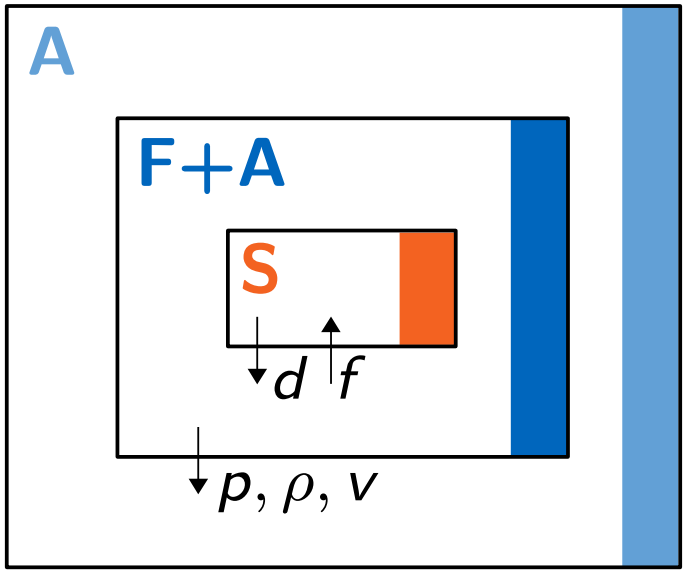
Scalable and Easy-to-use Coupling of Multi-Physics Simulations

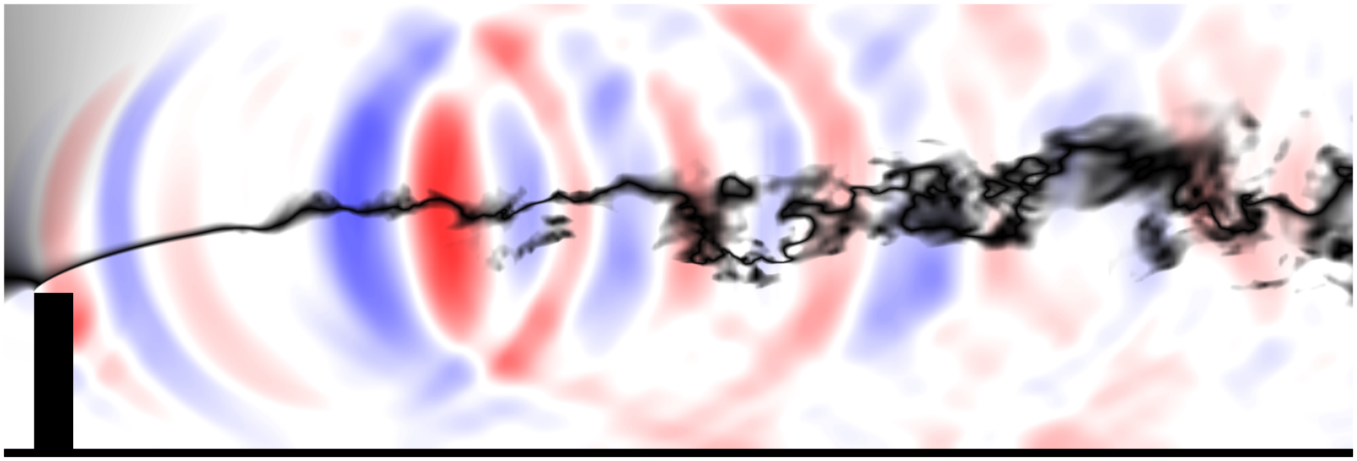
Benjamin Uekermann et al.,

Eindhoven University of Technology

The ExaFSA Challenge



- **S**: FEM structure solver
- **F+A**: Low-order FV solver, resolve geometries, resolve turbulent structures
- **A**: High-order DG solver, linearized Euler, transport phenomena, very large domain



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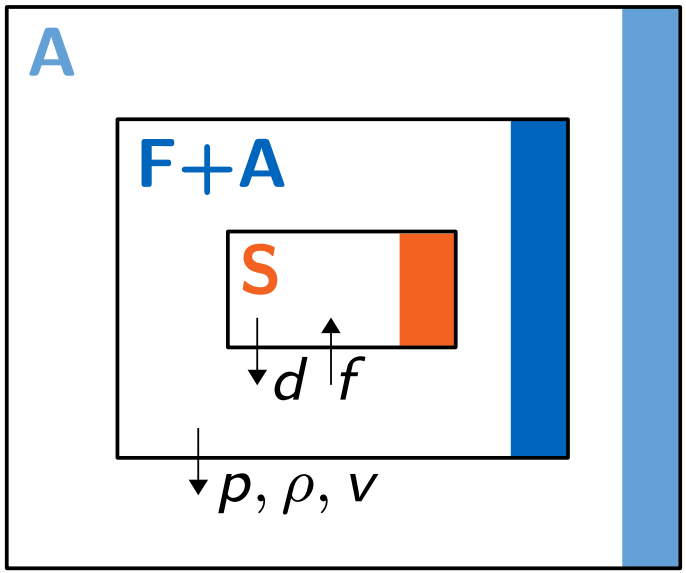

