

# A nonconforming substructuring method for first-order systems in space-time

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  - $\rightarrow$  there is no general answer!



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## Challenge:

Find discretization scheme

- that is versatile
- that is practical



- Domain  $\Omega \subset \mathbb{R}^{D}$ , time interval (0, *T*), space-time cylinder  $Q = \Omega \times (0, T)$
- Wave equation

 $\partial_t^2 \phi = \Delta \phi$  in Q, + initial/boundary conditions



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Solution with low regularity (1D case):

 $\Omega=(0,1), \quad \phi_0(\cdot):=\phi(\cdot,0)=1, \quad \partial_t\phi(\cdot,0)=0, \quad \text{homogeneous bnd conditions}$ 



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$$\phi(x,t) = \frac{1}{2} (\phi_0(x+t) + \phi_0(x-t))$$
$$= \frac{4}{\pi} \sum_{k=0}^{\infty} \frac{1}{2k+1} \cos\left((2k+1)\pi t\right) \sin\left((2k+1)\pi x\right)$$



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#### How to approximate low regularity solutions?



Figure: FDTD Scheme with 83 000 DoFs (space: 86, time: 969)



Figure: FDTD Scheme with 83 000 DoFs (space: 86, time: 969)



Figure: FDTD Scheme with 1 300 000 DoFs (space: 340, time: 3865)

 $\rightarrow$  CFL-condition fulfilled: c = 1,  $\frac{c\Delta t}{h} = 0.67$ 



• Set 
$$p = \partial_t \phi$$
,  $q = -\nabla \phi$   
 $\partial_t p + \nabla \cdot q = 0$   
 $\partial_t q + \nabla p = 0$  in  $Q$ 

+ initial/boundary conditions

observe:  $\partial_t^2 p = \Delta p$ 

Ω



$$\left.\begin{array}{l} \partial \quad \text{Set } p = \partial_t \phi, \, q = -\nabla \phi \\ \\ \partial_t p + \nabla \cdot q = 0 \\ \\ \partial_t q + \nabla p = 0 \end{array}\right\} \qquad \text{in}$$

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• Consider  $L(p,q) = \begin{pmatrix} \partial_t p + \nabla \cdot q \\ \partial_t q + \nabla p \end{pmatrix}$ defined on  $V \subsetneq L_2(Q)$  (closed wrt to the graph norm of *L*)



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Variational problem:

Given  $f \in L_2(Q)$ , find  $u \in V$ :  $(Lu, \varphi)_{L_2(Q)} = (f, \varphi)_{L_2(Q)} \quad \forall \varphi \in X = L_2(Q)$ 

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- Petrov-Galerkin setting
- inf-sup condition in  $V \times L_2(Q)$  holds



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observe:  $\partial_t^2 p = \Delta p$   
• Consider  $L(p,q) = \left(\frac{\partial_t p + \nabla \cdot q}{\partial_t q + \nabla p}\right)$ 

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- Petrov-Galerkin setting
- inf-sup condition in  $V \times L_2(Q)$  holds
- Space-Time Least Squares: test space X = L(V), solve:  $\min_{v \in V} \frac{1}{2} ||Lv f||^2_{L_2(Q)}$

#### What does Least-Squares yield?



Space-Time Least Squares:  $V_h \subset V$ , solve:  $\min_{v_h \in V_h} \frac{1}{2} ||Lv_h - f||^2_{L_2(Q)}$ 

# What does Least-Squares yield? Space-Time Least Squares: $V_h \subset V$ , solve: $\min_{v_h \in V_h} \frac{1}{2} ||Lv_h - f||^2_{L_2(Q)}$ $V_h = \mathbb{Q}_1(Q)^2$

Figure: Example plots for p (83 000 and 1 300 000 uniform space-time DoFs)



# Comparison in L<sub>1</sub>-Norms ( $T = 8 \cdot \frac{3}{\pi} \approx 7.64$ )



• Error:  $e_h = ||u - u_h||_{L_1(Q)} / ||u||_{L_1(Q)}$ 

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#### • Error: $e_h = ||u - u_h||_{L_1(Q)} / ||u||_{L_1(Q)}$

