Karlsruhe Institute of Technology

KaMPIng: Flexible and (Near) Zero-Overhead C++ Bindings for MPI

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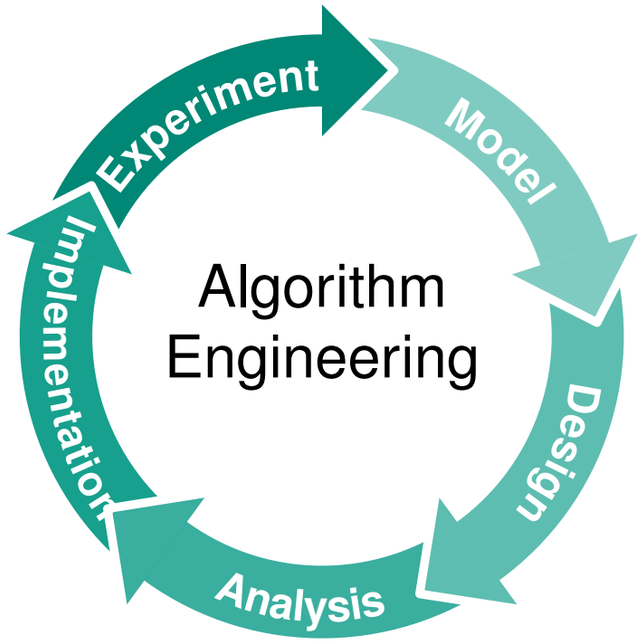
Tim Niklas Uhl, Matthias Schimek, Lukas Hübner, Demian Hespe,
Florian Kurpicz, Daniel Seemaier, Christoph Stelz, Peter Sanders

The Trail to HPC



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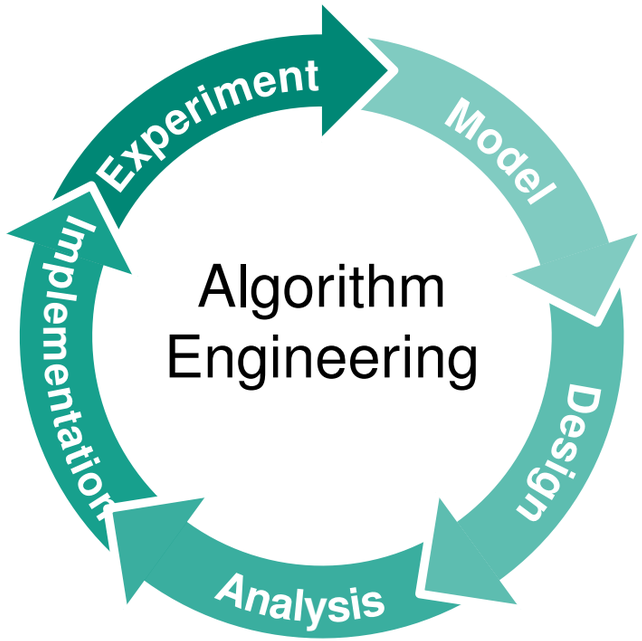

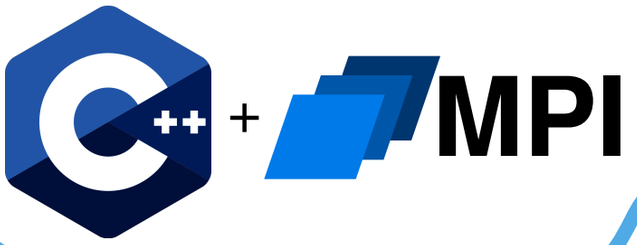

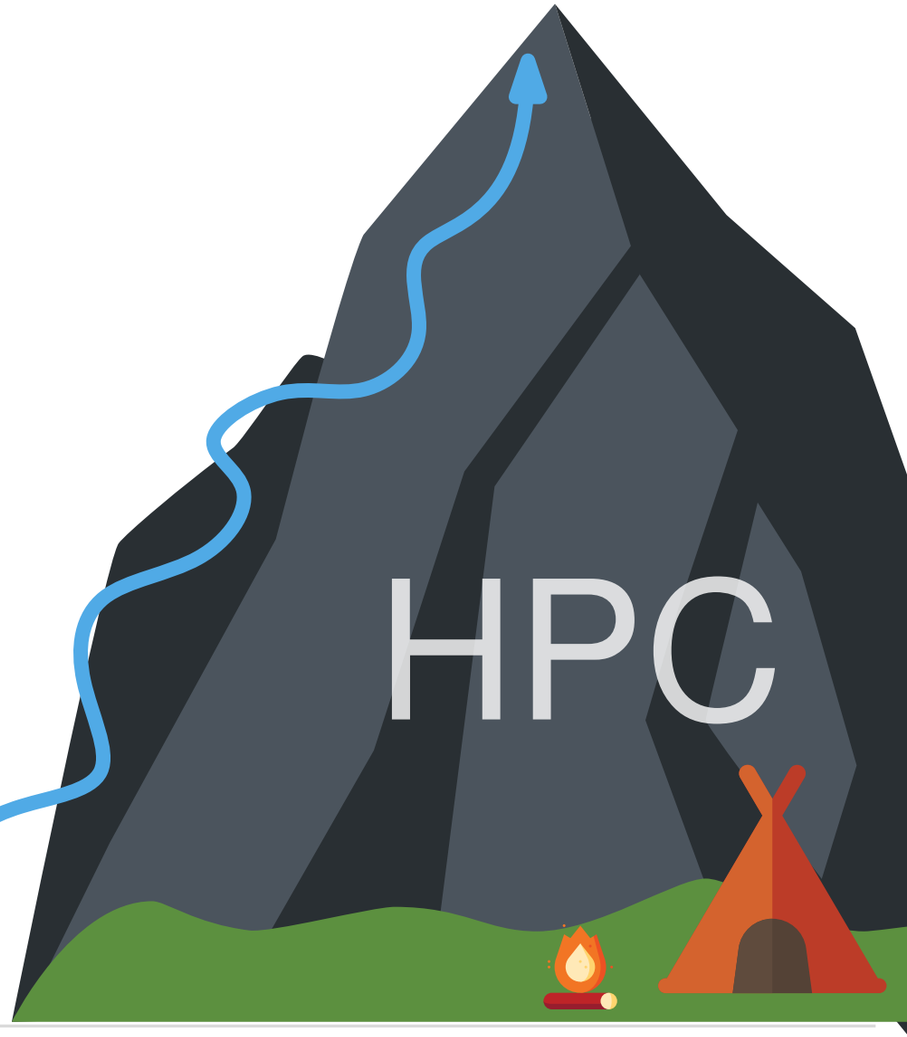

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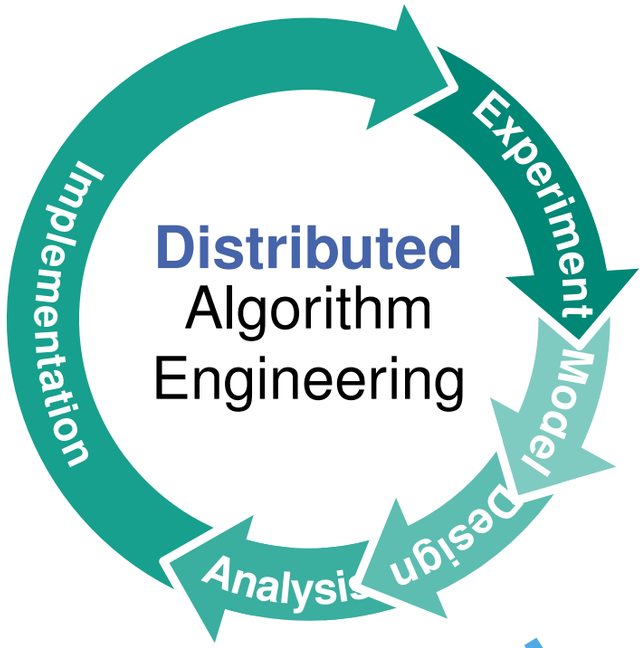

