A fast solver for the periodic Lippmann-Schwinger equation

Kai Sandfort

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associate member of the Workgroup of Inverse Problems, Department of Mathematics
leader of the Feasibility Study “Schnelle alternative Lösung von Streuproblemen mit unstetigen Materialparametern”
Outline

1 Introduction
   Scattering from a periodic inhomogeneity

2 Vainikko’s method
   Periodization of the problem
   Trigonometric collocation
   Modification for discontinuous contrasts

3 Numerical results

4 Outlook
Motivation: Scattering from a periodic inhomogeneity

Here: time-harmonic fields, TM mode, 2D projection

\[ R^2 \setminus \tilde{\Omega}, \ q = 0 \]
\[ R_+ \]
\[ \tilde{\Omega}, \ q \neq 0 \]
\[ -\pi \]
\[ +\pi \]
\[ R_- \]
\[ \partial \tilde{\Omega} \]

‘periodic’ \( \equiv \) ‘2\pi’-periodic in \( x_1 \)

\[ \tilde{\Omega} \]
periodic medium (Lipschitz)

\[ \Pi \]
unit cell

\[ R_{\pm} \]
semi-infinite rectangles in \( \Pi \)
above / below \( \tilde{\Omega} \)

\[ q \]
periodic contrast with
\[ q(x)\big|_{x_1=-\pi} = q(x)\big|_{x_1=+\pi} \]
\( (q \text{ sufficiently regular}) \)
Motivation: Scattering from a periodic inhomogeneity

\[ R^2 \setminus \Omega, \ q = 0 \]

\[ \partial \Omega, \ q \neq 0 \ -\pi \]

\[ \Omega, \ q \neq 0 \ +\pi \]

\[ R_+ \]

\[ R_- \]

Scattering problem: Find a periodic \( u_{\text{per}} : \Pi \to \mathbb{C} \) such that

\[ \Delta u_{\text{per}} + \kappa_0^2 (1 + q) u_{\text{per}} = 0, \quad u_{\text{per}} = u_{\text{per}}^i + u_{\text{per}}^s \quad \text{in} \ \Pi, \quad u_{\text{per}} \approx E_3 \]

\[ u_{\text{per}}^s(x) = \sum_{z \in \mathbb{Z}} u_{z}^{\pm} e^{i(z x_1 \pm \beta z x_2)} \quad \text{in} \ R_{\pm}, \quad \beta_z = \sqrt{\kappa_0^2 - |z|^2} \neq 0 \ \forall z \in \mathbb{Z}. \]
Motivation: Scattering from a periodic inhomogeneity

\[ \begin{array}{c}
\mathbb{R}^2 \setminus \tilde{\Omega}, \quad q = 0 \\
R^2 \setminus \tilde{\Omega}, \quad q \neq 0
\end{array} \]

\[ R_+, \quad R_- \]

\[ \tilde{\Omega}, \quad q \neq 0 \]

\[ -\pi \quad +\pi \]

\[ \partial \tilde{\Omega} \]

\[ \Pi \]

\[ \therefore \quad \text{equivalent to the periodic Lippmann-Schwinger equation} \]

\[ u_{\text{per}}(x) = u_{\text{per}}^i(x) + \kappa_0^2 \int_{\Omega} G_{\text{per}}(x - y) q(y) u_{\text{per}}(y) \, dy, \quad x \in \Omega. \]

\[ \Omega = \tilde{\Omega} \cap \Pi, \quad G_{\text{per}}: \text{periodic Green's function for } \Delta + \kappa_0^2 \text{id} \]
The periodic Lippmann-Schwinger equation

\[ u_{\text{per}}(x) = u_{\text{per}}^i(x) + \kappa_0^2 \int_{\Omega} G_{\text{per}}(x - y) q(y) u_{\text{per}}(y) \, dy, \quad x \in \Omega. \]

- \(1 + q \in L^{\infty}(\Omega)\) is the refraction index of the medium
- \(\text{pLS}\) is uniquely solvable in \(C_{\text{per}}(\Omega) \iff \text{pLS}\) with \(u_{\text{per}}^i \equiv 0\) has only trivial solution (Fredholm alternative)
- unique extension to \(\Pi \setminus \Omega\) by RHS of \(\text{pLS}\) yields \(u_{\text{per}}\) in \(\Pi\) (and in \(\mathbb{R}^2\))
- in \(\Pi \setminus \overline{\Omega}\), \(u_{\text{per}}\) is smooth (strict ellipticity), even analytic (analyticity inherited from \(G_{\text{per}}\))
The periodic Lippmann-Schwinger equation

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- \(1 + q \in L^\infty(\Omega)\) is the refraction index of the medium

