
# A Comprehensive Coupling Library for Large-scale Surface-coupled Multi-physics Problems

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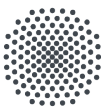
†Department of Mechanical Engineering, Eindhoven University of Technology

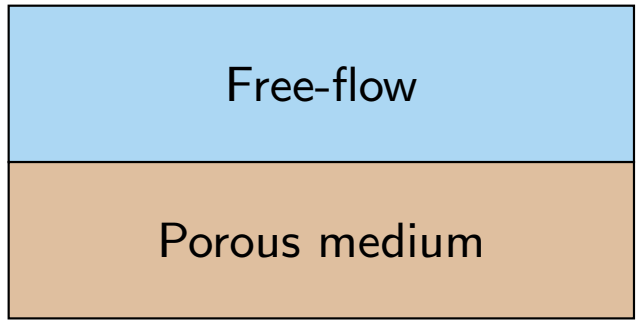


University of Stuttgart
Germany

March 11, 2019


# Interface-coupled problems

- Porous media and free flow



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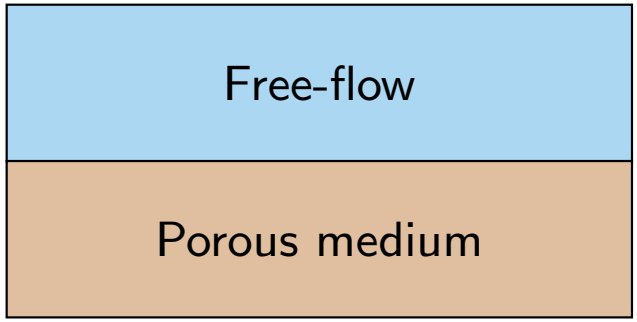
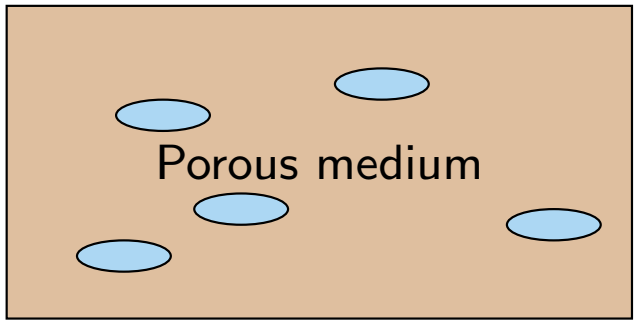



- Fractured porous media



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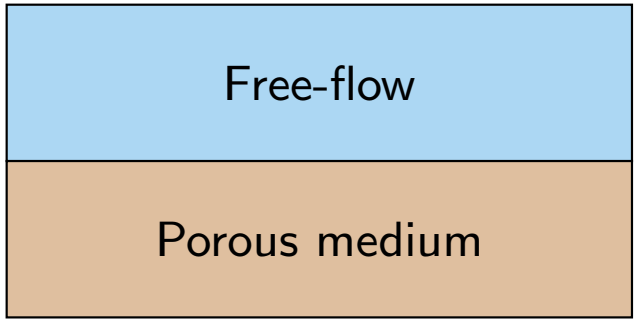


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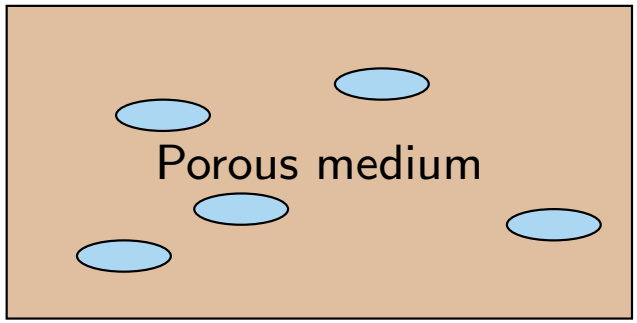
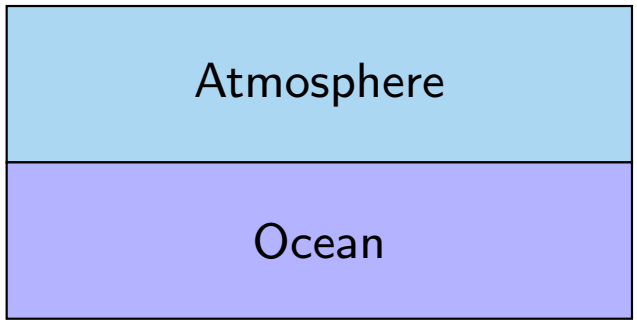



- Atmosphere and ocean



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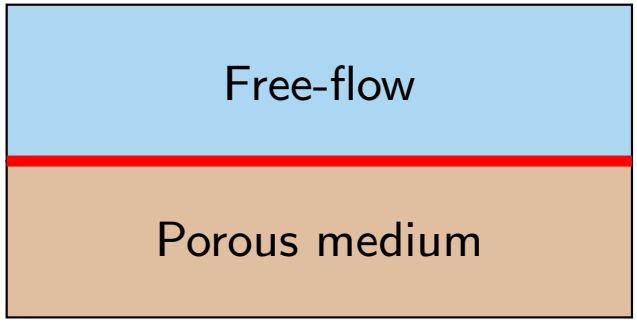


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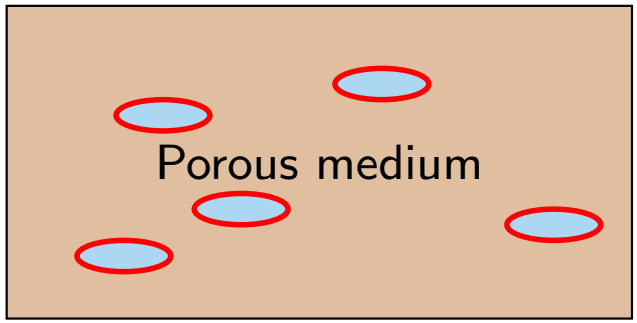


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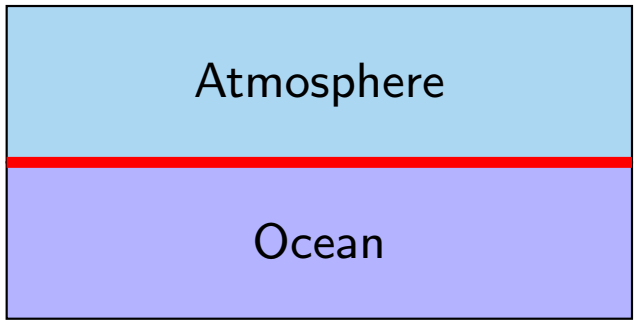

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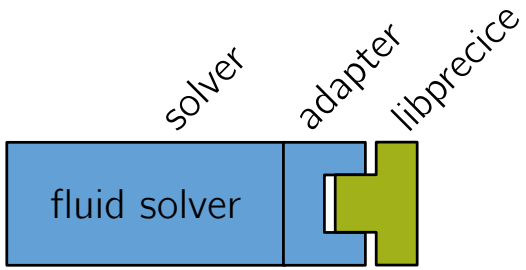
# Origin

## Fluid-structure interaction

https://vimeo.com/user79566151

# preCICE – A Plug-and-Play Coupling Library




OpenFOAM
SU2
foam-extend

# preCICE – A Plug-and-Play Coupling Library


OpenFOAM
SU2
foam-extend

CalculiX
Code_Aster
FEniCS
deal-ii
MBDyn

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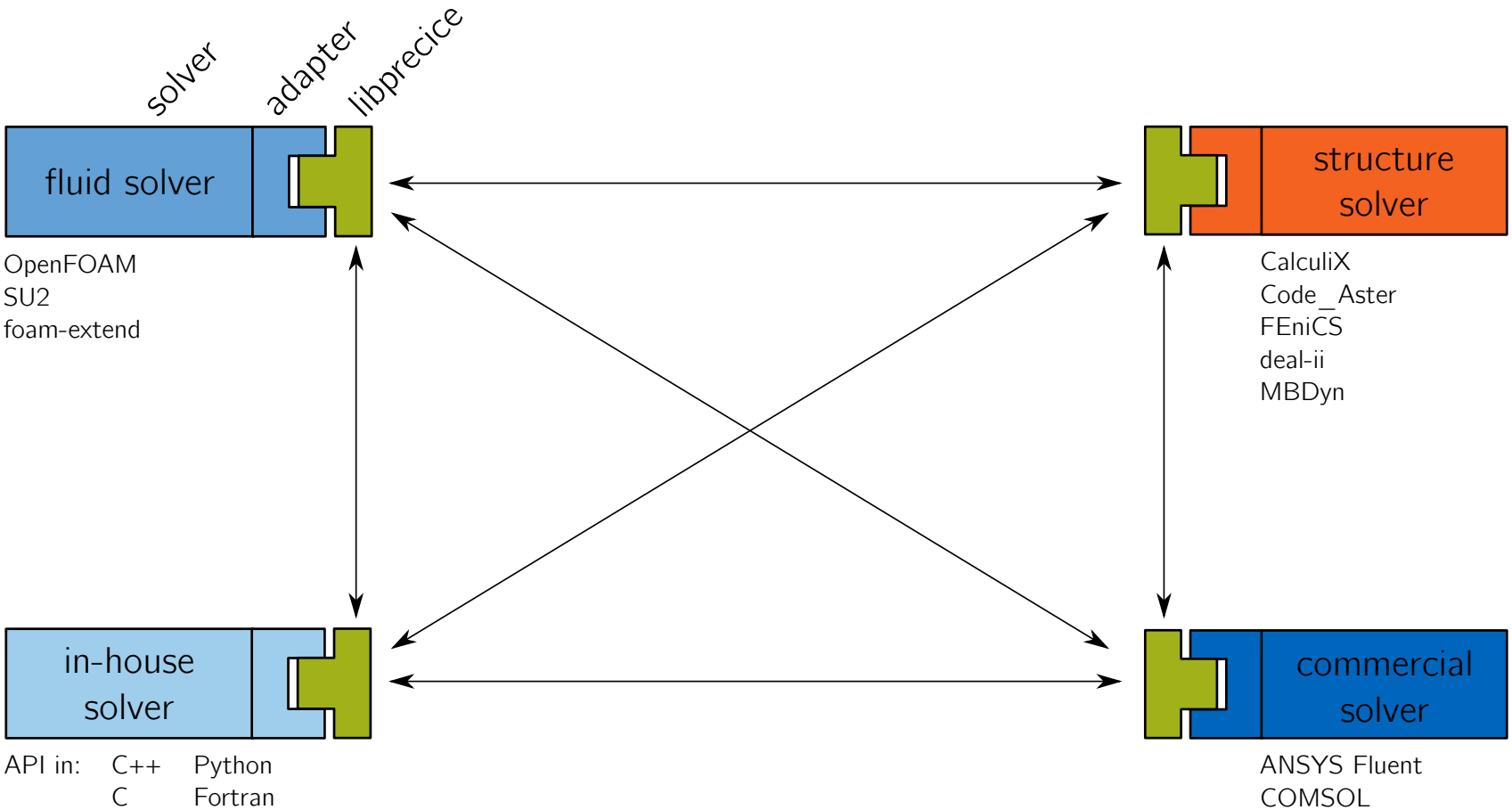

