Space-Time Modeling, Discretization and Solution of Coupled Problems in Incompressible Flow, Fluid-Structure Interaction and Porous Media

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Dec 05, 2023
Hot topics workshop:
Recent Progress in Deterministic and Stochastic Fluid-Structure Interaction, Dec 4-8, 2023
Berkeley, California, United States

Overview

Collaborators in this work

- Jan Philipp Thiele, WIAS, Berlin, Germany (space-time adaptivity Navier-Stokes)
- Julian Roth, Hannover, Germany (space-time model order reduction, Navier-Stokes)
- Hendrik Fischer, Hannover, Germany (space-time model order reduction)
- Thomas Richter, Magdeburg, Germany (space-time multirate schemes)
- Amélie Fau, ENS Paris-Saclay, France (space-time model order reduction)
- Ludovic Chamoin, ENS Paris-Saclay, France (space-time model order reduction)
- Mary F. Wheeler, Austin, USA (porous media discussions)
- Lukas Failer, Siemens, Germany (time adaptivity fluid-structure interaction)
- Philipp Junker, Hannover, Germany (space-time variational material modeling)

Motivation I: Interest

1. Elegant mathematical descriptions and **similar discretizations in space and time (generically implicit, A-stable schemes, numerical stability)** with the typical concepts at hand well-known from finite elements in space
2. Concerning temporal discretization, the integral form allows **natural information on the entire time interval** I_m rather than only at discrete time points t_{m-1} and t_m as for finite differences
3. **Flexible discretization** when using suitable FE libraries, i.e. no special treatment needed for higher temporal order if implemented as a weak form
4. **Higher-order basis functions**; and natural higher order regularity specifically when using splines such as in isogeometric analysis
5. Typical **Galerkin-based best approximation results, interpolation error estimates, and resulting a priori and a posteriori error estimates**
6. **Space-time adaptivity**
7. Global 'viewpoint' allows for (parallel) **space-time solution via multigrid**

Motivation II: Shortcomings

1. Heavy notation
2. More error-prone (in comparison to finite differences; specifically for dG in time) when implemented the first time
3. Higher cost in men/women power to derive schemes (by hand), which may become very technical, including sustainable implementations and documentation towards re-usable research software developments[1]
4. Without good (linear) solvers, costly to solve

[1] Thiele, 2023; `https://github.com/instatdealii/idealii`

Motivation III: Methodology

1. Describe spatial and temporal domains in a common setting
2. Apply similar discretizations, i.e., Galerkin FEM
3. FEM: geometry (elements), simple functions, set of degrees of freedom
4. $cG(s)$: continuous Galerkin, FEM polynomial degree $s \in \mathbb{N}_0$
5. $dG(r)$: discontinuous Galerkin, FEM polynomial degree $r \in \mathbb{N}_0$, more expensive than cG because more degrees of freedom
6. For certain polynomials degrees, relation to well-known finite difference schemes (later more details):
   - $r = 0$: variant of backward Euler, $\theta = 1$
   - $s = 1$: variant of Crank-Nicolson, $\theta = 0.5$

Model problem statement

1. Find $u : \bar{\Omega} \times \bar{I} \to \mathbb{R}^{\tilde{d}}$ such that

$$\begin{aligned} \partial_t u + \mathcal{A}(u) &= f && \text{in } \Omega \times I, \\ u &= u_D && \text{on } \Gamma_D \times I, \\ \mathcal{B}(u) &= g_N && \text{on } \Gamma_N \times I, \\ u &= u^0 && \text{in } \Omega \times \{0\}, \end{aligned} \tag{1}$$

with possibly nonlinear spatial operator $\mathcal{A}$, boundary operator $\mathcal{B}$ and sufficiently regular right-hand side f.

Examples of PDEs and PDE systems

1. **Heat equation:** $\partial_t u - \Delta_x u = f \qquad \text{in } \Omega \times I$
2. **Elastodynamics equation:** $\partial_{tt} u - \nabla_x \cdot \sigma(u) = 0 \qquad \text{in } \Omega \times I$
3. **Biot system in porous media:**

$$\begin{aligned} \partial_t(cp + \alpha(\nabla_x \cdot u)) - \frac{1}{\nu}\nabla_x \cdot (K\nabla_x p) &= 0 \qquad \text{in } \Omega \times I, \\ -\nabla_x \cdot \sigma(u) + \alpha \nabla_x p &= 0 \qquad \text{in } \Omega \times I, \end{aligned} \tag{2}$$

   1. with the isotropic stress tensor $\sigma(u) := \mu(\nabla_x u + (\nabla_x u)^T) + \lambda(\nabla_x \cdot u)I$,
   2. (constrained specific) storage coefficient $c \geq c^* > 0$, may depend on space, i.e., $c(x)$, and is linked to the compressibility $M > 0$,
   3. Biot-Willis constant $\alpha \in [0, 1]$,
   4. the permeability tensor K, fluid's viscosity ν,
   5. Lamé parameters $\lambda, \mu > 0$.

Discretization in time (heat equation) I

1. $dG(r)$ with polynomial degree $r \geq 0$ ($r = 0$ variant of backward Euler)
2. Why dG? Implicit, A-stable, finite element error estimates, 'global' view,
3. Let $\mathcal{T}_k := \{I_m := (t_{m-1}, t_m) \mid 1 \leq m \leq M\}$ be a partitioning of time, i.e. $\bar{I} = [0, T] = \bigcup_{m=1}^{M} \bar{I}_m$.
4. Broken continuous level function spaces

$$\tilde{X}(\mathcal{T}_k, V(\Omega)) := \{v \in L^2(I, L^2(\Omega)) \mid v|_{I_m} \in X(I_m, V(\Omega)) \quad \forall I_m \in \mathcal{T}_k\}$$

5. Due to these discontinuities, we define the limits of f at time t_m from above and from below for a function f as

$$f_m^{\pm} := \lim_{\epsilon \searrow 0} f(t_m \pm \epsilon),$$

6. Jump of the function value of f at time t_m as

$$[f]_m := f_m^+ - f_m^-.$$

Discretization in time (heat equation) II

Formulation (Time-discontinuous variational formulation of the heat equation)

Find $u \in \tilde{X}(\mathcal{T}_k, V(\Omega))$ *such that*

$$\tilde{A}(u)(\varphi) = \tilde{F}(\varphi) \qquad \forall \varphi \in \tilde{X}(\mathcal{T}_k, V(\Omega)),$$

where

$$\tilde{A}(u)(\varphi) := \sum_{m=1}^{M} \int_{I_m} (\partial_t u, \varphi) + (\nabla_x u, \nabla_x \varphi)\, \mathrm{d}t + \sum_{m=1}^{M-1} ([u]_m, \varphi_m^+) + (u_0^+, \varphi_0^+),$$

$$\tilde{F}(\varphi) := ((f, \varphi)) + (u^0, \varphi_0^+).$$

Fully discrete space-time system (heat)

Formulation

Find $u_{kh} \in X_k^{\mathrm{dG}(r)}(\mathcal{T}_k, V_h^s)$ *such that*

$$\tilde{A}(u_{kh})(\varphi_{kh}) = \tilde{F}(\varphi_{kh}) \quad \forall \varphi_{kh} \in X_k^{\mathrm{dG}(r)}(\mathcal{T}_k, V_h^s)$$

where

$$V_h^s := V_h^s(\mathcal{T}_h) := \left\{ v \in C(\bar{\Omega}) \middle| v|_K \in \mathcal{Q}_s(K) \quad \forall K \in \mathcal{T}_h \right\}$$

Recall:

1. Benefit from space-time formulation allows for consistent **space-time a posteriori error estimation**

→ Numerical examples later in this talk.

Fluids and solids in their standard systems

Equations for fluid flows (Navier Stokes) - Eulerian

$$\partial_t v + (v \cdot \nabla v) - \nabla \cdot \sigma(v,p) = 0, \quad \nabla \cdot v = 0, \quad \text{in } \Omega_f \times I, \quad +\text{bc and initial conditions}$$

with Cauchy stress tensor $\sigma(v,p) = -pI + \rho_f \nu_f (\nabla v + \nabla v^T)$.

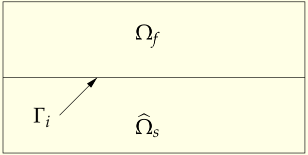
Equations for (nonlinear) elasticity - Lagrangian

$$\partial_t^2 \hat{u} - \hat{\nabla} \cdot (\hat{F}\widehat{\Sigma}(\hat{u})) = 0 \quad \text{in } \widehat{\Omega}_s \times I, \quad +\text{bc and initial conditions}$$

with the stress $\hat{F}\widehat{\Sigma}(\hat{u}) = 2\mu_s \hat{E} + \lambda_s \text{trace}(\hat{E}) I$, the strain $\hat{E} = (\widehat{F}\widehat{F}^T - I)$ and $\widehat{F} = I + \widehat{\nabla}\hat{u}$.

