Non Uniform Discrete Fourier Transform for adaptive acceleration of the Aitken-Schwarz DDM

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Aitken-Schwarz DDM for uniform grids

- 3D Poisson Pb 762Mdof/60s 5Mbit/s
  1256 proc 3 cray T3E
- FFT of Schwarz DDM artificial interfaces ⇒ needs regular discretization of the interfaces
- Aitken acceleration of Fourier modes
- Barberou, Garbey, Hess, Resch, Rossi, Toivanen and Tromeur-Dervout, J. of Parallel and Distributed Computing, special issue on Grid computing, 63(5) :564-577, 2003

Aim : extension of this method to non uniform meshes
Aitken-Schwarz DDM for uniform grids

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1. Aitken-Schwarz recall
2. New NUDFT formulation
3. NUDFT for Aitken-Schwarz method
4. Numerical results
5. Summary and Future Work
Outline

1. Aitken-Schwarz recall
2. New NUDFT formulation
3. NUDFT for Aitken-Schwarz method
4. Numerical results
5. Summary and Future Work
Acceleration of Schwarz Method for Elliptic Problems


- 1D additive Schwarz algorithm for linear differential operators:
  - \( L[u_{1}^{n+1}] = f \) in \( \Omega_1 \), \( u_{1}^{n+1}|_{\Gamma_1} = u_{2}^{n}|_{\Gamma_1} \),
  - \( L[u_{2}^{n+1}] = f \) in \( \Omega_2 \), \( u_{2}^{n+1}|_{\Gamma_2} = u_{1}^{n}|_{\Gamma_2} \).

- The interface error operator \( T \) is **linear**, i.e.
  - \( u_{1}^{n+1}|_{\Gamma_2} - U|_{\Gamma_2} = \delta_1 (u_{2}^{n}|_{\Gamma_1} - U|_{\Gamma_1}) \),
  - \( u_{2}^{n+1}|_{\Gamma_1} - U|_{\Gamma_1} = \delta_2 (u_{1}^{n}|_{\Gamma_2} - U|_{\Gamma_2}) \).

- Consequently
  - \( u_{1}^{2}|_{\Gamma_2} - u_{1}^{1}|_{\Gamma_2} = \delta_1 (u_{2}^{1}|_{\Gamma_1} - u_{2}^{0}|_{\Gamma_1}) \),
  - \( u_{2}^{2}|_{\Gamma_1} - u_{2}^{1}|_{\Gamma_1} = \delta_2 (u_{1}^{1}|_{\Gamma_2} - u_{1}^{0}|_{\Gamma_2}) \).

- Computation of \( \delta_{1/2} \):
  - \( L[v_{1/2}] = 0 \) in \( \Omega_{1/2} \), \( v_{1/2}|_{\Gamma_{1/2}} = 1 \), thus \( \delta_{1/2} = v_{\Gamma_{2/1}} \).

- Iff \( \delta_1 \delta_2 \neq 1 \) **Aitken-Schwarz** gives the solution with exactly 3 iterations and possibly 2 in the analytical case.
Acceleration of Schwarz Method for Elliptic Problems


- **1D additive Schwarz** algorithm for linear differential operators:
  \[ L[u_1^{n+1}] = f \text{ in } \Omega_1, \quad u_1^{n+1}|_{\Gamma_1} = u_2^n|_{\Gamma_1}, \]
  \[ L[u_2^{n+1}] = f \text{ in } \Omega_2, \quad u_2^{n+1}|_{\Gamma_2} = u_1^n|_{\Gamma_2}. \]

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- Consequently
  
  - \( u_2^2|_{\Gamma_2} - u_1^1|_{\Gamma_2} = \delta_1(u_2^1|_{\Gamma_1} - u_2^0|_{\Gamma_1}) \),
  
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- Iff \( \delta_1 \delta_2 \neq 1 \) *Aitken-Schwarz* gives the solution with exactly 3 iterations and possibly 2 in the analytical case.
1D additive Schwarz algorithm for linear differential operators:

\[ L[u_{11}^{n+1}] = f \text{ in } \Omega_1, \quad u_{11}^{n+1}\mid_{\Gamma_1} = u_{21}^n, \]
\[ L[u_{21}^{n+1}] = f \text{ in } \Omega_2, \quad u_{21}^{n+1}\mid_{\Gamma_2} = u_{12}^n. \]

the interface error operator \( T \) is \textit{linear}, i.e.

