SPPEXA APM 2016

Partitioned Multi-Physics on Distributed Data via preCICE

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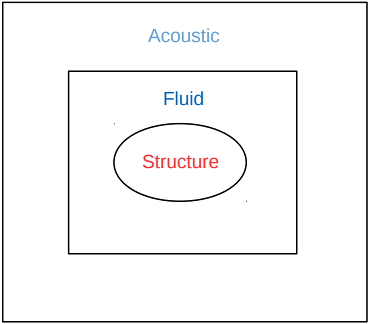
IAS TUM Institute for Advanced Study

Multi-Physics and Exa-Scale

- many exciting applications need multi-physics
- more compute power $\Rightarrow$ more physics?
- many sophisticated, scalable,
  single-physics, legacy codes
- our goal: minimal invasive coupling,
  no deterioration of scalability

Our Example: Fluid-Structure-Acoustic Interaction



- FEAP - FASTEST - Ateles
- OpenFOAM - OpenFOAM - Ateles
- glue-software: preCICE

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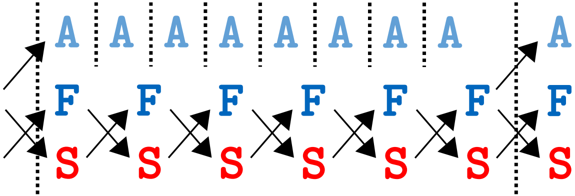

- implicit or explicit coupling
- subcycling

Agenda

This talk: glue-software preCICE
Next talk (Verena Krupp): application perspective

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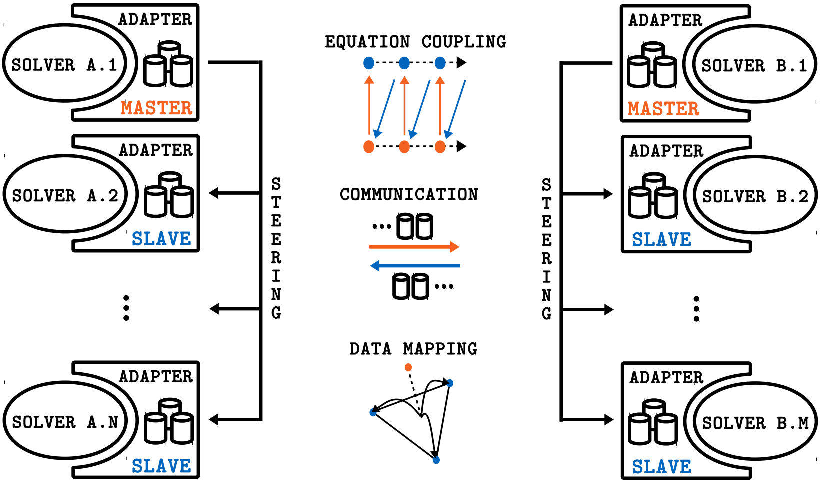
Next talk (Verena Krupp): application perspective

1. Very brief introduction to preCICE
2. Realization on Distributed Data
3. Performance on Distributed Data

preCICE

- **pre**cise **C**ode **I**nteraction **C**oupling **E**nvironment
- developed in Munich and Stuttgart
- library approach, minimal invasive
- high-level API in `C++`, `C`, `Fortran77/90/95`, `Fortran2003`
- once adapter written $\Rightarrow$ plug and play
- `https://github.com/precice/precice`

Big Picture



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SOLVER B.M
SLAVE

Coupled Solvers

Ateles (APES)	**CF**, **A**	in-house (U Siegen)
Alya System	**IF**, **S**	in-house (BSC)
Calculix	**S**	open-source (A*STAR)
CARAT	**S**	in-house (TUM STATIK)
COMSOL	**S**	commercial
EFD	**IF**	in-house (TUM SCCS)
FASTEST	**IF**	in-house (TU Darmstadt)
Fluent	**IF**	commercial
OpenFOAM	**CF**, **IF**, **S**	open-source (TU Delft)
Peano 1	**IF**	in-house (TUM SCCS)
SU2	**CF**	open-source

preCICE API

```
turn_on()

while time loop ≠ done do

   solve_timestep()

end while
turn_off()
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preCICE Config

