Transition Regime Models from Kinetic Equations

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Introduction

Traditionally kinetic equations are solved numerically either by particle methods, such as Monte Carlo (MC) or molecular dynamics (MD) methods, or by finite difference, finite element, or finite volume methods (FXMs). All of these methods become inefficient in regimes where collisions dominate, so-called small mean-free-path regimes, because kinetic equations become stiff.

In such regimes collisions typically drive the underlying kinetic densities toward local equilibria. This fact allows solutions of the kinetic equation to be approximated by solutions of a reduced system, typically a diffusion equation or a fluid dynamical system, that then can be solved efficiently by classical numerical methods.

Transition Regimes

The most difficult regimes to simulate are the so-called transition regimes. In these collisions are plentiful enough to make the full kinetic equation fairly stiff and expensive to solve, but are not plentiful enough to drive the underlying kinetic densities too close to local eqilibria.

Such regimes often arise in photon transport where there can be optically thin and optically thick regions in a given problem. In fact, the same point in a spatial domain can be optically thin to some frequencies of light while being optically thick to others.

Transition Regime Models

Transition regime models must be designed to bridge the gap between small mean-free-paths regimes in which traditional reduced models are accurate, and large mean-free-paths regimes in which kinetic equations can be solved efficiently by traditional numerical methods. They should:

- be able to recover traditional reduced models derived for small mean-free-path regimes;
- be more accurate than the reduced models in transition regimes, where the reduced models typically fail badly;
- be solved more efficiently than the full kinetic equation.

Uses of Transition Regime Models

Such a model can then be used either:

- as a stand-alone model for problems that lie completely within the transition regime,
- as a matching model between small mean-free-path regimes and large mean-free-path regimes in a hybrid simulation,
- as a preconditioner in a full transport simulation.

Two Traditional Approaches

Two long-standing approaches to systematically deriving transition regime models are moment closures and Chapman-Enskog expansions. Both these approaches have well-known shortcomings.

Moment closures yield large hyperbolic systems with relaxation terms that become stiff wherever in the diffusive regime, all of which increases their cost and complexity of their numerical implementation.

Beyond the first two in the sequence, Chapman-Enskog expansions generally yield equations that do not dissipate properly, that are not consistent with the stationary equation, or that are even ill-posed.

Both these approaches are usually presented so as to yield interior equations first, and treat the formulation of boundary conditions separately. They both typically fail to yield equations with an entropy.

Guiding Viewpoints

This talk will survey some recent advances in the development of transition regime models.

The approach advocated here adopts the guiding viewpoint that in a transition regime the particle density, while not necessarily in a local equilibrium, takes a form governed by balances in the kinetic equation rather than a form dominated by either boundary or initial conditions (except near the boundaries or the initial time).

It also adopts the viewpoint that expansions should not be the central tool for deriving transition regime models. Rather, expansions should be used to refine the approximations one makes within a larger framework that preserves the key structural features of the kinetic equation.

Framework

For linear kinetic equations we present a framework that has three components:

- either the stationary balance or the quasistationary balance temporal approximation,
- the small-gradient expansion as an interior spatial approximation,
- a natural framework for developing boundary conditions.

The resulting models share elements with both traditional moment closures and expansions. They will be formally well-posed, capture a correct stationary asymptotics, and properly dissipate.

Monoenergetic Photon Transport

We will illustrate our key ideas in the context of monoenergetic, photon transport through a stationary, isotropic medium that scatters, absorbs, and emits as a blackbody. The photon kinetic density $F = F(\omega, x, t)$ is a function of the direction $\omega \in \mathbb{S}^{D-1}$, the position $x \in \mathbb{R}^D$, and time t. It is governed by the transport equation

$$\partial_t F + \omega \cdot \nabla_x F + \kappa F - \mathcal{K}^S F = \kappa^A b\,. \tag{1}$$

Here the speed of light is set to 1; $b = b(x) > 0$ is the black-body emission; $\kappa^A = \kappa^A(x) > 0$ is the absorption coefficient; $\mathcal{K}^S = \mathcal{K}^S(x)$ is the scattering operator.

Scattering and Interaction

Here the scattering operator $\mathcal{K}^S = \mathcal{K}^S(x)$ is given by

$$\mathcal{K}^S(x) F(\omega, x, t) = \frac{1}{|\mathbb{S}^{D-1}|} \int_{\mathbb{S}^{D-1}} K^S(\omega \cdot \omega', x)\, F(\omega', x, t)\, \mathrm{d}\omega' \,, \quad (2)$$

where $K^S(\omega \cdot \omega', x) > 0$ is the scattering redistribution kernel; and $\kappa = \kappa(x)$ is the total interaction coefficient, which is given by

$$\kappa(x) = \kappa^A(x) + \frac{1}{|\mathbb{S}^{D-1}|} \int_{\mathbb{S}^{D-1}} K^S(\omega \cdot \omega', x)\, \mathrm{d}\omega \,. \quad (3)$$

Initial and Boundary Conditions

We consider the transport equation (1) to be posed over a domain $X \subset \mathbb{R}^D$. It must be supplemented by the initial condition,

$$F(\omega, x, 0) = F^{in}(\omega, x)\,, \tag{4}$$

and the boundary conditions

$$F(\omega, x, t) = F_B(\omega, x, t)\,, \quad \text{for } x \in \partial X \text{ and } \nu(x) \cdot \omega < 0\,. \tag{5}$$

Here $\nu(x)$ denotes the outward normal unit vector at the boundary point x, and $F_B(\omega, x, t)$ prescribes the density of incoming photons at the boundary point x.

