Toward Making the Kinetic Boltzmann Equation Tractable

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Deterministic Evaluation of the Collision Operator Using Fourier Galerkin Discretization in the Velocity Variable

Fourier-Galerkin Discretization

L. Pareschi and B. Perthame (1996):

$$Q[f](t,\vec{v}) = \int_{\mathbb{R}^3}\int_{\mathbb{S}^2} (f(t,\vec{v}')f(t,\vec{v}_1') - f(t,\vec{v})f(t,\vec{v}_1))B(|g|,w)\,dw\,d\vec{v}_1,$$

$$\vec{v}' = (\vec{v}+\vec{v}_1)/2 + \|\vec{g}\|\vec{w}/2, \qquad \vec{v}_1' = (\vec{v}+\vec{v}_1)/2 - \|\vec{g}\|\vec{w}/2\,,$$

Assume periodicity of the kernel (N runs over 3D),

$$\tilde{f}_N(\vec{v}) = \sum_{h=-N}^{N} \phi_{\vec{h}} \mathrm{e}^{\imath \vec{v}\cdot\vec{h}\pi/T}, \qquad \phi_{\vec{h}} = \frac{1}{(2\pi)^3}\int_{[-T,T]^3} f(\vec{v})e^{-\imath\vec{v}\cdot\vec{h}/T}d\vec{v}.$$

Upon substitution in $Q[f](t,\vec{v})$

$$Q[f](t,\vec{v}) = \sum_{h=-N}^{N}\sum_{k=-N}^{N}\phi_k\phi_h \int_{[-T,T]^3}\int_{\mathbb{S}^2} B(|g|,w)(\mathrm{e}^{\imath\vec{v}'\cdot\vec{h}\pi/T}e^{\imath\vec{v}_1'\cdot\vec{k}\pi/T} - \mathrm{e}^{\imath\vec{v}\cdot\vec{h}\pi/T}e^{\imath\vec{v}_1\cdot\vec{k}\pi/T})\,dw\,d\vec{v}_1,$$

Fourier-Galerkin Discretization

$$Q[f](t,\vec{v}) = \sum_{h=-N}^{N}\sum_{k=-N}^{N} \phi_k\phi_h \int_{[-T,T]^3}\int_{\mathbb{S}^2} B(|g|,w)(\mathrm{e}^{\imath\vec{v}'\cdot\vec{h}\pi/T} e^{\imath\vec{v}_1'\cdot\vec{k}\pi/T} - \mathrm{e}^{\imath\vec{v}\cdot\vec{h}\pi/T} e^{\imath\vec{v}_1\cdot\vec{k}\pi/T})\, dw\, d\vec{v}_1$$

$$= \sum_{h=-N}^{N}\sum_{\vec{k}=-N}^{N} \phi_{\vec{k}}\phi_{\vec{h}} \mathrm{e}^{\imath\vec{v}\cdot(\vec{h}+\vec{k})}\beta(\vec{h},\vec{k})$$

where

$$\beta(\vec{h},\vec{k}) = \int_{[-T,T]^3}\int_{\mathbb{S}^2} B(|g|,w)(\mathrm{e}^{\imath(\|g\|\vec{w}\cdot(\vec{h}-\vec{k})-\vec{g}\cdot(\vec{h}+\vec{k}))\pi/2T} - \mathrm{e}^{\imath\vec{g}\cdot\vec{k}\pi/T})\, dw\, d\vec{v}_1,$$

By re-organizing the double sum,

$$Q[f](t,\vec{v}) = \sum_{\vec{l}=-2N}^{2N} \mathrm{e}^{\imath\vec{v}\cdot\vec{l}} \left[\sum_{\substack{\vec{h},\vec{k}=-N \\ \vec{h}+\vec{k}=\vec{l}}}^{N} \phi_{\vec{k}}\phi_{\vec{h}}\beta(\vec{h},\vec{k}) \right] = \sum_{\vec{l}=-2N}^{2N} \mathrm{e}^{\imath\vec{v}\cdot\vec{l}}\hat{Q}_{\vec{l}}$$

