# On an Operator Projection Framework for Kinetic Equations

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# Outline

1. Review of Quadrature-Based Moment Equations
2. Quadrature-Based Cut-Off
3. Quadrature-Based Projection
4. Operator Projection Framework

# Review of Quadrature-Based Moment Equations

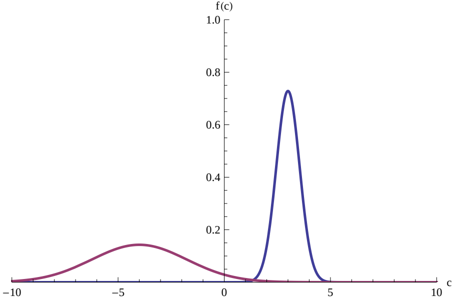
# Boltzmann Transport Equation

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

**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 (1D)




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

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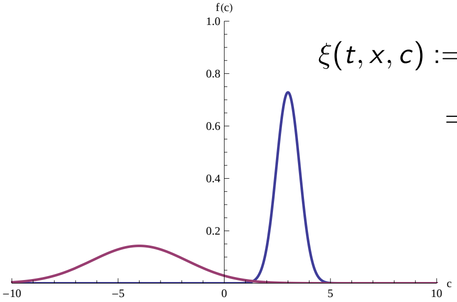


$$\xi(t,x,c) := \frac{c - v(t,x)}{\sqrt{\theta(t,x)}}$$

$$\Longrightarrow$$

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

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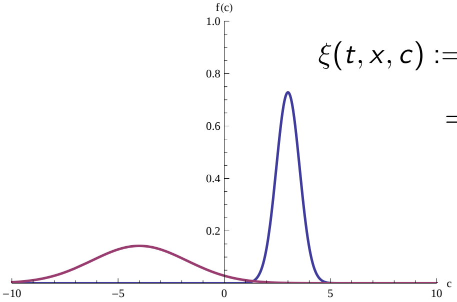


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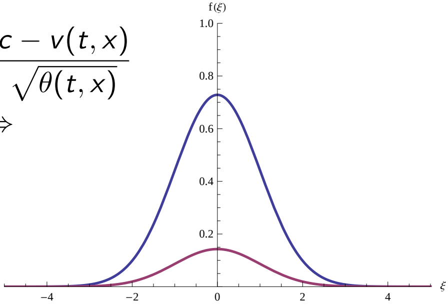


$$f(c) = \frac{\rho}{\sqrt{2\pi\theta}} \exp\left(-\frac{(c-v)^2}{2\theta}\right) \qquad f(\xi) = \frac{\rho}{\sqrt{2\pi\theta}} \exp\left(-\frac{\xi^2}{2}\right)$$

Lagrangian velocity space reduces numerical complexity

# Transformation of Boltzmann Equation

$$\frac{\partial}{\partial t} f(t,x,c) + c \frac{\partial}{\partial x} f(t,x,c) = 0$$

$$\Downarrow$$

$$D_t f + \sqrt{\theta}\xi\partial_x f + \partial_\xi f \left( -\frac{1}{\sqrt{\theta}} \left( D_t v + \sqrt{\theta}\xi\partial_x v \right) - \frac{1}{2\theta}\xi \left( D_t\theta + \sqrt{\theta}\xi\partial_x\theta \right) \right) = 0$$

- Additional terms from chain rule for $f$, with $\xi(t,x,c) := \frac{c - v(t,\mathbf{x})}{\sqrt{\theta(t,x)}}$
- Convective time derivative $D_t := \partial_t + v\partial_x$
- Additional equations for $v$ and $\theta$ from definition of moments

# Ansatz and Expansion

## Expansion

$$f(t,x,\xi) = \sum_{i=0}^{n} f_i(t,x)\mathcal{H}_i(\xi)$$

## Weight and basis function

$$w(\xi) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{\xi^2}{2}\right)$$

$$\mathcal{H}_k(\xi) = (-1)^k \frac{d^k w(\xi)}{d\xi^k} = w(\xi) He_k(\xi)$$

# Quadrature-Based Moment Equations

## Standard approach by GRAD [5]

Multiplication with test function $He_k(\xi)$ and integration over $\xi$

$$\int_{\mathbb{R}} \cdot \quad He_k(\xi) d\xi$$

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Multiplication with test function $He_k(\xi)$ and integration over $\xi$

$$\int_{\mathbb{R}} \cdot \quad He_k(\xi) d\xi$$

## Quadrature-Based Moment Method (QBME) [1]

Substitute integration by Gaussian quadrature

$$\int_{\mathbb{R}} \cdot \quad He_k(\xi) d\xi \approx \sum_{k=0}^{n} w_k \quad \cdot \, |_{\xi_k} \; He_k(\xi_k)$$