Coupling conditions on $\Gamma_i, \hat{\Gamma}_i$

$$v_f = \hat{v}_s \quad \text{and} \quad \sigma(v,p) n_f = \widehat{F}\widehat{\Sigma}(\hat{u}) \hat{n}_s.$$



Function spaces (I)

1. For the function spaces in the (fixed) reference domains $\widehat{\Omega}, \widehat{\Omega}_f, \widehat{\Omega}_s$, we define spaces for spatial discretization first.
2. First we define
$$\hat{V} := H^1(\widehat{\Omega})^d, \quad \hat{V}^0 := H_0^1(\widehat{\Omega})^d.$$
3. Next, in the fluid domain, we define further:
$$\begin{aligned}
\hat{L}_f &:= L^2(\widehat{\Omega}_f),\\
\hat{L}_f^0 &:= L^2(\widehat{\Omega}_f)/\mathbb{R},\\
\hat{V}_f^0 &:= \{\hat{v}_f \in H^1(\widehat{\Omega}_f)^d : \hat{v}_f = 0 \text{ on } \hat{\Gamma}_{\text{in}} \cup \hat{\Gamma}_D\},\\
\hat{V}_{f,\hat{u}}^0 &:= \{\hat{u}_f \in H^1(\widehat{\Omega}_f)^d : \hat{u}_f = \hat{u}_s \text{ on } \hat{\Gamma}_i, \quad \hat{u}_f = 0 \text{ on } \hat{\Gamma}_{\text{in}} \cup \hat{\Gamma}_D \cup \hat{\Gamma}_{\text{out}}\},\\
\hat{V}_{f,\hat{u},\hat{\Gamma}_i}^0 &:= \{\hat{\psi}_f \in H^1(\widehat{\Omega}_f)^d : \hat{\psi}_f = 0 \text{ on } \hat{\Gamma}_i \cup \hat{\Gamma}_{\text{in}} \cup \hat{\Gamma}_D \cup \hat{\Gamma}_{\text{out}}\}.
\end{aligned}$$
4. In the solid domain, we use
$$\hat{L}_s := L^2(\widehat{\Omega}_s)^d, \quad \hat{V}_s^0 := \{\hat{u}_s \in H^1(\widehat{\Omega}_s)^d : \hat{u}_s = 0 \text{ on } \hat{\Gamma}_D\}.$$

Function spaces (II)

1. As **trial spaces** for a space-time model, we define

$$\widehat{X} = \{U = (\hat{v}, \hat{u}_f, \hat{u}_s, \hat{p}_f) | \; \hat{v} \in L^2(I, \{\hat{v}^D + \hat{V}^0\}), \partial_t \hat{v} \in L^2(I, H(\widehat{\Omega})_d^*), \hat{u}_f \in L^2(I, \{\hat{u}_f^D + \hat{V}^0_{f,\hat{u}}\}),$$
$$\partial_t \hat{u}_f \in L^2(I, H(\widehat{\Omega}_f)_d^*), \hat{u}_s \in L^2(I, \{\hat{u}_s^D + \hat{V}_s^0\}), \partial_t \hat{u}_s \in L^2(I, H(\widehat{\Omega}_s)_d^*), \hat{p}_f \in L^2(I, \hat{L}_f^0)\}$$

2. As **test spaces** for a space-time model, we use

$$\widehat{X}^0 = \{U = (\hat{v}, \hat{u}_f, \hat{u}_s, \hat{p}_f) | \; \hat{v} \in L^2(I, \hat{V}^0), \partial_t \hat{v} \in L^2(I, H(\widehat{\Omega})_d^*), \hat{u}_f \in L^2(I, \hat{V}^0_{f,\hat{u},\hat{\Gamma}_i}),$$
$$\partial_t \hat{u}_f \in L^2(I, H(\widehat{\Omega}_f)_d^*), \hat{u}_s \in L^2(I, \hat{V}_s^0), \partial_t \hat{u}_s \in L^2(I, H(\widehat{\Omega}_s)_d^*), \hat{p}_f \in L^2(I, \hat{L}_f^0)\}$$

ALE: arbitrary Lagrangian-Eulerian

ALE:

1. Use ALE_{fx}: arbitrary Lagrangian Eulerian, where fluid equations (incompressible Navier-Stokes) is transformed to a fixed (arbitrary) reference domain $\widehat{\Omega}$
2. Construct mesh motion model to extend displacements to flow domain $\widehat{\Omega}_f$ in order to realize ALE transformation: $\mathcal{A}(\hat{x}, t) : \widehat{\Omega}_f \to \Omega_f$
3. Deformation gradient $\widehat{F} := \widehat{\nabla} \mathcal{A}(\hat{x}, t)$ and determinant $\hat{J} := det(\widehat{F})$.

Variational-monolithic coupling:

1. Realize coupling conditions in an implicit way on the continuous level:

$$\hat{v}_f = \hat{v}_s \quad \text{on } \hat{\Gamma} \quad \text{(built into function spaces!)}$$

$$\langle \hat{J} \hat{\sigma}_f \widehat{F}^{-T} \hat{n}_f, \varphi \rangle_{\hat{\Gamma}} + \langle \widehat{F} \widehat{\Sigma} \hat{n}_s, \varphi \rangle_{\hat{\Gamma}} = 0 \quad \forall \varphi \in V$$

2. Geometric condition due to ALE:

$$\hat{u}_f = \hat{u}_s \quad \text{on } \hat{\Gamma} \quad \text{(built into function spaces!)}$$

A space-time fluid-structure interaction model

Proposition (Variational-monolithic space-time ALE-FSI in $\widehat{\Omega}$)

Find a global vector-valued velocity, vector-valued displacements and a scalar-valued fluid pressure, i.e., $\hat{U} := (\hat{v}, \hat{u}_f, \hat{u}_s, \hat{p}_f) \in \widehat{X}$ *such that*

$$\text{Fluid/solid momentum} \begin{cases} \int_I \Big((\hat{J}\hat{\varrho}_f \partial_t \hat{v}, \hat{\psi}^v)_{\widehat{\Omega}_f} + (\hat{\varrho}_f \hat{J}(\widehat{F}^{-1}(\hat{v}-\hat{w})\cdot\widehat{\nabla})\hat{v}), \hat{\psi}^v)_{\widehat{\Omega}_f} + (\hat{J}\hat{\sigma}_f \widehat{F}^{-T}, \widehat{\nabla}\hat{\psi}^v)_{\widehat{\Omega}_f} \\ -\langle \hat{\varrho}_f \nu_f \hat{J}(\widehat{F}^{-T}\widehat{\nabla}\hat{v}^T \hat{n}_f)\widehat{F}^{-T}, \hat{\psi}^v\rangle_{\hat{\Gamma}_{out}} + (\hat{\varrho}_s \partial_t \hat{v}, \hat{\psi}^v)_{\widehat{\Omega}_s} + (\widehat{F}\widehat{\Sigma}, \widehat{\nabla}\hat{\psi}^v)_{\widehat{\Omega}_s} \Big)\, dt \\ +(\hat{J}\hat{\varrho}_f(\hat{v}(0)-\hat{v}_0), \hat{\psi}^v(0))_{\widehat{\Omega}_f} + \hat{\varrho}_s(\hat{v}(0)-\hat{v}_0, \hat{\psi}^v(0))_{\widehat{\Omega}_s} = 0 \end{cases}$$

$$\text{Fluid mesh motion} \left\{ \int_I (\hat{\sigma}_{mesh}, \widehat{\nabla}\hat{\psi}^u_f)_{\widehat{\Omega}_f}\, dt \quad = 0 \right.$$

$$\text{Solid momentum, 2nd eq.} \left\{ \int_I \Big(\hat{\varrho}_s (\partial_t \hat{u}_s - \hat{v}|_{\widehat{\Omega}_s}, \hat{\psi}^u_s)_{\widehat{\Omega}_s} \Big)\, dt + \hat{\varrho}_s(\hat{u}_s(0) - \hat{u}_{s,0}, \hat{\psi}^u_s(0)) \quad = 0 \right.$$

$$\text{Fluid mass conservation} \left\{ \int_I \Big((\widehat{div}\,(\hat{J}\widehat{F}^{-1}\hat{v}), \hat{\psi}^p_f)_{\widehat{\Omega}_f} \Big)\, dt \quad = 0 \right.$$

for all $\hat{\Psi} = (\hat{\psi}^v, \hat{\psi}^u_f, \hat{\psi}^u_s, \hat{\psi}^p_f) \in \widehat{X}^0$. *In compact form, the above problem reads: Find* $\hat{U} \in \widehat{X}$ *such that*

$$\hat{A}(\hat{U})(\hat{\Psi}) = 0 \quad \forall \hat{\Psi} \in \widehat{X}^0$$

where the FSI equations are combined in the semi-linear form $\hat{A}(\hat{U})(\hat{\Psi})$.