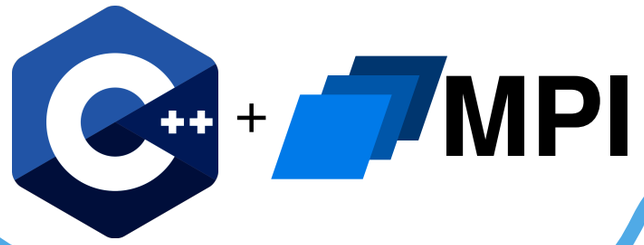

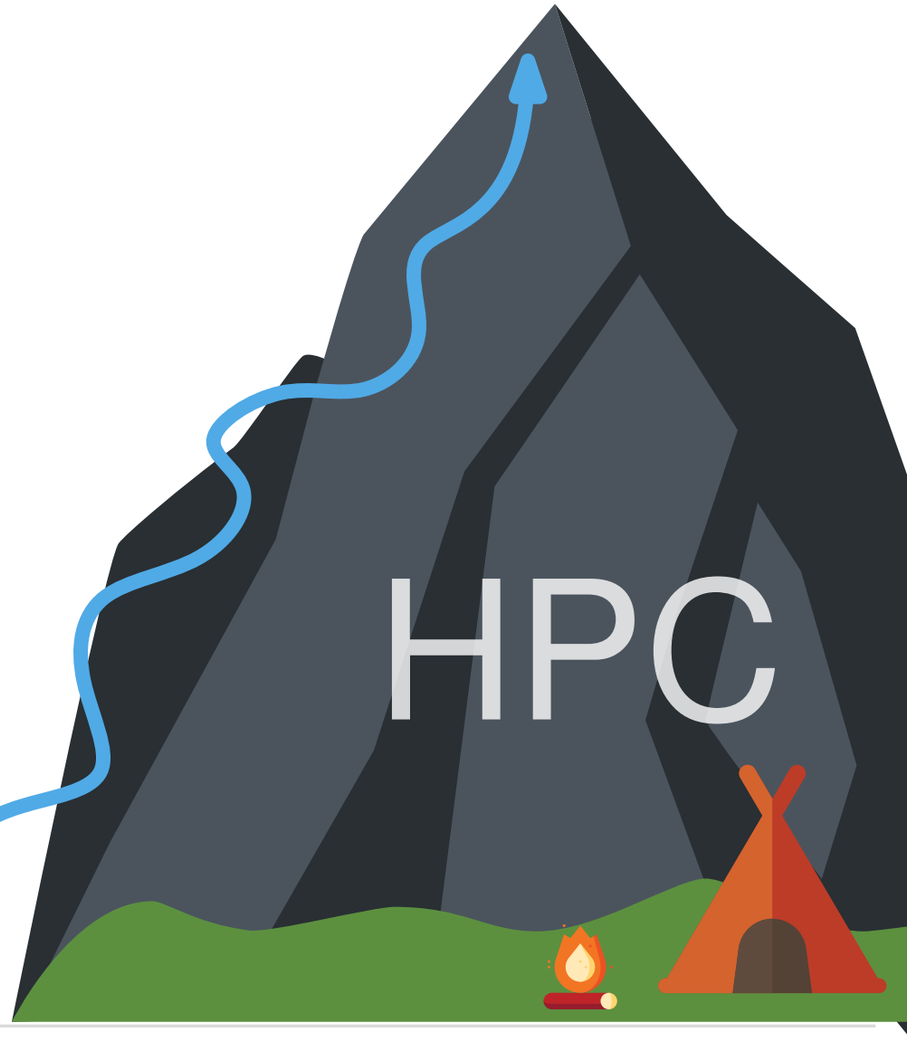

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The baggage of using C++ + MPI

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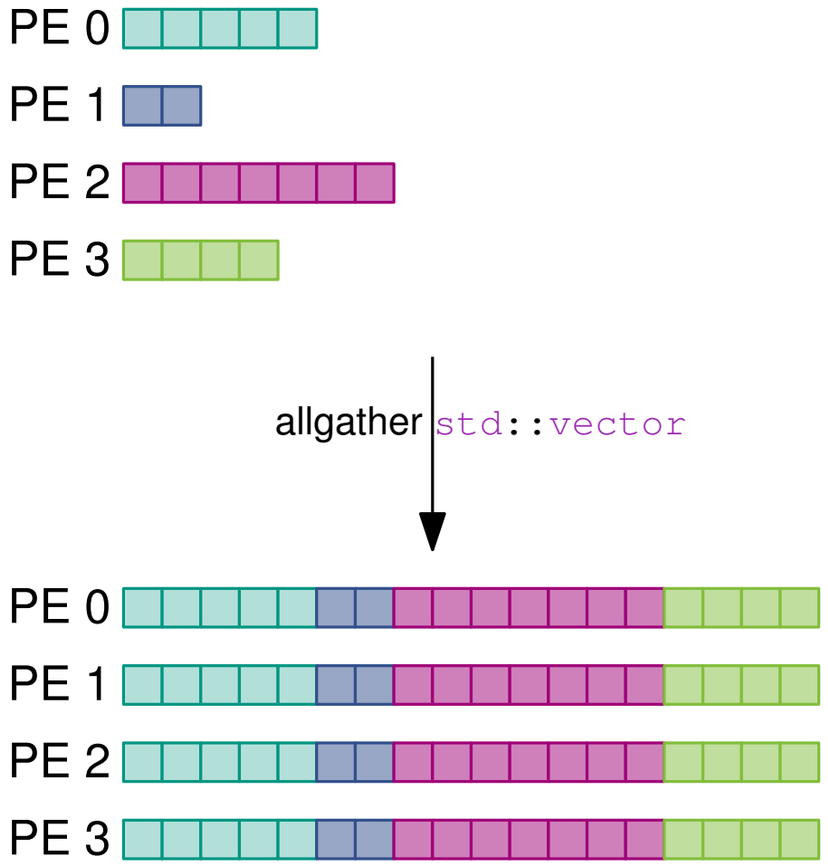

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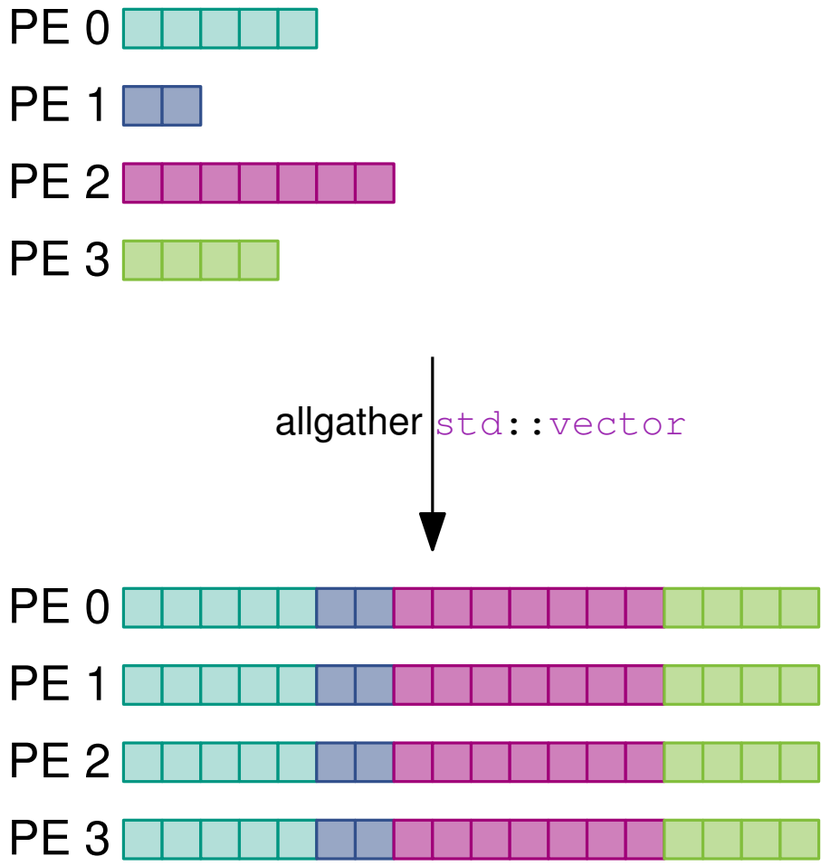
The baggage of using C++ + MPI

