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Macroscopic description of arbitrary Knudsen number flow using Boltzmann–BGK kinetic theory. Part 2

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We extend our previous analysis of closed-form equations for finite Knudsen number flow and scalar transport that result from the Boltzmann–Bhatnagar–Gross–Krook (BGK) kinetic theory with constant relaxation time. Without approximation, we obtain closed-form equations for arbitrary spatial dimension and flow directionality which are local differential equations in space and integral equations in time. These equations are further simplified for incompressible flow and scalars. The particular case of no-flow scalar transport admits analytical solutions that exhibit ballistic behaviour at short times while behaving diffusively at long times. It is noteworthy that, even with constant relaxation time BGK microphysics, quite complex macroscopic descriptions result that would be difficult to obtain using classical constitutive models or continuum averaging.

Key words: general fluid mechanics, non-continuum effects, non-Newtonian flows

1. Introduction

In Chen, Orszag & Staroselsky (2007) (hereafter referred to as Part 1), we derived macroscopic flow equations for arbitrary Knudsen number (Kn) with the only assumptions being that the microscopic dynamics is given by Boltzmann–Bhatnagar–Gross–Krook (BGK) kinetic theory with a single relaxation time and that statistical equilibrium existed in the infinite past. These results demonstrate the existence of such a closed-form macroscopic dynamical description of microscopic dynamics, following the seminal work of Cercignani (1969, 1975) (cf. also the early work of Shen 1963). While the equations that are presented in Part 1 are integral equations in both space and time, we further reduced them to local differential equations in space for the case of isothermal unidirectional flow. An exact analytical solution of the latter equations was also presented in Part 1 for the non-monotonic flow flux in a channel with accurate prediction of the minimum mass flux as a function of Knudsen number. However, the closed macroscopic representation derived in Part 1 for arbitrary flow situations has a less revealing form. In the present work, we extend our previous analysis of closed-form equations for finite-Knudsen-number flow resulting from the same Boltzmann–BGK kinetic equation. Without approximation, we obtain a new

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set of closed-form continuum equations for arbitrary spatial dimension and flow directionality, which are local differential equations in space and integral equations in time. This new macroscopic representation reveals clearer macroscopic physics and its relationship to conventionally familiar flow structures. It is noteworthy that, even with constant relaxation time BGK microphysics, quite complex macroscopic descriptions (Chen *et al.* 2003) result that would be difficult to obtain using classical constitutive models or continuum averaging.

In addition, we obtain a closed-form macroscopic description of transport of 'colour' tracers by general flows of arbitrary Knudsen number within the framework of the Boltzmann–BGK microdynamics. The colour tracers have, microscopically, identical particle properties but are just labelled according to an internal colour label σ. The particle distribution for a given tracer is thus defined as $f_\sigma(\boldsymbol{x}, \boldsymbol{v}, t)$, while a 'colour blind' particle distribution function is simply a summation of the former over all possible tracers,

$$f(\boldsymbol{x}, \boldsymbol{v}, t) = \sum_\sigma f_\sigma(\boldsymbol{x}, \boldsymbol{v}, t).$$

Here $f = f(\boldsymbol{x}, \boldsymbol{v}, t)$ is the single-particle distribution function which represents the density of particles in phase space $(\boldsymbol{x}, \boldsymbol{v})$ at time t.

Once again, the colour blind distribution f obeys the BGK collision model (Bhatnagar, Gross & Krook 1954)

$$\partial_t f + \boldsymbol{v} \cdot \nabla f = -\frac{f - f^{eq}}{\tau}, \tag{1}$$

where the (constant) relaxation time is τ, and the local kinetic equilibrium distribution function f^{eq} is the Maxwell–Boltzmann distribution,

$$f^{eq}(\boldsymbol{x}, \boldsymbol{v}, t) = \frac{\rho(\boldsymbol{x}, t)}{(2\pi\theta(\boldsymbol{x}, t))^{D/2}} \exp\left[-\frac{(\boldsymbol{v} - \boldsymbol{u}(\boldsymbol{x}, t))^2}{2\theta(\boldsymbol{x}, t)}\right]. \tag{2}$$

Macroscopic flow variables, like the fluid velocity, are moments of f:

$$\left\{\begin{array}{c} \rho(\boldsymbol{x}, t) \\ \rho\boldsymbol{u}(\boldsymbol{x}, t) \\ \rho(u^2(\boldsymbol{x}, t) + D\,\theta(\boldsymbol{x}, t)) \end{array}\right\} = \int \mathrm{d}\boldsymbol{v} \left\{\begin{array}{c} 1 \\ \boldsymbol{v} \\ \boldsymbol{v}^2 \end{array}\right\} f(\boldsymbol{x}, \boldsymbol{v}, t) = \int \mathrm{d}\boldsymbol{v} \left\{\begin{array}{c} 1 \\ \boldsymbol{v} \\ \boldsymbol{v}^2 \end{array}\right\} f^{eq}(\boldsymbol{x}, \boldsymbol{v}, t), \tag{3}$$

where $\rho, \boldsymbol{u}$ and θ, denote, respectively, density, fluid velocity and temperature. D is the dimension of phase space $(\boldsymbol{v})$. Notwithstanding some well-known limitations such as unity Prandtl number, the Boltzmann–BGK kinetic model has been used broadly for study of high Kn as well as high Mach number (*Ma*) flow problems (cf. Xu, Martinelli & Jameson 1994). It is noteworthy that, even for gas dynamics at high *Ma*, in which the relaxation time τ clearly depends on thermodynamic properties, the constant τ BGK model is still quite useful to provide insight and clarity for the more general problem.

2. General formulation of hydrodynamics at arbitrary Kn

Equation (1) may be solved by the method of characteristics so that, assuming that the solution, as $t \to -\infty$, the distribution function f approaches the equilibrium distribution f^{eq},

$$f(\boldsymbol{x}, \boldsymbol{v}, t) = \int_{-\infty}^{t} \frac{\mathrm{d}t'}{\tau} \mathrm{e}^{-(t-t')/\tau} f^{eq}(\boldsymbol{x} - \boldsymbol{v}(t - t'), \boldsymbol{v}, t'), \tag{4}$$

which may be rewritten as

$$f(\boldsymbol{x},\boldsymbol{v},t)=\int_0^\infty \mathrm{e}^{-s} f^{eq}(\boldsymbol{x}-\boldsymbol{v}\tau s,\boldsymbol{v},t-\tau s)\,\mathrm{d}s. \tag{5}$$

As shown in Part 1, substitution of the exact solution (5) into (3) already reveals the existence of closed-form macroscopic equations for ρ, $\boldsymbol{u}$, θ at all Kn in a general flow situation in d-dimensional physical space. Indeed, (5) embodies both the equilibrium and non-equilibrium parts of $f(\boldsymbol{x},\boldsymbol{v},t)$ and is determined (non-locally in time and space) by the inhomogeneity in the macroscopic variables ρ, $\boldsymbol{u}$, and θ. This inhomogeneous (and nonlinear in ρ, $\boldsymbol{u}$, and θ) solution should be distinguished from that of the linearized analysis based on a homogeneous absolute equilibrium (Cercignani 1969).

