# Improving the Efficiency of Quasi-optical Analysis and Design of Terahertz Systems

Marcin L. Gradziel<sup>1</sup>, David White<sup>2</sup>, J.A. Murphy<sup>1</sup>, S. Withington<sup>3</sup>

1. Department of Experimental Physics, National University of Ireland Maynooth, Ireland

2. Department of Computing, Institute of Technology, Tallaght, Dublin, Ireland

3. Astrophysics, Cavendish Laboratory, Madingley Road, Cambridge CB3 OHE

### Introduction

The aim of long wavelength analysis is to understand the unique behaviour of terahertz (300 GHz - 30 THz) quasioptical systems, and since most THz systems have small Fresnel numbers, a modal approach to analysis is appropriate. In this paper in particular we discuss the extension of a powerful approach based on Singular Value Decomposition (SVD) [1] for improving the efficiency of the application of Gaussian Beam Mode Analysis (GBMA) to complex optical systems. We compare the efficiency of the SVD approach with the overlap integral approach, and also validate the technique by comparison with test cases computed using physical optics code. This work was inspired by the need for efficient numerical schemes as part of the development of a software package for quasi-optical analysis and design of terahertz systems at NUI Maynooth (MODAL).

GBMA is particularly suited to analysing long wavelength systems and has been applied extensively in the design and analysis of both coherent and partially coherent quasi-optical systems in the millimeter and submillimeter wavebands [2]. Beam Modes can be thought of as the beam-guide analog of conventional waveguide modes, where a beam guide consists of a number of refocussing elements which ensure that the propagating beam remains quasi-collimated. The strength of Gaussian beam-mode analysis is that it is straightforward to model propagation through beam guide systems with apertures, mirrors and lenses, and build them up in a modular way, while at the same time keeping track of the evolution of the beam. Generally the source fields can be represented to high accuracy by a finite sum of only a few beam modes underlining the potential efficiency of the modal description.

However realistic optical components disturb the pure modal propagation through truncation and aberrational effects just as a step does in a waveguide. At such optical components power is scattered between modes and for a high accuracy description of beam propagation one needs to keep track of this scattering [3]. However, when there is a significant amount of power scattering between modes the number of integrations required to derive a scattering matrix in a straightforward way can be quite prohibitive. This has limited the efficiency with which GMBA has been applied to practical optical configurations.

An example of this is the calculation of Gaussian-mode scattering matrices at focussing mirrors [4]. If an off-axis mirror is treated as an inclined phase transforming plane, then it is necessary to determine the mode coefficients of the scattered field over the plane, but Gaussian-beam modes are only orthogonal over planes that are orthogonal to the direction of propagation and the direct evaluation of the scattering matrix turns out to be computationally extremely intensive. In fact many scattering matrices suffer from this kind of limitation [5]. Therefore such systems could be analysed much more efficiently if a more economical numerical method for determining the expansion coefficients over complex surfaces was available [6].

#### **Modal Analysis**

In Gaussian Beam Mode (GBM) theory a monochromatic coherent beam can be represented by a scalar field E, which can be written as a linear combination of independently propagating modes  $\Psi_m$ . The field at any plane z is then given by:

$$E(\mathbf{x}, \mathbf{y}, \mathbf{z}) = \sum A_m \Psi_m(\mathbf{x}, \mathbf{y}; W(\mathbf{z}), R(\mathbf{z})), \tag{1}$$

where W and R are beam parameters that depend on z and  $A_m$  are the mode coefficients [7]. To analyse optical systems in 3-D it is most convenient to use the Hermite-Gaussian modes  $\Psi_{\mu,\nu}(x, y, z)$  of the form:

$$\Psi_{\mu,\nu}(x, y, z) = \sqrt{\frac{1}{\pi W(z)^2 \mu! \nu! 2^{\mu+\nu-1/2}}} H_{\mu}\left(\frac{\sqrt{2}x}{W(z)}\right) H_{\nu}\left(\frac{\sqrt{2}y}{W(z)}\right) \exp\left(-\frac{x^2+y^2}{W(z)^2}\right) \\ \times \exp\left(-jk\left(\frac{x^2+y^2}{2R(z)}\right)\right) \exp(-jkz) \exp\left(j(\mu+\nu+1)\Delta\Phi_0(z)\right),$$

$$(2)$$

where all the symbols have their usual significance and where  $H_i(s)$  is the Hermite polynomial of order *i* [7]. The beam width parameter *W*, phase radius of curvature *R* and phase slippage term  $\Delta \Phi_0$  are functions of position *z*, which is taken to be zero at a waist of the mode. The Hermite-Gaussian modes propagate through an optical system without scattering and the output field at the image plane can be reconstructed by resumming the modes using (1).

