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CM4
Collaboratory on Mathematics for
Mesoscopic Modeling of Materials

Multiscale Universal Interface

A Concurrent Framework for Coupling Heterogeneous Solvers

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Brown University

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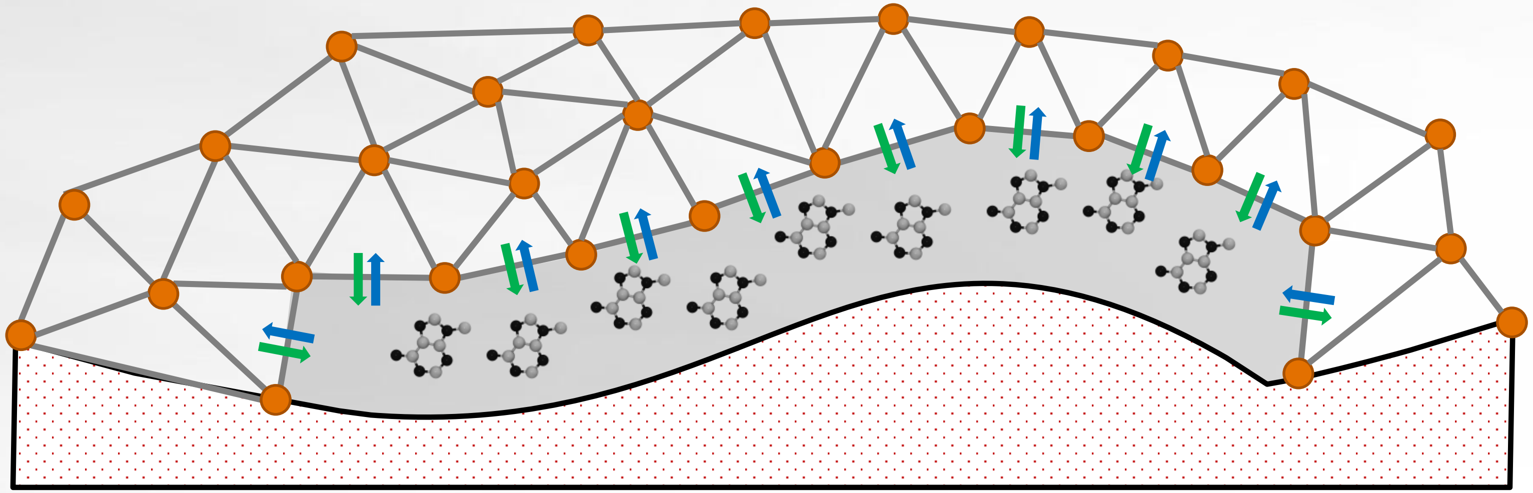
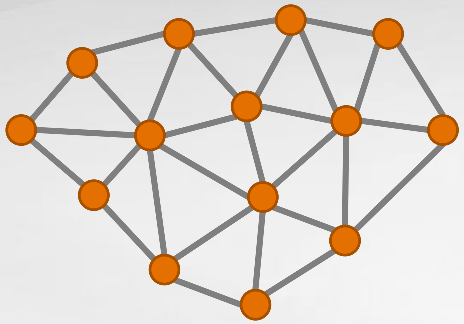
Multiscale Simulations by Domain Decomposition

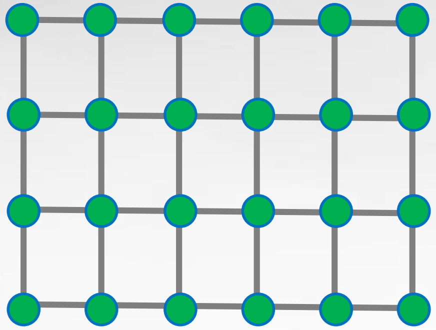
- Each solver handles a subdomain and use the other as boundary

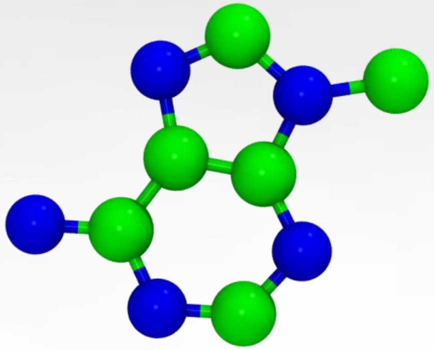


Diversity in Current Coupling - I

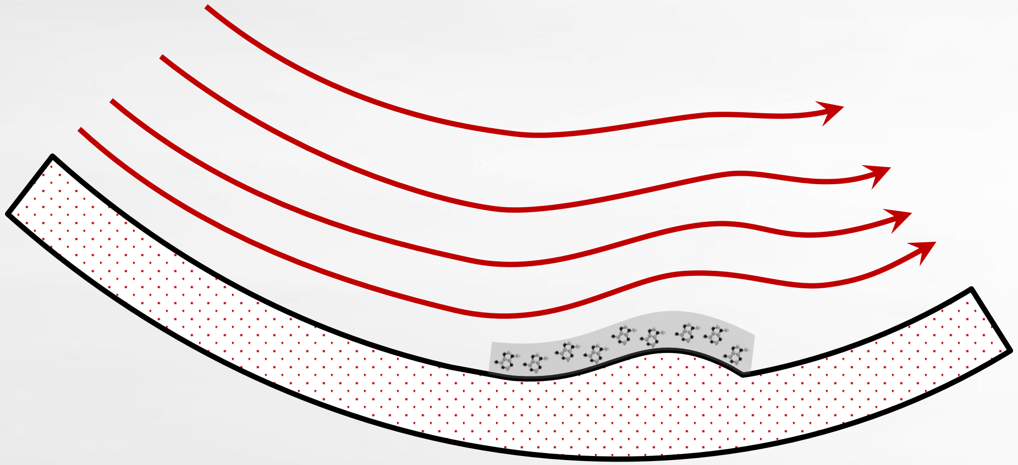
- Equation
  - Newton’s
  - Schrödinger's
  - etc.