- **pLS** is uniquely solvable in \(C_{\text{per}}(\Omega)\) \(\iff\) **pLS** with \(u_{\text{per}}^i \equiv 0\) has only trivial solution (Fredholm alternative)

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My talk in a nutshell

**object of interest:** periodic Lippmann-Schwinger equation \( pLS \)

**aim:** its efficient numerical treatment

**tools:** method by Prof. em. Gennadi Vainikko and my enhancement
Choose $r > 0$ so that $\overline{\Omega} \subset C_r = \{ x \in \Pi : |x_2| < r \}$. Consider restrictions of $G_{\text{per}}, u_{\text{per}}^i$, and $q$ to $\overline{C_{2r}}$. Extend to $\mathbb{R}^2$ as $(2\pi, 4r)$-biperiodic functions. Denote extensions by $K_{\text{ext}}, u_{\text{ext}}^i$, and $q_{\text{ext}}$, respectively.
For $v_{\text{ext}} = q_{\text{ext}} u_{\text{ext}}$ and $x \in C_{2r}$, we get the $(2\pi, 4r)$-biperiodic L.-S. eqn.

$$v_{\text{ext}}(x) = (q_{\text{ext}} u_{\text{ext}}^i)(x) + \kappa_0^2 q_{\text{ext}}(x) \int_{C_{2r}} K_{\text{ext}}(x - y) v_{\text{ext}}(y) \, dy.$$
• **Fourier expansion** of $K_{\text{ext}}$ w.r.t. trigonometric basis $\{\varphi_j\}_{j \in \mathbb{Z}^2}$ of $L^2(C_{2r})$

• It holds $(\Delta + \kappa_0^2) \varphi_j = \lambda_j \varphi_j$. Assume $\lambda_j \neq 0$ for all $j \in \mathbb{Z}^2$.

• By Green’s representation theorem, we obtain

$$\hat{K}_{\text{ext}}(j) = -\frac{\tilde{c}}{\lambda_j} \left(1 - (-1)^j e^{i \beta h^{2r}}\right) \quad \Rightarrow \quad \hat{K}_{\text{ext}}(j) = \mathcal{O}(|j|^{-2}),$$

$\tilde{c}$: normalization constant.

**exploited:** problem-specific periodicity in $x_1$!
- Fourier expansion of $K_{\text{ext}}$ w.r.t. trigonometric basis $\{\varphi_j\}_{j \in \mathbb{Z}^2}$ of $L^2(C_{2r})$

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**exploited**: problem-specific periodicity in $x_1$!
Trigonometric collocation for smooth contrast

Define

$$\mathbb{Z}_N^2 = \left\{ j \in \mathbb{Z}^2 : -\frac{N}{2} < j_k \leq \frac{N}{2}, \ k = 1, 2 \right\},$$

$$\mathcal{T}_N = \text{span} \left\{ \varphi_j, \ j \in \mathbb{Z}_N^2 \right\}.$$

Define interpolation projection $Q_N : C_{\text{per}}(C_{2r}) \to \mathcal{T}_N$ by

$$(Q_N v_{\text{per}})(j \odot h_N) = v_{\text{per}}(j \odot h_N), \quad j \in \mathbb{Z}_N^2,$$

where $h_N = (2\pi, 4r)/N$ and $\odot$ denotes componentwise multiplication.
Trigonometric collocation for smooth contrast

For \( q \in H^2_{\text{per}}(C_{2r}) \), solve \( \text{bpLS} \) by collocation

\[
\nu_N = Q_N(q_{\text{ext}} u_{\text{ext}}^i) + \kappa_0^2 Q_N(q_{\text{ext}} \mathcal{K} \nu_N), \tag{bpLS-C}
\]

where \( \mathcal{K} : L^2(C_{2r}) \rightarrow H^2_{\text{per}}(C_{2r}) \) is given by

\[
(\mathcal{K} \nu_{\text{per}})(x) = \int_{C_{2r}} K_{\text{ext}}(x - y) \nu_{\text{per}}(y) \, dy.
\]

**Note:** \( (\mathcal{K} \varphi_j)(x) = \widetilde{c}^{-1} \widetilde{K}_{\text{ext}}(j) \varphi_j(x), \ j \in \mathbb{Z}^2, \) by convolution theorem

\( \widehat{\nu}_N(j), \ j \in \mathbb{Z}^2_N, \) are computed by fast Fourier transform (FFT)
Trigonometric collocation for smooth contrast

