Partitioned Methods for Multifield Problems

Rang, 3.4.2017

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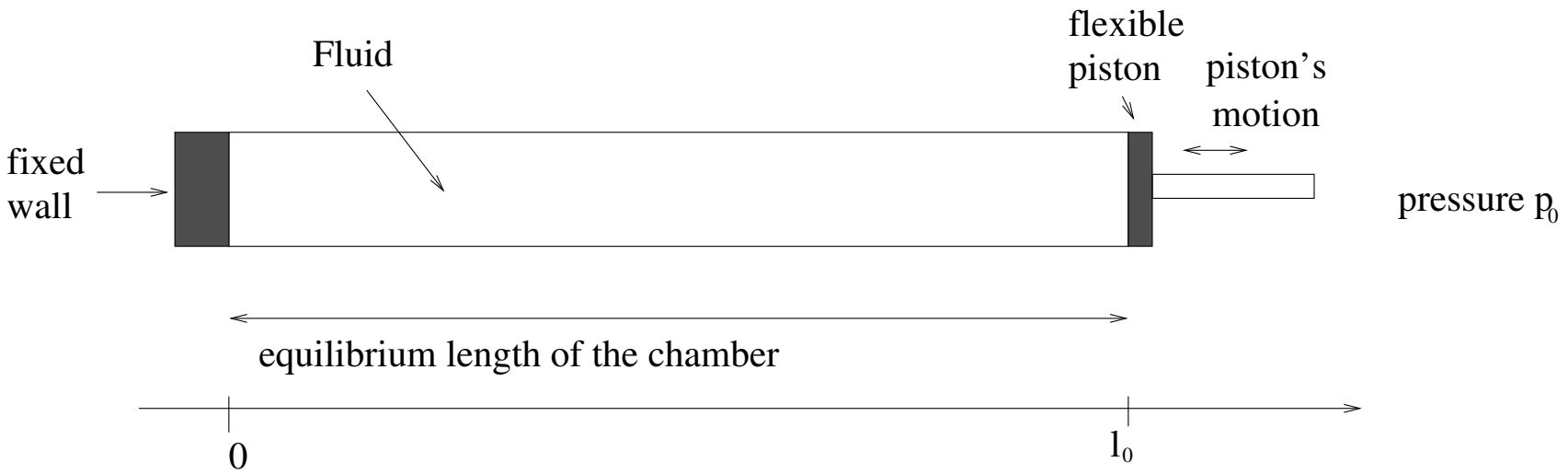


One-dimensional piston problem

Fluid (mass and momentum equation conservation equations):

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho u) = 0$$
$$\frac{\partial}{\partial t}(\rho u) + \frac{\partial}{\partial x}(\rho u^2 + p) = 0$$

- ρ ... gas density
- u ... flow velocity
- p ... pressure
- Moreover $\frac{\partial p}{\partial \rho} = c^2$

One-dimensional piston problem

linear dynamic equilibrium of the piston:

$$m\ddot{q} + d\dot{q} + Kq = p(l_0 + q) - p_0$$

- m ... mass
- d ... damping
- K ... stiffness
- q ... displacement
- $\dot{q}$ ... velocity
- $\ddot{q}$ ... acceleration

One-dimensional piston problem

- equilibrium state: uniform pressure p_0, inside and outside the piston chamber, a uniform gas density ρ_0, a zero flow velocity $u_0 = 0$ and a chamber length equal to l_0
- boundary conditions:

$$\rho(t,0)u(t,0) = 0, \quad u(t, l_0 + q) = \dot{q}$$

- initial conditions:

$$u(0,x) = u_0(x), \rho(0,x) = \rho_0(x), q(0,x) = q_0(x), \dot{q}(0,x) = \dot{q}_0(x)$$

Discretisation in space and time

- spatial discretisation for the fluid part: finite difference scheme with upwinding (finite volumes)
- Semi-discretisation in space:

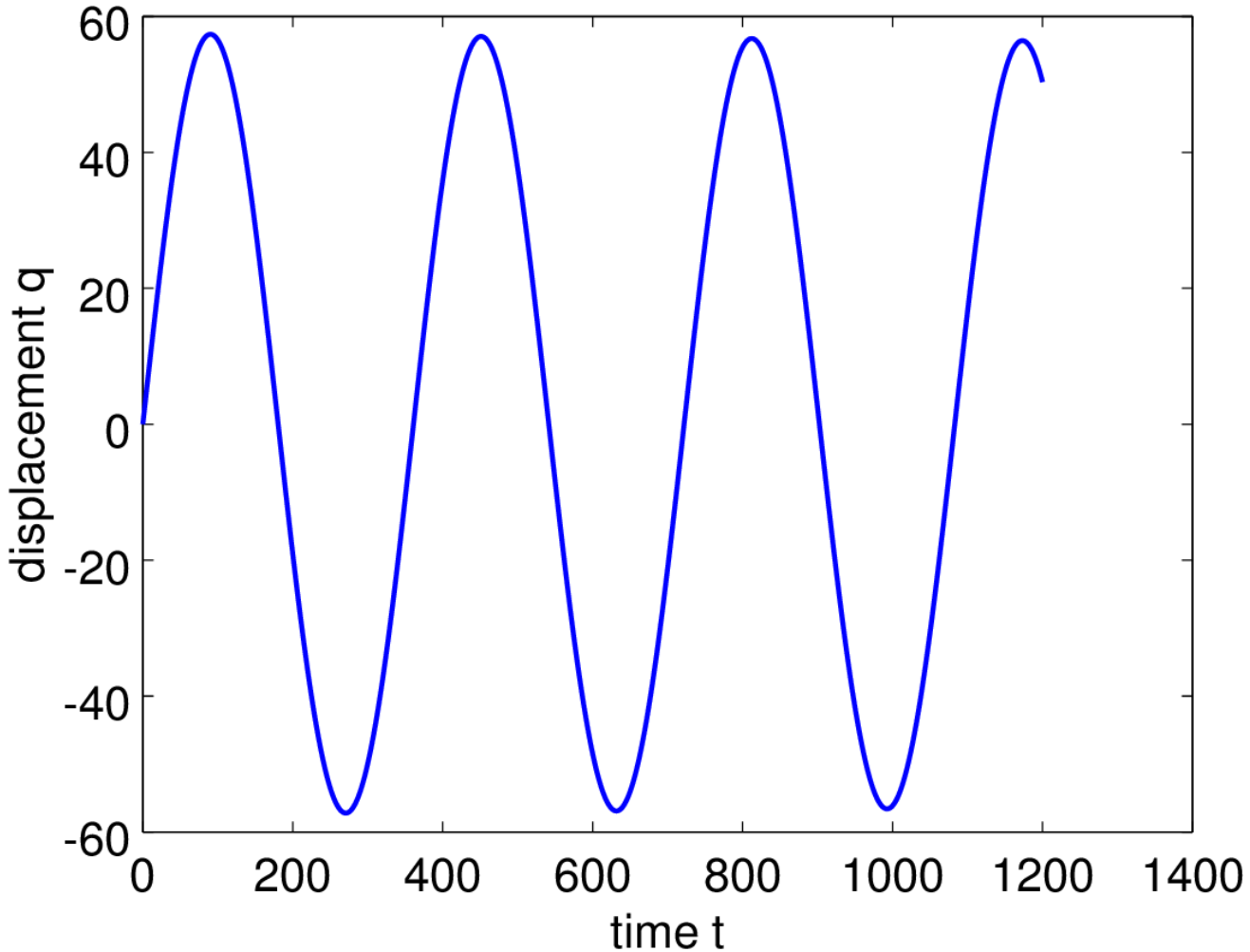
$$\begin{pmatrix} \dot{\mathbf{u}} \\ \dot{\mathbf{v}} \end{pmatrix} = \begin{pmatrix} A & B \\ C & D \end{pmatrix} \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix} + \begin{pmatrix} \mathbf{f}(t) \\ \mathbf{g}(t) \end{pmatrix}$$

- time discretisation for the fluid and structural part: implicit Euler method

Discretised system:

$$\begin{pmatrix} I - \tau A & -\tau B \\ -\tau C & I - \tau D \end{pmatrix} \begin{pmatrix} \mathbf{u}_{m+1} \\ \mathbf{v}_{m+1} \end{pmatrix} = \begin{pmatrix} \mathbf{u}_m \\ \mathbf{v}_m \end{pmatrix} + \tau \begin{pmatrix} \mathbf{f}(t_{m+1}) \\ \mathbf{g}(t_{m+1}) \end{pmatrix}$$

