Operator preconditioning for EMI equations

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3rd MICROCARD Workshop

5th July 2023, Strasbourg



 $\begin{aligned} -\nabla \cdot (K_0 \nabla u_0) &= 0 & \text{ in } \Omega_0, \\ -\nabla \cdot (K_1 \nabla u_1) &= 0 & \text{ in } \Omega_1, \\ -K_0 \nabla u_0 \cdot \nu + K_1 \nabla u_1 \cdot \nu &= 0 & \text{ on } \Gamma, \\ u_0 - u_1 + \varepsilon K_0 \nabla u_0 \cdot \nu &= f & \text{ on } \Gamma. \end{aligned}$

Goal: Construct scalable and K_i , ε -robust solvers for linear systems

Find $u_h \in W_h$ such that $A_h u_h = b_h$ $= R^n : \mathbf{A} \mathbf{u} = \mathbf{b}$



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Construction reflects origin of A_h in a continuous problem, $W_h \approx W$





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Goal: Construct scalable and K_i , ε -robust solvers for linear systems

Find $u_h \in W_h$ such that $A_h u_h = b_h$ $aggree R^n$: Au = b

Construction reflects origin of A_h in a continuous problem, $W_h \approx W$



Mapping properties of A established via studying well-posedness

Stable discretization yields $\operatorname{cond}(\mathcal{B}_h\mathcal{A}_h) \leq C \neq C(h, \varepsilon, K_i)$

Mardal, K., Winther, R. (2011). Preconditioning discretizations of systems of PDEs. NUMER LINEAR ALGEBR. Kuchta, M., Mardal, K. A. (2020). Iterative solvers for EMI models. Modeling Excitable Tissue The EMI Framework, 70.

The many ways of EMI



Poisson-like formulation



$$-\nabla \cdot (K_0 \nabla u_0) = 0 \quad \text{in } \Omega_0,$$

$$-\nabla \cdot (K_1 \nabla u_1) = 0 \quad \text{in } \Omega_1, \quad \text{for all } U_0 = 0$$

$$-K_0 \nabla u_0 \cdot \nu + K_1 \nabla u_1 \cdot \nu = 0 \quad \text{on } \Gamma, \quad \text{for all } U_0 = 0$$

$$\underbrace{u_0 | \Gamma - u_1 | \Gamma}_{= \llbracket u \rrbracket} + \varepsilon K_0 \nabla u_0 \cdot \nu = f \quad \text{on } \Gamma. \quad \text{for all } U_0 = 0$$

QApply Robin condition in integration by parts

With Γ -discontinous test/trial functions: Find $u = [u_0, u_1] \in W$ such that

$$\int_{\Omega_0} K_0 \nabla u_0 \cdot \nabla v_0 + \int_{\Omega_1} K_1 \nabla u_1 \cdot \nabla v_1 + \varepsilon^{-1} \int_{\Gamma} \llbracket u \rrbracket \llbracket v \rrbracket = \varepsilon^{-1} \int_{\Gamma} f\llbracket v \rrbracket \quad \forall v \in W$$

Equivalent operator equation Au = b in W'

$$\underbrace{\begin{bmatrix} -K_0\Delta_0 + \varepsilon^{-1}T'_0T_0 & -\varepsilon^{-1}T'_0T_1 \\ -\varepsilon^{-1}T'_1T_0 & -K_1\Delta_1 + \varepsilon^{-1}T'_1T_1 \end{bmatrix}}_{\mathcal{A}} \begin{bmatrix} u_0 \\ u_1 \end{bmatrix} = b$$

Well-posedness in $W = H^1(\Omega_0) \times H^1_0(\Omega_1)$ by Lax-Milgram theorem

Do standard norms yield ε -robust preconditioners?

$$\mathcal{A} = \begin{bmatrix} -\mathbf{K}_0 \Delta_0 + \varepsilon^{-1} T_0' T_0 & -\varepsilon^{-1} T_0' T_1 \\ -\varepsilon^{-1} T_1' T_0 & -\mathbf{K}_1 \Delta_1 + \varepsilon^{-1} T_1' T_1 \end{bmatrix}$$

Norm of W due (almost) standard inner-product

$$\|u\|_{W}^{2} = \int_{\Omega_{0}} K_{0} \nabla u_{0} \cdot \nabla v_{0} + \int_{\Omega_{0}} K_{0} u_{0} v_{0} + \int_{\Omega_{1}} K_{1} \nabla u_{1} \cdot \nabla v_{1}$$

Choice of inner product induces a concrete Riesz operator

$$\mathcal{B} = \begin{bmatrix} -K_0 \Delta_0 + K_0 I_0 & \\ & -K_1 \Delta_1 \end{bmatrix}^{-1}$$



$$\mathcal{A} = \begin{bmatrix} -\mathbf{K}_0 \Delta_0 + \varepsilon^{-1} T_0' T_0 & -\varepsilon^{-1} T_0' T_1 \\ -\varepsilon^{-1} T_1' T_0 & -\mathbf{K}_1 \Delta_1 + \varepsilon^{-1} T_1' T_1 \end{bmatrix}$$

