

Concepts for designing modern C++ interfaces for MPI

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```
asserting_cast<size_t>(recv_buf.size() + 1);
recv_buf.resize_if_requested(compute_recv_size);
KASSERT(
    // if the recv type is user provided
    // recv buffer
    !recv_type_has_to_be_deduced || recv_type_is_user_provided,
    "Recv buffer is not large enough to receive"
) assert::light;

// These KASSERTs are required to avoid a false positive
KASSERT(send_buf.data() != nullptr, assert::light);
KASSERT(recv_buf.data() != nullptr, assert::light);

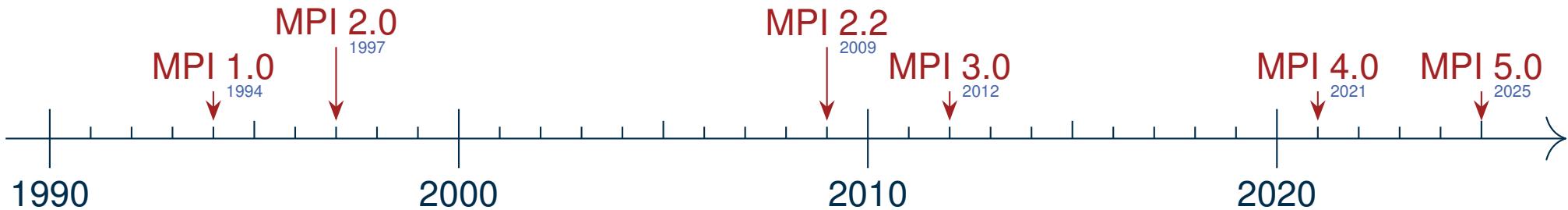
[[maybe_unused]] int err = MPI_Alltoall(
    send_buf.data(),
    send_count.get_single_element(),
    send_type.get_single_element(),
    recv_buf.data(),
    recv_count.get_single_element(),
    recv_type.get_single_element(),
    mpi_communicator()
) assert::light;

error_hook(err, MPI_RESULT_STATUS(recv_buf),
    MPI_RESULT_TYPE(recv_type),
    MPI_RESULT_COUNT(recv_count),
    MPI_RESULT_SOURCE(recv_source),
    MPI_RESULT_DEST(recv_dest));

