Some more comments on the normal equations: With a focus on discretisation of partial differential equations

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UNIVERSITY OF OXFORD
Mathematical Institute

THE NORMAL EQUATION

Let us consider the following linear system of equations

$$\underline{\underline{A}}\,\underline{x} = \underline{b}, \qquad \underline{\underline{A}} \in \mathbb{R}^{n\times n}, \quad \underline{x}, \underline{b} \in \mathbb{R}^n.$$

$$\boxed{A^T \neq A}$$

In order to solve the system, we can consider the normal equation, i.e.

$$\boxed{B := \underline{\underline{A}}^T \underline{\underline{A}}\,\underline{x} = \underline{\underline{A}}^T \underline{b}}$$

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- Unfortunately the condition number of $\underline{\underline{A}}^T\underline{\underline{A}}$ is the square of the condition number of $\underline{\underline{A}}$.
- We now have a symmetric positive definite system, that can be solved using CG (**CGNE**).

HOW CAN WE PRECONDITION THE NORMAL EQUATIONS?

SIREV Vol. 64, Iss. 3, 2022 (A. Wathen),

Good preconditioners – Classical Definition

$\underline{\underline{P}}$ is a good preconditioner if $\underline{\underline{P}}^{-1}\underline{\underline{A}}$ has clustered eigenvalues.

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$$A = \begin{bmatrix} b_0 & & \\ & \ddots & \\ & & b_{n-1} \end{bmatrix}, \qquad P = \begin{bmatrix} & & b_0 \\ & \iddots & \\ b_{n-1} & & \end{bmatrix}.$$

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$$P^{-1}A = \begin{bmatrix} & & 1 \\ & \iddots & \\ 1 & & \end{bmatrix}, \qquad G^{-1}B = \begin{bmatrix} (b_0/b_{n-1})^2 & & \\ & \ddots & \\ & & (b_{n-1}/b_0)^2 \end{bmatrix}.$$

HOW CAN WE PRECONDITION THE NORMAL EQUATIONS?

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Gratton–Gürol–Simon–Toint

If the matrix P is such that $\|I - A\,P^{-1}\|_2 \leq \sqrt{2} - 1 - \delta$, then

$$\Lambda(G^{-1}B) \subset (\sqrt{2}\delta + \delta^2, 2 - \sqrt{2}\delta - \delta^2).$$

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$$\Lambda(G^{-1}B) \subset (\sqrt{2}\delta + \delta^2, 2 - \sqrt{2}\delta - \delta^2).$$

We consider the matrix $T := I - AP^{-1}$, and expand $G^{-1}B$ as

$$G^{-1}B = P^{-1}P^{-T}A^TA \sim P^{-T}A^TAP^{-1} = I - T - T^T + T^TT.$$

Since $\Lambda(G^{-1}B) \subset [-\|G^{-1}B\|_2, \|G^{-1}B\|_2]$, we can easily see that

$$-1 - 2\|T\|_2 - \|T\|_2^2 \leq \lambda \leq 1 + 2\|T\|_2 + \|T\|_2^2.$$

Substituing $\|I - AP^{-1}\|_2 \leq \sqrt{2} - 1 - \delta$ we obtained the desired result.

CROSS PRECONDITIONING

We would like to give a different intuition of good preconditioners for normal equations. To this aim we consider the previously observed similarity,

$$G^{-1}B = P^{-1}P^{-T}A^TA \sim P^{-T}A^TAP^{-1} = (AP^{-1})^T(AP^{-1}).$$

Hence, the closer the matrix AP^{-1} is to an orthogonal matrix, the closer $G^{-1}B$ is to the identity matrix.

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Cross preconditioning

We say that the preconditioner P is a good **left** preconditioner for the normal equations if it is a good **right** preconditioner for $\underline{\underline{A}}$, in the sense that $\underline{\underline{AP}}^{-1}$ has clustered singular values.