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Choice of inner product induces a concrete Riesz operator

$$C(\varepsilon) \neq C \leq \inf_{v} \frac{\langle Av, v \rangle}{\|v\|_{W}} \quad \mathcal{B} = \begin{bmatrix} -K_{0}\Delta_{0} + K_{0}I_{0} & \\ & -K_{1}\Delta_{1} \end{bmatrix}^{-1}$$



1

 $\|u\|_W = \sqrt{\langle \mathcal{B}^{-1}u, u \rangle}$

$$\mathcal{A} = \begin{bmatrix} -\mathbf{K}_0 \Delta_0 + \varepsilon^{-1} T_0' T_0 & -\varepsilon^{-1} T_0' T_1 \\ -\varepsilon^{-1} T_1' T_0 & -\mathbf{K}_1 \Delta_1 + \varepsilon^{-1} T_1' T_1 \end{bmatrix}$$

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 Ω_0

 $||u||_W = \sqrt{\langle \mathcal{B}^{-1}u, u \rangle}$

$$\mathcal{A} = \begin{bmatrix} -\mathbf{K}_0 \Delta_0 + \varepsilon^{-1} T_0' T_0 & -\varepsilon^{-1} T_0' T_1 \\ -\varepsilon^{-1} T_1' T_0 & -\mathbf{K}_1 \Delta_1 + \varepsilon^{-1} T_1' T_1 \end{bmatrix}$$

Norm of W due (almost) standard inner-product

$$\|u\|_{W}^{2} = \int_{\Omega_{0}} K_{0} \nabla u_{0} \cdot \nabla v_{0} + \int_{\Omega_{0}} K_{0} u_{0} v_{0} + \int_{\Omega_{1}} K_{1} \nabla u_{1} \cdot \nabla v_{0}$$

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Choice of inner product induces a concrete Riesz operator



$$\mathcal{A} = \begin{bmatrix} -K_0 \Delta_0 + \varepsilon^{-1} T'_0 T_0 & -\varepsilon^{-1} T'_0 T_1 \\ -\varepsilon^{-1} T'_1 T_0 & -K_1 \Delta_1 + \varepsilon^{-1} T'_1 T_1 \end{bmatrix}$$

Norm of W due diagonal of ${\mathcal A}$



$$\|u\|_{W}^{2} = \int_{\Omega_{0}} K_{0} \nabla u_{0} \cdot \nabla v_{0} + \int_{\Gamma} \varepsilon^{-1} u_{0} v_{0} + \int_{\Omega_{0}} K_{0} u_{0} v_{0} + \int_{\Omega_{1}} K_{1} \nabla u_{1} \cdot \nabla v_{1} + \int_{\Gamma} \varepsilon^{-1} u_{1} v_{1}$$

Choice of inner product induces Riesz operator

$$\mathcal{B} = \begin{bmatrix} -K_0 \Delta_0 + \varepsilon^{-1} T_0' T_0 + K_0 I_0 \\ -K_1 \Delta_1 + \varepsilon^{-1} T_1' T_1 \end{bmatrix}^{-1}$$

$$\mathcal{A} = \begin{bmatrix} -\mathbf{K}_0 \Delta_0 + \varepsilon^{-1} T_0' T_0 & -\varepsilon^{-1} T_0' T_1 \\ -\varepsilon^{-1} T_1' T_0 & -\mathbf{K}_1 \Delta_1 + \varepsilon^{-1} T_1' T_1 \end{bmatrix}$$

Norm of W due diagonal of A

$$\|u\|_{W}^{2} = \int_{\Omega_{0}} K_{0} \nabla u_{0} \cdot \nabla v_{0} + \int_{\Gamma} \varepsilon^{-1} u_{0} v_{0} + \int_{\Omega_{0}} K_{0} u_{0} v_{0} + \int_{\Omega_{1}} K_{1} \nabla u_{1} \cdot \nabla v_{1} + \int_{\Gamma} \varepsilon^{-1} u_{1} v_{1}$$
Choice of inner product induces Riesz operator
$$\|u\|_{W} = \sqrt{\langle \mathcal{B}^{-1} u, u \rangle}$$

Choice of inner product induces Riesz operator

$$\mathcal{B} = \begin{bmatrix} -K_0 \Delta_0 + \varepsilon^{-1} T'_0 T_0 + K_0 I_0 \\ -K_1 \Delta_1 + \varepsilon^{-1} T'_1 T_1 \end{bmatrix}^{-1} \sup_{\substack{\langle Au, v \rangle \\ \|u\|_W \|v\|_W}} \leq C \neq C(\varepsilon)$$

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$$\mathcal{A} = \begin{bmatrix} -\mathbf{K}_0 \Delta_0 + \varepsilon^{-1} T_0' T_0 & -\varepsilon^{-1} T_0' T_1 \\ -\varepsilon^{-1} T_1' T_0 & -\mathbf{K}_1 \Delta_1 + \varepsilon^{-1} T_1' T_1 \end{bmatrix}$$

