Report on EPSRC Senior Research Fellowship
Grant number SF/000169, held by
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There is not room in this report to list all the publications. They are given on my web site at http://www.dur.ac.uk/peter.bettess/public/fellow/publsrf.htm In this report the numbering of the references refers to the numbering in that list. I gave a presentation summarising much of the work at a conference in Reading University in September, 2004. The powerpoint presentation is available to download from http://www.dur.ac.uk/peter.bettess/public/fellow/reading05.ppt If difficulties are encountered in accessing these files, please let me know.

1. Background / Context

Wave problems are of great importance. They permeate the world in which we live and have an influence on everything from atomic processes, through Schrödinger's wave equation, to waves in the ocean and earthquake waves. The fellowship was devoted to ways in which waves could be modelled on the computer more efficiently. This is because many wave systems are too complicated to be modelled using conventional finite elements, simply because too many variables are involved and the system matrices become too large.

The work was originally planned to tackle two main areas:

- infinite elements for short wave problems
- special finite elements for short wave problems

Subsequently the work developed another dimension. The ideas that had worked with finite elements were applied to boundary elements.

- boundary elements for short wave problems

Although this last concept was not in the original proposal this work turned out to be the most fruitful of all. This will be explained later. For some boundary integral wave scattering problems the errors with the new plane wave basis methods were *ten million* times smaller than those for conventional boundary elements. Other more peripheral ideas were also explored. There was a collaboration with the Department of Physics at Durham, to work on Schrödinger's wave equation, and a collaboration with the Ecole Centrale de Nantes, France, to work on ground vibrations caused by trains. Another development was the extension of the theory of the special short wave finite elements to include *wave refraction.* None of these had been in the original proposal.

2. Key Advances and Supporting Methodology

2.1 Infinite elements for short waves

I rate the work on infinite elements as not very successful at all. I had originally planned to extend the concepts currently used in infinite elements to include multiple wave directions. I also wanted to develop conjugated and unconjugated infinite elements of these new types. The necessary theory was worked out. Some of the work was done in conjunction with a researcher on an EPSRC grant number GR/M41018. Her name was Rie Sugimoto. Between us we tried a number of new formulations for the infinite wave elements. Unfortunately although all these elements had more free parameters, (and thus one would have expected them to be more accurate), in all cases they gave worse answers than the conventional wave infinite elements with a single wave direction. We checked our theory and coding exhaustively. One concern was that the integration scheme was not accurate for the case of additional wave directions. We developed and thoroughly tested a brute force and ignorance scheme which used very large numbers of Gauss-Legendre integration points. Although this integration scheme was impractical as the computer execution times were excessive, it did give the same results for the element matrices in the case where there was a single outgoing wave direction. This is the case in the classical wave infinite element, for which efficient integration schemes are available. We were able to confirm that all the terms in the infinite element matrix were identical using the two integration schemes. So we were confident that the integrations were working for the multiple direction infinite wave elements. However the results obtained with these elements were worse than those obtained with elements which only had a single wave direction. (To our surprise this remained true, even when the single, radial, wave direction was included in the set of wave directions in the infinite element. The effect may be connected with ill-conditioning of the element matrix, although this is speculation.) I was not able to discover the reason for this unsatisfactory behaviour of the elements. Whether there is a programming error, or whether it is due to some conceptual mistake, I could not determine.

The one success in this field that we obtained was that we demonstrated that it was possible to link the new plane wave basis short wave finite elements with classical infinite elements for waves. Papers were published giving results obtained using this linking[11,24]. Despite all these problems Rie Sugimoto was able to get enough results to successfully complete her Ph.D. She went on to a post as a research associate at the Institute of Sound and Vibration in Southampton University. In terms of key advances, this part of the fellowship yielded next to none.

2.2 Finite elements for short waves

This part of the fellowship involved extending special finite elements which incorporate short waves to three dimensions and to developing schemes for integrating the element matrices rapidly. It was also intended that adaptivity schemes would be developed. These would enable the rapid selection of optimal wave directions in these finite elements.

