On some geometric and algebraic aspects of domain decomposition methods

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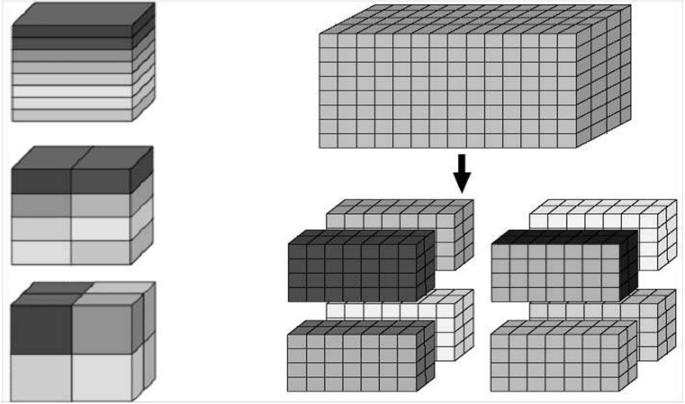
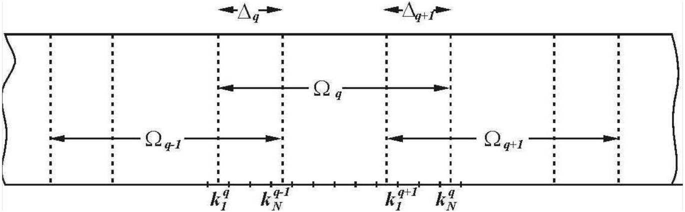
Examples of 1D-, 2D- and 3D- domain decomposition



1D-domain decomposition with overlapping



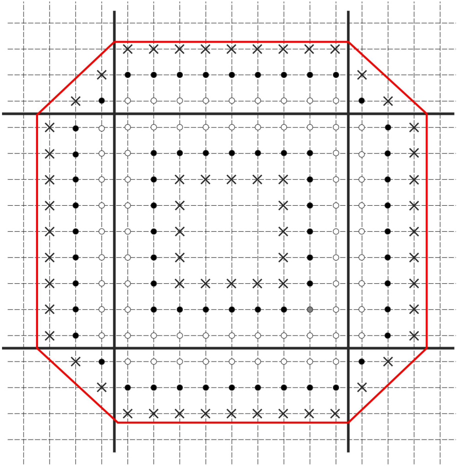
$\Omega = \bigcup_{q=1}^{P} \Omega_q$ - computational domain,

$\Omega_q = \{k_1^q, ..., k_N^q\}$ - q-th subdomain,

Δ_q, Δ_{q+1} - overlapping,

$k_1^q = k_N^{q-1},\ k_1^{q+1} = k_N^q$ - non-overlapping

$$\bar{\Omega}_p \equiv \Omega_p \bigcup \Gamma_p^1 \dots \bigcup \Gamma_p^\Delta,$$



Boundary Value Problem

$$Lu = f(\vec{r}), \quad \vec{r} \in \Omega; \qquad lu|_{\Gamma} = g,$$

Notations

$$\Omega = \bigcup_{q=1}^{P} \Omega_q, \quad \bar{\Omega} = \Omega \bigcup \Gamma, \quad \bar{\Omega}_q = \Omega_q \bigcup \Gamma_q,$$

$$\Gamma_q = \bigcup_{q' \in \omega_q} \Gamma_{q,q'}, \quad \Gamma_{q,q'} = \Gamma_q \bigcap \bar{\Omega}_{q'}, \quad q' \neq q,$$

Ω_0 – **external domain**, $\bar{\Omega}_0 = \Omega_0 \bigcup \Gamma$,

$\Gamma_{q,0} = \Gamma_q \bigcap \bar{\Omega}_0 = \Gamma_q \bigcap \Gamma$ – **external boundary of** Ω_q,

