Preconditioning vs. Deflation

Studying SIPG matrices for diffusion problems with strong variations



Kees Vuik

Paulien van Slingerland

Oil Reservoir Simulation

Layered structures yield challenging problems



Methods

DG Methods

DG methods are like FVMs, but then based on piecewise polynomials



DG for elliptic problems: [Arnold et al., 2002], [Rivière, 2008]

Problem

DG matrices are ill-conditioned and relatively large

2D Laplace problem with 3×3 mesh elements:



DG matrix with p = 0



Condition number: $\kappa(A) = O(h^{-2})$

Condition number

The condition number increases with the polynomial degree p





Coarse Corrections

The main idea is to speed up CG using coarse corrections based on p = 0



Original idea of spectral multigrid: [Rønquist and Patera, 1987]

Two-Level Preconditioner

The coarse corrections are combined with two smoothing steps

Computing $z = P_{\text{prec}}r$:

 $\begin{aligned} z^{(1)} &= \omega M^{-1} r & \text{smoothing} \\ z^{(2)} &= z^{(1)} + Q(r - Az^{(1)}) & \text{coarse correction} \\ z &= z^{(2)} + \omega M^{-T}(r - Az^{(2)}) & \text{smoothing} \end{aligned}$

Requirement: $M + M^T - \omega A$ is SPD

This preconditioner yields scalable CG convergence as was shown for p = 1 in [Dobrev et al., 2006] using [Falgout et al., 2005]

ADEF2 Deflation Variant

We can switch to deflation by simply skipping a smoothing step

Computing $z = P_{ADEF2}r$: $z^{(1)} = \omega M^{-1}r$ smoothing $z^{(2)} = z^{(1)} + Q(r - Az^{(1)})$ coarse correction $z = z^{(2)} + \omega M^{-T}(r - Az^{(2)})$ smoothing Requirement: $M + M^{T} - \omega A$ is SPD M is SPD

This operator is not symmetric ... (cf. next slide)

BNN deflation variant

BNN is symmetric, but more expensive due to two coarse solves

Computing $z = P_{BNN}r$:

 $\begin{aligned} z^{(1)} &= Qr & \text{coarse correction} \\ z^{(2)} &= z^{(1)} + \omega M^{-1} (r - A z^{(1)}) & \text{smoothing} \\ z &= z^{(2)} + Q (r - A z^{(2)}) & \text{coarse correction} \end{aligned}$

Requirement: M is SPD

ADEF2 and BNN yield the same CG iterates

assuming we preprocess the start vector: $x_0 \mapsto Qb + (I - AQ)^T x_0$ [Tang et al., 2009]

Theoretical Results

Theory The preconditioner yields scalable CG convergence

Theorem:

Suppose that A is the SPD result of a coercive SIPG discretization for a diffusion problem $-\nabla(K\nabla u) = f$ on a regular mesh with $p \ge 1$. Then:

 $\kappa_2(P_{\mathrm{prec}}^{-1}A) \lesssim 1,$

i.e. $\kappa_2(P_{\text{prec}}^{-1}A) \leq C$ for some constant C independent of h.

Shown for p = 1 in [Dobrev et al., 2006] using [Falgout et al., 2005]

Assumptions: The diffusion and SIPG penalty parameter are bounded M is nonsingular and $M + M^T - \omega A$ is SPD $\Rightarrow P_{\text{prec}}$ is SPD $h^{2-d}v^T M^T (M + M^T - \omega A)^{-1} M v \leq v^T v$ for all vectors v

A similar result is true for BNN deflation

Theorem:

Suppose that A is the SPD result of a coercive SIPG discretization for a diffusion problem $-\nabla(K\nabla u) = f$ on a regular mesh with $p \ge 1$. Then:

 $\kappa_2(P_{\mathrm{BNN}}^{-1}A) \lesssim 1,$

i.e. $\kappa_2(P_{\text{BNN}}^{-1}A) \leq C$ for some constant C independent of h.