Rotational Invariance

The fact that emission, absorption, and scattering are rotationally invariant processes in a stationary, isotropic medium implies that the emission b, the absorption coefficient κ^A, and the total interaction coefficient κ are independent of ω. It also implies that for each x the spherical harmonic tensors $Y^m(\omega)$ are eigenfunctions of scattering operator $\mathcal{K}^S(x)$.

We introduce the so-called total interaction operator $\mathcal{K}(x)$ by

$$\mathcal{K}F = \kappa F - \mathcal{K}^S F\,. \tag{6}$$

The spherical harmonic tensors are eigenfunctions of $\mathcal{K}(x)$ with

$$\mathcal{K}(x)Y^m = \kappa_m(x)Y^m\,. \tag{7}$$

Here $\kappa_0 = \kappa^A$ and $\kappa^A < \kappa_m \leq \kappa$ for $m \geq 1$.

Classical Diffusion Approximation

The classical reduced model for the transport equation is the diffusion equation

$$\partial_t \rho - \tfrac{1}{D} \nabla_x \cdot \left[\frac{1}{\kappa_1} \nabla_x \rho \right] + \kappa^A \rho = \kappa^A \beta \,,$$

where

$$\rho(x,t) = \langle F \rangle = \frac{1}{|\mathbb{S}^{D-1}|} \int F(\omega, x, t) \, \mathrm{d}\omega \,.$$

This is best derived through a matched asymptotic analysis that leads to boundary conditions of the form

$$\rho + \frac{\lambda}{\kappa_1} \nu \cdot \nabla_x \rho = \beta_B \,,$$

where ν is the outward unit normal of the domain boundary.

Expansion in Spherical Harmonics

Define the m^{th} order moment of F by

$$\begin{aligned}\rho^m(x,t) &= \langle Y^m(\,\cdot\,)\, F(\,\cdot\,,x,t)\rangle \\ &= \frac{1}{|\mathbb{S}^{D-1}|}\int_{\mathbb{S}^{D-1}} Y^m(\omega)\, F(\omega,x,t)\,\mathrm{d}\omega\,.\end{aligned}$$

This is a symmetric traceless m^{th} order tensor. One can show that

$$F(\omega) = \rho + \sum_{m=1}^{\infty} \frac{D(D+2)\cdots(D+2m-2)}{m!}\, Y^m(\omega)\cdot\rho^m\,,$$

Spherical Harmonic Tensors

Recall the first six spherical harmonic tensors are

$$
\begin{aligned}
Y^0(\omega) &= 1\,, \\
Y^1(\omega) &= \omega\,, \\
Y^2(\omega) &= \omega^{\vee 2} - \tfrac{1}{D}\,\delta\,, \\
Y^3(\omega) &= \omega^{\vee 3} - \tfrac{3}{D+2}\,\delta \vee \omega\,, \\
Y^4(\omega) &= \omega^{\vee 4} - \tfrac{6}{D+4}\,\delta \vee \omega^{\vee 2} + \tfrac{3}{(D+4)(D+2)}\,\delta^{\vee 2}\,, \\
Y^5(\omega) &= \omega^{\vee 5} - \tfrac{10}{D+6}\,\delta \vee \omega^{\vee 3} + \tfrac{15}{(D+6)(D+4)}\,\delta^{\vee 2} \vee \omega\,,
\end{aligned}
$$

Here δ denotes the metric tensor, $\vee$ denotes the symmetric tensor product, and $\Omega^{\vee k}$ denotes the k-fold symmetric tensor product of a tensor Ω with itself (so that $\delta^{\vee 2} = \delta \vee \delta$ and $\omega^{\vee 3} = \omega \vee \omega \vee \omega$).

Classical Moment Equations

The zeroth moment of the transport equation is

$$\partial_t \rho + \nabla_x \cdot \rho^1 + \kappa^A \rho = \kappa^A \beta \,,$$

where $\rho = \rho^0$, while the m^{th} moment for $m \geq 1$ is

$$\partial_t \rho^m + \nabla_x \cdot \langle \omega \, Y^m(\omega) \, F \rangle + \langle Y^m(\omega) \, \mathcal{K} F \rangle = 0 \,.$$

Evaluating the divergence and interaction terms above leads to

$$\partial_t \rho^m + \nabla_x \cdot \rho^{m+1} + \frac{m}{D+2m-2} \Big[\nabla_x \vee \rho^{m-1} - \frac{m-1}{D+2m-4} \delta \vee (\nabla_x \cdot \rho^{m-1}) \Big] + \kappa_m \rho^m = 0 \,.$$