These points can be made clearer by presenting a conventional hydrodynamic equation representation. By taking moments (3) of (1), we get

$$\partial_t\rho u_\alpha+\partial_\beta\sigma_{\alpha\beta}=0,\quad \partial_t[\rho(u^2+D\theta)]+\partial_\beta q_\beta=0. \tag{6}$$

Here $\partial_t\equiv\partial/\partial t$, subscripts α, β denote Cartesian components and $\partial_\beta\equiv\partial/\partial x_\beta$. The fluxes are defined as

$$\sigma_{\alpha\beta}\equiv\int \mathrm{d}\boldsymbol{v}\; v_\alpha v_\beta f;\quad q_\alpha\equiv\int \mathrm{d}\boldsymbol{v}\; v^2 v_\alpha f. \tag{7}$$

Upon combining (6) and (7) with (5), a closed-form macroscopic description is established:

$$\partial_t\rho(\boldsymbol{x},t)u_\alpha(\boldsymbol{x},t)=-\partial_\beta\int_0^\infty \mathrm{d}s\;\mathrm{e}^{-s}\int \mathrm{d}\boldsymbol{v}\; v_\alpha v_\beta\frac{\rho(\boldsymbol{x}-\boldsymbol{v}\tau s,t-\tau s)}{(2\pi\theta(\boldsymbol{x}-\boldsymbol{v}\tau s,t-\tau s))^{D/2}} \times\exp\left[-\frac{(\boldsymbol{v}-\boldsymbol{u}(\boldsymbol{x}-\boldsymbol{v}\tau s,t-\tau s))^2}{2\theta(\boldsymbol{x}-\boldsymbol{v}\tau s,t-\tau s)}\right], \tag{8}$$

$$\partial_t[\rho(\boldsymbol{x},t)(\boldsymbol{u}^2(\boldsymbol{x},t)+D\theta(\boldsymbol{x},t))]=-\partial_\alpha\int_0^\infty \mathrm{d}s\;\mathrm{e}^{-s}\int \mathrm{d}\boldsymbol{v}\; v^2 v_\alpha \times\frac{\rho(\boldsymbol{x}-\boldsymbol{v}\tau s,t-\tau s)}{(2\pi\theta(\boldsymbol{x}-\boldsymbol{v}\tau s,t-\tau s))^{D/2}}\exp\left[-\frac{(\boldsymbol{v}-\boldsymbol{u}(\boldsymbol{x}-\boldsymbol{v}\tau s,t-\tau s))^2}{2\theta(\boldsymbol{x}-\boldsymbol{v}\tau s,t-\tau s)}\right]. \tag{9}$$

Of course, this system should be augmented by mass conservation which has the same form as for $Kn=0$:

$$\partial_t\rho(\boldsymbol{x},t)=-\partial_\beta\int \mathrm{d}\boldsymbol{v}\; v_\beta f=-\partial_\beta\int \mathrm{d}\boldsymbol{v}\; v_\beta f^{eq}=-\partial_\beta(\rho(\boldsymbol{x},t)u_\beta(\boldsymbol{x},t)). \tag{10}$$

As in Part 1, (8)–(10) are a self-contained set of integro-differential equations for the macroscopic fields ρ, $\boldsymbol{u}$ and θ that are valid for all Kn. As mentioned in § 1, the system (8)–(10) does not appeal to the intuition of a fluid dynamicist. For instance, as a clear signature of the past history of particles, (8)–(10) explicitly contains integration over the microscopic velocity $\boldsymbol{v}$ (even though it is just a dummy variable). Part 1 of this paper contains a conversion of the macroscopic equations (8)–(10) into a set of integro-differential equations in space that are perhaps still complicated, difficult to manipulate, and not intuitive looking.

In this paper, we go further and obtain a closed-form macroscopic description by carrying out the integration over the microscopic velocity $\boldsymbol{v}$, resulting in differential-in-$\boldsymbol{x}$ equations of motion. To do this, we note first that all spatial arguments on the right-hand side of (8) can be made equal to $\boldsymbol{x}$ by using the spatial shift operator: $F(x+a)=\exp(a\partial_x)F(x)$ and rewriting (8) as

$$\partial_t\rho(\boldsymbol{x},t)u_\alpha(\boldsymbol{x},t) = -\partial_\beta\int_0^\infty \mathrm{d}s\,\mathrm{e}^{-s}\int \mathrm{d}\boldsymbol{v}\; v_\alpha v_\beta \exp\left[-\tau s\boldsymbol{v}\cdot\frac{\partial}{\partial\boldsymbol{x}}\right] \times\frac{\rho(\boldsymbol{x},t-\tau s)}{(2\pi\theta(\boldsymbol{x},t-\tau s))^{D/2}}\exp\left[-\frac{(\boldsymbol{v}-\boldsymbol{u}(\boldsymbol{x},t-\tau s))^2}{2\theta(\boldsymbol{x},t-\tau s)}\right]. \quad (11)$$

At a first glance, not much is gained in this way, since the operator $\exp[-\tau s\boldsymbol{v}\cdot(\partial/\partial\boldsymbol{x})]$ does not commute with the rest of the expression, making the whole formula intractable. Indeed, it is not possible to combine the two exponentials in (11) and compute it as a Gaussian integral over the phase space $\boldsymbol{v}$, as could have done if $\partial/\partial\boldsymbol{x}$ were just a scalar and not an operator. Note in this regard that the only reason we could exactly compute such a Gaussian integral in Part 1 is that for the special case of unidirectional flow, the shift operator $\partial/\partial z$ commutes with $u_z(x,y)$.