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std::vector<double> get_whole_vector(std::vector<double> const& v_local,
                                     MPI_Comm comm) {
  int size;
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  rc[rank] = v_local.size();
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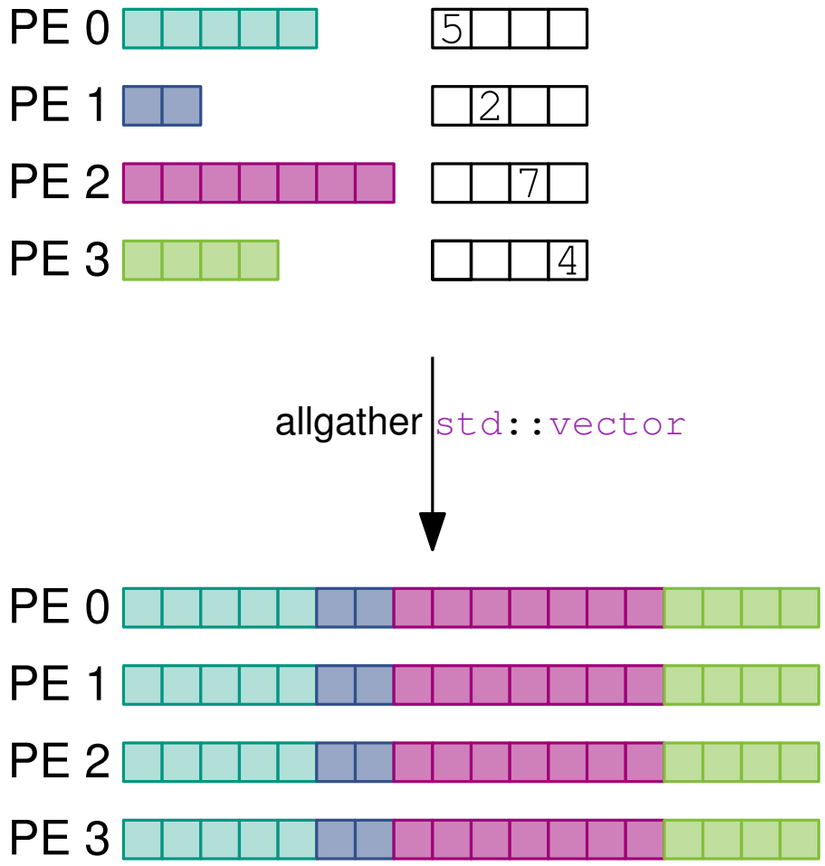


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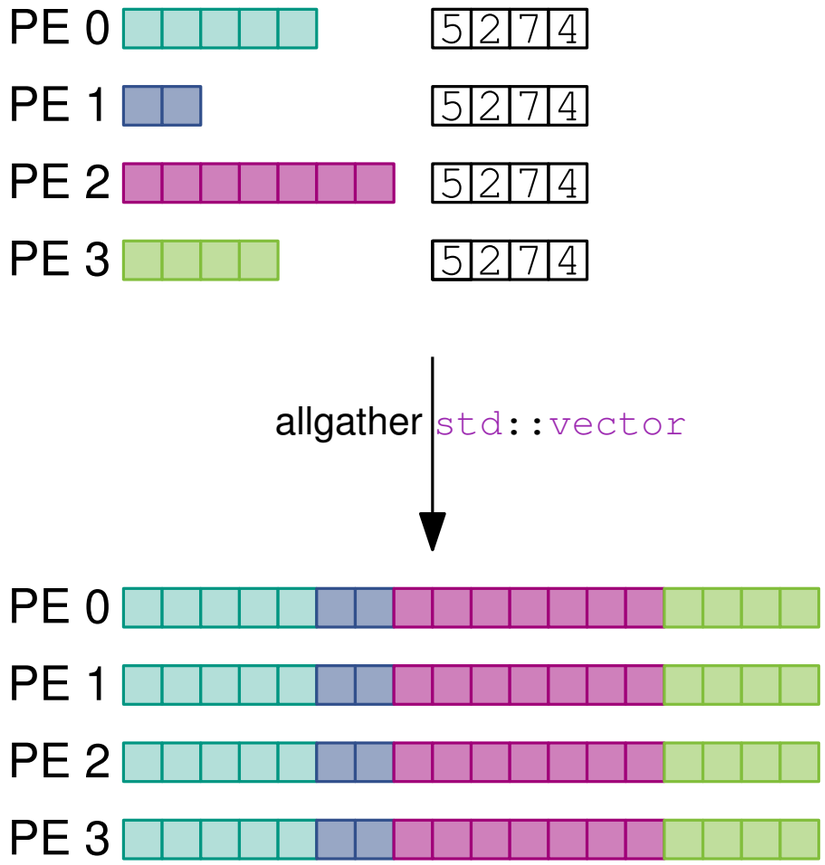


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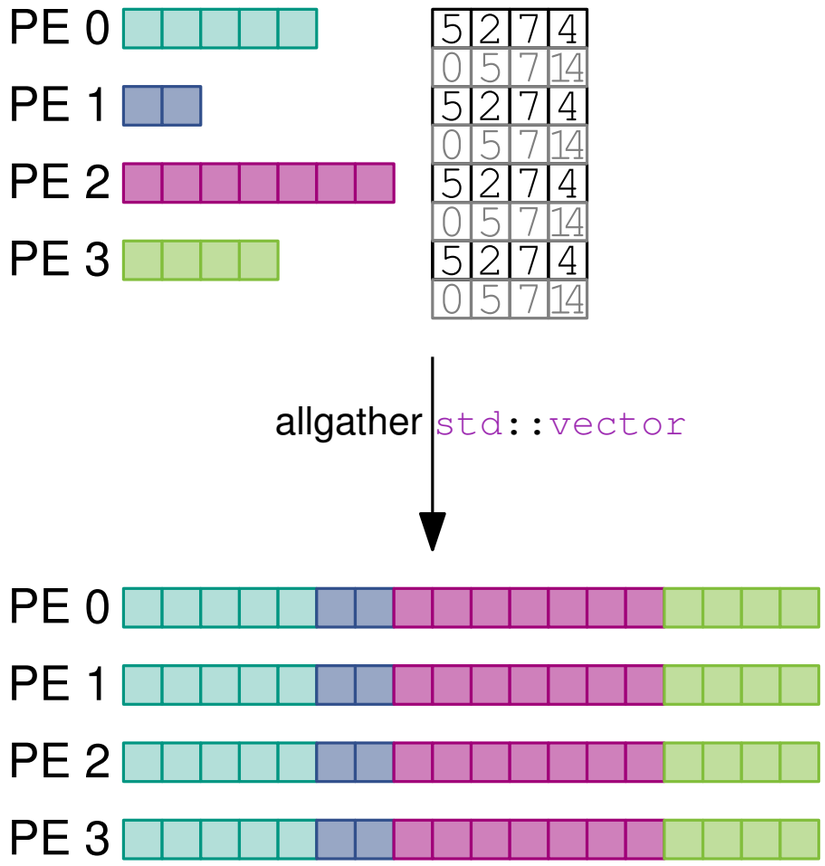


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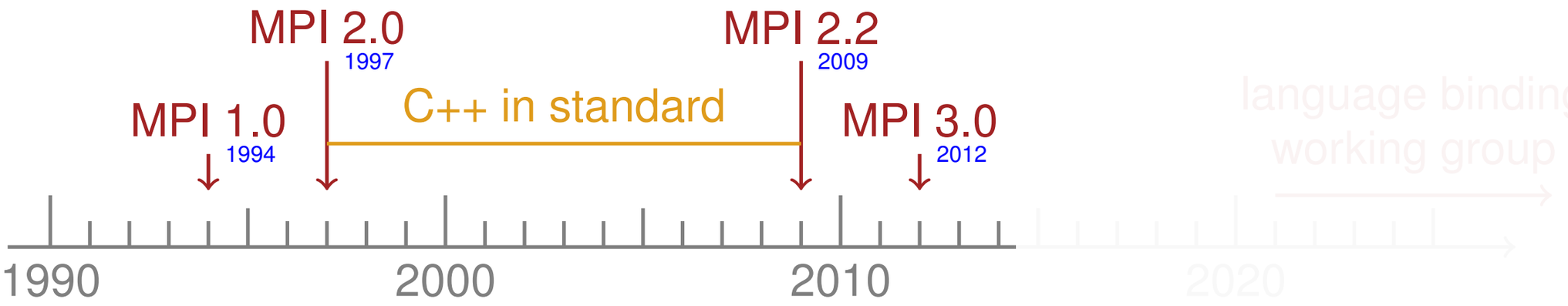
A Walk Through the History of MPI and C++