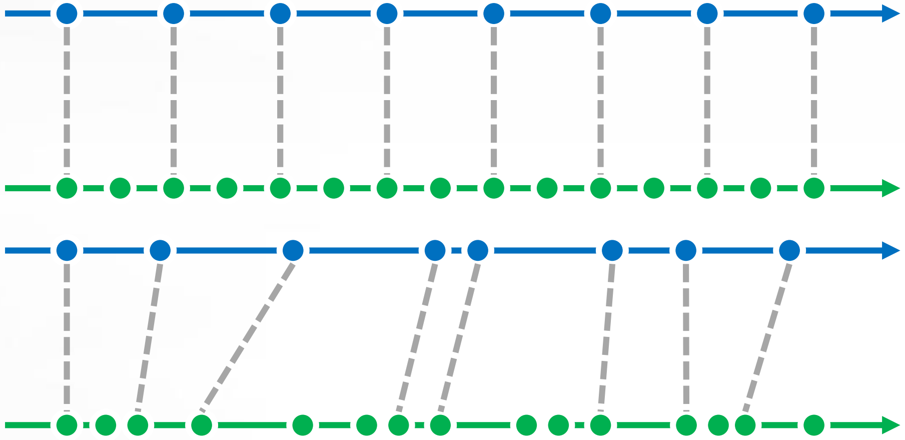




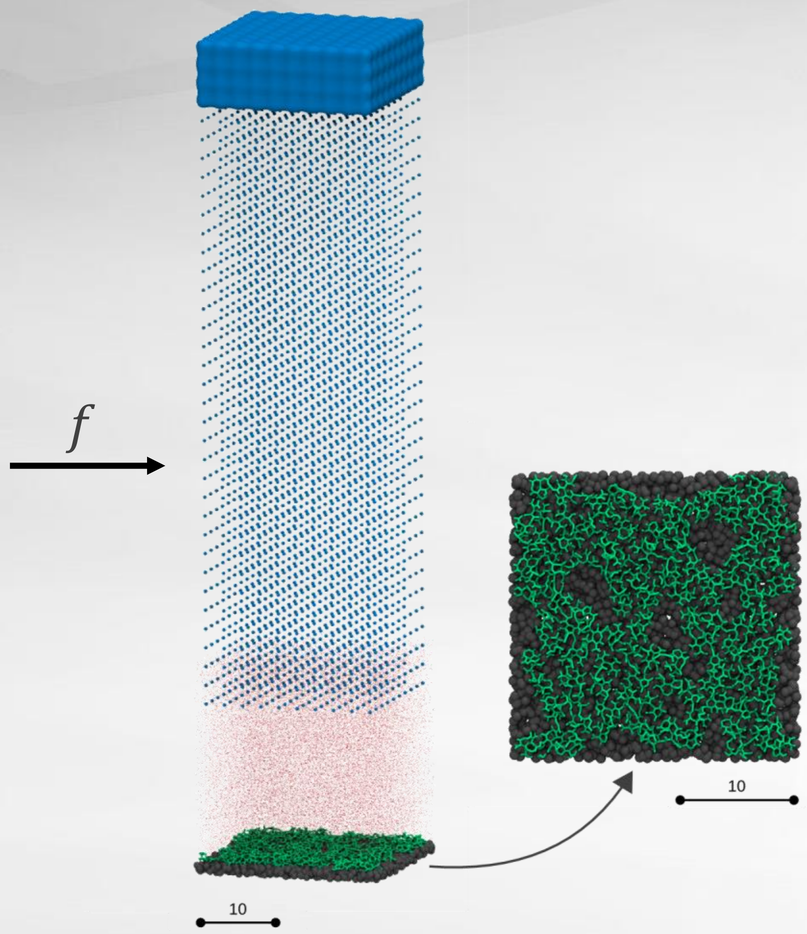


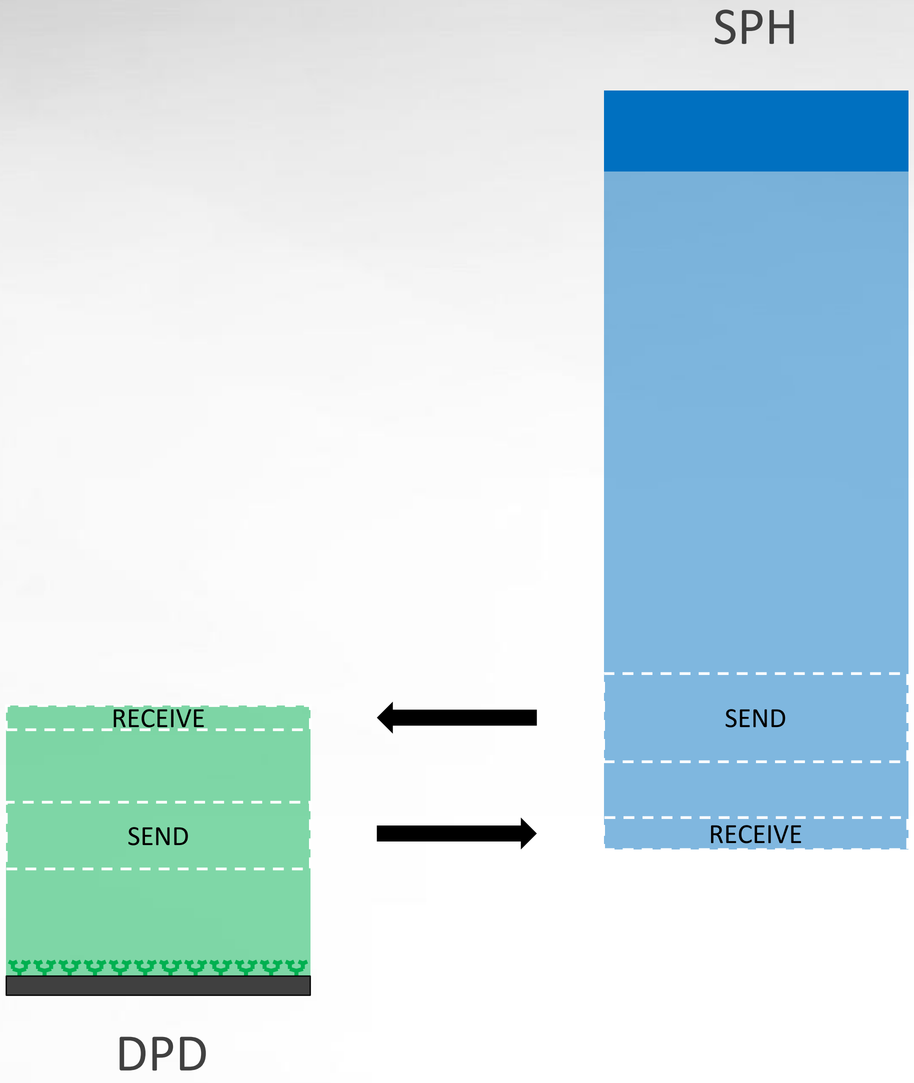
- Discretization / Geometry
- Time stepping: uniform, staggered, variable