- Integration schemes for plane wave basis finite elements for waves. I collaborated with Joe Shirron in the U.S.A. and we were able to effectively develop all the integration schemes that I had originally proposed. Howevever this work took much longer and was much more complicated than I originally anticipated.
- Adaptivity for plane wave basis finite elements for waves
- Link infinite and short wave elements into one computer program

2.2.1 Wave finite element integrations

This was a feature that was emphasized in the original proposal. I spent a great deal of time and effort on this aspect of the work, so would like to discuss it in some detail. One of the problems with the method which was investigated is that integrals of the form

$$\int_{\Omega} f(x,y)\exp(ik_x x)\exp(ik_y y)d\Omega \qquad \text{or} \qquad \int_0^y \int_0^{1-x} f(x,y)\exp(ik_x x)\exp(ik_y y)dydx \tag{1}$$

arise. There are also corresponding integrals in three dimensions. k_x and k_y are the vector components of the local wave number. This is *not* the wave number of the problem, but arises from the product of two plane waves. The values of k_x and k_y can range from large and negative, to large and positive, including the value of zero. (The last case arises when two waves travelling in opposite directions, cancel each other.) The above integration is relatively simple, although it does require integration by parts or some other device to deal with the higher order terms in the polynomial $f(x,y)$. However it is very difficult to write a general analytical solution which is valid for *all* values of k_x and k_y, and to program this. The reason for the difficulty is that the analytical integral

$$\int \exp(ikx)dx = -\frac{i}{k}\exp(ikx) \tag{2}$$

clearly breaks down when $k = 0$ and gives numerical problems when $k \approx 0$. The physical interpretation of this mathematical effect is that when one of the wave directions is perpendicular to an edge of an element, then the variation *along* that edge (or *across* that face) is no long in the form of a wave. This gives rise to many special cases, especially in three dimensional elements, where special cases arise for waves perpendicular to all faces and all edges of any element! For a general hexahedron for example, 19 special cases arise. (The waves can be perpendicular to any of the 6 faces and any of the 12 edges, and the final case is when there are no waves at all present.) When a special case arises, the exponential must be replaced by the series representation of the exponential,

$$\exp(ikx) \approx 1 + ikx + (ikx)^2/2! + \ldots (ikx)^n/n! \ldots \tag{3}$$

and then the integration can be carried out successfully. But this can only be done when the argument, kx is small, and judgements have to be made as to when the exponential form and the series form are to be used, and how many terms to retain in the series form in the above equation. This all makes the conceptually simple integrations very complicated when a computer program must be written. It took me three attempts to analyse this problem and to develop suitable integration schemes for general two and three dimensional elements. The final algorithm used the divergence theorem to transform the integrals over a three dimensional domain into integrals over the surfaces of the solid element. These in turn were transformed into integrals over the edges of each face. Finally each edge integral was transformed into two functions to be evaluated at the ends of the edge. Throughout account had to be taken of the degenerate forms. The resulting integration code was developed using the Maple computer algebra software. It was essential to use a computer algebra code, because the resulting expressions had to be differentiated, so as to obtain the integrals for the higher powers of x, y and z. Once this had been done, and the final expressions for the integrals had been obtained in closed form, the Maple code was used to generate Fortan code, which executed sufficiently rapidly to be inserted in the finite element program. The Maple code was far too slow to do this. The Fortran code was subjected to numerical tests, by substituting specific values for the element co-ordinates, wave directions and wave number. The values it obtained were compared with those obtained by the Maple code, when run with specific numerical values, instead of variables. The aggreement was within the limits of the double precision, i.e. about 10^{-15}.

Papers was published on the earliest integration scheme[1,21,22]. But since then the method has been improved greatly. The description above is of the latest version. This work has been communicated to our industrial partners, but not published. A device due to Joe Shirron greatly simplified some of these integration procedures. This device can be explained as follows. Suppose we have found a closed form expression for an exponential integral, which we denote by W_{00}.

$$W_{00} = \int_{\Omega} \exp\left[i(k_x x + k_y y)\right] d\Omega \tag{4}$$

The integral, W_{10} can easily be obtained by observing that

$$W_{10} = \int_{\Omega} x \exp\left[i(k_x x + k_y y)\right] d\Omega = -i\frac{\partial W_{00}}{\partial x} \tag{5}$$

This can easily be generalised to higher powers of x and y and to three dimensions. The computer algebra code, Maple, will readily find the higher derivatives. (The alternative method, that of repeated integration by parts, is more difficult to follow. Moreover the computer algebra codes are much slower at integrations. Naturally the results are the same.)

