Algorithms for Casimir Force Prediction

(ESA Contract 15615/01/NL/LvH)

Summary Report

May 2003

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Summary Report

1. INTRODUCTION.

The project to develop algorithms to calculate the Casimir force (Contract 15615/01/NL/LvH) ran from December 2001 to March 2003 and was carried out at the Space Science and Technology Department of the Rutherford Appleton Laboratory. The final presentation was made at Estec on 14th March 2003
During that time all progress reports, minutes of meetings and other project deliverables were sent to ESA and also made available on a password protected FTP server.
The contents of the server will be made available to ESA on a CD .

2. THE AIM

The aim of the contract was to perform a study summarising the current status of the theoretical understanding and experimental work on vacuum fluctuations and Casimir force. This study was then used as a knowledge base from which to develop a modelling and simulation tool to calculate the Casimir force in general situations.

3. THE LITERATURE SURVEY

As part of the process of summarising current status, a thorough literature survey was conducted. A document summarising this survey was prepared and reported in August 2002.
The document reviewed the history of the Casmir force and the various experimental investigations and measurements. Theoretical approaches to calculating the force both in particular analytic cases and in the generality of cases, for which analytic solutions are not available, were also reviewed.

A further short document was prepared which addressed the effect of the Casimir force on Micro-electromechanical systems (MEMS) and Nano-electromechanical systems NEMS, giving the range and strength of the force in relation to other forces to which microstructures are exposed.

Both documents and the contents of the literature survey were made available on a password protected FTP server. Documents were filed under 18 primary headings to give a database of 160 documents (146Mbyte) on all aspects of the Casimir force ranging from theoretical, to measurements and MEMS applications.

4. THE PFF DOCUMENT

A ~2000 word (3 page) semi popular account of the Casimir force and its relevance to MEMS and space applications was prepared for the ESA journal Preparing For the Future. The article outlined the origins of the Casimir force and described the calculation process and included a description of the relevance to Micro electromechanical systems (MEMS) and also speculated on the use of the Casimir force for future Star Drives.

5. THE WEB SITE

A 14-page web site was prepared which outlined the features of the Casimir force described in the PFF and User Example documents, and included descriptions of the algorithm and user interface. In addition to the technical contents the site also includes a biography of the Dutch physicist H.B.G. Casimir.

The web site files, which are currently held on a server at RAL, will be made available to ESA on a CD so that the web site may be based at ESTEC.

6. THE SOFTWARE

The software was written in IDL and uses IDL graphics to display the geometry, intermediate calculation steps as well as the final result. The algorithm was discussed and described in the User example report and a description is also included as section 9 of this report.

An initial version of the software was made available to ESA at the final presentation and an updated version in which some minor bugs have been removed will be sent on CD.

7. THE USER EXAMPLE

An example geometry was supplied by ESA and calculated using the tool developed in this programme. The results were presented at the final presentation and discussed in the Example User Case Report. This 24 page report details the process of running the computational tool and discusses the strengths and limitations of the algorithm selected.

8. THE FUTURE

In the process of carrying out this study it became clear that computational resources were one of the limitations on the complexity of problem that could be addressed. In the intervening year clusters of parallel computers have become available at a reasonable price and the use of these devices would mean that the computational time limit would be greatly relaxed.

Further developments in the algorithm, particularly through work on the Lifshitz formalism, which makes use of the enhanced computing power of parallel processing, will enable other limitations of the additive principle approach to be addressed.

9. DEVELOPMENT OF THE ALGORITHM.

9.1 General Aim and the Casimir Effect

The present numerical code has been developed to be a user-friendly tool for the calculation and estimate of the retarded Casimir force in condensed matter structures with complex geometries.

The Casimir force is evidence of the quantum character of the physical world which seldom reveals itself at a macroscopic level. The simplest form of the Casimir effect was predicted in 1948 by H.B.G. Casimir and consists in the attraction between a pair of neutral, parallel, conducting plates placed in the vacuum. Recently, the Casimir force has been verified experimentally by Lamoreaux and Mohideen & Roy, thus adding it to the list of macroscopic quantum effects, which includes Superconductivity, Bose-Einstein Condensation and the Hall effect.

