EUROPEAN COMMISSION

RESEARCH DG

MARIE CURIE MOBILITY ACTIONS

INDIVIDUAL DRIVEN ACTIONS
FINAL SCIENTIFIC/MANAGEMENT REPORT

FINAL ACTIVITY AND MANAGEMENT REPORT

annexes:

- *list of participation in conferences;*
- *list of publications;*

Type of Marie Curie action:	IEF
Contract No.:	237397
Title of the Project[1]:	Nonlinear spectral problems and wave propagation in crystals
Duration of fellowship/appointment/training period (Start Date – End Date[1]):	01/01/2010 - 31/12/2011

1 Pre filled when applicable

1. PUBLIC OUTREACH: PUBLISHABLE SUMMARY OF WORK PERFORMED AND RESULTS

Non-linear spectral problems frequently occur when damping effects or frequency dependencies are included in a mathematical model. Prominent examples are plasmon resonances and band gaps in dielectric and metallic photonic crystals. Such crystal structures that are designed for controlling propagation of electromagnetic waves have numerous applications including telecommunication, solar cells and integrated circuits. The fellow studied photonic crystals theoretically and developed mathematical theory and numerical software. In the lossless case (no dispersion/absorption) the spectral properties are known and the convergence of a Galerkin approximation of the underlying operator is well established. However, the impact of material losses and the frequency dependence of the material parameters are in many cases crucial for the value of metallic photonic crystals and metamaterials at optical frequencies. A model with frequency dependent material parameters leads to a nonlinear dependence on the spectral parameter. That is, the resonances in the system are given by an nonlinear operator function. Basic questions such as the discreetness of the spectrum and convergence of a Galerkin approximation of the operator function was not known before the start of the project.

In his work, Christian Engström addresses these and other problems based on operator theory and approximation theory for non-compact operators. Moreover he applies a novel set of numerical techniques, which make it possible to simulate a broad range of problems in nano-optics. The software provide physicists and engineers with a new simulation tool for dielectric and metallic photonic crystals. The mathematical analysis and the numerical methods in the project are highly relevant since they assure that the numerical algorithms are reliable.

List of Keywords

photonic crystals, Galerkin approximation, operator function, nano-optics, resonances

Websites where additional information may be found

2. REPORT ON WORK PERFORMED AND RESULTS

The aims of the proposed research (as stated in the proposal) were

1. Spectral analysis and linearization of polynomial operator pencils
2. Galerkin discretization error analysis for quadratic eigenvalue problems
3. Computation of eigenvalues of matrix pencils that preserve the symmetry of the spectrum and computation of eigenspaces
4. Perturbation analysis of self-adjoint polynomial operator pencils
5. Application of the developed analytical and numerical tools to photonic crystals through the development of high performance software to compute plasmon resonances and band gaps in dielectric and metallic photonic crystals

Full details of The work performed and the results of the research are given below

1. Spectral analysis and linearization of polynomial operator pencils

The fellow addressed the spectral problems of operator pencils in [A8, C1] and proved for several classes of non-linearity that the spectrum consists of at most countable many isolated eigenvalues of finite multiplicity. Moreover, he proved in [A8] that all eigenvalues have a non-zero imaginary part even if one component has no losses. The analysis of Lorentz permittivity model shows that all eigenvalues are real when the permittivity is real. The fellow addressed several linearization techniques of operator pencils in [A8, A9, A10, A11, C1, C2]. In particular, the conditioning of linearizations was studied and a new linearization of rational eigenvalue problems was proposed. Figure 1 illustrates a computation of band gaps in a lossless two-dimensional photonic crystal with a frequency dependent material model.

