

The effect of approximate coarsest-level solves on the convergence of multigrid V-cycle methods

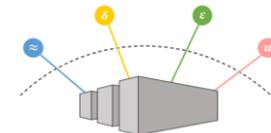
Petr Vacek, Erin Carson, Kirk M. Soodhalter
Charles University in Prague

Sparse Days Meeting 2024, Cerfacs, France

June 17, 2024



FACULTY
OF MATHEMATICS
AND PHYSICS
Charles University



inEXASCALE

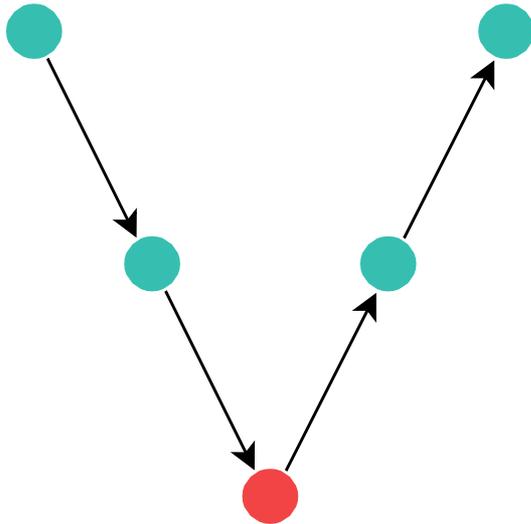
We acknowledge funding from ERC Starting Grant No. 101075632, Charles University PRIMUS project no. PRIMUS/19/SCI/11, the Exascale Computing Project (17-SC-20-SC), a collaborative effort of the U.S. Department of Energy Office of Science and the National Nuclear Security Administration.

Introduction

Find x : $Ax = b$.

x^{prev}

x^{new}



● smoothing

● solving on the coarsest level

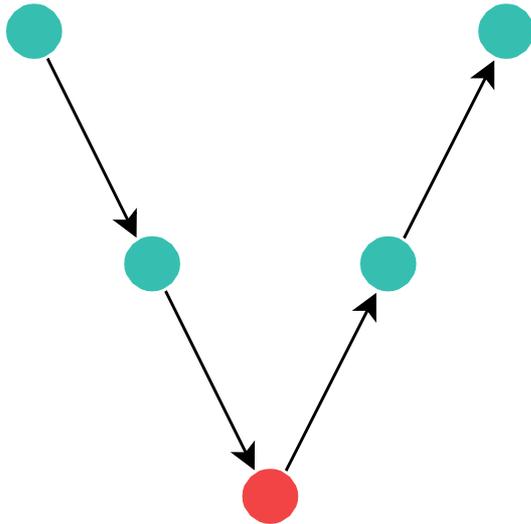
Find v_0 : $A_0 v_0 = f_0$.

Introduction

Find x : $Ax = b$.

x^{prev}

x^{new}



● smoothing

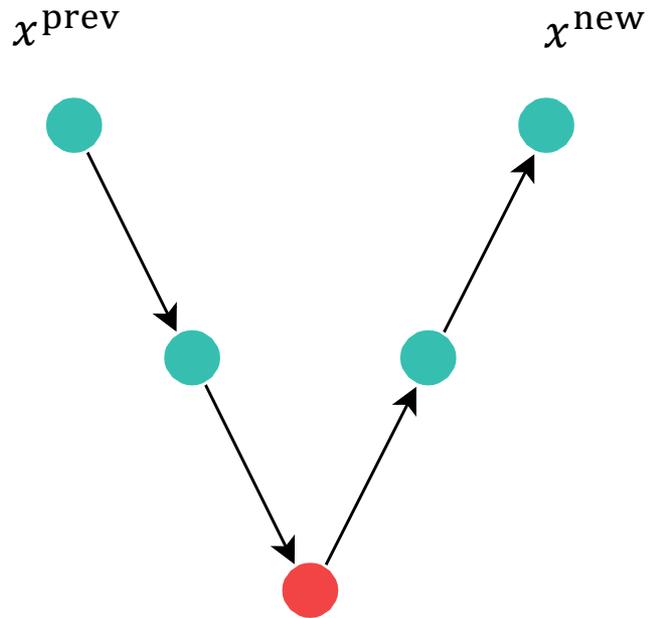
● solving on the coarsest level

direct solver based on LU decomposition

Find v_0 : $A_0 v_0 = f_0$.

Introduction

Find x : $Ax = b$.



Find v_0 : $A_0 v_0 = f_0$.

$$v_{0,\text{in}} \approx v_0$$

● smoothing

● solving on the coarsest level

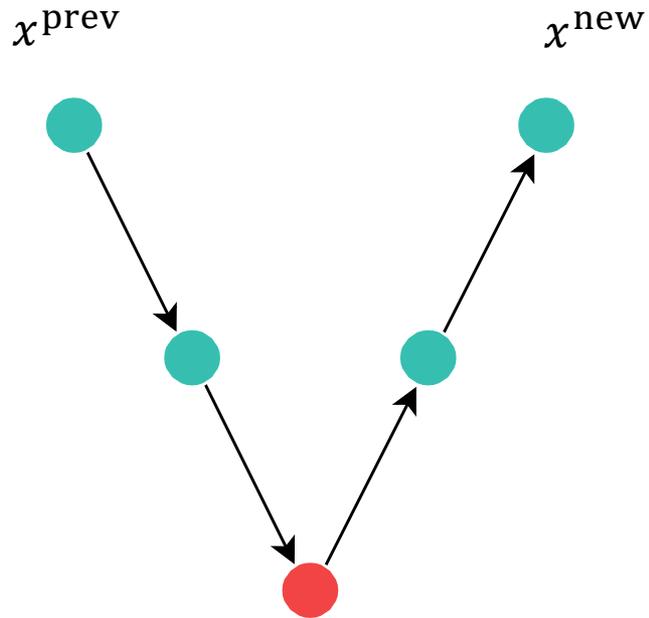
direct solver based on LU decomposition

Krylov subspace methods

Block Low Rank direct solver

Introduction

Find x : $Ax = b$.



