Hyperbolic Approximation of Kinetic Equations Using Quadrature-Based Projection Methods

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September 25th, 2013

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Outline

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2. Transformation and Projections
3. Abstract Framework
4. Applications and Results
5. Conclusion and Further Work
Introduction
Motivation 1

Goal

derive model equations for flow problems involving rarefied gases

Knudsen number $Kn = \frac{\lambda}{L}$

- $Kn \leq 0.1$: continuum model; Navier-Stokes Equation and extensions
- $Kn \geq 0.1$: rarefied gas; Boltzmann Equation or Monte-Carlo simulations
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Knudsen number

distinguish flow regimes by orders of the Knudsen number $Kn = \frac{\lambda}{L}$

- $\lambda$ is the mean free path length
- $L$ is a reference length
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Motivation 2

Applications for large $Kn = \frac{\lambda}{L}$

- small $L$: micro-scale applications, Knudsen pump
- large $\lambda$: rarefied gases, atmospheric reentry flights
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Tasks
- calculation of shock layer thickness
- accurate prediction of heat flux
Boltzmann Equation

PDE for particles' *probability density function* $f(t, x, c)$

- describes change of $f$ due to transport and collisions
- usually seven-dimensional phase space in 3D
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\[
\frac{\partial}{\partial t} f(t, x, c) + c_i \frac{\partial}{\partial x_i} f(t, x, c) = S(f)
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Simplifications

- no external force
- neglect collision operator \( S \)
- mostly consider only 1D case
Aims and Challenges

Aims

- perform adaptive discretization of velocity space
- investigate different basis functions for the ansatz of $f$
- derive hyperbolic PDE systems for discretized variables

Challenges

- adaptive discretization is difficult in velocity space
- simple Hermite ansatz by Grad is not globally hyperbolic
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- adaptive discretization is difficult in velocity space
- simple Hermite ansatz by $\text{GRAD}$ is not globally hyperbolic
Transformation and Projections
Transformation of Velocity Variable

\[ f(c) = \frac{\rho}{\sqrt{2\pi}\theta} \exp \left( -\frac{(c-v)^2}{2\theta} \right) \]
Transformation of Velocity Variable

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\[ \xi(t, x, c) := \frac{c-v(t, x)}{\sqrt{\theta(t, x)}} \]
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\[ f(\xi) = \frac{\rho}{\sqrt{2\pi\theta}} \exp\left( -\frac{\xi^2}{2} \right) \]
Transformation of Boltzmann Equation

\[
\frac{\partial}{\partial t} f(t, x, c) + c_i \frac{\partial}{\partial x_i} f(t, x, c) = 0
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Transformation of Boltzmann Equation

\[ \frac{\partial}{\partial t} f(t, x, c) + c_i \frac{\partial}{\partial x_i} f(t, x, c) = 0 \]

\[ \Downarrow \]

\[ D_t f + \sqrt{\theta} \xi \partial_x f + \partial_\xi f \left( -\frac{1}{\sqrt{\theta}} \left( D_t v + \sqrt{\theta} \xi \partial_x v \right) - \frac{1}{2\theta} \xi \left( D_t \theta + \sqrt{\theta} \xi \partial_x \theta \right) \right) = 0 \]
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- additional terms from chain rule for \( f \), with \( \xi(t, x, c) := \frac{c - v(t, x)}{\sqrt{\theta(t, x)}} \)
- convective time derivative \( D_t := \partial_t + v \partial_x \)
- additional variables \( v \) and \( \theta \)
Macroscopic variables $\rho, v, \theta$ are *moments* of the PDF $f$

\[
\rho = \int_{\mathbb{R}} f(t, x, c) dc
\]
\[
\rho v = \int_{\mathbb{R}} c \cdot f(t, x, c) dc
\]
\[
\rho \theta = \int_{\mathbb{R}} (c - v)^2 f(t, x, c) dc
\]
Macroscopic variables \( \rho, \nu, \theta \) are *moments* of the PDF \( f \)

\[
\begin{align*}
\rho &= \int_{\mathbb{R}} f(t, x, c) dc \\
\rho \nu &= \int_{\mathbb{R}} c \cdot f(t, x, c) dc \\
\rho \theta &= \int_{\mathbb{R}} (c - \nu)^2 f(t, x, c) dc
\end{align*}
\]