Norm of W due diagonal of A

$$\|u\|_{W}^{2} = \int_{\Omega_{0}} K_{0} \nabla u_{0} \cdot \nabla v_{0} + \int_{\Gamma} \varepsilon^{-1} u_{0} v_{0} + \int_{\Omega_{0}} K_{0} u_{0} v_{0} + \int_{\Omega_{1}} K_{1} \nabla u_{1} \cdot \nabla v_{1} + \int_{\Gamma} \varepsilon^{-1} u_{1} v_{1}$$
Choice of inner product induces Biesz operator
$$\|u\|_{W} = \sqrt{\langle \mathcal{B}^{-1} u, u \rangle}$$

Choice of inner product induces Riesz operator

$$\mathcal{B} = \begin{bmatrix} -K_0 \Delta_0 + \varepsilon^{-1} T'_0 T_0 + K_0 I_0 \\ -K_1 \Delta_1 + \varepsilon^{-1} T'_1 T_1 \end{bmatrix}^{-1} \\ c(\varepsilon) = C \leq \inf_V \frac{\langle Av, v \rangle}{\|v\|_W} \leq C \neq C(\varepsilon) \\ sup_v \sup_u \frac{\langle Au, v \rangle}{\|v\|_W \|v\|_W} \leq C \neq C(\varepsilon)$$

 Ω_0

$$\mathcal{A} = \begin{bmatrix} -K_0 \Delta_0 + \varepsilon^{-1} T'_0 T_0 & -\varepsilon^{-1} T'_0 T_1 \\ -\varepsilon^{-1} T'_1 T_0 & -K_1 \Delta_1 + \varepsilon^{-1} T'_1 T_1 \end{bmatrix}$$
Norm of *W* due diagonal of *A*

$$||u||_W^2 = \int_{\Omega_0} K_0 \nabla u_0 \cdot \nabla v_0 + \int_{\Gamma} \varepsilon^{-1} u_0 v_0 + \int_{\Omega_0} K_0 u_0 v_0 + \int_{\Omega_1} K_1 \nabla u_1 \cdot \nabla v_1 + \int_{\Gamma} \varepsilon^{-1} u_1 v_1$$
Choice of inner product induces Riesz operator
$$||u||_W = \sqrt{\langle \mathcal{B}^{-1} u, u \rangle}$$

$$\mathcal{B} = \begin{bmatrix} -K_0 \Delta_0 + \varepsilon^{-1} T'_0 T_0 + K_0 I_0 & -K_1 \Delta_1 + \varepsilon^{-1} T'_1 T_1 \end{bmatrix}^{-1}$$

$$\mathcal{C}(\varepsilon) = C \leq \inf_{v} \frac{\langle Av, v \rangle}{||v||_W} = 250$$

ConjGrad ite 100 \mathbb{P}_1 - \mathbb{P}_1 elements $K_0 = 0, K_1 = 2$ 50relative tolerance 10⁻¹⁰ maximum iterations 250 0 preconditioner by LU

150

 10^{3}

 10^{4} System size u>

Iterations affected by ε

-6

-8

 $10^6 \log_{10} \varepsilon^{-10}$

F

 10^{5}

Poisson-like formulation with "energy" Riesz map

$$\mathcal{A} = \begin{bmatrix} -\mathbf{K}_0 \Delta_0 + \varepsilon^{-1} \mathbf{T}_0' \mathbf{T}_0 & -\varepsilon^{-1} \mathbf{T}_0' \mathbf{T}_1 \\ -\varepsilon^{-1} \mathbf{T}_1' \mathbf{T}_0 & -\mathbf{K}_1 \Delta_1 + \varepsilon^{-1} \mathbf{T}_1' \mathbf{T}_1 \end{bmatrix}$$

 ${\mathcal A}$ induces inner product on ${\it W}$

 $||u||_W^2 = \langle Au, u \rangle$ so that $1 \cdot ||u||_W^2 \le \langle Au, u \rangle$, $\langle Au, v \rangle \le \overline{1 \cdot ||u||_W ||v||_W}$ The Riesz map preconditioner is then $\mathcal{B} = \mathcal{A}^{-1}$ *Is it easy to invert?*



Poisson-like formulation with "energy" Riesz map

$$\mathcal{A} = \begin{bmatrix} -K_0 \Delta_0 + \varepsilon^{-1} T'_0 T_0 & -\varepsilon^{-1} T'_0 T_1 \\ -\varepsilon^{-1} T'_1 T_0 & -K_1 \Delta_1 + \varepsilon^{-1} T'_1 T_1 \end{bmatrix}$$

 \mathcal{A} induces inner product on W



(default) point smoother System size

ConjGrad iterations

6

(block) Schwarz smoother

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Poisson-like formulation with "energy" Riesz map

$$\mathcal{A} = \begin{bmatrix} -K_0 \Delta_0 + \varepsilon^{-1} T_0' T_0 & -\varepsilon^{-1} T_0' T_1 \\ -\varepsilon^{-1} T_1' T_0 & -K_1 \Delta_1 + \varepsilon^{-1} T_1' T_1 \end{bmatrix}$$