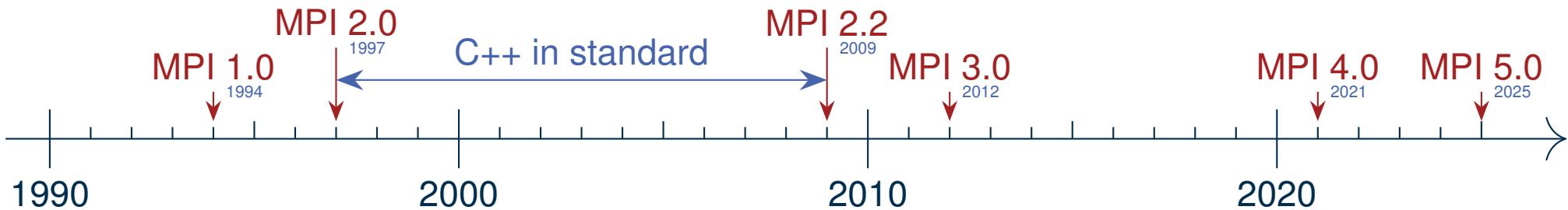
```



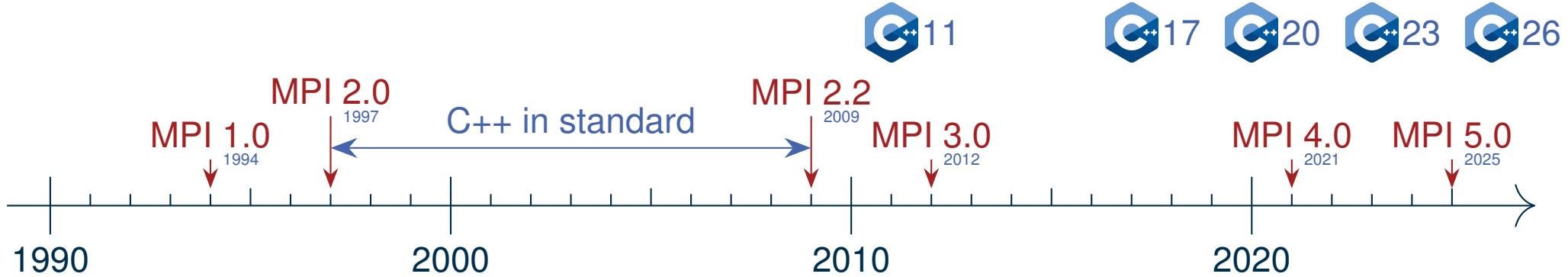
A Brief History of MPI and C++



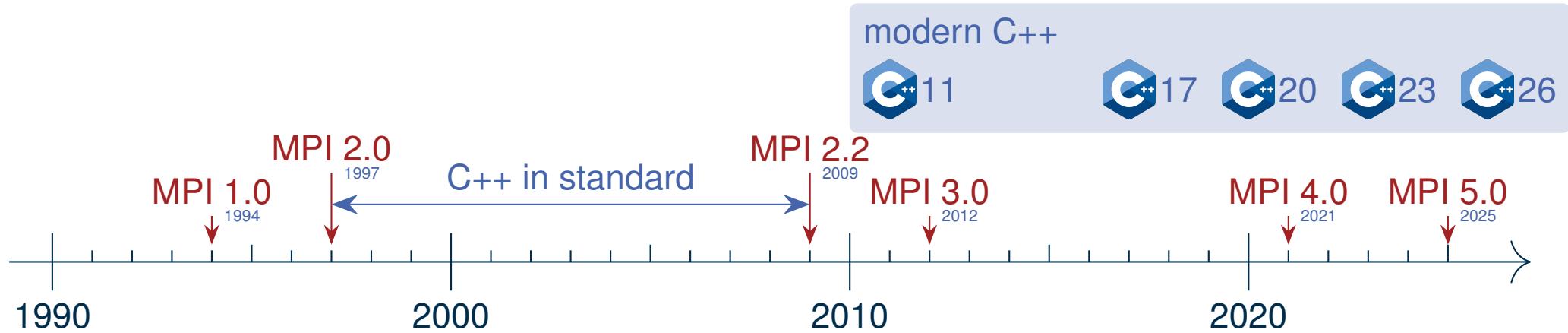
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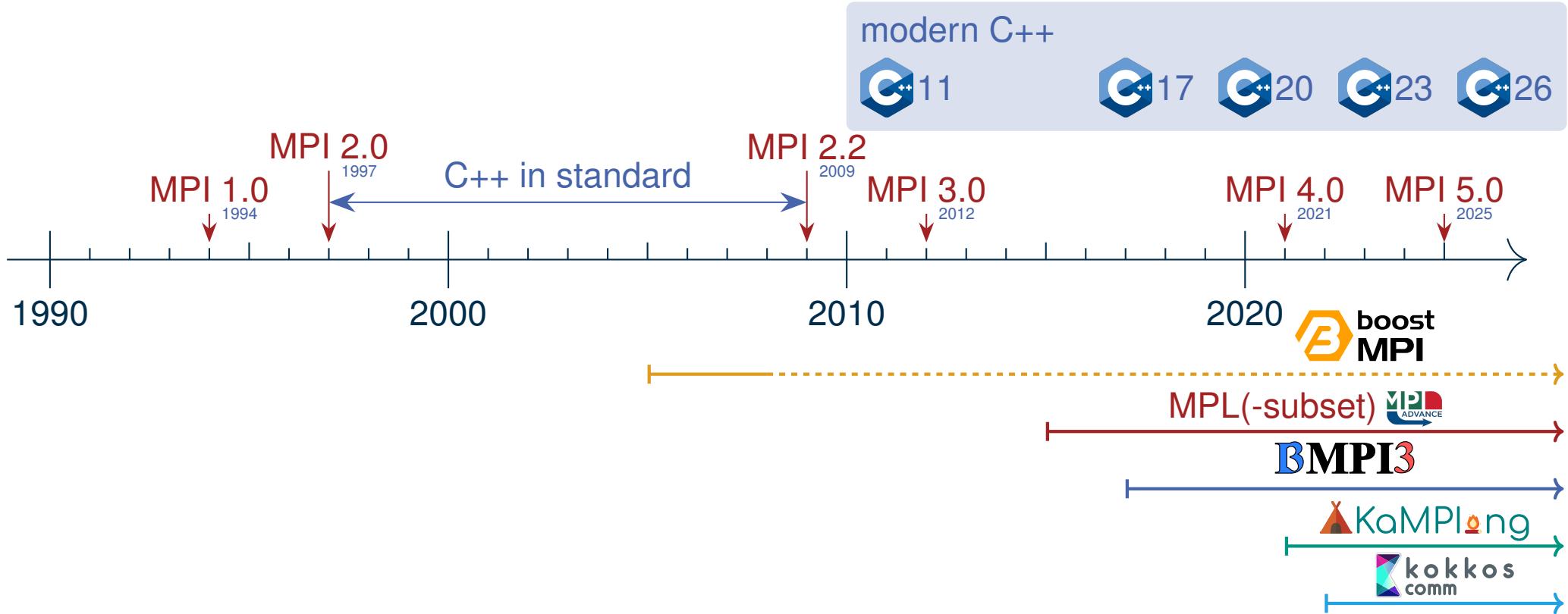