To be shown in this presentation

Assumptions: The diffusion and SIPG penalty parameter are bounded M is SPD and $2M - \omega A$ is SPD $\Rightarrow P_{BNN}$ is SPD $h^{2-d}v^T M v \leq v^T v$ for all vectors v

Special case

The required smoothing conditions are satisfied for block Jacobi smoothing



Assumption: the damping parameter $\omega \leq 1$ (strictly for the preconditioning variant)

Proof Overview

We show that $\kappa_2(P^{-1}A)\lesssim 1$ for BNN deflation without relaxation $(\omega=1)$

Step 1: Writing $E = I - P^{-1}A$, we have (with $\lambda_{\max}(E) < 1$):

$$\kappa_2(\mathsf{P}^{-1}\mathsf{A}) \leq rac{1-\lambda_{\min}(\mathsf{E})}{1-\lambda_{\max}(\mathsf{E})}$$

Step 2: Next, there exists a constant $K \ge 1$ such that:

$$-1 \leq \lambda_{\sf min}(E) \leq \lambda_{\sf max}(E) \leq 1 - rac{1}{\kappa}$$

Step 3: The proof is completed by showing:

$$K \lesssim 1$$

Proof: Step 1 We show that $\kappa_2(P^{-1}A) \leq rac{1-\lambda_{\min}(E)}{1-\lambda_{\max}(E)}$

$$\lambda_{\max}(E) = \max_{y \neq 0} \frac{y^T A E y}{y^T A y}, \qquad \lambda_{\min}(E) = \min_{y \neq 0} \frac{y^T A E y}{y^T A y}$$

Proof: $E := I - P^{-1}A$ has the same spectrum as $A^{\frac{1}{2}}EA^{-\frac{1}{2}} = I - A^{\frac{1}{2}}P^{-1}A^{\frac{1}{2}}$ (symmetric) $\lambda_{\max}(E) = \max_{x \neq 0} \frac{x^{T}A^{\frac{1}{2}}EA^{-\frac{1}{2}x}}{x^{T}x} \stackrel{y = A^{-\frac{1}{2}x}}{=} \max_{y \neq 0} \frac{y^{T}AEy}{y^{T}Ay}$ Similarly: $\lambda_{\min}(E) = ... = \min_{y \neq 0} \frac{y^{T}AEy}{y^{T}Ay}$

Proof: Step 1 We show that $\kappa_2(P^{-1}A) \leq \frac{1-\lambda_{\min}(E)}{1-\lambda_{\max}(E)}$

$$\lambda_{\max}(E) = \max_{y \neq 0} \frac{y^T A E y}{y^T A y}, \qquad \lambda_{\min}(E) = \min_{y \neq 0} \frac{y^T A E y}{y^T A y}$$
$$\frac{1}{1 - \lambda_{\min}(E)} A \le P \le \frac{1}{1 - \lambda_{\max}(E)} A$$

 $\begin{array}{ll} \textbf{Proof:} & \text{For all } y \colon \lambda_{\min}(E) \ y^T A y \leq y^T A E y \leq \lambda_{\max}(E) \ y^T A y \\ & \text{Shorter notation: } \lambda_{\min}(E) \ A \leq A E \leq \lambda_{\max}(E) \ A \\ & \text{Rewriting yields: } \frac{1}{1 - \lambda_{\min}(E)} \ A \leq P \leq \frac{1}{1 - \lambda_{\max}(E)} \ A \end{array}$

Proof: Step 1 We show that $\kappa_2(P^{-1}A) \leq \frac{1-\lambda_{\min}(E)}{1-\lambda_{\max}(E)}$

$$\lambda_{\max}(E) = \max_{y \neq 0} \frac{y^T A E y}{y^T A y}, \qquad \lambda_{\min}(E) = \min_{y \neq 0} \frac{y^T A E y}{y^T A y}$$

$$\frac{1}{1 - \lambda_{\min}(E)} A \leq P \leq \frac{1}{1 - \lambda_{\max}(E)} A$$

$$We \text{ conclude:}$$

$$\kappa_2(P^{-1}A) \leq \frac{1 - \lambda_{\min}(E)}{1 - \lambda_{\max}(E)}$$

 $\begin{array}{ll} \textbf{Proof:} & \text{Known: } c_1A \leq P \leq c_2A \quad \Rightarrow \quad \kappa_2(P^{-1}A) \leq \frac{c_2}{c_1} & (\text{cf. e.g. [Vassilevski, 2008]}) \\ & \text{The proof is completed using } c_1 = \frac{1}{1 - \lambda_{\min}(E)} \text{ and } c_2 = \frac{1}{1 - \lambda_{\max}(E)} \\ \end{array}$