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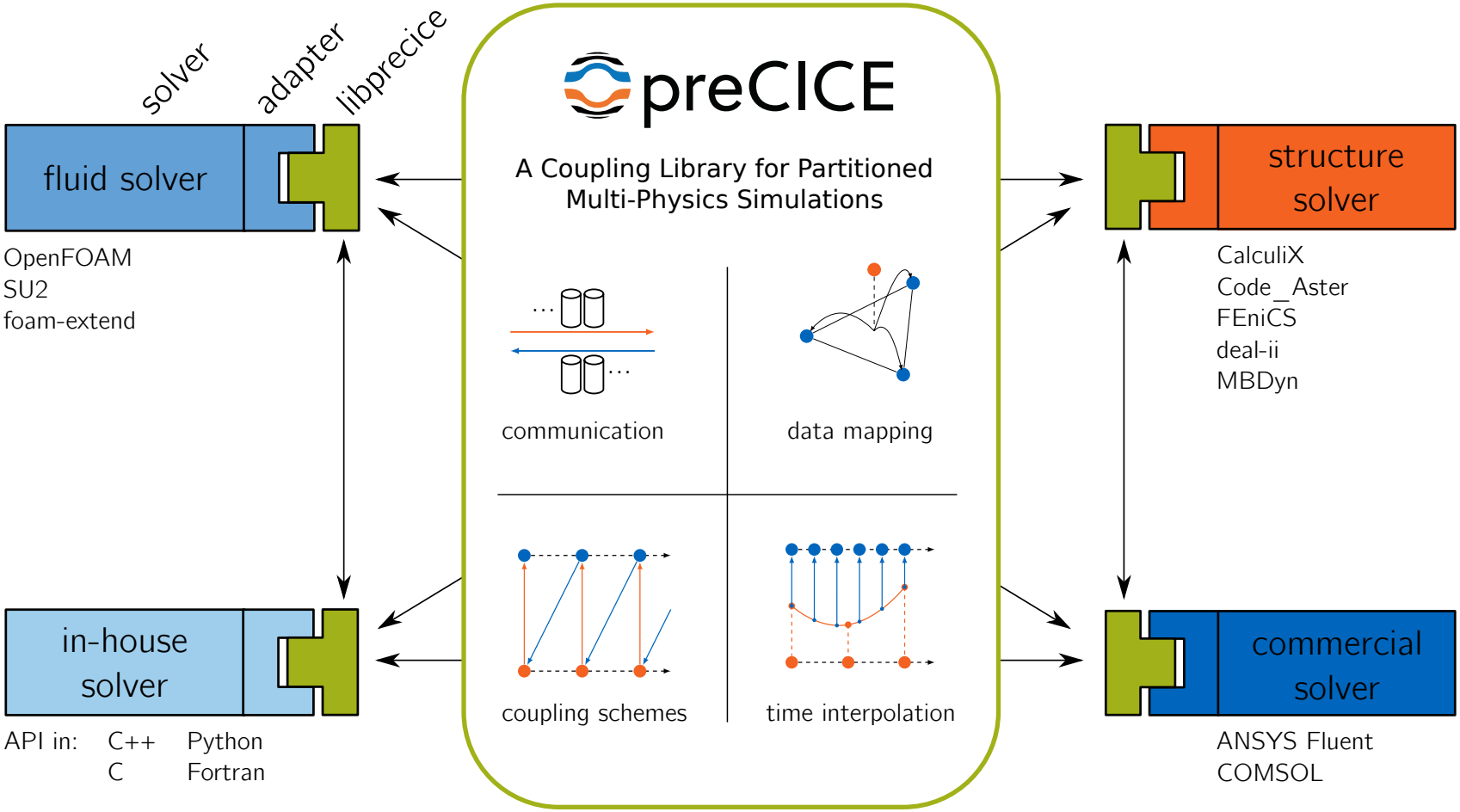
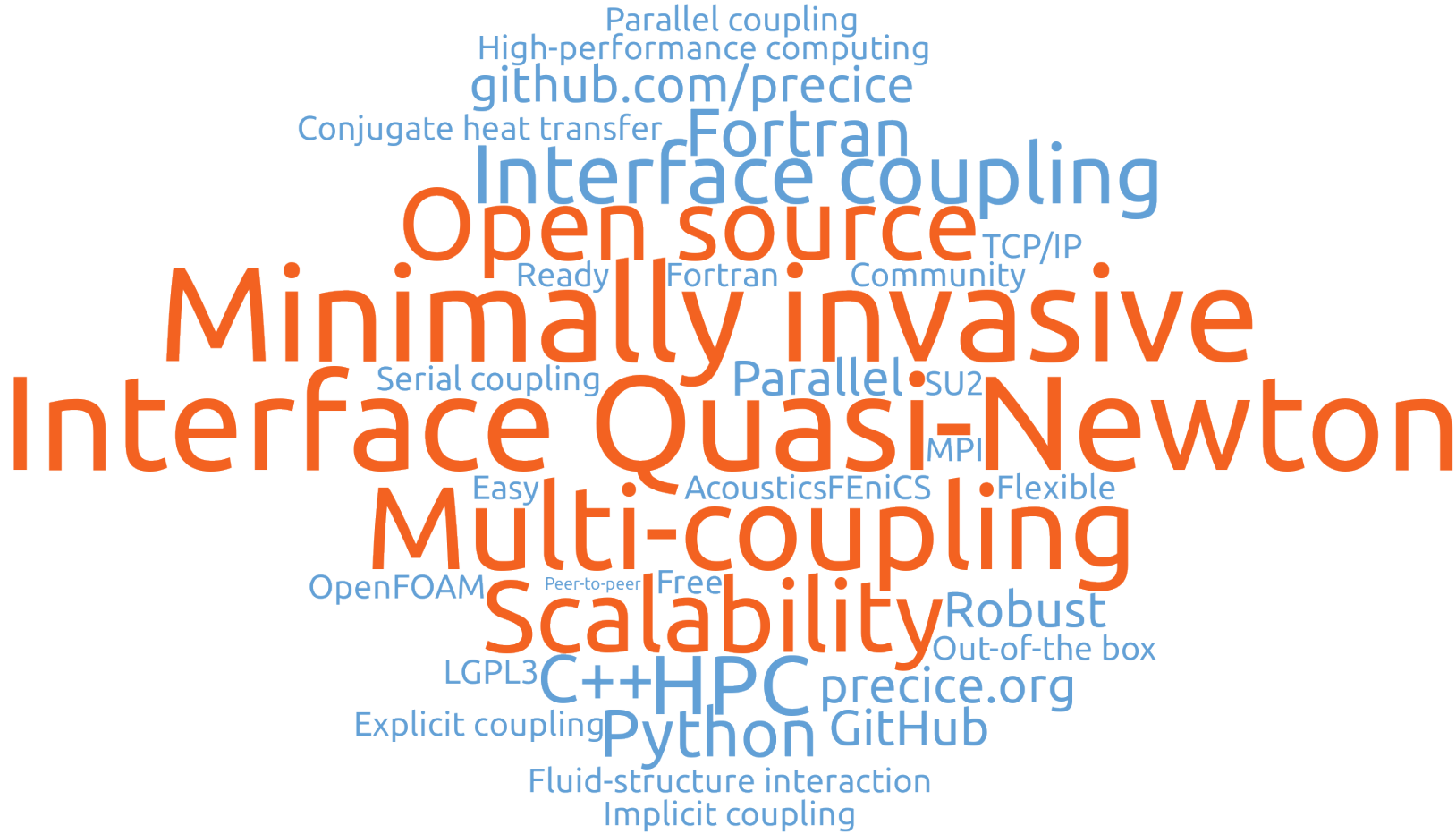
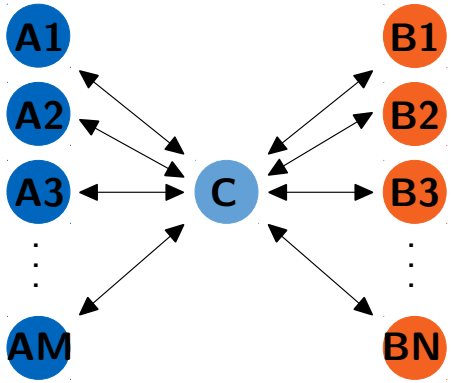


# Features


Parallel coupling
High-performance computing
github.com/precice
Conjugate heat transfer
Fortran
Interface coupling
Open source
TCP/IP
Ready
Fortran
Community
Minimally invasive
Serial coupling
Parallel
SU2
Interface Quasi-Newton
MPI
Easy
AcousticsFEniCS
Flexible
Multi-coupling
OpenFOAM
Peer-to-peer
Free
Scalability
Robust
Out-of-the box
LGPL3
C++HPC
precice.org
Explicit coupling
Python
GitHub
Fluid-structure interaction
Implicit coupling