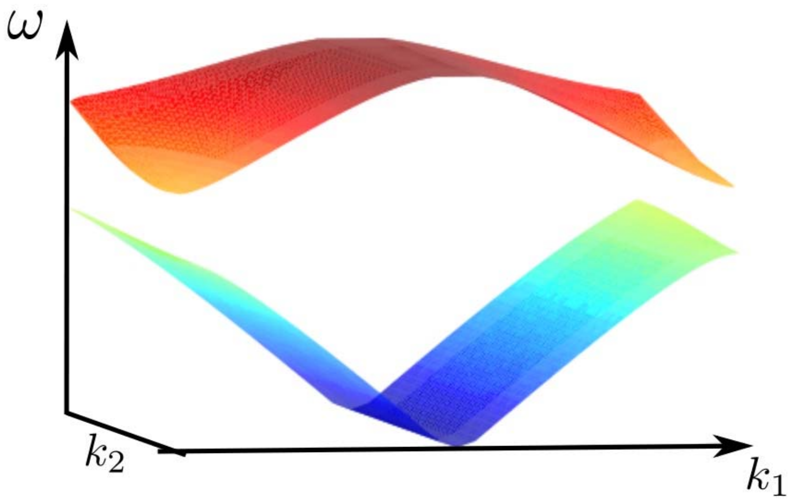

Figure 1. The spectral surfaces for a frequency dependent material model. No wave can propagate in the frequency range in between the two surfaces.

All deliverables were fulfilled in this part of the project.

2. Galerkin discretization error analysis for quadratic eigenvalue problems

The fellow addressed Galerkin discretization error analysis for quadratic and rational eigenvalue problems in [C1, C2] and a third paper is in preparation. He proved convergence of the spectral approximation and provided convergence rates. Moreover, he derived a computable residual estimate of a finite element approximation. The derived residual estimate was successfully used in numerical computations of band structures. Furthermore, the fellow compared [A10] numerically the p-version of a continuous finite element method (p-FEM, implemented in CONCEPTS) with a discontinuous Galerkin code (p-SIP) and an in physics commonly used code (MPB from MIT). Figure 2 illustrates the superior convergence of the high-order finite element codes p-SIP and p-FEM [A10].

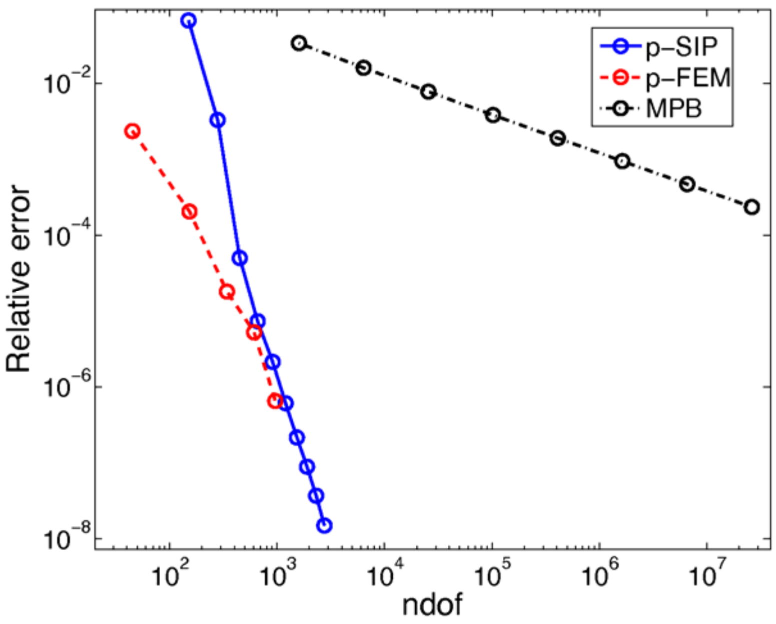

Figure 2. Convergence of the p-version of two finite element methods (p-SIP, p-FEM) and the MIT Photonic-Bands (MPB) package.
ndof – number of degrees of freedom,

All deliverables were fulfilled in this part of the project.

3. Computation of eigenvalues of matrix pencils that preserve the symmetry of the spectrum and computation of eigenspaces

The fellow addressed the computation of eigenvalues of matrix pencils that preserve the symmetry in [A11]. By taking the rich structure of these eigenvalue problems into account, we arrive at linearizations of reduced size, which considerably reduces the computational effort in terms of memory and execution time.

All deliverables were fulfilled in this part of the project.

4. Perturbation analysis of self-adjoint polynomial operator pencils

The fellow addressed the topic in [C2]. He used perturbation theory for generalized Rayleigh quotients and developed *a posteriori* approximation error estimation techniques.
Moreover the fellow considered the perturbation of a selfadjoint operator pencil by a non-selfadjoint operator function. This question was addressed in the end of the project and a paper is in preparation. Figure 3 shows that perturbation analysis is a very useful for determine the impact of losses in a photonic crystal.

