# Is the BGK equation only a toy model ?

Mario Pulvirenti

Dipartimento di Matematica, Universita' di Roma, Sapienza
and International Research Center on the Mathematics and Mechanics of
Complex Systems MeMoCS, University of L'Aquila, Italy.
Accademia Nazionale dei Lincei

June 19-23, 2023

# The model

In 1953 Bhatnagar, Gross and Krook proposed a new kinetic equation giving a tool of analysis, more efficient than the Boltzmann equation, when the Knudsen number is small compared to the macroscopic scales, but not enough to use the hydrodynamical picture. Now starting from the Boltzmann equation, we are led to perform complex dynamical calculations (e.g., numerically) to obtain precise information on the local equilibria driving the hydro description. Therefore we replace the two-body collision by an instantaneous thermalization on a local Maxwellian, constructed with the empirical parameters given by the dynamics itself. The equation for the one-particle distribution function $f = f(x, v, t)$ proposed reads

$$(\partial_t f + v \cdot \nabla_x f)(x, v, t) = \varrho(\varrho M_f - f)(x, v, t)\,,$$

$$M_f(x, v, t) = \frac{1}{(2\pi T(x,t))^{3/2}} \exp\left(-\frac{|v - u(x,t)|^2}{2T(x,t)}\right)\,,$$

$$\varrho(x,t) = \int dv\, f(x,v,t)\,, \quad \varrho\, u(x,t) = \int dv\, f(x,v,t) v\,,$$

$$\varrho(|u|^2 + 3T)(x,t) = \int dv\, f(x,v,t)|v|^2\,.$$

Here, we fix the space dimension $d = 3$, $(x, v)$ denotes position and velocity of a typical particle, and $t$ is the time. The Maxwellian $M_f$ has hydrodynamic parameters (density, mean velocity and temperature) obtained from local averages of $f$ itself. Same qualitative and hydrodynamic behaviour of the Boltzmann equation. No details of the interaction. Useful because, with respect to the Boltzmann equation, it is a simpler and more flexible tool to perform computations.
Extensive literature (mathematical and applied) concerning BGK : numerical methods, hydrodynamic limits, applications to gas mixtures ......

Here we present a (formal and preliminary) analysis by P. Butta' , S. Simonella and P. (2023) in which, we try to derive BGK starting from a stochastic system, the non-homogeneous Kac model, which is a continuous version of the Direct Simulation Bird's scheme. This is equivalent to the Boltzmann eq.n in a natural scaling limit. Real mechanical particle systems are too difficult due to the lack of ergodic results. The problem now is how to modify the scaling in order to outline a quick thermalization, leaving a finite mean free path. To show that, in some sense BGK is not only a toy model. Previous results: Assuming BGK prove the convergence of suitable (stochastic) particle scheme: Butta', Hauray, P. ARMA '21; Butta',P. KRM '22; Mustafa', Wennberg (linear) JSP '20.

Summarizing:
1) Consider the non-homogeneous Kac model for a stochastic $N$-particle system.
2) In some Mean-Field scaling limit we derive the Boltzmann equation.
3) Modify the scaling by reinforcing the interaction (toward hydrodynamics), but leaving finite the mean-free path.
4) Derive BGK.

Comments: 2) is well known....in some sense. Very difficult in the low-density limit.

Consider a partition of $\mathbb{T}^3$ ($3-d$ torus of side 1) in cubic cells $\Delta$ with equal volume $|\Delta|$. Consider a system of $N$ particles evolving freely in $\mathbb{T}^3$ up to an exponential time of suitable intensity. Then extract a pair of particles randomly. If they fall in the same cell $\Delta$, they perform a collision. Otherwise, nothing happens.
Notation: $Z_N = (X_N, V_N) = (z_1, \dots, z_N)$ denotes a configuration of the system, being $z_i = (x_i, v_i)$ position and velocity of the $i$-th particle. The generator of this process reads ($\Phi = \Phi(Z_N)$ a test function)

$$\mathcal{L}\Phi(Z_N) = V_N \cdot \nabla_{X_N}\Phi(Z_N) + \frac{1}{N|\Delta|}\sum_{i<j}\int d\omega\, B(\omega; v_i - v_j)\chi_{i,j} \times \{\Phi(X_N, V_N^{i,j}) - \Phi(X_N, V_N)\},$$

where $\chi_{i,j} = 1$ if $i$ and $j$ belong to the same cell and 0 otherwise.