$\Delta_{q,q'} = \Omega_q \bigcap \Omega_{q'}$ – **overlapping**,

$\Gamma_{q,q'} = \Gamma_{q',q}$ – **non-overlapping** $(\Delta_{q,q'} = 0)$

Generalized Schwarz Decomposition

$$
\begin{aligned}
&Lu_q(\vec{r}) = f_q, \quad \vec{r} \in \Omega_q, \\
&l_{q,q'}(u_q)\big|_{\Gamma_{q,q'}} = g_{q,q'} \equiv l_{q',q}(u_{q'})\big|_{\Gamma_{q',q}}, \\
&q' \in \omega_q, \quad l_{q,0}u_q|_{\Gamma_{q,0}} = g, \quad q = 1, ..., P,
\end{aligned}
$$

$$
\begin{aligned}
&\alpha_q u_q + \beta_q \frac{\partial u_q}{\partial n_q}\Big|_{\Gamma_{q,q'}} = g_{q,q'} \equiv \alpha_{q'} u_q + \beta_{q'} \frac{\partial u_{q'}}{\partial n_{q'}}\Big|_{\Gamma_{q',q}}, \\
&|\alpha_q| + |\beta_q| > 0, \quad \alpha_q \cdot \beta_q \geq 0,
\end{aligned}
$$

Iterations:

$$
Lu_q^n = f_q, \quad l_{q,q'}u_q^n|_{\Gamma_{q,q'}} = l_{q',q}u_{q'}^{n-1}|_{\Gamma_{q',q}},
$$

Example:

Dirichlet Boundary Value Problem for Poisson Equation in the Square

$$-\Delta u = f, \quad u|_\Gamma = g, \; \Omega = [0 \times 1]^3; \; \Omega^h = \{i, j, k\},$$

$$(Au^h)_{i,j,k} = 6u^h_{i,j,k} - u^h_{i-1,j,k} - u^h_{i,j-1,k} -$$

$$-u^h_{i+1,j,k} - u^h_{i,j+1,k} - u^h_{i,j,k-1} - u^h_{i,j,k+1} = f^h_{i,j,k};$$

$$i, j, k = 1, ..., M, \;\; f^h = \{f^h_{i,j,k}\}, \;\; u^h = \{u^h_{i,j,k}\} \in \mathcal{R}^{M^3},$$

Notations for 1D Grid Decomposition

$$N = \mathbf{dim}(\Omega_q^h),\ \ m = \mathbf{dim}(\Delta_q^h),\ \ q = 1, ..., P,$$

$$N = k_N^q - k_1^q + 1, \quad m = k_N^q - k_1^{q+1} + 1, \quad M = PN - (P-1)m,$$

$$u_q = (u_1^{k^q}, ..., u_N^{k^q})^T), \quad u_l^{k^q} = \{u_l^{i,j,k^q};\ i, j, = 1, ..., M\} \in \mathcal{R}^{M^2},$$

Block Tridiagonal Systems

$$-A_{q,q-1}u_{q-1} + A_{q,q}u_q - A_{q,q+1}u_{q+1} = f_q, \quad q = 1, ..., P,$$

$$A_{1,0} = A_{P,P+1} = 0, \quad A_{q,q}, A_{q,q\pm1} = A_{q\pm1,q}^T \in \mathcal{R}^{M^2N, M^2N}$$

Block Jacobi Method

$$n = 1, 2 \ldots - \textbf{number of iterations},$$
$$A_{q,q} u_q^n = \bar{f}_q^{n-1} \equiv f_q + \hat{f}_q^{n-1} + \check{f}_q^{n-1},$$
$$\hat{f}_q^{n-1} = A_{q,q-1} u_{q-1}^{n-1}, \; \check{f}_q^{n-1} = A_{q,q+1} u_{q+1}^{n-1},$$

$$(A_{q,q} u_q^n)_k = \begin{cases} (C - \theta I) u_{k_1^q}^n - u_{k_1^q - 1}^n = f_{k_1^q} + v_{q-1}^{n-1}, \\ v_{q-1}^{n-1} = u_{k_1^q - 1}^{n-1} - \theta u_{k_1^q}^{n-1}, \qquad k = k_1^q, \\ (C - \theta I) u_{k_N^q}^n - u_{k_N^q + 1}^n = f_{k_N^q} + w_{q+1}^{n-1}, \\ w_{q+1}^{n-1} = u_{k_N^q + 1}^{n-1} - \theta u_{k_N^q}^{n-1}, \qquad k = k_N^q, \\ -u_{k-1}^n + C u_k^n - u_{k+1}^n = f_k, \\ k = k_1^q + 1, \ldots, k_N^q - 1, \end{cases}$$

