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Appendix A

Experimental Results

Results from the experiments performed in Chapter 3 are presented here.

A.1 Exponential Horn

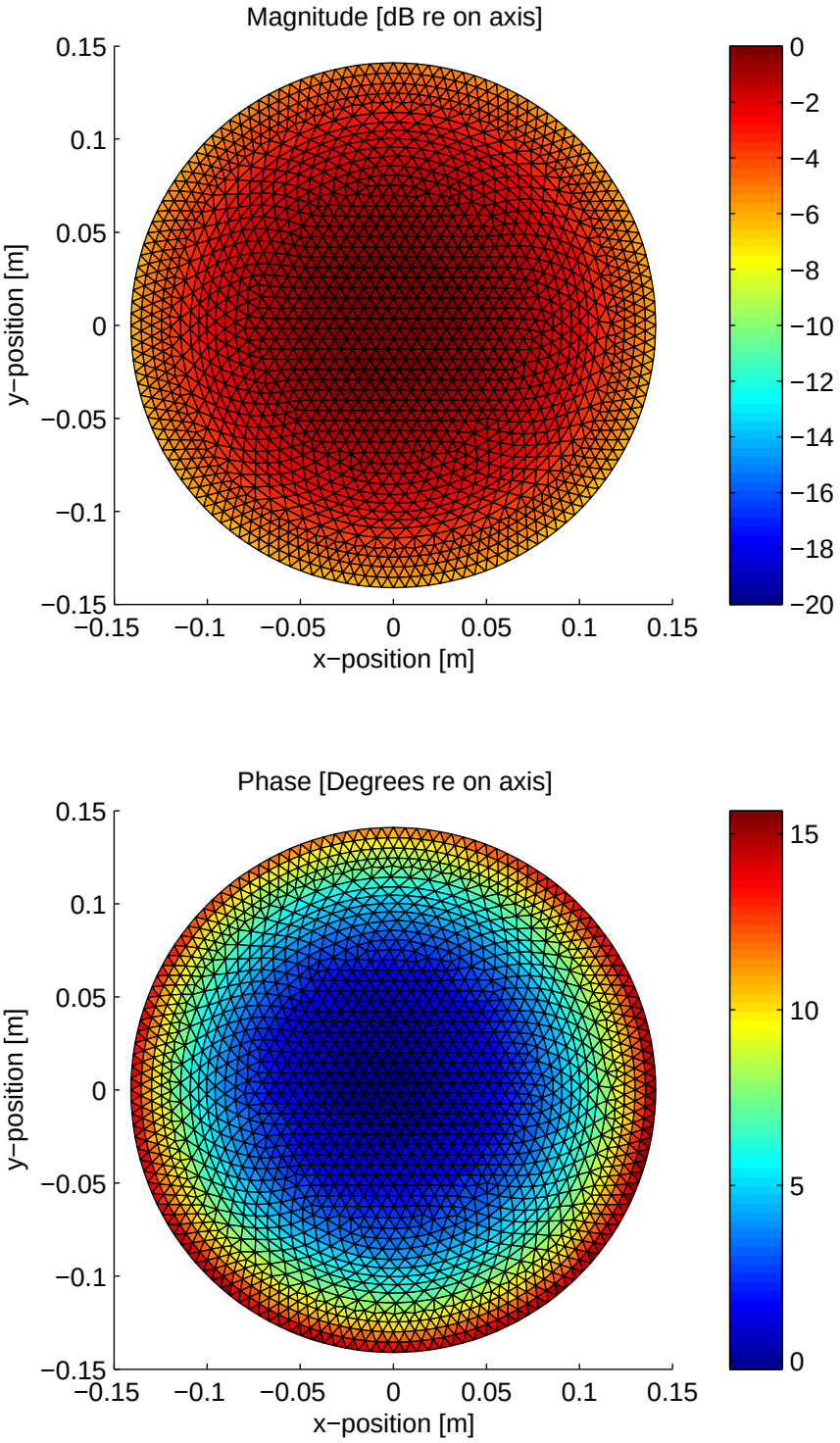


Figure A.1: Exponential horn, frequency 410 *Hz*

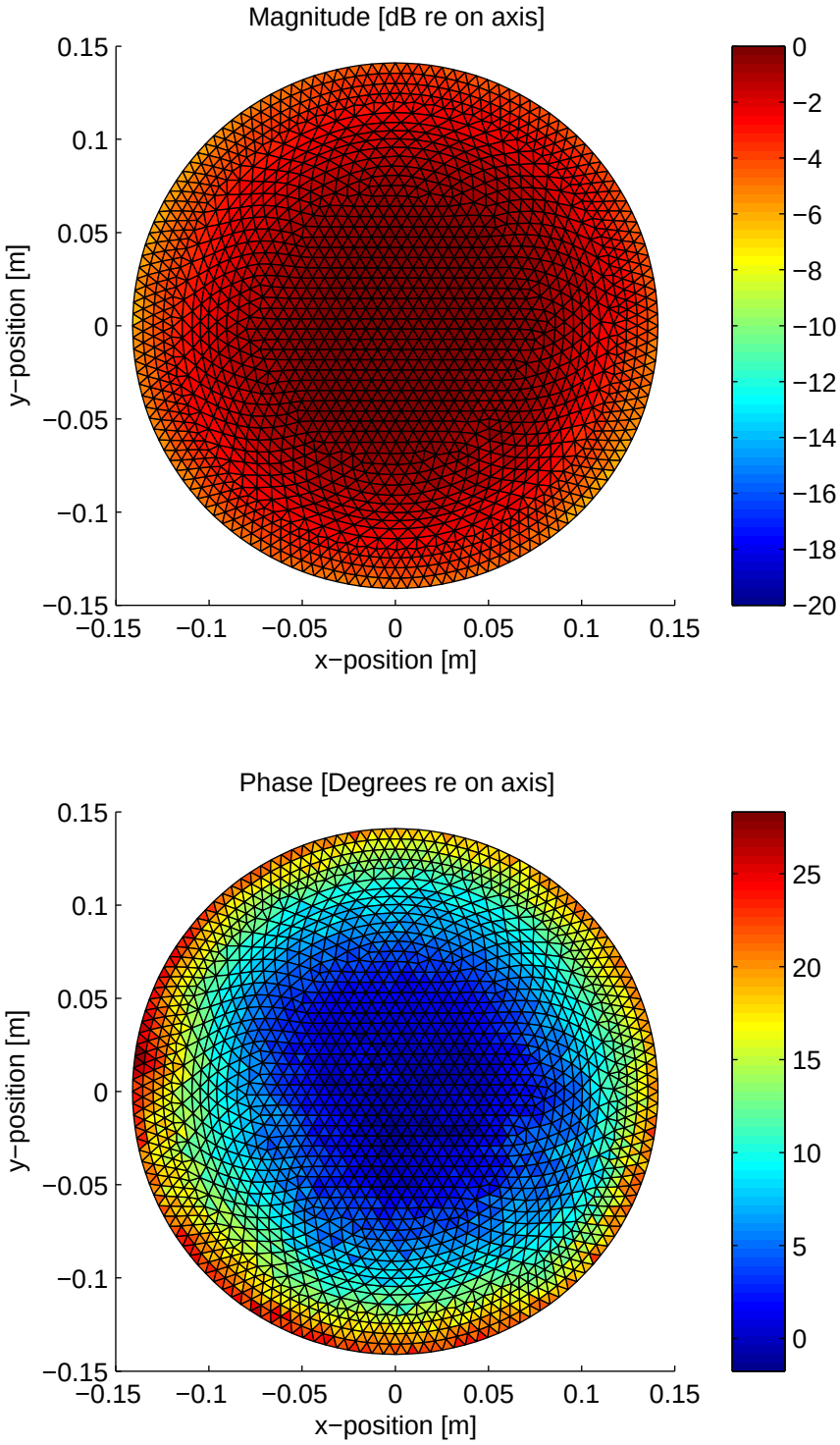


Figure A.2: Exponential horn, frequency 710 *Hz*

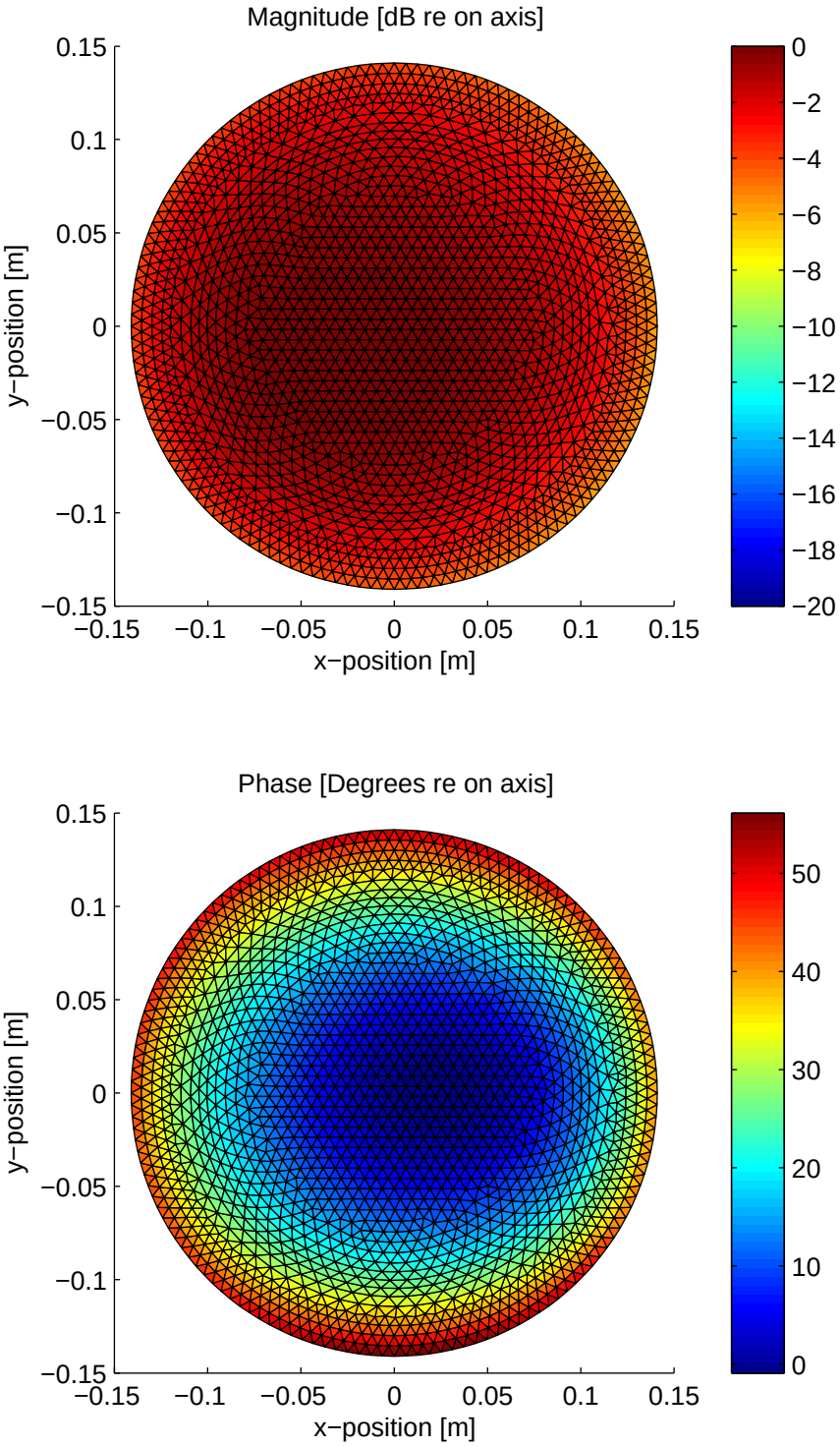


Figure A.3: Exponential horn, frequency 1320 *Hz*

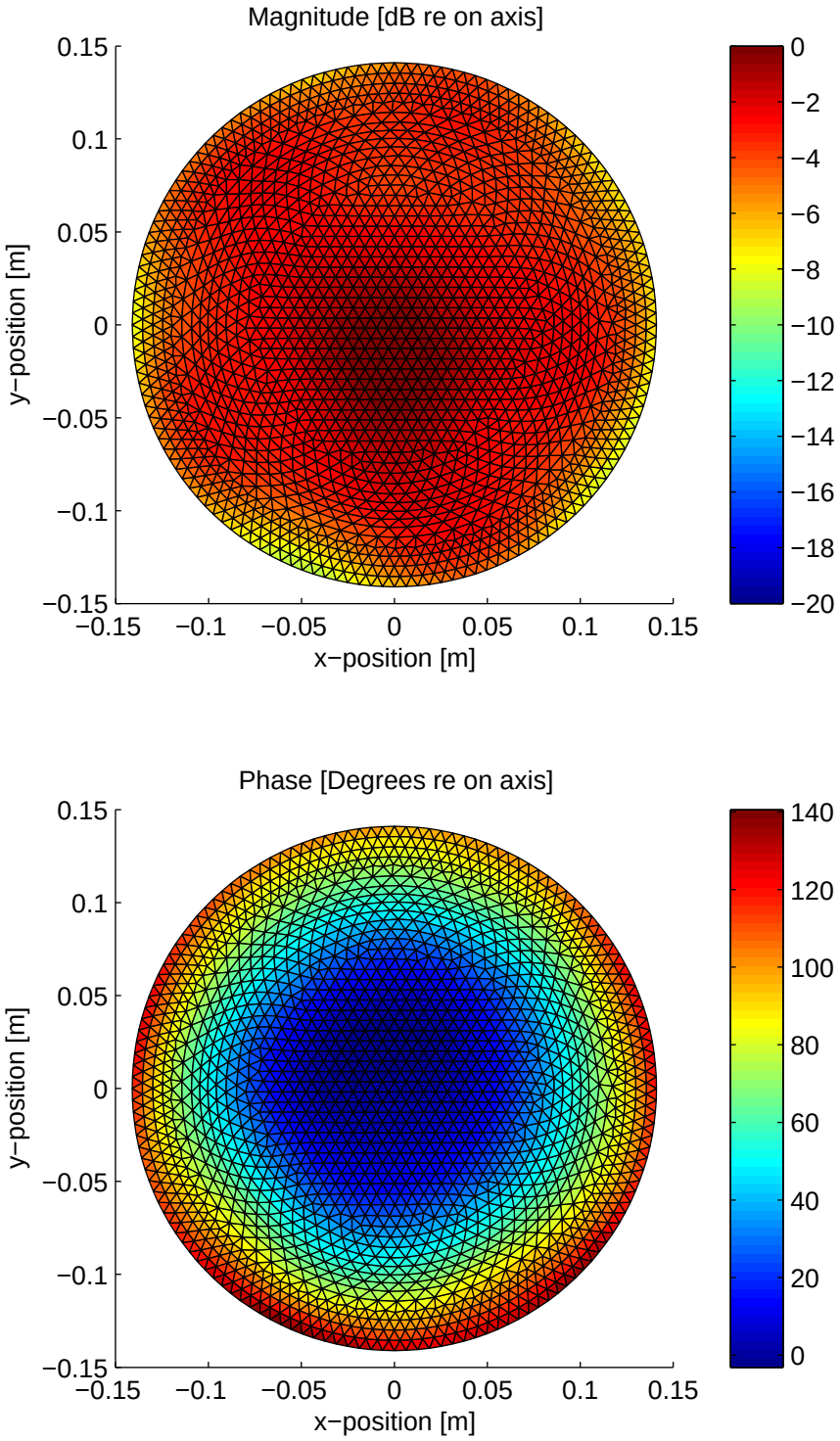


Figure A.4: Exponential horn, frequency 2840 *Hz*

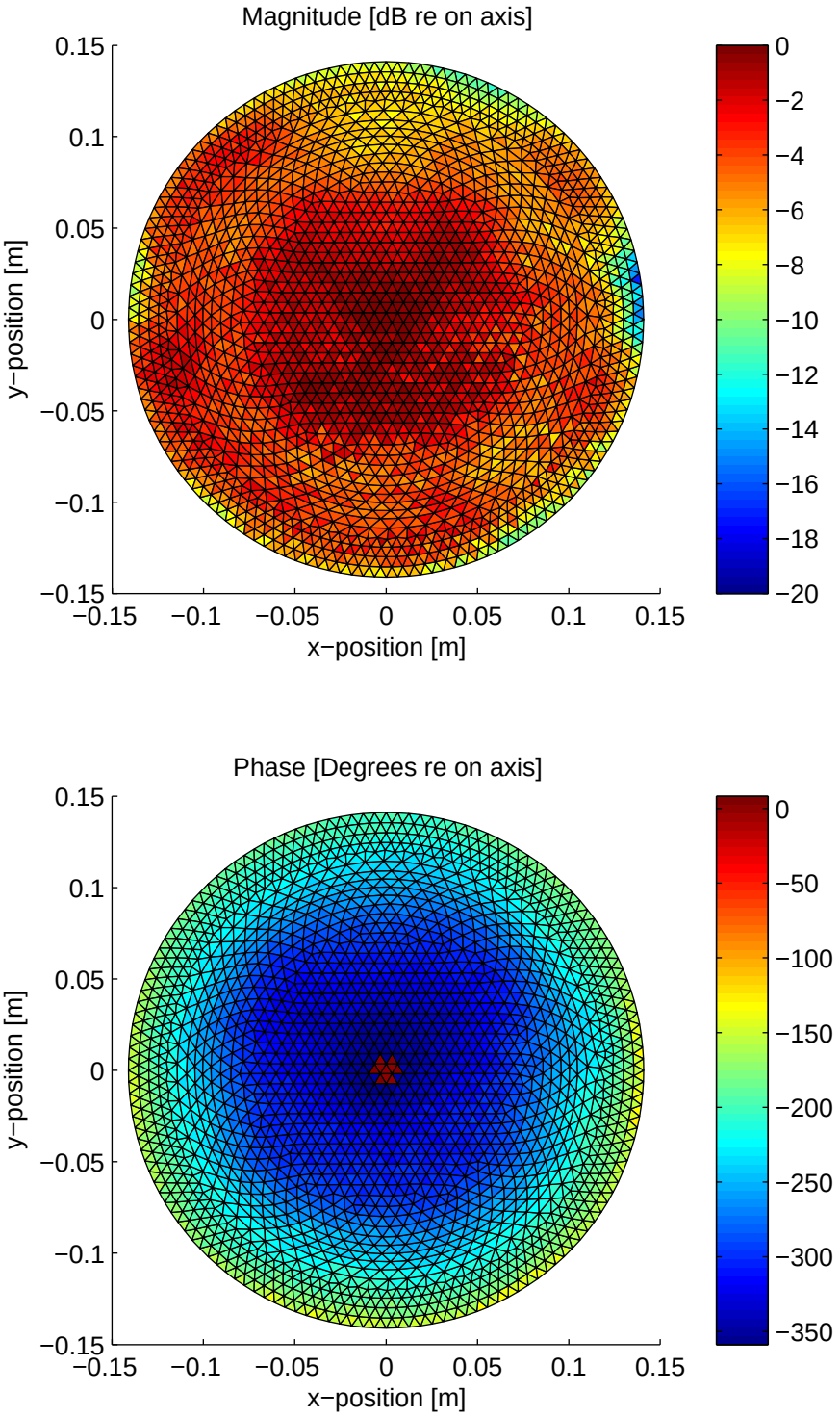


Figure A.5: Exponential horn, frequency 4360 *Hz*

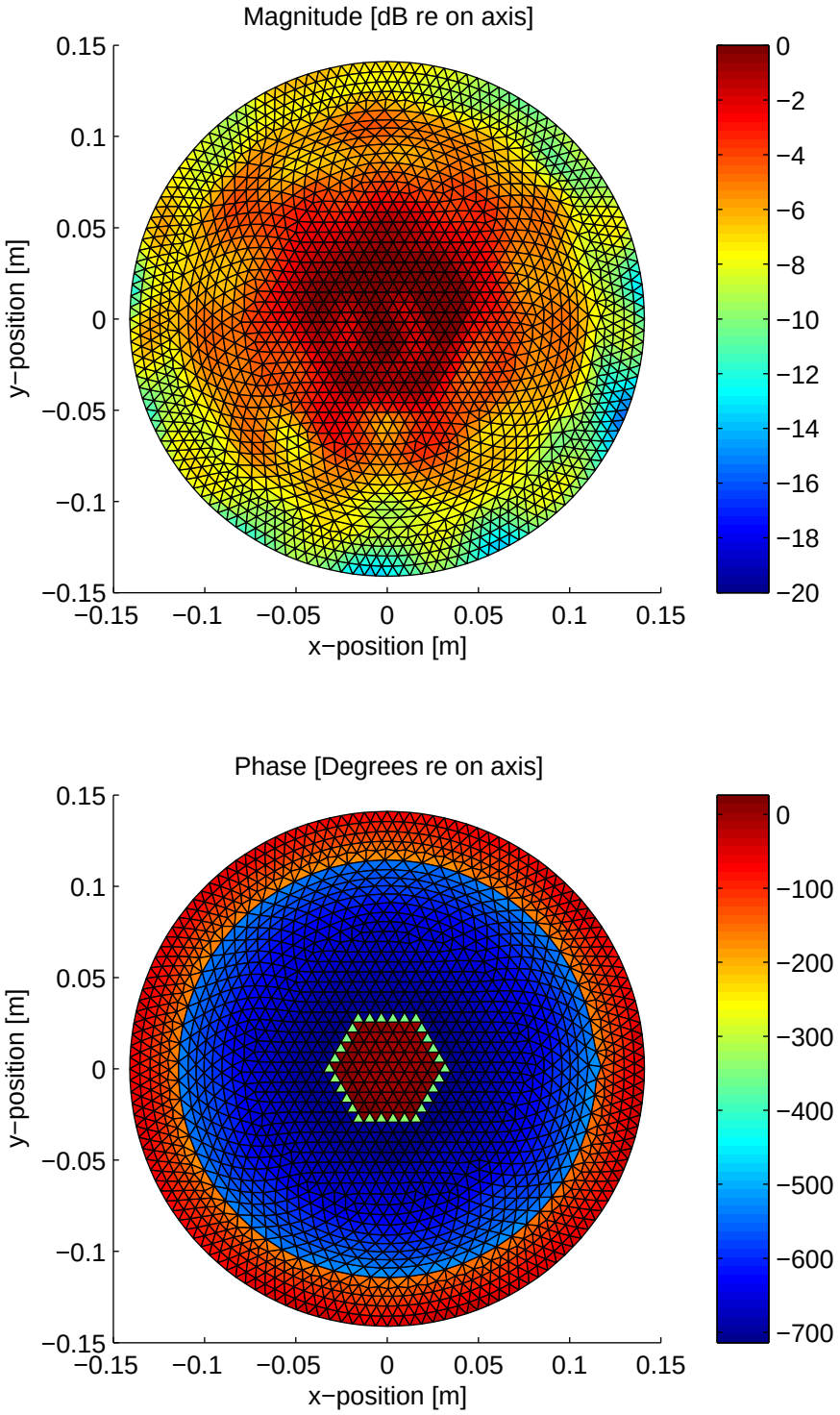


Figure A.6: Exponential horn, frequency 7400 *Hz*

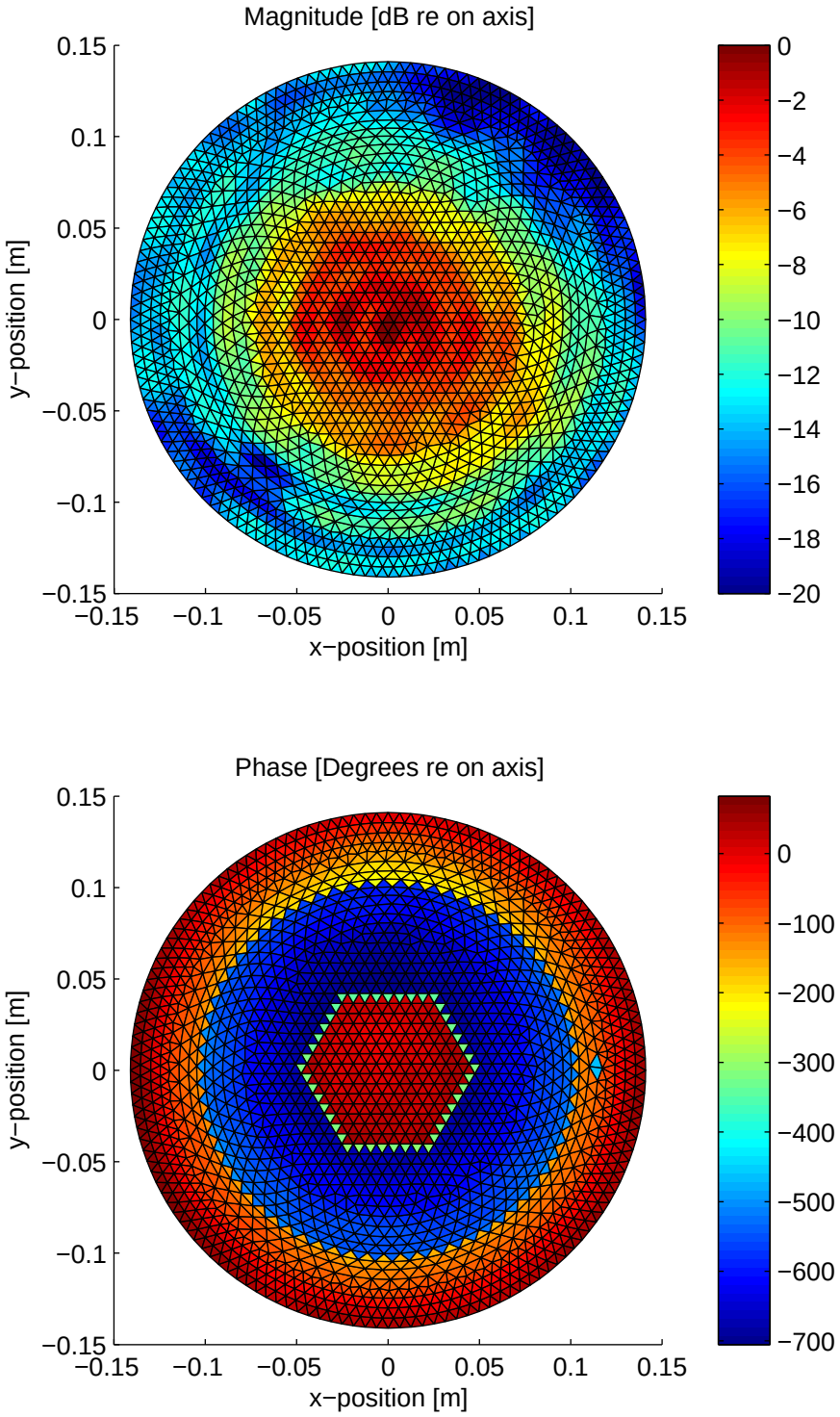


Figure A.7: Exponential horn, frequency 10440 *Hz*

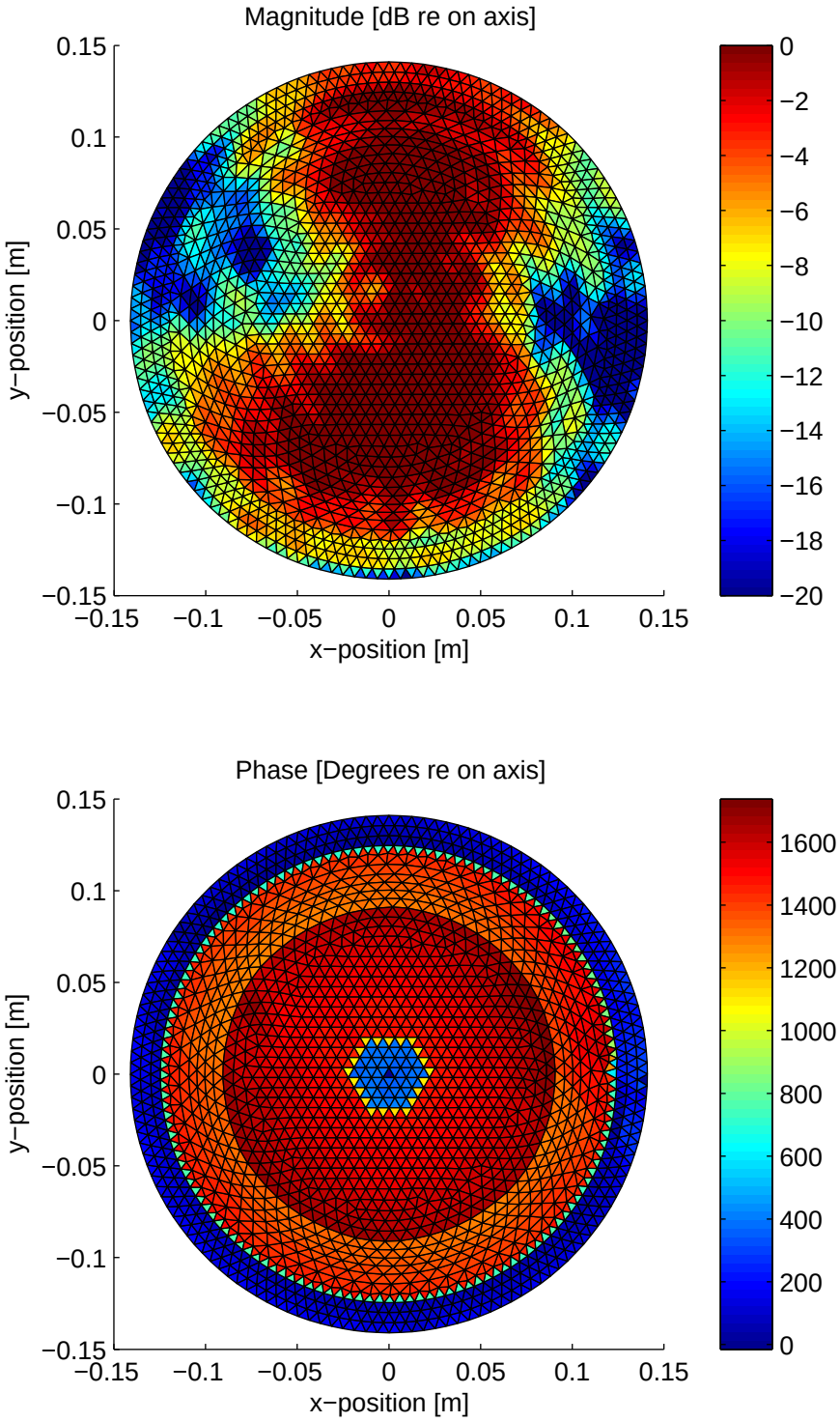


