Computational Aspect of Series Solution of Helmholtz Equation

BY ZHIJUN ZENG

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1 Neumann Series

Consider the 2- dimensional Helmholtz equation in inhomogeneous medium subject to the Sommerfeld radiation condition at infinity

$$\begin{aligned} \Delta u + k^2 (1 + q(x)) u &= f(x), \quad x \in \mathbb{R}^2, \\ \lim_{r \to \infty} \sqrt{r} \left(\frac{\partial u}{\partial r} - i k u \right) &= 0, \quad r = |x|. \end{aligned}$$

Suppose Ω is a rectangle in $\mathbb{R}^2$, then consider the problem:

$$\begin{aligned} \Delta u + k^2 u &= g(x), \quad \text{in} \quad \Omega, \\ \frac{\partial u}{\partial n} - i k u &= 0, \quad \text{on} \quad \partial \Omega. \end{aligned}$$

One can define a solution operator

$$G: g \to u$$

Then for the heterogeneous equation, we can derive a series solution. Indeed,

$$\Delta u_{n+1} + k^2 u_{n+1} = f - k^2 \mathrm{qu}_n$$

By the linearity of G

$$u_{n+1} = G(f) - k^2 G(\mathrm{qu}_n)$$

By defining $u_0 = G(f)$, we have

$$u_{n+1} = u_0 - (k^2 \mathrm{Gq}) u_n$$

Then

$$u_N = \sum_{i=0}^{N} (-k^2 \mathrm{Gq})^N u_0$$

1.1 Convergence of Neumann Series

2 Born series

For inhomogeneous Helmholtz equation

$$\Delta u + k^2 (1 + q(x)) u = f(x), \quad x \in \mathbb{R}^2,$$

The scattering potential is $V(x) = k^2(1+q(x)) - k^2 - i\varepsilon = k^2 q(x) - i\varepsilon$, then

$$\Delta u + k^2(1+i\varepsilon)u = f(x) - V(x)u(x)$$

The aforementioned solution operator is defined explicitly by the Green function

$$u(x) = \int g_0(x-y)[V(y)u(y) - f(y)]\mathrm{dy}$$

where

$$\Delta g(x) + k^2(1+i\varepsilon)g(x) = -\delta(x)$$

we know that $\hat{g}(\xi) = \frac{1}{|p|^2 - k^2 - i\varepsilon}$. By defining the similiar $G: u \rightarrow \int g_0(x-y)u(y)\mathrm{dy}$

$$u = \mathrm{GVu} - \mathrm{Gf}$$

set $u_0 = -\mathrm{Gf}$, then

$$u = [1 + \mathrm{GV} + \cdots + \mathrm{GV}^N +]u_0$$

2.1 Convergence Result

Omit

3 Convergent Born Series

By introducing an preconditioner γ, the equation is modified as

$$\gamma u = \gamma \mathrm{GVu} - \gamma \mathrm{Gf}$$

and by defining $M = \gamma \mathrm{GV} - \gamma + 1$,

$$u = \mathrm{Mu} - \gamma \mathrm{Gf}$$

then

$$u = [1 + M + M^2 + \cdots] - \gamma \mathrm{Gf}$$

Here we choose $\gamma(x) = \frac{i}{\varepsilon}V(x), \varepsilon \geqslant \max_x |k(x)^2 q(x)|$

For implementation, we discretize the potential map $V(x)$ and $u(x)$ on 2-d grid with $\Delta x = \frac{\lambda}{4}$, with λ an arbitrarily chosen wavelength of 1 distance unit. The iterative algorithm is

$$u_{k+1}(x) = u_k(x) - \frac{i}{\varepsilon}V(x)(u_k(x) - \mathrm{ifft}[\tilde{g}_0(x)\mathrm{fft}[V(x)u_k(x) - f(x)]])$$

3.1 Convergence Analysis

A sufficient condition is $\rho(M) < 1$. We first prove that $\rho(M) \leqslant 1$. The fourier transform of the green function is

$$\frac{1}{|\mathbf{p}|^2 - k_0^2 - i\,\epsilon} = \frac{i}{2\,\epsilon}\left(1 - \frac{|\mathbf{p}|^2 - k_0^2 + i\,\epsilon}{|\mathbf{p}|^2 - k_0^2 - i\,\epsilon}\right),$$