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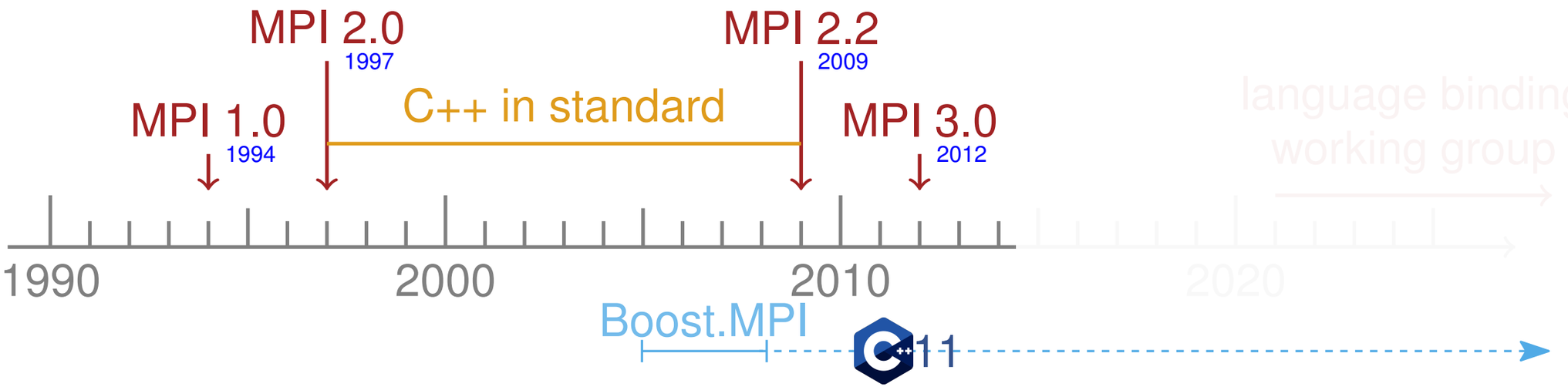

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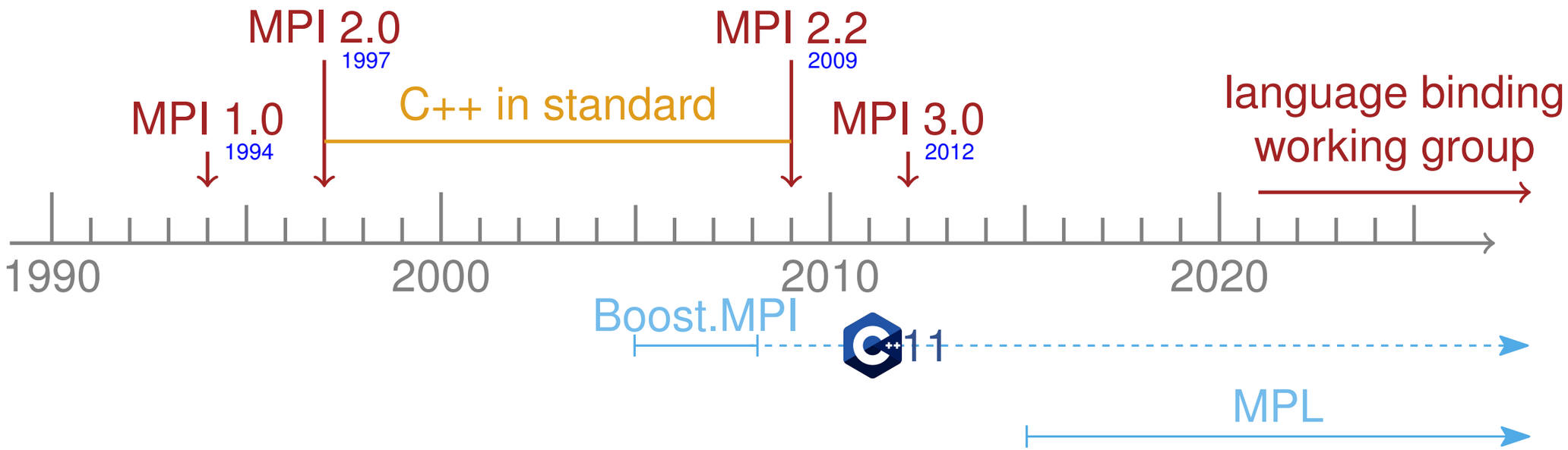

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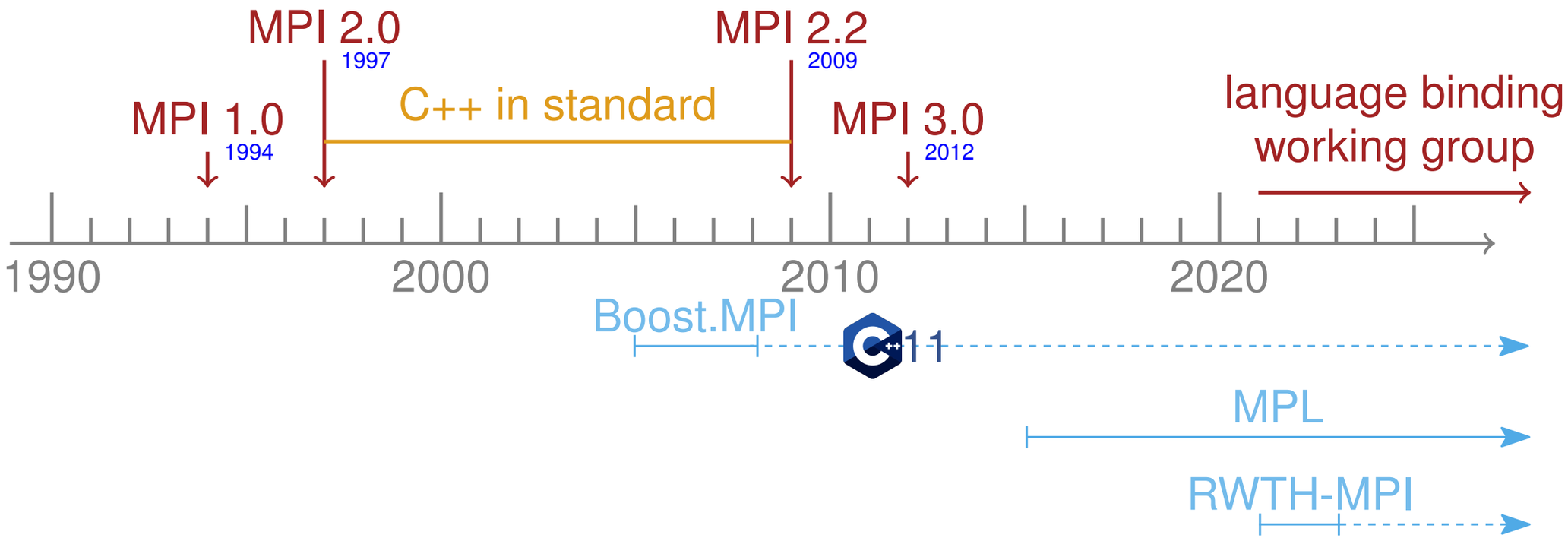

