

Multiscale Universal Interface

A Concurrent Framework for Coupling Heterogeneous Solvers

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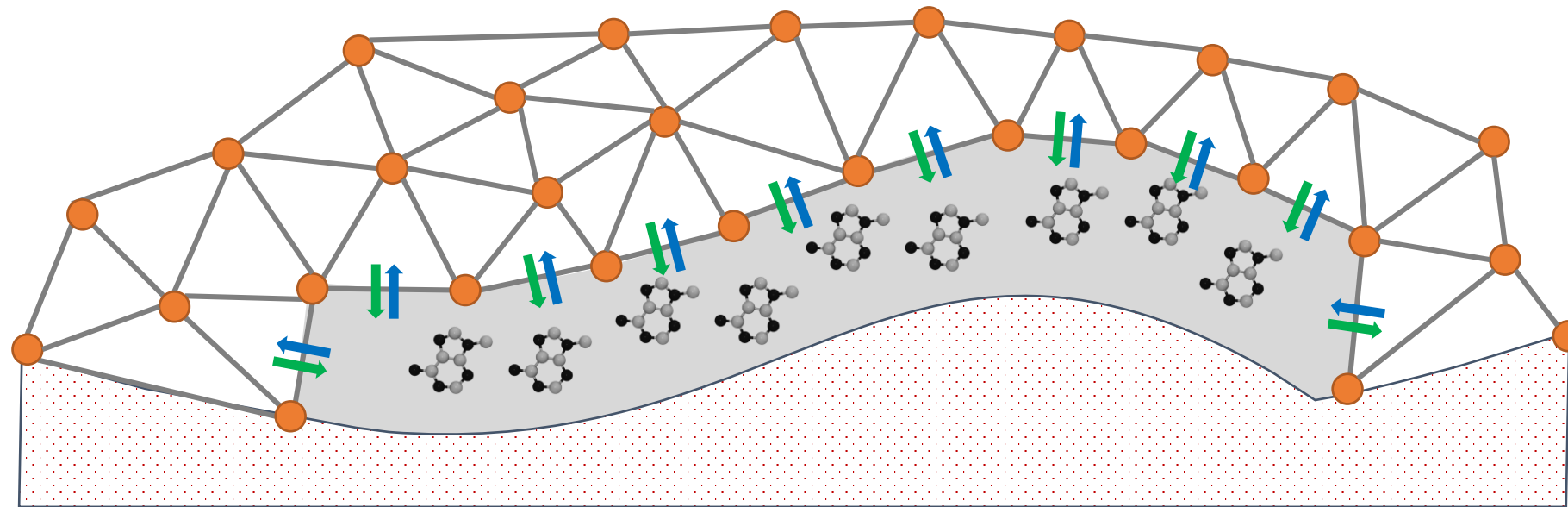
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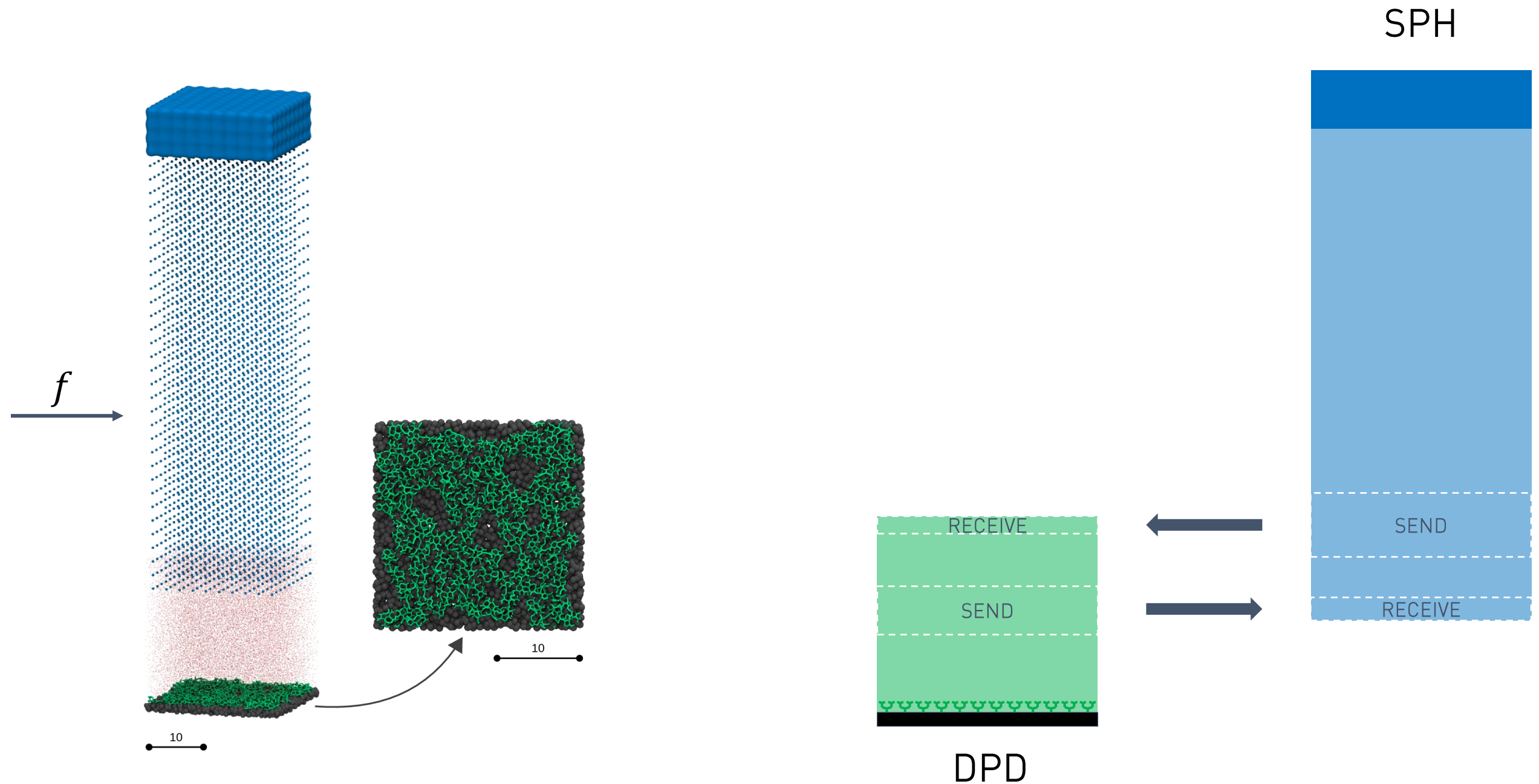
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Multiscale Simulations by Domain Decomposition