Equivalent formulation - start for space-time discretization

Proposition

Find $\hat{U} := (\hat{v}, \hat{u}_f, \hat{u}_s, \hat{p}_f) \in \widehat{X}$ *such that*

$$
\begin{aligned}
&\int_I (\hat{J}\hat{\varrho}_f \partial_t \hat{v}, \hat{\psi}^v)_{\widehat{\Omega}_f}\, dt + \int_I (\hat{\varrho}_s \partial_t \hat{v}, \hat{\psi}^v)_{\widehat{\Omega}_s}\, dt + \int_I (\hat{\varrho}_s \partial_t \hat{u}_s, \hat{\psi}^u_s)_{\widehat{\Omega}_s}\, dt \\
&+ \hat{A}_{notimeder}(\hat{U})(\hat{\Psi}) \\
&+ (\hat{J}\hat{\varrho}_f(\hat{v}(0) - \hat{v}_0), \hat{\psi}^v(0))_{\widehat{\Omega}_f} + \hat{\varrho}_s(\hat{v}(0) - \hat{v}_0, \hat{\psi}^v(0))_{\widehat{\Omega}_s} + \hat{\varrho}_s(\hat{u}_s(0) - \hat{u}_{s,0}, \hat{\psi}^u_s(0))
\end{aligned}
$$

where $\hat{A}_{notimeder}(\hat{U})(\hat{\Psi})$ *(here notimeder stands for 'no time derivatives') contains all terms from the previous proposition that are not initial conditions and contain no time derivatives.*

Galerkin in time discretization (I)

1. Let
$$\bar{I} = \{0\} \cup I_1 \cup \ldots \cup I_M$$
2. Half-open subintervals $I_m := (t_{m-1}, t_m]$ and the time step size, i.e., temporal discretization parameter, $k_m := t_m - t_{m-1}$ for $m = 1, \ldots, M$
3. The time points (i.e., temporal edges in the FEM context) are
$$0 = t_0 < \ldots < t_m < \ldots t_M = T.$$
4. Let $r \in \mathbb{N}_0$ be the temporal polynomial degree. We define the semi-discrete space
$$\tilde{X}_k^r := \{\hat{U}_k \in \widehat{X} |\ U_k|_{I_m} \in P_r(I_m, \widehat{X}),\ \hat{U}_k(0) \in L^2(\widehat{\Omega})\},$$
where k stands for the temporal discretization parameter
5. For setting up the $dG(r)$ method, we need to account for the jumps and introduce further for $\hat{U}_k \in \tilde{X}_k^r$:
$$\hat{U}_{k,m}^{\pm} := \lim_{s \to 0} \hat{U}_k(t_m \pm s), \quad [\hat{U}_k]_m := \hat{U}_{k,m}^{+} - \hat{U}_{k,m}^{-}.$$

Galerkin in time discretization (II)

Proposition ($dG(r)$ semi-discretization of FSI)

Find $U_k \in \tilde{X}_k^r$ *such that*

$$\sum_{m=1}^{M} \int_{I_m} (\hat{J}\hat{\varrho}_f \partial_t \hat{v}_k, \hat{\psi}^v)_{\widehat{\Omega}_f} + (\hat{\varrho}_s \partial_t \hat{v}_k, \hat{\psi}^v)_{\widehat{\Omega}_s} + (\hat{\varrho}_s \partial_t \hat{u}_{k,s}, \hat{\psi}_s^u)_{\widehat{\Omega}_s} \, dt$$
$$+ \hat{A}_{notimeder}(\hat{U}_k)(\hat{\Psi})$$
$$+ \sum_{m=0}^{M-1} (\hat{J}\hat{\varrho}_f [\hat{v}_k]_m, \hat{\psi}_m^{v,+})_{\widehat{\Omega}_f} + (\hat{\varrho}_s [\hat{v}_k]_m, \hat{\psi}_m^{v,+})_{\widehat{\Omega}_s} + (\hat{\varrho}_s [\hat{u}_k]_m, \hat{\psi}_m^{u,+})_{\widehat{\Omega}_s}$$
$$+ (\hat{J}\hat{\varrho}_f \hat{v}_{k,0}^-, \hat{\psi}_0^{v,-})_{\widehat{\Omega}_f} + (\hat{\varrho}_s \hat{v}_{k,0}^-, \hat{\psi}_0^{v,-})_{\widehat{\Omega}_s} + (\hat{\varrho}_s \hat{u}_{k,0}^-, \hat{\psi}_0^{u,-})_{\widehat{\Omega}_s}$$
$$= (\hat{J}\hat{\varrho}_f \hat{v}_0, \hat{\psi}_0^{v,-})_{\widehat{\Omega}_f} + (\hat{\varrho}_s \hat{v}_0, \hat{\psi}_0^{v,-})_{\widehat{\Omega}_s} + (\hat{\varrho}_s \hat{u}_0, \hat{\psi}_0^{u,-})_{\widehat{\Omega}_s}$$

for all $\hat{\Psi} \in \tilde{X}_k^r$ *and where* $\hat{A}_{notimeder}(\hat{U})(\hat{\Psi})$ *is defined as before.*

Galerkin in time discretization (III)

1. **Temporal discretization**: Due to the dG test functions, the schemes will decouple to each time interval I_m and known time-stepping schemes are obtained:
   - $dG(0)$ vs. backward Euler, $\theta = 1$: For $r = 0$, we deal with the $dG(0)$ scheme, first order in time, which is a variant of the backward Euler scheme (see below) for $\theta = 1$.
   - $cG(1)$ vs. Crank-Nicolson, $\theta = 0.5$: Using $cG(1)$ trial functions and $dG(0)$ test functions, yields a scheme similar to the Crank-Nicolson scheme, which is actually used in computations with dynamics since $dG(0)$ is strongly A-stable and will damp physical oscillations.
2. **Spatial discretization**: based on classical continuous cG finite elements ; here at t_m: $(\hat{v}, \hat{u}, \hat{p}_f) \in Q_c^2 \times Q_2^2 \times Q_c^1$ (Taylor-Hood due to LBB for the flow part)

Goal functional and optimization problem

1. Let a **goal functional**[2] $J : \tilde{X}(\mathcal{T}_k, V(\Omega)) \to \mathbb{R}$ of the form

$$J(u) = \int_0^T J_1(u(t))\,\mathrm{d}t + J_2(u(T)), \tag{3}$$

be given, which represents some physical quantity of interest (QoI).

2. Here, T denotes the end time as before.
3. **Objective:** reduce the difference between the quantity of interest of some (unknown) solution and some numerical approximation:

$$\min J(u) - J(\tilde{u}), \quad \text{subject to the given PDE(s) } A(\cdot)(\cdot) = F(\cdot) \tag{4}$$

4. $A(\cdot)(\cdot)$: space-time weak form, e.g., heat, porous media, Navier-Sokes, FSI
5. $F(\cdot)$: given right hand side data, e.g., forces, boundary data, initial data

[2] Becker, Rannacher, 1996/2001; Bangerth, Rannacher, 2003; Schmich, Vexler, 2008

Overall interest and specifications

Overall interest in a posteriori error estimation:

⇒ A **robust, time-adaptive, procedure** to calculate functionals of interest with **sufficient accuracy** allowing for the **automated adjustment of time step sizes** where necessary.

⇒ A (global) **error estimator and not only an error indicator**. Therefore, we obtain a guess η about the unknown true error $J(u) - J(\tilde{u})$. Consequently, we know to which accuracy we have computed a certain physical quantity without knowing its exact (analytical) value $J(u)$.

Specific interest in this talk:

1. full discretization estimates for heat, Navier-Stokes, i.e.,

$$\min J(u) - J(u_{kh})$$

2. temporal error control for FSI, i.e.,

$$\min J(u) - J(u_k)$$

3. model error control for heat, porous media (Biot system), i.e.,

$$\min J(u^{fine}) - J(u^{course})$$

Lagrangian and optimality system

1. Formulate Lagrangian, compute stationary points, yielding primal and adjoint solutions
2. Lagrangian:

$$\mathcal{L}_\square : X_k^{\mathrm{dG}(0)}(\mathcal{T}_k, V_h^\square) \times X_k^{\mathrm{dG}(0)}(\mathcal{T}_k, V_h^\square) \to \mathbb{R},$$
$$(U^\square, Z^\square) \mapsto J(U^\square) - A(U^\square)(Z^\square) + F(Z^\square)$$

   with $\square \in \{\text{exact}, \text{discrete}\}$.