# Scalability

## Server-based concept




- All communication through central server
- Interface computations on server (in sequential)
- $\Rightarrow$ Coupling becomes bottleneck for overall simulation already on moderate parallel systems

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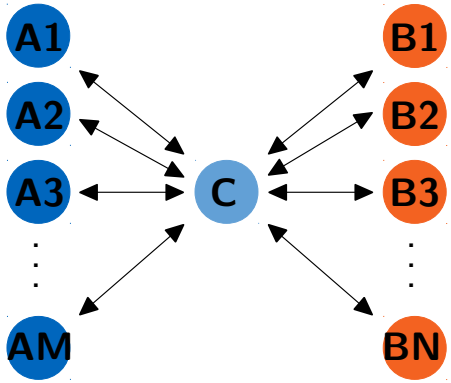


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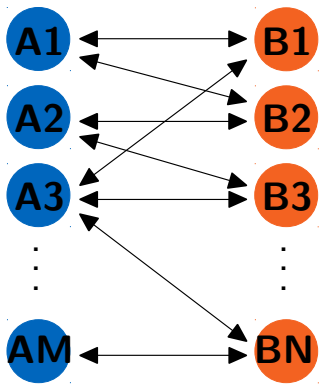
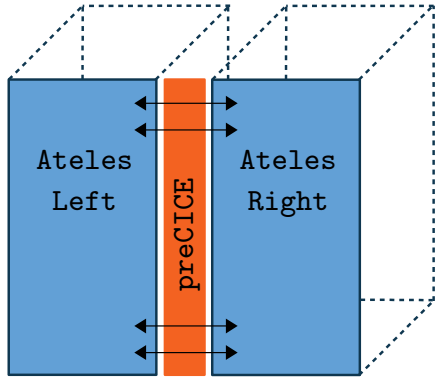
## Our peer-to-peer concept

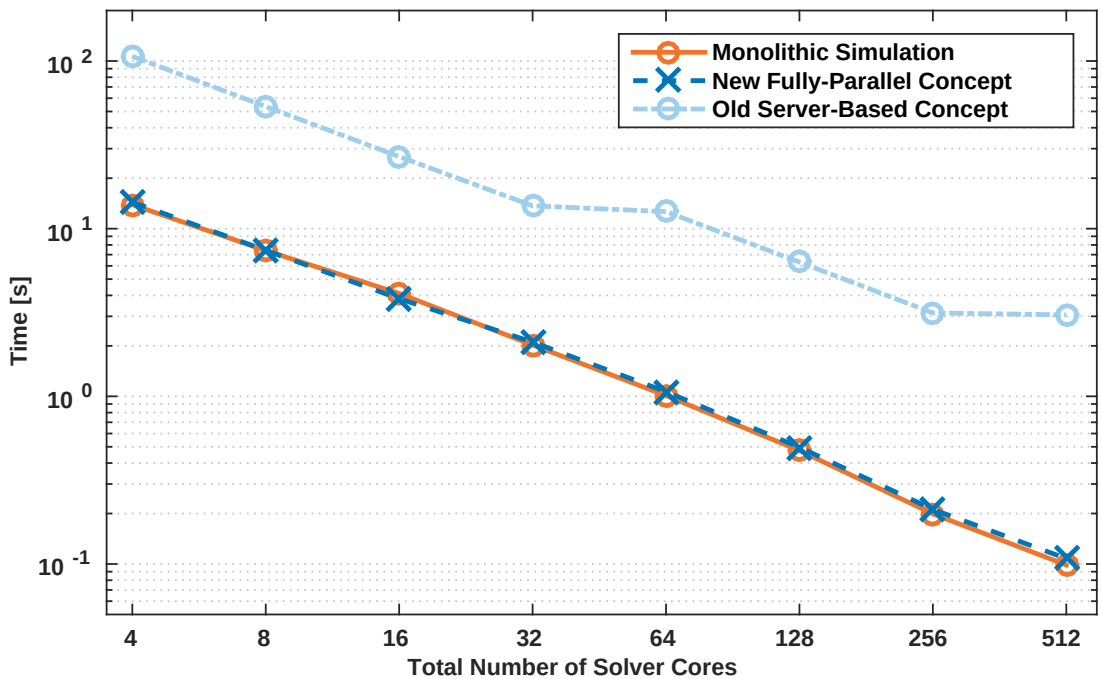



- No central entity
- $\Rightarrow$ Easier to handle (user does not need to care about server)
- $\Rightarrow$ No scaling issues

# Scalability

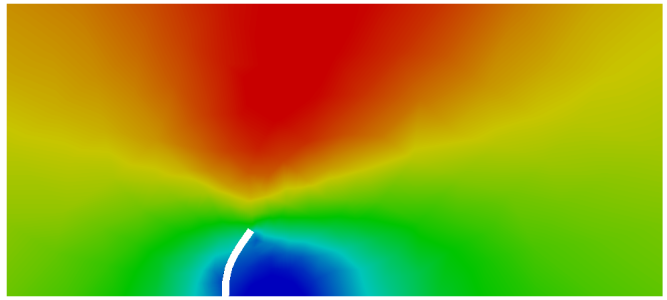
- Travelling density pulse (Euler equations) through artificial coupling interface
- DG solver Ateles (U Siegen), $7.1 \cdot 10^6$ dofs
- Nearest neighbor mapping and communication



# Different couplings

- Fluid solver: $F : d \mapsto f$
- Structure solver: $S : f \mapsto d$
- Solve fixed-point problem: $(S \circ F)(d) \overset{!}{=} d$



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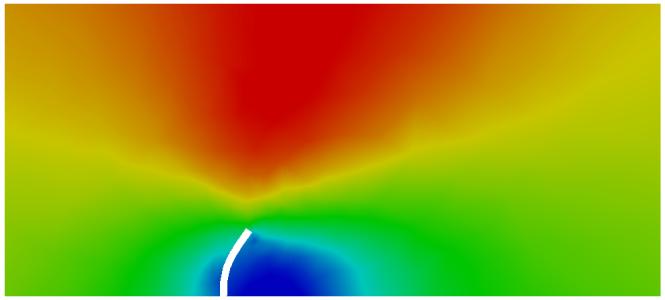
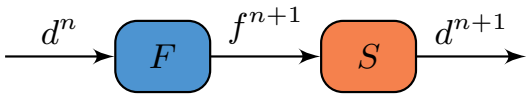


**explicit**

**serial**



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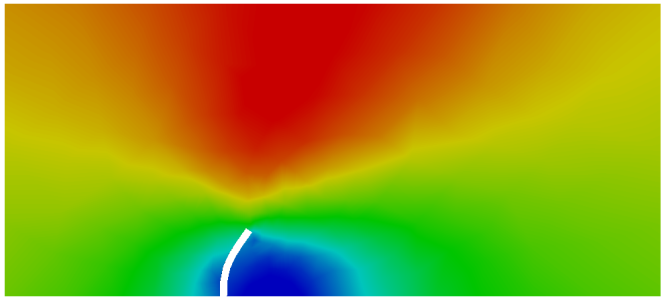

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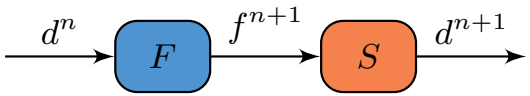
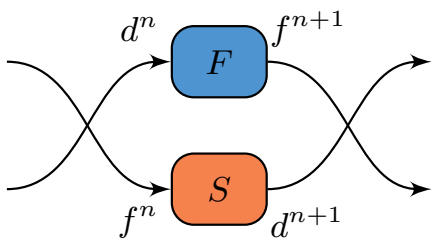



**parallel**



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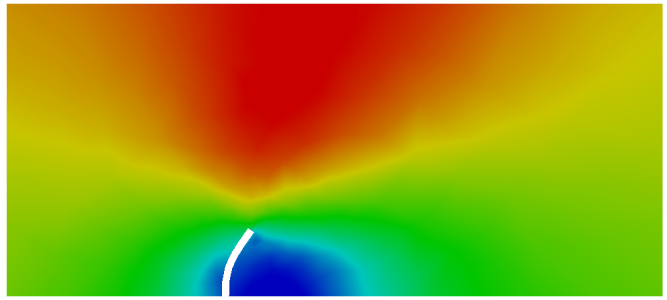

**explicit**

**implicit** (iterative)

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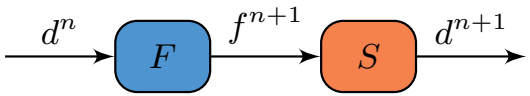


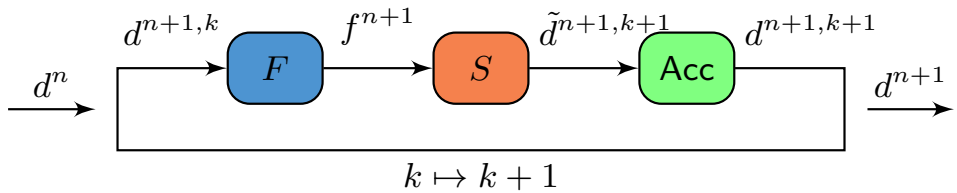


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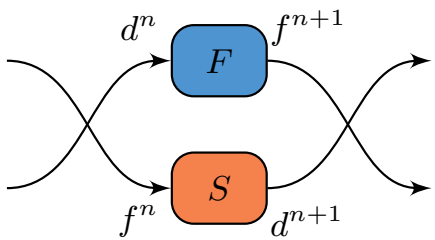

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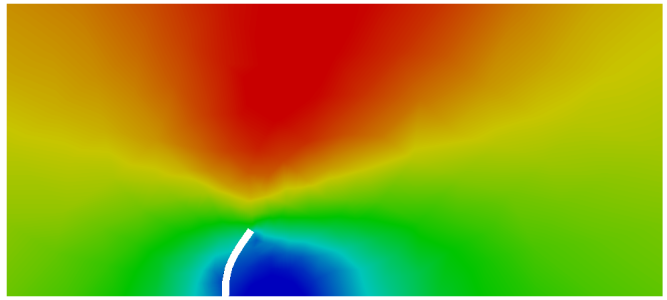