Proof: Step 2 We show that $-1 \le \lambda_{\min}(E) \le \lambda_{\max}(E) \le 1 - \frac{1}{K}$

Recall: Restriction operator *R*: defined such that $A_0 = RAR^T$ is the SIPG matrix for p = 0Coarse correction operator: $Q = R^T A_0^{-1} R$

Proof: Step 2 We show that $-1 \le \lambda_{\min}(E) \le \lambda_{\max}(E) \le 1 - \frac{1}{K}$

• Define for any SPD matrix D:

$$\Theta_D = (I - \overline{\pi}_A)(I - A^{\frac{1}{2}}D^{-1}A^{\frac{1}{2}})(I - \overline{\pi}_A)$$

$$K_D = \sup_{v \neq 0} \frac{\|(I - \pi_D)v\|_D^2}{\|v\|_A^2}$$

$$\bar{\pi}_A = A^{\frac{1}{2}} Q A^{\frac{1}{2}}$$
$$\pi_D = R^T (R D R^T)^{-1} R D$$

• E has the same spectrum as Θ_M

Proof: Known: $E = I - P^{-1}A = (I - QA)(I - M^{-1}A)(I - QA)$ [Tang et al., 2010] At the same time: $A^{-\frac{1}{2}}\Theta_M A^{\frac{1}{2}} = (I - QA)(I - M^{-1}A)(I - QA)$

$\begin{array}{c} \textbf{Proof: Step 2} \\ \text{We show that } -1 \leq \lambda_{\min}(E) \leq \lambda_{\max}(E) \leq 1 - \frac{1}{\mathcal{K}} \end{array}$

► Define for any SPD matrix D:

$$\Theta_D = (I - \bar{\pi}_A)(I - A^{\frac{1}{2}}D^{-1}A^{\frac{1}{2}})(I - \bar{\pi}_A)$$

$$K_D = \sup_{v \neq 0} \frac{\|(I - \pi_D)v\|_D^2}{\|v\|_A^2}$$
► E has the same spectrum as Θ_M

$$\bar{\pi}_A = A^{\frac{1}{2}} Q A^{\frac{1}{2}}$$
$$\pi_D = R^T (R D R^T)^{-1} R D$$

 $\blacktriangleright \ 0 < D_1 \leq D_2 \quad \Rightarrow \quad \Theta_{D_1} \leq \Theta_{D_2}$

$$\begin{array}{ll} \textbf{Proof:} & D_1 \leq D_2 \Rightarrow I - A^{\frac{1}{2}} D_1^{-1} A^{\frac{1}{2}} \leq I - A^{\frac{1}{2}} D_2^{-1} A^{\frac{1}{2}} \\ & QAQ = Q \Rightarrow \bar{\pi}_A^2 = (A^{\frac{1}{2}} QA^{\frac{1}{2}}) (A^{\frac{1}{2}} QA^{\frac{1}{2}}) = A^{\frac{1}{2}} QA^{\frac{1}{2}} = \bar{\pi}_A \text{ is a symmetric projection} \\ & \Theta_{D_1} = (I - \bar{\pi}_A) (I - A^{\frac{1}{2}} D_1^{-1} A^{\frac{1}{2}}) (I - \bar{\pi}_A) \leq (I - \bar{\pi}_A) (I - A^{\frac{1}{2}} D_2^{-1} A^{\frac{1}{2}}) (I - \bar{\pi}_A) = \Theta_{D_2} \end{array}$$