Fourier-Galerkin Discretization

Approach:

1. Compute $\phi_{\vec{h}}$ from $f(\vec{v})$ using fast Fourier transform in $O(n^3 \log n)$ operations;
2. Compute the Fourier transform of the collision operator

$$\hat{Q}_{\vec{l}} = \sum_{\substack{\vec{h},\vec{k}=-N \\ \vec{h}+\vec{k}=\vec{l}}}^{N} \phi_{\vec{k}} \phi_{\vec{h}} \beta(\vec{h}, \vec{k})$$

   in $O(n^6)$ operations.
3. Compute $Q[f](t, \vec{v})$ from $\hat{Q}_{\vec{l}}$ using inverse Fourier transform in $O(n^3 \log n)$ operations.

The method has complexity of $O(n^6)$ operations.

Fast Method Based on Carleman Representation

A. Bobylev and S. Rjasanow (1999). Carleman representation

$$Q[f](\vec{v}) = \int_{\mathbb{R}^3}\int_{\mathbb{S}^2} (f(t,\vec{v}')f(t,\vec{v}_1') - f(t,\vec{v})f(t,\vec{v}_1))B(|g|,w)\,dw\,d\vec{v}_1$$

$$= \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \delta\Big((\vec{z},\vec{u}) + \frac{1}{2}\|\vec{z}\|^2\Big)\Big(f\Big(\vec{v}+\frac{1}{2}\vec{z}\Big)f\Big(\vec{v}_1-\frac{1}{2}\vec{z}\Big)$$

$$- f(\vec{v})f(\vec{v}_1))B(|g|,z)\,d\vec{v}_1\,d\vec{z}$$

$$= 4\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \delta\Big((\vec{z},\vec{y})\Big)\Big(f(\vec{v}+\vec{z})f(\vec{v}+\vec{y}) - f(\vec{v})f(\vec{v}+\vec{y}+\vec{z})B(|g|,z)\,d\vec{y}\,d\vec{z}$$

Switch to spherical coordinates, assume hard spheres molecules

$$\vec{y} = \rho_1\vec{e}_1, \quad \vec{z} = \rho_2\vec{e}_2, \quad \vec{e}_{1,2} \in \mathbb{S}^2$$

After additional transformation rewrite in ray-transform form

$$Q(\vec{v}) = 4\int_{\mathbb{S}^2}\int_{\mathbb{S}^2} \delta\Big((\vec{e}_1,\vec{e}_2)\Big)\Big((\int_0^\infty \rho_1 f(\vec{v}+\rho_1\vec{e}_1)d\rho_1)(\int_0^\infty \rho_2 f(\vec{v}+\rho_2\vec{e}_2)d\rho_2)$$

$$- f(\vec{v})\int_0^\infty\int_0^\infty \rho_1\rho_2 f(\vec{v}+\rho_1\vec{e}_1+\rho_2\vec{e}_2)\,d\rho_1\,d\rho_2\Big)de_1\,de_2$$

Fast Fourier-Galerkin Method

To derive Fast Fourier-Galerkin Method, we need to re-write the

$$\int_{\mathbb{R}^3}\int_{S^2} \quad \text{as} \quad \int_{\mathbb{R}^3}\int_{\mathbb{R}^3}$$

To do so, we can use Dirac delta-function

$$f(\xi) = \int \delta(x-\xi) f(x)\, dx$$

In particular, up to possibly a scalar factor

$$\int_{S^2} f(x,y,z)\, d\sigma = C \int_{\mathbb{R}^3} f(x,y,z)\delta(\sqrt{x^2+y^2+z^2}-1)\, dx\, dy\, dz$$

Fast Fourier-Galerkin Method

F. Filbet, C. Mouhot and L. Pareschi (2006), L. Pareschi and C. Mouhot (2003,2006). Use Carleman representation in Fourier-Galerkin method.

