Kinetic Models for Multiscale Problems

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1 General comments

Besides the four organizers there were five additional "core" participants hosted at the institute. In alphabetical order: Chi-Kun Lin (presently University of Calgary), Dietmar Oelz (Technical University Vienna), Christian Schmeiser (Technical University Vienna), Giovanni Russo (University of Catania) and Holger Teismann (Acadia University). In addition there were two observers, hosted elsewhere in Banff but fully integrated in the scientific activities: Jean Dolbeault (Université Paris Dauphine) and Horst Lange (University of Cologne). There were thus a total of 11 participants.

Each participant gave one or two seminar style presentations on current research. Abstracts of these presentations may be found on the website of Peter Markowich:

http://homepage/univie.ac.at/peter.markowich/

A brief list of the presented topics, in the order in which they were presented, follows:

- R. Illner: Fokker-Planck type models for multilane traffic flow
- S. Jin: Computation of semi-classical limits and multivalued solutions of PDEs
- C.-K. Lin: On coupled nonlinear Schroedinger equations, and From compressible to incompressible fluid equations
- J. Dolbeault: Entropy/ entropy production methods for degenerate drift-diffusion equations, and Comments on stability and control of quantum equations
- H. Lange: Limitations of controllability for linear and nonlinear Schrödinger equations
- H. Teismann: An overview of controllability results for Schrödinger equations. The significance of coherent states.
- P. Markowich: Bose-Einstein condensates
- L. Pareschi: Analytical and numerical results for the Boltzmann equation for Bosons; Bose-Einstein condensation

- G. Russo: Implicit-explicit numerical methods for nonlinear hyperbolic systems
- C. Schmeiser: Mathematical models for chemotaxis, and Dimension reduction for the Gross-Pitaevski equation
- D. Oelz: Nonlinear Diffusion equations as macroscopic limits of generalized BGK models, and Numerical studies on chemotaxis

These lectures happened in a very informal setting and without serious time constraints, such that detailed discussions were possible during the talks. Everybody attended all lectures and participated in the discussions. Research sessions typically happened immediately after the lectures. These sessions were exceptionally fruitful and entailed many continued and new collaborations. Several research papers were completed or significantly advanced during the workshop. Details are given in the sequel.

2 Central research topics

Among the many research subjects which were considered during the workshop, the following saw the most efforts and progress.

J. Dolbeault, P. Markowich, D. Oelz and C. Schmeiser continued joint work on the mean free path limit of a Boltzmann-type equation with general equilibrium function and a relaxation time approximation collision operator (a generalized BGK model) This advances the theory of diffusion limits, a theory with fundamental roots in a paper by C. Bardos, R. Santos and R. Sentis (Diffusion approximation and computation of the critical size, *Trans. Amer. Math. Soc.* **284** (1984), no. 2, 617–649). In this project a Boltzmann-type equation with a non-linear relaxation time approximation collision operator involving a general equilibrium function is considered. Under parabolic scaling a rigorous convergence proof of solutions to a macroscopic limit was obtained. The analysis employs compensated compactness theory.

Different choices for the local equilibrium lead to different macroscopic equations. Most notably, non-linear diffusion equations ranging from fast diffusion to porous medium equations are reproduced as macroscopic limits by employing different types of equilibrium functions with decreasing rates of decay in terms of energy. The resulting paper is available as a preprint [1].

Chemotaxis was studied by D. Oelz and C. Schmeiser on the kinetic level with particular emphasis on diffusion limits and microscopic modelling of the motion of bacteria. It is conceivable that finite-time blow-up can be avoided on this level by careful modelling of reorientation processes.

Peter Markowich and Lorenzo Pareschi finished work on the numerical solution of the ergodic approximation of the quantum Boltzmann equation. The main difficulty here was finding an efficient scheme which maintains entropy growth, mass conservation and is at the same time able to reproduce a generalized Bose-Einstein equilibrium. The devised scheme is based on appropriate discretisation of the three dimensional integral in the collision operator and was found to be competitive with a Monte-Carlo method. It can be used for both the homogeneous gas dynamics Boltzmann equation and for the Boltzmann equation for Fermions.

Shi Jin and Peter Markowich further completed a paper (with additional authors Sparber, Zheng and Huang) on the numerical solution of the Dirac-Maxwell system. The scheme is based on a spectral discretisation in position space combined with a time splitting method. Test examples are presented in the semiclassical and non-relativistic regimes, focusing on electon-phonon coupling.

Lorenzo Pareschi and Giovanni Russo continued their analysis of stability and accuracy of IMEX-Runge Kutta schemes. Implicit-explicit (IMEX) Runge-Kutta schemes are a very effective tool for the numerical solution of hyperbolic systems with stiff relaxation. Under mild assumptions on the system coefficients, they provide numerical schemes that are accurate in the limit of both very large and very small relaxation parameters. However, for intermediate values of the parameter the accuracy of such schemes is not known theoretically. Numerical tests show degradation of the accuracy for values of the relaxation parameter of the order of the time step. During the Focussed Research Group workshop, asymptotic analysis was used to obtain an estimate of the uniform order of accuracy for the various IMEX-RK schemes developed by the authors. One of the aims of the stability analysis is to exploit the stabilization effect introduced by the dissipative term, when it is treated by an L-stable space discretization. The larger the stabilization, the less severe the restriction on the time step, resulting in a more efficient scheme.

