Fast Iterative Solvers for Reaction-Diffusion Control Models of Chemical and Biological Processes

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17th IMA Leslie Fox Prize Meeting,
University of Strathclyde, 22 June 2015

PDE-Constrained Optimization

- A general PDE-constrained optimization problem may be written as

$$\begin{aligned} \min_{y,f} \quad & \frac{1}{2}\|y-\widehat{y}\|^2_{L_2(\Omega)} + \frac{\beta}{2}\|f\|^2_{L_2(\Omega)} \\ \text{s.t.} \quad & \mathcal{L}y = f, \quad \text{in } \Omega, \\ & y = g, \quad \text{on } \partial\Omega. \end{aligned}$$

- Applications in far-reaching areas such as flow control, semiconductor design, electromagnetic inverse problems, weather forecasting, medical imaging and finance.

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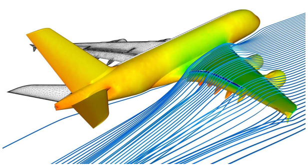
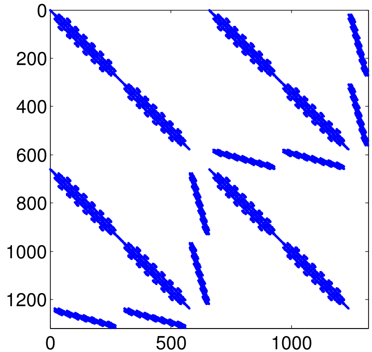
- Applications in far-reaching areas such as flow control, semiconductor design, electromagnetic inverse problems, weather forecasting, medical imaging and finance.

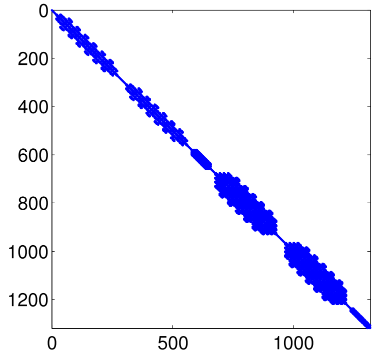
	Flow control	**Image processing**	**Chemical reactions**
State	Velocity and pressure of fluid	Image post-processing	Concentrations of reactants
Control	Energy put into system	Data-driven terms in processing	Rate at which reactants inserted



PDE-Constrained Optimization

- Problems clearly defined, but in general extremely difficult to solve.
- Using a finite element method → matrix system of very high dimension.
- Very effective approach for solving these systems is to construct iterative methods which are accelerated by powerful preconditioners.
- When solving matrix system $\mathcal{A}\mathbf{x} = \mathbf{b}$, a good preconditioner $\mathcal{P}$ will be cheap to apply & such that $\mathcal{P}^{-1}\mathcal{A}$ has desirable properties.
- Many advantages: can exploit sparsity and structure of matrices, don't have to store the entire system, can solve large problems rapidly & in parallel.





Matrix $\mathcal{A}$ & Preconditioner $\mathcal{P}$

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Saddle Point Systems

- For the problems we consider, the matrices are of *saddle point* structure:

$$\mathcal{A} = \begin{bmatrix} A & B^\top \\ B & -C \end{bmatrix}.$$

- Two preconditioners are [Kuznetsov, 1995], [Murphy, Golub & Wathen, 2000]:

$$\mathcal{P}_D = \begin{bmatrix} A & 0 \\ 0 & S \end{bmatrix}, \qquad \mathcal{P}_T = \begin{bmatrix} A & 0 \\ B & -S \end{bmatrix}.$$

- Here, $S = C + BA^{-1}B^\top$ is the (negative) *Schur complement.*
- Excellent spectral properties: if $\mathcal{P}_D^{-1}\mathcal{A}$ and $\mathcal{P}_T^{-1}\mathcal{A}$ are nonsingular [Murphy, Golub & Wathen, 2000], [Ipsen, 2001]:

$$\lambda(\mathcal{P}_D^{-1}\mathcal{A}) \in \left\{1, \frac{1}{2}(1 \pm \sqrt{5})\right\}, \qquad \text{if } C = 0,$$
$$\lambda(\mathcal{P}_T^{-1}\mathcal{A}) \in \{1\}, \qquad \text{generally.}$$

- In general A, S are not practical preconditioners, so devise approximations $\widehat{A}$, $\widehat{S}$.

$$\begin{aligned}\min_{y,f} \quad & \frac{1}{2}\|y-\widehat{y}\|^2_{L_2(\Omega)} + \frac{\beta}{2}\|f\|^2_{L_2(\Omega)} \\ \text{s.t.} \quad & -\nabla^2 y = f, \quad \text{in } \Omega, \\ & \qquad\; y = g, \quad \text{on } \partial\Omega.\end{aligned}$$

$$\min_{y,f} \quad \frac{1}{2}\|y-\widehat{y}\|^2_{L_2(\Omega)} + \frac{\beta}{2}\|f\|^2_{L_2(\Omega)}$$
$$\text{s.t.} \quad -\nabla^2 y = f, \quad \text{in } \Omega,$$
$$y = g, \quad \text{on } \partial\Omega.$$

Distributed Poisson Control

- Differentiating (with respect to **y**, **f**, **p**) the cost functional:

$$\mathcal{L}(\mathbf{y},\mathbf{f},\mathbf{p}) = \frac{1}{2}(\mathbf{y}-\widehat{\mathbf{y}})^\top M(\mathbf{y}-\widehat{\mathbf{y}}) + \frac{\beta}{2}\mathbf{f}^\top M\mathbf{f} + \mathbf{p}^\top(K\mathbf{y} - M\mathbf{f} - \mathbf{g}),$$

where M is a finite element *mass matrix*, and K a *stiffness matrix*, gives

$$\left[\begin{array}{cc|c} M & 0 & K \\ 0 & \beta M & -M \\ \hline K & -M & 0 \end{array}\right] \left[\begin{array}{c} \mathbf{y} \\ \mathbf{f} \\ \mathbf{p} \end{array}\right] = \left[\begin{array}{c} M\widehat{\mathbf{y}} \\ \mathbf{0} \\ \mathbf{g} \end{array}\right].$$

$$\min_{y,f} \quad \frac{1}{2}\|y-\widehat{y}\|_{L_2(\Omega)}^2 + \frac{\beta}{2}\|f\|_{L_2(\Omega)}^2$$
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- This is a saddle point system with

$$A = \left[\begin{array}{cc} M & 0 \\ 0 & \beta M \end{array}\right], \qquad S = KM^{-1}K + \frac{1}{\beta}M.$$

- We may precondition A using Chebyshev semi-iteration to approximate M^{-1}.

Approximating the Schur Complement – Matching Strategy

- We aim to capture both terms of the Schur complement by writing

$$S = KM^{-1}K + \frac{1}{\beta}M, \qquad \widehat{S} = \left(K + \frac{1}{\sqrt{\beta}}M\right) M^{-1} \left(K + \frac{1}{\sqrt{\beta}}M\right).$$

- This ensures that [Pearson & Wathen, 2012]:

$$\boxed{\lambda(\widehat{S}^{-1}S) \in \left[\frac{1}{2}, 1\right]}$$

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- Our preconditioner requires four ingredients:
  1. Saddle point approximation,
  2. Approximation of mass matrix by Chebyshev semi-iteration,
  3. Matching strategy for Schur complement,
  4. Effective multigrid method for $K + \frac{1}{\sqrt{\beta}}M$ to apply $\widehat{S}$.
- Only $\sim$ 15 iterations required for 6 digits of accuracy using MINRES.

J. W. Pearson and A. J. Wathen, *A New Approximation of the Schur Complement in Preconditioners for PDE-Constrained Optimization*, Numerical Linear Algebra with Applications, 2012.

Extension to Time-Dependent Problems

- When solving an analogous time-dependent (heat equation control) problem:

$$\begin{aligned} \min_{y,f} \quad & \frac{1}{2}\int_0^T \int_\Omega (y(\mathbf{x},t) - \widehat{y}(\mathbf{x},t))^2 \ \mathrm{d}\Omega\mathrm{d}t + \frac{\beta}{2}\int_0^T \int_\Omega (f(\mathbf{x},t))^2 \ \mathrm{d}\Omega\mathrm{d}t, \\ \text{s.t.} \quad & y_t - \nabla^2 y = f, \quad \text{for } (\mathbf{x},t) \in \Omega \times [0,T], \\ & y = g, \quad \text{on } \partial\Omega \times [0,T], \\ & y = y_0, \quad \text{at } t = 0, \end{aligned}$$

one is faced with a system of the form:

$$\left[\begin{array}{cc|c} \tau\mathcal{M}_{1/2} & 0 & \mathcal{K}^\top \\ 0 & \beta\tau\mathcal{M}_{1/2} & -\tau\mathcal{M} \\ \hline \mathcal{K} & -\tau\mathcal{M} & 0 \end{array}\right] \left[\begin{array}{c} \mathbf{y} \\ \mathbf{f} \\ \mathbf{p} \end{array}\right] = \left[\begin{array}{c} \tau\mathcal{M}_{1/2}\widehat{\mathbf{y}} \\ \mathbf{0} \\ \mathbf{g} \end{array}\right],$$

where

$$\mathcal{K} = \left[\begin{array}{cccc} M+\tau K & & & \\ -M & M+\tau K & & \\ & \ddots & \ddots & \\ & & -M & M+\tau K \end{array}\right],$$

$$\mathcal{M}_{1/2} = \text{blkdiag}\left(\frac{1}{2}M, M, ..., M, \frac{1}{2}M\right), \qquad \mathcal{M} = \text{blkdiag}\left(M, ..., M\right).$$

Extension to Time-Dependent Problems

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$$\min_{y,f} \quad \frac{1}{2}\int_0^T \int_\Omega (y(\mathbf{x},t)-\widehat{y}(\mathbf{x},t))^2 \ \mathrm{d}\Omega\mathrm{d}t + \frac{\beta}{2}\int_0^T \int_\Omega (f(\mathbf{x},t))^2 \ \mathrm{d}\Omega\mathrm{d}t,$$

$$\text{s.t} \qquad \begin{aligned} y_t - \nabla^2 y &= f, && \text{for } (\mathbf{x},t)\in\Omega\times[0,T], \\ y &= g, && \text{on } \partial\Omega\times[0,T], \\ y &= y_0, && \text{at } t=0, \end{aligned}$$

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- We construct our preconditioner as follows [Pearson, Stoll & Wathen, 2012]:

$$S = \frac{1}{\tau}\mathcal{K}\mathcal{M}_{1/2}^{-1}\mathcal{K}^\top + \frac{\tau}{\beta}\mathcal{M}\mathcal{M}_{1/2}^{-1}\mathcal{M}, \quad \widehat{S} = \frac{1}{\tau}\left(\mathcal{K}+\frac{\tau}{\sqrt{\beta}}\mathcal{M}\right)\mathcal{M}_{1/2}^{-1}\left(\mathcal{K}+\frac{\tau}{\sqrt{\beta}}\mathcal{M}\right)^\top$$

$$\hookrightarrow \quad \mathcal{P} = \left[\begin{array}{ccc} \tau\mathcal{M}_{1/2} & 0 & 0 \\ 0 & \beta\tau\mathcal{M}_{1/2} & 0 \\ 0 & 0 & \frac{1}{\tau}\left(\mathcal{K}+\frac{\tau}{\sqrt{\beta}}\mathcal{M}\right)\mathcal{M}_{1/2}^{-1}\left(\mathcal{K}+\frac{\tau}{\sqrt{\beta}}\mathcal{M}\right)^\top \end{array}\right].$$

$$S_G = XX^\top + YY^\top \qquad X,\ Y \text{ real}$$
$$\widehat{S}_G = (X+Y)(X+Y)^\top \qquad S_G,\ \widehat{S}_G \text{ invertible}$$

$$\rightarrow \quad \boxed{\lambda(\widehat{S}_G^{-1} S_G) \geqslant \frac{1}{2}}$$

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Uses of Matching Strategy

- Complex valued linear algebraic systems [Axelsson et al., 2014], [Bai et al., 2013].
- Cahn-Hilliard models in imaging [Bosch, Stoll & Benner, 2014], [Boyanova, Do-Quang & Neytcheva, 2012].
- Phase Field Crystal equation in soft matter physics [Praetorius & Voigt, 2015].

