Numerical and Asymptotic Analysis of Singularly Perturbed PDEs of Kinetic Theory

N. Parumasur, J. Banasiak and J.M. Kozakiewicz

University of KwaZulu-Natal, Durban, 4041, South Africa parumasurn1@ukzn.ac.za

1. Introduction

We consider the numerical solution of various equations occurring in kinetic theory. The numerical algorithm is applied in conjuction with a modified asymptotic procedure. Various mathematical derivations and numerical algorithms are provided for the following singularly perturbed models of kinetic theory

$$\partial_t u + \mathcal{A}u + \mathcal{S}u + \frac{1}{\varepsilon}\mathcal{C}u = 0 \tag{1}$$

where u is the particle distribution, ∂_t is the time derivative and the operators $\mathcal{A}$, $\mathcal{S}$, and $\mathcal{C}$ describe attenuation, streaming and collisions of particles, respectively. We begin by outlining the features of a modified asymptotic method [4, 1] which is quite useful when solving (1).

Let $\mathcal{P}$ be a bounded operator in the Banach space X having zero as its simple isolated eigenvalue and the corresponding eigenspace V. Then X can be expressed as a direct sum $X = V \oplus W$, where both V and W are invariant subspaces of the operator $\mathcal{C}$ and $\mathcal{C}$ is one-to-one from W onto itself. Let $\mathcal{P}$ be the spectral projection associated with the eigenvalue $\lambda = 0$ so that

$$V = \mathcal{P}X, \qquad W = \mathcal{Q}X,$$

where $\mathcal{Q} = \mathcal{I} - \mathcal{P}$ is the complementary projection. We use a projection method [4] to write (1) as a system of evolution equations in subspaces V and W. Applying the projections $\mathcal{P}$ and $\mathcal{Q}$ on both sides of (1), successively, we obtain

$$\begin{aligned} \partial_t v &= \mathcal{P}(\mathcal{A}+\mathcal{S})\mathcal{P}v + \mathcal{P}(\mathcal{A}+\mathcal{S})\mathcal{Q}w \\ \varepsilon\partial_t w &= \varepsilon\mathcal{Q}(\mathcal{A}+\mathcal{S})\mathcal{Q}w + \varepsilon\mathcal{Q}(\mathcal{S}+\mathcal{A})\mathcal{P}v + \mathcal{Q}\mathcal{C}\mathcal{Q}w, \end{aligned} \tag{2}$$

with the initial conditions

$$v(0) = \overset{o}{v},\ w(0) = \overset{o}{w},$$

where $\overset{o}{v} = \mathcal{P}\ \overset{o}{u}$, $\overset{o}{w} = \mathcal{Q}\ \overset{o}{u}$. Taking into account that the projected operators $\mathcal{PSP}$, $\mathcal{PAQ}$ and $\mathcal{QAP}$ vanish for most types of linear equations we obtain the following form of (2)

$$\begin{aligned} \partial_t v &= \mathcal{PAP}v + \mathcal{PSQ}w \\ \varepsilon\partial_t w &= \varepsilon\mathcal{QSP}v + \varepsilon\mathcal{QSQ}w + \varepsilon\mathcal{QAQ}w + \mathcal{QCQ}w \\ v(0) &= \overset{o}{v},\ w(0) = \overset{o}{w}, \end{aligned} \tag{3}$$

Next we apply the modified asymptotic approach to (3). We represent the solution of (3) as a sum of the bulk and the initial layer parts:

$$v(t) = \bar{v}(t) + \tilde{v}(\tau), \quad w(t) = \bar{w}(t) + \tilde{w}(\tau), \tag{4}$$

where the variable τ in the initial layer part is given by $\tau = t/\varepsilon$. The bulk solution will be considered as a function of ρ of order zero and the function $\bar{w}^{(N)}$ will be assumed to be of the form

$$\bar{w}^{(N)}(t) = \sum_{n=0}^{N} \varepsilon^n \mathcal{W}_n \rho(t), \tag{5}$$

where the superscript N indicates the order of the approximation and $\mathcal{W}$ are time-independent bounded linear operators from V to W. Substituting this expansion into the first equation in (3) yields

$$\partial_t \rho = \mathcal{PAP}\rho + \sum_{n=0}^{N} \varepsilon^n \mathcal{PSQ}(\mathcal{W}_n \rho). \tag{6}$$