 ${\mathcal A}$ induces inner product on ${\it W}$



 $\|u\|_W^2 = \langle Au, u \rangle$ so that $\mathbf{1} \cdot \|u\|_W^2 \leq \langle Au, u \rangle$, $\langle Au, v \rangle \leq \mathbf{1} \cdot \|u\|_W \|v\|_W$ The Riesz map preconditioner is then $\mathcal{B} = \mathcal{A}^{-1}$ *Is it easy to invert?* B by HYPRE BoomerAMG V-cycle 30 250ConjGrad iterations ConjGrad iterations 252002015015 100 -6-610 50-8-8-10-10 $10^6 \log_{10} \varepsilon$ $10^6 \log_{10} \varepsilon$ 10^{3} 10^{4} 10^{5} 10^{3} 10^{4} 10^{5} (default) point smoother System size System size (block) Schwarz smoother Handling $\varepsilon \ll 1$ requires AMG smoothers capturing kernel of metric perturbation $\mathcal{M}_{v}(\mathbf{u}_{0}(\mathbf{v}))$ length scale² $| u_1(v) |$ diffusion = $\mathcal{A} = \begin{bmatrix} -K_0 \Delta_0 & \\ & -K_1 \Delta_1 \end{bmatrix} + \varepsilon^{-1} \begin{bmatrix} T_0' T_0 & -T_0 T_1 \\ -T_1' T_0 & T_1' T_1 \end{bmatrix}$

Budisa, A., et al. (2023). AMG methods for metric-perturbed coupled problems. arXiv:2305.06073.

Poisson-Lagrange formulation



$$-\nabla \cdot (K_0 \nabla u_0) = 0 \quad \text{in } \Omega_0,$$

$$-\nabla \cdot (K_1 \nabla u_1) = 0 \quad \text{in } \Omega_1,$$

$$-K_0 \nabla u_0 \cdot \nu + K_1 \nabla u_1 \cdot \nu = 0 \quad \text{on } \Gamma,$$

$$u_0 | \mathbf{r} - u_1 | \mathbf{r} + \varepsilon \underbrace{K_0 \nabla u_0 \cdot \nu}_{=-\lambda:\Gamma \to \mathbb{R}} = f \quad \text{on } \Gamma.$$

 $\$ Lagrange multiplier λ enforces Robin

Saddle point problem for $x = [u_0, u_1, \lambda] \in W$ with operator

$$\mathcal{A} = \begin{bmatrix} -K_0 \Delta_0 & T_0' \\ & -K_1 \Delta_1 & -T_1' \\ T_0 & -T_1 & -\varepsilon I_{\Gamma} \end{bmatrix}$$

Well-posedness in $W = H^1(\Omega_0) \times H^1_0(\Omega_1) \times H^{-1/2}(\Gamma)$ by Brezzi theory

Are fractional spaces really needed?

Poisson-Lagrange formulation



$$-\nabla \cdot (K_0 \nabla u_0) = 0 \quad \text{in } \Omega_0,$$

$$-\nabla \cdot (K_1 \nabla u_1) = 0 \quad \text{in } \Omega_1,$$

$$-K_0 \nabla u_0 \cdot \nu + K_1 \nabla u_1 \cdot \nu = 0 \quad \text{on } \Gamma,$$

$$u_0 | \Gamma - u_1 | \Gamma + \varepsilon \underbrace{K_0 \nabla u_0 \cdot \nu}_{=-\lambda:\Gamma \to \mathbb{R}} = f \quad \text{on } \Gamma.$$

Solution Lagrange multiplier λ enforces Robin

Saddle point problem for $x = [u_0, u_1, \lambda] \in W$ with operator

$$\mathcal{A} = \begin{bmatrix} -K_0 \Delta_0 & T'_0 \\ & -K_1 \Delta_1 & -T'_1 \\ T_0 & -T_1 & -\varepsilon I_{\Gamma} \end{bmatrix}$$

Well-posedness in $W = H^1(\Omega_0) \times H^1_0(\Omega_1) \times H^{-1/2}(\Gamma)$ by Brezzi theory

Are fractional spaces really needed?

Assume $H^1(\Omega_0) \times H^1_0(\Omega_1) \times L^2(\Gamma)$ leading to Riez map

$$\mathcal{B} = \begin{bmatrix} -K_0 \tilde{\Delta}_0 & \\ & -K_1 \Delta_1 & \\ & & I_{\Gamma} \end{bmatrix}^{-1}$$

For convenience let $\tilde{\Delta}_0 = \Delta_0 - I_0$

\mathbb{P}_1 - \mathbb{P}_1 - \mathbb{P}_1 ele	ements, k	$K_0 = 1, K$	í ₁ = 2, рі	reconditio	oner by LU
εh	2-4	2 ⁻⁵	2 ⁻⁶	2 ⁻⁷	2 ⁻⁸
1	23	23	23	22	22
10^{-2}	86	89	91	92	85
10^{-4}	143	183	237	250	250

