Partial Differential Equations
in Kinetic Theories (KIT)
INI-Thematic Programme Final Report

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A. Basic Theme & Background:

Kinetic equations occur naturally in the modelling of the collective motion of large individual particle ensembles such as molecules in rarefied gases, beads in granular materials, charged particles in semiconductors and plasmas, dust in the atmosphere, cells in biology, or the behaviour of individuals in economical trading ... Although such a variety of applications seems at first sight overwhelmingly broad, there are important common mathematical features in the kinetic theories of all these applications. Generally, huge interacting particle systems cannot efficiently be described by the individual dynamics of all particles due to complexity but clearly some input from the microscopic behaviour is needed in order to bridge from microscopic dynamics to the macroscopic world, typically described in terms of averaged quantities. This leads to classical equations of mathematical physics: the Boltzmann equation of rarified gas dynamics, the fermionic and bosonic Boltzmann equations and the relativistic Vlasov-Maxwell system of particle physics, the quantistic Wigner-Poisson system, to name just a few.

Kinetic theory has produced as a spin-off many new mathematical tools in the last 20 years: renormalized solutions of transport equations by R. DiPerna and P. L. Lions, averaging lemmas by the French kinetic school, entropy dissipation tools which have been extended methodologically and used far beyond kinetic theory, are just some highlights of new analytical PDE methods stemming from kinetic theory. Another landmark in this field was the proof of the hydrodynamic limit process of the renormalized solutions of the Boltzmann equation towards (weak) Leray solutions of the Navier-Stokes equations by F. Golse and L. Saint-Raymond. On the other hand, kinetic theory has different scientific viewpoints ranging from applied mathematical and physical modelling to stochastic analysis, numerical analysis of PDEs and in many important cases extensive numerical simulations.

While modern computers are still inadequate in simulating dynamics in micro- and nano-technologies, kinetic equations provide models that can capture important features of microscopic or quantum phenomena with a computational cost manageable by today's computing facilities. Indeed, the mesoscopic kinetic theory, connecting the microscopic and even quantum scale to the hydrodynamic scales, plays a central role in developing these modern computational methods.

*UK-based participants will be marked with an asterisk.

B. Chosen Specific Directions & Main Objectives:

The main objective of this program was aimed at advancing **Partial Differential Equations (PDEs) research in kinetic theories** and its impact in the applied sciences highlighting selected modern application areas. This effort was understood from a global perspective of research in PDEs bringing together mathematical modelling, analysis, numerical schemes and simulation in a feedback loop of synergies. Therefore, the main key objective was fostering the mathematical knowledge of Boltzmann and Vlasov-type models together with bridging them towards scientists applying them in specific application areas.

For this programme we chose three exemplary newly emerging areas of application for kinetic theories. This choice was aimed at facilitating the embedding of our programme into UK and specific local (Cambridge) scientific strengths in fluid dynamics, mathematical modelling of biological flows and quantum mechanics. These three topics represented and still do very active and fast-paced growing areas of kinetic research.

The three selected emerging application areas of kinetic theories were:

1. ***Kinetic modelling in biology:*** Various kinetic models have been proposed for the description of chemotaxis, collective motion of individuals (swarming), blood coagulation, tumour growth and neuroscience. They include running & tumble kernels, Keller-Segel equations, coagulation-fragmentation models just to name a few. From a more mathematical analysis viewpoint they are modelled through nonlinear drift-diffusion or Fokker-Planck equations. The main questions treated were long-time asymptotics, free-energy functionals, probability tools, refined estimates for mathematical fluid equations…
2. ***Coupled Fluid-Particle Models:*** Fluid-kinetic coupling appears naturally in many applications such as: motion of swimming bacteria in a fluid, polymers, and aerosols/sprays with applications ranging from Diesel engines to drug delivery by means of aerosols in human lungs. Their analysis includes tools related to core mathematical techniques in general kinetic theory such as: entropy estimates, scaling limits, simplified asymptotic equations, closures, approximated models...
3. ***PDE Models for Quantum Fluids:*** Quantum fluid modelling attracts lot of attention, mainly due to the phenomena of Bose-Einstein condensation. Kinetic equations, relying mainly on the Wigner transformation, can also be applied to quantum fluid dynamics. Recently hybrid kinetic-quantum mechanical models, coupling the Gross-Pitaevskii equation to the boson Boltzmann equation became a hot topic.

