Discrete Dipole Approximation of Volume Integral Equations: A perfect method for perfect equations?

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IRMAR -IASBS

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An integral equation with simple discretization:

Consider the following integral equation

$$\lambda u(x) - \int_{\Omega} K(x,y)u(y)\mathrm{d}y = f(x), \quad x \in \Omega$$

and imagine the following system of equations as its discretization

$$\lambda u_m - \sum_{x_n \in \Omega, n \neq m} h^m K(x_m, x_n)u_n = f(x_m), \quad x_m \in \Omega$$

where $h = 1/N$

Discrete Dipole Approximation (DDA)

Let $\Omega = \bigcup_{i=i}^{N} \Omega_i$, $x_i \in \Omega_i$, collocate Eq. (asli) at points x_i and approximate the integrals by one-point quadrature rule, then:

$$\boxed{\mathscr{A}_\kappa \mathbf{E}(x_i) \simeq \left(\frac{1}{N}\right)^3 \sum_{j \neq i} k(x_i, x_j)\mathbf{E}(x_j) + \alpha_i^{-1}\mathbf{E}(x_i)},$$

where

$$k(x,y) = -(\nabla \operatorname{div} + \kappa^2) G_\kappa(x-y) = -(D^2 + \kappa^2) G_\kappa(x-y).$$

The idea of DDA is introduced in:

PURCELL, E. M., AND PENNYPACKER, R. P: Scattering and absorption of light by non spherical dielectric grains. *ApJ, 186, pp.705-714*, (1973)

with Clausius-Mossotti polarizability as α_i's:

$$\alpha_i^{\mathrm{CM}} = \frac{3d^3}{4\pi}\frac{\varepsilon_i - 1}{\varepsilon_i + 2}, \qquad = \frac{3V}{4\pi N}\frac{\varepsilon_i - 1}{\varepsilon_i + 2}$$

$\varepsilon_i = \varepsilon(x_i)$, dielectric function at location x_i, $d^3 = V/N$ and $V = \mathrm{Vol}(\Omega)$.

Another option for α_i's in order to answer the question: " for what polarizability α will an infinite lattice of polarizable points have the same dispersion relation as a continuum of refractive index $m = \sqrt{\varepsilon}$? ",

$$\alpha_i^{\mathrm{LDR}} = \frac{\alpha^{\mathrm{CM}}}{1 + \frac{\alpha^{\mathrm{CM}}}{d^3}\left[(b_1 + m^2 b_2 + m^2 b_3 S)(kd)^2 - (2/3)\mathrm{i}(kd)^3\right]},$$

with

$$b_1 = -1.891531;\ b_2 = 0.1648469;\ b_3 = -1.7700004;\ S = \sum_{j=1}^{3} (a_j e_j)^3,$$

is discussed in:

DRAINE, B. T., AND GOODMAN J.: Beyond Clausius-Mossotti-Wave propagation on a polarizable point lattice and the discrete dipole approximation. *ApJ, 405, pp. 685-697*, (1993).

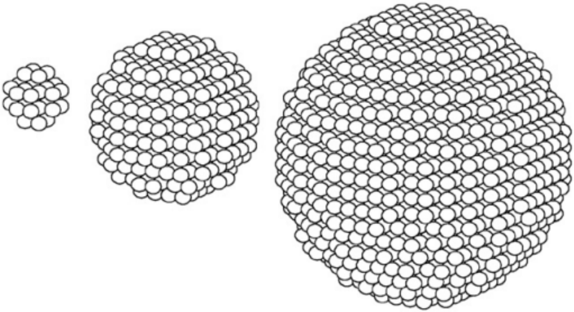

Figure: Pseudospheres made from 32, 552 and 3112 dipoles, arranged in cubic lattic

LOKE, V. AND MENGÜÇ, M PINAR AND NIEMINEN, TIMO A: Discrete-dipole approximation with surface interaction: Computational toolbox for MATLAB. *JQSRT, 112, pp. 1711–1725*, (2011).

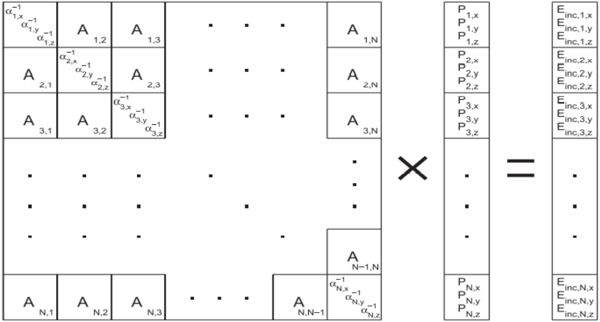

Figure: Coefficient Matrix

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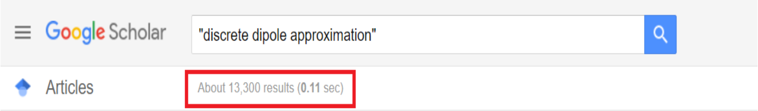
```julia
function  TMat(k,N)
  Np = N+1;   Np3 = Np^3;
  Line = collect(range(0,1,length=Np));
  Point = zeros(Np3,3); # Point(m,:)=x_m
  m = 0;
  for i in 1:Np for j in 1:Np for l in 1:Np
          m = m+1;
          Point[m,:] = [Line[i]; Line[j]; Line[l]]
  end end end
TM11 = complex(zeros(Np3,Np3));
TM12 = similar(TM11); TM13 = similar(TM11);
TM21 = similar(TM11); TM22 = similar(TM11); TM23 = similar(TM11);
TM31 = similar(TM11); TM32 = similar(TM11); TM33 = similar(TM11);
   for m in 1:Np3  for n in 1:Np3
          Kmn = K(k,Point[m,:]-Point[n,:]);
          TM11[m,n] = Kmn[1,1];          TM12[m,n] = Kmn[1,2];          TM13[m,n] = Kmn[1,3];
          TM21[m,n] = Kmn[2,1];          TM22[m,n] = Kmn[2,2];
          TM23[m,n] = Kmn[2,3];          TM31[m,n] = Kmn[3,1];
          TM32[m,n] = Kmn[3,2];          TM33[m,n] = Kmn[3,3];
   end end
   TM = [TM11 TM12 TM13; TM21 TM22 TM23; TM31 TM32 TM33];
   # multiply by element area
   h = 1/N;     TM = h^3*TM;    return TM
end
```