MinRes iterations are unbounded in ε

Intersection spaces for Poisson-Lagrange formulation

$$\mathcal{A} = \begin{bmatrix} -K_0 \Delta_0 & T'_0 \\ & -K_1 \Delta_1 & -T'_1 \\ T_0 & -T_1 & -\varepsilon I_{\Gamma} \end{bmatrix} : W_i \to W'_i$$

Different function space setting via LM space





Intersection spaces for Poisson-Lagrange formulation

$$\mathcal{A} = \begin{bmatrix} -K_0 \Delta_0 & T_0' \\ & -K_1 \Delta_1 & -T_1' \\ T_0 & -T_1 & -\varepsilon I_{\Gamma} \end{bmatrix} : W_i \to W_i'$$

Different function space setting via LM space





Fractional and intersection spaces yield ε -robustness (At the price of dealing with $-\Delta_r^{-1/2}$)



Darcy-like formulation - dealing with strong coupling





Well-posed saddle point problem for $[\sigma, u] \in H(\operatorname{div}, \Omega) \times L^2(\Omega)$

(Mass)-conservative mixed method

$$\mathcal{A} = \begin{bmatrix} \mathcal{K}^{-1}I + \varepsilon \mathcal{T}'_{\nu}\mathcal{T}_{\nu} & -\nabla \\ \nabla \cdot \\ \mathcal{A} \to \text{Darcy as } \varepsilon \to 0 \end{bmatrix}$$

Darcy-like formulation - dealing with strong coupling



 $\sigma_{0} + K_{0} \nabla u_{0} = 0, \ \nabla \cdot \sigma_{0} = 0 \quad \text{in } \Omega_{0},$ $\sigma_{1} + K_{1} \nabla u_{1} = 0, \ \nabla \cdot \sigma_{1} = 0 \quad \text{in } \Omega_{1}, \quad \stackrel{\text{G}}{\supset}$ $\sigma_{0} \cdot \nu - \sigma_{1} \cdot \nu = 0 \quad \text{on } \Gamma, \quad \stackrel{\text{G}}{\supset}$ $u_{0}|_{\Gamma} - u_{1}|_{\Gamma} - \varepsilon \sigma_{0} \cdot \nu = f \quad \text{on } \Gamma. \quad \stackrel{\text{G}}{\triangleleft}$ $\underbrace{\mathfrak{Q} \text{ Seek flux } \sigma \in H(\operatorname{div}, \Omega), \ \sigma|_{\Omega_{i}} = \sigma_{i}, \ u \in L^{2}(\Omega), u|_{\Omega_{i}} = u_{i}}$ $\underbrace{\mathfrak{Q} \text{ Apply Robin in integration by parts}}$

Well-posed saddle point problem for $[\sigma, u] \in H(\text{div}, \Omega) \times L^2(\Omega)$



Darcy-like formulation - dealing with strong coupling



 $\sigma_0 + K_0 \nabla u_0 = 0, \quad \nabla \cdot \sigma_0 = 0$ in Ω_0 , $= \Omega_0 \cup \Omega_1$ $\sigma_1 + K_1 \nabla u_1 = 0, \quad \nabla \cdot \sigma_1 = 0$ in Ω_1 . on Γ. $\sigma_0 \cdot \nu - \sigma_1 \cdot \nu = 0$ C $u_0|_{\Gamma} - u_1|_{\Gamma} - \varepsilon \sigma_0 \cdot \nu = f$ on Γ. 𝔅 Seek flux $\sigma \in H(\operatorname{div}, \Omega)$, $\sigma|_{\Omega_i} = \sigma_i$, $u \in L^2(\Omega)$, $u|_{\Omega_i} = u_i$ Apply Robin in integration by parts Well-posed saddle point problem for $[\sigma, u] \in H(\text{div}, \Omega) \times L^2(\Omega)$ (Mass)-conservative mixed method



Könnö, J. et al (2011). Mixed FEM for problems with Robin boundary conditions. SINUM, 49(1), 285-308

Darcy-Lagrange formulation to avoid non-standard H(div) norm



$$\sigma_{0} + K_{0} \nabla u_{0} = 0, \ \nabla \cdot \sigma_{0} = 0 \quad \text{in } \Omega_{0},$$

$$\sigma_{1} + K_{1} \nabla u_{1} = 0, \ \nabla \cdot \sigma_{1} = 0 \quad \text{in } \Omega_{1},$$

$$\sigma_{0} \cdot \nu - \sigma_{1} \cdot \nu = 0 \quad \text{on } \Gamma,$$

$$\underbrace{u_{0}|_{\Gamma} - u_{1}|_{\Gamma}}_{=\lambda} -\varepsilon \sigma_{0} \cdot \nu = f \quad \text{on } \Gamma.$$

$$\underbrace{\mathcal{O} \text{Solve explicitely for pressure jump } \lambda, f = f(\lambda, \cdots)$$
problem for $[\sigma, u, \lambda] \in H(\text{div}, \Omega) \times L^{2}(\Omega) \times H^{1/2}(\Gamma)$

$$\Box = \begin{bmatrix} K^{-1}(I - \nabla \nabla \cdot) \end{bmatrix}$$

$$\mathcal{A} = \begin{bmatrix} K^{-1}I & -\nabla & T'_{\nu} \\ \nabla \cdot & & \\ T_{\nu} & & \varepsilon^{-1}I_{\Gamma} \end{bmatrix} \quad \mathcal{B} = \begin{bmatrix} K^{-1}(I - \nabla \nabla \cdot) \\ KI \\ & \varepsilon^{-1}I_{\Gamma} - \overline{K}\Delta_{\Gamma}^{1/2} \end{bmatrix}^{-1}$$