3. Optimality system:

$$\mathcal{L}'_\square = 0$$

4. Primal problem:

$$\mathcal{L}'_{\square,Z}(U^\square, Z^\square)(\delta Z^\square) = -A(U^\square)(\delta Z^\square) + F(\delta Z^\square) = 0 \qquad \forall \delta Z^\square \in X_k^{\mathrm{dG}(0)}, \quad \square \in \{\text{exact}, \text{discrete}\}$$

5. Adjoint problem:

$$\mathcal{L}'_{\square,U}(U^\square, Z^\square)(\delta U^\square) = J'_U(U^\square)(\delta U^\square) - A(\delta U^\square)(Z^\square) = 0$$
$$\forall \delta U^\square \in X_k^{\mathrm{dG}(0)}(\mathcal{T}_k, V_h^\square), \quad \square \in \{\text{exact}, \text{discrete}\}.$$

Error representation and error estimator

1. **Adjoint problem** (heat), linear (always!), primal solution enters, running backwards in time: Find $z \in X_k^{\mathrm{dG}(r)}(\mathcal{T}_k, V_h)$ such that

$$\sum_{m=1}^{M} \int_{I_m} (\delta u, -\partial_t z) + (\nabla_x \delta u, \nabla_x z)\, \mathrm{d}t - \sum_{m=1}^{M-1} (\delta u_m^-, [z]_m) + (\delta u_M^-, z_M^-) = J_u'(u)(\delta u).$$

2. It holds (based on Becker, Rannacher, 2001):

$$J(u) - J(\tilde{u}) = -\tilde{A}(\tilde{u})(z - i_h z) + \tilde{F}(z - i_h z) + R^{(2)}.$$

3. **A posteriori error estimator**

$$\eta := -\tilde{A}(\tilde{u})(z - i_h z) + \tilde{F}(z - i_h z).$$

4. Quality measure by **effectivity index**:

$$I_{eff} := \left| \frac{\eta}{J(u) - J(\tilde{u})} \right|$$

5. Ideally $I_{eff} \sim 1$ (rigorous reliability and efficiency for discretization errors Endtmayer, Langer, Wick; SISC, 2020; key tool in the proof: saturation assumption on goal functional)

Failer/Wick (JCP, 2018): Adaptive time step control

1. $J(U)$ can be a point value, deformation, drag, lift, temperature evaluation etc. but not necessarily in the entire domain!

Proposition (Goal-oriented error estimator with primal part)

Let $\hat{U} \in X$ the unknown, exact, solution and $\hat{U}_{kh} \in X_{kh}^{r,s}$ the space-time fully discrete solution. Furthermore, let $\hat{Z}$ the exact adjoint solution and $\hat{Z}_{kh} \in X_{kh}^{r,s}$ the discrete adjoint. It holds the a posteriori error estimate

$$J(\hat{U}) - J(\hat{U}_{kh}) = \frac{1}{2}\rho(\hat{U}_{kh})(\hat{Z} - \hat{Z}_{kh}) + R^{(2)},$$

where

$$\rho(\hat{U}_{kh})(\hat{Z} - \hat{Z}_{kh}) := -A(\hat{U}_{kh})(\hat{Z} - \hat{Z}_{kh})$$

where $A(\hat{U}_{kh})(\hat{Z} - \hat{Z}_{kh})$ is our space-time FSI formulation.

2. Idea of the proof: take Lagrangian, use trapezoidal rule, insert continuous and disdrete problem statements
3. Difficulty: $\hat{Z}$ still unknown; use higher-order approximation $\hat{Z}^{high}$.

Adaptive time step control: error estimator

- We want to use global error estimator for steering algorithms during computations

Proposition

The localized error estimator readsfor M time intervals (only temporal part U_k!)

$$J(\hat{U}) - J(\hat{U}_k) \approx \eta := \sum_{m=1}^{M} \eta_m = \frac{1}{2}\left(-A(\hat{U}_k, \hat{Z}_k^{(2)} - \hat{Z}_k^{(1)})\right) + \tilde{R}^{(2)}$$

- Idea of the proof: follows naturally from the dG properties or alternatively from a partition-of-unity (see next slide)
- As just before, check by computing the effectivity index (now w.r.t. temporal error):

$$I_{eff} = \frac{\eta}{J(\hat{U}) - J(\hat{U}_k)}$$

where η is a computable error estimator and $J(\hat{U}) - J(\hat{U}_k)$ is the true error for some known 'exact' solution $\hat{U}$

Full space-time error control: partition-of-unity localication [3]

1. Now: space-time localization techniques to localize error contributions in time as well as space:

$$\eta = \sum_{m=1}^{M} \sum_{n=1}^{N} \eta_{mn},$$

where M number of temporal elements and N number of spatial elements.

Proposition (PU)

Let V_{PU} a discrete finite element space. For a function $\chi \in V_{PU}$, it holds

$$\sum_{m=1}^{M} \sum_{n=1}^{N} \chi_{mn} \equiv 1. \tag{5}$$

Proof: Follows immediately from the properties of the finite element functions.

[3] Thiele, Wick; J. Sci. Comput. 2023; in revised review

Full space-time error control: heat equation

Proposition (Primal joint error estimator for the heat equation)

For the space-time formulation of the heat equation, we have the following a posteriori joint error estimator with partition-of-unity localization:

$$|J(u) - J(u_{kh})| \leq |\eta_{joint}| := \left|\sum_m \eta_{kh}^m\right|, \qquad \text{with } \eta_{kh}^m := \sum_{i \in \mathcal{T}_h^m} \eta_{kh}^{i,m}, \tag{6}$$

with the error indicators

$$\begin{aligned} \eta_{kh}^{i,m} := & \int_{I_m} (f, (\tilde{z} - z_{kh})\chi_{i,m})_H \, \mathrm{d}t - \int_{I_m} (\nabla u_{kh}, \nabla((\tilde{z} - z_{kh})\chi_{i,m}))_H \, \mathrm{d}t \\ & - \int_{I_m} (\partial_t u_{kh}, (\tilde{z} - z_{kh})\chi_{i,m})_H \, \mathrm{d}t - ([u_{kh}]_{m-1}, (\tilde{z}^+(t_{m-1}) - z_{kh}^+(t_{m-1}))\chi_{i,m})_H. \end{aligned} \tag{7}$$

Proof: Thiele, Wick, 2023: use main error theorem, use space-time weak forms, plug-in PU, seperate temporal and spatial error contributions, apply triangle inequality.

Motivation: Reduced order modeling

1. Another method to significantly reduce computational cost, when problem must be run numerous times (100x, 1000x, ...)

→ Parameter estimation (Bayesian inversion), optimal control, optimal experimental design

2. Complementary to parallel computing and adaptivity
3. Idea[4]:
   - Compute full-order model (everything we had before),
   - select snapshots based on SVD (singular value decomposition), here POD (proper orthogonal decomposition),
   - construct reduced (finite element) basis
4. Our contribution: let goal-oriented error estimator decide on enrichment of reduced basis in order to obtain a desired accuracy in $J(u_{kh})$

---

[4] e.g., P. Benner and A. Cohen and M. Ohlberger and K. Willcox; Model Reduction and Approximation: Theory and Algorithms, SIAM, 2015

Goal functional and optimization problem

1. Let a **time-distributed goal functional** $J : \tilde{X}(\mathcal{T}_k, V(\Omega)) \to \mathbb{R}$ of the form

$$J(u) = \int_0^T J_1(u(t))\, \mathrm{d}t, \tag{8}$$

be given, which represents some physical quantity of interest (QoI).