Proof: Step 2 We show that $-1 \le \lambda_{\min}(E) \le \lambda_{\max}(E) \le 1 - \frac{1}{K}$

► D - A SPSD $\Rightarrow \lambda_{\max}(\Theta_D) \le 1 - \frac{1}{K_D}$ with $K_D \ge 1$

Proof: Step 2 We show that $-1 \le \lambda_{\min}(E) \le \lambda_{\max}(E) \le 1 - \frac{1}{K}$

• *E* has the same spectrum as Θ_M

$$\bullet \quad 0 < D_1 \le D_2 \quad \Rightarrow \quad \Theta_{D_1} \le \Theta_{D_2}$$

- ► D A SPSD $\Rightarrow \lambda_{\max}(\Theta_D) \le 1 \frac{1}{K_D}$ with $K_D \ge 1$
- Using that 2M A is SPD completes the proof (with $K_{2M} \ge 1$):

$$-1 \leq \lambda_{\min}(E) \leq \lambda_{\max}(E) \leq 1 - rac{1}{K_{2M}}$$

 $\begin{array}{ll} \textbf{Proof:} & 2M - A > 0 \Rightarrow M \geq \frac{1}{2}A \Rightarrow \Theta_M \geq \Theta_{\frac{1}{2}A} = -(I - \bar{\pi}_A)^2 \Rightarrow \lambda_{\min}(\Theta_M) \geq -1 \\ & M \leq 2M \Rightarrow \Theta_M \leq \Theta_{2M} \Rightarrow \lambda_{\max}(\Theta_M) \leq 1 - \frac{1}{K_{2M}} \mbox{ (with } K_{2M} \geq 1) \\ & \text{Using that } E \mbox{ has the same spectrum as } \Theta_M \mbox{ completes the proof} \end{array}$

Proof: Step 3 We show that $K \lesssim 1$

For all v:
$$\|(I - \pi_{2M})v\|_{2M}^2 \le h^{d-2}\|(I - \pi_I)v\|_2^2$$

Proof: Recall the assumption: $h^{2-d} w^T M w \leq w^T w$ for all vectors $w \pi_D$ is the projection onto the coarse space $\operatorname{Range}(R^T)$ in the *D*-norm $\|(I - \pi_{2M})v\|_{2M}^2 \leq \|(I - \pi_I)v\|_{2M}^2 = h^{d-2}\|(I - \pi_I)v\|_{h^{2-d}2M}^2 \leq h^{d-2}\|(I - \pi_I)v\|_2^2$

Proof: Step 3 We show that $K \lesssim 1$

► For all
$$v: ||(I - \pi_{2M})v||_{2M}^2 \le h^{d-2} ||(I - \pi_I)v||_2^2$$

► For all $w \in \text{Range} (I - \pi_I): w^T w \le h^{2-d} w^T A w$

Info: This can be shown using properties of the SIPG method (we omit the proof) The main idea is to construct a block diagonal matrix D (independent of h) such that $w^T w \leq w^T D w \leq h^{2-d} w^T A w$ (coercivity is also used)

Proof: Step 3 We show that $K \lesssim 1$

► For all
$$v$$
: $\|(I - \pi_{2M})v\|_{2M}^2 \le h^{d-2}\|(I - \pi_I)v\|_2^2$
► For all $w \in \text{Range} (I - \pi_I)$: $w^T w \le h^{2-d} w^T A w$
► We conclude that

$$\mathcal{K} := \mathcal{K}_{2M} := \sup_{v \neq 0} \frac{\|(I - \pi_{2M})v\|_{2M}^2}{\|v\|_A^2} \lesssim 1$$

Info: For all v: $\|(I - \pi_{2M})v\|_{2M}^2 \le h^{d-2}\|(I - \pi_I)v\|_2^2 \le \|(I - \pi_I)v\|_A^2 \le \|v\|_A^2$ (The last inequality follows because π_I is a projection) Substitution into the definition of K completes the proof

Proof Overview

We show that $\kappa_2(P^{-1}A)\lesssim 1$ for BNN deflation without relaxation $(\omega=1)$