$$Q(\vec{v}) = 8 \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} B\left(\|\vec{x}+\vec{y}\|, -\frac{\vec{x}\cdot(\vec{x}+\vec{y})}{\|\vec{x}\|\|\vec{x}+\vec{y}\|} \right) \frac{1}{\|\vec{x}+\vec{y}\|}$$

$$\delta(\vec{x}\cdot\vec{y})[f(\vec{v}+\vec{y})f(\vec{v}+\vec{x}) - f(\vec{v})f(\vec{v}+\vec{x}+\vec{y})]\, d\vec{x}d\vec{y}.$$

Approximate

$$\tilde{f}_N(\vec{v}) = \sum_{h=-N}^{N} \phi_{\vec{h}} e^{\imath \vec{v}\cdot\vec{h}}, \qquad \phi_{\vec{h}} = \frac{1}{(2\pi)^3} \int_{[-\pi,\pi]^3} f(\vec{v}) e^{-\imath \vec{v}\cdot\vec{h}} d\vec{v}.$$

Substituting into collision operator, transforming

$$\hat{Q}_k = \sum_{\substack{l,m=-N \\ l+m=k}}^{N} \hat{\beta}(l,m)\hat{f}_l\hat{f}_m, \quad k=-N,\dots,N$$

where

$$\hat{\beta}(l,m) = \int_{[-\pi,\pi]^3} \int_{[-\pi,\pi]^3} \tilde{B}(x,y)\delta(\vec{x}\cdot\vec{y})[e^{\imath l\cdot x}e^{\imath m\cdot y} - e^{\imath m\cdot(x+y)}]\, dx\, dy$$

Fast Fourier-Galerkin Method

The fast approach is obtained by recognizing that $l + m = k$ indicates convolution,

$$\hat{Q}_k = \sum_{\substack{l,m=-N \\ l+m=k}}^{N} \hat{\beta}(l,m)\hat{f}_l\hat{f}_m = \sum_{m=-N}^{N} \hat{\beta}(k-m,m)\hat{f}_{k-m}\hat{f}_m$$

By splitting

$$\hat{\beta}(l,m) \approx \sum_{p=1}^{A} \alpha_p(l)\alpha'_p(m)$$

we obtain

$$\hat{Q}_k = \sum_{p=1}^{A}\sum_{m=-N}^{N} (\alpha_p(k-m)\hat{f}_{k-m})(\alpha'_p(m)\hat{f}_m)$$

which is $O(AN\log N)$ operations.

Fast Fourier-Galerkin Method

To find a good splitting for $\hat{\beta}(l, m)$ the authors turned to Carleman representation. Assume $B(\|g\|, w) = b(\theta, \varepsilon)\|g\|^{\alpha}$, then $\tilde{B}(x, y) = a(x)b(x)$ and

$$\beta(l, m) = \frac{1}{4}\int_{\mathbb{S}^2}\int_{\mathbb{S}^2}\delta(e{\cdot}e')\Big[\int_{[-\pi,\pi]} \mathrm{e}^{\imath\rho(l\cdot e)}\,d\rho\Big]\Big[\int_{[-\pi,\pi]} \mathrm{e}^{\imath\rho'(m\cdot e')}\,d\rho'\Big]\,de\,de'$$

By discretizing $\int_{\mathbb{S}^2}\int_{\mathbb{S}^2}$ the desired splitting is obtained for $\beta(l, m)$

$O(AN\log N)$ operations, $O(An^3)$ memory: Wu, White, Scanlon, Reese, and Zhang (2013) (extended to L-J and more); Gamba, Haack and Hu (2014)

2D: Filbet and Russo (2003); Liu, Xu, Sun, and Cai (2014) (UGKS);

Internal Energy/Polyatomic: Munafo, Haack, Gamba, and Magin (2012); Liu, Yu, Xu and Zhong (2014) (UGKS);