- S: FEM structure solver
- F+A: Low-order FV solver, resolve geometries, resolve turbulent structures
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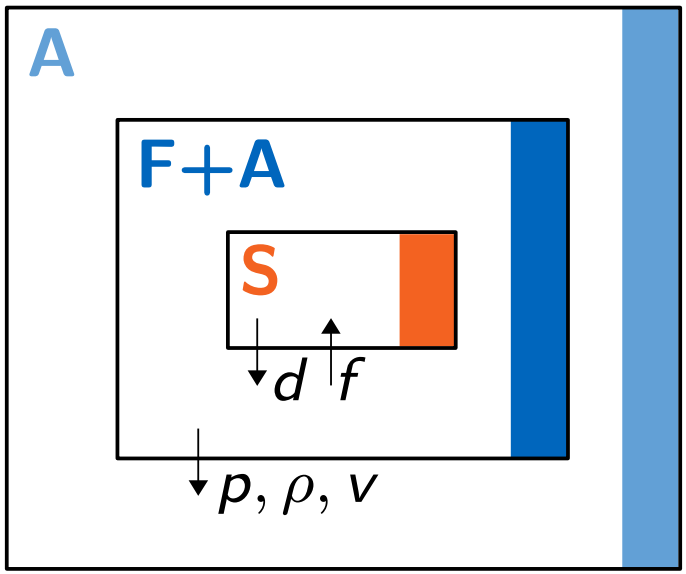
- Taylored numerical methods necessary for each subdomain
  $\Rightarrow$ partitioned approach
- Multi-scale $\Rightarrow$ HPC

The ExaFSA Challenge



- **S**: FEAP or CalculiX
- **F+A**: FASTEST (TU Darmstadt, Thorsten Reimann, Dörte Sternel)
- **A**: Ateles (U Siegen, Verena Krupp, Neda Ebrahimi Pour, Harald Klimach, Sabine Roller)
- **Performance Portability**: Xevolver (Tohoku, Hiro Takizawa, Ryusuke Egawa et al.)

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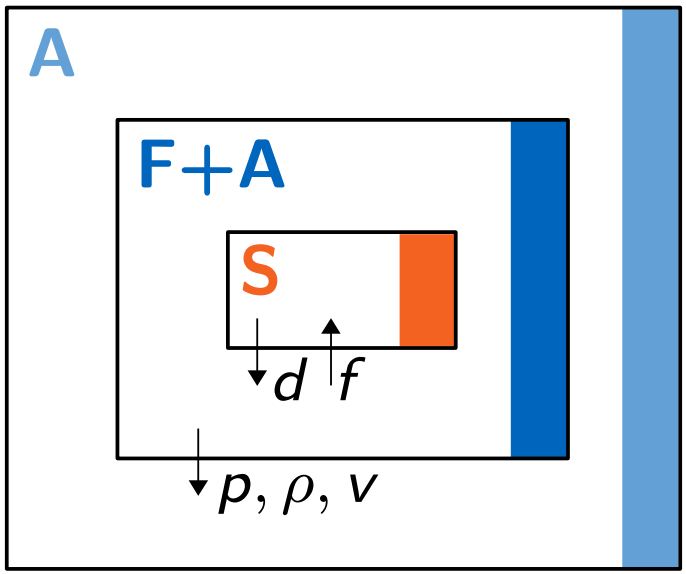

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Coupling: preCICE

- . . . has to be scalable and easy-to-use
- 1. **Easy-to-use Coupling**: flexible and minimally-invasive integration into existing legacy codes
- 2. **Scalable Coupling**: don't deteriorate the scalability of the coupled single-physics solvers by the coupling

preCICE Contributors

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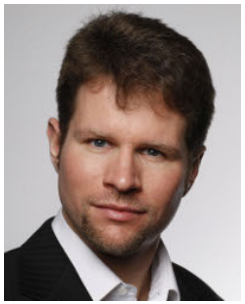

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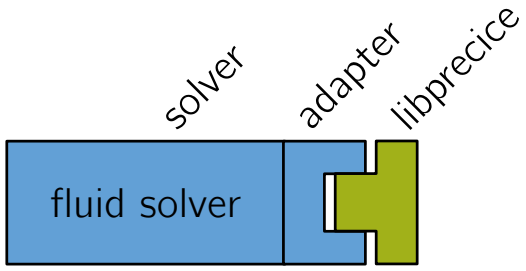
1. Easy-to-use Coupling

Easy-to-use: We need a library approach (. . . not a framework)



OpenFOAM
SU2
foam-extend

Easy-to-use: We need a library approach (. . . not a framework)