The strongest Casimir force results from the interaction of quantum electromagnetic fields with macroscopic background objects occupying the same region of space. This interaction changes the properties of the field given that it must satisfy some form of boundary conditions or constraints, which arise from the presence of the background objects. The field and its observables are then distorted away from spatial homogeneity that characterizes them in an empty space. As a result the field fluctuations are altered causing a pressure restitution force on the object. Within this scope the Casimir force can be understood as an unbalance of the radiation pressure produced by the virtual photons on the classical objects. These forces are called the Casimir forces and its strength depends on the electromagnetic and optical properties of the objects, as well as on the geometry of the boundary conditions imposed.
The Casimir force and related Zero-Point Fluctuation effects play an important role in different areas of both scientific research and technological and industrial development, thus increasing the need for fast and easy to use methods of calculation of this effect. In particular, one can distinguish the field of condensed matter physics where direct applications of this quantum effect are currently under development. In areas such as thin film physics, the Casimir effect should be taken into account in the determination of surface tension and latent heat, MEMS and NEMS, where the Casimir force plays an important role in stiction control, and surface physics, where the Casimir effect is a determinant in bulk and surface critical phenomena.

9.2 Calculation Methods for the Casimir Force

Different models have been proposed throughout the past fifty years to calculate the Casimir force for different configurations, geometries and considering different practical aspects such as thermal and finite conductivity corrections. Unfortunately there is no general method to calculate the Casimir force, instead for each specific configuration there exists a specific method.

The analytical methods developed give the most complete and insightful description of the Casimir effect, but they pose many difficulties as they result in infinite quantities such as the total vacuum energy. Most of the research during the past fifty years was concerned with the development of different techniques to deal with such infinite quantities, which have been developed in a highly mathematical context, and which do not take into account the practical framework associated with physical and technological implementation.

The calculation of the Casimir effect in situations with real practical use is limited by the lack of an efficient and numerically fast method of determining the eigenmode structure of the field for several configurations, geometries and boundary conditions. Most of the configurations previously analyzed deal with simple and highly symmetrical geometries, such as spheres, cylinders or plates, where the determination of the complete set of eigenmodes of the field is trivial. For technological applications of the Casimir force it is necessary to consider more complicated shapes where the determination of the eigenmodes of the system is not possible exactly.

A practical solution for these problems is to use the approximated methods which are easily modelled numerically and can be applied in a wide range of configurations. Presently there exist two main numerical methods for the calculation of the Casimir force in complex geometries: the lattice QED techniques and the phenomenological methods, such as Proximity force method.

The lattice QED can mimic and reproduce, in a detailed way, both global and local features of continuum Casimir systems with simple geometries, while failing to produce meaningful results for most highly complex systems.

In terms of computational power, adequate choices of lattice geometry can increase the efficiency of the method, reducing the number of grid points and enhancing the precision of the calculations. Nevertheless such choices are still limited by the complexity of the physical objects considered. Also some authors have noted that not all lattice descriptions of the Casimir effect in a lattice lead automatically to the correct continuum.

The Proximity force method considers the sum of the contributions of small surface elements which compose two close objects, assuming that they behave as infinitesimal parallel plates. This phenomenological approach is limited to objects with surfaces that have a small degree of non-parallelism and requires careful parameterisation of each system.

Finally, there is the method based on the Additive Principle. This is the most versatile and easy to use method to calculate the Casimir force in complex geometries, and it can take into account some of the physical properties (the atomic polarizability) of the materials of the object. The numerical implementation of the method is fairly simple and requires computational resources compatible with presently commercially available workstations. Moreover, it is a fairly fast algorithm as each run takes less than a day, which is considered numerically fast and it can provide numerically accurate results (numerical errors have been estimated as being less than 10^{-12}). For these reasons the algorithm based on the Additive Principle was considered the best choice for the method used in the present implementation.

Table 1: Comparisons of the basic Casimir force calculation algorithms.

	Lattice QED	**Proximity Force**	**Additive Theorem**
Range of configurations	Wide but with limitations.	Quasi-parallel geometries only.	Complex geometries.
Material properties of objects	No references found.	Atomic polarizability.	Atomic polarizability.
Repulsive Force	No references found.	No	No
Numerical resources	Large	Works on PC	Works on PC
Numerical accuracy	In some cases gives wrong answer.	Good	Good (numerical error~10^{-12})
Speed of calculations	Slow, needs many runs to produce final result.	Fast (less than a day)	Fast (less than a day)
Implementation and algorithm	Complex, lattice must be adapted to configuration.	Fairly complex.	Fairly simple.