## QBME result

Globally hyperbolic equations

# Further work on QBME

## Further work on QBME

- Extension of framework to multi-dimensional case
- Hyperbolicity proof for multi-dimensional case
- Development of diagram notation to visualize QBME derivation

## Problems

- Multi-dimensional systems not rotationally invariant
- Depends on existence of Gaussian quadrature rule
- Generalization to other equations, weights, basis functions

# Quadrature-Based Cut-Off

# Towards a Quadrature-Based Cut-Off

$$D_t f + \sqrt{\theta}\xi\partial_x f + \partial_\xi f \left( -\frac{1}{\sqrt{\theta}} \left( D_t v + \sqrt{\theta}\xi\partial_x v \right) - \frac{1}{2\theta}\xi \left( D_t \theta + \sqrt{\theta}\xi\partial_x \theta \right) \right) = 0$$

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## Use recursion formulas for basis function

- Basis function: $\mathcal{H}_k(\xi) := \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{\xi^2}{2}\right) He_k(\xi)$
- Derivative of basis function: $\frac{\partial \mathcal{H}_k(\xi)}{\partial \xi} = -\mathcal{H}_{k+1}(\xi)$
- $\xi$ multiplication: $\xi \cdot \mathcal{H}_k(\xi) = \mathcal{H}_{k+1}(\xi) + k\mathcal{H}_{k-1}(\xi)$

## Properties of Gaussian quadrature rule

Gaussian quadrature points are zeros of $\mathcal{H}_{n+1}(\xi)$, i.e. $\mathcal{H}_{n+1}(\xi_k) = 0$

# Cut-Off Procedure

## Use recursion formulas for basis function

- Expand $f$ with basis functions
- Insert expanded $f$ into transformed Boltzmann equation
- Perform calculations using recursion formulas and derivative
- Do a projection using multiplication and integration or quadrature

## Properties of Gaussian quadrature rule

Gaussian quadrature points are zeros of $\mathcal{H}_{n+1}(\xi)$, i.e. $\mathcal{H}_{n+1}(\xi_k) = 0$

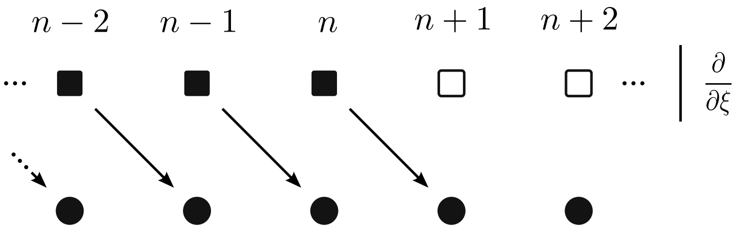
## Remember

$$\frac{\partial \mathcal{H}_k(\xi)}{\partial \xi} = -\mathcal{H}_{k+1}(\xi), \qquad \xi \cdot \mathcal{H}_k(\xi) = \mathcal{H}_{k+1}(\xi) + k\mathcal{H}_{k-1}(\xi)$$

# Cut-Off in Grad's method

| | | | | | | |
|---|---|---|---|---|---|---|
| | $n-2$ | $n-1$ | $n$ | $n+1$ | $n+2$ | |
| … | ■ | ■ | ■ | □ | □ | … |

# Cut-Off in GRAD's method



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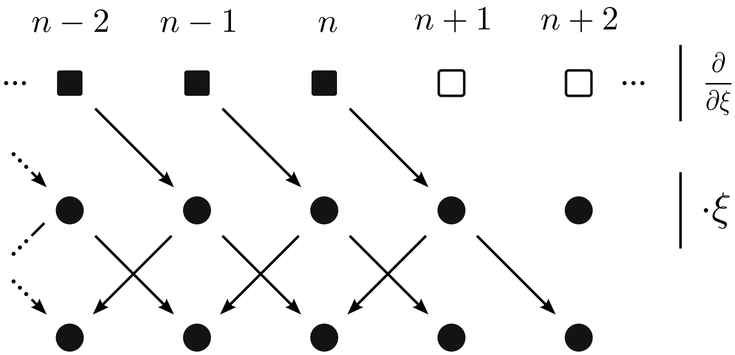