Outstanding problems in general kinetic theory that remained to be clarified at time of application of this program were among others: convergence and equilibration rates in inhomogeneous Boltzmann-type problems, mean-field limits, weakly inhomogeneous situations, weak relaxation for Vlasov-models related to Landau damping, asymptotic preserving schemes, Bose-Einstein condensation modelling, Bohmian measures for Wigner-Poisson...

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C. Structure of the Programme:

The organisers with the initial help of the Scientific Advisory Committee formed by: **Y. Guo** (Brown, USA), **R. Illner** (Victoria, Canada), **B. Perthame** (Paris VI, France), **A Stuart** *(*Warwick), **J.F. Toland** (Bath) and **G. Toscani** (Pavia, Italy), coordinated more than 120 invited researchers for long-stays. As it can be checked in the web page, the final list includes a large part of the most prominent researchers in kinetic theory world-wide, and we can state that most of them were involved in one way or another. At the beginning of the program (August 25^{th} – September 3^{rd}) we organized a series of **lectures/tutorials** in specific trends of current interest for KIT's practitioners to trigger the collaboration between the researchers just landed in the program, particularly the newcomers and the junior participants. There were three workshops related to the program:

1. ***Workshop on*** Fluid-Kinetic Modelling in Biology, Physics and Engineering **6-10 September 2010, organized by J.A.** Carrilo **(ICREA-UAB, Barcelona) and A. Jüngel (TU-Wien, Austria):** This workshop included in part general talks in Partial Differential Equations in kinetic theories and secondly was in part devoted to new applications of kinetic modelling in the fields of mathematical biology, mathematical physics and engineering. Some of the application fields covered were swarming, coagulation processes and biological flows.
2. ***Workshop on*** PDEs in Kinetic Theories: Kinetic Description of Biological Models (A Satellite Meeting at ICMS, Edinburgh) **8-12 November 2010, organized by N. Bournaveas* (Edinburgh) and E. Tadmor (Maryland, USA):** The main objective of this satellite workshop at the ICMS (Edinburgh) was to bring together leading researchers to review the recent developments in research on mathematical modelling, analysis, numerical schemes and simulation of kinetic equations in general and of models in Biology in particular.
3. ***Workshop on*** PDE Models for Quantum Fluids **13-17 December 2010, organized by S. Jin (Wisconsin) and P.A. Markowich* (Cambridge*)*:** the recent advances in the mathematical understanding of Bose-Einstein condensation were the main theme of this workshop. Quantum fluid modelling in vortex dynamics, mixing of scales in random phase approximations, lattice and multi-component condensates modelled by coupled systems of nonlinear Schrödinger equations and Wigner-like kinetic equations were also treated.

During the duration of the programme a weekly seminar working group was organized in which we had the participation of many long-participants not having the opportunity to give a talk during the workshops. We should mention that the timing of our programme could not be better since at its beginning, we were thrilled by the fantastic news of the award of the Fields medal to one of the leading researchers in kinetic theory, C. Villani. He gave a wide-audience talk at the Mathematics department of the University of Cambridge sponsored by our program with a great success of attendance by young undergraduates. He also participated in our weekly seminar. His

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recent work mentioned in the laudation of the Fields medal in collaboration with **C. Mouhot*** (Cambridge) was object of special attention during the program, since C. Mouhot gave us a 10-hour course on Landau damping specifying the details of such landmark work.

D. Outcome and Achievements:

As we expected this programme was useful to create sufficient critical mass in events and brainpower, i.e. research visits of interested junior and senior scientists, for improving the visibility of UK research in PDE analysis as requested by recent IRMs. Therefore, we emphasized PhD and postdoctoral stays to attract young talented UK and international researchers to these fields as well as contacts with other UK researchers of enough close areas such as Fluid Dynamics (**J.L. Rodrigo***), Mathematical Analysis (**J. Bennet***) or Applied PDEs and asymptotics (**J. King***). Finally, the thematic program attracted 97 Visiting Fellows, 34 Programme participants and 4 Affiliate participants.

The long-term effects of such highlights as the two talks of the Field's medal ***C. Villani*** in attracting good undergraduate students to PDE Analysis are hard to measure but certainly, they will contribute to it particularly in the steadily-growing local group of PDEs in the University of Cambridge. As mentioned already the course on Landau damping offered by ***C. Mouhot**** giving all the details in this achievement in kinetic theory is another highlight of the program.