Figure A.8: Exponential horn, frequency 12260 *Hz*

A.2 Conical Horn

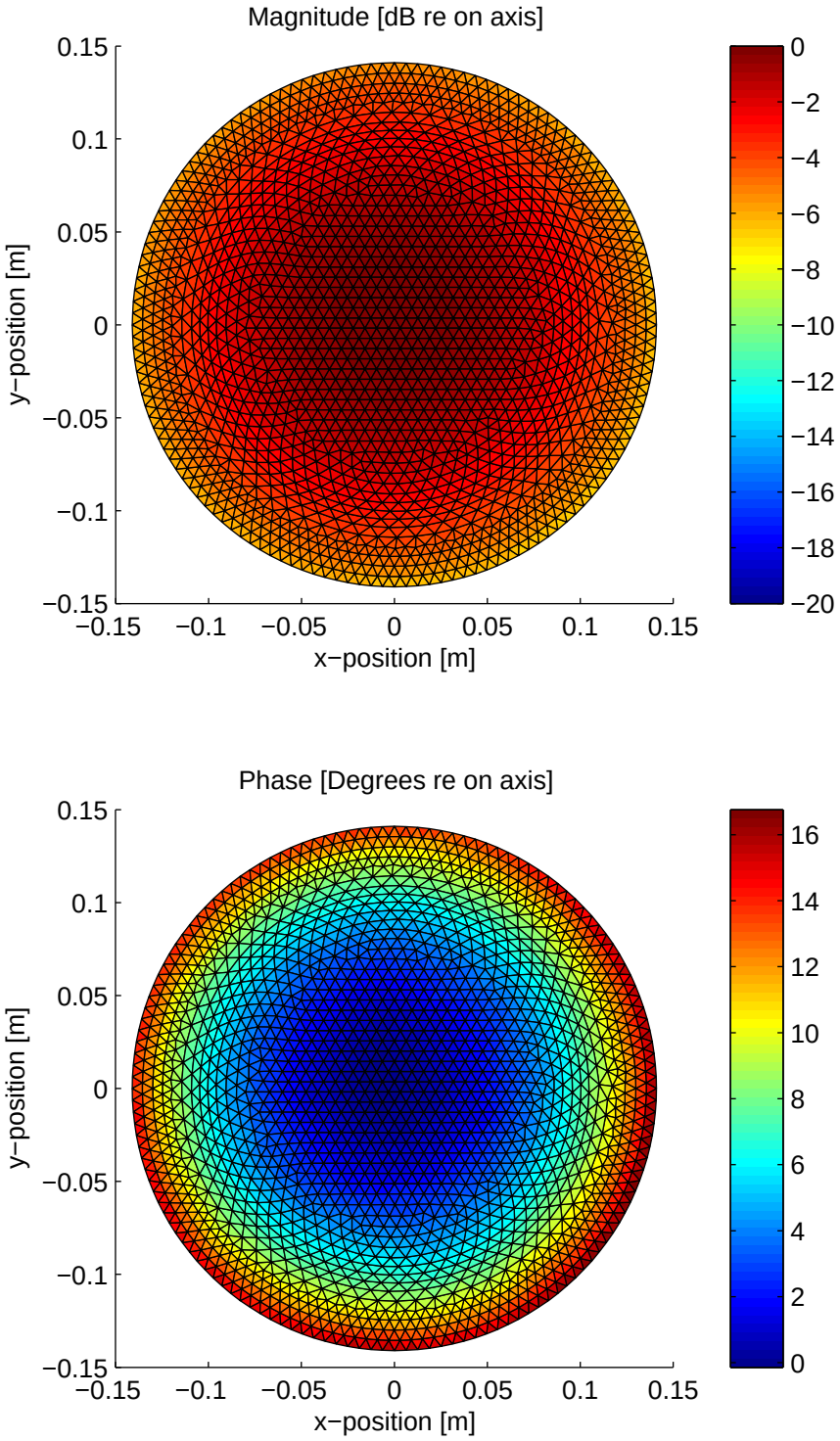


Figure A.9: Conical horn, frequency 410 *Hz*

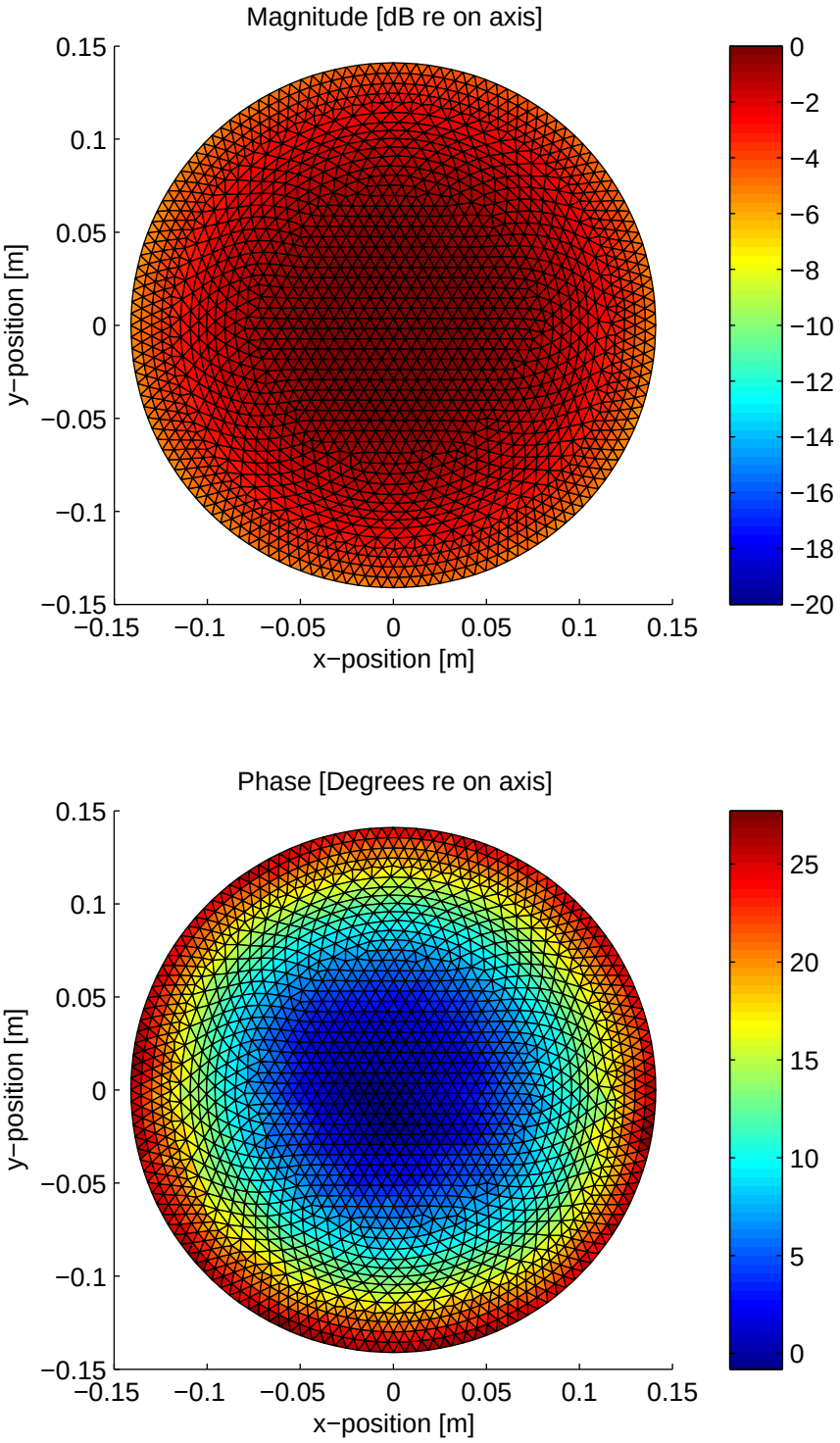


Figure A.10: Conical horn, frequency 710 *Hz*

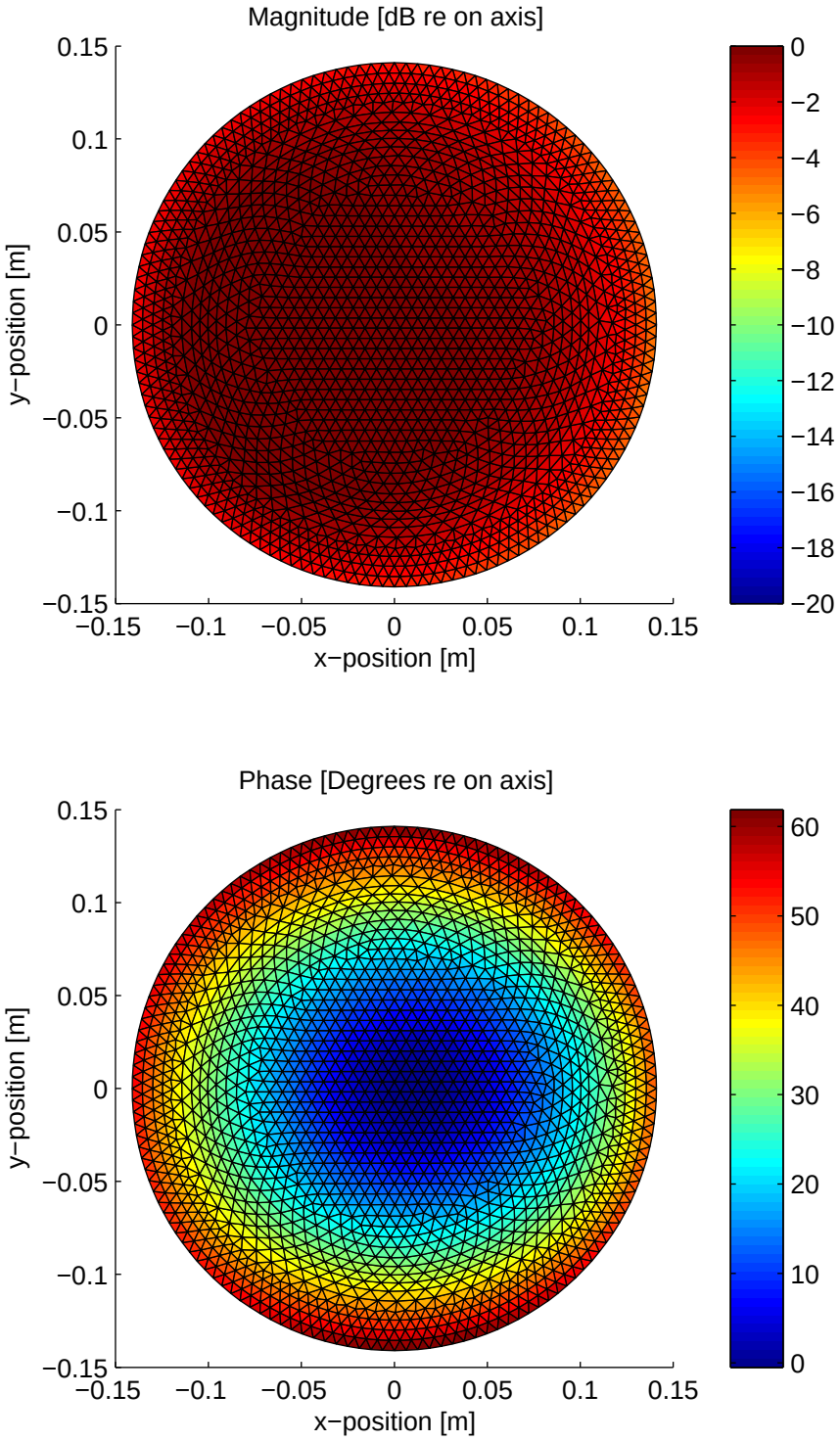


Figure A.11: Conical horn, frequency 1320 *Hz*

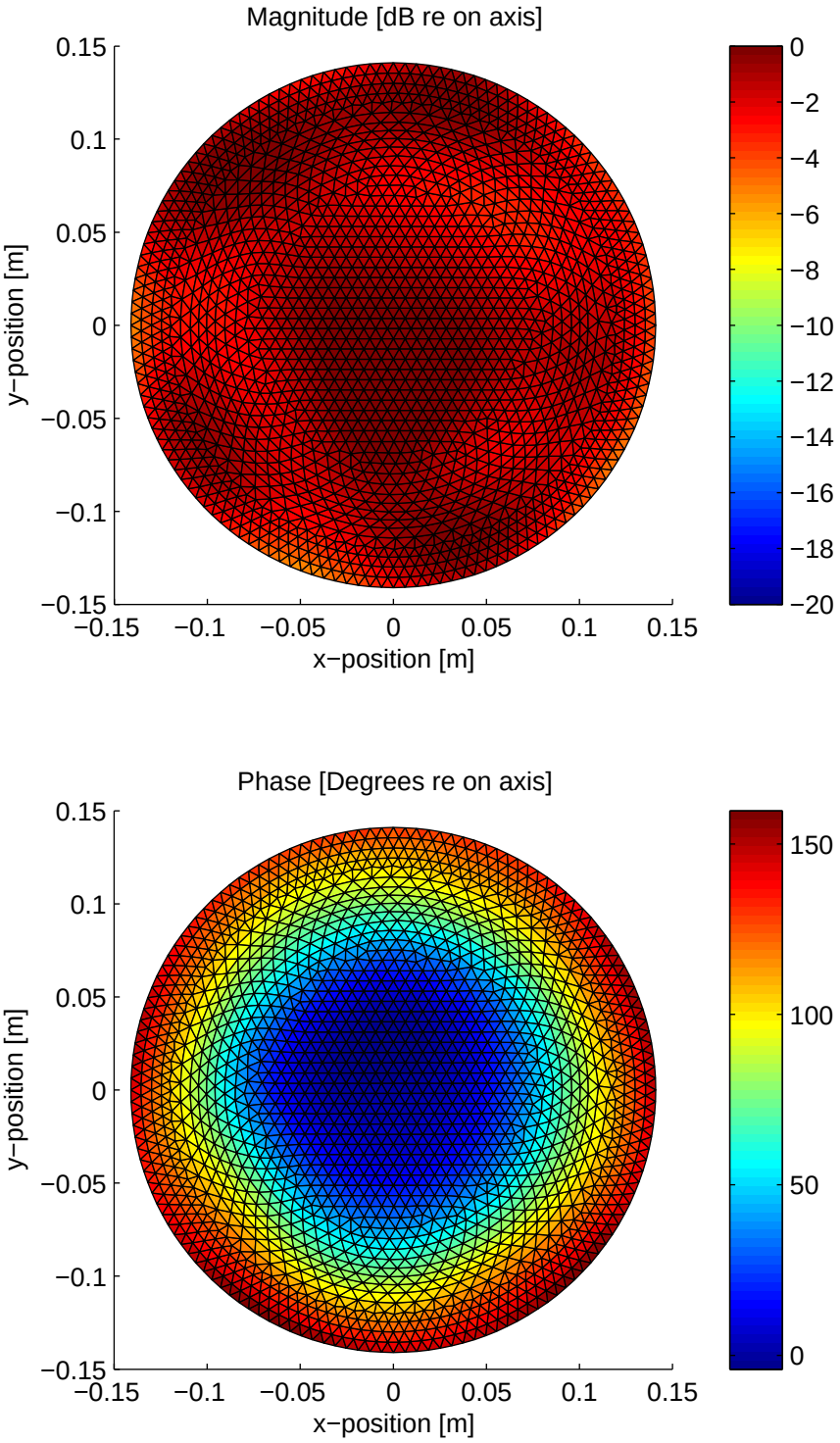


Figure A.12: Conical horn, frequency 2840 *Hz*

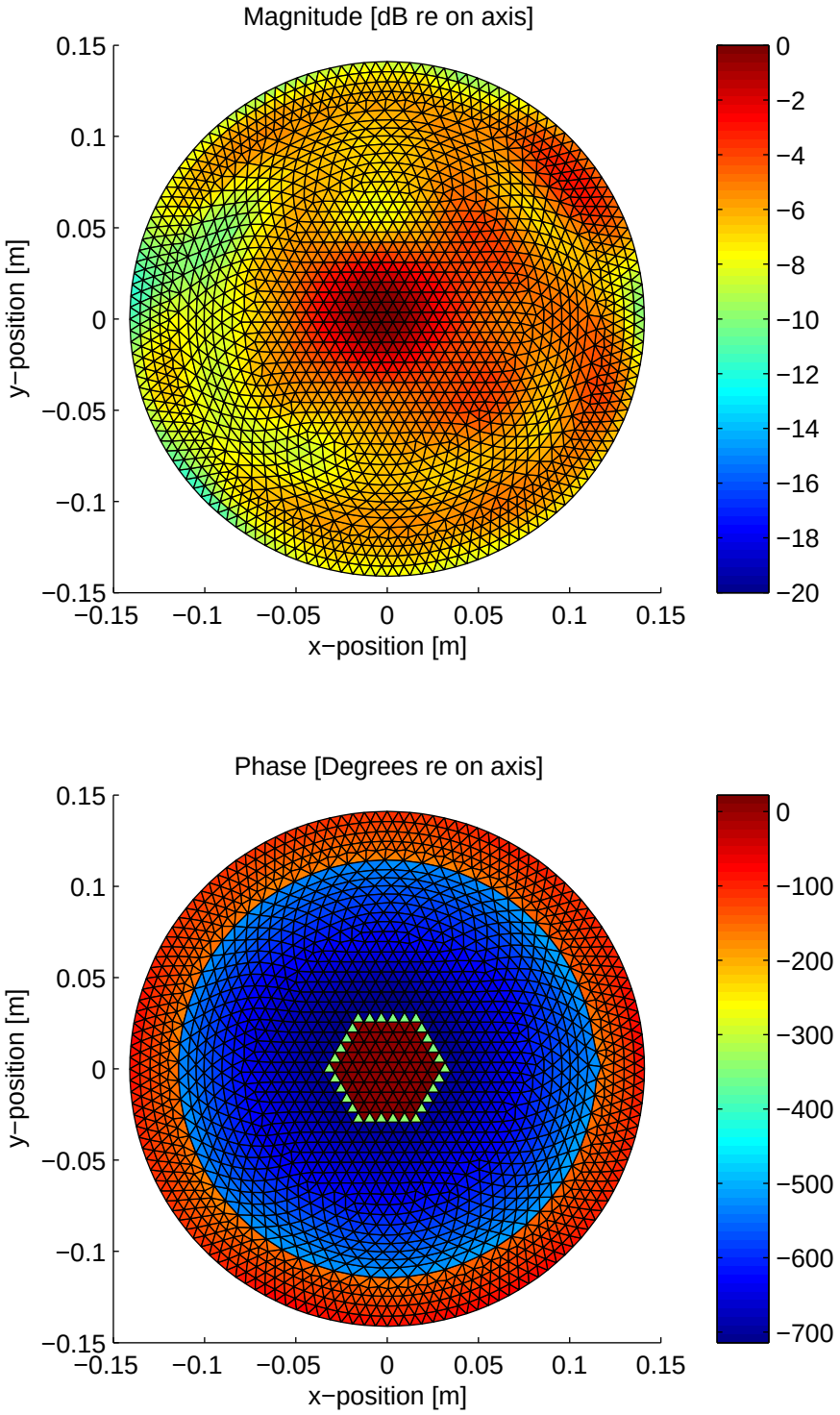


Figure A.13: Conical horn, frequency 4360 *Hz*

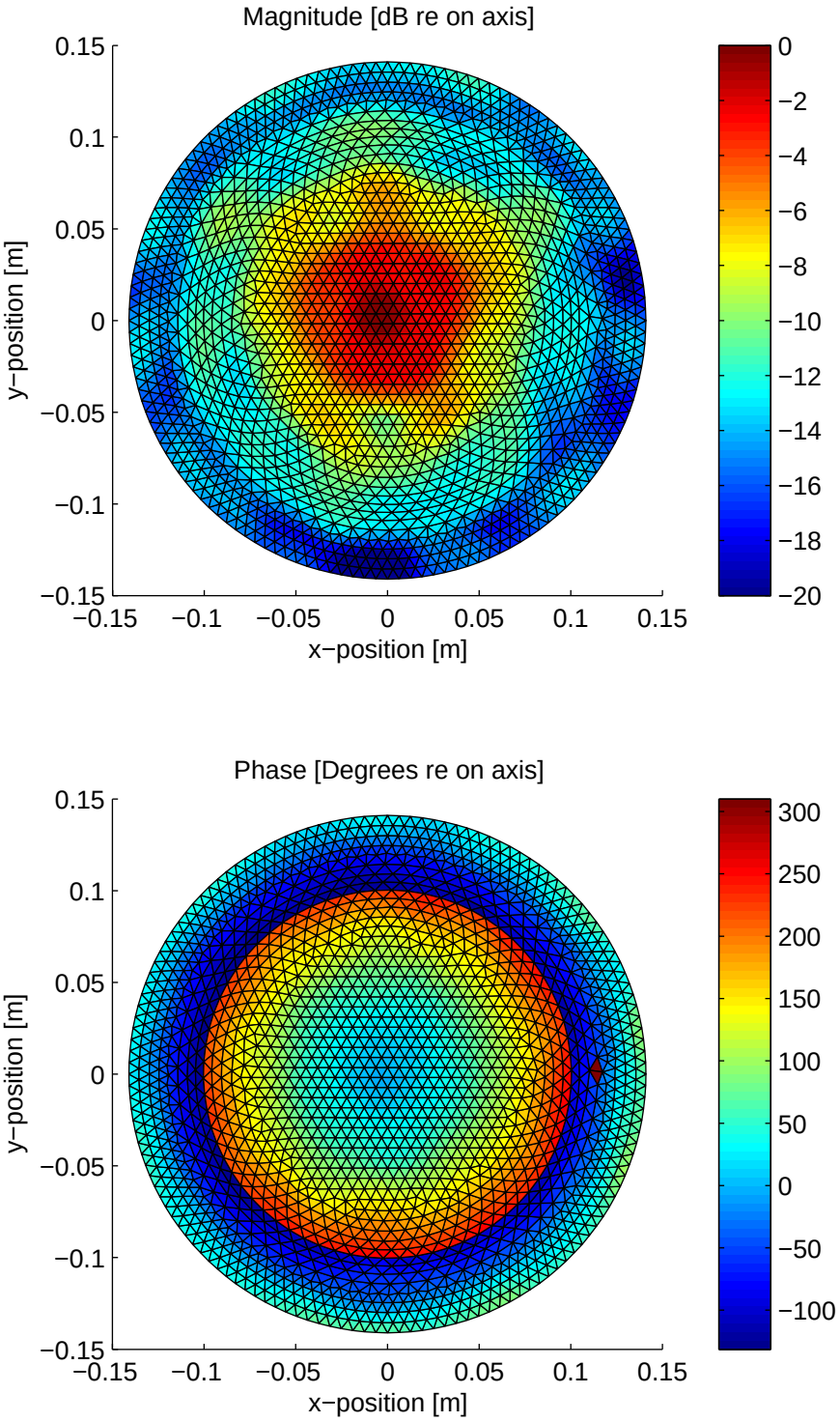


Figure A.14: Conical horn, frequency 7400 Hz

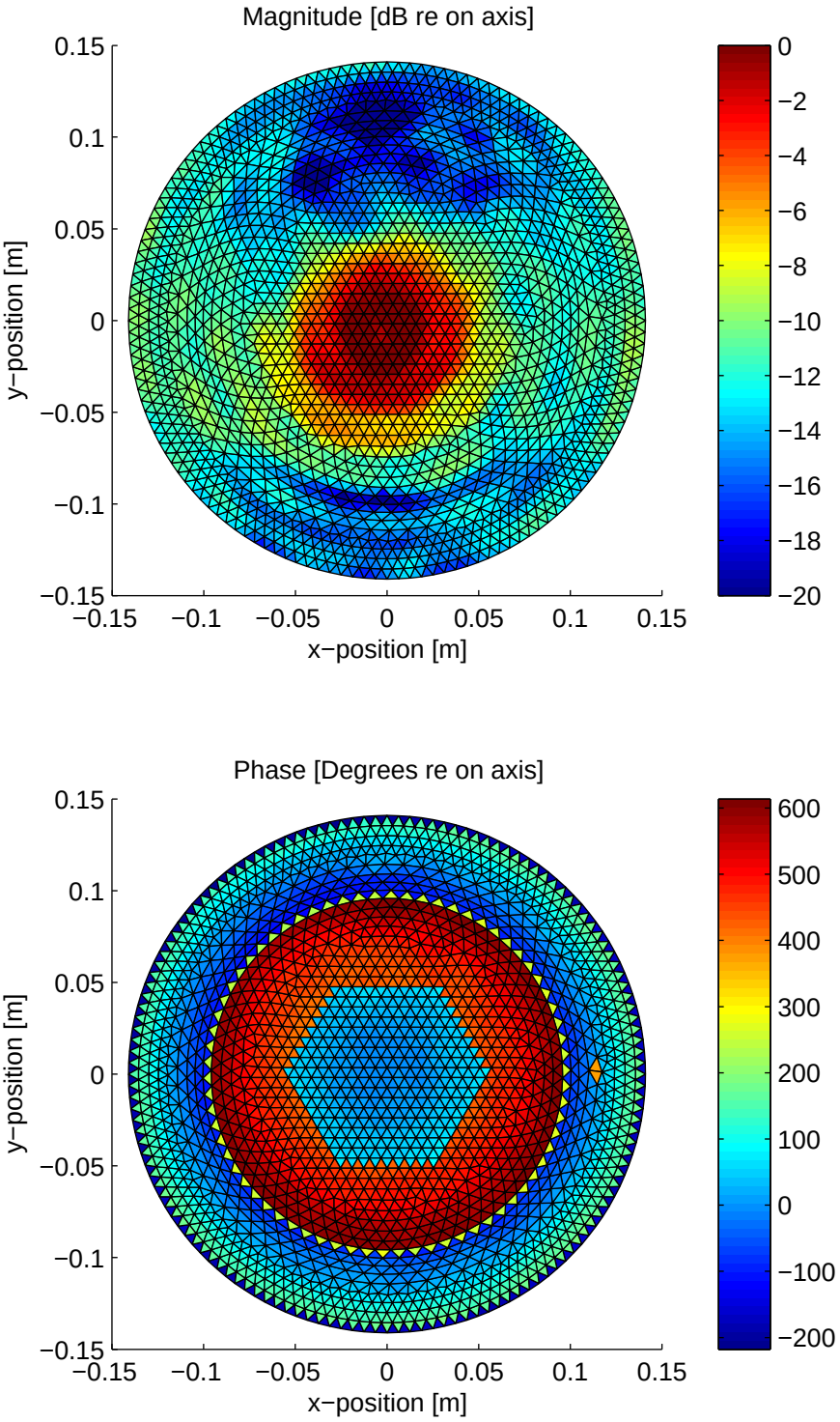


Figure A.15: Conical horn, frequency 10440 *Hz*

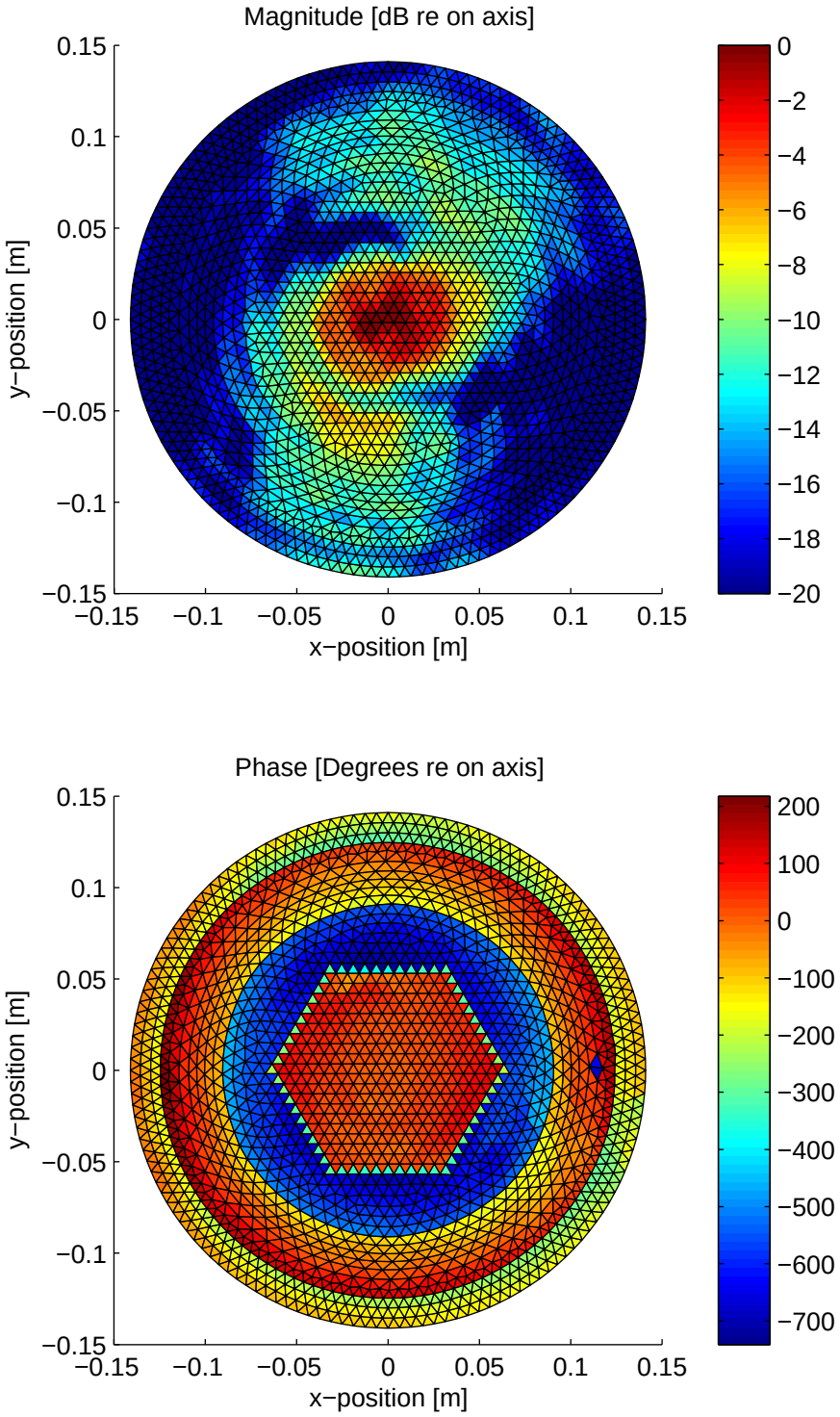


Figure A.16: Conical horn, frequency 12260 *Hz*

Appendix B

Optimisation techniques