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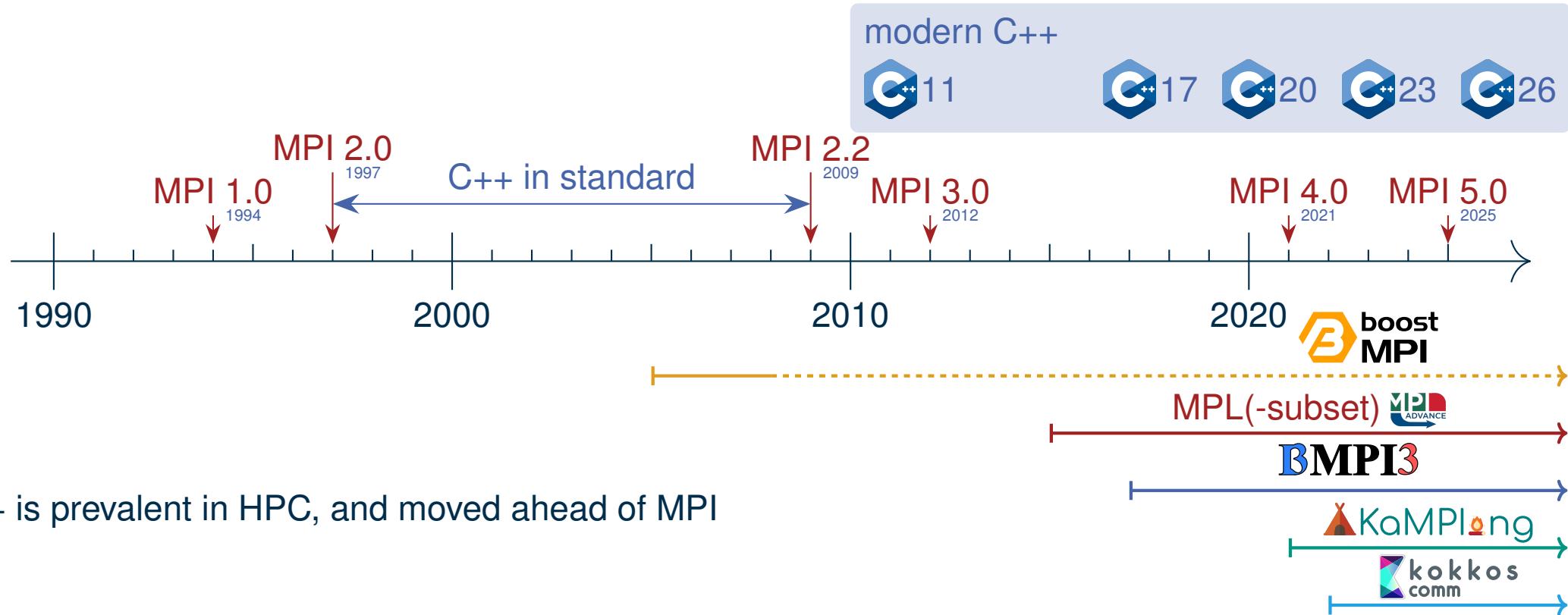
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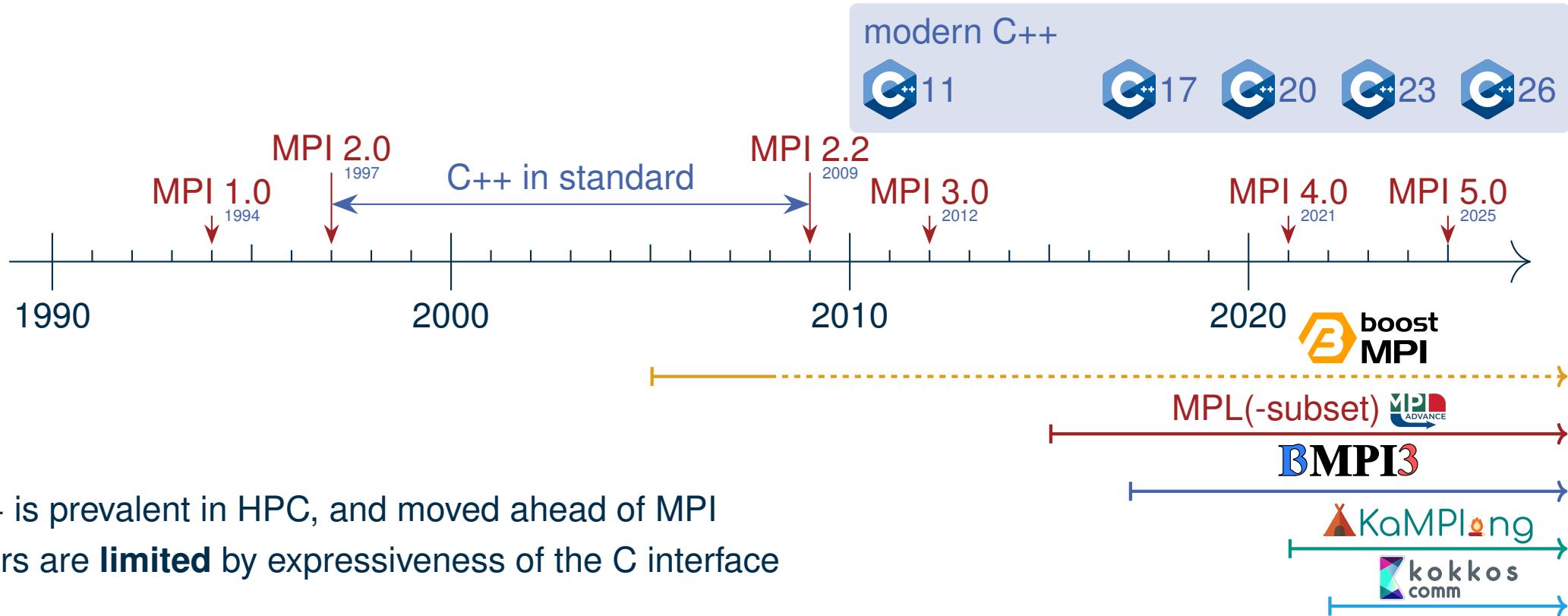
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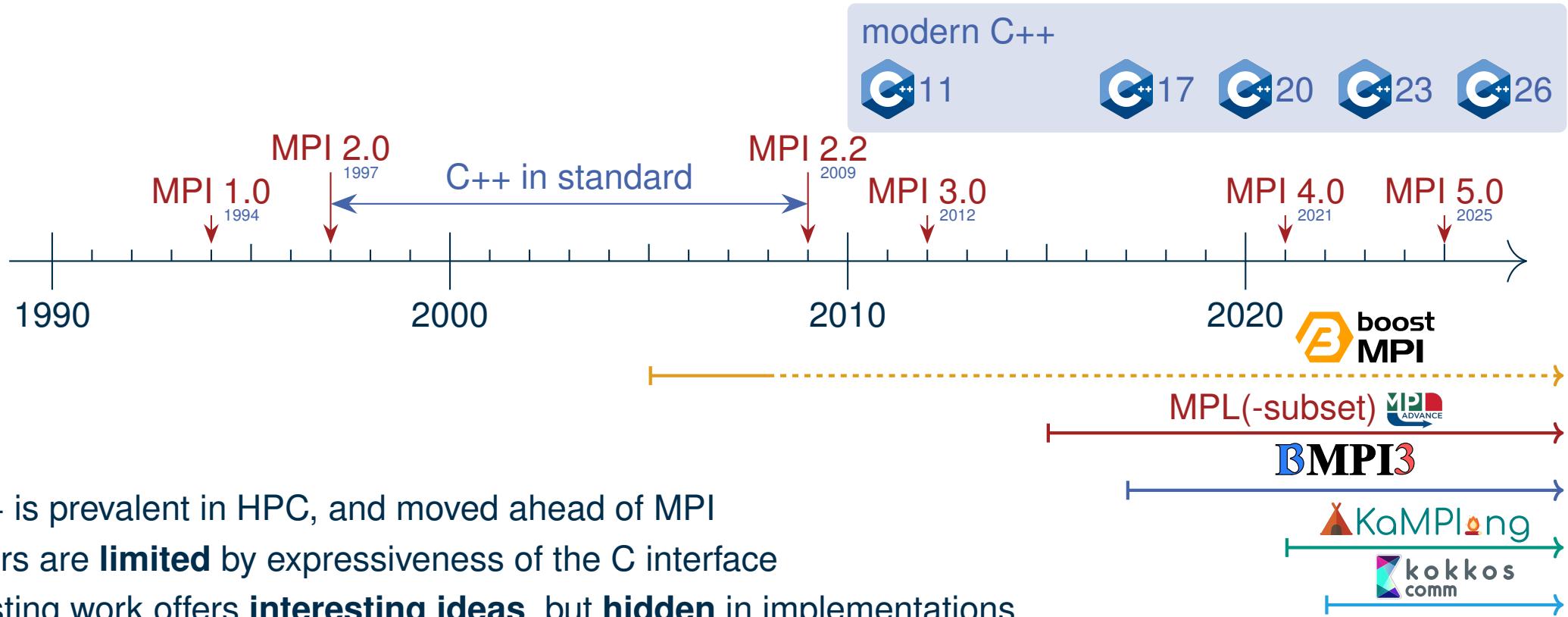