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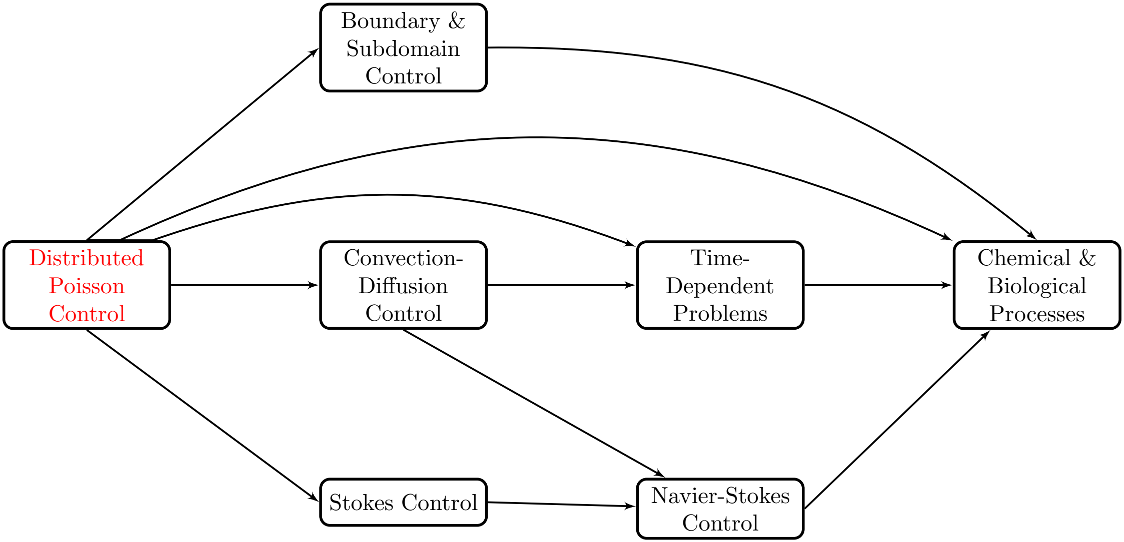
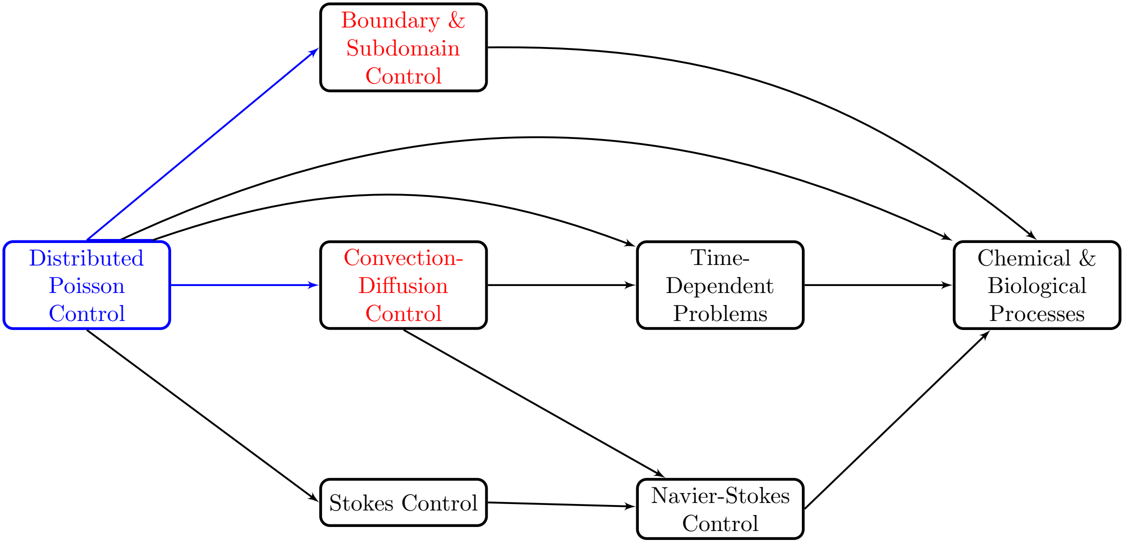
- Phase Field Crystal equation in soft matter physics [Praetorius & Voigt, 2015].
- Interior point methods for linear (and quadratic) programming:

$$\mathcal{A} = \begin{bmatrix} A_1 & 0 & B_1^\top \\ 0 & A_2 & B_2^\top \\ B_1 & B_2 & 0 \end{bmatrix}, \qquad A_1 < A_2.$$

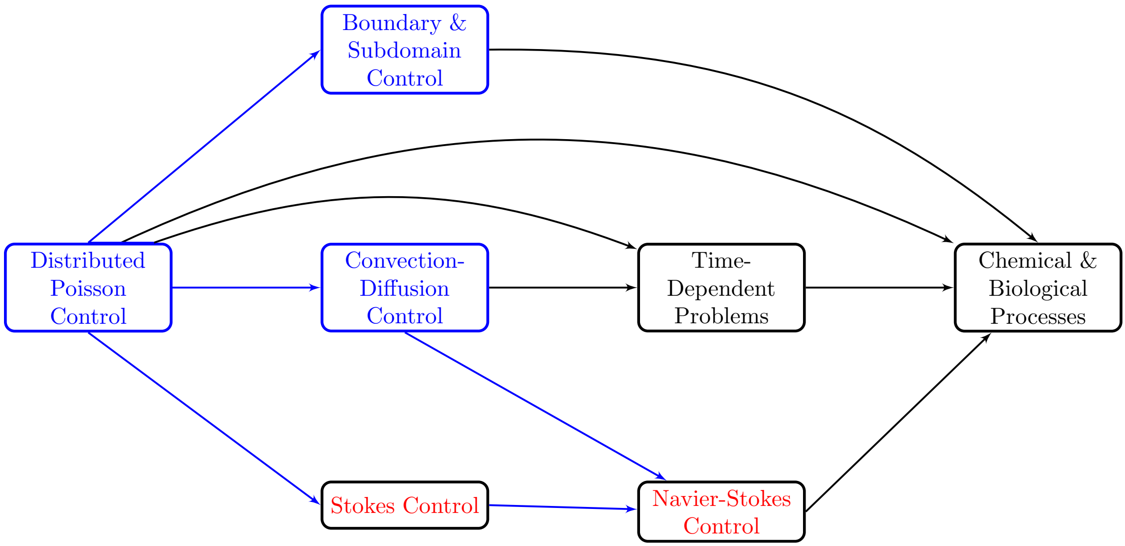
The Schur complement may be approximated as follows:

$$S = B_1 A_1^{-1} B_1^\top + B_2 A_2^{-1} B_2^\top \quad \rightarrow \quad \widehat{S} = \left(B_1 + \widehat{D}\right) A_1^{-1} \left(B_1 + \widehat{D}\right)^\top,$$
$$\widehat{D} A_1^{-1} \widehat{D} \approx \operatorname{diag}\left(B_2 A_2^{-1} B_2^\top\right).$$


Boundary & Subdomain Control
Distributed Poisson Control
Convection-Diffusion Control
Time-Dependent Problems
Chemical & Biological Processes
Stokes Control
Navier-Stokes Control

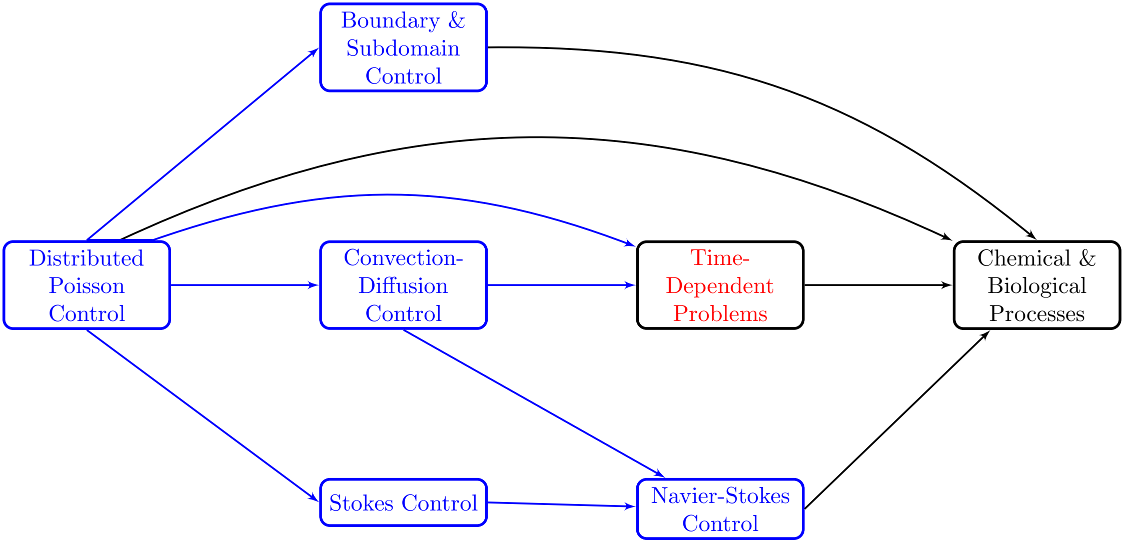


JWP and A. J. Wathen, *Fast Iterative Solvers for Convection-Diffusion Control Problems*, Electronic Transactions on Numerical Analysis, 2013.

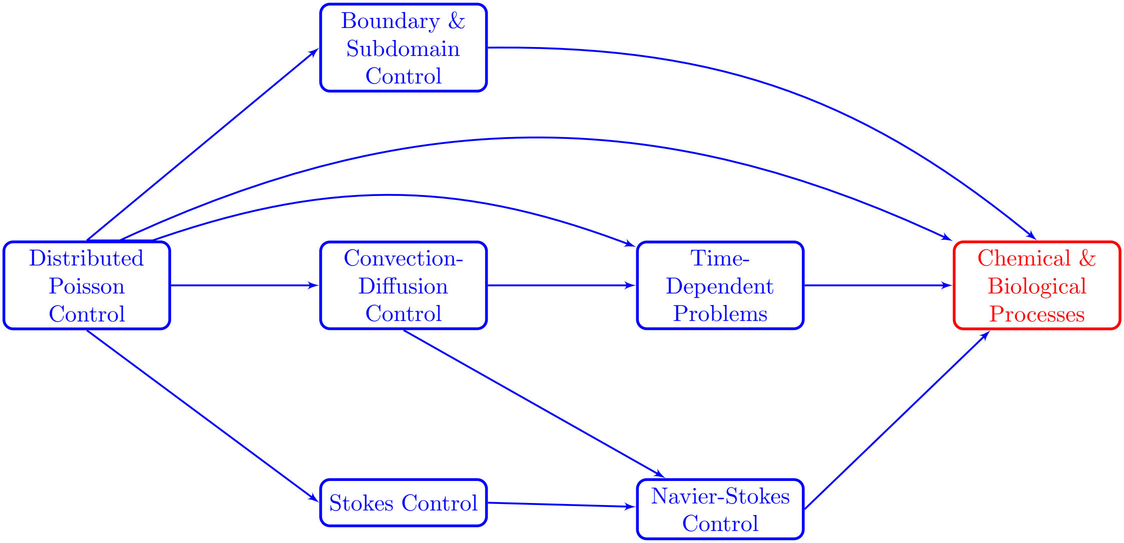


JWP, *On the Development of Parameter-Robust Preconditioners and Commutator Arguments for Solving Stokes Control Problems*, Electronic Transactions on Numerical Analysis, 2015.

JWP, *Preconditioned Iterative Methods for Navier-Stokes Control Problems*, Journal of Computational Physics, 2015.



JWP, M. Stoll and A. J. Wathen, *Regularization-Robust Preconditioners for PDE-Constrained Optimization Problems*, SIAM Journal on Matrix Analysis and Applications, 2012.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Control

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Reaction-Diffusion Control from Chemical Processes

- A problem which we are now keen to consider is the following optimal control problem involving reaction-diffusion equations. We wish to minimize

$$\mathcal{J}(u,v,c)=\frac{\alpha_u}{2}\left\|u-\widehat{u}\right\|^2_{L_2(Q)}+\frac{\alpha_v}{2}\left\|v-\widehat{v}\right\|^2_{L_2(Q)}+\frac{\alpha_c}{2}\left\|c\right\|^2_{L_2(\Sigma)},$$

subject to the following PDE constraints:

$$\begin{aligned}
u_t-D_1\nabla^2u+k_1u &= -\gamma_1uv, && \text{in } Q:=\Omega\times[0,T],\\
v_t-D_2\nabla^2v+k_2v &= -\gamma_2uv, && \text{in } Q,\\
D_1\frac{\partial u}{\partial n} &= c, && \text{on } \Sigma:=\partial\Omega\times[0,T],\\
D_2\frac{\partial v}{\partial n}+\epsilon v &= 0, && \text{on } \Sigma,\\
u(\mathbf{x},0) &= u_0(\mathbf{x}), && \text{in } \Omega,\\
v(\mathbf{x},0) &= v_0(\mathbf{x}), && \text{in } \Omega.
\end{aligned}$$

- We may also incorporate the control constraints:

$$c\in C_{ad}:=\{c\in L_\infty(\Sigma):\ c_a\leqslant c\leqslant c_b \text{ a.e. on } \Sigma\}.$$

- Examined in e.g. [Barthel, John & Tröltzsch, 2010], [Griesse & Volkwein, 2006].

