Hydrodynamic Limits for Linear Transport with Multiplying Boundary Conditions

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Congress in honor of Carlo Cercignani on his 65th birthday

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UT-BATTELLE

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Statement of the Problem

Investigate the hydrodynamic limit of a suitably rescaled linear transport equation in a slab with *multiplying boundary conditions* as the scaling parameter tends to zero

Recover the corresponding diffusion equation with appropriate initial and *boundary conditions*

Motivation

- **Fundamental: Unify theoretical framework**

  Understand occurrence and evolution of dissipation in various regimes of the dynamical evolution (Newtonian → kinetic → Euler hydrodynamic → Navier - Stokes hydrodynamic → etc.)

- **Practical: Simplify description and analysis**

  Assess validity of various diffusion approximations for applications in nuclear reactor physics, porous rock transport, capillary transport, cell multiplication, etc.

- **Computational: reduce computational complexity, stabilize algorithms**

  Develop solvers for parabolic instead of hyperbolic PDEs

Background

Over the last 50 years, this type of results have been obtained for various deterministic and stochastic transport equations with dissipative and conservative B.C.

Asymptotic Results – Hydrodynamic Limits

Formal derivations **(Hilbert, Chapman-Enskog, Scharf, Cercignani, Larsen & Keller, etc.)**

Probabilistic methods – Homogeneization **(Bensoussan, Papanicolaou & Lions, Ellis & Pinsky, Lebowitz, Spohn, Babowsky, etc.)**

Functional analytic methods **(Bardos, Sentis, Angelescu & V.P., Mokhtar-Kharroubi, etc.)**

Background (cont'd)

Functional analytic methods:

1) No "small scaling parameter" expansion

Use spectral properties to show the asymptotic equivalence between the two descriptions:

$$\lim_{t\to\infty} \left\| \int (\textit{transport solution})dv - (\textit{diffusion solution}) \right\| = 0$$

2) Asymptotic expansion in a small scaling parameter

Carry out formal expansion and use functional analytic methods to show:

$$\lim_{\varepsilon\to 0} \left\| \int (\textit{main term in } \varepsilon\text{-expansion of transport solution})dv - (\textit{diffusion solution}) \right\| = 0$$

New Features and Difficult Aspects in a Nutshell

- **Multiplying boundary conditions**
- **Evolution semigroup is not a contraction**
- **In fact, the solution of the transport equation grows exponentially in time**
- **In the asymptotic limit, this growth becomes uncontrollable**
- **As a result, the corresponding diffusion equation cannot be derived, not even formally**

Technical Steps to Address This Problem

1. Set the transport problem with multiplying B.C. as a well posed evolution problem
2. Determine the evolution generated by and the spectral properties of the transport operator
3. Determine the correct scaling and compensating factors to ensure well-posedness in the limit
4. Carry out the formal asymptotic expansion
5. Estimate initial and boundary layer terms
6. OBTAIN MAIN RESULT: The bulk term in the asymptotic expansion satisfies a diffusion equation completely determined by the original transport problem, including initial and boundary conditions.

Model Transport Problem

$$\frac{\partial \varphi}{\partial t} = -\mu \frac{\partial \varphi}{\partial x} - C\varphi := T\varphi$$

$$C\varphi(\mu) = \varphi(\mu) - P\varphi(\mu) = \varphi(\mu) - \frac{1}{2}\int_{-1}^{1} \varphi(\mu')\, d\mu'$$

$$\varphi(-a,\mu) = \alpha\, \varphi(-a,-\mu) \text{ for } \mu > 0,$$

$$\varphi(a,-\mu) = \alpha\, \varphi(a,\mu) \text{ for } \mu > 0;$$

Consider evolution problem in the Hilbert space

$$H := L^2([-a,a]\times[-1,1])$$

$\alpha < 1$ - dissipative B.C.

$\alpha = 1$ - conservative B.C.

$\alpha > 1$ - multiplying B.C.

