# Математические и технологические проблемы распараллеливания крыловских итерационных процессов

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ПАВТ, 2013
Челябинск

# Содержание

- Вопросы обоснования, сходимости, устойчивости и оптимизации крыловских алгоритмов
- Алгебра-геометрические аспекты предобуславливания СЛАУ
- Математические и технологические вопросы декомпозиции областей
- Принципы ускорения крыловских итерационных процессов
- О программных реализациях параллельных алгебраических решателей

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$$Au = f, \quad A = \{a_{i,j}\} \in \mathcal{R}^{N,N},$$

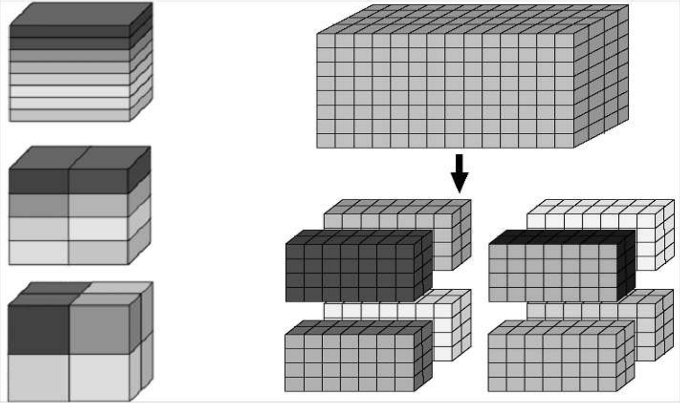
$$A = \{A_p \in \mathcal{R}^{N_p,N},\ p = 1, ..., P\}, \quad N_1 + ... + N_p = N,$$

$$A_{p,p} u_p + \sum_{\substack{q=1 \\ q \neq p}}^{P} A_{p,q} u_q = f_p, \quad p = 1, ..., P, \quad A_{p,q} \in \mathcal{R}^{N_p,N_q},$$

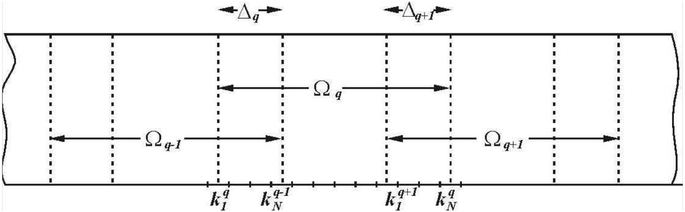
$$a_{i,i} u_i + \sum_{\substack{j \in \omega_i \\ j \neq i}} a_{i,j} u_j = f_i, \quad i \in \Omega^h,$$

$$A_{p,p} u_p^n = f_p - \sum_{\substack{q=1 \\ q \neq p}}^{P} A_{p,q} u_q^{n-1} \equiv g_p^{n-1}$$

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



## 1D-domain decomposition with overlapping




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

$$\Omega_q = \{K_1^q, ..., K_N^q\} \text{ - } q\text{-th subdomain,}$$

$$\Delta_q, \Delta_{q+1} \text{ - overlapping,}$$

$$K_1^q = K_N^{q-1},\ K_1^{q+1} = K_N^q \text{ - non-overlapping}$$

# Boundary Value Problem

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

**Notations**

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

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

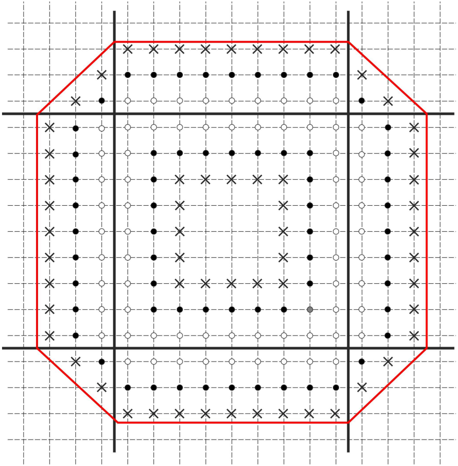
$\Omega_0$ – **external domain**, $\bar{\Omega}_0 = \Omega_0 \bigcup \Gamma$,

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

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

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

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



$$(\bar{A}_{p,p} + \theta \bar{D}_p)\bar{u}_p = \bar{f}_p - \sum_{\substack{q=1 \\ q \neq p}}^{P} \bar{A}_{p,q}\bar{u}_q + \theta \bar{D}_p \bar{u}_p,$$

$$\bar{D}_p e = \sum_{\substack{q=1 \\ q \neq p}}^{P} \bar{A}_{p,q} e, \quad e = (1, ..., 1)^T \in \mathcal{R}^{\bar{N}_p},$$

$$B_p = block\text{-}diag\{\bar{A}_{p,p} + \theta \bar{D}_p\},$$

$$u^n = u^{n-1} + B^{-1}(f - Au^{n-1}) = u^{n-1} + B^{-1} r^{n-1},$$

$$B^{-1} = B_{AS}^{-1} = \sum_{p=1}^{P} \bar{B}_p^{-1},$$

$$\bar{B}_p^{-1} = W_p^T B_p^{-1} W_p, \;\; W_p = (w_1, ..., w_{\bar{N}_p})^T \in \mathcal{R}^{\bar{N}_p, N}$$