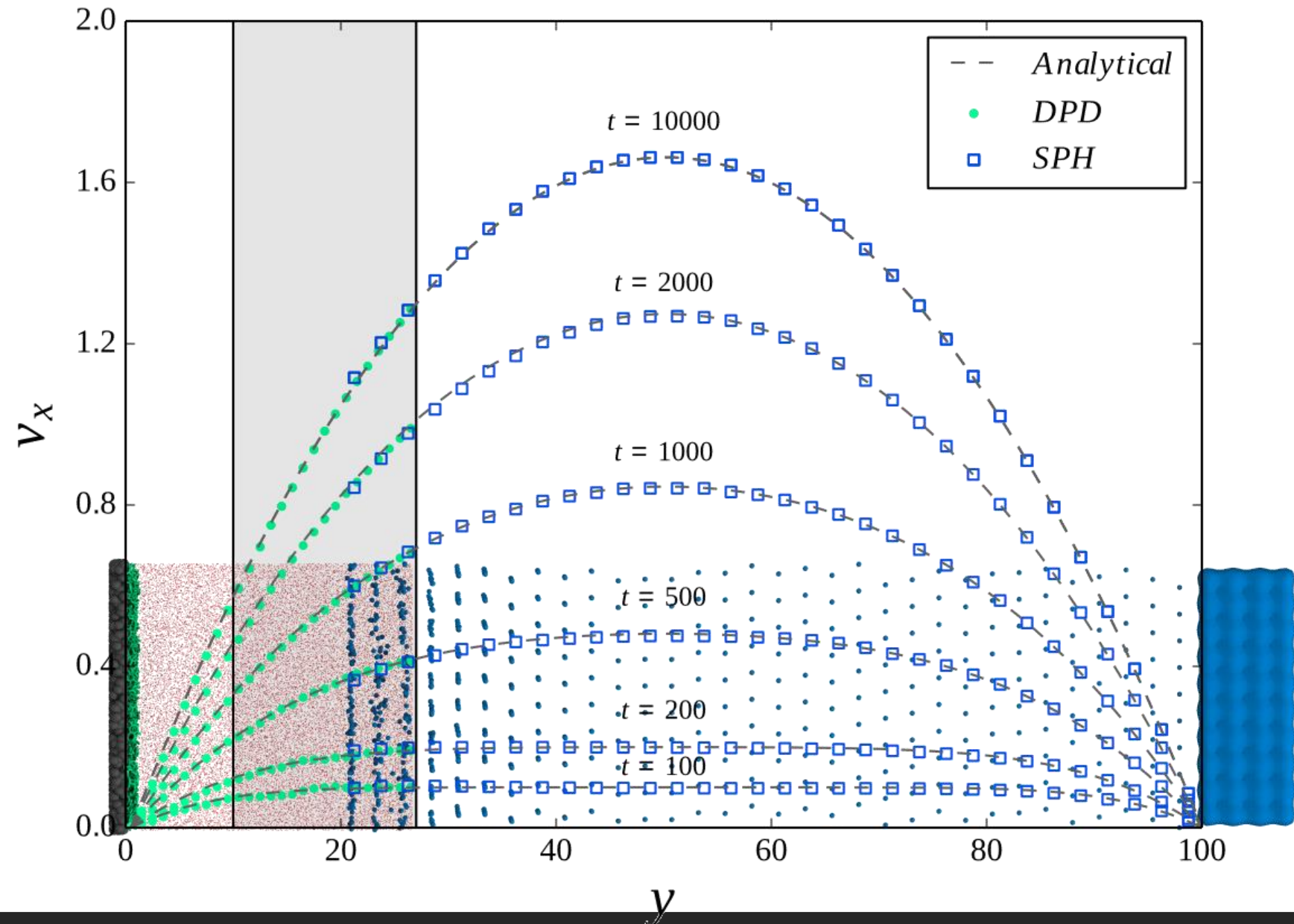
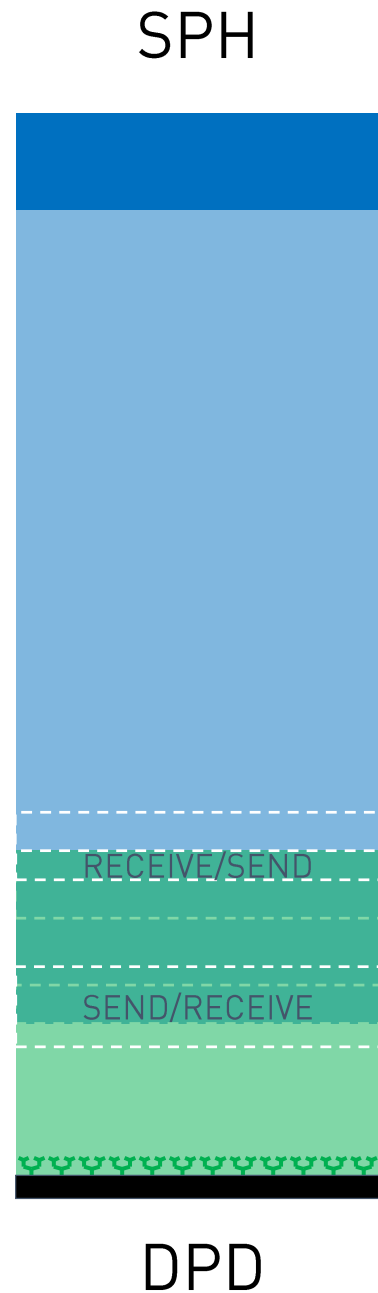
- Each solver handles a subdomain and use the other as boundary



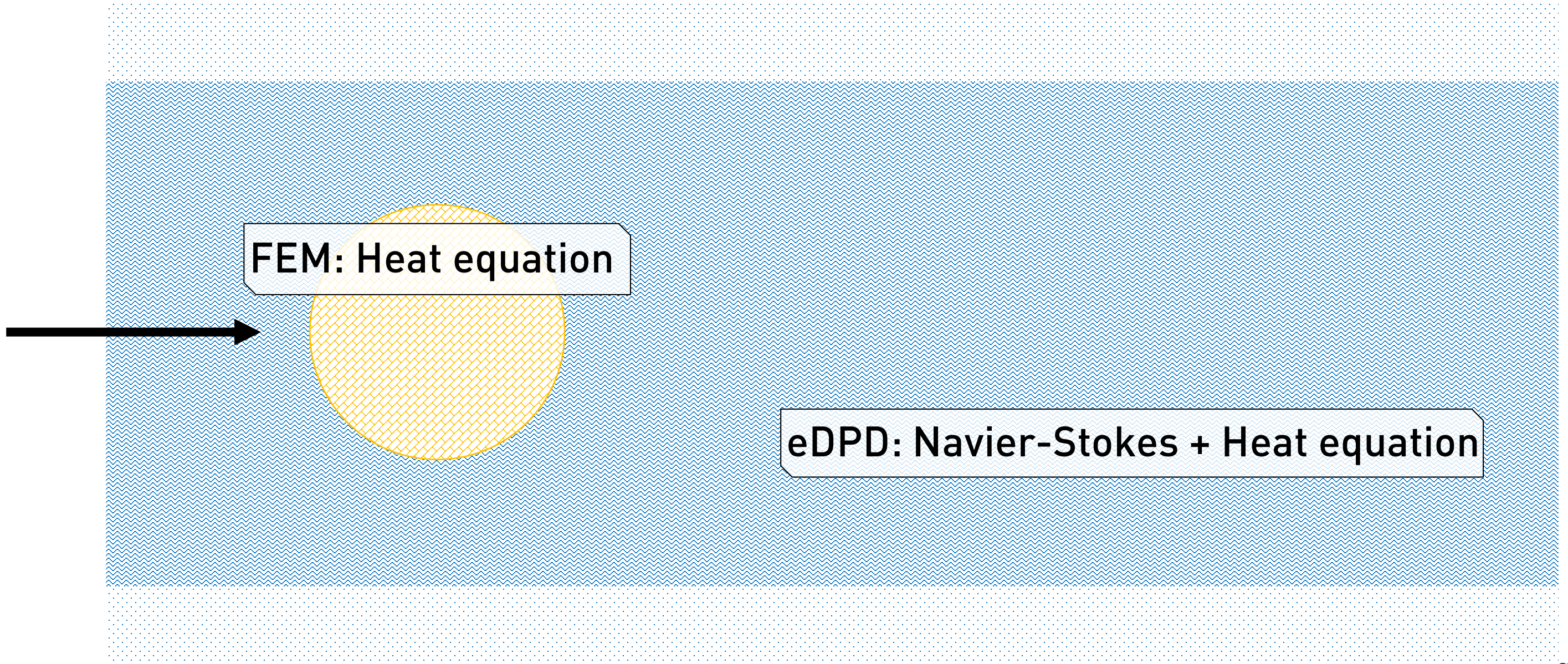
Example: Grafted Surface



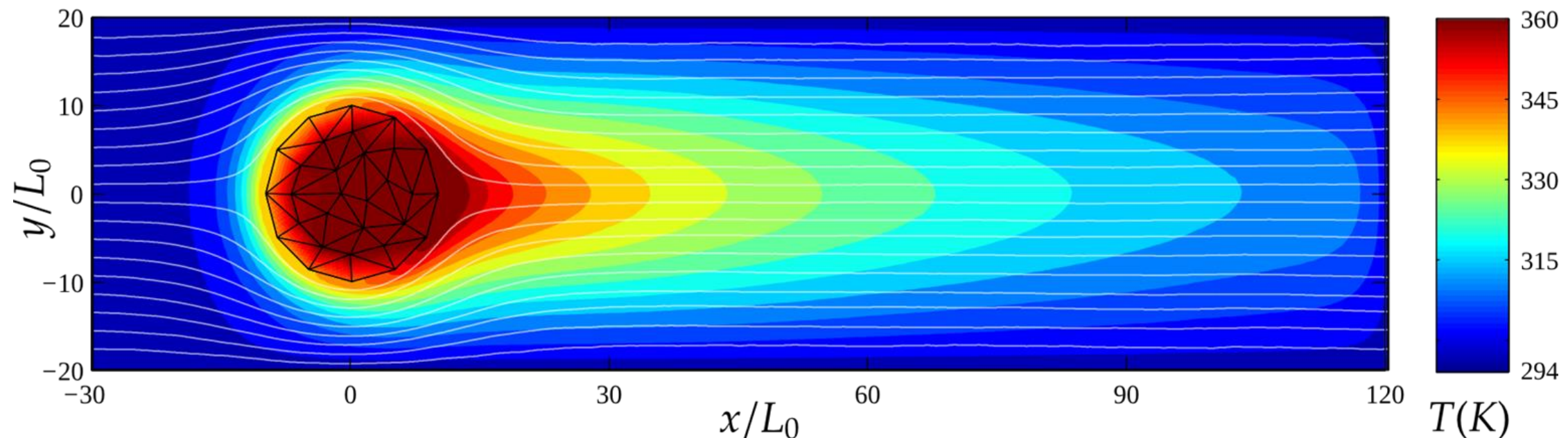
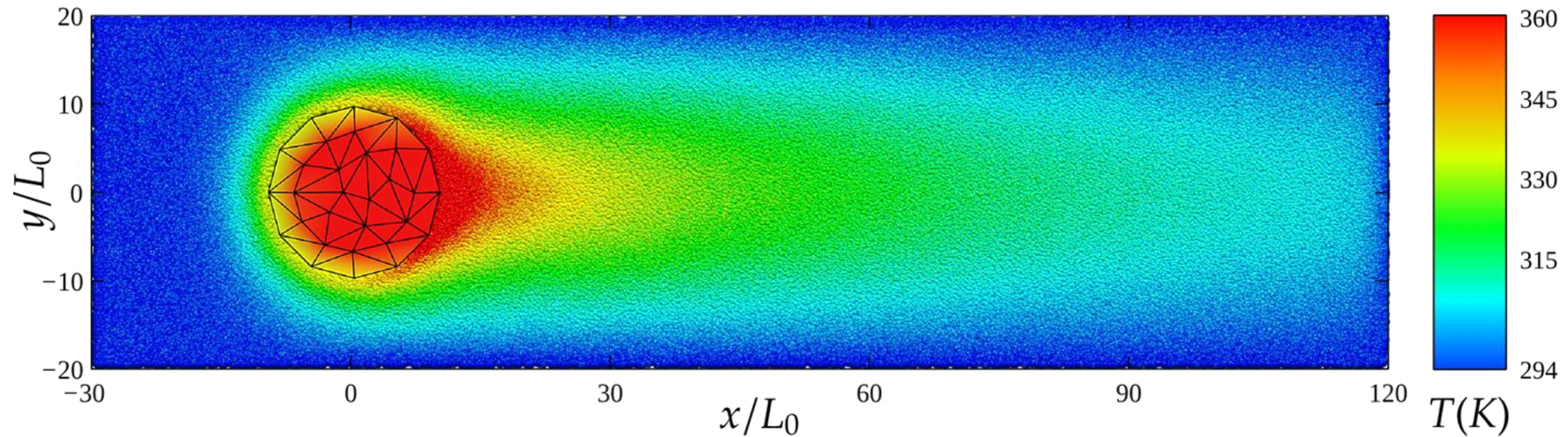
Example : Grafted Surface