Moment Equations

More explicitly, for $m = 1$ through $m = 4$ these equations are

$$\partial_t \rho^1 + \nabla_x \cdot \rho^2 + \tfrac{1}{D} \nabla_x \rho + \kappa_1 \rho^1 = 0\,,$$

$$\partial_t \rho^2 + \nabla_x \cdot \rho^3 + \tfrac{2}{D+2} \Big[\nabla_x \vee \rho^1 - \tfrac{1}{D} \delta \, (\nabla_x \cdot \rho^1) \Big] + \kappa_2 \rho^2 = 0\,,$$

$$\partial_t \rho^3 + \nabla_x \cdot \rho^4 + \tfrac{3}{D+4} \Big[\nabla_x \vee \rho^2 - \tfrac{2}{D+2} \delta \vee (\nabla_x \cdot \rho^2) \Big] + \kappa_3 \rho^3 = 0\,,$$

$$\partial_t \rho^4 + \nabla_x \cdot \rho^5 + \tfrac{4}{D+6} \Big[\nabla_x \vee \rho^3 - \tfrac{3}{D+4} \delta \vee (\nabla_x \cdot \rho^3) \Big] + \kappa_4 \rho^4 = 0\,.$$

Spherical Harmonic Moment Closures

The P-n moment closure retains the moment equations through order n and sets $\rho^m = 0$ for every $m > n$. Traditionally one takes n to be odd. The P-1 closure yields the system

$$\begin{aligned} \partial_t \rho + \nabla_x \cdot \rho^1 + \kappa^A \rho &= \kappa^A \beta \,, \\ \partial_t \rho^1 + \tfrac{1}{D} \nabla_x \rho + \kappa_1 \rho^1 &= 0 \,, \end{aligned}$$

while the P-3 closure yields the system

$$\begin{aligned} \partial_t \rho + \nabla_x \cdot \rho^1 + \kappa^A \rho &= \kappa^A \beta \,, \\ \partial_t \rho^1 + \nabla_x \cdot \rho^2 + \tfrac{1}{D} \nabla_x \rho + \kappa_1 \rho^1 &= 0 \,, \\ \partial_t \rho^2 + \nabla_x \cdot \rho^3 + \tfrac{2}{D+2} \Big[\nabla_x \vee \rho^1 - \tfrac{1}{D} \delta \left(\nabla_x \cdot \rho^1 \right) \Big] + \kappa_2 \rho^2 &= 0 \,, \\ \partial_t \rho^3 + \tfrac{3}{D+4} \Big[\nabla_x \vee \rho^2 - \tfrac{2}{D+2} \delta \vee \left(\nabla_x \cdot \rho^2 \right) \Big] + \kappa_3 \rho^3 &= 0 \,. \end{aligned}$$

When $D = 3$ there are $(n+1)^2$ equations in the P-n system.

Boundary Conditions

The reason n is traditionally taken to be odd when making the P-n closure is that for those cases boundary conditions have been developed that give satisfactory results. One example is the Marshak boundary conditions for $n = 2l + 1$, which are obtained by taking moments of boundary condition (5) of the form

$$\int_{\nu\cdot\omega<0} |\nu\cdot\omega|\, Y^{2k}(\omega)\, F^n(\omega,x,t)\, \mathrm{d}\omega = \int_{\nu\cdot\omega<0} |\nu\cdot\omega|\, Y^{2k}(\omega)\, F_B(\omega,x,t)\, \mathrm{d}\omega\,,$$

for $k = 0, \cdots, l$, where $F^n(\omega,x,t)$ is the P-n approximate

$$F^n(\omega,x,t) = \rho + \sum_{m=1}^{n} \frac{D(D+2)\cdots(D+2m-2)}{m!}\, Y^m(\omega)\cdot\rho^m\,.$$

Temporal Approximations: General Setting

We consider a setting of linear kinetic equations for densities F that belong to a Hilbert space $\mathbb{H}$ whose inner product is denoted $(\cdot\,|\,\cdot)_{\mathbb{H}}$. More specifically, we consider kinetic equations that fall into the abstract form

$$\partial_t F + \mathcal{L}F = B\,, \qquad F(0) = F^{in}\,, \tag{8}$$

where $\mathcal{L}$ is a densely defined, closed linear operator over $\mathbb{H}$ with domain $\mathrm{Dom}(\mathcal{L})$ such that

$$(G\,|\,\mathcal{L}\,G)_{\mathbb{H}} \geq 0 \qquad \text{for every } G \in \mathrm{Dom}(\mathcal{L})\,, \tag{9}$$

while $B \in C([0,\infty);\mathbb{H})$ and $F^{in} \in \mathbb{H}$. We assume moreover that $B(t) \in \mathrm{Range}(\mathcal{L})$ for every $t > 0$.

Reduced Description

We will develop reduced models for f that belong to a "smaller" Hilbert space $\mathbb{M}$ with inner product $(\cdot\,|\,\cdot)_{\mathbb{M}}$. We think of f as moments of the kinetic density F. We therefore *assume* that there is a bounded linear operator $\mathcal{M} : \mathbb{H} \to \mathbb{M}$ such that

$$\mathcal{M}\mathcal{M}^T : \mathbb{M} \to \mathbb{M} \text{ is positive definite}. \tag{10}$$

Here the bounded linear operator $\mathcal{M}^T : \mathbb{M} \to \mathbb{H}$ is the adjoint of $\mathcal{M}$. Our assumption implies that $\mathcal{M}\mathcal{M}^T$ has a bounded inverse. We define the bounded linear operator $\mathcal{E} : \mathbb{M} \to \mathbb{H}$ by

$$\mathcal{E} = \mathcal{M}^T(\mathcal{M}\mathcal{M}^T)^{-1}\,. \tag{11}$$

One sees that

$$\mathcal{M}\mathcal{E} = \mathcal{I}\,, \quad \text{and} \quad \mathcal{E}^T\mathcal{E} = (\mathcal{M}\mathcal{M}^T)^{-1} \text{ is positive definite}. \tag{12}$$

Here $\mathcal{I}$ denotes the identity (on $\mathbb{M}$) while $\mathcal{E}^T$ denotes the adjoint of $\mathcal{E}$.