Jean Dolbeault and Reinhard Illner continued work on entropy methods for (linear) drift-diffusion equations with time-dependent and locally vanishing drift and diffusion coefficents (thus leading to degeneracies in the diffusion). Problems of this nature emerged in the traffic models which Reinhard Illner presented at the workshop; related problems arise in the analysis of flashing ratchets. Many open mathematical questions emerge naturally in this theory, among them the validity of generalized Hardy-Poincare inequalities, the description of asymptotic behaviour of the system if the roots of the diffusion and drift coefficients experience periodic oscillations, and others. A comprehensive paper about these matters was essentially completed during the workshop [2].

Finally, Reinhard Illner, Horst Lange and Holger Teismann completed work on a comprehensive article on the limitations of exact controllability of linear and nonlinear Schroedinger equations, with the Hartree equation and the Gross-Pitaevski equation as the most relevant examples. In particular, a result on non-controllability (complementing the knowledge on optimal control) for the Hartree equation was obtained. The paper is presently undergoing final revisions.

3 Concluding observations

1. The workshop united a small group of researchers with a strong common mathematical culture and very varied applied interests. Such a variety of domains of applications is common among applied mathematicians and especially among people involved in multiscale modelling.

2. The main applications considered at the workshop were:

   - New classes of kinetic traffic flow models, leading to original research on nonlinear and nonlocal degenerate drift-diffusion equations (Dolbeault, Illner).
   - Bose-Einstein condensation: the condensation mechanism, the dynamics of the condensate, and numerical methods (Markowich, Pareschi, Russo, Schmeiser). The numerical methods presented by Russo (IMEX) essentially apply to all the topics considered in the meeting (they are derived to treat multiscale problems).
   - quantum control (Dolbeault, Illner, Lange, Teismann)
   - multiscale models in biology, in particular the phenomenon of chemotaxis (Markowich, Oelz, Schmeiser)
   - Scaling limits in kinetic theory and fluid dynamics (Dolbeault, Jin, Markowich, Lin, Oelz, Schmeiser).

3. The format of a small foccused research group was universally found to be ideal: long presentations, enough time for detailed discussions, and time and space for active research (there are numerous articles in preparation as a consequence; new projects are being planned)

The workshop was a resounding success.

References

[1] J. Dolbeault, P. Markowich, D. Oelz and C. Schmeiser, Mean free path limit of a Boltzmann-type equation with general equilibrium function and relaxation time approximation collision operator. *in preparation.*

[2] Ph. Bartier, J. Dolbeault, R. Illner and M. Kowalczyk, A qualitative study of linear drift-diffusion equations with time-dependent or vanishing coefficients, *in preparation.*

[3] R. Illner, H. Lange and H. Teismann, Limitations in quantum control, *in preparation.*

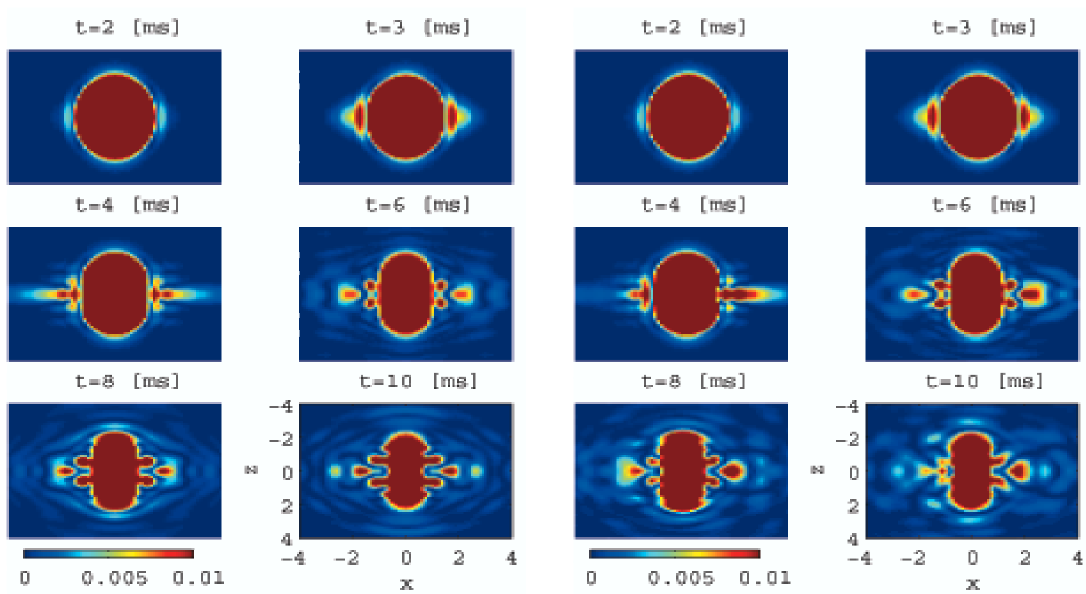

Figure 1: Jets in Bose-Einstein condensates