Then we modify the M as

$$M = \frac{-V}{2\,\epsilon^2}\left[1 - F^{-1}\frac{|\mathbf{p}|^2 - k_0^2 + i\,\epsilon}{|\mathbf{p}|^2 - k_0^2 - i\,\epsilon}F\right]V - \frac{i\,V}{\epsilon} + 1,$$
$$= \frac{1}{2\,\epsilon^2}\,[-V^2 + VUV - 2\,i\,\epsilon\,V + 2\,\epsilon^2]$$

where $U \equiv F^{-1}\frac{|\mathbf{p}|^2 - k_0^2 + i\epsilon}{|\mathbf{p}|^2 - k_0^2 - i\epsilon}F$ is a unitary operator.

We first show that $|<x, \mathrm{Mx}>| \leqslant <x, x>$. By Cauchy-Schwartz, $|<x, \mathrm{VUVx}>| = |<V^{\mathrm{T}}x, \mathrm{UVx}>| \leqslant \sqrt{<\mathrm{UVx}, \mathrm{UVx}>}\sqrt{<V^{\mathrm{T}}x, V^{\top}x>} = <\mathrm{Vx}, \mathrm{Vx}>$, result in

$$|\langle x, M\,x\rangle| \leq \frac{1}{2\,\epsilon^2}|\langle x, [2\,\epsilon^2 - 2\,i\,\epsilon\,V - V^2]\,x\rangle| + \frac{1}{2\,\epsilon^2}\langle Vx, Vx\rangle$$

To complete the proof, define $\Delta = V + i\varepsilon = k^2 q(x)$, we need

$$|2\varepsilon^2 - 2i\varepsilon V - V^2| + |V|^2 \leqslant 2\epsilon^2$$

everywhere. We can rewrite this as

$$|\varepsilon^2 - \Delta(x)^2| + |\Delta(x) - i\varepsilon|^2 \leqslant 2\varepsilon^2$$

Since we have $\varepsilon \geqslant |\Delta|$

which can be written as

$$\left|\epsilon^2 - |\Delta(\mathbf{r})|^2 - 2i\Delta(\mathbf{r})\mathrm{Im}\{\Delta(\mathbf{r})\}\right| + |\Delta(\mathbf{r})|^2 + \epsilon^2 - 2\epsilon\mathrm{Im}\{\Delta(\mathbf{r})\} \leq 2\epsilon^2.$$

A slightly stricter criterion follows from triangle inequality

$$\left|\epsilon^2 - |\Delta(\mathbf{r})|^2\right| + 2|\Delta(\mathbf{r})|\mathrm{Im}\{\Delta(\mathbf{r})\} + |\Delta(\mathbf{r})|^2 + \epsilon^2 - 2\epsilon\mathrm{Im}\{\Delta(\mathbf{r})\} \leq 2\epsilon^2,$$

4 Born Series For Wave Equation

Consider

$$m(x)\frac{\partial^2 u}{\partial^2 t} - \Delta u = f(x, t)$$

Let

$$\frac{1}{c(x)^2} = m(x), \frac{1}{c_0^2(x)} = m_0(x)$$

Then perturbate

$$m(x) = m_0(x) + \varepsilon m_1(x)$$

is equivalent to

$$c(x) = c_0(x) + \varepsilon c_1(x), \frac{1}{c(x)^2} \sim \frac{1}{c_0^2(x)} - 2\varepsilon\frac{c_1(x)}{c_0(x)^2}$$

The wavefield is splits into

$$u(x,t) = u_0(x,t) + u_{\mathrm{sc}}(x,t)$$

$$m_{_0}(x)\frac{\partial^2 u_0}{\partial^2 t} - \Delta u_0 = f(x,t)$$

and

$$m_0(x)\frac{\partial^2 u_{\mathrm{sc}}}{\partial^2 t} - \Delta u_{\mathrm{sc}} = -\varepsilon m_1(x)\frac{\partial^2 u}{\partial t^2}$$