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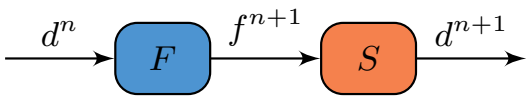


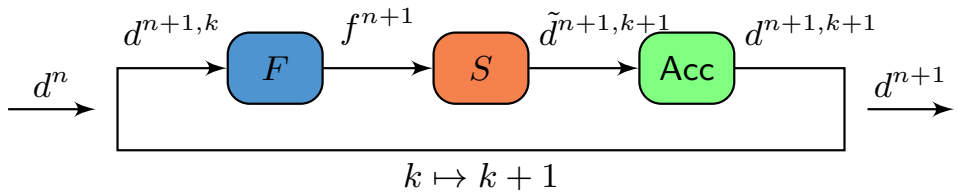


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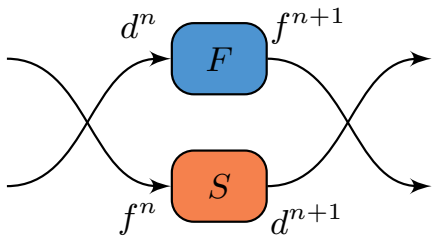
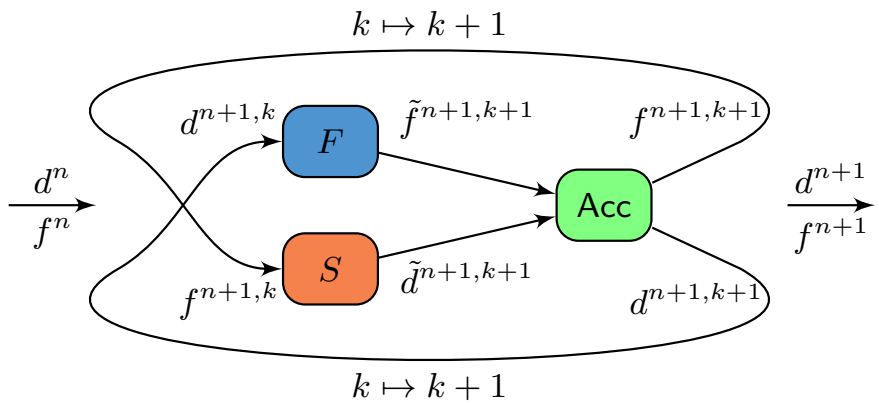


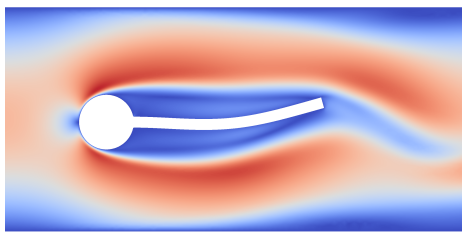
**Explicit** serial coupling

https://vimeo.com/user79566151

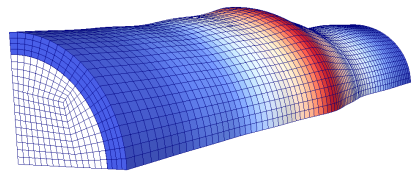
# Quasi-Newton Coupling (Accelerator/Postprocessing)

Coupled problem: $F : d \mapsto f,\ S : f \mapsto d \quad \rightsquigarrow \quad (S \circ F)(d) \overset{!}{=} d$

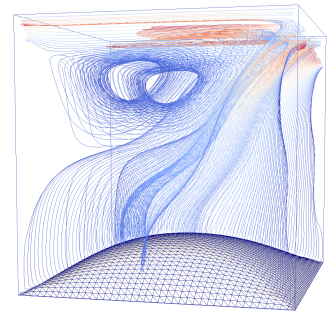
FSI3



3D-tube



Driven cavity



| Mean Iterations | Aitken | Quasi-Newton |
|---|---|---|
| FSI3 | 17.0 | 3.3 |
| 3D-tube | Div. | 7.5 |
| Driven cavity | 7.4 | 2.0 |

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# Infrastructure

We are on GitHub: `https://github.com/precice`

- Main developers: University of Stuttgart and TU Munich
- LGPL3 license
- User documentation in the wiki

# Building

## Dependencies

- Eigen, Boost (version $\geq$ 1.60), libxml2
- Optional: PETSc, Python (incl. Numpy), MPI

## The easy way

- **NEW in 1.4**: Debian package available
- Ubuntu 18.04: All dependencies available through distribution
- Ubuntu 16.04: All dependencies available except Boost

## Still doable

- macOS
- Other Linux distributions

## Experimental

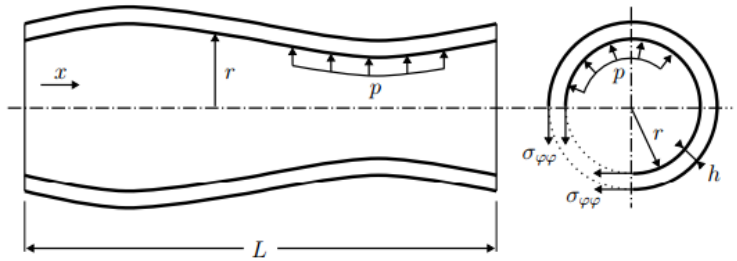
- Conda, Docker, Debian package, Spack
- Windows

# Tutorials

`https://github.com/precice/precice/wiki`

## 1D Elastic Tube

- Simple provided solvers
- Learn about API and configuration



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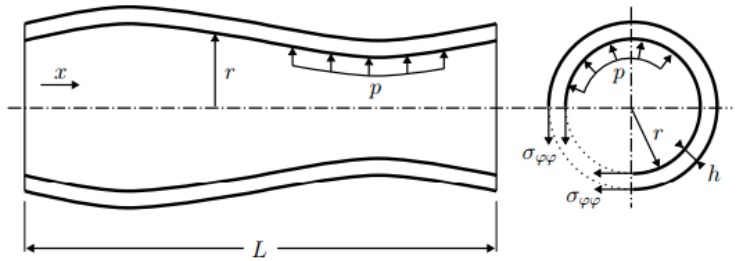
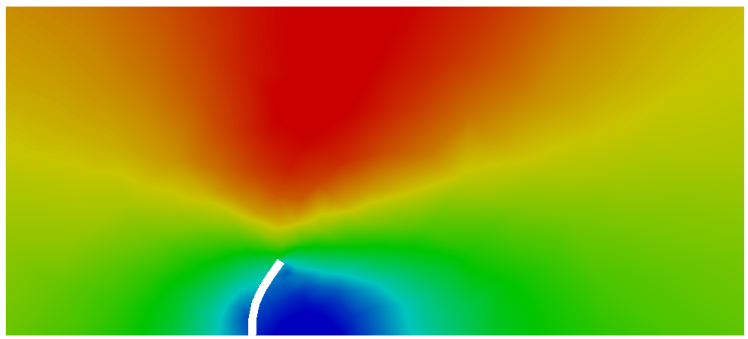



## Flexible beam

- Fluid-structure interaction
- Couple SU2 to CalculiX
- Learn about coupling schemes
- Also interactive version available in browser `http://run.coplon.de/`



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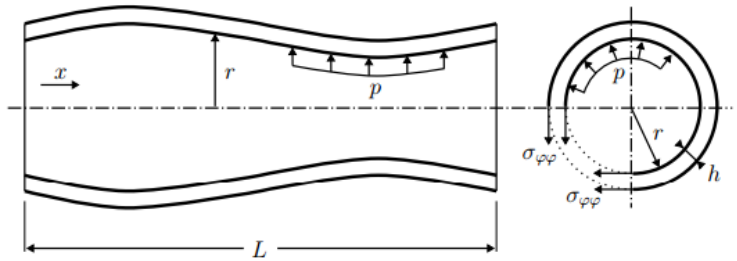


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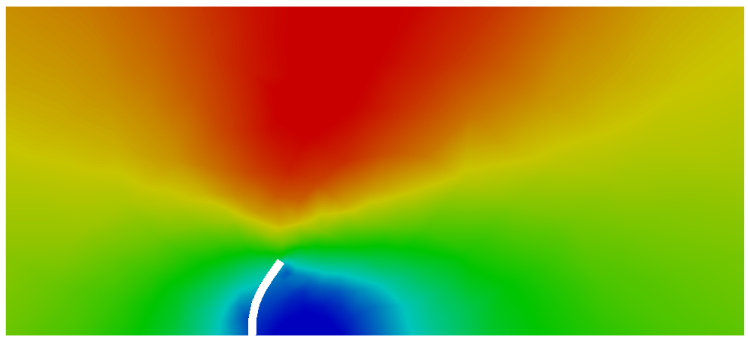

## More tutorials in the wiki!

- Conjugate heat transfer
- Structure-structure interaction
- ...