Step 1: Writing $E = I - P^{-1}A$, we have (with $\lambda_{\max}(E) < 1$):

$$\kappa_2(\mathsf{P}^{-1}\mathsf{A}) \leq rac{1-\lambda_{\min}(\mathsf{E})}{1-\lambda_{\max}(\mathsf{E})}$$

Step 2: Next, there exists a constant $K \ge 1$ such that:

$$-1 \leq \lambda_{\sf min}(E) \leq \lambda_{\sf max}(E) \leq 1 - rac{1}{\kappa}$$

Step 3: The proof is completed by showing:

$$K \lesssim 1$$

Numerical Experiments

Poisson Problem

Both two-level methods yield fast & scalable CG convergence

degree	p=2				p=3			
mesh	N=20 ²	N=40 ²	N=80 ²	N=160 ²	N=20 ²	N=40 ²	N=80 ²	$N = 160^{2}$
size A	2400	9600	38400	153600	4000	16000	64000	256000
Jacobi	301	581	1049	1644	325	576	1114	1903
block Jacobi (BJ)	205	356	676	1190	206	357	696	1183
two-level prec., 2x BJ	36	38	39	40	49	52	53	54
two-level defl., 1x BJ	32	33	33	34	36	37	37	38



CG stopping criterion: $\frac{||b-Ax_k||_2}{||b||_2} \leq 10^{-6}$ Diagonal-scaling is applied beforehand

Layered Problem

Not so fast & scalable anymore ...

degree	p=2				p=3			
mesh	N=20 ²	$N = 40^{2}$	N=80 ²	N=160 ²	N=20 ²	$N = 40^{2}$	N=80 ²	$N = 160^{2}$
size A	2400	9600	38400	153600	4000	16000	64000	256000
Jacobi	1671	4311	9069	15924	2569	5070	9083	15656
block Jacobi (BJ)	933	2253	4996	9656	1398	2960	5660	9783
two-level prec., 2x BJ	415	1215	2534	3571	1089	2352	4709	8781
two-level defl., 1x BJ	200	414	531	599	453	591	667	698

$$K = 1$$
$$K = 10^{-3}$$
$$K = 1$$
$$K = 10^{-3}$$
$$K = 1$$

CG stopping criterion: $\frac{||b-Ax_k||_2}{||b||_2} \leq 10^{-6}$ Diagonal-scaling is applied beforehand

SIPG Penalty Parameter σ

Sufficiently large for stabilty, but as small as possible for proper conditioning



[Epshteyn and Rivière, 2007]

[Dryja, 2003]

Layered Problem Revisited

Both two-level methods now yield fast & scalable convergence

degree		p=2				р	=3	
mesh	N=20 ²	N=40 ²	N=80 ²	N=160 ²	N=20 ²	N=40 ²	N=80 ²	$N = 160^{2}$
size A	2400	9600	38400	153600	4000	16000	64000	256000
Jacobi	975	1264	1567	2314	1295	1490	1921	3110
block Jacobi (BJ)	243	424	788	1285	244	425	697	1485
two-level prec., 2x BJ	46	43	43	44	55	56	56	57
two-level defl., 1x BJ	43	45	45	46	47	48	48	48

$$K = 1$$
$$K = 10^{-3}$$
$$K = 1$$
$$K = 10^{-3}$$
$$K = 1$$

CG stopping criterion: $\frac{||b-Ax_k||_2}{||b||_2} \le 10^{-6}$ Diagonal-scaling is applied beforehand