Orthogonal Projections

It follows from (10-12) that $\mathrm{Range}(\mathcal{E})$, the range of $\mathcal{E}$, is a closed linear subspace of $\mathbb{H}$, and that $\mathcal{P} = \mathcal{E}\mathcal{M}$ is the orthogonal projection of $\mathbb{H}$ onto $\mathrm{Range}(\mathcal{E})$.

Let $\widetilde{\mathbb{H}}$ denote the orthogonal complement of $\mathrm{Range}(\mathcal{E})$. Then $\widetilde{\mathcal{P}} = \mathcal{I} - \mathcal{P}$ is the orthogonal projection of $\mathbb{H}$ onto $\widetilde{\mathbb{H}}$.

We orthogonally decompose F and B as

$$\begin{aligned} F &= \mathcal{E}f + \widetilde{F}\,, \quad \text{where} \quad f = \mathcal{M}F\,, \\ B &= \mathcal{E}b + \widetilde{B}\,, \quad \text{where} \quad b = \mathcal{M}B\,. \end{aligned} \tag{13}$$

Clearly, $\mathcal{E}f$ and $\mathcal{E}b$ are in $\mathrm{Range}(\mathcal{E})$ while $\widetilde{F}$ and $\widetilde{B}$ are in $\widetilde{\mathbb{H}}$.

Example: Photon Transport

In the context of the monoenergetic, photon transport equation we identify the space $\mathbb{H}$ as $\mathsf{L}^2(\mathrm{d}\omega\,\mathrm{d}x)$, the operator $\mathcal{M}$ as the mapping from F to a subset of its moments,

$$f = \mathcal{M}F = \left(\rho, \rho^1, \cdots, \rho^n\right),$$

the space $\mathbb{M}$ as $\mathsf{L}^2(\mathrm{d}x; \mathcal{T}^n)$ with

$$\left(f \,|\, g\right)_{\mathbb{M}} = \rho^0 \cdot \gamma^0 + \sum_{m=1}^{n} \frac{D(D+2)\cdots(D+2m-2)}{m!}\, \rho^m \cdot \gamma^m \,,$$

and $\mathcal{E}$ as the spherical harmonic expansion associated with f,

$$\mathcal{E}f = \rho + \sum_{m=1}^{n} \frac{D(D+2)\cdots(D+2m-2)}{m!}\, \mathrm{Y}^m(\omega) \cdot \rho^m \,.$$

Then $\mathcal{E}f = \mathcal{P}F = F^n$ is the P-n approximate to F, while $\widetilde{F} = \widetilde{\mathcal{P}}F = F - F^n$.

Decomposition of the Dynamics

Equation (8) then decomposes as

$$\partial_t f + \mathcal{M}\mathcal{L}\mathcal{E} f + \mathcal{M}\mathcal{L}\widetilde{F} = b\,, \qquad f(0) = f^{in}\,, \tag{14}$$

$$\partial_t \widetilde{F} + \widetilde{\mathcal{L}}\widetilde{F} + \widetilde{\mathcal{P}}\mathcal{L}\mathcal{E} f = \widetilde{B}\,, \qquad \widetilde{F}(0) = \widetilde{F}^{in}\,, \tag{15}$$

where $\widetilde{\mathcal{L}} = \widetilde{\mathcal{P}}\mathcal{L}\widetilde{\mathcal{P}}$ is a restriction of $\mathcal{L}$ to $\widetilde{\mathbb{H}}$. The initial data above are obtained from F^{in} by

$$f^{in} = \mathcal{M}F^{in}\,, \qquad \widetilde{F}^{in} = \widetilde{\mathcal{P}}F^{in}\,. \tag{16}$$

We think of $\mathcal{E}f$ as the moment expansion of F and of $\widetilde{F}$ as the deviation of F from $\mathrm{Range}(\mathcal{E})$. We will therefore refer to (14) as the moment equation and to (15) as the deviation equation.

Truncation Closure

We obtain the so-called *truncation closure* by setting $\widetilde{F} = 0$ in (14), which formally yields the reduced model

$$\partial_t f + \mathcal{M}\mathcal{L}\mathcal{E} f = b\,, \qquad f(0) = f^{in}\,. \tag{17}$$

This seems to be the simplest closure one can make. When we think of $\mathcal{E}$ as an expansion in terms of linearly independent polynomials then this closure is just the associated Galerkin approximation. This is the most common way in which moment equations have been closed. The P-n closure has this form.

Local Temporal Approximations

In order to improve upon the truncation closure we must find better approximations for $\widetilde{F}$. Recall that our guiding viewpoint, we seek temporal approximations that are local in time — in other words, that have no memory.

