Hyperbolic Moment Equations
Using Quadrature-Based Projection Methods

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Outline

Boltzmann Transport Equation

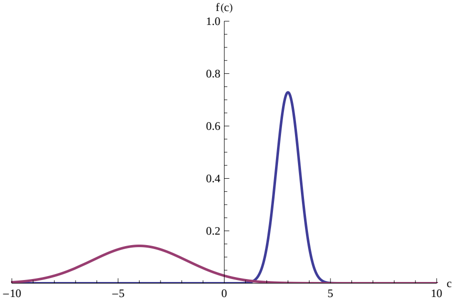
Boltzmann Transport Equation

$$\frac{\partial}{\partial t} f(t, \mathbf{x}, \mathbf{c}) + c_i \frac{\partial}{\partial x_i} f(t, \mathbf{x}, \mathbf{c}) = S(f)$$

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

- Describes change of f due to transport and collisions
- Collision operator S
- $\mathbf{x} \in \mathbb{R}^d, \mathbf{c} \in \mathbb{R}^d$
- No external force

Transformation of Velocity Variable



$$f(c) = \frac{\rho}{\sqrt{2\pi\theta}} \exp\left(-\frac{(c-v)^2}{2\theta}\right)$$

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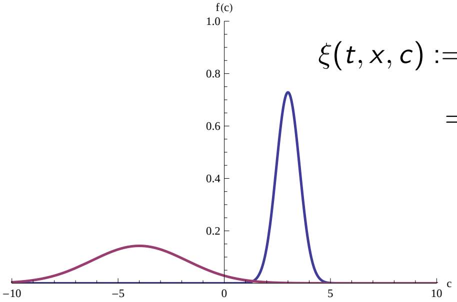

$$\xi(t,x,c) := \frac{c - v(t,x)}{\sqrt{\theta(t,x)}}$$

$$\Longrightarrow$$

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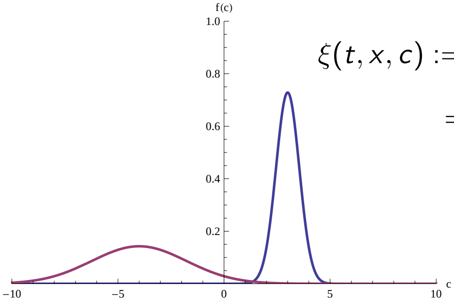

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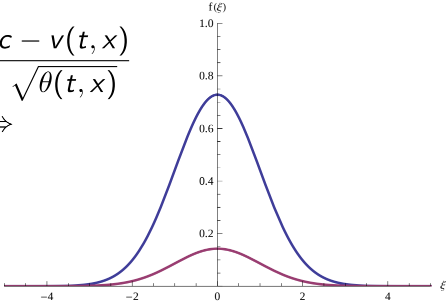
$$\Longrightarrow$$



$$f(c) = \frac{\rho}{\sqrt{2\pi\theta}} \exp\left(-\frac{(c-v)^2}{2\theta}\right) \qquad f(\xi) = \frac{\rho}{\sqrt{2\pi\theta}} \exp\left(-\frac{\xi^2}{2}\right)$$

Lagrangian velocity space reduces numerical complexity

Transformed Boltzmann Transport Equation

Transformation: $\xi(t, \mathbf{x}, \mathbf{c}) := \frac{\mathbf{c} - \mathbf{v}(t,\mathbf{x})}{\sqrt{\theta(t,\mathbf{x})}}$

Scaled distribution function: $f(t, \mathbf{x}, \boldsymbol{\xi}) = \frac{\rho}{\sqrt{\theta}^d} \widetilde{f}(t, \mathbf{x}, \boldsymbol{\xi})$

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$$\left(\frac{1}{\rho} D_t \rho - \frac{d}{2\theta} D_t \theta\right) \widetilde{f} + D_t \widetilde{f} +$$
$$\sqrt{\theta} \xi_j \left(\left(\frac{1}{\rho} \partial_{x_j} \rho - \frac{d}{2\theta} \partial_{x_j} \theta\right) \widetilde{f} + \partial_{x_j} \widetilde{f} \right) +$$
$$\partial_{\xi_j} \widetilde{f} \left(-\frac{1}{\sqrt{\theta}} \left(D_t v_j + \sqrt{\theta} \xi_i \partial_{x_i} v_j \right) - \frac{1}{2\theta} \xi_j \left(D_t \theta + \sqrt{\theta} \xi_i \partial_{x_i} \theta \right) \right) = 0.$$

Compatibility Conditions

Macroscopic variables $\rho, \mathbf{v}, \theta$ are *moments* of the PDF f

$$
\begin{aligned}
\rho(t,\mathbf{x}) &= \int_{\mathbb{R}^d} f(t,\mathbf{x},\mathbf{c})\, d\mathbf{c}, \\
\rho(t,\mathbf{x})\mathbf{v}(t,\mathbf{x}) &= \int_{\mathbb{R}^d} \mathbf{c} f(t,\mathbf{x},\mathbf{c})\, d\mathbf{c}, \\
d \cdot \rho(t,\mathbf{x})\theta(t,\mathbf{x}) &= \int_{\mathbb{R}^d} |\mathbf{c}-\mathbf{v}|^2 f(t,\mathbf{x},\mathbf{c})\, d\mathbf{c}.
\end{aligned}
$$