OpenFOAM
SU2
foam-extend

CalculiX
Code_Aster
FEniCS
deal-ii
MBDyn

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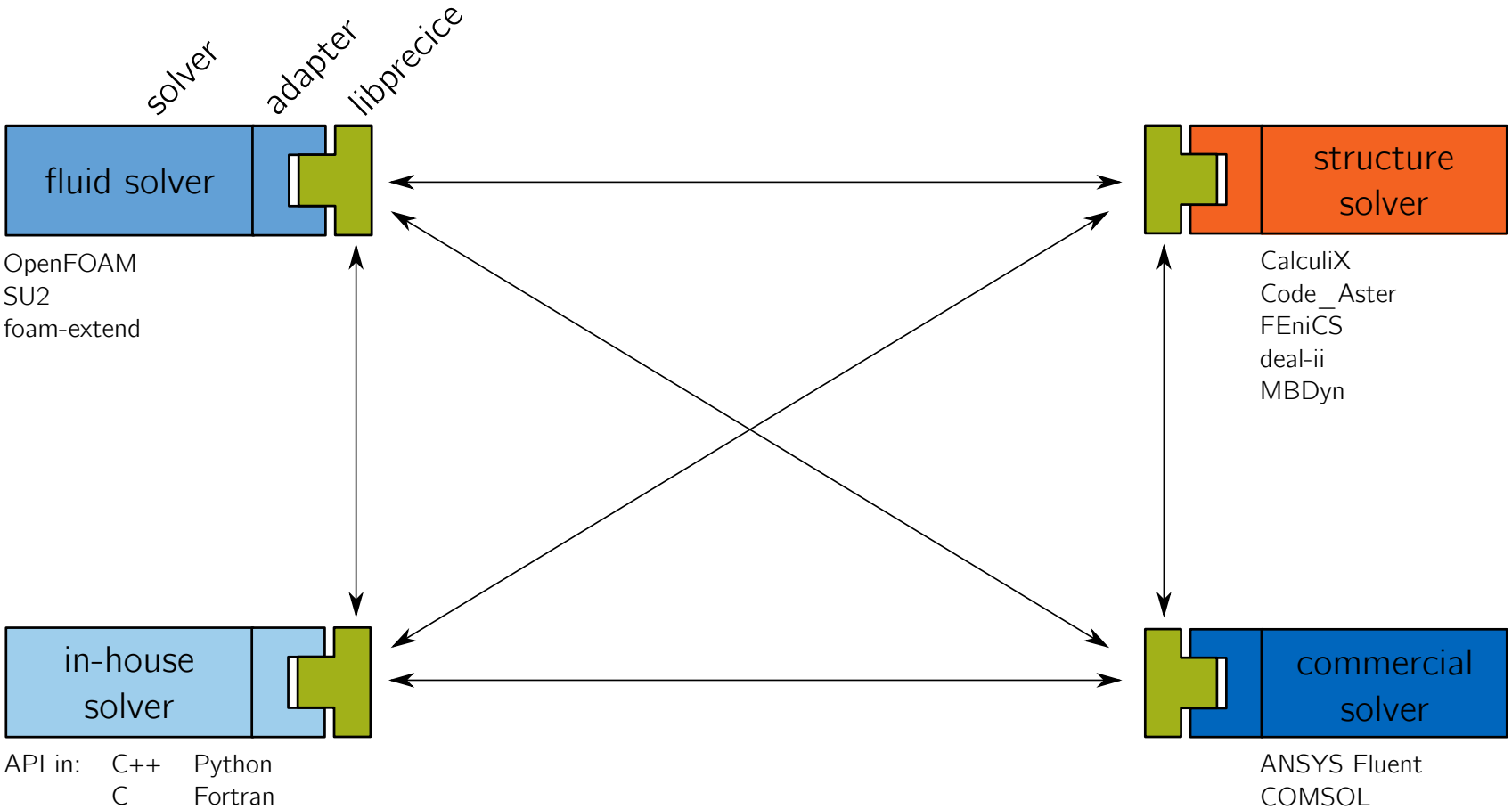
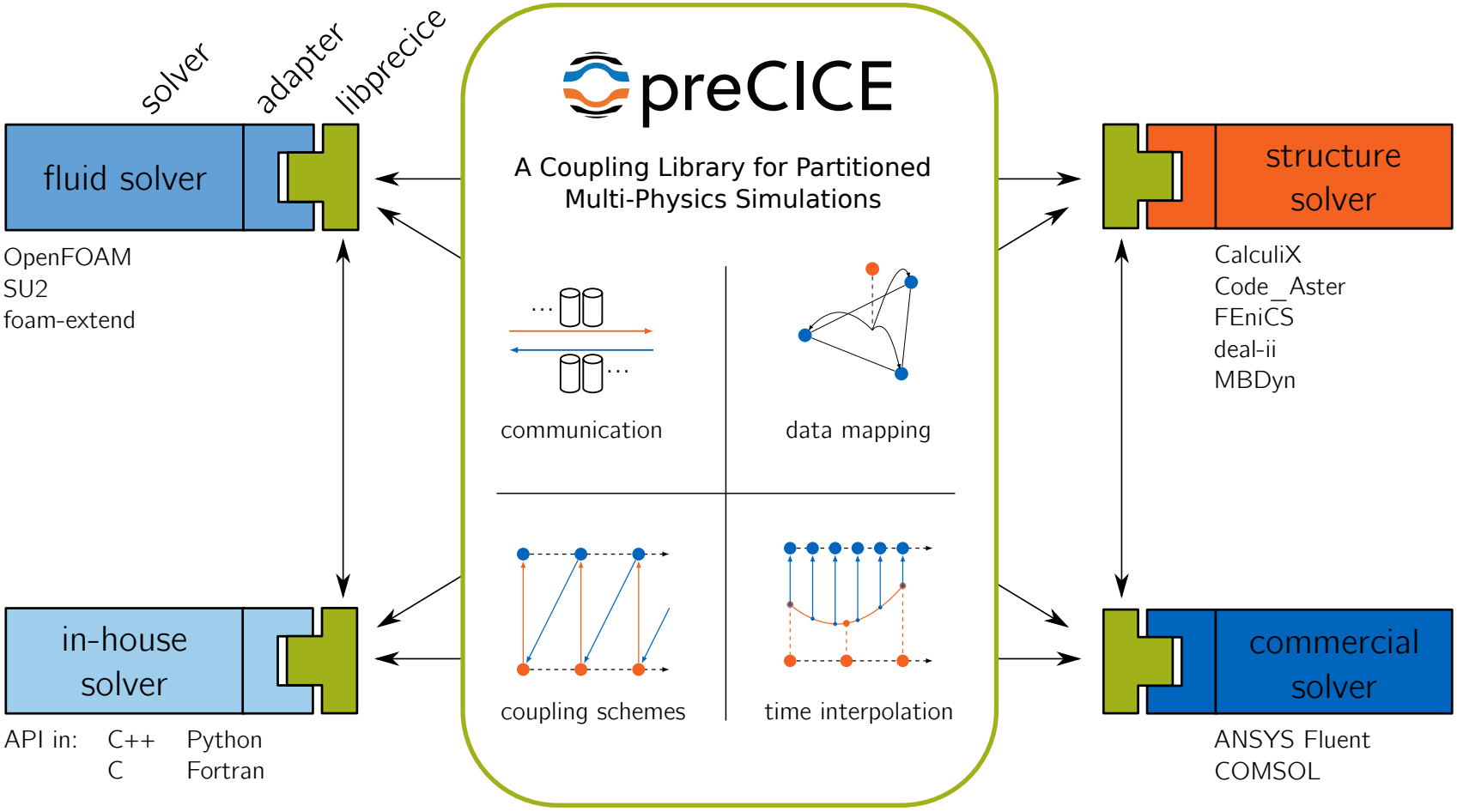