Figure: A piece of Julia code for DDA matrix

- ⋆ ✓ It is the simplest method that one can apply to numerically solve an IE. Open source codes are available in Fortran(DDSCAT), MATLAB(DDA-SI), Python(PyDDA), C(ADDA), C++(DDScat), ...
- ⋆ ✓ It is quite easy to understand in comparison with BEM, FEM or even FDM.
- ⋆ ✓ Convolution structure of the operator; Toeplitz matrix in the discretized level; application of FFT method.
  One can see the last development in:

  GROTH, S. P., ATHANASIOS G. P., AND JACOB K. W.: Accelerating the discrete dipole approximation via circulant preconditioning. *Journal of Quantitative Spectroscopy and Radiative Transfer, 420, (2020)*

- ⋆ ✓ It is very popular: 9/30/2022



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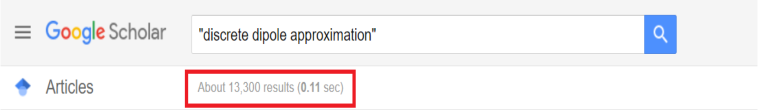

DDA: the pros and cons

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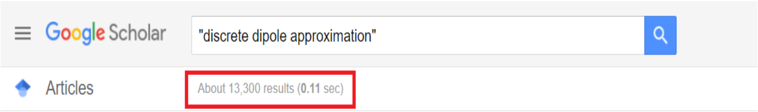

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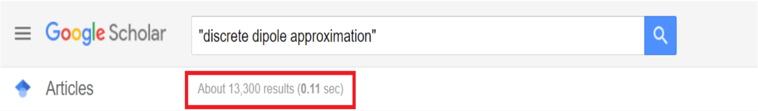


DDA: the pros and cons

but among physicists not mathematicians!

1 hit in NA (MR1375267) published 1996!

12 hits from 2014-2022, there is no document before!

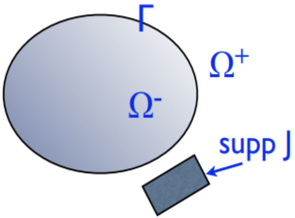
- ⋆ In continuous level: $\mathscr{A}_\kappa$ is a strongly singular operator. So compared to boundary integral operators, it is less discussed.

$\Omega \subset \mathbb{R}^3$, bounded domain:

Time-harmonic Maxwell Equations:

$$\textbf{curl}\,\mathbf{E} - \mathrm{i}\kappa\,\mu\,\textbf{curl}\,\mathbf{H} = 0; \quad \textbf{curl}\,\mathbf{H} + \mathrm{i}\kappa\,\varepsilon\,\mathbf{E} = \mathbf{J}$$

$\varepsilon = \varepsilon_r$ in Ω, $\quad \varepsilon = 1$ in $\mathbb{R}^3 \setminus \overline{\Omega}$,
$\eta = 1 - \varepsilon_r$: has compact support
$\mu = \mu_r$ in Ω, $\mu = 1$ in $\mathbb{R}^3 \setminus \overline{\Omega}$,
$\nu = 1 - \frac{1}{\mu_r}$



Supp $\mathbf{J}$ compact in $\mathbb{R}^3 \setminus \Omega$
Transition condition on the boundary $\Gamma = \partial\Omega$:
$[\mathbf{E} \times \mathbf{n}]_\Gamma = 0, \quad [\mathbf{n}.\mu\mathbf{H}]_\Gamma = 0, \quad [\mathbf{H} \times \mathbf{n}]_\Gamma = 0, \quad [\mathbf{n}.\varepsilon\mathbf{E}]_\Gamma = 0$

+ Sommerfeld Radiation Condition

$$\textbf{curl}\,\frac{1}{\mu}\,\textbf{curl}\,\mathbf{E} - \kappa^2\,\varepsilon\,\mathbf{E} = \mathbf{J}$$

$$\Downarrow$$

$$\textbf{curl curl}\,\mathbf{E} - \kappa^2\,\mathbf{E} = \mathrm{i}\kappa\,\mathbf{J} - \kappa^2(1-\varepsilon)\,\mathbf{E} + \textbf{curl}\,(1-\frac{1}{\mu})\,\textbf{curl}\,\mathbf{E}$$

$$= \mathrm{i}\,\kappa\,\mathbf{J} - \kappa^2\eta\,\chi_\Omega\,\mathbf{E} + \textbf{curl}\,\nu\,\chi_\Omega\,\textbf{curl}\,\mathbf{E}$$

It is seen that

$$(\textbf{curl curl} - \kappa^2\mathbb{I})(\frac{1}{\kappa^2}\nabla\,\mathrm{div} + \mathbb{I}) = -(\Delta + \kappa^2\mathbb{I})$$

so **E** is obtained from the convolution with the fundamental solution

$$g_\kappa(x) = (\frac{1}{\kappa^2}\nabla\,\mathrm{div} + \mathbb{I})G_\kappa(x), \quad G_\kappa(x) = \frac{\exp(\mathrm{i}\kappa|x|)}{4\pi|x|}$$

We get an VIE for the electric part **E**:

$$\mathbf{E} = \kappa^2 g_\kappa * (\eta\, \chi_\Omega\, \mathbf{E}) + g_\kappa * (\mathbf{curl}\ \nu\, \chi_\Omega\ \mathbf{curl}\ \mathbf{E}) + \mathrm{i}\kappa g_\kappa * \mathbf{J},$$

or

$$\mathbf{E}(x) = \kappa^2 \int_\Omega g_\kappa(x-y)\eta(y)\mathbf{E}(y)\mathrm{d}y + \int_\Omega g_\kappa(x-y)\ \mathbf{curl}\ \nu(y)\ \mathbf{curl}\ \mathbf{E}(y)\mathrm{d}y$$
$$+\mathrm{i}\kappa \int_\Omega g_\kappa(x-y)\mathbf{J}(y)\mathrm{d}y,$$