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QR decomposition

We can construct an ideal preconditioner using the QR decomposition of $\underline{\underline{A}}$, i.e.

$$\underline{\underline{P}} = \underline{\underline{R}},\ \underline{\underline{A}} = \underline{\underline{Q}}_{QR}\underline{\underline{R}}.$$

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Polar decomposition

We can construct an ideal preconditioner using the polar decomposition of $\underline{\underline{A}}$, i.e.

$$\underline{\underline{P}} = (\underline{\underline{A}}^T\underline{\underline{A}})^{\frac{1}{2}}, \ \underline{\underline{A}} = \underline{\underline{Q}}_{P}\underline{\underline{P}}.$$

APPLICATIONS TO FINITE DIFFERENCE SCHEMES

1

ADVECTION DIFFUSION ODE – CROSS PRECONDITIONING

We consider the classical advection-diffusion ODE in one dimension, i.e.

$$-\nu\ddot{u} + \beta\dot{u} = f \text{ in } (a, b) \subset \mathbb{R},$$
$$u(a) = 0,\ u(b) = 1,\ \nu, \beta \in \mathbb{R}_{\geq 0}.$$

R. J. LeVeque, Finite Difference Methods for Ordinary and Partial Differential Equations, 2007 ,*SIAM*.

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For the moment we will consider neither diffusion nor advection-dominated regimes, i.e. $\nu \approx \beta$, and discretisation over an equi-spaced mesh of step-size h. Such a discretisation results in the matrix

$$\underline{\underline{A}} = \text{tridiag}\left(-\frac{\nu}{h^2} - \frac{\beta}{2h}, \frac{2\nu}{h^2}, -\frac{\nu}{h^2} + \frac{\beta}{2h}\right)$$

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n	QR	RQ	$Q(A^TA)^{1/2}$	$(AA^T)^{1/2}Q$
10	2	12	2	4
100	2	-	2	6
1000	2	-	2	7

Table: Comparison of the number of iterations for different preconditioners for the left preconditioned normal equation. The CGNE method was terminated when the absolute residual was less than 10^{-12}. If the method did not converge in 1000 iterations, we marked the number of iterations with a dash.

ADVECTION DIFFUSION ODE – UPWINDING

In the case of advection–dominated regimes, i.e. $\nu \ll \beta$, it is better to opt for an upwinding scheme. In fact, in the advection–dominated regime we might observe the appearance of boundary layers, that are not well resolved by the standard central difference scheme.

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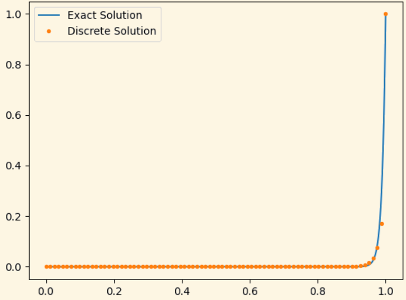

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The discretisation of this scheme results in the linear system

$$A = \text{tridiag}\left(-\frac{\nu}{h^2} - \frac{\beta}{h}, \frac{2\nu}{h^2} + \frac{\beta}{h}, -\frac{\nu}{h^2}\right).$$

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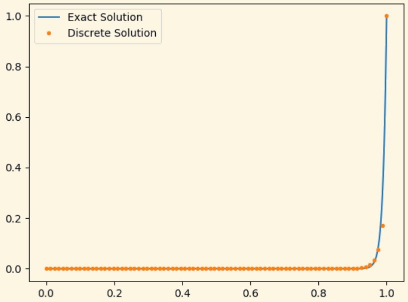

ADVECTION DIFFUSION ODE – CROSS PRECONDITIONING

In the case of advection-dominated regimes, i.e. $\nu \ll \beta$, we can think of preconditioning $\underline{\underline{A}}$ with P defined as