The picture of what has to be done becomes clearer upon solving the deviation equation (15) for $\widetilde{F}$ in terms of f and $\widetilde{B}$, and substituting the result into the moment equation (14). The solution $\widetilde{F}$ of the deviation equation can be expressed in terms of $\widetilde{\mathcal{S}}(t)$, the contraction semigroup over $\widetilde{\mathbb{H}}$ generated by $-\widetilde{\mathcal{L}}$, as

$$\widetilde{F}(t) = \widetilde{\mathcal{S}}(t)\widetilde{F}^{in} + \int_0^t \widetilde{\mathcal{S}}(t-t')\Big(\widetilde{B}(t') - \widetilde{\mathcal{P}}\mathcal{L}\mathcal{E}f(t')\Big)\,\mathrm{d}t' \qquad (18)$$

Master Equation

We then make the change of variables $t' \mapsto t - t'$ in the above time integral and substitute the result into the moment equation (14) to obtain the master equation

$$\begin{aligned} &\partial_t f + \mathcal{M}\mathcal{L}\mathcal{E} f - \mathcal{M}\mathcal{L}\int_0^t \widetilde{\mathcal{S}}(t')\widetilde{\mathcal{P}}\mathcal{L}\mathcal{E} f(t-t')\,\mathrm{d}t' \\ &\qquad = b - \mathcal{M}\mathcal{L}\int_0^t \widetilde{\mathcal{S}}(t')\widetilde{B}(t-t')\,\mathrm{d}t' - \mathcal{M}\mathcal{L}\widetilde{\mathcal{S}}(t)\widetilde{F}^{in}\,, \\ &f(0) = f^{in}\,. \end{aligned} \tag{19}$$

We now wish to identify approximations in which the terms involving time integrals above are replaced by terms that only depend locally on t and in which the term involving $\widetilde{F}^{in}$ can be dropped.

Stiffness Assumption

In order to justify such approximations we *assume* that $\mathcal{E}$ has been chosen so that

$$\left(\tilde{G} \,|\, \tilde{\mathcal{L}}\tilde{G}\right)_{\mathbb{H}} \geq \frac{1}{T}\,\|\tilde{G}\|_{\mathbb{H}}^2 \quad \text{for every } \tilde{G} \in \mathrm{Dom}(\tilde{\mathcal{L}})\,, \tag{20}$$

where T be a timescale over which $\tilde{B}(t)$ does not vary significantly and over which $f(t)$ does not vary significantly, except possibly after an initial layer.

The bound (20) implies that the semigroup $\tilde{\mathcal{S}}$ satisfies

$$\left\|\tilde{\mathcal{S}}(t)\tilde{G}\right\|_{\mathbb{H}} \leq e^{-t/T}\|\tilde{G}\|_{\mathbb{H}} \quad \text{for every } \tilde{G} \in \tilde{\mathbb{H}}\,. \tag{21}$$

Laplace's Approximation

Because $\widetilde{\mathcal{S}}(t)$ decays to zero over the timescale T, we may therefore drop the term in (19) involving $\widetilde{F}^{in}$ outside an initially layer of order T. Moreover, because we have assumed $f(t)$ and $\widetilde{B}(t)$ do not vary significantly over the timescale T, we may therefore localize the time integrals in (19) by using Taylor approximations obtained by truncating the expansions

$$\begin{aligned} f(t-t') &\sim f(t) - t'\partial_t f(t) + t'^2 \partial_t^2 f(t) - \cdots . \\ \widetilde{B}(t-t') &\sim \widetilde{B}(t) - t'\partial_t \widetilde{B}(t) + t'^2 \partial_t^2 \widetilde{B}(t) - \cdots . \end{aligned} \tag{22}$$

These are essentially the Laplace approximations of the time integrals in (19).

First Order Evolution

We will moreover require the resulting approximate evolution equation for f to be first order. This last requirement is based in part on the feeling that any regime described by an approximation that leads to a higher order equation can probably be described better by an approximation for a larger collection of moments that leads to a first order system. This means we will only consider the zeroth-order Taylor approximation

$$f(t-t') \approx f(t)\,, \qquad \widetilde{B}(t-t') \approx \widetilde{B}(t)\,, \tag{23}$$

and the first-order Taylor approximation

$$f(t-t') \approx f(t) - t'\partial_t f(t)\,, \quad \widetilde{B}(t-t') \approx \widetilde{B}(t) - t'\partial_t \widetilde{B}(t)\,. \tag{24}$$

The first of these we dub the *stationary balance approximation* and study below. The second of these we dub the *quasistationary balance approximation*.

Stationary Balance Approximation

We use the zeroth-order Taylor approximation (23) to approximate $\widetilde{F}(t)$ given by (18) as

$$\begin{aligned}\widetilde{F}(t) &= \widetilde{\mathcal{S}}(t)\widetilde{F}^{in} + \int_0^t \widetilde{\mathcal{S}}(t')\Big(\widetilde{B}(t-t') - \widetilde{\mathcal{P}}\mathcal{L}\mathcal{E}f(t-t')\Big)\,\mathrm{d}t' \\ &\approx \int_0^\infty \widetilde{\mathcal{S}}(t')\,\mathrm{d}t'\,\Big(\widetilde{B}(t) - \widetilde{\mathcal{P}}\mathcal{L}\mathcal{E}f(t)\Big) \\ &= \widetilde{\mathcal{L}}^{-1}\Big(\widetilde{B}(t) - \widetilde{\mathcal{P}}\mathcal{L}\mathcal{E}f(t)\Big)\,.\end{aligned} \tag{25}$$