Example : Conjugate Heat Transfer

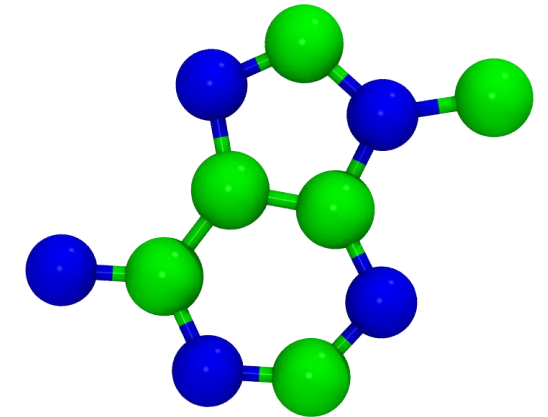
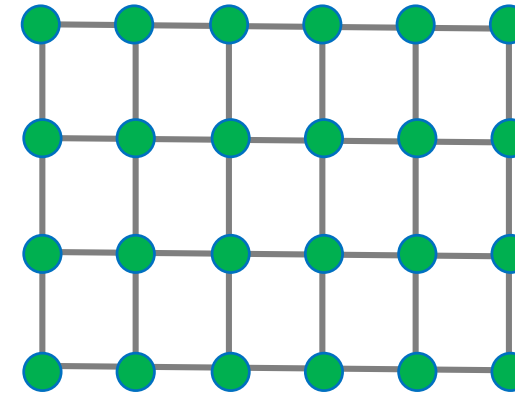
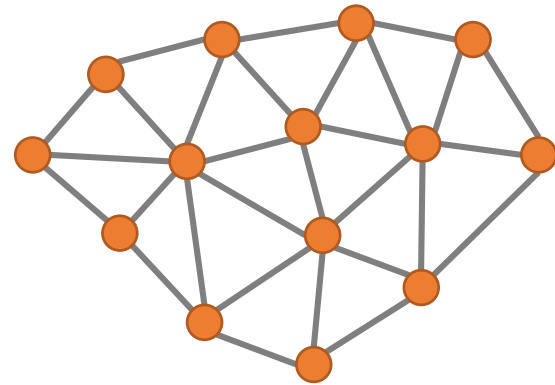


Example : Conjugate Heat Transfer

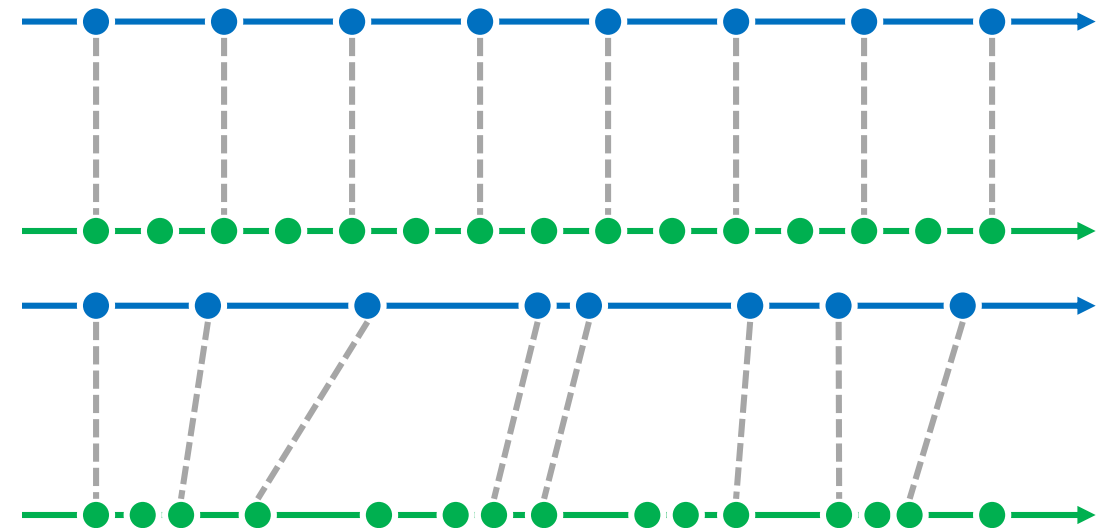
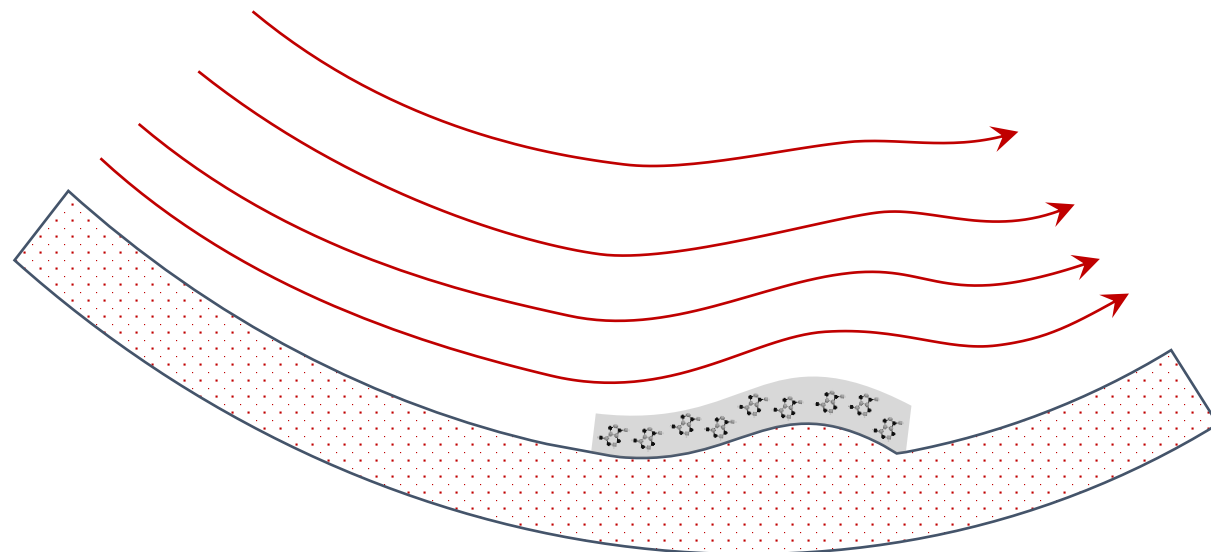


Diversity in Current Coupling - I

- Equation
 - Newton's
 - Schrödinger's
 - etc.