2. Here, T denotes the end time as before.

3. **Objective:** reduce the difference between the quantity of interest of a fine solution u^{fine} and a coarse solution u^{coarse}, i.e.,

$$\min J(u^{\text{fine}}) - J(u^{\text{coarse}}), \quad \text{subject to the given PDE(s) } \tilde{A}(\cdot)(\cdot) = \tilde{F}(\cdot) \tag{9}$$

4. **Enrichment[5] of the reduced basis depending on the temporal evolution of the goal functional[6]**

[5] Fischer, Roth et al. 2023a, 2023b on arXiv

[6] For coarsening, see Meyer/Matthies; Comp. Mech. 2003

Tensor-product space-time POD-ROM

1. General spatial FEM space V_h is replaced by a problem-specific low-dimensional space $V_N = \text{span}\{\varphi_N^1, \ldots, \varphi_N^N\}$
2. Use (incremental) POD.
3. Variational formulation:

Formulation

Find $u_N \in \tilde{X}(\mathcal{T}_k, V_N)$ such that

$$\tilde{A}(u_N)(\varphi) = \tilde{F}(\varphi) \qquad \forall \varphi \in \tilde{X}(\mathcal{T}_k, V_N).$$

Slabwise assemply I (FOM tensor-product space-time modeling)

1. Define (time) slabs:

$$S_l^n := \Omega \times \left(\bigcup_{m=l}^{n} I_m \right),$$

   where $1 \leq l \leq n \leq M$

2. Space-time basis by tensor-product ansatz $\varphi_{kh}(t,x) = \varphi_k(t)\varphi_h(x)$

3. Full-order solution on slab S_l^n is given by

$$\begin{pmatrix} A & & & & 0 \\ B & A & & & \\ & B & A & & \\ & & \ddots & \ddots & \\ 0 & & & B & A \end{pmatrix} \begin{pmatrix} U_l \\ U_{l+1} \\ U_{l+2} \\ \vdots \\ U_n \end{pmatrix} = \begin{pmatrix} F_l - BU_{l-1} \\ F_{l+1} \\ F_{l+2} \\ \vdots \\ F_n \end{pmatrix} \tag{10}$$

4. Idea to formulate 'big' space-time system matrix inspired by Gander, Neumüller, SISC, 2016, who developed space-time multigrid solvers.

Slabwise assemply II (ROM)

1. The reduced basis matrix can be formed by the concatenation of the reduced basis vectors, viz.

$$Z_N = \begin{bmatrix} \varphi_N^1 & \dots & \varphi_N^N \end{bmatrix} \in \mathbb{R}^{\#\text{DoFs}(\mathcal{T}_h)\times N}. \tag{11}$$

2. Subsequently, the slabwise discretization for the space-time slab S_l^n with $n-l+1$ time intervals is obtained in analogy to the full-order model

3. We arrive at

$$\begin{pmatrix} A_N & & & & 0 \\ B_N & A_N & & & \\ & B_N & A_N & & \\ & & \ddots & \ddots & \\ 0 & & & B_N & A_N \end{pmatrix} \begin{pmatrix} U_{N_l} \\ U_{N_{l+1}} \\ U_{N_{l+2}} \\ \vdots \\ U_{N_n} \end{pmatrix} = \begin{pmatrix} F_{N_l} - B_N U_{N_{l-1}} \\ F_{N_{l+1}} \\ F_{N_{l+2}} \\ \vdots \\ F_{N_n} \end{pmatrix} \tag{12}$$

4. In brevity $A_N U_{N,S_l^n} = F_{N,S_l^n}$

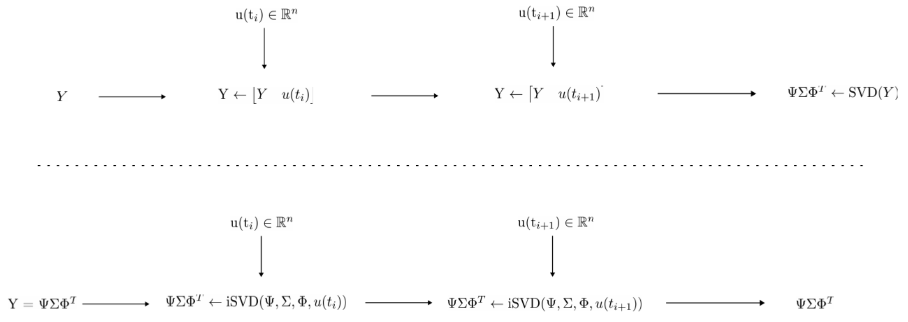
5. Reduced components

$$A_N = Z_N^T A Z_N, \quad B_N = Z_N^T B Z_N, \quad F_{N_i} = Z_N^T F_i, \quad l \le i \le n. \tag{13a}$$

Incremental POD

1. Update already existing truncated SVD
2. According to modifications in the snapshot matrix
3. Append additional snapshots to the initial snapshot matrix

→ Additive rank-b modification of the SVD[7]



[7] M. Brand; 2006 and 2006; Kühl, Fischer, Hinze, Rung; 2023

MORe DWR algorithm I

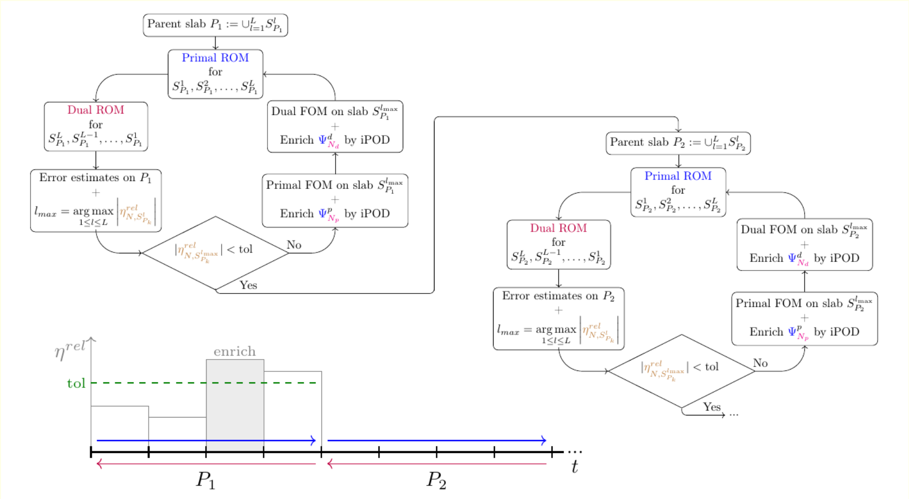
Algorithm 2 MORe DWR algorithm

Input: Initial condition $U_0 := U(t_0)$, primal and dual reduced basis matrices $\Psi^p_{N_p}$ and $\Psi^d_{N_d}$, energy threshold $\varepsilon \in [0,1]$ and error tolerance tol > 0.

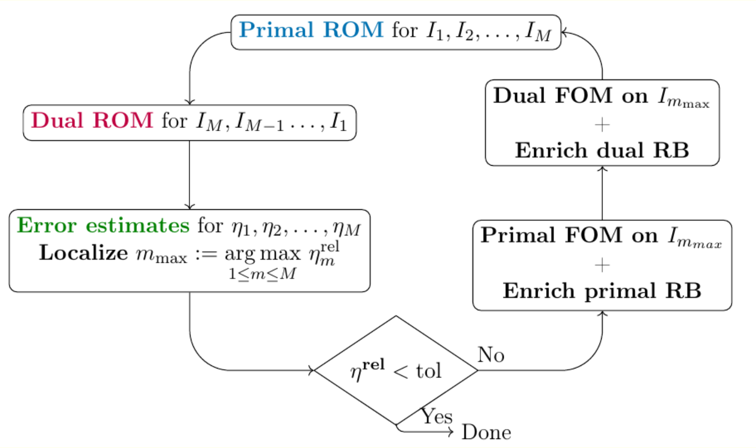
Output: Primal and dual reduced basis matrices $\Psi^p_{N_p}$ and $\Psi^d_{N_d}$ and reduced primal solutions U_{N_p, I_m} for all $1 \leq m \leq M$.

```
for k = 1, 2, ..., K do                                                   ▷ Loop over parent slabs
    while η_max > tol do
        for l = 1, 2, ..., L do                                           ▷ Primal ROM on k-th parent slab
            Solve reduced primal system (8): A_{N_p} U_{N_p, S^l_{P_k}} = F_{N_p, S^l_{P_k}}
        for l = L, L − 1, ..., 1 do                                       ▷ Dual ROM on k-th parent slab
            Solve reduced dual system (25): A'_{N_d} Z_{N_d, S^l_{P_k}} = J_{N_d, S^l_{P_k}}
        for l = 1, 2, ..., L do                                           ▷ Error estimates on k-th parent slab
            Compute error estimate: η^{rel}_{N, S^l_{P_k}} (U_{N_p, S^l_{P_k}}, Z_{N_d, S^l_{P_k}})
        η_max = max_{1≤l≤L} |η^{rel}_{N, S^l_{P_k}}|
        if η_max > tol then
            l_max = arg max_{1≤l≤L} |η^{rel}_{N, S^l_{P_k}}|
            Solve primal full-order system (3): A U_{S^{l_max}_{P_k}} = F_{S^{l_max}_{P_k}}
            Update primal reduced basis: Ψ^p_{N_p} = iPOD(Ψ^p_{N_p}, Σ_{N_p}, [U_{S^{l_max}_{P_k}}(t_1), ..., U_{S^{l_max}_{P_k}}(t_{r+1})], ε)
            Solve dual full-order system (24): A' Z_{S^{l_max}_{P_k}} = J_{S^{l_max}_{P_k}}
            Update dual reduced basis: Ψ^d_{N_d} = iPOD(Ψ^d_{N_d}, Σ_{N_d}, [Z_{S^{l_max}_{P_k}}(t_1), ..., Z_{S^{l_max}_{P_k}}(t_{r+1})], ε)
            Update reduced system components and error estimator w.r.t (9)

——— Validation loop ———                                                   ▷ This is an optional validation of the model.

for k = 1, 2, ..., K do                                                   ▷ Primal ROM on whole temporal domain
    for l = 1, 2, ..., L do
        Solve primal reduced system: A_{N_p} U_{N_p, S^l_{P_k}} = F_{N_p, S^l_{P_k}}
for k = K, K − 1, ..., 1 do                                               ▷ Dual ROM on whole temporal domain
    for l = L, L − 1, ..., 1 do
        Solve dual reduced system: A'_{N_d} Z_{N_d, S^l_{P_k}} = J_{N_d, S^l_{P_k}}
for k = 1, 2, ..., K do                                                   ▷ Error estimates on whole temporal domain
    for l = 1, 2, ..., L do
        Compute slab estimate: η^{rel}_{N, S^l_{P_k}} (U_{N_p, S^l_{P_k}}, Z_{N_d, S^l_{P_k}})
```