Compatibility Conditions

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\begin{aligned}
1 &= \int_{\mathbb{R}^d} \widetilde{f}(\boldsymbol{\xi})\, d\boldsymbol{\xi}, \\
\mathbf{0} &= \int_{\mathbb{R}^d} \boldsymbol{\xi}\widetilde{f}(\boldsymbol{\xi})\, d\boldsymbol{\xi}, \\
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\end{aligned}
$$

Ansatz

$$
\widetilde{f}(t, \mathbf{x}, \xi) = \sum_{i=0}^{n} \alpha_i(t, \mathbf{x}) \Phi_i(\xi)
$$

Hyperbolicity

Hyperbolicity

Definition: Hyperbolicity

The PDE system of the form

$$\frac{\partial}{\partial t}\mathbf{u} + \mathbf{A}(\mathbf{u})\frac{\partial}{\partial x}\mathbf{u} = 0$$

is *globally hyperbolic* if matrix **A** is diagonalizable with real eigenvalues for every **u**.

Hyperbolicity necessary for

- Well-posedness of the initial value problem and stable solutions
- Physical solutions with real-valued propagation speed

Failure of Classical Methods

Discrete Velocity Method

Ansatz: Discrete point evaluations of transformed Boltzmann Equation

Projection: $\int_{\mathbb{R}^d} \cdot \ \delta(\boldsymbol{\xi} - \boldsymbol{\xi}_{\mathbf{j}}) d\boldsymbol{\xi}$

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Grad's Method [Grad, 1949]

Ansatz: $\widetilde{f}(t, \mathbf{x}, \boldsymbol{\xi}) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{\boldsymbol{\xi}^2}{2}\right) \sum_{i=0}^{n} \alpha_i(t, \mathbf{x}) He_i(\boldsymbol{\xi})$

Projection: $\int_{\mathbb{R}^d} \cdot \; He_j(\boldsymbol{\xi}) d\boldsymbol{\xi}$

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Methods are not globally hyperbolic, imaginary eigenvalues

Hyperbolic Approximation

Quadrature-based Projection Method [Koellermeier et al., 2014]

Ansatz: $\widetilde{f}(t, \mathbf{x}, \xi) = \sum_{i=0}^{n} \alpha_i(t, \mathbf{x}) \Phi_i(\xi)$

Projection: $\int_{\mathbb{R}^d} \cdot \quad \Psi_j(\xi) d\xi \approx \sum_{k=0}^{n} w_k \quad \cdot \, |_{\xi_\mathbf{k}} \quad \Psi_j(\xi_\mathbf{k})$

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Global Hyperbolicity

PDE system is globally hyperbolic, eigenvalues can be precomputed under some simple conditions on $\Phi_i, \Psi_i, \xi_\mathbf{k}$ and w_k

Hermite Basis and Gauss-Hermite Quadrature

Hermite Basis and Gauss-Hermite Quadrature

Quadrature-based Projection Method

Grad ansatz: $\Phi_i(\xi) = \frac{1}{\sqrt{2\pi}} e^{-\xi/2} He_i(\xi), \quad \Psi_i(\xi) = He_i(\xi)$

Gauss-Hermite quadrature: Points ξ_k are roots of $He_{N+1}(\xi), w_k$ are corresponding weights

Hermite Basis and Gauss-Hermite Quadrature

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Global Hyperbolicity

- Global hyperbolicity has been analytically proven in 1D and general d-dimensional case
- Eigenvalues contain roots of Hermite polynomials:

$$\lambda_k = \sqrt{\theta}\, \xi_k + v$$

Comparison to Grad and Cai in 1D

Grad's Method [Grad, 1949]

Ansatz: Expansion in Hermite ansatz functions

Projection: Exact integration

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Cai's Method [Cai et al. 2014]

Ansatz: Arbitrary basis function
Regularization: Cut-off higher terms during computations
Additional terms only in last equation

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Ansatz: Expansion in Hermite ansatz functions
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Cai's Method [Cai et al. 2014]

Ansatz: Arbitrary basis function
Regularization: Cut-off higher terms during computations
Additional terms only in last equation

Quadrature-based projection Method [Koellermeier et al., 2014]

Ansatz: Arbitrary basis function
Regularization: Corresponding Gaussian-quadrature rule
Additional terms in last two equations, includes Cai's regularisation terms

Summary and Further Work

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Results

- Development of abstract framework
- Derivation of hyperbolicity conditions and eigenvalues
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Quadrature-based projection methods derive globally hyperbolic PDE systems from the transformed Boltzmann Equation

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Quadrature-based projection methods derive globally hyperbolic PDE systems from the transformed Boltzmann Equation

Further Work

- Different expansions, basis functions, quadrature formulas
- Use of sparse-tensor product approximations
- Numerics for the (non-conservative) hyperbolic PDE system

