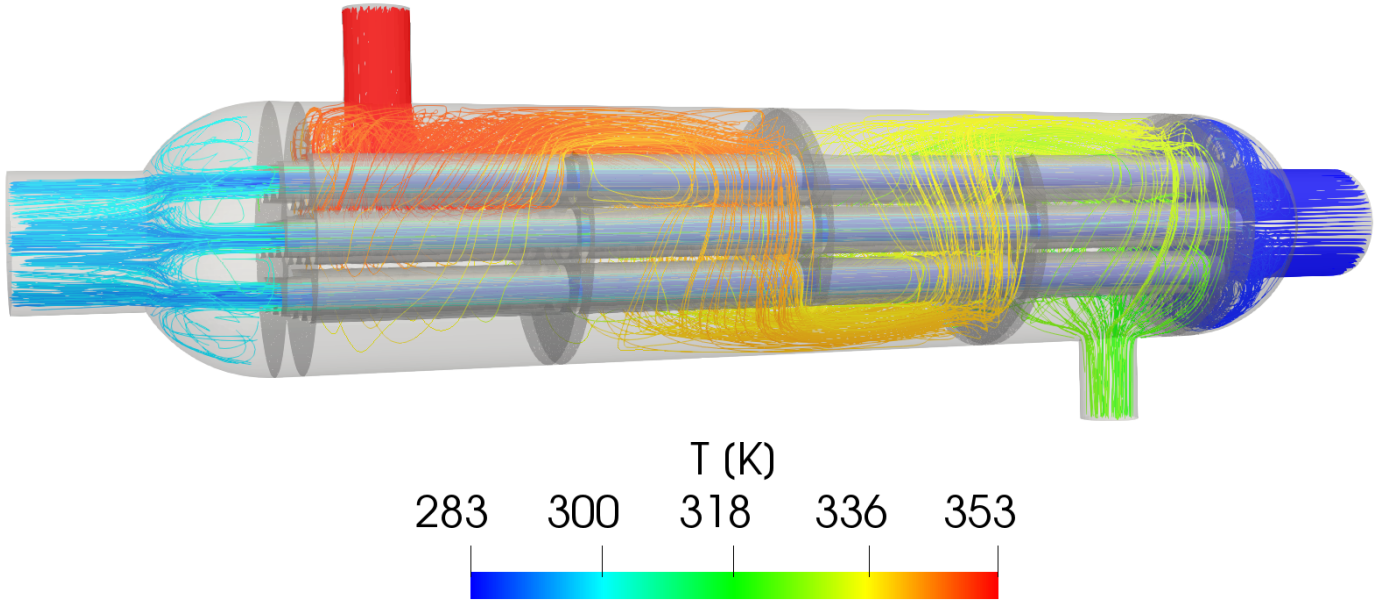
A Coupling Library for Partitioned Multi-Physics Simulations

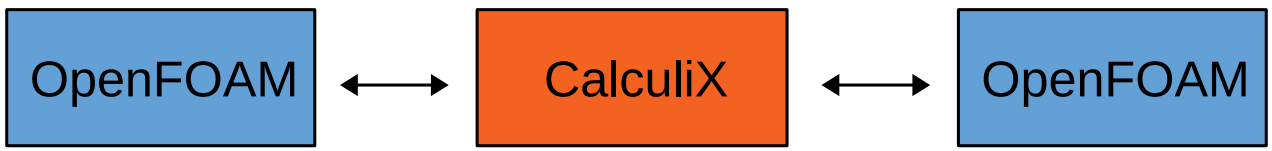
1. What is preCICE?
2. How to get started?
3. How can I couple my own code?

