Mathematical and Numerical modeling of Transport Problems

Faculty :	N. Ben Abdallah, C. Besse (50%), P. Degond, F. Deluzet, M. Lemou, F. Méhats, L. Mieussens, M.H. Vignal (50%), Y. Qiu.
PhD :	J.P. Bourgade (Degond, Mieussens), N. Crouseilles (Degond, Lemou), A. El Ayyadi (Degond), J. Kéfi (Ben Abdallah), A. Mellet (Degond), C. Parzani (Degond, Vignal), O. Pinaud (Ben Abdallah, Méhats), E. Polizzi (Ben Abdallah), R. Talaalout (Degond, Vignal), O. Saut (Besse, Degond), M.L. Tayeb (Ben Abdallah)
Ex. PhD :	V. Latocha (Degond, 01), P. Omnés (Degond, 99), F.P. Peyrard (Degond, 98), D. Reignier (Bidégaray, Degond, 00).

The team activity concerns the study of particle transport in various situations (fluids, plasmas, gas discharges, semiconductors, polymers, etc) of interest for industry or applied sciences. Through collaborations with reknown physics groups and contracts with industrial partners (e.g. CEA, CNES, Astrium, IEMN, CPAT), physically accurate models able to run on a standard workstation are derived by means of asymptotic analysis tools and numerically implemented. The team developed durable interdisciplinary and bilateral research actions, it is a participant team of the TMR network "Asymptotic methods in kinetic theory" (EEC, 1998-2001) and most of its members form, together with the 'electromagnestism' team, the joint CNRS-CEA research unit (LRC) recently funded by the CEA and coordinated by P. Degond.

Asymptotic analysis techniques such as macroscopic limits have been successfully developed by the team to derive a hierarchy of models including generalized diffusion and hydrodynamic equations. These techniques also allow the design of interface conditions to couple the various models, thus reducing the cost of numerical simulations. The generalized diffusion models (such a the ET and SHE models, see next section) derived by the team, have been succesfully used to describe particle transport in many contexts (e.g. Spatial Technologies, astrophysics and hot plamsas, polymers, kinetic turbulence). Further developments will be done at the numerical and analytical levels. Semiclassical limits tools are used by the team to connect quantum transport models to classical transport models and to derive new adiabatic models for semiconductors which include both quantum and classical features. Numerical simulations of these models as well as their mathematical analysis will be done. The numerical simulations are sustained by the development of efficient numerical methods (entropic algorithms, euelerian methods for kinetic equations, wavelet and multipole methods for collision integrals, atrificial boundary conditions, etc).

The targetted applications of the above developments include Spatial Technologies (arcs on satelites, ion propellors, current contracts with ESA, Astrium, CNES, ONERA), Astrophysics problems (in connection with current contracts with the CEA, the LRC lab. and with the future Plasma Physics institute of Bordeaux) and Cathodic spot plasmas and hot plasmas (LRC, development of hybrid kinetic-fluid models) ; Kinetic turbulence models developed by the team will be numerically simulated and their fluid counterparts will be used for ionosphere modeling (LRC). Adiabatic models will be used for simulating ulstrashort transistor and single electron memories (SPM-STIC action with LETI) and broken gap and spin devices (IEMN).

A hierarchy of models for transport problems

A common feature to the various actions conducted within our team consists in the combined use of asymptotic and numerical methods, the aim is to obtain reduced models capable of accurately describing the physics with the lowest possible numerical cost.

One way of achieving this goal is by revisiting macroscopic limits of kinetic models for particle systems (like the Navier-Stokes limit of the Boltzmann equation in gases), or semi-classical limits of quantum systems. To this aim, standard asymptotic methods (like e.g. the Hilbert or Chapman-enskog expansion method, boundary layer correctors, Wigner transforms, etc) are used on novel situations (like diffusion systems driven by collisions with the boundary, see figure 2 or adiabatic quantum-kinetic models for partially confined nanostructures). Mathematically rigorous frameworks are set, in which convergence results are proven, numerical approximations are investigated and implemented and the results are confronted with experiments or other models.

- Macroscopic limits: from kinetics to diffusion and hydrodynamics. A series of work is devoted to 'non-standard' diffusion models, like the SHE (Spherical Harmonics Expansion) or ET (Energy-Transport) models. In general, collisions contribute to relax a particle system (described by a kinetic equation) towards a local thermodynamical equilibrium. The equilibrium evolves in time according to the macroscopic model, the numerical resolution of which is less expensive. However, in most situations of physical interest, standard macroscopic models provide too coarse descriptions of the physics to be useful. By a close inspection of the collision mechanisms, it is possible to derive intermediate models between the kinetic and macroscopic ones, evolving on a mesoscopic scale. These models are related to 'partial equilibria' depending on a larger set of parameters than the usual macroscopic models.

The SHE and ET models are two examples of such models, which proved to be particularly suitable to plasmas and semiconductors. They have been applied to several industrial problems (Plasma Opening Switch (contract with CEA, PhD thesis of F. Deluzet), surface discharges on solar pannels of satelites (contract with ONERA, CNES and Astrium company, PhD thesis of C. Parzani and R. Talaalout, [28]), plasma propellors for satellites (collaboration with CNES and the French Research Group (GDR) on ionic propulsion, PhD thesis of Latocha [19]), semiconductors devices and superlattices, etc, (see following pages).