$$(C - \theta I)u^n)_k)_{i,j} = \{(6 - \theta)u^n_{i,j,k} - u^n_{i-1,j,k} - u^n_{i+1,j,k} - $$
$$- u^n_{i,j-1,k} - u^n_{i,j+1,k}\},$$

$$C \in \mathcal{R}^{M^2},\ \theta \in [0,1],\ u^{n-1}_{k^q_1} \in \Omega_{q-1},\ u^{n-1}_{k^q_N} \in \Omega_{q+1},$$

$\theta = 0 -$ **Dirichlet Boundary Condition**,

$\theta = 1 -$ **Neumann Boundary Condition**,

$0 < \theta < 1 -$ **Robin Boundary Condition**,

$\theta -$ **compensation parameter**

Iterations in Trace Spaces

$$v_q = C_{q,q-1} u_q, \quad w_q = C_{q,q+1} u_q, \quad A_{q,q\pm1} = Q_{q,q\pm1} C_{q,q\pm1},$$

$$v_q^n = \hat{B}_{q,q-1} w_{q-1}^{n-1} + \hat{B}_{q,q+1} v_{q+1}^{n-1} + \hat{g}_q, \quad q = 2, \ldots, P,$$

$$w_q^n = \check{B}_{q,q-1} w_{q-1}^{n-1} + \check{B}_{q,q+1} v_{q+1}^{n-1} + \check{g}_q, \quad q = 1, \ldots, P-1,$$

$$\hat{B}_{1,0} = \hat{B}_{P,P+1} = 0,$$

$$\hat{g}_q = C_{q,q-1} A_{q,q}^{-1} f_q, \quad \check{g}_q = C_{q,q+1} A_{q,q}^{-1} f_q,$$

$$\hat{B}_{q,q\pm1} = C_{q,q-1} A_{q,q}^{-1} Q_{q,q\pm1}, \quad \check{B}_{q,q\pm1} = C_{q,q+1} A_{q,q}^{-1} Q_{q\pm1},$$

$C_{q,q\pm1} \in \mathcal{R}^{M^2 N, M^2}$ – **extension matrices,**

$Q_{q,q\pm1} \in \mathcal{R}^{M^2, M^2 N}$ – **reduction matrices**

Preconditioned Equation in Trace Space

$$s = (w_1, v_2, ..., w_{p-1}, v_p)^T,$$

$$As = f_{tr}; \quad s, f_{tr} \in \mathcal{R}^{N_{tr}},$$

$$n = 0, 1, ... : s^{n+1} = s^n + B_n^{-1}(f_{tr} - As^n),$$

$$s^{n+1} = T_n s^n + g^n, g^n = B_n^{-1} f_{tr},$$

$$T_n = I - B_n^{-1} A$$

$$s^n \to s : \bar{A}_n s \equiv (I - T_n)s = g^n$$

Conjugate Direction Methods

$CG: \ \nu = 0 \qquad\qquad CR: \ \nu = 1$

$$r^0 = g - \bar{A}s^0 = \hat{s}^1 - s^0, \ \ \hat{s}^1 = Ts^0 + g, \ \ p^0 = r^0,$$

$$s^{n+1} = s^n + \alpha_n^{(\nu)} p^n, \ \ \alpha_n^{(\nu)} = \rho_n^{(\nu)} / \delta_n^{(\nu)},$$

$$\rho_n^{(\nu)} = (\bar{A}^\nu r^n, r^n), \ \ \delta_n^{(\nu)} = (\bar{A}p^n, \bar{A}^\nu p^n),$$

$$r^{n+1} = r^n - \alpha_n^{(\nu)} \bar{A} p^n, \ \ p^{n+1} = r^{n+1} + \beta_n^{(\nu)} p^n, \ \ \beta_n^{(\nu)} = \rho_{n+1}^{(\nu)} / \rho_n^{(\nu)},$$

two-level : $(r_{in}^{n_q}, r_{in}^{n_q})/(f_q^n, f_q^n) \leq (\varepsilon_{in}^{(n)})^2, \ \ (r^n, r^n) \leq \varepsilon_{ex}^2 (g, g)$