1. What is preCICE?

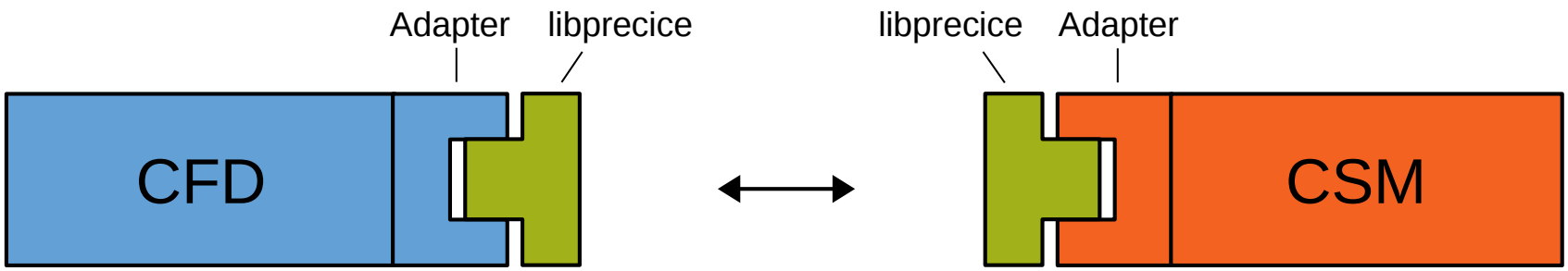
Example: Shell-And-Tube Heat Exchanger



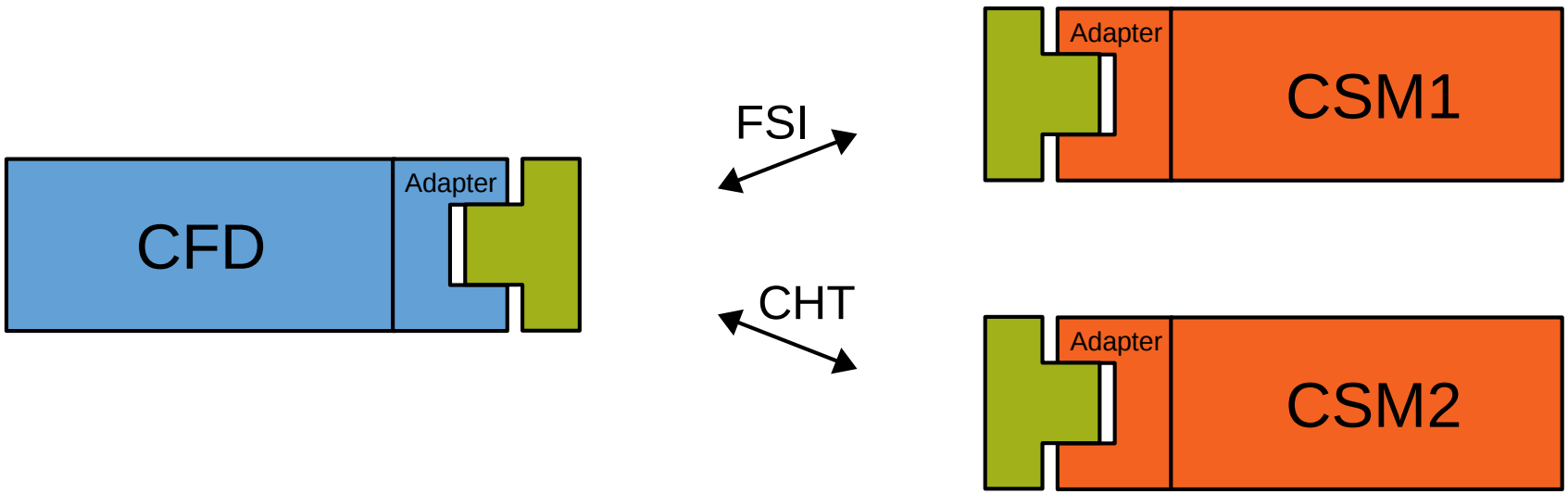
- Partitioned coupling: Usage of three independent solvers
- Reuse of existing solvers



