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Grid-enabled electromagnetic optimisation (GEM) for industrial use

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Abstract. We have developed a tool for parametric electromagnetic design studies using industrial analysis code for the design search and optimisation of photonic crystals. This software tool allows engineering users to transparently access Grid compute components for an end-to-end design of a photonic device using computational electromagnetics. In this paper, we give an overview of the industrial application background, present some aspects of the interface developed, and discuss some of the issues involved in the computational tasks and the storage of metadata.

1 Introduction

Industrial engineering applications frequently require resources which are often not available to or accessible from small or medium sized enterprises (SME). This can be due to the high acquisition and/or maintenance cost of large computer systems or that of specialised software applications or due to the sporadic nature of the load placed on such a resource which does not justify its outright acquisition.

Grid technology [1] addresses these needs by enabling large-scale resource sharing over the web and thus offers SMEs the possibility of cost-effectively using software services and compute resources on an as-needed or on-demand basis.

We concentrate on the field of Computational Electromagnetics (CEM) within the area of Engineering Design Search and Optimisation, in which companies endeavour to find product designs which optimally fulfil certain objectives and respect constraints placed on them.

Grid-enabled Electromagnetic Optimisation (GEM, [2]) is a DTI-funded project in collaboration with Mesophotonics Ltd [3], a laboration with Mesophotonics Ltd [3], a start-up company working on the design, fabrication and characterisation of next-generation planar photonic devices. We will demonstrate the use of Grid resources for parametric studies of photonic crystals design.

This paper is organised as follows. Section 2 gives a brief overview of the application background, in section 3 we detail some of the technology used. Section 4 discusses the user interface and issues we encountered are discussed in section 5 before we present further work in section 6.

2 Application

Mesophotonics Ltd is a company specialising in the development and manufacturing of optical components for state-of-the-art communication devices. Their expertise and interest lies primarily in the computational and experimental investigation of Photonic Crystals (PCs) and the exploration of the characteristic light transmission properties for subsequent commercialisation.

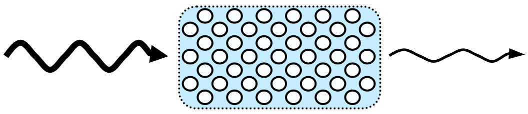

Figure 1 The geometrical design of a photonic crystal determines its light transmission properties.

A typical example of a PC is shown in figure 1. The base material is a silicon substrate with periodic changes in the dielectric constant, which can be obtained by, for example, etching a silicon wafer using a predefined geometrical pattern. The geometry used determines the transmission and reflection properties of the crystal for electromagnetic waves with wave lengths corresponding to that of visible and infrared light. These PCs can be used as components for filters, splitters or other optical devices.

Suppose an engineer wants to optimise the electromagnetic transmission properties of such a PC. There exist designs which exhibit a reduction of light propagation within a specific frequency range, called a photonic bandgap (PBG) of the crystal. For certain applications, it is desirable to obtain a large bandgap in the frequency spectrum.

The size of the bandgap for a number of design geometries can be investigated by sampling the parameters r and d across a range of values. Every design point gives rise to a different frequency spectrum $f(r,d)$ for the transmission of light; and after post-processing this spectrum, we obtain differing band gap values $b(r,d)$ for the corresponding geometries.

This approach can be seen as initial design search, from which further local design optimisation can be carried out at a later stage. The number of designs and the number of parameters varied for each design can be large and thus gives rise to many solutions and large amounts of data. All of these solutions – if good or poor – yield valuable information for later design optimisation and need to be preserved in a design data base. They may also be re-used in the design of future devices.

The analysis of the frequency spectrum for a given geometry is the computationally most expensive part as it involves a full finite difference time domain (FDTD) based analysis with a subsequent Fourier transformation of the obtained time spectrum.

To sample the large space of possible design parameters, we employ the LP-tau Design of Experiment (DoE) method, which can at present be accessed through a web interface and will be available as a grid service in due course.

The computation currently takes place on a pool of Condor-enabled desktop computers or – if a Linux executable can be used – on Globus-enabled resources.

2.1 Application Scenarios

(a) A software engineer at the company has developed analysis software and would like to use a Design of Experiment service to obtain optimal distribution of design points. The computation using his executable should be carried out efficiently on a cluster of machines within or outside the company and the resulting data and metadata shall be stored in a database.