Here $\widetilde{\mathcal{L}}^{-1}$ is the inverse of $\widetilde{\mathcal{L}}$ over $\widetilde{\mathbb{H}}$, which uniquely extends to all $\mathbb{H}$ by requiring that $\widetilde{\mathcal{L}}^{-1}\mathcal{E} = 0$. This extension is the unique psuedo-inverse of $\widetilde{\mathcal{L}}$ over $\mathbb{H}$ that satisfies

$$\widetilde{\mathcal{L}}^{-1}\widetilde{\mathcal{L}} \subset \widetilde{\mathcal{P}}\,, \qquad \widetilde{\mathcal{L}}\widetilde{\mathcal{L}}^{-1} = \widetilde{\mathcal{P}}\,. \tag{26}$$

Stationary Balance

The approximation (25) can be restated as $\widetilde{F} \approx \widetilde{F}_S$ where $\widetilde{F}_S$ solves the equation

$$\widetilde{\mathcal{L}}\widetilde{F}_S + \widetilde{\mathcal{P}}\mathcal{L}\mathcal{E}f = \widetilde{B}\,, \tag{27}$$

Time is parametric in this equation through f and $\widetilde{B}$.

The designation *stationary balance approximation* reflects the fact that (27) is the stationary equation associated with the deviation equation (15).

One can also arrive at this approximation by arguing the deviation equation is stiff, whereby after the initial layer its solution will be well-approximated by $\widetilde{F}_S$.

Stationary Balance Master

In the stationary balance approximation the master equation is approximated by

$$\begin{aligned} \partial_t f + \mathcal{M}\mathcal{L}\mathcal{E} f - \mathcal{M}\mathcal{L}\widetilde{\mathcal{L}}^{-1}\mathcal{L}\mathcal{E} f &= b - \mathcal{M}\mathcal{L}\widetilde{\mathcal{L}}^{-1}\widetilde{B}\,, \\ f(0) &= f^{in}\,. \end{aligned} \tag{28}$$

One can show that this equation is always dissipative.

Equation (28) is not a very practical closure in the context of kinetic equations. This is because it involves the operator $\widetilde{\mathcal{L}}^{-1}$ which, being the inverse of a stationary kinetic operator, is an integral operator. We therefore view (28) as an intermediate closure from which we will derive other closures based on various spatial approximations.

Spatial Approximation: General Setting

Now assume $\mathcal{L}$ has the decomposition

$$\mathcal{L} = \mathcal{A} + \mathcal{K}\,, \tag{29}$$

where $\mathcal{A}$ and $\mathcal{K}$ are densely defined, closed linear operators over $\mathbb{H}$ such that

$$\mathcal{A}^T = -\mathcal{A}\,, \quad \text{and} \quad \mathcal{K}^T = \mathcal{K} \geq 0\,. \tag{30}$$

Finally, we assume that for every $t > 0$

$$B(t) \in \text{ Range}(\mathcal{K}) \cap \text{ Range}(\mathcal{L})\,. \tag{31}$$

We will refer to $\mathcal{A}$ as the advection operator, to $\mathcal{K}$ as the collision operator. We define $\widetilde{\mathcal{K}} = \widetilde{\mathcal{P}}\mathcal{K}\widetilde{P}$ and $\widetilde{\mathcal{A}} = \widetilde{\mathcal{P}}\mathcal{A}\widetilde{\mathcal{P}}$, so that $\widetilde{\mathcal{L}} = \widetilde{\mathcal{A}} + \widetilde{\mathcal{K}}$.

Relation Between $\mathcal{K}$ and $\mathcal{E}$

We will assume that the range of $\mathcal{E}$ is an invariant subspace of $\mathcal{K}$ that is a direct sum of the eigenspaces corresponding to its smallest eigenvalues. We then have that

$$\mathcal{K}\mathcal{E} = \mathcal{E}k\,, \qquad \text{where } k = \mathcal{M}\mathcal{K}\mathcal{E}\,.$$

It follows that $\mathcal{K}$ decomposes as

$$\mathcal{K} = \mathcal{E}k\mathcal{M} + \tilde{\mathcal{K}}\,,$$

and that $\tilde{\mathcal{K}}\mathcal{E} = 0$. We also assume that $\tilde{\mathcal{K}}$ is invertible over $\tilde{\mathbb{H}}$. This inverse has a unique extension $\tilde{\mathcal{K}}^{-1}$ over $\mathbb{H}$ such that

$$\tilde{\mathcal{K}}^{-1}\tilde{\mathcal{K}} = \tilde{\mathcal{K}}\,\tilde{\mathcal{K}}^{-1} = \tilde{\mathcal{P}}\,,$$
$$\tilde{\mathcal{K}}^{-1}\mathcal{E} = 0\,, \qquad \mathcal{M}\tilde{\mathcal{K}}^{-1} = 0\,.$$

Example: Transport Equation

In the context of the monoenergetic, photon transport equation we identify

$$\mathcal{A} = \omega \cdot \nabla_x \,, \qquad \mathcal{K} = \kappa - \mathcal{K}^S \,.$$

Note that $\mathcal{K}$ is symmetric over $\mathbb{H} = \mathsf{L}^2(\mathrm{d}\omega\, \mathrm{d}x)$. Of course, whether $\mathcal{A}$ is antisymmetric or not depends on the boundary conditions. In most physical problems these boundary conditions would be dissipative, and consequently $\mathcal{A}$ would not be antisymmetric.