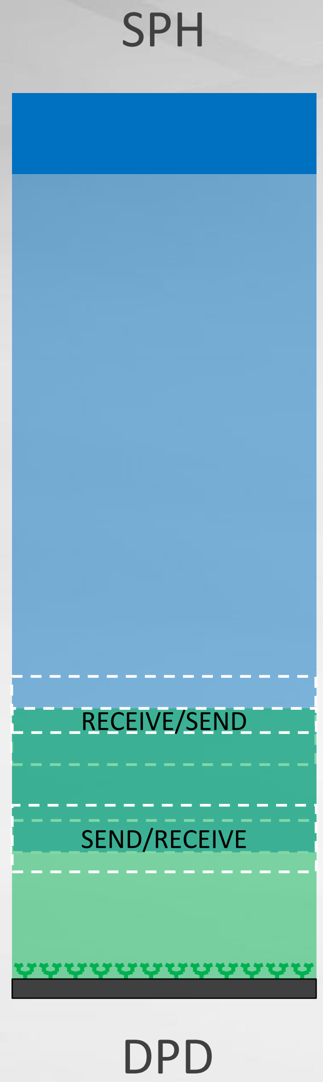


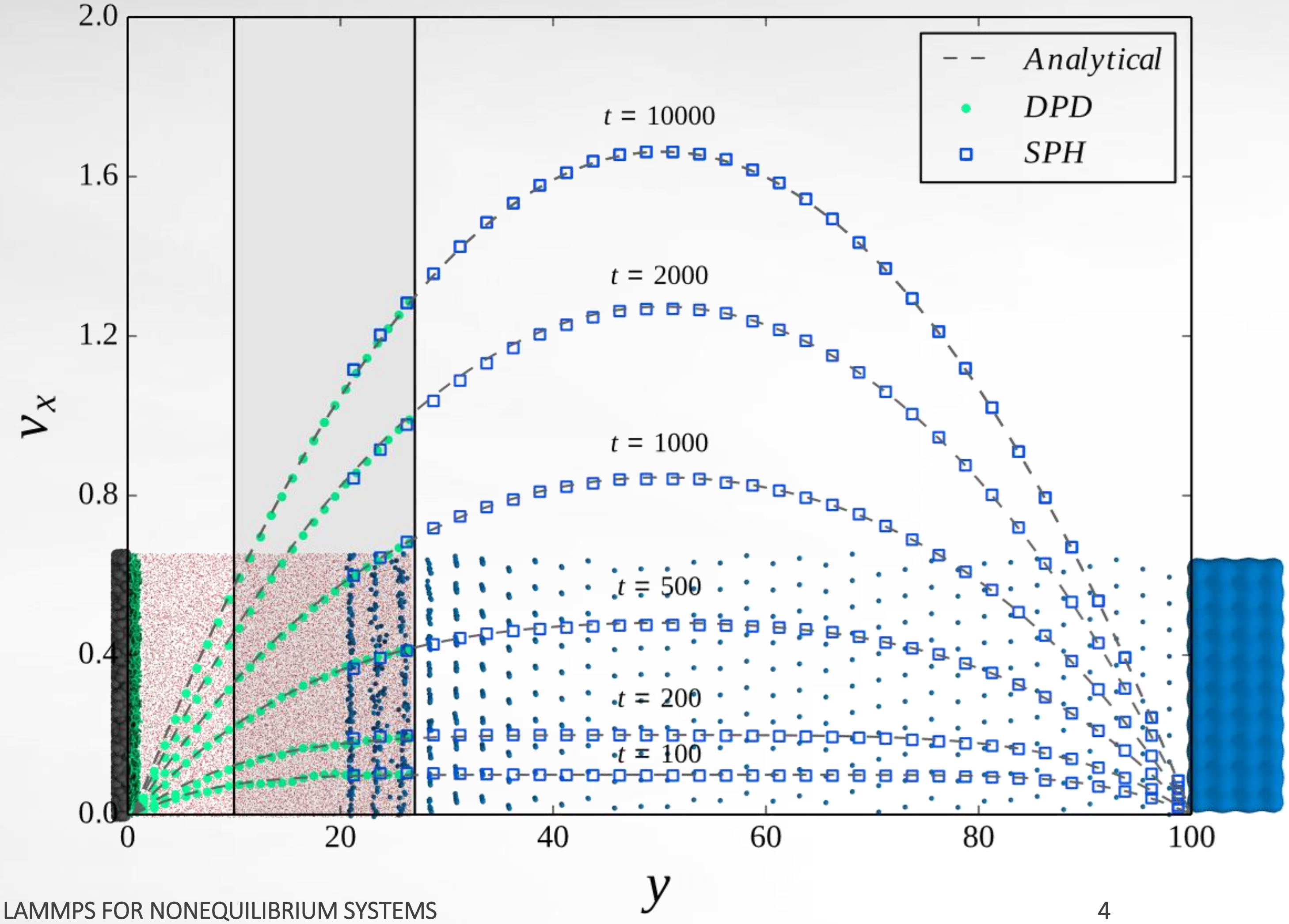
Example: Grafted Surface





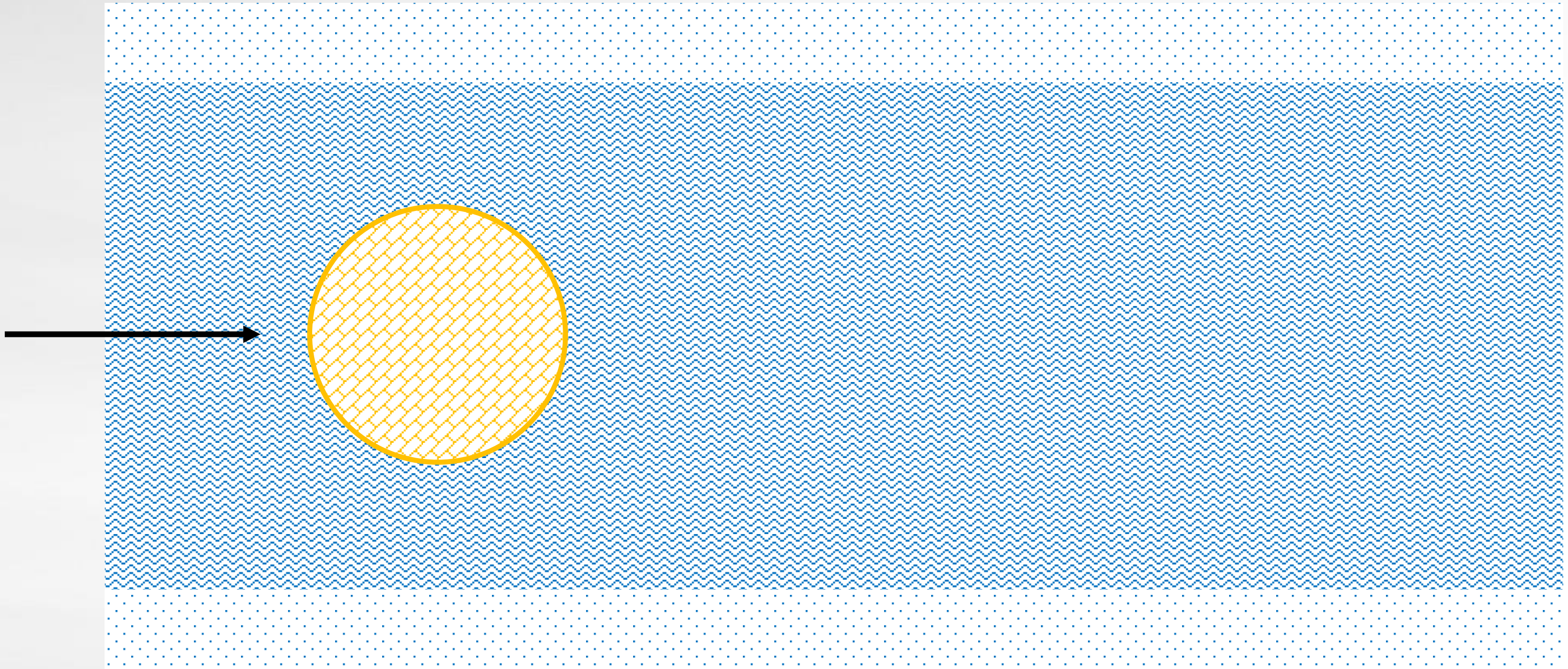
Example : Grafted Surface



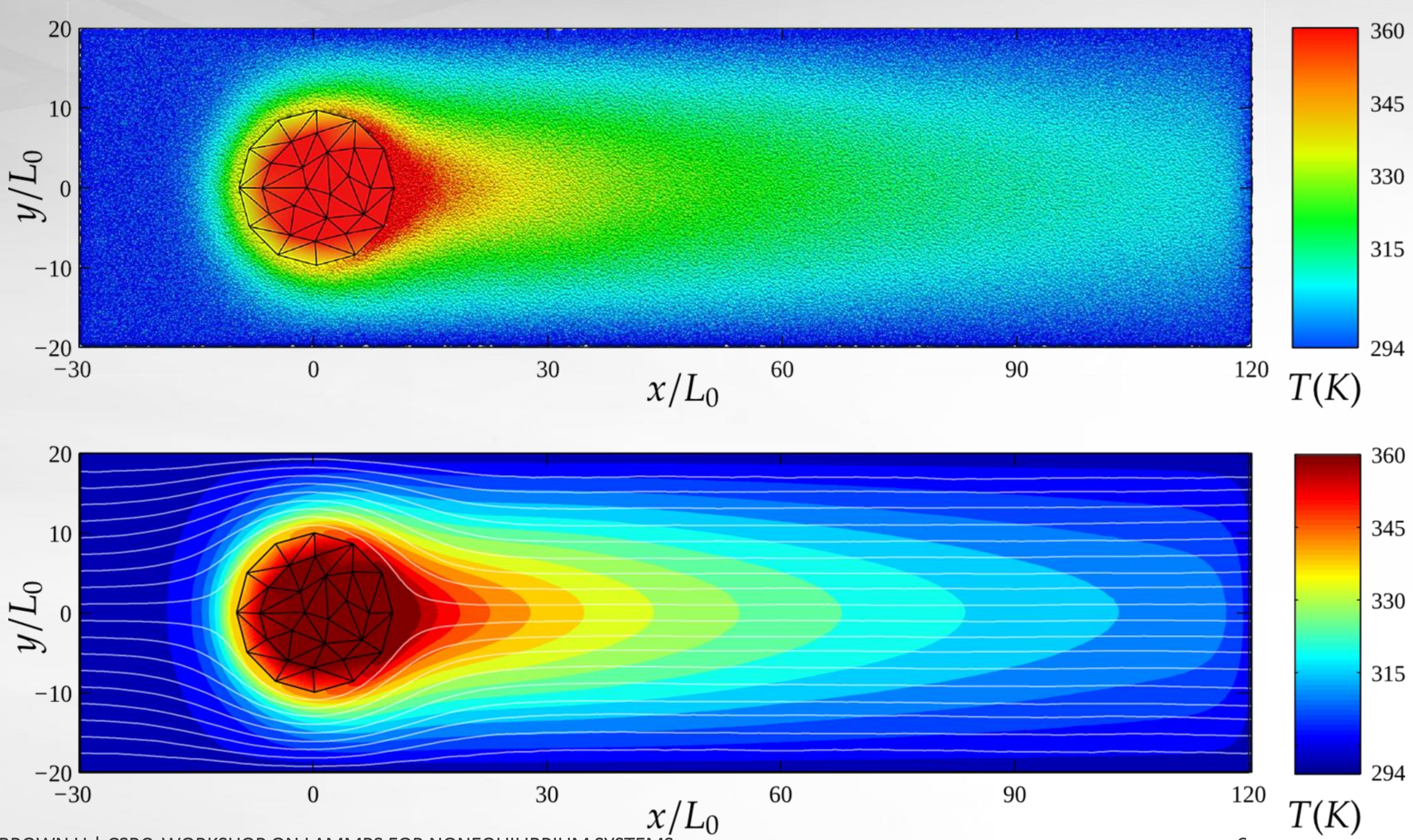


Example : Conjugate Heat Transfer

- FEM: Heat equation
- eDPD: Navier-Stokes + Heat equation



Example : Conjugate Heat Transfer

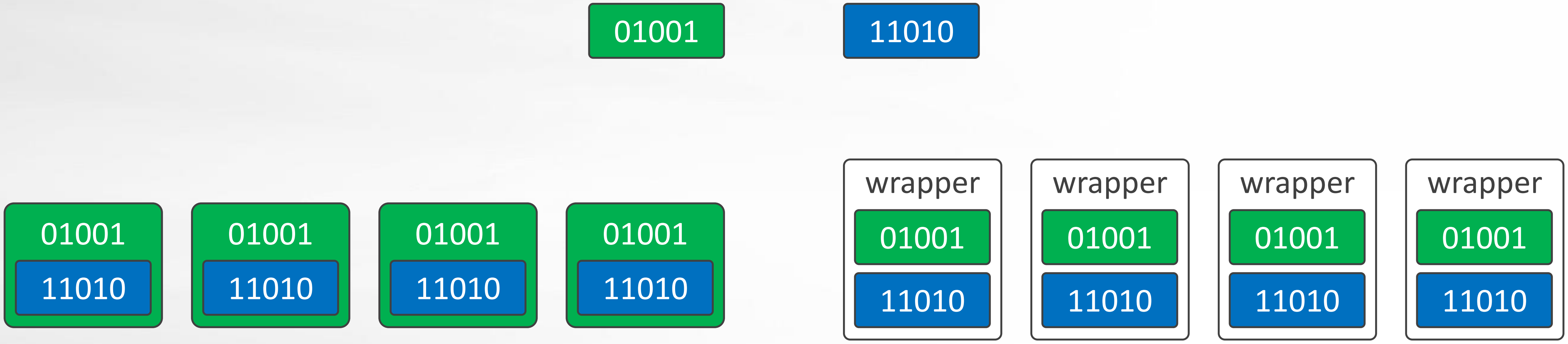


