Highly Oscillatory Problems

Final Report

1 Basic theme and background information

High oscillation plays crucial role in a wide range of phenomena in science and engineering and it represents formidable mathematical and computational challenge. Its understanding calls for an extensive array of distinct mathematical techniques and numerical algorithms.

Traditionally, research into high oscillation was problem-oriented or technique-oriented. This led to an impressive, yet fairly disjoint, body of knowledge. The wish to create a shared space for different workers in the area of high oscillation motivated the Isaac Newton Institute HOP programme, the first ever with the organising principle of high oscillation at its core. We brought together 119 professionals, mostly in different areas associated with the computation of high oscillation (e.g. multiresolution methods, homogenisation, geometric numerical integration, calculations in electromagnetics and acoustics, highly oscillatory quadrature, Riemann–Hilbert techniques, discretizations of the Schrödinger equation, exponential integrators), but also in the theory underlying high oscillation (e.g. in asymptotics and in random-matrix theory) and in application areas. Significantly larger number of participants took part in the workshops organised at INI and in satellite workshops.

Our main challenge was to bring together different mathematical traditions and create, at the first instance, shared language and ultimately a comprehensive theory of high oscillation and its computation. Thus, we have carefully selected our participants as leading practitioners of all different aspects of the craft, as well as a good number of the most promising young colleagues. Yet, we have also taken care, both in our invitations and in the ethos we have strived to create, to ensure that participants are willing not just to *tell,* but also to *listen.* The programme represented for all of us a very steep learning curve and we are the better for it.

Several "master problems" served as a useful focus in our deliberations:

The Schrödinger equation: In its different settings, the Schrödinger equation is the basic model of wave phenomena, of cardinal importance in quantum and plasma physics and in chemistry. High oscillation is endemic, and it joins with a wide array of other phenomena that render analysis and computation so very challenging, including nonlinearity, large potentials, integrability, (de)focusing, and Hamiltonicity. No wonder that this equation has been recently approached with a very wide range of computational techniques: homogenisation, multiresolution, nonlinear optics approximation, symplectic and multisymplectic methods, Wigner measures, splitting methods and much more.

Electromagnetic and acoustic scattering: A major inverse problem, replete with applications, is to identify the shape of an object from waves (electromagnetic or acoustic) that it reflects and scatters. This can be reduced to the computation of the Helmholtz equation in an "exterior" large domain and involves high oscillation, typically in a wide range of frequencies. It is exceedingly sensitive to the geometry of the underlying (and in principle unknown!) object. State-of-the-art approach converts the Helmholtz equation to integral equations with highly oscillating kernels, defined on the boundary of the domain. This, in turn, is converted to the quadrature of highly oscillating multivariate integrals.

Symplectic long-term integration: One of the great triumphs of geometric numerical integration has been the current generation of very sophisticated symplectic solvers for Hamiltonian problems but the main remaining challenge (of critical importance in celestial mechanics and in accelerator physics) is their very long-term behaviour and error accumulation – by "long term" we mean regime that involves huge number of oscillations and it is essential that the qualitative properties of the underlying system remain true, at least in some ergodic sense. This has been treated with a measure of success by ideas from backward error analysis, modulated Fourier expansions, exponential integrators and mollifiers.

The above three problems were central to our joint deliberations but the HOP programme involved many more themes.

As an aside, we have enjoyed ongoing communication and discussions with colleagues from the parallel programme ("Analysis on Graphs and Applications"). The two themes and the language employed by the two groups were sufficiently similar to allow for cross fertilization and synergy.

This is the place to acknowledge the outstanding facilities of the Isaac Newton Institute and the exemplary helpfulness and competence of its staff. Among the four of us, we have an experience, both as organisers and participants, of most similar establishments worldwide – it is not an exaggeration to state that INI is absolutely the best. ***We wish, in both our and our colleagues' names, to express profound appreciation and thanks to the INI staff for all they have done for the HOP programme.***

