BGK-type models for chemically reacting gas mixtures

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The Bhatnagar-Gross-Krook (BGK, in short) model

$$\partial_t f + v \cdot \nabla_x f = \tilde{Q}(f) := \nu(M - f),$$

where

$$M(x, v, t) := n(x, t) \left(\frac{m}{2\pi k T(x, t)} \right)^{\frac{3}{2}} \exp\left(-\frac{m|v - U(x, t)|^2}{2kT(x, t)} \right)$$

with

$$n(x, t) := \int_{\mathbb{R}^3} f(x, v, t) dv, \quad U(x, t) := \int_{\mathbb{R}} v f(x, v, t) dv,$$

$$T(x, t) := \frac{m}{3kn(x, t)} \int_{\mathbb{R}} |v - U(x, t)|^2 f(x, v, t) dv.$$

This model is a good approximation for the Boltzmann equation.

Conservation of mass, momentum and energy

$$\int_{\mathbb{R}^3} (M - f)(1, v, |v|^2) dv = 0 \quad \Longrightarrow \quad \int_{\mathbb{R}^6} f(1, v, |v|^2) dv dx : \text{ conserved.}$$

Hence BGK model is a reasonable, low-cost approximation to the Boltzmann equation:

$$\partial_t f + v \cdot \nabla_x f = Q(f, f)$$
$$:= \int_{\mathbb{R}^3 \times \mathbb{S}^2} (f(w^*)f(v^*) - f(w)f(v))\sigma(\omega.w - v, \|w - v\|)\|w - v\| dw d\omega,$$

where

$$v^* := v + ((w - v) \cdot \omega)\omega, \quad w^* := w + ((v - w) \cdot \omega)\omega.$$

The Boltzmann equation for chemical reaction

Consider the following chemical reaction for molecules A^i (i=1,2,3,4):

$$A^1 + A^2 \rightleftharpoons A^3 + A^4.$$

The Boltzmann equation reads as [Rossani-Spiga (1999)]

$$\partial_t f_i + v \cdot \nabla_x f_i = I_i + J_i,$$

where

$$I_i := \sum_{l=1}^{4} \int d\mathbf{w} \int V I_{il}^{il}(V, \mathbf{\Omega} \cdot \mathbf{\Omega}')[f_i(\mathbf{v}_{il}) f_l(\mathbf{w}_{il}) - f_i(\mathbf{v}) f_l(\mathbf{w})] d\mathbf{\Omega}'$$

and

$$J_i := \iint U(V - \epsilon_{12}) V I_{12}^{34}(V, \mathbf{\Omega} \cdot \mathbf{\Omega}')[\left(\frac{\mu_{12}}{\mu_{34}}\right)^3 f_3(\mathbf{v}_1) f_4(\mathbf{w}_1) - f_1(\mathbf{v}) f_2(\mathbf{w})] d\mathbf{w} d\mathbf{\Omega}'.$$

Given constants

- m_i: the mass for each species with $M = m_1 + m_2 = m_3 + m_4$
- $\mu_{ij} := \frac{m_i m_j}{m_i + m_j}$ $(i, j = 1, 2, 3, 4)$ denote the reduced mass
- E_i: the energy of chemical bond with $\Delta E = -\sum_{i=1}^{4} \lambda_i E_i$, where we denote $\lambda_1 = \lambda_2 = -\lambda_3 = -\lambda_4 = 1$.