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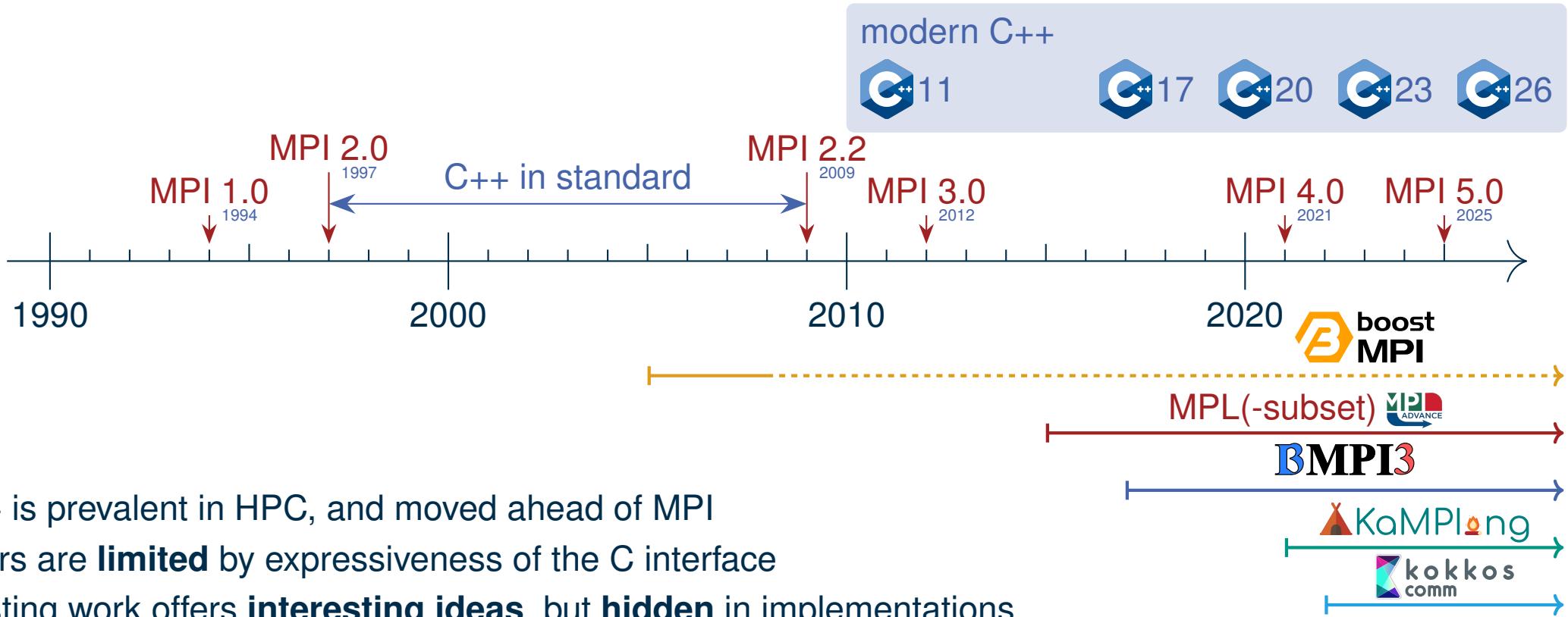
A Brief History of MPI and C++



A Brief History of MPI and C++



A Brief History of MPI and C++



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++

Modeling Objects

- MPI users interact with **objects**
 - communicators, data types, requests, groups, info objects,
...
 - via **opaque handles** in C

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 - ... and move semantics

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■ ... and move semantics