Stochastic evaluation of the collision integral

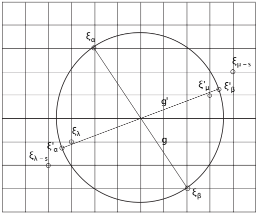
Korobov quasi-stochastic multidimensional integration:

$$\int_0^1 \dots \int_0^1 h(x_1,\dots,x_s)\,dx_1\dots dx_s = \frac{1}{p}\sum_{k=1}^{P} h\Big(\Big\{\frac{a_1 k}{p}\Big\},\dots,\Big\{\frac{a_s k}{p}\Big\}\Big) - R_p[h],$$

p is prime, a_i r.p. with p. If h has Fourier series, coefficients decaying with power α, then $|R_p[h]| \leq C_1(\alpha,s)\frac{\ln^{\alpha s} p}{p^{\alpha}}$. Any dimensionality!

Cheremissine (2003) used Korobov schemes for collision integral.

$$I_p = \frac{1}{4}\int_{R^3}\int_{R^3}\int_0^{2\pi}\int_0^{b^*} (\delta' + \delta'_1 - \delta - \delta')(f' f'_1 - f f_1)|g|\,b\,db\,d\varepsilon\,.$$



$$\delta(\xi_{\alpha_\nu} - \xi_\gamma) = (1 - r_\nu)\delta(\xi_{\lambda_\nu} - \xi_\gamma) + r_\nu\delta(\xi_{\lambda_\nu + s} - \xi_\gamma)\,,$$

$$\delta(\xi_{\beta_\nu} - \xi_\gamma) = (1 - r_\nu)\delta(\xi_{\mu_\nu} - \xi_\gamma) + r_\nu\delta(\xi_{\mu_\nu + s} - \xi_\gamma)\,,$$

Related approaches: Morris, Varghese, and Goldstein (2008,2011), Arslanbekov, Kolobov, and Frolova (2013) (UFS);

Approach Based on the Fourier Transform

R. Kirsch and S. Rjasanow (2007), I.M. Gamba and Tharkabhushaman (2009,2010). The Fourier transform of the collision operator,

$$\hat{Q}(\vec{\xi}) = \int_{\mathbb{R}^3} \mathrm{e}^{-\imath \vec{xi}\cdot\vec{v}} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} (f(\vec{v}')f(\vec{v}_1') - f(\vec{v})f(\vec{v}_1))B(\|g\|, \vec{w})\, d\vec{w}\, d\vec{v}_1 d\vec{v},$$

Assuming $B(\|g\|, \vec{w}) = C(\vec{w})\|g\|^{\lambda}$,using substitutions of variables, properties of exponentials, and properties of the Fourier transform:

$$\hat{Q}(\vec{\xi}) = \int_{\mathbb{R}^3} \hat{f}(\vec{\zeta} - \vec{\xi})\hat{f}(\vec{\xi})\hat{G}(\vec{\xi}, \vec{\zeta})d\vec{\xi},$$

where $\hat{f}(\vec{\zeta})$ is the Fourier transform of $f(\vec{v})$ and

$$\hat{G}(\vec{\xi}, \vec{\zeta}) = \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} \mathrm{e}^{-\imath \vec{\xi}\cdot\vec{g}} \mathrm{e}^{\imath \frac{\beta}{2} \vec{\zeta}\cdot\vec{g}} \|g\|^{\lambda} \left[C(\vec{w}) \mathrm{e}^{\imath \frac{\beta}{2} \|g\| \vec{\zeta}\cdot\vec{w}} - 1 \right] d\vec{w}\, d\vec{g}$$

Complexity $O(k^6)$, memory $O(k^6)$.

Approach Based on the Fourier Transform

$$\hat{Q}(\vec{\xi}) = \int_{\mathbb{R}^3} \hat{f}(\vec{\zeta} - \vec{\xi})\hat{f}(\vec{\xi})\hat{G}(\vec{\xi}, \vec{\zeta})d\vec{\xi},$$

$O(k^6)$ operations and memory: Kirsch and Rjasanov (2007), Gamba and Tharkabhushanam (2009, 2010), Haack and Gamba (2012)

Internal Energy/ Polyatomic: Munafo, Haack, Gamba, and Magin (2012)

Main constraint is memory. $k = 32$ is a hard barrier for the method.