Macroscopic fields

(a) Single component macroscopic fields:

$$\begin{aligned} \rho^{(i)} &:= m_i n^{(i)} := m_i \int_{\mathbb{R}^3} f_i dv, \\ \rho^{(i)} U^{(i)} &:= m_i \int_{\mathbb{R}^3} v f_i dv, \\ 3n^{(i)} kT^{(i)} &:= m_i \int_{\mathbb{R}^3} |v - U^{(i)}|^2 f_i dv. \end{aligned} \tag{1}$$

(b) Global macroscopic fields:

$$\begin{aligned} &n = \sum_{i=1}^{4} n^{(i)}, \qquad \rho = \sum_{i=1}^{4} \rho^{(i)}, \qquad U = \frac{1}{\rho} \sum_{i=1}^{4} \rho^{(i)} U^{(i)}, \\ &nkT = \sum_{i=1}^{4} n^{(i)} kT^{(i)} + \frac{1}{3} \sum_{i=1}^{4} \rho^{(i)} (|U^{(i)}|^2 - |U|^2). \end{aligned} \tag{2}$$

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Modeling setup

Consider the BGK-type equation

$$\partial_t f_i + v \cdot \nabla_x f_i = Q_i := \nu_i \big(\mathcal{M}_i - f_i \big)$$

with

$$\mathcal{M}_i := n_i \left(\frac{m_i}{2\pi k T_i} \right)^{3/2} \exp\left(- \frac{m_i |v - U_i|^2}{2kT_i} \right)$$

Goal: Define the following terms ‘reasonably’:

- n_i, U_i and T_i $(i = 1, 2, 3, 4)$
- ν_i $(i = 1, 2, 3, 4)$

Key idea

Consider the Boltzmann equation for the chemical reaction, constructed in [Rossani-Spiga (1999)]:

$$\partial_t f_i + v \cdot \nabla_x f_i = I_i + J_i := \text{mechanical} + \text{chemical collision operator.}$$

Idea: Define n_i, U_i and T_i $(i = 1, 2, 3, 4)$ so that they satisfy

$$\int Q_i dv = \int I_i dv + \int J_i dv, \quad \int m_i v Q_i dv = \int m_i v I_i dv + \int m_i v J_i dv,$$
$$\int \frac{m_i}{2}|v|^2 Q_i dv = \int \frac{m_i}{2}|v|^2 I_i dv + \int \frac{m_i}{2}|v|^2 J_i dv.$$

This extends the method in [Andries-Aoki-Perthame (2002)], in which a BGK-type model for a mixture of gases (without chemical reaction) was derived.

Exchange relations of the mechanical collision operator

For some given constants χ_{ij}, we have

$$\int I_i dv = 0, \quad \int m_i v I_i dv = 2\sum_{j=1}^{4} \chi_{ij}\mu^{ij} n^{(i)} n^{(j)} (U^{(j)} - U^{(i)}),$$

$$\int \frac{m_i}{2}|v|^2 I_i dv = 6k \sum_{j=1}^{4} \chi_{ij} \frac{\mu^{ij}}{m_i + m_j} n^{(i)} n^{(j)} (T^{(j)} - T^{(i)})$$

$$+ 2\sum_{j=1}^{4} \chi_{ij} \frac{\mu^{ij}}{m_i + m_j} n^{(i)} n^{(j)} (m_i U^{(i)} + m_j U^{(j)})(U^{(j)} - U^{(i)}).$$

Exchange relations of the chemical collision operator

With

$$\mathcal{S} := \nu_{12}^{34} \frac{2}{\sqrt{\pi}} \Gamma\left(\frac{3}{2}, \frac{\Delta E}{kT}\right) \left[n^{(3)} n^{(4)} \left(\frac{m_1 m_2}{m_1 m_2}\right)^{3/2} e^{\Delta E/kT} - n^{(1)} n^{(2)} \right],$$

we compute

$$\int J_i dv = \lambda_i \mathcal{S}, \quad \int m_i v J_i dv = \lambda_i \mathcal{S} m_i U,$$

$$\int \frac{m_i}{2} |v|^2 J_i dv = \lambda_i \mathcal{S} \left[\frac{1}{2} m_i |U|^2 + \frac{3}{2} kT + \frac{M - m_i}{M} kT \frac{(\Delta E/kT)^{3/2} e^{-\Delta E/kT}}{\Gamma(\frac{3}{2}, \frac{\Delta E}{kT})} - \frac{1 - \lambda_i}{2} \frac{M - m_i}{M} \Delta E \right].$$

Here $\Gamma(s, x) := \int_x^\infty t^{s-1} e^{-t} dt$ is the upper incomplete gamma function.