Optimality Conditions

- On the continuous level, we consider the Lagrangian

$$\begin{aligned}\mathcal{L}(u,v,c,p,q) = {} & \frac{\alpha_u}{2}\|u-\widehat{u}\|^2_{L_2(Q)} + \frac{\alpha_v}{2}\|v-\widehat{v}\|^2_{L_2(Q)} + \frac{\alpha_c}{2}\|c\|^2_{L_2(\partial Q)} \\ & + \int_Q p_\Omega\big(u_t - D_1\nabla^2 u + k_1 u + \gamma_1 uv\big) \\ & + \int_Q q_\Omega\big(v_t - D_2\nabla^2 v + k_2 v + \gamma_2 uv\big) \\ & + \int_{\partial Q} p_{\partial\Omega}\left(D_1\frac{\partial u}{\partial n} - c\right) + \int_{\partial Q} q_{\partial\Omega}\left(D_2\frac{\partial v}{\partial n} + \epsilon v\right).\end{aligned}$$

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- Differentiating with respect to p, q gives the *state equations*:

$$u_t - D_1\nabla^2 u + k_1 u = -\gamma_1 uv, \qquad v_t - D_2\nabla^2 v + k_2 v = -\gamma_2 uv.$$

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& + \int_Q p_\Omega\big(u_t - D_1\nabla^2 u + k_1 u + \gamma_1 uv\big) \\
& + \int_Q q_\Omega\big(v_t - D_2\nabla^2 v + k_2 v + \gamma_2 uv\big) \\
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- Differentiating with respect to p, q gives the *state equations*:

$$u_t - D_1\nabla^2 u + k_1 u = -\gamma_1 uv, \qquad v_t - D_2\nabla^2 v + k_2 v = -\gamma_2 uv.$$

- Differentiating with respect to u, v gives the *adjoint equations*:

$$
\begin{aligned}
-p_t - D_1\nabla^2 p + k_1 p + \gamma_1 pv + \gamma_2 qv + \alpha_u u &= \alpha_u\widehat{u}, \\
-q_t - D_2\nabla^2 q + k_2 q + \gamma_2 qu + \gamma_1 pu + \alpha_v v &= \alpha_v\widehat{v}.
\end{aligned}
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- Differentiating with respect to u, v gives the *adjoint equations*:

$$\begin{aligned}-p_t - D_1\nabla^2 p + k_1 p + \gamma_1 pv + \gamma_2 qv + \alpha_u u &= \alpha_u \widehat{u}, \\ -q_t - D_2\nabla^2 q + k_2 q + \gamma_2 qu + \gamma_1 pu + \alpha_v v &= \alpha_v \widehat{v}.\end{aligned}$$

- Differentiating with respect to c gives the *gradient equation*:

$$\alpha_c c - p = 0, \quad \text{on } \partial Q.$$

Newton Iteration – Matrix System

- In matrix form, the Newton system is written as

$$\begin{bmatrix} \alpha_u \mathrm{Id} & \gamma_1\bar{p}+\gamma_2\bar{q} & 0 & \mathcal{D}_u' & \gamma_2\bar{v} \\ \gamma_1\bar{p}+\gamma_2\bar{q} & \alpha_v \mathrm{Id} & 0 & \gamma_1\bar{u} & \mathcal{D}_v' \\ 0 & 0 & \alpha_c D_1^{-1}\mathrm{Id} & -D_1^{-1}\mathrm{Id} & 0 \\ \mathcal{D}_u & \gamma_1\bar{u} & -D_1^{-1}\mathrm{Id} & 0 & 0 \\ \gamma_2\bar{v} & \mathcal{D}_v & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} s_u \\ s_v \\ s_c \\ s_p \\ s_q \end{bmatrix} = b,$$

where

$$\mathcal{D}_u = \frac{\partial}{\partial t} - D_1\nabla^2 + k_1\mathrm{Id} + \gamma_1\bar{v}, \qquad \mathcal{D}_u' = -\frac{\partial}{\partial t} - D_1\nabla^2 + k_1\mathrm{Id} + \gamma_1\bar{v},$$
$$\mathcal{D}_v = \frac{\partial}{\partial t} - D_2\nabla^2 + k_2\mathrm{Id} + \gamma_2\bar{u}, \qquad \mathcal{D}_v' = -\frac{\partial}{\partial t} - D_2\nabla^2 + k_2\mathrm{Id} + \gamma_2\bar{u}.$$

- The vector b represents the terms from the previous iteration:

$$\begin{bmatrix} \alpha_u\widehat{u} - \left(-\bar{p}_t - D_1\nabla^2\bar{p} + k_1\bar{p} + \gamma_1\bar{p}\bar{v} + \gamma_2\bar{q}\bar{v} + \alpha_u\bar{u}\right) \\ \alpha_v\widehat{v} - \left(-\bar{q}_t - D_2\nabla^2\bar{q} + k_2\bar{q} + \gamma_2\bar{q}\bar{u} + \gamma_1\bar{p}\bar{u} + \alpha_v\bar{v}\right) \\ -(\alpha_c\bar{c} - \bar{p}) \\ -\left(\bar{u}_t - D_1\nabla^2\bar{u} + k_1\bar{u} + \gamma_1\bar{u}\bar{v}\right) \\ -\left(\bar{v}_t - D_2\nabla^2\bar{v} + k_2\bar{v} + \gamma_2\bar{u}\bar{v}\right) \end{bmatrix}.$$

Newton Iteration – Matrix System

- Applying a finite element method at the Newton step, we obtain the matrix:

$$\begin{bmatrix} \tau\alpha_u \mathbf{M} & \tau(\gamma_1 \mathbf{M}_p + \gamma_2 \mathbf{M}_q) & 0 & \mathbf{L}_{u,C}^\top & \tau\gamma_2 \mathbf{M}_v \\ \tau(\gamma_1 \mathbf{M}_p + \gamma_2 \mathbf{M}_q) & \tau\alpha_v \mathbf{M} & 0 & \tau\gamma_1 \mathbf{M}_u & \mathbf{L}_{v,C}^\top \\ 0 & 0 & \tau\alpha_c D_1^{-1} \mathbf{M}_\Gamma & -\tau D_1^{-1} \mathbf{N}^\top & 0 \\ \mathbf{L}_{u,C} & \tau\gamma_1 \mathbf{M}_u & -\tau D_1^{-1} \mathbf{N} & 0 & 0 \\ \tau\gamma_2 \mathbf{M}_v & \mathbf{L}_{v,C} & 0 & 0 & 0 \end{bmatrix},$$

  where

$$\begin{aligned} \mathbf{L}_{u,C} &= \mathbf{M}_E + \tau D_1 \mathbf{K} + \tau k_1 \mathbf{M} + \tau\gamma_1 \mathbf{M}_v, \\ \mathbf{L}_{v,C} &= \mathbf{M}_E + \tau D_2 \mathbf{K} + \tau k_2 \mathbf{M} + \tau\gamma_2 \mathbf{M}_u. \end{aligned}$$

- Here $\mathbf{M}$ and $\mathbf{K}$ are block diagonal matrices with mass and stiffness matrices for each time-step, $\mathbf{M}_\Gamma$ is associated boundary mass matrix, $\mathbf{N}$ the trace operator mapping onto the boundary, and $\mathbf{M}_E$ mass matrices from time-stepping.
- All other $\mathbf{M}_\psi = \text{blkdiag}(M_\psi, \ldots, M_\psi)$ are obtained from evaluating integrals of the form $[M_\psi]_{ij} = \int \psi \phi_i \phi_j$ for each matrix entry.

Newton Iteration – Matrix System

$$\begin{bmatrix} \tau\alpha_u\mathbf{M} & \tau(\gamma_1\mathbf{M}_p+\gamma_2\mathbf{M}_q) & 0 & \mathbf{L}_{u,C}^\top & \tau\gamma_2\mathbf{M}_v \\ \tau(\gamma_1\mathbf{M}_p+\gamma_2\mathbf{M}_q) & \tau\alpha_v\mathbf{M} & 0 & \tau\gamma_1\mathbf{M}_u & \mathbf{L}_{v,C}^\top \\ 0 & 0 & \tau\alpha_c D_1^{-1}\mathbf{M}_\Gamma & -\tau D_1^{-1}\mathbf{N}^\top & 0 \\ \mathbf{L}_{u,C} & \tau\gamma_1\mathbf{M}_u & -\tau D_1^{-1}\mathbf{N} & 0 & 0 \\ \tau\gamma_2\mathbf{M}_v & \mathbf{L}_{v,C} & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \mathbf{s}_u \\ \mathbf{s}_v \\ \mathbf{s}_c \\ \mathbf{s}_p \\ \mathbf{s}_q \end{bmatrix} = \mathbf{b}$$

- The vector $\mathbf{b}$ represents the discretization of

$$\begin{bmatrix} \int \alpha_u\widehat{u} - \int\left(-\bar{p}_t - D_1\nabla^2\bar{p} + k_1\bar{p} + \gamma_1\bar{p}\bar{v} + \gamma_2\bar{q}\bar{v} + \alpha_u\bar{u}\right) \\ \int \alpha_v\widehat{v} - \int\left(-\bar{q}_t - D_2\nabla^2\bar{q} + k_2\bar{q} + \gamma_2\bar{q}\bar{u} + \gamma_1\bar{p}\bar{u} + \alpha_v\bar{v}\right) \\ -\int(\alpha_c\bar{c} - \bar{p}) \\ -\int\left(\bar{u}_t - D_1\nabla^2\bar{u} + k_1\bar{u} + \gamma_1\bar{u}\bar{v}\right) \\ -\int\left(\bar{v}_t - D_2\nabla^2\bar{v} + k_2\bar{v} + \gamma_2\bar{u}\bar{v}\right) \end{bmatrix},$$

at each time-step.

$$\left[\begin{array}{ccc|cc}
\tau\alpha_u\mathbf{M} & \tau(\gamma_1\mathbf{M}_p+\gamma_2\mathbf{M}_q) & 0 & \mathbf{L}_{u,C}^\top & \tau\gamma_2\mathbf{M}_v \\
\tau(\gamma_1\mathbf{M}_p+\gamma_2\mathbf{M}_q) & \tau\alpha_v\mathbf{M} & 0 & \tau\gamma_1\mathbf{M}_u & \mathbf{L}_{v,C}^\top \\
0 & 0 & \tau\alpha_c D_1^{-1}\mathbf{M}_\Gamma & -\tau D_1^{-1}\mathbf{N}^\top & 0 \\
\hline
\mathbf{L}_{u,C} & \tau\gamma_1\mathbf{M}_u & -\tau D_1^{-1}\mathbf{N} & 0 & 0 \\
\tau\gamma_2\mathbf{M}_v & \mathbf{L}_{v,C} & 0 & 0 & 0
\end{array}\right]$$

Preconditioning the Matrix System – $(1,1)$-block

- Let us apply saddle point theory when approximating the $(1,1)$-block, and take

$$\widehat{A}=\tau\left[\begin{array}{ccc}
\alpha_u\mathbf{M}-\alpha_v^{-1}(\gamma_1\mathbf{M}_p+\gamma_2\mathbf{M}_q)\mathbf{M}^{-1}(\gamma_1\mathbf{M}_p+\gamma_2\mathbf{M}_q) & 0 & 0 \\
\gamma_1\mathbf{M}_p+\gamma_2\mathbf{M}_q & \alpha_v\mathbf{M} & 0 \\
0 & 0 & \alpha_c D_1^{-1}\mathbf{M}_\Gamma
\end{array}\right].$$

- We replace $\mathbf{M}^{-1}$ with $[\mathrm{diag}(\mathbf{M})]^{-1}$, and apply Chebyshev semi-iteration to approximate $\mathbf{M}_\Gamma^{-1}$.
- Preconditioner will be non-symmetric → apply BICG, GMRES, or other non-symmetric solver.