Some unpublished work has also been done on the case where edges or faces of a solid element are curved. When the edges of the element are curved the Jacobian is no longer a constant. (The mapping is not affine.) However the Jacobian can be approximated as a series, in terms of co-ordinate parameters. (These would typcially be the offsets of midside nodes). This has the effect of simply requiring higher orders of x and y in the element, and thus higher order integration rules. Preliminary results showed that while the integrations are more difficult for such cases, some progress is possible.

For rectangular and cuboid elements Joe Shirron contributed a very elegant scheme which uses a property of spherical bessel functions and Legendre polynomials to give a method for integrating the element matrices very rapidly. The computer code is also very simple, being less than 60 lines. I programmed and tested Shirron's theory and it works. So rectangular and cuboid element matrices can be formed extremely rapidly and efficiently.

2.2.2 Adaptivity and error indicators

Efforts were made throughout the term of the fellowship to develop adaptivity schemes. These would enable the wave directions to be selectively improved. Typically after the first solution to the problem would be studied, and better wave directions would be chosen at all nodes. The solution would be repeated and the directions refined, until the accuracy of the solution was known and acceptable. Several methods were tried. One in particular gave good results for some special cases, but for more general cases gave only poor results. I was not able to obtain any adaptivity results that were of publishable quality. No suitable error indicators were found either. This was a disappointment.

Some work was successful on the related problem of the conditioning of the element matrices. This was published[10,14].

2.2.3 Conclusions

The work on the special short wave finite elements was broadly successful. Despite some problems by the end of the project a finite element code had been developed and tested. It had solved a large range of short wave scattering problems in two and three dimensions. The integration schemes had been tested for a significant range of element types, and had shown the expected behaviour, i.e. the integration execution time was independent of the wavenumber. Results can be seen in the papers listed on the form and in the references in the list mentioned at the start of this report and in the powerpoint presentation, which is available for downloading on the web.

2.3 Boundary elements for short waves

I carried out this work in conjunction with my colleague, Dr. Jon Trevelyan, also of the School of Engineering at the University of Durham and our joint research associate, Dr. Emmanuel Perrery-Debain. I had originally had the idea, before starting the fellowship, that the concept of using plane waves might work just as well with boundary elements as with finite elements for wave problems. My colleague, Dr. Jon Trevelyan, is an expert on boundary elements. Between us we developed a proposal for the EPSRC on this topic. This at first found little support from the EPSRC and it was only on the third submission that it was funded. The title of the grant was: Development of Special Boundary elements for diffraction of very short waves (Principal investigator Dr. Jon Trevelyan, myself as co-investigator). As the title suggests this work involves the development of new types of boundary elements for unbounded problems, which will include the wave shapes in the boundary element shape functions. The project ran from 2000 to 2003. The project involved collaboration with British Aerospace, Bristol. The EPSRC code number is GR/N09879. The total project value was £135,087. We appointed a researcher, Dr. Perrey-Debain. It turned out that the idea was successful, beyond our wildest dreams. It only required a relatively simple extension of the boundary element concept to include a set of plane waves, multiplied by the conventional boundary element polynomials. In our case these were quadratic polynomials. The integrations over the element domains are now more complicated, since they involve the product of not only the Green's function and a polynomial, (which is true of conventional boundary elements), but also plane waves. These integrals were found by using many Gauss-Legendre integration points. It is also a process which is easy to execute in parallel on suitable computer hardware. The results obtained by the new elements were startling. The code included the conventional elements as a special case. For problems of scattering of waves by a cylinder or a sphere, the errors for a frequency of practical interest, and for the same number of equations to solve, dropped by a factor of 10^7 for many cases. Alternatively the same accuracy could be obtained and the frequency could be increased by a factor of 3 in two dimensions and more in three dimensions.

Dr. Perrey-Debain, while supervised by Dr. Trevelyan and myself rapidly established two dimension results and he followed these with three dimensional scattering results. After that he extended his work to two dimensional elastic scattering problems. The equations of elasticity are much more complicated than the Helmholtz equation of course. Not only is the variable now the vector displacement at a point instead of a scalar potential, but a minimum of two wave speeds are always present. The displacement field had to be partitioned into pressure (or dilatational) and shear wave components, each with their own wave number. However despite the additional complexities, the method proved again very successful, with similar error reductions when using the plane wave solution space. Excellent comparisons were obtained with theoretical solutions for elastic waves scattered by circular and elliptical cavities. The project was very fruitful in terms of publications[9,13,17,18,20,23,25,26,27,29,30,33,35,36,38,39,41].