```
<coupling-scheme:parallel-explicit>
    <participants first="FLUID" second="ACOUSTIC" />
    <timestep-length value="1e-4" />
    <exchange data="Density"   mesh="AcousticSurface" from="FLUID" to="ACOUSTIC"/>
    <exchange data="Velocity"  mesh="AcousticSurface" from="FLUID" to="ACOUSTIC"/>
</coupling-scheme:parallel-explicit>

<coupling-scheme:parallel-implicit>
    <participants first="FLUID" second="STRUCTURE"/>
    <timestep-length value="1e-3"/>
    <exchange data="Forces"        mesh="WetSurface" from="FLUID" to="STRUCTURE"/>
    <exchange data="Displacements" mesh="WetSurface" from="STRUCTURE" to="FLUID"/>
    <rel-conv-measure data="Displacements" mesh="WetSurface" limit="1e-3"/>
    <post-processing:IQN-ILS>
        <data name="Forces" mesh="WetSurface">
        <data name="Displacements" mesh="WetSurface">
    </post-processing:IQN-ILS>
</coupling-scheme:parallel-implicit>
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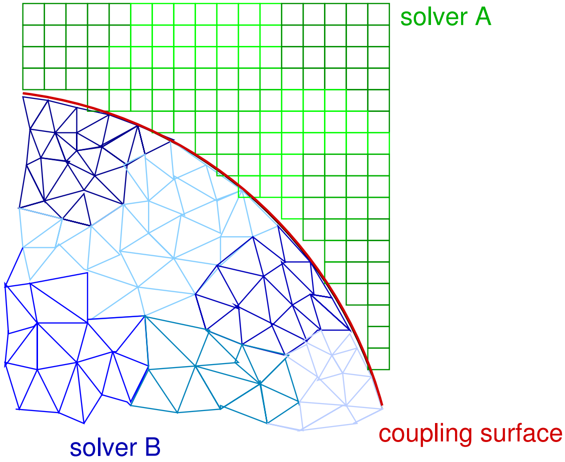
Communication on Distributed Data



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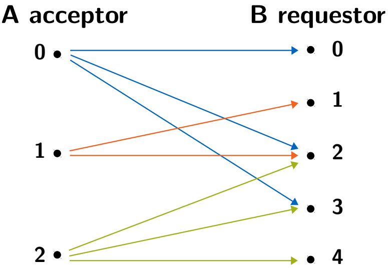
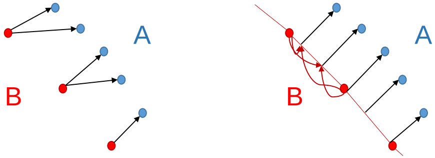


- kernel: 1:N communication based on either TCP/IP or MPI Ports
  ⇒ no deadlocks at initialization (independent of order at B)
- asynchronous communication (preferred over threads)
  ⇒ no deadlocks at communication

Interpolation on Distributed Data

Projection-based Interpolation

- first or second order
- example: consistent mapping from B to A
- parallelization: almost trivial



nearest neighbour mapping   nearest projection mapping

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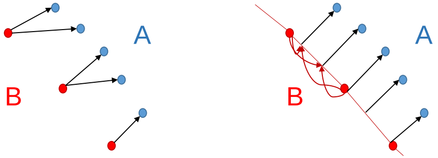


nearest neighbour mapping nearest projection mapping

Radial Basis Function Interpolation

- higher order
- parallelization: far from trivial (realized with `PETSc`)

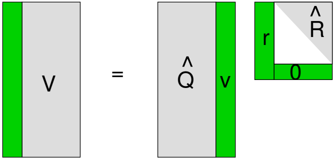
Fixed-Point Acceleration on Distributed Data