$$B_c^{-1} = W_c^T A_c^{-1} W_c, \quad A_c = W_c A W_c^T \in \mathcal{R}^{N_c, N_c},$$

$$B^{-1} = B_{AS}^{-1} + B_c^{-1}, \quad W_c \in \mathcal{R}^{N_c, N},$$

**Deflation**

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

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

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

# Conjugate Direction Methods

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

$$r^0 = \bar{f} - \bar{A}\bar{u}^0 = \hat{u}^1 - \bar{u}^0, \ \ \hat{u}^1 = T\bar{u}^0 + \bar{f}, \ \ p^0 = r^0,$$

$$\bar{u}^{n+1} = \bar{u}^n + \alpha_n^{(s)} p^n, \ \ \alpha_n^{(s)} = \rho_n^{(s)}/\delta_n^{(s)}, \ \ \rho_n^{(s)} = (\bar{A}^s r^n, r^n),$$

$$\delta_n^{(s)} = (\bar{A}p^n, \bar{A}^{(s)} p^n),$$

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

$$(r_{in}^{n_q}, r_{in}^{n_q})/(f_q^n, f_q^n) \le (\varepsilon_{in}^{(n)})^2, \ \ (r^n, r^n) \le \varepsilon_{ex}^2 (\bar{f}, \bar{f})$$

# Two – side Block Jacobi

$$Au = f, \quad A = D - C = (A^t), \quad D = \{A_{p,p}\},$$

$$Du = Cu + f, \quad D = L_D U_D = (L_D L_D^t),$$

$$U_D u = L_D^{-1} C U_D^{-1} U_D u + L_D^{-1} f,$$

$$\bar{A}\bar{u} \equiv (I - \bar{T})\bar{u} = \bar{f}, \quad u = U_D^{-1}\bar{u},$$

$$\bar{u}^n = \bar{T}\bar{u}^{n-1} + \bar{f}, \quad \bar{u}^n = U_D u^n,$$

$$\bar{T} = L_D^{-1} C U_D^{-1} (= \bar{T}^t), \quad \bar{f} = L_D^{-1} f$$

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

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

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

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

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

$$\bar{H}_n = \{h_{k,n}\} = \begin{bmatrix} H_n \\ e_n^t \end{bmatrix} \in \mathcal{R}^{n+1,n}, \quad H_n \in \mathcal{R}^{n,n},$$

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

**FOM, A-FOM, GMRES, A-GMRES**

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

$$
\alpha_q u_q + \beta_q \frac{\partial u_q}{\partial n_q}\Big|_{\Gamma_{q,q'}} = g_{q,q'} \equiv \alpha_{q'} u_q + \beta_{q'} \frac{\partial u_{q'}}{\partial n_{q'}}\Big|_{\Gamma_{q',q}},
$$

$$
|\alpha_q| + |\beta_q| > 0, \quad \alpha_q \cdot \beta_q \geq 0,
$$

**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 Grid Decomposition

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

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

$$u_q = (u_{k_1^q}, ..., u_{k_N^q})^T, \quad u_{k_l^q} = \{u_{i,j,k_l^q}; \; i, j, = 1, ..., M\} \in \mathcal{R}^{M^2},$$

**Block Tridiagonal Systems**

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

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

# Block Jacobi Method

$n = 1, 2 \ldots$ – **number of iterations**,

$$A_{q,q} u_q^n = \bar{f}_q^{n-1} \equiv f_q + \hat{f}_q^{n-1} + \check{f}_q^{n-1},$$

$$\hat{f}_q^{n-1} = A_{q,q-1} u_{q-1}^{n-1}, \; \check{f}_q^{n-1} = A_{q,q+1} u_{q+1}^{n-1},$$

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

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

$$C \in \mathcal{R}^{M^2},\ \theta \in [0,1],\ u^{n-1}_{k_1^q} \in \Omega_{q-1},\ u^{n-1}_{k_N^q} \in \Omega_{q+1},$$

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

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

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

$\theta$ – **compensation parameter**

# Iterations in Trace Spaces

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

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

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

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

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

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

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

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

# Preconditioned Equation in Trace Space

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

$$g = (\check{g}_1, \hat{g}_2, ..., \check{g}_{p-1}, \hat{g}_p)^T,$$

$$s^n = Ts^{n-1} + g, \qquad n = 1, 2, ...,$$

$$s^n \to s : \; \bar{A}s \equiv (I - T)s = g,$$

$$g, \; s \in \mathcal{R}^{2M^2N}, \quad \bar{A}, T \in \mathcal{R}^{2M^2N, 2M^2N},$$

**Acceleration by Krylov Methods**

# 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,**

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

$P_q = B_q A, \; P_q^2 = P_q$ - **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,**

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

# Parallel Implementation

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

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

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

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

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

# Theoretical Speedup

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

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

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

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

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

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

# Технические требования к библиотеке

а. Состав решаемых задач и алгоритмов.
б. Принципы организации интерфейса.
в. Проблема переиспользования программ.
г. Внутренняя структура и организация библиотеки.
д. Развиваемость функционального и системного наполнения.
е. Многоязычность и платформонезависимость.
ж. Сопровождение и документируемость.