Diversity in Concurrent Coupling - II

- Solver: C, C++, Fortran, Python, …
- Scheme
- Parallelization: Serial, OpenMP, MPI, …

- The majority of existing code
  - was not developed to be coupled
  - need refactoring/invasive development

- Existing solutions largely rely on embedding or metacode



EMBEDDED

METACODE

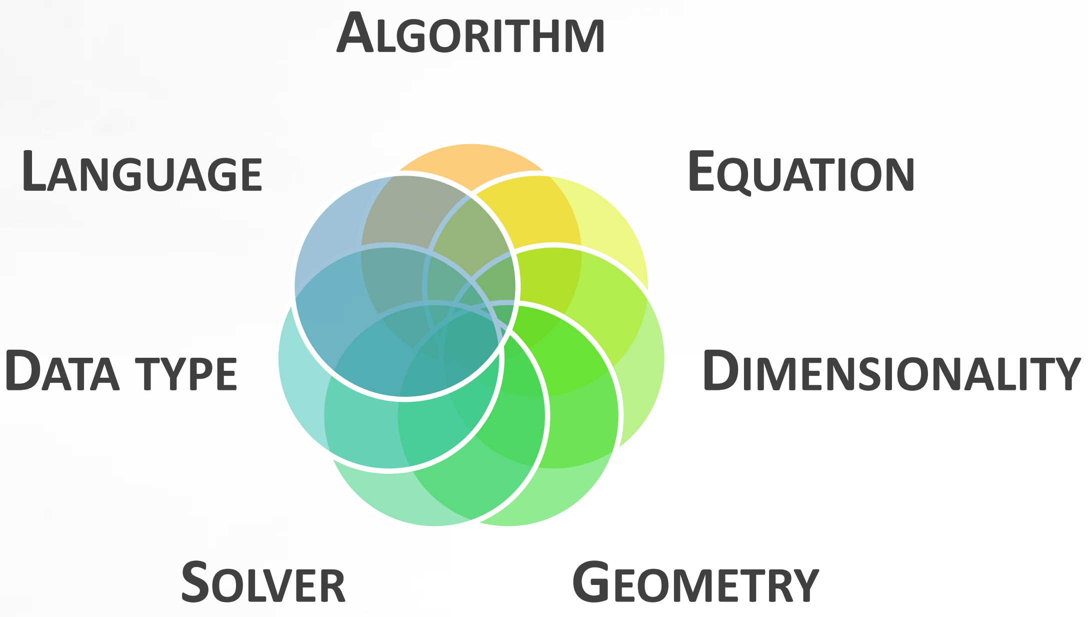
Multiscale Universal Interface (MUI) 01001 MUI