Easy-to-use: We need a library approach (...not a framework)



Easy-to-use: We need a high-level API

```
1     precice::SolverInterface
2     precice("FluidSolver",rank,size);
3     precice.configure("precice-config.xml");
4     precice.setMeshVertices();
5     precice.initialize();
6
7     while (precice.isCouplingOngoing()) { // main time loop
8         solve();
9
10        precice.writeBlockVectorData();
11        precice.advance();
12        precice.readBlockVectorData();
13
14        endTimeStep(); // e.g. write results, increase time
15    }
16
17    precice.finalize();
```

Timesteps, most arguments and less important methods omitted. Full example in the wiki.

Easy-to-use: We need ready-to-use adapters

→ **Our flagship: The OpenFOAM Adapter**

```
/* Start the solver */

Info<<"\nStarting time loop\n"<< endl;
while (runTime.run()) {
  #include "readTimeControls.H"
  #include "compressibleCourantNo.H"
  #include "setDeltaT.H"

  runTime++;

  /* solve the equations */
  #include "rhoEqn.H"
  while (pimple.loop())
  {
      ...
  }

  runTime.write();
}

/* Finalize */
```

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```

```
// system/controlDict OpenFOAM config file
functions
{
  preCICE_Adapter
  {
    type preciceAdapterFunctionObject;
    libs ("libpreciceAdapterFunctObj.so");
  }
}
```

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    type preciceAdapterFunctionObject;
    libs ("libpreciceAdapterFunctObj.so");
  }
}
```