Evolution Generated by the Streaming Operator

Proposition. The streaming operator, $A\varphi = -\mu \frac{\partial \varphi}{\partial x} - \varphi$, generates a non-unitary group, whose action can be computed by explicitly accounting by for the boundary conditions (image method):

$$e^{tA}\varphi(x,\mu) = e^{-t}\varphi_0(x-\mu t,\mu)$$

$$+e^{-t}\sum_{k\in\mathbb{Z}}\alpha(\mu)^{2k+1}\varphi_0(-x-(4k+2)a-\mu t,-\mu) \; +e^{-t}\sum_{k\in\mathbb{Z}}\alpha(\mu)^{2k+2}\varphi_0(x+(4k+4)a-\mu t,-\mu)$$

$$+e^{-t}\sum_{k\in\mathbb{Z}}\alpha(\mu)^{2k+1}\varphi_0(-x+(4k+2)a-\mu t,-\mu) + e^{-t}\sum_{k\in\mathbb{Z}}\alpha(-\mu)^{2k+2}\varphi_0(x-(4k+4)a-\mu t,-\mu)$$

where

$$\alpha(\mu) = \alpha \text{ if } \mu > 0 \text{ and } \alpha(\mu) = \alpha^{-1} \text{ if } \mu < 0,$$

$\varphi(z) = 0$ if the value of z falls outside the interval [-a,a].

For $\alpha \le 1$, the evolution semigroup is (strictly) contractive

For $\alpha > 1$, the evolution semigroup is exponentially bounded !

Spectral Properties of the Transport Operator

- **"Standard" procedure**

  - Calculate resolvent of the streaming operator as the Laplace transform of the semigroup

  - Determine singularities of the resolvent and nature thereof

  - Use Gohberg & Krein - type results on relatively compact perturbations to determine spectrum of the resolvent of the complete transport operator

Spectrum of the Transport Operator

Rescaled Transport Equation

$$\frac{\partial \varphi_\varepsilon}{\partial t} = -\frac{1}{\varepsilon}\mu\frac{\partial \varphi_\varepsilon}{\partial x} - \frac{1}{\varepsilon^2}C\varphi_\varepsilon := T_\varepsilon \varphi_\varepsilon$$

$$C\varphi_\varepsilon(\mu) = \varphi_\varepsilon(\mu) - P\varphi_\varepsilon(\mu) = \varphi_\varepsilon(\mu) - \frac{1}{2}\int_{-1}^{1}\varphi_\varepsilon(\mu')\,d\mu'$$

$$\varphi_\varepsilon(-a,\mu) = \alpha\,\varphi_\varepsilon(-a,-\mu) \text{ for } \mu > 0,$$

$$\varphi_\varepsilon(a,-\mu) = \alpha\varphi_\varepsilon(a,\mu) \text{ for } \mu > 0; \qquad \alpha > 1$$

Evolution problem in the Hilbert space

$$H := L^2([-a,a]\times[-1,1])$$

This scaling makes the evolution unbounded and uncontrollable !

Spectrum of Rescaled Transport Operator

$$\left(\alpha > 1; \quad \varepsilon \to 0 \right)$$

Fully Rescaled Transport Equation

$$\frac{\partial \varphi_\varepsilon}{\partial t} = -\frac{1}{\varepsilon}\mu\frac{\partial \varphi_\varepsilon}{\partial x} - \frac{1}{\varepsilon^2}C\varphi_\varepsilon$$

$$C\varphi_\varepsilon(\mu) = \varphi_\varepsilon(\mu) - P\varphi_\varepsilon(\mu) = \varphi_\varepsilon(\mu) - \frac{1}{2}\int_{-1}^{1}\varphi_\varepsilon(\mu')d\mu'$$

$$\varphi_\varepsilon(-a,\mu) = (1+\varepsilon\beta)\,\varphi_\varepsilon(-a,-\mu) \text{ for } \mu > 0,$$

$$\varphi_\varepsilon(a,-\mu) = (1+\varepsilon\beta)\varphi_\varepsilon(a,\mu) \text{ for } \mu > 0; \qquad \beta>0$$

Evolution problem in the Hilbert space

$$H := L^2([-a,a]\times[-1,1])$$

Full scaling makes the evolution unbounded, but controllable !