However, it is still possible to perform the required integration in the general case without manipulation of non-commuting operators. In order to do that, we assign a different spatial argument $\boldsymbol{y}$ to all the functions to the right of the differential operator and rewrite (8) and (11) as

$$\begin{aligned}\partial_t\rho(\boldsymbol{x},t)u_\alpha(\boldsymbol{x},t) &= -\partial_\beta\int_0^\infty \mathrm{d}s\,\mathrm{e}^{-s}\int\mathrm{d}\boldsymbol{y}\int \mathrm{d}\boldsymbol{v}\; v_\alpha v_\beta \exp\left[-\tau s\boldsymbol{v}\cdot\frac{\partial}{\partial\boldsymbol{x}}\right]\\ &\quad\cdot\delta(\boldsymbol{x}-\boldsymbol{y})\frac{\rho(\boldsymbol{y},t-\tau s)}{(2\pi\theta(\boldsymbol{y},t-\tau s))^{D/2}}\exp\left[-\frac{(\boldsymbol{v}-\boldsymbol{u}(\boldsymbol{y},t-\tau s))^2}{2\theta(\boldsymbol{y},t-\tau s)}\right]\\ &= -\partial_\beta\int_0^\infty \mathrm{d}s\,\mathrm{e}^{-s}\int\mathrm{d}\boldsymbol{y}\;B_{\alpha\beta}(\boldsymbol{y},t-\tau s)\,\delta(\boldsymbol{x}-\boldsymbol{y}).\end{aligned}\quad (12)$$

Now everything commutes within the scope of Gaussian integration over $\boldsymbol{v}$ because ρ, $\boldsymbol{u}$, and θ are now functions of $\boldsymbol{y}$, not $\boldsymbol{x}$, and the operator

$$B_{\alpha\beta}\equiv\frac{\rho(\boldsymbol{y},t-\tau s)}{(2\pi\theta(\boldsymbol{y},t-\tau s))^{D/2}}\int\mathrm{d}\boldsymbol{v}\;v_\alpha v_\beta\exp\left[-\tau s\boldsymbol{v}\cdot\frac{\partial}{\partial\boldsymbol{x}}-\frac{(\boldsymbol{v}-\boldsymbol{u}(\boldsymbol{y},t-\tau s))^2}{2\theta(\boldsymbol{y},t-\tau s)}\right] \quad (13)$$

is readily evaluated. To do this, we note that

$$\langle v_{\alpha_1}\ldots v_{\alpha_n}\rangle\equiv\int\frac{\mathrm{d}\boldsymbol{v}}{(2\pi\theta)^{D/2}}\,v_\alpha\ldots v_{\alpha_n}\exp\left[-\frac{\boldsymbol{v}^2}{2\theta}+\boldsymbol{p}\cdot\boldsymbol{v}\right]=\frac{\partial^n Z(\boldsymbol{p})}{\partial p_{\alpha_1}\ldots\partial p_{\alpha_n}}, \quad (14)$$

where the generating function Z is given by

$$Z(\boldsymbol{p})\equiv\int\frac{\mathrm{d}\boldsymbol{v}}{(2\pi\theta)^{D/2}}\exp\left[-\frac{\boldsymbol{v}^2}{2\theta}+\boldsymbol{p}\cdot\boldsymbol{v}\right]=\exp\left[\frac{\theta\boldsymbol{p}^2}{2}\right]. \quad (15)$$

We also note that (15) holds for all mathematical objects $\boldsymbol{p}$ that commute with all $\boldsymbol{v}$ and θ numbers. Using (14) and (15), we compute (13) by differentiation with respect to $\boldsymbol{p}$ with the choice

$$p_\gamma=-\tau s\partial_\gamma+\frac{u_\gamma(\boldsymbol{y},t-\tau s)}{\theta(\boldsymbol{y},t-\tau s)}, \quad (16)$$

so that

$$B_{\alpha\beta}=\exp\left[\frac{\theta\tau^2s^2\partial_\gamma^2}{2}-\partial_\gamma\tau s u_\gamma\right]\rho(\theta\delta_{\alpha\beta}+u_\alpha u_\beta\;-\theta\tau s u_\beta\partial_\alpha-\theta\tau s u_\alpha\partial_\beta+\theta^2\tau^2s^2\partial_\alpha\partial_\beta).$$

In this way, we obtain

$$\partial_t(\rho(x,t)u_\alpha(\boldsymbol{x},t)) = -\partial_\beta \int_0^\infty \mathrm{d}s\ \mathrm{e}^{-s} \int_R \mathrm{d}\boldsymbol{y}\ \exp\left[\frac{\theta(\boldsymbol{y},t-\tau s)\tau^2 s^2 \partial_\gamma^2}{2} - \partial_\gamma \tau s u_\gamma(\boldsymbol{y},t-\tau s)\right]$$
$$\times \rho(\boldsymbol{y},t-\tau s)[\theta(\boldsymbol{y},t-\tau s)\delta_{\alpha\beta} + u_\alpha(\boldsymbol{y},t-\tau s)u_\beta(\boldsymbol{y},t-\tau s)$$
$$-\theta(\boldsymbol{y},t-\tau s)\tau s\left(u_\alpha(\boldsymbol{y},t-\tau s)\partial_\beta + u_\beta(\boldsymbol{y},t-\tau s)\partial_\alpha\right)$$
$$+\theta^2(\boldsymbol{y},t-\tau s)\tau^2 s^2 \partial_\alpha\partial_\beta]\ \delta(\boldsymbol{x}-\boldsymbol{y}). \tag{17}$$

Finally, in (17), $\boldsymbol{y}$ can be integrated out resulting in a local-in-$\boldsymbol{x}$ differential form of the momentum equation:

$$\partial_t(\rho(\boldsymbol{x},t)u_\alpha(\boldsymbol{x},t)) = -\boldsymbol{P}\ \partial_\beta \int_0^\infty \mathrm{d}s\ \mathrm{e}^{-s}\ \exp\left[-\partial_\gamma \tau s u_\gamma(\boldsymbol{x},t-\tau s)\right.$$
$$\left. + (1/2)\theta(\boldsymbol{x},t-\tau s)\tau^2 s^2 \partial_\gamma^2\right]\ \rho(\boldsymbol{x},t-\tau s)[\theta(\boldsymbol{x},t-\tau s)\delta_{\alpha\beta}$$
$$+u_\alpha(\boldsymbol{x},t-\tau s)u_\beta(\boldsymbol{x},t-\tau s) - \theta(\boldsymbol{x},t-\tau s)\tau s\left(\partial_\beta u_\alpha(\boldsymbol{x},t-\tau s)\right.$$
$$\left.+\ \partial_\alpha u_b(\boldsymbol{x},t-\tau s)\right) + \tau^2 s^2 \partial_\alpha\partial_\beta\theta^2(\boldsymbol{x},t-\tau s)]. \tag{18}$$