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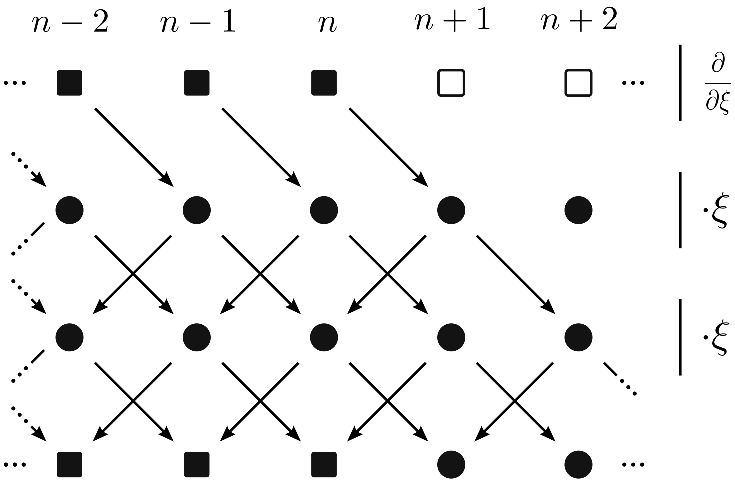

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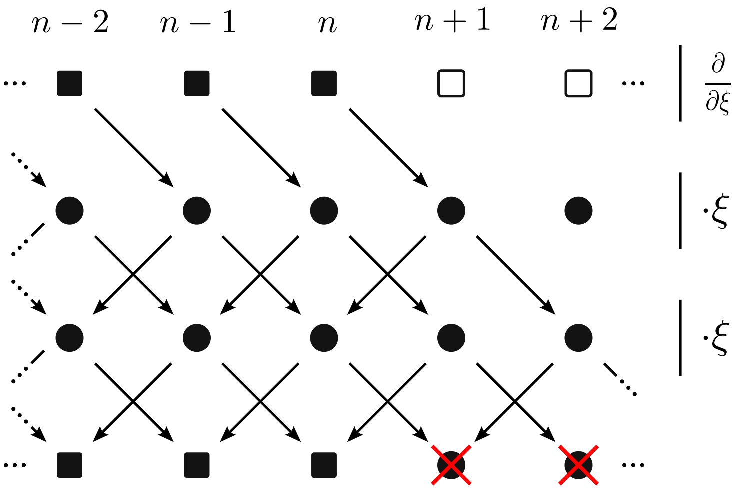
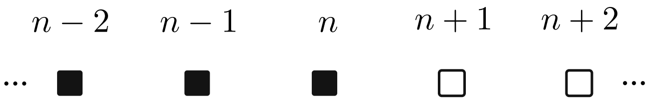


# Cut-Off in Quadrature-Based Method



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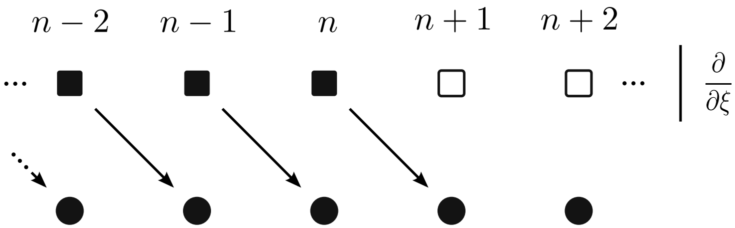

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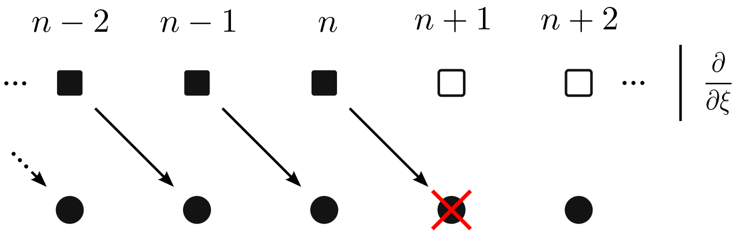