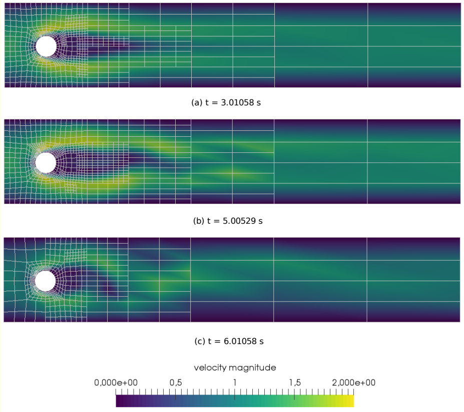
MORe DWR algorithm I: two consecutive parent slabs



MORe DWR algorithm II



Schäfer, Turek, 2D-3 benchmark in incompressible flow around a cylinder: spatial and temporal refinement



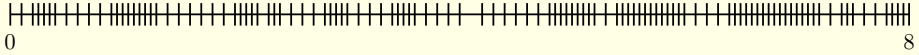


Figure: Left: spatial refinement. Right: temporal refinement.

Drag and lift evaluations

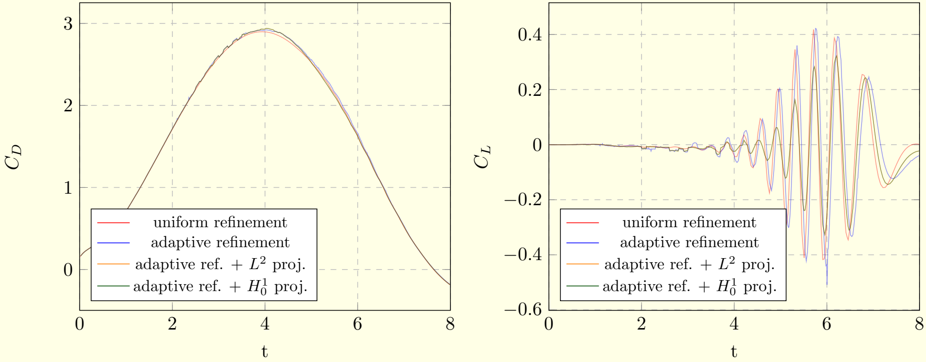


Figure: Left: drag evaluation. Right: lift evaluation. Little oscillations are due to dynamic mesh refinement with non-robustness of pressure (Besier, Wollner, 2011) and treated with additional projections.

Performance studies

#DoF(primal)	#DoF(adjoint)	M	η_k	η_h	η	$J(U)-J(U_{kh})$	I_{eff}
17,800	96,600	20	$-9.3298 \cdot 10^{-6}$	$3.8542 \cdot 10^{-1}$	$3.8541 \cdot 10^{-1}$	$5.5752 \cdot 10^{-1}$	0.69
63,454	350,922	36	$-1.4015 \cdot 10^{-7}$	$2.6505 \cdot 10^{-1}$	$2.6505 \cdot 10^{-1}$	$2.6642 \cdot 10^{-1}$	0.99
230,032	1,294,482	64	$8.9182 \cdot 10^{-4}$	$-1.2571 \cdot 10^{-2}$	$1.1679 \cdot 10^{-2}$	$1.2586 \cdot 10^{-1}$	0.09
828,744	4,706,883	113	$-1.1615 \cdot 10^{-1}$	$7.6888 \cdot 10^{-2}$	$3.9265 \cdot 10^{-2}$	$2.5449 \cdot 10^{-2}$	1.54
3,004,686	17,251,722	199	$4.3194 \cdot 10^{-3}$	$1.9094 \cdot 10^{-2}$	$2.3414 \cdot 10^{-2}$	$1.9674 \cdot 10^{-2}$	1.19

Table 12: Adaptive refinement of mixed order on dynamic meshes for Navier–Stokes 2D-3 with divergence-free L^2 projection.

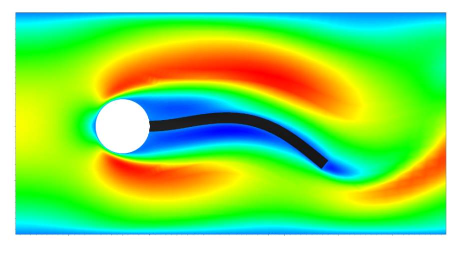
#DoF(primal)	#DoF(adjoint)	M	η_k	η_h	η	$J(U)-J(U_{kh})$	I_{eff}
17,800	96,600	20	$-9.1676 \cdot 10^{-6}$	$3.8548 \cdot 10^{-1}$	$3.8547 \cdot 10^{-1}$	$5.5768 \cdot 10^{-1}$	0.69
63,690	352,278	36	$1.4710 \cdot 10^{-6}$	$2.6493 \cdot 10^{-1}$	$2.6493 \cdot 10^{-1}$	$2.6667 \cdot 10^{-1}$	0.99
234,878	1,322,502	64	$7.5795 \cdot 10^{-4}$	$-4.4232 \cdot 10^{-3}$	$3.6653 \cdot 10^{-3}$	$1.2633 \cdot 10^{-1}$	0.03
834,710	4,741,881	113	$-2.3546 \cdot 10^{-3}$	$-7.6972 \cdot 10^{-2}$	$7.9327 \cdot 10^{-2}$	$1.9651 \cdot 10^{-2}$	4.04
3,044,708	17,485,449	199	$3.0977 \cdot 10^{-3}$	$9.0900 \cdot 10^{-3}$	$1.2188 \cdot 10^{-2}$	$6.5227 \cdot 10^{-3}$	1.87

Table 13: Adaptive refinement of mixed order on dynamic meshes for Navier–Stokes 2D-3 with divergence-free H_0^1 projection.

Figure: Performance of adaptive refinements in terms of error reductions, estimator behavior and effectivity indices. Results from Roth, Thiele, Köcher, Wick, CMAM, 2023.

Adaptive time step control in FSI: computations [8]

- Code verification: test code with the help of a manufactured solution (rarely possible!) or with a computationally-obtained referenced solution $\hat{U}_{ref} =: \hat{U}$.
- In this work: up to 1 444 384 **time steps** are used to obtain a numerically-obtained U; wall clock time > 31 **days** (serial computation in time and space)
- Numerical test: **FSI-2 benchmark (Hron/Turek, 2006)**
- Elastic beam immersed in a fluid (Navier-Stokes)



[8] Failer, Wick, JCP, 2018.

Adaptive time step control in FSI: results

- Goal functional: $J(\hat{U}) := \int_I \int_{\hat{\Gamma}_i \cup \hat{\Gamma}_{cyl}} -\hat{\sigma}_f \hat{n} e_1 \, d\hat{x} \, dt$
- Time step refinements after selected refinement rounds:

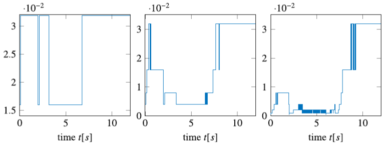


Fig. 8. Section 6.3.2: time step size k_m plotted over time t after 1 (left), 3 (middle) and 6 (right) adaptive refinements for the FSI-3 benchmark using the DWR time discretization error estimator with respect to $\mathcal{J}_3(U)$.