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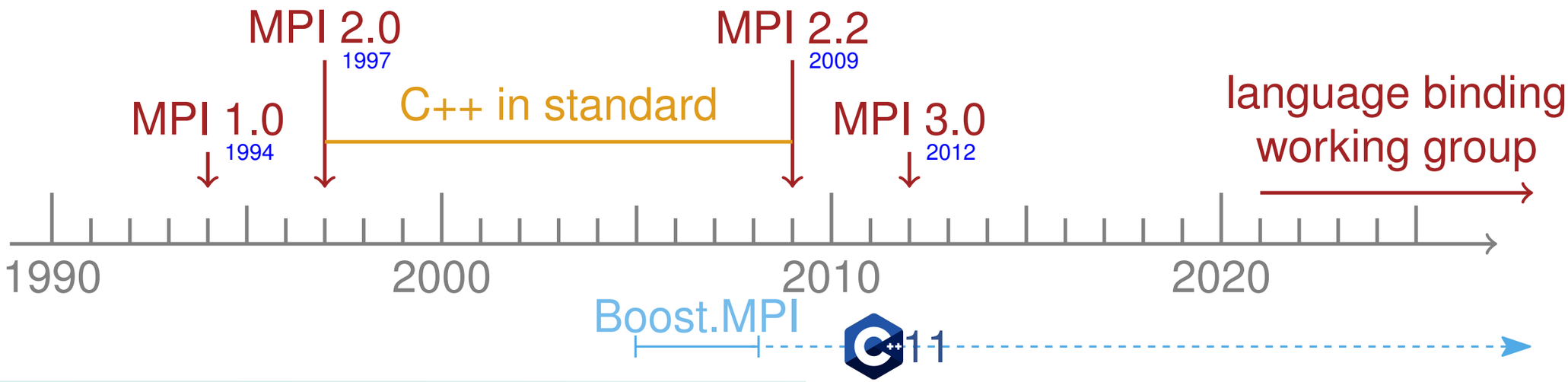
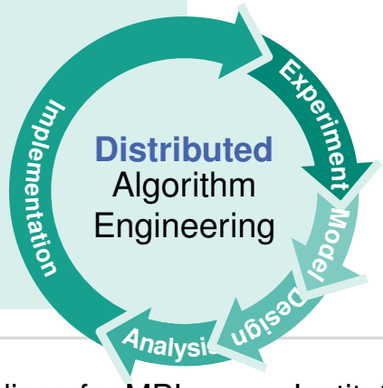


Example

```
// ...

boost::mpi::all_gatherv(comm, v_local, v_global);

// ...
for (auto& elem : v_global) {
  process(elem);
}
```



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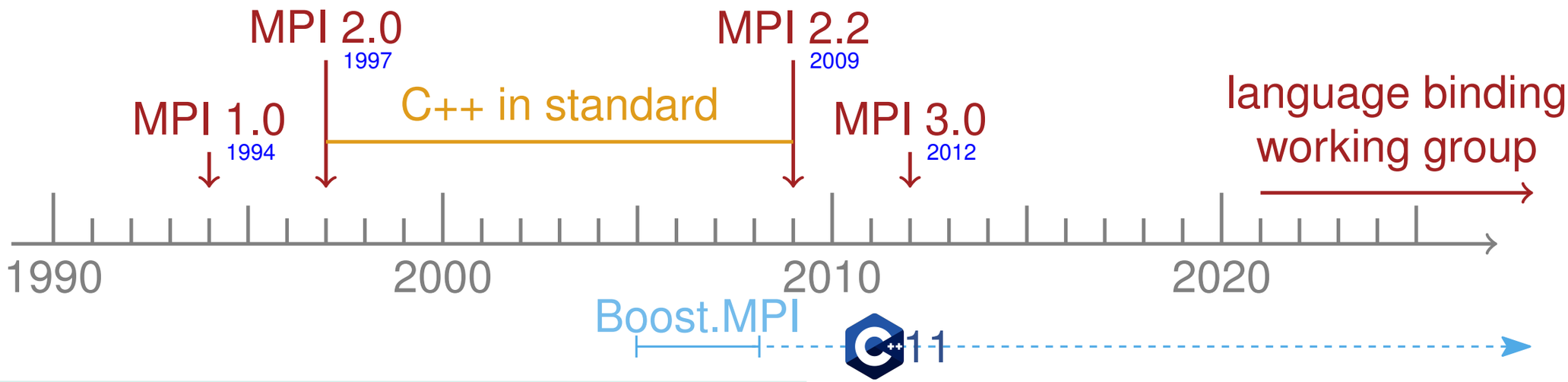
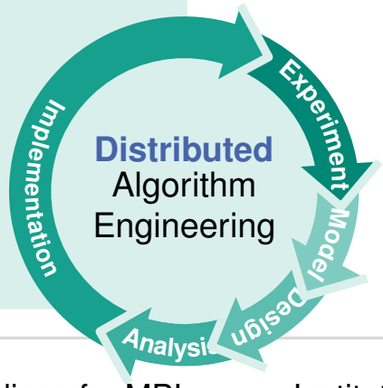


Example

```
// ...
std::vector<int> sizes;
boost::mpi::all_gather(comm, v_local.size(), sizes);
boost::mpi::all_gatherv(comm, v_local, v_global, sizes);
// ...
for (auto& elem : v_global) {
  process(elem);
}
```



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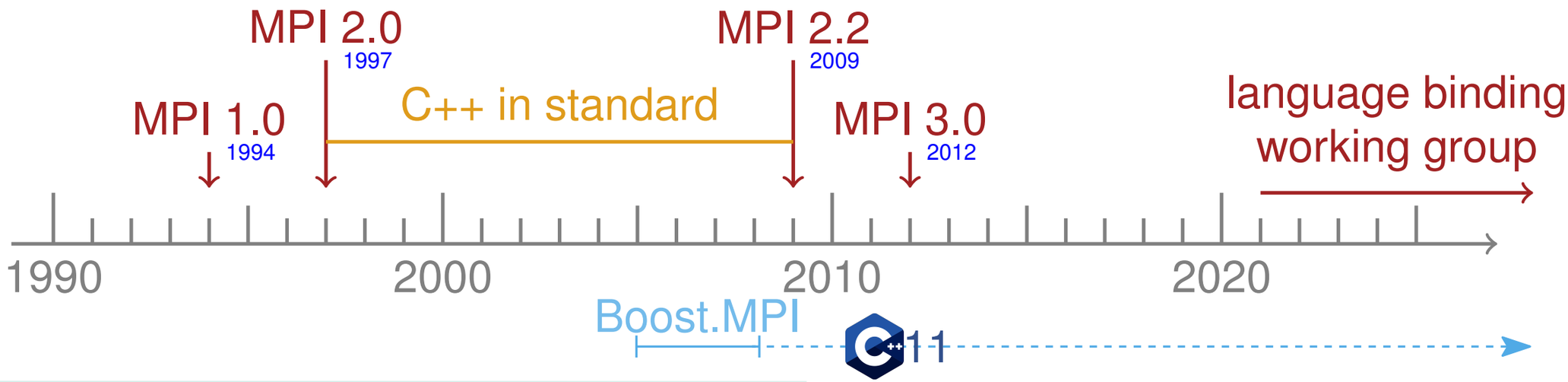
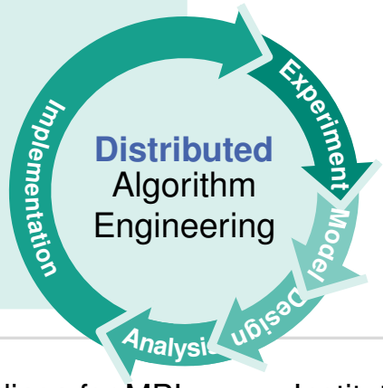


Example

```
std::vector<int> displs;
std::vector<int> sizes;
boost::mpi::all_gather(comm, v_local.size(), sizes);
boost::mpi::all_gatherv(comm, v_local, v_global, sizes);
// ...
for (auto& elem : v_global) {
  process(elem, heuristic(elem_rank));
}
```