By utilizing the Green's function, we obtain

$$u_{sc}(x,t) = -\varepsilon \int_0^t \int_{\mathbb{R}^n} G(x,y;t-s)\, m_1(y)\frac{\partial^2 u}{\partial t^2}(y,s)\, d\, y\, d\, s.$$

We denote this equation as $u_{\mathrm{sc}} = -\varepsilon \mathrm{Gm}_1 \frac{\partial^2 u}{\partial t^2}$, which is equivalent to

$$u = u_0 - \varepsilon \mathrm{Gm}_1 \frac{\partial^2 u}{\partial t^2}$$

This is called Lippmann-Schwinger equation. We can formally write this into

$$u = \left[I + \mathrm{Gm}_1 \frac{\partial^2}{\partial t^2}\right]^{-1} u_0$$

If $\left\|\mathrm{Gm}_1 \frac{\partial^2}{\partial t^2}\right\| < 1$ then we can write the Inverse Operator into a Neumann Series

$$u = \sum_{i=0}^{\infty} \left(-\varepsilon \mathrm{Gm}_1 \frac{\partial^2}{\partial t^2}\right)^i u_0$$

We naturally summarize the expansion

$$u = u_0 + \varepsilon u_1 + \varepsilon^2 u_2 + \ldots$$

The approximation $u_{\mathrm{sc}} = \varepsilon u_1 = -\varepsilon \mathrm{Gm}_1 \frac{\partial^2 u_0}{\partial t^2}$ is called the Born approximation. We can return to the PDE based on Green's function:

$$m_{_0}(x)\frac{\partial^2 u_1}{\partial^2 t} - \Delta u_1 = m_1 \frac{\partial^2 u_0}{\partial^2 t}$$

This is the primary reflection.

4.1 Convergence Analysis

We treat the wave equation in first order hyperbolic system

$$M\frac{\partial w}{\partial t} - \mathrm{Lw} = f, L^* = -L$$

where

$$w = \begin{pmatrix} \partial u / \partial t \\ \nabla u \end{pmatrix}, M = \begin{pmatrix} m(x) & \\ & 1 \end{pmatrix}, L = \begin{pmatrix} 0 & \nabla \cdot \\ \nabla & 0 \end{pmatrix}, f = \begin{pmatrix} f \\ 0 \end{pmatrix}$$

The conserved energy is $E = <w, \mathrm{Mw}>$. Consider a background medium M_0 such that $M = M_0 + \varepsilon M_1$, then let $w = w_0 + \varepsilon w_1 + \cdots$.We have

$$w = w_0 - \varepsilon \mathrm{GM}_1 \frac{\partial w}{\partial t}$$

where the Green function is $G = \left(M_0 \frac{\partial}{\partial t} - L\right)^{-1}$. The Neumann series of interest is

$$w = w_0 - \varepsilon\, G\, M_1 \frac{\partial\, w_0}{\partial\, t} + \varepsilon^2\, G\, M_1 \frac{\partial}{\partial\, t}\, G\, M_1 \frac{\partial\, w_0}{\partial\, t} + \dots$$

Here we define $w_1 = -\mathrm{GM}_1 \frac{\partial w_0}{\partial t}$, then we have a PDE

$$M_0 \frac{\partial\, w_0}{\partial\, t} - L\, w_0 = f, \quad M_0 \frac{\partial\, w_1}{\partial\, t} - L\, w_1 = -M_1 \frac{\partial\, w_0}{\partial\, t}$$

The weak scattering condition insist that $\varepsilon \|w_1\|_* \leqslant \|w_0\|_*$. We define the norm as

$$\|w\|_* = \max_{0 \le t \le T} \sqrt{\langle w, M_0\, w\rangle} = \max_{0 \le t \le T} |\sqrt{M_0}\, w|$$