(b) The engineer would like to use a commercial solver and analysis package to compare results, which is available on the web exposed via a Grid service. The design point data is already stored in the database.

(c) The engineer selects a specific design and would like to optimise this using an Optimisation Service on the Grid. The computation will take place both locally for the objective function and through a compute service for obtaining updates of the design point.

(d) A new engineer wants advice about how to run a design search and what resources to use. The knowledge-based advice service will help and guide setting up the components based on the knowledge extracted from previous senior engineers' tasks.

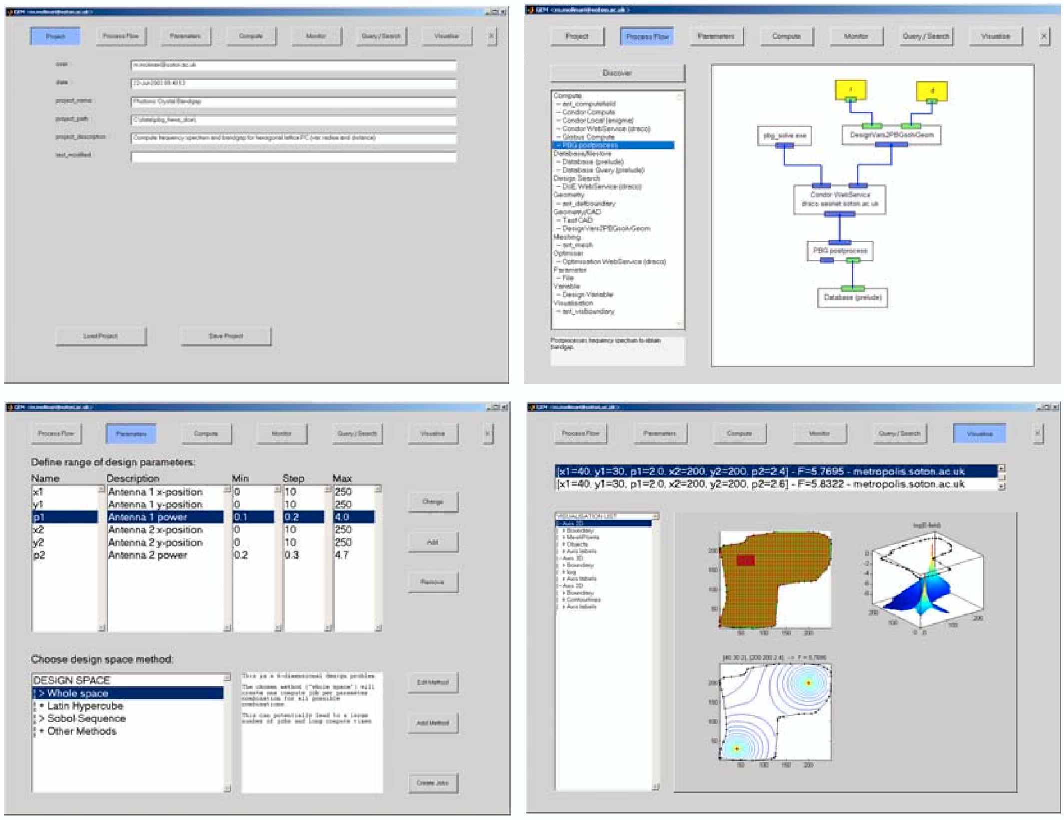

Figure 2. Graphical user interface/portal for (a) project definition, (b) process flow editing with Grid component insertion, (c) design parameter definition and (d) visualisation capabilities.

3 Middleware

For initial parametric studies of the designs, we have employed Matlab [4] as a problem solving environment and used the Grid interface functionality developed by the Geodise project [5].

As the XML based SOAP is the protocol used for web service interconnects, we have developed and integrated the XML Toolbox for Matlab [6] to be able to convert the proprietary Matlab structures into XML and vice versa.

4 User Interface

Computational Grids make it possible to access a wide range of distributed engineering applications and services. However, the consumption of these services remains difficult due to the lack of high-level tools to support engineers. One way of integrating Grid computing into engineering applications is by providing interface functions which seamlessly and transparently integrate access to Grid resources. The Geodise project provides such interfaces for the Matlab problem solving environment for access to compute as well as database resources.