Here we have introduced the 'left-ordering' operator $\boldsymbol{P}$ that sends all differential operators to the leftmost part of any expression (where, in fact, they all commute with each other), according to the Taylor expansion

$$\boldsymbol{P}\Phi\left(\frac{\partial}{\partial \boldsymbol{x}}, \boldsymbol{x}\right) \equiv \prod_{\alpha=1}^{d} \sum_{n_\alpha=0}^{\infty} \frac{1}{n_\alpha!}\left(\frac{\partial}{\partial x_\alpha}\right)^{n_\alpha} \left[\frac{\partial^{n_\alpha}}{\partial z_\alpha^{n_\alpha}}\Phi(\mathbf{z},\boldsymbol{x})\right]_{\mathbf{z}=0}. \tag{19}$$

The definition of the left-ordering operator $\boldsymbol{P}$ ensures that for each operator Φ and each function A:

$$\int_R \mathrm{d}\boldsymbol{y}\ \Phi\left(\frac{\partial}{\partial \boldsymbol{x}}, \boldsymbol{y}\right) \delta(\boldsymbol{x}-\boldsymbol{y})A(\boldsymbol{y}) = \boldsymbol{P}\Phi\left(\frac{\partial}{\partial \boldsymbol{x}}, \boldsymbol{x}\right) A(\boldsymbol{x}).$$

In this way, expressions like (18) are uniquely defined in terms of operator algebra. (The properties of $\boldsymbol{P}$ are considered in more detail in the Appendix.) The following compact rewriting of (18) perhaps makes a better connection with conventional hydrodynamics:

$$\partial_t(\rho u_\alpha) + \boldsymbol{P}\boldsymbol{M}_0\partial_\beta\rho u_\beta u_\alpha = -\boldsymbol{P}\boldsymbol{M}_0\partial_\alpha\rho\theta + \boldsymbol{P}\boldsymbol{M}_1\left(\partial_\beta\rho\nu\,\partial_\beta u_\alpha + \partial_\alpha\rho\varsigma\,\partial_\beta u_\beta\right)$$
$$-\boldsymbol{P}\boldsymbol{M}_2\tau\partial_\beta^2\partial_\alpha\rho\eta\theta, \tag{20}$$

where $\varsigma = \nu = \eta \equiv \tau\theta$ and

$$\boldsymbol{M}_n A(\boldsymbol{x},t) \equiv \int_0^\infty \mathrm{d}s\ s^n \mathrm{e}^{-s} \exp\left[-\tau s\boldsymbol{u}(\boldsymbol{x},t-\tau s)\cdot\nabla + (1/2)\theta(\boldsymbol{x},t-\tau s)\tau^2 s^2\nabla^2\right] A(\boldsymbol{x},t-\tau s). \tag{21}$$

Similar analysis yields a local equation for the temperature θ and the mass conservation equation (10) is, as noted above, the same as for small Kn. Indeed, the resulting equation for θ is included in

$$\partial_t\left[\rho(\boldsymbol{x},t)(\boldsymbol{u}^2(\boldsymbol{x},t) + D\,\theta(\boldsymbol{x},t))\right] = -\boldsymbol{P}\nabla\int_0^\infty \mathrm{d}s\ \mathrm{e}^{-s}\exp\left[\frac{\theta\tau^2 s^2\nabla^2}{2} - \tau s\boldsymbol{u}\cdot\nabla\right]$$
$$\times\rho(\boldsymbol{u}-\theta\tau s\nabla)\left[\theta(D+2) + (\boldsymbol{u}-\tau s\nabla\theta)^2\right] \tag{22}$$

that can be also rewritten in a more intuitive way:

$$\begin{aligned}
&\partial_t(\rho h) + \boldsymbol{PM}_0\nabla\cdot(\rho h\boldsymbol{u}) = (\partial_t + \boldsymbol{u}\cdot\nabla)p + \boldsymbol{PM}_1\nabla\cdot\rho\eta\nabla h \\
&\quad + \boldsymbol{PM}_1\rho\nu\left(\partial_\beta u_\alpha + \partial_\alpha u_\beta - \frac{2}{d}\nabla\cdot\boldsymbol{u}\right)\partial_\alpha u_\beta - \boldsymbol{PM}_1\tau\nabla(\boldsymbol{u}\cdot\nabla T)\cdot\rho\boldsymbol{u} + \boldsymbol{PM}_2\tau\nabla\rho\eta\cdot\nabla T \\
&\quad - \boldsymbol{PM}_2\tau^2\nabla(\nabla T)^2\cdot\rho\boldsymbol{u} + \boldsymbol{PM}_3\tau^2\nabla\rho\eta\cdot\nabla(\nabla T)^2 + \boldsymbol{P}(1-\boldsymbol{M}_1)\nabla\cdot\left(\rho\frac{u^2}{2}\boldsymbol{u} + \rho\eta\nabla\frac{u^2}{2}\right),
\end{aligned} \tag{23}$$

where $h = C_pT \equiv (D+2)T/2$ is the specific enthalpy and $p = \rho T$.

All terms except the last one in (20) and the last five (the last two terms on the second and the three on the third lines) in (23) are the same as in classical hydrodynamics, apart from the $\boldsymbol{P}$ and $\boldsymbol{M}_n$ operators. However, the other terms are new for $Kn \neq 0$. Indeed, these additional terms vanish at $Kn \to 0$ ($\tau \to 0$), while the operators $\boldsymbol{M}_0 = \boldsymbol{M}_1 \to 1$, as is evident from (21). Since (20) and (23) are an exact macroscopic consequence of the microscopic Boltzmann–BGK system (1) and (2), they may be useful for systematic analysis of macroscopic fluid behaviour for arbitrary Kn.

3. General formulation of scalar transport at arbitrary Kn

Now we analyse generalized transport of a passive colour field, denoted $A(\boldsymbol{x}, t)$, under the same kinetic Boltzmann–BGK framework. The master BGK equation for the non-equilibrium single-particle density $f_\sigma(\boldsymbol{x}, \boldsymbol{v}, t)$ of colour σ is

$$\partial_t f_\sigma + \boldsymbol{v}\cdot\nabla f_\sigma = -\frac{f_\sigma - f_\sigma^{eq}}{\tau_\sigma}. \tag{24}$$