# How to couple my own code?

```
precice::SolverInterface precice("FluidSolver",rank,size);
precice.configure("precice-config.xml");
precice.setMeshVertices();
precice.initialize();

while (precice.isCouplingOngoing()) { // main time loop
solve();

precice.writeBlockVectorData();
precice.advance();
precice.readBlockVectorData();

endTimeStep(); // e.g. write results, increase time
}

precice.finalize();
```

- Timesteps, most arguments, and less important methods omitted.
- Full example in the wiki.
- API in C++, C, Fortran, and Python

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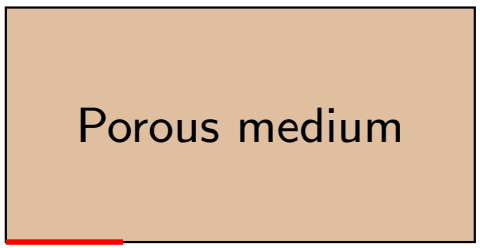
# Coupled flow and poromechanics



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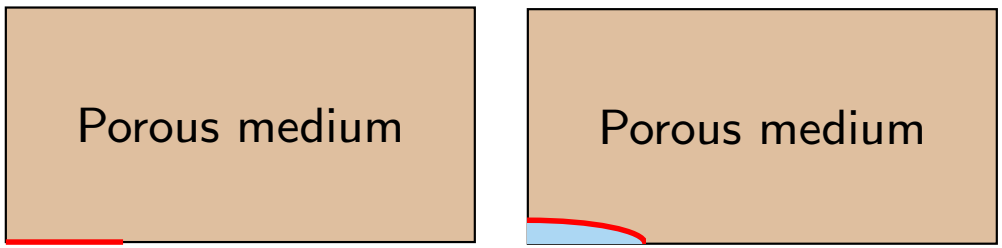

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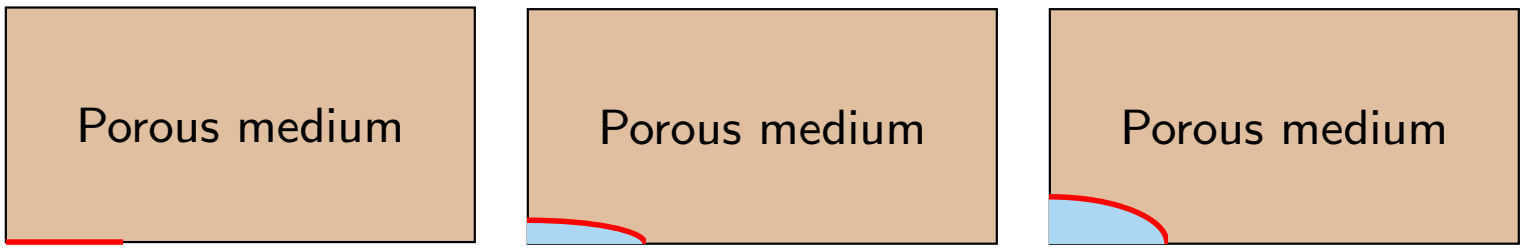

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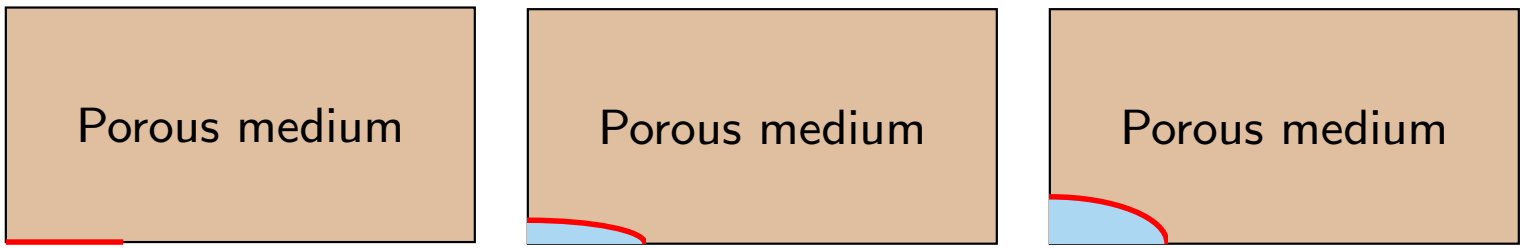
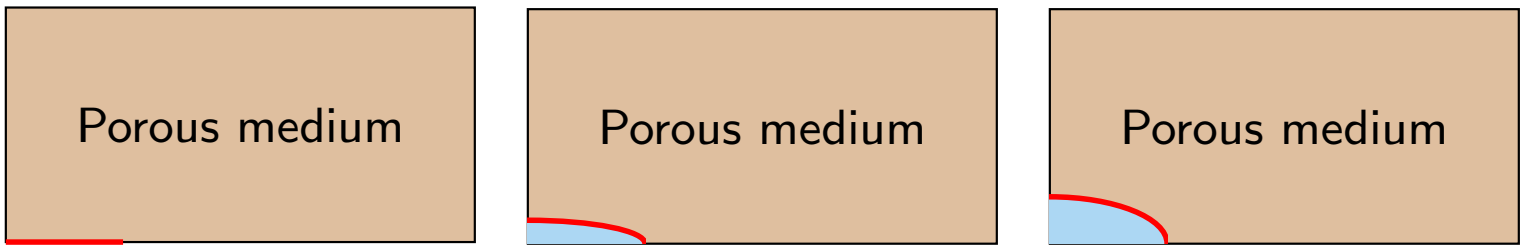