References

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Hermite Polynomials 1D

$$He_n(\xi) := \frac{1}{\sqrt{n!}}\widetilde{He}_n(\xi), \quad \text{for} \quad n \in \mathbb{N}.$$

Orthonormality w.r.t. the scalar product:

$$\langle \phi, \psi \rangle_w = \int_{-\infty}^{+\infty} \phi(\xi)\psi(\xi)w(\xi)d\xi, \quad \text{for} \quad w(\xi) := \frac{1}{\sqrt{2\pi}}e^{-\xi^2/2}.$$

Recursion formulas:

$$\begin{aligned}
\xi He_n(\xi) &= \sqrt{n+1}He_{n+1}(\xi) + \sqrt{n}He_{n-1}(\xi), \\
He_n'(\xi) &= \sqrt{n}He_{n-1}(\xi), \\
\frac{d}{d\xi}\Big(He_n(\xi)w(\xi)\Big) &= -w(\xi)\sqrt{n+1}He_{n+1}(\xi), \\
\xi\frac{d}{d\xi}\Big(He_n(\xi)w(\xi)\Big) &= -w(\xi)\sqrt{n+1}\Big(\sqrt{n+2}He_{n+2}(\xi) + \sqrt{n+1}He_n(\xi)\Big).
\end{aligned}$$

Multi-dimensional Expansion

$$\widetilde{f}(t,x,\xi) = \sum_{\alpha_i \leq N_i} \kappa_{\boldsymbol{\alpha}}(t,\mathbf{x})\phi_{\boldsymbol{\alpha}}(\boldsymbol{\xi}),$$

Basis functions are tensor product of 1D Hermite functions:

$$\phi_{\boldsymbol{\alpha}}(\boldsymbol{\xi}) = \prod_{i=1}^{d} \phi_{\alpha_i}(\xi_i), \quad \phi_i(x) = He_i(x)\frac{1}{\sqrt{2\pi}}e^{-x^2/2} \quad \psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi}) = \prod_{i=1}^{d} He_i(\xi_i),$$

Recursion formulas:

$$\begin{aligned} \frac{\partial \Phi_{\boldsymbol{\alpha}}}{\partial \xi_i} &= -\sqrt{\alpha_i + 1}\Phi_{\boldsymbol{\alpha}+\mathbf{e_i}}, \\ \xi_i \frac{\partial \Phi_{\boldsymbol{\alpha}}}{\partial \xi_i} &= -\sqrt{\alpha_i + 1}\left(\sqrt{\alpha_i + 2}\Phi_{\boldsymbol{\alpha}+2\mathbf{e_i}} + \sqrt{\alpha_i + 1}\Phi_{\boldsymbol{\alpha}}\right). \end{aligned}$$

Gauss-Hermite Quadrature

Multi-dimensional Gauss-Hermite quadrature

$$\int_{\mathbb{R}^d} g(\boldsymbol{\xi})\mathbf{d}\boldsymbol{\xi} \approx \sum_{i_1=0}^{N_1} \cdots \sum_{i_d=0}^{N_d} g\left((\xi_1)_{i_1}, \ldots, (\xi_d)_{i_d}\right) w_{1,i_1} \cdot \ldots w_{d,i_d},$$

Quadrature points $(\xi_i)_j$ and weights $w_{i,j}$:

$$\begin{aligned} (\xi_i)_j &= j\text{-th root of } He_{N_i+1}(\xi), \\ w_{i,j} &= j\text{-th weight of quadrature formula in direction } i. \end{aligned}$$

Compact notation for quadrature formula

$$\int_{\mathbb{R}^d} g(\boldsymbol{\xi})\mathbf{d}\boldsymbol{\xi} \approx \sum_{k=1}^{N} g\left(\boldsymbol{\xi}_{\mathbf{k}}\right) w_k.$$

Hyperbolicity Conditions

Emerging PDE system after compatibility conditions:

$$\boldsymbol{\Psi}^T \mathbf{W} \mathbf{A}_{\boldsymbol{\beta}} \boldsymbol{\Lambda}_{\beta} \frac{D}{Dt}\mathbf{u} + \sum_{i=1}^{d} \boldsymbol{\Psi}^T \mathbf{W} \boldsymbol{\Xi}_{\mathbf{i}} \mathbf{A}_{\boldsymbol{\beta}} \boldsymbol{\Lambda}_{\beta} \sqrt{\theta} \frac{\partial}{\partial x_i}\mathbf{u} = 0 \qquad (1)$$

Hyperbolicity conditions:

$$\begin{aligned}
&(1)\ \text{Regularity of matrix } \boldsymbol{\Psi}, \\
&(2)\ \text{Regularity of matrix } \mathbf{W} \text{ or equivalently } \omega_i \neq 0,\ \forall i = 0, \dots, n, \\
&(3)\ \text{Regularity of matrix } \boldsymbol{\Lambda}_{\beta}, \\
&(4)\ \text{Regularity of matrix } \mathbf{A}_{\boldsymbol{\beta}} \text{ or equivalently } rank \mathbf{A}_{\boldsymbol{\beta}} = n+1.
\end{aligned} \qquad (2)$$