Let

Dielectric problem: $\mu \equiv \text{const}, \nu = 0$

then

$$\mathbf{E}(x) = -(\nabla\,\mathrm{div} + \kappa^2 \mathbb{I}_d) \int_\Omega G_\kappa(x-y)\eta(y)\mathbf{E}(y)\mathrm{d}y + \mathbf{E}^{\mathrm{inc}}(x).$$

We get

$$\boxed{\mathbf{E}(x) - \mathscr{A}_\kappa(\eta \mathbf{E})(x) = \mathbf{E}^{\text{inc}}(x)}$$

with

$$(\mathscr{A}_\kappa u)(y) = -(\nabla \operatorname{div} + \kappa^2 \mathbb{I}_d) \int_\Omega G_\kappa(x-y)u(y)\mathrm{d}y.$$

Applying Fourier transform on $\mathscr{A}_\kappa$:

$$\sigma_\kappa(\xi) := \mathscr{F}\{\mathscr{A}_\kappa u\}(\xi) = \frac{\xi\xi^T - \kappa^2 \mathbb{I}_d}{|\xi|^2 - \kappa^2} \hat{u}(\xi),$$

the inversion Fourier transform gives:

$$\boxed{(\mathscr{A}_\kappa u)(x) = (2\pi)^{-d} \int_{\mathbb{R}^d} \sigma_\kappa(\xi)\hat{u}(\xi)\exp(-\mathrm{i}\xi . x)\mathrm{d}\xi}.$$

So $\mathscr{A}_\kappa$ has a inverse Fourier representation with specific kernel called symbol of the operator. Such operators are called pseudo-differential operators.

The operator $\mathscr{A}_\kappa$ can be represented as a strongly singular integral operator:

$$\boxed{\mathscr{A}_\kappa \mathbf{E}(x) = \text{p.v.} \int_\Omega \nabla_x \nabla_y G_\kappa(x-y)\mathbf{E}(y)\mathrm{d}y + \frac{1}{3}\mathbf{E}(x)},$$

where p.v denotes the Cauchy Principle Value:

$$T_\kappa \mathbf{E}(x) := \text{p.v.} \int_\Omega \nabla_x \nabla_y G_k(x-y)\mathbf{E}(y)\mathrm{d}y = \lim_{\varepsilon \to 0} \int_{\Omega \setminus B_\varepsilon(x)} \nabla_x \nabla_y G_\kappa(x-y)\mathbf{E}(y)\mathrm{d}y.$$

Is the problem

$$\mathbf{E} - \mathscr{A}_\kappa(\eta \mathbf{E}) = \mathbf{E}^{\text{inc}} \qquad \text{(asli)}$$

or its equivalence

$$\frac{1}{\eta}\mathbf{E} - \mathscr{A}_\kappa \mathbf{E} = \mathbf{E}^{\text{inc}}$$

well-posed in the sense of Hadamard (existence, uniqueness and stability)?

Some properties of $\mathscr{A}_\kappa$

- ✓ The operator $\mathscr{A}_\kappa$ can be extended to $\mathbf{L}^2(\Omega)$ as a bounded operator;
- ✓ $\mathscr{A}_\kappa - \mathscr{A}_0$ is a compact operator in $\mathbf{L}^2(\Omega)$;

Let spectrum:

$$\boxed{\mathrm{Sp}(T) := \{\lambda \in \mathbb{C} \mid (\lambda \mathbb{I} - T)^{-1} \text{ does not exits}\}}$$

and essential spectrum

$$\boxed{\mathrm{Sp}_{\mathrm{ess}}(T) := \{\lambda \in \mathbb{C} \mid (\lambda \mathbb{I} - T) \text{ is not Fredholm}\}}$$

then
✓ Let $\Sigma := \mathrm{Sp}_{\mathrm{ess}}(\frac{1}{2}\mathbb{I} + K') \subset (0,1)$, then for Lipschitz Γ:
$\mathrm{Sp}_{\mathrm{ess}}(\mathscr{A}_0) = \{0,1\} \bigcup \Sigma$ and for smooth Γ: $\mathrm{Sp}_{\mathrm{ess}}(\mathscr{A}_0) = \{0, 1/2, 1\}$. K' is

boundary integral operator adjoint to the Helmholtz double layer potential operator.

DDA: the questions

- ⋆ DDA as a popular method between physicists and engineers is really accurate as it is shown by numerical examples?
- ⋆ Is it a consistent, convergent and stable method?
- ⋆ Is there any estimation for the rate of convergence?

YURKIN, M. A., VALERI P. M., AND A. G. HOEKSTRA: Convergence of the discrete dipole approximation. I. Theoretical analysis, *JOSA A, 23(10)*, pp. 2578-2591 (2006).

$$\|(\mathscr{A}_\kappa \mathbf{E})(\mathbf{x}_i) - \mathscr{A}_\kappa^{\mathrm{DDA}}(\mathbf{E})_i\|_{L^1(\overline{\Omega})} = ch + \mathscr{O}\left(h^2 \log(h)\right) \text{ for } \mathbf{E} \in C^4(\overline{\Omega})$$

Lax equivalence theorem:

For a consistent numerical algorithm:

stability $\Leftrightarrow$ convergence

Q: Is DDA stable?