This appendix describes the optimisation techniques used in this thesis. It discusses global verses local optimisation, gradient based, non-gradient based global optimisation techniques, surrogate modelling, space filling sampling and global optimisation techniques for expensive objective function evaluations.

B.1 Global optimisation

Global optimisation strives to find the global minimum of an objective function, i.e. to minimise a function $f(x)$, you must find a value of $x = x^*$ such that $f(x^*) < f(x)$ for all x. Most optimisation techniques strive to find a local minimum, a point $x = x^*$ such that $f(x^*) < f(x)$ for $|x - x^*| \leq \delta$, where $\delta > 0$ (i.e. for all x in a bounded region near x^*). In many real world problems both local and global minima simultaneously exist. As an example, consider the simple function (from Sasena 2002)

$$f(x) = -\sin(x) - \exp\left(\frac{x}{100}\right) + 10 \tag{B.1}$$

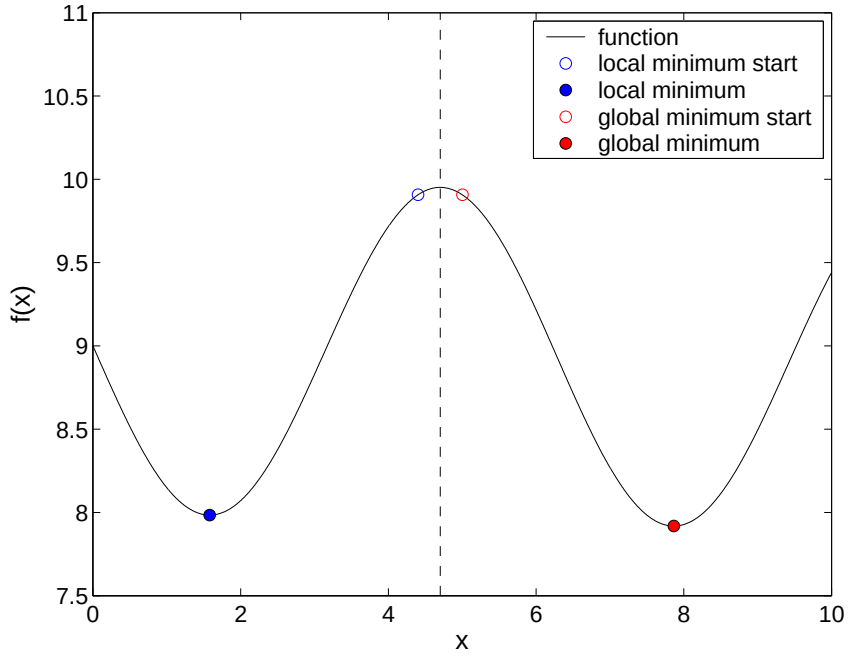