**Ansatz**

\[
f(t, x, \xi) = \frac{\rho}{\sqrt{2\pi \theta}} \exp \left( -\frac{\xi^2}{2} \right) \sum_{i=0}^{n} \alpha_i(t, x) \Phi_i(\xi)
\]
Continuous Projection

\[ P^C_j(g) = \int_{\mathbb{R}} g(t, x, \xi) \tilde{\Phi}_j(\xi) d\xi \]

**Interpretation**

multiplication by test function \( \tilde{\Phi}_j \) and exact integration over velocity space

**Example: GRAD-Hermite Ansatz**

use Hermite polynomials for ansatz \( \Phi_i \) and test functions \( \tilde{\Phi}_j \)
Result of continuous projection

- System of equations $D_t u + A \partial_x u = 0$
- unknowns $u = (\rho, v, \theta, \alpha_3, \ldots, \alpha_n)^T$
- not globally hyperbolic
Result of continuous projection

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- unknowns \( u = (\rho, v, \theta, \alpha_3, \ldots, \alpha_n)^T \)
- not globally hyperbolic

Characteristic polynomial of \( A \)

\[
\chi_A (\lambda) = \gamma \Phi_{n+1} (\lambda) + \delta_1 \alpha_{n-1} + \delta_2 \alpha_n
\]

\( \Rightarrow \) hyperbolicity depends on coefficients \( \alpha \)
Quadrature-based Projection

\[ P_j^Q(g) = \sum_{k=0}^{n} w_k g(t, x, \xi_k) \tilde{\Phi}_j(\xi_k) \]

Interpretation

substitute exact integral in continuous projection by quadrature formula
Quadrature-based Projection

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**Interpretation**

substitute exact integral in continuous projection by quadrature formula

**Example: Gauss-Hermite quadrature**

- \( \Phi \) are orthogonal Hermite polynomials
- quadrature points \( \xi_k \) are roots of \( \Phi_{n+1} \)
- quadrature weights \( w_k \) are chosen such that quadrature is exact for polynomials up to degree \( 2n + 1 \)
Success of Quadrature-based Projection methods

Result of quadrature-based projection

- System of equations \( D_t u + \tilde{A} \partial_x u = 0 \)
- unknowns \( u = (\rho, v, \theta, \alpha_3, \ldots, \alpha_n)^T \)
- globally hyperbolic
Success of Quadrature-based Projection methods

Result of quadrature-based projection

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- unknowns \( u = (\rho, v, \theta, \alpha_3, \ldots, \alpha_n)^T \)
- globally hyperbolic

Characteristic polynomial of \( \tilde{A} \)

\[
\chi_{\tilde{A}} (\lambda) = \gamma \Phi_{n+1} (\lambda)
\]

\( \Rightarrow \) hyperbolic system independent of \( \alpha \)
Abstract Framework
Open questions

- Why does quadrature-based projection lead to global hyperbolicity?
- Is there a generalization to 2D or 3D?
- Are there analogous results for more classes of basis functions?
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- Is there a generalization to 2D or 3D?
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Aims

- development of abstract setting for expansion and projection methods of transformed Boltzmann Equation
- derivation of conditions for global hyperbolicity
Example Shifted Boltzmann Equation

\[ D_t f + \xi \partial_x f + \partial_\xi f (-D_t v - \xi \partial_x v) = 0, \quad \xi(t, x, c) := c - v(t, x) \]
Example Shifted Boltzmann Equation

\[ D_t f + \xi \partial_x f + \partial_\xi f \left( -D_t v - \xi \partial_x v \right) = 0, \quad \xi(t, x, c) := c - v(t, x) \]

\[ \downarrow \]

\[ (-\partial_\xi f \cdot 1) D_t \begin{pmatrix} v \\ f \end{pmatrix} + \xi (\partial_\xi f \cdot 1) \partial_x \begin{pmatrix} v \\ f \end{pmatrix} = 0 \]
Example Shifted Boltzmann Equation