2.4 Wave refraction

In the original proposal for the fellowship I had only envisaged tackling problems in which the wave speed was constant. About three quarters of the way through the project I realised that there was the potential to extend the concept to the case where the wave speed varied linearly in a certain domain, and also to the case where there was a jump in the wave speed. The first can occur in the case of surface waves on water, where there are gradual changes in the water depth. The latter can occur where there is a sudden change in depth, or where acoustic waves move from a zone of one density to a zone with another density, for example. In the case of linear variation of wave speed, the waves will follow circular arcs. I was able to sketch out the necessary theory to extend the method to this case. A paper giving the theory was published, but the resources were not available to obtain any results[32]. In the case of jumps in wave speeds, the theory for matching the wave potentials at the interface, using Lagrange Multipliers was developed with Dr. Omar Laghrouche. This was also programmed. Good results were obtained for a number of cases for which the analytical solution was known. The theory and results have been published[38].

We have good contacts with a group at the Institute of Sound and Vibration at Southampton University led by Professor Jeremy Astley. During my fellowship, he spent a term at Durham University, as the Pemberton Visiting Fellow at University College. An outcome of this collaboration was a joint publication. Later Astley was able to tackle the associated problem of wave refraction caused by flow. He has recently published two papers which extend the plane wave basis finite element method to refraction in the presence of a flow. The main application is jet engine noise propagation, where the noise is superposed on a flow field.

2.5 Quantum Mechanics and Schrödingers Equation

During the term of the fellowship I collaborated with the Departemnt of Physics at Durham University. They were interested in the use of finite element methods to model Schrödingers Equation. We carried out some preliminary studies. We were able to model the lowest energy modes of the hydrogen atom. This indicated that the method was viable. We also succesfully applied infinite elements to a simple quantum mechanics problem. This was the first application of infinite elements to the solution of Schrödingers equation that I am aware of. A paper resulted from this work[16].

2.6 Railway track vibration, shock waves etc.

For a number of years I have had a successful collaboration with the Ecole Centrale de Nantes. They are interested in the vibration caused by trams and railway trains. Clearly our work on waves was of interest to them. We obtained two years of Alliance funding through the British Council for exchange visits. Several staff from Durham visited the Ecole Centrale de Nantes and their staff visited Durham. Researchers and final year undergraduates were also exchanged for longer periods. Collaborative papers were published with Professor Le Houedec and Professor Peseux of Nantes[12,40]. There are some interesting practical problems which arise with fast trains running on foundations of soft soil. The train speed can become a significant fraction of the wave speed in the soil. This can lead to large displacements of the ground and large stresses in the rails. If the train could travel as fast as the elastic wave, there would be a kind of sonic boom effect. Fortunately the trains do not travel so rapidly, but it is easy to see the importance of the problem for fast trains. I was the external assessor of a PhD thesis dealing with experimental and numerical studies of trains in the Somme valley and sat on the PhD jury, One of the French visiting students was very helpful in developing the integration methods for our special finite elements.

3. Project Plan Review

Some aspects of the project followed the plans that I had laid out. This included the work on infinite elements (even though relatively unsuccesful) and the work on the integration of the finite element matrices. The work on plane wave basis boundary elements, on Schrödinger's equation and on the ground vibrations, with ECN, were not in the original plan. However I felt that is was right to pursue promising research opportunities as they arose.

4. Research Impact and Benefits to Society

The impact of this research will clearly be long term. It should lead to a better understanding of problems involving the scattering of waves. It is also part of the progress towards the prediction of short wave effects in detail. This work has obvious applications in acoustics. For example it is leading to better modelling of the propagation of noise from aero-engines, and thus to quieter aircraft, both for passengers and those on the ground. There are defence applications, in the prediction of radar signatures of aeroplanes and ships. There are medical applications in imaging processes, and even therapeutic applications where waves can be focussed on a tumour for example. Developments in the modelling of Schrödinger's equation can lead to the prediction of the properties of a molecule before it is created.

5. Explanation of Expenditure

There was no deviation from the planned expenditure, which was entirely spent on my salary.

6. Further Research or Dissemination Activities

During the term of the fellowship I submitted five EPSRC proposals, as either PI or co-investigator. These all covered interesting developments in the general research area of short wave modelling.