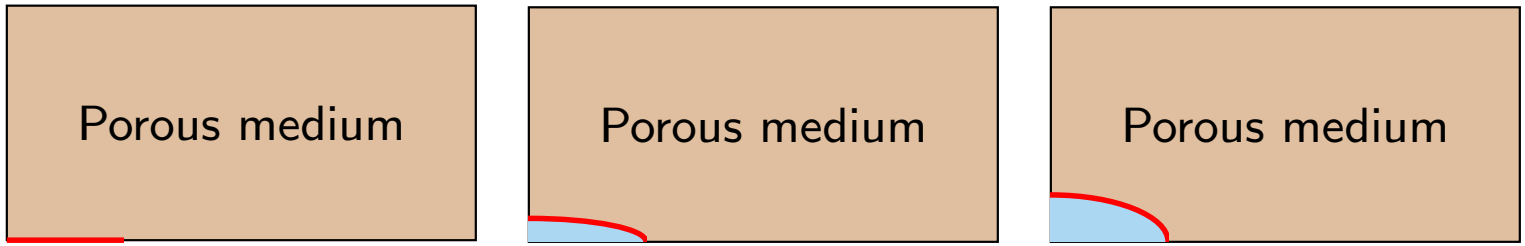

1. Poromechanics solver

# Coupled flow and poromechanics

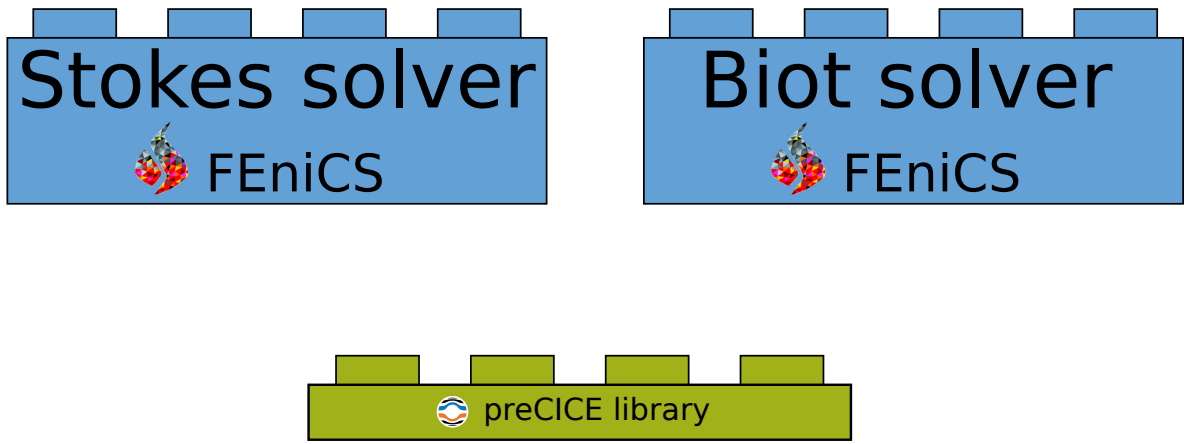



1. Poromechanics solver
2. Flow solver

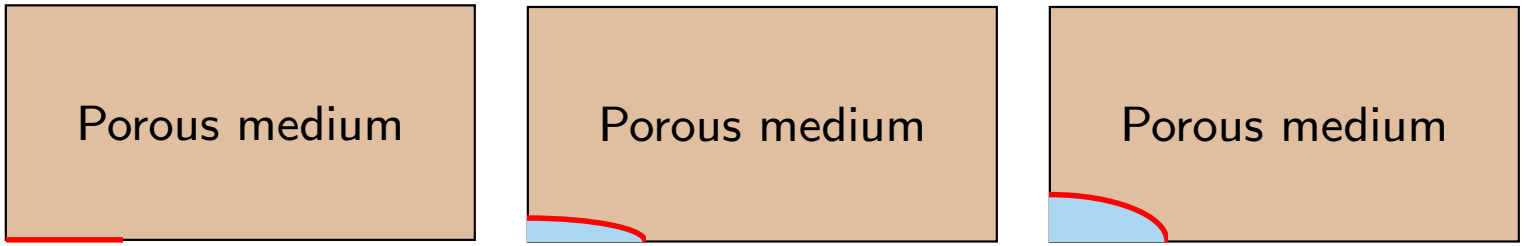
# Coupled flow and poromechanics



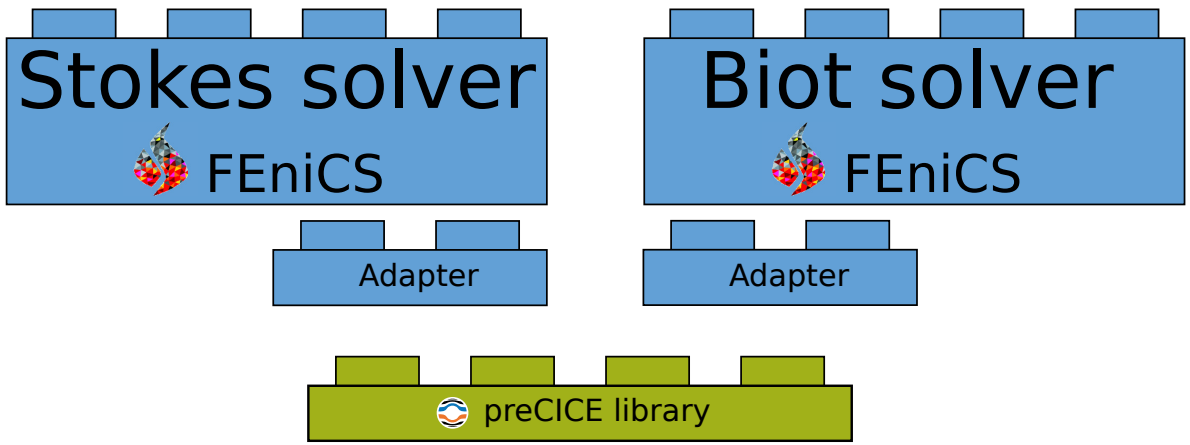

1. Poromechanics solver
2. Flow solver



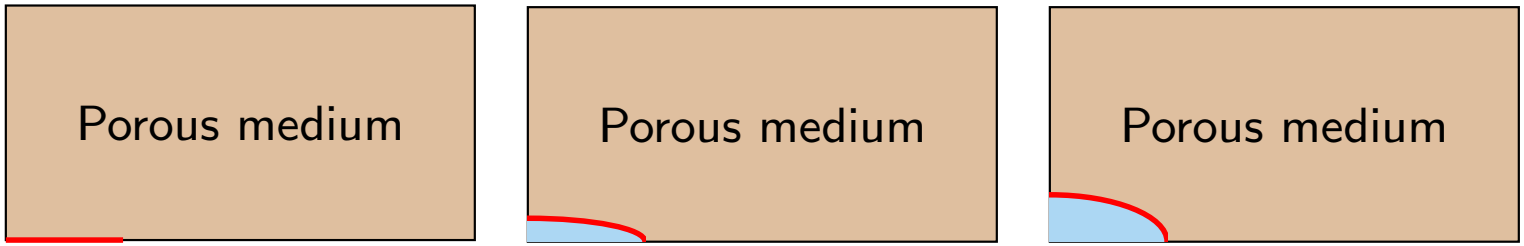
# Coupled flow and poromechanics



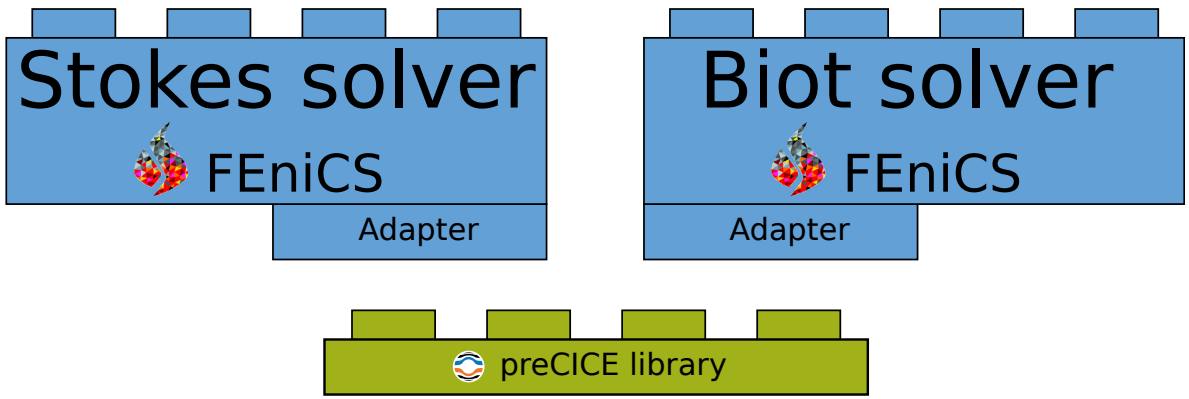

1. Poromechanics solver
2. Flow solver



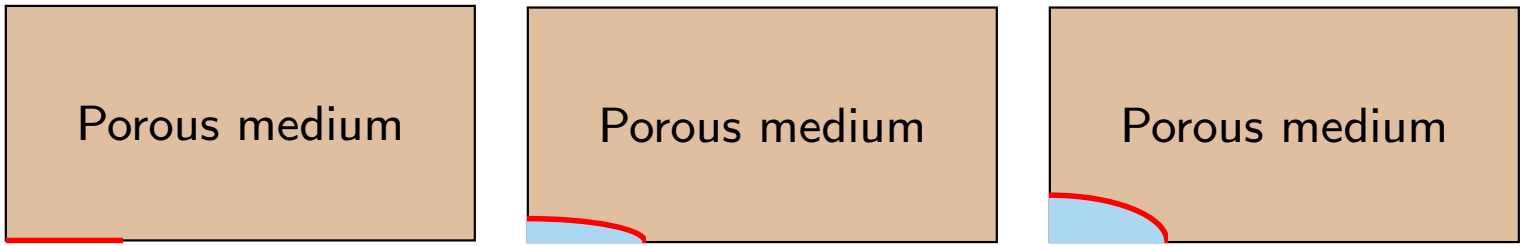
# Coupled flow and poromechanics



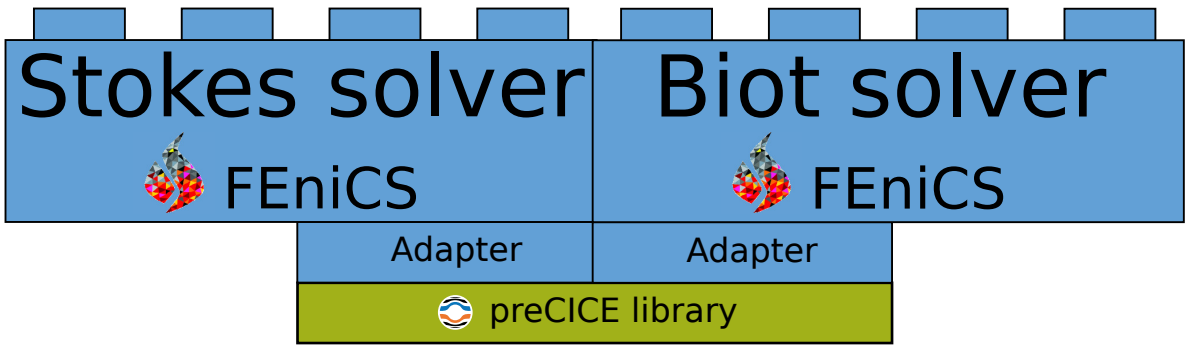

1. Poromechanics solver
2. Flow solver



# Coupled flow and poromechanics




1. Poromechanics solver
2. Flow solver

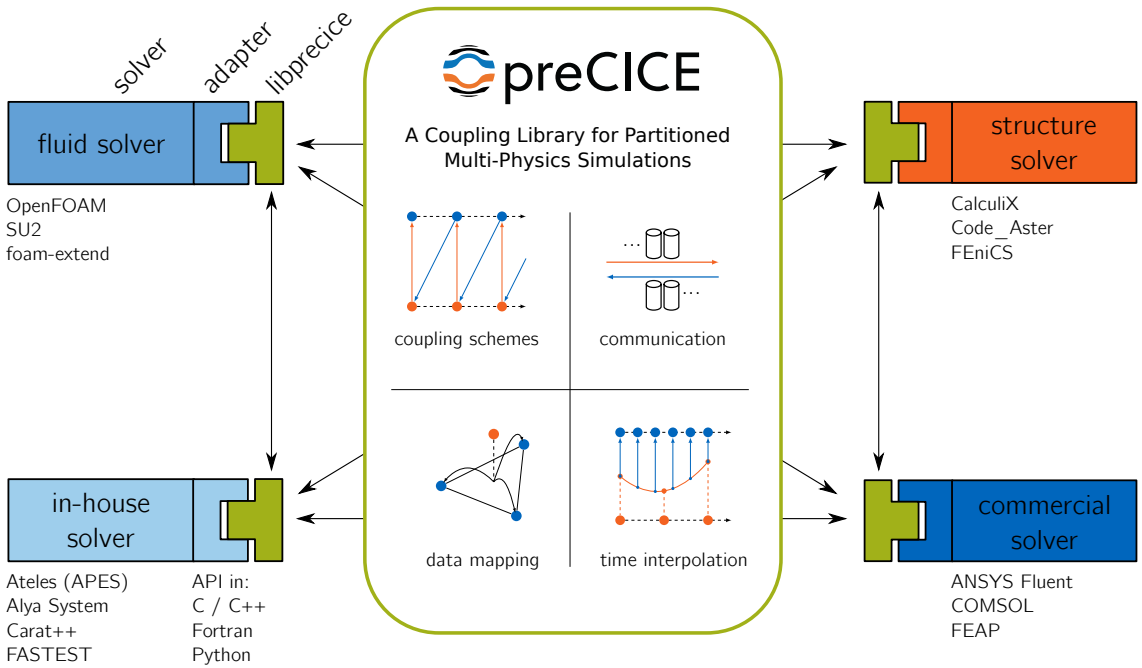


# Pressure over the fracture (Biot)

# Table of contents

## Summary

- Black box coupling tool
- Coupling arbitrary number of solvers
- Suitable for strongly coupled problems
- Good scalability
- Minimally invasive



# Roadmap

## Current Developments v1.4 (just released)

- Debian package
- Building with cmake

## Current Developments Adapters

- Fluid-fluid module for the OpenFOAM adapter
- Update of Fluent adapter
- Official adapters for dealii, FEniCS, and Nutils

## Long-term Goals v2.0

- 3D-1D and 3D-2D data mapping
- Parallel initialization $\rightarrow$ support of very large cases
- Support of re-meshing and dynamically changing coupling interfaces
- Consistent time interpolation

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- www.precice.org
- github.com/precice
- @preCICE_org
- Mailing-list, Gitter
- Literature Guide on wiki

SPPEXA DFG EuroTech Universities SFB 1313 Interface-Driven Multi-Field Processes in Porous Media

TUM TU/e Universität Stuttgart

# Thank you for your attention!

alexander.jaust@ipvs.uni-stuttgart.de

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- Literature Guide on wiki

SPPEXA DFG EuroTech Universities SFB 1313 Interface-Driven Multi-Field Processes in Porous Media