In practise


60
40
20
0
-20
-40
-60
displacement q
0
200
400
600
800
1000
1200
1400
time t

In practise

- Discretisation of each subproblem leads to large systems.
- Sub-problems are solved with different software (Example FSI: OpenFOAM for the fluid part and FEAP for the structural part)
- Possibilities for computing the numerical solution:
  - monolythical approach: solve the whole problem with one method (software)
  - partitioned approach: solve each subproblem separately

Direct vs. iterative (I)

direct/monolithic approach

- solve the whole problem with one software package
- In practise: difficult to implement
- large discretised problem
- problem may be instable

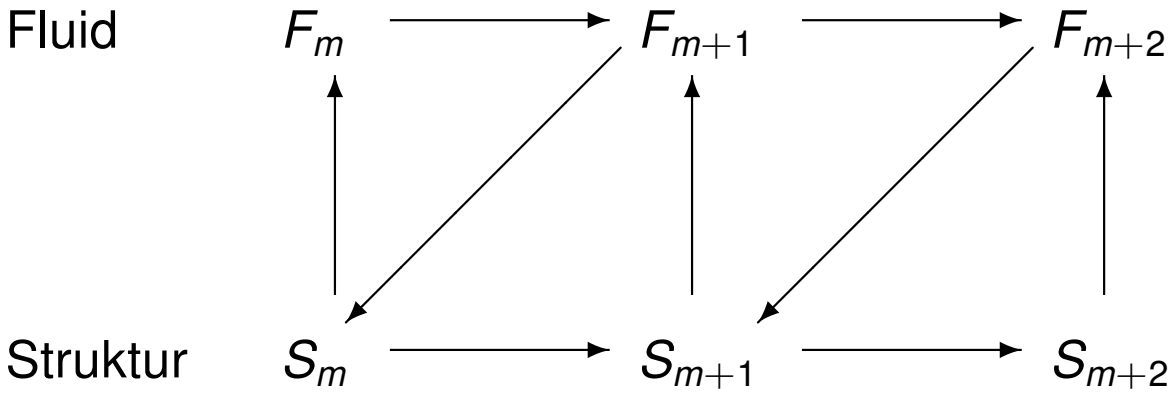
Direct vs. iterative (II)

modular approach (partitioned methods)

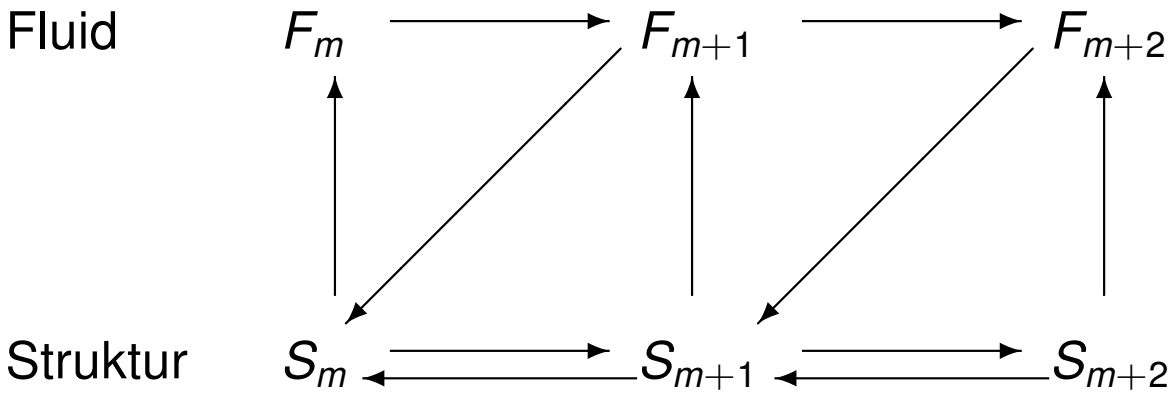
- solve the subproblems with different codes
- Advantages:
  - existing software can be used
  - the best codes for the subproblems can be used
  - each subproblem is better conditioned as the whole problem
- Disadvantages:
  - different discretisations on the interface
  - numerical results depends on the coupling, i.e. on the iterative solution of the subsystems