We have developed a user interface on top of the Geodise high level routines, which provides a straightforward to access and integrate Grid services for parametric CEM studies.

Figure 2 shows examples of this Matlab based (and hence operating system independent) user interface. The GEM portal starts up with the project definition screen for the engineer, where details such as user name, project name and information can be entered. The process flow editor then allows integrating Grid and local components into the solution architecture. At present, all services are represented by XML files containing service descriptions, in future these will be discovered and retrieved at run-time. The parameter definition screen lets the user choose the range of design variables and select parameters for a DoE (if not requested from the DoE Grid service).

Archive Design Data:

```
% create proxy for access to Grid resources
gd_createproxy;

% define design metadata common to all designs
m.model = 'pbg_design';

% do computation for 1000 design points
for i=1:1000

 % create design point (r,d)
 [m.param.r, m.param.d] = designpoint(i);
 infile  = ['geometry_', num2str(N), '.cad'];
 outfile = ['spectrum_', num2str(N), '.dat'];

 % call routine that creates geometry file
 create_pbg_geometry_file( infile, m.param );

 % archive geometry definition and metadata
 gd_archive( infile, m );

 % Grid-compute frequency spectrum for design
 compute_pbg( m.param, infile, outfile );

 % post-process result and obtain bandgap
 m.result.bandgap = postprocess_pbg(outfile);

 % archive spectrum results and metadata
 gd_archive( outfile, m );

end
```

Query results:

```
% find all designs with bandgap bigger than 99
M = gd_query( 'model = pbg_design & …
               result.bandgap > 99.7' )
M: 4x1 struct array with fields
      standard, access, model, param, result
```

Now, `M` is a vector of structures containing the metadata of all PBG designs with bandwidth larger than 99. In this case, four designs match the query. The associated files can be retrieved and viewed:

Retrieve results:

```
gd_retrieve( {M.standard.fileID}, …
             '/home/Eng007/pbg_files/' )
diplay_freqSpect('/home/Eng007/pbg_files/*')
```

Figure 3. Matlab script for interaction with databases on the Grid.

The local directory tree with all data necessary for a submission for the analysis is then created in the background and the engineer can start the computation on the compute screen, where resources can be further specified.

The monitoring pane allows the inspection of the job queue and execution as well as the results while the job is running remotely. After jobs have finished, the engineer will be able to query job details and results from a Xindice database, where metadata about the runs and designs has been stored. A visual examination of the results will be possible via the visualisation pane.

Figure 3 shows cut-outs from a created Matlab script which can be used to create PBG designs, store the related metadata in a database on the Grid and query this data later to retrieve designs with specific properties.

5 Issues encountered

In an industrial environment, resources can be very scarce. The Grid offers the possibility of incorporating unavailable resources in the business workflow. Not only the (horizontal) computational workflow which we have been looking at in this paper is important, also the overall inclusion of Grid technology in the vertical business workflow which ranges from an initial design idea via computational electromagnetics to sharing of manufacturing data to the product which then needs to be verified experimentally. The results of the experiment as well as the performance of the product in the final application are all aspects which are important to the industrial partner and can be associated with future Grid technology.

Of high importance for commercial entities is the security of code and analysis results when being executed or transferred across the internet and such issues are addressed by, for example, WS security [7].

Amongst some of the interoperability issues we have faced, one was to overcome the proprietary data formats of existing software packages. During the course of this project, we developed for example the XML Toolbox for Matlab to be able to convert proprietary data type formats into an open standard XML format. This was necessary to enable us to create and use generic parameter description for a seamless combination of heterogeneous components and to subsequently be able to store XML (meta-)data in a native XML database.

In addition offer almost all currently accessible Globus-enabled resources on the UK Grid Linux-based operating systems whereas most of the software used in SMEs is Microsoft Windows based, i.e. there are issues with usage of these resources.

6 Conclusion & Future Work

We have used locally available Web Services and a Condor pool to perform parametric studies for computational electromagnetics problems in an SME.

We are currently concerned with the integration of web service access and functionality within a Web portal, i.e. webpages through which engineers can access/use the services.

Future work will also include the set-up of a repository of electromagnetic analysis codes and the deployment of a metadata-based design exploration system using current web standards such as WebDAV.

We will further expose solver and optimisation software via GridService specification compliant interfaces (OGSI.NET) and test these for application in a commercial environment.

Acknowledgements

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