```
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

```
class Comm {...};
```

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...
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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);
```

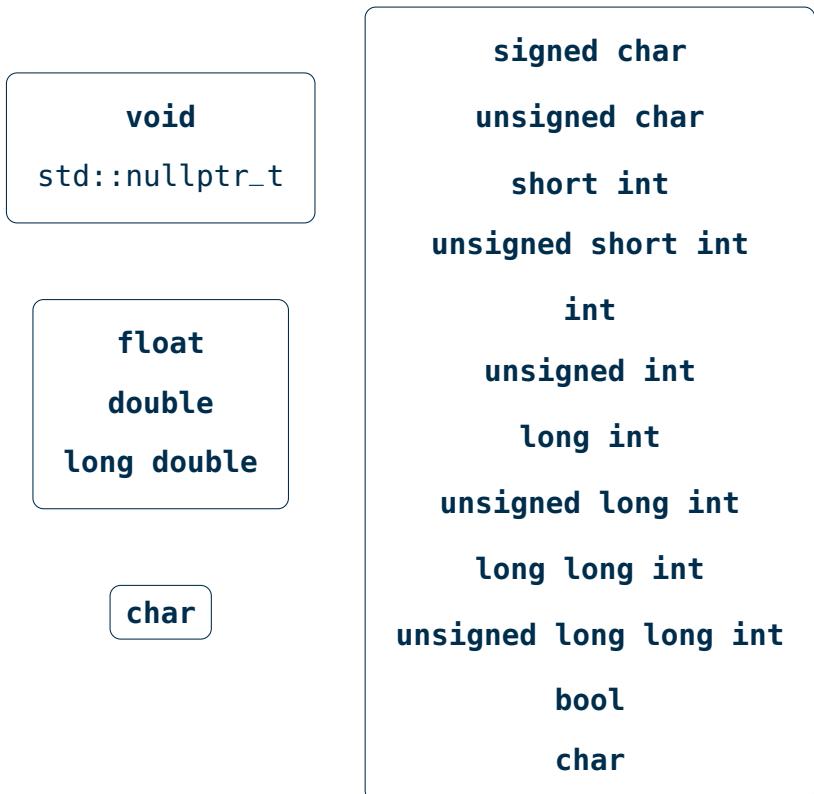
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 - communicators, data types, requests, groups, info objects, ...
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 - but that sometimes conflicts with MPI's implicit global state
- **session model** aligns well with object oriented design

