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Preface

High oscillation is everywhere and it is difficult to compute. The conjunction of these two statements forms the rationale of this volume and it is therefore appropriate to deliberate further upon them.

Rapidly oscillating phenomena occur in electromagnetics, quantum theory, fluid dynamics, acoustics, electrodynamics, molecular modelling, computerised tomography and imaging, plasma transport, celestial mechanics – and this is a partial list! The main reason to the ubiquity of these phenomena is the presence of signals or data at widely different scales. Typically, the slowest signal is the carrier of important information, yet it is overlayed with signals, usually with smaller amplitude but with considerably smaller wavelength (cf. the top of Fig. 1). This presence of different frequencies renders both analysis and computation considerably more challenging. Another example of problems associated with high oscillation is provided by the wave packet at the bottom of Fig. 1 and by other phenomena which might appear dormant (or progress sedately, at measured pace) for a long time, only to demonstrate suddenly (and often unexpectedly) much more hectic behaviour.

The difficulty implicit in high oscillation becomes a significant stumbling block once we attempt to produce reliable numerical results. In principle, the problem can be alleviated by increasing the resolution of the computation (the step size, spatial discretization parameter, number of modes in an expansion, the bandwidth of a filter), since high oscillation is, after all, an artefact of resolution: zoom in sufficiently and all signals oscillate slowly. Except that such 'zooming in' requires huge computer resources and the sheer volume of computations, even were it possible, would have led to an unacceptable increase of error because of the roundoff error accumulation.

The situation is reminiscent, yet very different, of the phenomenon of *transient behaviour,* commonly associated with stiff ordinary differential equations or with boundary layers for singularly perturbed partial differential equations. In those cases a differential system undergoes a brief but very intensive change over a small domain of the independent variables. Away from this domain the solution settles down to its asymptotic behaviour, typically at an exponential rate. In that case it is enough to

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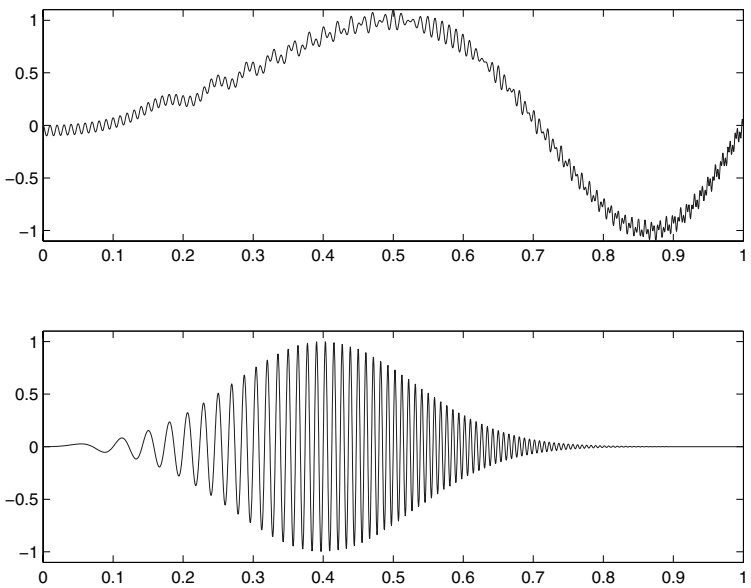

Fig. 1 Two highly oscillatory signals.

filter the contribution of transiency (or use a numerical method that dampens transient components). Not so with high oscillation, because this is a persistent phenomenon which stretches out over a large part of the computational domain. We cannot banish it by mesh refinement in the domain of rapid change and then just apply a stable algorithm. In a sense, the entire computational domain is in a transient phase.

Numerical analysis of differential equations is, at its very core, based upon Taylor expansions. Although often disguised by the formalism of order or of Sobolev-space inequalities, Taylor expansions are the main organising principle in the design of numerical methods and a criterion for their efficacy. Thus, typically numerical error scales as a derivative (or an elementary differential, or a norm of the derivative...). And this is precisely why standard numerical methods experience severe problems in the presence of high oscillation.