• LM space
$$H^{1/2} \cap \varepsilon^{-1}L^2$$

• unlike with Poisson, L^2 part can dominate for $\varepsilon \ll 1$

Darcy-Lagrange formulation to avoid non-standard H(div) norm



60r

40

20

ΩЩ

 10^{3}

 $10^{\bar{4}}$

 10^{5}

System size

 10^{6}

MinRes iterations

 $\sigma_0 + K_0 \nabla u_0 = 0, \quad \nabla \cdot \sigma_0 = 0$ in Ω_0 . $\sigma_1 + K_1 \nabla u_1 = 0, \quad \nabla \cdot \sigma_1 = 0$ in Ω_1 . $\sigma_0 \cdot \nu - \sigma_1 \cdot \nu = 0$ on Γ , $\underbrace{u_0|_{\Gamma}-u_1|_{\Gamma}}_{\varepsilon\sigma_0}-\varepsilon\sigma_0\cdot\nu=f$ on Γ. Solve explicitly for pressure jump λ , $f = f(\lambda, \cdots)$ Well-posed saddle point problem for $[\sigma, u, \lambda] \in H(\operatorname{div}, \Omega) \times L^2(\Omega) \times H^{1/2}(\Gamma)$ $\int K^{-1}(I - \nabla \nabla \cdot)$ $\begin{bmatrix} \mathcal{K}^{-1}\mathcal{I} & -\nabla & \mathcal{T}'_{\nu} \\ \nabla \cdot & & \\ \mathcal{T}_{\nu} & \varepsilon^{-1}\mathcal{I}_{\Gamma} \end{bmatrix}$ $\mathcal{A} = |$ $\mathcal{B} =$ ΚI $\varepsilon^{-1}I_{\Gamma} - \overline{K}\Delta_{\Gamma}^{1/2}$ • LM space $H^{1/2} \cap \varepsilon^{-1}L^2$ -2• unlike with Poisson, L^2 part can dominate for $\varepsilon \ll 1$ -4Full robustness with fractional and intersection spaces -6-8

-10

 \mathbb{RT}_0 - \mathbb{P}_0 - \mathbb{P}_0 elements

 $\log_{10}\varepsilon$

Multiplier formulations and scaling block-diagonal preconditioners



In the bulk multiplier-free formulations require no-black-box solvers for low-rank perturbations

Solvers for bulk unknowns in Lagrange formulations

Standard operators in bulk blocks in Poisson-Lagrange and Darcy-Lagrange

$$\mathcal{B}_{P} = \begin{bmatrix} -K_{0}\tilde{\Delta}_{0} & & \\ & -K_{1}\Delta_{1} & \\ & & -\overline{K}^{-1}\Delta_{\Gamma}^{-1/2} + \varepsilon I_{\Gamma} \end{bmatrix}^{-1} \mathcal{B}_{D} = \begin{bmatrix} K^{-1}(I - \nabla\nabla\cdot) & & \\ & KI & \\ & & -\overline{K}\Delta_{\Gamma}^{1/2} + \varepsilon^{-1}I_{\Gamma} \end{bmatrix}^{-1}$$

Black-box algorithms applicable for their approximations



Scalabity hinges on performant solvers for (small) LM block

Kolev, T. V., Vassilevski, P. S. (2012). Parallel auxiliary space AMG solver for H(div) problems. SISC

Rational approximation for fractional order Riesz maps

Babuška problem $-\Delta u + u = f$ in Ω with u = g in $\lambda = \partial \Omega$

Precondition
$$\mathcal{A} = \begin{bmatrix} -\Delta + I & T' \\ T & 0 \end{bmatrix}$$
 by $\mathcal{B} = \begin{bmatrix} -\Delta + I & 0 \\ 0 & (-\Delta_{\Gamma})^{-1/2} \end{bmatrix}^{-1}$

Preconditioner requires solving $\langle (-\Delta_{\Gamma})^{-1/2}p,q \rangle = \langle b,q \rangle$ in Q_h



Spectral realization $A^s = (MU)\Lambda^s (MU)^T$, s.t. $AU = MU\Lambda$ and $U^T MU = I$

Rational approximation for fractional order Riesz maps

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- Spectral realization $A^s = (MU)\Lambda^s (MU)^T$, s.t. $AU = MU\Lambda$ and $U^T MU = I$
- Rational approximation for f, $f(x) = (x^s)^{-1}$ $f(A) = c_0 M^{-1} + \sum_{i=1}^{N} (c_i A + p_i M)^{-1}, \quad \mathbb{R} \ni p_i > 0$

N controlled by accuracy ε_{RA} not dim Q_h

Budisa, A., et al. (2022). Rational approximation preconditioners for multiphysics problems. arXiv:2209.11659. Budisa, A., et al. (2022). HAZniCS–Software Components for Multiphysics Problems. arXiv:2210.13274.