Exchange relations of the BGK operator

Now, from

$$\int Q_i dv = \nu_i(n_i - n^{(i)}), \quad \int m_i v Q_i dv = \nu_i m_i (n_i U_i - n^{(i)} U^{(i)}),$$
$$\int \frac{m_i}{2}|v|^2 Q_i dv = \nu_i \left[\frac{3}{2} n_i k T_i - \frac{3}{2} n^{(i)} k T^{(i)} + \frac{1}{2} m_i n_i |U_i|^2 - \frac{1}{2} m_i n^{(i)} |U^{(i)}|^2\right],$$

we can define n_i, U_i and T_i $(i = 1, 2, 3, 4)$ so that they satisfy

$$\int Q_i dv = \int I_i dv + \int J_i dv, \quad \int m_i v Q_i dv = \int m_i v I_i dv + \int m_i v J_i dv,$$
$$\int \frac{m_i}{2}|v|^2 Q_i dv = \int \frac{m_i}{2}|v|^2 I_i dv + \int \frac{m_i}{2}|v|^2 J_i dv.$$

Collision frequencies

For given constants $\nu_{ij} \geq \chi_{ij}$, we define

$$\nu_1 = \sum_{j=1}^{4} \nu_{1j} n^{(j)} + \frac{2}{\sqrt{\pi}} \Gamma\left(\frac{3}{2}, \frac{\Delta E}{kT}\right) \nu_{12}^{34} n^{(2)},$$

$$\nu_2 = \sum_{j=1}^{4} \nu_{2j} n^{(j)} + \frac{2}{\sqrt{\pi}} \Gamma\left(\frac{3}{2}, \frac{\Delta E}{kT}\right) \nu_{12}^{34} n^{(1)},$$

$$\nu_3 = \sum_{j=1}^{4} \nu_{3j} n^{(j)} + \frac{2}{\sqrt{\pi}} \Gamma\left(\frac{3}{2}, \frac{\Delta E}{kT}\right) \left(\frac{\mu^{12}}{\mu^{34}}\right)^{3/2} e^{\Delta E/kT} \nu_{12}^{34} n^{(4)},$$

$$\nu_4 = \sum_{j=1}^{4} \nu_{4j} n^{(j)} + \frac{2}{\sqrt{\pi}} \Gamma\left(\frac{3}{2}, \frac{\Delta E}{kT}\right) \left(\frac{\mu^{12}}{\mu^{34}}\right)^{3/2} e^{\Delta E/kT} \nu_{12}^{34} n^{(3)}.$$

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Problem

Consider the stationary problem in a slab

$$v_1 \frac{\partial f_i}{\partial x} = \frac{\nu_i}{\tau}(\mathcal{M}_i - f_i) \text{ on } [0,1] \times \mathbb{R}^3, \quad (i = 1,2,3,4) \tag{3}$$

subject to the boundary data:

$$f_i(0,v) = f_{i,L}(v), \text{on } v_1 > 0, \quad f_i(1,v) = f_{i,R}(v), \text{on } v_1 < 0,$$

Definition

(f_1, f_2, f_3, f_4) is a mild solution for (3) if for each $i = 1,2,3,4$, we have

$$\begin{aligned} f_i = &\left(e^{-\frac{1}{\tau|v_1|}\int_0^x \nu_i(y)dy} f_{i,L}(v) + \frac{1}{\tau|v_1|}\int_0^x e^{-\frac{1}{\tau|v_1|}\int_y^x \nu_i(z)dz} \nu_i \mathcal{M}_i dy \right) 1_{v_1>0} \\ &+ \left(e^{-\frac{1}{\tau|v_1|}\int_x^1 \nu_i(y)dy} f_{i,R}(v) + \frac{1}{\tau|v_1|}\int_x^1 e^{-\frac{1}{\tau|v_1|}\int_x^y \nu_i(z)dz} \nu_i \mathcal{M}_i dy \right) 1_{v_1<0}. \end{aligned}$$

Main theorem

Denote the norm $\|\cdot\|_{L^1_2}$ by $\|f\|_{L^1_2} = \int_{\mathbb{R}^3} |f(x,v)|(1+|v|^2)dv$.