The equilibrium colour distribution is

$$f_\sigma^{eq}(\boldsymbol{x}, \boldsymbol{v}, t) = \frac{\rho_\sigma(\boldsymbol{x}, t)}{(2\pi\theta(\boldsymbol{x}, t))^{D/2}}\exp\left[-\frac{(\boldsymbol{v} - \boldsymbol{u}(\boldsymbol{x}, t))^2}{2\theta(\boldsymbol{x}, t)}\right], \tag{25}$$

where $\rho_\sigma(\boldsymbol{x}, t) = \int \mathrm{d}\boldsymbol{v}\, f_\sigma(\boldsymbol{x}, \boldsymbol{v}, t) = \int \mathrm{d}\boldsymbol{v}\, f_\sigma^{eq}(\boldsymbol{x}, \boldsymbol{v}, t)$ is the number density of particles of specific colour σ. Notice that in the above, both the fluid velocity and temperature are independent of colour σ, reflecting the 'passiveness' of the scalar. Obviously, the overall particle distribution function and number density are results of summation over those of all colours,

$$\begin{aligned}
f(\boldsymbol{x}, \boldsymbol{v}, t) &= \sum_\sigma f_\sigma(\boldsymbol{x}, \boldsymbol{v}, t), \\
\rho(\boldsymbol{x}, t) &= \int \mathrm{d}\boldsymbol{v}\, f(\boldsymbol{x}, \boldsymbol{v}, t) = \int \mathrm{d}\boldsymbol{v} \sum_\sigma f_\sigma(\boldsymbol{x}, \boldsymbol{v}, t) = \sum_\sigma \rho_\sigma(\boldsymbol{x}, t).
\end{aligned}$$

It can be easily shown that by summing over colour σ, (24) reduces to (1), and the equilibrium distribution function (25) reduces to (2), provided the relaxation time $\tau_\sigma (= \tau)$ is the same for all different colours. This confirms that 'colour blind' hydrodynamics is indeed independent of the scalar (colour) distribution. Integrating (24) along characteristics, we obtain

$$f_\sigma(\boldsymbol{x}, \boldsymbol{v}, t) = \int_0^\infty \mathrm{e}^{-s} f_\sigma^{eq}(\boldsymbol{x} - \boldsymbol{v}\tau_\sigma s, \boldsymbol{v}, t - \tau_\sigma s)\,\mathrm{d}s. \tag{26}$$

Integrating (24) over $\int \mathrm{d}\boldsymbol{v}$ yields

$$\partial_t \rho_\sigma(\boldsymbol{x}, t) + \partial_\beta J_\beta^{(\sigma)} = 0, \tag{27}$$

where

$$\boldsymbol{J}^{(\sigma)}(\boldsymbol{x}, t) \equiv \int \mathrm{d}\boldsymbol{v}\ \boldsymbol{v} f_\sigma(\boldsymbol{x}, \boldsymbol{v}, t) \neq \int \mathrm{d}\boldsymbol{v}\ \boldsymbol{v}\ f_\sigma^{eq}(\boldsymbol{x}, \boldsymbol{v}, t), \tag{28}$$

$$\int \mathrm{d}\boldsymbol{v}\ \boldsymbol{v}\ f_\sigma^{eq}(\boldsymbol{x}, \boldsymbol{v}, t) = \rho_\sigma(\boldsymbol{x}, t)\boldsymbol{u}(\boldsymbol{x}, t). \tag{29}$$

Due to the overall mass and momentum conservation,

$$\left.\begin{aligned} \rho(\boldsymbol{x}, t) &= \sum_\sigma \rho_\sigma(\boldsymbol{x}, t), \\ \sum_\sigma \boldsymbol{J}^{(\sigma)}(\boldsymbol{x}, t) &= \rho(\boldsymbol{x}, t)\boldsymbol{u}(\boldsymbol{x}, t). \end{aligned}\right\} \tag{30}$$

The macroscopic colour field $A(\boldsymbol{x}, t)$ is naturally defined as a colour-weighted density:

$$A(\boldsymbol{x}, t) \equiv \sum_\sigma \sigma \rho_\sigma(\boldsymbol{x}, t), \tag{31}$$

and thus (27) yields

$$\partial_t A + \nabla \cdot \sum_\sigma \sigma \boldsymbol{J}^{(\sigma)}(\boldsymbol{x}, t) = 0 \tag{32}$$

which is a generalized continuity equation for colour density at arbitrary Kn. In order to obtain an explicit closed-form equation for colour density, we substitute (26) into (32) to get

$$\begin{aligned} \boldsymbol{J} = \sum_\sigma \sigma \boldsymbol{J}^{(\sigma)} = \sum_\sigma \sigma \int_0^\infty \mathrm{d}s\ \mathrm{e}^{-s} \int \mathrm{d}\boldsymbol{v}\ \boldsymbol{v} \exp[-\tau_\sigma s \boldsymbol{v} \cdot \nabla] \\ \times \frac{\rho_\sigma(\boldsymbol{x}, t - \tau_\sigma s)}{(2\pi\theta(\boldsymbol{x}, t - \tau_\sigma s))^{D/2}} \exp\left[-\frac{(\boldsymbol{v} - \boldsymbol{u}(\boldsymbol{x}, t - \tau_\sigma s))^2}{2\theta(\boldsymbol{x}, t - \tau_\sigma s)}\right]. \end{aligned} \tag{33}$$

Next we assume that $\tau_\sigma \equiv \tau$ for all colours so that $\sum_\sigma$ can be performed inside the integrals yielding the integro-differential equation:

$$\begin{aligned} \partial_t A(\boldsymbol{x}, t) = -\partial_\beta \int_0^\infty \mathrm{d}s\ \mathrm{e}^{-s} \int \mathrm{d}\boldsymbol{v}\ v_\beta \exp[-\tau s \boldsymbol{v} \cdot \nabla] \\ \times \frac{A(\boldsymbol{x}, t - \tau s)}{(2\pi\theta(\boldsymbol{x}, t - \tau s))^{D/2}} \exp\left[-\frac{(\boldsymbol{v} - \boldsymbol{u}(\boldsymbol{x}, t - \tau s))^2}{2\theta(\boldsymbol{x}, t - \tau s)}\right]. \end{aligned} \tag{34}$$

Equation (34) can be transformed according to the above procedure into

$$\begin{aligned} \partial_t A(\boldsymbol{x}, t) = &- \partial_\beta \int_0^\infty \mathrm{d}s\ \mathrm{e}^{-s} \int \mathrm{d}\boldsymbol{y} \int \mathrm{d}\boldsymbol{v}\ v_\beta \exp[-\tau s \boldsymbol{v} \cdot \nabla] \delta(\boldsymbol{x} - \boldsymbol{y}) \\ &\times \frac{A(\boldsymbol{y}, t - \tau s)}{(2\pi\theta(\boldsymbol{y}, t - \tau s))^{D/2}} \cdot \exp\left[-\frac{(\boldsymbol{v} - \boldsymbol{u}(\boldsymbol{y}, t - \tau s))^2}{2\theta(\boldsymbol{y}, t - \tau s)}\right] \\ \equiv &- \partial_\beta \int_0^\infty \mathrm{d}s\ \mathrm{e}^{-s} \int \mathrm{d}\boldsymbol{y}\ q_\beta\ \delta(\boldsymbol{x} - \boldsymbol{y}) \equiv -\partial_\beta J_\beta(\boldsymbol{x}, t), \end{aligned} \tag{35}$$