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Normal preconditioning

For the normal equations we can think of preconditioning with $\underline{\underline{P}}^T\underline{\underline{P}}$. In fact the matrix $\underline{\underline{P}}^T\underline{\underline{P}}$ is close to discretising $-\beta^2\ddot{u}$ and the $\underline{\underline{A}}^T\underline{\underline{A}}$ can be thought of as discretising the *normal PDE*:

$$-\nu^2 u^{(4)} - \beta^2\ddot{u} = g, \text{ in } (a,b) \subset \mathbb{R}.$$

ADVECTION DIFFUSION ODE – CHOLESKY-QR

Since as $\nu \to 0$ we know that $\underline{\underline{P}}^T \underline{\underline{P}}$ approaches $\underline{\underline{A}}^T \underline{\underline{A}}$, we can think of $\underline{\underline{P}}$ as an approximate Cholesky factor of $\underline{\underline{A}}^T \underline{\underline{A}}$. From **Cholesky-QR** we know that the Cholesky factor of $\underline{\underline{A}}^T \underline{\underline{A}}$ is the R factor of the QR decomposition of $\underline{\underline{A}}$, hence $\underline{\underline{P}}$ is a good **cross left preconditioner** for the normal equations.

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ν	$\underline{\underline{P}}$ (GMRES)	$\underline{\underline{R}}^T \underline{\underline{R}}$ (CGNE)	$\underline{\underline{P}}^T \underline{\underline{P}}$ (CGNE)
$1 \cdot 10^{-2}$	199	217	216
$5 \cdot 10^{-3}$	97	108	109
$1 \cdot 10^{-3}$	17	19	19

Table: Comparison of the number of iterations for different preconditioners for the left preconditioned normal equation. The CGNE and GMRES methods were terminated when the absolute residual was less than 10^{-5}

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n	$\underline{\underline{R}}^T \underline{\underline{R}}$ (CGNE)	$\underline{\underline{P}}^T \underline{\underline{P}}$ (CGNE)
1250	36	37
2500	69	69
5000	134	136
10000	249	251

Table: The CGNE methods were terminated when the absolute residual was less than 10^{-5}

APPLICATIONS TO THE FINITE ELEMENT METHOD

2

ADVECTION DIFFUSION PDE

We consider the classical advection-diffusion PDE in two dimensions, i.e.

$$\mathcal{L}u := -\nu\Delta u + \underline{\beta} \cdot \nabla u = f \text{ in } \Omega \subset \mathbb{R}^d,$$
$$u = g \text{ on } \partial\Omega, \text{ with } \nu \ll \|\beta\|, \nabla \cdot \beta = 0.$$

H. Elman, D. Silvester, A. Wathen, Finite Elements and Fast Iterative Solvers, 2005, *Oxford University Press*

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Finite Element Discretisation

Fix a discrete space $V_h \subset H_0^1(\Omega)$ and look for $u_h \in V_h$ such that

$$(\hat{\mathcal{L}}u_h, v_h) = \nu(\nabla u_h, \nabla v_h)_{L^2(\Omega)} + (\beta\cdot\nabla u_h, v_h)_{L^2(\Omega)} = (f, v_h)_{L^2(\Omega)} \text{ for any } v_h \in V_h.$$

THE NORMAL EQUATIONS

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We now need to understand what are the normal equations associated with the linear system,

$$A\,\underline{x} = \underline{b}, \text{ with } A_{ij} = (\hat{\mathcal{L}}\varphi_i, \varphi_j)_{L^2(\Omega)} \text{ and } b_j = (f, \varphi_j)_{L^2(\Omega)}.$$

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The first thing we need to understand is what is $\underline{\underline{A}}^T$, in fact $\underline{\underline{A}}^T$ is neither **Hilbert adjoint** of A nor the **Banach adjoint** seen as the operator $A : V_h \subset H_0^1(\Omega) \to H^{-1}(\Omega) \subset V_h'$.