- Computation of effectivity indices:

M	1128	1482	2322	4176	5844	10518
$J(\hat{U}_{kh})$	$2.896 \cdot 10^3$	$3.048 \cdot 10^3$	$3.117 \cdot 10^3$	$3.130 \cdot 10^3$	$3.129 \cdot 10^3$	$3.129 \cdot 10^3$
$J(\hat{U}_{kh}) - J(\hat{U}_{ref})$	$2.3 \cdot 10^2$	$8.1 \cdot 10^1$	$1.2 \cdot 10^1$	$7.0 \cdot 10^{-1}$	$7.4 \cdot 10^{-1}$	$4.6 \cdot 10^{-1}$
I_{eff}	1.01	1.01	1.00	0.97	1.02	1.04

Table: Effectivity indices I_{eff} for DWR time discretization error estimator with respect to $J(U)$ on adaptively refined time grids.

2+1D heat equation [9]

1. Spatial domain $\Omega = (0,1)^2$ and temporal domain $I = (0,10)$
2. Moving heat source of oscillating temperature that rotates around the midpoint of the spatial domain Ω
3. For this, we use the right-hand side function

$$f(t,x) := \begin{cases} \sin(4\pi t) & \text{if } (x_1 - p_1)^2 + (x_2 - p_2)^2 < r^2, \\ 0 & \text{else,} \end{cases}$$

   with $x = (x_1, x_2)$, midpoint $p = (p_1, p_2) = (\frac{1}{2} + \frac{1}{4}\cos(2\pi t), \frac{1}{2} + \frac{1}{4}\sin(2\pi t))$ and radius of the trajectory $r = 0.125$.

4. Goal functional (distributed in time):

$$J(u) := \frac{1}{10}\int_0^{10}\int_\Omega u(t,x)^2 \, dx \, dt$$

[9] Fischer, Roth, Wick, Chamoin, Fau, 2023, arXiv.

FOM solution

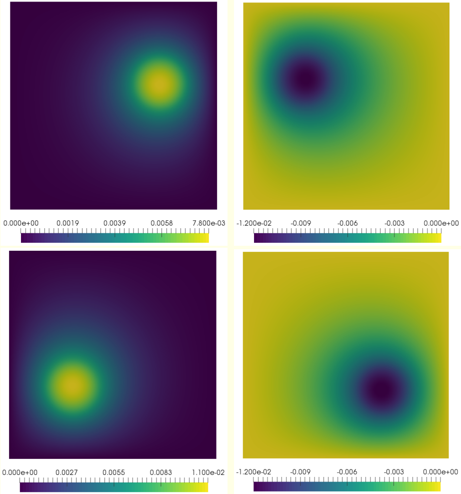


Figure: Full-order solution snapshots for the 2+1D heat equation.

Goal functional evolution, error estimator, true error

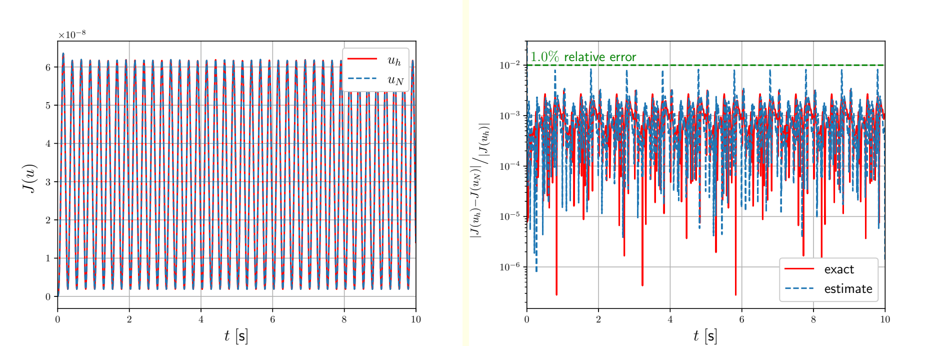


Figure: Temporal evolution of the time interval-wise relative error estimator compared to the true error for the 2+1D heat equation.

Summary of performances

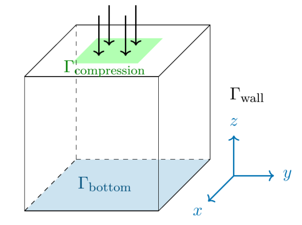
Tolerance	Relative error	Speedup	FOM solves	Basis size	Prediction	Effectivity
0.1%	0.0019%	7.7	150	92 | 78	0 | 35 | 0 | 2013	0.7524
1%	0.0017%	27.5	80	55 | 44	0 | 1 | 0 | 2047	0.2771
2%	0.0628%	29.6	66	47 | 36	0 | 9 | 0 | 2039	3.9181
5%	0.9162%	44.8	44	33 | 25	0 | 1 | 0 | 2047	1.2254
10%	0.9243%	50.0	38	31 | 23	79 | 28 | 17 | 1924	1.5474

Table: Incremental reduced-order modeling summary for the 2+1D heat equation depending on the tolerance in the goal functional.

1. Column 5: POD basis sizes for the primal and dual problem
2. Column 6: (sorted according to the severity; first bad, ..., fourth best)

$$\begin{aligned} &\text{error} > \text{tol} \wedge \text{estimate} < \text{tol} \quad | \quad \text{error} < \text{tol} \wedge \text{estimate} > \text{tol} \quad | \\ &\text{error} > \text{tol} \wedge \text{estimate} > \text{tol} \quad | \quad \text{error} < \text{tol} \wedge \text{estimate} < \text{tol}. \end{aligned}$$

Footing problem in a 3D porous medium (Biot equations)



Goal functional:

$$J(U) := \int_I \int_{\Gamma_{\text{compression}}} p \, \mathrm{d}x \, \mathrm{d}t.$$

Initial and boundary conditions:

$$\begin{aligned}
p(0) = p^0 = 0 \quad & \text{in } \Omega \times \{0\}, \\
u(0) = u^0 = 0 \quad & \text{in } \Omega \times \{0\}, \\
\frac{K}{\nu} \nabla_x p \cdot n = 0 \quad & \text{on } \partial\Omega \setminus \Gamma_{\text{bottom}} \times I, \\
\sigma(u) \cdot n = -\bar{t} e_z \quad & \text{on } \Gamma_{\text{compression}} \times I, \\
\sigma(u) \cdot n = 0 \quad & \text{on } \Gamma_{\text{top}} \setminus \Gamma_{\text{compression}} \times I, \\
p = 0 \quad & \text{on } \Gamma_{\text{bottom}} \times I, \\
u = 0 \quad & \text{on } \Gamma_{\text{bottom}} \times I, \\
\sigma(u) \cdot n = 0 \quad & \text{on } \Gamma_{\text{wall}} \times I.
\end{aligned}$$

Parameter	Value
M	1.75×10^7 Pa
c	$1/M$
α	1 Pa m
ν	$1 \times 10^{-3}\,\mathrm{m}^2\,\mathrm{s}^{-1}$
K	$1 \times 10^{-13}\,\mathrm{m}^2$
ρ	$1\,\mathrm{kg}\,\mathrm{m}^{-3}$
$\bar{t}$	1×10^7 Pa m
μ	1×10^8
λ	$\frac{2}{3} \times 10^8$

Summary of performances [10]

TOL^{rel} [%]	e^{rel} [%]	speedup	FOM solves	ROM size	I_{eff}	I_{ind}
0.1	0.0971	8.6	220	4 / 55 + 53 / 28	0.999	1.207
0.5	0.5333	21.2	80	4 / 19 + 38 / 27	1.068	3.441
1	0.579	22.4	78	4 / 18 + 38 / 26	1.084	3.378
2	0.579	21.7	78	4 / 18 + 38 / 26	1.084	3.378
5	0.579	22.2	78	4 / 18 + 38 / 26	1.084	3.378
10	8.49	22.4	76	4 / 17 + 38 / 26	1.008	1.099
20	19.9	26.2	66	3 / 13 + 33 / 24	1.005	1.031

Table: Performance of MORe DWR method for the 3D footing problem, depending on the tolerance in the goal functional.

1. Column 5: primal (displacements, pressure) and adjoint (displacements, pressure)

[10] Fischer, Roth, Fau, Chamoin, Wheeler, Wick, 2023, arXiv.