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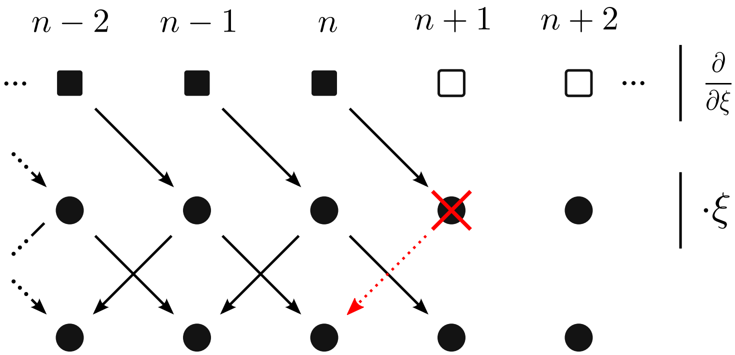

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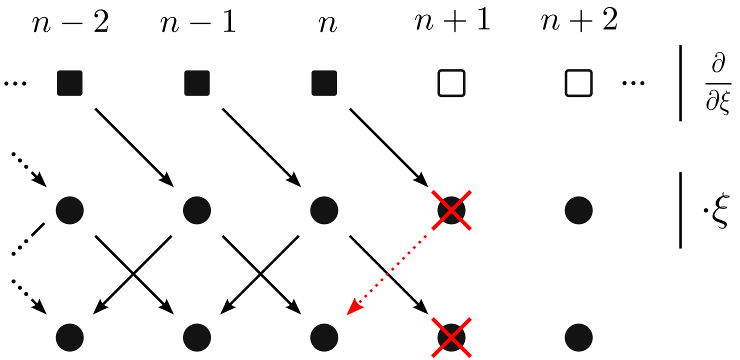

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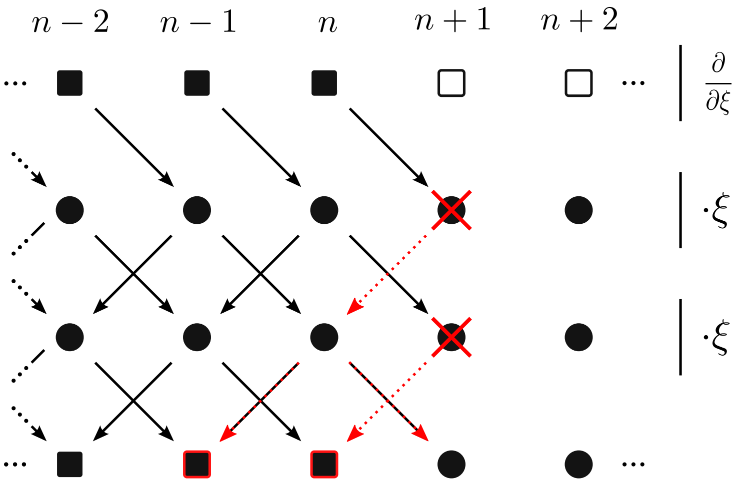

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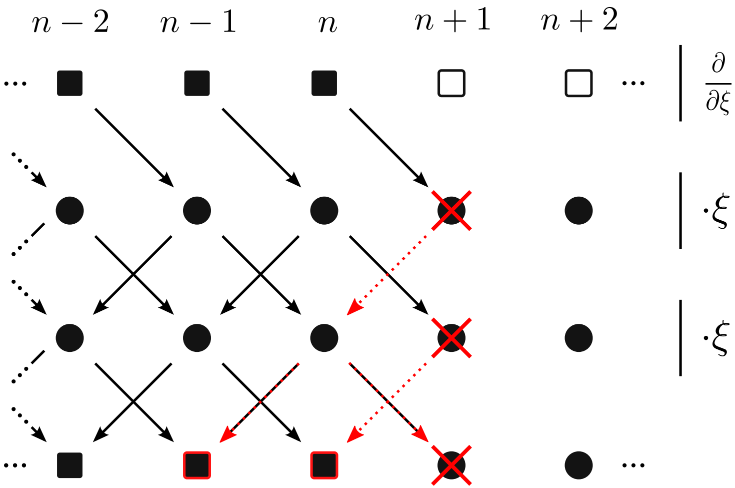
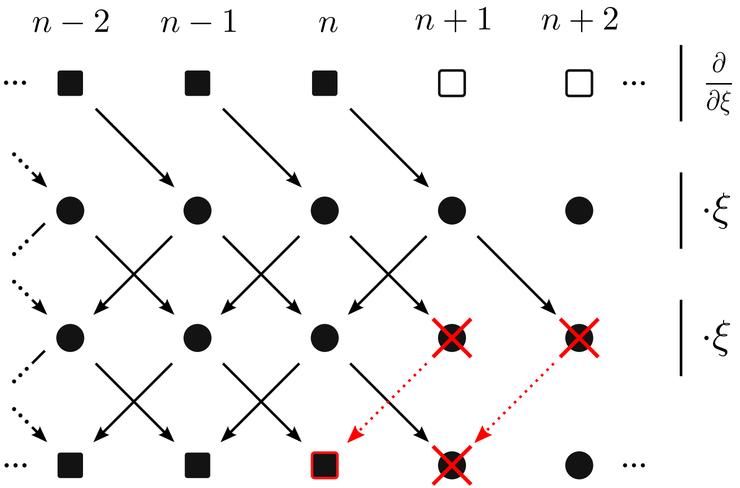