The team (N. Ben Abdallah, P. Degond, PhD theses of S. Génieys, V. Latocha, A. Mellet, N. Crouseilles, JP Bourgade, L. Tayeb, post doc of S. Mancini, K. Zhang, etc) has worked on the rigorous establishment of the models by Hilbert expansion and entropy methods [27, 20, 18, 16, 8, 3], and on the existence and uniqueness of solutions [17]. P. Degond and M. Lemou (cf also the PhD thesis of Peyrard) have translated this approach to hydrodynamics and applied it to turbulence modeling in [26, 26]. Homogenization problems, combined with diffusion approximation problems arise when the length scales related to the driving forces or to collision processes are comparable with the mean free path. This leads to new diffusion models pertaining with quantum semiconductor devices and superlattice structures (N. Ben Abdallah, P. Degond, PhD theses of A. Mellet, L. Tayeb, post doc of Zhang, etc) [7]...

- Local models. Physical and aritifical boundaries play an important role in the modeling and simulations of realistic devices. Boundary layers form when two models are coupled with

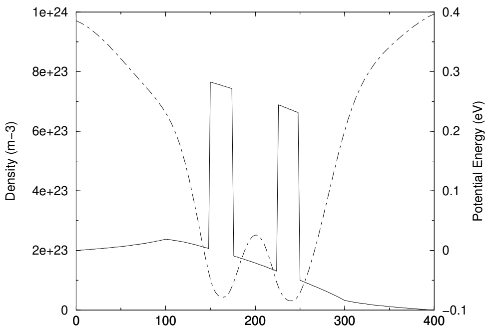


FIG. 1: Electrostatic energy and electron density in a resonant tunneling diode are plotted. The resonant state is responsible for the density peak in the well btween the two barriers .

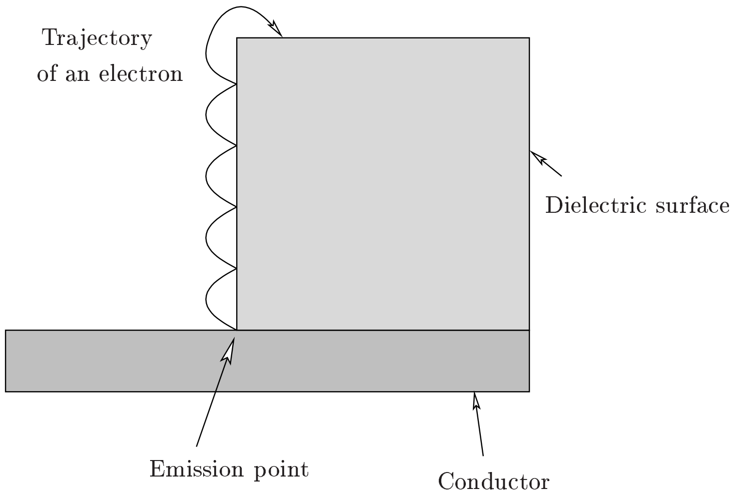


FIG. 2: Hopping of particles constrained to move close to a surface. The many bounces induce a diffusion motion parallel to the surface. This model applies to the ionic propellor for satellites and to surface discharges on the panels of satelite solar generators.

each other (see section 'model coupling') and are analyzed through boundary layer problems for kinetic equations (N. Ben Abdallah and H. Chaker P. Degond and C. Schmeiser, PhD thesis of A. El Ayyadi). Singularly perturbed boundary conditions, like those arising in the Child Langmuir asymptotics (N. Ben Abdallah, P. Degond and F. Méhats, see section 'POS' [5, 6]) lead to original free boundary models which apply to magnetic insulation problems.

- Quantum transport and waves. For nanoscale semiconductors like resonant intraband or interband tunneling diodes (see figure 1), ultrashort channel transistor or quantum waveguides, electrons can no longer be considered as particles but rather as waves. A series of work is devoted to the derivation and the analysis of quantum transport models valid at these lengthscales [9].

The first point concerns the modeling of open quantum systems whic interact with a reservoir. This is done through open boundary conditions for the scalar Schrödinger equation (N. Ben Abdallah, P. Degond, F. Méhats [4], PhD theses of J. Kéfi, O. Pinaud and E. Polizzi) and for the multiband Schrödinger equation (N. Ben Abdallah, PhD thesis of J. Kéfi). In the semiclassical limit, these boundary conditions lead to the standard inflow boundary conditions for kinetic equations (N. Ben Abdallah, P. Degond and I. Gamba [1, 4]). This opens the way to efficient classical/quantum coupling strategies (see next section).

The second point concerns the derivation and the analysis of adiabatic models, for 2D electron gases, which allow decouple the confinement directions (quantum) from the transport directions (which can be quantum or classical). This is done by using Wigner transform techniques (N. Ben Abdallah, F. Méhats) and results in numerically less expensive models (PhD theses of O. Pinaud and E. Polizzi). Numerical simulations have established the practical validity of these models.