Spectrum of Fully Rescaled Transport Operator

$$\left(\alpha = 1 + \varepsilon\beta; \quad \beta > 0; \quad \varepsilon \to 0 \right)$$

Spectrum of the Transport Operator

Proposition. ***The spectrum of the streaming operator,*** $A_\varepsilon, \sigma(A_\varepsilon)$ ***is located in the band*** $\left\{\lambda \in \mathrm{C}, -\frac{1}{\varepsilon^2} \le Re\lambda \le -\frac{1}{\varepsilon^2} + \frac{\ln\alpha}{2a\varepsilon}\right\}$ ***and is composed of the line*** $\left\{\lambda \in \mathrm{C}, Re\lambda = -\frac{1}{\varepsilon^2}\right\}$ ***and the segments*** $\bigcup_{k\in\mathbb{Z}} \left\{-\frac{1}{\varepsilon^2} + v\left(\frac{\ln\alpha}{2a\varepsilon} + i\frac{k\pi}{2a\varepsilon}\right),\ v \in [0,1]\right\}.$

The spectrum of the transport operator, T_ε, ***consists of*** $\sigma(A_\varepsilon)$, ***plus possibly a denumerable set of isolated eigenvalues with finite algebraic multiplicities. Moreover, for all*** $\varphi \in L^2([-a,a]\times[-1,1])$, ***the semigroup generated by*** T_ε ***satisfies the estimate***

$$\left\| e^{tT_\varepsilon}\varphi \right\|_{L^2} \le \alpha\, e^{\omega(\alpha,\varepsilon)t} \left\| \varphi \right\|_{L^2}$$

with the exponential bound $\omega(\alpha,\varepsilon) = \frac{\ln\alpha}{2a\varepsilon} + \frac{1}{2\varepsilon^2}\left(\alpha + \frac{1}{\alpha} - 2\right).$

Corollary

With the scaled restitution coefficient, $\alpha = 1 + \beta\varepsilon \, (\beta > 0)$,
the transport semigroup becomes exponentially bounded in time, uniformly in ε **, since**

$$\omega(1+\beta\varepsilon, \varepsilon) = \frac{\ln(1+\beta)}{2a\varepsilon} + \frac{1}{2\varepsilon^2}\left(1+\beta\varepsilon + \frac{1}{1+\beta\varepsilon} - 2 \to \frac{\beta}{2a} + \frac{\beta^2}{2} \, (\varepsilon \to 0).\right)$$

The exponential type depends on the slab size, and strength of boundary reflection

Since the type is finite, it can be compensated !

Introduce additional volume absorption to compensate for the boundary production, as a function of medium size

Rescaled and Compensated Inhomogeneous Transport Problem

$$\begin{cases} \dfrac{\partial \varphi_\varepsilon}{\partial t}(x,\mu,t) = -\varepsilon^{-1}\mu\dfrac{\partial \varphi_\varepsilon}{\partial x} - \varepsilon^{-2}C\varphi_\varepsilon - \gamma\,\varphi_\varepsilon + S \quad \text{on } (-a,a)\times(-1,1)\times \mathrm{R}_+ \\ \varphi_\varepsilon\ (-a,\mu,t) = (1+\beta\varepsilon)\,\varphi_\varepsilon(-a,-\mu,t) + \varepsilon S^-(\mu) \qquad \mu>0 \\ \varphi_\varepsilon\ (a,-\mu,t) = (1+\beta\varepsilon)\,\varphi_\varepsilon(a,\mu,t) + \varepsilon S^+(\mu) \qquad \mu>0 \\ \varphi_\varepsilon\ (x,\mu,0) = \varphi_0(x,\mu) \end{cases}$$

γ **is a positive constant,** $S^+, S^- \in L^2(0,1)$, **and** $\varphi_0 \in L^2([-a,a]\times[-1,1])$.