Consistency, stability, convergence

Let $Au = f$ and the discrete form as $A_N u_N = f_N := r_N f$:

$$\begin{array}{ccc} X & \xrightarrow{A} & X \\ \downarrow r_N & & \downarrow r_N \\ X_N & \xrightarrow{A_N} & X_N \end{array}$$

Consistency error (truncation error): $E_N[v] = A_N r_N v - r_N A v$
Discrete error: $e_N = r_N u - u_N$

$$\boxed{A_N e_N = A_N r_N u - A_N u_N = A_N r_N u - r_N f = A_N r_N u - r_N A u = E_N[u]}$$

$$\Downarrow$$

$$\boxed{\|e_N\| \leq \|(A_N)^{-1}\| \|E_N[u]\|}$$

If $\exists\, C > 0$ s.t $\|(A_N)^{-1}\| \leq C$, uniformly, then the method is stable and truncation error gives an estimation for discrete error.

DDA in 3D: Ω is unit cube; $h = 1/N$; N the number of dipoles

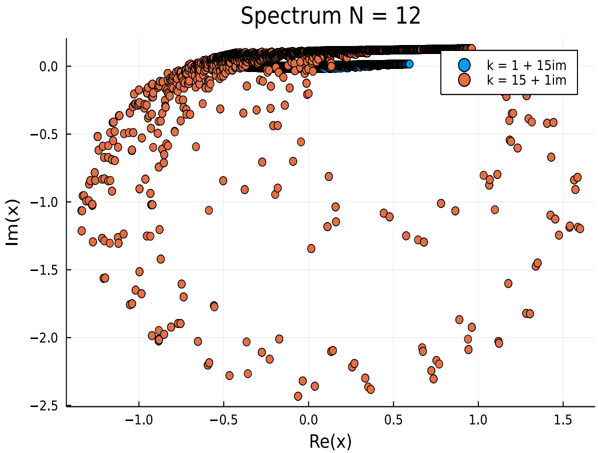


Figure: $k \equiv \kappa,\ \lambda = \frac{1}{\eta} - \frac{1}{3} = \frac{2+\varepsilon_r}{3(1-\varepsilon_r)}$

An example: convergence of the spectrum

DDA in 3D: Ω is unit cube; $h = 1/N$; N the number of dipoles

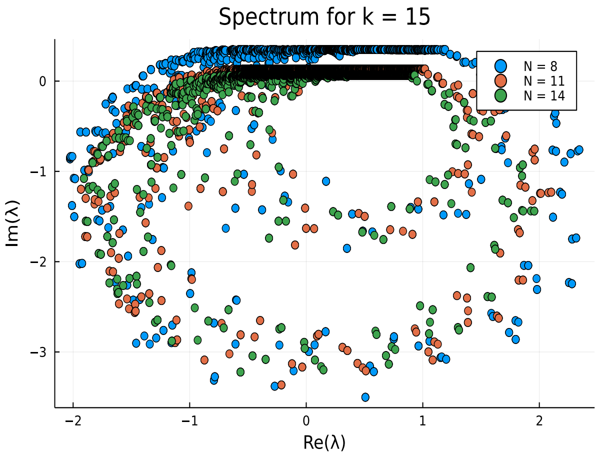


Figure: $k \equiv \kappa,\ \lambda = \frac{1}{\eta} - \frac{1}{3} = \frac{2+\varepsilon_r}{3(1-\varepsilon_r)}$

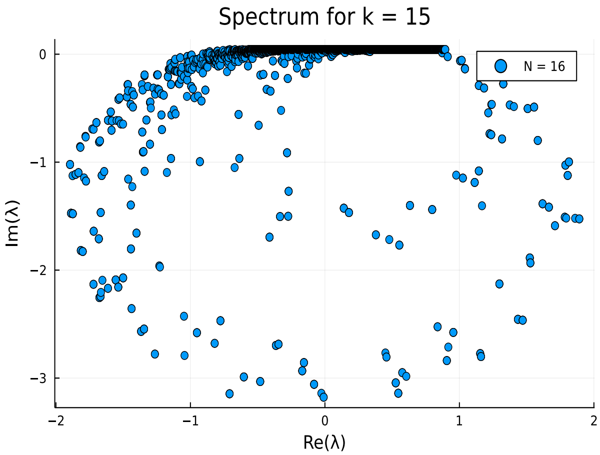


Figure: $k \equiv \kappa,\ \lambda = \frac{1}{\eta} - \frac{1}{3} = \frac{2+\varepsilon_r}{3(1-\varepsilon_r)}$

We have

$$\boxed{\Omega \subset \mathbb{R}^d, \quad K_\kappa = -(D^2+\kappa^2)G_\kappa \quad \text{and} \quad \mathscr{A}_\kappa u = K_\kappa * (\chi_\Omega u)}$$

and

$$T_\kappa u = \text{p.v.} \int_\Omega K_\kappa(x-y)u(y)\mathrm{d}y$$

and

$$\mathscr{A}_\kappa u = T_\kappa u + \frac{1}{d}u$$

then

$$\left(\frac{1}{\eta}\mathbb{I}_d - \mathscr{A}_\kappa\right)u = \underbrace{\left(\frac{1}{\eta} - \frac{1}{d}\right)u}_{\text{diagonal terms}} - T_\kappa u$$

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where

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$$\alpha_i^{\mathrm{CM}} = \frac{3d^3}{4\pi} \frac{\varepsilon_i - 1}{\varepsilon_i + 2}, = \frac{3}{4\pi N} \frac{\varepsilon_i - 1}{\varepsilon_i + 2} \qquad (1)$$

$\varepsilon_i = \varepsilon(x_i)$, dielectric function at location x_i, $d^3 = V/N$ and $V = \mathrm{Vol}(\Omega)$.

The discrete system

DDA system matrix:

$$T_N^\kappa = (N^{-d} K_\kappa(x_m - x_n))_{n,m\in\omega^N}, \;\; K_\kappa(0) = 0, \;\; \omega_N = \{n \in \mathbb{Z}^d \mid x_n = \frac{n}{N} \in \Omega\}.$$

To get an approximation for $\frac{1}{\eta}\mathbb{I}_d - \mathscr{A}_\kappa$, we see that

$$\frac{1}{\eta}\mathbb{I}_d - \mathscr{A}_\kappa = (\frac{1}{\eta} - \frac{1}{d})\mathbb{I}_d - T_\kappa,$$

for T_κ^N as an approximation for T_κ, $\lambda\mathbb{I} - T_\kappa^N$ is an approximation for $\frac{1}{\eta}\mathbb{I} - \mathscr{A}_\kappa$.