Arnoldi A^s-orthogonalization $(s = 0, 1)$

$$u^n = u^0 + y_1 v^n + \dots + y_n v^n, \quad (v^n, A^s v^k) = d_n^{(s)} \delta_{k,n},$$

$$d_n^{(s)} = (v^n, A^s v^n),$$

$$v^{n+1} = Av^n - \sum_{k=1}^{n} h_{k,n}^{(s)} v^k, \quad v^1 = r^0 = f - Au^0,$$

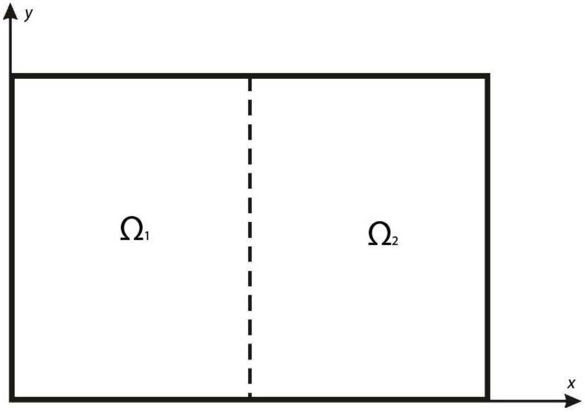
$$h_{k,n}^{(s)} = \frac{(Av^n, A^s v^k)}{(A^s v^k, v^k)}, \quad k = 1, \dots, n+1, \quad V_{n+1} = (v^1, \dots, v^{n+1})$$

$$\bar{H}_n = \{h_{k,n}\} = \left[\begin{array}{c} H_n \\ e_n^t \end{array} \right] \in \mathcal{R}^{n+1,n}, \quad H_n \in \mathcal{R}^{n,n},$$

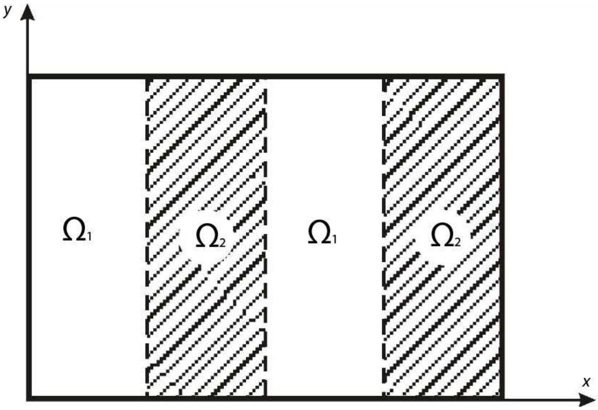
$$\mathcal{K}_{n+1}(r^0, A) = \mathrm{span}\{v^1, \dots, v^{n+1}\} = \mathrm{span}\{r^0, Ar^0, \dots, A^n r^0\}$$

FOM, A-FOM, GMRES, A-GMRES

Subdomains without overlapping



Even - Odd Decomposition



The Poincare - Steklov Operators (PSO)

$$P = 2,\ \Delta = 0: \quad -\Delta u_q = f_q, \quad u|_\Gamma = g,\ q = 1, 2,$$

$$-\Delta u = f, \quad u = u_1 \bigcup u_2; \quad \Gamma_{1,2} : u_1 = u_2, \quad -\frac{\partial u_1}{\partial n_1} = \frac{\partial u_2}{\partial n_2},$$

$$u_1 = u_2\big|_{\Gamma_{1,2}}, \Rightarrow -\Delta u_q^0 = f_q, \quad v_q \equiv u_q - u_q^0,\ q = 1, 2,$$

$$-\Delta v_q = 0, \quad v_q|_\Gamma = 0, \quad v_q|_{\Gamma_{1,2}} = u - u^0_{\Gamma_{1,2}},$$

$$\frac{\partial v_1}{\partial n_1} + \frac{\partial v_2}{\partial n_2} = \varphi \equiv -\Big(\frac{\partial u_1^0}{\partial n_1} + \frac{\partial u_2^0}{\partial n_2}\Big),$$