```
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);  
  
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`
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`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`

Modeling Data

Safe Type Mapping

fundamental types

```
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
```

```
std::array<int, 3>
```

```
double[5]
```

```
enum class MyEnum {...};
```

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

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Safe Type Mapping

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`double`
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`char`

`int`
`unsigned int`
`long int`
`unsigned long int`
`long long int`
`unsigned long long int`
`bool`
`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;
    }
};
```

`std::array<int, 3>`
`double[5]`

`enum class MyEnum { ... };`

```
struct MyType {
    int a;
    std::array<int, 3> b;
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```

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MPI data types

MPI_Type_contiguous
MPI_Type_vector
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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;
    }
};
```

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Safe Type Mapping

fundamental types

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double
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char

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        return type;
    }
};
```

trivially copyable types

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double[5]

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    }
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```

Modeling Data

Safe Type Mapping

fundamental types

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float  
double  
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signed char  
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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

Handling Memory Buffers

```
template<typename T>
int sendrecv(std::vector<T> const& s, int dest, ...) {
    return MPI_Sendrecv(s.data(), s.size(), MPI_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, ...) {
    return MPI_Sendrecv(s.data(), s.size(), MPI_INT, dest, ...);
}
```

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                  int recvtag,
                  MPI_Comm comm,
                  MPI_Status *status)
```

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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                  int source,
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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<DataBuffer SendBuf>
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send buffer recv buffer

```
template <typename T>
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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 =
    std::ranges::contiguous_range<T> &&
    std::ranges::sized_range<T> && mpi::Typed<T>;
```

Modeling Data

Handling Memory Buffers

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template<SendBuffer> SendBuf>
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send buffer
recv buffer

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```

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

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Handling Memory Buffers

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    std::ranges::sized_range<T> && mpi::Typed<T>;
```

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

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

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Handling Memory Buffers

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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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Problem: ad-hoc, limited to a fixed set of containers → **Solution:** define general concepts

```
template <typename Buf>
concept Typed = requires(Buf buf) {
    { mpi::type(buf) } -> std::same_as<MPI_Datatype>;
};
```

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

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

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

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Handling Memory Buffers

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template<SendBuffer SendBuf>
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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> &&
    std::ranges::sized_range<T> && mpi::Typed<T>;

template <typename T>
concept SendBuffer =
    DataBuffer<T> &&
    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::r...
```

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

```
template <typename Buf>
concept Typed = requires(Buf buf) {
    { mpi::type(buf) } -> std::same_as<MPI_Datatype>};

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Examples

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

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

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comm.send(std::span(buf, BUFSIZE), dest);

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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
comm.send(v | with_type(MY_MPI_TYPE), dest);

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// or constructing an appropriate type
Kokkos::View<int*> kv (...);
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thrust::device_vector<int> dv;
comm.send(thrust_adapter {dv}, dest);
```

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

```
    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);

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    thrust::device_vector<int> dv;
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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 Ownership

- Modeling data as **data buffers** allows for a better **ownership** model
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```
std::vector<int> recv_buf = {...};  
                                ^ transfer ownership to library  
recv_buf = comm.recv(std::move(recv_buf), ...);
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Modeling Data Ownership