Coupling algorithms

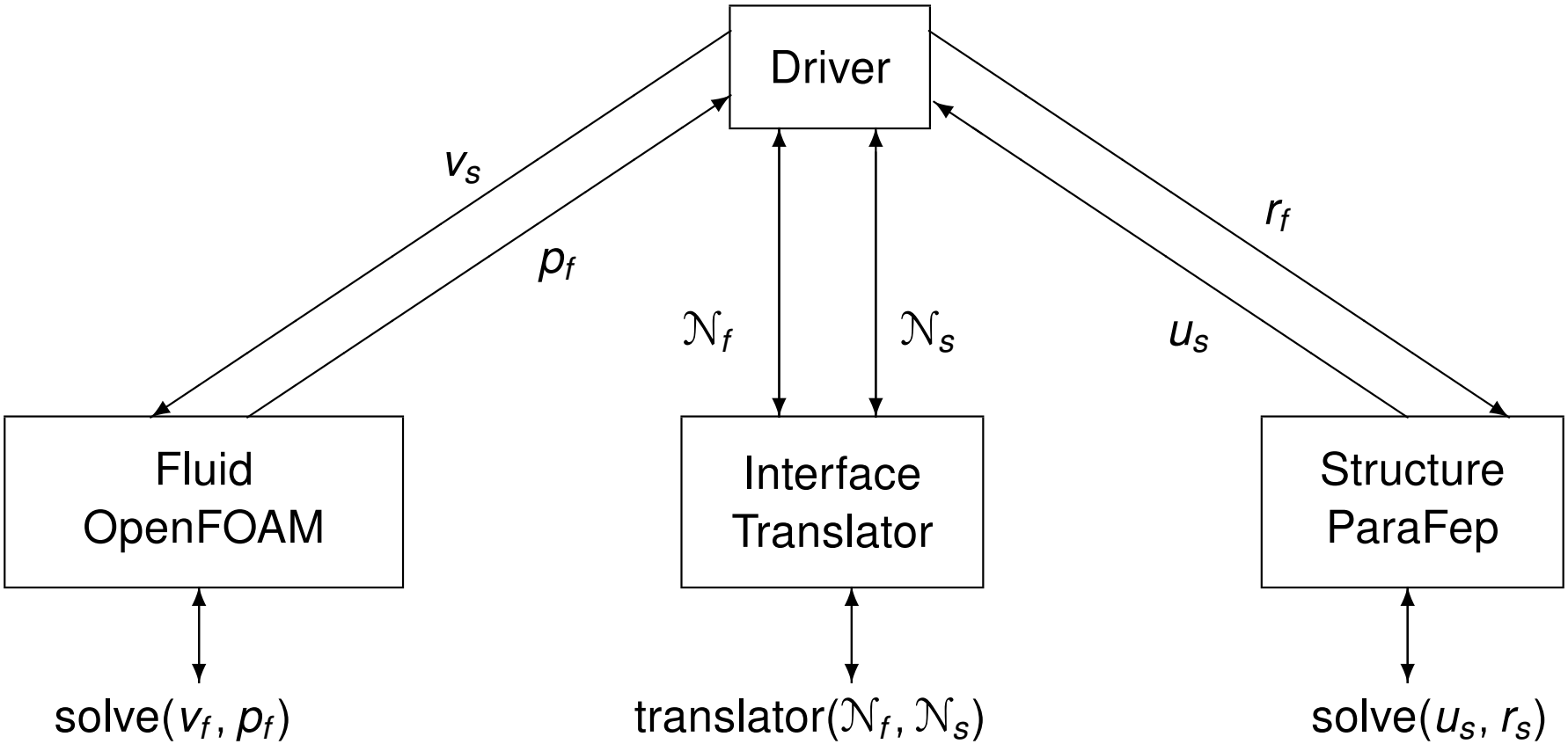
- staggered: weak (explicit)