\[ D_t f + \xi \partial_x f + \partial_{\xi} f \left( -D_t v - \xi \partial_x v \right) = 0 \, , \quad \xi(t, x, c) := c - v(t, x) \]

\[ \downarrow \]

\[ (-\partial_{\xi} f, 1) D_t \begin{pmatrix} v \\ f \end{pmatrix} + \xi (\partial_{\xi} f, 1) \partial_x \begin{pmatrix} v \\ f \end{pmatrix} = 0 \]

insert ansatz: \[ f(t, x, \xi) = \sum_{i=0}^{n} \alpha_i(t, x) \Phi_i(\xi) \]
Example Shifted Boltzmann Equation

\[ D_t f + \xi \partial_x f + \partial_\xi f \left( -D_t v - \xi \partial_x v \right) = 0 \, , \quad \xi(t, x, c) := c - v(t, x) \]

\[ \Downarrow \]

\[ \left( -\partial_\xi f , 1 \right) D_t \left( \begin{array}{c} v \\ f \end{array} \right) + \xi \left( \partial_\xi f , 1 \right) \partial_x \left( \begin{array}{c} v \\ f \end{array} \right) = 0 \]

insert ansatz: \( f(t, x, \xi) = \sum_{i=0}^{n} \alpha_i(t, x) \Phi_i(\xi) \)

\[ \Downarrow \]

\[ \left( -\partial_\xi \phi \cdot \alpha , \phi \right) D_t \left( \begin{array}{c} v \\ \alpha \end{array} \right) + \xi \left( \partial_x \phi \cdot \alpha , \phi \right) \partial_x \left( \begin{array}{c} v \\ \alpha \end{array} \right) = 0 \]
Example Shifted Boltzmann Equation

\[
(-\partial_\xi \phi \cdot \alpha, \phi) D_t \begin{pmatrix} \nu \\ \alpha \end{pmatrix} + \xi (\partial_x \phi \cdot \alpha, \phi) \partial_x \begin{pmatrix} \nu \\ \alpha \end{pmatrix} = 0
\]

apply projection: \( P_j^Q(g) = \sum_{k=0}^{n} w_k \tilde{\Phi}_j(\xi_k) g(t, x, \xi_k) \)
Example Shifted Boltzmann Equation

\[
(-\partial_{\xi}\phi \cdot \alpha, \phi) D_t \begin{pmatrix} v \\ \alpha \end{pmatrix} + \xi (\partial_x \phi \cdot \alpha, \phi) \partial_x \begin{pmatrix} v \\ \alpha \end{pmatrix} = 0
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apply projection: \( P^Q_j(g) = \sum_{k=0}^{n} w_k \tilde{\Phi}_j(\xi_k) g(t, x, \xi_k) \)

\[\downarrow\]

\[
\tilde{\Phi}_W (-D\Phi \alpha, \Phi) D_t \begin{pmatrix} v \\ \alpha \end{pmatrix} + \tilde{\Phi}_W \xi (-D\Phi \alpha, \Phi) \partial_x \begin{pmatrix} v \\ \alpha \end{pmatrix} = 0
\]

system of \( n + 1 \) equations
Example Shifted Boltzmann Equation

\[-\partial_{\xi} \phi \cdot \alpha, \phi \] 
\[\mathcal{T} \left( \begin{pmatrix} \nu \\ \alpha \end{pmatrix} \right) + \xi \left( \partial_{x} \phi \cdot \alpha, \phi \right) \partial_{x} \left( \begin{pmatrix} \nu \\ \alpha \end{pmatrix} \right) = 0\]

\[\tilde{\Phi} W \left( -D \Phi \alpha, \Phi \right) \mathcal{T} \left( \begin{pmatrix} \nu \\ \alpha \end{pmatrix} \right) + \tilde{\Phi} W \xi \left( -D \Phi \alpha, \Phi \right) \partial_{x} \left( \begin{pmatrix} \nu \\ \alpha \end{pmatrix} \right) = 0\]
Example Shifted Boltzmann Equation