Before stating the main result, we define the following projection operators:

$$\overline{P}\varphi = 2\int_0^1 \mu\varphi(\mu)\,d\mu,\ \varphi \in L^2_\mu(0,1), \quad P\varphi = \int_{-1}^{1}\varphi(\mu)\,d\mu,\ \varphi \in L^2_\mu(-1,1).$$

Main Result

Let $\gamma > \frac{\beta}{2a} + \frac{\beta^2}{2}$ ***and assume that the data,*** $P\varphi_0$ ***and PS, are sufficiently smooth. Then the solution,*** φ_ε ***, of the rescaled and compensated transport equation satisfies***

$$\left\| \varphi_\varepsilon - f \right\|_{L^2([-a,a]\times[-1,1])} \le \varepsilon M e^{\delta T}, \ \ for\ all\ t \in (0,T),$$

where T > 0, M and δ are two positive constants independent of T and ε, and f is the solution of the following diffusion problem in $H^1(-a,a)$:

$$\begin{cases} \dfrac{\partial f}{\partial t}(x,t) = \dfrac{1}{3}\dfrac{\partial^2 f}{\partial x^2} - \gamma f + PS & on\ (-a,a)\times \mathrm{R}_+ \\ \dfrac{4}{3}\dfrac{\partial f}{\partial n} = \beta f + \overline{P}S^-, & in\ x = -a \\ \dfrac{4}{3}\dfrac{\partial f}{\partial n} = \beta f + \overline{P}S^+, & in\ x = a \\ f(x,0) = P\varphi_0(x) \end{cases}$$

Sketch of the Proof - Asymptotic Expansion

Seek solution φ_ε of the rescaled transport problem in the form:

$$\varphi_\varepsilon = u_\varepsilon^0\left(x,\mu,t\right) + u_\varepsilon^i(x,\mu,\tau = \frac{t}{\varepsilon^2}) + u_\varepsilon^b(\xi = \frac{x}{\varepsilon},\mu,t) + w_\varepsilon\left(x,\mu,t\right)$$

where $u_\varepsilon^0, u_\varepsilon^i, u_\varepsilon^b$, and w_ε **denote respectively the interior (bulk), initial layer, boundary layer, and reminder terms. Each one of the first three terms in assumed to satisfy exactly the transport equation and is written as an asymptotic expansion in ε, namely:**

$$u_\varepsilon^0 = \sum_{n=0}^{\infty} \varepsilon^n u_n^0, \qquad u_\varepsilon^i = \sum_{n=0}^{\infty} \varepsilon^n u_n^i, \qquad u_\varepsilon^b = \sum_{n=0}^{\infty} \varepsilon^n u_n^b.$$

The leading term in the interior (bulk) term does not depend on μ.

The leading term in the initial layer term does not depend on x.

The leading term in the boundary layer term does not depend on t.

Separate Terms in Powers of ε

Separation in evolution equation

$$Cu_0^0 = 0; \quad Cu_1^0 = -\mu \frac{\partial u_0^0}{\partial x}; \quad Cu_2^0 = -(\frac{\partial u_0^0}{\partial t} + \mu \frac{\partial u_1^0}{\partial x} + \gamma u_0^0 - S)$$

Solvability condition for u_1^0 is trivially satisfied and the one for u_2^0 formally yields diffusion equation !

$$\frac{\partial u_0^i}{\partial \tau} + Cu_0^i = 0$$

$$\mu \frac{\partial u_{0,1}^b}{\partial \xi} + Cu_{0,1}^b = 0; \quad \mu \frac{\partial u_2^b}{\partial \xi} + Cu_2^b = -\gamma u_0^b - \frac{\partial u_0^b}{\partial \tau}$$

Initial data

$$u_0^0(x,\mu,0) + u_0^i(x,\mu,0) = f_0(x,\mu)$$

Boundary conditions

$$u_0^0(-a,\mu) + u_0^b(-\frac{a}{\varepsilon},\mu) = u_0^0(-a,-\mu) + u_0^i(-\frac{a}{\varepsilon},-\mu); \quad \mu > 0$$

$$u_0^0(a,-\mu) + u_0^b(\frac{a}{\varepsilon},-\mu) = u_0^0(a,\mu) + u_0^i(\frac{a}{\varepsilon},\mu)$$

etc.