Figure B.1: Plot showing both local and global minimum of Equation (B.1).

Figure B.1 shows a plot of this function, which contains the global minimum ($x = 7.86, f(x) = 7.92$) and a local minimum ($x = 1.58, f(x) = 7.98$).

B.2 Gradient based techniques

There are many different types of optimisation methods available to solve many different types of problems. A good overview of different optimisation techniques is given in the introductory textbook by Belegundu and Chandrupatla (1999). A popular method of optimisation makes use of both the objective function value and derivatives with respect to optimisation parameters. These gradient based optimisation methods search for local minima in objective function space, starting from an initial guess. There are many types of gradient based optimisation, and all methods answer two basic questions in their search for a minima: which is the best direction to find a minima?; and how far do I travel in this direction?

Sequential Quadratic Programming (SQP) is a popular gradient based technique that solves a locally quadratic approximation to the objective function surface to find the best direction (the Quadratic Programming algorithm), and then performs a line search to find out how far to move. The quadratic approximation is then made again around the new point and the operation is performed repeatedly until convergence (the Sequential part of the algorithm). The method is able to handle both linear and non-linear constraints. Belegundu and Chandrupatla (1999) Section 5.10 has a good introduction to Sequential Quadratic Programming. A robust implementation of SQP, based on the work of Schittkowski (1985), is found in the MATLAB optimisation toolbox function `fmincon` and used in this thesis.