Q1	260 000	1 100 000	4 200 00	0 1700	000 00	67 000 000
e <sub>h</sub>	0.340	0.255	0.192	0.1	141	0.103
$e_h/e_{h/2}$	1.3	334 1	.328	1.357	1.37	'4
$\log_2 e_h/e_{h/2}$	0.	415 C	).410	0.440	0.4	58
Q2	260 000	1 100 000	4 200 00	0 1700	000 00	67 000 000
e <sub>h</sub>	0.143	0.094	0.061	0.0	039	0.025
$e_h/e_{h/2}$	1.	522 1	.546	1.562	1.5	71
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DoFs per accuracy (estimate for uniform refinement)

e <sub>h</sub>	0.1	0.01	0.001
Q1	70 000 000	>1e12	>1e17
Q2	850 000	>1e9	>1e12



# How can this be improved?



• Least-Squares: solve:  $\min_{v_h \in V_h} \frac{1}{2} ||Lv_h - f||^2_{L_2(Q)}$ 

 $\longrightarrow$  which space  $V_h$ ?





Least-Squares:



 $\rightarrow$  which space  $V_h$ ?







Idea:

- approximate traces of  $v \in V$  on the skeleton
- 2 solve a local problem in each cell



How to represent traces?



for adjoint  $L^{ad}$ :  $W \longrightarrow L_2(R)$ 



• Observe  $\gamma_R v \in \gamma_R^{ad}(W|_R)'$  (dual space)



• Observe for 
$$v \in \prod_{R \in \mathcal{R}} V|_R$$

$$v \in V \qquad \Longleftrightarrow \qquad \langle \gamma v, \gamma^{ad} w \rangle := \sum_{R \in \mathcal{R}} \langle \gamma_R v|_R, \gamma_R^{ad} w|_R \rangle = 0 \quad \forall w \in W$$



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• Choose  $W_h \subset W, \quad V_R \subset V|_R$  and set  $V_{\mathcal{R}} = \prod_{R \in \mathcal{R}} V_R$ 



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## Substructuring – Approximation Space



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• On face  $F = \partial R \cap \partial R'$  we have for  $v_h \in V_h$   
 $\langle \gamma_R v_R, \gamma_R^{ad} w_R \rangle_F = -\langle \gamma_{R'} v_{R'}, \gamma_{R'}^{ad} w_{R'} \rangle_F \quad \forall w_h \in W_h \text{ (face bubbles)}$ 

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• Trace space:  $\hat{V}_h = \gamma^{ad}(W_h)'$  (dual space)  
• Representation of  $\hat{v}_h \in \hat{V}_h$ :  $\left( \langle \hat{v}_h, \gamma_R^{ad} w_F \rangle \right)_{F \subset \partial R, R \in \mathcal{R}}$  (by duality)



- Define  $J_R \colon V_R \longrightarrow \mathbb{R}, v_R \longmapsto \frac{1}{2} \|Lv_R f\|_{L_2(R)}^2$
- Problem: find  $v_h \in V_R$  with

$$\sum_{R \in \mathcal{R}} J_R(v_R) \longrightarrow \mathsf{Min!} \qquad \text{s.t.} \qquad \sum_{R \in \mathcal{R}} \langle \gamma_R v_R, \gamma_R^{\mathsf{ad}} w_R \rangle = 0 \quad \forall w_h \in W_h$$



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• Find saddle point of  $F_h$ :  $\hat{V}_h \times V_R \times W_h \longrightarrow \mathbb{R}$ 

$$F_{h}(\hat{v}_{h}, v_{h}, w_{h}) = \sum_{R \in \mathcal{R}} J_{R}(v_{R}) + \langle \gamma_{R} v_{R} - \hat{v}_{h}, \gamma_{R}^{ad} w_{R} \rangle$$