Peformance of rational approximation



Rational approximation $\varepsilon_{RA} = 10^{-12}$ leads to bounded^{*} iterations





Role of RA accuracy for iterations



Sufficient accuracy of RA is required for stable iterations, $\varepsilon_{RA} \leq 10^{-4}$



Number of RA poles grows slowly with ε_{RA}



Rational approximation for sum of fractional operators

$-\nabla \cdot (\sigma(u_0, p_0)) = f_0$	in Ω_0 ,
$ abla \cdot u_0 = 0$	in Ω_0 ,
$\sigma(u_0,p_0)=-p_0I+2\mu\varepsilon(u_0)$	in Ω_0 ,
$K^{-1}u_1 + \nabla p_1 = 0$	in Ω_1 ,
$\nabla \cdot u_1 = f_1$	in Ω ₁
$u_0\cdot\nu-u_1\cdot\nu=0$	on Γ



Multiplier space $\mu^{-1/2} H^{-1/2} \cap K^{1/2} H^{1/2}$





Holter K.E., et al. (2020). Robust preconditioning of monolithically coupled multiphysics problems. arXiv:2001.05527.

Ω₁ 0 = ¹α

 $u_0 = 0$

 Ω_0

Towards HPC



Towards HPC



Towards HPC



Discontinuous Galerkin method for EMI Poisson-formulation



$$-\nabla \cdot (K_0 \nabla u_0) = 0 \quad \text{in } \Omega_0, \quad \text{for } U_0 = 0$$
$$-\nabla \cdot (K_1 \nabla u_1) = 0 \quad \text{in } \Omega_1, \quad \text{for } U_0 = 0$$
$$-K_0 \nabla u_0 \cdot \nu + K_1 \nabla u_1 \cdot \nu = 0 \quad \text{on } \Gamma, \quad \text{for } U_0 = 0$$
$$\underbrace{u_0 | \Gamma - u_1 | \Gamma}_{u^+ - u^- = \llbracket u \rrbracket} + \varepsilon K_0 \nabla u_0 \cdot \nu = f \quad \text{on } \Gamma.$$

Q Discontinuity on *every* facet $F \in \mathcal{F}_h$

Seek
$$u \in W_h \not\subset W, u|_{\Omega_i} = u_i$$
 such that

$$\begin{split} &\sum_{T \in \Omega_h \cap \Omega_0} \int_T K_0 \nabla u_0 \cdot \nabla v_0 + \sum_{T \in \Omega_h \cap \Omega_1} \int_T K_1 \nabla u_1 \cdot \nabla v_1 + \sum_{F \in \mathcal{F}_h \cap \Gamma} \int_F \frac{1}{\varepsilon} (\llbracket u \rrbracket - f) \llbracket v \rrbracket \\ &- \sum_{F \in \mathcal{F}_h \setminus \Gamma} \int_F \{\!\!\{ K \nabla v \cdot v \}\!\!\} \llbracket u \rrbracket - \sum_{F \in \mathcal{F}_h \setminus \Gamma} \int_F \{\!\!\{ K \nabla u \cdot v \}\!\!\} \llbracket v \rrbracket + \sum_{F \in \mathcal{F}_h \setminus \Gamma} \int_F \frac{\overline{K} \gamma}{h} \llbracket v \rrbracket [\llbracket u \rrbracket - v] \forall v \in W_h \\ & \text{Stabilization } \gamma > 0 \text{ set for coercivity} \end{split}$$

Discontinuous Galerkin method for EMI Poisson-formulation



$$-\nabla \cdot (K_0 \nabla u_0) = 0 \quad \text{in } \Omega_0, \quad \nabla \cdot (K_1 \nabla u_1) = 0 \quad \text{in } \Omega_1, \quad \nabla \cdot (K_1 \nabla u_1) = 0 \quad \text{in } \Omega_1, \quad \nabla \cdot (K_1 \nabla u_1) = 0 \quad \text{on } \Gamma, \quad \nabla \cdot (K_0 \nabla u_0 \cdot \nu = 0) \quad \text{on } \Gamma, \quad \nabla \cdot (K_0 \nabla u_0 \cdot \nu = 0) \quad \text{on } \Gamma, \quad \nabla \cdot (K_0 \nabla u_0 \cdot \nu = 0)$$