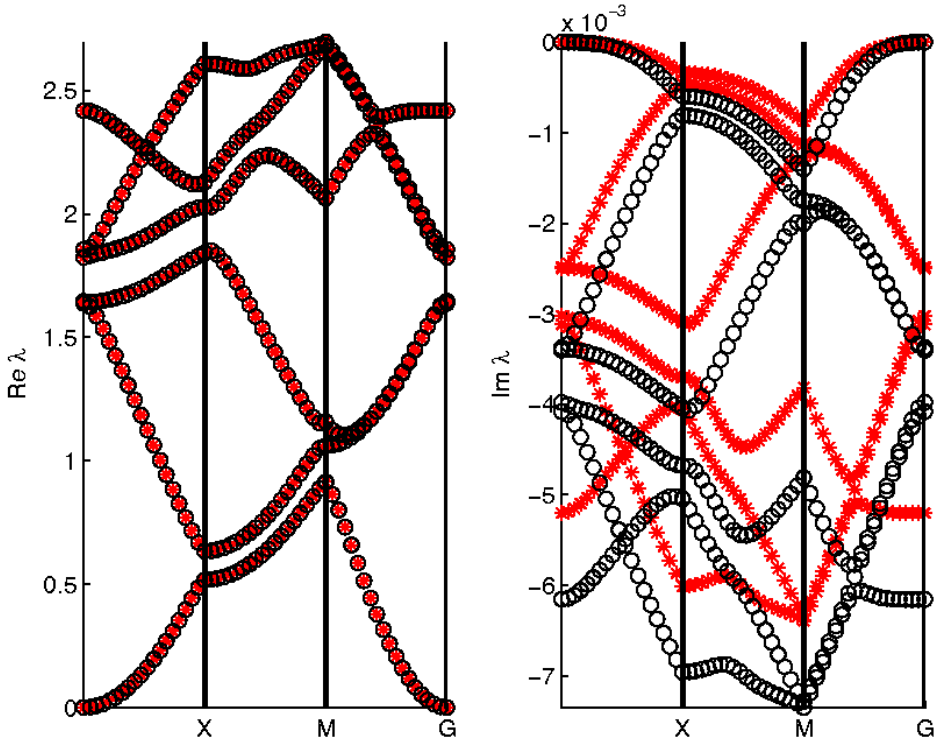

Figure 3. Left: the real part of the band structure (Reλ). The red stars are computed from the full (non-self adjoint operator function) problem and the black circles are computed by first solving a self-adjoint problem and then add a perturbation term. Right: The corresponding imaginary part of the band structure (Imλ). X, M and G represent the corner points of the reduced Brillouin zone, whereby X: (π,0), M: (π,π), G: (0,0).

All deliverables were fulfilled in this part of the project.

5. Application of the developed analytical and numerical tools to photonic crystals through the development of high performance software to compute plasmon resonances and band gaps in dielectric and metallic photonic crystals

The fellow developed a high-order discontinuous Galerkin code [A9] and adapted the continuous finite element code CONCEPTS to band structure calculations [A10, C1]. These two codes make it possible to obtain highly accurate eigenvalues from relatively small matrices. However, the matrix eigenvalue problem is nonlinear and there exist no general code that efficiently and robust compute the eigenvalues of nonlinear problems. We addressed this nonlinear matrix eigenvalue problem in [A11] and developed a new type of linearization that is very robust and result in much smaller matrix problems. The result is a high performance software for computation of the complex band structure in metallic photonic crystals.

All deliverables were fulfilled in this part of the project.

I enclose copies of

Christian Engström, *On the spectrum of a holomorphic operator-valued function with applications to absorptive photonic crystals*. Mathematical Models and Methods in Applied Sciences, 20 (8), 1319-1341, 2010.

Christian Engström and Mengyu Wang, *Complex dispersion relation calculations with the symmetric interior penalty method*. International Journal for Numerical Methods in Engineering, 84, 849-863, 2010.

Cedric Effenberger, Daniel Kressner and Christian Engström, *Linearization techniques for band structure calculations in absorbing photonic crystals*. International Journal for Numerical Methods in Engineering, 89, 180-191, 2012.