Many scientific developments have started as a result of this program; some of them are already reported as INI preprints (21 at 1st February 2010) and others will come in the near future. We are aware about a large number of collaborations through the individual scientific reports of each long-stay participant. We also are proud about the mixture of scientists of different origin and background such as applied mathematicians in mathematical biology problems, mathematical and numerical analysts of PDEs and designers and developers of numerical schemes and simulations. We expect that the synergies obtained from this mixture will be reflected in the large impact of the publications obtained or initiated from the discussions at the INI.

We extract here a few of these collaborations: ***K. Aoki and F. Golse*** have investigated the speed of approach to Maxwellian equilibrium for a collision-less gas enclosed in a vessel whose walls are kept at a uniform, constant temperature, assuming diffuse reflection of gas molecules on the vessel wall; ***C. Bardos and F. Golse*** initiated a programme to understand the effect of boundaries in the hydrodynamic limit of the Boltzmann or BGK equations leading to the incompressible Euler equations; ***S. Takata, T.-P. Liu and I.-K. Chen*** continued its collaboration on understanding singularities near the boundary in the thermal transpiration problem, ***J.J.L. Velázquez and B. Niethammer**** continued their collaboration in coagulation equations, ***J.J.L. Velázquez and M. Escobedo*** started the study of properties of the solutions of the Uehling-Uhlenbeck equation, ***A.***

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Bobylev, R. Esposito and R. Marra started a new collaboration on the 2d Boltzmann equation for hard discs in order to see which properties of 3d systems can be violated in 2d cases; ***M. Bostan and J.A. Carrillo*** started a collaboration in developing numerical schemes for strongly magnetized plasmas in the guiding centre approximation with finite Larmor radius regime; ***C. Schmeiser and M. Tang*** continued a cooperation on a model for bacterial swarming; ***G. Toscani*** worked in the problem of blow-up for the Bose-Einstein-Fokker-Planck equation giving a great talk, as Rotschild Professor, on the subject; ***M. J. Cáceres, J.A. Carrillo and B. Perthame*** have finished a work on qualitative properties of solutions to Fokker-Planck models in computational neuroscience; ***A. Tzavaras*** started two projects with D Stuart and S Demoulini on properties related to elasticity equations; ***R. Esposito, Y. Guo and R. Marra*** have worked in the relation between the microscopic Newton equations for a system of many particles and the Boltzmann equation in case a suitable Lipschitz external force is included generalizing Lanford's theorem; ***M. Geier, L. S. Luo and T. Ohwada*** started a prospective discussion on using the kinetic formulation to simulate the Navier Stokes equation in the context of the lattice Boltzmann method; ***L. Almazán, N. Brilliantov* and C. Salueña*** have analysed the kinetics of cluster formation in granular fluids and studied the transient pattern formation in granular fluids by means of granular hydrodynamics; ***I. Aranson and N. Brilliantov**** started to discuss about boundary conditions for active Brownian particles with applications in biological flows; ***F. Bolley, J.A. Cañizo and J.A. Carrillo*** have continued their collaboration in mean-field limits for collective behaviour of individuals; ***J.A. Carrillo, M. González and M. Gualdani*** have continued their collaboration related to Fokker-Planck models in computational neuroscience using ideas of free boundary problems; ***J.A. Carrillo, P. Gwiazda and A. Ulikowska*** continued their discussion on splitting methods applied to structure population models; ***P.A. Markowich*, T. Paul and C. Sparber*** finished a work on Bohmian measures related to the Wigner-Poisson and many-body Schrödinger equations; ***R. Erban* and J. Haskovec*** collaborated in kinetic models for swarming, ***A. Majorana*** finished a work proposing new numerical schemes of DG type for the Boltzmann equation; ***A. Majorana and F. Vecil*** are extending these ideas to nonlinear problems such as radiative transfer equations; ***J.A. Carrillo, S. Martin and V. Panferov*** discussed on finding particular solutions for the kinetic models of swarming; ***L. Mieussens and S. Taguchi*** started a collaboration in the design of an asymptotic preserving scheme for rarefied gas dynamic simulations in transitional regimes; ***C. Mouhot and S. Mischler*** continued their work in mean-field limits and rates of convergence for inhomogenous Boltzmann equations; ***T. Goudon and S. Jin*** started new collaborations on asymptotic preserving schemes for kinetic-fluid coupling simulation of multiphase flows.

Finally, on behalf of all the participants of this program, we want to profit this occasion to thank the staff and the direction of the INI for their welcoming atmosphere and the great working environment they have offered us during this period.

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