Attempts were to compress $\hat{G}(\vec{\xi}, \vec{\zeta})$ using the structure of the collision operator.

Gamba, Haack and Hu (2014) *A fast conservative spectral solver for the nonlinear Boltzmann collision operator.*

Gamba, Haack, Hauk and Hu (2016) *A fast spectral method for the Boltzmann collision operator with general collision kernels.*, $O(Mk^3 \log k)$ can do 0D with $k = 64$.

Compression of Kernel in the Fourier Galerkin

$$Q[f](t,\vec{v}) = \sum_{\substack{l,m=-N \\ l+m=k}}^{N} \hat{f}_{\vec{l}} \hat{f}_{\vec{m}} \hat{G}(\vec{l},\vec{m})$$

where $\hat{G}(\vec{l},\vec{m}) = G(\vec{l},\vec{m}) - G(\vec{m},\vec{m})$ and

$$\hat{G}(\vec{m},\vec{l}) = \int_{[-T,T]^3} \int_{\mathbb{S}^2} B(|g|,w)(\mathrm{e}^{\imath(\|g\|\vec{w}\cdot(\vec{h}-\vec{k})-\vec{g}\cdot(\vec{h}+\vec{k}))\pi/2T}\, dw\, d\vec{v}_1,$$

Seek an approximation to $G(\vec{l},\vec{m})$

$$G(\vec{l},\vec{m}) \approx \sum_{p=1}^{N_p} \alpha_p(\vec{l}+\vec{m})\beta_p(\vec{l})\beta_p(\vec{m})$$

To generate low rank approximation, rewrite

$$\hat{G}(\vec{m},\vec{l}) = \int_0^R \int_{S^2} F(\vec{l}+\vec{m},r,\sigma)\mathrm{e}^{\imath\vec{\sigma}\cdot(\vec{h}+\vec{k}))\pi/2T}\, d\sigma\, dr.$$

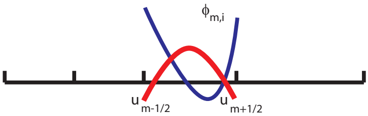
$$F(\vec{l}+\vec{m},r,w) = r^2 \int_{\mathbb{S}^2} B(|g|,w)\mathrm{e}^{\imath(r\vec{w}\cdot(\vec{h}-\vec{k}))\pi/2T}\, dw\, d\vec{v}_1$$

Nodal-Discontinuous Galerkin Approximations

The Galerkin approximation:

$$f(\vec{u})\Big|_{U_m} = \sum_{i=1}^{k} \hat{f}_{i,m}\varphi_{i,m}(\vec{u})$$

Discontinous Galerkin methods: domain is partitioned into $U_m = [u_{m-1/2}, u_{m+1/2}]$; typical choice $\int_R \varphi_{i,m}\varphi_{j,n}\, du = \delta_{ij}\delta_{mn}$.



To find $\hat{f}_{i,m}$, multiply by $\varphi_{i,m}(\vec{u})$, integrate and solve:

$$\hat{f}_{i,m} = \int_{U_m} f(\vec{u})\varphi_{i,m}(\vec{u})\, du = f(\kappa_{i,m}) \quad \text{up to truncation errors}$$

(Hesthaven and Warburton, 2007)

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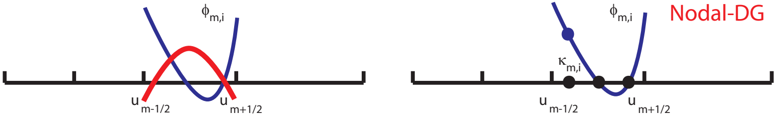

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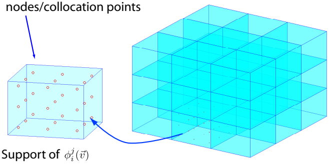
Nodal DG Discretizations in 3D Velocity Variable