MANAGEMENT REPORT

Please justify any deviations and/or modifications to the initial financial planning of the project.

3. ASSESSMENT BY THE SCIENTIST IN CHARGE ON THE FELLOW'S WORK DURING THE FELLOWSHIP

Dr. Christian Engström studies a class of nano-sized structures called photonic crystals that can be used to control the flow of light. Photonic crystals are periodic structures made of two or more materials with different electrodynamic properties. Such structures are frequently used in for example thin film optics and in integrated optics. In the lossless case (no absorption) the spectral properties for a fixed Floquet-Bloch wave vector k are known and the convergence of a Galerkin approximation of the underlying self-adjoint compact operator is well established. However, the impact of material losses and the frequency dependence of the material parameters are in many cases crucial for the value of metallic photonic crystals and metamaterials at optical frequencies. A model with frequency dependent material parameters leads to a nonlinear dependence on the spectral parameter. That is, the spectrum is given by an operator function. Basic questions such as the discreetness of the spectrum and convergence of a Galerkin approximation of the operator function was not known before the start of the project.

In his work, Christian Engström addresses these and other problems based on operator theory and approximation theory for non-compact operators. Moreover he applies novel set of numerical techniques, which make it possible to simulate a broad range of problems in nano-optics.

The work excels in several regards. First, Mr Engström proved for the first time that the spectrum for an important class of operator functions is discrete. Second, the work is highly original in the approaches taken to numerically compute the spectrum of rational operator functions. Third, Christian Engström has successfully developed a high-order finite element code and applied the code to several relevant physical problems.

The high quality of Christian Engströms work is confirmed by the fact that he published 7 papers related to the project in top journals in the field. Moreover, 5 conference papers were published in the proceeding of conferences.

The undersigned agree:

- that the Commission may publish information contained in this report **Yes** X **No** ☐

- to allow the Commission to divulge future contact details to national representatives or to organisations carrying out services for the Commission **Yes** X **No** ☐

Signatures:

Name of fellow: Christian Engström

Date: 31 January 2012

Signature of fellow:

Name of scientist in charge:

Date:

Signature of scientist in charge:

RESEARCH RESULTS (Summarise the results obtained by the contractor since the beginning of the project)**:**

Participation in conferences and other scientific events:

Please indicate the number of participation to scientific events by the beneficiary of the contract. List the participation on a separate sheet following the classification used below.

	Number			
	Active participation			Passive participation
	Oral	Poster	Of which were invited presentations (oral + poster)	
Conferences	8	1	1	1
Workshops				
Other Scientific Meetings				

Patents:

Please indicate the number and status of patents, which have been the direct results of the research project. List the patents on a separate sheet giving their complete reference number and briefly stating the applicability of each patent.

	Number of Patents		
	Application filed	Pending	Granted
National Patents:			
- Member States and/or Associated States			
- Third Countries:			
- US			
- Japan			
- Other			
European Patents (EP number):			
International Patents (WO number):			

Publications:

Please indicate the number of publications resulting directly from the project. List the publications on a separate sheet following the classification used below, indicating any invited contributions. In publications resulting from collaboration with other institutions, indicate name and country of institution.

	Number of Publications		
	As main author	Total	Of which were co-authored with researchers from other institutions
A. Peer Reviewed ***(incl. in press)***			
- Articles in Journals	3	7	4
- Chapters in Books			
- Articles in Conference Proceedings	1	5	4
- Books and Monographs			
B. Non-Peer Reviewed ***(incl. in press)***			
C. Submitted	2	2	
D. Manuscripts in preparation	2	2	

Teaching and Transfer of Knowledge:

Please indicate the number of hours of lectures, which have been delivered by the beneficiaries of the project and training courses, which have been organised by the contractor(s) on the research carried out in the project. List on a separate sheet the lectures and/or training courses delivered.

		Number of participants	
	Number of Hours	Early stage researchers	Other
Lectures			
Training Courses			

Other outcomes:

Please list other outcomes of the project than those mentioned above. Such outcomes may be further academic qualifications, spin-off companies, prizes, awards, media coverage, etc.

	Number	Type
Academic qualifications		
Prizes and Awards		
Spin-off companies		