When applied to optimisation of Equation B.1, SQP will find either the local minimum or the global minimum depending on which side of the local maximum ($x = 4.70$) the minimisation technique is started. The inability to find the global minimum from any starting point is a major failing of gradient methods such as SQP. They often have to be run many times from different starting positions, and a globally optimum solution is not guaranteed.

Gradient based methods also require the gradient of the function to be minimised. For analytic functions such as Equation B.1, calculation of the gradient is not difficult. For real engineering problems, such as those formulated in this thesis, the analytic gradient is not generally available. A number of approaches are used: numerical approximations to the gradient, automatic differentiation programs and adjoint formulations.

The gradient is generally evaluated numerically by either forward or central differences. A forward difference can be calculated thus

$$\frac{\partial f\left(\mathbf{x}^0\right)}{\partial x_i} = \frac{f\left(x_1^0, x_2^0, \ldots, x_i^0 + \varepsilon, \ldots, x_n^0\right) - f\left(\mathbf{x^0}\right)}{\varepsilon}, i = 1, \ldots, n$$

where $\mathbf{x}^0 = \left\{x_1^0, x_2^0, \ldots, x_i^0, \ldots, x_n^0\right\}$ is a vector of input parameters, and ε is the step size.

This approximation to the true gradient requires an additional function evaluation for each dimension considered, in addition to the original evaluation at $\mathbf{x}^0$. The value of the gradient is also dependent on the choice of step size ε. Most mesh based numerical techniques, such as those used in this thesis, can produce relatively large changes in function value for a small change in input, which makes numerically evaluated gradients problematic.

Automatic differentiation (Bischof et al., 1998) is an attractive scheme that provides source code for analytic gradients from the source code of the function itself. It does this by parsing the function source code and applying the chain rule automatically to the individual operations contained within. As can be imagined this is a significant task and these programs are not robust, not generally available and are limited to a single programming language. They are a topic of current research and look promising for future optimisation methods.

The adjoint technique (Noreland, 2002, Jameson, 1995, 2003, Ghayour and Baysal, 2000, Belegundu and Chandrupatla, 1999) can be used in certain problems to efficiently evaluate the gradient of the objective function. It uses a mathematical technique that forms an "adjoint" problem that calculates the gradient with the same cost as a single extra function evaluation, no matter the dimension of the minimisation to be performed. This technique has not been applied to the source superposition method before, and will not be considered further in this thesis.

B.3 Non-gradient based global optimisation techniques

The issues associated with gradient based methods such as local minimisation and difficult evaluation of the function gradient have been overcome by non-gradient based, non-deterministic global methods such as genetic algorithms (Goldberg, 1989, Deb, 2001) or simulated annealing (Ingber, 1993). It has been found that such techniques can require

many thousands (or even tens of thousands) of objective function evaluations. For expensive cost function evaluations, non-deterministic methods can lead to intractable solution times. One solution for the efficient calculation of such problems is parallel computing (Howard et al., 2004).

An alternative to non-deterministic global optimisation is the deterministic sampling DIRECT algorithm (Jones et al., 1993). This method requires no knowledge of the objective function gradient. It samples points in the domain, and then uses these points to decide where to sample next, with equal merit given to both local and global searches. For a proof of convergence of the algorithm in the dense sampling limit see Finkel and Kelley (2004).

The implementation of DIRECT used in this thesis is the MATLAB implementation of Finkel (2003), which allows constrained minimisation. When applied to minimising Equation B.1, the DIRECT algorithm finds an acceptable global minimum within 333 function evaluations. This is a much larger than the 20 function evaluations required to reach a global optimum for SQP (this is, of course, provided that the starting point of the SQP procedure is already near the global minimum). The DIRECT algorithm does find the global minimum basin in a small number of function evaluations, and this suggests a hybrid strategy where a small number of DIRECT iterations are performed to find a point near a global optimum and the SQP engaged to efficiently find the global minimum. The success at finding a true global minimum using this strategy will depend on the function optimised. Sasena (2002, Appendix A.3.4) describes an implementation of DIRECT that contains a local search option, using SQP but embedded in the DIRECT algorithm, which seems a promising augmentation to the DIRECT algorithm.

B.4 Surrogate modelling techniques

The idea of surrogate modelling techniques (or meta-modelling) is to replace the expensive cost function evaluation with a model that is both cheap to construct and evaluate. There are many such techniques available, including polynomial response surface methods (Myers and Montgomery, 1995), artificial neural networks (MacKay, 1992, Belegundu and Chandrupatla, 1999), Multivariate Adaptive Regression Spline (MARS) (Friedman, 1991), and the one used in this thesis, Kriging (Cressie, 1991, Santner et al., 2003).

Kriging techniques, developed in the geostatistics and spatial statistics fields, fits a surface to values from a set of data points. It models the variation of the unknown function $\hat{y}(x)$ as a constant value plus the variation of a normally distributed stochastic variable. The Kriging model used in this thesis is from the MATLAB DACE toolkit (Lophaven et al., 2002b), and allows the simple creation of a Kriging model with a wide variety of regression and correlation functions, with predictions of the mean function value, $\hat{y}(x)$, mean square error of the function, $\hat{\sigma}^2(x)$, the gradient of the function ,$\frac{\partial \hat{y}(x)}{\partial x}$, and also the gradient of the error, $\frac{\partial \hat{\sigma}^2(x)}{\partial x}$, from this model. This thesis uses a constant regression function and a general exponential correlation function (Lophaven et al., 2002b). The details of the modelling process are beyond the scope of this thesis, as there are many references to the derivation of the Kriging interpolation process (Cressie, 1991, Santner et al., 2003, Lophaven et al., 2002b, Jones, 2001, Jones et al., 1998).

As example of Kriging, Equation B.1 is predicted by a subset of points evaluated at $x = \{0, 3.4, 5.9, 6.7, 7.6, 10\}$. The Kriging approximation is shown in Figure B.2, the true value is shown in black, the blue dots are the points at which the function is calculated exactly. The red line is the Kriging approximation to the mean value of the prediction. Kriging also gives information about the error in prediction between the known values (at which the true function is known and the error goes to zero), and the orange envelope gives 95% confidence intervals for the prediction. It should be noted that the variance calculated

by the Kriging function is only a prediction of the true variance, and is underestimated by the usual Kriging techniques such as those found in the Matlab toolbox DACE (Lophaven et al., 2002b). The reasons behind this and a description of a more sophisticated statistical technique (bootstrapping) may be found in den Hertog et al. (2004). This underestimation may explain why the true value of the function plotted in Figure B.2 is actually outside the lower bound at $x \approx 1.5$. For the purpose of this thesis, the standard Kriging prediction of variance is deemed acceptable, as it is generally only used to find the next most likely position to sample.

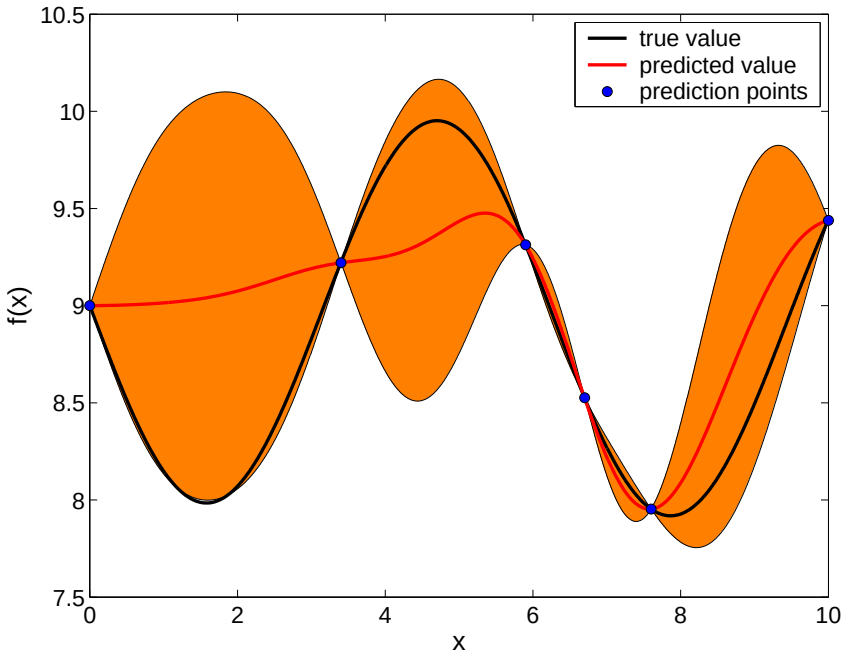


Figure B.2: Kriging approximation to Equation (B.1) with 95% *confidence interval for prediction from a subset of points.*

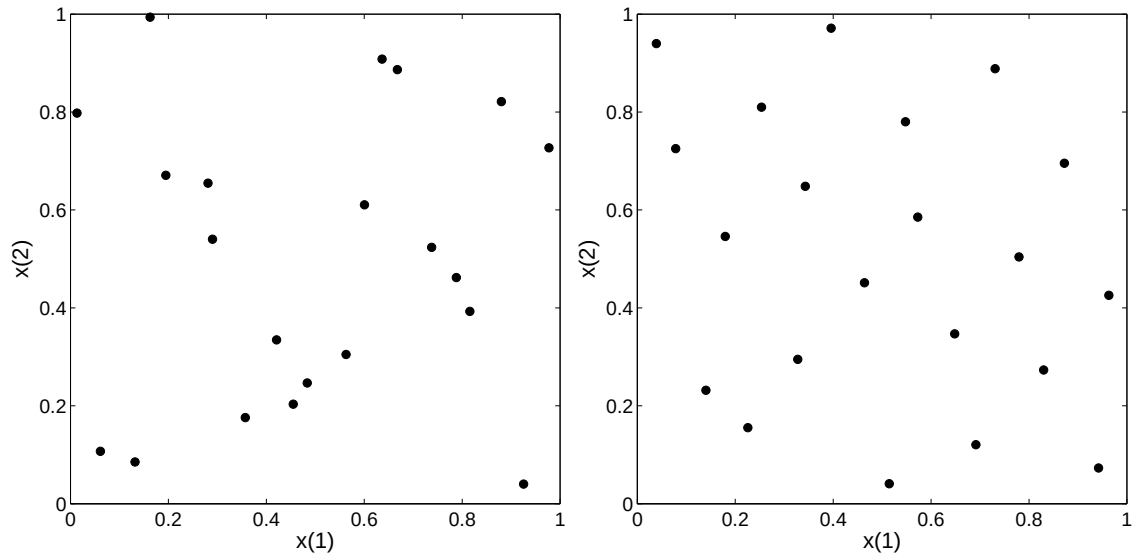
Kriging has been found to be a very useful tool for Design and Analysis of Computer Experiments (DACE), and for optimisation of expensive objective functions. The technique can become computationally expensive for a large number of data points ($n_p \geq 1000$).

B.5 Improved Distributed Latin Hypercube Sampling

When producing a Kriging model, it is imperative for the accuracy of the predictions made that the underlying points evenly sample the parameter space. A simple choice would be a regular grid of points, however this soon becomes prohibitively expensive as the number of dimensions increase. To find an even distribution of sample points in n dimensional space is not a trivial task, and is the topic of current research (Cioppa, 2002, Romero et al., 2003).

The technique of Latin Hypercube Sampling (LHS) was introduced by McKay et al. (1979) and is commonly used in DACE. A purely random (Monte-Carlo) sampling technique samples directly from the joint probability distribution of the input variables. For all cases considered in this thesis, the input variables are considered uniformly distributed (equally likely). This method is not very efficient when small numbers of samples are used to find the distribution of the output variables, and LHS was developed to overcome these shortcomings. LHS is a constrained Monte-Carlo sampling technique, that divides the input space up into a number of equally likely "bins". These bins are then sampled without replacement (Matlab function `randperm`) in each dimension and a point chosen within each bin. While this technique produces better sampling distributions that the Monte-Carlo sampling, it has been found to produce inferior distributions when a one dimensional uniform random distribution is projected onto more than one dimension (Beachkofski and Grandhi, 2002).

The Improved Distributed Latin Hypercube Sampling technique of Beachkofski and Grandhi (2002) overcomes this issue by trying to sample points such that the distance between them is close to the optimal spacing for the number of points. This technique can become computationally expensive for a large number of sample points ($n_p \geq 1000$). Figure B.3 shows a comparison between LHS and IHS for 21 sampled points. It is evident from visual inspection that the IHS has "less space" than LHS. The IHS method is used in this thesis to evenly sample points for the Kriging meta-models.



(a) Latin Hypercube Sampling (b) Improved Latin Hypercube Sampling

Figure B.3: Comparison between space filling sampling techniques with 21 points sampled.

B.6 Enhanced Global Optimisation (EGO)

There has been much research into finding a method of efficiently optimising functions in which the evaluation of the cost function is extremely expensive, where they are typically expensive numerical methods such as Computational Fluid Dynamics, FEA simulations or a combination of both (Booker et al., 1998). The work of Jones et al. (1998), refined by Sasena (2002) into the algorithm `superEGO`, has developed an efficient method for global optimisation, called Enhanced Global Optimisation[1].