For \( q \in H^2_{\text{per}}(C_2r) \), solve \( \text{bpLS} \) by collocation

\[
\nu_N = Q_N(q_{\text{ext}} u^i_{\text{ext}}) + \kappa_0^2 Q_N(q_{\text{ext}} K \nu_N), \tag{bpLS-C}
\]

where \( K : L^2(C_2r) \rightarrow H^2_{\text{per}}(C_2r) \) is given by

\[
(K \nu_{\text{per}})(x) = \int_{C_2r} K_{\text{ext}}(x - y) \nu_{\text{per}}(y) \, dy.
\]

Hence, we can

avoid numerical integration for \( \text{bpLS-C} \) and use cheap expressions!
**Theorem 1:** Assume \( q \in H^2_{\text{per}}(C_{2r}) \) and \( u^i_{\text{per}} \in H^2_{\text{per}}(C_{2r}) \). Let \( p_{\text{LS}} \) with \( u^i_{\text{per}} \equiv 0 \) be only trivially solvable.

Then, \( b_{\text{LS}} \) has a unique sol.n \( v_{\text{ext}} \in H^2_{\text{per}}(C_{2r}) \), and the collocation eqn. \( b_{\text{LS}} - C \) has a unique sol.n \( v_N \in \mathcal{I}_N \) for \( N \geq N_0 \), and

\[
\| v_N - v_{\text{ext}} \|_\lambda \leq c' N^{\lambda - 2} \| v_{\text{ext}} \|_2, \quad 0 \leq \lambda \leq 2.
\]

Here, \( \| \cdot \|_\mu \) denotes the norm of \( H^\mu_{\text{per}}(C_{2r}) \).
Modification for discontinuous contrasts

Assume \( q \in L^2(C_{2r}) \). Instead of

\[
v_{\text{ext}}(x) = (q_{\text{ext}} u_{\text{ext}}^i)(x) + \kappa_0^2 q_{\text{ext}}(x) \int_{C_{2r}} K_{\text{ext}}(x - y) v_{\text{ext}}(y) \, dy
\]

for \( v_{\text{ext}} = q_{\text{ext}} u_{\text{ext}} \) in \( C_{2r} \), consider

\[
u_{\text{per}}(x) = u_{\text{per}}^i(x) + \kappa_0^2 \int_{\Omega} G_{\text{per}}(x - y) q(y) u_{\text{per}}(y) \, dy
\]

for \( u_{\text{per}} \) in \( \Omega \) (total field).
Modification for discontinuous contrasts

Assume $q \in L^2(C_{2r})$. Instead of

$$v_{\text{ext}}(x) = (q_{\text{ext}} u_{\text{ext}}^i)(x) + \kappa_0^2 q_{\text{ext}}(x) \int_{C_{2r}} K_{\text{ext}}(x - y) v_{\text{ext}}(y) \, dy$$

for $v_{\text{ext}} = q_{\text{ext}} u_{\text{ext}}$ in $C_{2r}$, consider

$$u_{\text{per}}(x) = u_{\text{per}}^i(x) + \kappa_0^2 \int_{\Omega} G_{\text{per}}(x - y) q(y) u_{\text{per}}(y) \, dy$$

for $u_{\text{per}}$ in $\Omega$ (total field).

Recall $K_{\text{ext}} = G_{\text{per}}$ on $\overline{C_{2r}} \subset (2 \cdot \Omega) \cap \Pi$. 
Modification for discontinuous contrasts

\[
\begin{align*}
&u_{\text{per}}(x) = u'^{\text{per}}_{\text{per}}(x) + \kappa_0^2 \int_{\Omega} K_{\text{ext}}(x-y) q(y) u_{\text{per}}(y) \, dy, \quad x \in \Omega \\
&\text{ Define } \mathcal{P} u = \begin{cases} 
  u & \text{in } \Omega \\
  0 & \text{in } C_{2r} \setminus \Omega
\end{cases} \text{ and } \mathcal{R} u = u|_{\Omega}, \text{ then new integral operator } \tilde{\mathcal{K}} : L^2(\Omega) \to H^2_{\text{per}}(\Omega) \text{ by } \\
&\tilde{\mathcal{K}} = \mathcal{R} \circ \mathcal{K} \circ \mathcal{P}.
\end{align*}
\]

- Use extension operator \( E_{\text{per}} : H^2_{\text{per}}(\Omega) \to H^2_{\text{per}}(C_{2r}) \) to setup collocation

\[
\begin{align*}
u_N &= Q_N E_{\text{per}}(u'^{\text{per}}_{\text{per}}) + \kappa_0^2 Q_N E_{\text{per}} \tilde{\mathcal{K}}(q \mathcal{R} u_N).
\end{align*}
\]

**Purpose:** Good approx. by \( Q_N \) as restriction to \( \Omega \) of a function in \( T_N \)!
Modification for discontinuous contrasts

\[ u_{\text{per}}(x) = u_{i\text{per}}(x) + \kappa_0^2 \int_{\Omega} K_{\text{ext}}(x - y) q(y) u_{\text{per}}(y) \, dy, \quad x \in \Omega \]

- Define \( \mathcal{P} u = \begin{cases} u & \text{in } \Omega \\ 0 & \text{in } C_{2r} \setminus \Omega \end{cases} \) and \( \mathcal{R} u = u|_{\Omega} \), then new integral operator \( \mathcal{\tilde{K}} : L^2(\Omega) \to H^2_{\text{per}}(\Omega) \) by \( \mathcal{\tilde{K}} = \mathcal{R} \circ \mathcal{K} \circ \mathcal{P} \).