A rectangular velocity domain is partitioned into $K_i = U_j \times V_k \times W_l$. (Hesthaven and Warburton, 2007) Let $\kappa_{p,i}$, $p = 1, \ldots, s$ be the nodes of Legendre's quadrature on U_i. Define



$$\lambda_{p,i}(u) = \prod_{\substack{r=1,s \\ r \neq p}} \frac{u - \kappa_{r,i}}{\kappa_{p,i} - \kappa_{r,i}}$$

In three dimensions use $\phi_{j,i}(\vec{u}) = \lambda_{p,j}(u)\lambda_{q,k}(v)\lambda_{r,l}(w)$, j runs over all (p, q, r). Up to truncation errors of integration, the Galerkin coefficients are the nodal values of the function .

$$f(u)|_{K_i} = \sum_j f_{j,i}\phi_{j,i}(\vec{u}), \quad \text{where} \quad f_{j,i} = f(\kappa_{p,i}, \kappa_{q,i}, \kappa_{r,i}).$$

Nodal-DG discretizations are obtained by substituting the Galerkin approximation into the equation, multiplying by a basis function and integrating over the velocity domain:

$$\partial_t f_{p,i}(t, \vec{x}) + \kappa^u_{p,i}\partial_x f_{p,i}(t, \vec{x}) + \kappa^v_{p,i}\partial_y f_{p,i}(t, \vec{x}) + \kappa^w_{p,i}\partial_z f_{p,i}(t, \vec{x}) = \int_{V_i} \varphi_{p,i} Q(f, f)$$

The Bilinear Form of the Galerkin Projection

Galerkin projection of Q onto a basis function $\varphi(\vec{\xi})$

$$I_\varphi = \int_{R^3} \varphi(\vec{v}) \int_{R^3} \int_0^{2\pi} \int_0^{b_*} (f(\vec{v}')f(\vec{v}_1') - f(\vec{v})f(\vec{v}_1))|g|b\, db\, d\varepsilon\, d\vec{v}_1\, d\vec{v}$$

Replace it with (e.g., Kogan, 1995)

$$I_\varphi = \int_{R^3} \int_{R^3} \int_0^{2\pi} \int_0^{b_*} \frac{|g|}{2} f(t,\vec{x},\vec{v})f(t,\vec{x},\vec{v}_1)(\varphi(\vec{v}') + \varphi(\vec{v}_1') - \varphi(\vec{v}) - \varphi(\vec{v}_1))b\, db\, d\varepsilon\, d\vec{v}_1\, d\vec{v}$$

From first principles of rarefied gas dynamics it follows that the last equation can be re-written as

$$I_\varphi = \int_{R^3} \int_{R^3} f(t,\vec{x},\vec{v})f(t,\vec{x},\vec{v}_1)A(\vec{\xi},\vec{v}_1;\varphi)d\vec{v}_1\, d\vec{v}$$

where information about molecular collisions is encoded in

$$A(\vec{\xi},\vec{v}_1;\varphi) = \frac{|g|}{2} \int_0^{2\pi} \int_0^{b_*} (\varphi(\vec{v}') + \varphi(\vec{v}_1') - \varphi(\vec{v}) - \varphi(\vec{v}_1))b\, db\, d\varepsilon\, .$$

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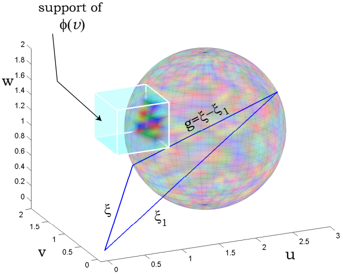
Collision Kernel. Shift Invariance

(Alekseenko and Josyula (2012), Also see Grohs, Hiptmair and Pintarelli (2015))

$$A(\vec{\xi}, \vec{\xi}_1; \varphi) = |g|^\alpha \int_{\mathbb{S}^2} \phi_{i;j}(\vec{v}')b_\alpha(\theta)\, d\sigma\,.$$