In summary we may characterise the various calculation methods as detailed in the above table. The table lists the attributes of QED and two phenomenological approaches to Casimir force calculations, and clearly shows that the Additive Theorem is the first choice for calculations of reasonably complex configurations, without resorting to parallel or other sophisticated computers.

9.3 The Algorithm

The numerical code developed at the Rutherford Appleton Laboratory uses an algorithm based on the Additive Theorem, which considers the sum of the retarded Casimir interactions of every two atoms or molecules composing the physical object. This method is of course very versatile since in principle it can be applied to bodies of arbitrary shape and also because the two atoms interaction is easy to calculate numerically and they do not generate infinite quantities.

The interaction between two neutral atoms due to the dipolar fluctuations of the electronic cloud is described by the following potential energy[1]:

$$E(R) = -C\sum_{l,m}\int_0^\infty du\,\frac{k_l k_m}{(k_l^2+u^2)(k_m^2+u^2)}\,\frac{e^{-2Ru}}{R^2}\times\left\{Q_\perp^2\left(1+\frac{1}{Ru}+\frac{1}{R^2u^2}\right)^2+4Q_z^2\left(\frac{1}{Ru}+\frac{1}{R^2u^2}\right)^2\right\}$$

,

with $Q_\perp^2=\left(q_l^x q_m^x\right)^2+\left(q_l^y q_m^y\right)^2$ and $Q_z^2=q_l^z q_m^z$ the dipole moments of each atom.

The asymptotic limits of this potential energy for short and long distances results in the London and the Casimir interactions, respectively:

$$E(R \to 0) = -C' \sum_{l,m} \frac{Q_\perp^2 + 4Q_z^2}{(k_l + k_m)} \frac{1}{R^6} \qquad \text{and}$$

$$E(R \to \infty) = -C'' \sum_{l,m} \frac{13Q_\perp^2 + 20Q_z^2}{k_l k_m} \frac{1}{R^7} .$$

The present implementation of the code explores the formal similarities between the calculation of the Casimir force and the calculation of the electric force produced by a distribution of charges and it is based on the determination of the values of a Casimir interaction energy between atoms or molecules A and B:

$$E_{A,B} = \xi \frac{\alpha_A \alpha_B}{\left|\vec{r}_A - \vec{r}_B\right|^7},$$

where α is the polarizability of each atom or molecule and $\xi = 23\hbar c / 4\pi$ is the interaction strength.

The code considers a cubic simulation box where the physical object is located. The physical object is then divided into a lattice of small cubic cells. The choice of the size of each matter cell depends on the degree of detail needed to describe the physical object. It should be noticed that an excessively small cell size would result in a large number of cells whose value may exceed the computational resources available. Also very small matters cells do not necessarily produce more accurate results due to the increase of accumulated numerical errors (such as those due to truncation). Therefore to establish a good cell size it is advisable to repeat the same simulation with different matter cell sizes and compare the results obtained.

Each matter cell *j* is assumed to be sufficiently small so that the Casimir potential field produced by it can be calculated as if all the atoms or molecules in the interior where placed at the geometrical centre of the cell and thus behaving as a point like source. The Casimir potential $\varphi_j(\vec{r})$ produced by each matter cell *j* is given according to:

$$\varphi_j(\vec{r}) = \xi \frac{n\alpha}{\left|\vec{r} - \vec{r}_j\right|^7},$$

where n is the number of atoms or molecules present in the matter cell and $\vec{r}_j$ is the geometrical centre of the matter cell. Notice that this Casimir potential field is here introduced simply as a notation and has no physical meaning.

The total Casimir potential produced in each point of space by the physical object in the interior of the simulation space is therefore the sum of the contributions of all matter cells, *i.e.*:

$$\varphi(\vec{r}) = \sum_j \varphi_j(\vec{r})$$

In practice, it is impossible to calculate the value of φ in all the points of space, instead φ is evaluated in an irregularly distributed grid of points $\{\vec{R}_j\}$ in the interior of the simulation box. This irregular grid is constructed in order to have a higher density of grid points in regions of space where the Casimir force is stronger thus increasing the accuracy of the results and reducing the time of calculation and computer memory use.

The energy of Casimir interaction between a cell *i* and the remaining cells of the physical object is given according to:

$$E_i = \alpha \varphi_j(\vec{r}_i).$$

The Casimir force acting on that matter cell is simply calculated as:

$$\vec{f}_i = -\vec{\nabla} E_i = -\alpha \vec{\nabla} \varphi_j(\vec{r}_i).$$

In order to calculate numerically the value of the differential operator ∇ in the previous expression the total Casimir potential is interpolated using a cubic spline over the grid $\{\vec{R}_j\}$.