Theorem 3. *(Convergence of the Born series) Assume that the fields w, w_0, w_1 are bandlimited with bandlimit*[3] *Ω. Consider these fields for $t \in [0, T]$. Then the weak scattering condition $\varepsilon \|w_1\|_* < \|w_0\|_*$ is satisfied, hence the Born series converges, as soon as*

$$\varepsilon\, \Omega T\, \|\frac{M_1}{M_0}\|_\infty < 1.$$

Proof. We compute

$$\begin{aligned}
\frac{d}{dt}\langle w_1, M_0 w_1\rangle &= 2\langle w_1, M_0 \frac{\partial w_1}{\partial t}\rangle \\
&= 2\langle w_1, L w_1 - M_1 \frac{\partial w_0}{\partial t}\rangle \\
&= -2\langle w_1, M_1 \frac{\partial w_0}{\partial t}\rangle \qquad \text{because } L^* = -L \\
&= -2\langle \sqrt{M_0} w_1, \frac{M_1}{\sqrt{M_0}} \frac{\partial w_0}{\partial t}\rangle.
\end{aligned}$$

Square roots and fractions of positive diagonal matrices are legitimate operations. The left-hand-side is also $\frac{d}{dt}\langle w_1, M_0 w_1\rangle = 2\|\sqrt{M_0} w_1\|_2 \frac{d}{dt}\|\sqrt{M_0} w_1\|_2$. By Cauchy-Schwarz, the right-hand-side is majorized by

$$2\|\sqrt{M_0} w_1\|_2\, \|\frac{M_1}{\sqrt{M_0}} \frac{\partial w_0}{\partial t}\|_2.$$

Hence

$$\frac{d}{dt}\|\sqrt{M_0} w_1\|_2 \le \|\frac{M_1}{\sqrt{M_0}} \frac{\partial w_0}{\partial t}\|_2.$$

$$\|\sqrt{M_0}w_1\|_2 \leq \int_0^t \|\frac{M_1}{\sqrt{M_0}}\frac{\partial w_0}{\partial t}\|_2(s)\,ds.$$

$$\begin{aligned}\|w_1\|_* = \max_{0\leq t\leq T}\|\sqrt{M_0}w_1\|_2 &\leq T\max_{0\leq t\leq T}\|\frac{M_1}{\sqrt{M_0}}\frac{\partial w_0}{\partial t}\|_2 \\ &\leq T\|\frac{M_1}{M_0}\|_\infty \max_{0\leq t\leq T}\|\sqrt{M_0}\frac{\partial w_0}{\partial t}\|_2.\end{aligned}$$

This last inequality is almost, but not quite, what we need. The right-hand side involves $\frac{\partial w_0}{\partial t}$ instead of w_0. Because time derivatives can grow arbitrarily large in the high-frequency regime, this is where the bandlimited assumption needs to be used. We can invoke a classical result known as Bernstein's inequality[4], which says that $\|f'\|_\infty \leq \Omega\|f\|_\infty$ for all Ω-bandlimited f. Then

$$\|w_1\|_* \leq \Omega T\|\frac{M_1}{M_0}\|_\infty\|w_0\|_*.$$

In view of our request that $\varepsilon\|w_1\|_* < \|w_0\|_*$, it suffices to require

$$\varepsilon\,\Omega T\,\|\frac{M_1}{M_0}\|_\infty < 1.$$

□

5 Neumann Series

For NSNO:

$$\Delta\, u + k^2\,(1+q(x))\,u = f(x), \quad x\in\mathbb{R}^2,$$
$$\lim_{r\to\infty}\sqrt{r}\left(\frac{\partial u}{\partial r} - i\,k\,u\right) = 0, \quad r = |x|.$$

Recall that

$$\Delta u_{n+1} + k^2 u_{n+1} = f - k^2 \mathrm{q} u_n$$

By the linearity of G

$$u_{n+1} = G(f) - k^2 G(\mathrm{q}u_n)$$

By defining $u_0 = G(f)$, we have

$$u_{n+1} = u_0 - (k^2\mathrm{Gq})u_n$$

Then

$$u_N = \sum_{i=0}^{N} (-k^2 \mathrm{Gq})^N u_0$$

In NSNO implementation,

$$u_{_0} = G_{\theta_1}(f), u_1 = G_{\theta_1}(-k^2 \mathrm{qu}_0), \ldots u_n = G_{\theta_1}(-k^2 \mathrm{qu}_{n-1})$$

And the solution is given by

$$\tilde{u}_n = \sum_{i=0}^{n} u_n$$

We can consider the G_{θ_i} as a series of self attention layer.