TUM TU/e Universität Stuttgart

# preCICE

preCICE = **Pre**cise **C**ode **I**nteraction **C**oupling **E**nvironment

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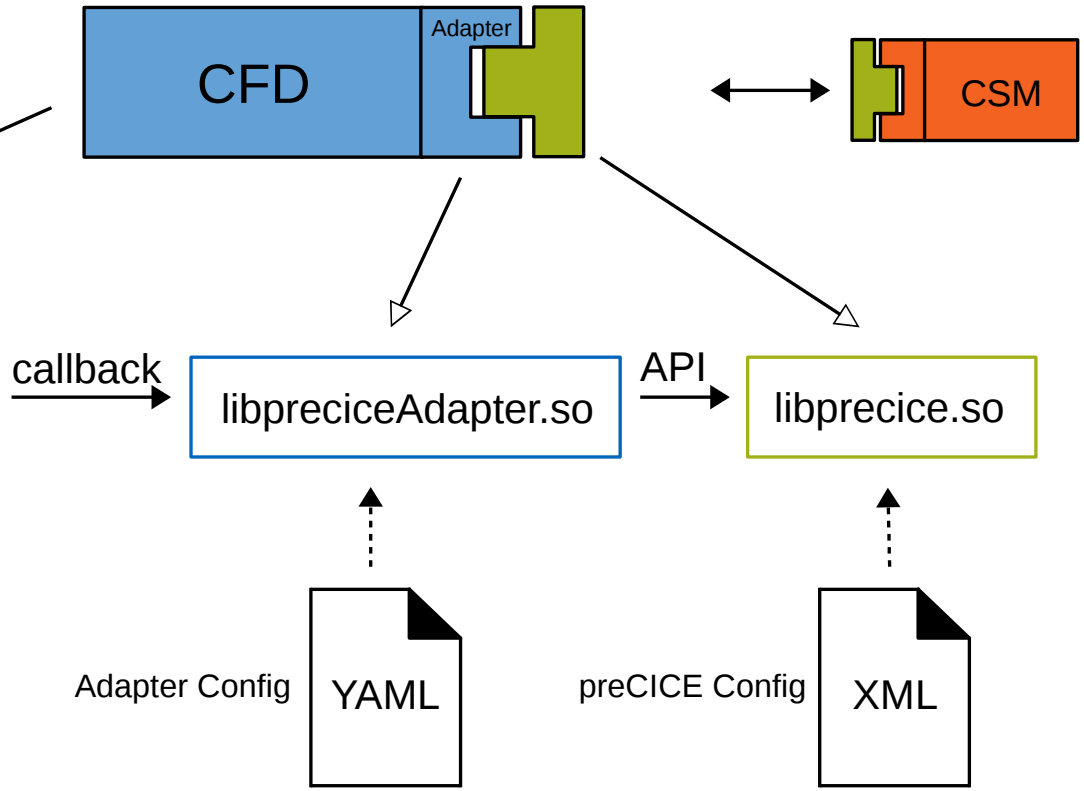
# Flow over a heated plate

# Table of contents

# The (new) OpenFOAM adapter

```
int main(int argc, char *argv[])
{
    #include "setRootCase.H"
    #include "createTime.H"
    #include "createMesh.H"
    ...

    while (runTime.loop())
    {
        Info<< "Time = " ... << endl;

        #include "CourantNo.H"

        // Momentum predictor

        fvVectorMatrix UEqn
        (
            fvm::ddt(U)
          + fvm::div(phi, U)
          - fvm::laplacian(nu, U)
        );

        if (piso.momentumPredictor())
        {
            solve(
                  UEqn
                  ==
                  -fvc::grad(p)
                 );
        }

        // --- PISO loop
        while (piso.correct())
        {
            ...
        }

        runTime.write();
    }

    Info<< "End\n" << endl;
    return 0;
}
```

myFoam



# Flow over a heated plate

Load adapter at runtime in `system/controlDict`:

```
functions
{
preCICE_Adapter
{
type preciceAdapterFunctionObject;
libs ("libpreciceAdapterFunctionObject.so");
}
}
```

Define coupling boundary in `system/blockMeshDict`:

```
interface
{
type wall;
faces
(
(4 0 1 5)
);
}
```

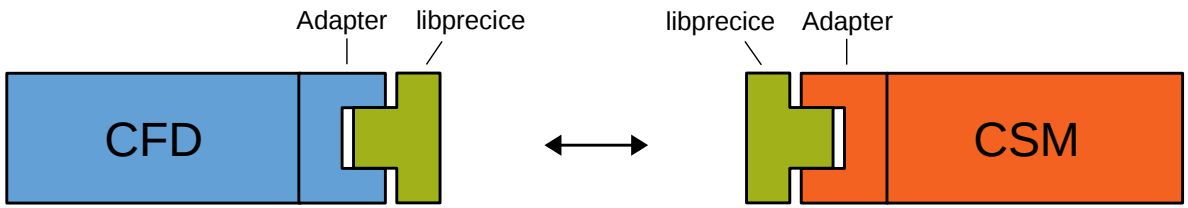
# Flow over a heated plate

Configure adapter in `precice-adapter-config.yml`:

```yaml
participant: Fluid

precice-config-file: /path/to/precice-config.xml

interfaces:
- mesh: Fluid-Mesh
patches: [interface]
write-data: Temperature
read-data: Heat-Flux
```

# Table of contents

# Coupling own code




1. Steering
2. Mesh and data access
3. Checkpointing (Implicit coupling, optional)

# 1. Steering

# API 1: Steering

```
turnOnSolver(); //e.g. setup and partition mesh



double dt; // solver timestep size




while (not simulationDone()){
  dt = beginTimeStep(); // e.g. compute adaptive dt

  computeTimeStep(dt);

  endTimeStep(); // e.g. update variables, increment time
}

turnOffSolver();
```

# API 1: Steering

```
turnOnSolver(); //e.g. setup and partition mesh
precice::SolverInterface precice("FluidSolver",rank,size);


double dt; // solver timestep size




while (not simulationDone()){
  dt = beginTimeStep(); // e.g. compute adaptive dt

  computeTimeStep(dt);

  endTimeStep(); // e.g. update variables, increment time
}

turnOffSolver();
```

# API 1: Steering

```
turnOnSolver(); //e.g. setup and partition mesh
precice::SolverInterface precice("FluidSolver",rank,size);
precice.configure("precice-config.xml");

double dt; // solver timestep size




while (not simulationDone()){
  dt = beginTimeStep(); // e.g. compute adaptive dt

  computeTimeStep(dt);

  endTimeStep(); // e.g. update variables, increment time
}

turnOffSolver();
```

# API 1: Steering

```
turnOnSolver(); //e.g. setup and partition mesh
precice::SolverInterface precice("FluidSolver",rank,size);
precice.configure("precice-config.xml");

double dt; // solver timestep size
double maxDt; // maximum precice timestep size



while (not simulationDone()){
  dt = beginTimeStep(); // e.g. compute adaptive dt

  computeTimeStep(dt);

  endTimeStep(); // e.g. update variables, increment time
}

turnOffSolver();
```

# API 1: Steering

```
turnOnSolver(); //e.g. setup and partition mesh
precice::SolverInterface precice("FluidSolver",rank,size);
precice.configure("precice-config.xml");

double dt; // solver timestep size
double maxDt; // maximum precice timestep size

maxDt = precice.initialize()

while (not simulationDone()){
  dt = beginTimeStep(); // e.g. compute adaptive dt

  computeTimeStep(dt);

  endTimeStep(); // e.g. update variables, increment time
}

turnOffSolver();
```

# API 1: Steering

```
turnOnSolver(); //e.g. setup and partition mesh
precice::SolverInterface precice("FluidSolver",rank,size);
precice.configure("precice-config.xml");

double dt; // solver timestep size
double maxDt; // maximum precice timestep size

maxDt = precice.initialize()

while (not simulationDone() && precice.isCouplingOngoing()){
  dt = beginTimeStep(); // e.g. compute adaptive dt

  computeTimeStep(dt);

  endTimeStep(); // e.g. update variables, increment time
}

turnOffSolver();
```

# API 1: Steering

```
turnOnSolver(); //e.g. setup and partition mesh
precice::SolverInterface precice("FluidSolver",rank,size);
precice.configure("precice-config.xml");

double dt; // solver timestep size
double maxDt; // maximum precice timestep size

maxDt = precice.initialize()

while (not simulationDone() && precice.isCouplingOngoing()){
  dt = beginTimeStep(); // e.g. compute adaptive dt
  dt = min(maxDt, dt);
  computeTimeStep(dt);

  endTimeStep(); // e.g. update variables, increment time
}

turnOffSolver();
```

# API 1: Steering

```
turnOnSolver(); //e.g. setup and partition mesh
precice::SolverInterface precice("FluidSolver",rank,size);
precice.configure("precice-config.xml");

double dt; // solver timestep size
double maxDt; // maximum precice timestep size

maxDt = precice.initialize()

while (not simulationDone() && precice.isCouplingOngoing()){
  dt = beginTimeStep(); // e.g. compute adaptive dt
  dt = min(maxDt, dt);
  computeTimeStep(dt);
  maxDt = precice.advance(dt); // communication, data mapping, ...
  endTimeStep(); // e.g. update variables, increment time
}

turnOffSolver();
```

# API 1: Steering

```
turnOnSolver(); //e.g. setup and partition mesh
precice::SolverInterface precice("FluidSolver",rank,size);
precice.configure("precice-config.xml");

double dt; // solver timestep size
double maxDt; // maximum precice timestep size

maxDt = precice.initialize()

while (not simulationDone() && precice.isCouplingOngoing()){
  dt = beginTimeStep(); // e.g. compute adaptive dt
  dt = min(maxDt, dt);
  computeTimeStep(dt);
  maxDt = precice.advance(dt); // communication, data mapping, ...
  endTimeStep(); // e.g. update variables, increment time
}
precice.finalize();
turnOffSolver();
```

# 2. Mesh and data access

# API 2: Mesh and data access

```
precice::SolverInterface precice("FluidSolver",rank,size);
precice.configure("precice-config.xml");









precice.initialize()



[...]
```

# API 2: Mesh and data access

```
precice::SolverInterface precice("FluidSolver",rank,size);
precice.configure("precice-config.xml");

int meshID = precice.getMeshID("FluidMesh");









precice.initialize()



[...]
```

# API 2: Mesh and data access

```
precice::SolverInterface precice("FluidSolver",rank,size);
precice.configure("precice-config.xml");

int meshID = precice.getMeshID("FluidMesh");
int vertexSize; // number of vertices at coupling interface









precice.initialize()



[...]
```

# API 2: Mesh and data access

```
precice::SolverInterface precice("FluidSolver",rank,size);
precice.configure("precice-config.xml");

int meshID = precice.getMeshID("FluidMesh");
int vertexSize; // number of vertices at coupling interface
// determine vertexSize









precice.initialize()









[...]
```

# API 2: Mesh and data access

```
1  precice::SolverInterface precice("FluidSolver",rank,size);
2  precice.configure("precice-config.xml");
3
4  int meshID = precice.getMeshID("FluidMesh");
5  int vertexSize; // number of vertices at coupling interface
6  // determine vertexSize
7  double* coords = new double[vertexSize*dim]; // coupling mesh (nodes)
8
9
10
11
12 precice.initialize()
13
14
15
16
17
18 [...]
```

# API 2: Mesh and data access

```
precice::SolverInterface precice("FluidSolver",rank,size);
precice.configure("precice-config.xml");

int meshID = precice.getMeshID("FluidMesh");
int vertexSize; // number of vertices at coupling interface
// determine vertexSize
double* coords = new double[vertexSize*dim]; // coupling mesh (nodes)
// determine coordinates



precice.initialize()



[...]
```

# API 2: Mesh and data access

```
precice::SolverInterface precice("FluidSolver",rank,size);
precice.configure("precice-config.xml");

int meshID = precice.getMeshID("FluidMesh");
int vertexSize; // number of vertices at coupling interface
// determine vertexSize
double* coords = new double[vertexSize*dim]; // coupling mesh (nodes)
// determine coordinates
int* vertexIDs = new int[vertexSize];



precice.initialize()









[...]
```

# API 2: Mesh and data access

```
precice::SolverInterface precice("FluidSolver",rank,size);
precice.configure("precice-config.xml");

int meshID = precice.getMeshID("FluidMesh");
int vertexSize; // number of vertices at coupling interface
// determine vertexSize
double* coords = new double[vertexSize*dim]; // coupling mesh (nodes)
// determine coordinates
int* vertexIDs = new int[vertexSize];
precice.setMeshVertices(meshID, vertexSize, coords, vertexIDs);

precice.initialize()



[...]
```

# API 2: Mesh and data access

```
precice::SolverInterface precice("FluidSolver",rank,size);
precice.configure("precice-config.xml");

int meshID = precice.getMeshID("FluidMesh");
int vertexSize; // number of vertices at coupling interface
// determine vertexSize
double* coords = new double[vertexSize*dim]; // coupling mesh (nodes)
// determine coordinates
int* vertexIDs = new int[vertexSize];
precice.setMeshVertices(meshID, vertexSize, coords, vertexIDs);

precice.initialize()

[...]

int forceID = precice.getDataID("Forces", meshID);

[...]
```

# API 2: Mesh and data access

```
precice::SolverInterface precice("FluidSolver",rank,size);
precice.configure("precice-config.xml");

int meshID = precice.getMeshID("FluidMesh");
int vertexSize; // number of vertices at coupling interface
// determine vertexSize
double* coords = new double[vertexSize*dim]; // coupling mesh (nodes)
// determine coordinates
int* vertexIDs = new int[vertexSize];
precice.setMeshVertices(meshID, vertexSize, coords, vertexIDs);

precice.initialize()

[...]

int forceID = precice.getDataID("Forces", meshID);
double* forces = new double[vertexSize*dim];
[...]
```

# API 2: Mesh and data access

```
precice::SolverInterface precice("FluidSolver",rank,size);
precice.configure("precice-config.xml");

int meshID = precice.getMeshID("FluidMesh");
int vertexSize; // number of vertices at coupling interface
// determine vertexSize
double* coords = new double[vertexSize*dim]; // coupling mesh (nodes)
// determine coordinates
int* vertexIDs = new int[vertexSize];
precice.setMeshVertices(meshID, vertexSize, coords, vertexIDs);

precice.initialize()

[...]

int forceID = precice.getDataID("Forces", meshID);
double* forces = new double[vertexSize*dim];
precice.writeBlockVectorData(forceID, vertexSize, vertexIDs, forces);
```

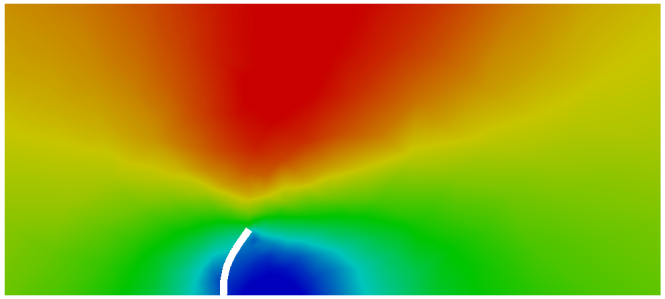
# preCICE configuration

```
<precice-configuration>

  <data:vector name="Forces" />
  <data:vector name="Displacements" />

  <mesh name="FluidMesh">
    <use-data name="Forces" />
    <use-data name="Displacements" />
  </mesh>

  <participant name="FluidSolver">
    <use-mesh name="FluidMesh" provide="yes" />
    <write-data name="Forces" mesh="FluidMesh" />

    [...]

  </participant>

  [...]
```

# 3. Checkpointing (for implicit coupling)

# Different couplings

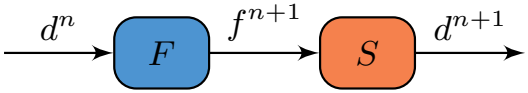
- Fluid solver: $F : d \mapsto f$
- Structure solver: $S : f \mapsto d$
- Solve fixed-point problem: $(S \circ F)(d) \overset{!}{=} d$

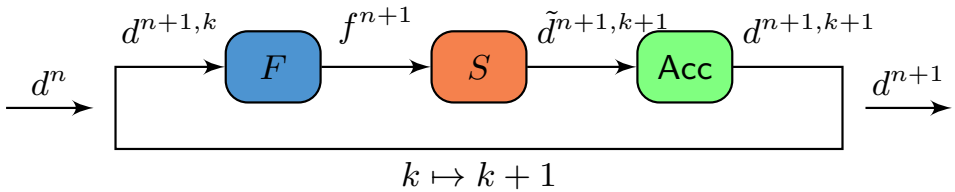


explicit

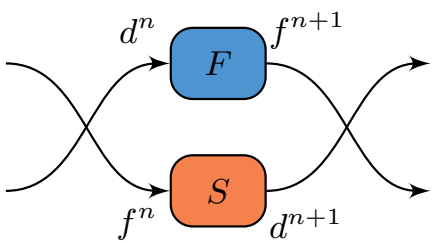
implicit

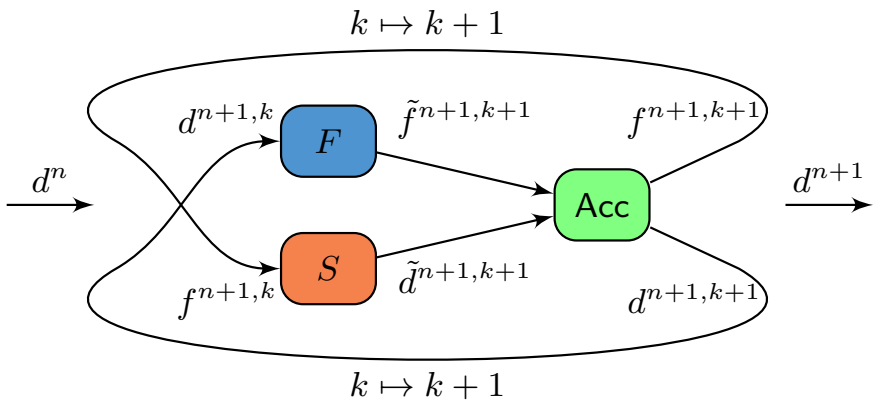
serial




parallel



# API 3: Implicit coupling

```
while (not simulationDone() && precice.isCouplingOngoing()){
  dt = beginTimeStep();
  computeTimeStep(dt);
  precice.advance(dt); // communication, data mapping, ...
  endTimeStep(); // e.g. update variables, increment time
}
```

# API 3: Implicit coupling

```
while (not simulationDone() && precice.isCouplingOngoing()){
  if(precice.isActionRequired("WriteIterationCheckpoint")){
    saveCheckpoint(); // save internal state of solver
    precice.fulfilledAction("WriteIterationCheckpoint");
  }

  dt = beginTimeStep();
  computeTimeStep(dt);
  precice.advance(dt); // communication, data mapping, ...









  endTimeStep(); // e.g. update variables, increment time

}
```

# API 3: Implicit coupling

```
while (not simulationDone() && precice.isCouplingOngoing()){
  if(precice.isActionRequired("WriteIterationCheckpoint")){
    saveCheckpoint(); // save internal state of solver
    precice.fulfilledAction("WriteIterationCheckpoint");
  }

  dt = beginTimeStep();
  computeTimeStep(dt);
  precice.advance(dt); // communication, data mapping, ...

  if(precice.isActionRequired("ReadIterationCheckpoint")){
    reloadCheckpoint(); // set variables back to checkpoint
    precice.fulfilledAction("ReadIterationCheckpoint");
  }
  else{ // timestep converged
    endTimeStep(); // e.g. update variables, increment time
  }
}
```