\[
(-\partial_{\xi} \phi \cdot \alpha, \phi) \frac{D_t}{\nu} \begin{pmatrix} \nu \\ \alpha \end{pmatrix} + \xi (\partial_x \phi \cdot \alpha, \phi) \partial_x \begin{pmatrix} \nu \\ \alpha \end{pmatrix} = 0
\]

\[
\tilde{\Phi} \mathbf{W} (-D \Phi \alpha, \Phi) \frac{D_t}{\nu} \begin{pmatrix} \nu \\ \alpha \end{pmatrix} + \tilde{\Phi} \mathbf{W} \xi (-D \Phi \alpha, \Phi) \partial_x \begin{pmatrix} \nu \\ \alpha \end{pmatrix} = 0
\]

\[
\xi := \text{diag} (\xi_0, \ldots, \xi_n), \quad \mathbf{W} := \text{diag} (w_0, \ldots, w_n)
\]

\[
\Phi := \begin{pmatrix} 
\Phi_0(\xi_0) & \cdots & \Phi_n(\xi_0) \\
\vdots & \ddots & \vdots \\
\Phi_0(\xi_n) & \cdots & \Phi_n(\xi_n)
\end{pmatrix}, \quad D\Phi := \begin{pmatrix}
\partial_{\xi} \Phi_0(\xi) & \cdots & \partial_{\xi} \Phi_n(\xi) \\
\vdots & \ddots & \vdots \\
\partial_{\xi} \Phi_0(\xi) & \cdots & \partial_{\xi} \Phi_n(\xi)
\end{pmatrix}
\]
Conditions for Hyperbolicity

use discrete compatibility condition to solve for one variable $\alpha_m$

\[
0 = \int_{\mathbb{R}} \xi f(t, x, \xi) d\xi \quad \alpha \rightarrow \hat{\alpha} = (\alpha_0, \ldots, \alpha_{m-1}, \alpha_{m+1}, \ldots, \alpha_n)^T
\]

\[
\tilde{\Phi}W \left( -D\Phi\hat{\alpha}, \hat{\phi} \right) D_t \left( \frac{\nu}{\hat{\alpha}} \right) + \tilde{\Phi}W\xi \left( -D\Phi\hat{\alpha}, \hat{\phi} \right) \partial_x \left( \frac{\nu}{\hat{\alpha}} \right) = 0
\]
Conditions for Hyperbolicity

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$$0 = \int_{\mathbb{R}} \xi f(t, x, \xi) d\xi \quad \alpha \rightarrow \hat{\alpha} = (\alpha_0, \ldots, \alpha_{m-1}, \alpha_{m+1}, \ldots, \alpha_n)^T$$

$$\tilde{\Phi} W \left( -\hat{D}\Phi \hat{\alpha}, \hat{\Phi} \right) D_t \left( \frac{v}{\hat{\alpha}} \right) + \tilde{\Phi} W \xi \left( -\hat{D}\Phi \hat{\alpha}, \hat{\Phi} \right) \partial_x \left( \frac{v}{\hat{\alpha}} \right) = 0$$

$$\Rightarrow \quad D_t \left( \frac{v}{\hat{\alpha}} \right) + \left( -\hat{D}\Phi \hat{\alpha}, \hat{\Phi} \right)^{-1} \xi \left( -\hat{D}\Phi \hat{\alpha}, \hat{\Phi} \right) \partial_x \left( \frac{v}{\hat{\alpha}} \right) = 0$$

Requirements

Regularity of matrices $\tilde{\Phi}, W, \left( -\hat{D}\Phi \hat{\alpha}, \hat{\Phi} \right)$
Hyperbolicity of the System

\[ D_t \left( \frac{v}{\hat{\alpha}} \right) + \left( -\hat{D}\Phi\hat{\alpha}, \hat{\Phi} \right)^{-1} \xi \left( -\hat{D}\Phi\hat{\alpha}, \hat{\Phi} \right) \partial_x \left( \frac{v}{\hat{\alpha}} \right) = 0 \]