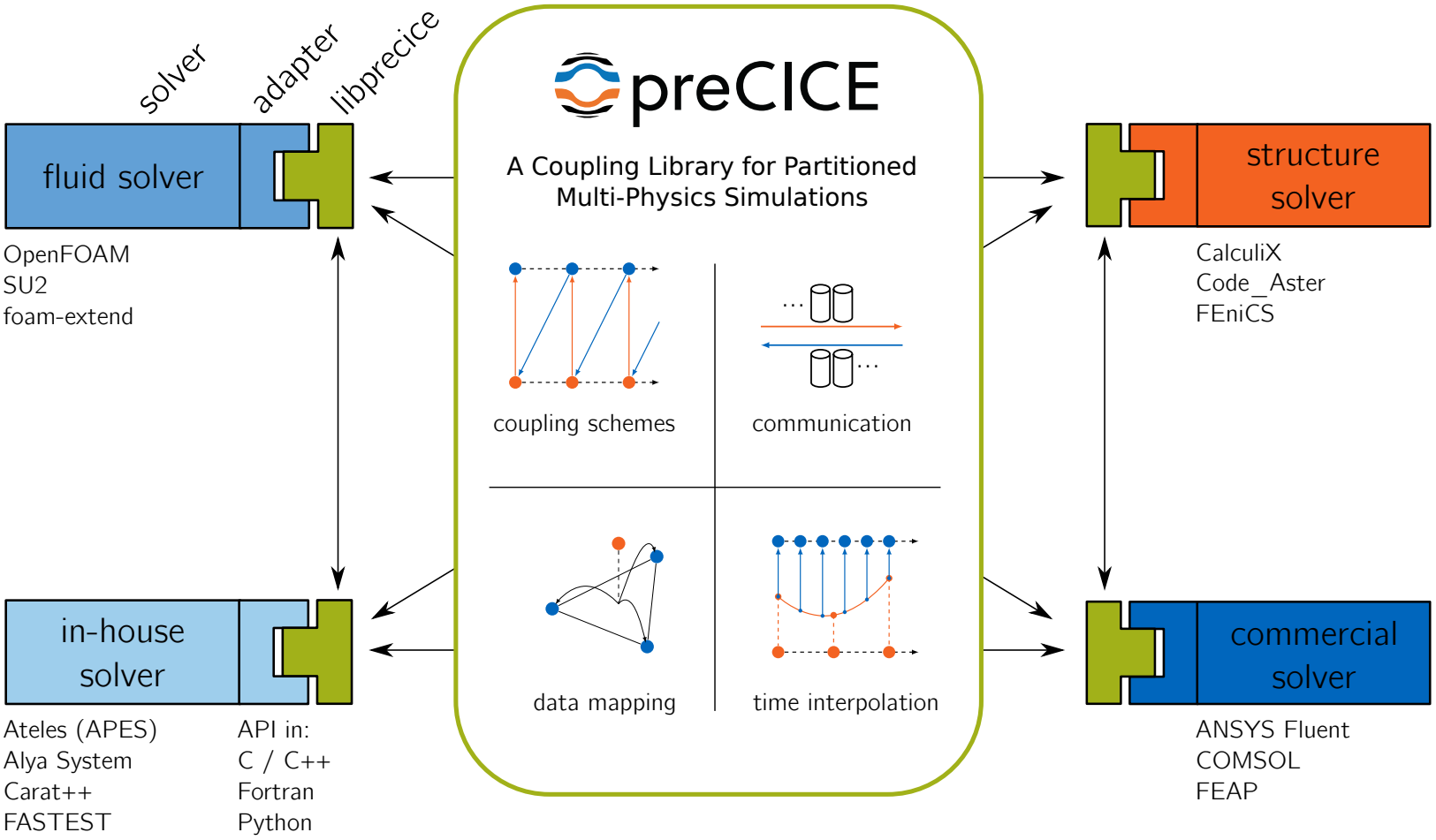
preCICE – A Plug-and-Play Coupling Library



preCICE – A Plug-and-Play Coupling Library



preCICE – A Plug-and-Play Coupling Library

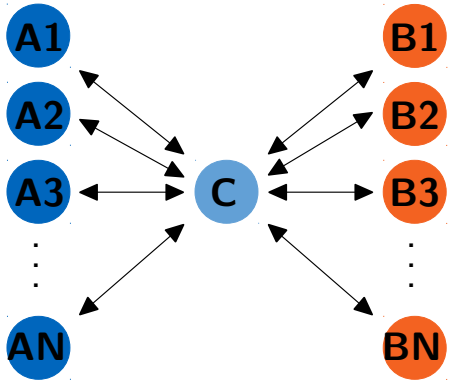


USPs

1. Scalability
2. Robust quasi-Newton coupling
3. Coupling of arbitrary many components
   (*arbitrary many = more than two*)
4. Minimally-invasive coupling
5. Open-source, community