where, by using (14)–(16) to perform the Gaussian integration over $\boldsymbol{v}$, $\mathbf{q}$ may be expressed as

$$q_\beta \equiv \frac{A(\boldsymbol{y}, t-\tau s)}{(2\pi\theta(\boldsymbol{y}, t-\tau s))^{D/2}} \int \mathrm{d}\boldsymbol{v}\; v_\beta \exp\left[-\partial_\gamma \tau s v_\gamma - \frac{(v_\gamma - \tau s\, u_\gamma(\boldsymbol{y}, t-\tau s))^2}{2\theta(\boldsymbol{y}, t-\tau s)}\right]$$
$$= A\; \frac{\partial Z(\boldsymbol{p})}{\partial p_\beta}\bigg|_{\boldsymbol{p}=-\tau s\nabla+\boldsymbol{u}/\theta} \exp\left[\frac{\boldsymbol{u}^2}{2\theta}\right] = A\; \exp\left[\frac{\theta\tau^2 s^2 \partial_\gamma^2}{2} - \partial_\gamma \tau s\, u_\gamma\right](-\theta\tau s\partial_\beta + u_\beta). \tag{36}$$

Integration of the right-hand side of (36) over $\boldsymbol{y}$ is done in the same way as in (17), making use of the left-ordering operator (19) and resulting in the dynamical equation for colour density:

$$\partial_t A(x,t) + \boldsymbol{PM}_0 \partial_\beta u_\beta A = \boldsymbol{PM}_1 \partial_\beta \eta \partial_\beta A \tag{37}$$

with the diffusion coefficient $\eta \equiv \tau\theta$. It is important to note that the generalized scalar transport equation is linear in $A(\boldsymbol{x}, t)$ regardless of the Knudsen number. Furthermore, it describes evolution of a passive scalar, because the macroscopic fluid velocity and temperature, given by (20) and (23) bear no signature of the scalar distribution.

4. Low-Mach-number hydrodynamics at arbitrary Kn

Isothermal/low Mach number and purely incompressible applications that can involve arbitrary Kn include the analysis of flows involving microscopic/nanoscopic geometries, biochemical flows, flows in disk drive systems, etc., but exclude aerospace applications (cf. Toschi & Succi 2005 and Zhou *et al.* 2006). In this section, we derive simplified forms of (29) and (37) that do not involve the left-ordering operator $\boldsymbol{P}$. These low Mach number equations are obtained by directly expanding the Gaussian exponential in f^{eq} in powers of Mach number $U/\sqrt{\theta}$, noting that pressure is introduced later as enforcing the kinematic constraint of incompressibility.

At constant temperature, (11) becomes

$$\partial_t \rho u_\alpha(\boldsymbol{x}, t) = -\,\partial_\beta \int_0^\infty \mathrm{d}s\; \mathrm{e}^{-s} \int \frac{\mathrm{d}\boldsymbol{v}}{(2\pi\theta)^{D/2}}\; v_\alpha v_\beta \exp\left[-\tau s \boldsymbol{v}\cdot\frac{\partial}{\partial \boldsymbol{x}}\right]$$
$$\times\, \rho(\boldsymbol{x}, t-\tau s)\exp\left[-\frac{(\boldsymbol{v}-\boldsymbol{u}(\boldsymbol{x}, t-\tau s))^2}{2\theta}\right] = -\,\partial_\beta \int_0^\infty \mathrm{d}s\; \mathrm{e}^{-s}\; B_{\alpha\beta}. \tag{38}$$

Expanding $B_{\alpha\beta}$ in powers of the Mach number gives

$$B_{\alpha\beta} = \int \frac{\mathrm{d}\boldsymbol{v}}{(2\pi\theta)^{D/2}}\; v_\alpha v_\beta \exp\left[-\partial_\gamma \tau s v_\gamma - \frac{(v_\gamma - u_\gamma(\boldsymbol{x}))^2}{2\theta}\right]\rho$$
$$= \int \frac{d\boldsymbol{v}}{(2\pi\theta)^{D/2}}\; v_\alpha v_\beta \exp\left[-\partial_\gamma \tau s v_\gamma - \frac{v^2}{2\theta}\right]\rho \exp\left[\frac{v_\mu u_\mu(\boldsymbol{x})}{\theta}\right]\exp\left[-\frac{u^2}{2\theta}\right]$$
$$= \int \frac{d\boldsymbol{v}}{(2\pi\theta)^{D/2}}\; v_\alpha v_\beta \exp\left[-\partial_\gamma \tau s v_\gamma - \frac{v^2}{2\theta}\right]\rho \sum_{n=0}^\infty \frac{1}{n!}\left(\frac{v_\mu u_\mu(x)}{\theta}\right)^n \sum_{m=0}^\infty \frac{1}{m!}\left(\frac{u^2}{2\theta}\right)^m$$
$$= \sum_{n=0}^\infty \frac{1}{n!}\boldsymbol{R}_{\alpha\beta\mu_1\ldots\mu_n}\rho\frac{u_{\mu_1}\ldots u_{\mu_n}}{\theta^n}\sum_{m=0}^\infty \frac{1}{m!}\left(\frac{u^2}{2\theta}\right)^m \equiv \sum_{n=0}^\infty\sum_{m=0}^\infty B^{nm}_{\alpha\beta}, \tag{39}$$

where the operator $\boldsymbol{R}_{\alpha\beta\mu_1\ldots\mu_n}$ is defined using (14), with, instead of (16), $p_\gamma = -\tau s \partial_\gamma$:

$$\boldsymbol{R}_{\alpha\beta\mu_1\ldots\mu_n} = \frac{\partial}{\partial p_\alpha}\frac{\partial}{\partial p_\beta}\frac{\partial}{\partial p_{\mu_1}}\cdots\frac{\partial}{\partial p_{\mu_n}}\exp\left[\frac{\theta \boldsymbol{p}^2}{2}\right]\bigg|_{\boldsymbol{p}=-\tau s\nabla}. \tag{40}$$