$$V_N = (v_1 \cdots v_i, \cdots v_j \cdots v_N), \quad V_N^{i,j} = (v_1 \cdots v_i', \cdots v_j' \cdots v_N)$$

where $(v_i, v_j) \rightarrow (v_i', v_j')$ describes a collision with impact parameter $\omega$.
$B$ is the given cross-section.
We denote by $W^N(Z_N, t)$ a symmetric probability distribution solution to the associated master equation,

$$(\partial_t + V_N \cdot \nabla_{X_N}) W^N(Z_N, t)$$
$$= \frac{1}{N|\Delta|} \sum_{i<j} \int d\omega\, B(\omega; v_i - v_j) \chi_{i,j} \{ W^N(X_N, V_N^{i,j}) - W^N(X_N, V_N) \} .$$

This process yields formally the Boltzmann equation in the combined limit $N \to \infty$ and $|\Delta| \to 0$. If $f_1^N$ and $f_2^N$ are the one and two particle marginals, for any test function $\varphi = \varphi(z)$,

$$\frac{d}{dt} \int dz_1 \, f_1^N \varphi = \int dz_1 \, f_1^N v_1 \cdot \nabla_x \varphi + \frac{N-1}{N|\Delta|} \int dz_1 \, dz_2 \int d\omega$$

$$B(\omega; v_1 - v_2) \times \chi_{1,2} f_2^N(z_1, z_2) \{\varphi(x_1, v_1') - \varphi(x_1, v_1)\} \, .$$

Therefore, under the assumption of propagation of chaos, letting first $N \to \infty$ and then $|\Delta| \to 0$ we recover the Boltzmann equation in the weak form.

How to modify the model to recover, at least formally, the BGK model?

Inspired from the original paper, we reinforce the interaction leaving finite the mean-free path. We introduce a time $\tau$, which will eventually converge to 0, and prescribe the dynamics in each time interval $[2n\tau, 2(n+1)\tau]$, $n \in \mathbb{N}$. All the particles move freely in the time interval $[2n\tau, (2n+1)\tau]$. During the time interval $[(2n+1)\tau, (2n+2)\tau]$, the particles contained in each cell $\Delta$ evolve according to the homogeneous Kac dynamics with probability $\tau N_\Delta / N$ and nothing happens with probability $1 - \tau N_\Delta / N$. $N_\Delta$ is the number of particles in $\Delta$. Moreover, we increase the number of collisions introducing a time-scale parameter $\epsilon$ in the Kac dynamics.

The evolution $W^N(t)$ is given by the product formula,

$$W^N(n\tau) = (S_0(\tau)K(\tau))^n W^N(0)\,,$$

where $S_0$ is the free stream operator and

$$K(\tau) = \prod_{\Delta} \left[ \frac{\tau N_\Delta}{N} S^\Delta(\tau) + \left(1 - \frac{\tau N_\Delta}{N}\right)\right],$$

with

$$S^\Delta(\tau) = \exp\left(\frac{\tau}{\epsilon}\mathcal{L}^\Delta_{\text{int}}\right)$$

and ($G = G(V_N)$ a test function)

$$\mathcal{L}^\Delta_{\text{int}} G(V_N) = \frac{1}{N|\Delta|}\sum_{i<j}\int d\omega\, B(\omega; v_i - v_j)\chi^\Delta_{i,j}\{G(V_N^{i,j}) - G(V_N)\}\,.$$

Above, $\chi^\Delta_{i,j} = 1$ iff $x_i, x_j \in \Delta$, and $\chi^\Delta_{i,j} = 0$ otherwise. Moreover, we assume $\epsilon \ll \tau \ll 1$.

We rewrite as a discrete time Duhamel formula with respect to the linear evolution $S_0$,

$$
\begin{aligned}
W^N(n\tau) &= S_0(\tau)(K(\tau)-1)W^N((n-1)\tau) + S_0(\tau)W^N((n-1)\tau) \\
&= \cdots \\
&= S_0(n\tau)W^N(0) + \sum_{k=1}^{n} S_0(k\tau)(K(\tau)-1)W^N[(n-k)\tau]\,.
\end{aligned}
$$

We next observe that

$$
K(\tau)-1 = \tau \sum_{\Delta} \frac{N_\Delta}{N}(S^\Delta(\tau)-1) + O(\tau^2)\,,
$$

and, for small $\tau$,

$$
W^N(n\tau) \approx S_0(n\tau)W^N(0) + \sum_{k=1}^{n} \tau S_0(k\tau) \sum_{\Delta} \frac{N_\Delta}{N}(S^\Delta(\tau)-1)W^N((n-k)\tau)
$$