Find v_0 : $A_0 v_0 = f_0$.

$$v_{0,\text{in}} \approx v_0$$

- smoothing
- solving on the coarsest level

direct solver based on LU decomposition
Krylov subspace methods

$$\frac{\|f_0 - A_0 v_{0,\text{in}}\|}{\|f_0\|} \leq \tau$$

Block Low Rank direct solver

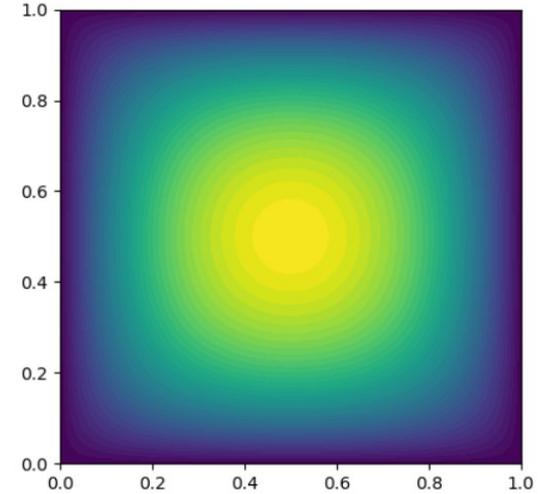
Motivational experiment

Poisson problem

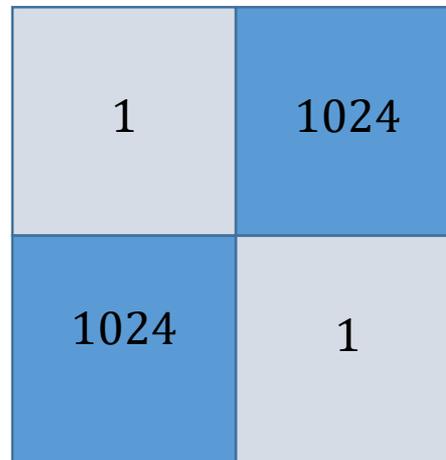
$$-\Delta u = 1 \text{ in } \Omega, \quad u = 0 \text{ on } \partial\Omega.$$

jump-1024 problem

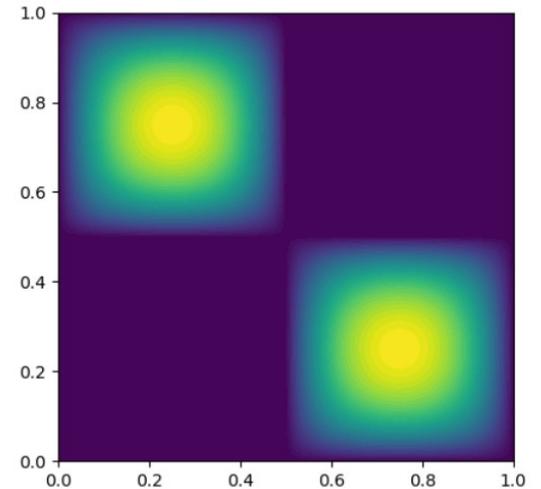
$$-\nabla \cdot (k(x)\nabla u) = 1 \text{ in } \Omega, \quad u = 0 \text{ on } \partial\Omega.$$



computed solution



coefficient $k(x)$



computed solution

Motivational experiment

Discretization

Galerkin FEM – continuous piecewise linear functions

uniform refinement

6 levels

coarsest-level: 1.52E+03 DoF

finest level: 1.64E+06 DoF

V-cycle method V(1,1)

smoother: symmetric Gauss-Seidel method

solver: MATLAB backslash or CG

zero initial approximation

$$\|x - x^{(n)}\|_A \leq \theta, \quad \theta = 10^{-4} \text{ or } \theta = 10^{-11}$$

Motivational numerical experiment

	Poisson problem		jump-1024 problem	
	condition number of the coarsest-level matrix			
	6.48E+02		1.66E+05	
	finest level tolerance θ		finest level tolerance θ	
	1.00E-04	1.00E-11	1.00E-04	1.00E-11
τ	V-cycles	total CG it.		
5.00E-01	5	68		
2.50E-01	3	62		
1.25E-01	3	71		
6.25E-02	2	63		
3.13E-02	2	71		
1.56E-02	2	79		
7.81E-03	2	88		
3.91E-03	2	96		
1.95E-03	2	100		
9.77E-04	2	106		
4.88E-04	2	110		
2.44E-04	2	115		
1.22E-04	2	120		
6.10E-05	2	125		
3.05E-05	2	129		
1.53E-05	2	132		
7.63E-06	2	135		
3.81E-06	2	139		
1.91E-06	2	152		
9.54E-07	2	158		
A\b	2			