In theory, if the field  $E_0$  is known at some reference plane  $z_0$ , the mode coefficients can be calculated by the appropriate overlap integrals of the general form:

$$A_{m} = \iint E_{0}(x, y, z_{0}) \Psi_{m}^{*}(x, y; W(z_{0}), R(z_{0})) dx dy.$$
(3)

Element boundaries are inherently accounted for, because the field is taken to be zero outside of the element aperture. For most applications the overlap integrals  $A_m$  have to be evaluated by numerical integration. This requires sampling of the field to be sufficiently fine to avoid numerical artefacts, such as aliasing. The minimum sampling period is given by the Nyquist's theorem ( $\lambda/2$ ), but in most cases finer sampling is needed to obtain convergence. This means that the evaluation of the overlap integrals is computationally intensive and therefore inherently slow.

Alternative fast methods of modal decomposition are desirable for optics design and analysis tools, that would still retain the accuracy of the overlap technique. We can attempt to fit a linear combination (coefficients  $\tilde{A}$ ) of the mode set functions  $\Psi_i$  to the known field E, sampled on a limited number of points  $r_j$ . In matrix formulation the approximate field  $\tilde{E}$  is given by:

$$\tilde{\boldsymbol{E}} = \begin{bmatrix} \tilde{\boldsymbol{E}}(\boldsymbol{r}_1) \\ \tilde{\boldsymbol{E}}(\boldsymbol{r}_2) \\ \vdots \\ \tilde{\boldsymbol{E}}(\boldsymbol{r}_N) \end{bmatrix} = \begin{bmatrix} \boldsymbol{\Psi}_1(\boldsymbol{r}_1) & \boldsymbol{\Psi}_2(\boldsymbol{r}_1) & \cdots & \boldsymbol{\Psi}_M(\boldsymbol{r}_1) \\ \boldsymbol{\Psi}_1(\boldsymbol{r}_2) & \boldsymbol{\Psi}_2(\boldsymbol{r}_2) & \cdots & \boldsymbol{\Psi}_M(\boldsymbol{r}_2) \\ \vdots & \vdots & \ddots & \vdots \\ \boldsymbol{\Psi}_1(\boldsymbol{r}_N) & \boldsymbol{\Psi}_2(\boldsymbol{r}_N) & \cdots & \boldsymbol{\Psi}_M(\boldsymbol{r}_N) \end{bmatrix} \begin{bmatrix} \tilde{\boldsymbol{A}}_1 \\ \tilde{\boldsymbol{A}}_2 \\ \vdots \\ \tilde{\boldsymbol{A}}_M \end{bmatrix} = \boldsymbol{\Psi} \tilde{\boldsymbol{A}}$$
(4)

and we determine the best approximation  $\tilde{A}$  by minimising the norm of the residual  $E - \tilde{E}$ :

$$|E - \tilde{E}| = |E - \Psi \tilde{A}| = \inf_{A \in \Omega_A} |E - \Psi A| \quad .$$
(5)

This approach, for the usual choice of the norm for the residual, reduces the problem of calculating the mode coefficients to a *linear least squares* (LLS) problem [8]. We can express it in a simple form using the Moore-Penrose pseudo-inverse  $\Psi^+$  of the *mode matrix*  $\Psi$ :

$$\tilde{A} = \Psi^+ E \tag{6}$$

Effective routines for solving LLS problems are readily available (e.g. LU decomposition, Gauss-Jordan elimination [1], [9]). SVD is one of the most powerful and interesting techniques that can be used to solve a LLS problem. The SVD method is based on the linear algebra theorem which states that any NxM matrix M can be written as the product of three matrices: a column-orthogonal NxM matrix U, a diagonal MxM matrix W, and a transpose of an orthogonal MxM matrix V[1]:

$$M = U W V^T . (7)$$

SVD allows the pseudo-inverse to be calculated as:

$$\boldsymbol{M}^{+} = \boldsymbol{V} \, \boldsymbol{W}^{-1} \, \boldsymbol{U}^{T} \tag{8}$$

even if some of the *singular values*  $w_i$  on the diagonal of the matrix W are zero. If that is the case, the corresponding elements in the inverted matrix  $W^{-1}$  need to be set to zero. SVD is numerically stable, handles both over- and under-determined systems, and provides diagnostic information about the mode set (through the singular values) [1].