JWP and M. Stoll, *Fast Iterative Solution of Reaction-Diffusion Control Problems Arising from Chemical Reactions*, SIAM Journal on Scientific Computing, 2013.

$$\left[\begin{array}{ccc|cc}
\tau\alpha_u\mathbf{M} & \tau(\gamma_1\mathbf{M}_p+\gamma_2\mathbf{M}_q) & 0 & \mathbf{L}_{u,C}^\top & \tau\gamma_2\mathbf{M}_v \\
\tau(\gamma_1\mathbf{M}_p+\gamma_2\mathbf{M}_q) & \tau\alpha_v\mathbf{M} & 0 & \tau\gamma_1\mathbf{M}_u & \mathbf{L}_{v,C}^\top \\
0 & 0 & \tau\alpha_c D_1^{-1}\mathbf{M}_\Gamma & -\tau D_1^{-1}\mathbf{N}^\top & 0 \\
\hline
\mathbf{L}_{u,C} & \tau\gamma_1\mathbf{M}_u & -\tau D_1^{-1}\mathbf{N} & 0 & 0 \\
\tau\gamma_2\mathbf{M}_v & \mathbf{L}_{v,C} & 0 & 0 & 0
\end{array}\right]$$

Preconditioning the Matrix System – Schur complement

- We now approximate

$$S=\frac{1}{\tau}\left[\begin{array}{cc}\mathbf{L}_{u,C} & \tau\gamma_1\mathbf{M}_u \\ \tau\gamma_2\mathbf{M}_v & \mathbf{L}_{v,C}\end{array}\right]\mathbf{A}_{(1,2)}^{-1}\left[\begin{array}{cc}\mathbf{L}_{u,C}^\top & \tau\gamma_2\mathbf{M}_v \\ \tau\gamma_1\mathbf{M}_u & \mathbf{L}_{v,C}^\top\end{array}\right]+\frac{\tau}{\alpha_c D_1}\left[\begin{array}{cc}\mathbf{N}\mathbf{M}_\Gamma^{-1}\mathbf{N}^\top & 0 \\ 0 & 0\end{array}\right],$$

  where

$$\mathbf{A}_{(1,2)}=\left[\begin{array}{cc}\alpha_u\mathbf{M} & \gamma_1\mathbf{M}_p+\gamma_2\mathbf{M}_q \\ \gamma_1\mathbf{M}_p+\gamma_2\mathbf{M}_q & \alpha_v\mathbf{M}\end{array}\right].$$

- We make use of our matching strategy derived earlier to write:

$$\widehat{S}=\frac{1}{\tau}\left[\begin{array}{cc}\mathbf{L}_{u,C}+\widehat{\mathbf{M}} & \tau\gamma_1\mathbf{M}_u \\ \tau\gamma_2\mathbf{M}_v & \mathbf{L}_{v,C}\end{array}\right]\mathbf{A}_{(1,2)}^{-1}\left[\begin{array}{cc}\mathbf{L}_{u,C}^\top+\widehat{\mathbf{M}} & \tau\gamma_2\mathbf{M}_v \\ \tau\gamma_1\mathbf{M}_u & \mathbf{L}_{v,C}^\top\end{array}\right].$$

$$S = \frac{1}{\tau}\left[\begin{array}{cc} \mathbf{L}_{u,C} & \tau\gamma_1\mathbf{M}_u \\ \tau\gamma_2\mathbf{M}_v & \mathbf{L}_{v,C} \end{array}\right]\mathbf{A}_{(1,2)}^{-1}\left[\begin{array}{cc} \mathbf{L}_{u,C}^\top & \tau\gamma_2\mathbf{M}_v \\ \tau\gamma_1\mathbf{M}_u & \mathbf{L}_{v,C}^\top \end{array}\right] + \frac{\tau}{\alpha_c D_1}\left[\begin{array}{cc} \mathbf{N}\mathbf{M}_\Gamma^{-1}\mathbf{N}^\top & 0 \\ 0 & 0 \end{array}\right]$$

$$\widehat{S} = \frac{1}{\tau}\left[\begin{array}{cc} \mathbf{L}_{u,C} + \widehat{\mathbf{M}} & \tau\gamma_1\mathbf{M}_u \\ \tau\gamma_2\mathbf{M}_v & \mathbf{L}_{v,C} \end{array}\right]\mathbf{A}_{(1,2)}^{-1}\left[\begin{array}{cc} \mathbf{L}_{u,C}^\top + \widehat{\mathbf{M}} & \tau\gamma_2\mathbf{M}_v \\ \tau\gamma_1\mathbf{M}_u & \mathbf{L}_{v,C}^\top \end{array}\right]$$

Preconditioning the Matrix System – Schur complement

- We select $\widehat{\mathbf{M}}$ such that

$$\frac{1}{\tau}\begin{bmatrix} \widehat{\mathbf{M}} & 0 \\ 0 & 0 \end{bmatrix}\begin{bmatrix} \alpha_u\mathbf{M} & \gamma_1\mathbf{M}_p + \gamma_2\mathbf{M}_q \\ \gamma_1\mathbf{M}_p + \gamma_2\mathbf{M}_q & \alpha_v\mathbf{M} \end{bmatrix}^{-1}\begin{bmatrix} \widehat{\mathbf{M}} & 0 \\ 0 & 0 \end{bmatrix} \approx \frac{\tau}{\alpha_c D_1}\begin{bmatrix} \mathbf{N}\mathbf{M}_\Gamma^{-1}\mathbf{N}^\top & 0 \\ 0 & 0 \end{bmatrix}.$$

$$S = \frac{1}{\tau}\begin{bmatrix} \mathbf{L}_{u,C} & \tau\gamma_1\mathbf{M}_u \\ \tau\gamma_2\mathbf{M}_v & \mathbf{L}_{v,C} \end{bmatrix} \mathbf{A}_{(1,2)}^{-1} \begin{bmatrix} \mathbf{L}_{u,C}^\top & \tau\gamma_2\mathbf{M}_v \\ \tau\gamma_1\mathbf{M}_u & \mathbf{L}_{v,C}^\top \end{bmatrix} + \frac{\tau}{\alpha_c D_1}\begin{bmatrix} \mathbf{N}\mathbf{M}_\Gamma^{-1}\mathbf{N}^\top & 0 \\ 0 & 0 \end{bmatrix}$$

$$\widehat{S} = \frac{1}{\tau}\begin{bmatrix} \mathbf{L}_{u,C} + \widehat{\mathbf{M}} & \tau\gamma_1\mathbf{M}_u \\ \tau\gamma_2\mathbf{M}_v & \mathbf{L}_{v,C} \end{bmatrix} \mathbf{A}_{(1,2)}^{-1} \begin{bmatrix} \mathbf{L}_{u,C}^\top + \widehat{\mathbf{M}} & \tau\gamma_2\mathbf{M}_v \\ \tau\gamma_1\mathbf{M}_u & \mathbf{L}_{v,C}^\top \end{bmatrix}$$

Preconditioning the Matrix System – Schur complement

- We select $\widehat{\mathbf{M}}$ such that

$$\frac{1}{\tau}\begin{bmatrix} \widehat{\mathbf{M}} & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \alpha_u\mathbf{M} & \gamma_1\mathbf{M}_p + \gamma_2\mathbf{M}_q \\ \gamma_1\mathbf{M}_p + \gamma_2\mathbf{M}_q & \alpha_v\mathbf{M} \end{bmatrix}^{-1} \begin{bmatrix} \widehat{\mathbf{M}} & 0 \\ 0 & 0 \end{bmatrix} \approx \frac{\tau}{\alpha_c D_1}\begin{bmatrix} \mathbf{N}\mathbf{M}_\Gamma^{-1}\mathbf{N}^\top & 0 \\ 0 & 0 \end{bmatrix}.$$

- This implies that

$$\frac{1}{\tau}\widehat{\mathbf{M}}\left(\alpha_u\mathbf{M} - \alpha_v^{-1}\mathbf{M}_{p,q}^{(1,2)}\right)^{-1}\widehat{\mathbf{M}} \approx \frac{\tau}{\alpha_c D_1}\mathbf{N}\mathbf{M}_\Gamma^{-1}\mathbf{N}^\top,$$

where $\mathbf{M}_{p,q}^{(1,2)} := (\gamma_1\mathbf{M}_p + \gamma_2\mathbf{M}_q)\mathbf{M}^{-1}(\gamma_1\mathbf{M}_p + \gamma_2\mathbf{M}_q)$.

- An efficient and accurate approximation is a diagonal matrix with

$$[\widehat{\mathbf{M}}]_{jj} = \frac{\tau}{\sqrt{\alpha_c D_1}}\left|\left[\left(\alpha_u\mathbf{M} - \alpha_v^{-1}\mathbf{M}_{p,q}^{(1,2)}\right)\right]_{jj}\right|^{1/2} \cdot [\mathbf{N}\mathbf{M}_\Gamma^{-1}\mathbf{N}^\top]_{jj}^{1/2}.$$

$$\left[\begin{array}{ccc|cc} \tau\alpha_u\mathbf{M} & 0 & 0 & \mathbf{L}_{u,C}^\top & \tau\gamma_2\mathbf{M}_v \\ 0 & \tau\alpha_v\mathbf{M} & 0 & \tau\gamma_1\mathbf{M}_u & \mathbf{L}_{v,C}^\top \\ 0 & 0 & \tau\alpha_c D_1^{-1}\mathbf{M}_\Gamma & -\tau D_1^{-1}\mathbf{N}^\top & 0 \\ \hline \mathbf{L}_{u,C} & \tau\gamma_1\mathbf{M}_u & -\tau D_1^{-1}\mathbf{N} & 0 & 0 \\ \tau\gamma_2\mathbf{M}_v & \mathbf{L}_{v,C} & 0 & 0 & 0 \end{array}\right]$$

Deriving $\widehat{S}$ – Gauss-Newton iteration

- Within the matching strategy, we select $\widehat{\mathbf{M}}$ such that

$$\frac{1}{\tau}\begin{bmatrix} \widehat{\mathbf{M}} & 0 \\ 0 & 0 \end{bmatrix}\begin{bmatrix} \alpha_u\mathbf{M} & 0 \\ 0 & \alpha_v\mathbf{M} \end{bmatrix}^{-1}\begin{bmatrix} \widehat{\mathbf{M}} & 0 \\ 0 & 0 \end{bmatrix} \approx \frac{\tau}{\alpha_c D_1}\begin{bmatrix} \mathbf{N}\mathbf{M}_\Gamma^{-1}\mathbf{N}^\top & 0 \\ 0 & 0 \end{bmatrix}.$$

- The resulting approximation $\widehat{\mathbf{M}}$ has diagonal entries given by

$$[\widehat{\mathbf{M}}]_{jj} = \tau\sqrt{\frac{\alpha_u}{\alpha_c D_1}}\,[\mathbf{M}]_{jj}^{1/2}\cdot[\mathbf{N}\mathbf{M}_\Gamma^{-1}\mathbf{N}^\top]_{jj}^{1/2}.$$

$$\left[\begin{array}{ccc|cc} \tau\alpha_u\mathbf{M} & \gamma_1\mathbf{M}_p+\gamma_2\mathbf{M}_q & 0 & \mathbf{L}_{u,C}^\top & \tau\gamma_2\mathbf{M}_v \\ \gamma_1\mathbf{M}_p+\gamma_2\mathbf{M}_q & \tau\alpha_v\mathbf{M} & 0 & \tau\gamma_1\mathbf{M}_u & \mathbf{L}_{v,C}^\top \\ 0 & 0 & \tau D_1^{-1}(\alpha_c\mathbf{M}_\Gamma+\varepsilon^{-1}\mathbf{G}_{\mathbb{A}}) & -\tau D_1^{-1}\mathbf{N}^\top & 0 \\ \hline \mathbf{L}_{u,C} & \tau\gamma_1\mathbf{M}_u & -\tau D_1^{-1}\mathbf{N} & 0 & 0 \\ \tau\gamma_2\mathbf{M}_v & \mathbf{L}_{v,C} & 0 & 0 & 0 \end{array}\right]$$

Deriving $\widehat{S}$ – Control constraints

- Within the matching strategy, we select $\widehat{\mathbf{M}}$ such that

$$\frac{1}{\tau}\left[\begin{array}{cc} \widehat{\mathbf{M}} & 0 \\ 0 & 0 \end{array}\right]\left[\begin{array}{cc} \alpha_u\mathbf{M} & \gamma_1\mathbf{M}_p+\gamma_2\mathbf{M}_q \\ \gamma_1\mathbf{M}_p+\gamma_2\mathbf{M}_q & \alpha_v\mathbf{M} \end{array}\right]^{-1}\left[\begin{array}{cc} \widehat{\mathbf{M}} & 0 \\ 0 & 0 \end{array}\right]$$
$$\approx \frac{\tau}{D_1}\left[\begin{array}{cc} \mathbf{N}(\alpha_c\mathbf{M}_\Gamma+\varepsilon^{-1}\mathbf{G}_{\mathbb{A}})^{-1}\mathbf{N}^\top & 0 \\ 0 & 0 \end{array}\right].$$

- The resulting approximation $\widehat{\mathbf{M}}$ has diagonal entries given by

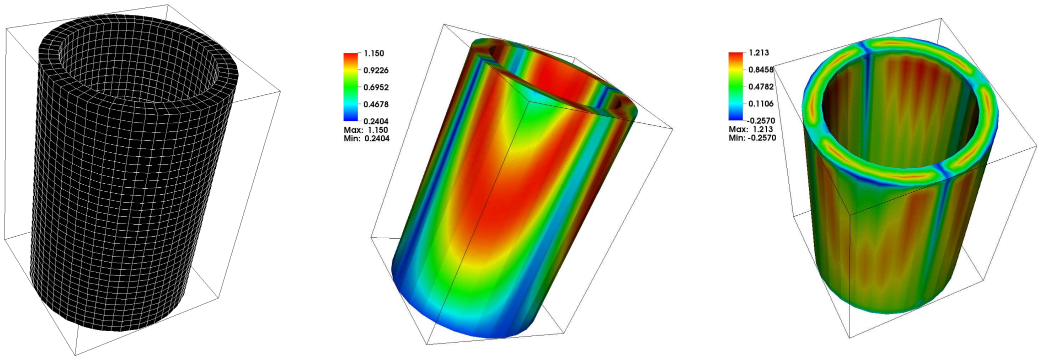
$$[\widehat{\mathbf{M}}]_{jj} = \frac{\tau}{\sqrt{\alpha_c D_1}}\left|\left[\left(\alpha_u\mathbf{M}-\alpha_v^{-1}\mathbf{M}_{p,q}^{(1,2)}\right)\right]_{jj}\right|^{1/2}\cdot\left[\mathbf{N}\left(\alpha_c\mathbf{M}_\Gamma+\varepsilon^{-1}\mathbf{G}_{\mathbb{A}}\right)^{-1}\mathbf{N}^\top\right]_{jj}^{1/2}.$$

$$\widehat{S} = \frac{1}{\tau} \begin{bmatrix} \mathbf{L}_{u,C} + \widehat{\mathbf{M}} & \tau\gamma_1 \mathbf{M}_u \\ \tau\gamma_2 \mathbf{M}_v & \mathbf{L}_{v,C} \end{bmatrix} \mathbf{A}_{(1,2)}^{-1} \begin{bmatrix} \mathbf{L}_{u,C}^\top + \widehat{\mathbf{M}} & \tau\gamma_2 \mathbf{M}_v \\ \tau\gamma_1 \mathbf{M}_u & \mathbf{L}_{v,C}^\top \end{bmatrix}$$