This technique uses a Kriging meta-model to predict the values of the objective function at a few, sparsely distributed sample points. Instead of trying to optimise the value of the mean prediction directly, information about the error in the prediction from the Kriging meta-model is utilised, and a optimisation performed on an auxiliary subproblem to pick the next position for the (expensive) function evaluation. Solving the Infill Selection Criteria (ISC) subproblem finds a position that is "most likely" to obtain a better function

[1] Originally called SPACE in Schonlau (1997).

evaluation, taking into account the error in the meta-model. Direct optimisation of the Kriging meta-model implicitly assumes that the meta-model accurately represents the objective function. Sasena (2002) developed the ideas of Schonlau by examining a variety of ISC, as well as extending the algorithm to constrained optimisation. He used the DIRECT method (Finkel, 2003) to optimise the ISC subproblem. Jones (2001) also gives a good overview of various ISC, including more sophisticated techniques that look ahead to include the potential error of the Kriging model in finding the next best sample.

To examine the performance of the EGO technique, the Kriging approximation to Equation B.1 shown in Figure B.2 will be optimised using the lower confidence bounding ISC (Sasena, 2002),

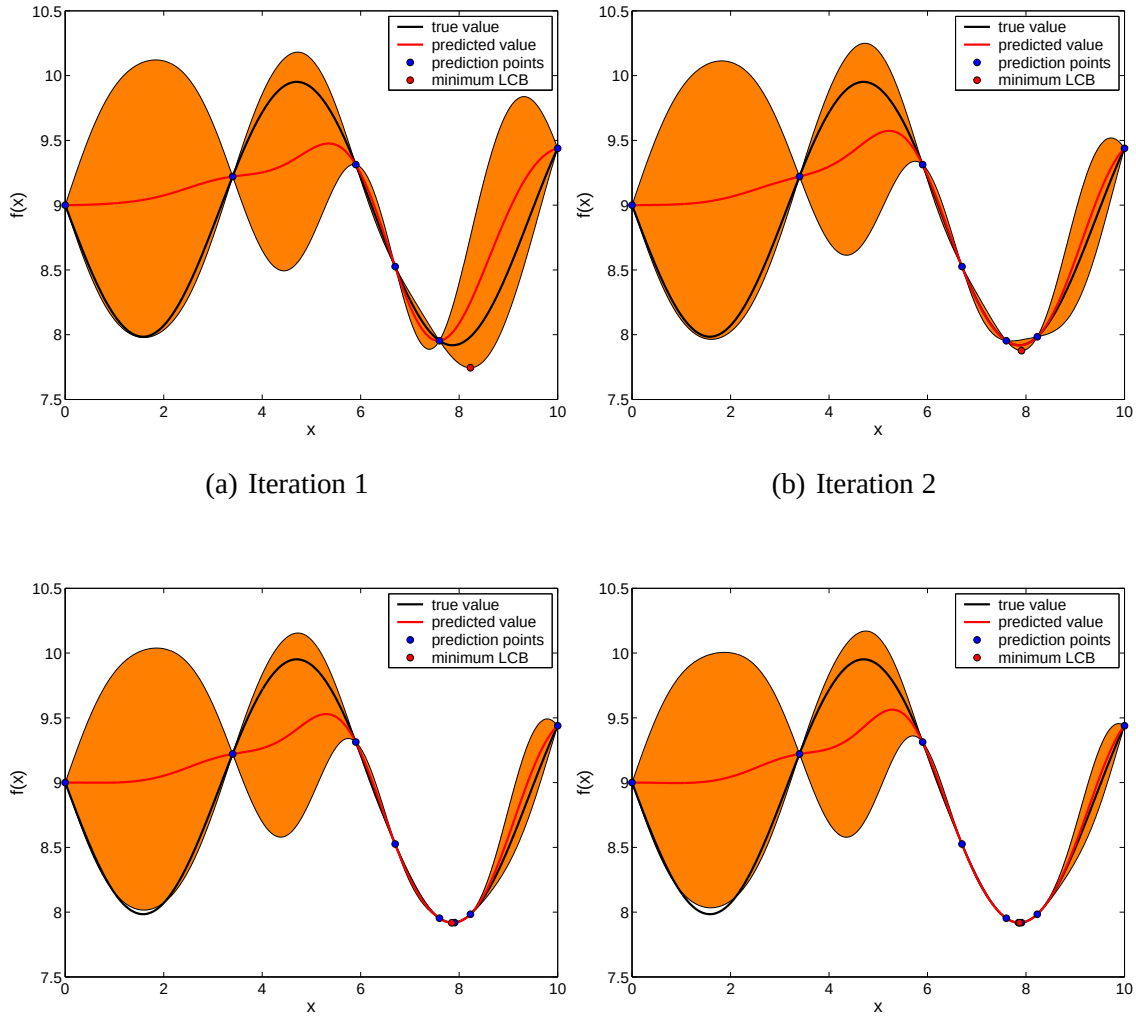
$$LCB = \hat{y} - b\hat{\sigma} \tag{B.2}$$

where $\hat{y}$ is the mean value and $\hat{\sigma}^2$ is the mean squared error of the prediction, and b is a user defined parameter describing the emphasis between local ($b = 2$) and global ($b = 2.5$) search.

Figure B.4 shows the results of 4 iterations for the local search, and Figure B.5 shows the global search results. The ISC minimum, used to select the next candidate for updating the Kriging meta-model, is shown as a red dot.

As the iteration proceeds for the search for the best next location, the ISC does not sample near the local minimum, and all selected points are near the global minimum. If the search is terminated at 4 iterations, then a total of 9 function evaluations have been completed, compared to 20 for SQP and 333 for DIRECT.

When $b = 2.5$ (Figure B.5), the search proceeds more globally. Figure B.5 (b) shows the second ISC selection near the local minimum. By Figure B.5 (d) the ISC selection is back near the global minimum, having removed uncertainty that the local minimum could have been a global one. To reach the same point as the locally biased search, the globally biased search required 12 function evaluations.



(a) Iteration 1

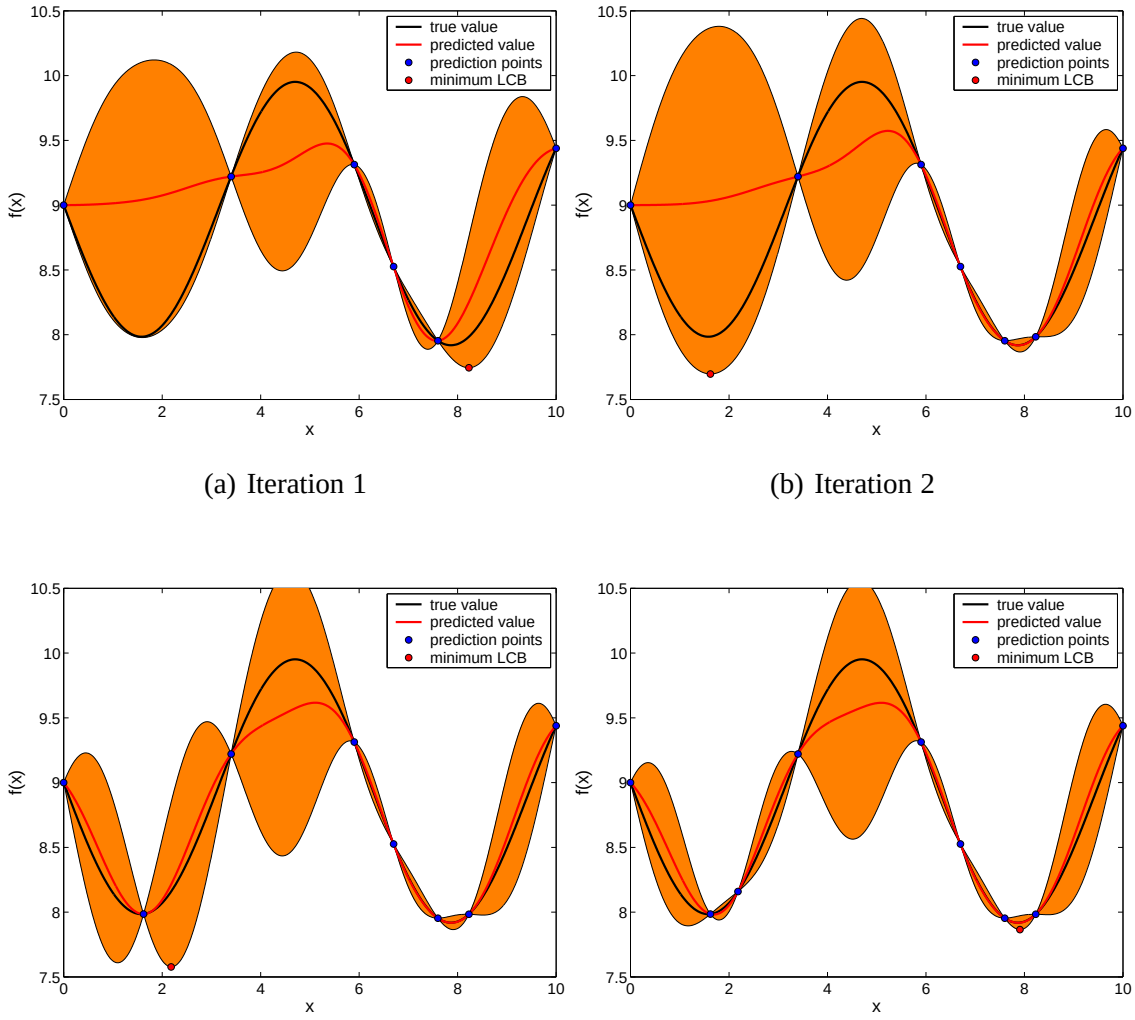
(b) Iteration 2

(c) Iteration 3

(d) Iteration 4

Figure B.4: EGO optimisation of Equation (B.1) using a lower confidence bounds ISC, with emphasis on local search ($b = 2$).

It should be clear that the optimisation procedure will still tend to a global minimum with a locally biased search, however if the initial sampling is too sparse, a potential global minimum may be missed. Jones (2001) states that a there is no guarantee of finding a global minimum if the lower confidence bound ISC is used with a constant parameter b. It may be prudent to focus on strategies that include a global search component, such as starting with large b early in the search, later transitioning to a local one with small b to speed up convergence, similar to the "cooling" schedule of Sasena (2002, Table 4.1). Alternatively cycling between various values of b throughout the optimisation process would



(a) Iteration 1 (b) Iteration 2

(c) Iteration 3 (d) Iteration 4

Figure B.5: EGO optimisation of Equation (B.1) using a lower confidence bounds ISC, with emphasis on global search ($b = 2.5$).

allow both a local and global search. Questions could then arise as to which values of b should be used. Adopting a technique similar to Jones (2001) in his "Enhanced Method 4", where in a single iteration a number of different values of b are tried, producing a number of potential sample sites. Many of these sample points will be the similar, and they can then be clustered into a number of distinct groups using a statistical technique such as the k-means test. A representative of each group is then sampled, leading to both local and global searching.

Alternative ISC are given in Schonlau (1997), Jones (2001) and Sasena (2002). One important criteria is the Expected Improvement (EI) function, as this contains both local and global search components. The improvement function is defined as the improvement of the current prediction, $\hat{y}(x)$, at point x over the minimum value of the current set of samples, f_{min}, i.e.

$$I = \max\left(f_{min} - \hat{y}(x), 0\right) \tag{B.3}$$

The expected improvement ISC, defined as the expectation of the improvement, is given by

$$EI = \mathbf{E}[I] = \left(f_{min} - \hat{y}(x)\right)\Phi\left(\frac{f_{min} - \hat{y}(x)}{s(x)}\right) + s(x)\,\phi\left(\frac{f_{min} - \hat{y}(x)}{s(x)}\right) \tag{B.4}$$

Where $\Phi(x)$ is the standard normal cumulative density function, $\phi(x)$ is the standard normal probability density function and $s(x)$ is the estimated standard deviation of the prediction at point x. This criteria contains two terms, a local term related to the difference between the current smallest value and the prediction and a global term related to the standard deviation. When the expected improvement has found many local values and the difference between the current smallest value and the prediction is small, the standard deviation will dominate and a global search will ensue. This behaviour is exemplified in Jones (2001, Figure 20).

Appendix C compares the interpretation by Sasena (2002) of the Regional Extreme (RE) criteria with the criteria originally proposed by Watson and Barnes (1995). It finds this new interpretation different, and that the original implementation, the minimisation of a "regional minimum extreme" is equivalent to Schonlau's expected improvement. It also finds that an alternative implementation of Sasena's criteria (which cannot be called a regional extreme criteria) may not find the global optimum. For these reasons the Regional Extreme Infill Sampling Criteria is not used in this thesis.

One good reason for Sasena's adoption of his "regional extreme" criteria is that its smooth variation helps the constrained minimisation technique used (the DIRECT global optimi-

sation technique) find a suitable solution easily. ISC such as the expected improvement have large plateaus with values close to zero, making constrained minimisation difficult Sasena (2002, Page 101). The RE of Sasena is not a good choice for finding a global optimum. The LCB criteria (Equation B.2) has a relatively smooth variation, although with points of inflection at the sample positions. Although not used in this thesis, it is suggested that the LCB criteria with multiple b values (similar to Jones (2001) in his "Enhanced Method 4") be tested for problems with constraints, and that constrained EGO is still very much a current research topic.