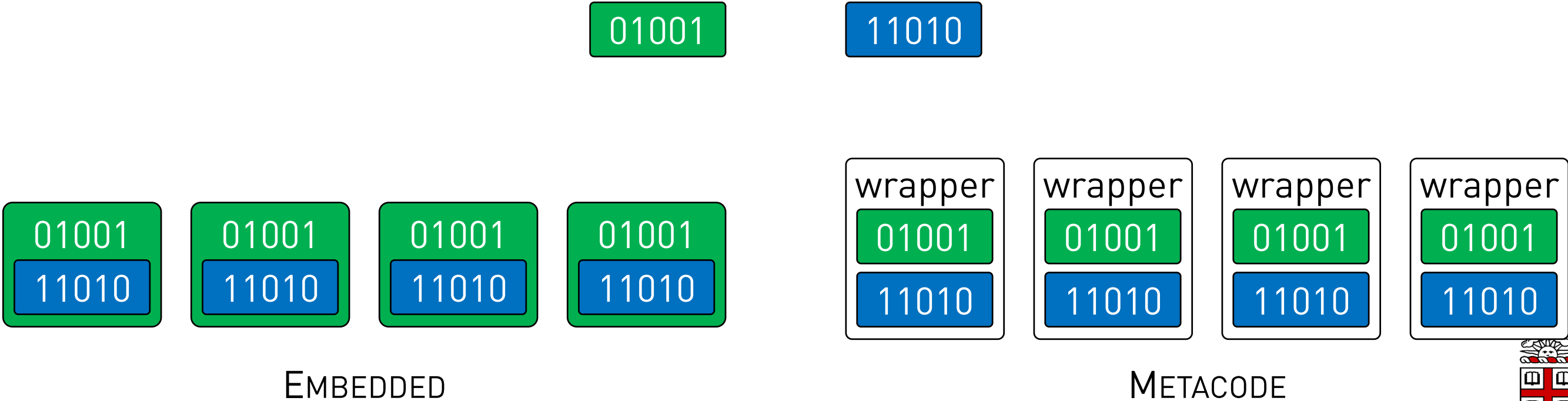


- Discretization / Geometry
- Time stepping: uniform, staggered, variable



Diversity in Concurrent Coupling - II

- Solver: C, C++, Fortran, Python, ...
 - Scheme
 - Parallelization: Serial, OpenMP, MPI, ...
 - Existing solutions largely rely on embedding or metacode
- The majority of existing code
 - was not developed to be coupled
 - need refactoring/invasive development



Multiscale Universal Interface (MUI)

IS

A plug-and-play platform for testing ideas on multiscale coupling.

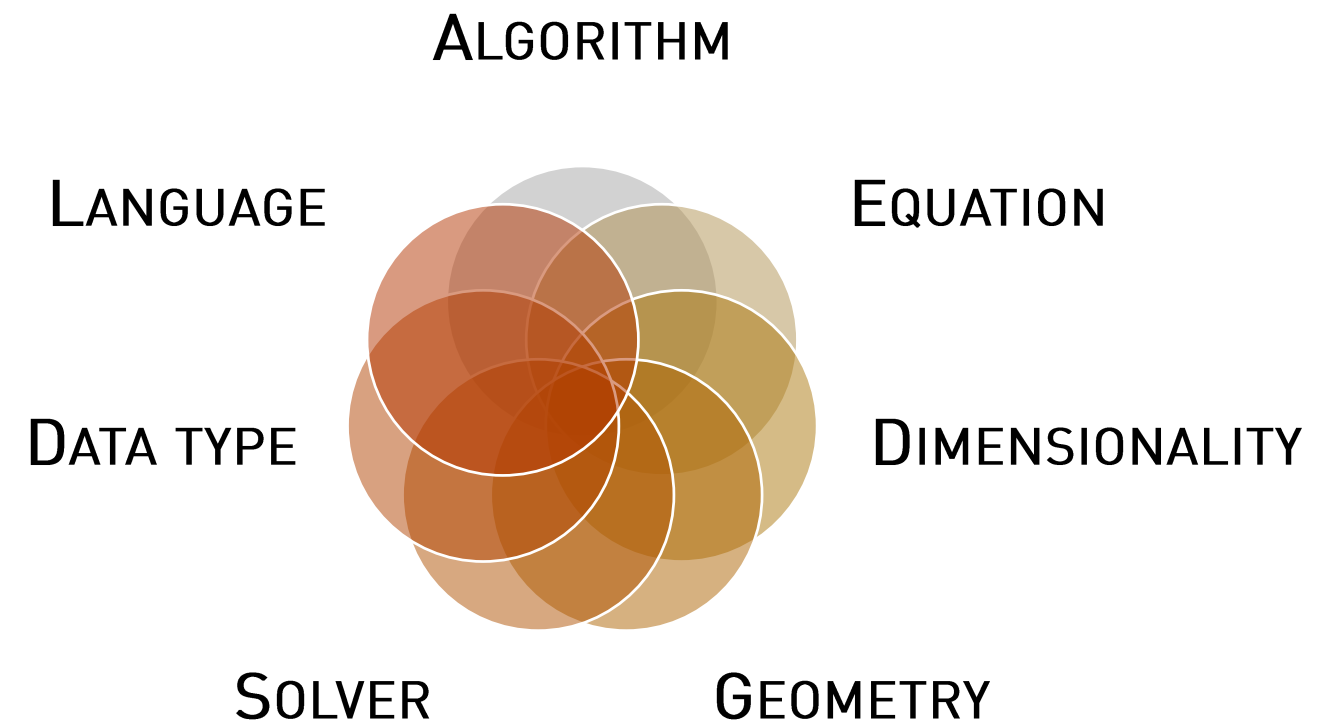
A communication layer for multi-solver information exchange.

A header-only C++ library that can be dropped into existing codes easily

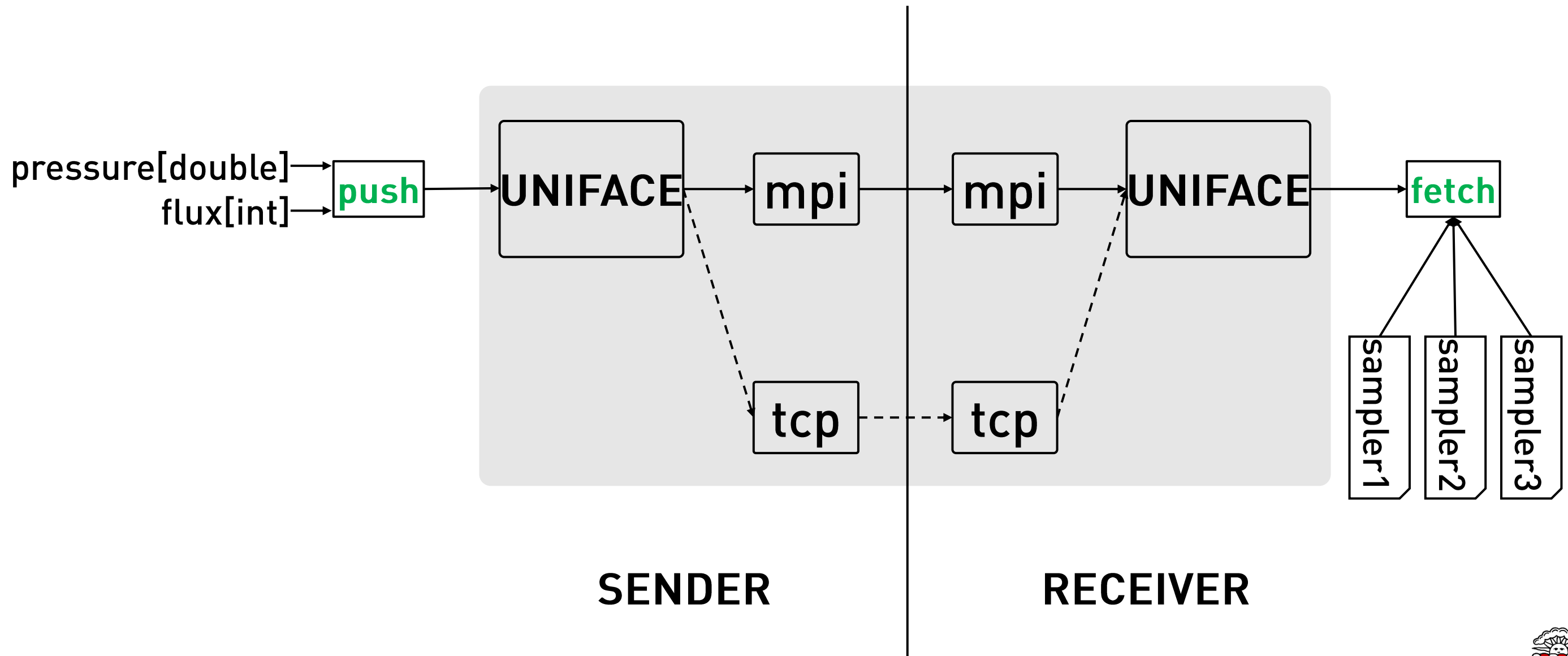
IS NOT

A specific coupling method that dictates which and how physical quantities get coupled.