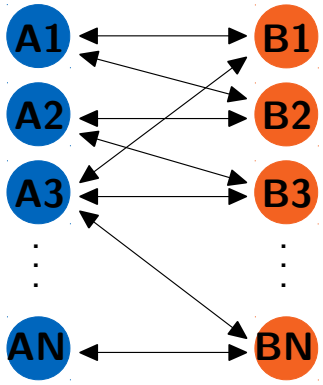
USP 1: Scalability

Server-Based Concept



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

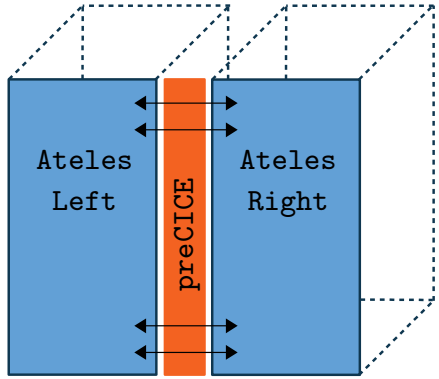
Our Peer-To-Peer Concept

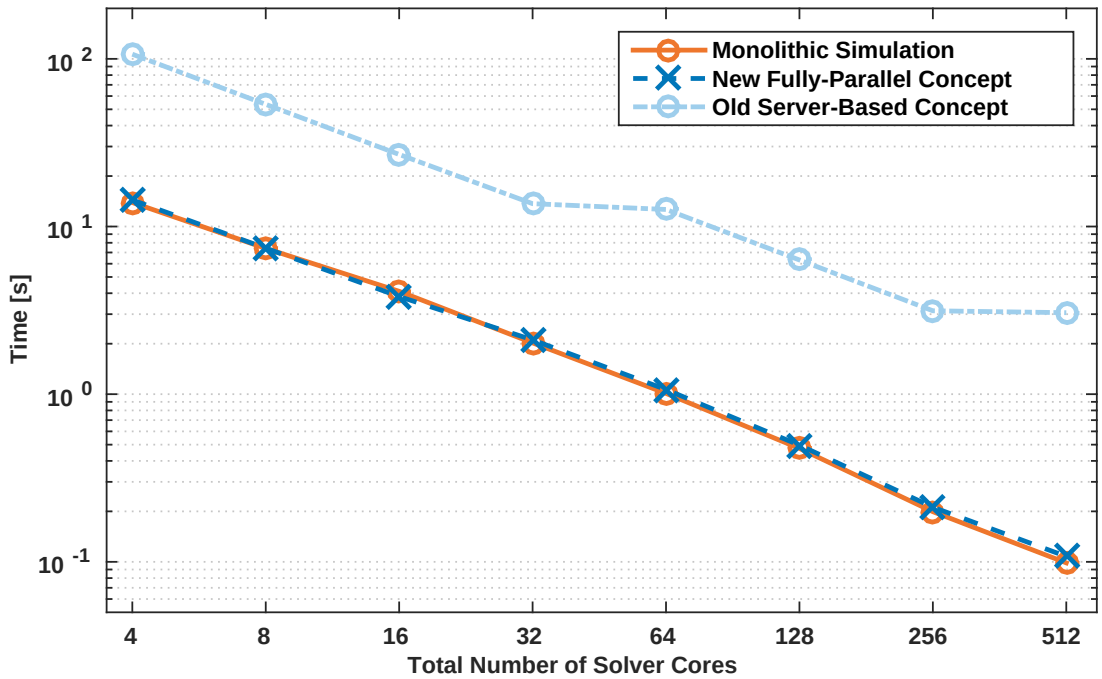


- No central entity
- $\Rightarrow$ Easier to handle (user does not need to care about server)
- $\Rightarrow$ No scaling issues