Some Observations

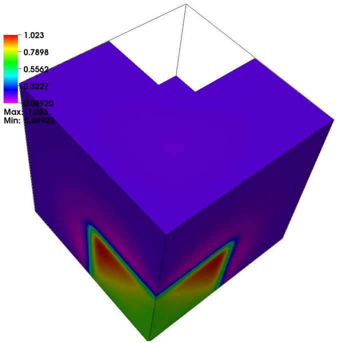
- To apply $\widehat{S}^{-1}$ in practice, use fixed number of iterations of an Uzawa scheme, coupled with algebraic multigrid routine to approximate the diagonal blocks.
- Good lower bound of $\lambda(\widehat{S}^{-1}S)$.
- Greater variation in upper bound due to range of parameters: mesh size h, τ, α_u, α_v, α_c, D_1, D_2, k_1, k_2, γ_1, γ_2, ϵ, c_a, c_b, ε.
- Best case scenario: when one term in S strongly dominates.
- Worst case scenario: when first term of S is (close to) indefinite.

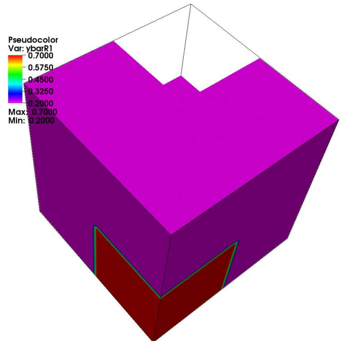
$$\widehat{u} = t\,|\sin(2x_1x_2x_3)| + 0.3, \quad \widehat{v} = 0, \quad k_1 = k_2 = D_1 = D_2 = 1, \quad \gamma_1 = \gamma_2 = 0.15$$

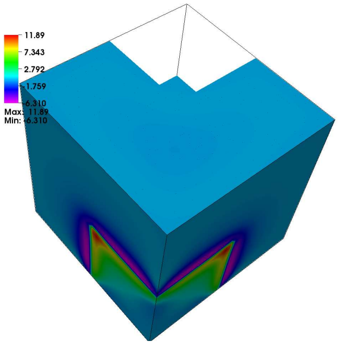


DoF	$\alpha_c = 10^{-3}$			$\alpha_c = 10^{-5}$		
	Time	Newton	Iterations	Time	Newton	Iterations
$538,240$	$1,995$	step 1	17	$1,726$	step 1	16
		step 2	20		step 2	16
		step 3	20		step 3	16
$3,331,520$	$14,757$	step 1	28	$14,904$	step 1	28
		step 2	31		step 2	27
		step 3	29		step 3	34

$$\widehat{u} = \begin{cases} 0.7 & \text{if } \mathbf{x} \in [0, \frac{1}{2}]^3 \\ 0.2 & \text{otherwise} \end{cases}, \quad \widehat{v} = 0, \quad k_1 = k_2 = D_1 = D_2 = 1, \quad \gamma_1 = \gamma_2 = 0.15$$

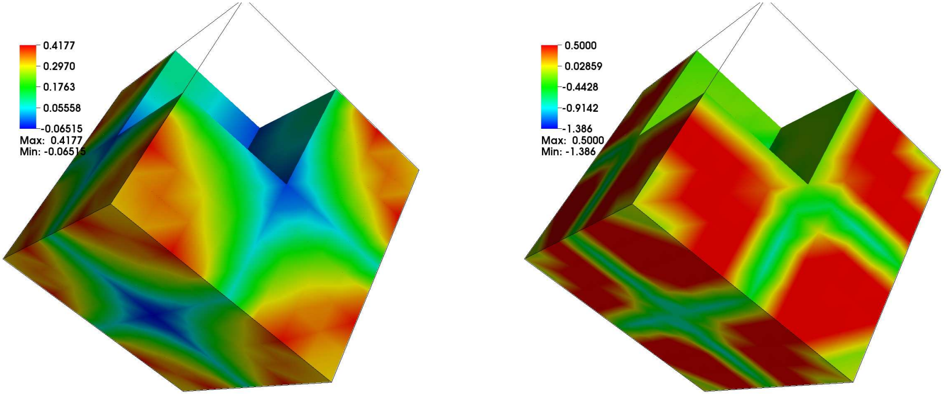






DoF	$\alpha_c = 10^{-3}$			$\alpha_c = 10^{-5}$		
	Time	Newton	Iterations	Time	Newton	Iterations
382, 840	2, 624	step 1	24	2, 819	step 1	29
		step 2	30		step 2	35
		step 3	33		step 3	33
2, 670, 200	19, 128	step 1	36	22, 976	step 1	46
		step 2	44		step 2	52
		step 3	44		step 3	53

$$\widehat{u} = t\,|\sin(2x_1x_2x_3)|, \quad \widehat{v} = 0, \quad k_1 = k_2 = D_1 = D_2 = 1, \quad \gamma_1 = \gamma_2 = 0.15, \quad c \leqslant 0.5$$



DoF	$\alpha_c = 10^{-3}$			$\alpha_c = 10^{-5}$		
	Time	Newton	Iterations	Time	Newton	Iterations
60, 920	1, 066	step 1	18	859	step 1	22
		step 2	21		step 2	26
		step 3	21			
382, 840	5, 498	step 1	26	13, 358	step 1	29
		step 2	36		step 2	33
		step 3	35		step 3	33

Table of Contents

Parameter Identification in Pattern Formation Processes

- Another important reaction-diffusion control problem concerns pattern formation processes. Here we wish to minimize

$$\mathcal{J}(u,v,a,b) = \frac{\beta_1}{2}\left\|u-\widehat{u}\right\|^2_{L_2(Q)} + \frac{\beta_2}{2}\left\|v-\widehat{v}\right\|^2_{L_2(Q)} + \frac{\nu_1}{2}\left\|a\right\|^2_{L_2(Q)} + \frac{\nu_2}{2}\left\|b\right\|^2_{L_2(Q)},$$

subject to PDE constraints given by the Gierer-Meinhardt equations

$$\begin{aligned}
u_t - D_u\nabla^2 u - \frac{ru^2}{v} + au &= r, && \text{in } Q,\\
v_t - D_v\nabla^2 v - ru^2 + bv &= 0, && \text{in } Q,\\
u(\mathbf{x},0) = u_0(\mathbf{x}), \quad v(\mathbf{x},0) &= v_0(\mathbf{x}), &&\\
\frac{\partial u}{\partial n} = \frac{\partial v}{\partial n} &= 0, && \text{on } \partial Q
\end{aligned}$$

Parameter Identification in Pattern Formation Processes

- Another important reaction-diffusion control problem concerns pattern formation processes. Here we wish to minimize

$$\mathcal{J}(u,v,a,b)=\frac{\beta_1}{2}\left\|u-\widehat{u}\right\|^2_{L_2(Q)}+\frac{\beta_2}{2}\left\|v-\widehat{v}\right\|^2_{L_2(Q)}+\frac{\nu_1}{2}\left\|a\right\|^2_{L_2(Q)}+\frac{\nu_2}{2}\left\|b\right\|^2_{L_2(Q)},$$

subject to PDE constraints given by the Gierer-Meinhardt equations

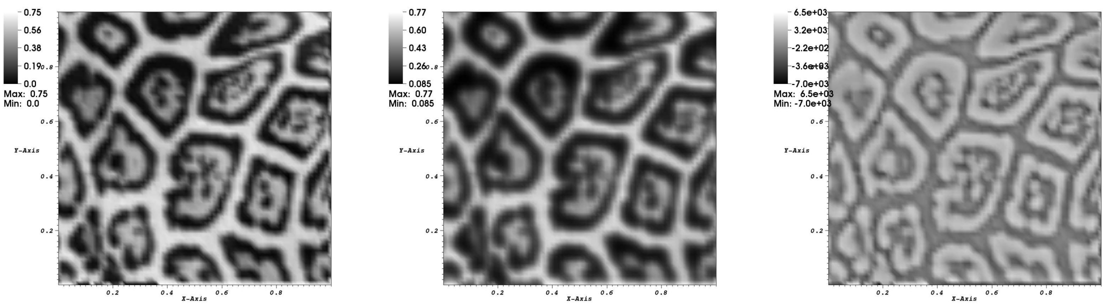
$$\begin{aligned} u_t-D_u\nabla^2u-\frac{ru^2}{v}+au&=r, && \text{in } Q,\\ v_t-D_v\nabla^2v-ru^2+bv&=0, && \text{in } Q,\\ u(\mathbf{x},0)=u_0(\mathbf{x}),\quad v(\mathbf{x},0)&=v_0(\mathbf{x}),\\ \frac{\partial u}{\partial n}=\frac{\partial v}{\partial n}&=0, && \text{on } \partial Q,\end{aligned}$$

or the Schnakenberg equations

$$\begin{aligned} u_t-D_u\nabla^2u+\gamma(u-u^2v)-\gamma a&=0, && \text{in } Q,\\ v_t-D_v\nabla^2v+\gamma u^2v-\gamma b&=0, && \text{in } Q,\\ u(\mathbf{x},0)=u_0(\mathbf{x}),\quad v(\mathbf{x},0)&=v_0(\mathbf{x}),\\ \frac{\partial u}{\partial n}=\frac{\partial v}{\partial n}&=0, && \text{on } \partial Q.\end{aligned}$$

Parameter Identification in Pattern Formation

$$
\begin{aligned}
\min_{u,v,a,b} \quad & \frac{\beta_1}{2}\|u-\widehat{u}\|^2_{L_2(Q)} + \frac{\beta_2}{2}\|v-\widehat{v}\|^2_{L_2(Q)} + \frac{\nu_1}{2}\|a(\mathbf{x},t)\|^2_{L_2(Q)} + \frac{\nu_2}{2}\|b(\mathbf{x},t)\|^2_{L_2(Q)} \\
\text{s.t.} \quad & u_t - D_u\nabla^2 u - \frac{ru^2}{v} + au = r, \qquad \text{in } Q, \\
& v_t - D_v\nabla^2 v - ru^2 + bv = 0, \qquad \text{in } Q, \\
& u(\mathbf{x},0) = u_0(\mathbf{x}), \quad v(\mathbf{x},0) = v_0(\mathbf{x}), \\
& \frac{\partial u}{\partial n} = \frac{\partial v}{\partial n} = 0, \qquad \text{on } \partial Q.
\end{aligned}
$$



Newton System – Schnakenberg Model

- The matrix system obtained from a finite element discretization at each Newton step is given by

$$\begin{bmatrix} \mathbf{A}_{u,S} & -2\tau\gamma\mathbf{M}_{u(q-p)} & 0 & 0 & -\mathbf{L}_{u,S}^{\top} & -2\tau\gamma\mathbf{M}_{uv} \\ -2\tau\gamma\mathbf{M}_{u(q-p)} & \mathbf{A}_{v,S} & 0 & 0 & \tau\gamma\mathbf{M}_{u^2} & -\mathbf{L}_{v,S}^{\top} \\ 0 & 0 & \tau\nu_1\mathbf{M} & 0 & \tau\gamma\mathbf{M} & 0 \\ 0 & 0 & 0 & \tau\nu_2\mathbf{M} & 0 & \tau\gamma\mathbf{M} \\ -\mathbf{L}_{u,S} & \tau\gamma\mathbf{M}_{u^2} & \tau\gamma\mathbf{M} & 0 & 0 & 0 \\ -2\tau\gamma\mathbf{M}_{uv} & -\mathbf{L}_{v,S} & 0 & \tau\gamma\mathbf{M} & 0 & 0 \end{bmatrix} \begin{bmatrix} \mathbf{s}_u \\ \mathbf{s}_v \\ \mathbf{s}_a \\ \mathbf{s}_b \\ \mathbf{s}_p \\ \mathbf{s}_q \end{bmatrix} = \mathbf{b},$$

  where

$$\begin{aligned} \mathbf{A}_{u,S} &= \tau\beta_1\mathbf{M} + 2\tau\gamma\mathbf{M}_{v(q-p)}, \\ \mathbf{A}_{v,S} &= \tau\beta_2\mathbf{M}, \\ \mathbf{L}_{u,S} &= \mathbf{M}_E + \tau D_u\mathbf{K} + \tau\gamma\mathbf{M} - 2\gamma\mathbf{M}_{uv}, \\ \mathbf{L}_{v,S} &= \mathbf{M}_E + \tau D_v\mathbf{K} + \tau\gamma\mathbf{M}_{u^2}, \end{aligned}$$

- Here $\mathbf{M}_E$ denotes the mass matrices appearing from time-stepping method.
- All other $\mathbf{M}_\psi = \text{blkdiag}(M_\psi, \ldots, M_\psi)$ are again obtained from evaluating integrals of the form $[M_\psi]_{ij} = \int \psi\phi_i\phi_j$ for each matrix entry.