The stability: $\|(\lambda\mathbb{I} - T_\kappa^N)^{-1}\| < M.$ Let $\tilde{a}(\xi) = \sum_{m\in\mathbb{Z}^d} a(m)e^{im.\xi}$, $a(m) = (2\pi)^{-d}\int_Q \tilde{a}(t)e^{-im.\xi}\mathrm{d}\xi$, then the quadratic form of the DDA system is

$$(u_N, (\lambda\mathbb{I} - T_\kappa^N)u_N)_{l^2(\omega^N)} = (2\pi)^{-d}\int_Q \overline{\tilde{u}_N(\xi)}(\lambda\mathbb{I} - \underbrace{\tilde{K}_\kappa^N(\xi)}_{:=F_\kappa^N(\xi)})\tilde{u}_N(\xi)\mathrm{d}\xi,$$

where $Q = [-\pi,\pi]^d \simeq \mathbb{R}^d \setminus (2\pi\mathbb{Z}^d)$. Let $\lambda = \frac{1}{\eta} - \frac{1}{d}$ and $\eta = 1 - \varepsilon_r$, then $\lambda = \frac{d-1+\varepsilon_r}{d(1-\varepsilon_r)}$. Especially, for $d = 3$, $\lambda = \frac{2+\varepsilon_r}{3(1-\varepsilon_r)}$.

$A : X \to X$ a bounded linear operator in Hilbert space H and $a(u,v) = (Au,v)$ the corresponding sesquilinear form

Definition: $W(A) = \{(Au,u) \mid u \in X,\ \|u\| = 1\}$

✓ $W(A)$ is convex;

✓ $\mathrm{Sp}(A) \subset \overline{W(A)} \subset \{z \in \mathbb{C} \mid |z| \le \|A\|\}$;

✓ (Au,u) is coercive iff $0 \notin \overline{W(A)}$, and coercivity constant $\gamma = \inf_{z \in W(A)} |z|$

✓ Let $X_N \subset X$ and $A_N : X_N \to X_N$ with $A_N = a(u,u)|_{X_N}$, then $W(A_N) \subset W(A)$ and furthermore for $\lambda \notin \overline{W(A)}$,

$$\|(\lambda \mathbb{I} - A_N)^{-1}\| \le \frac{1}{\mathrm{dist}(\lambda, W(A))}$$

Stability results for quasi static case: $\kappa = 0$

Theorem(Zachlin & Hochstenbach)

The numerical range of a Hermitian matrix T is a closed interval on the real axis, whose endpoint are formed by the extreme eigenvalue of T.

Due to symmetry and $\mathrm{Tr}(F_0(t)) = 0$, for $d = 2$, $F_0(t) = \begin{bmatrix} a(t) & b(t) \\ b(t) & -a(t) \end{bmatrix}$

Theorem A

There exits an interval $\Sigma := [\Lambda_-, \Lambda_+]$ such that $\Sigma = \cup_{N\in\mathbb{N}} W(T_0^N)$. Then for $\lambda \in \mathbb{C} \setminus \Sigma$, DDA metod $(\lambda\mathbb{I} - T_0^N)u = f$ is l^2-stable and

$$\|(\lambda\mathbb{I} - T_0^N)^{-1}\| \leq \frac{1}{\mathrm{dist}(\lambda, \Sigma)}.$$

It is seen that the spectrum of T_0 is $[-1/d, 1-1/d]$ which is contained in $[\Lambda_-, \Lambda_+]$, so for

$$\Lambda_- \leq \lambda < -1/d \quad \text{or} \quad 1 - 1/d < \lambda < \Lambda_+$$

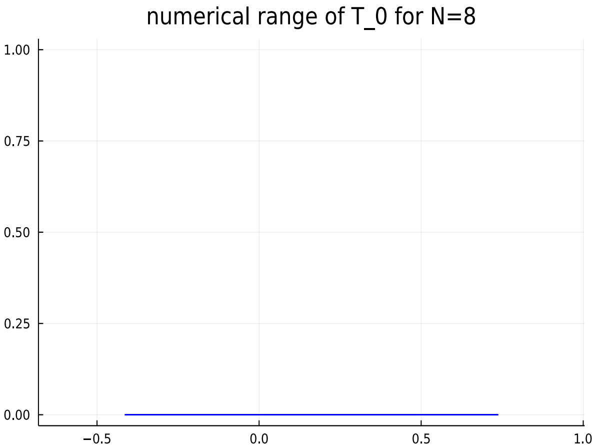
the VIE is well-posed in $L^2(\Omega)$ but DDA is unstable.

For $d = 2$

$$-\Lambda_- = \Lambda_+ \geq \Lambda_0 = \frac{\Gamma(1/4)^4}{32\pi^2} = 0.5471\ldots$$

for $d = 3$

$\Lambda_- \sim -0.42$ and $\Lambda_+ \sim 0.77$ Conjecture: $\Lambda_+ = \Lambda_0$



Stability results for $\kappa \in \mathbb{C} \setminus \mathbb{R}$

Theorem B

Let $\alpha \in \arg\ \kappa \in (-\pi, \pi) \setminus \{0\}$ and

$$W_\kappa = \{z \in \mathbb{C} \mid |z - \frac{1}{2}(z - \mathrm{i}\cot(2\alpha))| \leq \frac{1}{2|\sin(2\alpha)|},\ \mathrm{Im} z.Im(\kappa^2) < 0\}.$$