Motivational numerical experiment

τ	Poisson problem				jump-1024 problem	
	condition number of the coarsest-level matrix					
	6.48E+02				1.66E+05	
	finest level tolerance θ					
	1.00E-04		1.00E-11		1.00E-04	1.00E-11
	V-cycles	total CG it.		V-cycles	total CG it.	
5.00E-01	5	68		14	226	
2.50E-01	3	62		11	234	
1.25E-01	3	71		10	231	
6.25E-02	2	63		9	240	
3.13E-02	2	71		9	251	
1.56E-02	2	79		9	294	
7.81E-03	2	88		9	352	
3.91E-03	2	96		9	390	
1.95E-03	2	100		9	412	
9.77E-04	2	106		9	445	
4.88E-04	2	110		9	472	
2.44E-04	2	115		9	543	
1.22E-04	2	120		9	579	
6.10E-05	2	125		9	638	
3.05E-05	2	129		9	671	
1.53E-05	2	132		9	711	
7.63E-06	2	135		9	741	
3.81E-06	2	139		9	773	
1.91E-06	2	152		9	815	
9.54E-07	2	158		9	843	
A\b	2			9		

Motivational numerical experiment

τ	Poisson problem				jump-1024 problem			
	condition number of the coarsest-level matrix							
	6.48E+02				1.66E+05			
	finest level tolerance θ				finest level tolerance θ			
	1.00E-04		1.00E-11		1.00E-04		1.00E-11	
	V-cycles	total CG it.		V-cycles	total CG it.		V-cycles	total CG it.
5.00E-01	5	68	14	226	3	544	31	2319
2.50E-01	3	62	11	234	3	708	28	2506
1.25E-01	3	71	10	231	2	537	28	2694
6.25E-02	2	63	9	240	2	615	23	3008
3.13E-02	2	71	9	251	2	724	26	3328
1.56E-02	2	79	9	294	2	787	25	3956
7.81E-03	2	88	9	352	2	843	27	4199
3.91E-03	2	96	9	390	2	975	19	4415
1.95E-03	2	100	9	412	2	996	19	5113
9.77E-04	2	106	9	445	2	1032	17	5727
4.88E-04	2	110	9	472	2	1083	16	6249
2.44E-04	2	115	9	543	2	1107	16	6963
1.22E-04	2	120	9	579	2	1194	15	7541
6.10E-05	2	125	9	638	2	1312	9	6391
3.05E-05	2	129	9	671	2	1385	12	7936
1.53E-05	2	132	9	711	2	1428	9	6982
7.63E-06	2	135	9	741	2	1491	9	7220
3.81E-06	2	139	9	773	2	1537	10	8197
1.91E-06	2	152	9	815	2	1621	9	7664
9.54E-07	2	158	9	843	2	1688	9	7900
A\b	2		9		2		9	

Motivational numerical experiment

τ	Poisson problem				jump-1024 problem			
	condition number of the coarsest-level matrix							
	6.48E+02				1.66E+05			
	finest level tolerance θ				finest level tolerance θ			
	1.00E-04		1.00E-11		1.00E-04		1.00E-11	
	V-cycles	total CG it.		V-cycles	total CG it.		V-cycles	total CG it.
5.00E-01	5	68	14	226	3	544	31	2319
2.50E-01	3	62	11	234	3	708	28	2506
1.25E-01	3	71	10	231	2	537	28	2694
6.25E-02	2	63	9	240	2	615	23	3008
3.13E-02	2	71	9	251	2	724	26	3328
1.56E-02	2	79	9	294	2	787	25	3956
7.81E-03	2	88	9	352	2	843	27	4199
3.91E-03	2	96	9	390	2	975	19	4415
1.95E-03	2	100	9	412	2	996	19	5113
9.77E-04	2	106	9	445	2	1032	17	5727
4.88E-04	2	110	9	472	2	1083	16	6249
2.44E-04	2	115	9	543	2	1107	16	6963
1.22E-04	2	120	9	579	2	1194	15	7541
6.10E-05	2	125	9	638	2	1312	9	6391
3.05E-05	2	129	9	671	2	1385	12	7936
1.53E-05	2	132	9	711	2	1428	9	6982
7.63E-06	2	135	9	741	2	1491	9	7220
3.81E-06	2	139	9	773	2	1537	10	8197
1.91E-06	2	152	9	815	2	1621	9	7664
9.54E-07	2	158	9	843	2	1688	9	7900
A\b	2		9		2		9	

Can we analytically describe how the choice of the relative tolerance on the coarsest-level affects the convergence of the V-cycle method?

Motivational numerical experiment

τ	Poisson problem				jump-1024 problem							
	condition number of the coarsest-level matrix											
	6.48E+02				1.66E+05							
	finest level tolerance θ				finest level tolerance θ							
	1.00E-04		1.00E-11		1.00E-04		1.00E-11					
	V-cycles	total CG it.			V-cycles	total CG it.			V-cycles	total CG it.		
5.00E-01	5	68	14	226	3	544	31	2319				
2.50E-01	3	62	11	234	3	708	28	2506				
1.25E-01	3	71	10	231	2	537	28	2694				
6.25E-02	2	63	9	240	2	615	23	3008				
3.13E-02	2	71	9	251	2	724	26	3328				
1.56E-02	2	79	9	294	2	787	25	3956				
7.81E-03	2	88	9	352	2	843	27	4199				
3.91E-03	2	96	9	390	2	975	19	4415				
1.95E-03	2	100	9	412	2	996	19	5113				
9.77E-04	2	106	9	445	2	1032	17	5727				
4.88E-04	2	110	9	472	2	1083	16	6249				
2.44E-04	2	115	9	543	2	1107	16	6963				
1.22E-04	2	120	9	579	2	1194	15	7541				
6.10E-05	2	125	9	638	2	1312	9	6391				
3.05E-05	2	129	9	671	2	1385	12	7936				
1.53E-05	2	132	9	711	2	1428	9	6982				
7.63E-06	2	135	9	741	2	1491	9	7220				
3.81E-06	2	139	9	773	2	1537	10	8197				
1.91E-06	2	152	9	815	2	1621	9	7664				
9.54E-07	2	158	9	843	2	1688	9	7900				
A\b	2		9		2		9					

Can we analytically describe how the choice of the relative tolerance on the coarsest-level affects the convergence of the V-cycle method?