IS

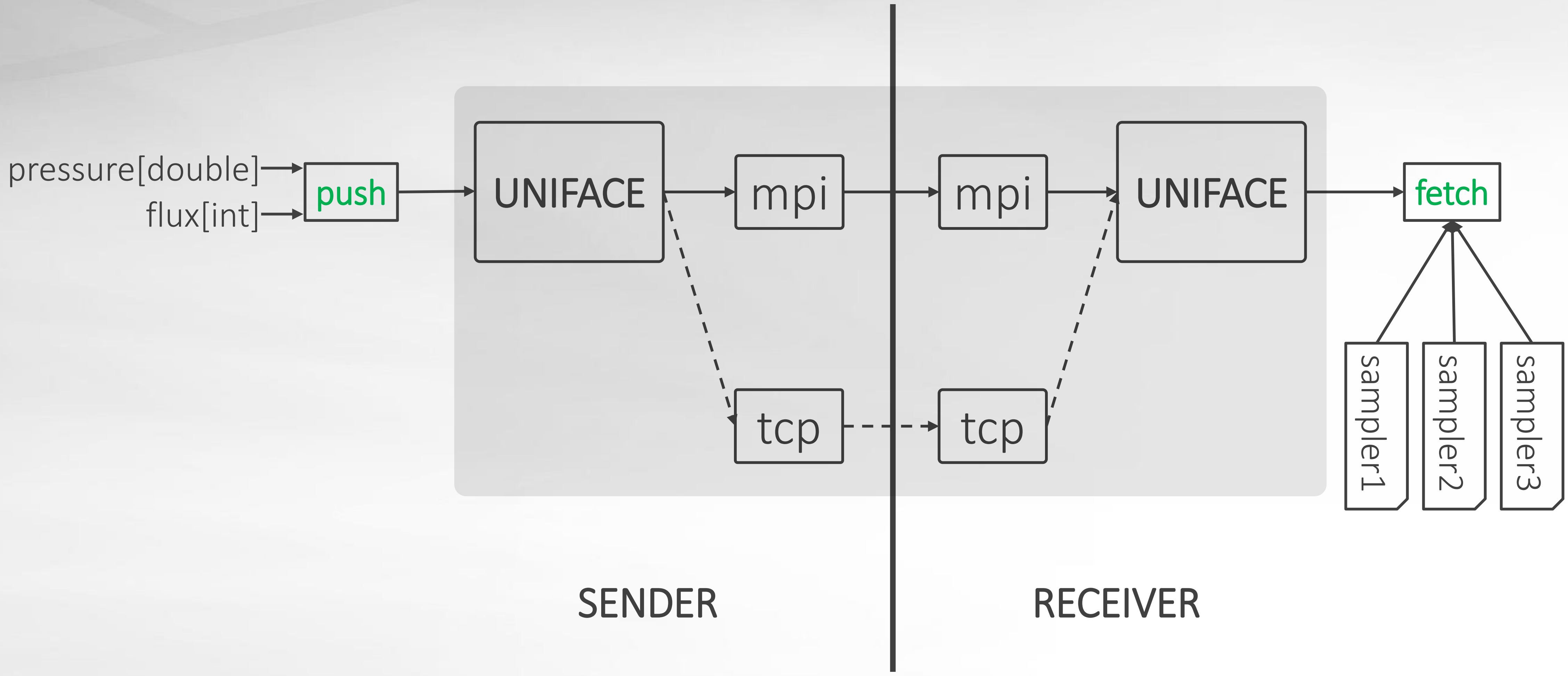
- **A plug-and-play platform** for testing ideas on multiscale coupling.
- **A communication layer** for multi-solver information exchange.
- **A header-only C++ library** that can be dropped into existing codes easily

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.

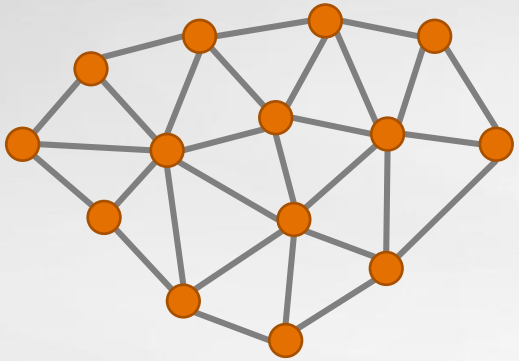


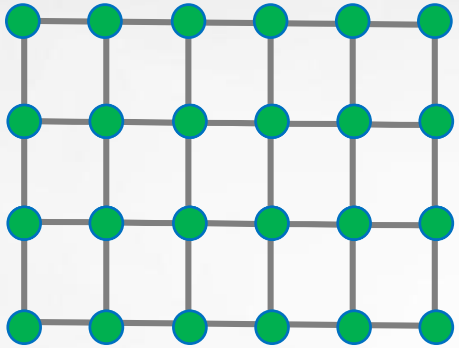
Workflow Overview

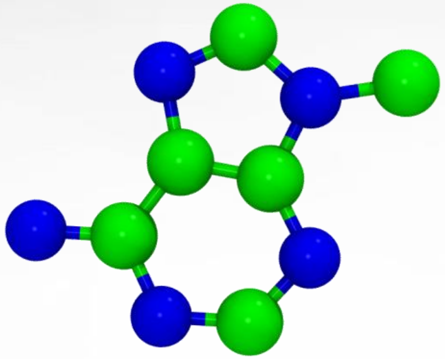


Abtraction: Data points

- Data point ≔ (location, type, value)