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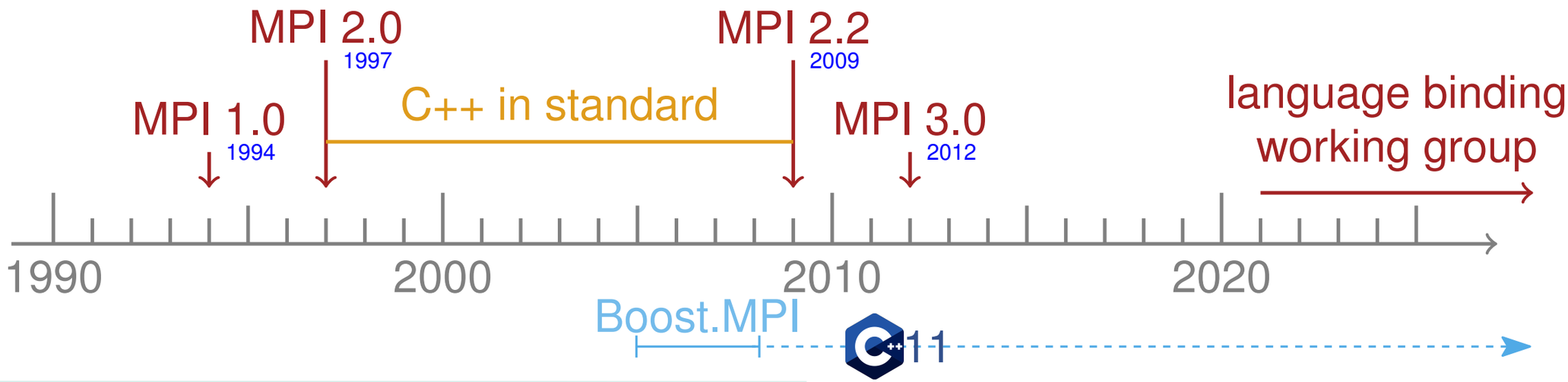

Example

```
std::vector<int> displs;
std::vector<int> sizes;
boost::mpi::all_gather(comm, v_local.size(), sizes);
std::exclusive_scan(sizes.begin(), sizes.end(), displs.begin(), 0);
boost::mpi::all_gatherv(comm, v_local, v_global, sizes, displs);
// ...
for (auto& elem : v_global) {
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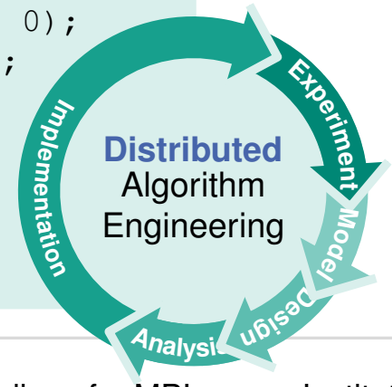

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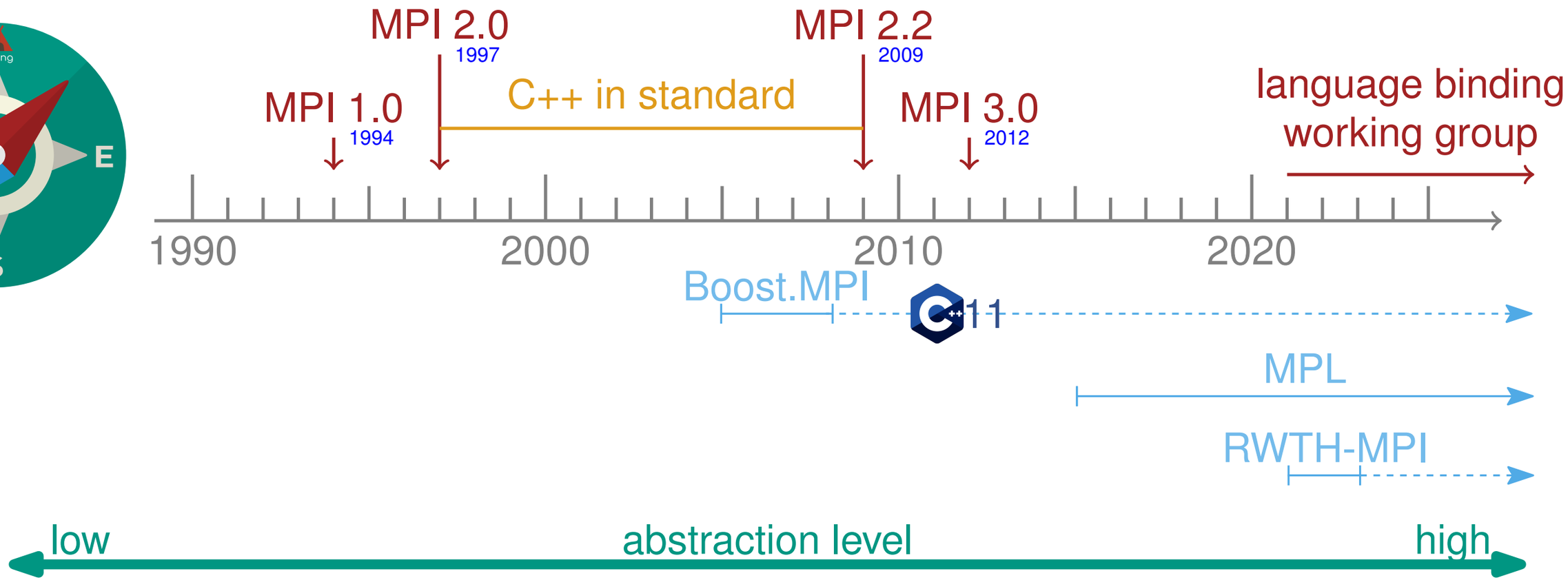

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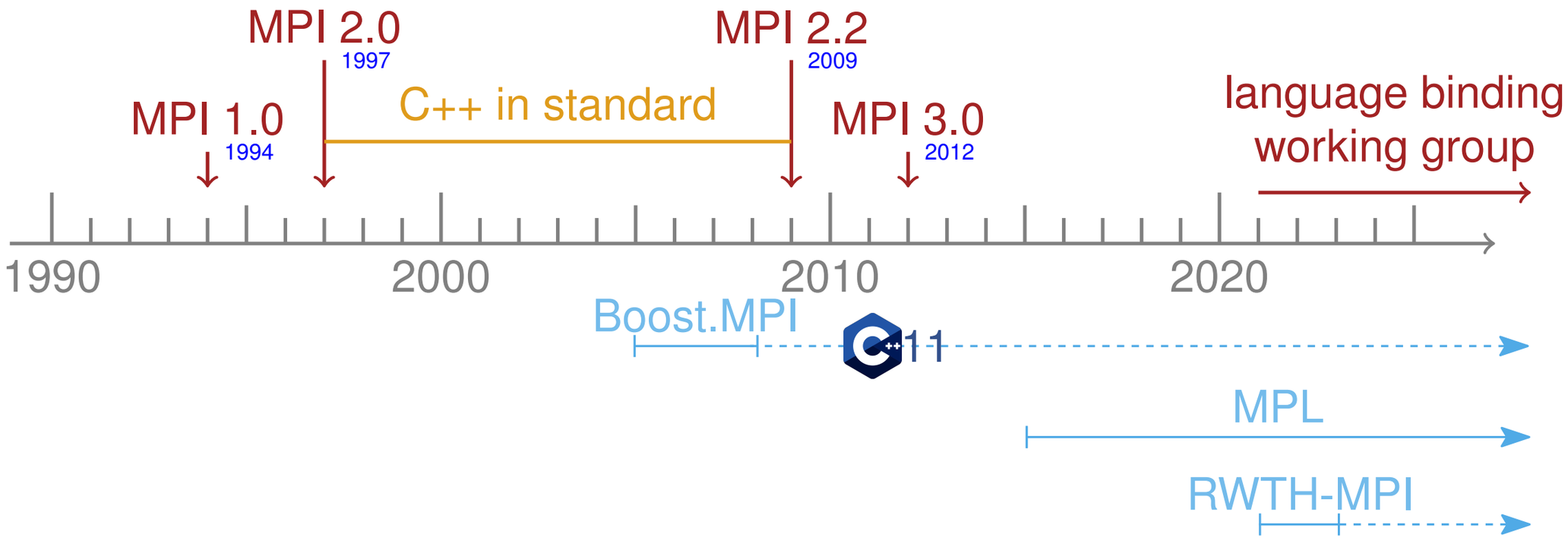

KaMPIng

Karlsruhe **MPI** **n**ext **g**eneration

A KaMPIng Trip

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```

low — abstraction level — high

Goals:

- ☐ zero-overhead **abstraction** over MPI
- ☐ covering whole abstraction **range**: rapid prototyping ↔ highly engineered algorithms
- ☐ flexible **parameter handling**, sensible defaults
- ☐ configurable **memory management**
- ☐ compatible with **move semantics**

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C-ish API

all other parameters can be inferred

parameter order?

low — abstraction level — high

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  rc[rank] = v_local.size();
  comm.allgather(send_recv_buf(rc));
  std::exclusive_scan(rc.begin(), rc.end(), rd.begin(), 0);
  std::vector<T> v_global(rd.back() + rc.back());
  comm.allgatherv(send_buf(v_local), recv_buf(v_global),
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  return v_global;
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all other parameters can be inferred

parameter order?

arbitrary parameter order!

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manual allocation

low — abstraction level — high

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automatic or manual allocation

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common idiom: boilerplate!

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  rc[rank] = v_local.size();
  comm.allgather(send_recv_buf(rc));
  std::exclusive_scan(rc.begin(), rc.end(), rd.begin(), 0);
  std::vector<T> v_global;
  comm.allgatherv(send_buf(v_local), recv_buf(v_global),
                  recv_counts(rc), recv_displs(rd));

  return v_global;
}
```

common idiom: boilerplate!