Model coupling

In many situations related to complex physical phenomena, the use of a single model throughout the entire device or region of interest is not possible. Often, this would necessitate a trade-off between physical accuracy and numerical efficiency which would never be satisfactory. Therefore, considerable effort has been put in the team on 'model coupling'. This strategy can be implemented in a large variety of ways. Coupling can be achieved via domain decomposition (e.g. in fluid-kinetic coupling, part of the domain is described by a fluid model, part of it by a kinetic model ; the same approach can be developed in classical-quantum coupling). Another approach is to use a velocity splitting of particles, rather than a position splitting. In hybrid models, the particle population is decomposed into two subpopulations, each of the populations being described by its own model: for instance, thermal particles can be described by a fluid model and suprathermal particles, by a kinetic model. Related to this straegy, the adiabatic approach consists in decomposing the particle wave function into a purely quantum part (e.g. describing a quantum confinement in one direction) and a semi-classical one (to account for a large delocalization in the other direction). The team has developed the various aspects mentioned above.

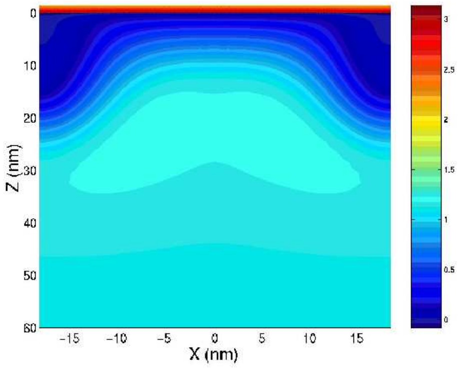


FIG. 3: The electrostatic potential in a Transistor. It can be seen at the top of the figure that the lengthscale in the vertical direction is much smaller than in the horizontal one..

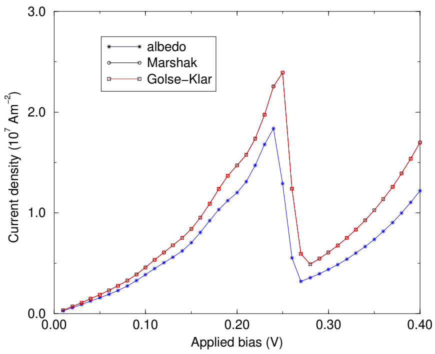


FIG. 4: Current versus Voltage characteristic curves of a Resonant Tunelling Diode obtained through three different quantum-kinetic coupling strategies.

Spatial domain decomposition : Kinetic-fluid coupling Fluid-kinetic coupling has been investigated by P. Degond and C. Schmeiser, in connection with the ET and SHE models (see section 'hierarchy of models'). The determination of the interface conditions between the classical and quantum region requires the resolution of half space kinetic problems (so-called 'Milne problems'), which are related to the construction of adequate boundary layer correctors. N. Ben Abdallah, I. Gamba and A. Klar have analyzed such Milne problem for high electric field and linear collision operators. The nonlinear case which includes Pauli exclusion terms has been treated by N. Ben Abdallah and H. Chaker.

Spatial domain decomposition : Classical-Quantum coupling The classical (kinetic) -quantum coupling problem by domain decomposition methods has been investigated by N. Ben Abdallah in the one-dimensional stationary framework [1], and has been later extended to the time-dependent case by N. Ben Abdallah, P. Degond and I. Gamba [4]. The first step in this series of works consists in writing open boundary conditions for the quantum regions by considering the classical regions as 'reservoirs' (see previous section). The semiclassical analysis of the 'quantum' zone by Wigner function techniques allows the derivation of interface conditions which involve the amplitude of the reflection-transmission coefficients (for stationary problems) as well as their phase (for time dependent problems). When the classical zones are collision dominated, these models naturally lead, through diffusion approximation, to coupling strategies between quantum and classical macroscopic models (e.g. drift-diffusion models, which is the most widely used models in the industry). This question has been investigated in the PhD thesis of A. El Ayyadi (supervised by P. Degond), see figure 4 and section 'nanostructures'. This work makes use of earlier work by P. Degond and C. Schmeiser on diffusion models for semiconductor heterostructures.

- Velocity domain decomposition : hybrid kinetic-fluid models. A second class of model coupling concerns the momentum splitting of particles. Hybrid kinetic-fluid models are being developed in the PhD thesis of N. Crouseilles (supervised by P. Degond and M. Lemou) within a contract with the CEA. The targetted applications concern hot plasmas, with a strong non equilibrium component. Low energy particles are in a local equilibrium, whereas high energy particles are purely kinetic. This leads to a new coupling strategy which necessitates both analytical efforts (connected with the moment hierarchy method of Levermore) and numerical ones.

- Velocity domain decomposition : adiabtic quantum-classical models. In the adiabatic models, the components of the momentum variable behave differently from one another. In the confinement direction, the particle wavelength and the geometrical length scale are of the same order of magnitude, while in the transport direction, the wavelength is much smaller than the geormetrical length scale (see figure 3). The semiclassical analysis (N. Ben Abdallah, F. Méhats leads to an adiabatic model in which the particles are in a quantum state in the confinement direction while the evolution in the transport directions is governed by kinetic equations. The spatial quantum/classical coupling strategies is being adapted to couple the adiabatic models to fully quantum models (N. Ben Abdallah and C. Negulescu). The approach will be applied to the modeling of single electron memories for which transport direction has succesive slices, with regions with large lengthscales (treated by the adiabatic model) seprated by small lengthscale regions (quantum dots, treated by a fully quantum model). Besides, taking into account the scattering mechanisms in the adiabatic models, diffusion approximations are being applied in order to derive macroscopic and mesoscopic adiabatic models (N. Ben Abdallah, F. Méhats).