Can we define coarsest-level stopping criteria that would yield a computed V-cycle approximation „close“ to the V-cycle approximation which would be obtained by solving the coarsest-level problems exactly?

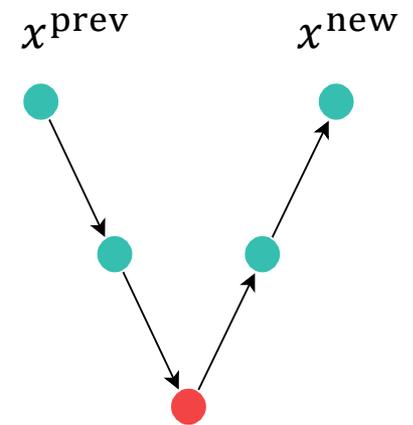
Setting

A - symmetric positive definite matrix

V-cycle method, $R_j = P_j^T$, $A_j = P_j^T A P_j$, Galerkin condition

V-cycle with exact solver converges

Find x : $Ax = b$.



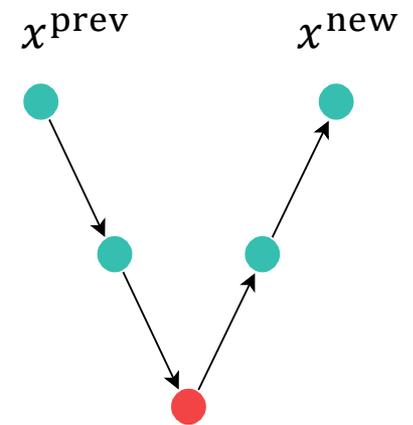
Find v_0 : $A_0 v_0 = f_0$.

$$v_{0,\text{in}} \approx v_0$$

Analysis

$$x - x_{\text{in}}^{\text{new}} = x - x_{\text{ex}}^{\text{new}} + x_{\text{ex}}^{\text{new}} - x_{\text{in}}^{\text{new}}$$

Find x : $Ax = b$.



Find v_0 : $A_0 v_0 = f_0$.

$$v_{0,\text{in}} \approx v_0$$

Analysis

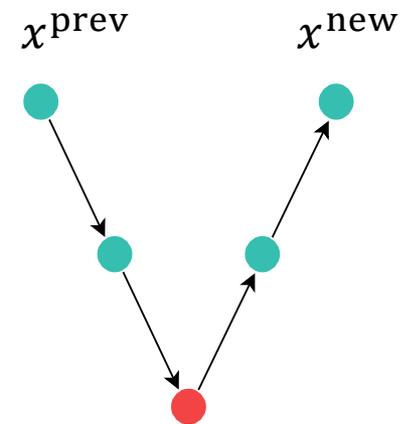
$$\begin{aligned}x - x_{\text{in}}^{\text{new}} &= x - x_{\text{ex}}^{\text{new}} + x_{\text{ex}}^{\text{new}} - x_{\text{in}}^{\text{new}} \\ &= E(x - x^{\text{prev}}) + S(v_0 - v_{0,\text{in}})\end{aligned}$$

error propagation
matrix of V-cycle with
exact solver

error of previous
approximation

error on the
coarsest-level

Find x : $Ax = b$.



Find v_0 : $A_0 v_0 = f_0$.

$$v_{0,\text{in}} \approx v_0$$

Analysis

$$\begin{aligned} x - x_{\text{in}}^{\text{new}} &= x - x_{\text{ex}}^{\text{new}} + x_{\text{ex}}^{\text{new}} - x_{\text{in}}^{\text{new}} \\ &= E(x - x^{\text{prev}}) + S(v_0 - v_{0,\text{in}}) \end{aligned}$$

error propagation
matrix of V-cycle with
exact solver

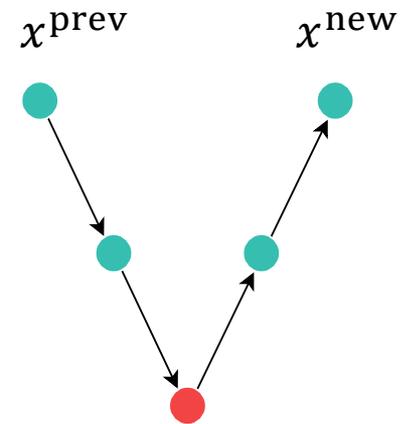
error of previous
approximation

error on the
coarsest-level

$$\|x - x_{\text{in}}^{\text{new}}\|_A \leq \|E\|_A \cdot \|x - x^{\text{prev}}\|_A + \underbrace{\|S\|_{A_0,A}}_{\leq 1} \cdot \|v_0 - v_{0,\text{in}}\|_{A_0}$$

$$\|S\|_{A_0,A} := \max_{v \in \mathbb{R}^{n_0}, v \neq 0} \frac{\|Sv\|_A}{\|v\|_{A_0}}$$

Find x : $Ax = b$.