Theorem

Suppose $f_{i,LR}, \frac{1}{|v_1|} f_{i,LR} \in L^1_2(\mathbb{R}^3_v)$. And suppose futher that for $j = 2, 3$

$$\int_{\mathbb{R}^2} f_{i,L} v_j dv_2 dv_3 = \int_{\mathbb{R}^2} f_{i,R} v_j dv_2 dv_3 = 0.$$

Then there exist two constants $\epsilon, L > 0$, depending only on the boundary data, such that if $\epsilon > \nu^{34}_{12} > 0$ and $\tau > L$, then there exists a unique mild solution (f_1, f_2, f_3, f_4) for (3).

The proof uses Banach fixed point argument, with the metric

$$d(F,G) = \sum_{i=1}^{4} \sup_{x \in [0,1]} ||f_i - g_i||_{L^1_2}.$$

Reactive temperatures can be negative

Proposition

For any given positive constants m_i, χ_{ij}, ν_{ij}, ν_{12}^{34} and ΔE $(i,j = 1,2,3,4)$, we can choose macroscopic parameters $n^{(i)} > 0$, $U^{(i)} \in \mathbb{R}^3$ and $T^{(i)} > 0$ $(i = 1,2,3,4)$ such that the corresponding reactive temperature T_3 is negative.

Sketch of proof: Take

$$n^{(1)} = n^{(2)} = n^{(3)} = n^{(4)} = \delta > 0, \quad U^{(1)} = U^{(2)} = U^{(3)} = U^{(4)} = 0,$$

$$T^{(1)} = T^{(2)} = T^{(4)} = \varepsilon > 0 \quad \text{and} \quad T^{(3)} = \eta > 0.$$

Then we have

$$\lim_{\varepsilon \searrow 0} \lim_{\eta \searrow 0} \frac{\nu_3}{\varepsilon} n_3 T_3 = -\infty.$$

A property of the incomplete gamma function

Lemma

For any $0 < x < \infty$, we have the following inequality:

$$0 < x\left(1 - \frac{\sqrt{x}e^{-x}}{\Gamma(\frac{3}{2}, x)}\right) < \frac{1}{2}.$$

For the left inequality, we employ the identity

$$\Gamma(s+1, x) = s\Gamma(s, x) + x^s e^{-x}, \quad s > 0$$

to obtain

$$x\left(1 - \frac{\sqrt{x}e^{-x}}{\Gamma(\frac{3}{2}, x)}\right) = \frac{\frac{1}{2}x\Gamma(\frac{1}{2}, x)}{\Gamma(\frac{3}{2}, x)} > 0.$$

For the right inequality, we use

$$\Gamma\left(\frac{1}{2}, x\right) = \int_x^\infty \frac{1}{\sqrt{t}} e^{-t} dt < \int_x^\infty \frac{\sqrt{t}}{x} e^{-t} dt = \frac{1}{x}\Gamma\left(\frac{3}{2}, x\right).$$

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Modeling setup

Consider the BGK-type equation

$$\partial_t f_i + v \cdot \nabla_x f_i = \tilde{Q}_i := \tilde{\nu}_i \big(\widetilde{\mathcal{M}}_i - f_i \big)$$

with

$$\widetilde{\mathcal{M}}_i := \tilde{n}^i \left(\frac{m_i}{2\pi k \tilde{T}} \right)^{3/2} \exp\left(- \frac{m_i |v - \tilde{U}|^2}{2k\tilde{T}} \right)$$