Perspectives. Further studies for diffusion and hydrodynamic limits will be done. This includes the determination of validity domains for the ET and SHE approximations, the extension of fluid limits to relativistic flows, to adiabatic models and to the anomalous diffusion as well as the study of homegenization problems for charged particles and rarefied gases. The hybrid models (fluid description of low energies and kinetic modeling of high energies), will be studied and applied to out of equilibrium plasmas. Quantum *Interactions* will receive a special care. Rate equations for laser-matter interaction (propagation in non centrosymmetric crystals), electron-phonon and surface roughness scattering, transition to classical transport, will be studied by semiclassical tools and Transfer matrix methods. Quantum-classical coupling strategies will be further studied in the time dependent and multidimensional case and fluid-quantum coupling will be investigated.

Nanostructures

N. Ben Abdallah, P. Degond, A. Elayyadi, J. Kéfi, F. Méhats, O. Pinaud, E. Polizzi

The objectives of this work is the simulation of nanoscale electronic devices, the operation of which involves quantum effects such as tunneling. The devices are in general composed of an active region, connected to particle reservoirs (source, drain) which 'send' the particles into the device according to an equilibrium profile.

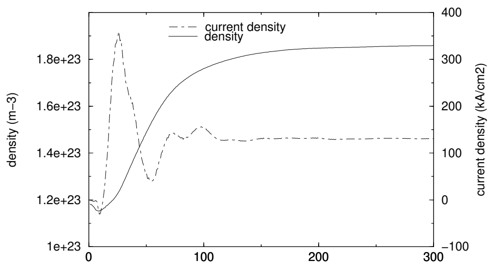


FIG. 5: Evolution of the current as a function of time in a resonant tunneling diode.

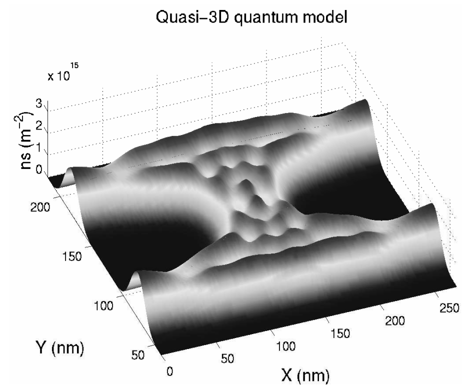


FIG. 6: Interference patterns for the surfacic particle density in a quantum coupler.

- Injection from reservoirs and boundary conditions (N. Ben Abdallah, P. Degond and F. Méhats, PhD theses of J. Kéfi, E. Polizzi and O. Pinaud). One way to model the inejction of particles from reservoirs consists in assuming that the particles are in a mixed state which is a statistical mixture of elementary scattering states ; each of them correspondng to an individual particle injected from the reservoir elementary state corresponding to a single wave originating from the reservoir. Open boundary conditions for the stationary Schrödinger equation were previously derived and analyzed by N. Ben Abdallah, P. Degond and P. Markowich for the one dimensional case and by N. Ben Abdallah in the multidimensional case [2]. They are currently analyzed in the time-dependent case (N. Ben Abdallah, P. degond, I. Gambba [4] F. Méhats, PhD thesis of O. Pinaud, see also the work of X. Antoine and C. Besse in the 'electromagnetism team'). Stationary and time dependent one dimensional simulations for the Resonant Tunneling Diode (RTD) have been realized in the PhD thesis of O. Pinaud (see figure 5). Stationary simulations are done in the multidimensional case in the PhD thesis of E. Polizzi and are being developed for multiband transport (PhD thesis of J. Kéfi).

- Collisions and quantum transport. (PhD thesis of A. El Ayyadi), Parts of a semiconductor device are purely classical and involve collision phenomena. Thereofore, a diffusion equation, deduced by a diffusion approximation of the kinetic-quantum model is used to model these zones. This results in a considerable saving in computer time, a drift-diffusion model being much cheaper than a kinetic one. Figure 4 in section 'Model-coupling' shows the current-voltage characteristic of an RTD by the hybrid diffusion-quantum model.

- Partially confined structures : adiabatic quantum models. (PhD thesis of E. Polizzi) For multidimensional devices such as split gate devices and Short channel transistor, the mixed state description of electrons is numerically expensive. In order to reduce the numerical simulation cost, an adiabatic quantum model which takes into account the partial confinement of electrons is derived and simulated (see Fig 6). This work is done in the framework of a collaboration with O. Vanbésien from the IEMN [10]. Analytical issues related to this model are studied in the PhD thesis of O. Pinaud.