Depends on φ and the collision model, **information on collisions**



Theorem. $A(\vec{v}, \vec{v}_1; \varphi)$ is invariant with respect to a shift, namely

$$A(\vec{v}+\vec{\eta}, \vec{v}_1+\vec{\eta}; \varphi(\vec{v}-\vec{\eta})) = A(\vec{v}, \vec{v}_1; \varphi)$$

(Alekseenko and Josyula (2012), Also see Grohs, Hiptmair and Pintarelli (2015))

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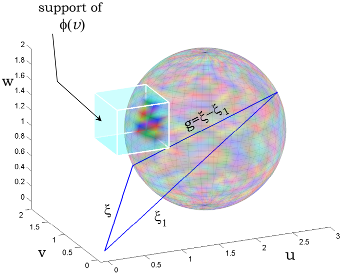

Theorem. $A(\vec{v}, \vec{v}_1; \varphi)$ is invariant with respect to a shift, namely

$$A(\vec{v} + \vec{\eta}, \vec{v}_1 + \vec{\eta}; \varphi(\vec{v} - \vec{\eta})) = A(\vec{v}, \vec{v}_1; \varphi)$$

Convolution Formulation of DG Galerkin Projection

Theorem. $A(\vec{v}, \vec{v}_1; \varphi)$ is invariant with respect to a shift, specifically

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Discrete Convolution Form

$$I(\vec{\xi}) = \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} f(\vec{v}-\vec{\xi})f(\vec{v}_1-\vec{\xi})A(\vec{v},\vec{v}_1;\varphi)\,d\vec{v}_1\,d\vec{v}$$

The convolution form is discretized in a finite velocity domain using native nodal-DG Gauss quadratures

$$I_{i;j} := I_i(\vec{\xi}_j) = \sum_{i',i''=1}^{s}\sum_{j'=1}^{M^3}\sum_{j''=1}^{M^3} f_{i';j'-j}f_{i'';j''-j}A_{i,i',i'';j',j''}$$

where $f_{i';j'-j} = f(t,\vec{x},\vec{v}_{i';j'-j})$, $A_{i,i',i'';j',j''} = A(\vec{v}_{i';j'},\vec{v}_{i'';j''};\phi_{i;c})(\omega_{i'}\Delta\vec{v}/8)(\omega_{i''}\Delta\vec{v}/8)$ and the three dimensional indices i' and i'' run over the velocity nodes within a single velocity cell and indices j' and j'' run over all velocity cells.

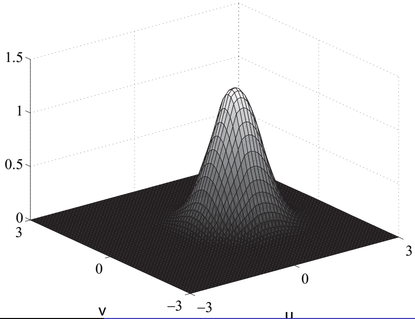
Some shifted indices $j'-j$ point outside of the velocity domain. In direct evaluation, missing values are replaced with zeros.

Extension to Circular Convolution

$$I_{i;j} := I_i(\vec{\xi}_j) = \sum_{i',i''=1}^{s} \sum_{j'=1}^{M^3} \sum_{j''=1}^{M^3} f_{i';j'-j} f_{i'';j''-j} A_{i,i',i'';j',j''}$$

There is a considerable wealth of theory on fast evaluation of discrete convolution. (Nussbaumer, 1982)

Most are related to circular convolution. This requires to extend the solution and kernel $A_{i,i',i'';j',j''}$ periodically.