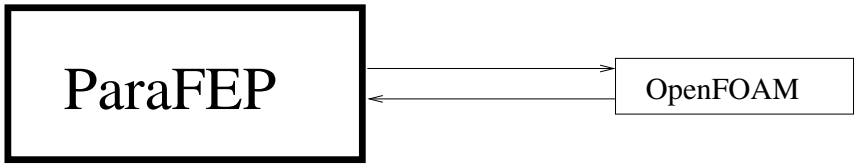
- block-Gauß-Seidel: strong, restricted

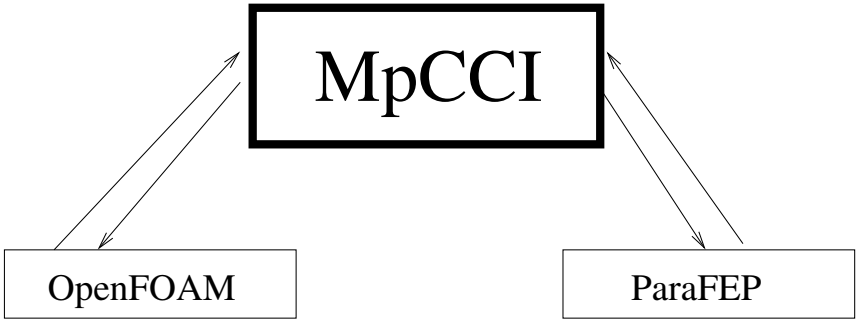


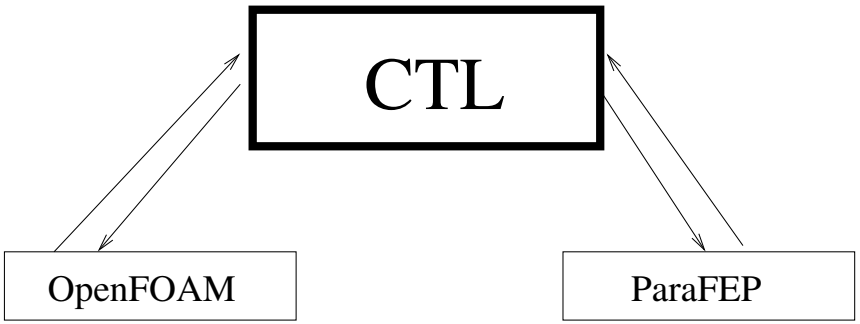
Interaction of Components



Communication

- 

- 

- 

OpenFOAM and ParaFEP are software components

MpCCI – Multiphysics Interfaces

- software tool for coupling multiphysic software
- developed by Fraunhofer SCAI
- for communication MPI is used
- only linear interpolation for non-matching meshes

Software Components

Criteria for software components:

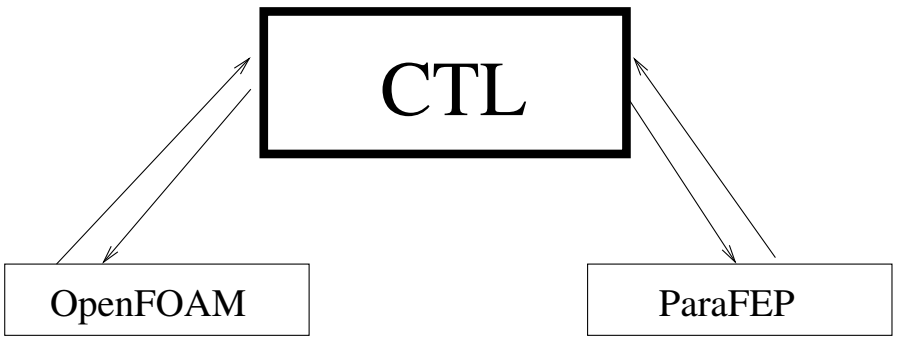
- Non-context-dependent $\rightarrow$ exchangeable
- Composable with other components
- Encapsulated i.e., only investigable through its interfaces
- A unit of independent deployment and versioning

Examples:

- linear solver
- CFD solver, CSD solver

Reasons to use Components

- Growing number of (freely) available libraries and programs worth to be re-used
- Exchangeable software units
- Avoids linking errors of incompatible libraries
- Longer lifetime of implementations



Example: Piston problem

- Monolythical system:

$$\begin{pmatrix} I-\tau A & -\tau B \\ -\tau C & I-\tau D \end{pmatrix} \begin{pmatrix} \mathbf{u}_{m+1} \\ \mathbf{v}_{m+1} \end{pmatrix} = \begin{pmatrix} \mathbf{u}_m \\ \mathbf{v}_m \end{pmatrix} + \tau \begin{pmatrix} \mathbf{f}(t_{m+1}) \\ \mathbf{g}(t_{m+1}) \end{pmatrix}$$

- Simplification: $\tau B\mathbf{v}_{m+1} \approx \tau B\mathbf{v}_m$ and $\tau C\mathbf{u}_{m+1} \approx \tau C\mathbf{u}_m$.
- Staggered system:

$$\begin{pmatrix} I-\tau A & 0 \\ 0 & I-\tau D \end{pmatrix} \begin{pmatrix} \mathbf{u}_{m+1} \\ \mathbf{v}_{m+1} \end{pmatrix} = \begin{pmatrix} I & \tau B \\ \tau C & I \end{pmatrix} \begin{pmatrix} \mathbf{u}_m \\ \mathbf{v}_m \end{pmatrix} + \tau \begin{pmatrix} \mathbf{f}(t_{m+1}) \\ \mathbf{g}(t_{m+1}) \end{pmatrix}$$