Hence, the low-Mach-number momentum equation is, up to terms of order u^2 (obtained by retaining the pairs $(n, m) = (0, 0)$, (0,1), (1,0), (2,0) in (39)), given by (38) with

$$\left.\begin{aligned}
B^{00}_{\alpha\beta} &= \exp\left[\frac{\lambda^2 s^2\nabla^2}{2}\right](\rho\theta\delta_{\alpha\beta} + s^2\lambda^2\partial_\alpha\partial_\beta\rho\theta),\\
B^{01}_{\alpha\beta} &= \exp\left[\frac{\lambda^2 s^2\nabla^2}{2}\right](\delta_{\alpha\beta} + s^2\lambda^2\partial_\alpha\partial_\beta)\frac{1}{2}\rho u^2,\\
B^{10}_{\alpha\beta} &= -\exp\left[\frac{\lambda^2 s^2\nabla^2}{2}\right]\left[\theta^2\tau s(\delta_{\mu\beta}\partial_\alpha + \delta_{\alpha\mu}\partial_\beta + \delta_{\alpha\beta}\partial_\mu)\rho\frac{u_\mu}{\theta} + \theta^3\tau^3 s^3\partial_\alpha\partial_\beta\partial_\mu\rho\frac{u_\mu}{\theta}\right],\\
B^{20}_{\alpha\beta} &= \frac{1}{2}\theta^2\exp\left[\frac{\lambda^2 s^2\nabla^2}{2}\right](\delta_{\mu\beta}\delta_{\nu\alpha} + \delta_{\alpha\mu}\delta_{\nu\beta} + \delta_{\mu\nu}\delta_{\alpha\beta})\rho\frac{u_\mu u_\nu}{\theta^2} + \frac{1}{2}\theta^3\tau^2 s^2\exp\left[\frac{\lambda^2 s^2\nabla^2}{2}\right]\\
&\quad\times(\delta_{\alpha\mu}\partial_\beta\partial_\nu + \delta_{\alpha\nu}\partial_\beta\partial_\mu + \delta_{\beta\mu}\partial_\alpha\partial_\nu + \delta_{\beta\nu}\partial_\alpha\partial_\mu + \delta_{\mu\nu}\partial_\alpha\partial_\beta + \delta_{\alpha\beta}\partial_\mu\partial_\nu)\rho\frac{u_\mu u_\nu}{\theta^2}\\
&\quad+\frac{1}{2}\theta^4\tau^4 s^4\exp\left[\frac{\lambda^2 s^2\nabla^2}{2}\right]\partial_\alpha\partial_\beta\partial_\mu\partial_\nu\rho\frac{u_\mu u_\nu}{\theta^2}\\
&= \exp\left[\frac{\lambda^2 s^2\nabla^2}{2}\right]\left[\rho u_\alpha u_\beta + \delta_{\alpha\beta}\frac{1}{2}\rho u^2 + \lambda^2 s^2\bigg(\partial_\alpha\partial_\mu\rho u_\beta u_\mu + \partial_\beta\partial_\mu\rho u_\alpha u_\mu\right.\\
&\quad\left.+\partial_\alpha\partial_\beta\frac{1}{2}\rho u^2 + \delta_{\alpha\beta}\partial_\mu\partial_\nu\frac{1}{2}\rho u_\mu u_\nu\bigg) + \lambda^4 s^4\partial_\alpha\partial_\beta\partial_\mu\partial_\nu\frac{1}{2}\rho u_\mu u_\nu\right],
\end{aligned}\right\} \tag{41}$$

where $\lambda = \tau\sqrt{\theta}$ is the mean free path. Adding up these contributions gives

$$\begin{aligned}
B_{\alpha\beta} = \exp\left[\frac{\lambda^2 s^2\nabla^2}{2}\right]\bigg\{&\rho u_\alpha u_\beta + (\delta_{\alpha\beta} + \lambda^2 s^2\partial_\alpha\partial_\beta)(\rho\theta + \rho u^2)\\
&-\theta\tau s(\partial_\alpha\rho u_\beta + \partial_\beta\rho u_\alpha) + \lambda^2 s^2\left(\partial_\beta\partial_\mu\rho u_\alpha u_\mu + \partial_\alpha\partial_\mu\rho u_\beta u_\mu + \frac{1}{2}\delta_{\alpha\beta}\partial_\mu\partial_\nu\rho u_\mu u_\nu\right)\\
&-\theta\tau\lambda^2 s^3\partial_\alpha\partial_\beta\partial_\mu\rho u_\mu + \frac{1}{2}\lambda^4 s^4\partial_\alpha\partial_\beta\partial_\mu\partial_\nu\rho u_\mu u_\nu\bigg\}.
\end{aligned} \tag{42}$$

Passive scalar diffusion in the low Ma limit is analysed in the same way. Rewrite (34) as

$$\begin{aligned}
\partial_t A(\boldsymbol{x}, t) = -\partial_\beta\int_0^\infty \mathrm{d}s\, \mathrm{e}^{-s}\int \mathrm{d}\boldsymbol{v}\frac{v_\beta}{(2\pi\theta)^{D/2}}\exp[-\tau s\boldsymbol{v}\cdot\nabla]&\\
\times\exp\left[-\frac{(\boldsymbol{v}-\boldsymbol{u}(\boldsymbol{x}, t-\tau s))^2}{2\theta}\right]A(\boldsymbol{x}, t-\tau s) = -\partial_\beta\int_0^\infty \mathrm{d}s\, \mathrm{e}^{-s} J_\beta.&
\end{aligned} \tag{43}$$

Repeating the steps leading to (42) gives

$$\begin{aligned}
J_\beta = \sum_{n=0}^\infty\frac{1}{n!}\frac{\partial}{\partial p_\beta}\frac{\partial}{\partial p_{\mu_1}}\cdots\frac{\partial}{\partial p_{\mu_n}}&\\
\times\exp\left[\frac{\theta\boldsymbol{p}^2}{2}\right]\bigg|_{\boldsymbol{p}=-\tau s\nabla}\frac{u_{\mu_1}\ldots u_{\mu_n}}{\theta^n}\sum_{m=0}^\infty\frac{1}{m!}\left(\frac{u^2}{2\theta}\right)^m A \equiv \sum_{n=0}^\infty\sum_{m=0}^\infty J^{nm}_\beta,&
\end{aligned} \tag{44}$$

and we need to retain only two expansion terms corresponding to $(n, m) = (0, 0)$ and $(1, 0)$:

$$J_\beta^{00} = -\theta\tau s \partial_\beta \exp\left[\frac{\theta\tau^2 s^2 \nabla^2}{2}\right] A, \quad J_\beta^{01} = \exp\left[\frac{\theta\tau^2 s^2 \nabla^2}{2}\right] (\theta\delta_{\beta\mu} + \theta^2\tau^2 s^2 \partial_\beta\partial_\mu)\frac{u_\mu}{\theta} A. \tag{45}$$