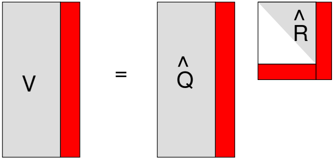
Anderson Acceleration (IQN-ILS)

Find $x \in D \subset \mathbb{R}^n : \; H(x) = x, \; H : D \to \mathbb{R}^n$

initial value x^0
$\tilde{x}^0 = H(x^0)$ and $R^0 = \tilde{x}^0 - x^0$
$x^1 = x^0 + 0.1 \cdot R^0$
for $k = 1 \ldots$ **do**
   $\tilde{x}^k = H(x^k)$ and $R^k = \tilde{x}^k - x^k$
   $V^k = [\Delta R_0^k, \ldots, \Delta R_{k-1}^k]$ with $\Delta R_i^k = R^i - R^k$
   $W_k = [\Delta \tilde{x}_0^k, \ldots, \Delta \tilde{x}_{k-1}^k]$ with $\Delta \tilde{x}_i^k = \tilde{x}^i - \tilde{x}^k$
   decompose $V^k = Q^k U^k$
   solve the first k lines of $U^k \alpha = -{Q^k}^T R^k$
   $\Delta \tilde{x} = W \alpha$
   $x^{k+1} = \tilde{x}^k + \Delta \tilde{x}^k$
end for

Fixed-Point Acceleration on Distributed Data





Insert Column

In: $\hat{Q} \in \mathbb{R}^{n \times m}$, $\hat{R} \in \mathbb{R}^{m \times m}$, $v \in \mathbb{R}^n$, Out: $Q \in \mathbb{R}^{n \times (m+1)}$, $R \in \mathbb{R}^{(m+1) \times (m+1)}$

for $j = 1 \dots m$ **do**

$r(j) = \hat{Q}(:, j)^T v$

$v = v - r(j) \cdot \hat{Q}(:, j)$

end for

$r(m+1) = \|v\|_2$

$Q(:, m+1) = r(m+1)^{-1} \cdot v$

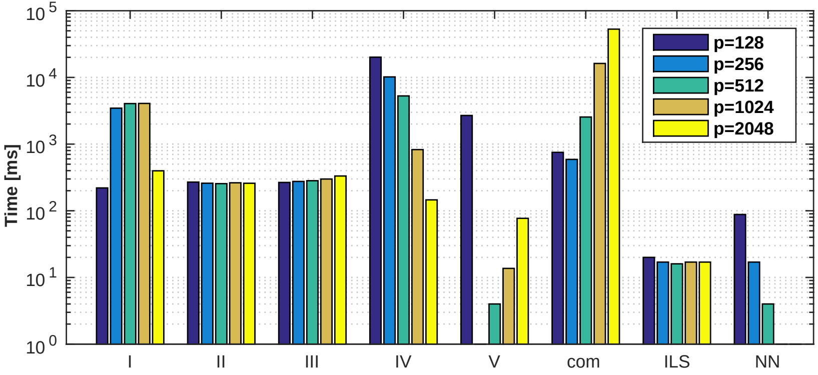
$R = \left[r, \begin{pmatrix} \hat{R} \\ 0 \end{pmatrix} \right]$

