SYMBOL-BASED ANALYSIS OF (TWO RELATED) MULTIGRID METHODS FOR ELECTROMAGNETIC SCATTERING PROBLEMS

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OVERVIEW

- Introduction to symbols and Toeplitz matrices
- Electromagnetic scattering problems
- Multigrid with finite elements
- Multigrid with the finite integration technique
- Outlook and perspective

THE SYMBOL

Take some 2π-periodic function $f(\theta) = \sum_{k \in \mathbb{Z}} \hat{f}_k e^{ik\theta}$ (the symbol) and construct the $n \times n$ Toeplitz matrix

$$T_n(f) = \begin{bmatrix} \hat{f}_0 & \hat{f}_{-1} & \cdots & \hat{f}_{-k} & \cdots & \cdots & \hat{f}_{-n+1} \\ \hat{f}_1 & \hat{f}_0 & \ddots & & \ddots & & \vdots \\ \vdots & \ddots & \ddots & \ddots & & \ddots & \vdots \\ \hat{f}_k & & \ddots & \ddots & \ddots & & \hat{f}_{-k} \\ \vdots & \ddots & & \ddots & \ddots & \ddots & \vdots \\ \vdots & & \ddots & & \ddots & \hat{f}_0 & \hat{f}_{-1} \\ \hat{f}_{n-1} & \cdots & \cdots & \hat{f}_k & \cdots & \hat{f}_1 & \hat{f}_0 \end{bmatrix} = \sum_{k \in \mathbb{Z}} J_n^{(k)} \cdot \hat{f}_k$$

In practice, we will often work with (real-valued) trigonometric polynomials and thus with banded matrices.

ONE LEVEL UP

Take the symbol

$$g(\underline{\theta}) = g(\theta_1, \theta_2) = \sum_{\underline{k} \in \mathbb{Z} \times \mathbb{Z}} \hat{g}_{\underline{k}} e^{ik_1\theta_1 + ik_2\theta_2}$$

and define the 2-level $\underline{n} \times \underline{n} = (n_1, n_2) \times (n_1, n_2)$ Toeplitz matrix as

$$\begin{aligned} T_{\underline{n}}(g) &= \sum_{\underline{k} \in \mathbb{Z} \times \mathbb{Z}} J_{n_1}^{(k_1)} \otimes J_{n_2}^{(k_2)} \cdot \hat{g}_{\underline{k}} \\ &= \sum_{\underline{k} \in \mathbb{Z} \times \mathbb{Z}} J_{\underline{n}}^{\underline{k}} \cdot \hat{g}_{\underline{k}} \end{aligned}$$

MATRIX-VALUED SYMBOLS

Consider the matrix-valued symbol symbol $\mathbf{h} : [-\pi, \pi]^d \to \mathbb{C}^{s\times s}$ defined by

$$\mathbf{h}(\underline{\theta}) = \sum_{\underline{k}\in\mathbb{Z}\times\mathbb{Z}} \hat{\mathbf{h}}_{\underline{k}} e^{i\underline{k}\cdot\underline{\theta}}$$

and define the d-level $\underline{n} \times \underline{n}$ block-Toeplitz matrix as

$$T_{\underline{n}}(\mathbf{h}) = \sum_{\underline{k}\in\mathbb{Z}\times\mathbb{Z}} J_{\underline{n}}^{\underline{k}} \otimes \hat{\mathbf{h}}_{\underline{k}}$$

A SIMPLE EXAMPLE

Let $g(\theta_1, \theta_2) = 4 - 2\cos\theta_1 - 2\cos\theta_2 = 4 - e^{-i\theta_1} - e^{i\theta_1} - e^{-i\theta_2} - e^{i\theta_2}$.

Then the $(4,3) \times (4,3)$ matrix $T_{(4,3)}(g)$ is given by

$$
\left[\begin{array}{ccc:ccc:ccc:ccc}
4 & -1 & & -1 & & & & & & & & \\
-1 & 4 & -1 & & -1 & & & & & & & \\
 & -1 & 4 & & & -1 & & & & & & \\
\hdashline
-1 & & & 4 & -1 & & -1 & & & & & \\
 & -1 & & -1 & 4 & -1 & & -1 & & & & \\
 & & -1 & & -1 & 4 & & & -1 & & & \\
\hdashline
 & & & -1 & & & 4 & -1 & & -1 & & \\
 & & & & -1 & & -1 & 4 & -1 & & -1 & \\
 & & & & & -1 & & -1 & 4 & & & -1 \\
\hdashline
 & & & & & & -1 & & & 4 & -1 & \\
 & & & & & & & -1 & & -1 & 4 & -1 \\
 & & & & & & & & -1 & & -1 & 4
\end{array}\right]
$$

- Corresponds to the 2-D Laplace operator with homogeneous boundary conditions on a 4×3 grid.
- Symbol is equivalent to the 5-point stencil:

$$
\begin{array}{ccc}
 & -1 & \\
-1 & 4 & -1 \\
 & -1 &
\end{array}
$$

- The symbol allows analysis of the spectrum.

SPECTRAL DISTRIBUTION OF MATRIX SEQUENCES

Definition

Let f be a trigonometric polynomial. A matrix sequence $\{A_n\}_n$ is said to be *spectrally distributed according to* f if, for all $G \in C_c(\mathbb{C})$,

$$\lim_{n\to\infty} \frac{1}{n} \sum_{j=1}^{n} G(\lambda_j(A_n)) = \frac{1}{2\pi} \int_{-\pi}^{\pi} G\big(f(\theta)\big) \mathrm{d}\theta.$$

In that case, we write $\{A_n\}_n \sim_\lambda f$.

SPECTRAL DISTRIBUTION EXPLAINED

$$\lim_{n\to\infty} \frac{1}{n} \sum_{j=1}^{n} G(\lambda_j(A_n)) = \frac{1}{2\pi} \int_{-\pi}^{\pi} G\big(f(\theta)\big) \mathrm{d}\theta.$$

Assume that $\lambda_j, f(\theta) \in \mathbb{R}$ and let

$$G(x) = \begin{cases} 1 & x \in [a, b], \\ 0 & \text{otherwise.} \end{cases}$$

Then:

- LHS: the proportion of eigenvalues of A_n in $[a, b]$
- RHS: the proportion of the domain $[-\pi, \pi]$ where the values of f lie in $[a, b]$.
- A sampling of the generating function f gives an approximation of the eigenvalues of A_n as $n \to \infty$.

SPECTRAL DISTRIBUTION OF TOEPLITZ MATRICES

Theorem (Szegő's First Limit Theorem)[1]

If f is a *univariate real-valued* trigonometric polynomial, then $\{T_n(f)\}_n \sim_\lambda f$.

[1]Grenander and Szegő, Toeplitz Forms and Their Applications, (1958).

EIGENVALUE DISTRIBUTION OF MULTILEVEL BLOCK-TOEPLITZ SEQUENCES

Definition

Let $\mathbf{h}(\underline{\theta}) : [-\pi, \pi]^d \to \mathbb{C}^{s\times s}$ be a multivariate matrix-valued trigonometric polynomial. Then a matrix sequence $\{A_{\underline{n}}\}_{\underline{n}}$ is said to be spectrally distributed according to $\mathbf{h}$ if, for all $G \in C_c(\mathbb{C})$,

$$\lim_{\underline{n}\to\infty} \frac{1}{s\cdot n_1\cdots n_d} \sum_{j=1}^{s\cdot n_1\cdots n_d} G(\lambda_j(A_n)) = \frac{1}{(2\pi)^d} \int_{[-\pi,\pi]^d} \frac{1}{s} \sum_{j=1}^{s} G\Big(\lambda_j\big(\mathbf{h}(\underline{\theta})\big)\Big) \mathrm{d}\underline{\theta}.$$

In that case, we write $\{A_{\mathbf{n}}\}_{\mathbf{n}} \sim_\lambda \mathbf{f}$.

Theorem[2]

If $\mathbf{h}$ is *Hermitian-valued*, then $\{T_n(\mathbf{h})\}_n \sim_\lambda \mathbf{h}$.

[2] Tilli, “A note on the spectral distribution of toeplitz matrices”, (1998).

ELECTROMAGNETIC SCATTERING PROBLEMS

MAXWELL'S EQUATIONS

We consider the scattering of electromagnetic waves within a bounded cavity $\Omega \in \mathbb{R}^3$ of linear isotropic material with perfectly conducting walls. The Maxwell equations lead to the following system of equations for the electric field $\mathbf{E} = \mathbf{E}(\mathbf{x}, t)$ and the magnetic field $\mathbf{H} = \mathbf{H}(\mathbf{x}, t)$.

$$\begin{aligned} \epsilon \frac{\mathrm{d}}{\mathrm{d}t}\mathbf{E} + \sigma\mathbf{E} - \mathbf{curl}\ \mathbf{H} = \mathbf{j} &\quad \text{in } \Omega \times [0, T] \\ \mu \frac{d}{dt}\mathbf{H} + \mathbf{curl}\ \mathbf{E} = 0 &\quad \text{in } \Omega \times [0, T] \\ \mathbf{E} \times \mathbf{n} = 0 &\quad \text{on } \partial\Omega \end{aligned}$$

By eliminating the magnetic field from Maxwell's equations and employing an implicit time-stepping scheme, we are left with a (space-continuous) problem:

$$\begin{aligned} \frac{1}{4}\Delta t^2 \mathbf{curl}\left(\frac{1}{\mu}\mathbf{curl}\ \mathbf{E}_n\right) + \left(\epsilon + \frac{1}{2}\sigma\Delta t\right)\mathbf{E}_n = \text{r.h.s} &\quad \text{in } \Omega, \\ \mathbf{E}_n \times \mathbf{n} = 0 \qquad &\quad \text{on } \partial\Omega. \end{aligned}$$

FINITE ELEMENT FORMULATION

The problem can be cast into a weak form by defining the Hilbert space

$$\mathbf{H}_0(\mathbf{curl}, \Omega) := \left\{ \eta \in \mathbf{L}^2(\Omega); \mathbf{curl}\eta \in \mathbf{L}^2(\Omega); \eta \times \mathbf{n} = 0 \text{ on } \partial\Omega \right\},$$

resulting in the following variational problem:

Find $\mathbf{E} \in \mathbf{H}_0(\mathbf{curl}, \Omega)$ such that $\forall \xi \in \mathbf{H}_0(\mathbf{curl}, \Omega)$,

$$(\alpha \mathbf{curl}\mathbf{E}, \mathbf{curl}\xi)_{\mathbf{L}^2(\Omega)} + (\beta \mathbf{E}, \xi)_{\mathbf{L}^2(\Omega)} = f(\xi).$$

To discretise the variational formulation in space, we use *Nédélec elements* (of the first kind, of order 1) on a regular hexahedral grid. They

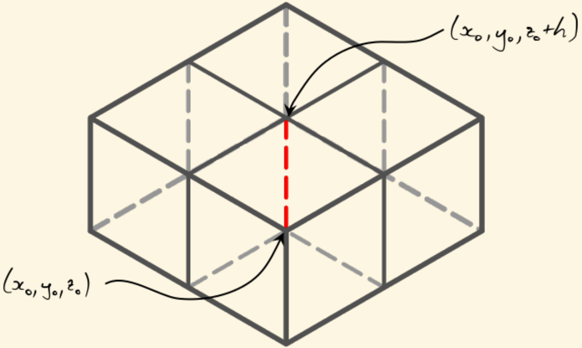
- are $\mathbf{H}(\mathbf{curl}, \Omega)$-conforming,
- ensure tangential continuity across element boundaries and
- are called "edge elements".

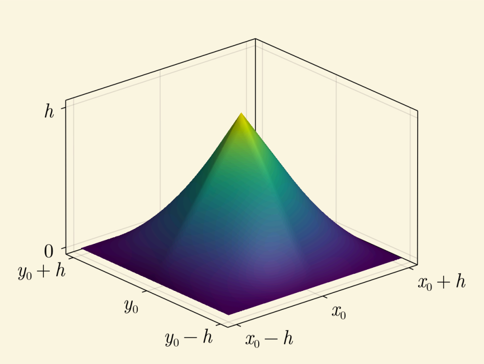
DISCRETISATION WITH NÉDÉLEC ELEMENTS

Degrees of freedom: line integrals along the edges e of the grid $\boldsymbol{\xi} \mapsto \int_e \boldsymbol{\xi}(\mathbf{r}) \cdot \mathrm{d}\mathbf{r}$.

For an edge extending from (x_0, y_0, z_0) to $(x_0, y_0, z_0 + h)$, the corresponding basis function is given by

$$\xi(x,y,z) = \frac{1}{h} \begin{pmatrix} 0 \\ 0 \\ (1 - \frac{1}{h}|x - x_0|)(1 - \frac{1}{h}|y - y_0|) \end{pmatrix} \qquad \text{if} \qquad \begin{matrix} x_0 - h \leq & x & \leq x_0 + h, \\ y_0 - h \leq & y & \leq y_0 + h, \\ z_0 \quad \leq & z & \leq z_0 + h, \end{matrix}$$





STRUCTURED STIFFNESS MATRIX

- The stiffness matrix of the finite element formulation can almost be represented by a multilevel block-Toeplitz matrix.
- A small-rank correction is needed to account for the boundary condition.
- The symbol which generates this matrix has two terms corresponding to the two terms in the bi-linear form of the variational formulation.

$$\mathbf{f}(\underline{\theta}) + h^2\mathbf{g}(\underline{\theta})$$

$$= \frac{\alpha}{3}\begin{bmatrix} 9-(1+2\cos(\theta_2))(1+2\cos(\theta_3)) & -2\left(1-e^{-i\theta_1}\right)\left(1-e^{i\theta_2}\right)\left(1+\frac{1}{2}\cos(\theta_3)\right) & -2\left(1-e^{-i\theta_1}\right)\left(1-e^{i\theta_3}\right)\left(1+\frac{1}{2}\cos(\theta_2)\right) \\ -2\left(1-e^{i\theta_1}\right)\left(1-e^{-i\theta_2}\right)\left(1+\frac{1}{2}\cos(\theta_3)\right) & 9-(1+2\cos(\theta_1))(1+2\cos(\theta_3)) & -2\left(1-e^{-i\theta_2}\right)\left(1-e^{i\theta_3}\right)\left(1+\frac{1}{2}\cos(\theta_1)\right) \\ -2\left(1-e^{i\theta_1}\right)\left(1-e^{-i\theta_3}\right)\left(1+\frac{1}{2}\cos(\theta_2)\right) & -2\left(1-e^{i\theta_2}\right)\left(1-e^{-i\theta_3}\right)\left(1+\frac{1}{2}\cos(\theta_1)\right) & 9-(1+2\cos(\theta_1))(1+2\cos(\theta_2)) \end{bmatrix}$$

$$+ \frac{4\beta h^2}{9}\begin{bmatrix} \left(1+\frac{1}{2}\cos\theta_2\right)\left(1+\frac{1}{2}\cos\theta_3\right) & & \\ & \left(1+\frac{1}{2}\cos\theta_1\right)\left(1+\frac{1}{2}\cos\theta_3\right) & \\ & & \left(1+\frac{1}{2}\cos\theta_1\right)\left(1+\frac{1}{2}\cos\theta_2\right) \end{bmatrix}$$

SPECTRAL DISTRIBUTION

The stiffness matrix $A_\mathbf{n}$ can be written as

$$\begin{aligned} A_n &= T_n(\mathbf{f}) + h^2 T_n(\mathbf{g}) + R_n \\ &= F_n + h^2 G_n + R_n \end{aligned}$$

where

- $T_n(\mathbf{f})$ is the part generated by the main part of the generating symbol,
- $||h^2 T_n(\mathbf{g})||_2 \rightarrow 0$ as $n \rightarrow \infty$, and
- R_n is a small-rank matrix as $n \rightarrow \infty$ and results from the boundary condition.

From the theory of locally Toeplitz matrices, it follows that $A_n \sim_\lambda \mathbf{f}$. This characterisation is not enough when analysing the multigrid methods.

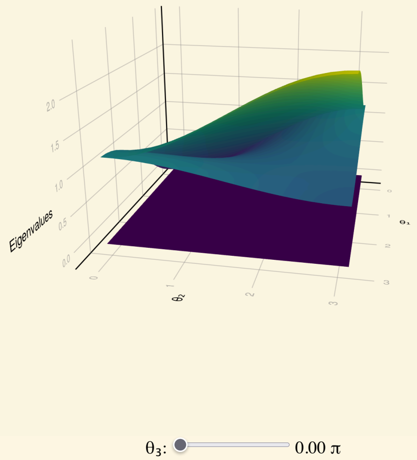
EIGENVALUES OF THE MAIN SYMBOL

We can explicitly compute the eigenvalues of the symbol $f(\underline{\theta})$, which again are functions of $\underline{\theta}$.

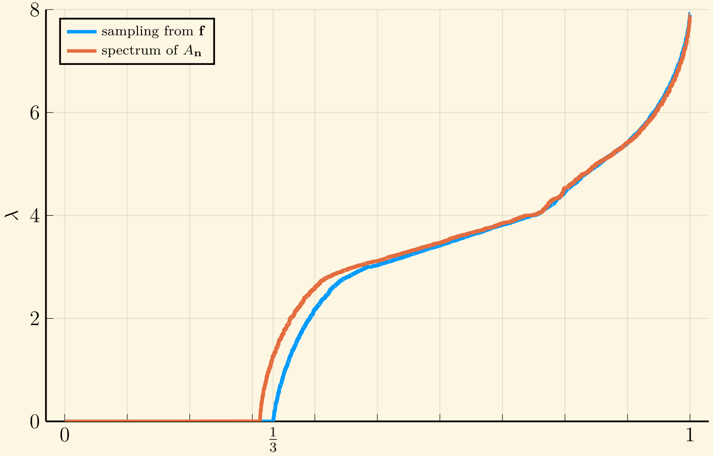
$$\lambda_0(\underline{\theta}) \equiv 0$$
$$\lambda_+(\underline{\theta}) = b(\underline{\theta}) + \sqrt{d(\underline{\theta})}$$
$$\lambda_-(\underline{\theta}) = b(\underline{\theta}) - \sqrt{d(\underline{\theta})}$$

- Invariant under permutation of θ_i.
- Even in all θ_i.
- The eigenvector corresponding to λ_0 is

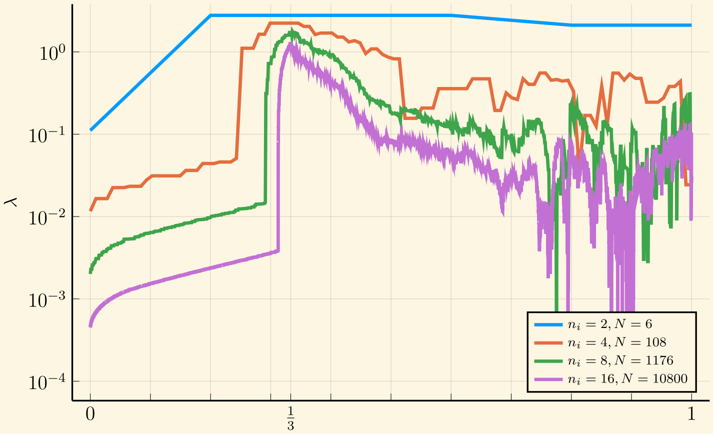
$$\begin{bmatrix} 1 - e^{-i\theta_1} \\ 1 - e^{-i\theta_2} \\ 1 - e^{-i\theta_3} \end{bmatrix}$$



SAMPLING OF THE SYMBOL (N = 10800)



SAMPLING OF THE SYMBOL



HIPTMAIR METHOD

The *two-grid method* iteratively approximates the solution to $A_n x_n = b_n$ as follows:

1. $\tilde{x}_n \leftarrow \mathcal{V}_{n,\text{pre}}(A_n, b_n, x_n^{(j)})$	pre-smoothing
2. $r_n \leftarrow b_n - A_n \tilde{x}_n$	residual
3. $r_k \leftarrow P_{n,k}^H r_n$	restrict residual to coarse grid
4. $A_k = P_{n,k}^H A_n P_{n,k}$	restrict operator to coarse grid
5. Solve $A_k y_k = r_k$	exact solve
6. $\hat{x}_n \leftarrow \tilde{x}_n + P_{n,k} y_k$	prolongate correction to fine grid
7. $x_n^{(j+1)} \leftarrow \mathcal{V}_{n,\text{post}}(A_n, b_n, \hat{x}_n)$	post-smoothing

Multigrid method: recursively applying the algorithm at step 5.

- The simple smoothers (Gauss-Seidel, Richardson), work poorly for our problem.
- Hiptmair developed a problem-specific smoother[3] to remedy convergence issues.

[3] Hiptmair, "Multigrid method for Maxwell's equations", (1998).

ITERATION MATRIX FOR THE HIPTMAIR SMOOTHER

1. Stationary iteration on $A_n x_n = b_n$ — on original space
2. $\rho_n \leftarrow b_n - A_n x_n$ — residual
3. $\tilde{\rho}_n \leftarrow T_n^H \rho$ — transfer to problematic subspace
4. $y_n \leftarrow 0$
5. Stationary iteration on $\Delta_n y_n = \tilde{\rho}$ — on problematic subspace
6. return $x_n + T_n \tilde{\rho}$ — add correction term

Gauss-Seidel is commonly used. Since we have good spectral information about A (and Δ), we can also use the modified Richardson method.

The Hiptmair smoother is again a stationary method. The Richardson method allows for easier symbolic analysis of the iteration matrix V:

$$V = I - (\omega_1 T D_\Delta^{-1} T^H G + \omega_2 D_A^{-1} A)$$

T is generated by the eigenvector $[1 - e^{-i\theta_1}, 1 - e^{-i\theta_2}, 1 - e^{-i\theta_3}]^T$ corresponding to λ_0.