Relaxation

Using ωM^{-1} rather than M^{-1} benefits the preconditioning variant only

degree		р	=2			р	=3	
mesh	N=20 ²	N=40 ²	N=80 ²	N=160 ²	N=20 ²	N=40 ²	N=80 ²	N=160 ²
two-level prec. ($\omega = 1$)	46	43	43	44	55	56	56	57
$(\omega = 0.9)$	34	34	34	37	38	40	40	42
$(\omega = 0.8)$	32	33	34	34	36	36	37	39
$(\omega = 0.7)$	31	33	33	33	34	35	36	36
$(\omega = 0.6)$	32	32	33	34	35	35	36	36
$(\omega = 0.5)$	34	34	34	35	37	36	37	38
two-level defl. ($\omega = 1$)	43	45	45	46	47	48	48	48
$(\omega = 0.9)$	43	45	45	46	47	48	48	48
$(\omega = 0.8)$	43	45	45	46	47	48	48	48
$(\omega = 0.7)$	43	45	45	46	47	48	48	48
$(\omega = 0.6)$	43	45	45	46	47	48	48	48
$(\omega = 0.5)$	43	45	45	46	47	48	48	48

CPU Time

Deflation is still fast due to 30% lower costs per iteration



Coarse Systems

Coarse systems can be solved by applying CG again with a high tolerance

degree		р	=2		p=3			
mesh	N=20 ²	N=40 ²	N=80 ²	$N = 160^{2}$	N=20 ²	$N = 40^{2}$	N=80 ²	$N = 160^{2}$
direct	43	45	45	46	47	48	48	48
$TOL = 10^{-4}$	43	45	45	46	47	48	48	48
$TOL = 10^{-3}$	43	45	45	46	47	48	48	48
$TOL = 10^{-2}$	43	45	45	46	47	48	48	48
$\mathrm{TOL} = 10^{-1}$	55	60	81	51	48	48	54	79

Outer loop: two-level deflation, $\frac{||b-A_{x_k}||_2}{||b||_2} \leq 10^{-6}$

Inner loop: AMG * preconditioner, $\frac{||b-Ax_k||_2}{||b||_2} \leq \text{TOL}$

*HSL, a collection of Fortran codes for large-scale scientific computation. See http://www.hsl.rl.ac.uk/

Inner iterations

The HSL-CG solver yields fast convergence

Average # inner iterations ($\mathrm{TOL}=10^{-2}$):

degree	p=2					р	=3	
mesh	N=20 ²	N=40 ²	N=80 ²	$N = 160^{2}$	N=20 ²	N=40 ²	N=80 ²	$N = 160^{2}$
$TOL = 10^{-2}$	2.0	2.5	2.4	3.2	2.0	2.1	2.6	3.1

SIPG Convergence

A diffusion-dependent penalty parameter yields better accuracy



 $p = 3, u(x, y) = \cos(10\pi x)\cos(10\pi y)$

mesh elements

Test Case II Sand inclusions

degree	p=2					р	=3	
mesh	N=20 ²	N=40 ²	N=80 ²	$N = 160^{2}$	N=20 ²	N=40 ²	N=80 ²	$N = 160^{2}$
two-level prec. $(\omega = 1)$	44	44	48	46	53	53	56	58
two-level prec. ($\omega = 0.7$)	28	30	30	30	32	32	34	34
two-level defl. $(\omega = 1)$	38	42	42	42	43	46	47	48



Test case taken from [Vuik et al., 2001]

Test Case III Groundwater

degree	p=2					р	=3	
mesh	N=20 ²	N=40 ²	N=80 ²	N=160 ²	N=20 ²	N=40 ²	N=80 ²	N=160 ²
two-level prec. ($\omega = 1$)	53	54	52	52	63	67	68	68
two-level prec. ($\omega = 0.7$)	36	38	38	38	39	41	42	42
two-level defl. $(\omega = 1)$	52	54	54	54	58	59	59	60



Test case taken from [Vuik et al., 2001]

Conclusion

Both two-level variants yield fast and scalable CG convergence

- ► The SIPG penalty parameter can best be chosen diffusion-dependent
- Coarse systems can be solved by applying AMG-CG again in an inner loop
- Without relaxation, deflation is faster due to lower smoothing costs and faster convergence
- With relaxation, the preconditioner can become equally fast

Further Research

- Compare preconditioning and deflation theoretically
- Study more challenging test cases

Contact c.vuik@tudelft.nl



http://ta.twi.tudelft.nl/users/vuik/