Given's rotations $G_{i,j}$ s.t. $R = G_{1,2} \dots G_{m,m+1} R$ upper triangle

$Q = Q G_{m,m+1} \dots G_{1,2}$

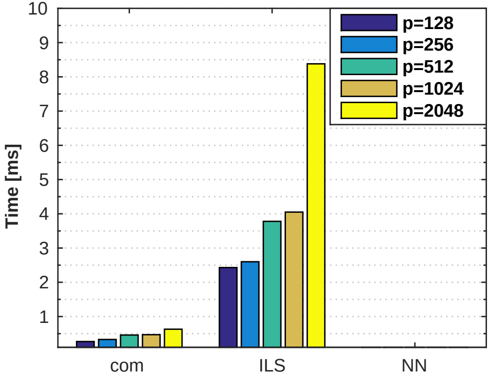
Performance Tests, Initialization

#DOFs at interface: $2.6 \cdot 10^5$, strong scaling



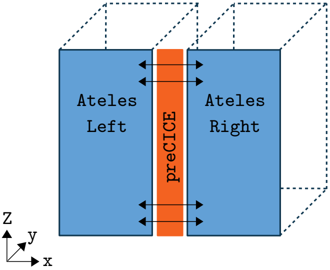
Performance Tests, Work per Timestep

#DOFs at interface: $2.6 \cdot 10^5$, strong scaling



Performance Tests, Traveling Pulse

DG solver Ateles, Euler equations,
#DOFs: total: $5.9 \cdot 10^9$, at interface: $1.1 \cdot 10^7$,
NN mapping and communication
strong scaling from 128 to 16384 processors per participant.



Joint work with V. Krupp et al. (Universität Siegen)

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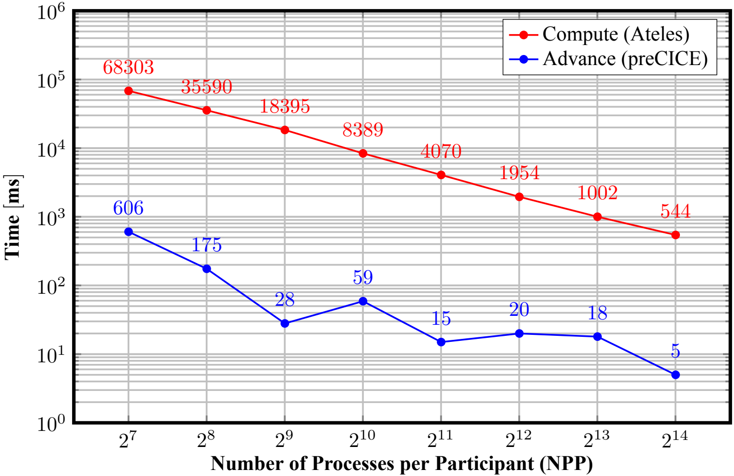

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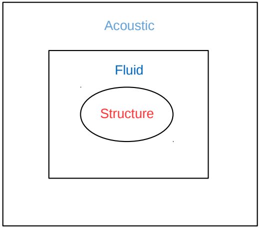

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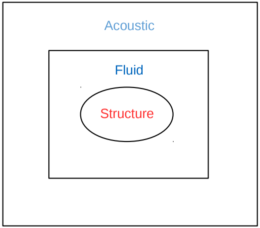
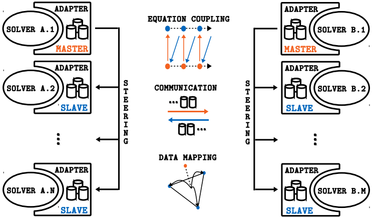

Acoustic
Fluid
Structure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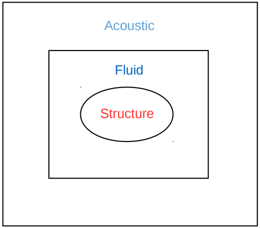

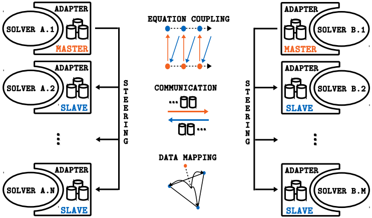


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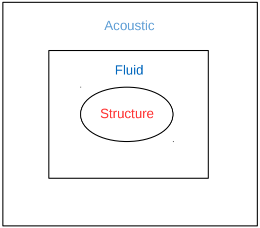

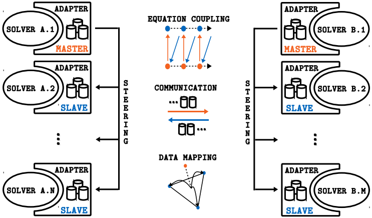

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