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In fact, A^T is an operator itself of the form $A^T : V_h \subset H_0^1(\Omega) \to H^{-1}(\Omega) \subset V_h'$ which corresponds to the discretisation of the **Hilbert adjoint** of $\mathcal{L}$, i.e.

$$A_{ij}^T = A_{ji} = (\hat{\mathcal{L}}\varphi_j, \varphi_i)_{L^2(\Omega)} = (\varphi_j, \hat{\mathcal{L}}^*\varphi_i)_{L^2(\Omega)} = (\hat{\mathcal{L}}^*\varphi_i, \varphi_j)_{L^2(\Omega)},$$

THE NORMAL EQUATIONS – PRIMAL DUAL ERROR

If we consider the classical normal equations, i.e. $\underline{\underline{A}}^T \underline{\underline{A}}\,\underline{x} = \underline{\underline{A}}^T \underline{b}$.

Primal Dual Error

We notice that there is a primal dual error in the classical formulation of the normal equations.

$$V_h \subset H^1_0(\Omega) \xrightarrow{A} H^{-1} \subset V_h' \qquad\qquad V_h \subset H^1_0(\Omega) \xrightarrow{A^T} H^{-1} \subset V_h'$$

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To make sense of the normal equations we need to consider a Riesz map $T : V_h' \to V_h$.

$$V_h \subset H_0^1(\Omega) \xrightarrow{A} H^{-1} \subset V_h' \xrightarrow{\quad T \quad} V_h \subset H_0^1(\Omega) \xrightarrow{A^T} H^{-1} \subset V_h'$$

THE NORMAL EQUATIONS

The Riesz map gives rise to a discrete operator $T : V_h' \to V_h$, which is **symmetric and positive definite**. Therefore if we consider the normal equations with respect to the Riesz map, i.e.

$$\underline{\underline{A}}^T T \underline{\underline{A}}\,\underline{x} = \underline{\underline{A}}^T T \underline{b},$$

we can rewrite them using a Cholesky factorisation of T, i.e. $T = C^T C$.

$$(CA)^T (CA)\underline{x} = (CA)^T C\underline{b},$$

hence the previous normal equation are associated with the linear system $CA\underline{x} = C\underline{b}$.

- The normal equations are still symmetric and positive definite. Hence we can solve them using CGNE. The cross-preconditioning idea is still applicable.
- The condition number of the normal equations is the square of the condition number of the original system.

THE NORMAL EQUATIONS – L^2-RIESZ MAP

We can consider as Riesz map the L^2-Riesz map, i.e.

$$(Tf, v_h)_{L^2(\Omega)} = \langle f, v_h \rangle \text{ for any } v_h \in V_h,\ f \in V_h'$$

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Using the L^2-Riesz map the new normal is approximating, in the limit $\nu \to 0$, the problem: find $u \in H_0^1(\Omega)$ such that

$$(\beta \otimes \beta \nabla u, \nabla v)_{L^2(\Omega)} = (g, v)_{L^2(\Omega)} \text{ for any } v \in H_0^1(\Omega).$$

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ν	CGNE Iterations
$1 \cdot 10^{-2}$	4231
$5 \cdot 10^{-3}$	3803
$2.5 \cdot 10^{-3}$	3327
$1.25 \cdot 10^{-3}$	2419

Table: The CGNE methods were terminated when the absolute residual was less than 10^{-5}.

Due to the function space involved in the weak form, **we chose the wrong Riesz map**.

$$\subset H_0^1(\Omega) \longrightarrow H^{-1} \subset L^{2'} \xrightarrow{T^{-1}} L^2 \not\subset H_0^1(\Omega) \longrightarrow H^{-1} \subset V_h$$

THE NORMAL EQUATIONS – H^1-RIESZ MAP

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ν	32×32	64×64	128×128
$1 \cdot 10^{-2}$	2	2	2
$5 \cdot 10^{-3}$	3	3	3
$2.5 \cdot 10^{-3}$	3	3	3
$1.25 \cdot 10^{-3}$	3	3	3

Table: The CGNE methods were terminated when the absolute residual was less than 10^{-5}.