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• Local Operators  $A_R$ ,  $B_R$ ,  $C_R$  and linear form  $\ell_R$ :

$$\begin{split} J_R(v_R) &= \frac{1}{2} \langle A_R v_R, v_R \rangle - \langle \ell_R, v_R \rangle, \quad \langle B_R w_R, v_R \rangle = \langle \gamma_R v_R, \gamma_R^{ad} w_R \rangle = \langle B'_R v_R, w_R \rangle \\ &\langle C_R \hat{v}_h, w_R \rangle = \langle \hat{v}_R, \gamma_R^{ad} w_R \rangle = \langle C'_R w_R, \hat{v}_h \rangle \end{split}$$



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• System: 
$$A_R u_R + B_R \mu_R = \ell_R \in V'_R,$$
  $\sum_{R \in \mathcal{R}} C'_R \mu_R = 0 \in \hat{V}'_h.$ 



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 $B'_R u_R = C_R \hat{u}_h \in W'_R,$   $\sum_{R \in \mathcal{R}} C'_R \mu_R = 0 \in \hat{V}'_h.$ 



• Global system:  $\hat{S}_h \hat{u}_h = \hat{\ell}_h$  with

$$\hat{S}_{h} = \sum_{R \in \mathcal{R}} \begin{pmatrix} 0 \\ C_{R} \end{pmatrix}' \begin{pmatrix} A_{R} & B_{R} \\ B'_{R} & 0 \end{pmatrix}^{-1} \begin{pmatrix} 0 \\ C_{R} \end{pmatrix}, \quad \hat{\ell}_{h} = \sum_{R \in \mathcal{R}} \begin{pmatrix} 0 \\ C_{R} \end{pmatrix}' \begin{pmatrix} A_{R} & B_{R} \\ B'_{R} & 0 \end{pmatrix}^{-1} \begin{pmatrix} \ell_{R} \\ 0 \end{pmatrix}$$



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• Local system for  $R \in \mathcal{R}$ :

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- Result:  $\hat{S}_h$  is sparse and symmetric, positive definite



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- **Result:**  $\hat{S}_h$  is sparse and symmetric, positive definite
- Assemble  $\underline{\hat{S}}_h \in \mathbb{R}^{\dim W_h \times \dim W_h}$  and  $\underline{\hat{\ell}}_h \in \mathbb{R}^{\dim W_h}$ 
  - For each cell *R* assemble  $\underline{A}_R$ ,  $\underline{B}_R$  and obtain  $\begin{pmatrix} \underline{A}_R & \underline{B}_R \\ B'_R & 0 \end{pmatrix}^{-1}$



• Global system:  $\hat{S}_h \hat{u}_h = \hat{\ell}_h$  with

$$\hat{S}_{h} = \sum_{R \in \mathcal{R}} \begin{pmatrix} 0 \\ C_{R} \end{pmatrix}' \begin{pmatrix} A_{R} & B_{R} \\ B'_{R} & 0 \end{pmatrix}^{-1} \begin{pmatrix} 0 \\ C_{R} \end{pmatrix}, \quad \hat{\ell}_{h} = \sum_{R \in \mathcal{R}} \begin{pmatrix} 0 \\ C_{R} \end{pmatrix}' \begin{pmatrix} A_{R} & B_{R} \\ B'_{R} & 0 \end{pmatrix}^{-1} \begin{pmatrix} \ell_{R} \\ 0 \end{pmatrix}$$

- Local system for  $R \in \mathcal{R}$ :  $A_R u_R + B_R \mu_R = \ell_R \quad \in V'_R,$  $B'_R u_R = C_R \hat{u}_h \in W'_R$
- **Result:**  $\hat{S}_h$  is sparse and symmetric, positive definite

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 and  $\underline{\hat{\ell}}_h \in \mathbb{R}^{\dim W_h}$ 

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- <u>C</u><sub>R</sub> and <u>C</u>'<sub>R</sub> are selection operators
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#### $\longrightarrow$ well suited for parallel implementation!



