TU Wien WS 2016
Institute for Analysis and Scientific Computing
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9. Exercise sheet for the course "Modeling with PDEs"
(Hydrodynamic and drift-diffusion models, related equations)

Exercise 1. The following system of PDEs is called the *bipolar model*:

$$\partial_t n + q^{-1}\mathrm{div}_x J_n = -R(n,p), \qquad J_n = -q\mu_n(U\nabla_x n + n\nabla_x V), \tag{1}$$
$$\partial_t p - q^{-1}\mathrm{div}_x J_p = -R(n,p), \qquad J_p = q\mu_p(U\nabla_x p - p\nabla_x V), \tag{2}$$
$$R(n,p) = \frac{np - n_i^2}{\tau_p(n+n_d) - \tau_n(p+p_d)}, \tag{3}$$
$$-\varepsilon_s \Delta V = q(n - p - C). \tag{4}$$

Here n, p are the electron and hole densities (resp.), q is the electron charge, U is the reference potential, $C = C(x)$ is the so-called *doping profile*, τ_n, τ_p are the carrier life times, and

$$n_d = N_c e^{(E_t - E_c)/k_B T}, \qquad p_d = N_v e^{(E_v - E_t)/k_B T}, \qquad n_i = \sqrt{n_d p_d}.$$

The quantities N_c, N_v are the carrier effective densities of states, n_i is the intrinsic density, and E_t is the so-called *trap energy level*. The function $R(n,p)$ in (3) is called *Shockley-Read-Hall recombination-generation term*.

(i) A thermal equilibrium state is a time-independent solution (n,p,V) to (1)–(4) with zero current flow, i.e.
$$\partial_t n = \partial_t p = 0, \quad J_n = J_p = 0.$$
For a generic equilibrium state, write n, p as functions only of the intrinsic density n_i, the a-dimensional potential V/U, and an integration constant. Write the equation satisfied by V.

(ii) Consider (1)–(4) in a bounded domain Ω with the following Dirichlet boundary conditions:
$$n = n_D, \quad p = p_D, \quad V = V_D \quad \text{on } \partial\Omega, \tag{5}$$
where n_D, p_D, V_D are given functions. Under the assumptions that the densities are in equilibrium (recall point (i)) on $\partial\Omega$ and the total space charge $n_D - p_D - C$ vanish on $\partial\Omega$, write n_D, p_D, V/U are functions only of C and n_i.

Exercise 2. Use the hints written at p. 21 of the lecture notes (about the Boltzmann equations) to derive the hydrodynamic model:

$$\partial_t n + \mathrm{div}(n\overline{v}) = 0, \tag{6}$$
$$\partial_t(n\overline{v}) + \mathrm{div}(n\overline{v}\otimes\overline{v}) + \frac{k_B}{m}\nabla(nT_e) + \frac{nqE}{m} = \int_{\mathbb{R}^3} vQ(f)dv, \tag{7}$$
$$\partial_t\mathcal{E} + \mathrm{div}\left(n\overline{v}\left(\frac{5}{2}k_B T_e + \frac{m|\overline{v}|^2}{2}\right)\right) + qn\overline{v}\cdot E = \int_{\mathbb{R}^3}\frac{m|v|^2}{2}Q(f)dv, \tag{8}$$

where n is the concentration, $\overline{v}$ is the velocity, $\mathcal{E} = n\left(\frac{m|\overline{v}|^2}{2} + \frac{3}{2}k_B T_e\right)$ is the energy density, T_e is the effective temperature.

Exercise 3. The so-called *low-density* collision operator $Q_\ell(f)$ is defined as

$$Q_\ell(f)(v) = \frac{1}{\tau(x)}\left(\mathcal{M}\int_{\mathbb{R}^3} f(v')dv' - f(v)\right),$$

where $\tau(x) > 0$ is the relaxation time, $\mathcal{M}$ is the "global Maxwellian"

$$\mathcal{M}(v) = \left(\frac{m}{2\pi k_B T_L}\right)^{3/2} e^{-m|v|^2/2k_B T_L},$$

and $T_L > 0$ is the (constant) lattice temperature.

(i) Rewrite (6)–(8) with $Q = Q_\ell$.

(ii) Consider now the system of equations:

$$\partial_t n + \operatorname{div}(n\overline{v}) = 0, \tag{9}$$

$$\partial_t(n\overline{v}) + \operatorname{div}(n\overline{v}\otimes\overline{v}) + \frac{k_B}{m}\nabla(nT_e) + \frac{nqE}{m} = -\frac{n\overline{v}}{\tau_p}, \tag{10}$$

$$\partial_t\mathcal{E} + \operatorname{div}\left(n\overline{v}\left(\frac{5}{2}k_B T_e + \frac{m|\overline{v}|^2}{2}\right) - \kappa n T_e \nabla T_e\right) + qn\overline{v}\cdot E = -\frac{n}{\tau_e}\left(\frac{\mathcal{E}}{n} - \frac{3}{2}k_B T_L\right), \tag{11}$$

where τ_p, τ_e are ($x-$dependent) relaxation times for momentum and energy, respectively, and $\kappa = \kappa(x) > 0$ is the heat conductivity. How do (9)–(11) relate with (6)–(8)? Rewrite (9)–(11) in terms of the a-dimensional variables x_s, t_s, n_s, J_s, V_s, T_s defined as

$$x = \lambda x_s, \quad t = \tau t_s, \quad n = C_m n_s, \quad J = J_0 J_s, \quad V = UV_s, \quad T = T_L T_s,$$

where λ is the reference length (device diameter), C_m is the reference particle density, $U = k_B T_L/q$ is the reference potential, $J_0 = qC_M\lambda/\tau$ is the reference current density and $\tau = m^*\lambda/\tau_p k_B T_L$ is the reference time.

(iii) Define the a-dimensional parameters $\alpha = \tau_p/\tau$, $\beta = \tau_e/\tau$. Take the limit $\alpha \to 0$ in the scaled version of (9)–(11); this limit system is called (scaled) *energy-transport model*. If you take the limit $\beta \to 0$ in the scaled energy-transport model what do you obtain?

The exercises will be reviewed in class on January 18th, 2017.