USP 1: 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

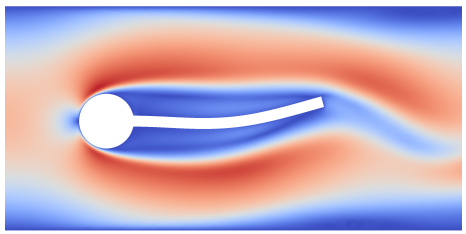




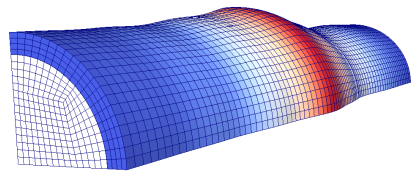
USP 2: Quasi-Newton Coupling

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

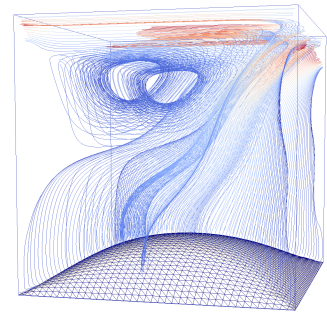
FSI3



3D-Tube



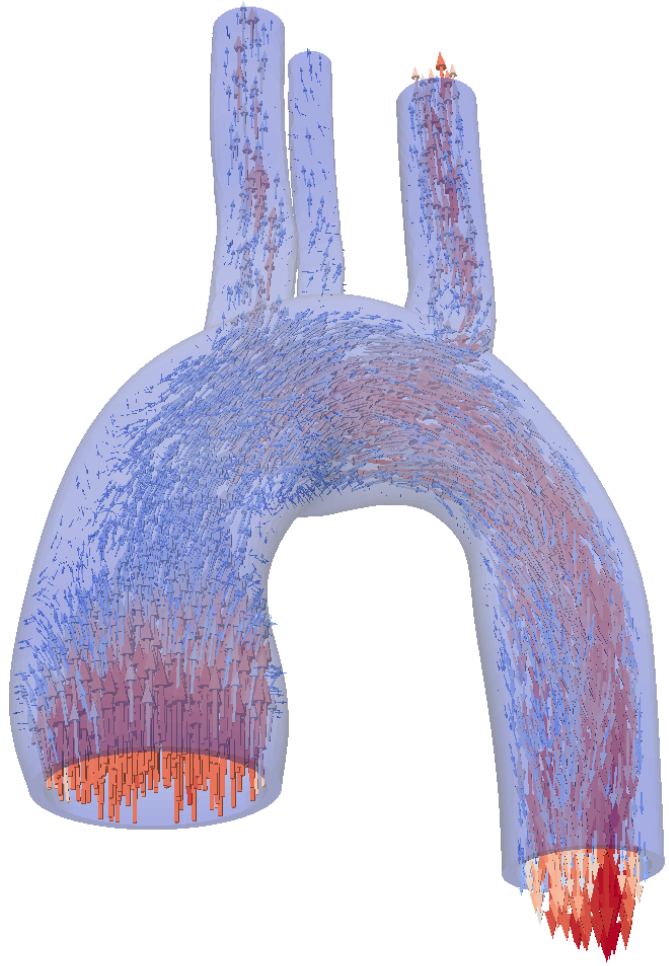
Driven Cavity



Mean Iterations	Aitken	Quasi-Newton
FSI3	17.0	3.3
3D-Tube	Div.	7.5
Driven Cavity	7.4	2.0

USP 2: Quasi-Newton Coupling

- Quasi-Newton can even handle biomedical applications, such as an Aortic bloodflow
- Stable coupling (no added-mass instabilities)
- Six times less iterations than Aitken