- Use extension operator \( \mathbb{E}_{\text{per}} : H^2_{\text{per}}(\Omega) \to H^2_{\text{per}}(C_{2r}) \) to setup collocation

\[ u_N = Q_N \mathbb{E}_{\text{per}} (u_{i\text{per}}) + \kappa_0^2 Q_N \mathbb{E}_{\text{per}} \mathcal{\tilde{K}}(q \mathcal{R} u_N). \]

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Illustration of the extension by $E_{\text{per}} : H^2_{\text{per}}(\Omega) \rightarrow H^2_{\text{per}}(C_{2r})$

(left) data points in $\Omega$, (right) extension to $C_{2r}$ with data and guiding points
Theorem 2: Assume \( q \in L^2(C_{2r}) \) and \( u^i_{per} \in H^2_{per}(C_{2r}) \). Let \( \text{pLS} \) with \( u^i_{per} \equiv 0 \) be only trivially solvable. Then, \( \text{pLS} \) has a unique sol.n \( u_{per} \in H^2_{per}(\Omega) \), and the collocation eqn. \( E-\text{pLS}-C \) has a unique sol.n \( u_N \in \mathcal{T}_N \) for \( N \geq N_0 \), and

\[
\|u_N - E_{per}u_{per}\|_\lambda \leq c'' N^{\lambda-2} \|E_{per}u_{per}\|_2, \quad 0 \leq \lambda \leq 2.
\]

Cost: extremely efficient eval. of \( \mathcal{K} \) applied to \( \varphi_j \in \mathcal{T}_N \) not applicable!
For piecewise constant \( q = \sum_{i=1}^{L} q_i \text{id}_{C_i} \):

For some \( N_0 \geq N \), precompute "generalized Fourier coefficients"

\[
\hat{K}_{\text{ext}}^{(i)}(x, j) = \int_{\tilde{C}_i} G_{\text{per}}(x - y) \varphi_j(y) \, dy, \quad j \in \mathbb{Z}_{N_0}^2,
\]

on grid \( \mathbb{Z}_{N_0}^2 \odot h_{N_0} \ni x \). Use again Green's representation theorem.

Assume that any valid \( C_i \) meets \( C_i = \bigcup_{k \in \mathcal{I}_i} \tilde{C}_k \).
Projection errors for piecewise constant $q$

(left) piecewise constant $q$, (right) error in the orthogonal ($P_N$) and in the interpolation ($Q_N$) projection of $q$
Projection errors for smooth $q$

(left) smooth $q$, (right) error in the orthogonal and in the interpolation projection of $q$
Error in the solution $v_N$ to the collocation $\text{bpLS-C}$

$\log_2(\text{rel. error of } v_N)$

$\log_2(\text{rel. error of } u_N)$

error in $v_N$ w.r.t. $v_{128}$ *(Theorem 1 applies!)*
Projection errors for smoothly extended $q$

*left* smoothly extended $q$,  *right* error in the orthogonal and in the interpolation projection of the extension
Error in the solution $u_N$ to the collocation E-pLS-C

error in $u_N$ w.r.t. $u_{64}$ (Theorem 2 applies!)
Evolution of $v_N$ (for exemplary $u_{per}^i$)

$V_{16}$

$V_{32}$

$V_{64}$
Evolution of $u_N$ cropped to $\Omega$ (for same $u_{\text{per}}^i$)
Outlook

- setup of a solver for full time-harmonic EM case with $\mu_r \equiv 1$, i.e. for

$$u_{\text{per}}(x) = u_{\text{per}}^i(x) + \text{curl} \int_{\Omega} G_{\text{per}}(x - y) \left( 1 - \frac{1}{\varepsilon_r(y)} \right) \text{curl} u_{\text{per}}(y) \, dy$$

with $x \in \Omega$. Here: $u_{\text{per}} \equiv H$ (total magnetic field)

- error estimation for collocation sol.n to above eqn.
- error analysis for two-grid collocation solver for above eqn.
- acceleration of computation of generalized Fourier coefficients
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Thank you!

Reference: