MPT-Calculator: A Python-NGSolve Implementation of Magnetic Polarizabiltiy Tensor Accelerated by POD

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1 Introduction

The purpose of this document is to provide an overview on how to install and use the MPT-Calculator, which is a high order finite element method (FEM) implementation using NGSolve [13, 16, 11] for computing the magnetic polarizability tensor for object characterisation in metal detection. In the case of frequency sweeps, this is accelerated by the Proper Orthogonal Decomposition (POD) technique. We begin, in Section 2, with an overview of the underlying mathematical theory describing the eddy current model and forward and inverse problems of metal detection. The formulae for the explicit calculation of the magnetic polarizability description of conducting permeable objects are included in this section along with references to the technical details. The installation of the program is described in Section 3. Then, in Section 4, an overview of the structure of the code is provided. In Section 5 a description of how to create your own geometry file is provided and then in Section 6 a series of examples that can be obtained with the software are included.

2 The eddy-current model and asymptotic expansion

We briefly discuss the eddy-current model along with stating the asymptotic expansion that forms the basis of the magnetic polarizability description of conducting objects in metal detection.

2.1 Eddy-current model

The eddy current model is a low frequency approximation of the Maxwell system that neglects the displacement currents, which is valid when the frequency is small and the conductivity of the body is high. A rigorous justification of the model involves the topology of the conducting body [3]. The eddy current model is described by the system

$$\nabla \times \boldsymbol{E}_{\alpha} = \mathrm{i}\omega \mu \boldsymbol{H}_{\alpha},\tag{1a}$$

$$\nabla \times \boldsymbol{H}_{\alpha} = \boldsymbol{J}_0 + \sigma \boldsymbol{E}_{\alpha}. \tag{1b}$$

where E_{α} and H_{α} are the electric and magnetic interaction fields, respectively, J_0 is an external current source, $i := \sqrt{-1}$, ω is the angular frequency, μ is the magnetic permeability and σ is the electric conductivity. We will use the eddy current model for describing the forward and inverse problems in the metal detection problem.

2.1.1 Metal Detection Forward Problem

In the forward (or direct) problem, the position and materials of the conducting body B_{α} are known. The object has a high conductivity, $\sigma = \sigma_*$, and a permeability, $\mu = \mu_*$. The conducting body is assumed to buried in soil, which is assumed to be of a much lower conductivity so that $\sigma \approx 0$ and have a permeability $\mu = \mu_0 := 4\pi \times 10^{-7} \text{H/m}$. A background field is generated by a solenodial current source J_0 with support in the air above the soil, which has $\sigma = 0$ and $\mu = \mu_0$. The region around the object is $B_{\alpha}^c := \mathbb{R}^3 \backslash B_{\alpha}$ as shown in Figure 1.

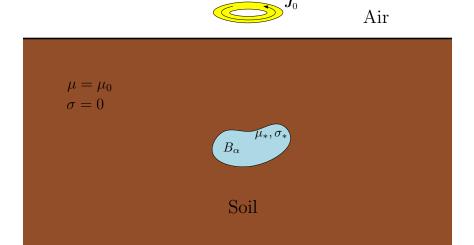


Figure 1: A diagram showing a hidden conducting object B_{α} surrounded by it's compliment B_{α}^{c} which is made up of soil and air.

The forward model is described by the system (1), which hold in \mathbb{R}^3 , with

$$\mu(\boldsymbol{x}) = \begin{cases} \mu_* & \boldsymbol{x} \in B_{\alpha} \\ \mu_0 & \boldsymbol{x} \in B_{\alpha}^c \end{cases}, \sigma(\boldsymbol{x}) = \begin{cases} \sigma_* & \boldsymbol{x} \in B_{\alpha} \\ 0 & \boldsymbol{x} \in B_{\alpha}^c \end{cases}, \tag{2}$$

and the regions B_{α} and B_{α}^{c} are coupled by the transmission conditions

$$[\mathbf{n} \times \mathbf{E}_{\alpha}]_{\Gamma_{\alpha}} = [\mathbf{n} \times \mathbf{H}_{\alpha}]_{\Gamma_{\alpha}} = \mathbf{0}, \tag{3}$$

which hold on $\Gamma_{\alpha} := \partial B_{\alpha}$. In the above, $[u]_{\Gamma_{\alpha}} := u|_{+} - u|_{-}$ denotes the jump, the + refers to just outside of B_{α} and the - to just inside and n denotes a unit outward normal to Γ_{α} .

The electric interaction field in (1) is non-physical and, to ensure uniqueness of this field, the condition $\nabla \cdot \mathbf{E}_{\alpha} = 0$ is imposed in B_{α}^{c} . Furthermore, we also require that $\mathbf{E}_{\alpha} = O(1/|\mathbf{x}|)$ and $\mathbf{H}_{\alpha} = O(1/|\mathbf{x}|)$ as $|\mathbf{x}| \to \infty$, denoting that the fields go to zero at least as fast as $1/|\mathbf{x}|$, although, in practice, this can faster.

2.1.2 Metal Detection Inverse Problem

In the metal detection inverse problem, one wishes to determine the location, shape and material properties of the conducting object B_{α} , described above, from measurements of $(\mathbf{H}_{\alpha} - \mathbf{H}_{0})(\mathbf{x})$ at locations \mathbf{x} in the air. Here, \mathbf{H}_{0} denotes the background magnetic and is the magnetic field that result from the solution of (1) without the presence of the object B_{α} , i.e. \mathbf{E}_{0} and \mathbf{H}_{0} are the solution of (1) with $\sigma = 0$ and $\mu = \mu_{0}$ in \mathbb{R}^{3} . Similar to above, we also require that $\mathbf{E}_{0} = O(1/|\mathbf{x}|)$ and $\mathbf{H}_{0} = O(1/|\mathbf{x}|)$ as $|\mathbf{x}| \to \infty$, denoting that the fields go to zero at least as fast as $1/|\mathbf{x}|$, although, in practice, this can faster.

Practical metal detectors measure a voltage perturbation, which corresponds to $\int_S \boldsymbol{n} \cdot (\boldsymbol{H}_{\alpha} - \boldsymbol{H}_0)(\boldsymbol{x}) d\boldsymbol{x}$ over an appropriate surface S [7]. For very small coils, this voltage perturbation corresponds to $\boldsymbol{m} \cdot (\boldsymbol{H}_{\alpha} - \boldsymbol{H}_0)(\boldsymbol{x})$ where \boldsymbol{m} is magnetic dipole moment of the coil [7].

2.2 The asymptotic expansion

The forward problem described in Section 2.1.1, implies that if we know B_{α} , σ_* and μ_* we can solve (1) to determine E_{α} and H_{α} . However, to do this repeatably for each new object is computationally expensive. Instead, we seek an approximation in the form of trying approximate the perturbation $(H_{\alpha} - H_{0})(x)$ at some point x exterior to B_{α} .

To do this, following [4, 5] we define $B_{\alpha} := \alpha B + z$ where B is a unit size object, α is the object size and z is the object's translation from the object as shown in Figure 2.

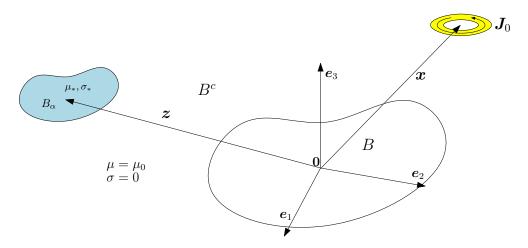


Figure 2: A diagram showing the physical description of B_{α} with respect to the coordinate axes.

Then, using results obtained by Ammari, Chen, Chen, Garnier and Volkov [4], Ledger and Lionheart [5] have derived the asymptotic expansion

$$(\boldsymbol{H}_{\alpha} - \boldsymbol{H}_{0})(\boldsymbol{x})_{i} = (\boldsymbol{D}_{\boldsymbol{x}}^{2} G(\boldsymbol{x}, \boldsymbol{z}))_{ij} (\mathcal{M})_{jk} (\boldsymbol{H}_{0}(\boldsymbol{z}))_{k} + O(\alpha^{4}), \tag{4}$$

which holds as $\alpha \to 0$. In the above, $G(x, z) = 1/4\pi |x - z|$ is the free space Laplace Green's function, $D_x^2 G$ denotes the Hessian of G and Einstein summation convention of the indices is implied. The term \mathcal{M} is the symmetric rank 2 magnetic polarizability tensor, which describes the shape and material properties of the object B_{α} and is independent of the object's position, but is frequency dependent. We will sometimes write $\mathcal{M}[\alpha B, \omega]$ to emphasise this. The above formulation, and the definition of \mathcal{M} below, are presented for the case of a single homogenous object B, the extension to multiple inhomogeneous objects can be found in [9, 8].

Let us now turn our attention to the computation of the coefficients of \mathcal{M} in (4), which describes the shape and material properties of B_{α} . From the following, will be able compute a library of such tensors for different choices of αB since \mathcal{M} is independent of z, this, in turn, will lend itself to the application of dictionary based classification algorithms [9] for the solution of the inverse problem stated in Section 2.1.2.

2.3 Calculating the Magnetic Polarizability Tensor

In the following, we state the explicit formulae for the computation of the coefficients of \mathcal{M} , which have been derived in [8]. Earlier, Ledger and Lionheart [5, 6, 7] have also derived other equivalent formulations, but those below lead to a more natural FEM implementation (using NGSolve).