Newton System – Schnakenberg Model

- The matrix system obtained from a finite element discretization at each Newton step is given by

$$\begin{bmatrix} \mathbf{A}_{u,S} & -2\tau\gamma\mathbf{M}_{u(q-p)} & 0 & 0 & -\mathbf{L}_{u,S}^{\top} & -2\tau\gamma\mathbf{M}_{uv} \\ -2\tau\gamma\mathbf{M}_{u(q-p)} & \mathbf{A}_{v,S} & 0 & 0 & \tau\gamma\mathbf{M}_{u^2} & -\mathbf{L}_{v,S}^{\top} \\ 0 & 0 & \tau\nu_1\mathbf{M} & 0 & \tau\gamma\mathbf{M} & 0 \\ 0 & 0 & 0 & \tau\nu_2\mathbf{M} & 0 & \tau\gamma\mathbf{M} \\ -\mathbf{L}_{u,S} & \tau\gamma\mathbf{M}_{u^2} & \tau\gamma\mathbf{M} & 0 & 0 & 0 \\ -2\tau\gamma\mathbf{M}_{uv} & -\mathbf{L}_{v,S} & 0 & \tau\gamma\mathbf{M} & 0 & 0 \end{bmatrix} \begin{bmatrix} \mathbf{s}_u \\ \mathbf{s}_v \\ \mathbf{s}_a \\ \mathbf{s}_b \\ \mathbf{s}_p \\ \mathbf{s}_q \end{bmatrix} = \mathbf{b}.$$

- The vector $\mathbf{b}$ denotes the discrete representation of

$$\begin{bmatrix} \beta_1 \int(\hat{u}-\bar{u}) + \int(-\bar{p}_t - D_u\nabla^2\bar{p} + 2\gamma\bar{u}\bar{v}(\bar{q}-\bar{p}) + \gamma\bar{p}) \\ \beta_2 \int(\hat{v}-\bar{v}) + \int(-\bar{q}_t - D_v\nabla^2\bar{q} + \gamma\bar{u}^2(\bar{q}-\bar{p})) \\ -\int(\nu_1\bar{a} + \gamma\bar{p}) \\ -\int(\nu_2\bar{b} + \gamma\bar{q}) \\ \int(\bar{u}_t - D_u\nabla^2\bar{u} + \gamma(\bar{u}-\bar{u}^2\bar{v}) - \gamma\bar{a}) \\ \int(\bar{v}_t - D_v\nabla^2\bar{v} + \gamma\bar{u}^2\bar{v} - \gamma\bar{b}) \end{bmatrix}.$$

$$\left[\begin{array}{cccc|cc} \mathbf{A}_{u,S} & -2\tau\gamma\mathbf{M}_{u(q-p)} & 0 & 0 & -\mathbf{L}_{u,S}^{\top} & -2\tau\gamma\mathbf{M}_{uv} \\ -2\tau\gamma\mathbf{M}_{u(q-p)} & \mathbf{A}_{v,S} & 0 & 0 & \tau\gamma\mathbf{M}_{u^2} & -\mathbf{L}_{v,S}^{\top} \\ 0 & 0 & \tau\nu_1\mathbf{M} & 0 & \tau\gamma\mathbf{M} & 0 \\ 0 & 0 & 0 & \tau\nu_2\mathbf{M} & 0 & \tau\gamma\mathbf{M} \\ \hline -\mathbf{L}_{u,S} & \tau\gamma\mathbf{M}_{u^2} & \tau\gamma\mathbf{M} & 0 & 0 & 0 \\ -2\tau\gamma\mathbf{M}_{uv} & -\mathbf{L}_{v,S} & 0 & \tau\gamma\mathbf{M} & 0 & 0 \end{array}\right] \left[\begin{array}{c} \mathbf{s}_u \\ \mathbf{s}_v \\ \mathbf{s}_a \\ \mathbf{s}_b \\ \mathbf{s}_p \\ \mathbf{s}_q \end{array}\right] = \mathbf{b}$$

Preconditioning the Matrix System – $(1,1)$-block

- We approximate the $(1,1)$-block by:

$$\widehat{A} = \left[\begin{array}{cccc} \widehat{\mathbf{A}}_1 & 0 & 0 & 0 \\ -2\tau\gamma\mathbf{M}_{u(q-p)} & \mathbf{A}_{v,S} & 0 & 0 \\ 0 & 0 & \tau\nu_1\mathbf{M} & 0 \\ 0 & 0 & 0 & \tau\nu_2\mathbf{M} \end{array}\right],$$

where $\widehat{\mathbf{A}}_1$ is a Schur complement approximation defined by

$$\widehat{\mathbf{A}}_1 = \mathbf{A}_{u,S} - (2\tau\gamma)^2\mathbf{M}_{u(q-p)}\mathbf{A}_{v,S}^{-1}\mathbf{M}_{u(q-p)}.$$

M. Stoll, JWP and P. K. Maini, *Fast Solvers for Optimal Control Problems from Pattern Formation*, submitted to Journal of Computational Physics, 2014.

$$S = \begin{bmatrix} -\mathbf{L}_{u,S} & \tau\gamma\mathbf{M}_{u^2} \\ -2\tau\gamma\mathbf{M}_{uv} & -\mathbf{L}_{v,S} \end{bmatrix} \mathbf{A}_{(1,2)}^{-1} \begin{bmatrix} -\mathbf{L}_{u,S}^{\top} & -2\tau\gamma\mathbf{M}_{uv} \\ \tau\gamma\mathbf{M}_{u^2} & -\mathbf{L}_{v,S}^{\top} \end{bmatrix} + \tau\gamma^2 \begin{bmatrix} \nu_1^{-1}\mathbf{M} & 0 \\ 0 & \nu_2^{-1}\mathbf{M} \end{bmatrix}$$

$$\widehat{S} = \begin{bmatrix} -\mathbf{L}_{u,S} + \widehat{\mathbf{M}}_1^{(1)} & \tau\gamma\mathbf{M}_{u^2} \\ -2\tau\gamma\mathbf{M}_{uv} & -\mathbf{L}_{v,S} + \widehat{\mathbf{M}}_2^{(1)} \end{bmatrix} \mathbf{A}_{(1,2)}^{-1} \begin{bmatrix} -\mathbf{L}_{u,S}^{\top} + \widehat{\mathbf{M}}_1^{(2)} & -2\tau\gamma\mathbf{M}_{uv} \\ \tau\gamma\mathbf{M}_{u^2} & -\mathbf{L}_{v,S}^{\top} + \widehat{\mathbf{M}}_2^{(2)} \end{bmatrix}$$

Preconditioning the Matrix System – Schur complement

- We choose $\widehat{\mathbf{M}}_1^{(1)}$, $\widehat{\mathbf{M}}_1^{(2)}$, $\widehat{\mathbf{M}}_2^{(1)}$, $\widehat{\mathbf{M}}_2^{(2)}$ such that [Stoll, Pearson & Maini, 2014]:

$$\begin{bmatrix} \widehat{\mathbf{M}}_1^{(1)} & 0 \\ 0 & \widehat{\mathbf{M}}_2^{(1)} \end{bmatrix} \mathbf{A}_{(1,2)}^{-1} \begin{bmatrix} \widehat{\mathbf{M}}_1^{(2)} & 0 \\ 0 & \widehat{\mathbf{M}}_2^{(2)} \end{bmatrix} \approx \tau\gamma^2 \begin{bmatrix} \nu_1^{-1}\mathbf{M} & 0 \\ 0 & \nu_2^{-1}\mathbf{M} \end{bmatrix}.$$

$$S = \begin{bmatrix} -\mathbf{L}_{u,S} & \tau\gamma\mathbf{M}_{u^2} \\ -2\tau\gamma\mathbf{M}_{uv} & -\mathbf{L}_{v,S} \end{bmatrix} \mathbf{A}_{(1,2)}^{-1} \begin{bmatrix} -\mathbf{L}_{u,S}^{\top} & -2\tau\gamma\mathbf{M}_{uv} \\ \tau\gamma\mathbf{M}_{u^2} & -\mathbf{L}_{v,S}^{\top} \end{bmatrix} + \tau\gamma^2 \begin{bmatrix} \nu_1^{-1}\mathbf{M} & 0 \\ 0 & \nu_2^{-1}\mathbf{M} \end{bmatrix}$$

$$\widehat{S} = \begin{bmatrix} -\mathbf{L}_{u,S} + \widehat{\mathbf{M}}_1^{(1)} & \tau\gamma\mathbf{M}_{u^2} \\ -2\tau\gamma\mathbf{M}_{uv} & -\mathbf{L}_{v,S} + \widehat{\mathbf{M}}_2^{(1)} \end{bmatrix} \mathbf{A}_{(1,2)}^{-1} \begin{bmatrix} -\mathbf{L}_{u,S}^{\top} + \widehat{\mathbf{M}}_1^{(2)} & -2\tau\gamma\mathbf{M}_{uv} \\ \tau\gamma\mathbf{M}_{u^2} & -\mathbf{L}_{v,S}^{\top} + \widehat{\mathbf{M}}_2^{(2)} \end{bmatrix}$$

Preconditioning the Matrix System – Schur complement

- We choose $\widehat{\mathbf{M}}_1^{(1)}$, $\widehat{\mathbf{M}}_1^{(2)}$, $\widehat{\mathbf{M}}_2^{(1)}$, $\widehat{\mathbf{M}}_2^{(2)}$ such that [Stoll, Pearson & Maini, 2014]:

$$\begin{bmatrix} \widehat{\mathbf{M}}_1^{(1)} & 0 \\ 0 & \widehat{\mathbf{M}}_2^{(1)} \end{bmatrix} \mathbf{A}_{(1,2)}^{-1} \begin{bmatrix} \widehat{\mathbf{M}}_1^{(2)} & 0 \\ 0 & \widehat{\mathbf{M}}_2^{(2)} \end{bmatrix} \approx \tau\gamma^2 \begin{bmatrix} \nu_1^{-1}\mathbf{M} & 0 \\ 0 & \nu_2^{-1}\mathbf{M} \end{bmatrix}.$$

- Examining the diagonal blocks leads to approximations such that

$$\mathbf{M}_1^{(1)}\hat{\mathbf{A}}_1^{-1}\mathbf{M}_1^{(2)} \approx \frac{\tau\gamma^2}{\nu_1}\mathbf{M}, \qquad \hat{\mathbf{A}}_1 = \mathbf{A}_{u,S} - (2\tau\gamma)^2\mathbf{M}_{u(q-p)}\mathbf{A}_{v,S}^{-1}\mathbf{M}_{u(q-p)},$$

$$\mathbf{M}_2^{(1)}\hat{\mathbf{A}}_2^{-1}\mathbf{M}_2^{(2)} \approx \frac{\tau\gamma^2}{\nu_2}\mathbf{M}, \qquad \hat{\mathbf{A}}_2 = \mathbf{A}_{v,S} - (2\tau\gamma)^2\mathbf{M}_{u(q-p)}\mathbf{A}_{u,S}^{-1}\mathbf{M}_{u(q-p)}.$$

$$S = \begin{bmatrix} -\mathbf{L}_{u,S} & \tau\gamma\mathbf{M}_{u^2} \\ -2\tau\gamma\mathbf{M}_{uv} & -\mathbf{L}_{v,S} \end{bmatrix} \mathbf{A}_{(1,2)}^{-1} \begin{bmatrix} -\mathbf{L}_{u,S}^\top & -2\tau\gamma\mathbf{M}_{uv} \\ \tau\gamma\mathbf{M}_{u^2} & -\mathbf{L}_{v,S}^\top \end{bmatrix} + \tau\gamma^2 \begin{bmatrix} \nu_1^{-1}\mathbf{M} & 0 \\ 0 & \nu_2^{-1}\mathbf{M} \end{bmatrix}$$

$$\widehat{S} = \begin{bmatrix} -\mathbf{L}_{u,S} + \widehat{\mathbf{M}}_1^{(1)} & \tau\gamma\mathbf{M}_{u^2} \\ -2\tau\gamma\mathbf{M}_{uv} & -\mathbf{L}_{v,S} + \widehat{\mathbf{M}}_2^{(1)} \end{bmatrix} \mathbf{A}_{(1,2)}^{-1} \begin{bmatrix} -\mathbf{L}_{u,S}^\top + \widehat{\mathbf{M}}_1^{(2)} & -2\tau\gamma\mathbf{M}_{uv} \\ \tau\gamma\mathbf{M}_{u^2} & -\mathbf{L}_{v,S}^\top + \widehat{\mathbf{M}}_2^{(2)} \end{bmatrix}$$