Goal: Define the following terms 'reasonably':

- $\tilde{n}_i$ $(i = 1, 2, 3, 4)$, $\tilde{U}$ and $\tilde{T}$
- $\tilde{\nu}_i$ $(i = 1, 2, 3, 4)$

Conservation laws

The seven conservation laws

$$\int (\tilde{Q}_i + \tilde{Q}_j) dv = 0, \quad (i,j) = (1,3), (1,4), (2,4),$$

$$\sum_{i=1}^{4} \int m_i v \tilde{Q}_i dv = 0, \quad \sum_{i=1}^{4} \int (\frac{1}{2} m_i |v|^2 + E_i) \tilde{Q}_i dv = 0$$

leads to the seven equations

$$\tilde{n}_i = n^{(i)} + \lambda_i \frac{\tilde{\nu}_1}{\tilde{\nu}_i} (\tilde{n}_1 - n^{(1)}), \quad i = 2,3,4, \quad \tilde{U} = \frac{\sum_{i=1}^{4} \tilde{\nu}_i m_i n^{(i)} U^{(i)}}{\sum_{i=1}^{4} \tilde{\nu}_i m_i n^{(i)}},$$

$$\tilde{T} = \frac{\sum_{i=1}^{4} \tilde{\nu}_i n^{(i)} \left[\frac{1}{2} m_i (|U^{(i)}|^2 - |\tilde{U}|^2) + \frac{3}{2} k T^{(i)} \right] + \Delta E \tilde{\nu}_1 (\tilde{n}_1 - n^1)}{\frac{3}{2} k \sum_{i=1}^{4} \tilde{\nu}_i n^{(i)}}.$$

Once $\tilde{n}_1$ is determined, the other terms are automatically determined.

Mass action law

The mass action law

$$\frac{\tilde{n}_1 \tilde{n}_2}{\tilde{n}_3 \tilde{n}_4} = \left(\frac{\mu^{12}}{\mu^{34}}\right)^{\frac{3}{2}} \exp\left(\frac{\Delta E}{k\tilde{T}}\right)$$

yields the following definition. $\tilde{n}_1$ is the unique root of the equation in x:

$$\frac{\tilde{\nu}_3\tilde{\nu}_4}{\tilde{\nu}_1\tilde{\nu}_2} \frac{\tilde{\nu}_1 x[\tilde{\nu}_2 n^{(2)} + \tilde{\nu}_1(x - n^{(1)})]}{[\tilde{\nu}_3 n^{(3)} - \tilde{\nu}_1(x - n^{(1)})][\tilde{\nu}_4 n^{(4)} - \tilde{\nu}_1(x - n^{(1)})]} e^{-\frac{\Delta E}{kF(x)}} = \left(\frac{\mu^{12}}{\mu^{34}}\right)^{\frac{3}{2}}, \tag{4}$$

where the function $F(x)$ is defined as

$$F(x) := \frac{\sum_{i=1}^{4} \tilde{\nu}_i n^{(i)} \left[\frac{1}{2} m_i(|U^{(i)}|^2 - |\tilde{U}|^2) + \frac{3}{2} kT^{(i)}\right] + \Delta E \tilde{\nu}_1(x - n^1)}{\frac{3}{2} k \sum_{i=1}^{4} \tilde{\nu}_i n^{(i)}}.$$

Well-definedness

LHS of (4) is strictly increasing in the domain defined by the constraint of positivity for $\tilde{n}_i$ $(i = 1, 2, 3, 4)$ and $\tilde{T}$, i.e.,

$$x > 0, \quad x > n^{(1)} - \frac{\tilde{\nu}_2}{\tilde{\nu}_1} n^{(2)}, \quad x < n^{(1)} + \frac{\tilde{\nu}_3}{\tilde{\nu}_1} n^{(3)}, \quad x < n^{(1)} + \frac{\tilde{\nu}_4}{\tilde{\nu}_1} n^{(4)},$$

$$x > n^{(1)} - \frac{1}{\tilde{\nu}_1} \frac{1}{\Delta E} \sum_{i=1}^{4} \tilde{\nu}_i n^{(i)} \Big[\frac{1}{2} m_i (|U^{(i)} - \tilde{U}|^2) + \frac{3}{2} k T^{(i)} \Big].$$