Expressing the time derivative $\partial_t \rho$ in (6) in powers of ε and comparing terms of the same power in ε yields at first order

$$\mathcal{W}_0 = 0, \quad \mathcal{W}_1 = -(\mathcal{QCQ})^{-1}\mathcal{QSP}. \tag{7}$$

The operator $\mathcal{W}_1$ can be evaluated since $\mathcal{QCQ}$ is invertible on the subspace $\mathcal{W}$. Using (7) in (6) gives the equation

$$\partial_t \rho = \mathcal{PAP}\rho - \varepsilon\mathcal{PSQ}(\mathcal{QCQ})^{-1}\mathcal{QSP}\rho. \tag{8}$$

A similar procedure yields the initial layer terms

$$\tilde{v}_0(\tau) \equiv 0, \qquad \tilde{v}_1(\tau) = \mathcal{PSQ}(\mathcal{QCQ})^{-1} e^{\tau \mathcal{QCQ}}\ \overset{o}{w},$$

and the initial condition for (8)

$$\bar{v}(0) = \overset{o}{v}\ -\varepsilon\mathcal{PSQ}(\mathcal{QCQ})^{-1}\ \overset{o}{w}\ . \tag{9}$$

In our presentation we apply the procedure to a wide range of problems of kinetic theory. However due to limited space we only present the case of the linear Boltzmann equation of semiconductor theory. Further details are also available in the following [1],[3].

2. Linear Boltzmann Equation of Semiconductor Theory

Here we apply our numerical methods to the model [2]. Thus we consider the linear Boltzmann equation which describes time evolution of the spatially dependent electron distribution function $u(x, \mu, t)$ under the influence of spatially uniform constant electric field and use the scaling corresponding to a weak external field. Then the equation is of the form

$$\varepsilon \partial_t u(x,\mu,t) + \varepsilon\mu\partial_x u(x,\mu,t) + \varepsilon a \partial_\mu u(x,\mu,t) = -u(x,\mu,t) + m(\mu)\int_{-\infty}^{+\infty} u(x,\mu',t)d\mu' \qquad (10)$$

with the initial condition

$$u(x,\mu,0) = \overset{0}{u},$$

where $0 \le x \le 2\pi$, $\mu \in \mathbf{R}$, a is the acceleration due to the electric field, and

$$m(\mu) = \sqrt{\frac{\beta}{\pi}}\exp\left(-\beta\mu^2\right) \qquad (11)$$

is the Maxwellian distribution normalized to satisfy $\int_{-\infty}^{+\infty} m(\mu)\, d\mu = 1$. The parameter β is defined by $\beta = m/(2Tk)$, where T is the temperature of the background, m the mass of the particles and k the Boltzmann constant.

Equation (10) is considered in the space

$$\mathcal{X} = L_1(R \times R)$$

We assume periodic boundary conditions with respect to x to avoid the boundary layer effects. Dividing (10) by ε we get

$$\partial_t u(x,\mu,t) = -\mu\partial_x u(x,\mu,t) - a\partial_\mu u(x,\mu,t) - \frac{1}{\varepsilon}u(x,\mu,t) + \frac{1}{\varepsilon}m(\mu)\int_{-\infty}^{+\infty} u(x,\mu',t)d\mu'. \qquad (12)$$

It is clear from this formulation that the field is weaker than the scattering mechanism. Here

$$\mathcal{A}u(x,\mu) = 0,$$

the streaming operator is of the form

$$\mathcal{S}u(x,\mu) = -\mu\partial_x u(x,\mu) - a\partial_\mu u(x,\mu),$$

and the collision operator is given by

$$\mathcal{C}u(x,\mu) = -u(x,\mu) + m(\mu)\int_{-\infty}^{+\infty} u(x,\mu')d\mu'.$$