# What can we do with that?





# Comparison in L<sub>1</sub>-Norms ( $T = 8 \cdot \frac{3}{\pi} \approx 7.64$ )



#### • Error: $e_h = ||u - u_h||_{L_1(Q)} / ||u||_{L_1(Q)}$

Q1	260 000	1 100 000	4 200 00	0 17000	000	67 000 000
e <sub>h</sub>	0.340	0.255	0.192	0.14	11	0.103
$e_h/e_{h/2}$	1.:	334	1.328	1.357	1.37	4
$\log_2 e_h/e_{h/2}$	0.	.415	0.410	0.440	0.4	58
Q2	260 000	1 100 000	4 200 00	0 17000	000	67 000 000
e <sub>h</sub>	0.143	0.094	0.061	0.03	39	0.025
$e_h/e_{h/2}$	1.	.522	1.546	1.562	1.5	71
$\log_2 e_h/e_{h/2}$	0.	.605	0.629	0.643	0.6	52

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$e_h/e_{h/2}$	1	.522	1.546	1.562	2 1.5	571
$\log_2 e_h/e_{h/2}$	0	.605	0.629	0.643	0.6	52
ncLS	330 000	1 300 000	5 300 0	00 2	1 000 000	84 000 000
e <sub>h</sub>	0.051	0.030	0.018	3	0.010	0.006
$e_h/e_{h/2}$	1	.692	1.694	1.694	1.6	693
$\log_2 e_h/e_{h/2}$	0	.758	0.761	0.761	0.7	'60

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DoFs per accuracy (estimate for uniform refinement)

e <sub>h</sub>	0.1	0.01	0.001	
Q1	70 000 000	>1e12	>1e17	
Q2	850 000	>1e9	>1e12	
ncLS	54 000	2e7	>1e10	



ad-hoc marking of faces



uniform grid



ad-hoc marking of faces



- uniform grid
- choose  $W_h \longrightarrow$  choose DoFs on each face



ad-hoc marking of faces



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- choose  $(V_R)_{R \in \mathcal{R}} \longrightarrow$  ensure local inf-sup-conditions



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- choose  $(V_R)_{R \in \mathcal{R}} \longrightarrow$  ensure local inf-sup-conditions

ncLS (uniform)	330 000	1 300 000	5 300 000	21 000 000	84 000 000
e <sub>h</sub>	0.050664	0.029965	0.017685	0.010438	0.006167
$e_h/e_{h/2}$	1.690	0786 1.69	94362 1.69	4260 1.692	637
$\log_2 e_h/e_{h/2}$	0.75	7694 0.76	60742 0.76	0655 0.759	273
ncLS (heterogenous)	180 000	720 000	2 900 000	12000000	46 000 000
e <sub>h</sub>	0.061163	0.031287	0.018011	0.010614	0.006620
$e_h/e_{h/2}$	1.954	4922 1.73	37079 1.69	6971 1.603	246
$\log_2 e_h/e_{h/2}$	0.96	7111 0.79	96663 0.76	2962 0.680	996

#### Similar accuracy with half number of DoFs



Result: discretization that



Result: discretization that

is flexible



Result: discretization that

- is flexible
- can exploit parallel computers



Result: discretization that

- is flexible
- can exploit parallel computers
- Paid: increased local costs



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Future extensions



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Future extensions

numerical analysis



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#### Future extensions

- numerical analysis
- multi-level preconditioner
- built-in error estimator
- other error functions  $J_R$  are possible



#### Result: discretization that

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- can exploit parallel computers

Paid: increased local costs (we don't care!)

#### Future extensions

- numerical analysis
- multi-level preconditioner
- built-in error estimator
- other error functions  $J_R$  are possible
- use as a forward-solver for full waveform inversion
- higher dimensions (2D, 3D)



## Conformity based error estimator



Assume the conformity error is dominant, i.e.

$$\sup_{R\in\mathcal{R}}\inf_{v_{R}\in V_{R}}\|u-v_{R}\|_{V_{R}}\ll\inf_{v\in V}\|u_{h}-v\|_{V},$$

with exact solution  $u \in V$  and approximation  $(u_R)_R \in V_h$ 

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•  $v_h \in V_h$  is just discretely conforming, i.e.

$$\sum_{R \in \mathcal{R}} \langle \gamma_R \mathbf{v}_R, \gamma_R^{ad} \mathbf{w}_R \rangle = 0 \quad \forall \mathbf{w}_h \in \mathbf{W}_h$$
## Conformity based error estimator



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#### • $v_h \in V_h$ is just discretely conforming, i.e.