The range of LHS of (4) for the above domain is $(0, \infty)$. Hence $\tilde{n}_i$ $(i = 1, 2, 3, 4)$ and $\tilde{T}$ are well-defined, and their positivity are guaranteed.

Collision frequencies

For given constants ν_{ij}s and ν_{34}^{12}, we set

$$\tilde{\nu}_1 = \sum_{j=1}^{4} \nu_{1j} n^{(j)} + \left(\frac{\mu^{34}}{\mu^{12}}\right)^{3/2} e^{-\Delta E/kT} \nu_{34}^{12} n^{(2)},$$

$$\tilde{\nu}_2 = \sum_{j=1}^{4} \nu_{2j} n^{(j)} + \left(\frac{\mu^{34}}{\mu^{12}}\right)^{3/2} e^{-\Delta E/kT} \nu_{34}^{12} n^{(1)},$$

$$\tilde{\nu}_3 = \sum_{j=1}^{4} \nu_{3j} n^{(j)} + \nu_{34}^{12} n^{(4)},$$

$$\tilde{\nu}_4 = \sum_{j=1}^{4} \nu_{4j} n^{(j)} + \nu_{34}^{12} n^{(3)}.$$

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Problem

Consider the stationary problem in a slab

$$v_1 \frac{\partial f_i}{\partial x} = \frac{\tilde{\nu}_i}{\tau}\left(\widetilde{\mathcal{M}}_i - f_i\right) \text{ on } [0,1]\times\mathbb{R}^3, \quad (i = 1,2,3,4) \tag{5}$$

subject to the boundary data:

$$f_i(0,v) = f_{i,L}(v), \text{on } v_1 > 0, \quad f_i(1,v) = f_{i,R}(v), \text{on } v_1 < 0,$$

Definition

(f_1, f_2, f_3, f_4) is a mild solution for (5) if for each $i = 1,2,3,4$, we have

$$\begin{aligned} f_i = &\left(e^{-\frac{1}{\tau|v_1|}\int_0^x \tilde{\nu}_i(y)dy} f_{i,L}(v) + \frac{1}{\tau|v_1|}\int_0^x e^{-\frac{1}{\tau|v_1|}\int_y^x \tilde{\nu}_i(z)dz}\tilde{\nu}_i\mathcal{M}_i dy\right)1_{v_1>0} \\ &+ \left(e^{-\frac{1}{\tau|v_1|}\int_x^1 \tilde{\nu}_i(y)dy} f_{i,R}(v) + \frac{1}{\tau|v_1|}\int_x^1 e^{-\frac{1}{\tau|v_1|}\int_x^y \tilde{\nu}_i(z)dz}\tilde{\nu}_i\mathcal{M}_i dy\right)1_{v_1<0}. \end{aligned}$$

Main theorem

Theorem

Suppose $f_{i,LR}, \frac{1}{|v_1|} f_{i,LR} \in L^1_2(\mathbb{R}^3_v)$*. And suppose futher that for* $j = 2, 3$

$$\int_{\mathbb{R}^2} f_{i,L} v_j dv_2 dv_3 = \int_{\mathbb{R}^2} f_{i,R} v_j dv_2 dv_3 = 0.$$

Then there exists a constant $L > 0$*, depending only on the boundary data, such that if* $\tau > L$*, then there exists a unique mild solution* (f_1, f_2, f_3, f_4) *for (5).*

Again, the proof uses Banach fixed point argument.