Find v_0 : $A_0 v_0 = f_0$.

$$v_{0,\text{in}} \approx v_0$$

Analysis

$$\begin{aligned} x - x_{\text{in}}^{\text{new}} &= x - x_{\text{ex}}^{\text{new}} + x_{\text{ex}}^{\text{new}} - x_{\text{in}}^{\text{new}} \\ &= E(x - x^{\text{prev}}) + S(v_0 - v_{0,\text{in}}) \end{aligned}$$

error propagation
matrix of V-cycle with
exact solver

error of previous
approximation

error on the
coarsest-level

$$\|x - x_{\text{in}}^{\text{new}}\|_A \leq \|E\|_A \cdot \|x - x^{\text{prev}}\|_A + \underbrace{\|S\|_{A_0,A}}_{\leq 1} \cdot \|v_0 - v_{0,\text{in}}\|_{A_0}$$

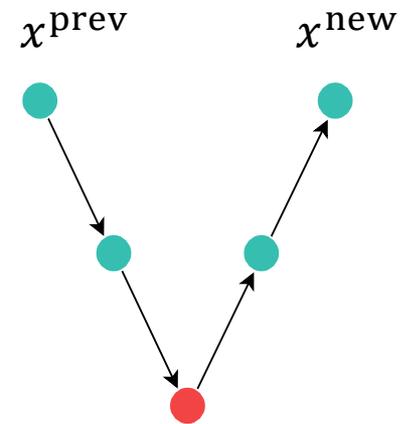
Relative coarsest-level accuracy assumption

$$\text{Let } \gamma > 0: \|v_0 - v_{0,\text{in}}\|_{A_0} \leq \gamma \cdot \|x - x^{\text{prev}}\|_A$$

Result:

$$\|x - x_{\text{in}}^{\text{new}}\|_A \leq (\|E\|_A + \gamma \cdot \|S\|_{A_0,A}) \|x - x^{\text{prev}}\|_A$$

Find x : $Ax = b$.



Find v_0 : $A_0 v_0 = f_0$.

$$v_{0,\text{in}} \approx v_0$$

Coarsest-level solver with relative residual tolerance

$$\frac{\|f_0 - A_0 v_{0,\text{in}}\|}{\|f_0\|} \leq \tau$$

$$\|x - x_{\text{in}}^{\text{new}}\|_A \leq \left(\|E\|_A + \tau \cdot \|T\| \cdot \|S\|_{A_0, A} \cdot \sqrt{\|A\| \cdot \|A_0^{-1}\|} \right) \|x - x^{\text{prev}}\|_A$$

Analysis

$$\begin{aligned} x - x_{\text{in}}^{\text{new}} &= x - x_{\text{ex}}^{\text{new}} + x_{\text{ex}}^{\text{new}} - x_{\text{in}}^{\text{new}} \\ &= E(x - x^{\text{prev}}) + S(v_0 - v_{0,\text{in}}) \end{aligned}$$

error propagation
matrix of V-cycle with
exact solver

error of previous
approximation

error on the
coarsest-level

$$\|x - x_{\text{in}}^{\text{new}}\|_A \leq \|E\|_A \cdot \|x - x^{\text{prev}}\|_A + \underbrace{\|S\|_{A_0,A}}_{\leq 1} \cdot \|v_0 - v_{0,\text{in}}\|_{A_0}$$

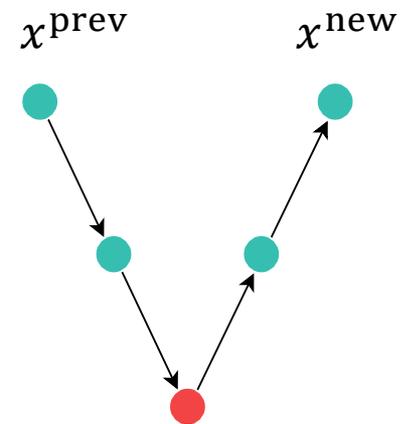
Absolute coarsest-level accuracy assumption

$$\text{Let } \epsilon > 0: \|v_0 - v_{0,\text{in}}\|_{A_0} \leq \epsilon$$

Result:

$$\|x_{\text{ex}}^{(n)} - x_{\text{in}}^{(n)}\|_A \leq \frac{\epsilon \cdot \|S\|_{A_0,A}}{1 - \|E\|_A} \leq \frac{\epsilon}{1 - \|E\|_A}$$

Find x : $Ax = b$.



Find v_0 : $A_0 v_0 = f_0$.

$$v_{0,\text{in}} \approx v_0$$

New coarsest-level stopping criterion

Can we define coarsest-level stopping criteria that would yield a computed V-cycle approximation „close“ to the V-cycle approximation which would be obtained by solving the coarsest-level problems exactly?

Ingredients:

Upper bound on the error of the coarsest level solver $\|v_0 - v_{0,\text{in}}\|_{A_0} \leq \eta(v_{0,\text{in}})$

Estimate of the convergence rate $\|E\|_A \leq \alpha$

Stop the coarsest-level solver when

$\frac{\eta(v_{0,\text{in}})}{(1-\alpha)} \leq \theta$, where θ is a parameter chosen by the user.