A driver/wrapper that requires the exposure of certain programming interfaces from the solver.

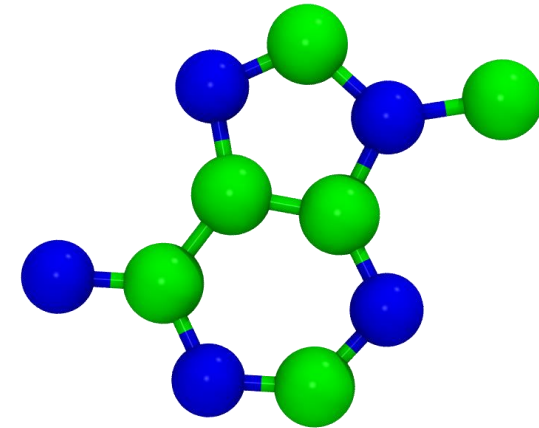
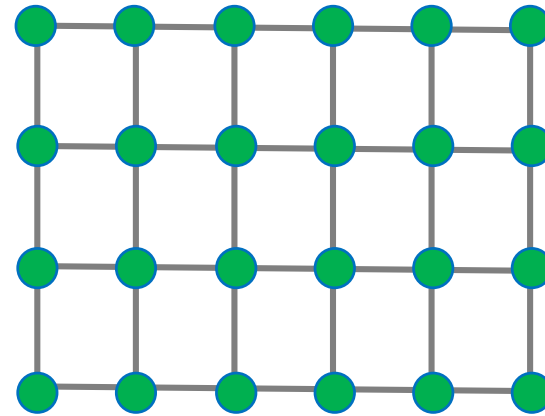
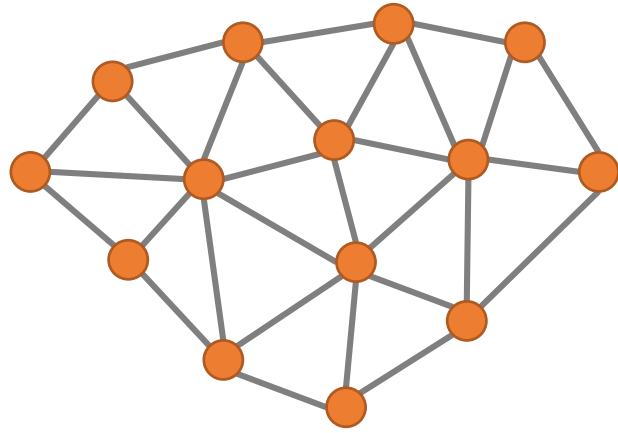


Workflow Overview



Abstraction: Data points

- Data point := (location, type, value)



- Location: Vector Expression Templates
 - arbitrary dimension
 - real/complex coordinate
 - automatic SIMDization
- Value: arbitrary type
 - C++ templates
 - Type list metaprogramming

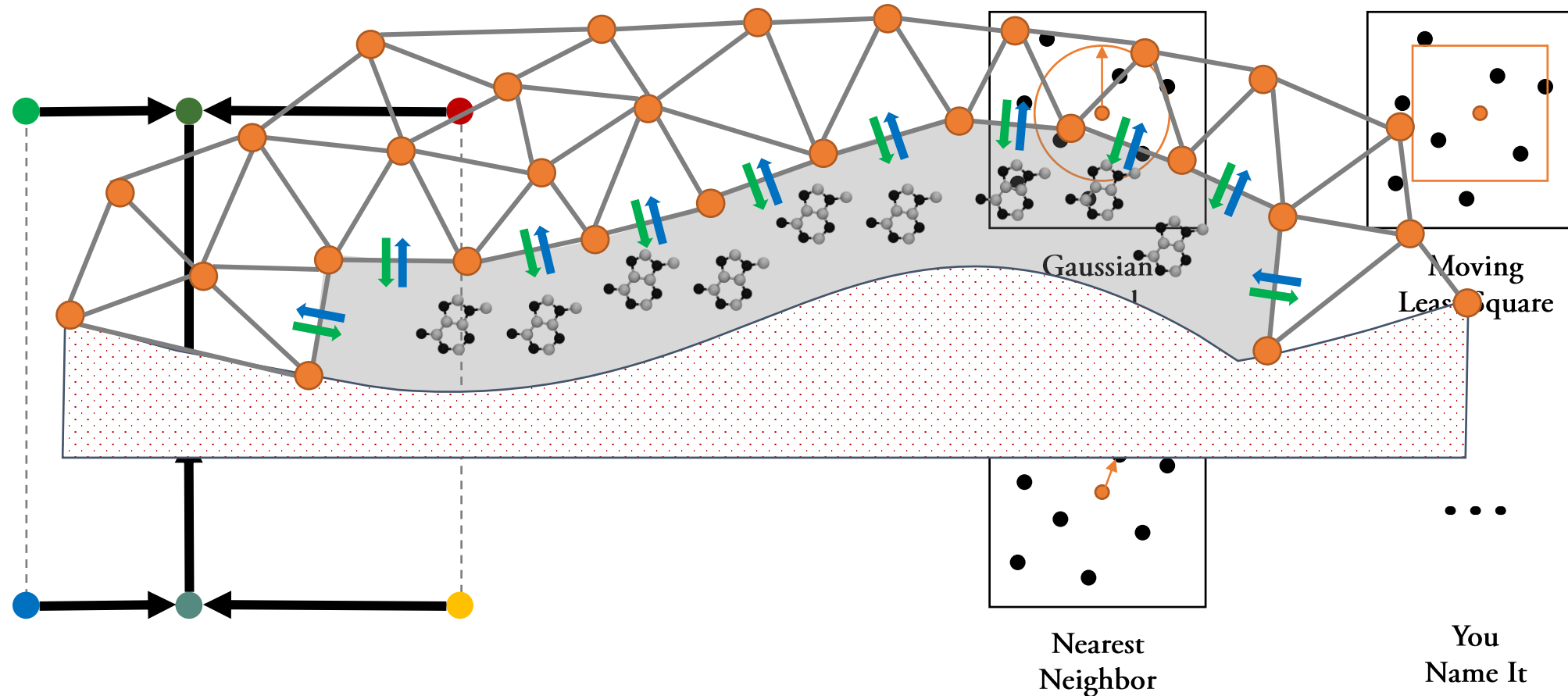
Abstraction: Sampling

- Texture Sampler

- Hardware-implemented
- Interpolate continuous color surface from discrete pixels