#### Mode set considerations

In all practical cases, we try to reduce the computational complexity of the propagation problem by representing the field using as few modes as possible. The choice of W and R are crucial in this case. Often they are chosen such that the power in the fundamental mode is maximised i.e.  $|A_0|^2$ . In the case of a uniformly illuminated aperture (top hat) we get W=0.891a, where *a* is the aperture radius. *R* is chosen to match the radius of curvature of the beam (i.e. infinity for a plane wave). With this choice, however, the remaining power is spread over a large number of higher order modes. Individually, they contribute little power, but all of them are required to accurately approximate the field.

The more appropriate choice of W should therefore take into account the form of the higher order modes. As the mode number increases, its spatial frequency spread is higher and hence it will perform better in modelling an edge. The choice of W should reflect this. The modes can be characterised in terms of their *effective extent*. Because of the gaussian envelope, the effective extent of the mode is finite, and is approximately given by  $W\sqrt{1.5 N}$ . Figure 1 shows the mode profile and its extent for N=10 and N=20.



Figure 1: The effective extent of the 10<sup>th</sup> and 20<sup>th</sup> order Hermite-Gaussian modes.

To accurately reproduce the discontinuity at the aperture edge, we match the position of the last zero crossing of the mode to the extent of the aperture. If we look just at the position of the last zero crossing, the extent of the mode is approximately given by  $W \sqrt{0.75 N}$ . This gives us the following rule for selecting W:

$$W = \frac{a}{\sqrt{0.75 N}} \tag{9}$$

We have to remember however, that the actual extent of the highest order mode is  $W\sqrt{1.5 N}$  rather than  $W\sqrt{0.75 N}$ . As a result, we must ensure that in any fitting routine the field is explicitly set to zero at all points outside the aperture, at least as far as  $W\sqrt{1.5 N}$ . This suppresses spurious side-lobes that would otherwise emerge there.

## Examples

First we will consider the modal decomposition of a top hat field of unit amplitude with an aperture of radius a = 1, in one dimension, using N = 50 modes. Figure 2 shows a comparison of the reconstruction (here using accurate overlap integrals) with W selected using both approaches discussed above.



Figure 2: Top hat reconstruction using 50 modes. *W* was chosen to maximise power in the fundamental mode (i), and using mode extent matching (ii).

In figures 3 and 4 we show the results of modal reconstruction of a top hat field and a corrugated horn field, respectively. The aperture radius was 2.5 mm. The decomposition was done using both the overlap integral approach and the faster SVD technique. Selected mode amplitudes are also presented.



Figure 3: Comparison between SVD and overlap integral calculations: top hat field reconstruction. Selected non-zero mode coefficients are listed in the table.



Figure 4: Corrugated horn mouth reconstruction and selected non-zero mode coefficients for 15 modes using SVD and overlap approaches.

# Quasi-optical analysis

SVD approach to modal field decomposition can be used in quasi-optical analysis of optical systems in the terahertz region of the spectrum. In its simplistic version, where only one element is considered at a time, the method can be summarised as follows:

- The mode set to be used to decompose the source field needs to be determined. This has been discussed earlier in this paper. It is worth mentioning however that in the case of multi-element optical systems system-wide factors (optical throughput of the system) can be taken into the account to optimise the mode set.
- Source field decomposition using SVD approach.
- Propagation of the source field to the next optical element (mirror) using simple propagation characteristics of the Gaussian Beam Modes. This can be done very easily since only the mode parameters W and R evolve. Mode amplitudes are unchanged.
- Re-composition of the field at the next element. This element becomes the new source and the whole loop can be repeated.

We keep track of W and R of the fundamental mode to aid the mode set selection. Only these parameters and the size the current element (aperture) are used in the selection of the mode set. The throughput of the system is not considered (we take one element at a time). The method itself is general, and can be applied to both on-axis and off-axis elements. The determination of the optimal mode set however, is more difficult for off-axis systems.