Our point is illustrated in Fig. 2 by the function

$$f(x) = \frac{\sin 2\pi x}{1+2x} + \tfrac{1}{10}\mathrm{Ai}(-100x),$$

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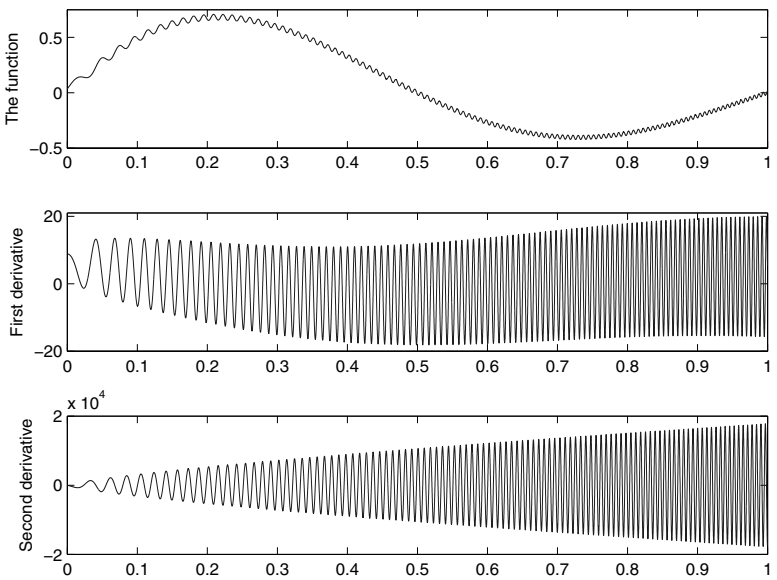

Fig. 2 A highly oscillatory function and its derivatives.

where $\mathrm{Ai}(\cdot)$ is the Airy function. Note that the function f itself is basically a gently decaying sinusoid, with small-amplitude, yet increasingly rapid oscillations superimposed. For all intents and purposes, it is the sinusoid that is likely to describe whatever natural phenomenon we attempt to model. Yet, once we start differentiating f, the amplitude associated with the highly oscillating Airy function is magnified rapidly. Suppose that f is a solution of a differential equation which we attempt to discretize by any classical numerical method: multistep or Runge–Kutta, say. The error of a pth-order method scales like a $(p+1)$st power of the step size times the $(p+1)$st derivative (or a linear combination of elementary differentials including the derivative in question). This imposes severe restrictions on the step size, which rapidly lead to unacceptable computational cost.

No wonder, thus, that high oscillation in computation has been at worst disregarded and eliminated from the mathematical model by fiat, at best approached by a fairly unstructured bag of tricks and *ad hoc* ideas. The motivation for the six-months' long programme on "Highly

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oscillatory problems: Computation, theory and applications" at the Isaac Newton Institute of Mathematical Sciences (January–July 2007) was to provide an overarching setting for research focusing on high oscillation. Thus, rather than dealing with highly oscillatory phenomena separately in each application, we have attempted to provide a broader, synergistic approach, with high oscillation – its analysis and computation – at the centre of attention.

At the outset of the programme we have identified a number of significant threads and challenges in high oscillation research to provide a focus for our deliberations:

Homogenization Many large scale physical problems involve highly oscillatory solutions that involve many non-separable scales. Examples include applications from environmental and geosciences, combustion, fluid dynamics, plasma physics, materials science, and biological applications. A key mathematical difficulty is that the problem has no scale separation, so traditional asymptotic methods fail to yield useful models. New systematic multiscale analysis needs to be developed that can account for interaction of infinitely many non-separable scales. Such analysis will shed useful light in designing accurate and reliable multiscale models. One approach is to develop a new homogenization theory that applies to nonlinear dynamic problems without scale separation. This can be achieved by using the two-scale analysis iteratively in space and incrementally in time.

Future advances in multiscale modeling and computation require rigorous mathematical analysis to quantify modelling error across scales, approximation error within each scale, uncertainty error, and to address the well-posedness of the multiscale model. An important issue is to derive a rigorous microscopic interface condition that connects large scales to small scales, or connects continuum model to subgrid microscopic model. It is in general easier to derive a local interface condition for elliptic or diffusion equations, because there is a strong localization of small scale interaction for diffusion dominated processes. Deriving accurate interface condition for convection-dominated transport or hyperbolic problems is more difficult due to the nonlocal memory effect: in this case, small scales are propagated along characteristics. Upscaling the saturation equation for two-phase flow in heterogeneous porous media is considerably more difficult mathematically than solving the pressure equation. While various *ad hoc* upscaling models have been proposed by engineers, there is still lack of a systematic derivation of

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upscaling models for two-phase flow with rigorous error control. Upscaling the nonlinear convection-dominated transport problem provides an excellent prototype problem for developing a dynamic multiscale computational method with error control.

Asymptotic theory In recent years substantial progress has been made in the analysis of *Riemann–Hilbert (RH)* problems containing highly oscillatory integrals. Such RH problems arise in a variety of mathematical formulations including inverse scattering, initial-boundary value problems for linear and integrable nonlinear partial differential equations, the isomonodromy method, orthogonal polynomials and random matrices. The question of extracting useful asymptotic information from these formulations, reduces to the question of studying the asymptotic behaviour of RH problems involving highly oscillatory integrals. The latter question can be rigorously investigated using the nonlinear steepest descent asymptotic technique introduced in the beginning of the 90's by P. Deift and X. Zhou.