Hamilton principle resulting into space-time modeling

1. Thermodynamically consistent Hamilton functional
2. Hamilton principle yields thermo-mechanically coupled models
3. State variables: displacements u, (velocities) v, internal variables α, and temperature θ
4. Specifically internal variables α are parts of new material models

[11] Junker, Wick, Comp. Mech., 2023

Hamilton principle resulting into space-time modeling

1. Thermodynamically consistent Hamilton functional
2. Hamilton principle yields thermo-mechanically coupled models
3. State variables: displacements u, (velocities) v, internal variables α, and temperature θ
4. Specifically internal variables α are parts of new material models
5. **Holistic space-time Hamilton principle yields direct (formal) mathematically consistent space-time settings**

→ **Unifying framework** for wave propagation, visco-elasticity, elasto-plasticity, gradient-enhanced damage / fracture[11]

→ Time t does **not have a specified direction**; **seems to contradict causality**

→ $u(0) = u_0$ and $v(0) = v_0$ become to $v(0) = v_0$ and $v(T) = v_T$ (assumption mechanical equilibrium; acceleration zero)

6. Current work (interest in this workshop): incompressible flow, thixotropy (time-dependent shear thinning property)

[11] Junker, Wick, Comp. Mech., 2023

Space-time system: stationarity conditions of extended Hamilton functional

$$
\begin{aligned}
&\int_I \left(\int_\Omega \frac{\partial \Psi}{\partial \varepsilon} : \delta\varepsilon \, dx - \int_\Omega b^* \cdot \delta u \, dx - \int_{\partial\Omega} t^* \cdot \delta u \, dx \right) dt \\
&- \int_I \int_\Omega \rho \partial_t u \cdot \partial_t \delta u \, dx \, dt - \int_I \int_{\partial\Omega_{D,u}} c_u (u - u^*) \delta u \, ds \, dt + \int_{\partial I} \int_\Omega \rho \partial_t u^* \cdot \partial u \, dx \, ds = 0 \quad \forall \delta u \\
&\int_I \left(\int_\Omega \frac{\partial \Psi}{\partial \alpha} \cdot \delta\alpha \, dx + \int_\Omega \frac{\partial \Psi}{\partial \nabla\alpha} : \delta\nabla\alpha \, dx + \int_\Omega p^{diss,*} \cdot \delta\alpha \, dx \right) dt \\
&- \int_I \int_{\partial\Omega_{D,\alpha}} c_\alpha (\alpha - \alpha^*) \cdot \delta\alpha \, ds \, dt - \int_\Omega \tilde{r}(\alpha - \alpha_0^*) \cdot \delta\alpha \, dx|_{t=0} = 0 \quad \forall \delta\alpha \\
&\int_I \int_\Omega \int \frac{1}{\theta} \left(\kappa \partial_t \theta + \nabla \cdot q^* - \theta \frac{\partial^2 \Psi}{\partial\theta \partial\varepsilon(u)} : \partial_t \varepsilon(u) + \left(\frac{\partial \Psi}{\partial \alpha} - \theta \frac{\partial^2 \Psi}{\partial\theta\partial\alpha} \right) \cdot \partial_t \alpha \right) \delta\theta \, dt \, dx \, dt \\
&- \int_I \int_{\partial\Omega_{D,\theta}} c_\theta (\theta - \theta^*) \delta\theta \, dx \, dt - \int_\Omega \kappa (\theta - \theta_0^*) \delta\theta \, dx|_{t=0} \\
&- \int_I \int_{\partial\Omega_{N,\theta}} \int \frac{1}{\theta} n q^* \delta\theta \, dt \, ds \, dt = 0 \quad \forall \delta\theta
\end{aligned}
$$

Strong form to 'see something' I

1. Find $u : \Omega \times I \to \mathbb{R}^d, v : \Omega \times I \to \mathbb{R}^d$ such that

$$\rho \partial_t v - \nabla \cdot p^{diss,*} - \nabla \cdot \frac{\partial \Psi^f}{\partial (\nabla u + \nabla u^T)} + \nabla p = b^* \quad \text{in } \Omega \times I,$$

$$\rho \partial_t u - \rho v - \frac{\partial \Psi^f}{\partial v} - \nabla \cdot \frac{\partial \Psi^f}{\partial (\nabla v + \nabla v^T)} = 0.$$

2. Non-conservative forces and dissipation function:

$$p^{diss,*} = \frac{\partial \Delta^{diss}}{\partial (\nabla v + \nabla v^T)}, \quad \Delta^{diss} = \frac{1}{2}\mu \|(\nabla v + \nabla v^T)\|^2 + \frac{1}{2}\lambda (\nabla \cdot v)^2$$

3. Free energy density: $\Psi^f := \Psi^f(\nabla u, \nabla v, \gamma, \nabla \gamma, \theta)$

Strong form to 'see something' II: two models

1. **Model 1 (classical Navier-Stokes)**. Set $\Psi^f = 0$. Find $u : \Omega \times I \to \mathbb{R}^d, v : \Omega \times I \to \mathbb{R}^d$ such that

$$\rho \partial_t v - \nabla \cdot (\mu(\nabla v + \nabla v^T) + \lambda \nabla \cdot v I) + \nabla p = b^* \quad \text{in } \Omega \times I,$$
$$\rho \partial_t u - \rho v = 0 \quad \text{in } \Omega \times I.$$

2. **Model 2**. Let the fluid potential be given by

$$\Psi^f = \mu_\gamma e^{-\gamma} \frac{d}{dt} \frac{1}{2} \|(\nabla u + \nabla u^T)\|^2 + \frac{1}{2} c \gamma^2$$

and the dissipation function as

$$\Delta^{diss} = \frac{1}{2} \mu \|(\nabla v + \nabla v^T)\|^2 + \frac{1}{2} \lambda (\nabla \cdot v)^2 + \frac{1}{2} \eta (\partial_t \gamma)^2.$$

Find $u : \Omega \times I \to \mathbb{R}^d, v : \Omega \times I \to \mathbb{R}^d$ and the internal variable, i.e., viscosity parameter, $\gamma : \Omega \times I \to \mathbb{R}$ such that

$$\rho \partial_t v - \nabla \cdot ((\mu + \mu_\gamma e^{-\gamma})(\nabla v + \nabla v^T) + \lambda \nabla \cdot v I) + \nabla p = b^* \quad \text{in } \Omega \times I,$$
$$\rho \partial_t u - \rho v + \nabla \cdot (\mu_\gamma e^{-\gamma} (\nabla u + \nabla u^T)) = 0 \quad \text{in } \Omega \times I,$$
$$\eta \partial_t \gamma - \mu_\gamma e^{-\gamma} \frac{d}{dt} \frac{1}{2} \|(\nabla u + \nabla u^T)\|^2 + c\gamma = 0 \quad \text{in } I.$$

First numerical simulations

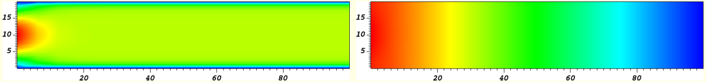


Figure: Model 1: left x-velocity, right pressure.

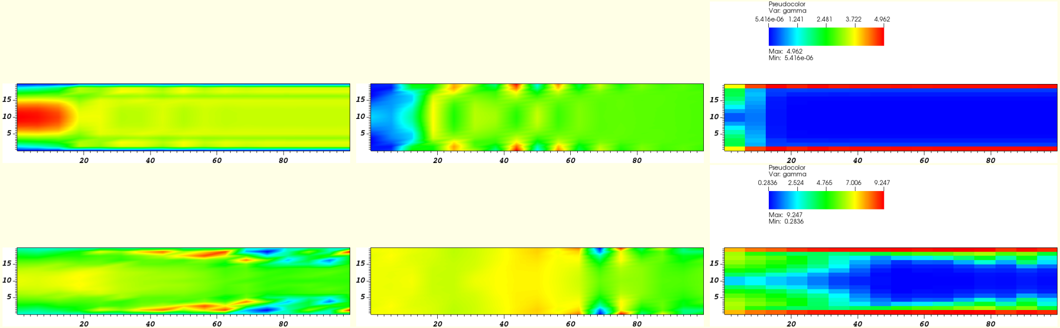


Figure: Model 2: left x-velocity v_x, middle pressure p, and viscosity γ at time $t = 100$ (top row) and $t = 400$ (bottom row).

Current questions from us (Junker, Wick)

1. Relevance of this model?
2. Relationship to known non-Newtonian flow models?
3. Correct functional framework / function spaces?
4. Sign $+\nabla \cdot (\mu_\gamma e^{-\gamma}(\nabla u + \nabla u^T))$?

Conclusions

Conclusions

1. Space-time formulations of single PDEs and coupled systems
2. Space-time Galerkin finite element discretizations
3. A posteriori goal-oriented error control with the dual-weighted residual method for time-distributed functionals (quantities of interest)
4. Incremental POD model order reduction by refining POD basis with previous error estimator
5. Variational material modeling

Key references of this work

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The end

Thank you very much!