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THE NORMAL EQUATIONS – PRECONDITION USING THE MASS MATRIX AND AMG

Mathematical Institute

Find $u_h \in V_h$ such that $\nu^{-1}(\beta u_h, \beta v_h)_{L^2(\Omega)}$, for any $v_h \in V_h$.

ν	32×32	64×64	128×128	256×256	512×512
$1 \cdot 10^{-2}$	9	14	21	24	26
$5 \cdot 10^{-3}$	13	13	19	28	33
$2.5 \cdot 10^{-3}$	19	17	17	25	37
$1.25 \cdot 10^{-3}$	27	24	21	22	33

Table: Comparison of the number of iterations for the CGNE method preconditioned by the inversion via PETSc GAMG, for different values of ν and different mesh sizes. The wind is fixed to $\beta = (1, 0)$ and as right-hand side we consider the function $f(x, y) \equiv 1$. The CGNE method was terminated when the absolute residual was less than 10^{-5}.

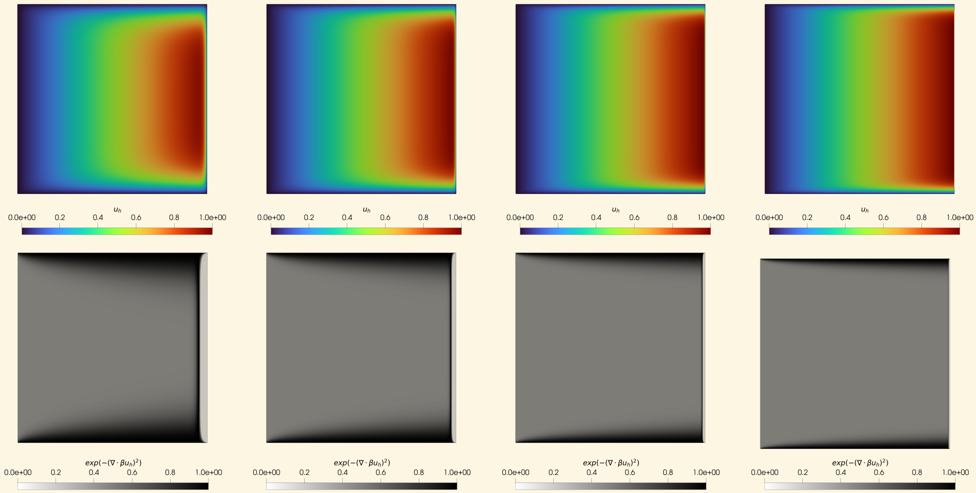

Figure: The discrete solution u_h of the advection-diffusion equation (1) for different value of ν at the finest mesh size 512×512, together with $exp(-|\nabla \cdot \beta u_h|^2)$.

THE NORMAL EQUATIONS – PRECONDITION USING THE MASS MATRIX AND AMG

Oxford Mathematical Institute

Find $u_h \in V_h$ such that $\nu^{-1}(\beta u_h, \beta v_h)_{L^2(\Omega)}$, for any $v_h \in V_h$.

ν	32×32	64×64	128×128	256×256
$1 \cdot 10^{-2}$	10	15	20	23
$5 \cdot 10^{-3}$	11	15	22	30
$2.5 \cdot 10^{-3}$	17	16	21	32
$1.25 \cdot 10^{-3}$	26	24	23	30

Table: Comparison of the number of iterations for the CGNE method preconditioned by the inversion via PETSc GAMG, for different values of ν and different mesh sizes. The wind is fixed to $\sqrt{2}\beta = (1, 1)$ and as right-hand side we consider the function $f(x, y) \equiv 1$. The CGNE method was terminated when the absolute residual was less than 10^{-5}.