PSO: $\dfrac{\partial v_q}{\partial n_q} = S_q^{-1} v_q = S_q^{-1}(u_q - u^0_{\Gamma_{1,2}}),$

$$\Gamma_{1,2} : Au \equiv (S_1^{-1} + S_2^{-1})u = \psi,$$

$$\psi = (S_1^{-1} + S_2^{-1})u^0_{\Gamma_{1,2}} - \Big(\frac{\partial u_1^0}{\partial n_1} + \frac{\partial u_2^0}{\partial n_2}\Big)$$

$$\bar{A}u \equiv BAu = B\psi, \quad B = S_1 + S_2,$$

$$\bar{A} = (S_1 + S_2)(S_1^{-1} + S_2^{-1}) = I + S_1 S_2^{-1} + I + S_2 S_1^{-1} =$$

$$= A_1 + A_2, \quad A_1 = I + S_1 S_2^{-1}, \quad A_2 = I + S_2 S_1^{-1},$$

$$A_1 A_2 = A_1 + A_2 = A_2 A_1 \quad \textbf{(commutative operators)}$$

Eigenvalue Problems

$$\bar{A}w_k = \lambda_k w_k, \quad \lambda_k(S_1 S_2^{-1}) = \lambda_k^{-1}(S_2 S_1^{-1}),$$

$$\lambda_k(\bar{A}) = 2 + \lambda_k(S_1 S_2^{-1}) + \lambda_k(S_2 S_1^{-1}), \; k = 1, 2, \ldots$$

Block Cimmino Algorithm

$$Au \equiv \begin{bmatrix} A_1 \\ \vdots \\ A_p \end{bmatrix} u = \begin{bmatrix} f_1 \\ \vdots \\ f_p \end{bmatrix} \equiv f, \quad A \in \mathcal{R}^{N,N}; u, f \in \mathcal{R}^N,$$

A_q - **block rows**

$$A_k u = f_k, \quad f_k \in \mathcal{R}^M, \quad A_k \in \mathcal{R}^{M,N}, \quad k = 1, ..., p, \; N = PM,$$

$$v_k^n = A_k^+ r_k^n, r_k^n = f_k - A_k u^n, \quad A^+ = A_k^T (A_k A_k^T)^{-1},$$

$$u^{n+1} = u^n + \omega \sum_{k=1}^{N} v_k^n, \quad n = 0, 1, ...$$

ω - **iterative parameter**

Generalized Pseudo-Inverse Matrix

$$A_k^{+G} = G^{-1} A_k^T (A_k G^{-1} A_k^T)^{-1}, \quad G_k \in \mathcal{R}^{M,M} - s.p.d.$$

$$\begin{bmatrix} G & A_k^T \\ G & 0 \end{bmatrix} \begin{bmatrix} w_k^n \\ v_k^n \end{bmatrix} = \begin{bmatrix} 0 \\ r_k^n \end{bmatrix},$$

$$G w_k^n = -A^T v_k^n, \quad v_k^n = A_k^{+G} r_k^n.$$

$Q = A_k^{+G} A_k$ - **orthogonal projector onto the range of** A_k^T.