- Remark: system is decoupled

Mixed problems

- adjectives ”coupled” and ”mixed” are often used in the context of numerical solution of PDEs.
- mixed problem (Zienkiewicz, 1984): Mixed formulations are those applicable to a single domain in which equations and boundary conditions describing the physical phenomenon and used for the numerical solution contain a number of dependent variables which could be reduced by elimination, still maintaining a solvable problem.
- This definition implies that an irreducible formulation can be found for each mixed formulation.

Example (heat diffusion problem)

- Let q be the flux and T be the temperature.
- Consider

$$\begin{aligned} q &= -k\nabla T, \quad \text{in } \Omega \\ \nabla \cdot q &= Q, \quad \text{in } \Omega \\ q_n &= \bar{q}_n, \quad \text{on } \Gamma_q, \\ T &= \bar{T}, \quad \text{on } \Gamma_T. \end{aligned}$$

- If we discretise the variables q and T we get a mixed formulation. Inserting q into the second equation leads to

$$-\nabla \cdot (k\nabla T) = Q,$$

which is now an irreducible formulation of the problem.

Coupled problems

Coupled formulations are those applicable to multiple domains and dependent variables which usually (but not always) describe different physical phenomena and in which

- neither domain can be solved separately from the other
- neither set of dependent variables can be explicitly eliminated.

(see Zienkiewicz, 1984)

Examples

- Coupled ODEs
- Coupling via the domain (Brusselator)
- Coupling via the boundary (Schwarz method, FSI)
- Coupling of DAEs with PDEs (high frequency integrated circuits)

A simplified model of a nuclear reactor

- Literature: Strehmel and Weiner, 1984
- $N(t)$ ... average density of neutrons
- $T_b(t)$ ... temperature of fuel
- $C_i(t)$ ... nuclear concentrations.
- system of ODEs:

$$\dot{N}(t) = \frac{1}{l}\left(\gamma(T_B(t) - T_B(0))N(t) + \sum_{i=1}^{6} \beta_i(C_i(t) - N(t))\right),$$

$$\dot{T}_B(t) = \frac{1}{C}(dN(t) - K(T_B(t) - T_M)),$$

$$\dot{C}_i(t) = \lambda_i(N(t) - C_i(t)), \quad i = 1, \ldots, 6.$$

- quantities γ, d, K, T_m, β_i, C, l and $\lambda_i \in [-3, 0)$ are given and independent from t.

Stiff and and non-stiff components in an ODE

- Consider the ODE (see Watkins and Hansonsmith, 1983)

$$\dot{y}_i = i - \frac{1}{10}\sum_{j=1}^{n} y_j - \frac{1}{100} y_{i-1} y_{i+1} + c_i y_i, \quad y_i(0) = 10, \quad i = 1, \ldots, n,$$

- $y_{n+1} = y_1$ and $y_0 = y_n$
- coefficients c_i are chosen in such a way that the ODE has $k < n$ stiff components.
- Example: Let $n = 20$, $c_{20} = -1000$, and $c_i = 1/10$, $i = 1, \ldots, 19$.

Coupling via the domain: The Brusselator

- Let $\Omega = (0,1)^2$ be a domain and $(0, T]$ be some time interval.
- Consider the reaction-diffusion equation (Brusselator with diffusion, see Hairer and Wanner, 1996)

$$\begin{aligned}
\dot{u} &= 1 + u^2 v - 4.4u + \alpha \Delta u, \quad \text{in } (0, T] \times \Omega \\
\dot{v} &= 3.4u - u^2 v + \alpha \Delta v, \quad \text{in } (0, T] \times \Omega \\
\frac{\partial u}{\partial \nu} &= \frac{\partial v}{\partial \nu} = 0, \quad \text{in } (0, T] \times \partial\Omega \\
u(0, x, y) &= 0.5 + y, \quad (x, y) \in \Omega, \\
v(0, x, y) &= 1 + 5x, \quad (x, y) \in \Omega
\end{aligned}$$

- $\alpha = 2 \cdot 10^{-3}$.