Now, let $f_1^N$ be the one-particle marginal,

$$f_1^N(t) = f_1^N(z_1, t) = \int dZ_{1,N}\, W^N(Z_N, t)\,,$$

being $dZ_{1,N} = dz_2 \cdots dz_N$. Then we get

$$f_1^N(n\tau) = s_0(n\tau) f_1^N(0) + \sum_{k=1}^{n} \tau s_0(k\tau) Q W^N((n-k)\tau)\,,$$

where $s_0$ is the one-particle free stream operator and

$$QW^N(t) = QW^N(z_1, t) = \int dZ_{1,N} \sum_{\Delta} \frac{N_\Delta}{N} (S^\Delta(\tau) - 1) W^N(Z_N, t)\,.$$

Now, for $\epsilon \ll \tau$, the mixing property of the Kac model implies

$$S^{\Delta_1}(\tau)\Pi_t^N(V_N^{\Delta_1}|X_N, V_N^{\Delta_1^c}) \approx \mu_{\mathcal{E}_{\Delta_1}^N, \mathcal{P}_{\Delta_1}^N}(V_N^{\Delta_1}),$$

where $\mu_{\mathcal{E}_{\Delta_1}^N, \mathcal{P}_{\Delta_1}^N}$ is the microcanonical measure associated to the empirical energy and momentum in $\Delta_1$,

$$\mathcal{E}_{\Delta_1}^N = \frac{1}{2N_{\Delta_1}} \sum_{j:\, x_j \in \Delta_1} v_j^2, \quad \mathcal{P}_{\Delta_1}^N = \frac{1}{N_{\Delta_1}} \sum_{j:\, x_j \in \Delta_1} v_j$$

and $\Pi_t^N(V_N^{\Delta_1}|X_N, V_N^{\Delta_1^c})$ is the conditional expectation of $W^N(t)$. Indeed as $\epsilon \to 0$ (time goes to infinity) the solutions of the homogeneous Kac model do converge to the microcanonical (uniform) distribution.

On the other hand, letting $\pi^N_{\Delta_1} = N_{\Delta_1}/N$ be the empirical density in $\Delta_1$, we expect that, with large $R^N_t(X_N) = \int W^N dV_N$-probability when increasing $N$,

$$\pi^N_{\Delta_1} \approx \varrho^N_{\Delta_1}(t) := \int_{\Delta_1} dx\, \varrho^N_1(x,t)$$

(where $\varrho^N_1(x,t) := \int v\, f^N_1(x,v,t)$) and that the $v_j$'s are asymptotically independent. Therefore, by the law of large numbers, we expect also

$$\mathcal{E}^N_{\Delta_1} \approx E^N_{\Delta_1}(t) := \frac{1}{\varrho^N_{\Delta_1}(t)} \int_{\Delta_1} dx \int v\, f^N_1(x,v,t) \frac{v^2}{2} \,,$$

$$\mathcal{P}^N_{\Delta_1} \approx P^N_{\Delta_1}(t) := \frac{1}{\varrho^N_{\Delta_1}(t)} \int_{\Delta_1} dx \int dv\, f^N_1(x,v,t) v \,.$$

We can compute $QW^N(z_1, t)$. But we can also use the equivalence of the ensembles (Canonical=Grandcanonical=Microcanonical) as $N \to \infty$.
At the end one obtains

$$QW^N(z_1, t) \approx \varrho^N_{\Delta_1}(t) \left( \varrho^N_1(x_1, t) M_{P^N_{\Delta_1}(t), T^N_{\Delta_1}(t)}(v_1) - f^N_1(z_1, t) \right).$$

where $M_{P^N_{\Delta_1}(t), T^N_{\Delta_1}(t)}$ is the maxwellian with local momentum and temperature $P^N_{\Delta_1}, T^N_{\Delta_1}$.

Therefore taking the limits $\epsilon \to 0$, $N \to \infty$, and finally $\tau \to 0$, the (limit) one-particle marginal $f$ solves the integral equation,

$$f(x,v,t) = f_0(x-vt,v) + \int_0^t ds\, \varrho_{\Delta_x}(\varrho M_{P_{\Delta_x},T_{\Delta_x}} - f)(x-vs,v,t-s)\,,$$

where $\Delta_x$ is the cell containing $x$ and $\varrho_\Delta$, $P_\Delta$, $T_\Delta$ are defined as $\varrho_\Delta^N$, $P_\Delta^N$, $T_\Delta^N$ with $f_1^N$ replaced by $f$.
Finally, taking also the limit $|\Delta| \to 0$, we recover the equation

$$f(x,v,t) = f_0(x-vt,v) + \int_0^t ds\, (\varrho(\varrho M_f - f))(x-vs,v,t-s)\,,$$

which is the mild formulation of BGK eq.n via the Duhamel formula.

At moment everything is reasonable but formal. We need....to rigorize it!

PIERO, best wishes!