2 Structure

The regular "flow" of the programme included typically 3–5 seminar talks each week, of which the Wednesday afternoon talk was on a more general theme and suitable for wider audience. Discussion meetings on matters of interest were often convened, sometimes in an *ad hoc* manner. Two workshops were organised at INI, each with > 60 participants: "The theory of highly oscillatory problems" (26–30 March) and "Effective computational methods for highly oscillatory problems: The interplay between mathematical theory and applications" (2–6 July), and they were complemented by four satellite events ("The future of computational acoustics", Arup Acoustics, London, 22–23 February; "Applying geometric integrators", ICMS, Edinburgh, 24–27 April; "Multi-resolution and high oscillation for evolutionary problems: Blow-up and Hamiltonian systems", University of Bath, 11–12 June; and "High frequency wave propagation and scattering", University of Reading, 24–26 July), as well as a one-day INI event on "Oscillatory integrals and integral equations in high frequency scattering and wave propagation" (19 June).

As a general rule, the two INI workshops were devoted to a wide range of topics spanning the entire subject area of high oscillation and they served the double purpose of reporting latest advances to the experts, while educating novices (who were often experts in other aspects of the subject). They also attracted significant numbers of participants, many of them research students and young researchers, who used this as an opportunity to learn about the subject matter as a whole. On the other hand, the satellite workshops were more focused, at research level, on particular aspects of high oscillation.

3 Outcome and achievements

It in the nature of programmes like HOP that papers are completed, new research produced.... The massively interdisciplinary nature of HOP puts the emphasis not on mathematical output *per se* but on collaborations across disciplines which have been initiated during the programme and that have already produced useful results. Herewith, in no particular order, several such new collaborations:

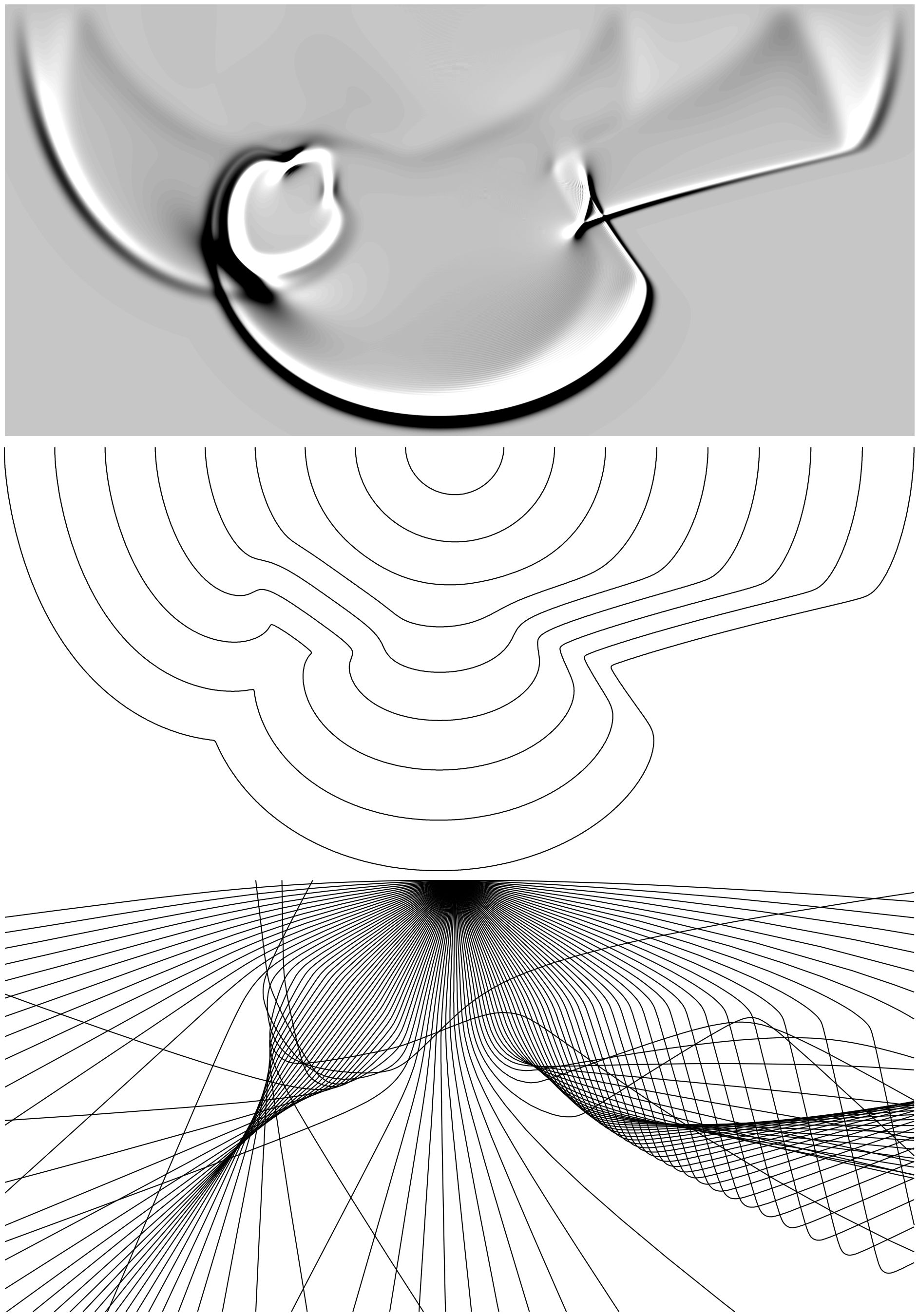


Figure 1: An initially circular wave propagating downwards through a heterogeneous medium. Top figure shows a snapshot of a resolved numerical solution of the wave equation. Middle and bottom figures show solution to the eikonal and ray tracing equations respectively. (Courtesy of O Runborg)

Example: Anisotropic Pendulum

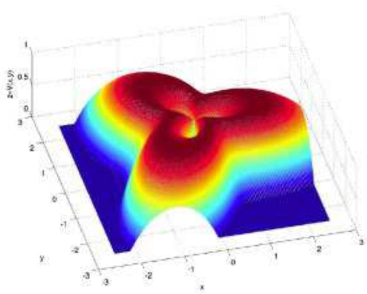
$$H(x,y,p_x,p_y) = \frac{1}{2}(p_x^2+p_y^2) + \frac{\kappa(c_3)}{2}(r-l(c_3))^2, \qquad r=\sqrt{x^2+y^2},$$

where

$$c_3 = \cos(3\theta)$$

$$\cos\theta = c = \frac{x}{r}, \qquad c_3 = 4c^3-3c.$$

$$\kappa(c_3) = \kappa_0(1-\frac{1}{2}\varepsilon c_3), \qquad l(c_3) = l_0(1+\frac{1}{2}\varepsilon c_3).$$



(upside down potential surface)

$\kappa_0 = 10 \qquad l_0 = 1$

School of Mathematics

- *Computation of Painlevé transcendents* F. Bornemann (Munich) & P. Deift (NYU)
  Following a chance remark in Deift's Rotschild Professor Seminar, a new research effort commenced, to devise effective and very accurate methods to compute Painlevé functions: because of their highly oscillatory nature, their computation with standard methods is suboptimal. There are already very promising results for Painlevé II, with more in the pipeline. This is of deep relevance to random-matrix theory.

- *Numerical methods for multiscale PDEs on perforated domains* A. Abdulle (Edinburgh) & V.H. Hoang (Cambridge)
  The effective equation includes "strange terms", which render analysis and computation difficult. Thus, classical multiscale methods are not effective and the new approach requires considerably more evolved hierarchies of multiscale discretization.

- *Round-off error of implicit symplectic Runge–Kutta methods* E. Hairer (Geneva) & R.I. McLachlan (Massey University)
  Following upon an observation that the round-off error does not behave as expected, namely as random walk, and that it carries statistical bias, Hairer and McLachlan identified the mathematical mechanism, analysed it and, consequently, were able to develop an implementation that removes the bias. This is of great importance in situations, e.g. in astronomy, when very long-term, very accurate and reliable numerical solution is sought.

- *Long-time analysis of analytical and numerical solutions of nonlinear wave equations.* D. Cohen (Trondheim), E. Hairer (Geneva) & Ch. Lubich (Tübingen)
  Based on the technique of modulated Fourier expansions, this work refines recent results by Bourgain and Bambusi on the long-time behaviour of the analytic solution, and extends them to semi- and full discretisations of nonlinear wave equations. This yields the first

rigourously proved result on the conservation of energy, momentum and harmonic actions over time intervals that are much longer than the natural time scale of the problem.