```
// 0/T OpenFOAM config file
interface
{
  type              fixedValue;
  value             uniform 300;
}
// other types: fixedGradient, mixed
```

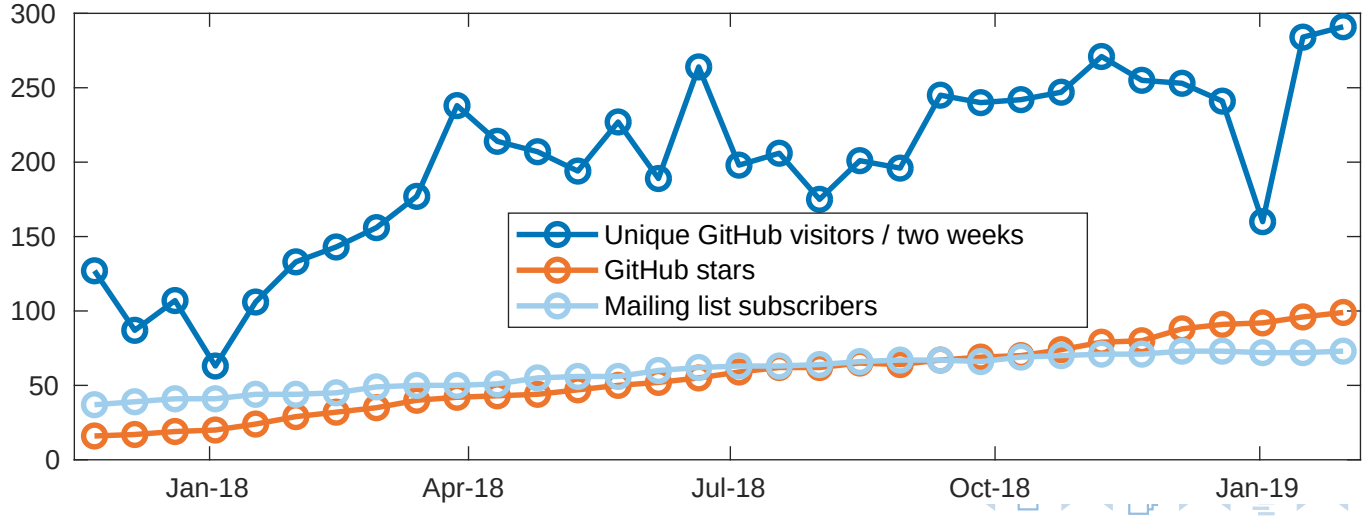
Coupling boundary patches, problem & solver type:
`precice-adapter-config.yml`

It's starting to pay off, our users:

- LSM & STS, U Siegen, Germany
- SC & FNB, TU Darmstadt, Germany
- SCpA, CIRA, Italy
- Cardiothoracic Surgery, UFS, South Africa
- A*STAR, Singapore
- NRG, Petten, The Netherlands
- Aerodynamics & Wind Energy (KITE Power), TU Delft, The Netherlands
- Mechanical and Aeronautical Eng., University of Manchester, UK
- University of Strathclyde, Glasgow, UK
- FAST, KIT, Germany
- AIT, Vienna, Austria
- IAG, University of Stuttgart, Germany
- CTTC UPC, Barcelona, Spain