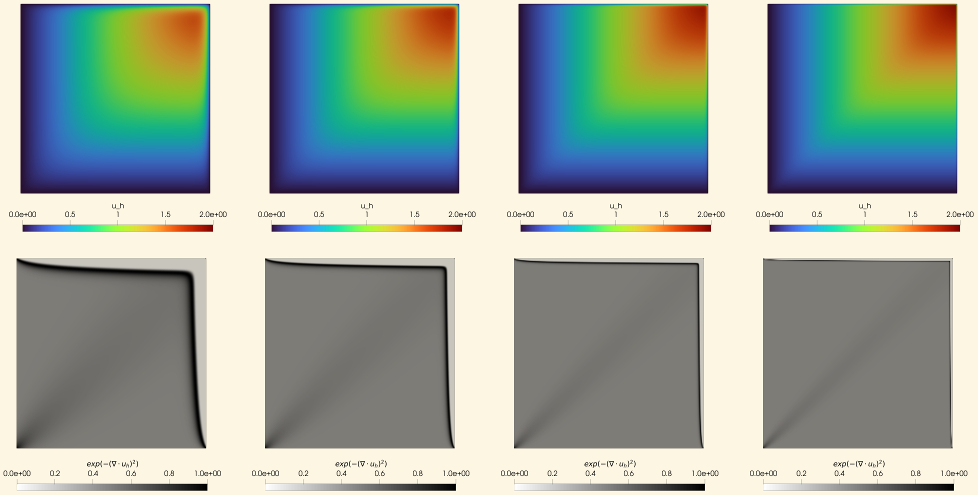

Figure: The discrete solution u_h of the convection-diffusion equation (1), with $\sqrt{2}\underline{\beta} = (1,1)$, for different values of ν at the finest mesh size 512×512, together with $exp(-|\nabla \cdot \beta u_h|^2)$.

THE NORMAL EQUATIONS – PROJECTED MASS MATRIX AND SSOR

Find $u_h \in V_h$ such that $\nu^{-1}(\Pi_\nabla \beta u_h, \Pi_\nabla \beta v_h)_{L^2(\Omega)}$, for any $v_h \in V_h$.

ν	32×32	64×64	128×128
$1 \cdot 10^{-2}$	14	22	40
$5 \cdot 10^{-3}$	16	21	33
$2.5 \cdot 10^{-3}$	22	22	29
$1.25 \cdot 10^{-3}$	30	30	34

Table: Comparison of the number of iterations for the CGNE method preconditioned by symmetric successive over-relaxation, for different values of ν and different mesh sizes. The wind is fixed to $\sqrt{2}\beta = (1,1)$ and as right-hand side we consider the function $f(x,y) \equiv 1$. The CGNE method was terminated when the absolute residual was less than 10^{-5}.

THE NORMAL EQUATIONS – PROJECTED MASS MATRIX AND GMG

Find $u_h \in V_h$ such that $\nu^{-1}(\Pi_\nabla \beta u_h, \Pi_\nabla \beta v_h)_{L^2(\Omega)}$, for any $v_h \in V_h$.

ν	32×32	64×64	128×128
$1 \cdot 10^{-2}$	4	5	8
$5 \cdot 10^{-3}$	4	5	7
$2.5 \cdot 10^{-3}$	5	5	7
$1.25 \cdot 10^{-3}$	7	7	7

Table: Comparison of the number of iterations for the CGNE method preconditioned by geometric multigird with SOR smoothing, for different values of ν and different mesh sizes. The wind is fixed to $\sqrt{2}\beta = (1,1)$ and as right-hand side we consider the function $f(x,y) \equiv 1$. The CGNE method was terminated when the absolute residual was less than 10^{-5}.

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- **We should reconsider the use of normal equations for solving linear systems arising from PDEs.**

FUTURE WORK

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- Understand how to efficiently compute the polar decomposition so that we can construct a good **cross preconditioner** starting from the normal PDE, for LSQR type methods.

THANK YOU!
Lorenzo now accepts questions.

Some more comments on the normal equations: With a focus on discretisation of partial differential equations

L. Lazzarino, Y. Nakatsukasa, Umberto Zerbinati*