Upper and lower bounds for the BGK-parameters

Note that

$$\tilde{n}_1 = F^{-1}_{\mathbf{n},\mathbf{n},\tilde{\boldsymbol{\nu}},\tilde{\boldsymbol{\nu}},\boldsymbol{T},\boldsymbol{V}}\left(\frac{3}{2}\log\left(\frac{\mu_{12}}{\mu_{34}}\right)\right),$$

where

$$\begin{aligned} F_{\mathbf{x},\mathbf{y},\boldsymbol{\mu},\boldsymbol{\eta},\boldsymbol{\alpha},\boldsymbol{\beta}}(z) &:= \log\frac{\mu_3\mu_4}{\eta_2} + \log z + \log(\mu_2 x_2 + \mu_1 z - \eta_1 y_1) \\ &- \log(\eta_3 y_3 - \mu_1 z + \eta_1 y_1) - \log(\eta_4 y_4 - \mu_1 z + \eta_1 y_1) \\ &- \frac{\frac{3}{2}\Delta E\sum_{i=1}^{4}\eta_i y_i}{\sum_{i=1}^{4}\mu_i x_i\left[\frac{1}{2}m_i(\beta_i^2) + \frac{3}{2}k\alpha_i\right] + \Delta E(\mu_1 z - \eta_1 y_1)}, \end{aligned}$$

and

$$\mathbf{n} = (n^{(i)})_{i=1,2,3,4},\ \tilde{\boldsymbol{\nu}} = (\tilde{\nu}_i)_{i=1,2,3,4}, \mathbf{T} = (T^{(i)})_{i=1,2,3,4},$$
$$\mathbf{V} = (|U^{(i)} - \tilde{U}|^2)_{i=1,2,3,4}.$$

Upper and lower bounds for the BGK-parameters

For fixed z, the function $(\mathbf{x},\mathbf{y},\boldsymbol{\mu},\boldsymbol{\eta},\boldsymbol{\alpha},\boldsymbol{\beta}) \mapsto F_{\mathbf{x},\mathbf{y},\boldsymbol{\mu},\boldsymbol{\eta},\boldsymbol{\alpha},\boldsymbol{\beta}}(z)$ is decreasing in $x_i, \mu_i, \alpha_i, |\beta_i|$ $(i = 1,2,3,4)$, and increasing in y_i, η_i $(i = 1,2,3,4)$. Hence the function $G : (\mathbb{R}_+)^{20} \times \mathbb{R}^4 \to \mathbb{R}_+$ defined as

$$G(\mathbf{x},\mathbf{y},\boldsymbol{\mu},\boldsymbol{\eta},\boldsymbol{\alpha},\boldsymbol{\beta}) = F^{-1}_{\mathbf{x},\mathbf{y},\boldsymbol{\mu},\boldsymbol{\eta},\boldsymbol{\alpha},\boldsymbol{\beta}}\left(\frac{3}{2}\log\left(\frac{\mu_{12}}{\mu_{34}}\right)\right)$$

is decreasing in $x_i, \mu_i, \alpha_i, |\beta_i|$ $(i = 1,2,3,4)$, and increasing in y_i, η_i $(i = 1,2,3,4)$. Therefore, we obtain

$$\begin{aligned} 0 &< G(\mathbf{n}^M,\mathbf{n}^m,\boldsymbol{\nu}^{\boldsymbol{M}},\boldsymbol{\nu}^{\boldsymbol{m}},\mathbf{T}^M,\mathbf{V}^M) \le \tilde{n}_1 = G(\mathbf{n},\mathbf{n},\tilde{\boldsymbol{\nu}},\tilde{\boldsymbol{\nu}},\mathbf{T},\mathbf{V}) \\ &\le G(\mathbf{n}^m,\mathbf{n}^M,\boldsymbol{\nu}^{\boldsymbol{m}},\boldsymbol{\nu}^{\boldsymbol{M}},\mathbf{T}^m,\mathbf{0}) \end{aligned}$$