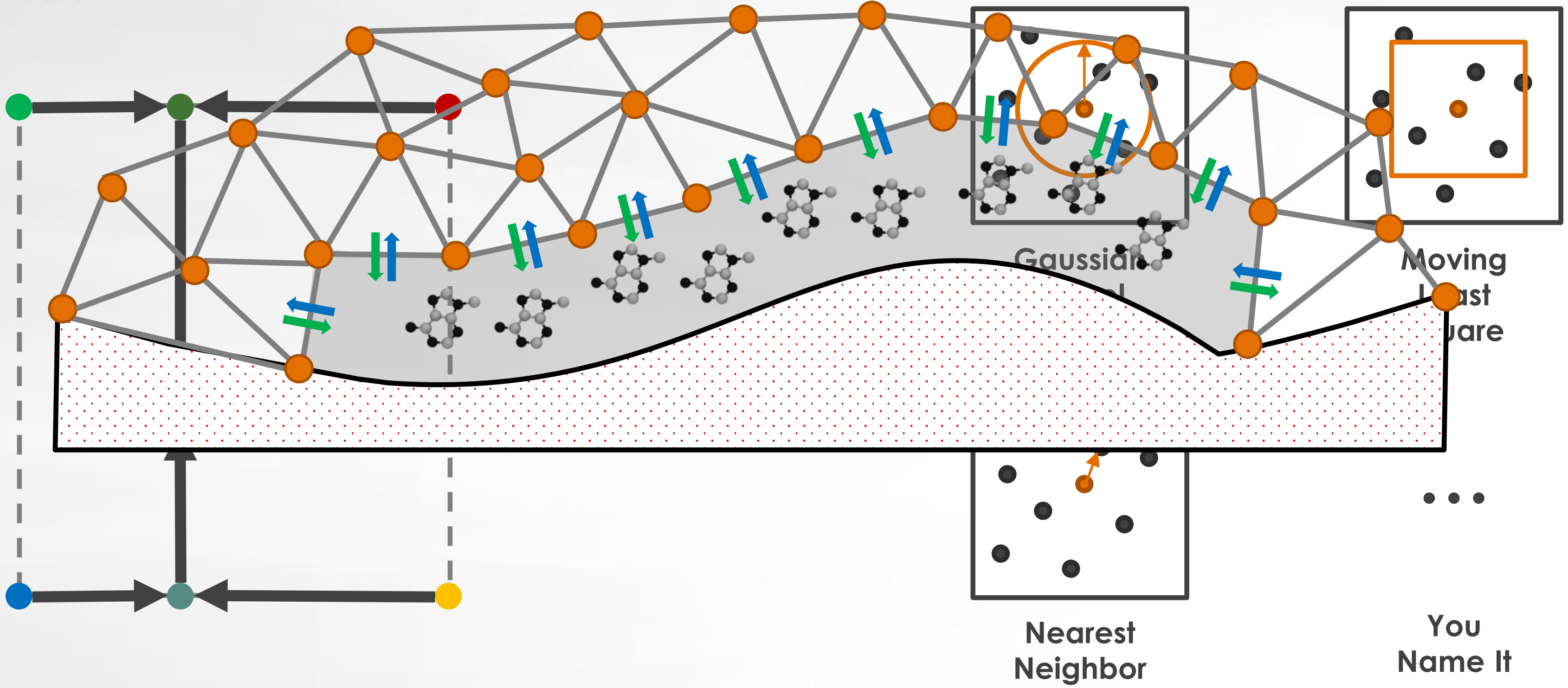




- Location: Vector Expression Templates
  - arbitrary dimension
  - real/complex coordinate
  - automatic SIMDization
- Value: arbitrary type
  - C++ templates
  - Type list metaprogramming

Abstraction: Sampling

- Texture Sampler
  - Hardware-implemented
  - Interpolate continuous color surface from discrete pixels
- Data sampler
  - C++ functors
  - Can implement any interpolation

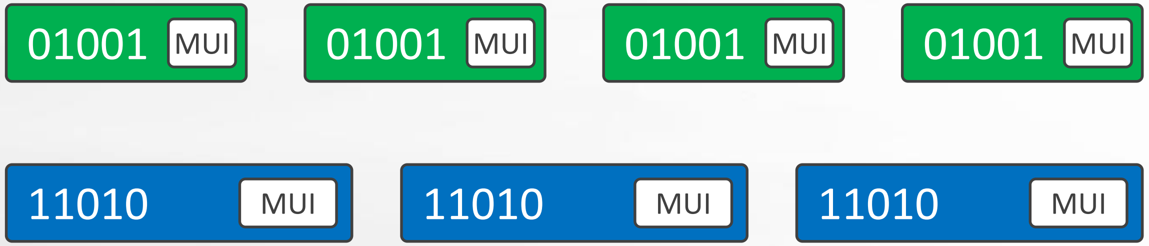


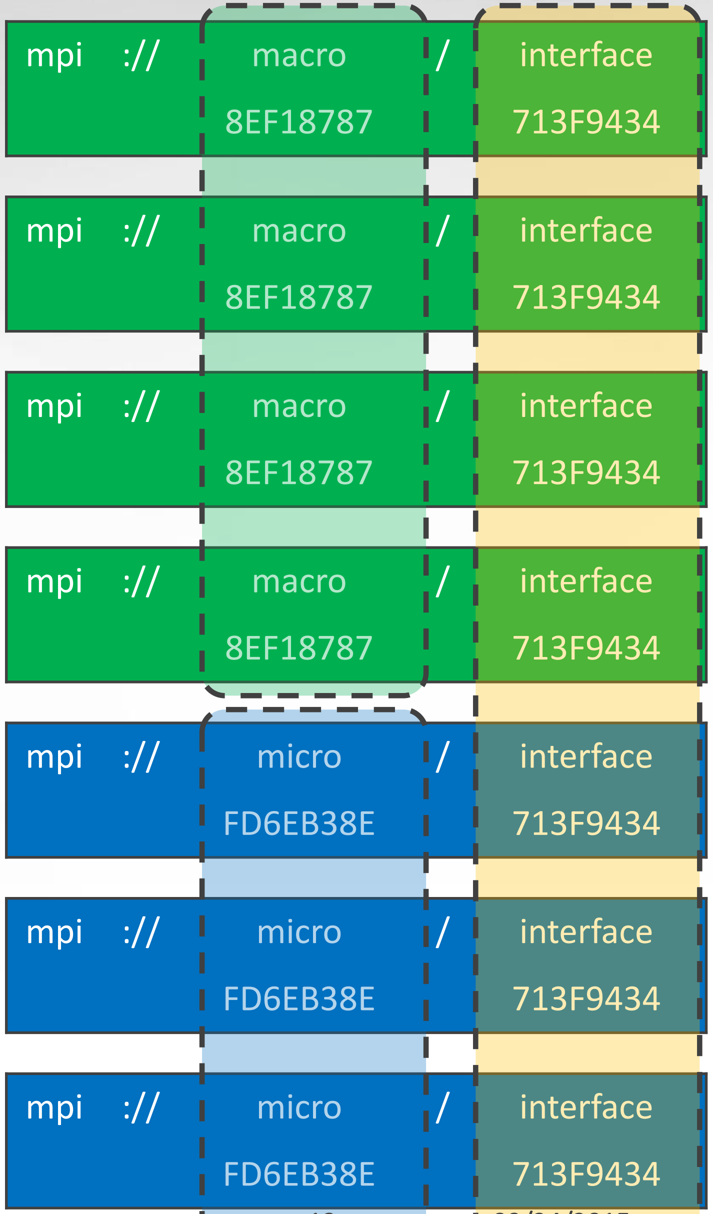
Sampler Design

```
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;
      }
```

Parallelization: MPI MPMD

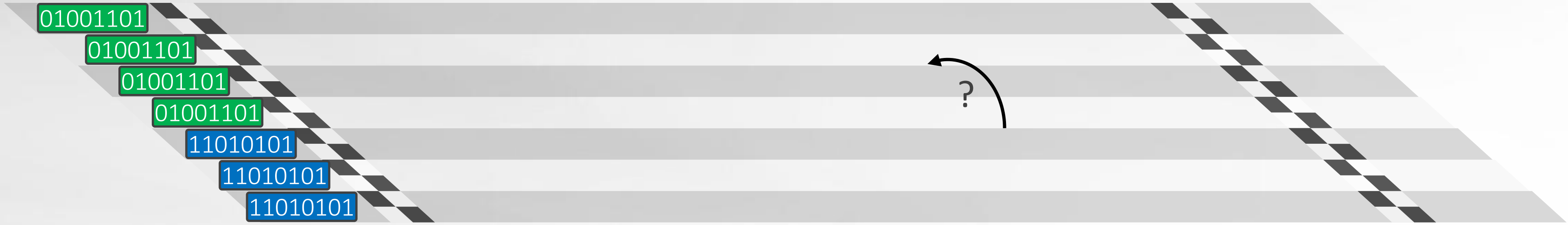
- Solvers compiled separately, runs concurrently
- MPMD syntax: mpirun -np N1 solver1 : -np n2 solver2
- URI: `protocol://domain/interface`
  - Use hash function to digitize the string
- Fetch method thread-safe
- TCP communicator in progress