Numerical methods in kinetic and quantum theory

X. Antoine, C. Besse, M. Lemou

-Fast Multipole Methods (M. Lemou, in collaboration with O. Bokanowski (Paris VII)) The Fast Multipole Method (FMM) was first introduced by Greengard and Rokhlin to rapidly compute binary interactions in a system of particles with a controled accuracy. This is equivalent to a fast computation of a two-variables integral. Using this idea, we have developed multipole methods to obtain conservative approximations of collisional operators in kinetic theory. However in quantum theory, the correlations between particles are stronger and make prohibitive any direct computation. Thus, we have extended the multipole method to the computation of multi-variable integrals. If m is the number of particles (or variables) and N is the number of discretization points of each varaiable, then the extended multipole method only requires a computational cost proportional to $(-\log \epsilon)^{\mu_m} N$ instead of N^m, ϵ being the desired accuracy, and μ_m is a constant (see Fig 7).

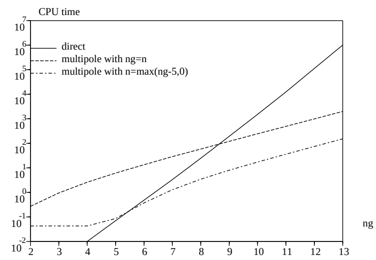


FIG. 7: CPU time (in logarithmic scale) vs $\log N$, using the FMM for computing multivariable integrals.

-Multiwavelet Methods X. Antoine, M. Lemou
An alternative strategy to the FMM consists in the use of wavelet schemes. In this work, we have used multiwavelet techniques to construct conservative and entropic approximations of kinetic collisional operators (see Fig 8). This approach allows a high accuracy with a reduced computational cost, and can easily be extended to collisional operators with more complex sructures (involving relativistic and quantum effects for instance). Furthermore, an important aspect of the method is its easy implementation compared with the multipole methods where the recursive evaluation of moments requires an additional heavy handling and a higher computational cost.

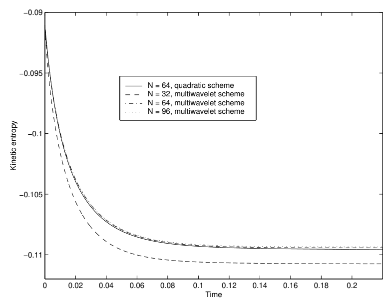


FIG. 8: Decay of entropy for the Fokker-Planck-Landau operator

-Numerical scheme for dispersive systems (C. Besse in collaboration with D. Lannes (Bordeaux I) and S. Descombes (ENS Lyon)) Numerical schemes for dispersive equations must preserve conserved quantities such as the energy and the hamiltonian and ensure the stability and convergence. For the nonlinear Schrödinger equation, two directions are investigated: the relaxation scheme [11] and the splitting scheme [12, 13]. The study of the instabilities of short wave-long wave resonances in the context of 3D water waves involves an operator of the type $\partial_x^{-1}\partial_y^2$ which leads to strong numerical difficulties. The numerical analysis of the scheme and numercial experiments are performed [14].

Plasma mathematical models in space technology

P. Degond, Ph. Guillaume, V. Latocha, R. Talaalout, M.H. Vignal

Plasma problems are almost ubquitous in space technology. Indeed, the environment of any satelite orbiting the earth is a plasma. The team has worked on two related problems:

- Ionic propulsion: (P. Degond, Ph. Guillaume, PhD thesis of V. Latocha, Post doc. of S. Mancini). The first studied problem is the modeling of the Stationary Plasma Thruster, a propulsion device first implemented by russian teams, and now developped by the 'Société Européenne de Propulsion', in a cooperation with academic teams within the 'GDR Propulsion Ionique'. Within this program, P. Degond has supervised the PhD thesis of V. Latocha, in collaboration with L. Garrigues and JP Boeuf (Laboratoire de Décharges dans les gaz, UPS). In these works, a diffusion model in the position-energy variables (a 'SHE' model) for the electrons in the SPT has been derived from kinetic theory, using collisions with the boundary as dominant collision mechanism (see section 'hierarchy of models' and [15], [27], [20]). The numerical results show an extremely good agreement with fully kinetic simulations by Monte-Carlo methods (developped in Boeuf's team), together with a tremendous gain of computer time (see Figure 9) and [19]). V. Latocha has also studied an elliptic problem with a very anisotropic diffusion matrix arising from the resolution of the continuity equation. An expansion in terms of the matrix anisotropy allows to solve a better conditioned problem (in collaboration with Ph. Guillaume).

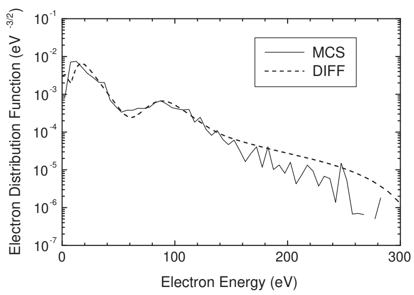


FIG. 9: Electron energy distribution function in a Stationary Plasma Thruster near the anode. Comparison using the (SHE) diffusion model (DIFF) and a Monte Carlo simulation of the full kinetic model (MCS). The diffusion model runs in a couple of minutes on a standard workstation. The kinetic one takes several hours.