The use of surrogate models with probabilistic ISC has the potential to reduce the number of objective function evaluations significantly, provided the evaluation of the objective function is expensive. However the cost of fitting the Kriging model and the DIRECT optimisation of the ISC subproblem may not warrant the extra overhead if the cost function evaluation is cheap. The crossover point between using EGO and DIRECT will be problem dependent.

Appendix C

Regional Extreme Infill Sampling Criteria

The Regional Extreme (RE) Infill Sampling Criteria (ISC) of Sasena (2002) is quoted as,

$$\begin{aligned} RE_S &= \hat{y}(x) + (f_{min} - \hat{y}(x))\,\Phi\left(\frac{f_{min}-\hat{y}(x)}{s(x)}\right) \\ &\quad + s(x)\,\phi\left(\frac{f_{min}-\hat{y}(x)}{s(x)}\right) \end{aligned} \tag{C.1}$$

Where $\hat{y}(x)$ is the current prediction at point x, f_{min} is the minimum value of the current set of samples, $\Phi(x)$ is the standard normal cumulative density function, $\phi(x)$ is the standard normal probability density function and $s(x)$ is the estimated standard deviation of the prediction. This criteria can be written in terms of the current prediction, $\hat{y}(x)$, at point x plus the expected improvement (Equation B.4) at that point,

$$RE_S = \hat{y}(x) + EI \tag{C.2}$$

For a minimisation problem, this form of ISC is inconsistent, as the EI term is generally positive, and large when either the probability of a point being better than the current

minimum point is large, or the standard deviation is high. The addition of a positive term that describes the improvement to the mean value of the prediction in a minimisation problem will not find a value near the best expected value.

Sasena (2002) reports that the RE criteria performs well on the problems considered. One hypothesis for this is that the RE ISC in effect minimises the value of the predictor $\hat{y}(x)$ as the magnitude of the EI may be many times smaller. The relative magnitudes of the mean value and EI depends on the function to be minimised, and the ability to find a global minimum depends on the initial sampling and the accuracy of the initial Kriging model. For the example given in Sasena Figure 4.5, (and reproduced in Figure (B.2) of this thesis) the EI is very small in comparison to the mean value of the predictor. A minimisation of the mean value of the predictor may not find a global optimum for the same reasons that Jones (2001) found the LCB criteria may not, because minimising the predictor is the same as minimising the LCB criteria for $b = 0$.

Further evidence of the anomalous performance of the RE ISC is given in Siah et al. (2004) where the RE criteria fails to find improvement after a number of iterations, and the value of the predictor is then optimised directly. The reasons behind this poor performance need to be further investigated, but is beyond the scope of the current study.

Referring to the original paper of Watson and Barnes (1995), their second criteria, a regional extreme, is derived for finding a regional maximum extreme. The derivation is repeated here. Given a known constant β and a normally distributed continuous random variable Z with mean μ, standard deviation σ and probability density function

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{\frac{-(x-\mu)^2}{2\sigma^2}} \tag{C.3}$$

find the expected value of the maximum of Z or β, i.e.

$$\mathbf{E}[\max(Z,\beta)] = \int_{-\infty}^{\infty} \max(t,\beta)\, f(t)\, dt \tag{C.4}$$

Following the definition of the max function, and that β is a constant, the integral in Equation C.4 can be partitioned into two integrals,

$$\int_{-\infty}^{\infty} \max(t,\beta)\, f(t)\, dt = \int_{\beta}^{\infty} t\, f(t)\, dt + \int_{-\infty}^{\beta} \beta\, f(t)\, dt \tag{C.5}$$

Next, using

$$\int_{-\infty}^{\infty} t\, f(t)\, dt = \int_{-\infty}^{\beta} t\, f(t)\, dt + \int_{\beta}^{\infty} t\, f(t)\, dt \tag{C.6}$$

we can write,

$$\mathbf{E}[\max(Z,\beta)] = \int_{-\infty}^{\infty} t\, f(t)\, dt - \int_{-\infty}^{\beta} t\, f(t)\, dt + \int_{-\infty}^{\beta} \beta\, f(t)\, dt \tag{C.7}$$

The first integral term is just the mean value μ of the random variable Z. We want to express the second two integrals in terms of the standard normal probability density function,

$$\phi(x) = \frac{1}{\sqrt{2\pi}} e^{\frac{-x^2}{2}} \tag{C.8}$$

and the standard normal cumulative density function,

$$\Phi(x) = \int_{-\infty}^{x} \frac{1}{\sqrt{2\pi}} e^{\frac{-t^2}{2}} dt \tag{C.9}$$

where the standard normal distribution has a mean of 0 and a standard distribution of 1. To do this, we will introduce the transformations

$$x = \frac{t-\mu}{\sigma} \tag{C.10}$$

$$dx = \frac{dt}{\sigma} \tag{C.11}$$

and define ξ, the value of β normalised by the distribution mean and standard deviation as

$$\xi = \frac{\beta - \mu}{\sigma} \tag{C.12}$$

Substituting transformation C.12, as well as the definition of the probability density function (C.3) into C.7 gives

$$\begin{aligned}
\mathbf{E}\left[\max\left(Z,\beta\right)\right] &= \mu - \int_{-\infty}^{\frac{\beta-\mu}{\sigma}} \frac{t}{\sigma}\frac{1}{\sqrt{2\pi}}e^{\frac{-x^2}{2}}dx\,\sigma + \int_{-\infty}^{\frac{\beta-\mu}{\sigma}} \frac{\beta}{\sigma}\frac{1}{\sqrt{2\pi}}e^{\frac{-x^2}{2}}dx\,\sigma & \text{(C.13)}\\
&= \mu + \sigma\left(\int_{-\infty}^{\xi}\frac{\beta}{\sigma}\phi\left(x\right)dx - \int_{-\infty}^{\xi}\frac{t}{\sigma}\phi\left(x\right)dx\right) & \text{(C.14)}\\
&= \mu + \sigma\left(\int_{-\infty}^{\xi}\frac{\beta-\mu}{\sigma}\phi\left(x\right)dx - \int_{-\infty}^{\xi}\frac{t-\mu}{\sigma}\phi\left(x\right)dx\right) & \text{(C.15)}\\
&= \mu + \sigma\left(\int_{-\infty}^{\xi}\xi\phi\left(x\right)dx - \int_{-\infty}^{\xi}x\phi\left(x\right)dx\right) & \text{(C.16)}
\end{aligned}$$

Knowing that ξ is a constant, the first integral becomes a standard cumulative density function. The second integral can be shown to be

$$\int_{-\infty}^{\xi} x\phi\left(x\right)dx = -\phi\left(\xi\right) \tag{C.17}$$

This gives

$$\begin{aligned}
\mathbf{E}\left[\max\left(Z,\beta\right)\right] &= \mu + \sigma\left(\xi\Phi\left(\xi\right) + \phi\left(\xi\right)\right) & \text{(C.18)}\\
&= \mu + \left(\beta-\mu\right)\Phi\left(\xi\right) + \sigma\phi\left(\xi\right) & \text{(C.19)}
\end{aligned}$$

Replacing the general random variable Z with the random variable Y that describes the Kriging prediction, and β with the maximum value of the current sample set f_{max} leads to

$$\begin{aligned}
RE_{max} &= \hat{y} + \left(f_{max} - \hat{y}\right)\Phi\left(\frac{f_{max}-\hat{y}}{s}\right) + s\phi\left(\frac{f_{max}-\hat{y}}{s}\right) & \text{(C.20)}\\
&\neq \hat{y} + EI & \text{(C.21)}
\end{aligned}$$

$$\neq \quad RE_S \tag{C.22}$$

which is the same as Equation C.1 with f_{min} replaced by f_{max}, but not equal to the prediction added to the expected improvement, which is Sasena's regional extreme (Equation C.2) as the expected improvement involves the minimum existing sample value, not the maximum.

Similarly, we can work out the regional minimum extreme, as suggested by Watson and Barnes (1995),

$$\begin{aligned}
\mathbf{E}\left[\min\left(Z,\beta\right)\right] &= \int_{-\infty}^{\infty} \min\left(\xi,\beta\right)\phi\left(\xi\right)d\xi && \text{(C.23)}\\
&= \int_{-\infty}^{\beta} t\phi\left(t\right)dt + \int_{\beta}^{\infty} \beta\phi\left(t\right)dt && \text{(C.24)}\\
&= \mu - \int_{\beta}^{\infty} t\phi\left(t\right)dt + \int_{\beta}^{\infty} \beta\phi\left(t\right)dt && \text{(C.25)}\\
&= \mu + \sigma\left(\int_{\xi}^{\infty} \xi\phi\left(x\right)dx - \int_{\xi}^{\infty} x\phi\left(x\right)dx\right) && \text{(C.26)}\\
&= \mu + \sigma\left(\xi\left(1-\Phi\left(\xi\right)\right) - \phi\left(\xi\right)\right) && \text{(C.27)}\\
&= \beta - \sigma\left(\xi\Phi\left(\xi\right) + \phi\left(\xi\right)\right) && \text{(C.28)}\\
&= \beta - \left(\left(\beta-\mu\right)\Phi\left(\xi\right) + \sigma\phi\left(\xi\right)\right) && \text{(C.29)}
\end{aligned}$$

This gives

$$\begin{aligned}
RE_{min} &= f_{min} - \left(\left(f_{min}-\hat{y}\right)\Phi\left(\frac{f_{min}-\hat{y}}{s}\right) + s\phi\left(\frac{f_{min}-\hat{y}}{s}\right)\right) && \text{(C.30)}\\
&= f_{min} - EI && \text{(C.31)}
\end{aligned}$$

So the regional minimum extreme is equal to the negative of the expected improvement criteria, plus a constant value (f_{min}). Minimisation of this function will lead to the same minimum as maximising the expected improvement.

In conclusion, the interpretation by Sasena (2002) of the Regional Extreme (RE) criteria

has been compared with the criteria originally proposed by Watson and Barnes (1995). It finds this new interpretation different, and that the original implementation, the minimisation of a “regional minimum extreme” is equivalent to Schonlau’s expected improvement. It also finds that an alternative implementation of Sasena’s criteria (which cannot be called a regional extreme criteria) may not find the global optimum.

Appendix D

Bézier curves

The Béezier spline is specified by two vectors, with the curve tangent to the head of each vector, and the “strength” of attachment to the vector determined by the length of the vector.

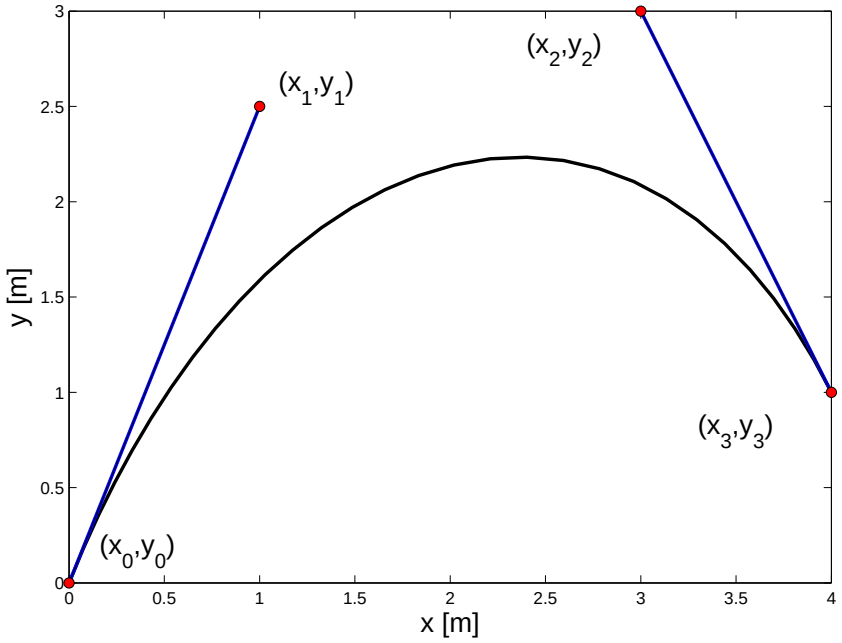


Figure D.1: Bézier curve (black line) with control vectors (blue lines).

The position of the curve is given by the cubic polynomials $x(t) = a_x t^3 + b_x t^2 + c_x t + x_0$ and $y(t) = a_y t^3 + b_y t^2 + c_y t + y_0$, where t varies between 0 and 1 between the start (x_0, y_0)

and end (x_3, y_3) points. (Plant, 1996). The coefficient values can be calculated from the given points as;

$$\begin{aligned} c_x &= 3(x_1 - x_0) \\ b_x &= 3(x_2 - x_1) - c_x \\ a_x &= x_3 - x_0 - c_x - b_x \end{aligned} \tag{D.1}$$

and

$$\begin{aligned} c_y &= 3(y_1 - y_0) \\ b_y &= 3(y_2 - y_1) - c_y \\ a_y &= y_3 - y_0 - c_y - b_y \end{aligned} \tag{D.2}$$