Preconditioning the Matrix System – Schur complement

- We choose $\widehat{\mathbf{M}}_1^{(1)}$, $\widehat{\mathbf{M}}_1^{(2)}$, $\widehat{\mathbf{M}}_2^{(1)}$, $\widehat{\mathbf{M}}_2^{(2)}$ such that [Stoll, Pearson & Maini, 2014]:

$$\begin{bmatrix} \widehat{\mathbf{M}}_1^{(1)} & 0 \\ 0 & \widehat{\mathbf{M}}_2^{(1)} \end{bmatrix} \mathbf{A}_{(1,2)}^{-1} \begin{bmatrix} \widehat{\mathbf{M}}_1^{(2)} & 0 \\ 0 & \widehat{\mathbf{M}}_2^{(2)} \end{bmatrix} \approx \tau\gamma^2 \begin{bmatrix} \nu_1^{-1}\mathbf{M} & 0 \\ 0 & \nu_2^{-1}\mathbf{M} \end{bmatrix}.$$

- This motivates selecting diagonal matrices with

$$[\widehat{\mathbf{M}}_1^{(1)}]_{jj} = \sqrt{\frac{\tau}{\nu_1}}\,\gamma \cdot [\mathbf{M}]_{jj}^{1/2} \cdot \left|[\hat{\mathbf{A}}_1]_{jj}\right|, \qquad [\widehat{\mathbf{M}}_1^{(2)}]_{jj} = \sqrt{\frac{\tau}{\nu_1}}\,\gamma \cdot [\mathbf{M}]_{jj}^{1/2},$$

$$[\widehat{\mathbf{M}}_2^{(1)}]_{jj} = \sqrt{\frac{\tau}{\nu_2}}\,\gamma \cdot [\mathbf{M}]_{jj}^{1/2} \cdot \left|[\hat{\mathbf{A}}_2]_{jj}\right|, \qquad [\widehat{\mathbf{M}}_2^{(2)}]_{jj} = \sqrt{\frac{\tau}{\nu_2}}\,\gamma \cdot [\mathbf{M}]_{jj}^{1/2}.$$

Newton System – Gierer-Meinhardt Model

- The matrix system obtained from a finite element discretization at each Newton step is given by

$$\begin{bmatrix} \mathbf{A}_{u,GM} & -2\tau r\mathbf{M}_{up/v^2} & -\tau\mathbf{M}_p & 0 & -\mathbf{L}_{u,GM}^\top & 2\tau r\mathbf{M}_u \\ -2\tau r\mathbf{M}_{up/v^2} & \mathbf{A}_{v,GM} & 0 & -\tau\mathbf{M}_q & -\tau r\mathbf{M}_{u^2/v^2} & -\mathbf{L}_{v,GM}^\top \\ -\tau\mathbf{M}_p & 0 & \tau\nu_1\mathbf{M} & 0 & -\tau\mathbf{M}_u & 0 \\ 0 & -\tau\mathbf{M}_q & 0 & \tau\nu_2\mathbf{M} & 0 & -\tau\mathbf{M}_v \\ -\mathbf{L}_{u,GM} & -\tau r\mathbf{M}_{u^2/v^2} & -\tau\mathbf{M}_u & 0 & 0 & 0 \\ 2\tau r\mathbf{M}_u & -\mathbf{L}_{v,GM} & 0 & -\tau\mathbf{M}_v & 0 & 0 \end{bmatrix} \begin{bmatrix} \mathbf{s}_u \\ \mathbf{s}_v \\ \mathbf{s}_a \\ \mathbf{s}_b \\ \mathbf{s}_p \\ \mathbf{s}_q \end{bmatrix} = \mathbf{b},$$

  where

$$\begin{aligned} \mathbf{A}_{u,GM} &= \tau\beta_1\mathbf{M} + 2\tau r\mathbf{M}_{p/v} + 2\tau r\mathbf{M}_q, \\ \mathbf{A}_{v,GM} &= \tau\beta_2\mathbf{M} + 2\tau r\mathbf{M}_{u^2p/v^3}, \\ \mathbf{L}_{u,GM} &= \mathbf{M}_E + \tau D_u\mathbf{K} - 2\tau r\mathbf{M}_{u/v} + \tau\mathbf{M}_a, \\ \mathbf{L}_{v,GM} &= \mathbf{M}_E + \tau D_v\mathbf{K} + \tau\mathbf{M}_b. \end{aligned}$$

Newton System – Gierer-Meinhardt Model

- The matrix system obtained from a finite element discretization at each Newton step is given by

$$\begin{bmatrix} \mathbf{A}_{u,GM} & -2\tau r\mathbf{M}_{up/v^2} & -\tau\mathbf{M}_p & 0 & -\mathbf{L}_{u,GM}^\top & 2\tau r\mathbf{M}_u \\ -2\tau r\mathbf{M}_{up/v^2} & \mathbf{A}_{v,GM} & 0 & -\tau\mathbf{M}_q & -\tau r\mathbf{M}_{u^2/v^2} & -\mathbf{L}_{v,GM}^\top \\ -\tau\mathbf{M}_p & 0 & \tau\nu_1\mathbf{M} & 0 & -\tau\mathbf{M}_u & 0 \\ 0 & -\tau\mathbf{M}_q & 0 & \tau\nu_2\mathbf{M} & 0 & -\tau\mathbf{M}_v \\ -\mathbf{L}_{u,GM} & -\tau r\mathbf{M}_{u^2/v^2} & -\tau\mathbf{M}_u & 0 & 0 & 0 \\ 2\tau r\mathbf{M}_u & -\mathbf{L}_{v,GM} & 0 & -\tau\mathbf{M}_v & 0 & 0 \end{bmatrix} \begin{bmatrix} \mathbf{s}_u \\ \mathbf{s}_v \\ \mathbf{s}_a \\ \mathbf{s}_b \\ \mathbf{s}_p \\ \mathbf{s}_q \end{bmatrix} = \mathbf{b}.$$

- The vector $\mathbf{b}$ here denotes the discrete representation of

$$\begin{bmatrix} \beta_1 \int(\widehat{u}-\bar{u}) + \int(-\bar{p}_t - D_u\nabla^2\bar{p} - 2r\frac{\bar{u}}{\bar{v}}\bar{p} + \bar{a}\bar{p} - 2r\bar{u}\bar{q}) \\ \beta_2 \int(\widehat{v}-\bar{v}) + \int(-\bar{q}_t - D_v\nabla^2\bar{q} + r\frac{\bar{u}^2}{\bar{v}^2}\bar{p} + \bar{b}\bar{q}) \\ \int(\bar{u}\bar{p} - \nu_1\bar{a}) \\ \int(\bar{v}\bar{q} - \nu_2\bar{b}) \\ \int(\bar{u}_t - D_u\nabla^2\bar{u} - \frac{r\bar{u}^2}{\bar{v}} + \bar{a}\bar{u} - r) \\ \int(\bar{v}_t - D_v\nabla^2\bar{v} - r\bar{u}^2 + \bar{b}\bar{v}) \end{bmatrix}.$$

$$\left[\begin{array}{cccc|cc} \mathbf{A}_{u,GM} & -2\tau r\mathbf{M}_{up/v^2} & -\tau\mathbf{M}_p & 0 & -\mathbf{L}_{u,GM}^\top & 2\tau r\mathbf{M}_u \\ -2\tau r\mathbf{M}_{up/v^2} & \mathbf{A}_{v,GM} & 0 & -\tau\mathbf{M}_q & -\tau r\mathbf{M}_{u^2/v^2} & -\mathbf{L}_{v,GM}^\top \\ -\tau\mathbf{M}_p & 0 & \tau\nu_1\mathbf{M} & 0 & -\tau\mathbf{M}_u & 0 \\ 0 & -\tau\mathbf{M}_q & 0 & \tau\nu_2\mathbf{M} & 0 & -\tau\mathbf{M}_v \\ \hline -\mathbf{L}_{u,GM} & -\tau r\mathbf{M}_{u^2/v^2} & -\tau\mathbf{M}_u & 0 & 0 & 0 \\ 2\tau r\mathbf{M}_u & -\mathbf{L}_{v,GM} & 0 & -\tau\mathbf{M}_v & 0 & 0 \end{array}\right] \left[\begin{array}{c} \mathbf{s}_u \\ \mathbf{s}_v \\ \mathbf{s}_a \\ \mathbf{s}_b \\ \mathbf{s}_p \\ \mathbf{s}_q \end{array}\right] = \mathbf{b}$$

Preconditioning the Matrix System – $(1,1)$-block

- We use saddle point theory to approximate the $(1,1)$-block by:

$$\widehat{A} = \left[\begin{array}{cccc} \widehat{\mathbf{A}}_1 & 0 & 0 & 0 \\ 0 & \widehat{\mathbf{A}}_2 & 0 & 0 \\ -\tau\mathbf{M}_p & 0 & \tau\nu_1\mathbf{M} & 0 \\ 0 & -\tau\mathbf{M}_q & 0 & \tau\nu_2\mathbf{M} \end{array}\right].$$

$$\left[\begin{array}{cccc|cc} \mathbf{A}_{u,GM} & -2\tau r\mathbf{M}_{up/v^2} & -\tau\mathbf{M}_p & 0 & -\mathbf{L}_{u,GM}^\top & 2\tau r\mathbf{M}_u \\ -2\tau r\mathbf{M}_{up/v^2} & \mathbf{A}_{v,GM} & 0 & -\tau\mathbf{M}_q & -\tau r\mathbf{M}_{u^2/v^2} & -\mathbf{L}_{v,GM}^\top \\ -\tau\mathbf{M}_p & 0 & \tau\nu_1\mathbf{M} & 0 & -\tau\mathbf{M}_u & 0 \\ 0 & -\tau\mathbf{M}_q & 0 & \tau\nu_2\mathbf{M} & 0 & -\tau\mathbf{M}_v \\ \hline -\mathbf{L}_{u,GM} & -\tau r\mathbf{M}_{u^2/v^2} & -\tau\mathbf{M}_u & 0 & 0 & 0 \\ 2\tau r\mathbf{M}_u & -\mathbf{L}_{v,GM} & 0 & -\tau\mathbf{M}_v & 0 & 0 \end{array}\right]\left[\begin{array}{c} \mathbf{s}_u \\ \mathbf{s}_v \\ \mathbf{s}_a \\ \mathbf{s}_b \\ \mathbf{s}_p \\ \mathbf{s}_q \end{array}\right] = \mathbf{b}$$

Preconditioning the Matrix System – $(1,1)$-block

- We use saddle point theory to approximate the $(1,1)$-block by:

$$\widehat{A} = \left[\begin{array}{cccc} \widehat{\mathbf{A}}_1 & 0 & 0 & 0 \\ 0 & \widehat{\mathbf{A}}_2 & 0 & 0 \\ -\tau\mathbf{M}_p & 0 & \tau\nu_1\mathbf{M} & 0 \\ 0 & -\tau\mathbf{M}_q & 0 & \tau\nu_2\mathbf{M} \end{array}\right].$$

- We seek $\widehat{\mathbf{A}}_1$ and $\widehat{\mathbf{A}}_2$ that satisfy:

$$\left[\begin{array}{cc} \widehat{\mathbf{A}}_1 & 0 \\ 0 & \widehat{\mathbf{A}}_2 \end{array}\right] \approx \mathbf{A}_{(1,2)} - \left[\begin{array}{cc} \tau\nu_1^{-1}\mathbf{M}_p\mathbf{M}^{-1}\mathbf{M}_p & 0 \\ 0 & \tau\nu_2^{-1}\mathbf{M}_q\mathbf{M}^{-1}\mathbf{M}_q \end{array}\right].$$

$$\left[\begin{array}{cccc|cc} \mathbf{A}_{u,GM} & -2\tau r\mathbf{M}_{up/v^2} & -\tau\mathbf{M}_p & 0 & -\mathbf{L}_{u,GM}^\top & 2\tau r\mathbf{M}_u \\ -2\tau r\mathbf{M}_{up/v^2} & \mathbf{A}_{v,GM} & 0 & -\tau\mathbf{M}_q & -\tau r\mathbf{M}_{u^2/v^2} & -\mathbf{L}_{v,GM}^\top \\ -\tau\mathbf{M}_p & 0 & \tau\nu_1\mathbf{M} & 0 & -\tau\mathbf{M}_u & 0 \\ 0 & -\tau\mathbf{M}_q & 0 & \tau\nu_2\mathbf{M} & 0 & -\tau\mathbf{M}_v \\ \hline -\mathbf{L}_{u,GM} & -\tau r\mathbf{M}_{u^2/v^2} & -\tau\mathbf{M}_u & 0 & 0 & 0 \\ 2\tau r\mathbf{M}_u & -\mathbf{L}_{v,GM} & 0 & -\tau\mathbf{M}_v & 0 & 0 \end{array}\right] \left[\begin{array}{c} \mathbf{s}_u \\ \mathbf{s}_v \\ \mathbf{s}_a \\ \mathbf{s}_b \\ \mathbf{s}_p \\ \mathbf{s}_q \end{array}\right] = \mathbf{b}$$