- MUI Data sampler

- C++ functors
- Can implement any interpolation



Sampler Design

```
template<typename O_TP, typename I_TP=O_TP, typename CONFIG=default_config>
class sampler_gauss {
public:
    using OTYPE      = O_TP;
    using ITYPE      = I_TP;
    using REAL       = typename CONFIG::REAL;
    using INT        = typename CONFIG::INT;
    using point_type = typename CONFIG::point_type;

    sampler_gauss( REAL r_, REAL h_ ) :
        r(r_), h(h_),
        nh(std::pow(2*PI*h,-0.5*CONFIG::D)) {}

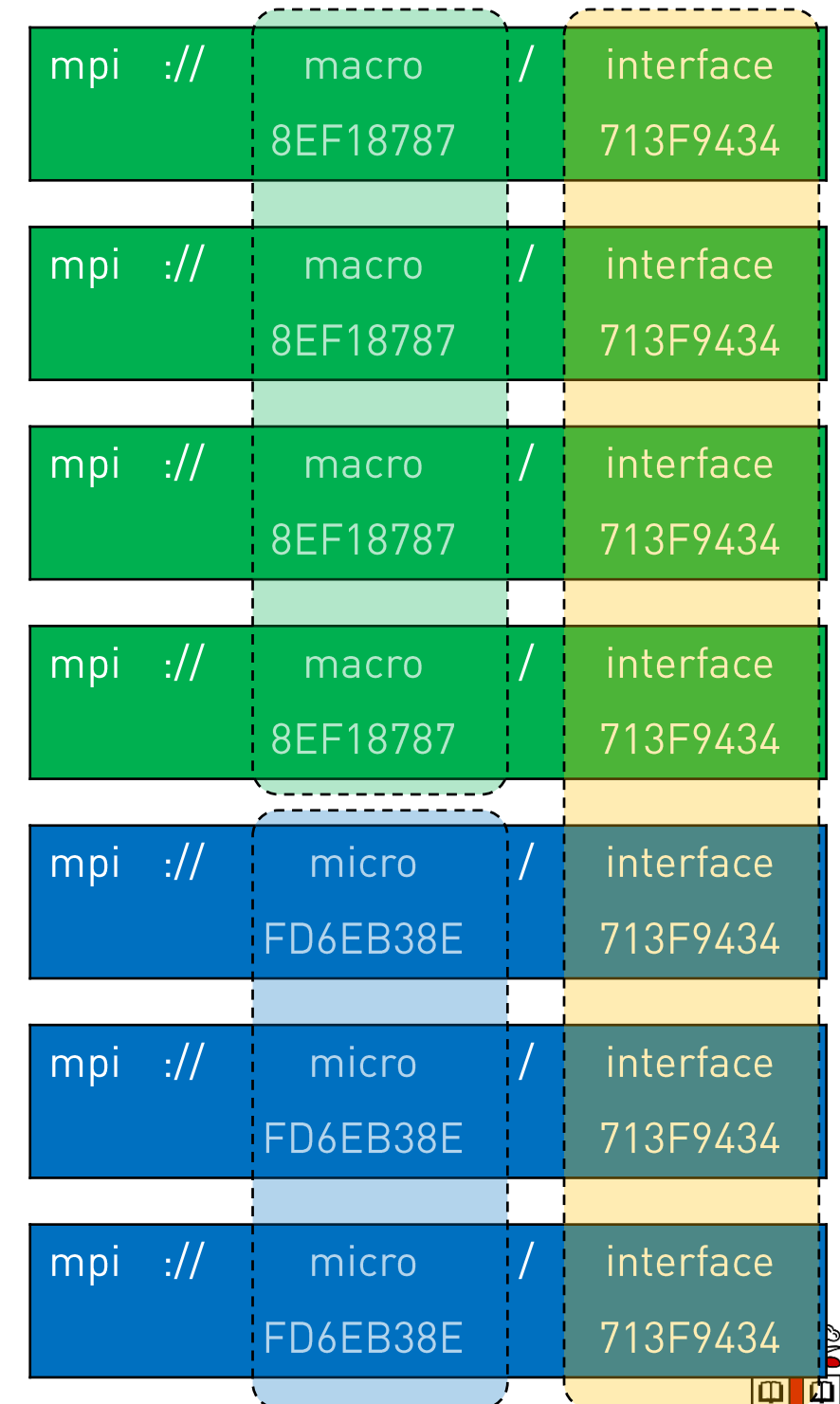
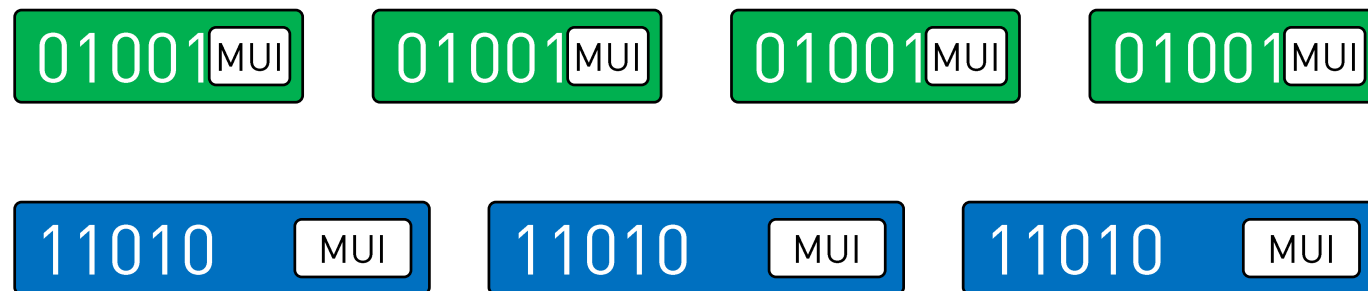
    template<template<typename,typename> class CONTAINER>
    inline OTYPE filter( point_type focus,
                        const CONTAINER<ITYPE,CONFIG> &data_points ) const {

        REAL wsum = 0;
        OTYPE vsum = 0;
        for(INT i = 0 ; i < data_points.size() ; i++) {
            auto d = (focus-data_points[i].first).normsq();
            if ( d < r*r ) {
                REAL w = nh * std::exp( (-0.5/h) * d );
                vsum += data_points[i].second * w;
                wsum += w;
            }
        }
        if ( wsum ) return vsum / wsum;
        else return 0.;
    }
};
```



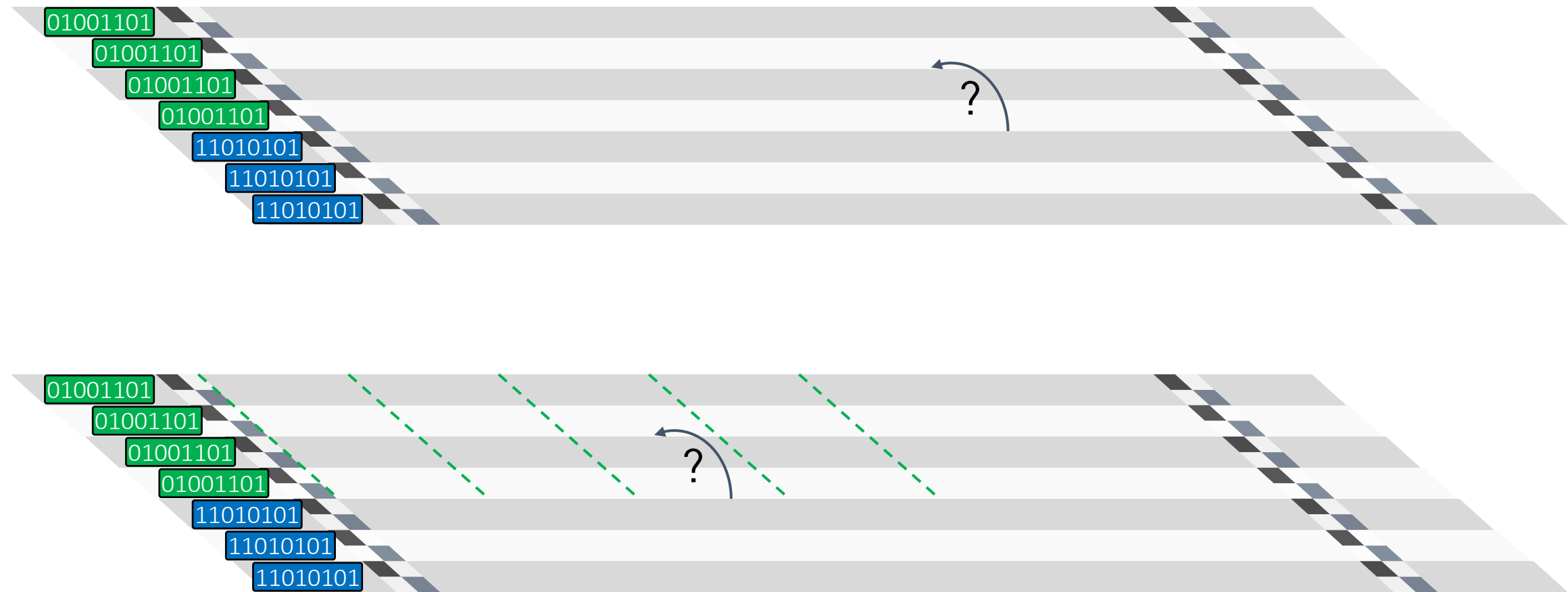
Parallelization: MPI MPMD

- Solvers compiled separately, runs concurrently
- MPMD syntax: `mpirun -np N1 solver1 : -np n2 solver2`
- URI: `protocol://domain/interface`
 - Use hash function to digitize the string
- Fetch method thread-safe