A Priori Estimates for the Diffusion Equation

Proposition. **For** $Pf_0,\ PS \in L^2(-a,a),$ **the diffusion equation**

$$\begin{cases} \dfrac{\partial f}{\partial t}(x,t) = \dfrac{1}{3}\dfrac{\partial^2 f}{\partial x^2} - \gamma f + PS \qquad on\,(-a,a)\times \mathrm{R}_+ \\ \dfrac{4}{3}\dfrac{\partial f}{\partial n} = \beta f + \bar{P}S^-, \quad in\ x = -a \\ \dfrac{4}{3}\dfrac{\partial f}{\partial n} = \beta f + \bar{P}S^+, \quad in\ x = a \\ f(x,0) = P\varphi_0(x) \end{cases}$$

admits a solution in $H^1(-a,a)$ **Additional smoothness in I.C. and sources Translates in corresponding additional smoothness of the solution and one can show that**

$$\| \partial^i f / \partial x_i \|_{L^2} \le M e^{\delta t}, \qquad i = 1,\ldots,5$$

Remark. **Conditions to ensure smoothness are not optimal.**

Proof. **A priori estimates for weak solutions of parabolic equations**

Boundary Layer Term - Milne Problem

Proposition. For $f \in L^2(0,1)$, the systems

$$(+/-)\mu \frac{\partial \varphi}{\partial x} + C\varphi = 0 \qquad (x,\mu) \in (0,\infty)\times(-1,1)$$

$$\varphi(0,\mu) = \varphi(0,-\mu) + f(\mu), \qquad \mu > 0$$

$$\lim_{x\to\infty} \varphi(x,\mu) = 0$$

admit solutions in $L^p((-1,1);L^\infty(0,\infty)),\ 1 \le p < \infty$, if and only if

$$\int_0^1 \mu\, f(\mu)\, d\mu = 0 .$$

Moreover, there exists a constant M>0, such that

$$\| \varphi \|_{L^p((-1,1);L^\infty(0,\infty))} \le M \| f \|_{L^2(0,1)}; \qquad \| \varphi \|_{L^2(0,1)} \le M \| f \|_{L^2(0,1)} .$$

B.C. and I.C. for the Diffusion Equation

- **Use asymptotic expansion, solution to the Milne problem, and solvability conditions of terms of various orders to derive boundary and initial conditions for the diffusion equation**

$$u_0^0(x,0) = \frac{1}{2}\int_{-1}^{1} f_0(x,\mu)\,d\mu$$

$$\frac{4}{3}\frac{\partial u_0^0}{\partial n} + \beta u_0^0 + \overline{P}S^{+/-} = 0$$

- **Estimate remainder**

Main Result

Let $\gamma > \frac{\beta}{2a} + \frac{\beta^2}{2}$ ***and assume that the data,*** $P\varphi_0$ ***and PS, are sufficiently smooth. Then the solution,*** φ_ε ***, of the rescaled and compensated transport equation satisfies***

$$\left\| \varphi_\varepsilon - f \right\|_{L^2([-a,a]\times[-1,1])} \le \varepsilon M e^{\delta T}, \ \ for\ all\ t \in (0,T),$$

where T > 0, M and δ are two positive constants independent of T and ε, and f is the solution of the following diffusion problem in $H^1(-a,a)$:

$$\begin{cases} \dfrac{\partial f}{\partial t}(x,t) = \dfrac{1}{3}\dfrac{\partial^2 f}{\partial x^2} - \gamma f + PS & on\ (-a,a)\times \mathrm{R}_+ \\ \dfrac{4}{3}\dfrac{\partial f}{\partial n} = \beta f + \overline{P}S^-, & in\ x = -a \\ \dfrac{4}{3}\dfrac{\partial f}{\partial n} = \beta f + \overline{P}S^+, & in\ x = a \\ f(x,0) = P\varphi_0(x) \end{cases}$$

Summary and Open Problems

- First rigorous result on the diffusion limit for linear transport with multiplying B.C. in L^2
- Results carry out, essentially unchanged, to the Banach spaces L^p, $1 < p$

$$\lim_{\varepsilon\to 0}\omega(1+\beta\varepsilon,\varepsilon)=\frac{\beta}{2a}+\frac{\beta^2}{2}(p+p') \quad 1<p<\infty; \quad \omega=\frac{\beta}{2a}+\frac{\beta^2}{2\varepsilon} \quad p=1$$

- Physically relevant case p = 1 is still open for multiplying B.C. The difficulty is purely technical and has to do with the fact that L^1 is not reflexive
- General geometries may require modifications in techniques