\[ u_{11}^{n+1}\mid_{\Gamma_2} - U_{\mid_{\Gamma_2}} = \delta_1(u_{21}^n\mid_{\Gamma_1} - U_{\mid_{\Gamma_1}}), \]
\[ u_{21}^{n+1}\mid_{\Gamma_1} - U_{\mid_{\Gamma_1}} = \delta_2(u_{12}^n\mid_{\Gamma_2} - U_{\mid_{\Gamma_2}}). \]

Consequently

\[ u_{21}^2\mid_{\Gamma_2} - u_{11}^1\mid_{\Gamma_2} = \delta_1(u_{21}^1\mid_{\Gamma_1} - u_{21}^0\mid_{\Gamma_1}), \]
\[ u_{21}^2\mid_{\Gamma_1} - u_{12}^1\mid_{\Gamma_1} = \delta_2(u_{12}^1\mid_{\Gamma_2} - u_{12}^0\mid_{\Gamma_2}). \]

Computation of \( \delta_{1/2} \):

\[ L[v_{1/2}] = 0 \text{ in } \Omega_{1/2}, \quad v_{\mid_{\Gamma_{1/2}}} = 1. \text{ thus } \delta_{1/2} = v_{\mid_{\Gamma_{2/1}}}. \]

iff \( \delta_1 \delta_2 \neq 1 \) Aitken-Schwarz gives the solution with \textit{exactly 3 iterations} and possibly 2 in the analytical case.
The algorithm in 2D or 3D writes:

- **step 1**: reconstruct $P$ from data given by two Schwarz iterates.

- **step 2**: apply one additive Schwarz iterate to the Poisson problem with block solver of choice i.e. multigrids, FFT etc...

- **step 3**:
  - compute the Fourier expansion $\hat{u}^n_{\mid \Gamma_i}$, $n = 0, 1$ of the traces on the artificial interface $\Gamma_i$, $i = 1..nd$ for the initial boundary condition $u^0_{\mid \Gamma_i}$ and the Schwarz iterate solution $u^1_{\mid \Gamma_i}$.
  - apply generalized Aitken acceleration based on
    
    $$\hat{u}^\infty = (Id - P)^{-1} (\hat{u}^1 - P\hat{u}^0)$$
    
    in order to get $\hat{u}^\infty_{\mid \Gamma_i}$.
  - recompose the trace $u^\infty_{\mid \Gamma_i}$ in physical space.

- **step 4**: compute in parallel the solution in each subdomains $\Omega_j$, with new inner BCs and blocksolver of choice.
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- **step3**: compute the Fourier expansion $\hat{u}_n^{\Gamma_i}, n = 0, 1$ of the traces on the artificial interface $\Gamma_i, i = 1..nd$ for the initial boundary condition $u^{0}_{|\Gamma_i}$ and the Schwarz iterate solution $u^{1}_{|\Gamma_i}$.
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Methods for non-uniform interface meshes (up to now):

- **Projection technique**: spectral interpolation of the interface traces on a third regular grid + classical FFT
  

- **Analysis of the error operator**, solving for eigenvalues and eigenvectors, chosen as generalized Fourier basis
  
  Baranger, Garbey and Oudin-Dardun *Generalized Aitken-like acceleration of the Schwarz method*, Lecture Notes in Computational Science and Engineering, pages 505-512, 2004. Based on an a priori approximation of the error operator $P$. No available tool to know how the eigenvalues of the approximate $P$ are close to the eigenvalues of true $P$. 
1. Aitken-Schwarz recall

2. New NUDFT formulation

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4. Numerical results

5. Summary and Future Work
Define a set of basis functions $\Phi = (\phi_l(x_j))_{0 \leq j \leq N}$ strictly related to the nonuniform mesh and orthogonal with respect to a sesquilinear form $[[.,.]]$, i.e $[[\phi_l, \phi_k]] = 0$, if $l \neq k$.