However, given the viewpoint adopted here that in transition regimes the form of the density should be governed by balances in the kinetic equation rather than boundary conditions, we will at first avoid these complications by considering spatial domains with either no boundaries (like a periodic domain or the whole space) or only boundaries of symmetry (like a specular reflecting boundary).

Small Gradient Expansion

We will use the fact that the collisional physics is dominant to construct closures by considering $\widetilde{\mathcal{A}}$ to be a formal perturbation of $\widetilde{\mathcal{K}}$. We therefore consider the formal Neuman series expansion

$$\begin{aligned}\widetilde{\mathcal{L}}^{-1} &= \left(\widetilde{\mathcal{K}} + \widetilde{\mathcal{A}}\right)^{-1} = \sum_{k=0}^{\infty} \left(-\widetilde{\mathcal{K}}^{-1}\mathcal{A}\right)^{k} \widetilde{\mathcal{K}}^{-1} \\ &= \widetilde{\mathcal{K}}^{-1} - \widetilde{\mathcal{K}}^{-1}\mathcal{A}\,\widetilde{\mathcal{K}}^{-1} + \left(\widetilde{\mathcal{K}}^{-1}\mathcal{A}\right)^{2}\widetilde{\mathcal{K}}^{-1} - \cdots .\end{aligned} \tag{32}$$

Here we have simplified the terms in the expansion by using the fact that

$$\widetilde{\mathcal{K}}^{-1}\widetilde{\mathcal{A}}\,\widetilde{\mathcal{K}}^{-1} = \widetilde{\mathcal{K}}^{-1}\mathcal{A}\,\widetilde{\mathcal{K}}^{-1} .$$

Of course, because $\mathcal{A}$ is unbounded, this series cannot converge.

Small Gradient Approximations

Rather, we will truncate the series to define the sequence of formal approximations to $\widetilde{F}_S$ given by

$$\widetilde{F}_S^{(n)} = \sum_{k=0}^{n} \Big(- \widetilde{\mathcal{K}}^{-1} \mathcal{A} \Big)^k \widetilde{\mathcal{K}}^{-1} \mathcal{A} \mathcal{E} f \, . \tag{33}$$

These approximations will be asymptotic provided $\mathcal{E}$ is smooth enough. This will be the case whenever n is such that one has sufficiently smooth solutions to the associated system

$$\partial_t f + \mathcal{M} \, \mathcal{A} \mathcal{E} f + k f + \mathcal{M} \mathcal{A} \widetilde{F}_S^{(n)} = 0 \, . \tag{34}$$

At a minimum therefore, such a system should be well-posed. One can show that this is the case for $n = 0, 1, 4, 5, 8, 9, \ldots$. In fact, for these values of n the system is dissipative.

Boundary Layer Corrections

The small gradient approximations are interior approximation. They generally do not yield solutions that are consistent with the given boundary conditions. However, we can view the small gradient approximation as the first step toward constructing a uniform approximation to the stationary balance equation

$$(\widetilde{\mathcal{A}} + \widetilde{\mathcal{K}})\widetilde{F}_S = \widetilde{B} - \widetilde{\mathcal{P}}\mathcal{A}\mathcal{E}f \ ,$$

We can then try to construct boundary layer correctors that match the interior solution given by a small gradient approximation to the given boundary conditions.

While this procedure has not been carried out in general, when it is applied to the diffusion approximations it yields the classical boundary conditions obtained by matched asymptotics.

Classical Diffusion Approximation

Diffusion approximations truncate the above series at $n = 0$. The classical diffusion approximation is

$$\partial_t \rho + \nabla_x \cdot \rho^1 + \kappa^A \rho = \kappa^A \beta \,,$$
$$\frac{1}{D} \nabla_x \rho + \kappa_1 \rho^1 = 0 \,,$$

which can be reduced to the classical diffusion equation

$$\partial_t \rho - \frac{1}{D} \nabla_x \cdot \left[\frac{1}{\kappa_1} \nabla_x \rho \right] + \kappa^A \rho = \kappa^A \beta \,.$$

One can think of this as the diffusion correction to the P-0 approximation.

Diffusion Correction to P-1 Approximation

The diffusion correction to the P-1 approximation is

$$\begin{aligned}
\partial_t \rho + \nabla_x \cdot \rho^1 + \kappa^A \rho &= \kappa^A \beta \,, \\
\partial_t \rho^1 + \nabla_x \cdot \rho^2 + \tfrac{1}{D} \nabla_x \rho + \kappa_1 \rho^1 &= 0 \,, \\
\tfrac{2}{D+2} \Big[\nabla_x \vee \rho^1 - \tfrac{1}{D} \delta \left(\nabla_x \cdot \rho^1 \right) \Big] + \kappa_2 \rho^2 &= 0 \,,
\end{aligned}$$

which can be reduced to the system

$$\begin{aligned}
\partial_t \rho + \nabla_x \cdot \rho^1 + \kappa^A \rho &= \kappa^A \beta \,, \\
\partial_t \rho^1 - \tfrac{2}{D+2} \nabla_x \cdot \left[\frac{1}{\kappa_2} \Big[\nabla_x \vee \rho^1 - \tfrac{1}{D} \delta \left(\nabla_x \cdot \rho^1 \right) \Big] \right& \\
+ \tfrac{1}{D} \nabla_x \rho + \kappa_1 \rho^1 &= 0 \,.
\end{aligned}$$