**System matrix A**

hyperbolicity requires real eigenvalues of system matrix

\[ A := \left( -\hat{D}\Phi\hat{\alpha}, \hat{\Phi} \right)^{-1} \xi \left( -\hat{D}\Phi\hat{\alpha}, \hat{\Phi} \right) \]

matrix A is obtained by similarity transformation of \( \xi \)

\[ \Rightarrow \text{matrix A has eigenvalues } \xi_k \in \mathbb{R} \]
Hyperbolicity of the System

\[ D_t \left( \begin{pmatrix} v \\ \alpha \end{pmatrix} \right) + \left( -\hat{D}\hat{\Phi}\hat{\alpha}, \hat{\Phi} \right)^{-1} \xi \left( -\hat{D}\hat{\Phi}\hat{\alpha}, \hat{\Phi} \right) \partial_x \left( \begin{pmatrix} v \\ \alpha \end{pmatrix} \right) = 0 \]

System matrix \( A \)

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Conditions for hyperbolicity

Regularity of matrices \( \tilde{\Phi}, \ W, \left( -\hat{D}\hat{\Phi}\hat{\alpha}, \hat{\Phi} \right) \)
Applications and Results
Applications 1: Proof of Hyperbolicity

Hyperbolicity of Hermite ansatz with quadrature

Use Hermite polynomials for $\Phi_i$, $\tilde{\Phi}_j$ and Gauss-Hermite quadrature for projections (1D, shifted Boltzmann Equation)
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Hyperbolicity of Hermite ansatz with quadrature

Use Hermite polynomials for $\Phi_i$, $\tilde{\Phi}_j$ and Gauss-Hermite quadrature for projections (1D, shifted Boltzmann Equation)

Check hyperbolicity conditions

- matrix $\tilde{\Phi}$ is invertible for all $n$
- matrix $\mathbf{W}$ is has positive diagonal entries and is invertible
- matrix $(-\hat{D}\Phi\hat{\alpha}, \hat{\Phi})$ has rank $n + 1$ and is invertible
Applications 1: Proof of Hyperbolicity

Hyperbolicity of Hermite ansatz with quadrature

Use Hermite polynomials for $\Phi_i$, $\tilde{\Phi}_j$ and Gauss-Hermite quadrature for projections (1D, shifted Boltzmann Equation)

Check hyperbolicity conditions

- matrix $\tilde{\Phi}$ is invertible for all $n$
  property of Hermite basis and quadrature formula
- matrix $W$ is has positive diagonal entries and is invertible
  property of quadrature formula
- matrix $\left(-\hat{D}\phi\hat{\alpha}, \phi\right)$ has rank $n + 1$ and is invertible
  property of Hermite basis and quadrature formula
Applications 2: Calculation of Eigenvalues

Hermite ansatz and quadrature

1D \( \lambda_k = \xi_k \)

3D for \( \|\beta\|_2 = 1 \):

\[
\lambda_k = \sum_{i=1}^{3} \beta_i (\xi_k)_i
\]
Applications 2: Calculation of Eigenvalues

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3D for \( \|\beta\|_2 = 1 \):

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Further Results

Transformed Boltzmann Equation

- Extension of transformation to multiple dimensions
- Compatibility conditions in multiple dimensions for different basis functions
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Transformed Boltzmann Equation
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Framework
- Extension to multiple dimensions
- Extension to fully transformed Boltzmann Equation including temperature scaling
- Derivation of general hyperbolicity conditions
Conclusion and Further Work
Conclusion

Abstract framework enables deeper understanding of the methods and is the starting point for further investigation.

Quadrature-based projection methods can be used to derive globally hyperbolic PDE systems from the transformed Boltzmann Equation.
Further Work

Next steps

- Extension of framework and proofs for more basis functions, general Gauss-quadrature, multiple dimensions
- Use of sparse-tensor product approximations
- Numerics for the hyperbolic PDE system

Start as PhD student in October

A Novel Approach for the Approximation of Kinetic Equations - Stable Projections and High-Resolution Numerics of Real Applications
Thank you for your attention