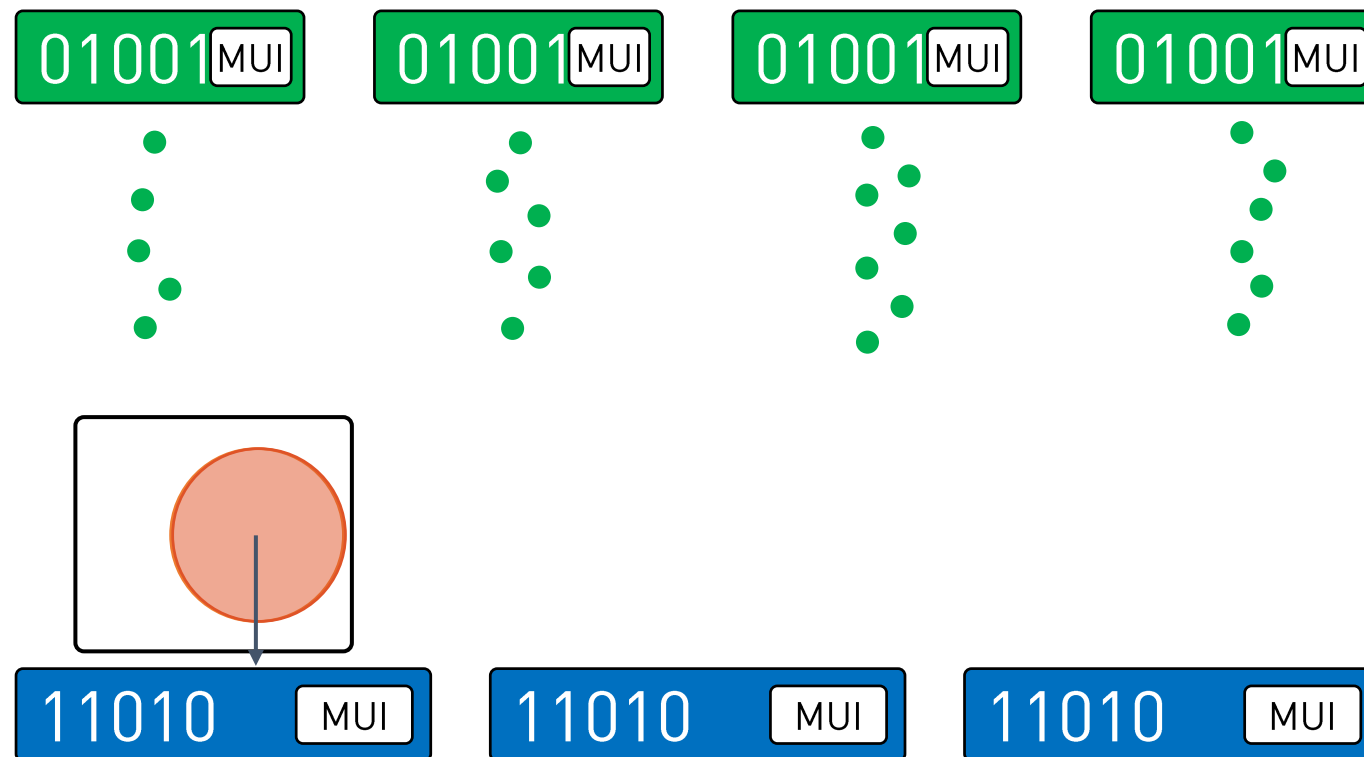
Time coherence

- MUI does not implicitly enforce solvers synchronization
 - In addition: time stepping may not align

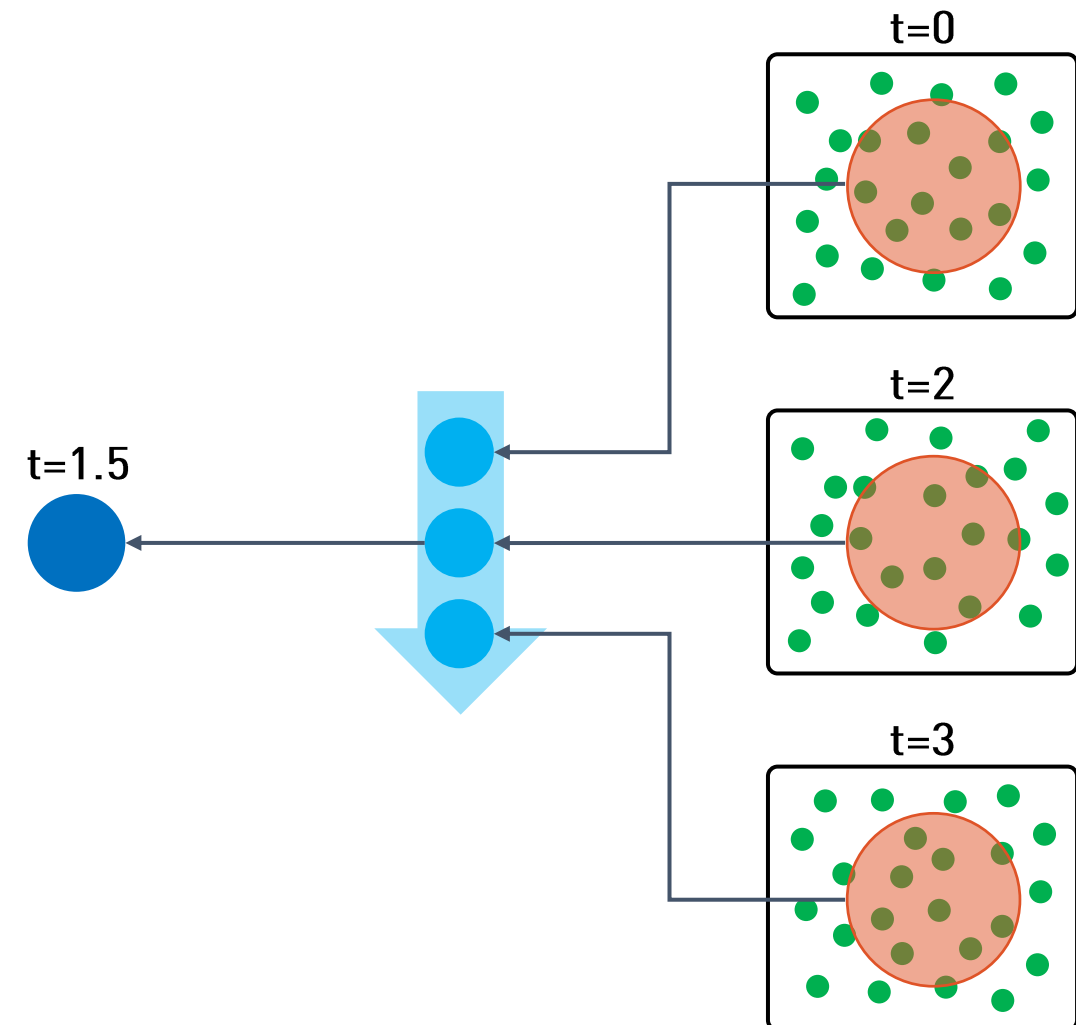


Time coherence

- Time frames
 - points of same timestamp merged as frames
 - tagged by timestamp
 - sampling performed on frames

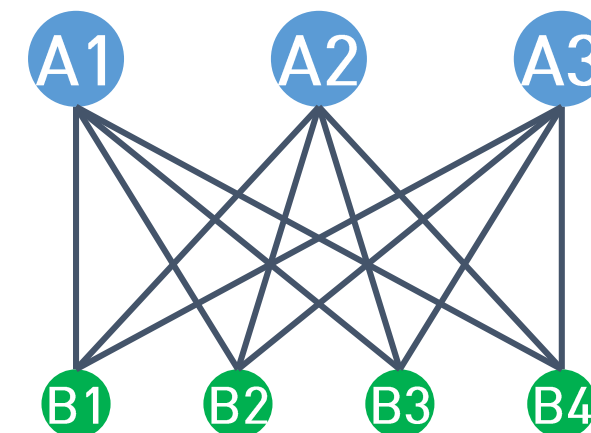
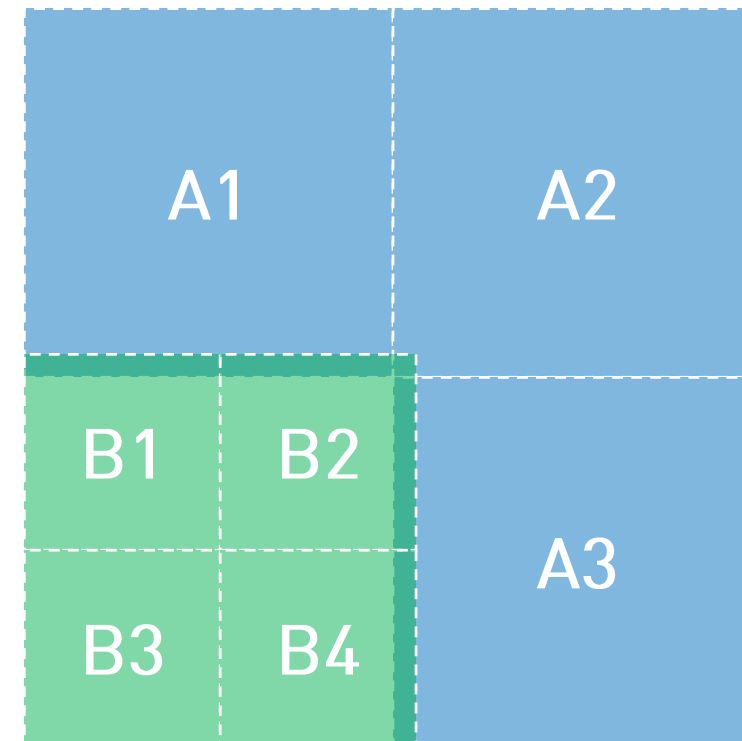