? Discontinuity on *every* facet $F \in \mathcal{F}_h$

Seek $u \in W_h \not\subset W, u|_{\Omega_i} = u_i$ such that

$$\sum_{T \in \Omega_h \cap \Omega_0} \int_T K_0 \nabla u_0 \cdot \nabla v_0 + \sum_{T \in \Omega_h \cap \Omega_1} \int_T K_1 \nabla u_1 \cdot \nabla v_1 + \sum_{F \in \mathcal{F}_h \cap \Gamma} \int_F \frac{1}{\epsilon} (\llbracket u \rrbracket - t) \llbracket v \rrbracket$$
$$- \sum_{F \in \mathcal{F}_h \setminus \Gamma} \int_F \{ [K \nabla v \cdot v] \} \llbracket u \rrbracket - \sum_{F \in \mathcal{F}_h \setminus \Gamma} \int_F \{ [K \nabla u \cdot v] \} \llbracket v \rrbracket + \sum_{F \in \mathcal{F}_h \setminus \Gamma} \int_F \frac{K_\gamma}{h} \llbracket v \rrbracket \llbracket u \rrbracket \quad \forall v \in W_h$$
Stabilization $\gamma > 0$ set for

coercivity

- - (- K h E)

With Γ -only-discontinous test/trial functions: Find $u = [u_0, u_1] \in W = H^1(\Omega_0) \times H^1(\Omega_1)$ such that

$$\int_{\Omega_0} K_0 \nabla u_0 \cdot \nabla v_0 + \int_{\Omega_1} K_1 \nabla u_1 \cdot \nabla v_1 + \int_{\Gamma} \frac{1}{\varepsilon} (\llbracket u \rrbracket - f) \llbracket v \rrbracket = 0 \quad \forall v \in W$$

Solution operator A_h with familiar structure, large "interface" - $T_{i,h}$ couples on every facet

$$\begin{bmatrix} -\kappa_{0,h}\Delta_{0,h} + \varepsilon_h^{-1}T'_{0,h}T_{0,h} & -\varepsilon_h^{-1}T'_{0,h}T_{1,h} \\ -\varepsilon_h^{-1}T'_{1,h}T_{0,h} & -\kappa_{1,h}\Delta_{1,h} + \varepsilon_h^{-1}T'_{1,h}T_{1,h} \end{bmatrix} \begin{bmatrix} u_0 \\ u_1 \end{bmatrix} = b$$

Discontinuous Galerkin method for EMI Poisson-formulation

- EOC for $W_h = \{ v \in L^2(\Omega_h), v |_T \in \mathbb{P}^k(T) \}$
- System size $\propto \Omega_h$ -element count
- conservative method (electric charge)
- runs in parallel in any FEniCS
- standard solvers seem to work

Riesz maps wrt





Masri, R., et al. (in prep 2023). Discontinuous Galerkin method for EMI equations

Performance of DG EMI-Poisson solver

Parametrized cylindrical "myocyte" cell defined in Gmsh



Periodicity of "tile" mesh enables building (layers of) sheets (no meshing)

n _{EMI}	2 ²	4 ²	8 ²	16 ²	32 ²	64 ²	128 ²	256 ²	
$ \Omega_{h} /10^{3}$	7	26	106	423	690	6 793	27 050	108 200	$h \approx 4 \mu m$
T _{gen} [s]	0.004	0.006	0.01	0.04	0.16	0.65	2.7	10.5	
T _{save} [s]	0.004	0.02	0.06	0.23	1.01	4.04	16.02	63.1	
HDF5 [MB]	1.1	4.3	17	68	271	1100	4300	17000	

Performance of DG EMI-Poisson solver

Parametrized cylindrical "myocyte" cell defined in Gmsh



Periodicity of "tile" mesh enables building (layers of) sheets (no meshing)

	n_E	MI	22	42	82	164	322	642	1282	256 ²	
	$ \Omega_h $	/10 ³	7	26	106	423	690	6 793	27 050	108 200	$h \approx 4$
	Tger	ן [s]	0.004	0.006	0.01	0.04	0.16	0.65	2.7	10.5	- 🖊
	Tsav	e [S]	0.004	0.02	0.06	0.23	1.01	4.04	16.02	63.1	- /_ .
	HDF5	[MB]	1.1	4.3	17	68	271	1100	4300	17000	
Preli	minary s	caling	g: 32p	rocs,	128G	B RAI	M ^{Pdisc}	1 elemen	ts		
	n _{EMI}	2 ²	4 ²	8 ²	16 ²	32 ²	64 ²	dim	$W_{h}/10^{3}$	n _{iters}	T _{KSP} [s]
	$\dim W_h/10^3$	26	106	423	1 690	6762	27 049		3 588	58	194
	n _{iters}	47	48	48	48	47	47	- (6 762	47	185
	T _{KSP} [s]	0.12	0.35	145	155	185	323	- 2	7 576	34	298
KSP=B-s	setup+ConjGra	id							Decement		!

BoomerAMG with point smoother relative tolerance 10^{-8}

• "Balance" the EMI solver tree



• "Balance" the EMI solver tree



• "Balance" the EMI solver tree



- How critical is parameter robustness in practice?
- (DG) solvers in real applications
- Coupling EMI and mechanics

• "Balance" the EMI solver tree



- How critical is parameter robustness in practice?
- (DG) solvers in real applications
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Thank you for your attention!

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