Additive Schwarz Methods

$$\Omega = \Omega_q \bigcup \tilde{\Omega}_q, \quad \tilde{\Omega}_q = \Omega / \Omega_q - \textbf{complement}$$

$$\textbf{subdomain to} \quad \Omega_q, \quad q = 1, ..., P,$$

$$u = \begin{bmatrix} u_q \\ \tilde{u}_q \end{bmatrix}, \quad u_q = R_q u, \ R_q = [0 \ I \ 0] - \textbf{restriction operator},$$

$$R_q^T - \textbf{extension operator}, \ A = A^T :$$

$B_q = R_q^T (R_q A R_q^T)^{-1} R_q = B_q^T$ - **preconditioning operator,**

$u^{n+1} = u^n + \sum_{q=1}^{p} B_q (f - Au^n)$,

$P_q = B_q A, \ P_q^2 = P_q$ - **orthogonal projector in the A-inner product:**

$$(P_q u, v)_A = u^T P_q^T A v = u^T A B_q A v = (U, P_q v)_A$$

Coarse Grid Correction

$$A_f u_F = f_f, \quad u_f, f_f \in \mathcal{R}^{N_f}, \quad A_f \in \mathcal{R}^{N_f, N_f},$$

$$R \in \mathcal{R}^{N_f, N_f}, \quad N_c \ll N_f, \quad A_c \in \mathcal{R}^{N_c, N_c},$$

$$u_f^{n+1} = u_f^n + (B_c + B_f)(f_f - A_f u_f),$$

$$B_c = R^T A_c^{-1} R \in \mathcal{R}^{N_f, N_f}, \quad B_f = \sum_{q=1}^{P} B_q$$

Galerkin version:

$R^T = R_0^T$ - **interpolation matrix,**

$$A_c = R_0 A R_0^T, \quad B_c = R_0^T (R_0 A R_0^T) R_0$$

Deflation

$$W_d^T r^0 = 0, \quad W_d^T A p^0 = 0, \quad (w_1, ..., w_m) = W_d,$$

$$u^0 = u^{-1} + W_d A_d^{-1} W_d^T r^{-1}, \quad r^0 = f - A u^0,$$

$$p^0 = [I - W_d A_d^{-1}(A W_d^T)] r^0, \quad A_d = W_d^T A W_d$$

Parallel Implementation

$$v_q^0 = C_{q,q-1} u_q^0 = \{u^0_{i,j,k_N^{q-1}+1} - \theta u^0_{i,j,k_N^{q-1}};\, i,j, = 1, ..., M\},$$

$$w_q^0 = C_{q,q+1} u_q^0 = \{u^0_{i,j,k_1^{q+1}-1} - \theta u^0_{i,j,k_1^{q+1}};\, i,j, = 1, ..., M\},$$

$$v_q^0, w_q^0 : \Omega_q \to \Omega_{q\pm1}; \quad v_{q+1}^0, w_{q-1}^0 : \Omega_{q\pm1} \to \Omega_q,$$

$$A_{q,q}\hat{u}_q^1 = \bar{f}_q = \left[f_k^q = \begin{cases} f_{k_1^q} + w_{q-1}^0, & k = k_1^q, \\ f_{k_N^q} + v_{q+1}^0, & k = k_N^q, \\ f_k, & k = k_1^q + 1, ..., k_N^q - 1. \end{cases} \right]$$

$$t^n \equiv \bar{A}p^n = p^n - q^n, \qquad q^n = Tp^n,$$

Theoretical Speedup

$$S_P = T_1/T_P, \qquad E_P = S_P/P,$$

$$T_P = T_P^a + T_P^c \approx \tau_a V_a + N_a(\tau_0 + \tau_c V_c),$$

$$T_a^{(1)} = C_1 M^2 N^{\gamma+1} |ln \varepsilon_{in}| \tau_a,$$

$$T_a^{(3)} \approx 20M^2 + C_2,$$

$$T_P^c \leq C_3(\tau_0 + 2\tau_c M^2 N),$$

$$S_P = T_P^a \cdot P/(T_P^a + T_P^c) \approx P, \qquad E_P \approx 1,$$

Model problems 1.