Compute the associated interface operator $P_{[[.,.]]}$.

Approximate $P_{[[.,.]]}$ with $P^*_{[[.,.]]}$ through a posteriori estimates of Fourier coefficients behavior.

Instead of:

Approximate in the physical space $P$ with $P^*$.

Compute eigenvalues and eigenvectors of matrix $P^*$.

Take eigenvectors as basis functions for generalized Fourier decomposition.
NonUniform Fourier Transform formulation

Definition

Let \((x_i)_{0 \leq i \leq N}\) and \(z_i = \frac{2\pi i}{N}\) such that \(x_i = z_i + \epsilon_i\), and

\[
\phi_l(x) = \begin{cases} 
\psi_l(x) = \exp(ilx), & 0 \leq l \leq N/2 \\
D^{-N} \exp(i(N - l)x), & N/2 + 1 \leq l \leq N,
\end{cases}
\]

\(D = \text{diag}(\epsilon_i)_{0 \leq i \leq N}\)

\[\Rightarrow \phi_{N-l}(x) = \overline{\phi_l(x)}.\]

Definition

Define sesquilinear form on \(S_N = \text{span}\{\phi_l(x), 0 \leq l \leq N\}\), using Hermite integration formula:

\[
[[f, g]] = \sum_{l=0}^{N} \gamma_l f(x_l) \overline{g(x_l)} + \sum_{l=0}^{N} \beta_l (f'(x_l) \overline{g(x_l)} + f(x_l) \overline{g'(x_l)})
\]

\(\{\gamma_l\}\) and \(\{\beta_l\}: [[\phi_l, \phi_k]] = \delta_{lk} \Rightarrow \text{solve one L.S. (size 2N)}.\)
NonUniform Fourier Transform formulation

\[ H = \left( \left[ \phi_l, \phi_k \right] \right)_{l,k=0,...,N} = Id \Rightarrow [\ : , : ] \text{ hermitian} \]

**Definition**

The discrete Fourier coefficients of \( f \) are given by:

\[ \tilde{f}_k = \left[ f, \Phi_k \right], \quad k = -N/2, ..., N/2 \]

\[ \tilde{f} = M_1 f + M_2 f', \quad M_1, M_2 \in \mathcal{M}_{N+1}(\mathbb{C}) \]

\[ M_1(k, l) = \gamma_l \phi_k(x_l) + \beta_l \phi'_k(x_l), \quad M_2(k, l) = \beta_l \phi_k(x_l) \]

**Proposition**

\[ \Pi_N^F(f(x)) = \sum_{l=0}^{N} \tilde{f}_k \phi_k(x), \quad \text{is exact } \forall f \in \mathbb{T}^{N/2}([0, 2\pi[) \]
Problem: in the applications one is given the vector $f$ which represents the values of a function $f(x)$ on the points $(x_i)_{0 \leq i \leq N}$. No information is given on the vector $f'$ which is needed in definition 3.

Solution: we determine the vector $f'$ implicitly by imposing

$$\frac{d}{dx}(\prod_{i=0}^{N-1}(f(x)))|_{x=x_i} = f'(x_i), \quad l = 0, \ldots, N - 1$$
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$$
\frac{d}{dx}(\prod_N^F(f(x)))|_{x=x_l} = f'(x_l), \quad l = 0, ..., N - 1
$$
In an algebraic form, if we note $M_\phi$ the matrix whose elements are :

$$M_\phi(l, k) = \phi'_k(x_l)$$

then the vector $f'$ is obtained by solving the algebraic system :

$$(id_{N+1} - M_\phi M_2)f' = M_\phi M_1 f$$

where $id_N$ is the identity matrix in $\mathcal{M}_{N+1}(\mathbb{C})$. 
Given a nonuniform mesh \((x_i)_{0 \leq i \leq N}\), define the basis functions and solve one L.S. (size 2N) to determine the two sets \(\{\gamma_l\}\) and \(\{\beta_l\}\).

Solve the algebraic system (size N):

\[
(id_{N+1} - M_\phi M_2)f' = M_\phi M_1 f
\]

to determine \(f'\) implicitly.