#### **Test systems**

To test the SVD approach to quasi-optical system analysis, we applied it to the simple one- and two- ellipsoidal mirror test cases. Curvature of the mirrors was chosen to be significant to emphasise some of the potential problems. The simulated feed was a corrugated conical horn with an aperture radius of 2.5 mm and a slant of 15.4 mm. The wavelength chosen for the tests was 0.625 mm. The polarisation was perpendicular to the plane of the system (relevant for the benchmark PO calculations, see below). Other details of the geometry of the test systems are shown in figure 5.



Figure 5: Geometry of the test cases. Please note that the systems are not drawn to scale.

The results of the SVD analysis of the test cases are shown in figures 6-9, in terms of two orthogonal cuts across the selected output plane (shown in the figures). Several combinations of the following parameters of the SVD method were tested:

- number of field sampling points: 40x40, 20x20, 10x10,
- number of modes used for decomposition: 10 or 15, and
- number of additional zero field points beyond the element (expressed in terms of the *padding* parameter extent of the added part of the grid as a fraction of the extent of the main element sampling grid).



Figure 6: Symmetric cut across the output plane of the first test system (single ellipsoidal mirror). The power is normalised to the vector PO result at the centre. In the legend, the numbers in brackets are the mirror grid sizes in points. The field at the source mouth was always represented on a 24x24 main grid.



Figure 7: Asymmetric cut across the output plane of the first test system (single ellipsoidal mirror). Other details as in figure 6.

The SVD results were compared to results of Physical Optics (PO) calculations, in two versions:

- 1. Simplified scalar approach (Fresnel-Kirchhoff diffraction, polarisation not accounted for) on a 40x40 grid. These results were included as an example of an approximate PO calculation (that could be used in an interactive design package). The calculation time was comparable to the most computationally intensive SVD case tested here (15x15 modes on 40x40 grid with 0.5 padding).
- 2. Full vector approach (typical PO [10], as implemented in GRASP8 [11]). These results, calculated on a bigger grid (120x120 PO points, which is in our case big enough to ensure convergence), constitute a benchmark the other results can be compared to.



Figure 8: Symmetric cut across the output plane of the second test system (two ellipsoidal mirrors). Other details as in figure 6.



Figure 9: Asymmetric cut across the output plane of the second test system (two ellipsoidal mirrors). Other details as in figure 6.

All results were generated using MODAL, a design and analysis package being developed in-house in Maynooth [12]. This allowed all methods to be applied using exactly the same definition of geometry of the system. The accuracy of the vector PO engine in Modal favourably compares to that of GRASP8.

# Analysis of the test results

Several general observations can be made if one analyses the SVD results:

• Apart from the 10x10 grid case, the SVD results agree rather well with the accurate PO calculation, down to -20 dB. The big advantage of the SVD method is its speed - here SVD calculations were a factor of 20-1000 faster (depending on the parameters) than the vector PO calculation.

- The SVD approach can yield a completely wrong result, if the field sampling is too coarse. This becomes a real problem if the phase changes quickly across the mirror, because aliasing effects can lead to physically incrrect results. In our test calculations the 10x10 grid case was included specifically to illustrate this issue. In other systems such grid size can be perfectly adequate.
- SVD results are much more regular than the scalar PO results, and do not suffer from spatial aliasing for small grid sizes (apart from 10x10 case, as discussed above).
- Increasing the number of modes (10x10 -> 15x15) to some extent improves the field reproduction, but gains are not very significant here.
- Adding zero field points around the main grid slightly improves the reproduction of the field in the centre of the beam, and also reduces the appearance of extra side-lobes.

### Conclusions

Fast methods based on SVD Gaussian Beam Mode decomposition are potentially a very useful tool for analysing quasioptical systems. There are many potential problems however that need to be studied in greater detail, before SVD approach to modal analysis reaches sufficient maturity to be considered a reliable method of quasi-optical analysis. The aspects of the SVD method that we aim to address in the near future include:

- optimisation of the mode set,
- minimum density of field sampling points,
- weighting of field sampling points in the fitting procedure,
- optimal number, and distribution, of the added zero field points,
- handling of polarisation.

Our view is that significant progress can be made in these areas. However, even at this early stage of its development, the SVD approach is useful in practical applications. In particular it can be implemented in designer tools, where it can be used to quickly generate useful results at the system design stage.

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