automatic or manual allocation

low — abstraction level — high

Goals:

- ☐ zero-overhead **abstraction** over MPI
- ☐ covering whole abstraction **range**: rapid prototyping ↔ highly engineered algorithms
- ☐ flexible **parameter handling**, sensible defaults
- ☐ configurable **memory management**
- ☐ compatible with **move semantics**

A KaMPIng Trip

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return by reference

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return by reference or by value

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A KaMPIng Trip

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```

```cpp
// avoid implicit allocation
comm.allgatherv(send_buf(v_local),
                recv_counts_out<no_resize>(some_buf));

// pass buffer ownership to calls
rc = comm.allgatherv(send_buf(v_local), recv_buf(v_global),
                     recv_counts_out<resize_to_fit>(std::move(rc)));

// retrieve auxiliary data
auto [recvbuf, displs] = comm.allgatherv(send_buf(v_local),
                                         recv_displs_out());
```

low — abstraction level — high

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Equipped with More Features

Flexible Type System

- automatic type deduction
- type reflection
- opt-in serialization

```
using dict = std::unordered_map<std::string, std::string>;
dict data = ...;
comm.send(send_buf( kamping:: as_serialized(data)));

dict recv_dict = comm.recv(
  send_buf( kamping:: as_deserializable<dict>())
);
```

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);
```

Safety Features

preventing programming errors for

- non-blocking communication
- inplace operations
- invalid arguments

```
std::vector<int> v = ...;
auto r1 = comm.isend(
    send_buf_out(std::move(v)), destination(1)
);