The zero-order approximation of the equation (10), obtained by putting $\varepsilon = 0$, is

$$-u(x,\mu) + m(\mu)\int_{-\infty}^{+\infty} u(x,\mu')d\mu' = \mathcal{C}u(x,\mu) = 0. \qquad (13)$$

A unique (up to a multiplicative constant) solution to this equation is the Maxwellian (11). Thus the hydrodynamic space is the eigenspace spanned by $m(\mu)$ and the projection operators are

$$\mathcal{P}u(x,\mu) = m(\mu)\int_{-\infty}^{+\infty} u(x,\mu')d\mu' = v(x,\mu) = m(\mu)c(x)$$

where $c(x) = \int_{-\infty}^{+\infty} u(x,\mu')d\mu'$ is the particle number density, and

$$\mathcal{Q}u(x,\mu) = u(x,\mu) - m(\mu)\int_{-\infty}^{+\infty} u(x,\mu')d\mu' = w(x,\mu).$$

Thus $\mathcal{C}$ can be written as

$$\mathcal{C}u = -u + \mathcal{P}u = -\mathcal{Q}u.$$

By applying the compressed method we are able to obtain the equation for diffusion approximation ρ.

First we derive the explicit forms of the operators involved. We have

$$\begin{aligned}
\mathcal{Q}\mathcal{S}\mathcal{P}v(x,\mu) &= \mathcal{Q}\mathcal{S}v(x,\mu) = \mathcal{Q}\mathcal{S}m(\mu)c(x) \\
&= \mathcal{Q}\left(-\mu\partial_x m(\mu)c(x) - a\partial_\mu m(\mu)c(x)\right) \\
&= \mathcal{Q}\left(-\mu m(\mu)\partial_x c(x) - ac(x)\partial_\mu m(\mu)\right) \\
&= -\mu m(\mu)\partial_x c(x) - ac(x)\partial_\mu m(\mu) \\
&\quad + \ m(\mu)\partial_x c(x)\int_{-\infty}^{+\infty}\mu m(\mu)\,d\mu + ac(x)\int_{-\infty}^{+\infty}\partial_\mu m(\mu)\,d\mu \\
&= -\mu m(\mu)\partial_x c(x) - ac(x)\partial_\mu m(\mu)
\end{aligned}$$

where the integrals vanish since $\mu m(\mu)$ and $\partial_\mu m(\mu)$ are odd functions.

Operator $\mathcal{Q}\mathcal{C}\mathcal{Q}$ is derived as follows. First

$$\mathcal{C}\mathcal{Q}u = -\mathcal{Q}\mathcal{Q}u = -\mathcal{Q}u,$$

as $\mathcal{Q}$ is a projection, and thus

$$\mathcal{Q}\mathcal{C}\mathcal{Q}u = \mathcal{Q}(-\mathcal{Q}u) = -\mathcal{Q}u = \mathcal{C}u.$$

To obtain $(\mathcal{Q}\mathcal{C}\mathcal{Q})^{-1}$ we solve the Fredholm equation

$$u(x,\mu) = m(\mu)\int_{-\infty}^{+\infty} u(x,\mu')\,d\mu' - f(x,\mu) \tag{14}$$

in QX, which is the same as

$$u = \mathcal{P}u - f. \tag{15}$$

If u is such that (15) is satisfied, then

$$\mathcal{Q}f = \mathcal{Q}(-u + \mathcal{P}u) = -u + \mathcal{P}u = f.$$

This is the solvability condition for (14). Hence

$$f - \mathcal{Q}f = \mathcal{P}f = 0.$$

We are looking for the solution satisfying u in the range of Q. Thus

$$u = \mathcal{Q}u$$

and

$$\mathcal{P}u = \mathcal{P}\mathcal{Q}u = 0$$

or, explicitly

$$m(\mu) \int_{-\infty}^{+\infty} u(x,\mu)\, d\mu = 0.$$

Thus

$$u = (\mathcal{Q}\mathcal{C}\mathcal{Q})^{-1} f = f$$

and

$$(\mathcal{Q}\mathcal{C}\mathcal{Q})^{-1}\mathcal{Q}\mathcal{S}\mathcal{P}\, v(x,\mu) = -\mu m(\mu)\partial_x c(x) - ac(x)\partial_\mu m(\mu).$$