- Chrono sampler
 - Interpolate spatial results from time frames



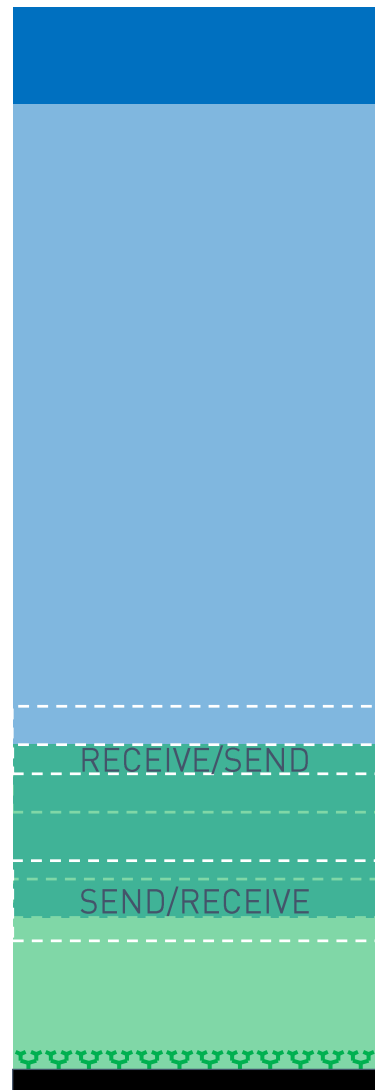
Selective Communication

- By default MPI broadcast all data points to all peer ranks
 - $O(N^2)$ messages!
- In many situations the interpolation algorithm is local
- Regions of interest
 - Hint for MPI to cut unnecessary messages
 - Arbitrary Boolean operations of boxes, spheres, and points
 - Use validity period for moving boundary



Example Revisited: Grafted Surface

SPH



DPD

```

/***** DPD *****/
For t = 0:dt:T
  For each particle i
    If WithinSendRegion(i)
      MUI::Push("v_x", coord[i], vel_x[i])
    MUI::Commit(t)

  Force Eval, Integrate...

  t_SPH = Floor(t, 50dt)
  For each particle i
    If WithinReceiveRegion(i)
      S_s = Quintic(r_SPH, h_SPH)
      S_t = ExactTime
      v_x[i] = MUI::Fetch
                ("v_x", coord[i], t_SPH, S_s, S_t)
    If t % 50dt = 0
      MUI::Forget(t-50dt)
  
```

```

/***** SPH *****/
For t = 0:50dt:T
  For each particle i
    If WithinSendRegion(i)
      MUI::Push("v_x", coord[i], vel_x[i])
    MUI::Commit(t)

  Force Eval, Integrate...

  For each particle i
    If WithinReceiveRegion(i)
      S_s = Quintic(r_DPD, h_DPD)
      S_t = AverageOver(50dt)
      v_x[i] = MUI::Fetch
                ("v_x", coord[i], t, S_s, S_t)

  MUI::Forget(t)
  
```



Warming Up: Common C++/C++11 Techniques in MUI

Templates

Template programming is the mechanism in C++ for writing code that is independent of any particular type.

Function template

```
template<class T> swap( T &a, T &b ) {  
    T tmp = a; a = b; b = tmp;  
}
```

Class template

```
template<class T> struct adder {  
    T sum = 0;  
    T accumulate( T v ) {  
        return sum += v;  
    }  
};
```

The `using` keyword

The `using` keyword can either be used as an enhanced version of `typedef`, or to bring classes/functions from another namespace into the current one.

```
// brings in iostream etc.  
using namespace std;  
  
// create type alias  
using real = double;  
  
// create class alias  
using real_adder = adder<real>;  
  
// create templated alias  
template<class T, int N> struct fft;  
template<class T> using fft_48pts =  
fft<T,48>;
```

Functors

A functor is basically a class which defines the operator `()`. It can instantiate objects which **look like** functions, while in addition can store states.

```
struct RNG {  
    int state = 0x0;  
    double operator () (bool peek =  
false) {  
        if (peek) return state;  
        else return peek = peek *  
0x1234 + 0x4321;  
    }  
};  
  
auto log3 = [&] (double x) {  
    return log(x) / log(3.0);  
};  
double a = log3( 9.0 ); // a = 2
```



Hands-on Practice: Environment Setup

Pre-configured Amazon EC2 Server

`ssh -CX user@ytang.dyndns.org` OR `52.53.243.39`

user = `summer00`, `summer01`, ..., `summer47` pick your lucky number!

initial password: `cm4summerschool` change it upon login to claim your account!

Once logged in: `cp -r /opt/hands_on ~`

Alternatively: use any system with a C++11 compiler and an MPI implementation and download example via SCP:

```
scp -r summer@ytang.dyndns.org:/opt/hands_on Local_path
```



Hands-on Practice: MUI Library Structure

LICENSE-Apache-v2

LICENSE-GPL-v3

wrapper_c

wrapper_f

sampler_exact.h

sampler_gauss.h

sampler.h

sampler_mov_avg.h

sampler_nn.h

sampler_null.h

sampler_pseudo_n2_linear.h

sampler_pseudo_nn.h

sampler_shepard_quintic.h

sampler_sph_quintic.h

sampler_sum_quintic.h

chrono_sampler_exact.h

chrono_sampler_gauss.h

chrono_sampler_mean.h

chrono_sampler_null.h

chrono_sampler_sum.h

comm_factory.h

comm.h

comm_mpi.h

comm_mpi_nxn.h

comm_mpi_smart.h

comm_tcp.h

config.h

dim.h

dynstorage.h

exception.h

geometry.h

lib_dispatcher.h

lib_factory.h

lib_mpi_hepler.h

lib_mpi_multidomain.h

lib_mpi_split.h

lib_singleton.h

lib_uri.h

message.h

mui.h

point.h

reader.h

reader_variable.h

README.md

span.h

spatial_storage.h

stream.h

stream_ordered.h

stream_string.h

stream_tuple.h

stream_unordered.h

stream_vector.h

uniface.h

util.h

bin.h

virtual_container.h



Hands-on Practice: Hello World

```
#include "../mui/mui.h"
int main( int argc, char ** argv ) {
    using namespace mui;
    uniface1d interface( argv[1] );
    printf( "domain %s pushed value %s\n", argv[1], argv[2] );
    interface.push( "data", 0, atof( argv[2] ) );
    interface.commit( 0 );
    double v = interface.fetch( "data", 0, 0,
                               sampler_exact1d<double>(),
                               chrono_sampler_exact1d() );
    printf( "domain %s fetched value %lf\n", argv[1], v );
    return 0;
}
```

```
// Include the MUI header file

// Bring in the MUI classes and functions
// Instantiate a interface object which implicitly initialize MPI

// Push a single data point at coordinate 0
// Commit the data points as frame 0
// Fetch the data point from coordinate 0 and time frame 0
// as provided by the other 'solver'

// Note how MUI implicitly handles MPI finalization
```

```
mpic++ -std=c++11 hello.cpp -o hello
```

```
mpirun -np 1 ./hello mpi://solver1/ifs 0.618 : -np 1 ./hello mpi://solver2/ifs 1.414
```



MUI Key Classes & Methods

mui::uniface[1d|2d|3d]

The MUI controller class that manages all coupling activities

mui::uniface::push(name, position, value)

Push data into the interface buffer

mui::uniface::commit(timestamp)

Send all data points in buffer as a time frame

mui::uniface::fetch(name, position, time, sampler_spatial, sampler_temporal)

Interpolate data from a timeframe / across several time frames

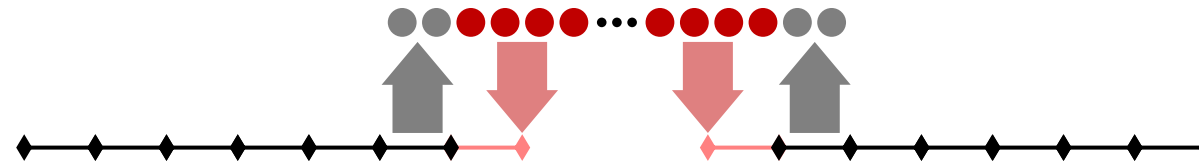
sampler_[gauss|exact|moving_avg|...][1d|2d|3d]

chrono_sampler_[gauss|exact|mean|...]

The MUI samplers



Hands-on Practice: 1D FDM-SPH Coupling



Finite Difference

```
for k steps
| push 'send' grid points
| commit
| fetch 'receive' grid points
| for all i:
| |  $u_i = u_i + k / h^2 * Du$ 
| end
end
```

Smoothed Particle Hydrodynamics

```
for k steps
| push 'send' particles
| commit
| fetch 'receive' particles
| for all i
| | for all j
| | |  $flux_{ij} = \dots$ 
| | end
| end
end
```



Hands-on Practice: 1D FDM-FDM Coupling



Fine

```
for k steps
| push 4 points near the boundary
| commit
| fetch 1 point from the coarse solver
| for all i:
| |  $u_i = u_i + k / h^2 * Du$ 
| end
end
```

Coarse

```
for k steps
| push 1 point near the boundary
| commit
| interpolate 1 point from the fine
solver using a Gaussian kernel
| for all i:
| |  $u_i = u_i + k / h^2 * Du$ 
| end
end
```



Thank you!

Acknowledgement

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Reference

Tang, Kudo, Bian, Li & Karniadakis. *Journal of Computational Physics*, 2015