v = r1.wait(); // v  moved back after completion

auto r2 = comm.irecv<int>(recv_count(42));
// data returned after completion
std::optional<std::vector<int>> data = r2.test();
```

Equipped with More Features

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using dict = std::unordered_map<std::string, std::string>;
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Extensibility

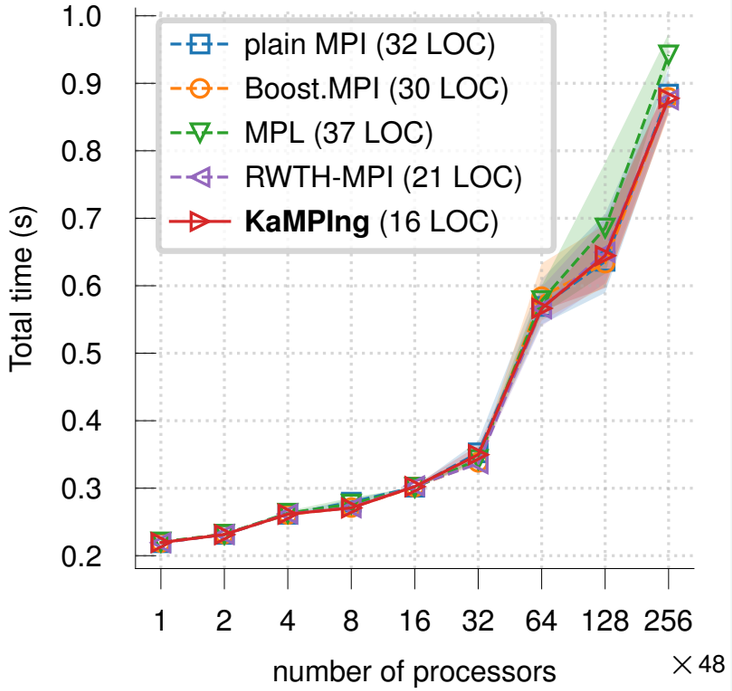
Plugins for

- specialized collectives
- fault tolerance
- STL-style algorithms

KaMPIng Out in the Wild

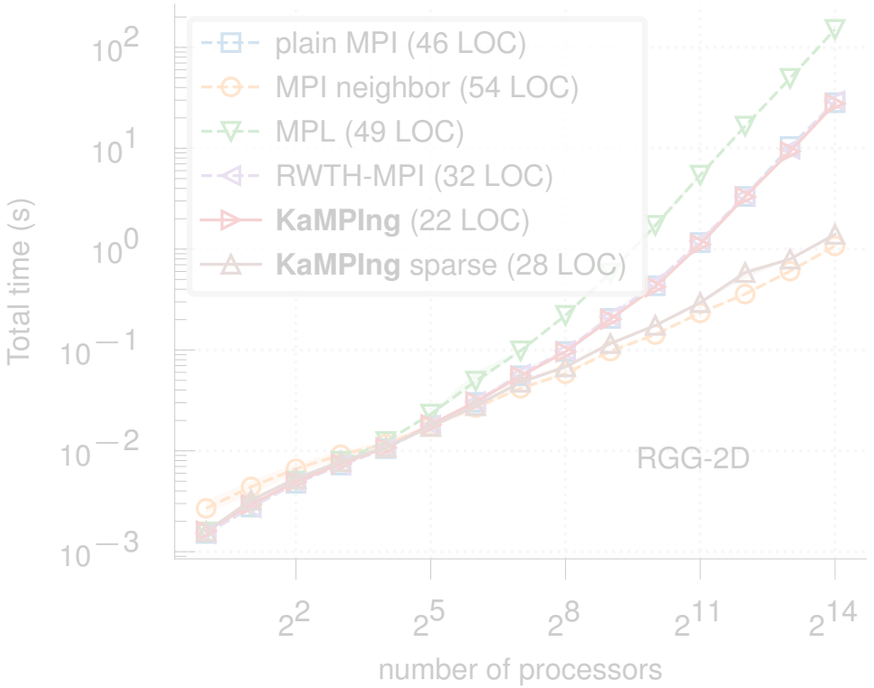
Karlsruhe Institute of Technology

Sorting
Sample Sort:



Suffix Sorting: $<$ 200 LOC

Graph Algorithms
BFS:



Graph Partitioning: 15% less code

Bioinformatics
Phylogenetic Inference:

- over 50 000 citations
- over 700 lines of custom MPI wrapper

compile time 1:15min + 0:15min

binary size +2.5%

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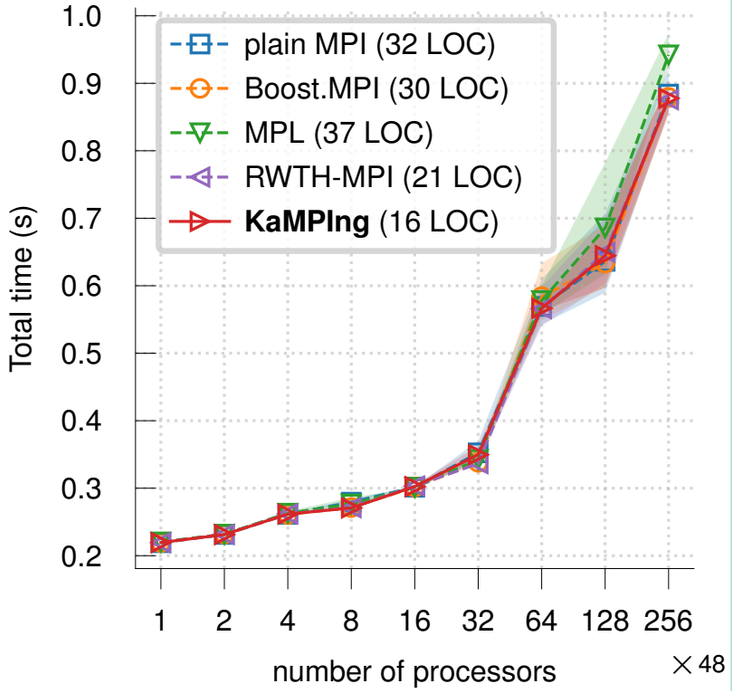

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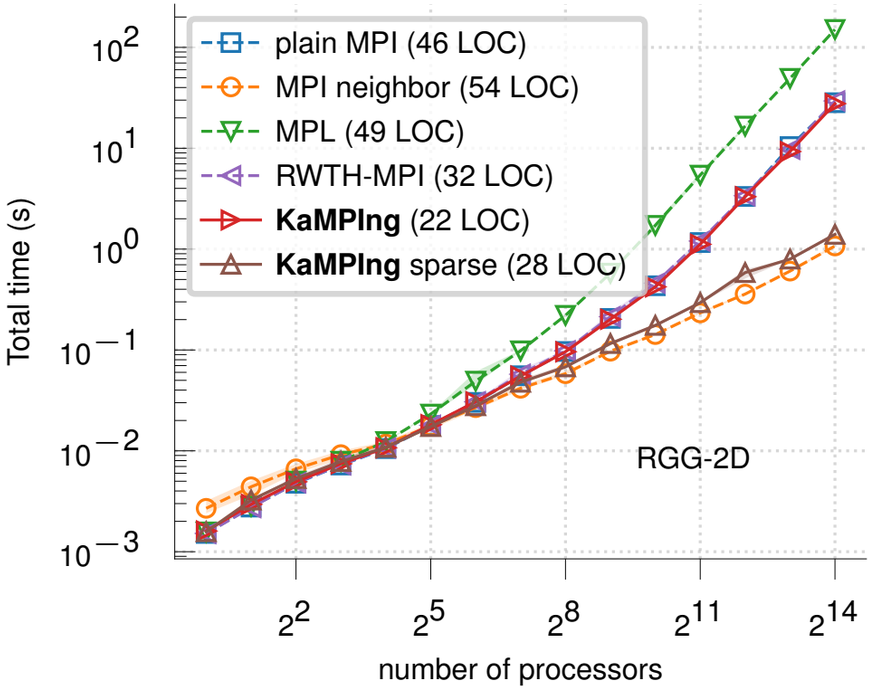

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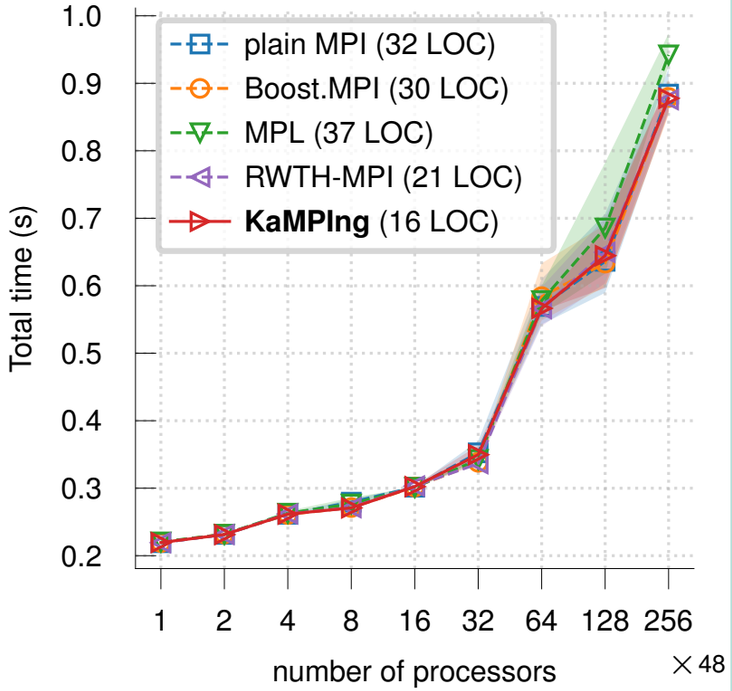

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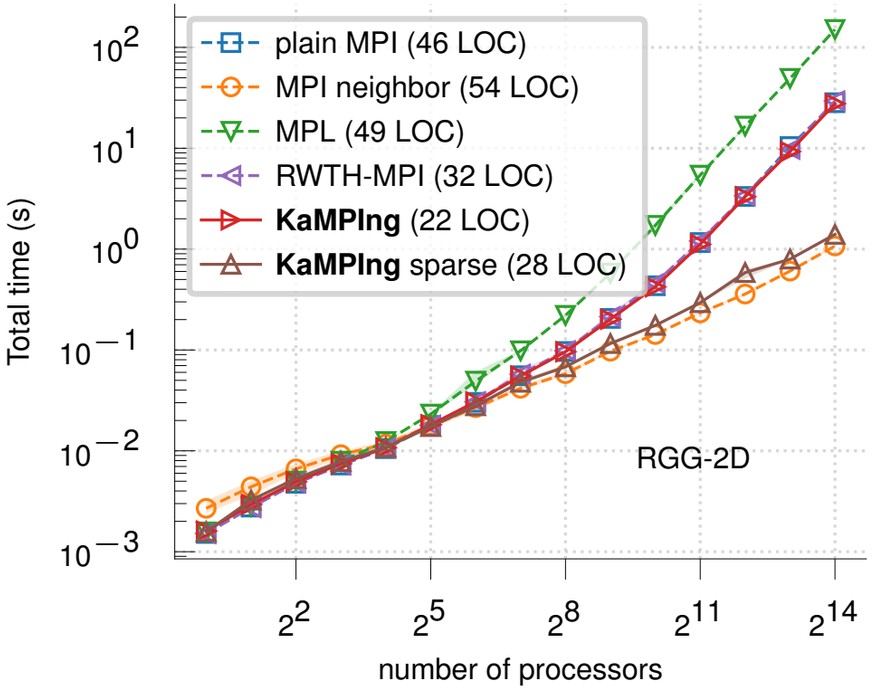

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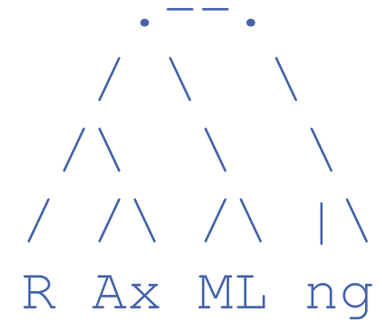

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Join the KAmp Today!

original RAxML-NG code

```
template<typename T>
static void mpi_broadcast(T& obj) {
  if (_num_ranks > 1) {
    size_t size = master() ?
      BinaryStream::serialize(
        _parallel_buf.data(),
        _parallel_buf.capacity(),
        obj)
      : 0;
    mpi_broadcast((void *) &size, sizeof(size_t));
    mpi_broadcast((void *) _parallel_buf.data(), size);
    if (!master()) {
      BinaryStream bs(_parallel_buf.data(), size);
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Get started!

CMake

```
FetchContent_Declare(
  kamping
  GIT_REPOSITORY https://github.com/kamping-site/kamping.g
  GIT_TAG v0.1.1
)

FetchContent_MakeAvailable(kamping)

target_link_libraries(myapp PRIVATE kamping::kamping)
```

C++

```
#include <kamping/communicator.hpp>
#include <kamping/collectives/bcast.hpp>

kamping::Communicator comm(my_comm);
comm.bcast(...);
```

github.com/kamping-site/kamping

Join the KAmp Today!

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Packing Up: The Journey Ahead

- **low-to-high-level** C++ bindings for MPI
- no **runtime-overhead**
- reduce boilerplate and error-proneness in MPI applications
  - default parameters
  - safety guarantess
  - fine-grained memory management
- base for a future **standard library** of distributed algorithms and data structures

github.com/kamping-site/kamping

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