- Discharges on satelites: (P. Degond, M.H. Vignal, PhD thesis of R. Talaalout) in cooperation with D. Payan and F. Severin (CNES), within contracts with ONERA, ESA, CNES and Astrium. Future satelite solar generators will operate under high voltage in order to meet high power demands. In these conditions discharges and arcs may occur and damage the generator. In order to understand the physics of these phenomena, a research program has been launched. R. Talaalout has started his PhD thesis supervised by P. Degond and M.H. Vignal within this program. The physical process can be split in two steps. The first one is the creation of a high density plasma near the solar cell by an avalanche breakdown mechanism. The second one is the transition to an electrical arc. A model describing the avalanche breakdown has been proposed. It is composed of an Energy-Transport model for electrons hopping along the surface of the cell, coupled with hydrodynamic models for neutrals and positive ions. Figure 10 shows the avalanche phenomenon : the electron density along the surface increases with time (see [28] for other numerical results). The future of this program consists in modeling the transition to the arc.

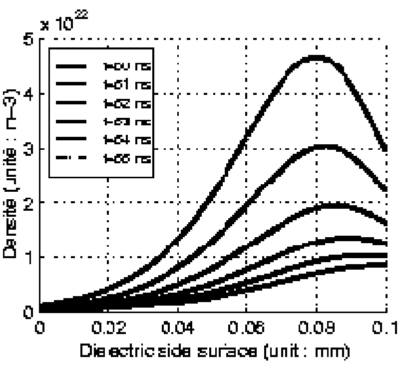


FIG. 10: Electron density along the dielectric.

Plasma Opening Switch

N. Ben Abdallah, P. Degond, F. Deluzet, F. Méhats

Plasma opening switches (POS) consist in plasma bridges between two concentric electrodes and are used to compress electromagnetic pulses. Their operation involves two phases. During the first one, the *conduction phase*, the magnetic field penetrates into the plasma, which acts as a short-circuit. Then the *opening phase* starts when complex plasma-waves interactions lead to a sudden drop of the POS conductance.

- Large scale global model and simulations (PhD thesis of F. Deluzet, supervised by N. Ben Abdallah and P. Degond). Charge separation effects are determinant in the POS operation. In order to simulate both the conduction and the opening phases, a global collisional bi-fluid model was developped. Hydrodynamic equations are considered for ions, while the Energy-Transport is used for electrons. These equations are coupled with Maxwell's system.

The two-dimensional numerical simulations rely on Finite Differences for Maxwell's equations and a Particle In Cell (PIC) method for the fluid equations. Due to the dielectric relaxation scale, we developed an implicit coupling method of Maxwell's equations with the electron Energy-Transport model.

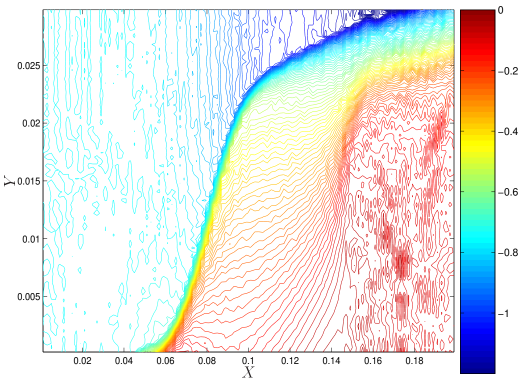


FIG. 11: Fast magnetic field diffusion. The magnetic field intensity (in Tesla) is represented in the interelectrode area.

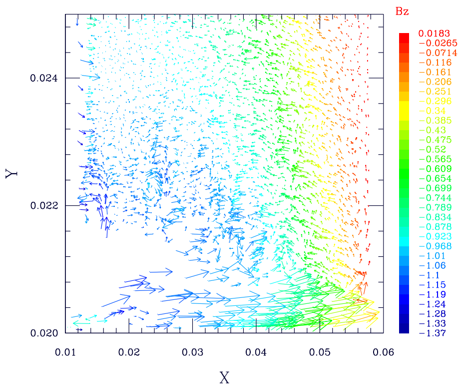


FIG. 12: Electron magnetic insulation. The electron velocities (m/s) are plotted at the particle positions. The color indicates the magnetic field intensity.

- Two local models

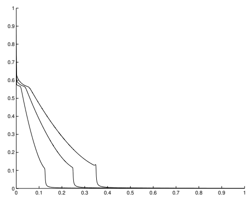
During the conduction phase, the plasma is quasineutral and ions are motionless. An asymptotic degenerate diffusion model with a nonlinear oblique derivative boundary condition has been studied in [30] by F. Méhats and J.-M. Roquejoffre (fluid mechanics group, see also pages "Asymptotic Methods in Fluid Mechanics"). It shows a **fast penetration of the magnetic field**, which was confirmed by the global simulations of F. Deluzet (see FIG.11).

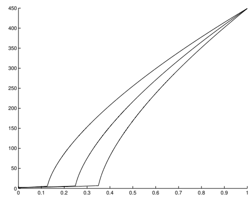
During the opening phase, the major phenomenon which prevents the electrons from conducting the current inside the POS is the **magnetic insulation**. For large magnetic fields, the Lorentz force curves the electron trajectories thus confining them inside a sheath near the cathode, as illustrated on the global simulation results (the bottom left of FIG.12). In [5, 6], N. Ben Abdallah, P. Degond and F. Méhats have analyzed this phenomenon by the so-called Child-Langmuir asymptotics and derived various limit problems involving free boundaries. Exact solutions of these models have been calculated, which enables to estimate the width of the electron sheath as a function of the applied magnetic field.

