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European Mathematical Society

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ISAAC NEWTON INSTITUTE FOR MATHEMATICAL SCIENCES

RESEARCH CONFERENCES

ESF Mathematics Conference in Partnership with EMS and ERCOM

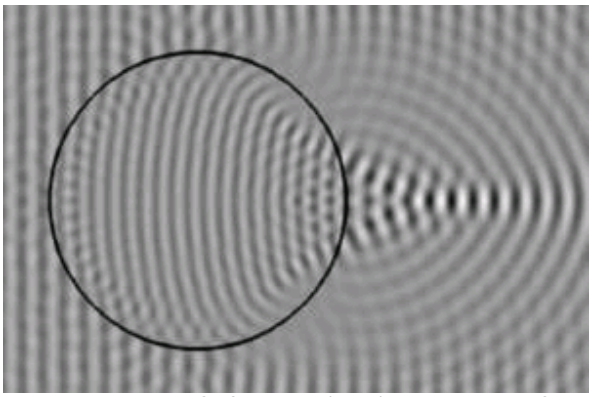
Highly Oscillatory Problems: From Theory to Applications

12-17 September 2010

The Isaac Newton Institute, Cambridge, UK

Chaired by:
- Arieh Iserles, Cambridge University, UK

Co-Chair:
- Claude Le Bris - Ecole Nationale des Ponts et Chaussées, Champs-sur-Marne, FR



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Conference Highlights

Please provide a brief summary of the conference and its highlights in non-specialist terms (especially for highly technical subjects) for communication and publicity purposes. (ca. 400-500 words)

The purpose of the conference was to bring together computational experts and workers in application areas under the common denominator of an interest in highly oscillatory phenomena and their computation. Thus, the range of both invited and submitted talks was very wide indeed, ranging from pure mathematics to application areas. Specific highlights include

• Jesús María Sanz-Serna (Universidad Valladolid, Spain) and Andrew Stuart (Warwick University) talked about their joint research on Markov-Chain Monte Carlo (MCMC) methods. Such methods have been used for 50 years, mostly in theoretical physics and engineering, to investigate very complicated and highly dimensional phenomena, typically in a situation when all other methods fail: it is fair to comment that MCMC methods account for a large share of time spent in high-performance computing calculations. Yet, their analysis from computational standpoint is deeply unsatisfactory. The Sanz-Serna–Stuart work in pioneering in the insight it provides on the MCMC method, in particular in highly dimensional setting. This insight is essential not just in understanding how the method works but also in improving it.

• Edriss Titi (Weizmann Institute) lectured about his work on differential equations exhibiting motion at two different scales. The dynamics of such equations is very intricate. In this talk Titi pioneered the use of *Young measures* in their investigation: essentially, monitoring how much time the trajectory spends in each small portion of the phase space. This allows to identify the types of motion that we can expect from both the slow and the fast components of the solution. The slow motion typically approaches a limit, while the fast, highly oscillatory motion is much more complicated but it is possible to identify its qualitative and topological features.

• Highly oscillatory phenomena feature strongly in the modeling of waves, the subject of the lecture by Ilaria Perugia (Universita degli studi di Pavia). The main problem, with fundamental applications in radar and sonar transmissions, medical imaging and oil exploration is that of scattering: how to deduce the shape of an object from the way it reflects incoming waves. A major approach to this problem is via finite element methodology, in particular discontinuous Galerkin method. In her talk Perugia analysed different versions of such methods and introduced a range of criteria that allow us to choose the correct approach in different situations.

• A major source of highly oscillatory problems is molecular dynamics. The main issue here is to descirbe the underlying geometry and dynamics as large molecules, e.g. proteins and DNA fold under the influence of physical forces. The problem is extremely challenging, because of the interplay of forces at the macro (van der Waals forces, gravity) and micro (quantum mechanics) level, but the prizes are immense: this is the key to the translation of knowledge from genomics to biology and medicine of organisms, with huge implications in medicine and biotechnology. In her talk, Caroline Lasser (Technische Universität München) described recent breakthroughs in our understanding of computational aspects of molecular dynamics.

x I hereby authorize ESF – and the conference partners to use the information contained in the above section on 'Conference Highlights' in their communication on the scheme.

Scientific Report

Executive Summary

(2 pages max)

This conference can be seen as a follow-up to the highly successful six-months research programme on “Highly oscillatory problems” at the Isaac Newton Institute in 2007. While lively research on high oscillation has been taking place in many areas of applied mathematics, science and engineering, it was typically done in a disjoint manner. Similar methodologies have been introduced in different areas without any connection being made among the people concerned and the flow of new ideas across disciplines was at best sclerotic, at worse non-existent. The INI programme was the first-ever to assemble a large number of professionals under the banner and the organizing principle of high oscillation.

Designing the ESF conference, we attempted to build upon the success of the INI programme, not least in building a community of professionals working in the computation of highly oscillatory phenomena, while trying to extend both the human and thematic scope. Thus, 11 of the invited speaker took part in the INI programme, 7 were new. Thematically, we have extended the scope to cover issues in computational dynamics, stochastic computation and in theoretical partial differential equations. We have also made a conscious effort to reach new audiences. The limited funding for non-invited participants was focused exclusively on two categories: young researchers and researchers from poorer countries.

The conference was a resounding success, not just in the wide range of excellent talks and posters, but also in the very active and enthusiastic extent of informal scientific interactions. There is no doubt that the professionalism of ESF personnel and the outstanding facilities at the Isaac Newton Institute have contributed a great deal, but so did the right format of the conference and its thematic focus.

Scientific Content of the Conference

(1 page min.)