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with exact solution  $u \in V$  and approximation  $(u_R)_R \in V_h$ 

■ Idea: choose 
$$\tilde{W}_h = \text{span}\{\tilde{w}_F^1, \dots, \tilde{w}_F^N \colon F \subset \Gamma_h \text{ mesh-face}\} \subset W \setminus W_h$$

$$\eta_{F} = \sum_{n} \left| \langle \gamma_{R} u_{h}, \gamma_{R}^{\text{ad}} \tilde{w}_{F}^{n} \rangle - \langle \gamma_{R'} u_{h}, \gamma_{R'}^{\text{ad}} \tilde{w}_{F}^{n} \rangle \right| \qquad (\text{error estimator})$$

for  $F = \partial R \cap \partial R'$ 

# Conformity based error estimator

Assume the conformity error is dominant, i.e.

S F

$$\sup_{P \in \mathcal{R}} \inf_{v_R \in V_R} \|u - v_R\|_{V_R} \ll \inf_{v \in V} \|u_h - v\|_V,$$



### Convergence for a smooth solution



Use smooth initial value

$$p_0(x,0) = egin{cases} \cos\left(rac{s-m}{w}
ight)^2, & |s-m| < w \ 0, & ext{else}, \end{cases}$$

with 
$$w = 0.3 \cdot \frac{3}{\pi}, m = 0.85 \cdot \frac{3}{\pi}.$$

• Error: 
$$e_h = ||u - u_h||_{L_2(Q)}$$

ncLS	11 000	42 000	170 000	660 000	2600000
e <sub>h</sub>	1.4e-3	3.8e-4	1.0e-4	2.9e-5	8.0e-6
$e_h/e_{h/2}$	3.7	75 3.67	7 3.60	3.58	
$\log_2 e_h/e_{h/2}$	1.9	91 1.87	7 1.85	1.84	

#### What can we expect?

- $\quad \bullet \ \ N^{\mathrm{DG}}_{\rho} = 2 \cdot \dim \mathbb{Q}_{\rho}(R), \qquad \|e\|_{L_2(Q)} \leq Ch^{\rho+1/2}$
- $N_1^{\text{DG}} = 8$ , rate:  $\le 1.5$   $N_2^{\text{DG}} = 18$ , rate:  $\le 2.5$
- Here:  $N_{3,3}^{\text{ncLS}} = 10$ , rate:  $1.5 \le 1.84 \le 2.5$

## Local Operators for the Wave Equation



• For  $u_R = (p_1, q_1), v_R = (p_2, q_2)$  it holds

$$\begin{aligned} \langle A_R u_R, v_R \rangle &= (Lu_R, Lv_R)_{L_2(R)} \\ &= \left( \begin{pmatrix} \partial_t p_1 + \nabla \cdot q_1 \\ \partial_t q_1 + \nabla p_1 \end{pmatrix}, \begin{pmatrix} \partial_t p_2 + \nabla \cdot q_2 \\ \partial_t q_2 + \nabla p_2 \end{pmatrix} \right)_{L_2(R)} \\ \langle \ell_R v_R \rangle &= (f, Lv_R)_{L_2(R)} \end{aligned}$$

• For  $v_R = (p, q)$ ,  $w_R = (\phi, \psi)$  we have

$$\begin{aligned} \langle \mathcal{B}_{R} \mathbf{w}_{R}, \mathbf{v}_{R} \rangle &= \langle \gamma_{R} \mathbf{v}_{R}, \gamma_{R}^{\text{ad}} \mathbf{w}_{R} \rangle \\ &= \left( (\mathbf{p}, \mathbf{q}), (\phi, \psi) \right)_{\mathcal{C} \times \{t_{n}\}} - \left( (\mathbf{p}, \mathbf{q}), (\phi, \psi) \right)_{\mathcal{C} \times \{t_{n-1}\}} \\ &+ \left\langle (\mathbf{p}, \mathbf{q} \cdot \mathbf{n}), (\psi \cdot \mathbf{n}, \phi) \right\rangle_{\partial \mathcal{C} \times (t_{n-1}, t_{n})} \end{aligned}$$