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} + p\frac{\partial u}{\partial x} + q\frac{\partial u}{\partial y} + r\frac{\partial u}{\partial z} = f(x, y, z),$$

$$(x, y, z) \in \Omega,\ u|_\Gamma = g(x, y, z)$$

$$\Omega = [0;1]^3,\ u(x, y, z) = x^2 + y^2 + z^2,\ u^0 = 0,\ \varepsilon = 10^{-7}$$

Model problem 2.

$$\nabla \times \left(\frac{1}{\mu_r}\nabla \times \vec{E}\right) - k_0^2 \dot{\varepsilon}_r \vec{E} = 0,\ k_0 = \omega\sqrt{\varepsilon_0 \mu_0},$$

waveguide: $0 < x < a = 72, 0 < y < b = 34, 0 < z < c = 200$

$\mu_r = 1,\ \dot{\varepsilon}_r = 1 - 0.1i,\ \omega = 6\pi \cdot 10^9 hz,$

$z = 200 : \vec{E}_0 \times \vec{n} = \vec{e}_y \sin(\pi \times /a) \times \vec{n};\ \vec{E}|_\Gamma = \vec{E}_0 = 0,\ z \neq 200,$

$$\vec{E} = \vec{e}_y \sin\left(\frac{\pi x}{a}\right)\frac{\sin \gamma z}{\sin \gamma c}$$

Problems 1, h=1/(M+1)

$$p = q = r = 0, \ \ \varepsilon_{in} = \varepsilon_e = 10^{-3}, P = 2$$

M	29				99			
	a	b	c	d	a	b	c	d
$\theta = 0$	21	6	11	4	64	10	33	7
	659	292	399	214	5542	1197	3094	920
$\theta = 0.25$	16	5	10	4	49	9	29	7
	534	259	377	218	4430	1157	2803	990
$\theta = 0.5$	11	4	8	3	33	8	23	6
	402	220	321	172	3164	1102	2325	990
$\theta = 0.75$	5	3	5	3	17	6	14	5
	251	175	252	198	1844	961	1583	861

$$a : \Delta = 2, Jac; \ b : \Delta = 2, CG; \ c : \Delta = 4, Jac; \ d : \Delta = 4, CG$$

Problem 2, $\varepsilon = 10^{-7}, \Delta = 0$

grid	N	N_{nz}		number of nodes			
				2	4	8	16
$8 \times 4 \times 20$	**21664**	**423392**	N_b	**1540**	**4678**	**10708**	**23052**
			n	**9**	**13**	**21**	**258**
			t_{fac}	**0,19**	**0,17**	**0,15**	**0,36**
			t_{tot}	**0,51**	**0,47**	**0,67**	**6,19**
$15 \times 7 \times 40$	**149874**	**3117779**	N_b	**5210**	**16646**	**37670**	**78446**
			n	**13**	**18**	**25**	**38**
			t_{fac}	**2,56**	**1,26**	**0,63**	**0,40**
			t_{tot}	**5,88**	**4,00**	**3,12**	**3,15**
$29 \times 14 \times 80$	**1196026**	**25795767**	N_b	**20562**	**67084**	**151032**	**318108**
			n	**18**	**26**	**34**	**49**
			t_{fac}	**108**	**39,9**	**14,9**	**5,29**
			t_{tot}	**173**	**85,6**	**43,3**	**32,94**

Problems 1, $\varepsilon_e = 10^{-7}, \theta = 0$

PARDISO+FGMRES

$t(P = 1) = 15.9, 276, 969$

grid/Δ	0	1	2	3	4
64^3 $P = 2$	**48** **5.4**	**25** **4.3**	**18** **4.1**	**14** **3.9**	**11** **3.9**
64^3 $P = 8$	**66** **3.4**	**35** **2.4**	**26** **4.2**	**20** **2.7**	**17** **2.9**
128^3 $P = 2$	**70** **178**	**38** **164**	**27** **181**	**21** **147**	**18** **131**
128^3 $P = 8$	**94** **52**	**51** **42**	**38** **44**	**30** **44**	**25** **49**

KRYLOV: integrated DDM environment

- interdisciplinary multiphysics problems
- different matrix structures & formats
- various DDM approaches
- direct & preconditioned iterative methods
- scalable parallelism (CPU, GPGPU)
- not group but community project