1. Development of special boundary elements for diffraction of very short waves, with Dr. Jon Trevelyan as PI (funded).
2. Development of special finite elements for electromagnetic scattering of very short waves, Jointly with Department of Civil Engineering University of Wales, Swansea, and BAE Systems, Bristol (funded).
3. The application of plane wave basis boundary elements and fast multipole methods to Maxwell's equations, in conjunction with BAE systems (not funded).
4. Finite element methods for electronic structure calculations, in conjunction with the Department of Physics, University of Durham (not funded).
5. Special Plane Wave Basis Finite Elements for Refraction of Waves in Shallow Water (submitted twice, not funded on either occasion)
6. Adaptivity and Integration Schemes in the Plane Wave Basis BEM for Helmholtz problems (funded on second submission)

I was also successful in getting Alliance funding, through the British Council, for links with Ecole Centrale de Nantes. This was to collaborate on ground vibrations.

There is great scope for further extension of the work done during the fellowship. The methods can be extended to other wave equations, to waves undergoing refraction due to inhomogeneous materials of flow of the wave medium and to completely transient wave problems. If we could predict all wave effects at any scale with arbitrary precision the scientific and engineering benefits would be immense.

My researchers and I presented results at numerous conferences. The resulting publications are listed on the web site given above.

Publications and other dissemination

The research was disseminated in the usual way, through web pages, presentations at conferences, presentations to industrial collaborators and, most importantly, by published papers in high impact factor journals. As seen in the IGR there were a large number of publications, particularly in IJNME which has the highest impact factor in the field. In addition I suggested to the Royal Society that a Theme Issue of the Philosophical Transactions could be devoted to short wave modelling. This suggestion was externally refereed and accepted by the editor, Prof. J.M.T. Thompson. I subsequently edited the issue with help from two of my researchers. The issue was published by the Royal Society early in 2004. This issue has, I think, helped to spread information about my research and that of leading researchers round the world. I am also writing two chapters which will appear in the sixth edition of the very popular book *The Finite Element Method for Fluid Dynamics* by O.C. Zienkiewicz and R.L. Taylor. These chapters give detailed overviews of recent developments in the modelling of short waves, and will, I hope, bring the latest developments to a wider audience.

Single most valuable outcome

In my view this was the outstanding results obtained using the plane wave basis boundary elements. To reduce the errors of a numerical method by a factor of 10 million, when using the same number of variables is unprecedented. This breakthrough will continue to have repercussions in the future, I am sure.

Career Progression

Throughout the term of the fellowship I stayed in the same post, that is Professor of Civil Engineering at the University of Durham. At the end of the term I have decided to retire, because my wife has retired from her post. My colleague, Dr. Jon Trevelyan was promoted to senior lecturer during the term of my fellowship, thanks, at least in part to the research that we have achieved together. One of my researchers, Dr. Omar Laghrouche has been appointed to a permanent lecturership in engineering at Heriot-Watt University Edinburgh. Both Dr. Rie Sugimoto and Dr. Emmanuel Perrey-Debain have been appointed to research associate positions at Southampton Universtiy and Manchester University respectively.

Conclusions

There were two main disappointments in the fellowship. The first was the lack of success with the infinite elements. Considering that I have quite a lot of experience in this field, this came as a surprise. The second was my inability to find a reasonable error indicator and an adaptivity strategy. I was also taken aback at the difficulties which arose in automating the element integrations, although I now regard that problem as solved. But these setbacks were counter balanced by the unexpected successes with the special wave boundary elements, which was a real bonus. I was also pleased with the work on the more general problem of varying wave speed. I was also pleased with the collaborations on Schrödinger's equation and with the group in France. Overall I think the fellowship was very successful, although it has developed in a different way from what I expected at the start. I am extremely grateful to the EPSRC. The fellowship was the opportunity of a lifetime. I must add that the fellowship freed me to get on with the research, I benefitted enormously from the contributions of my team of researchers, namely my colleague, Dr. Jon Trevelyan, and my researchers: Dr. Emmanuel Perrey-Debain, Dr. Omar Laghrouce and Dr. Rie Sugimoto. Without them I would have achieved less than half as much.

In the self assessment sheet, I have ticked a range of boxes. This is because some of the work went very well, (like the boundary elements), and I think it is internationally leading. Other aspects went much less well (like the infinite elements), and I think it does not deserve a high rating.

If any aspect of this report requires expansion or clarification, I would be very happy to do this.

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