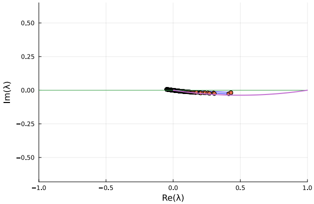
The compact bounded set $[\Lambda_-, \Lambda_+] + W_\kappa$ is bounded set for the spectrum of the VIE and it bounds the numerical range

Corollary

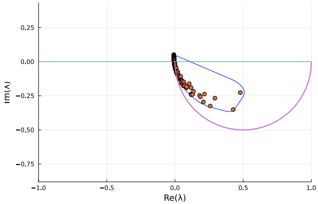
Let $\lambda \in \mathbb{C} \setminus ([\Lambda_-, \Lambda_+] + W_\kappa)$. Then the sequence of matrices $(\lambda \mathbb{I} - T_\kappa^N)_{N \in \mathbb{N}}$ is l^2-stable in the following sense: Given any $\varepsilon > 0$ that satisfies $\varepsilon < d_\kappa := \mathrm{dist}(\lambda, [\Lambda_-, \Lambda_+])$, there exists $N_0 \in \mathbb{N}$ such that for $N \geq N_0$ the matrix $\lambda \mathbb{I} - T_\kappa^N$ is invertible, and for the l^2-matrix norm we have the estimate

$$\|(\lambda \mathbb{I} - T_\kappa^N)^{-1}\| \leq \frac{1}{d_\kappa - \varepsilon}$$

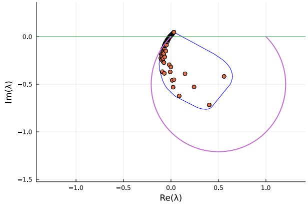
Ω is unit cube, $|\kappa| = 5$ and $N = 8$
Matrix $T_\kappa^N - T_0^N$: eigenvalues, numerical range, and proven bounds



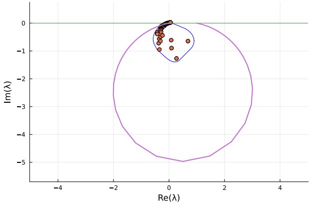
$\kappa = 0.37 + 4.99i$



$\kappa = 3.53 + 3.53i$



$\kappa = 4.62 + 1.91i$



$\kappa = 4.97 + 0.5i$

Stability results for real κ: imaginary part of DDA matrix

Theorem C

Let

$$\mu_+(\kappa) = \frac{d-1}{2^d\Gamma(\frac{d}{2})\pi^{d/2-1}}\kappa^d \quad (d=2, \mu_+(\kappa) = \frac{\kappa^2}{8} \text{ and } d=3, \frac{\kappa^3}{6\pi})$$

then

$$W(\mathrm{Im}(T_\kappa^N)) \subset [\mu_-^N, \mu_+^N],$$

with $\mu_+^N = \mu_+(\kappa)N^{-d}$ and $\lim_{N\to\infty}\mu_-^N = -\mu_+(\kappa)|\Omega|$.

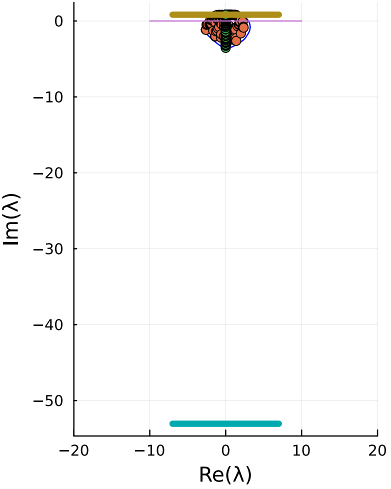
Corollay

If $\lambda \in \mathbb{C}$ is such that either $\mathrm{Im}\lambda > 0$ or $\mathrm{Im}\lambda < -\mu_+(\kappa)|\Omega|$, then for large enough N the matrix $\lambda\mathbb{I} - T_\kappa^N$ is invertible, and the l^2 matrix norms $\|(\lambda\mathbb{I} - T_\kappa^N)^{-1}\|$ are bounded uniformly in N. The invertibility holds if either $\mathrm{Im}\lambda > \mu_+(\kappa)N^{-d}$ or $\mathrm{Im}\lambda < -\mu_+(\kappa)\frac{|\omega^N|-1}{N^d}$.

κ real: bounds for the imaginary part of the numerical range

Ω unit cube, $\kappa = 10$

Eigenvalues, numerical range, and proven bounds:



κ real: bounds for the imaginary part of the numerical range

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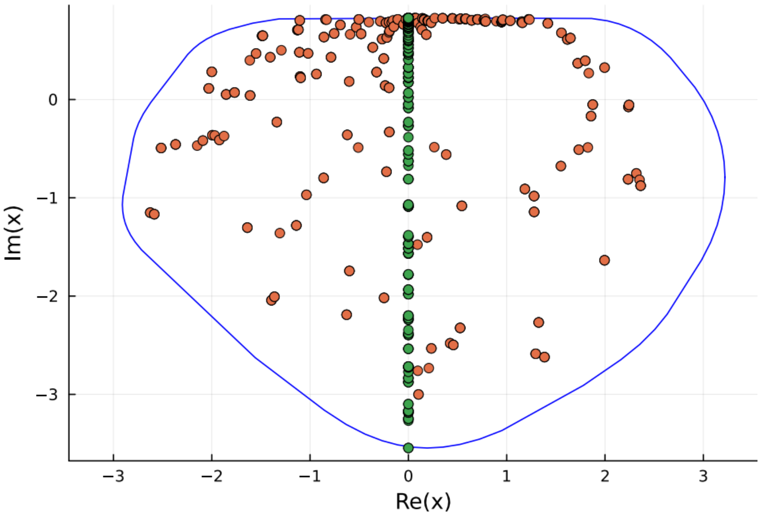
Eigenvalues, numerical range, and proven bounds:



For operator

$$\mathscr{A}_\kappa = \mathscr{A}_0 + \underbrace{(\mathscr{A}_\kappa - \mathscr{A}_0)}_{\text{compact}}$$

the principle part is $\mathscr{A}_0$ and $\mathscr{A}_0 u = -D^2 G_0 * (\chi_\Omega u)$
The kernel $K(x) = -D^2 g_0(x)$ and

$$G_0(x) = \begin{cases} -\frac{1}{2\pi}\log|x|, & d = 2 \\ \frac{1}{4\pi|x|}, & d = 3 \end{cases}$$

K is homogenous of degree $-d$

VIE: $\lambda u - Tu = f$ with $Tu(x) = \text{p.v}\int_\Omega K(x-y)u(y)\mathrm{d}y$
Discretization: $\lambda u_n - N^{-d}\sum_{m,n\in\omega^N m\neq n} K(x_n - x_m)u_m = f_n, n \in \omega^N$
$\Omega \subset \mathbb{R}^d$ is a bounded domain and $\omega^n = \{n \in \mathbb{Z}^d | x_n \in \Omega\}$
System matrix

$$T^N = (t_{mn})_{m,n\in\omega^N = \mathbb{Z}^d \cap N\Omega}, \quad t_{mn} = \begin{cases} N^{-d}K(x_m - x_n) = K(m-n), & m \neq n \\ 0, & m = n \end{cases}$$

Analysis ($\kappa = 0$): Toeplitz structure

The elements of t_{mn} of the system matrix are independent of N.
Let $T^\infty = (K(m-n))_{m,n\in\mathbb{Z}^d}, \quad K(0) = 0.$
T^N is Finite Section of the infinite block Toeplitz matrix.
Diagonalization via Fourier series leads to symbol

$$\tilde{t}(\xi) = \sum_{m\neq 0} K(m) e^{im.\xi}$$

Parseval and convolution theorems for Fourier series:

$$(u, T^N u)_{l^2(\omega^N)} = (2\pi)^{-d} \int_Q \overline{\tilde{u}}^T(\xi)\tilde{t}(\xi)\tilde{u}(\xi)\mathrm{d}\xi$$

Lemma

$$W(T^N) \subset W(T^\infty) \subset \overline{\text{conv}} \cup_{\xi\in Q} W(t(\tilde{\xi}))$$

Fourier series is not absolutely convergent. ⚠
Are there some bounds for $\tilde{t}(\xi)$?

Recall Poisson summation formula:

$$\sum_{m\in\mathbb{Z}^d} f(m)\exp(\mathrm{i}m.t) = \sum_{n\in\mathbb{Z}^d} \mathscr{F}\{f\}(t+2n\pi)$$

then

$$\tilde{t}(\xi) = \sum_{n\in\mathbb{Z}^d} \sigma(\xi+2n\pi) \text{ for } \sigma(\xi) = \mathscr{F}\{K\}(\xi) = \frac{\xi\xi^T}{|\xi|^2}.$$

$\sigma(\xi)$ is homogeneous of degree zero (the kernel is homogenous of degree $-d$), we have thus replaced a slowly converging Fourier series by a lattice sum that does not converge at all ⚠

Remedy for slowly converging or diverging lattice sums: Ewald's method.

EWALD, PAUL PETER Ewald summation. *Ann. Phys, 369, pp. 1–2*, (1921).

The idea is to split f into $f = f^F + f^p$ such that f^F and Fourier transform of f^P are rapidly decreasing at infinity.

Thus the Fourier series for f^F is absolutely convergent and the Poisson sum for f^P is also absolutely convergent, hence

$$\sum_{m\in\mathbb{Z}^d} f(m)e^{\mathrm{i}m.t} = \sum_{m\in\mathbb{Z}^d} f^F(m)e^{\mathrm{i}m.t} + \sum_{k\in\mathbb{Z}^d} \mathscr{F}\{f^P\}(\xi + 2\pi k)$$

and both sums on the right converge absolutely and boundedness of $\mathscr{F}\{f\}$ follows. Applying this for $f(x) = K(x)$, Theorem A is proved:

Theorem A

There exits an interval $\Sigma := [\Lambda_-, \Lambda_+]$ such that $\Sigma = \cup_{N\in\mathbb{N}} W(T_0^N)$. Then for $\lambda \in \mathbb{C} \setminus \Sigma$, DDA metod $(\lambda\mathbb{I} - T_0^N)u = f$ is l^2-stable and

$$\|(\lambda\mathbb{I} - T_0^N)^{-1}\| \leq \frac{1}{\mathrm{dist}(\lambda, \Sigma)}.$$

Details for the case $d = 3$: We write

$$K_\kappa(x) = -(D^2 + \kappa^2)G_\kappa(x) = (K_{\kappa,ij})_{i,j=1,2,3}$$

as integral (Mellin transform) of Gaussians

$$K_\kappa(x) = (K_{\kappa,ij})_{i,j=1,2,3},$$

with

$\frac{1}{2\pi^{d/2}} \int_0^\infty (2z^2\delta_{ij} - 4z^4 x_i x_j - \kappa^2\delta_{ij}) z^{d-1} \exp(-|x|^2 z^2 + \frac{\kappa^2}{4z^2}) \mathrm{d}z, \quad \mathrm{Re}\,\kappa^2 < 0$

For $\beta > 0$, we split the integral over z at $z = \beta$:

$$K_\kappa = K_\kappa^F + K_\kappa^P,$$

with

$$K_{\kappa,ij}^F = \frac{1}{2\pi^{3/2}} \int_{\beta^2}^\infty (2z^2\delta_{ij} - 4z^4 x_i x_j - \kappa^2\delta_{ij}) z^2 \exp(-|x|^2 z^2 + \frac{\kappa^2}{4z^2}) \mathrm{d}z.$$