- *Summary of the conference sessions focusing on the scientific highlights*
- *Assessment of the results and their potential impact on future research or applications*

The very wide range of talks and sessions reflects the broad sweep of high oscillation, theoretical, computational and applied, and the manner it pervades many subject areas in science and engineering.

• Ilaria Perugia (Pavia) on the computation of highly oscillatory waves scattered off rigid three-dimensional objects;

• Edriss Titi (Weizmann Institute) on the dynamics of two-time-scale systems where the fast motion exhibits high oscillations;

• Daan Huybrechs (Louven) on novel ways to approximate functions on tetrahedral exploiting highly oscillatory phenomena;

• Irene Fonseca (Carnegie Mellon) on the analysis and homogenization of nonlinear partial differential equations with high oscillation;

• Peter Markowich (Cambridge) on the analysis of the Schrödinger equation using Wigner and

Boehmian measures;

• Assyr Abdulle (EPFL Lausanne) on the numerical integration of homogenization problems fpr partial differential equations;

• Yalchin Efendiev (Texas A&M) on multiscale methods for partial differential equations;

• Caroline Lasser (TU Munich) on computational methods in molecular quantum dynamics and in the modeling of macromolecules;

• Christian Lubich (Tübingen) on symplectic numerical methods and modulated Fourier expansions;

• Tony Lelievre (Ecole des Ponts, Paris) on the computation of thermodynamical features in molecular dynamics;

• Jesús María Sanz-Serna (Valladolid) on the mathematical and computational analysis of the Markov Chain Monte Carlo method;

• Andrew Stuart (Warwick) on the Markov Chain Monte Carlo method in a large number of dimensions;

• Houman Owhadi (Caltech) on computational homogenization of partial differential equations with non-separated scales;

• Thanasis Fokas (Cambridge) on new transform method, based upon the dbar equation, and its many numerical consequences;

• Isabelle Terrasse (Aerospatiale Paris) on the wide range of high frequency problems in practical aeronautics and aircraft design and their computational treatment;

• Dario Bambusi (Milan) on the existence of solitary waves in symplectic discretizations of Hamiltonian problems.

However, it would be wrong to restrict the attention just to hour-long invited talks. Some of the highlights of the conference were in 30 mins talks by young and highly promising researchers, like Gil Ariel (Bar Ilan) on the heterogeneous homogenization method with three different frequencies, Timo Betcke (Reading) on matrix analysis approaches to high-frequency scattering, Sheehan Olver (Oxford) on the computation of Painléve equations, Carola Schönlieb (Cambridge) on high-frequency problems in image reconstruction and Euan Spence (Bath) on the theory of boundary integral operators in high frequency scattering.

Forward Look

(1 page min.)

- *Assessment of the results*
- *Contribution to the future direction of the field – identification of issues in the 5-10 years & timeframe*
- *Identification of emerging topics*

The primary purpose of the original Isaac Newton Institute programme was to commence a "grand conversation' among the disparate body of professionals with an interest in the computation of highly oscillatory phenomena. It is important to see the ESF conference as a major next step, not just to keep the conversation going but to broaden it and bring on board new people and new themes. It is clear that this goal has been attained.

As to the road forward, the most immediate test is whether the idea of oscillation-centred research, bringing together workers from different areas of applied mathematics, science and engineering, will bed down. For example, there are several main international conferences in applied and computational mathematics and their proceedings are centred in large measure upon minisymposia and workshops. Will there be such minisymposia in high oscillation? There has already been impact of this kind on the 2009 Scientific Computing and Differential equations conference in Beijing and the forthcoming conferences on Foundations of Computational Mathematics (Budapest) and EquaDiff'11 (Loughborough) will have workshops devoted to high oscillation. A forthcoming Oberwolfach workshop on geometric numerical integration will be devoted in large measure to highly oscillatory phenomena. There is much less impact, however, on the annual SIAM conference, which probably reflects the fact that the whole idea of high oscillation as a major organizing principle for applied mathematical and computational research is thriving much stronger in Europe than in United States.

Another test is whether the informal networks, many of which owe their existence to the INI programme, will continue to thrive. Here, again the omens are good. The new EU-funded CriSP project, bringing together universities in Norway, UK, Australia and New Zealand, is devoted in large measure to high oscillation. Following the INI programme, a major partnership between Reading and Bath Universities, with many external participants, has been forged in the area of electromagnetic and acoustic scattering. The challenge is to continue and develop similar networks and partnerships: more are in the works and their success depends on the cooperation of diverse funding agencies.

In the longer term there is the need for further formal gatherings and conferences, perhaps for another longer research programme. It is at the moment probably premature to elaborate the specifics of such events.

- Is there a need for a foresight-type initiative?

Definitely. HOP (highly oscillatory problems) and their computational aspects are ripe for a foresight-type initiative for a number of reasons:

1. This is by its very nature multidisciplinary research, disregarding demarcation lines and cutting across areas in mathematics, science and engineering.
2. The subject matter is of fundamental importance to a wide raft of issues in the modeling of natual and engineering phenomena, in particular in areas where wave-like behaviour is at issue: from fluid mechanics to electromagnetics, acoustics, electronics, oil exploration and reservoir modeling, quantum chemistry, molecular and protein modeling…
3. The core of research into high oscillation is in Europe. This is the broad geographic area with arguably the highest concentration of researchers in the subject – certainly, with the best and stronger networks binding together workers on different aspects of the subject. It is vital to build upon this success.

Atmosphere and Infrastructure

- *The reaction of the participants to the location and the organization, including networking, and any other relevant comments*

The feedback from participants has been most satisfying and gratifying. Both the conference venue at the Isaac Newton Institute and the accommodation in Fitzwilliam College were excellent and the ESF organizational support very professional and efficient.

Date & Author:

8 February 2012

A. Iserles