Free Surfaces

C. Besse, P. Degond, F. Deluzet, K. Domelevo, C. Parzani, M.-H. Vignal

- Explosive erosion of a cathode (P. Degond, MH Vignal, PhD thesis of C. Parzani): collaboration in progress with J. Segre and F. Assous from CEA/DAM-Ile de France. In some electron beam devices, the emitter cathode is made of a material which presents a network of micro points (such as point cathodes or velvet cathodes). The goal is to extract currents greater than the Child Langmuir (C-L) current, which is the theoretical limit for plane cathodes. These cathodes operate by the vaporization of the points and the creation of a plasma near the cathode. This plasma expands in the vacuum and forms an effective cathode at the interface between the plasma and the vacuum. As this effective cathode moves towards the anode, the extracted current increases (due to the C-L law) and allows to extract larger currents than with a conventional diode. The aim of our work is to find a mathematical model of this phenomenon which gives accurate results for a small numerical cost. Thanks to a formal asymptotic analysis, we were able to derive a simplified model from a bifluid Euler model (for the electrons and the ions) coupled with the Poisson equation. This simpler model consists of a quasi-neutral model for the plasma coupled through a transition layer to a C-L model for the electron beam. The comparison of these models is in progress. On the following figures, we can see the density (on the first one) and the velocity (on the second one) at different times in the gap between the cathode (x=0) and the anode (x=1). These results are given by the bifluid model.





- Plasma turbulence (C. Besse, P. Degond, F. Deluzet): collaboration in progress with G. Gallice and C. Tessieras from CEA-CESTA within an industrial contract. The ionosphere plays a key role in radioelectric waves propagation for earth-to-earth or earth-to-satellite telecommunications. Nethertheless, the ionospheric plasma is subject to instabilities which make it a random environment and penalize communications. Our goal is the modeling of these ionospheric irregularities by means of the dynamo model. This model consists of the non-standard, nonlinear coupling of a hyperbolic equation with an elliptic one. We have investigated the instability of discontinuous steady states which explains the formation of the irregularities. In numerical simulations, a sub-grid modeling of the short scale irregularities is necessary since the length scale of the inhomogeneities becomes smaller as time proceeds. Inspired by the statistical approach to turbulence of fluids mechanics, we have proposed a model which takes into account the small turbulent scales by means of a diffusion. The implementation of this model is in progress. Theoretical analyses of the model are planned.

- Crystal growth (C. Besse, K. Domelevo, C. Galusinski (Bordeaux 1)): This is a transverse activity with the fluid mechanics group. Electric fields can affect the growth of ice crystals. The electric effects are interesting because electric fields influence the way water molecules diffuse through the air in the vicinity of the ice surface. If we charge up a growing crystal, then electrostatics dictates that strong electric fields will be set up around the crystal. The fields and field gradients will be particularly strong near any sharp points on the crystal. Since water molecules have an intrinsic electric polarizability, the electric fields tend to polarize the water molecules. If the field also has a strong gradient, then the polarized molecules are attracted in the direction of stronger fields. We analyze dendrite growth in the presence of an applied voltage and establish a model.

Kinetic modeling of fluids

P. Degond, M. Lemou, L. Mieussens

- Kinetic modeling of turbulent flows (P. Degond, M. Lemou). In a first work, an extension of classical compressible fluid models, in which the fluid internal energy is a measure-valued quantity, is derived from kinetic theory [26, 22]. The so obtained fluid models contain more phenomenology than the standard models (e.g. richer structures of the viscosity and heat flux). This can help to understand the fluid turbulence from kinetic theory.

Then in a second work, we have focused on the kinetic modeling of turbulent incompressible flows. The kinetic model involves a relaxation time which is tuned in a such a way that both the molecular viscosity and the Kolmogorov law for turbulence can be described. Starting from this kinetic model, we then derive $k - \epsilon$ type models of turbulent flows, and compare with the standard equations. Finally, moment systems derived form this kinetic model have been investigated [23, 21].

- Viscoelastic fluid models from kinetic theory (P. Degond, M. Lemou, co-operation with M. Picasso). This work concerns the description of the visco-elastic tensor of a non-Newtonian fluid from kinetic theory. The used kinetic equation is a Fokker-Planck model corresponding to the so called dumbbells theory for dilute solutions of polymers. We show how asymptotic expansions (as Chapman Enskog expansion) can be used to obtain general expressions for the stress tensor, and then to recover the well known results of Bird et al [25, 24].

- Modeling rarefied gas flows by BGK models (L. Mieussens). The aim of this work is to obtain fast and robust numerical methods for computing gas flows in rarefied or transitional regimes. The main ingredient is a conservative and entropic approximation of the BGK relaxation operator, for which we have a convergence result [32], and a linearized implicit scheme [31].

We have developped a code that can compute rarefied gas flows from subsonic to hypersonic regimes, in 1D, plane 2D and axisymmetric 3D geometries in space, and 3D in velocity. The code is particularly well suited for steady flows (see figures 14 and 13).