Then $\|x_{\text{ex}}^{(n)} - x_{\text{in}}^{(n)}\|_A \leq \theta$,
 $\|x - x_{\text{in}}^{(n)}\|_A \leq \|x - x_{\text{ex}}^{(n)}\|_A + \theta$

Numerical Experiments

Stop the coarsest-level solver when

$$\frac{\eta(v_{0,in})}{(1-\alpha)} \leq \theta$$

$$\|E\|_A < \alpha = 2/3$$

$$\theta = 10^{-4} \text{ or } 10^{-11}$$

(GR) Gauss-Radau bound
on A-norm of the error in CG
 [Meurant, Tichý2023]

τ	Poisson problem, 6 levels				jump-1024 problem, 6 levels				
	condition number coarsest-level matrix								
	6.48E+02				1.66E+05				
	finest level tolerance θ				finest level tolerance θ				
	1.00E-04		1.00E-11		1.00E-04		1.00E-11		
	V-cycles	total CG it.		V-cycles	total CG it.	V-cycles	total CG it.	V-cycles	total CG it.
5.00E-01	5	68	14	226	3	544	31	2319	
2.50E-01	3	62	11	234	3	708	28	2506	
1.25E-01	3	71	10	231	2	537	28	2694	
6.25E-02	2	63	9	240	2	615	23	3008	
3.13E-02	2	71	9	251	2	724	26	3328	
1.56E-02	2	79	9	294	2	787	25	3956	
7.81E-03	2	88	9	352	2	843	27	4199	
3.91E-03	2	96	9	390	2	975	19	4415	
1.95E-03	2	100	9	412	2	996	19	5113	
9.77E-04	2	106	9	445	2	1032	17	5727	
4.88E-04	2	110	9	472	2	1083	16	6249	
2.44E-04	2	115	9	543	2	1107	16	6963	
1.22E-04	2	120	9	579	2	1194	15	7541	
6.10E-05	2	125	9	638	2	1312	9	6391	
3.05E-05	2	129	9	671	2	1385	12	7936	
1.53E-05	2	132	9	711	2	1428	9	6982	
7.63E-06	2	135	9	741	2	1491	9	7220	
3.81E-06	2	139	9	773	2	1537	10	8197	
1.91E-06	2	152	9	815	2	1621	9	7664	
9.54E-07	2	158	9	843	2	1688	9	7900	
GR	2	82	9	674	2	743	9	6489	

Conclusions

New approach for analyzing the effects of approximate coarsest-level solves on the convergence of multigrid V-cycle methods

New coarsest-level stopping strategy tailored to multigrid methods

Future work:

Algebraic multigrid methods

CG preconditioned by multigrid with inexact coarsest level solver

P. V., E. Carson and K. M. Soodhalter, The Effect of Approximate Coarsest-Level Solves on the Convergence of Multigrid V-Cycle Methods, SIAM Journal on Scientific Computing (accepted; in press), <https://arxiv.org/abs/2306.06182>

A posteriori error estimates based on multilevel decompositions with large problems on the coarsest level

Petr Vacek, Jan Papež and Zdeněk Strakoš

Multilevel a posteriori error estimate [Rüde 1993]

$$-\Delta u = f \text{ in } \Omega, \quad u = 0 \text{ on } \partial\Omega$$

$$Ax = b, \text{ FEM P1 discretization}$$

$$\hat{x} \approx x$$

$$r_j = P_j^T (b - A\hat{x})$$

$$\eta_J = \left(\sum_{j=1}^J r_j^T \text{diag}(A_j)^{-1} r_j + r_0^T A_0^{-1} r_0 \right)^{\frac{1}{2}}$$

Multilevel a posteriori error estimate [Rüde 1993]

$$-\Delta u = f \text{ in } \Omega, u = 0 \text{ on } \partial\Omega$$

$$Ax = b, \text{ FEM P1 discretization}$$

$$\hat{x} \approx x$$

$$r_j = P_j^T (b - A\hat{x})$$

$$\eta_J = \left(\sum_{j=1}^J r_j^T \text{diag}(A_j)^{-1} r_j + r_0^T A_0^{-1} r_0 \right)^{\frac{1}{2}}$$

$$c\eta_J \leq \|x - \hat{x}\|_A \leq C\eta_J$$

Multilevel a posteriori error estimate [Rüde 1993]

$$-\Delta u = f \text{ in } \Omega, u = 0 \text{ on } \partial\Omega$$

$$Ax = b, \text{ FEM P1 discretization}$$

$$\hat{x} \approx x$$

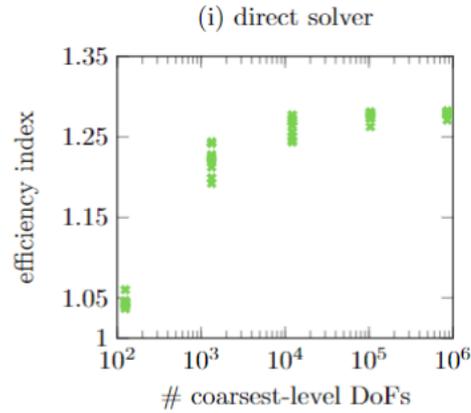
$$r_j = P_j^T (b - A\hat{x})$$

$$\eta_J = \left(\sum_{j=1}^J r_j^T \text{diag}(A_j)^{-1} r_j + r_0^T A_0^{-1} r_0 \right)^{\frac{1}{2}}$$

$$c\eta_J \leq \|x - \hat{x}\|_A \leq C\eta_J$$

Numerical experiment

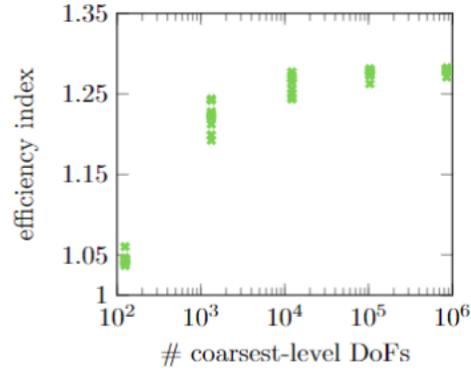
$$I = \frac{C \left(\sum_{j=1}^J r_j^T \text{diag}(A_j)^{-1} r_j + r_0^T A_0^{-1} r_0 \right)^{\frac{1}{2}}}{\|x - \hat{x}\|_A}$$