Compute Fourier coefficients through matrix-vector products:

\[
\tilde{f} = M_1 f + M_2 f'
\]
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<table>
<thead>
<tr>
<th>N</th>
<th>$\varepsilon = h_u/8$</th>
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<td>2.96E+8</td>
<td>7.30E+10</td>
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</table>

Tab.: $\|f - \Pi_N^F(f)\|_{\infty}$ and $\text{cond}_2([., .])$ for $f(x) = \exp(-40(x - (2\pi/3))^2)$, with $h_u = 2\pi/N$. 

Given a nonuniform cartesian 2D mesh $\mathbf{x} \times \mathbf{y} := \{(x_i, y_j)_{0 \leq i, j \leq N} \subset \mathbb{R}^2$ define the basis functions, the sesquilinear form:

$$[[f, g]] = \sum_{j=0}^{N} \gamma_j \left( \sum_{l=0}^{N} \alpha_l(fg)(x_j, y_l) + \sum_{l=0}^{N} \eta_l \partial_y(fg)(x_j, y_l) \right) +$$

$$\sum_{j=0}^{N} \beta_j \left( \sum_{l=0}^{N} \alpha_l \partial_x(fg)(x_j, y_l) + \sum_{l=0}^{N} \eta_l \partial_{xy}(fg)(x_j, y_l) \right)$$

Fourier coefficients computed algebraically by previously solving implicitly for $\partial_x f$, $\partial_y f$ and $\partial_{xy} f$. 

**NUDFT algorithm 2D**
Given a nonuniform cartesian 2D mesh \( \mathbf{x} \times \mathbf{y} := \{(x_i, y_j)_{0 \leq i,j \leq N} \} \subset \mathbb{R}^2 \) define the basis functions, the sesquilinear form:

\[
[[f, g]] = \sum_{j=0}^{N} \gamma_j \left( \sum_{l=0}^{N} \alpha_l \overline{g}(x_j, y_l) + \sum_{l=0}^{N} \eta_l \partial_y(f \overline{g})(x_j, y_l) \right) + \sum_{j=0}^{N} \beta_j \left( \sum_{l=0}^{N} \alpha_l \partial_x(f \overline{g})(x_j, y_l) + \sum_{l=0}^{N} \eta_l \partial_{xy}(f \overline{g})(x_j, y_l) \right)
\]

Fourier coefficients computed algebraically by previously solving implicitly for \( \partial_x f, \partial_y f \) and \( \partial_{xy} f \).
Numerical results 2D

<table>
<thead>
<tr>
<th>N</th>
<th>$\epsilon = h_u/2$</th>
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<th>$\epsilon = 2h_u$</th>
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<tbody>
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<td>$2^7$</td>
<td>1.1E-13</td>
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<td>9.5E-7</td>
<td>2.09E+3</td>
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<tr>
<td></td>
<td>1.5E+3</td>
<td>8E+3</td>
<td>2.5E+6</td>
<td>2.2E+12</td>
</tr>
<tr>
<td>$2^8$</td>
<td>2.62E-13</td>
<td>1.48E-10</td>
<td>8E-4</td>
<td>3E+6</td>
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<td>6E+3</td>
<td>5E+5</td>
<td>1.7E+10</td>
<td>1E+14</td>
</tr>
</tbody>
</table>

**Table:** $\|f - \Pi^F_N(f)\|_\infty$ and $\text{cond}_2([. , .])$ for $f(x, y) = \cos^2(x) \cos(y)$, with $h_u = 2\pi/N$. 
Advantages of NUDFT

- **Advantages:**
  - Better performance than FFT on nonuniform meshes when applied to Aitken-Schwarz DDM
  - $O(N^2)$ operations → cheaper in time in comparison with the $O(N^3)$ operations to solve for the eigenvalues and eigenvectors of the full interface operator
  - Adaptive approximation of the trace transfer operator $P$, based on a posteriori error estimates of Fourier modes convergence

- **Gridding:** interpolation and use of the FFT on an oversampled grid

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- Adaptive approximation of the trace transfer operator $P$, based on a posteriori error estimates of Fourier modes convergence