Diffusion Correction to P-2 Approximation

The diffusion correction to the P-2 approximation is

$$
\begin{aligned}
\partial_t \rho + \nabla_x \cdot \rho^1 + \kappa^A \rho &= \kappa^A \beta \,, \\
\partial_t \rho^1 + \nabla_x \cdot \rho^2 + \tfrac{1}{D} \nabla_x \rho + \kappa_1 \rho^1 &= 0 \,, \\
\partial_t \rho^2 + \nabla_x \cdot \rho^3 + \tfrac{2}{D+2} \Big[\nabla_x \vee \rho^1 - \tfrac{1}{D} \, \delta \, (\nabla_x \cdot \rho^1) \Big] + \kappa_2 \rho^2 &= 0 \,, \\
\tfrac{3}{D+4} \Big[\nabla_x \vee \rho^2 - \tfrac{2}{D+2} \, \delta \vee (\nabla_x \cdot \rho^2) \Big] + \kappa_3 \rho^3 &= 0 \,,
\end{aligned}
$$

Diffusion Correction to P-2 Approximation-2

which combines into the system

$$\partial_t \rho + \nabla_x \cdot \rho^1 + \kappa^A \rho = \kappa^A \beta \,,$$
$$\partial_t \rho^1 + \nabla_x \cdot \rho^2 + \tfrac{1}{D} \nabla_x \rho + \kappa_1 \rho^1 = 0 \,,$$
$$\partial_t \rho^2 - \tfrac{3}{D+4} \nabla_x \cdot \left[\frac{1}{\kappa_3} \Big[\nabla_x \vee \rho^2 - \tfrac{2}{D+2} \, \delta \vee (\nabla_x \cdot \rho^2) \Big] \right]$$
$$+ \tfrac{2}{D+2} \Big[\nabla_x \vee \rho^1 - \tfrac{1}{D} \, \delta \, (\nabla_x \cdot \rho^1) \Big] + \kappa_2 \rho^2 = 0 \,.$$

Boundary conditions are naturally inherited from the P-3 approximation.

Beyond Diffusion Approximations

When the stationary balance approximation is applied to the diffusion correction to the P-1 approximation gives

$$\partial_t \rho + \nabla_x \cdot \rho^1 + \kappa^A \rho = \kappa^A \beta \,,$$

$$\kappa_1 \rho^1 - \tfrac{2}{D+2} \nabla_x \cdot \left[\frac{1}{\kappa_2} \Big[\nabla_x \vee \rho^1 - \tfrac{1}{D} \delta \left(\nabla_x \cdot \rho^1 \right) \Big] \right] = -\tfrac{1}{D} \nabla_x \rho \,.$$

This can be viewed as a non-local modification of the classical equation.

Stationary Balance to P-3 Approximation

The stationary balance approximation can be applied to the P-3 approximation to find a correction to the P-1 approximation:

$$\partial_t \rho + \nabla_x \cdot \rho^1 + \kappa^A \rho = \kappa^A \beta \,,$$

$$\partial_t \rho^1 + \nabla_x \cdot \rho^2 + \tfrac{1}{D} \nabla_x \rho + \kappa_1 \rho^1 = 0 \,,$$

$$\nabla_x \cdot \rho^3 + \tfrac{2}{D+2} \Big[\nabla_x \vee \rho^1 - \tfrac{1}{D} \, \delta \, (\nabla_x \cdot \rho^1) \Big] + \kappa_2 \rho^2 = 0 \,,$$

$$\tfrac{3}{D+4} \Big[\nabla_x \vee \rho^2 - \tfrac{2}{D+2} \, \delta \vee (\nabla_x \cdot \rho^2) \Big] + \kappa_3 \rho^3 = 0 \,.$$

Stationary Balance to P-3 Approximation-2

These combine into the system

$$\partial_t \rho + \nabla_x \cdot \rho^1 + \kappa^A \rho = \kappa^A \beta \,,$$
$$\partial_t \rho^1 + \nabla_x \cdot \rho^2 + \tfrac{1}{D} \nabla_x \rho + \kappa_1 \rho^1 = 0 \,,$$

where ρ^2 is the solution of the elliptic equation

$$-\tfrac{3}{D+4} \nabla_x \cdot \left[\frac{1}{\kappa_3} \Big[\nabla_x \vee \rho^2 - \tfrac{2}{D+2} \delta \vee (\nabla_x \cdot \rho^2) \Big] \right] + \kappa_2 \rho^2$$
$$= \tfrac{2}{D+2} \Big[\nabla_x \vee \rho^1 - \tfrac{1}{D} \delta \, (\nabla_x \cdot \rho^1) \Big] \,.$$

Boundary conditions are naturally inherited from the P-3 approximation.

Conclusion: Nonlinear Extensions

These ideas have partial extensions to nonlinear settings. Specifically, corrections to the compressible Navier-Stokes system have been developed that formally dissipate the Euler entropy. There are three approximations:

1. Small Deviation (a kind of linearization),

2. Material-Frame Stationary Balance (a temporal approximation),

3. Small Gradient Expansion (a spatial approximation).