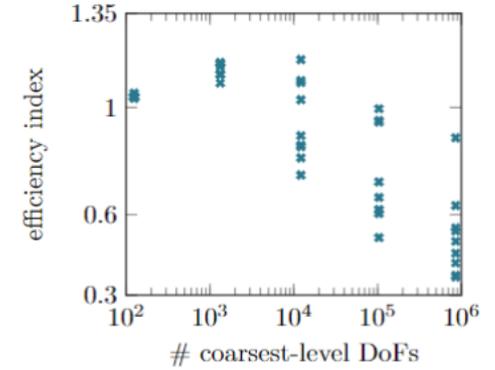
Numerical experiment

$$I = \frac{C \left(\sum_{j=1}^J r_j^T \text{diag}(A_j)^{-1} r_j + r_0^T A_0^{-1} r_0 \right)^{\frac{1}{2}}}{\|x - \hat{x}\|_A}$$

(i) direct solver



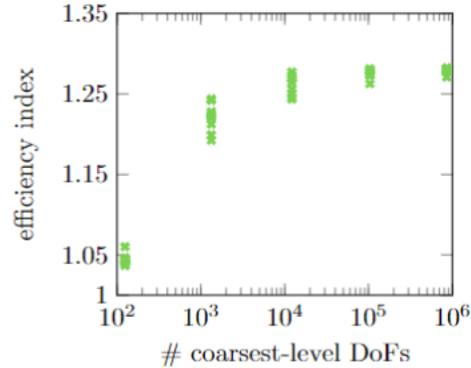
(ii) 4 iterations of CG



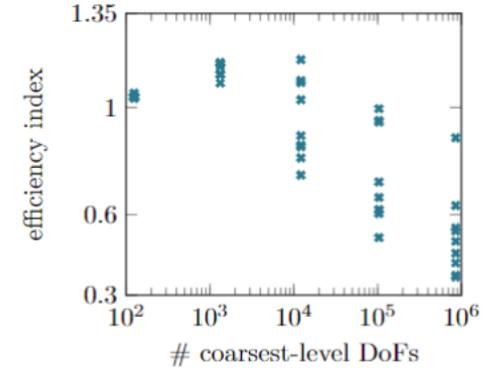
Numerical experiment

$$I = \frac{C \left(\sum_{j=1}^J r_j^T \text{diag}(A_j)^{-1} r_j + r_0^T A_0^{-1} r_0 \right)^{\frac{1}{2}}}{\|x - \hat{x}\|_A}$$

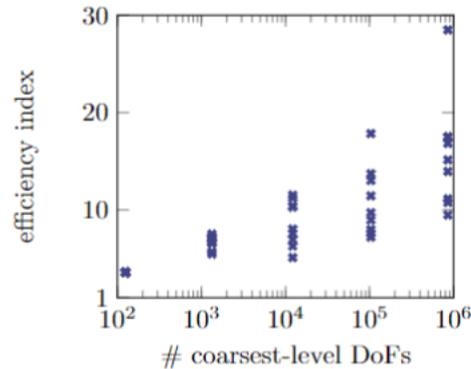
(i) direct solver



(ii) 4 iterations of CG



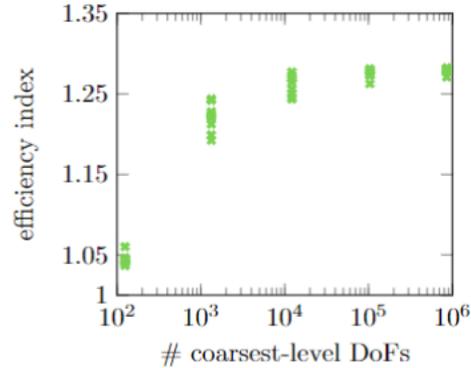
(iii) diagonal approximation



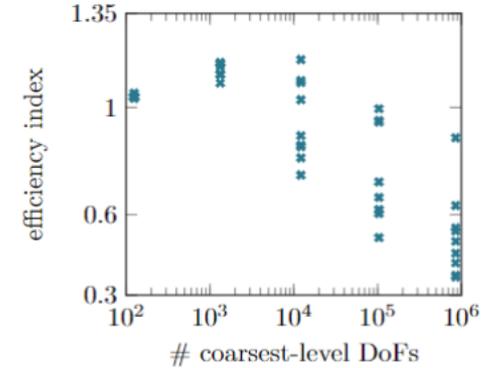
Numerical experiment

$$I = \frac{C \left(\sum_{j=1}^J r_j^T \text{diag}(A_j)^{-1} r_j + r_0^T A_0^{-1} r_0 \right)^{\frac{1}{2}}}{\|x - \hat{x}\|_A}$$