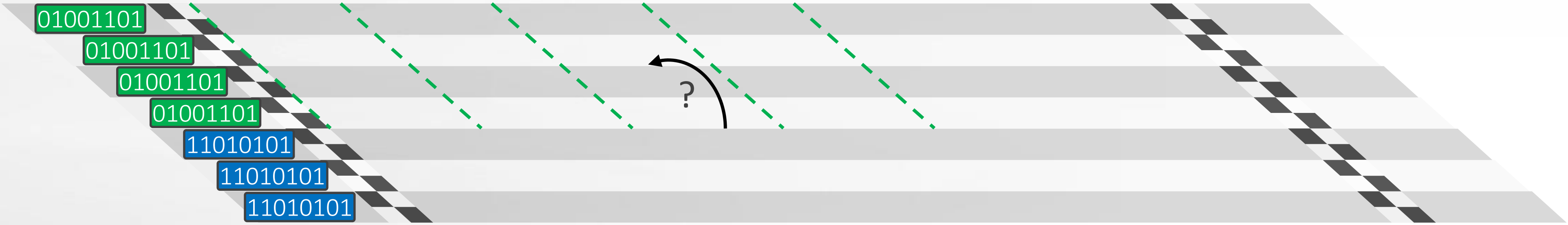



mpi :// macro 8EF18787 / interface 713F9434
mpi :// macro 8EF18787 / interface 713F9434
mpi :// macro 8EF18787 / interface 713F9434
mpi :// macro 8EF18787 / interface 713F9434
mpi :// micro FD6EB38E / interface 713F9434
mpi :// micro FD6EB38E / interface 713F9434
mpi :// micro FD6EB38E / interface 713F9434

Time coherence

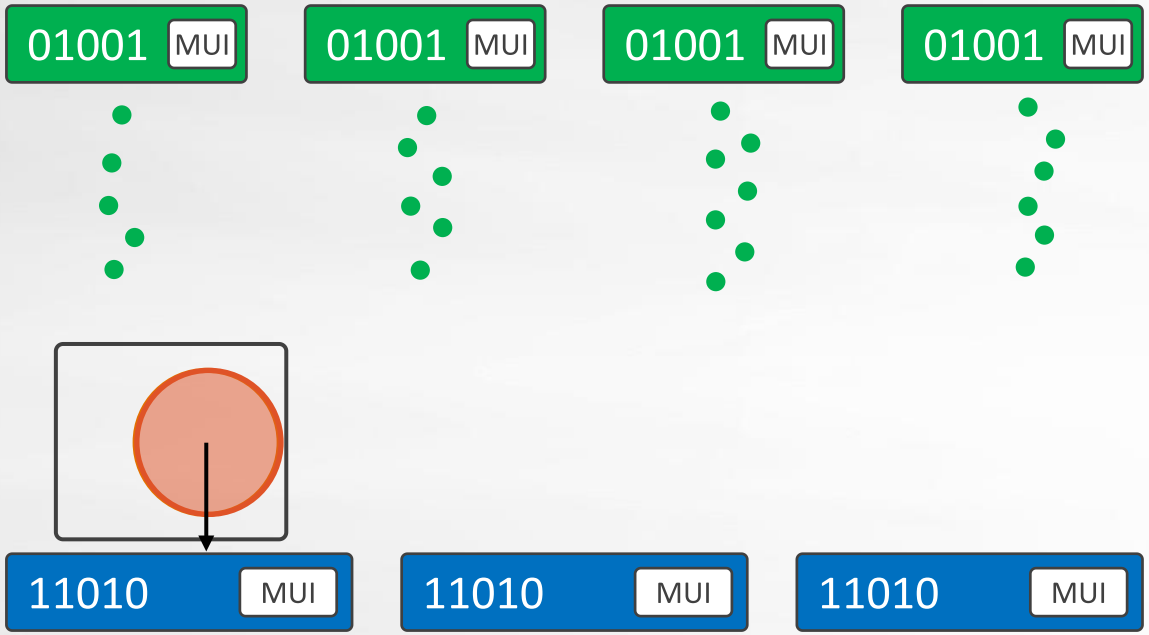
- MUI does not implicitly enforce solvers synchronization
  - In addition: time stepping may not align