Then

$$\begin{aligned}
& \mathcal{P}\mathcal{S}\mathcal{Q}(\mathcal{Q}\mathcal{C}\mathcal{Q})^{-1}\mathcal{Q}\mathcal{S}\mathcal{P}\, v(x,\mu) \\
= \;& \mathcal{P}\mathcal{S}\mathcal{Q}\, \left(-\mu m(\mu)\partial_x c(x) - ac(x)\partial_\mu m(\mu)\right) \\
= \;& \mathcal{P}\mathcal{S}\left[-\mu m(\mu)\partial_x c(x) - ac(x)\partial_\mu m(\mu) + m(\mu)\partial_x c(x)\int_{-\infty}^{+\infty} \mu' m(\mu') d\mu'\right. \\
& \left. +\; ac(x)m(\mu)\int_{-\infty}^{+\infty} \partial_{\mu'} m(\mu') d\mu'\right] \\
= \;& \mathcal{P}\mathcal{S}\, \left(-\mu m(\mu)\partial_x c(x) - ac(x)\partial_\mu m(\mu)\right) \\
= \;& \mathcal{P}\left[\mu^2 \partial_{xx}^2 c(x) m(\mu) + a\mu\partial_x c(x)\partial_\mu m(\mu) + a^2 \partial_x c(x)\partial_\mu(\mu m(\mu)) + a^2 c(x)\partial_{\mu\mu}^2 m(\mu)\right] \\
= \;& m(\mu)\left[\partial_{xx}^2 c(x)\int_{-\infty}^{+\infty} \mu^2 m(\mu)\, d\mu + a\partial_x c(x)\int_{-\infty}^{+\infty} \mu\partial_\mu m(\mu)\, d\mu\right. \\
& \left. +\; a^2 c(x)\int_{-\infty}^{+\infty} \partial_\mu(\mu m(\mu))\, d\mu\right] \\
= \;& m(\mu)\left[\frac{1}{2\beta}\partial_{xx}^2 c(x) - a\partial_x c(x)\int_{-\infty}^{+\infty} m(\mu)\, d\mu\right] \\
= \;& m(\mu)\left[\frac{1}{2\beta}\partial_{xx}^2 c(x) - a\partial_x c(x)\right].
\end{aligned}$$

where we used $\int_{-\infty}^{+\infty} \partial_\mu(\mu m(\mu))\, d\mu = 0$ since $\mu m(\mu) \to 0$ as $\mu \to \pm\infty$.

Thus we obtain the diffusion approximating equation

$$\partial_t \rho = -\varepsilon \mathcal{P}\mathcal{S}\mathcal{Q}(\mathcal{Q}\mathcal{C}\mathcal{Q})^{-1}\mathcal{Q}\mathcal{S}\mathcal{P}\rho = \varepsilon m(\mu)\left(\frac{1}{2\beta}\partial_{xx}^2 \rho - a\partial_x \rho\right). \tag{16}$$

or dropping the Maxwellian $m(\mu)$, to obtain the scalar density.

$$\partial_t c(x,t) = \varepsilon \left(\frac{1}{2\beta} \partial_{xx}^2 c(x,t) - a \partial_x c(x,t) \right). \tag{17}$$