Gridding: interpolation and use of the FFT on an oversampled grid

At interfaces $\Gamma_1$ and $\Gamma_2$, the Fourier coefficients of the error of additive Schwarz algorithm can be rearranged on the form:

\[
\hat{e}_1^{(n+2)}(\Gamma_1) = P_{[\ldots]} \hat{e}_1^{(n)}(\Gamma_1) \\
\hat{e}_2^{(n+2)}(\Gamma_2) = P_{[\ldots]} \hat{e}_2^{(n)}(\Gamma_2)
\]

Numerically, $P_{[\ldots]}$ is computed by applying two Schwarz iterates for each Fourier mode of the interface solution (computed through the NUDFT), as a relation between all the modes at the two iterates.
Numerical computation of the interface operator $P$

- Take one basis function on the interface (blue line):

- Applying NUDFT to the basis function, obtain a symmetric decomposition:
Numerical computation of the interface operator $P$

- With 2 Schwarz iterates determine how this function is modified by the additive Schwarz algorithm:

- Applying NUDFT, compute the influence of one Fourier mode on all modes:

- Fill $k$-column of matrix $P_{[,\cdot]}$, not symmetric.
Validation of the NUDFT for the construction of the interface operator $P$

Uniform grids: NUDFT $\rightarrow$ FFT

$P_{[[.,.]]}$ diagonal and $\|P_{[[.,.]]} - P_{an}\|_{\infty} = O(10^{-12})$
Adaptive construction of matrix $P$

- Nonuniform cartesian grids and/or non separable differential operator
- $P$ is no longer diagonal
- we can approximate $P[[.,]]$ using only the most important modes, then accelerate only these modes through the equation:

$$
\tilde{v}_\infty = (Id - P^*[[.,]])^{-1}(\tilde{v}^{n+1} - P^*[[.,]]\tilde{v}^n)
$$

where $\tilde{v}$ is the subset of $\tilde{u}$ used to approximate $P[[.,]]$ with $P^*[[.,]]$. Other modes are not accelerated.

$P^*[[.,]]$ columns can be built in parallel and the number of columns computed during the Schwarz iterates can be set according to the computer architecture.
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Outline

1. Aitken-Schwarz recall
2. New NUDFT formulation
3. NUDFT for Aitken-Schwarz method
4. Numerical results
5. Summary and Future Work
Solution of 2D convection-diffusion equation with Aitken-Schwarz DDM: the trace of the iterate solutions on the irregular mesh are projected on a Fourier orthogonal basis. The Fourier modes are accelerated through the Aitken technique.

\[ \nabla \cdot (a(x, y) \nabla u(x, y)) = f(x, y), \quad \text{on } \Omega = [0, 1]^2 \]
\[ u(x, y) = 0, \quad (x, y) \in \partial \Omega \]
\[ a(x, y) = a_0 + (1 - a_0)(1 + \tanh((x - (3h \ast y + 1/2 - h))/\mu))/2, \]
and \( a_0 = 10^1, \mu = 10^{-2} \).
Numerical results

**Figure:** acceleration using sub-blocks of $P_{[[..]]}$ with 90 points on the interface, overlap $= 5$ and $\epsilon = h_u/2$. Black line refers to results in Baranger, Garbey and Oudin-Dardun *The Aitken-Like Acceleration of the Schwarz Method on Non-Uniform Cartesian Grids*, Technical Report Number UH-CS-05-18, 2005.
**Numerical results**

**Fig.:** influence of the approximation of the interface operator $P_{[[..]]}$ on the convergence of the interface error
Convergence of AS in random porous media

\( K \) follows a log-normal random process

\[
\nabla \cdot (K(x, y)\nabla u) = f, \text{ on } \Omega \\
u = 0, \text{ on } \partial \Omega
\]

\( K(x, y) \in [0.0091, 242.66] \)

Convergence of AS

Work under progress in collaboration with J-R De Dreuzy and J. Erhel SAGE/IRISA
Summary and Future Work

- Extend ASDDM to nonuniform cartesian meshes by means of the NUDFT technique
- Reduce the numerical complexity by adaptively approximating the trace transfer operator $P$
- Validate the technique in the 2D case and DD in stripes
- Works also for Nonuniform non matching cartesian grids
- Under investigation: NUDFT $\rightarrow$ NUFFT