- Joint work with Juan-Carlos Cajas (Barcelona Supercomputing Center)
- Geometry by Jordi Martorell

Contributors

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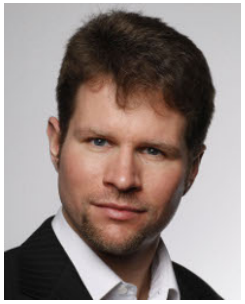

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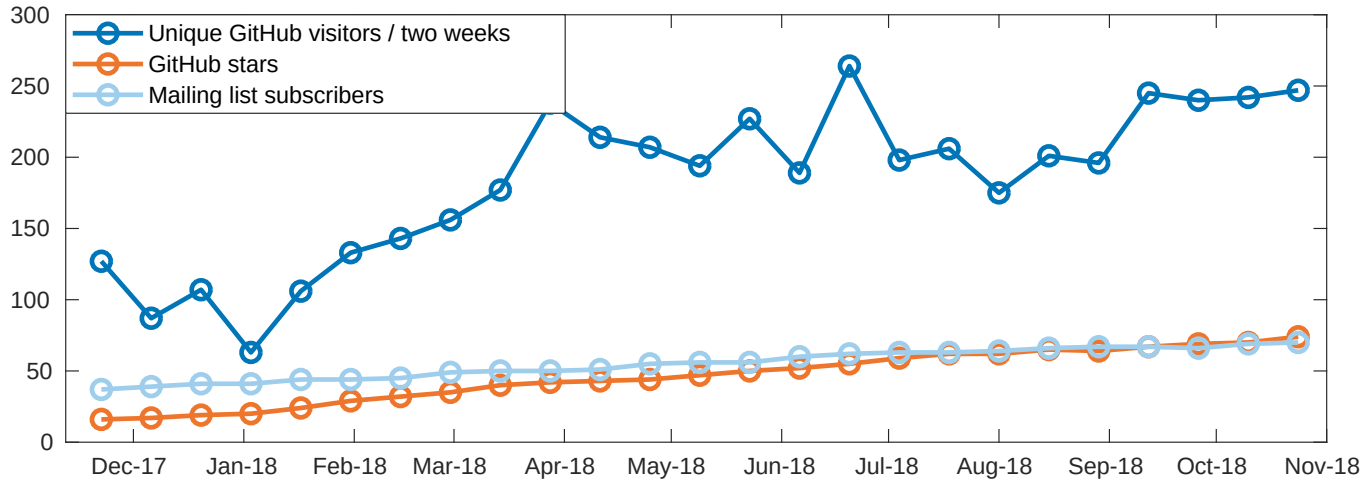


2. How to get started?

Infrastructure

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

- 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

- Ubuntu 18.04: All dependencies available through distribution
- Ubuntu 16.04: All dependencies available except Boost