- *Computation of highly-oscillatory integral equations* H. Brunner (Memorial University), A. Iserles (Cambridge) & S.P. Nørsett (NTNU Trondheim)
  Iserles and Nørsett are experts in highly oscillatory quadrature, while Brunner is the world leading expert in computational integral equations. They have combined their effort to address an important and challenging set of problems: computation of Fredholm and Volterra problems with highly oscillatory kernel and of their spectra. Major progress, combining methods of highly oscillatory quadrature, numerical linear algebra and asymptotics, has been already noted in the computation of spectra of Fredholm operators.

- *Riemann–Hilbert techniques for spectral problems* P. Deift (NYU) & A. Its (Indiana)
  Motivated by a problem in laser theory (the Fox–Li equation) and by intriguing numerical results of Iserles and Nørsett, Deift and Its applied Riemann–Hilbert techniques with great measure of success. Their work generalises to considerably broader class of problems and is of great potential significance to laser engineering.

- *Generalised Dirichlet–Neumann map in polygonal domains and its computation* T. Fokas (Cambridge) & S. Fulton (Clarkson University)
  This work addressed a long-standing challenge, but its completion at INI was directly thanks to interdisciplinary interaction. It turns out that an important observation is that the correct expansion basis consists of modified Fourier functions, which have been introduced in a different context by Iserles & Nørsett.

- *Spectra of travelling waves and the Evans function* V. Ledoux (Ghent), S. Malham (Heriot-Watt), Jitse Niesen (Melbourne) & V. Thummler (Bielefeld)
  This is fundamental problem in fluid flow and it has been approached by a mixture of techniques from CFD and from geometric numerical integration, working with Grassmannians associated with stable and unstable manifolds. The results are very promising and a multidimensional generalisation is also close to fruition.

- *Combination of modified Fourier expansion with polynomial subtraction and the hyperbolic cross* D. Huybrechs (Louven), A. Iserles (Cambridge) & S.P. Nørsett (NTNU Trondheim)
  Expansion in modified Fourier functions (and, in greater generality, in Laplace–Neumann eigenfunctions) enjoys marked advantage over standard Fourier expansion in the case of non-periodic functions, because rapid oscillation of basis functions allows for very effective calculation of the coefficients. This can be generalized to arbitrary multivariate parallelepipeds, but in that case it is possible to combine two further mechanisms: Krylov's polynomial subtraction, which accelerates the decay of expansion coefficients, and the hyperbolic cross, which means that only very small subset of coefficients need be calculated. The outcome in $d \geq 1$ dimensions is an $O(n(\log_2 n)^{d-1})$ method.

- *Highly oscillatory quadrature for electromagnetics and acoustics problems* O. Bruno (Caltech), S. Chandler-Wilde (Reading), M. Ganesh (Colorado), I. Graham (Bath), D. Huybrechs (Leuven) & S. Vandewalle (Leuven) This is a textbook example of "parallel universe": while workers in electromagnetics reduced their problems to the computation of highly oscillatory integrals, yet did the latter with mostly *ad hoc* methods, while another group of mathematicians developed considerably more effective techniques for the computation of such integrals. Bringing the two together is a non-trivial task but much of it has been already accomplished and it is of crucial importance to an important set of applications.

Only constraints of space prevent us from providing a list twice as long, but hopefully this is enough to sketch the extent of collaborationx1 and cross-fertilization.

4 Publications

We are planning a volume in INI series, composed of survey papers highlighting different aspects of the HOP programme. This will be the first-ever volume bringing together such a wide range of themes under the common denominator of high oscillation and we expect it to be a major resource. The programme also produced a large number of publications, many available in the INI series, and is likely to produce considerably more.

5 Prospects for the future

The INI programme established an enduring HOP community and brought together a large number of professionals in computation, theory and applications under a new heading. As organisers, we consider it vital for the programme to be a beginning of a considerably longer journey, rather than a one-off event, useful as it might have been. Although we would have welcomed a follow-up week-long workshop at INI in a year's time, say, we realise that INI has already done its share. We are hopeful that, following the foundations laid at the HOP programme, there will be more future concerted activity on high oscillation in UK and elsewhere and will be delighted to keep INI informed.

B. Engquist T. Fokas E. Hairer A. Iserles