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Modeling setup

Consider the BGK-type equation

$$\partial_t f_i + v \cdot \nabla_x f_i = \tilde{Q}_i^M + \tilde{Q}_i^C := \nu^M(\mathcal{M}_i^M - f_i) + \nu_i^C(\mathcal{M}_i^C - f_i)$$

with

$$\mathcal{M}_i^M := n^{(i)} \left(\frac{m_i}{2\pi k T^*}\right)^{3/2} \exp\left(-\frac{m_i|v - U_i^*|^2}{2kT^*}\right)$$

and

$$\mathcal{M}_i^C := \tilde{n}^i \left(\frac{m_i}{2\pi k \tilde{T}}\right)^{3/2} \exp\left(-\frac{m_i|v - \tilde{U}|^2}{2k\tilde{T}}\right)$$

Goal: Define the following terms 'reasonably':

- U_i^*, T^*, ν^M $(i = 1, 2, 3, 4)$
- $\tilde{n}_i$, $\tilde{U}$, $\tilde{T}$, ν_i^C $(i = 1, 2, 3, 4)$

Mechanical collision operator

Given symmetric non-positive matrix $L^* = (L^*_{ij})$ having 0 as a simple eigenvalue, we set

$$\underline{U} = (U_1, \dots, U_4)^T := \mathbf{U} + N^{-1}\left(I + \frac{1}{\nu^M}(L^*)^\dagger\right)N(\bar{\mathbf{U}} - \mathbf{U})$$

$$T^* := T - \frac{1}{3nk}\left\|\left(I + \frac{1}{\nu^M}(L^*)^\dagger\right)N(\bar{\mathbf{U}} - \mathbf{U})\right\|_2^2$$

where $\mathbf{U} = (U, U, U, U)^T$, $\bar{\mathbf{U}} = (U^{(1)}, \dots, U^{(4)})^T$ and $N = \mathrm{diag}(\sqrt{\rho^{(1)}}, \dots, \sqrt{\rho^{(4)}})$. For $\nu^M \geq \|(L^*)^\dagger\|$, we have $T^* > 0$.

Characterization of the mechanical collision operator

Theorem [Brull-Pavan-Schneider (2012)]

$(\mathcal{M}_i^M)_{i=1,2,3,4}$ is a unique solution to the minimization problem

$$\text{argmin}_{\mathbf{g}\in K(\mathbf{f})} \sum_{i=1}^{4} \int (g_i \log g_i - g_i) dv,$$

where $K(\mathbf{g})$ is a set of some admissible class of functions $\mathbf{f}$, including the conservation of mass, momentum and energy.

Chemical collision operator

We define $\tilde{n}_i$, $\tilde{U}$, $\tilde{T}$ the same way as in the Groppi-Rjasanow-Spiga model. For a given constant ν_{12}^{34}, we set

$$
\begin{aligned}
\nu_1^C &= \frac{2}{\sqrt{2\pi}} \nu_{12}^{34} \Gamma\left(\frac{3}{2}, \frac{\Delta E}{kT}\right) n^{(2)}, \\
\nu_2^C &= \frac{2}{\sqrt{2\pi}} \nu_{12}^{34} \Gamma\left(\frac{3}{2}, \frac{\Delta E}{kT}\right) n^{(1)}, \\
\nu_3^C &= \frac{2}{\sqrt{2\pi}} \left(\frac{\mu^{12}}{\mu^{34}}\right)^{3/2} e^{\Delta E/kT} \nu_{12}^{34} \Gamma\left(\frac{3}{2}, \frac{\Delta E}{kT}\right) n^{(4)}, \\
\nu_4^C &= \frac{2}{\sqrt{2\pi}} \left(\frac{\mu^{12}}{\mu^{34}}\right)^{3/2} e^{\Delta E/kT} \nu_{12}^{34} \Gamma\left(\frac{3}{2}, \frac{\Delta E}{kT}\right) n^{(3)}.
\end{aligned}
$$

Thank you