- Amirkabir U. of Technology, Iran

Upcoming:

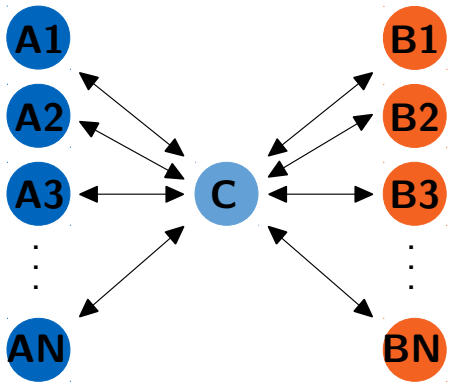
- GRS, Garching, Germany
- MTU Aero Engines, Munich, Germany
- Numerical Analysis, Lund, Sweden
- Helicopter Technology & Astronautics, TUM, Germany
- ATA Engineering Inc., USA
- BITS Pilani, India
- Aviation, MSU Denver, USA



2. Scalable Coupling

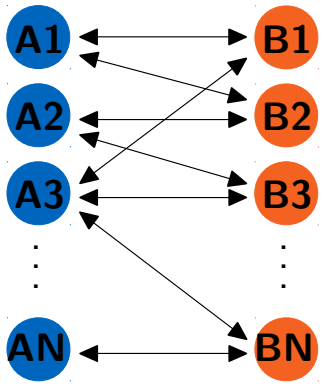
Communication Layout

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

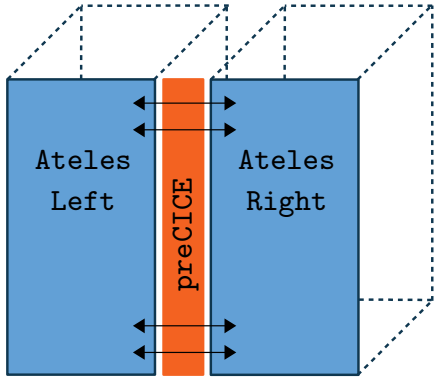
Our Peer-To-Peer Concept

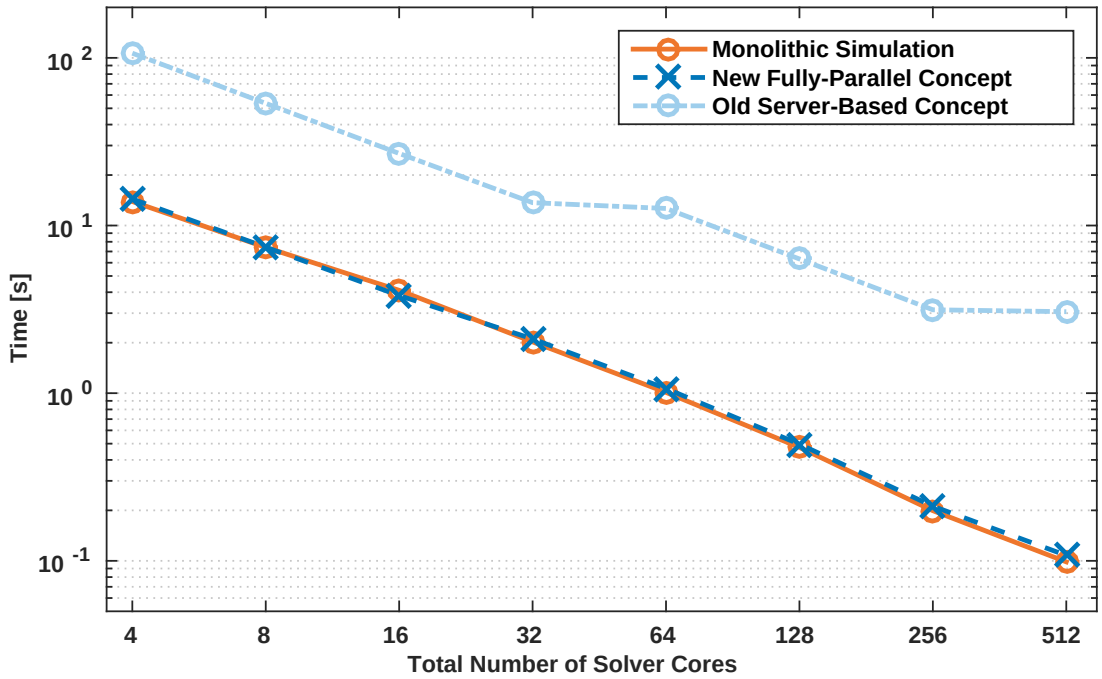


- No central entity
- Interface computations in parallel
- $\Rightarrow$ No scaling issues

Simple Scaling Test

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





Simple Scaling Test (cont.)