Following [8], we write $\mathcal{M} = (\mathcal{M})_{ij} e_i \otimes e_j$ where e_i denotes the *i*th orthonormal unit vector and use the splitting $(\mathcal{M})_{ij} := (\mathcal{N}^0)_{ij} + (\mathcal{R})_{ij} + \mathrm{i}(\mathcal{I})_{ij}$ with

$$(\mathcal{N}^0[\alpha B])_{ij} := \alpha^3 \delta_{ij} \int_B (1 - \mu_r^{-1}) d\boldsymbol{\xi} + \frac{\alpha^3}{4} \int_{B \cup B^c} \tilde{\mu}_r^{-1} \nabla \times \tilde{\boldsymbol{\theta}}_i^{(0)} \cdot \nabla \times \tilde{\boldsymbol{\theta}}_j^{(0)} d\boldsymbol{\xi}, \tag{5a}$$

$$(\mathcal{R}[\alpha B, \omega])_{ij} := -\frac{\alpha^3}{4} \int_{B \cup B^c} \tilde{\mu}_r^{-1} \nabla \times \boldsymbol{\theta}_j^{(1)} \cdot \nabla \times \overline{\boldsymbol{\theta}_i^{(1)}} \, \mathrm{d}\boldsymbol{\xi}, \tag{5b}$$

$$(\mathcal{I}[\alpha B, \omega])_{ij} := \frac{\alpha^3}{4} \int_{B} \nu \left(\boldsymbol{\theta}_j^{(1)} + (\tilde{\boldsymbol{\theta}}_j^{(0)} + \boldsymbol{e}_j \times \boldsymbol{\xi}) \right) \cdot \left(\overline{\boldsymbol{\theta}_i^{(1)} + (\tilde{\boldsymbol{\theta}}_i^{(0)} + \boldsymbol{e}_i \times \boldsymbol{\xi})} \right) d\boldsymbol{\xi}. \tag{5c}$$

In the above,

$$\tilde{\mu}_r(\boldsymbol{\xi}) := \left\{ \begin{array}{ll} \mu_r := \mu_*/\mu_0 & \boldsymbol{\xi} \in B \\ 1 & \boldsymbol{\xi} \in B^c \end{array} \right.,$$

and $\nu := \alpha^2 \omega \mu_0 \sigma_*, \, \delta_{ij}$ is the Kronecker delta and the overbar denotes the complex conjugate. The

computation of (5) rely on the solution of the transmission problems [8]

$$\nabla \times \tilde{\mu}_r^{-1} \nabla \times \boldsymbol{\theta}_i^{(0)} = \mathbf{0} \qquad \text{in } B \cup B^c, \tag{6a}$$

$$\nabla \cdot \boldsymbol{\theta}_i^{(0)} = 0 \qquad \text{in } B \cup B^c, \tag{6b}$$

$$[\boldsymbol{n} \times \boldsymbol{\theta}_i^{(0)}]_{\Gamma} = \mathbf{0}$$
 on Γ , (6c)

$$[\boldsymbol{n} \times \tilde{\mu}_r^{-1} \nabla \times \boldsymbol{\theta}_i^{(0)}]_{\Gamma} = \mathbf{0} \qquad \text{on } \Gamma,$$
 (6d)

$$\boldsymbol{\theta}_i^{(0)} - \boldsymbol{e}_i \times \boldsymbol{\xi} = \boldsymbol{O}(|\boldsymbol{\xi}|^{-1})$$
 as $|\boldsymbol{\xi}| \to \infty$, (6e)

and

$$\nabla \times \tilde{\mu}_r^{-1} \nabla \times \boldsymbol{\theta}_i^{(1)} - \mathrm{i}\nu (\boldsymbol{\theta}_i^{(0)} + \boldsymbol{\theta}_i^{(1)}) = \mathbf{0} \qquad \text{in } B \cup B^c, \tag{7a}$$

$$\nabla \cdot \boldsymbol{\theta}_{i}^{(1)} = 0 \qquad \text{in } B^{c}, \tag{7b}$$

$$[\boldsymbol{n} \times \boldsymbol{\theta}_i^{(1)}]_{\Gamma} = \mathbf{0}$$
 on Γ , (7c)

$$[\mathbf{n} \times \tilde{\mu}_r^{-1} \nabla \times \boldsymbol{\theta}_i^{(1)}]_{\Gamma} = \mathbf{0} \qquad \text{on } \Gamma, \tag{7d}$$

$$\boldsymbol{\theta}_i^{(1)}(\boldsymbol{\xi}) = \boldsymbol{O}(|\boldsymbol{\xi}|^{-1})$$
 as $|\boldsymbol{\xi}| \to \infty$. (7e)

Note also that $\tilde{\boldsymbol{\theta}}_i^{(0)} := \boldsymbol{\theta}_i^{(0)} - \hat{\boldsymbol{e}}_i \times \boldsymbol{\xi}$. In order to obtain a discrete approximation using the FEM, we need to introduce a finite computational domain Ω such that $B \subset \Omega$, whose boundary $\partial \Omega$ is placed sufficiently far from the object B.

The tensor $\mathcal{N}^0[\alpha B]$ describes the magnetostatic characterisation of αB and is independent of ω . The frequency dependent $\mathcal{R}[\alpha B, \omega]$ tensor vanishes at low frequency and $\mathcal{N}^0[\alpha B] + \mathcal{R}[\alpha B, \omega] = \text{Re}(\mathcal{M}[\alpha B, \omega])$ describes the frequency behaviour of the real part of the tensor. Similarly, $\mathcal{I}[\alpha B, \omega] = \text{Im}(\mathcal{M}[\alpha B, \omega])$ describes the frequency behaviour of the imaginary part of the tensor, which vanishes at low frequencies and tends to 0 as the upper limiting frequency of the eddy current model is reached [8].

In order to compute the tensor coefficients in (5) we need to solve (6) and (7) (repeatably for each ω) and this will be achieved by computing approximate solutions using a range of different numerical schemes

- 1. A hp FEM discretisation of the transmission problems (6) and (7) using NGSolve [13, 16, 11] to compute $\mathcal{M}[\alpha B, \omega]$ for a single frequency.
- 2. A hp FEM discretisation of the transmission problems (6) and (7) using NGSolve [13, 16, 11] for performing the computation of $\mathcal{M}[\alpha B, \omega]$ over a range of frequencies.
- 3. A Proper Orthogonal Decomposition (POD) reduced order model, which greatly accelerates the computation of the full order model in 2. for computing $\mathcal{M}[\alpha B, \omega]$ over a range of frequencies.
- 4. Certificates computed at run time, which indicate the accuracy of the POD outputs with respect to the full order solution over a range of frequencies.

A detailed description of the numerical implementation of these schemes can be found in [15].

In particular, we advocate a hp FEM discretisation using $\boldsymbol{H}(\text{curl})$ conforming elements for the transmission problems (6) and (7) due to the superior performance it overs over a traditional h-version of the FEM, in which only the mesh is refined. In the hp-version, the polynomial order of the elements can be increased, as well as refining the finite element grid, in order to obtain accurate solutions. In practice, it is often sufficient to generate a suitable mesh, which has local refinement around sharp edges and corners and increase the polynomial degree in order to obtain accurate solutions for the magnetic polarizability tensor coefficients. As an illustration, we present in Figure 3 convergence curves of $\|\mathcal{N}_{hp}^0 - \mathcal{N}^0\|_F / \|\mathcal{N}^0\|_F$ and $\|\mathcal{M}_{hp} - \mathcal{M}\|_F / \|\mathcal{M}\|_F$ computed for a conducting sphere of radius $\alpha = 0.01$ m, $\sigma_* = 6 \times 10^6 \text{S/m}$, $\mu_* = 1.5\mu_0$, which has an analytical solution [14], where hp denotes the tensor coefficients obtained by a hp FEM discretisation. The solutions obtained on a sequence of meshes with 12074, 22392, 26751, 48418, 54092, 123788 unstructured tetrahedral elements of order p = 0 (h-refinement) are compared with those obtained on a fixed mesh of 12074 unstructured tetrahedral elements using of order p = 0, 1, 2, 3, in turn (p-refinement). We observe the downward sloping behaviour of the p-refinement convergence curve, which illustrates that exponential convergence is being obtained, compared to the slower algebraic rate with h-refinement.

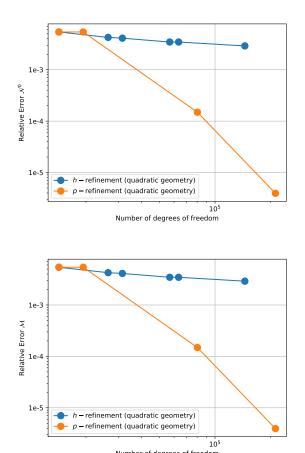


Figure 3: Conducting sphere of radius $\alpha = 0.01$ m, $\sigma_* = 6 \times 10^6$ S/m, $\mu_* = 1.5\mu_0$: Convergence curves of $\|\mathcal{N}_{hp}^0 - \mathcal{N}^0\|_F / \|\mathcal{N}^0\|_F$ and $\|\mathcal{M}_{hp} - \mathcal{M}\|_F / \|\mathcal{M}\|_F$ for h and p refinement

The following describes the installation and use MPT-Calculator, which implements the above schemes.

3 Installation

Due to the code being written in python and using NGSolve the user is required to install both of these in order to use the MPT-Calculator. Please follow the instructions available at https://ngsolve.org/in order to install the high order finite element and meshing library NGSolve [13, 16, 11] released under the LPLG license and ensure a compatible version of Python 3 is installed which is available at https://www.python.org. The code has been tested on version 6.2.1910 of NGSolve and version 3.7.1 of Python 3 [2]. The code has been tested on version 10.13.6 of MAC OS and 18.04 of Ubuntu.

Along with these installations, the MPT-Calculator relies on a number of python packages, which the user is required to install they are as follows sys, numpy, os, time, multiprocessing, cmath, subprocess, matplotlib. On a MAC or Linux they can be installed from the command line using the command

pip3 install "package to be installed"

where "package to be installed" is replaced with the appropriate package name. Finally the user is required to download or clone the repository of this MPT-Calculator from github.

4 Overview and structure of the code

Let us now discuss the layout of the code and the files which are designed to be edited. The user is expected interact with 3 files main.py, Settings.py and PlotterSettings.py, these files along with a geometry

file (.geo file) (see Section 5) allow the user to produce an array of different frequency sweeps for many different objects. In this section we discuss the layout of the folder system in place, how each of the input files can used and edited by the user to produce a frequency sweep along with how and where the results are saved. The structure of the code can be seen in Figure 4

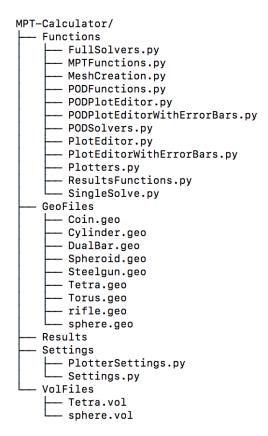


Figure 4: Image displaying the structure of the main folder of the FrequencySweepCode.

We next discuss how to use the input files of the code.