6 GMRES for Helmholtz

The Helmholtz problem is

$$\begin{aligned} \Delta\, u + k^2\,(1 + q(x))\, u &= f(x), \quad x \in \mathbb{R}^2, \\ \lim_{r \to \infty} \sqrt{r} \left(\frac{\partial\, u}{\partial\, r} - i\, k\, u \right) &= 0, \quad r = |x|. \end{aligned}$$

The Neumann Series propose that

$$\Delta u + k^2 u = f - k^2 \mathrm{qu}$$

by defininig a solution operator for

$$G \colon g \rightarrow u \qquad \Delta u + k^2 u = g(x)$$

We have

$$u + k^2 \mathrm{Gqu} = \mathrm{Gf}$$

The GMRES want to solve

$$(I + k^2 \mathrm{Gq}) u = \mathrm{Gf}$$

By denotes

$$\mathrm{Gf} = u_0$$

Then recall

算法 (GMRES)

1. Compute $\boldsymbol{r}_0 = \boldsymbol{b} - A\boldsymbol{x}_0$, $\beta = \|\boldsymbol{r}_0\|_2$, and $\boldsymbol{v}_1 = \boldsymbol{r}_0/\beta$
2. for $j = 1, 2, \cdots, m$ do
3. Compute $\boldsymbol{w}_j = A\boldsymbol{v}_j$
4. for $i = 1, \cdots, j$ do
5. $h_{ij} = (\boldsymbol{w}_j, \boldsymbol{v}_i)$
6. $\boldsymbol{w}_j = \boldsymbol{w}_j - h_{ij}\boldsymbol{v}_i$
7. end for
8. $h_{i+1,j} = \|\boldsymbol{w}_j\|_2$
9. if $h_{j+1,j} = 0$ set $m = i$ goto 12 % lucky breakdown
10. $\boldsymbol{v}_{j+1} = \boldsymbol{w}_j / h_{j+1,j}$
11. end for
12. Define the $(m+1) \times m$ Hessenberg matrix $\overline{H}_m = \{h_{ij}\}$
13. Compute y_m as the minimizer of $\|\beta\boldsymbol{e}_1 - \overline{H}_m\boldsymbol{y}_m\|_2$ and set $\boldsymbol{x}_m = \boldsymbol{x}_0 + V_m\boldsymbol{y}_m$

1. $r_0 = u_0$-$(I + k^2\text{Gq})u_0 = -k^2\text{Gqu}_0$, $\beta = \|-k^2\text{Gqu}_0\|_2$, $v_1 = \frac{-k^2\text{Gqu}_0}{\|-k^2\text{Gqu}_0\|}$
2. (Step1)$w_1 = (I + k^2\text{Gq})v_1 = v_1 + k^2\text{Gqv}_1$,$h_{11} = (w_1, v_1)$, $w_1 = w_1 - h_{11}v_1$,
3. $h_{21} = \|w_1\|_2$, $v_2 = \frac{w_1}{h_{21}}$
4. (Step2)$w_2 = (I + k^2\text{Gq})v_2 = v_2 + k^2\text{Gqv}_2$,$h_{12} = (w_2, v_1)$, $w_2 = w_2 - h_{12}v_1$, $h_{22} = (w_2, v_2)$, $w_2 = w_2 - h_{22}v_2$
5. $h_{32} = \|w_2\|_2$, $v_3 = \frac{w_2}{h_{32}}$
6. (Step3)$w_3 = (I + k^2\text{Gq})v_3 = v_3 + k^2\text{Gqv}_3$,$h_{13} = (w_3, v_1)$, $w_3 = w_3 - h_{13}v_1$, $h_{23} = (w_3, v_2)$, $w_3 = w_3 - h_{23}v_2$,$h_{33} = (w_3, v_3)$, $w_3 = w_3 - h_{33}v_3$
7. $h_{43} = \|w_3\|_2$, $v_4 = \frac{w_3}{h_{43}}$
8. $\ldots$
9. Solve $\|\bar{H}_m y_m - \beta e_1\|$ to obtain y_m and sum up $u_m = u_0 + V_m y_m$

Bi-CG stablized