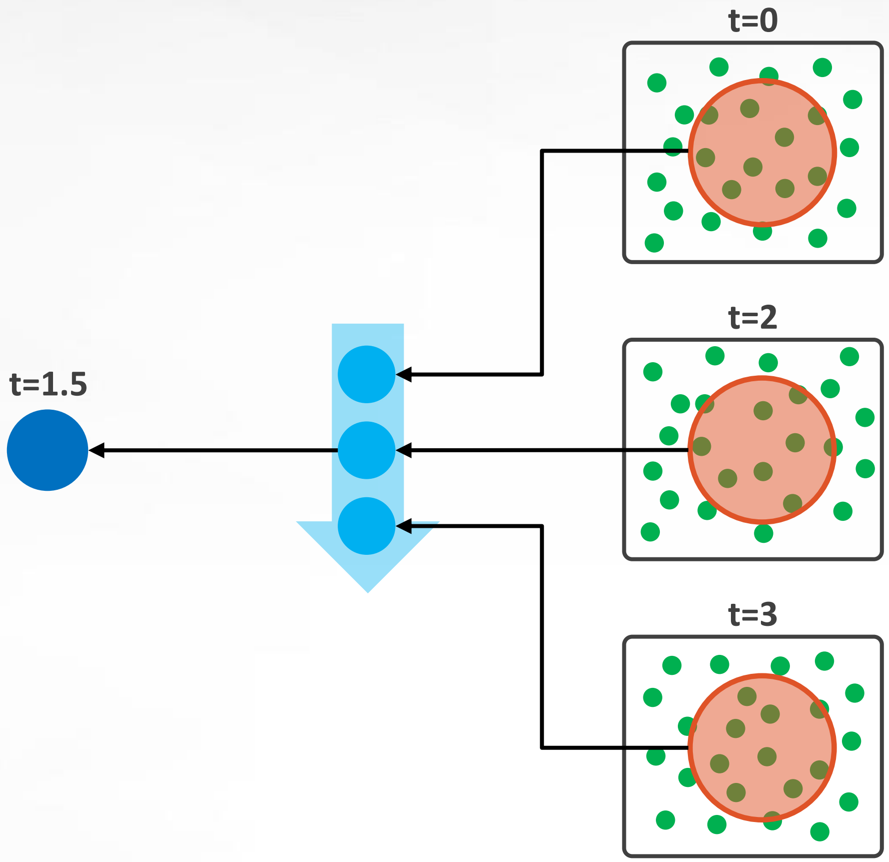


Time coherence

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

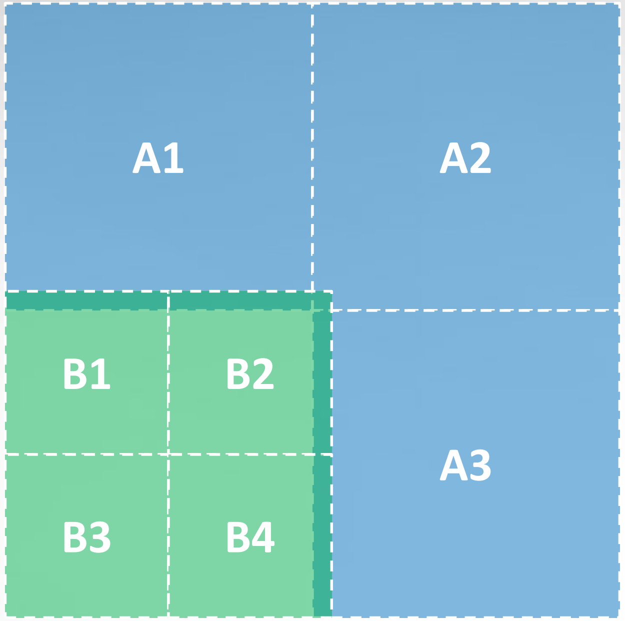


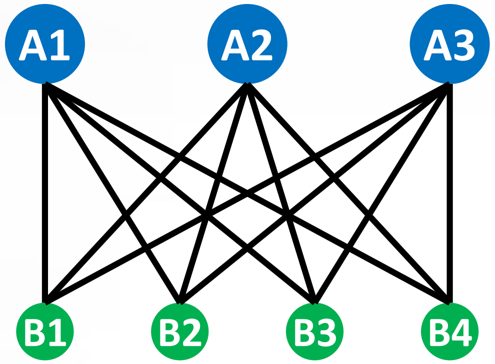
- Chrono sampler
  - Interpolate spatial results from time frames



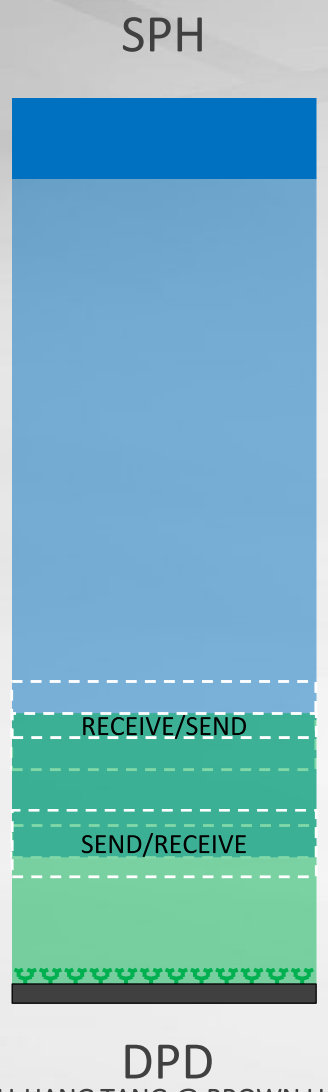
Selective Communication

- By default MUI 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 MUI to cut unnecessary messages
  - Arbitrary Boolean operations of boxes, spheres, and points
  - Use validity period for moving boundary





Example Revisited: Grafted Surface



```
/*********** 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)
```

MUI Functionality in LAMMPS

```
#include "fix.h"
#include <mui/mui.h>

class FixMUI : public Fix {
public:
  FixMUI(class LAMMPS *, int, char **);

  virtual ~FixMUI() {
    if ( interface ) delete interface;
  }
  int setmask() {
    return POST_INTEGRATE | END_OF_STEP;
  }

  virtual void post_integrate();
  virtual void end_of_step();

protected:
  mui::uniface3d *interface;
  double send_upper, send_lower;
  double recv_upper, recv_lower;
  double sample_rc;
};

FixMUI::FixMUI(LAMMPS *lmp, int narg, char **arg)
```

```
  nevery = 1;
}

// the PUSH part
void FixMUI::post_integrate()
{
  for (int i = 0; i < atom->nlocal; i++) {
    if ( atom->x[i][1] >= send_lower && atom-
>x[i][1] <= send_upper ) {
      interface->push( "v_x", mui::point3d(atom-
>x[i]), atom->v[i][0] );
    }
  }
  double t = update->ntimestep * update->dt;
  interface->commit( t );
  interface->barrier( t-1 );
  interface->forget( t-1 );
}

void FixMUI::end_of_step()
{
  mui::sampler_shepard_quintic<double>
quintic(sample_rc);
  mui::chrono_sampler_exact<>        texact(0);
```

Thank you!

Reference & Acknowledgement

Yu-Hang Tang, Shuhei Kudo, Xin Bian, Zhen Li, George Em Karniadakis, Multiscale Universal Interface: A Concurrent Framework for Coupling Heterogeneous Solvers, *Journal of Computational Physics*, manuscript in revision.

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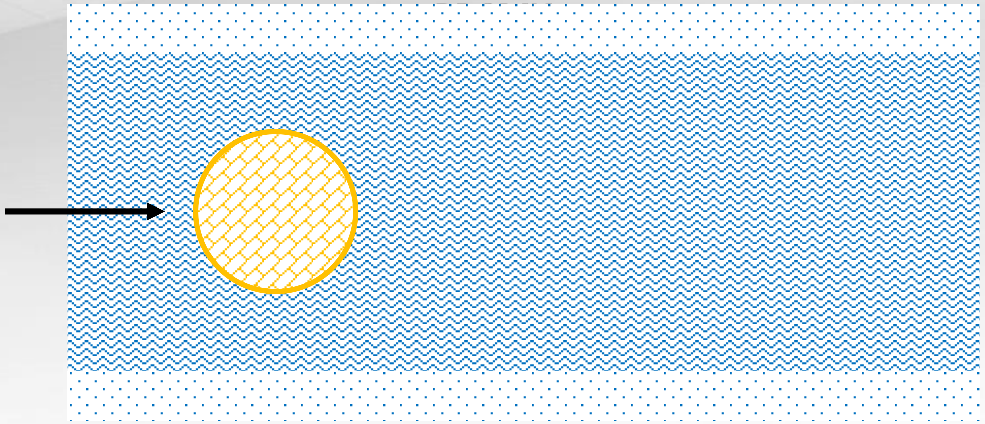
Language compatibility

- MUI is written in C++11
  - C and Fortran wrapper included
- Compatible compilers

Compiler	Version	Command
GCC	4.8.3	-std=c++11
Clang	3.5.0	-std=c++11
Intel C++	15.0	-std=c++11 /Qstd=c++11
NVCC	7.0	-std=c++11

Example Revisited: Heat Transfer



- FEM: Heat equation
- eDPD: Navier-Stokes + Heat equation

```
/********** eDPD **********/
For t = 0:dt:T
  $t_{FEM}$ = Floor(t,10dt)
  For each particle i
    If WithinCutoffOfCylinder(i)
      $S_s$ = Linear
      $S_t$ = ExactTime
      $T_{wall}$ = MUI::Fetch
            ("T", coord[i], $t_{FEM}$, $S_s$, $S_t$)
      q = CalculateFlux(T[i], $T_{wall}$)
      MUI::Push("q", coord[i], -q/Cv)
  MUI::Commit(t)
  If t % 10dt = 0 then MUI::Forget(t-10dt)
  Force Eval, Integrate...
```

```
/********** FEM **********/
For t = 0:10dt:T
  For each boundary vertex i
    MUI::Push("T", coord[i], T[i])
  MUI::Commit(t)

  For each boundary vertex i
    $S_s$ = VoronoiMean(Vertices)
    $S_t$ = SumOver(10dt)
    f[i] = MUI::Fetch
          ("q", coord[i], t, $S_s$, $S_t$)
  MUI::Forget(t)
  Solve for Next Step
```