Still doable

- macOS
- Other Linux distributions

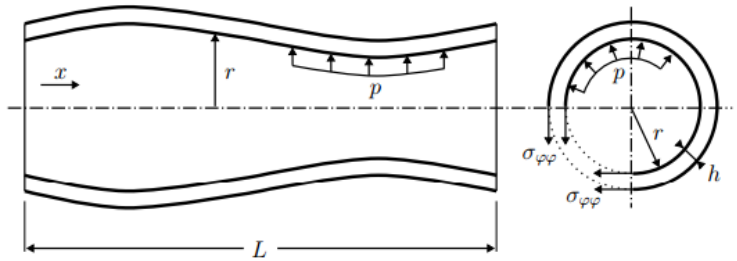
Experimental

- Conda, Docker, Debian package, Spack
- Windows

Tutorials

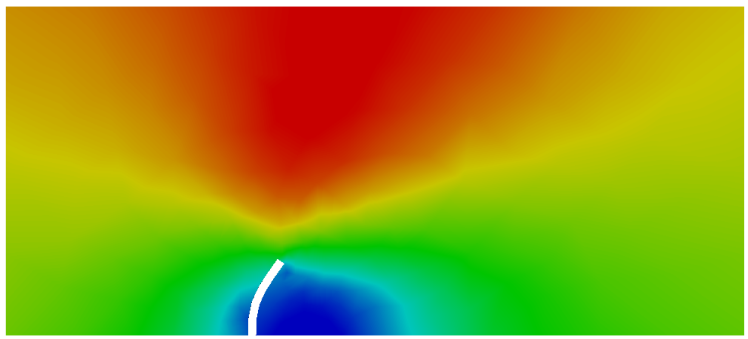
1D Elastic Tube

- Simple provided solvers
- Learn about API and configuration



Flexible beam

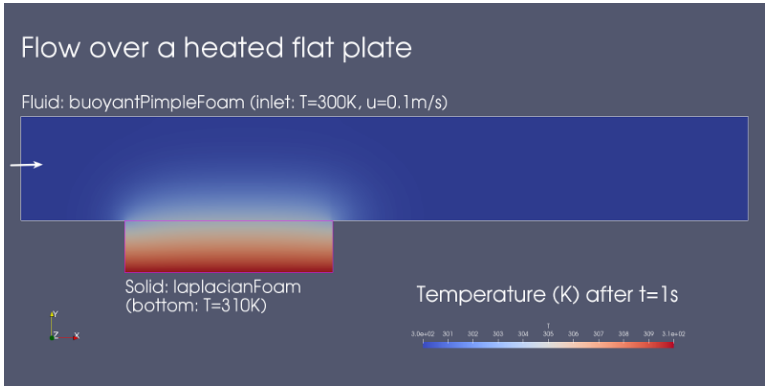
- Fluid-structure interaction
- Couple SU2 to CalculiX
- Learn about coupling schemes
- Also interactive version available in browser `http://run.coplon.de/`



Tutorials

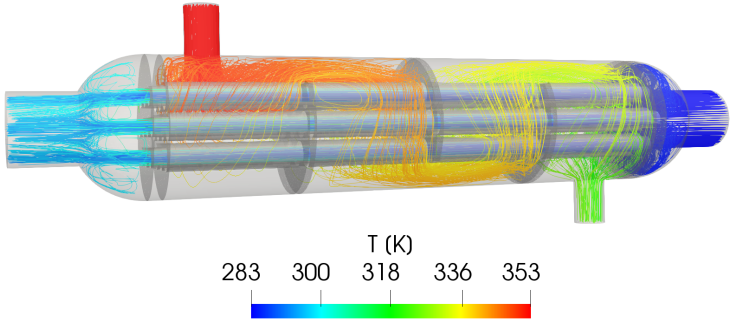
Flow over a Heated Plate

- Conjuagte-heat transfer
- Couple two OpenFOAM solvers
- Learn about OpenFOAM adapter