The Brusselator

Simulation of a PFBC plant

- model of a Pressurized Fluidized Bed Combustor (PFBC) (see Artlich and Mackens, 1995)
- Let $\Omega \subset \mathbb{R}^2$ be a domain. In practise, Ω is a two dimensional vertical section of the reactor.
- model consists of an enthalpy balance for the temperature T and two mass balances for the oxygen concentration C_{O_2} and the carbon concentration C_C.

$$
\begin{aligned}
-\nabla \cdot (D \nabla C_C) + k_C(T) C_C C_{O_2} &= 0 \quad \text{in } \Omega \\
\frac{\partial}{\partial x_2} C_{O_2} + b_1 k_C(T) C_C C_{O_2} &= 0 \quad \text{in } \Omega \\
-c_1 \nabla \cdot (D \nabla T) - c_2 \nabla \cdot (T D \nabla C_C) & \\
+c_3 \frac{\partial}{\partial x_2} T + c_4 (T - T_{KM}) \xi(x_2) &= c_5 k_C(T) C_C C_{O_2} \quad \text{in } \Omega
\end{aligned}
$$

Simulation of a PFBC plant

- $b_1, c_1, \ldots, c_4$ are some constants
- $D \in \mathbb{R}^{2,2}$ is the so-called diffusion tensor
- $k_C(T)$ is some given function.
- boundary conditions: For the mass balance we use Neumann boundary conditions whereas for the enthalpy balance we use Robin boundary condition, i.e. a combination of Dirichlet and Neumann boundary conditions.
- The oxygen mass balance is an ODE.
- It can be solved explicitly.
- In dependence of the temperature and the carbon concentration and we obtain

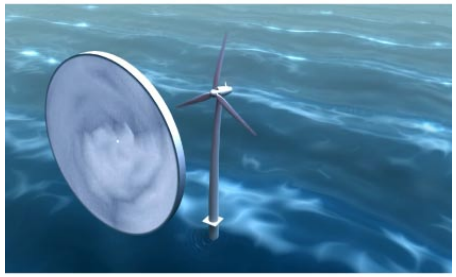
$$C_{O_2}(C_C, T, x) = C_{O_2,0} \exp\left(-b_1 \int_0^{x_2} k_C(T(x_1, s)) C_C(x_1, s) ds\right).$$

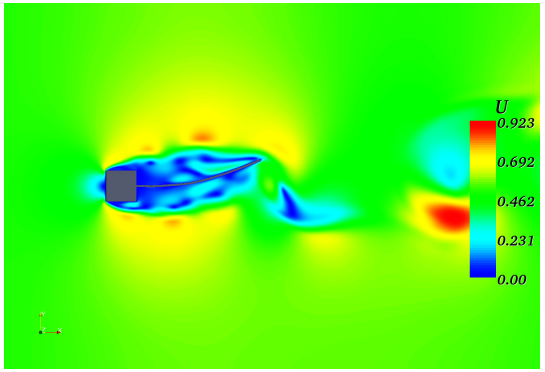
Fluid Structure Interaction

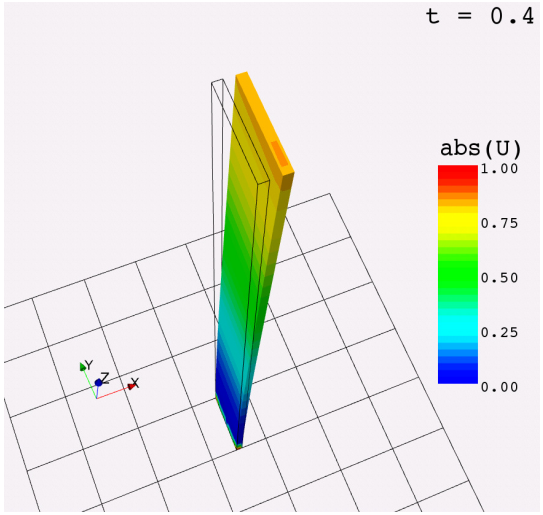
- motion of an incompressible fluid is described with the help of the incompressible Navier-Stokes equations
- In the case of fluid-structure interaction the fluid domain changes w.r.t. to time since the structure is moving in time $\rightarrow$ ALE approach
- The equations of the structure should be formulated in the case of fluid-structure interaction problems in such a way that large deformations of the structure are possible. Therefore we use equations of geometric non-linear elasto-dynamics which are represented in a Lagrangian formulation.
- coupling via the boundary conditions

Examples of FSI problems

- aerodynamics, hydrodynamics
- flutter of the Tacoma suspension bridge, ...
- offshore wind craft turbines, tsunamis, ...