To determine the total force acting on the physical object it is then necessary to sum over all its matter cells:

$$\vec{f} = \sum_i \vec{f}_i$$

In the actual code the calculations are done using the natural units defined according to $\xi\alpha^2 = 1$ and the matter cell size is renormalizes to 1, hence the value of the Casimir force obtained from the code does not depend on the nature of the material nor the actual dimensions of the physical object. To introduce these aspects in the calculation and to obtain the real value of the force $\vec{F}$ it is necessary for the value of the Casimir force obtained from the code $\vec{f}$ to be multiplied by the scaling factor:

$$\vec{F} = \frac{\xi\alpha^2}{a^7}\vec{f},$$

where *a* is the actual size of each matter cell.

9.4 Limitations and Advantages

Within the scale of the contract a fully general calculation, in a reasonable time, on a pc is not possible, for the reasons described above. However, as a calculation tool for MEMS and NEMS type of structures the code developed is valuable albeit with some limits and restrictions in its current implementation.

Currently, the calculation of the Casimir force is only possible for structures made of a single material- the calculation is performed using renormalized units in which all materials are alike and afterwards the results are reconverted back to S.I. units to give an idea of the likely strength of the force.

For most materials electric polarizability is dominant over the magnetic polarizability and the renormalization factor is positive, this implies that Casimir force predicted by this method is always attractive independently of the geometry. This limitation is due to the fact that this method does not consider high order corrections of the theory which require more computational power to be calculated.

The calculation is time consuming and only performed in one Z plane for each single run. To calculate the TOTAL force for a 100x100 parallel plate would require around 33 different runs to be summed together. This is because the code is performed in one Z plane for the X and Y components of the force, but in THREE Z planes in order to get the Z component of the force. However, if we call on the symmetry of the object and assume that the top half of the plate is going to be identical with the bottom half – or vice versa), this full calculation could be reduced to around 17 runs and would only be performed from the edge of the plate to the centre plane (in Y). This could still be a fairly time demanding procedure however, so prior optimisation would certainly be recommended before embarking on the "final" full calculation.

The definition of structures is currently limited to a relatively small range of shapes and these shapes cannot currently be "angled" to one another. Tests performed with spheres suggests that this may not be an important issue, but there is always likely to be some limitations when converting "smooth" shapes into cubic volume elements – in effect, an inclined shape is going to be modelled as a surface with a high degree of "surface roughness" compared to the same shape aligned parallel to the normal cubic grid structure. This limitation means that the code is actually applicable to exactly those planar structures most likely to be encountered in MEMS fabrications.

A "feature" of the code is the built-in requirement for the "surfaces" of the working volume to be vacuum. So, after creating the structure the code will automatically reset all 6 faces of the working volume back to vacuum. This is related to needing a vacuum point "outside" a matter point in order for the code to be sure it knows where the matter ends.

It is important that this limitation be borne in mind as it could lead to some confusion later on.
The code is also not temperature dependent. The code makes no allowance for finite temperature effects – the calculation is essentially performed at absolute zero.

Finally, the code does not consider “shielding”. The code calculates the total effect of each matter grid element on all other matter grid elements assuming that any intervening matter grid element will have no effect on the interaction. This means that intervening structures would also have no “dilution” effect on the force (they would, of course, have an additive effect on the total force).

The advantages of the IDL implementation of the algorithm are that the interface is very user friendly. It is relatively easy to build up quite complex structures and the code instantly updates after each new shape component is added to the overall structure. The code does give a relatively quick view of the overall “surface” of the Casimir potential when it performs its “coarse grid” calculation (used in deriving the full adaptive mesh used to calculate the final Casimir force components). The code also displays the final Casimir force in its various components (X, Y and Z directions) so the effects of changing component shapes or dimensions can be seen quite easily. The algorithm is ideally suited to comparing “similar” geometries – *i.e*. parallel plates of different dimensions and thickness (although the thickness of the plates is more connected with how well the code can “resolve” the asymptotic nature of the Casimir force). Also, the fact that the code is written in IDL should mean that it will run on a variety of computer platforms without any significant modifications (the modifications required would be to simple details like fonts and the initial definition of the graphical window – nothing that would affect the details of the calculation itself!).

References

[1]Casimir & Polder, Phys. Rev., vol. 73, 1948