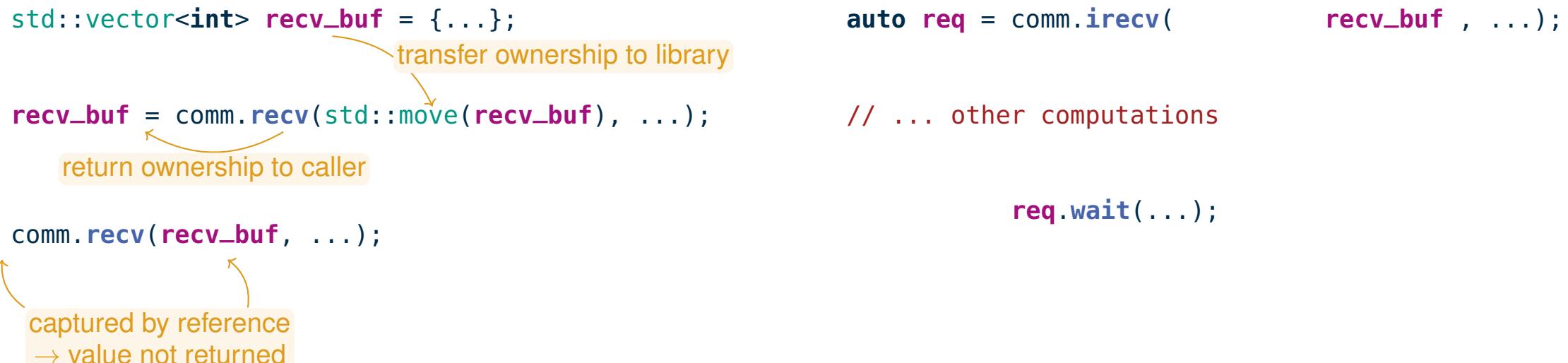
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comm.recv(recv_buf, ...);  
                                ^ captured by reference  
                                → value not returned
```

Modeling Data Ownership

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

```
std::vector<int> recv_buf = {...};  
auto req = comm.irecv(           recv_buf , ...);  
  
recv_buf = comm.recv(std::move(recv_buf), ...);    // ... other computations  
                                                 // return ownership to caller  
  
comm.recv(recv_buf, ...);  
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// ... other computations  
req.wait(...);  
  
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captured by reference  
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transfer ownership to library

return ownership to caller

access to recv_buf prohibited

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mpi::request<std::vector<int>>  
auto req = comm.irecv(std::move(recv_buf), ...);  
                                ↑  
                                // ... other computations  
                                ↑  
                                access to  
                                recv_buf  
                                prohibited  
req.wait(...);
```

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// ... other computations  
  
recv_buf = req.wait(...);  
                                ↑  
                                return ownership  
  
std::optional<std::vector<int>> result = req.test(...);
```

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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} catch (const mpi::exception& e) {
    std::cerr << "Recv_failed:" << e.what() << "\n";
}
```

Errors via std::expected

```
std::expected<result> result = comm.recv(std::vector<int>(recv_size), src, tag);
if (result) {
    std::vector buf = std::move(*result);
    // [...]
} 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?

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Acknowledgments

This project has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation program (grant agreement No. 882500).

PSAAP Funding in part is acknowledged from these NSF Grants OAC-2514054, CNS-2450093, CCF-2405142, and CCF-2412182 and the U.S. Department of Energy's National Nuclear Security Administration (NNSA) under the Predictive Science Academic Alliance Program (PSAAP-III), Award DE-NA0003966.

AAC work performed under the auspices of the US Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344, and supported by the Center for Non-Perturbative Studies of Functional Materials Under Non-Equilibrium Conditions (NPNEQ) funded by the Computational Materials Sciences Program of the US Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division. This work was also performed under the auspices of the US Department of Energy's Pacific Northwest National Laboratory, operated by Battelle Memorial Institute under contract DE-AC05-76RL01830.

Any opinions, findings, and conclusions or recommendations expressed in this material are those of the authors and do not necessarily reflect the views of the National Science Foundation, or the U.S. Department of Energy's National Nuclear Security Administration.