Preconditioning the Matrix System – $(1,1)$-block

- We use saddle point theory to approximate the $(1,1)$-block by:

$$\widehat{A} = \left[\begin{array}{cccc} \widehat{\mathbf{A}}_1 & 0 & 0 & 0 \\ 0 & \widehat{\mathbf{A}}_2 & 0 & 0 \\ -\tau\mathbf{M}_p & 0 & \tau\nu_1\mathbf{M} & 0 \\ 0 & -\tau\mathbf{M}_q & 0 & \tau\nu_2\mathbf{M} \end{array}\right].$$

- We then replace $\mathbf{A}_{(1,2)}$ by its own saddle point approximation to write:

$$\begin{aligned} \widehat{\mathbf{A}}_1 &= \mathbf{A}_{u,GM} - (2\tau r)^2\mathbf{M}_{up/v^2}\mathbf{A}_{v,GM}^{-1}\mathbf{M}_{up/v^2} - \tau\nu_1^{-1}\mathbf{M}_p\mathbf{M}^{-1}\mathbf{M}_p, \\ \widehat{\mathbf{A}}_2 &= \mathbf{A}_{v,GM} - \tau\nu_2^{-1}\mathbf{M}_q\mathbf{M}^{-1}\mathbf{M}_q. \end{aligned}$$

$$S = \begin{bmatrix} -\mathbf{L}_{u,GM} & -\tau r \mathbf{M}_{u^2/v^2} \\ 2\tau r \mathbf{M}_u & -\mathbf{L}_{v,GM} \end{bmatrix} \mathbf{A}_{(1,2)}^{-1} \begin{bmatrix} -\mathbf{L}_{u,GM}^\top & 2\tau r \mathbf{M}_u \\ -\tau r \mathbf{M}_{u^2/v^2} & -\mathbf{L}_{v,GM}^\top \end{bmatrix} + \tau \begin{bmatrix} \nu_1^{-1}\mathbf{M}_u \mathbf{M}^{-1} \mathbf{M}_u & 0 \\ 0 & \nu_2^{-1}\mathbf{M}_v \mathbf{M}^{-1} \mathbf{M}_v \end{bmatrix}$$

$$\widehat{S} = \begin{bmatrix} -\mathbf{L}_{u,GM} + \widehat{\mathbf{M}}_1^{(1)} & \tau r \mathbf{M}_{u^2/v^2} \\ -2\tau r \mathbf{M}_u & -\mathbf{L}_{v,GM} + \widehat{\mathbf{M}}_2^{(1)} \end{bmatrix} \mathbf{A}_{(1,2)}^{-1} \begin{bmatrix} -\mathbf{L}_{u,GM}^\top + \widehat{\mathbf{M}}_1^{(2)} & -2\tau r \mathbf{M}_u \\ \tau r \mathbf{M}_{u^2/v^2} & -\mathbf{L}_{v,GM}^\top + \widehat{\mathbf{M}}_2^{(2)} \end{bmatrix}$$

Preconditioning the Matrix System – Schur complement

- We choose $\widehat{\mathbf{M}}_1^{(1)}$, $\widehat{\mathbf{M}}_1^{(2)}$, $\widehat{\mathbf{M}}_2^{(1)}$, $\widehat{\mathbf{M}}_2^{(2)}$ such that [Stoll, Pearson & Maini, 2014]:

$$\begin{bmatrix} \widehat{\mathbf{M}}_1^{(1)} & 0 \\ 0 & \widehat{\mathbf{M}}_2^{(1)} \end{bmatrix} \mathbf{A}_{(1,2)}^{-1} \begin{bmatrix} \widehat{\mathbf{M}}_1^{(2)} & 0 \\ 0 & \widehat{\mathbf{M}}_2^{(2)} \end{bmatrix} \approx \tau \begin{bmatrix} \nu_1^{-1}\mathbf{M}_u \mathbf{M}^{-1} \mathbf{M}_u & 0 \\ 0 & \nu_2^{-1}\mathbf{M}_v \mathbf{M}^{-1} \mathbf{M}_v \end{bmatrix}.$$

$$S = \begin{bmatrix} -\mathbf{L}_{u,GM} & -\tau r \mathbf{M}_{u^2/v^2} \\ 2\tau r \mathbf{M}_u & -\mathbf{L}_{v,GM} \end{bmatrix} \mathbf{A}_{(1,2)}^{-1} \begin{bmatrix} -\mathbf{L}_{u,GM}^\top & 2\tau r \mathbf{M}_u \\ -\tau r \mathbf{M}_{u^2/v^2} & -\mathbf{L}_{v,GM}^\top \end{bmatrix} + \tau \begin{bmatrix} \nu_1^{-1}\mathbf{M}_u \mathbf{M}^{-1} \mathbf{M}_u & 0 \\ 0 & \nu_2^{-1}\mathbf{M}_v \mathbf{M}^{-1} \mathbf{M}_v \end{bmatrix}$$

$$\widehat{S} = \begin{bmatrix} -\mathbf{L}_{u,GM} + \widehat{\mathbf{M}}_1^{(1)} & \tau r \mathbf{M}_{u^2/v^2} \\ -2\tau r \mathbf{M}_u & -\mathbf{L}_{v,GM} + \widehat{\mathbf{M}}_2^{(1)} \end{bmatrix} \mathbf{A}_{(1,2)}^{-1} \begin{bmatrix} -\mathbf{L}_{u,GM}^\top + \widehat{\mathbf{M}}_1^{(2)} & -2\tau r \mathbf{M}_u \\ \tau r \mathbf{M}_{u^2/v^2} & -\mathbf{L}_{v,GM}^\top + \widehat{\mathbf{M}}_2^{(2)} \end{bmatrix}$$

Preconditioning the Matrix System – Schur complement

- We choose $\widehat{\mathbf{M}}_1^{(1)}$, $\widehat{\mathbf{M}}_1^{(2)}$, $\widehat{\mathbf{M}}_2^{(1)}$, $\widehat{\mathbf{M}}_2^{(2)}$ such that [Stoll, Pearson & Maini, 2014]:

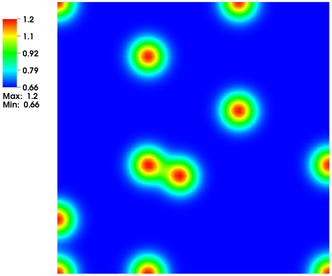
$$\begin{bmatrix} \widehat{\mathbf{M}}_1^{(1)} & 0 \\ 0 & \widehat{\mathbf{M}}_2^{(1)} \end{bmatrix} \mathbf{A}_{(1,2)}^{-1} \begin{bmatrix} \widehat{\mathbf{M}}_1^{(2)} & 0 \\ 0 & \widehat{\mathbf{M}}_2^{(2)} \end{bmatrix} \approx \tau \begin{bmatrix} \nu_1^{-1}\mathbf{M}_u \mathbf{M}^{-1} \mathbf{M}_u & 0 \\ 0 & \nu_2^{-1}\mathbf{M}_v \mathbf{M}^{-1} \mathbf{M}_v \end{bmatrix}.$$

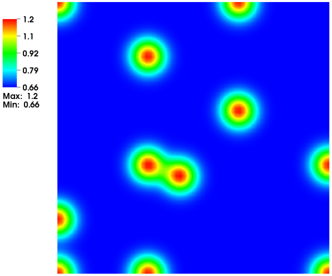
- We again examine the diagonal blocks, and select approximations such that

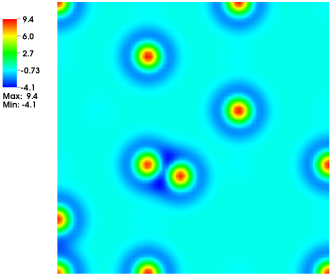
$$\mathbf{M}_1^{(1)} \hat{\mathbf{A}}_1^{-1} \mathbf{M}_1^{(2)} \approx \frac{\tau}{\nu_1} \mathbf{M}_u \mathbf{M}^{-1} \mathbf{M}_u, \qquad \hat{\mathbf{A}}_1 = \mathbf{A}_{u,GM} - (2\tau r)^2 \mathbf{M}_{up/v^2} \mathbf{A}_{v,GM}^{-1} \mathbf{M}_{up/v^2},$$

$$\mathbf{M}_2^{(1)} \hat{\mathbf{A}}_2^{-1} \mathbf{M}_2^{(2)} \approx \frac{\tau}{\nu_2} \mathbf{M}_v \mathbf{M}^{-1} \mathbf{M}_v, \qquad \hat{\mathbf{A}}_2 = \mathbf{A}_{v,GM} - (2\tau r)^2 \mathbf{M}_{up/v^2} \mathbf{A}_{u,GM}^{-1} \mathbf{M}_{up/v^2}.$$

$$\beta_1 = 1, \quad \beta_2 = 10, \quad D_u = 1, \quad D_v = 10, \quad \gamma = 50$$

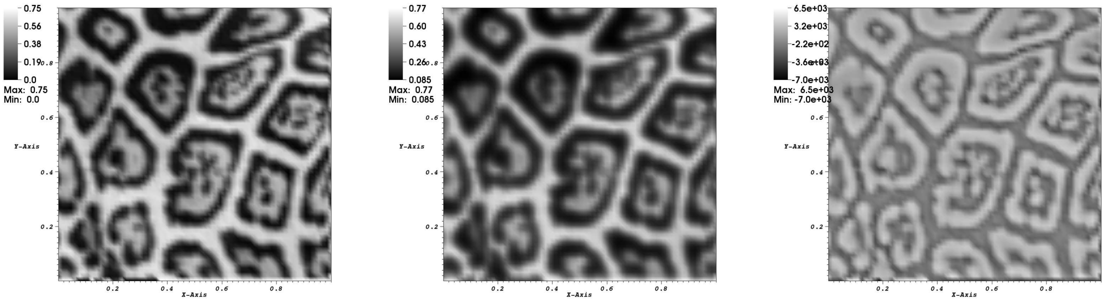






DoF	$\nu_1 = \nu_2 = 10^{-2}$		$\nu_1 = \nu_2 = 10^{-4}$		$\nu_1 = \nu_2 = 10^{-6}$	
	Newton	Iterations	Newton	Iterations	Newton	Iterations
43,740	step 1	11	step 1	13	step 1	9
	step 2	11	step 2	12	step 2	9
	step 3	11	step 3	12	step 3	9
	step 4	11	step 4	12		
	step 5	11	step 5	12		
294,780	step 1	11	step 1	13	step 1	11
	step 2	11	step 2	12	step 2	11
	step 3	11	step 3	12	step 3	11
	step 4	11	step 4	12	step 4	11
	step 5	11	step 5	12		
2,156,220	step 1	11	step 1	13	step 1	11
	step 2	11	step 2	12	step 2	11
	step 3	11	step 3	12	step 3	11
	step 4	11	step 4	12	step 4	11
	step 5	11	step 5	12		

$$\beta_1 = 10^2, \quad \beta_2 = 10^2, \quad D_u = 1, \quad D_v = 10, \quad r = 10^{-5}$$



DoF	$\nu_1 = \nu_2 = 10^{-2}$		$\nu_1 = \nu_2 = 10^{-4}$		$\nu_1 = \nu_2 = 10^{-6}$	
	Newton	Iterations	Newton	Iterations	Newton	Iterations
507,000	step 1	18	step 1	16	step 1	16
	step 2	20	step 2	15	step 2	15
	step 3	20	step 3	15	step 3	15
	step 4	20	step 4	15	step 4	15
	step 5	20	step 5	15		
1,996,920	step 1	23	step 1	17	step 1	17
	step 2	23	step 2	18	step 2	16
	step 3	24	step 3	18	step 3	16
	step 4	23	step 4	18	step 4	16
	step 5	23	step 5	18		

Conclusions

- PDE-constrained optimization is a diverse and important field.
- Have built framework for examining problems motivated by applications.
- Matrix systems have highly complex structure $\rightarrow$ carefully chosen preconditioners.
- Key is powerful approximations of $(1, 1)$-block and Schur complement.
- Image-driven: can "read in" data from nature.
- Fast and efficient solvers, often parallelizable.

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In the Future ...

- Efficient storage schemes for time-dependent nonlinear problems: data stored for each time-step.
- Pattern formation on more challenging/growing surfaces.
- Improved models using different norms.
- Tensor-train methodology & low-rank methods.

Thank you for your attention