- Travelling density pulse (Euler equations) through artificial coupling interface
- DG solver Ateles (U Siegen), $\mathbf{5.7 \cdot 10^7}$ dofs
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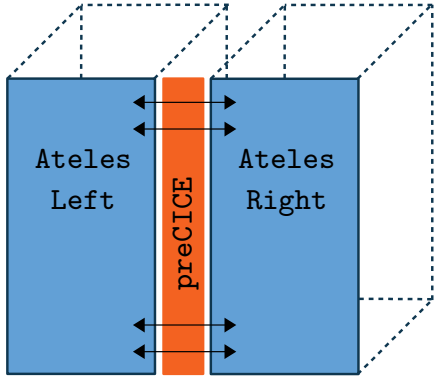

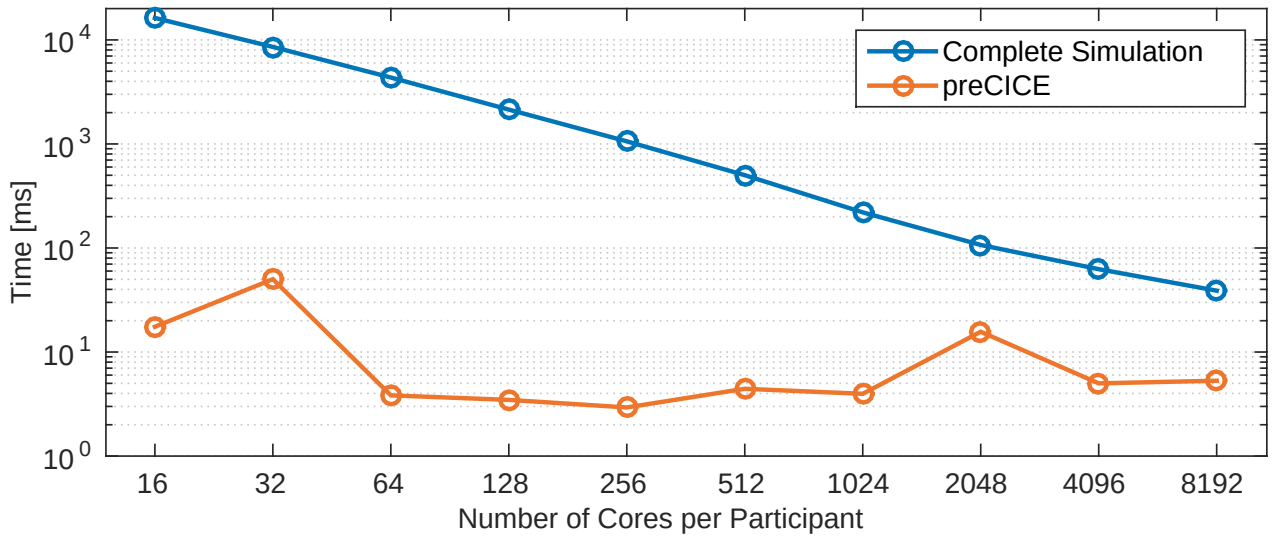

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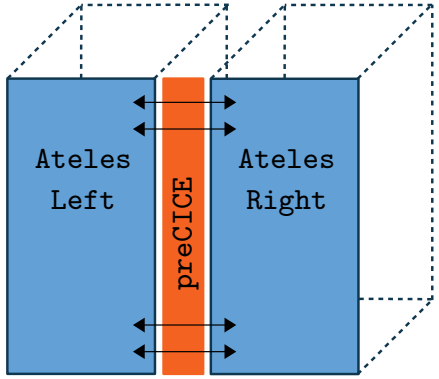
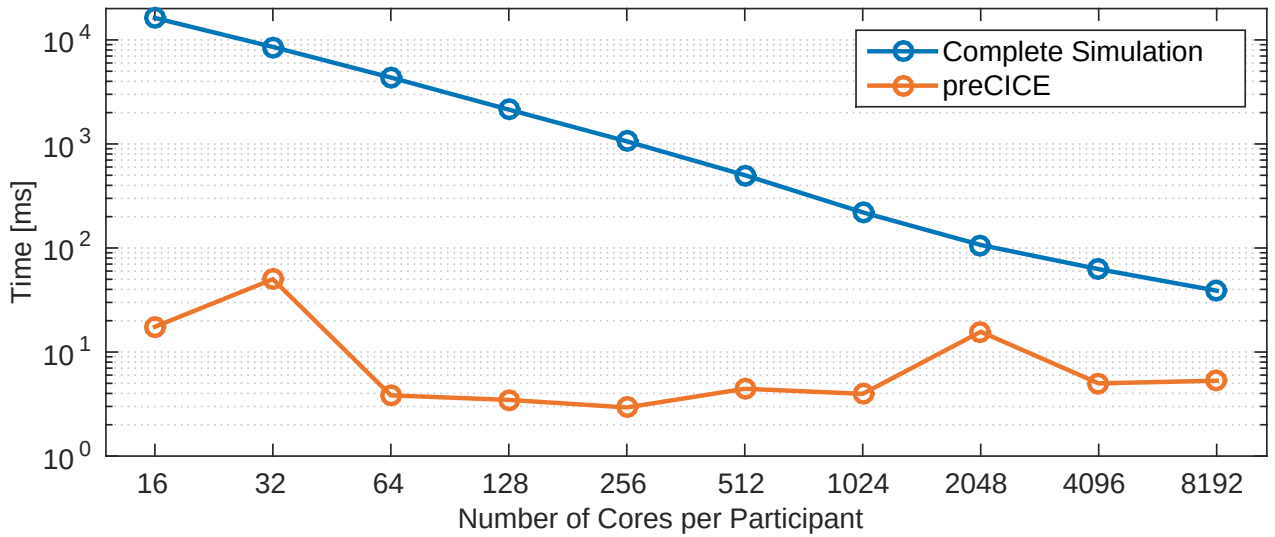
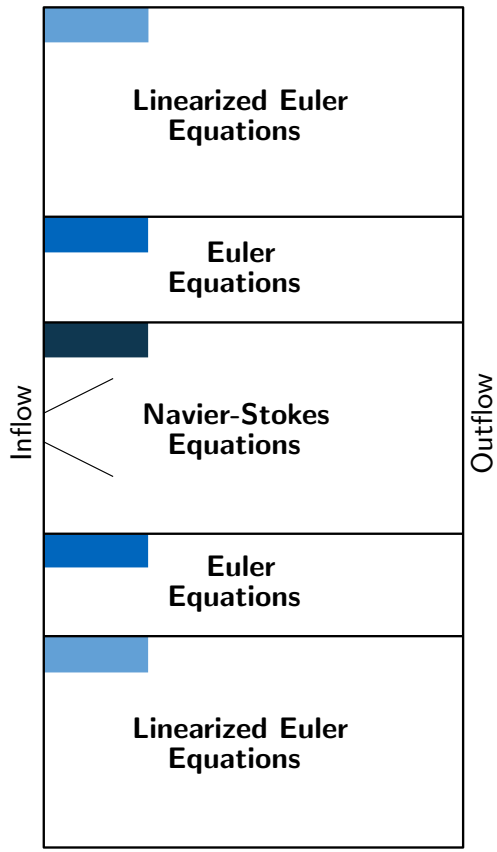


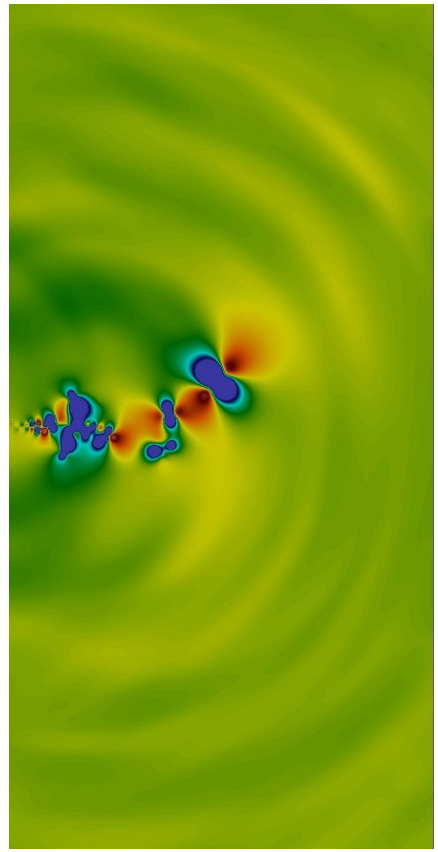


$\Rightarrow$ **Coupling does not deteriorate scalability**

Fluid-Acoustic Interaction

- Sub-sonic jet
- Explicit parallel coupling between three solver, all Ateles
- Linearized Euler 28x cheaper than Navier-Stokes

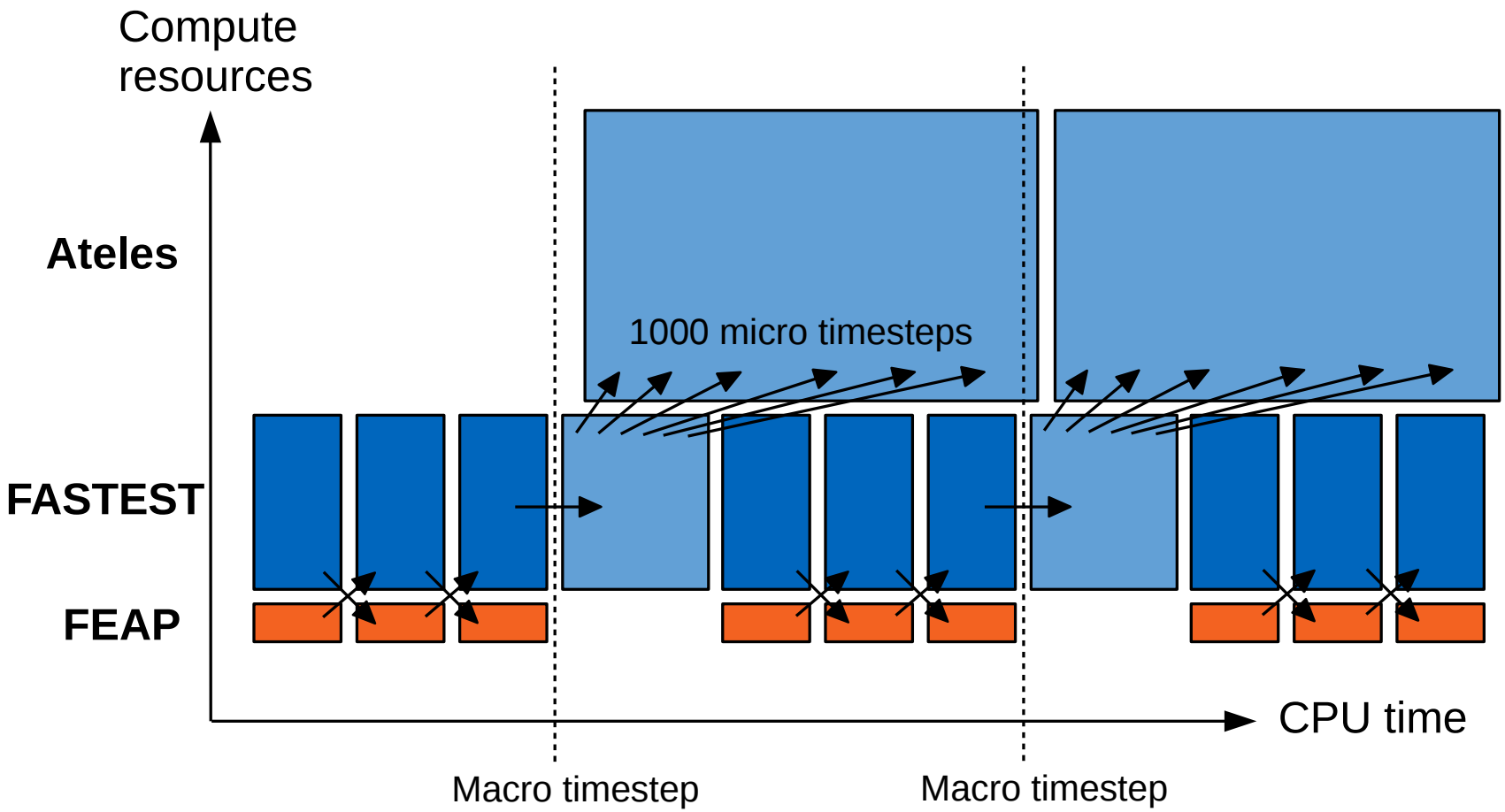




- Joint work with Verena Krupp et al.

Load-Balancing

- Difficult
- We need manual buffering for uni-directional coupling



- Joint work with Thorsten Reimann et al. and Neda Ebrahimi Pour et al.

Summary

- For challenging multiphysics, multiscale problems, we need an **easy-to-use** and **scalable** coupling approach
- **easy-to-use** = minimally-invasive integration in legacy codes
  - library approach (no framework approach)
  - high-level API
  - ready-to-use adapters for community codes
- **scalable** = don't deteriorate scalability of coupled solvers
  - peer-to-peer approach (no server approach)
  - tricks for load-balancing

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github.com/precice

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Figure: Doughnuts contributed by Gerasimos Chourdakis, TUM.