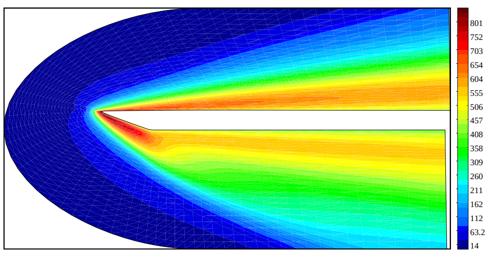


FIG. 13: Hypersonic flow past a flat plate ($Ma = 20, K_n = 0.014$), temperature contours

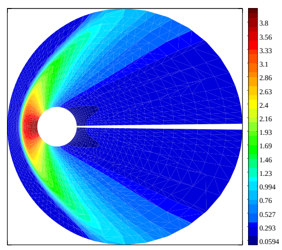


FIG. 14: Supersonic flow past a cylinder ($Ma = 4, K_n = 0.004$), pressure contours

In order to reach correct Prandtl number, the previous method has been extended to the Ellipsoidal-Statistical model [33], and in a joint work with H. Struchtrup (Victoria), we are investigating new BGK models with velocity-dependent collision frequency.

Finally, in collaboration with B. Dubroca (CEA-CESTA), we have also extended our method to polyatomic gases [29].

References

[1] N. Ben Abdallah. *J. Stat. Phys.*, 90(3-4):627–662, 1998.

[2] N. Ben Abdallah. *J. Math. Physics.*, 41(7):2241–2261, 2000.

[3] N. Ben Abdallah. and H. Chaker. *Math. Mod. Meth. Appl. Sci.*, 11(7):1253–1272, 2001.

[4] N. Ben Abdallah., P. Degond, and I. Gamba. *J. Math. Phys*, 2001. to appear.

[5] N. Ben Abdallah, P. Degond, and F. Méhats. *Physics of Plasmas*, 5(5):1522–1534, 1998.

[6] N. Ben Abdallah, P. Degond, and F. Méhats. *Asymptotic Analysis*, 20:97–132, 1999.

[7] N. Ben Abdallah, P. Degond, A. Mellet, and F. Poupaud. *Quarterly Appl. Math.* to appear.

[8] N. Ben Abdallah, L. Desvillettes, and S. Génieys. *J. Stat. Phys.*, 98(3-4):835–870, 2000.

[9] N. Ben Abdallah and J. Kefi. *C.R.Acad. Sci. Paris*, . t. 331 Série I:165–170, 2000.

[10] N. Ben Abdallah, E. Polizzi, O. Vanbésien, and D. Lippens. *J. of Appl. Phys.*, 87(12):8700–8706, 2000.

[11] C. Besse. *C. R. Acad. Sci. Paris Sér. I*, 326(12):1427–1432, 1998.

[12] C. Besse. In *Mathematical and numerical aspects of wave propagation, Santiago de Compostela 2000*, pages 605–609. SIAM, Philadelphia, 2000.

[13] C. Besse, B. Bidégaray, and S. Descombes. *SIAM J. Numer. Anal.* to appear.

[14] C. Besse and D. Lannes. *European Journal of Mechanic-B Fluids*, 20(5):627–650, 2001.

[15] P. Degond. *SIAM J. Applied Math*, 58:1138–1162, 1998.

[16] P. Degond. *Math. Methods and Models in the Applied Sciences*, 11:903–932, 2001.

[17] P. Degond, S. Génieys, and A. Jüngel. *Math. Methods in the Applied Sciences*, 21:1399–1413, 1998.

[18] P. Degond, T. Goudon, and F. Poupaud. *Indiana University Math. J.*, 49:1175–1198, 2000.

[19] P. Degond, V. Latocha, L. Guarrigues, and J. P. Boeuf. *Transp. Theory and Stat. Phys*, 27:203–221, 1998.

[20] P. Degond, V. Latocha, S. Mancini, and A. Mellet. *Methods and Applications of Analysis.* to appear.

[21] P. Degond and M. Lemou. Submitted.

[22] P. Degond and M. Lemou. *European J. Mech. B/fluids*, 20:303–327, 2001.

[23] P. Degond and M. Lemou. In *Magdebourg Proceedings, (Hyp 2000)*, 2001. to appear.

[24] P. Degond, M. Lemou, and M. Picasso. Submitted.

[25] P. Degond, M. Lemou, and M. Picasso. In *IMA-proceedings*, 2001. to appear.

[26] P. Degond, J. L. Lopez, and P. F. Peyrard. *Continuum Mechanics and Thermodynamics*, 10:153–178, 1998.

[27] P. Degond and S. Mancini. *Asymptotic Analysis*, 27:47–73, 2001.

[28] P. Degond, R. Talaalout, and M.H. Vignal. In *proceeding of the Workshop ESA-CNES*. ESTEC, Noordwijk the Netherlands, 2000.

[29] B. Dubroca and L. Mieussens. *ESAIM-Proceedings*, 10, CEMRACS 1999:127–139, 2001.

[30] F. Méhats and J.-M. Roquejoffre. *Analyse Non Linéaire, Annales de l'Institut Henri Poincaré*, 16(6):691–724, 1999.

[31] L. Mieussens. *Math. Models and Meth. Appl. Sci*, 8(10):1121–1149, 2000.

[32] L. Mieussens. *Computers Math. Applic.*, 41(1-2):83–96, 2001.

[33] L. Mieussens. *Journal of Computational Physics*, 162:429–466, 2001.