To find the corrected initial condition

$$\bar{\rho}(0) = \overset{0}{v} - \varepsilon \mathcal{PSQ} (\mathcal{QCQ})^{-1} \overset{0}{w},$$

we begin with finding

$$\begin{aligned}
& \mathcal{PSQ} (\mathcal{QCQ})^{-1} \overset{0}{w} \\
= \; & \mathcal{PSQ} \overset{0}{w} = \mathcal{PSQ} (\mathcal{Q} \overset{0}{u}) = \mathcal{PS} \left(\overset{0}{u} - m(\mu) \int_{-\infty}^{+\infty} \overset{0}{u} (x,\mu') \, d\mu' \right) \\
= \; & \mathcal{P} \left(-\mu \partial_x \overset{0}{u} (x,\mu) + \mu \partial_x m(\mu) \int_{-\infty}^{+\infty} \overset{0}{u} (x,\mu') \, d\mu' - a \partial_\mu \overset{0}{u} (x,\mu) \right. \\
& \left. + \; a \partial_\mu m(\mu) \int_{-\infty}^{+\infty} \overset{0}{u} (x,\mu') \, d\mu' \right) \\
= \; & \mathcal{P} \left[-\mu \partial_x \overset{0}{u} (x,\mu) + \mu m(\mu) \partial_x \int_{-\infty}^{+\infty} \overset{0}{u} (x,\mu') \, d\mu' - a \partial_\mu \overset{0}{u} (x,\mu) \right. \\
& \left. + \left(a \int_{-\infty}^{+\infty} \overset{0}{u} (x,\mu') \, d\mu' \right) \partial_\mu m(\mu) \right] \\
= \; & m(\mu) \int_{-\infty}^{+\infty} \left[- \int_{-\infty}^{+\infty} \mu \partial_x \overset{0}{u} (x,\mu) \, d\mu + \partial_x \int_{-\infty}^{+\infty} \overset{0}{u} (x,\mu') \, d\mu' \int_{-\infty}^{+\infty} \mu m(\mu) \, d\mu \right. \\
& \left. - \; a \int_{-\infty}^{+\infty} \partial_\mu \overset{0}{u} (x,\mu) \, d\mu + a \int_{-\infty}^{+\infty} \overset{0}{u} (x,\mu') \, d\mu' \int_{-\infty}^{+\infty} \partial_\mu m(\mu) \, d\mu \right] d\mu \\
= \; & -m(\mu) \int_{-\infty}^{+\infty} \mu \partial_x \overset{0}{u} (x,\mu) \, d\mu,
\end{aligned}$$

since as before $\int_{-\infty}^{+\infty} \mu m(\mu) = 0$, and also $\int_{-\infty}^{+\infty} \partial_\mu m(\mu) \, d\mu = 0$ $\int_{-\infty}^{+\infty} \partial_\mu \overset{0}{u} (x,\mu) \, d\mu = 0$ (under assumption that $\overset{0}{u} (x,\mu)$ goes to zero as $\mu \to \pm\infty$).

Thus

$$\bar{\rho}(0) = \overset{0}{v} (x) - \varepsilon m(\mu) \int_{-\infty}^{+\infty} \mu \partial_x \overset{0}{u} (x,\mu) \, d\mu$$

or

$$c(x,0) = c_0(x) - \varepsilon \int_{-\infty}^{+\infty} \mu \partial_x \overset{0}{u} (x,\mu) \, d\mu,$$

where $c_0(x) = \int_{-\infty}^{+\infty} \overset{0}{u} (x,\mu') d\mu'$ so that $\overset{0}{v} = m(\mu) c_0(x)$ and $\overset{0}{w} = \overset{0}{u} (x,\mu) - m(\mu) c_0(x)$.