# Cut-Off in CAI's Method



# Quadrature-Based Projection

# Towards a Quadrature-Based Projection [3]

$$\frac{\partial f}{\partial t} + c\frac{\partial f}{\partial x} = 0$$

- Use basis functions and recursion formulas
- Define unknowns $\mathbf{w} = (\rho, v, \theta, f_3, \ldots) \in \mathbb{R}^\infty$

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$$\mathbf{M}_1\mathbf{D}\frac{\partial \mathbf{w}}{\partial t} + \mathbf{M}_2\mathbf{M}_1\mathbf{D}\frac{\partial \mathbf{w}}{\partial x} = 0$$

# GRAD's Projection

$$\mathbf{M}_1 \mathbf{D} \frac{\partial \mathbf{w}}{\partial t} + \mathbf{M}_2 \mathbf{M}_1 \mathbf{D} \frac{\partial \mathbf{w}}{\partial x} = 0$$

# GRAD's Projection

$$(\mathbf{M}_1\mathbf{D})_N \frac{\partial \mathbf{w}_N}{\partial t} + (\mathbf{M}_2\mathbf{M}_1\mathbf{D})_N \frac{\partial \mathbf{w}_N}{\partial x} = 0$$

# GRAD's Projection

$$(\mathbf{M}_1\mathbf{D})_N \frac{\partial \mathbf{w}_N}{\partial t} + (\mathbf{M}_2\mathbf{M}_1\mathbf{D})_N \frac{\partial \mathbf{w}_N}{\partial x} = 0$$

## Define projection matrix and its *inverse*

$$\begin{aligned} \mathbf{P}_N &= (\mathbf{I}_N, \mathbf{0}) \in \mathbb{R}^{N\times\infty} \\ \mathbf{P}_N^T &= \begin{pmatrix} \mathbf{I}_N \\ \mathbf{0} \end{pmatrix} \in \mathbb{R}^{\infty\times N} \end{aligned}$$

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## Apply projection to parts of the equation

$$\begin{aligned} (\mathbf{M}_1\mathbf{D})_N &= \mathbf{P}_N (\mathbf{M}_1\mathbf{D}) \mathbf{P}_N^T \\ \mathbf{w}_N &= \mathbf{P}_N \mathbf{w} \end{aligned}$$

Only locally hyperbolic, loss of hyperbolicity possible

# Quadrature-Based Projection

$$\mathbf{M}_1 \mathbf{D} \frac{\partial \mathbf{w}}{\partial t} + \mathbf{M}_2 \mathbf{M}_1 \mathbf{D} \frac{\partial \mathbf{w}}{\partial x} = 0$$

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$$(\mathbf{M}_1)_N\,(\mathbf{D})_N\,\frac{\partial \mathbf{w}_N}{\partial t} + (\mathbf{M}_2)_N\,(\mathbf{M}_1)_N\,(\mathbf{D})_N\,\frac{\partial \mathbf{w}_N}{\partial x} = 0$$

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- Globally hyperbolic
- Changes last two equations

# CAI's Projection (HME)

$$(\mathbf{M}_1\mathbf{D})_N \frac{\partial \mathbf{w}_N}{\partial t} + (\mathbf{M}_2)_N (\mathbf{M}_1\mathbf{D})_N \frac{\partial \mathbf{w}_N}{\partial x} = 0$$

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- Globally hyperbolic
- Changes last equation
- Quadrature-based method can be written with different $\mathbf{P}_N$

# Operator Projection Framework

# Generalization of the framework

## Aim

Generalize projection procedure to include all methods in one framework that also allows derivation of new models