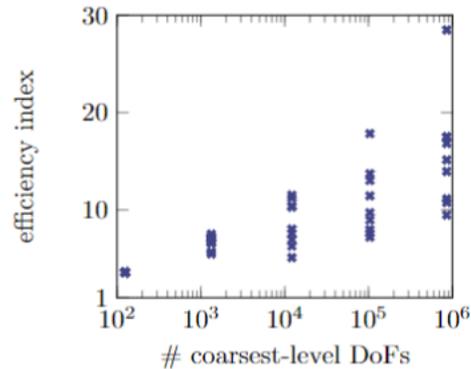
(i) direct solver



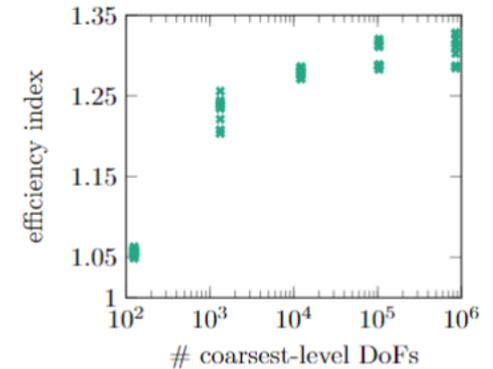
(ii) 4 iterations of CG



(iii) diagonal approximation

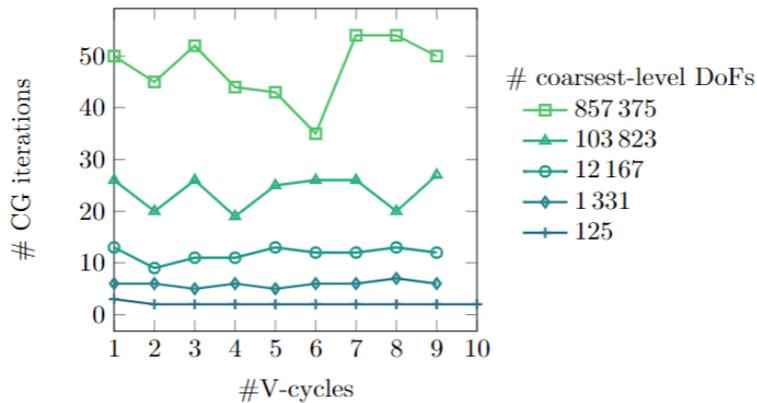


(iv) adaptive CG approximation

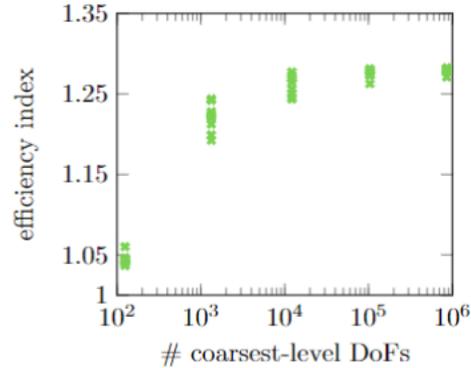


Numerical experiment

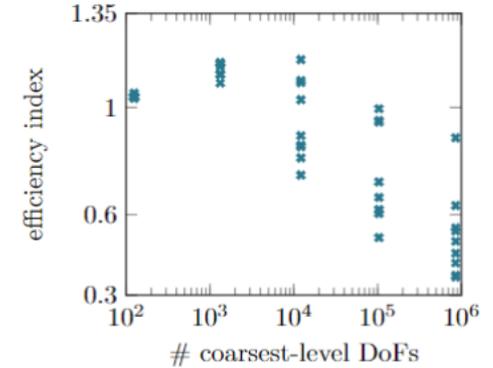
$$I = \frac{C \left(\sum_{j=1}^J r_j^T \text{diag}(A_j)^{-1} r_j + r_0^T A_0^{-1} r_0 \right)^{\frac{1}{2}}}{\|x - \hat{x}\|_A}$$



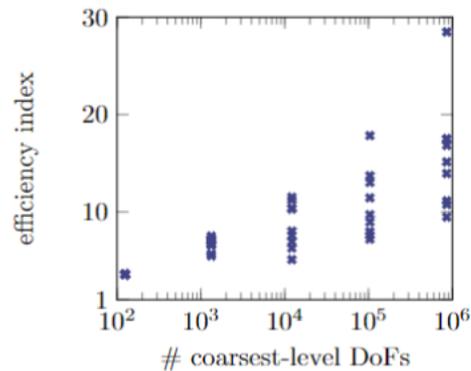
(i) direct solver



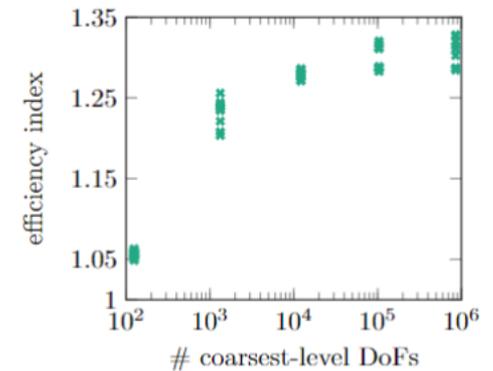
(ii) 4 iterations of CG



(iii) diagonal approximation



(iv) adaptive CG approximation



P. V., E. Carson and K. M. Soodhalter, The Effect of Approximate Coarsest-Level Solves on the Convergence of Multigrid V-Cycle Methods, SIAM Journal on Scientific Computing (accepted; in press), <https://arxiv.org/abs/2306.06182>

P. V., J. Papež and Z. Strakoš, A posteriori error estimates based on multilevel decompositions with large problems on the coarsest level, (submitted) May 2024, <https://arxiv.org/abs/2405.06532>



<https://sites.google.com/view/petrvacek>