Heat exchanger

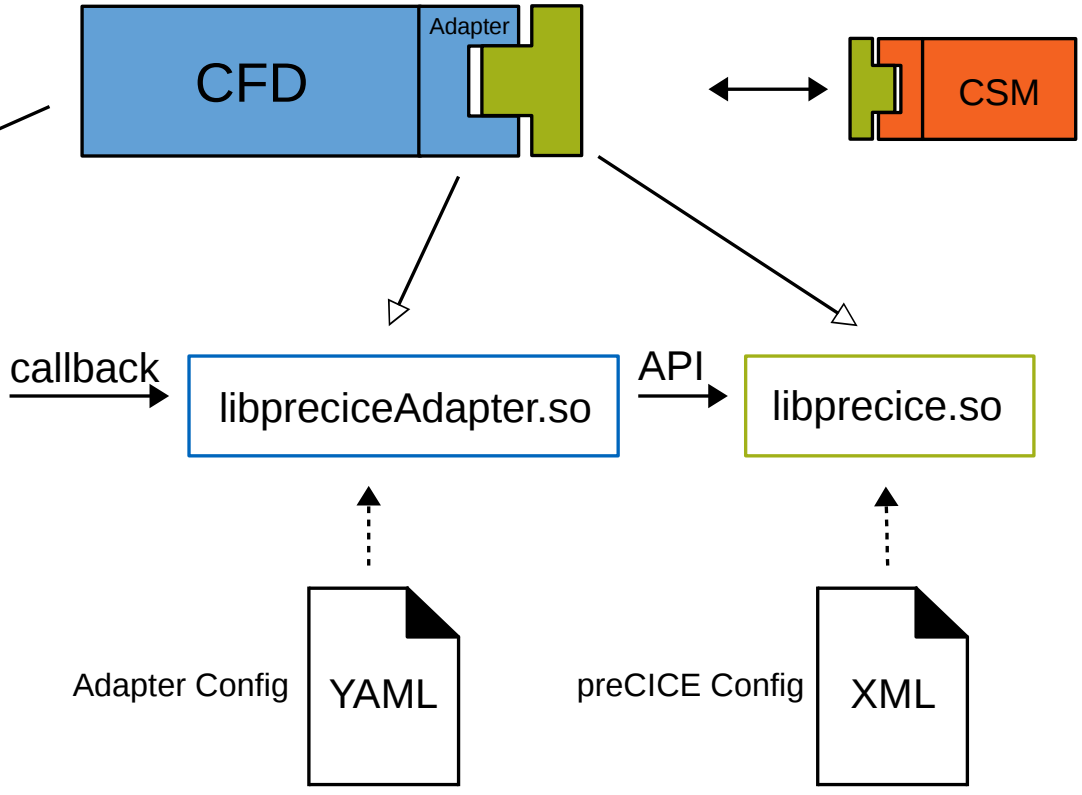
- Conjugate-heat transfer
- Couple two OpenFOAM instances with CalculiX
- Learn about multi coupling



The 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
```

Flow over a Heated Plate

3. How can I couple my own code?

API 1: Steering

```
1  turnOnSolver(); //e.g. setup and partition mesh
2
3
4
5  double dt; // solver timestep size
6
7
8
9
10 while (not simulationDone()){
11   dt = beginTimeStep(); // e.g. compute adaptive dt
12
13   computeTimeStep(dt);
14
15   endTimeStep(); // e.g. update variables, increment time
16 }
17
18 turnOffSolver();
```

API 1: Steering

```
1  turnOnSolver(); //e.g. setup and partition mesh
2  precice::SolverInterface precice("FluidSolver",rank,size);
3
4
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8
9
10 while (not simulationDone()){
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API 1: Steering

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

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();
```

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

```
1  precice::SolverInterface precice("FluidSolver",rank,size);
2  precice.configure("precice-config.xml");
3
4  int meshID = precice.getMeshID("FluidMesh");
5
6
7
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









precice.initialize()



[...]
```

API 2: Mesh and Data Access

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1  precice::SolverInterface precice("FluidSolver",rank,size);
2  precice.configure("precice-config.xml");
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4  int meshID = precice.getMeshID("FluidMesh");
5  int vertexSize; // number of vertices at coupling interface
6  // determine vertexSize
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8
9
10
11
12 precice.initialize()
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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)



precice.initialize()



[...]
```

API 2: Mesh and Data Access

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

API 2: Mesh and Data Access

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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");
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// 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>

  [...]
```

API 3: Implicit Coupling

```
1  while (not simulationDone() && precice.isCouplingOngoing()){
2
3
4
5
6
7    dt = beginTimeStep();
8    computeTimeStep(dt);
9    precice.advance(dt); // communication, data mapping, ...
10
11
12
13
14
15
16   endTimeStep(); // e.g. update variables, increment time
17
18 }
```

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
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  }

  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
  }
}
```

Roadmap

Current Developments

- Debian package
- FSI module for the OpenFOAM adapter
- Fluid-fluid module for the OpenFOAM adapter
- Structure-structure coupling with CalculiX

Long-term Goals

- 3D-1D and 3D-2D data mapping
- Parallel initialization and support of dynamically changing coupling interfaces
- Consistent time interpolation

Funding

More information

- Open-source project: `www.precice.org`
- Source code: `github.com/precice`

Contact us

- Mailing list
- Gitter chat room