Using the operators derived above we can find the formula for the initial layer corrector

$$\tilde{v}(x,\tau) = \mathcal{PSQ} (\mathcal{QCQ})^{-1} e^{\tau \mathcal{QCQ}} \overset{0}{w} (x,\mu) = e^{-\tau} m(\mu) \int_{-\infty}^{+\infty} \mu \partial_x \overset{0}{u} (x,\mu) \, d\mu.$$

For calculations the initial condition for the distribution function was

$$\overset{0}{u} (x,\mu) \; = f_0(\mu)(1 + A \sin x), \tag{18}$$

where $A \leq 1$ and the function f_0 satisfied

$$\int_{-\infty}^{+\infty} f_0(\mu)d\mu = 1 \quad \texttt{and} \quad \int_{-\infty}^{+\infty} \mu f_0(\mu)d\mu = s_0 \neq 0. \tag{19}$$

The last condition above ensures that this is a non-equilibrium initial value.
In particular, for the results presented below we have taken

$$f_0(\mu) = \begin{cases} 1 & for \quad 0 \leq \mu \leq 1 \\ 0 & for \quad other\, \mu \end{cases}$$

thus $s_0 = 0.5$ and we took $a = 0.6$, $A = 1/2$.
This gives the initial number density

$$c_0(x) = 1 + A \sin x, \tag{20}$$

and thus the corrected initial condition of the diffusion equation is

$$c(x, 0) = 1 + A \sin x - A\varepsilon s_0 \cos x \tag{21}$$

and the initial layer corrector is given by

$$\tilde{v}(x, \tau) = A s_0 m(\mu) e^{-\tau} \cos x, \tag{22}$$

where $\tau = t/\varepsilon$.

The sequence of calculations for the numerical results are as follows. First, we applied uncorrected initial condition to the diffusion approximation

$$\hat{c}(x, 0) = 1 + A \sin x; \tag{23}$$

then the error is given by

$$E = \int_0^1 |c(x, t) - \hat{c}(x, t)|\, dx. \tag{24}$$

Next, we applied the corrected initial value $c(x, 0)$ from (21), in which case the diffusion approximation yields the following error:

$$E_{IC} = \int_0^1 |c(x, t) - \bar{c}(x, t)|\, dx. \tag{25}$$

Next, we used the initial layer corrector (22) instead of the initial value corrector (21), and the resulting error, evaluated according to the formula

$$E_{IL} = \int_0^1 |c(x, t) - (\hat{c}(x, t) + \tilde{v}(x, t/\varepsilon)|\, dx \tag{26}$$

Table 1: Boltzmann equation of semiconductor theory: errors in diffusion approximation, $\varepsilon = 0.01$.

t	E	E_{IC}	E_{IL}	E_{ICIL}
0	2.2029e-016	5.0057e-002	5.0057e-002	2.2029e-016
1.0000e-003	7.2219e-004	4.9341e-002	4.9781e-002	2.9635e-004
5.0000e-003	3.4750e-003	4.6615e-002	4.8729e-002	1.4326e-003
5.0000e-002	2.3503e-002	2.7629e-002	4.1576e-002	1.0304e-002
5.0000e-001	5.9060e-002	4.8396e-002	5.9061e-002	4.8396e-002

is given in the table.

Finally, the error for the approximation with both correctors applied is evaluated according to the formula

$$E_{ICIL} = \int_0^1 |c(x,t) - [\bar{c}(x,t) + \tilde{v}(x,t/\varepsilon)]| \, dx. \tag{27}$$

The table gives the results for the calculations with $\varepsilon = 0.01$. It is observed that the best approximation is when we combine both correctors and the worst when we use only the initial layer corrector.

References

[1] J. Banasiak, J. Kozakiewicz, N. Parumasur, *Diffusion Approximation of Linear Kinetic Equations with Non-equilibrium Data – Computational Experiments*, Transport Theory Statist. Phys, **34**, (2005).

[2] L. Demeio and G. Frosali, *Diffusion Approximations of the Boltzmann Equation: Comparison results for linear model problems*, Atti Sem.Mat.Fis.Univ.Modena, Vol. XLVI (1998) 653-675.

[3] J. Kozakiewicz, *Singularly Perturbed Evolution Equations with Applications to Kinetic Theory - Analytical Methods and Numerical Investigations*, PhD thesis, University of KwaZulu-Natal, (2006).

[4] J. R. Mika, *New asymptotic expansion algorithm for singularly perturbed evolution equations*, Math. Methods Appl. Sci. **3** (1981) 172-188.