPI_Sendrecv(std::ranges::data(s), std::r
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concept Typed = requires(Buf buf) {
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template <typename Buf>
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MPI_Datatype type(Buf &buf) {
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        return buf.type();
    } else {
        type_traits<std::ranges::range_value_t<Buf>>(<
    }
}
```

Examples

```
std::vector<int> v = {...};
int dest = ...;
int* buf = {...};

// send a vector directly
comm.send(v, dest);

// send something from a raw pointer
comm.send(std::span(buf, BUFSIZE), dest);

// send a single element
comm.send(std::views::single {42}, dest);

// send only the first 4 elements
comm.send(v | std::views::take(4), dest);

// send with custom type
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// send a kokkos view, internally repacking data
// or constructing an appropriate type
Kokkos::View<int*> kv (...);
comm.send(kokkos_adapter {kv}, dest);

// accelerator support, adapting .data()
thrust::device_vector<int> dv;
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Modeling Data

Handling Memory Buffers

```
template<SendBuffer SendBuf>
int sendrecv(SendBuf&& s, int dest, ...) {
    return MPI_Sendrecv(std::ranges::data(s), std::r
```

Problem: ad-hoc, limited to a fixed set of containers

```
template <typename Buf>
concept Typed = requires(Buf buf) {
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Examples

```
std::vector<int> v = {...};
int dest = ...;
int* buf = {...};

// send a vector directly
comm.send(v, dest);

// send something from a raw pointer
comm.send(std::span(buf, BUFSIZE), dest);

// send a single element
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Modeling Data

Handling Memory Buffers

```
template<SendBuffer SendBuf>
int sendrecv(SendBuf&& s, int dest, ...) {
```

Collectives with varying counts

```
std::vector<int> send_buf = {...};
std::vector<int> recv_buf = {...};

// does not compile, send_buf
// needs members .sizev() and .displs()
comm.scatterv(send_buf, recv_buf, root);

// adapt data buffer with count information
comm.scatterv(
    mpi::vbuf {send_buf, scounts, sdisp},
    recv_buf,
    root
);

} else {
    type_traits<std::ranges::range_value_t<Buf>>()
}
}
```

Examples

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std::vector<int> v = {...};
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Modeling Data

Ownership

- Modeling data as **data buffers** allows for a better **ownership** model
- Clear **responsibility** for freeing memory

```
std::vector<int> recv_buf = {...};
```

```
recv_buf = comm.recv(std::move(recv_buf), ...);
```

Modeling Data

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```
std::vector<int> recv_buf = {...};  
  
recv_buf = comm.recv(std::move(recv_buf), ...);
```



A yellow callout box with the text "transfer ownership to library" is connected by a yellow arrow to the `std::move(recv_buf)` expression in the second line of code.

Modeling Data

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- Modeling data as **data buffers** allows for a better **ownership** model
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```
std::vector<int> recv_buf = {...};  
  
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transfer ownership to library

return ownership to caller

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std::vector<int> recv_buf = {...};  
  
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transfer ownership to library

return ownership to caller

captured by reference
→ value not returned

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- **Memory safety** guarantees for non-blocking communication **for free**

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std::vector<int> recv_buf = {...};  
  
recv_buf = comm.recv(std::move(recv_buf), ...);  
  
comm.recv(recv_buf, ...);
```

transfer ownership to library

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```
auto req = comm.irecv(recv_buf, ...);  
  
// ... other computations  
  
req.wait(...);
```

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std::vector<int> recv_buf = {...};  
  
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auto req = comm.irecv(  
  
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```

```
recv_buf , ...);
```

access to
recv_buf
prohibited

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comm.recv(recv_buf, ...);  
  
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req.wait(...);
```

Diagram annotations:

- `std::move(recv_buf)` in the first `recv` call: transfer ownership to library
- `recv_buf` in the second `recv` call: return ownership to caller
- `recv_buf` in the third `recv` call: captured by reference → value not returned
- `req` in the `wait` call: `mpi::request<std::vector<int>>`
- Between `comm.recv(recv_buf, ...);` and `req.wait(...);`: access to `recv_buf` prohibited

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comm.recv(recv_buf, ...);
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mpi::request<std::vector<int>>  
  
auto req = comm.irecv(std::move(recv_buf), ...);  
  
// ... other computations  
  
recv_buf = req.wait(...);  
  
std::optional<std::vector<int>> result = req.test(...);
```

access to recv_buf prohibited

return ownership

Handling Errors

- Meta-programming allows catching many (usage) errors at **compile-time**

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Errors via exceptions

```
try {  
    std::vector<int> buf = comm.recv(std::vector<int>(recv_size), src, tag);  
    // [...] computation  
} catch (const mpi::exception& e) {  
    std::cerr << "Recv_failed:_" << e.what() << "\n";  
}
```

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Errors via `std::expected`

```
std::expected result = comm.recv(std::vector<int>(recv_size), src, tag);  
if (result) {  
    std::vector buf = std::move(*result);  
    // [...] computation  
} else {  
    std::cerr << "Recv_failed:_"  
                << result.error().message() << "\n";  
    auto recovered_buffer = std::move(result).error().recv_buf();  
}
```

Conclusion

We started deriving **language support guidelines** for C++

Core aspects

- Object model
- Data representation
- Ownership
- Modeling and mapping types
- Idiomatic error handling

Future work

- Build a reference implementation (+ extensions for accelerators, libraries, ...)
- Concretize guidelines for non-blocking, one-sided, partitioned, ... communication
- Improve MPI's language interoperability, without sacrificing a C++ performance path

Open Question: How to bring C++ back to the MPI standard?

Sincere thanks to everyone who contributed to the MPI Languages WG discussions.

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Acknowledgments

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