## Inputs

- Kinetic equation, e.g. $\partial_t f + c\partial_x f = 0$
- Weight function and basis, e.g. $w(\xi) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{\xi^2}{2}\right)$, $\xi = \frac{c-v(t,x)}{\sqrt{\theta(t,x)}}$ and weighted Hermite polynomial basis $\mathcal{H}_i(\xi)$
- Projection operator, e.g. Cut-off
- Projection strategy, e.g. according to QBME or HME

# Projection Operator

## Expansion

$$f(t,x,\xi) = \sum_{i=1}^{\infty} f_i(t,x)\Phi_i(\xi) = \langle \mathbf{f}, \mathbf{\Phi} \rangle_\infty$$

## Projected expansion, e.g. cut-off

$$\mathcal{P}f(t,x,\xi) = \sum_{i=1}^{N} \widetilde{f}_i(t,x)\widetilde{\Phi_i}(\xi) = \langle \mathbf{Pf}, \mathbf{P\Phi} \rangle_N$$

## Example: Cut-off projection

$$\mathbf{P} = (\mathbf{I}_N, \mathbf{0}) \in \mathbb{R}^{N\times\infty}$$

# Step-by-step procedure I: Setup

1. Choose weight function $w(\xi)$ and basis $\mathbf{\Phi}$ of weighted polynomial space
2. Choose subspace and determine projection operator $\mathcal{P}$
3. Expand distribution function $f(t, x, \xi) = \langle \mathbf{f}, \mathbf{\Phi} \rangle_\infty$
4. Eliminate unknowns using definition of moments $\mathbf{f} \rightarrow \mathbf{w}$
5. Project distribution function $\mathcal{P}f(t, x, \xi) = \langle \mathbf{Pf}, \mathbf{P\Phi} \rangle_N$

# Step-by-step procedure II: Derivation

$$\partial_t f + c\partial_x f = 0$$

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$$\partial_t f + c\partial_x f = 0$$

6. Compute derivatives $\frac{\partial}{\partial s}\mathcal{P}f(t,x,\xi) = \langle \mathbf{D}\mathbf{P}^T \frac{\partial}{\partial s}\mathbf{P}\mathbf{w}, \mathbf{\Phi}\rangle_\infty$
7. Project derivatives $\mathcal{P}\frac{\partial}{\partial s}\mathcal{P}f(t,x,\xi) = \langle \mathbf{P}\mathbf{D}\mathbf{P}^T \frac{\partial}{\partial s}\mathbf{P}\mathbf{w}, \mathbf{P}\mathbf{\Phi}\rangle_N$
8. Multiply with velocity $c\mathcal{P}\frac{\partial}{\partial s}\mathcal{P}f(t,x,\xi) = \langle \mathbf{M}\mathbf{P}^T\mathbf{P}\mathbf{D}\mathbf{P}^T \frac{\partial}{\partial s}\mathbf{P}\mathbf{w}, \mathbf{\Phi}\rangle_\infty$
9. Project product $\mathcal{P}c\mathcal{P}\frac{\partial}{\partial s}\mathcal{P}f(t,x,\xi) = \langle \mathbf{P}\mathbf{M}\mathbf{P}^T\mathbf{P}\mathbf{D}\mathbf{P}^T \frac{\partial}{\partial s}\mathbf{P}\mathbf{w}, \mathbf{P}\mathbf{\Phi}\rangle_N$
10. Match coefficients to obtain regularized equations

$$\mathbf{P}\mathbf{D}\mathbf{P}^T \frac{\partial}{\partial t}\mathbf{P}\mathbf{w} + \mathbf{P}\mathbf{M}\mathbf{P}^T\mathbf{P}\mathbf{D}\mathbf{P}^T \frac{\partial}{\partial x}\mathbf{P}\mathbf{w} = 0$$

# Application of the framework

## Existing models

- Hyperbolic moment equations (HME) (CAI et al. [4])
- Anisotropic hyperbolic moment equations (AHME)
- GRAD 13 hyperbolic regularization
- Maximum entropy method
- Quadrature-based moment equations (QBME) (1D)

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## New models

- Regularization of GRAD's ordered moment systems (G13, G26, G45)
- multi-dimensional Quadrature-based moment equations
- ...

# Conclusion

# Summary and Further Work

## From quadrature to projection operators

- Includes almost all existing models
- Easy derivation of new models
- Global hyperbolicity and rotational invariance

## Further Work

- Numerics for the (non-conservative) hyperbolic PDE system

**Thank you for your attention**

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