It is shown that

$$K^F_{\kappa,ij}(x) = \frac{1}{4\pi^{3/2}} \sum_{q=0}^{\infty} \frac{(\kappa/2)^{2q}}{q!} (-4\beta^{4-2q} \frac{x_i x_j}{|x|^2} + ((2-4q)\delta_{ij} - 4(3/2-q)\frac{x_i x_j}{|x|^2}) I(3/2-q, \beta^2, r^2))$$

where $I(m,x,z) = z^{-m}\Gamma(m,zx)$.
For K^P_κ, we use the Fourier transformed (Poisson summation formula)

$$\mathscr{F}\{K^P_\kappa\}(\xi) = \frac{\xi\xi^T - \kappa^2 \mathbb{I}_d}{|\xi|^2 - \kappa^2} \exp(\frac{-|\xi|^2 + \kappa^2}{4\beta^2})$$

and $K^F_\kappa(0) = -K^P_\kappa(0)$ get the final Ewald summation:

$$F^N_\kappa(t) = \sum_{m\in\mathbb{Z}^d\setminus\{0\}} K_{\kappa/N}(m) e^{im.t} = \sum_{m\in\mathbb{Z}^d} K^F_{\kappa/N}(m) e^{im.t} + \sum_{n\in\mathbb{Z}^d} \mathscr{F}\{K^P_{\kappa/N}\}(t+2\pi n)$$

Homogenity: $\sigma_{\rho\kappa}(\rho\xi) = \sigma_\kappa(\xi)$ leads to $N^{-d}K_\kappa(m/N) = K_{\kappa/N}(m)$.

Ewald method in 3D: $\kappa = 0$

It is shown that

$$K^F_{\kappa,ij}(x) = \frac{1}{4\pi^{3/2}} \sum_{q=0}^{\infty} \frac{(\kappa/2)^{2q}}{q!} \Big(-4\beta^{4-2q} \frac{x_i x_j}{|x|^2} + ((2-4q)\delta_{ij} - 4(3/2-q)\frac{x_i x_j}{|x|^2}) I(3/2-q, \beta^2, r^2)\Big)$$

where $I(m,x,z) = z^{-m}\Gamma(m,zx)$.
For K^P_{κ}, we use the Fourier transformed (Poisson summation formula)

$$\mathscr{F}\{K^P_\kappa\}(\xi) = \frac{\xi\xi^T - \kappa^2 \mathbb{I}_d}{|\xi|^2 - \kappa^2} \exp\Big(\frac{-|\xi|^2 + \kappa^2}{4\beta^2}\Big)$$

It is now evident that both the Fourier sum with K^F and the lattice sum with K^P converge exponentially.

The characteristic function $\tilde{t}$ is a bounded 2π-periodic function on $\mathbb{R}^3$ whose values are real symmetric 3×3 matrices of trace 0 with elements

$$\tilde{t}_{ij}(\xi) = \sum_{m_1,m_2,m_3=-M}^{M} \frac{1}{4\pi^{3/2}}\left(-4\beta^4\frac{x_i x_j}{|x|^2} + (2\delta_{ij} - 6\frac{x_i x_j}{|x|^2})I(3/2,\beta^2,r^2)\right)e^{\mathrm{i}m.\xi}$$

$$+ \sum_{n_1,n_2,n_3=-N}^{N} \frac{(\xi_j + 2\pi n_j)(\xi_i + 2\pi n_i)}{|\xi + 2\pi n|^2} e^{-\frac{-|\xi+2n\pi|^2}{4\beta^2}} + R_{ij}^{(MN)}(\xi)$$

where in the first sum in the term with $m = (0,0,0)$ is understood to be $-(\frac{\beta}{\sqrt{\pi}})^3$. As $M, N \to \infty$, the remainders $R^{(MN)}$ converge to zero uniformly exponentially fast.

Lemma

$\tilde{t}_\kappa(\xi) = \sigma_\kappa(\xi) + v(\kappa,\xi)$ where v is continuous on $B_\pi(0) \times Q$ and

$$v(\kappa,\xi) = -\frac{1}{d} + \mathcal{O}(\kappa^2)$$

To bound $W(\sigma_\kappa(\xi))$, we notice that

$$\sigma_\kappa(\xi) = \frac{\xi\xi^T - \kappa^2\mathbb{I}_d}{|\xi|^2 - \kappa^2} = \mathbb{I}_d + \frac{|\xi|^2}{\kappa^2 - |\xi|^2}(\mathbb{I}_d - \frac{\xi\xi^T}{|\xi|^2})$$

so $W(\sigma_\kappa(\xi)) = \{1\} + \frac{|\xi|^2}{\kappa^2 - |\xi|^2}[0,1]$
Bound depending on arg $\kappa(-\pi,\pi) \setminus \{0\}$ lead to Theorem B

Lemma: Plane wave representation for the imaginary part

$$\text{Im } G_\kappa(x) = \frac{\kappa^{d-2}}{2^{d+1}\pi^{d-1}} \int_{\mathbb{S}^{d-1}} e^{\mathrm{i}\kappa\xi.x} \mathrm{d}s(\xi)$$

$$\text{Im } K_\kappa(x) = \frac{\kappa^{d-2}}{2^{d+1}\pi^{d-1}} \int_{\mathbb{S}^{d-1}} (\xi\xi^T - \mathbb{I}_d) e^{\mathrm{i}\kappa\xi.x} \mathrm{d}s(\xi)$$

Let $F(u(\xi)) := \sum_{m\in\omega_N} (u_m - (u_m.\xi)\xi) \exp(-\mathrm{i}\kappa\xi.m)$, then

$$\langle \bar{u}, \text{Im}\, T_\kappa^N u \rangle = \frac{-\kappa^d}{2^{d+1}\pi^{d-1}} \int_{\mathbb{S}^{d-1}} |F(u(\xi))|^2 \mathrm{d}s(\xi) + \mu_+(\kappa)\|u\|_{l^2}^2$$

and $0 \leq |\tilde{u}(\xi)|^2 \leq |\omega^N| \|u\|_{l^2}^2$ results Theorem C.

- M.Costabel, M. Dauge, K. Nedaiasl: Stability analysis of the DDA for Dielectric Scattering. *Oberwolfach Reports (vol. 43)*, (2022) 70-73.
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