Evaluating Circular Convolution in $O(n \log n)$

Let x_n and y_n be periodic sequences with period N. An N-point circular convolution is defined as (Nussbaumer, 1982)

$$z_l = \sum_{n=0}^{N-1} x_n y_{l-n} \,.$$

Discrete Fourier transform:

$$\mathcal{F}[x]_k = \sum_{n=0}^{N-1} W^{kn} x_n, \quad x_l = \frac{1}{N} \sum_{k=0}^{N-1} W^{-lk} \mathcal{F}[x]_k, \quad \text{where} \quad W = \mathrm{e}^{-\imath 2\pi/N} \,.$$

Application of the discrete Fourier transform (or any other number theoretical transform) yields

$$\mathcal{F}[z]_k = \mathcal{F}[x]_k \mathcal{F}[y]_k \,.$$

- $\mathcal{F}[x]_k$ and $\mathcal{F}[y]_k$ can be computed in $O(N \log N)$.
- $\mathcal{F}[z]_k$ are computed in $O(N)$ operations.
- Finally, the values of z_l are obtained in another $O(N \log N)$ operations.

Convolutions of non-periodic sequences are reduced to circular convolutions. A difficulty is aliasing.

Discrete Convolution Form

We extend the solution $f_{i;j}$ and kernel $A_{i,i',i'';j',j''}$ periodically in j, $j = 1 \dots, M$ — the cell number.

$$I_{i;j} := I_i(\vec{\xi}_j) = \sum_{i',i''=1}^{s} \sum_{j'=1}^{M^3} \sum_{j''=1}^{M^3} f_{i';j'-j} f_{i'';j''-j} A_{i,i',i'';j',j''}$$

Theorem Let f_{j_u,j_v,j_w} be a three-index sequence that is periodic in each index with period M and let $A_{j'_u,j'_v,j'_w,j''_u,j''_v,j''_w}$ be a M-periodic six-dimensional tensor. The multi-dimensional discrete Fourier transform of discrete collision operator can be represented as

$$\mathcal{F}[I]_{k_u,k_v,k_w} = M^3 \sum_{l_u,l_v,l_w=0}^{M-1} \mathcal{F}^{-1}[f]_{k_u-l_u,k_v-l_v,k_w-l_w} \mathcal{F}^{-1}[f]_{l_u,l_v,l_w}$$
$$\mathcal{F}[A]_{k_u-l_u,k_v-l_v,k_w-l_w,l_u,l_w,l_w}$$

The Algorithm

Use of DFT allows us to calculate the collision operator in $O(s^9 M^6)$ operations.

1. evaluate $\mathcal{F}^{-1}[f_i]_{k_u,k_v,k_w}$ in $O(s^3M^3 \log M)$ operations where s^3 is the number of velocity nodes in each velocity cell.
2. Next we directly compute the convolution in Forier space

$$\mathcal{F}[I_{i,i',i''}]_{k_u,k_v,k_w} = M^3 \sum_{l_u,l_v,l_w=0}^{M-1} \mathcal{F}^{-1}[f_{i'}]_{k_u-l_u,k_v-l_v,k_w-l_w} \mathcal{F}^{-1}[f_{i''}]_{l_u,l_v,l_w} \mathcal{F}[A_{i,i',i''}]$$

complexity of this step is $O(s^9 M^6)$.
3. Calculate $\mathcal{F}[I_i]_{k_u,k_v,k_w}$. in a complexity $O(s^9 M^3)$ operations.
4. Recover $\mathcal{F}^{-1}[\mathcal{F}[I_i]]_{j_u,j_v,j_w} = I_{i;j_u,j_v,j_w}$. in $O(s^3 M^3 \log M)$*operations*

Overall, the algorithm has the numerical complexity of $O(s^9 M^6)$. We note that $s = s_u = s_v = s_w$ can be kept fixed and the number of cells M^3 in velocity domain can be increased if more accuracy is desired.

Efficiency

	DFT		Direct		Speedup
M	time, s	α	time, s	α	
9	1.47E-02		1.25E-01		8.5
15	3.94E-01	6.43	4.91E+00	7.18	12.5
21	3.09E+00	6.14	7.80E+01	8.21	25.2
27	1.64E+01	6.65	6.05E+02	8.15	36.7

Table: CPU times for evaluating the collision operator directly and using the Fourier transform.