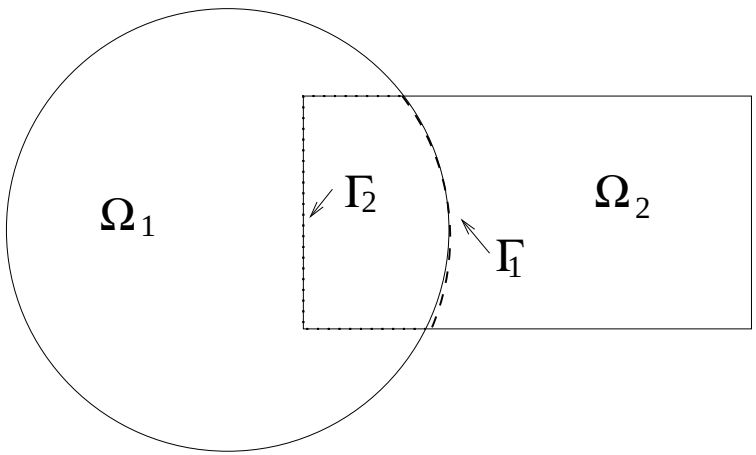


The classical alternating Schwarz method

- Let Ω be a domain. Consider the elliptic equation

$$\begin{cases} -\Delta u &= f, & \text{in } \Omega, \\ u &= g, & \text{on } \partial\Omega \end{cases}.$$

- Assume that $\Omega = \Omega_1 \cup \Omega_2$, where Ω_1 and Ω_2 are subdomains Ω with $\Omega_1 \cap \Omega_2 \neq \emptyset$.

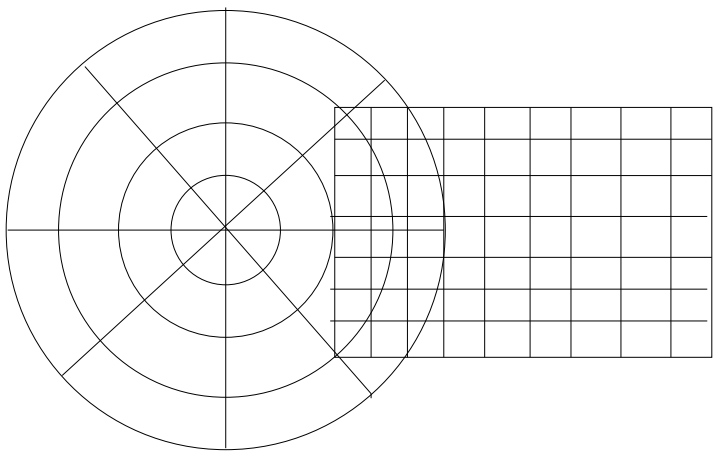


The classical alternating Schwarz method

- By Γ_i we denote the part of the boundary which is inside the domain Ω and is part of $\partial\Omega_i$. To be more precise we have

$$\Gamma_1 = \partial\Omega_1 \cap \Omega_2,$$
$$\Gamma_2 = \partial\Omega_2 \cap \Omega_1.$$

- Next we discretise our problem with Finite Elements and use a non-matching grid



The classical alternating Schwarz method

- First we choose an initial guess $u_2^{(0)}$ for the values on Γ_2.
- Then we solve for $n = 1, 2, 3, \ldots$ the elliptic equation in Ω_1.

$$\begin{cases} -\Delta u_1^{(n)} = f, & \text{in } \Omega_1, \\ u_1^{(n)} = g, & \text{on } \partial\Omega_1 \setminus \Gamma_1, \\ u_1^{(n)} = u_2^{(n-1)}|_{\Gamma_1} & \text{on } \Gamma_2 \end{cases}$$

- then the elliptic problem in in Ω_2

$$\begin{cases} -\Delta u_2^{(n)} = f, & \text{in } \Omega_2, \\ u_2^{(n)} = g, & \text{on } \partial\Omega_2 \setminus \Gamma_2, \\ u_2^{(n)} = u_1^{(n)}|_{\Gamma_2} & \text{on } \Gamma_1 \end{cases} .$$