ITERATION MATRIX FOR THE TWO-GRID METHOD

The iteration matrix for the two-grid method is given by

$$V_n \left(I - P_{n,k}(P_{n,k}^H A_n P_{n,k})^{-1} P_{n,k}^H\right) V_n.$$

With the usual (geometric) prolongation operator $P_{n,k}$, the symbol-based structure is preserved on the coarse grid:

$$P_{n,k}^H A_n P_{n,k} = F_k + h^2 G_k + R_k.$$

Because of the large null space of F, the term G is important in the inverse $(P_{n,k}^H A_n P_{n,k})^{-1}$:

$$(F + h^2 G)^{-1} = F^\dagger - F^\dagger G T (T^H G T)^{-1} T^H + \frac{1}{h^2} T (T^H G T)^{-1} T^H + \mathcal{O}(h^2)$$

This is challenging for the existing approaches to symbol-based analysis.

FINITE INTEGRATION TECHNIQUE

FIT

The finite integration technique[4] (FIT) uses

- the integral forms of Maxwell's equations and
- topological properties of the discretisation grid and its dual

to solve directly for integral quantities like:

- voltages along edges: $\hat{e} = \int_e \mathbf{E}(\mathbf{r}, t) \cdot \mathrm{d}\mathbf{r}$
- electric current through faces: $\hat{\hat{j}} = \iint_A \mathbf{J}(\mathbf{r}, t) \cdot \mathrm{d}\mathbf{A}$

In our setting, this leads to the (time-continuous) equation

$$C^T M_\mu C \hat{e} + M_\kappa \frac{\mathrm{d}}{\mathrm{d}t} \hat{e} + + M_\epsilon \frac{\mathrm{d}^2}{\mathrm{d}t^2} \hat{e} = -\frac{\mathrm{d}}{\mathrm{d}t} \hat{\hat{j}},$$

which can be discretised with an implicit time-stepping scheme. The resulting system matrix again has the form

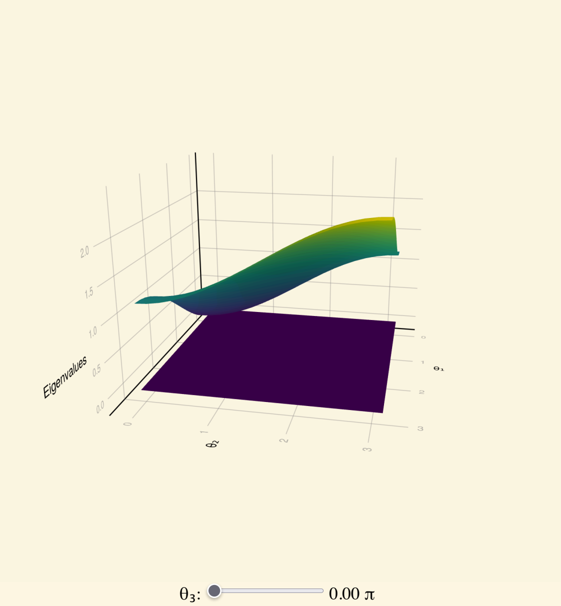
$$A'_n = T_n(\mathbf{f}') + h^2 T_n(\mathbf{g}') + R'_n.$$

[4]Weiland, "A Discretization Method for the Solution of Maxwell's Equations for Six-Component Fields", (1977).

SPECTRUM OF THE FIT OPERATOR

The eigenvalue functions are simpler than the finite element approach, but share characteristics.

$$\lambda_0(\underline{\theta}) \equiv 0$$
$$\lambda_1(\underline{\theta}) = \lambda_2(\underline{\theta}) = 6 - 2\cos\theta_1 - 2\cos\theta_2 - 2\cos\theta_3$$



OUTLOOK

We have a applied a symbol-based approach to analyse the spectrum of the system matrices and to provide a linear algebraic description of existing multigrid methods.

The goal is

- to consider different (non-geometric) prolongation and restriction operators and
- use a symbol-based approach to provide conditions for convergence of the resulting method.

The large null space of the dominant part of the system matrix prevents the direct application of existing symbol-based techniques[5].

[5]Bolten, Donatelli, Ferrari, Furci, "A symbol-based analysis for multigrid methods for block-circulant and block-Toeplitz systems", (2022).