4.1 User input files

The files (along with their file paths) the user is expected to interact with are

```
main.py
Settings/Settings.py
Settings/PlotterSettings.py.
```

Once the files have the desired inputs the simulation is run by entering the command

```
python3 main.py
```

to the command line from the main directory. The MPT-Calculator then runs the appropriate frequency sweep and saves the outputs in an output folder (see Section 4.2). We start this explanation with main.py.

4.1.1 main.py

The file main.py is the file with which the user is expected to have most interaction, it is the file which calls functions to generate a mesh, perform frequency sweeps and finally post process the data produced in the frequency sweep. In main.py, the user is greeted with an input section which should look similar to the image in Figure 5.

```
Geometry = "sphere.geo"
 #ffloat) scaling to be applied to the .geo file i.e. if you have defined
#a sphere of unit radius in a .geo file alpha = 0.01 would simulate a
#sphere with a radius of 0.01m ( or 1cm)
MeshSize = 1
#(int 1—5) this defines how fine the mesh should be for regions that do
#not have maxh values defined for them in the .geo file (1=verycoarse,
#The order of the elements in the mesh \mathbf{Order} = \mathbf{0}
#About the Frequency sweep (frequencies are in radians per second) #Minimum frequency (Powers of 10 i.e Start = 2 => 10***2) Start = 1
 #(float)
#Maximum frequency (Powers of 10 i.e Start = 8 => 10***8)
Points = 81
#I only require a single frequency
Single = False
#(boolean) True if single frequency is required
Omega = 133.5
roa = Irae
#(boolean) True if POD is to be used, the number of snapshots can be
#edited in in the Settings.py file
#Plot the POD points
PlotPod = True
 #(boolean) do you want to plot the snapshots (This requires additional
#calculations and will slow down sweep by around 2% for default settings)
 #(boolean) #I have multiple cores at my disposal and have enough spare RAM
# to run the frequency sweep in parrallel (Edit the number of cores to be
#used in the Settings.py file)
```

Figure 5: Image displaying the user input section of the file main.py

In this section we shall briefly explain what each of these inputs refer to and how to provide an input for each. For the first input Geometry the user is required to define the .geo (geometry) file which is to be used in the sweep see Section 5 for information on how to create geometry files) this input is a string and can be defined as follows

```
Geometry = "sphere.geo"
```

A frequency sweep would then be calculated the object defined in file sphere.geo. The object defined in this file is then scaled by the parameter α (meters), the input for this is a float and can be defined as follows

```
alpha = 0.01
```

This then defines how the object in the .geo file should be scaled. The next two options in the file relate to the mesh which is to be used in the simulation of the object. The variable MeshSize defines how refined the mesh used in the simulation should be, the input for this variable is an integer between 1 and 5 (1 being very coarse and 5 being very fine) and can be defined as follows

MeshSize = 3

The other key option when it comes to defining a mesh is the order of the elements (how complex the functions describing the solution are) this requires an integer input which is between 0 and 3 (0 being the fastest to run the least accurate and 3 being the slowest by most accurate) when running full simulations (not small tests) it is recommended that an order of 3 be used, this can be defined as follows

Order = 3

The next 3 inputs relate to the frequencies in radians/sec which should be included in the frequency sweep they are as follows, Start and Finish are the minimum and maximum frequencies which should be included (float) and Points is the number of logarithmically spaced frequencies to be sampled at (integer), n.b. these are the powers base 10 of the frequencies i.e. we create a frequency sweep for $10^{\text{Start}} - 10^{\text{Finish}}$ rad/s. For example if we defined the following

Start = 1 Finish = 8 Points = 8

We would run a frequency sweep for 8 logarithmically spaced points between 10^1 and 10^8 i.e. for the following frequencies

$$\omega = 10^1, 10^2, 10^3, 10^4, 10^5, 10^6, 10^7, 10^8 \text{ rad/s}.$$

Along with this there is also an option to run a simulation for a single frequency this may be done using the variable Single (boolean) and can be done as follows

Single = True

This then runs a simulation at the value defined for the variable Omega (float) n.b. this value is the frequency not the power of 10 of the frequency i.e. setting

Omega = 133.5

will run a simulation for $\omega=133.5$ rad/s not $\omega=10^{133.5}$ rad/s. If Single = False the frequency sweep will be run for the frequencies defined by Start, Finish and Points. Finally the user will find some options which affect how the frequency sweep will be produced. The first of these is whether or not to create a reduced order model (ROM) using the method of proper orthogonal decomposition (POD) the user may define whether to use this by editing the variable POD (boolean), if the user would like the frequency sweep to be produced using POD they set

POD = True

The POD works by producing a frequency sweep for a small number of frequencies (snapshots), it then uses the solutions to create an ROM which can then be used to produce a full frequency sweep containing many more points at a fraction of the computational cost. It is useful to note at this point that although POD works very well as the relative permeability μ_r of the object being simulated increases the POD becomes less accurate, see the spheroid example. This brings us to our next option, PlotPod (boolean) this option defines whether or not to plot points where the POD has taken snapshots. These points can be plotted by setting

PlotPod = True

Having these points plotted can be very useful as it gives a visual representation of the accuracy of the frequency sweep produced by POD compared with a full order frequency sweep. This brings us to our final user input in the main.py file which is the variable MultiProcessing this option decides whether to

produce the frequency sweep using multiple cores, by setting

MultiProcessing = True

The wall clock time will be reduced but the frequency sweep then requires more of the machines resources since it is running simulations on multiple cores. The default setting for the number of cores to be used is 2 but can be edited in the default settings section of Settings.py.

4.1.2 Settings/Settings.py

The second section which the users is able to interact with is the Settings.py file. This file contains settings related to how the frequency sweep is to be run, how the data should be saved and how NGSolve solves each of the finite element problems. An image of the file can be seen in Figure 6.

```
import numpy as np
from ngsolve import *
def DefaultSettings():
   CPUs = 4
   PODPoints = 13
   PODTol = 10**-4
   PODErrorBars = True
   return CPUs, PODPoints, PODTol, PODErrorBars
def SaverSettings():
   FolderName = "Default"
   return FolderName
def SolverParameters():
   Solver = "bddc"
   epsi = 10**-12
   Maxsteps = 5000
   Tolerance = 10**-10
   ngsglobals.msg_level = 0
   return Solver, epsi, Maxsteps, Tolerance
```

Figure 6: Image displaying the file Settings.py

The first section in this file is DefaultSettings these define how many cores the simulation should use and how many snapshots should be taken when using the POD option. The number of cores is set by editing the variable CPUs (integer) an example of this would be setting

```
CPUs = 4
```

which would produce a frequency sweep using 4 of the machines cores. It is useful to mention at this point that when using multiple cores the user is recommended to monitor memory usage especially when producing a frequency sweep for an object with a fine mesh on a machine with limited resources. The next two variables in the <code>DefaultSettings</code> section relate to the use of POD the first is <code>PODPoints</code> (integer), this defines how many snapshots should be taken when using the POD method, and can be set as

PODPoints = 13

This then creates an ROM using 13 snapshots (if POD = True in main.py). The other setting in the the DefaultSettings section is the variable PODTol (float) this variable sets at which point to truncate the singular value decomposition setting

```
PODTol = 10**-4
```

sets the truncation to the point at which the singular values drop below the 10^{-4} (for more explanation see [15]). Suggested values for PODPoints and PODTo1 are 13 and 10^{-4} respectively. Lastly the the setting

PODErrorBars = True

creates certificates for the outputs of the ROM. This gives the user an upper bound on the error introduced by using ROM.

The next section of Settings.py is the SaverSettings, this section allows the user to define a filepath within the folder Results to save the outputs of the frequency sweep. This is done by changing the variable FolderName (string) to the desired filepath within which save the outputs. An example of this would be

FolderName = MyShape/MyFrequencySweep

which would then store the output in Results/MyShape/MyFrequencySweep. Although this is an option, we recommend that FolderName = "Default", which, when set, produces a series of subfolders containing information relating to material properties scaling and frequencies in the sweep. This makes it very hard for the user to overwrite (and lose) existing data from other frequency sweeps, which will be done if the user forgets to change FolderName for a new frequency sweep.

The final section in Settings.py relates to how NGSolve solves each of the finite element problems. The default options work well for the frequency sweeps that are presented in the examples section. The default settings are as follows

```
Solver = "bddc"

epsi = 10**-12

Maxsteps = 5000

Tolerance = 10**-10

ngsglobals.msg_level = 0
```

These settings are optimised for meshes containing more than 20,000, 3rd order elements, see the examples section for further details. The options for the settings is as follows: The variable Solver (string)

can be set to either "bddc" or "local" this changes the preconditioner used by the iterative CG solver in NGSolve. For simulations using very coarse meshes or simulations with 0th order elements the "local" preconditioner is faster but for larger simulations setting

Solver = "bddc"

is recommended. The variable tolerance (float) sets the required relative residual for the iterative CG solver and controls the accuracy of the linear solve. For coarse discretisations, this does not need to be too small. For example, for full order sweeps, setting

Tolerance = 10**-6

often leads to satisfactory results, however, upon testing, we found that for the POD the solution needs to be calculated more accurately to capture the underlying behaviour of the solution. The variables epsi (float) (regularisation) and Maxsteps (integer) (the maximum number of iterations performed) are less important since provided that epsi is 1 order of magnitude smaller than tolerance a solution will be reached within the maximum number of iterations. Finally, the variable ngsglobals.msg_level (integer) relates to the information provided by NGSolve about solving the problems. We recommend that this be set to either 0 (for no information) or 3 (for information relating to the assembly and solving of the finite element problems). The next section explains how to use the PlotterSettings.py file.

4.1.3 Settings/PlotterSettings.py

To display the results of the frequency sweep a simple plotting function has been created¹, the settings of this function can be edited by changing the inputs of the PlotterSettings.py file. An image of the PlotterSettings.py file can be seen in Figure 7.

¹This is a basic visualisation tool, which allows the user to view results of the sweep. For a graph tailored to the users specification, use the data stored in the .csv files saved in the Data folder to produce their own plot.

```
import numpy as np
from ngsolve import *
#Function definition of the plotter settings
def PlotterSettings():
    EigsToPlot = [1,2,3]
    TensorsToPlot = [1,4,6,2,3,5]
   MainLineStyle = "-"
   MainMarkerSize = 4
    SnapshotLineStyle = "x"
    SnapshotMarkerSize = 8
    ErrorBarLineStyle = "--"
    ErrorBarMarkerSize = 4
    Title = True
    return Title, Show, EigsToPlot, TensorsToPlot, MainLineStyle,\
    MainMarkerSize, SnapshotLineStyle, SnapshotMarkerSize,\
     ErrorBarLineStyle, ErrorBarMarkerSize
```

Figure 7: Image displaying the file Settings.py

The first two inputs of the file EigsToPlot (list) and TensorsToPlot (list) relate to which lines are to be plotted on the graphs. With these options the user may change both the lines and the order in which the lines are to be plotted. The variable EigsToPlot defines which eigenvalues, sorted smallest to largest, are plotted. For example, setting

```
EigsToPlot = [3,2,1]
```

will plot all of the eigenvalues largest to smallest. The variable TensorsToPlot allows the user to choose

which coefficients of \mathcal{M} are to be plotted. Taking account of the symmetry of the tensor, the user has a choice of 6 independent coefficients to plot as referenced by the numbers in the following matrix

reference matrix =
$$\begin{bmatrix} 1 & 2 & 3 \\ 2 & 4 & 5 \\ 3 & 5 & 6 \end{bmatrix}$$
. (8)

For example, we may plot just diagonal coefficients of the matrix by setting

TensorsToPlot = [1,4,6]

For simplicity, a legend is created automatically for each of the lines in the plot, without additional inputs required from the user. The next 6 variables relate the style of lines being plotted. The variables MainLineStyle (string), SnapshotLineStyle (string) and ErrorBarLineStyle (string) define the line styles of the full frequency sweep and the line styles of the snapshots and certificate bounds (if PlotPod = True and/ or PODErrorBars = True), respectively. The plots are created using the matplotlib module of python and, thus, the available line styles are those supported by matplotlib [1]. The other variables relating to line style are MainMarkerSize (float), SnapshotMarkerSize (float) and ErrorBarMarkerSize (float), which define the size of the markers used in the plot for the full sweep, snapshots and certificate bounds, respectively. The recommended settings of these vary on the markers chosen, but the default settings for the line styles and markers are

```
MainLineStyle = "-"
MainMarkerSize = 4
SnapshotLineStyle = "x"
SnapshotMarkerSize = 8
ErrorBarLineStyle = "--"
ErrorBarMarkerSize = 4
```

The next vairable, Title (boolean), defines whether or not the plot includes a title and, again, the title is automatically created for each of the different plots with no user input required. The default setting is

Title = True

The final variable is Show (boolean), which defines whether or not to display the produced graphs once the frequency sweep is complete². The default setting is

Show = True

With this we conclude the section on how to interact with each of the input files. We next discuss how and where the output of the code is saved.

4.2 Output files

In this section, we discuss how the outputs for each of the different versions of the code are saved. As mentioned briefly in Section 4.1.2, the user may define which folder (or filepath) the outputs are saved in. However, when the code is run, it will generate subfolders to organise the results below this folder (or filepath), as described below. We start with the case of a single frequency simulation.

4.2.1 Single frequency output

In the case of a simulation with only one frequency, there is no need for a graphical representation, due to this the output folder has the structure shown in Figure 8.

 $^{^{2}}$ The graphs are automatically saved this option is whether to display them as well.

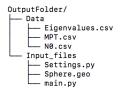


Figure 8: Image displaying the structure of the output folder for the case of a single frequency simulation.

Notice the inclusion of the folder Input_files, this folder contains a copy of the inputs files used to run the simulation. This allows the user to reproduce their results, if they so wish. The folder Data, contains the results for the computed \mathcal{M} , \mathcal{N}^0 , stored in MPT.csv and NO.csv, respectively, and their eigenvalues $\lambda_i(\mathcal{N}^0 + \mathcal{R})$ and $\lambda_i(\mathcal{I})$, stored in the file Eigenvalues.csv as the sum $\lambda_i(\mathcal{N}^0 + \mathcal{R}) + i\lambda_i(\mathcal{I})$ to reduce the number of output files. Let us next discuss the case of a full frequency sweep without using POD.

4.2.2 Full order frequency sweep output

In the case of the full order frequency sweep, the folder structure for the output folder can be seen in Figure 9.

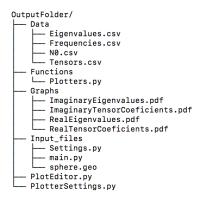


Figure 9: Image displaying the structure of the output folder for the full order frequency sweep.

The Functions folder contains the file Plotters.py, which contains the functions used for producing the plots. The folder Graphs contains the graphs displaying the results of the frequency sweep. The file Frequencies.csv contains a list of the frequencies for which the tensors have been calculated and Eigenvalues.csv contains the sum $\lambda_i(\mathcal{N}^0 + \mathcal{R}) + \mathrm{i}\lambda_i(\mathcal{I})$. The file Tensors.csv stores the MPTs coefficient as row vectors and stacks them so that each row corresponds to the same corresponding frequency in the row of the Frequencies.csv file and the eigenvalues in the row of the Eigenvalues.csv file. Finally, the files PlotEditor.py and PlotterSettings.py allow the user to replot and edit the graphs by editing the inputs in PlotterSettings.py in the same manner as in 4.1.3 and then running the file PlotEditor.py by entering the command

python3 PlotEditor.py

in the command line from the output folder. Next we discuss the case of a frequency sweep produced using POD.

4.2.3 POD frequency sweep output

In the case of a frequency sweep produced using POD there are two possible options for the structure of the output folder. If PlotPod = True and PODErrorBars = True, the folder will have the structure shown in Figure 10.

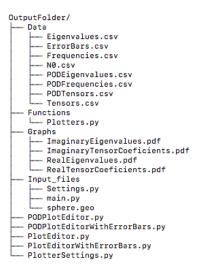


Figure 10: Image displaying the structure of the output folder for the frequency sweep using POD with the option of plotting the snapshot tensors.

The key differences to the full order solve are the inclusion of the data files PODFrequencies.csv, PODEigenv alues.csv, PODTensors.csv and ErrorBars.csv. These files contain the frequencies for the snapshots, the eigenvalues of the tensors calculated at the snapshots, the tensors calculated at the snapshots and the certificate bounds of the outputs, respectively. The other difference between this and the full order sweep is the inclusion of the extra plot editor files PODPlotEditor.py, PODPlotEditorWithErrorBars.py and PlotEditorWithErrorBars.py, which enables plots of both the snapshots and full frequency sweep to be reproduced.

In the case where PlotPod = False, the structure is as shown in Figure 10 except that the files PODEigenvalues.csv, PODTensors.csv and PODPlotEditor.py are not included in the folder. Similarly when PODErrorBars = False, we find the exclusion of the files ErrorBars.csv, PODPlotEditorWithErrorBars.py and PlotEditorWithErrorBars.py from the output folder. Finally when PlotPod = False and PlotEditorWithErrorBars.py = False we have the exclusion of PODEigenvalues.csv, PODTensors.csv and ErrorBars.csv along with PODPlotEditor.py, PODPlotEditorWithErrorBars.py and PlotEditorWithErrorBars.py.

The user may replot the graphs by entering the commands

```
python3 PlotEditorWithErrorBars.py
python3 PODPlotEditor.py
python3 PODPlotEditorWithErrorBars.py
```

in the output folder, to show a plot with the snapshots and/ or certificate bounds being displayed on the graph. Or if the command

```
python3 PlotEditor.py
```

is entered in the output folder, the graphs without the snapshots included is reproduced. With this we conclude our section on the overview and structure of the code. In the next section, we discuss how to create an object using a .geo file.

5 Creating your own geometry file

In this section we discuss how to create a geometry file (.geo), with the geometry file being interpreted by Netgen [12] (the meshing tool in NGSolve) we first explain how to create shapes and geometries using a .geo file.

Due to Netgen being the underlying interpreter of the .geo file we direct the user to the relevant Constructive Solid Geometry (CSG) documentation available at http://netgen-mesher.sourceforge.net/docs/ng4.pdf. With this knowledge of this, we next discuss how the requirements outlined in Section 2.3,

relating to the domain Ω , which contains the object B, can be specified. Finally we explain how to define material properties of the objects being simulated.

5.1 Truncating the domain

Since it is impossible to simulate an infinite computational domain we are required to create a truncated domain Ω whose boundary $\partial\Omega$ is sufficiently far from the object B. In order to do this in the .geo file we simply define a region which is much larger than the object and place the object at its centre. An example of this is presented in the .geo file shown in Figure 11 along with a visualisation of the of the geometry obtained in Netgen.

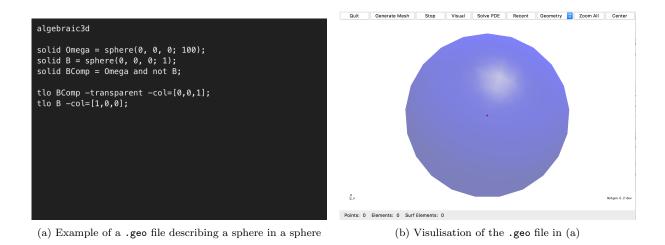


Figure 11: Example of a .geo file (a) describing a sphere of unit radius contained in a domain consisting of a sphere with a radius of 100, with (b) a visualisation of the constructed geometry using negten.

This example defines a unit sphere B contained in a domain Ω , which consists of a sphere with a radius of 100. Truncating the domain at a distance approximately 100 times the object size is sufficient for most cases. Next we discuss how to define the material properties of the different regions in the domain.

5.2 Defining material properties

To set the material parameters, the user is required to label each region defined as a Top Level Object (tlo). This is done by inserting a # after each toplevel object followed by a label for the material, it's relative permeability μ_r and it's conductivity σ_* . We define the material properties for the example presented in the Section 5.1 in the Figure 12.

```
algebraic3d

solid Omega = sphere(0, 0, 0; 100);
solid B = sphere(0, 0, 0; 1)-maxh=0.1;
solid BComp = Omega and not B;

tlo BComp -transparent -col=[0,0,1];#air
tlo B -col=[1,0,0];#sphere -mur=2 -sig=6E+06
```

Figure 12: Image displaying an example of a .geo file with material properties defined for it's regions.

In Figure 12, #sphere -mur=2 -sig=6e+06 labels the object B as "sphere" and defines it's material properties to be $\mu_r = 2$ and $\sigma_* = 6 \times 10^6 \mathrm{S/m}$. The inclusion of #air labels the non conducting region as "air", which is a protected material and, therefore, does not require the user to input a value for μ_r or σ_* . Lastly, note the inclusion of -maxh=0.1 when defining the geometry of B. This is an inbuilt function of Netgen for meshing purposes allowing the user to specify a maximum element size for each region in the domain. This is useful since it allows the user to refine the mesh in the conducting region of the domain.

Next, we specify the restrictions of the syntax for defining material properties. Any line which starts with tlo (which must have no spaces before) must also contain a material label defined as #material. On the same line, the user must define both μ_r and σ_* (unless the material is defined to be #air), to do this the user must provide the flag -mur=*** and -sig=*** with at least one space between the two flags, but no spaces before or either of the equal signs, and with *** replaced with value of the parameter. Note that σ_* should be specified in S/m. Some examples of this can be seen below, first the following examples are accepted,

```
tlo B -col=[1,0,0]; #sphere -mur=2 -sig=6E+06
tlo B -col=[1,0,0]; #sphere-mur=2 -sig=6E+06
tlo B -col=[1,0,0]; #sphere -mur=2 -sig=6E+06
```

However, the following examples will not work

```
tlo B -col=[1,0,0];#sphere -mur = 2 -sig = 6E+06
tlo B -col=[1,0,0];#sphere-mur=2 -sig=6E+06
tlo B -col=[1,0,0];#sphere -mur=2-sig=6E+06
tlo B -col=[1,0,0];#sphere
-mur=2-sig=6E+06
```

Due to there being a space before or after the equal signs in the first; to a space before the tlo in the second; to the lack of a space between the definition of -mur and -sig in the third and due to the split two lines in the last.

We next consider the case of an object made up of multiple conducting regions follow the examples in Ledger, Lionheart and Amad [9]. We define a conducting rectangular bar, B which is a $2 \times 1 \times 1$ block made up 2 distinct sections, contained in a domain bounded by a sphere with radius of 100, as defined in the .geo file shown in Figure 13. Note that B does not have units, the object αB has units with α being the size parameter specified in m and α is specified later.

```
algebraic3d

solid Omega = sphere (0, 0, 0; 100);
solid Block1 = orthobrick (-1,0,0;0,1,1) -maxh=0.15;
solid Block2 = orthobrick (0,0,0;1,1,1) -maxh=0.15;

solid Domain = Omega and not Block1 and not Block2;

tlo Domain -transparent -col=[0,0,1];#air
tlo Block1 -col=[1,0,0];#material1 -mur=1 -sig=1e+06
tlo Block2 -col=[0,1,0];#material2 -mur=2 -sig=1e+08
```

Figure 13: Image displaying an example of a .geo file which defines a bar constructed of 2 regions with different material properties contained in a domain consisting of a sphere with a radius of 100.

In Figure 13 we have defined two distinct regions Block1 and Block2 with materials "Material1" and "Material2" having different material properties, respectively.

We finish this section with an example of two unit spheres which are constructed using the same material. An example of the .geo file can be seen in Figure 14.

```
algebraic3d
solid Omega = sphere(0, 0, 0; 100);
solid Sphere1 = sphere(-1.5, 0, 0; 1)-maxh=0.1;
solid Sphere2 = sphere(1.5, 0, 0; 1)-maxh=0.1;
solid BComp = Omega and not Sphere1 and not Sphere2;
tlo BComp -transparent -col=[0,0,1];#air
tlo Sphere1 -col=[1,0,0];#sphere -mur=2 -sig=6E+06
tlo Sphere2 -col=[1,0,0];#sphere
```

Figure 14: Image displaying an example of a .geo file which defines a bar constructed of 2 regions with different material properties contained in a domain consisting of a sphere with a radius of 100.

This example demonstrates how we only need to define the material properties for **#sphere** once even though there are two regions to which it will be applied. This makes it easier to change material properties for a whole geometry when made up of multiple tlos. We expect this to be useful when working with more complex geometries such as that in the case of a rifle shell, which will be presented in Section 6.5. In the next Section we work through some specific examples.

6 Examples

In this section, we consider a set of examples in which the functionality of the MPT-Calculator is demonstrated. We start with the case of a sphere.

6.1 Sphere

For the case where B is a sphere of unit radius and αB is a sphere of radius $\alpha=0.01\mathrm{m}$ we shall create three different simulations, the first is a simulation consisting of a single frequency, the second a full order frequency sweep and the third a frequency sweep implementing the POD. All of these sphere examples are created using the sphere.geo file, shown in Figure 15, where Ω is chosen to be a ball of radius 200 containing the object B, $\sigma_* = 6 \times 10^6$ S/m and $\mu_* = 1.5\mu_0$.

```
algebraic3d
solid sphout = sphere (0, 0, 0; 200);
solid sphin = sphere (0, 0, 0; 1) -maxh=0.1;
solid rest = sphout and not sphin;
tlo rest -transparent -col=[0,0,1];#air
tlo sphin -col=[1,0,0];#sphere -mur=1.5 -sig=6E+06
```

Figure 15: Image displaying the Sphere.geo file used in all of the sphere frequency sweep examples in Section 6.1.

We start our examples session with a simulation of the sphere described in Figure 15 for a single frequency.

6.1.1 Single frequency sweep for a sphere

To set up this simulation, we used the **sphere.geo** file shown in Figure 15 along with the inputs displayed in Figure 16.

```
import numpy as np
from ngsolve import *
                                                                                                                                           def DefaultSettings():
                                                                                                                                                 #How many cores to be used (monitor memory consuption)
CPUs = 3
Geometry = "sphere.geo"
    string) Name of the .geo file to be used in the frequency sweep i.e.
"sphere.geo"
                                                                                                                                                  #How many snapshots should be taken PODPoints = 13
  iffloat) scaling to be applied to the .geo file i.e. if you have defined
ta sphere of unit radius in a .geo file alpha = 0.01 would simulate a
tsphere with a radius of 0.01m ( or 1cm)
                                                                                                                                                  #Tolerance to be used in the TSVD
PODTol = 10**-4
                                                                                                                                                  PODErrorBars = False
                                                                                                                                                  return CPUs, PODPoints, PODTol, PODErrorBars
                                                                                                                                            def SaverSettings():
                                                                                                                                                 FolderName = "Default"
#(string) This defines the folder (and potentially subfolders) the
#data will be saved in (if "Default" then a predetermined the data
#will be saved in a predetermined folder structure)
#Example input "MyShape/MyFrequencySweep"
                                                                                                                                                  return FolderName
                                                                                                                                          ## date of SolverParameters ():

#Parameters associated with solving the problem can edit this

#preconditioner to be used

Solver = "bddc"
Points = 81
#I only require a single frequency
Single = True
#(boolean) True if single frequency is required
Omega = 133.5
                                                                                                                                                  epsi = 10**-12
#(float) regularisation to be used in the problem
                                                                                                                                                  #(int) maximum number of iterations to be used in solving the problem
#the bddc will converge in most cases in less than 200 iterations
#the local will take more
 rou = raise
(|boolean) True if POD is to be used, the number of snapshots can be
#edited in in the Settings.py file
                                                                                                                                                  #Relative tolerance
Tolerance = 10**-10
                                                                                                                                                  ngsglobals.msg_level = 0
MultiProcessing = True
   (boolean) #I have multiple cores at my disposal and have enough spare RAP
to run the frequency sweep in parallel (Edit the number of cores to be
used in the Settings.py file)
                                                                                                                                                  return Solver,epsi,Maxsteps,Tolerance
```

(a) An image of main.py.

(b) An image of Settings.py.

Figure 16: Images displaying the inputs for the single frequency sweep for a sphere (a) image of the inputs in main.py (b) image of the inputs in Settings.py.

These inputs for main.py and Settings.py have been summarised in Table 1. As Single = True the following variables are not used: Start = 1, Finish = 8, Points = 81, PODPoints = 13, PODTol = 10**-4 and hence their values are arbitrary.

Geometry = "sphere.geo"	Single = True	PODTol = 10**-4
alpha = 0.01	Omega = 133.5	PODErrorBars = False
MeshSize = 2	Pod = False	FolderName = "Default"
Order = 3	PlotPod = False	Solver = "bddc"
Start = 1	MultiProcessing = True	epsi = 10**-12
Finish = 8	CPUs = 3	Maxsteps = 5000
Points = 81	PODPoints = 13	Tolerance = 10**-10
	ngsglobals.msg_level = 0	

Table 1: A table summarising the inputs for the simulation of the sphere with for a single frequency.

This means our interest lies in computing the characterisation for $\alpha B = 0.01B$ at a frequency of $\omega = 133.5 \,\mathrm{rad/s}$. Furthermore, the inputs led to a mesh of 26751 elements and a discretisation of p = 3. On a 2012 iMac with a 2.9 GHz quad core i5 processor with 16 GB 1600 MHz DDR3 memory the computation takes 1 minute and 20 seconds using 3 CPUs and results in the following for the \mathcal{N}^0 and \mathcal{M} ,

$$\mathcal{N}_{hp}^{0} = \left(\begin{array}{ccc} 1.80 \times 10^{-6} & 6.28 \times 10^{-14} & 2.59 \times 10^{-14} \\ 6.28 \times 10^{-14} & 1.80 \times 10^{-6} & 7.52 \times 10^{-14} \\ 2.59 \times 10^{-14} & 7.52 \times 10^{-14} & 1.80 \times 10^{-6} \end{array} \right),$$

$$\mathcal{M}_{hp} = \left(\begin{array}{cccc} 1.79 \times 10^{-6} + 6.97 \times 10^{-8} \mathrm{i} & 6.27 \times 10^{-14} + 4.88 \times 10^{-15} \mathrm{i} & 2.59 \times 10^{-14} + 2.01 \times 10^{-15} \mathrm{i} \\ 6.27 \times 10^{-14} + 4.88 \times 10^{-15} \mathrm{i} & 1.79 \times 10^{-6} + 6.97 \times 10^{-8} \mathrm{i} & 7.50 \times 10^{-14} + 5.84 \times 10^{-15} \mathrm{i} \\ 2.59 \times 10^{-14} + 2.01 \times 10^{-15} \mathrm{i} & 7.50 \times 10^{-14} + 5.84 \times 10^{-15} \mathrm{i} & 1.79 \times 10^{-6} + 6.97 \times 10^{-8} \mathrm{i} \end{array} \right).$$

The exact tensors for this object are known to be diagonal and multiple of identity [7, 14]. Specifically $(\mathcal{N})_{ii} = 1.80 \times 10^{-6}$ and $(\mathcal{M})_{ii} = 1.79 \times 10^{-6} + 6.97 \times 10^{-8}$ i to 2dp. By repeatably performing h or p refinement, the off diagonal terms tend to 0 and the diagonal entries of \mathcal{M}_{hp} and \mathcal{N}_{hp} to their exact values according to the convergence curves presented in Figure 3. In this case, the relative error $\|\mathcal{M} - \mathcal{M}_{hp}\|_F / \|\mathcal{M}\|_F = 2.72 \times 10^{-6}$. We also find the computed eigenvalues to be

$$\lambda(\mathcal{N}^0 + \mathcal{R}) = \begin{pmatrix} 1.79 \times 10^{-6} \\ 1.79 \times 10^{-6} \\ 1.79 \times 10^{-6} \end{pmatrix}, \quad \lambda(\mathcal{I}) = \begin{pmatrix} 6.97 \times 10^{-8} \\ 6.97 \times 10^{-8} \\ 6.97 \times 10^{-8} \end{pmatrix}.$$

We next consider the example of a full order frequency sweep once again for the sphere described by the .geo file in Figure 15.

6.1.2 Full order frequency sweep for a sphere

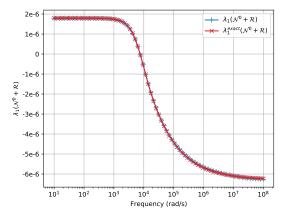
A frequency sweep is now performed for the sphere described by the sphere.geo file in Figure 15 along with the inputs represented in Table 2. As Single = False and Pod = False the following variables are not used Omega = 133.5, PODPoints = 13, PODTol = 10**-4 and hence their values are arbitrary.

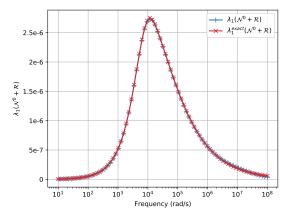
Geometry = "sphere.geo"	Single = False	PODTol = 10**-4
alpha = 0.01	Omega = 133.5	PODErrorBars = False
MeshSize = 2	Pod = False	FolderName = "Default"
Order = 3	PlotPod = False	Solver = "bddc"
Start = 1	MultiProcessing = True	epsi = 10**-12
Finish = 8	CPUs = 4	Maxsteps = 5000
Points = 81	PODPoints = 13	Tolerance = 10**-10
	ngsglobals.msg_level = 0	

Table 2: A table summarising the inputs for the simulation of a sphere for a full order frequency sweep.

This means our interest lies in computing the characterisation for $\alpha B = 0.01B$ at 81 frequencies in the range $10^1 \le \omega \le 10^8 \text{rad/s}$. Furthermore, the inputs lead to a mesh of 26751 elements and a discretisation

of p = 3. On a 2012 iMac with a 2.9 GHz quad core i5 processor with 16 GB 1600 MHz DDR3 memory the computation takes 1 hour and 4 minutes using 4 CPUs and produces the results shown in Figure 17.





- (a) A graph showing how $\lambda_1(\mathcal{N}^0 + \mathcal{R})$ changes with frequency.
- (b) A graph showing how $\lambda_1(\mathcal{I})$ changes with frequency.

Figure 17: Graphs displaying the eigenvalues of both the real and imaginary parts for \mathcal{M} calculated using a full order frequency sweep for a sphere compared with the exact values.

In Figure 17, we only show the first eigenvalues $\lambda_1(\mathcal{R}+\mathcal{N}^0)$ and $\lambda_1(\mathcal{I})$, this is due to the difference between $\lambda_1, \lambda_2, \lambda_3$ being negligible in each case. We also show the exact values of the eigenvalues, which corresponds to the diagonal coefficients of the tensors in this case [7, 14], in order to illustrate the performance of the sweep. Note that the code does not produce the exact value for $\lambda_1(\mathcal{R}+\mathcal{N}^0)$ and $\lambda_1(\mathcal{I})$ and these have been included afterwards for demonstration purposes. From a visual inspection, the simulation has obtained very good results and this is confirmed by a sweep of the relative error shown in Figure 18, which shows the maximum relative error is 0.006 over the sweep.

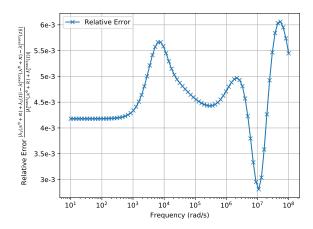


Figure 18: A graph showing how the relative error in the first eigenvalue changes due to frequency.

We next consider the case of a the reduced order frequency sweep using the POD.

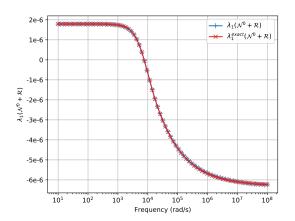
6.1.3 POD frequency sweep for a sphere

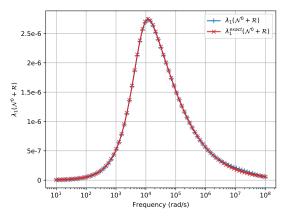
For this frequency sweep, the sphere described by the sphere.geo file in Figure 15 is simulated with the inputs as shown in Table 3. As Single = False the following variables are not used: Omega = 133.5 hence their values are arbitrary.

Geometry = "sphere.geo"	Single = False	PODTol = 10**-4
alpha = 0.01	Omega = 133.5	PODErrorBars = False
MeshSize = 2	Pod = True	FolderName = "Default"
Order = 3	PlotPod = True	Solver = "bddc"
Start = 1	MultiProcessing = True	epsi = 10**-12
Finish = 8	CPUs = 4	Maxsteps = 5000
Points = 81	PODPoints = 13	Tolerance = 10**-10
	ngsglobals.msg_level = 0	

Table 3: A table summarising the inputs for the simulation of a sphere for a reduced order frequency sweep.

This means our interest lies in computing the characterisation for $\alpha B = 0.01B$ at 81 output frequencies in the range $10^1 \le \omega \le 10^8 \text{rad/s}$ using the same mesh of 26751 elements and a p=3 discretisation. However, the result is now generated by using a POD technique in which 13 snapshots are chosen logarithmically (following the approach described in Section 4.1.1) in order to create to create the ROM. On a 2012 iMac with a 2.9 GHz quad core i5 processor with 16 GB 1600 MHz DDR3 memory the computation took 15 minutes and 45 seconds using 4 CPUs leading to the results shown in Figure 19.





- (a) A graph showing how $\lambda_1(\mathcal{N}^0 + \mathcal{R})$ changes with frequency.
- (b) A graph showing how $\lambda_1(\mathcal{I})$ changes with frequency.

Figure 19: Graphs displaying the eigenvalues of both the real and imaginary parts for \mathcal{M} calculated using a frequency sweep which implemented a POD for a sphere compared with the exact values.

Again only the first eigenvalues $\lambda_1(\mathcal{R} + \mathcal{N}^0)$ and $\lambda_1(\mathcal{I})$ are shown together with their exact values, added in a post-processing step. From Figure 19, we see that the sweep is very accurate and this is confirmed by showing the relative error as a function of frequency in Figure 20.

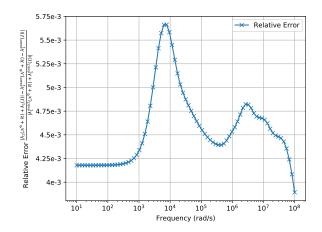
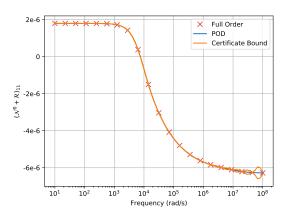
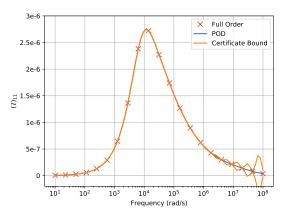


Figure 20: A graph showing how the relative error in the first eigenvalue changes due to frequency.

From Figure 20, we see that the performance is good, if not better, than the full order model, but only requires 13 full order model snapshots and took a quarter of the time of the full order model. However, if we set PODErrorBars =True then we obtain upper bounds on the difference between the full order and POD frequency sweeps. An example of this can be seen in Figure 21 this was run for 21 snapshots with a POD tolerance of 10^{-6} . Note that these certificate bounds are computed at run time with minimal additional computational cost. For further details of the cost break down and additional examples of certificate bounds see [15].





- (a) A graph showing how $(\mathcal{N}^0 + \mathcal{R})_{11}$ changes with frequency.
- (b) A graph showing how $(\mathcal{I})_{11}$ changes with frequency.

Figure 21: A graph showing the certificate bounds produced for the sphere with 21 snapshots with a POD tolerance of 10^{-6} .

For more detail about how the bounds are computed along with other examples please see [15]. With this we conclude the examples of the sphere, we next consider a simulation of a conducting permeable torus.

6.2 Torus

In this section, we consider the case where B is a torus with a major and minor radii of of 2 and 1, respectively, and the physical object αB is created from this object using the scaling $\alpha = 0.01$ m. We simulate a full order frequency sweep using the Torus.geo file shown in Figure 22, where Ω is chosen to be a ball of radius 100 containing the object B with material parameters $\sigma_* = 5.96 \times 10^6$ S/m and $\mu_* = 1.5\mu_0$.

```
algebraic3d
solid sphout = sphere (0, 0, 0; 100);
solid torin = torus (0, 0, 0; 1,0,0;2; 1) -maxh=0.4;
solid rest = sphout and not torin;
tlo rest -transparent -col=[0,0,1];#air
tlo torin -col=[1,0,0];#torus -mur=1.5 -sig=5.96E+06
```

Figure 22: An image showing the Torus.geo file used to simulate the torus.

To set up this simulation, we used the Torus.geo file shown in Figure 22 along with the inputs summarised in Table 4.

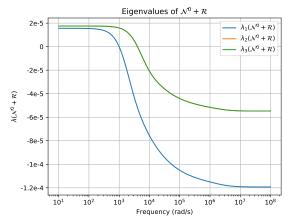
Geometry = "Torus.geo"	Single = False	PODTol = 10**-4
alpha = 0.01	Omega = 133.5	PODErrorBars = False
MeshSize = 3	Pod = False	FolderName = "Default"
Order = 3	PlotPod = True	Solver = "bddc"
Start = 1	MultiProcessing = True	epsi = 10**-12
Finish = 8	CPUs = 4	Maxsteps = 5000
Points = 81	PODPoints = 13	Tolerance = 10**-10
	ngsglobals.msg_level = 0	

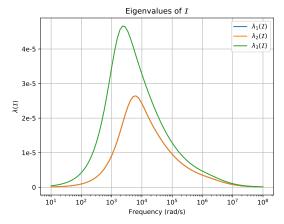
Table 4: A table summarising the inputs for the simulation of a torus for a reduced order frequency sweep.

This means our interest lies in computing the characterisation for $\alpha B = 0.01B$ at 81 frequencies in the range $10^1 \leqslant \omega \leqslant 10^8$ rad/s. Furthermore, the inputs lead to a mesh of 28953 elements and a discretisation of p=3. On a 2012 iMac with a 2.9 GHz quad core i5 processor with 16 GB 1600 MHz DDR3 memory the computation takes 1 hour 3 seconds using 4 CPUs (POD offers a considerable savings and comparable accuracy, see below). Using Order = 0 and the above settings has a run time of only 22 minutes 57 seconds, but with lower accuracy. In this case, the inputs in PlotterSettings.py are chosen to be as summarised in Table 5, which leads to the results shown in Figure 23.

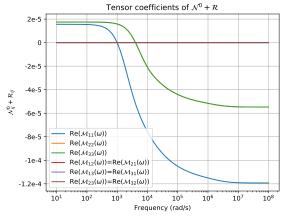
EigsToPlot = [1,2,3]	TensorsToPlot = $[1,4,6,2,3,5]$
MainLineStyle = "-"	MainMarkerSize = 4
SnapshotLineStyle = "x"	SnapshotMarkerSize = 8
ErrorBarLineStyle = ""	ErrorBarMarkerSize = 4
Title = True	Show = True

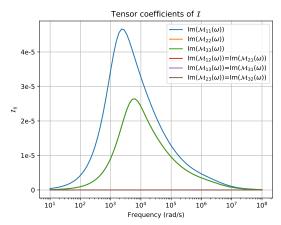
Table 5: A table summarising the inputs for the plots produced by the simulation of a torus using a reduced order frequency sweep.





- (a) A graph showing how $\lambda_i(\mathcal{N}^0 + \mathcal{R})$ changes with frequency.
- (b) A graph showing how $\lambda_i(\mathcal{I})$ changes with frequency.





- (c) A graph showing how $\mathcal{N}_{ij}^0 + \mathcal{R}_{ij}$ change with frequency.
- (d) A graph showing how \mathcal{I}_{ij} change with frequency.

Figure 23: Graphs displaying the eigenvalues and tensor coefficients of both the real and imaginary parts for \mathcal{M} calculated using a full order frequency sweep for a torus.

This means that the eigenvalues $\lambda_i(\mathcal{N}^0 + \mathcal{R})$, $\lambda_i(\mathcal{I})$, i = 1, 2, 3 are computed and shown as a function of frequency along with tensor coefficients $\mathcal{N}_{ij}^0 + \mathcal{R}_{ij}$, \mathcal{I}_{ij} for the combinations $(i, j) = \{(1, 1), (2, 2), (3, 3), (1, 2) = (2, 1), (1, 3) = (3, 1), (2, 3) = (3, 2)\}$. We note that the object has rotational and reflectional symmetries and so it has only 2 independent coefficients corresponding to tensor indices (1, 1) and (2, 2) = (3, 3) [5, 6].

Repeating the same simulation with Pod = True in Table 4 results in similar results, but only takes 14 minutes 38 seconds, which is a substantial saving.

With this we conclude our example of the torus, we next consider the example of a tetrahedron.

6.3 Tetrahedron

In this section, we consider the case where B is an irregular tetrahedron with vertices

$$(0,0,0), (7,0,0), (5.5,4.6,0), (3.3,2.0,0.5)$$

and αB is the irregular tetrahedron produced using the scaling $\alpha = 0.01 \text{m}$.

The geometry is described by Tetra.geo file as shown in Figure 24, where Ω is chosen to be a cube with sides of length 200 containing the object B and its material parameters are $\sigma_* = 5.96 \times 10^6$ S/m and $\mu_* = 2\mu_0$.

Figure 24: An image showing the Tetra.geo file used to simulate the torus.

The inputs for this simulation are summarised in Table 6.

Geometry = "Tetra.geo"	Single = False	PODTol = 10**-4
alpha = 0.01	Omega = 133.5	PODErrorBars = False
MeshSize = 3	Pod = True	FolderName = "Default"
Order = 3	PlotPod = True	Solver = "bddc"
Start = 1	MultiProcessing = True	epsi = 10**-12
Finish = 8	CPUs = 4	Maxsteps = 5000
Points = 81	PODPoints = 13	Tolerance = 10**-10
	ngsglobals.msg_level = 0	

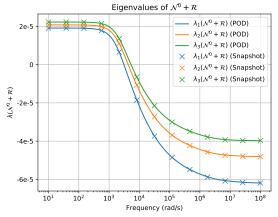
Table 6: A table summarising the inputs for the simulation of an irregular tetrahedron for a reduced order frequency sweep.

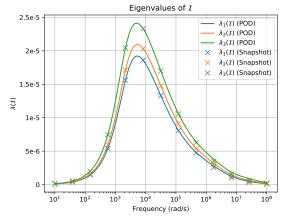
This means our interest lies in computing the characterisation for $\alpha B = 0.01B$ at 81 frequencies in the range $10^1 \le \omega \le 10^8$ rad/s. Furthermore, the inputs lead to a mesh of 20591 elements and a discretisation of p=3. In this case, a POD technique using 13 snapshots chosen logarithmically (following the approach described in Section 4.1.1) is used to create to create the ROM. On a 2012 iMac with a 2.9 GHz quad core i5 processor with 16 GB 1600 MHz DDR3 memory the computation takes 9 minutes and 48 seconds using 4 CPUs.

The inputs in PlotterSettings.py are summarised in Table 7 leading to the results shown in Figure 25.

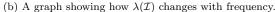
EigsToPlot = [1,2,3]	TensorsToPlot = [1,4,6,2,3,5]
MainLineStyle = "-"	MainMarkerSize = 4
SnapshotLineStyle = "x"	SnapshotMarkerSize = 8
ErrorBarLineStyle = ""	ErrorBarMarkerSize = 4
Title = True	Show = True

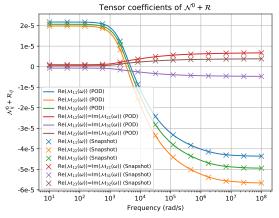
Table 7: A table summarising the inputs for the plots produced by the simulation of an irregular tetrahedron using a reduced order frequency sweep.

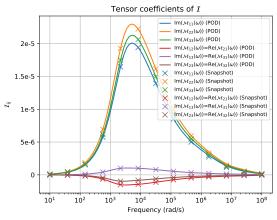




(a) A graph showing how $\lambda(\mathcal{N}^0 + \mathcal{R})$ changes with frequency.







(c) A graph showing how $\mathcal{N}_{ij}^0 + \mathcal{R}_{ij}$ change with frequency.

(d) A graph showing how \mathcal{I}_{ij} change with frequency.

Figure 25: Graphs displaying the eigenvalues and tensor coefficients of both the real and imaginary parts for \mathcal{M} calculated using a reduced order frequency sweep for a tetrahedron.

From Figure 25, we see that \mathcal{M} has 6 independent non-zero coefficients, due to the lack of rotational and reflectional symmetries in the (irregular) tetrahedron. With this we conclude our example of the tetrahedron, we next consider the case of a bar created using two regions.

6.4 Dual Bar

In this section we consider $B=B^{(1)}\cup B^{(2)}$ to be a bar created by joining two rectangular blocks with different parameters. The physical object αB is obtained by scaling B by $\alpha=0.01\mathrm{m}$. The geometry described by the DualBar.geo file in Figure 26, where Ω is chosen to be a ball of radius 100 containing the object B. Following the notation in [9], the material parameters of $B^{(1)}$ and $B^{(2)}$ are

$$\sigma_*^{(1)} = 10^6 \text{ S/m}$$
 and $\mu_*^{(1)} = \mu_0$
 $\sigma_*^{(2)} = 10^8 \text{ S/m}$ $\mu_*^{(2)} = \mu_0$

```
algebraic3d

solid rest = sphere (0, 0, 0; 100);
solid brick1 = orthobrick (-1,0,0;0,1,1) -maxh=0.12;
solid brick2 = orthobrick (0,0,0;1,1,1) -maxh=0.12;

solid domain = rest and not brick1 and not brick2;

tlo domain -transparent -col=[0,0,1];#air
tlo brick1 -col=[1,0,0];#mat1 -mur=1 -sig=1E+06
tlo brick2 -col=[0,1,0];#mat2 -mur=1 -sig=1E+08
```

Figure 26: An image showing the DualBar.geo file used to simulate the torus.

To set up this simulation, we used the Dualbar.geo file shown in Figure 26 along with the inputs summarised in Table 8

Geometry = "DualBar.geo"	Single = False	PODTol = 10**-5
alpha = 0.01	Omega = 133.5	PODErrorBars = False
MeshSize = 3	Pod = True	FolderName = "Default"
Order = 3	PlotPod = True	Solver = "bddc"
Start = 2	MultiProcessing = True	epsi = 10**-12
Finish = 7	CPUs = 4	Maxsteps = 5000
Points = 81	PODPoints = 9	Tolerance = 10**-10
	ngsglobals.msg_level = 0	

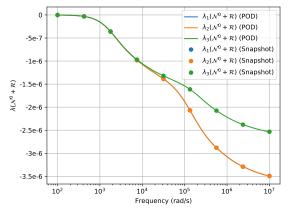
Table 8: A table summarising the inputs for the simulation of a bar containing two regions for a reduced order frequency sweep.

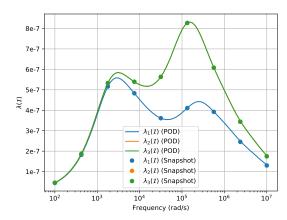
This means our interest lies in computing the characterisation for $\alpha B = 0.01B$ at 81 frequencies in the range $10^2 \le \omega \le 10^7$ rad/s. Furthermore, the inputs lead to a mesh of 30209 elements and a discretisation of p=3. In this case, a POD technique using 9 snapshots chosen logarithmically (following the approach described in Section 4.1.1) is used to create to create the ROM. On a 2012 iMac with a 2.9 GHz quad core i5 processor with 16 GB 1600 MHz DDR3 memory the computation takes 11 minutes and 30 seconds using 4 CPUs.

The inputs of PLotterSettings.py are summarised in Table 9 leading to the results shown in Figure 27.

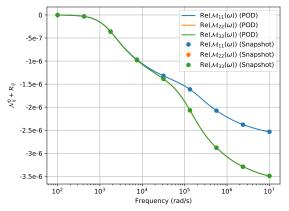
EigsToPlot = [1,2,3]	TensorsToPlot = [1,4,6]
MainLineStyle = "-"	MainMarkerSize = 4
SnapshotLineStyle = "o"	SnapshotMarkerSize = 6
ErrorBarLineStyle = ""	ErrorBarMarkerSize = 4
Title = False	Show = True

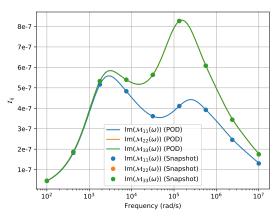
Table 9: A table summarising the inputs for the plots produced by the simulation of bar created using two regions using a reduced order frequency sweep.





- (a) A graph showing how $\lambda(\mathcal{N}^0 + \mathcal{R})$ changes with frequency.
- (b) A graph showing how $\lambda(\mathcal{I})$ changes with frequency.





- (c) A graph showing how $\mathcal{N}_{ij}^0 + \mathcal{R}_{ij}$ change with frequency.
- (d) A graph showing how \mathcal{I}_{ij} change with frequency.

Figure 27: Graphs displaying the eigenvalues and tensor coefficients of both the real and imaginary parts for \mathcal{M} calculated using a reduced order frequency sweep for a bar constructed of two regions.

In this case, we have chosen to plot only the non-zero coefficients of the tensors by changing the settings in PlotterSettings.py. With this we conclude our example of the bar of two regions, we next consider the case of a rifle shell.

6.5 Rifle shell casing

Finally, we consider αB to the be the rifle shell casing as defined in [10, 6] where B is defined such that $\alpha = 0.001$ m. The geometry for B is defined by the rifle.geo file in Figure 28, where Ω is chosen to be a cube with sides of length 2000 containing the shell B, which has material properties $\sigma_* = 1.5 \times 10^7$ S/m and $\mu_* = \mu_0$.

```
algebraic3d
 solid boxout = orthobrick (-1000, -1000, -1000; 1000, 1000, 1000);
solid cylinlinend = cylinder (0,0,-21.59;0,0, -21.09; 4.8)
and plane (0,0,-21.59; 0,0,-1)
and plane (0,0,-21.09; 0,0,1);
 solid cylin1out = cone (0,0,-21.09; 4.8; 0,0,10.54; 4.535)
and plane (0,0,-21.09;0,0, -1)
and plane (0,0,10.54;0,0, 1);
 solid conelout = cone (0,0,10.54; 4.535; 0,0,13.65; 3.215)
               and plane (0,0,10.54; 0,0,-1) and plane (0,0,13.65; 0,0,1);
           cylin2out = cylinder (0,0,13.65; 0,0, 21.59; 3.215)
and plane (0,0,13.65; 0,0,-1)
and plane (0,0,21.59; 0,0,1);
solid cylin1in = cone (0,0,-21.09; 4.3; 0,0,10.54; 4.035)
and plane (0,0,-21.09;0,0, -1)
and plane (0,0,10.54;0,0, 1);
solid conelin = cone (0,0,10.54; 4.035; 0,0,13.65; 2.715)
and plane (0,0,10.54; 0,0,-1)
and plane (0,0,13.65; 0,0,1);
           cylin2in = cylinder (0,0,13.65; 0,0, 21.59; 2.715) and plane (0,0,13.65; 0,0,-1) and plane (0,0,21.59; 0,0,1);
solid shell1 = cylin1out and not cylin1in -maxh=0.8;
solid shellend = cylin1inend -maxh=0.8;
solid shell2 = conelout and not conelin -maxh=0.8:
solid shell3 = cylin2out and not cylin2in -maxh=0.8;
solid rest1 = cylin1out and cylin1in;
solid rest2 = cone1out and cone1in;
solid rest3 = cylin2out and cylin2in;
 solid rest4 = boxout and not cylin1out and not cone1out and not cylin2out and not shellend;
 tlo rest1 -transparent -col=[0,0,1];#air
tlo rest2 -transparent -col=[0,0,1];#air
tlo rest3 -transparent -col=[0,0,1];#air
tlo rest4 -transparent -col=[0,0,1];#air
       shell1 -col=[1,0,0];#shell -mur=1 -sig=1.5E+07
shell2 -col=[1,0,0];#shell
shell3 -col=[1,0,0];#shell
shellend -col=[1,0,0];#shell
```

Figure 28: An image showing the rifle.geo file used to simulate the rifle shell casing.

To set up this simulation, we used the rfle.geo file show in Figure 28 along with the inputs summarised in Table 10.

Geometry = "rifle.geo"	Single = False	PODTol = 10**-4
alpha = 0.001	Omega = 133.5	PODErrorBars = False
MeshSize = 3	Pod = True	FolderName = "Default"
Order = 3	PlotPod = True	Solver = "bddc"
Start = 1	MultiProcessing = True	epsi = 10**-12
Finish = 9	CPUs = 4	Maxsteps = 5000
Points = 81	PODPoints = 9	Tolerance = 10**-10
	ngsglobals.msg_level = 0	

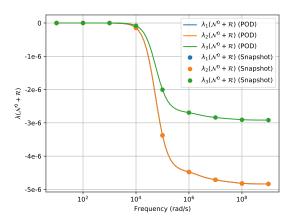
Table 10: A table summarising the inputs for the simulation of a rifle shell casing for a reduced order frequency sweep.

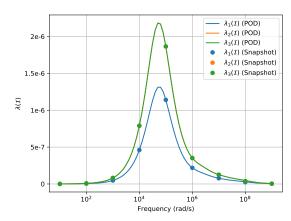
This means our interest lies in computing the charcterisation for $\alpha B = 0.001B$ at 81 frequencies in the range $10^1 \le \omega \le 10^9$ rad/s. Furthermore, the inputs lead to a mesh of 73082 elements and a discretisation of p=3. In this case, a POD technique using 9 snapshots chosen logarithmically (following the approach described in Section 4.1.1) is used to create to create the ROM. On a 2012 iMac with a 2.9GHz quad core i5 processor with 16 Gb 1600 MHz DDR3 memory the computation takes 35 minutes and 31 seconds using 4 CPUs.

The inputs of PlotterSettings.py are summarised in Table 11 leading to the results shown in Figure 29.

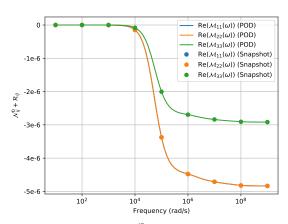
EigsToPlot = [1,2,3]	TensorsToPlot = [1,4,6]
MainLineStyle = "-"	MainMarkerSize = 4
SnapshotLineStyle = "o"	SnapshotMarkerSize = 6
ErrorBarLineStyle = ""	ErrorBarMarkerSize = 4
Title = False	Show = True

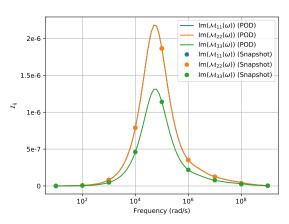
Table 11: A table summarising the inputs for the plots produced by the simulation of a rifle shell casing using a reduced order frequency sweep.





- (a) A graph showing how $\lambda(\mathcal{N}^0 + \mathcal{R})$ changes with frequency.
- (b) A graph showing how $\lambda(\mathcal{I})$ changes with frequency.





- (c) A graph showing how $\mathcal{N}_{ij}^0 + \mathcal{R}_{ij}$ change with frequency.
- (d) A graph showing how \mathcal{I}_{ij} change with frequency.

Figure 29: Graphs displaying the eigenvalues and tensor coefficients of both the real and imaginary parts for \mathcal{M} calculated using a reduced order frequency sweep for a rifle shell casing.

Once again we have only plotted the non-zero tensor coefficients. In Figure 29 (c) we note that the curve could be improved around $\omega=10^6$, although is still 'acceptable' if compared to the full order model. This suggests that we may wish to include some more additional snapshots in the reduced order model. Nevertheless, this 81 point frequency sweep for an object αB discretized by 73082 element mesh with p=3 using the POD is computed in considerably less time than the corresponding full order model.

Along with the .geo files for the examples which have been discussed in this article, there are a selection of other .geo files which are included with the download of the code.

7 Citation

If you use the tool, please refer to it in your work by citing the references

- [15] B. A. Wilson and P. D. Ledger, Efficient numerical schemes for the computation of the magnetic polarizability tensor, In preparation, 2019.
- [8], P. D. Ledger and W. R. B. Lionheart, The spectral properties of the magnetic polarizability tensor for metallic object characterisation, Math Meth Appl Sci., 2019, doi:10.1002/mma.5830
- [7] P. D. Ledger and W. R. B. Lionheart, An explicit formula for the magnetic polarizability tensor for object characterization, IEEE Trans Geosci Remote Sens., 56(6), 3520-3533, 2018.

as well as those of NGSolve:

- [13] J. Schöberl, C++11 Implementation of Finite Elements in NGSolve, ASC Report 30/2014, Institute for Analysis and Scientific Computing, Vienna University of Technology, 2014.
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