Another important development in asymptotic theory, which was the subject of a highly successful INI programme in 1995, is exponential asymptotics. It leads to considerably tighter and more powerful asymptotic estimates and tremendous speedup in the convergence of asymptotic series. In the specific context of scientific computation, this creates the prospect of techniques originating in exponential asymptotics for better computation of special functions, differential equations and integrals.

Symplectic algorithms The numerical solution of Hamiltonian differential equations is one of the central themes in *geometric numerical integration.* By interpreting the numerical approximation as the exact solution of a modified differential equation (backward error analysis), much insight into the long-time behaviour of symplectic and symmetric integrators is obtained. Unfortunately, in the presence of highly oscillatory solutions, this theory breaks down and new techniques have to be found. For some important situations (Fermi–Pasta–Ulam-like models for molecular dynamics simulations), where the high frequencies stem from a linear part in the differential equation, it is known that the exact flow has adiabatic invariants corresponding to actions (oscillatory energies divided by frequencies). The technique of *modulated Fourier expansions* has been developed to study the preservation of such adiabatic invariants by simulations. Numerical methods that nearly preserve the total energy and such adiabatic invariants are very important, because

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in realistic applications the solution is very sensitive to perturbations in initial values, so that it is not possible to control the global error of the approximation. Difficulties arise with resonant frequencies, numerical resonances, high dimensions as obtained with discretizations of nonlinear wave equations, and one is interested to get more insight in such situations. Problems where the high oscillations come from a time-dependent or nonlinear part of the differential equation are still more difficult to analyse and to treat numerically.

Integral expansion methods Changing locally the variables with respect to a rapidly-rotating frame of reference results in differential systems of the form $\partial u/\partial t = A(t)u + g(u)$, where the elements of the matrix A themselves oscillate rapidly, while g is, in some sense, small. Such systems can be computed very effectively by time-stepping methods that expand the solution by means of integral series: the main idea is that, integration being a smoothing operator, integral series converges significantly *faster* in the presence of oscillations. Two types of such methods have been recently the object of much attention. Firstly, Magnus, Cayley and Neumann expansions: the first two have been developed in the context of Lie-group methods and they possess remarkable structure-preserving features. The latter, known in physics as the Dyson expansion, is commonly dismissed as ineffective but it comes into its own in the presence of oscillations. The second (and related!) type of integral methods are *exponential integrators,* which represent the solution using variation of constants and employ, sometimes in succession, different discretization methods on the "linear but large" and "nonlinear but small" parts. Such methods have proved themselves in practice in the last few years but much work remains in harnessing them for the highly oscillatory setting.

Highly oscillatory quadrature Practical computation of integral expansions and exponential integrators with highly oscillatory kernels calls for efficient quadrature methods in one or several dimensions. Historically, this was considered very difficult and expensive – wrongly. Using appropriate asymptotic expansions and new numerical methods, it is possible to compute highly oscillating integrals very inexpensively indeed: rapid oscillation, almost paradoxically, renders quadrature much cheaper and more precise! The implications of such methods, which are presently subject to a very active research effort, are clear in the context of the above integral expansions. Wider implications are a matter of conjecture, as are the connections of these methods with exponential

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asymptotics, harmonic analysis and, in a multivariate setting, degree theory. Insofar as applications are concerned, highly oscillatory quadrature is central to calculations in electrodynamic and acoustic scattering and with wide range of other applications in fluid dynamics, molecular modelling and beyond.

The purpose of the INI programme was to bring together specialists in all these specialities (and beyond), to weave the distinct threads into a seamless theory of high oscillation. We have never laboured under the illusion that six months of an intensive exchange of ideas will somehow produce such a theory: rather more modestly, we have hoped at the first instance to open channels of communication, establish a dialogue and lay the foundations for future work. This, we believe, has been accomplished in a most outstanding manner.

The setting of the Isaac Newton Institute – its location, architecture, facilities and, perhaps most importantly, its very efficient and helpful staff – make it an ideal venue for collaborative projects. We have taken advantage of this to the fullest. For the first time ever high oscillation has been approached in a concerted manner not as an appendix to another activity or to an application but as a subject matter of its own. The eight review papers in this volume revisit in their totality the main themes of the programme. Carefully reading between the lines, it is possible to discern the impact of our six-months'-long conversation on different aspects of high oscillation research. We have every reason to believe that this impact is bound to progress and grow in leaps and bounds. The INI programme was a first step in what is a long journey toward the goal of *understanding* high oscillation in its analytic, computational and applied aspects. This volume is a first way-station on this journey.

This is the moment to thank the staff of the Isaac Newton Institute for their unstinting help and the 120 participants of the programme for their many contributions to its success.

We hope that this volume acts as a window to the fascinating world of computational high oscillation, sketching challenges, describing emerging methodologies and pointing the way to future research.

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