Skoltech

Skolkovo Institute of Science and Technology

Computational Science and Engineering II: Discretization

Introduction to Integral Equation Methods

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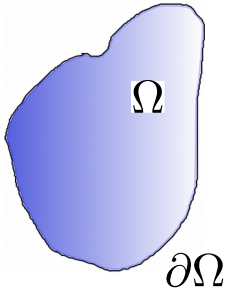
Skoltech, Moscow, 2018

What is an Integral Equation?

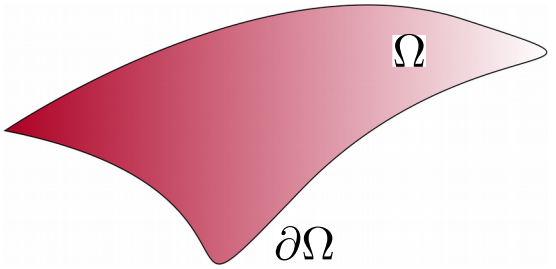
Unknown

$$\int_{\partial\Omega} \frac{q(x')}{|x-x'|}\,dx' = f(x), \quad x \in \partial\Omega$$

Simplest Integral Equation



Volume



Surface (Open or Closed)

The Green function

In general integral equations have the following form :

Green function

$$\int_{\partial\Omega} q(x')G(x-x')dx' = f(x), \quad x \in \partial\Omega$$

1) The Green function or fundamental solution of the respective PDE is the effect at the point **x** *from the source at point* **x'**.

2) The Green function can also incorporate the boundary conditions.

3) The Green function satisfies the following equation:

$$\mathcal{A}G(x-x') = \delta(x-x')$$

Where $\mathcal{A}$ *is the respective operator of the PDE*

We cannot find the analytical form of the Green function in every case!

Why Integral Equations?

- ***Automatically satisfy radiation conditions***
- *They allow higher-order approximations* $\quad \text{PWC} \rightarrow \text{PWL}$
- *We can do dimensionality reduction* $\quad \iiint \rightarrow \iint$
- *Unfortunately they are a very complex tool*
- *Dense matrices*
- ***In some cases the matrices are structured – Extreme memory compression***

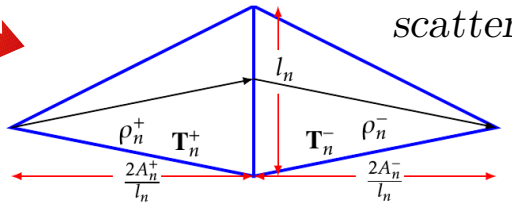
How to solve Integral Equations

***Discretization**: Select a finite-dimensional subspace, spanned by some basis function. Typically the basis functions are described over a mesh, meaning that one function can have a support of one (or more) element of the mesh.*

$$q(x') \approx \sum_{i=1}^{n} c_i \phi_i(x') \quad \text{where } c_i \text{ are the uknowns and } \phi_i \text{ are the basis functions}$$

Example

RWG basis function with common triangle edges as a support. Used for the approximation of the electric current on metallic scatterers



How to solve Integral Equations (II)

$$\int_{\partial\Omega} \frac{q(x')}{|x-x'|} dx' = f(x)$$

$$q(x') \approx \sum_{i=1}^{n} c_i \phi_i(x')$$

$$\sum_{i=1}^{N} q_i \int_{T_i} \frac{\phi_i(x')}{|x-x'|} dx' = f(x)$$

N is the number of elements

T_i is the support of ϕ_i

Two main methods exist:

1) ***Galerkin***

2) ***Petrov-Galerkin***

The idea is to find an appropriate set of ***testing functions*** *and project the above equation to it. With Galerkin method the testing functions are the same with the basis functions. In Petrov-Galerkin they are different.*

Galerkin Method

$$\sum_{i=1}^{N} q_i \int_{T_i} \frac{\phi_i(x')}{|x-x'|} dx' = f(x) \quad \longrightarrow \quad \sum_{i=1}^{N} q_i \int_{T_j} \int_{T_i} \frac{\phi_j(x)\phi_i(x')}{|x-x'|} dx'dx = \int_{T_j} f(x)\phi_j(x)dx$$

We project the testing functions ϕ_j with the Hilbert Space inner product

The scary equation it's a square system of linear equations $Aq = f$

The integral can be 4D (surfaces) or 6D (volume). Costly!

$$A_{ji} = \int_{T_j} \int_{T_i} \frac{\phi_j(x)\phi_i(x')}{|x-x'|} dx'dx \qquad f_j = \int_{T_j} f(x)\phi_j(x)dx$$

We can use LU,QR,SVD,GMRES,BICGSTAB,etc to solve it

Collocation Method

The testing functions are $\delta(x - x_j)$ and the basis functions are PWC

The square system can be simplified $\quad A_{ji} = \int\limits_{T_i} \frac{dx'}{|x - x'|}, \quad f_j = f(x_j)$

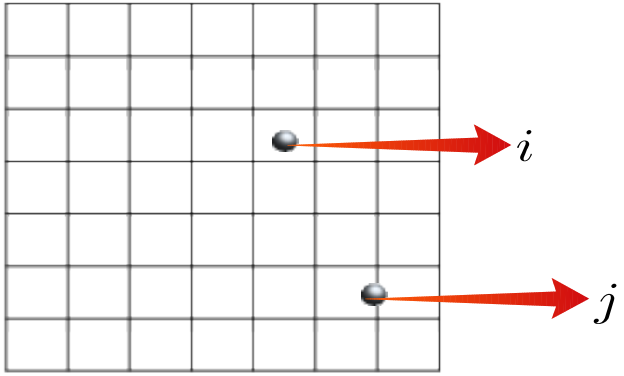
- The most common Petrov-Galerkin method.
- Each element is uniformly charged.
- Far simpler than Galerkin (the integral is 2D/3D)
- Not accurate enough since the basis and testing functions are specific

Nystrom Method

We can simplify even more our system with the so-called Nystrom method (simplification of the collocation method).

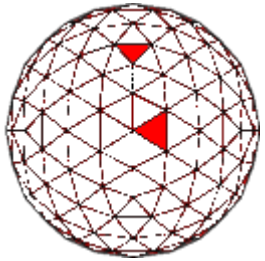
$$A_{ji} = \int_{T_i} \frac{dx'}{|x - x'|} \approx \frac{T_i}{|x_j - x_i'|} \text{ where } T_i \text{ is the area of the element}$$

If the x_j *is far away from* x_i *, then the approximation is good enough, otherwise it can be really bad. Therefore, we can apply the* ***locally corrected Nystrom method****, in which we use a different approximation in the close elements. Actually, we choose as a collocation point i, the center of the element and as j, the center of the side of the element. We can avoid singularities!*

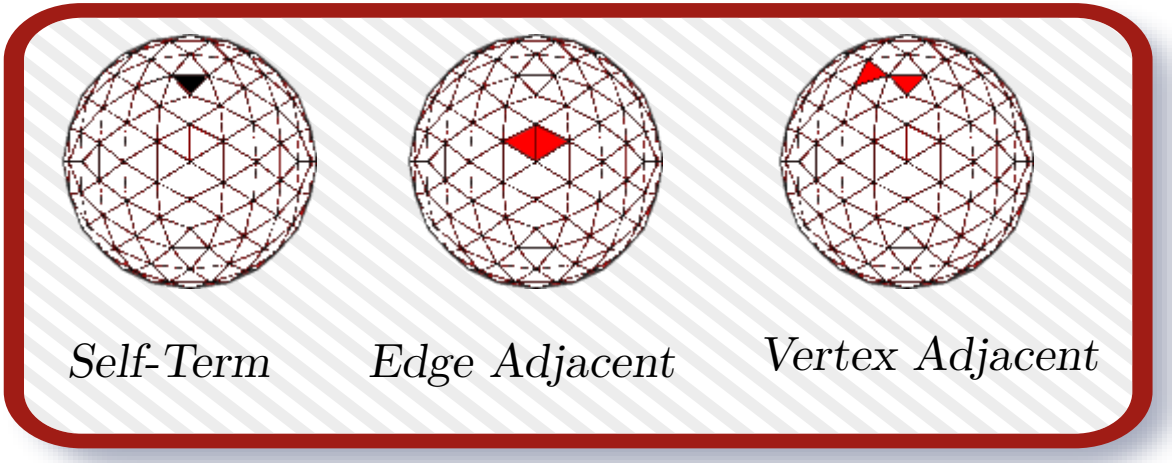


Computation of the Integrals

Consider the following cases with the Galerkin method



Classic Integration



Can be calculated analytically (impossible in many cases).
Or quadrature rules - trapezoidal integration.

All of these integrals are ***singular****. This is a very important topic about integral equations, and the appropriate calculation of these integrals is hard (more in CSE III). For now keep in mind the locally corrected Nystrom for these cases.*

An important property of IE

Example

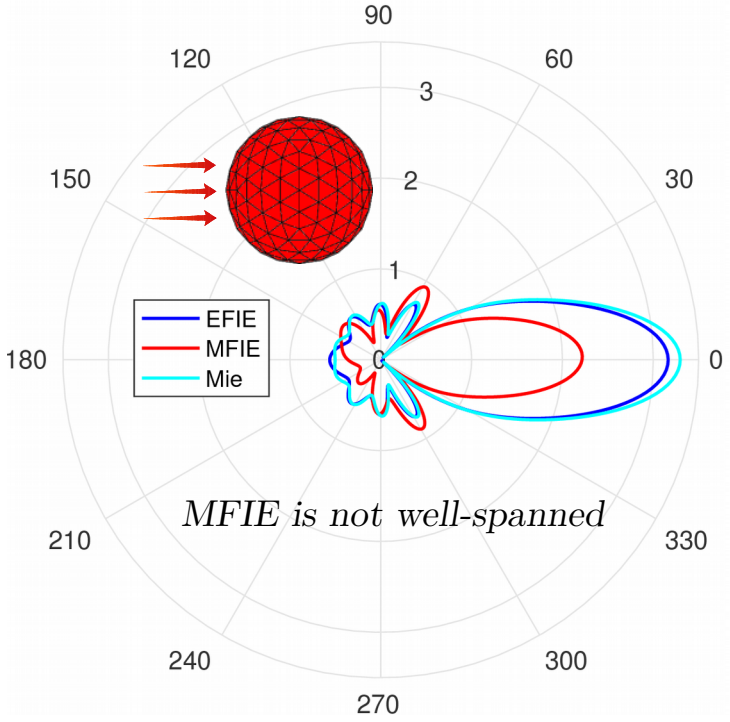
$$\text{EFIE:} 0 = \hat{n} \times \vec{E}_{inc}(\mathbf{r}) + j\omega\mu\hat{n} \times \int_S \bar{G}(\mathbf{r}, \mathbf{r}')\mathbf{J}_{eq}(\mathbf{r}')d\mathbf{r}'$$

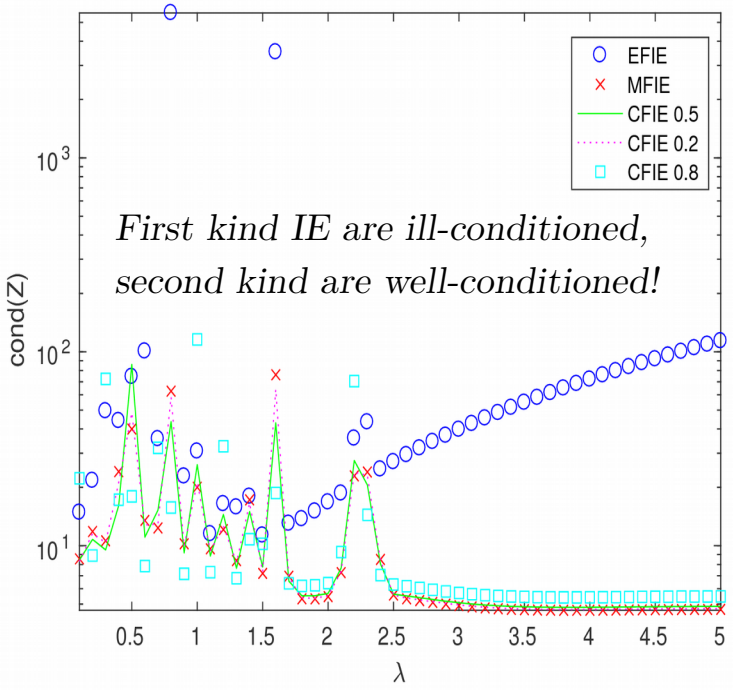
First Kind

Second Kind

$$\text{MFIE:} 0 = \hat{n} \times \vec{H}_{inc}(\mathbf{r}) - \frac{\mathbf{J}_{eq}(\mathbf{r}')}{2} + \hat{n} \times \nabla \times \int_{S-\delta S} \mathbf{J}_{eq}(\mathbf{r}') \times \nabla' g(\mathbf{r}, \mathbf{r}')d\mathbf{r}'$$

230 patches
Radius = 1
Wavelength = 1
RWG
DEMCEM





The condition number

The condition number measures how much the output value of a function can change if a small change in the input occurs

For a matrix A, the condition number is

$$\kappa(A) = ||A^{-1}|| \cdot ||A|| = \frac{\sigma_{\max}(A)}{\sigma_{\min}(A)}$$

$\kappa(A) = 10^k$ → *up to k digits of accuracy may be lost from the solution of a linear system $Ax = b$ with a direct solver (LU,SVD,QR,inverse,...)*

For iterative solvers the case is different, because the convergence rate is affected by the condition number!

$e_n \leq \kappa(A)^n$ → *Simplest Richardson iteration*

$$e_n \leq \left(\frac{\sqrt{\kappa(A)} - 1}{\sqrt{\kappa(A)} + 1} \right)^n$$ → *Chebyshev-accelerated Richardson iteration*

FFT-based Volume Integral Equations

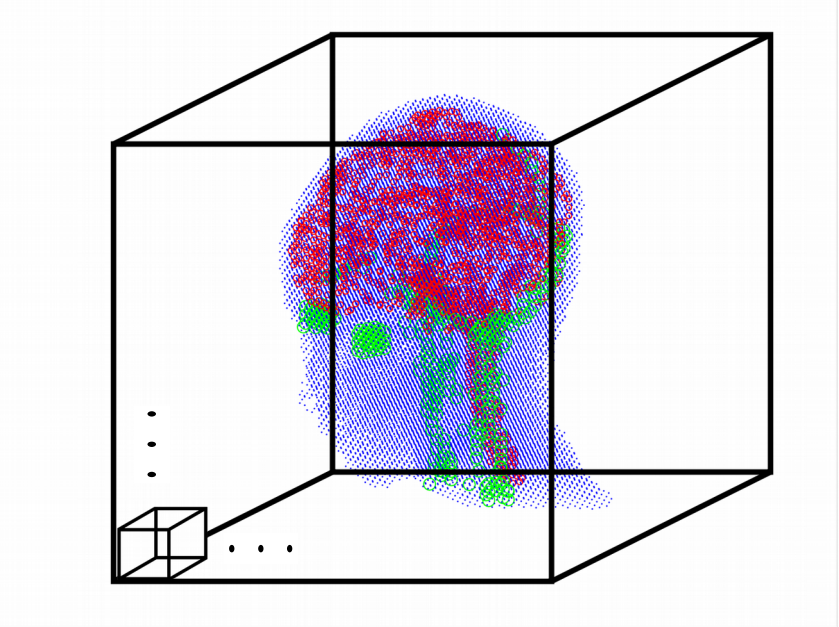
1) We want to solve more challenging problems, with millions of unknowns (n).

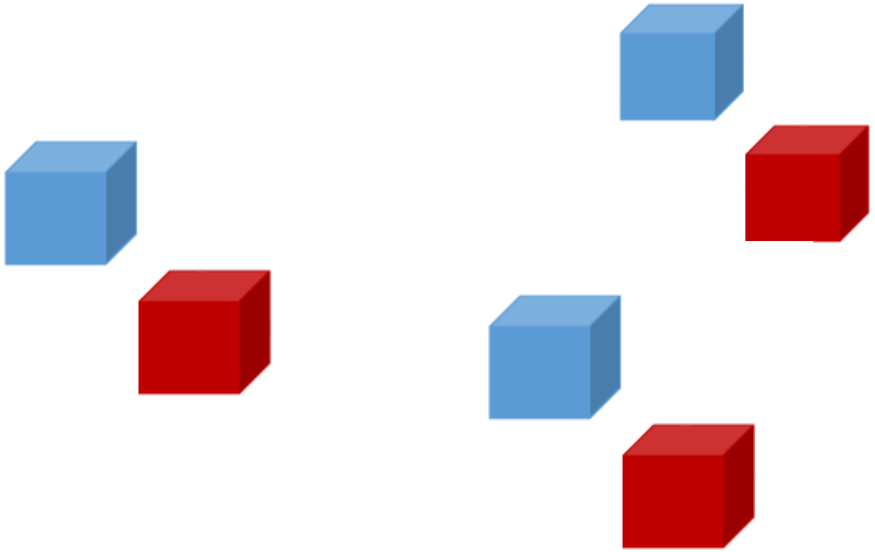
2) The Galerkin method leads to enormous dense matrices that require (in some cases) Peta Bytes $\mathcal{O}\{n^2\}$*!*

3) Even if we could store such matrices, it would be impossible to solve a linear system through LU decomposition $\mathcal{O}\{n^3\}$*!*

Toeplitz Structure

Let's see the special structure that the kernels of some integral equations have.





The Green function is the interaction between two separated elements. It is translationally invariant! This means that ***wherever*** *the two elements are placed their* ***interaction is the same****!*

The arising Galerkin matrix has a Toeplitz structure (Block Toeplitz with Toeplitz Blocks).

Back to Numerical Linear Algebra

Toeplitz

$$\begin{bmatrix} a_0 & a_{-1} & a_{-2} & \cdots & a_{-n+1} \\ a_1 & a_0 & a_{-1} & \cdots & \cdots \\ a_2 & a_1 & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ a_{n-1} & \cdots & \cdots & \cdots & a_0 \end{bmatrix}$$

Circulant

$$\begin{bmatrix} c_0 & c_{n-1} & c_{n-2} & \cdots & c_1 \\ c_1 & c_0 & c_{n-1} & \cdots & \cdots \\ c_2 & c_1 & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ c_{n-1} & \cdots & \cdots & \cdots & c_0 \end{bmatrix}$$

$$\mathcal{O}\{n^2\} \rightarrow \mathcal{O}\{n\}$$
$$\mathcal{O}\{n^3\} \rightarrow \mathcal{O}\{n \log n\}$$

Vector of unknowns

Element-wise product

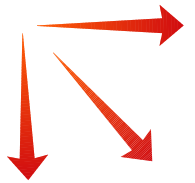
$$Cx = \text{ifft}\left(\text{fft}(c) \circ \text{fft}(x)\right)$$

Circulant matrix

Circulant defining vector. First row (or column of C matrix).
For 2D cases, the defining vector is formulated as a defining matrix, and for 3D as a defining tensor.

Circulant Embedding of Toeplitz Matrices

$$\begin{bmatrix} a_0 & a_{-1} & a_{-2} & \cdots & \cdots & a_{-n+1} \\ a_1 & a_0 & a_{-1} & \cdots & \cdots & \cdots \\ a_2 & a_1 & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & a_{-1} & a_{-2} \\ \cdots & \cdots & \cdots & a_1 & a_0 & a_{-1} \\ a_{n-1} & \cdots & \cdots & a_2 & a_1 & a_0 \end{bmatrix}$$



$$\begin{bmatrix} \begin{bmatrix} a_0 & a_{-1} & a_{-2} & \cdots & \cdots & a_{-n+1} \\ a_1 & a_0 & a_{-1} & \cdots & \cdots & \cdots \\ a_2 & a_1 & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & a_{-1} & a_{-2} \\ \cdots & \cdots & \cdots & a_1 & a_0 & a_{-1} \\ a_{n-1} & \cdots & \cdots & a_2 & a_1 & a_0 \end{bmatrix} & \begin{bmatrix} 0 & a_{n-1} & a_{-2} & \cdots & a_2 & a_1 \\ a_{-n+1} & \cdots & \cdots & \cdots & \cdots & a_2 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ a_{-2} & \cdots & \cdots & a_1 & a_0 & a_{n-1} \\ a_{-1} & a_{-2} & \cdots & \cdots & a_{-n+1} & 0 \end{bmatrix} \\ \begin{bmatrix} 0 & a_{n-1} & a_{-2} & \cdots & a_2 & a_1 \\ a_{-n+1} & \cdots & \cdots & \cdots & \cdots & a_2 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ a_{-2} & \cdots & \cdots & a_1 & a_0 & a_{n-1} \\ a_{-1} & a_{-2} & \cdots & \cdots & a_{-n+1} & 0 \end{bmatrix} & \begin{bmatrix} a_0 & a_{-1} & a_{-2} & \cdots & \cdots & a_{-n+1} \\ a_1 & a_0 & a_{-1} & \cdots & \cdots & \cdots \\ a_2 & a_1 & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & a_{-1} & a_{-2} \\ \cdots & \cdots & \cdots & a_1 & a_0 & a_{-1} \\ a_{n-1} & \cdots & \cdots & a_2 & a_1 & a_0 \end{bmatrix} \end{bmatrix}$$

Step by Step Algorithm

- $A_{circ}(1:M, 1:N) = A;$
- $A_{circ}(M+1, :) = 0;$
- $A_{circ}(:, N+1) = 0;$
- $A_{circ}(M+2:2M, :) = A(M:-1:2, :);$
- $A_{circ}(:, N+2:2N) = A(:, N:-1:2);$
- $A_{circ}(M+2:2M, N+2:2N) = A(M:-1:2, N:-1:2);$

1) Embed the defining Toeplitz matrix or tensor to a defining circulant one
2) Pad with zeros the vector (matrix or tensor) of unknowns so it will have the same size with the defining circulant array.
3) Apply ***fft*** *on the above two arrays and implement an element-wise multiplication*
4) Apply ***ifft*** *to the result and reduce the size to the original one.*

Other "good" properties of the IE matrices

1) In the case of 2D SIE the arising matrix doesn't have a Toeplitz structure, since we are using triangles and the mesh is a bit "random". Although the off-diagonal blocks of the matrix are low-rank because they correspond to interaction between remote elements. This is the main idea behind the Fast Multipole Method (FMM) which leads to a huge compression of the system (more on CSE III).

2) In the case of VIE the matrix has the Toeplitz structure, but in some cases when we use higher-order approximations for our basis functions (for example 12 unknowns per voxel) the required memory might be Terra-bytes. Although the arising arrays have a low multilinear rank, since we are dealing again with interactions between remote elements. The storage memory can be reduced with SVD or Cross Approximation based methods through a plethora of tensor decompositions (more on scientific articles).