Upon substitution of (42) into (38) and (45) into (43) and (44), we obtain the low-Mach-number equations for the flow

$$\left.\begin{aligned} \partial_t \rho u_\alpha(\boldsymbol{x}, t) + \boldsymbol{M}_0^l \partial_\beta \rho u_\alpha u_\beta &= -\partial_\alpha p + \boldsymbol{M}_1^l \nabla^2 \rho \nu u_\alpha - \lambda^2 \boldsymbol{M}_2^l \big(\partial_\mu^2 \partial_\beta \rho u_\alpha u_\beta \\ &\quad + \partial_\mu \partial_\nu \partial_\alpha \rho u_\nu u_\mu\big), \\ p \equiv \left(\boldsymbol{M}_0^l + \lambda^2 \nabla^2 \boldsymbol{M}_2^l\right)&(\rho\theta + \rho u^2) - \left(\boldsymbol{M}_1^l + \lambda^2 \nabla^2 \boldsymbol{M}_3^l\right) \rho \varsigma_\beta u_\beta \\ + \lambda^2 \left(\boldsymbol{M}_2^l + \lambda^2 \nabla^2 \boldsymbol{M}_4^l\right)& \partial_\mu \partial_\nu \rho u_\nu u_\mu \end{aligned}\right\} \tag{46}$$

and for the scalar

$$\partial_t A(\boldsymbol{x}, t) + \boldsymbol{M}_0^l \nabla(\boldsymbol{u} A) = \boldsymbol{M}_1^l \nabla^2 \eta A - \lambda^2 \nabla^2 \boldsymbol{M}_2^l \partial_\mu^2 \partial_\beta u_\beta A, \tag{47}$$

where the low-Mach-number form of the operator (21) is $\boldsymbol{M}_n^l$:

$$\boldsymbol{M}_n^l B(\boldsymbol{x}, t) \equiv \int_0^\infty \mathrm{d}s\, s^n \mathrm{e}^{-s} \exp\left(\frac{1}{2} s^2 \lambda^2 \nabla^2\right) B(\boldsymbol{x}, t - \tau s). \tag{48}$$

Notice that the left-ordering operator $\boldsymbol{P}$ is no longer present in (46)–(47) above. Equations system (46) represent a low (not zero) *Ma* approximation and should thus be used together with the continuity equation (10). A truly incompressible, simplified form is achieved by setting $\rho = \text{const.}$ and removing the pressure equation from (46). Then, the pressure is determined by the purely kinematic constraint that a pressure field p is required to ensure that the velocity field is divergence-free; in exact correspondence with the $Kn = 0$, incompressible Navier–Stokes equations:

$$\left.\begin{aligned} \partial_t u_\alpha(\boldsymbol{x}, t) + \boldsymbol{M}_0^l (\nabla \cdot \boldsymbol{u}) u_\alpha = -\frac{1}{\rho}\partial_\alpha p + \boldsymbol{M}_1^l \nu \nabla^2 u_\alpha - \lambda^2 \boldsymbol{M}_2^l \big(\partial_\mu^2 \partial_\beta u_\alpha u_\beta + \partial_\nu u_\mu \partial_\mu \partial_\alpha u_\nu\big), \\ \nabla \cdot \boldsymbol{u} = 0. \end{aligned}\right\} \tag{49}$$

Equations (49) describe, in closed form, arbitrary Kn flow with density $\rho = \text{const.}$ and temperature $\theta = \text{const.}$ It is interesting to note that, besides higher derivative terms typical of hyperviscous and diffusion effects, equations (46), (47) and (49) include the so-called nonlinear tensorial diffusion terms representative of the physics in finite Knudsen number regimes, away from the Newtonian linear stress–strain relationship. A similar (though less general) result for the fluid momentum equation is obtained via higher order [O(Kn^2)] Chapman–Enskog expansion (Chen *et al.* 2004).

5. Finite-time phenomena and generalized diffusion processes for scalar transport at arbitrary *Kn*

Let us now discuss the macroscopic description of the BGK kinetic system (1) at finite times. By that we mean evolution from an initial state $f(\boldsymbol{x}, \boldsymbol{v}, t) = f_0(\boldsymbol{x}, \boldsymbol{v})$ at $t = 0$, as opposed to the case when equilibrium is assumed in infinite past, $t \to -\infty$, as analysed above and in our previous work (Chen *et al.* 2007). In this case, (1) can still be solved by characteristics for free space but instead of (4)–(5) we now get

$$f(\boldsymbol{x}, \boldsymbol{v}, t) = f_0(\boldsymbol{x} - \boldsymbol{v}t, \boldsymbol{v}) \mathrm{e}^{-t/\tau} + \int_0^{t/\tau} \mathrm{e}^{-s} f^{eq}(\boldsymbol{x} - \boldsymbol{v}\tau s, \boldsymbol{v}, t - \tau s)\, \mathrm{d}s. \tag{50}$$

If the system is in equilibrium at $t=0$, $f_0(\boldsymbol{x},\boldsymbol{v})=f^{eq}(\boldsymbol{x},\boldsymbol{v},t=0)$, then (50) can be recast as

$$f(\boldsymbol{x},\boldsymbol{v},t)=\int_0^{t/\tau+\varepsilon} \mathrm{e}^{-s} f^{eq}(\boldsymbol{x}-\boldsymbol{v}\tau s,\boldsymbol{v},t-\tau s)\left[1+\tau^{-1}\delta(t-\tau s)\right]\mathrm{d}s \tag{51}$$

where $\varepsilon=0+$ is a positive infinitesimal number.

Equation (51) indicates that every formula derived above for the macroscopic dynamics at arbitrary Kn with equilibrium in the infinite past applies nearly unchanged to the initial value problem in which equilibrium is assumed at $t=0$, with the only modification being

$$\int_0^{\infty}\mathrm{d}s \to \int_0^{t/\tau+\varepsilon}\mathrm{d}s\,[1+\tau^{-1}\delta(t-\tau s)], \tag{52}$$

which needs to be made wherever integration over the past history is performed. This means that the general equations (20), (23) and (37) stay the same but they should be used together with the operators $\boldsymbol{M}$ defined as

$$\boldsymbol{M}_n A(\boldsymbol{x},t)\equiv\int_0^{t/\tau+\varepsilon}\mathrm{d}s\,[1+\tau^{-1}\delta(t-\tau s)]\,s^n\mathrm{e}^{-s}\exp\left[-\tau s\boldsymbol{u}(\boldsymbol{x},t-\tau s)\cdot\nabla + \frac{1}{2}\theta(\boldsymbol{x},t-\tau s)\tau^2 s^2\nabla^2\right]A(\boldsymbol{x},t-\tau s) \tag{53}$$

instead of (21). Similarly the low-Mach-number/incompressible equations (46), (47) and (49) stay the same but should be used together with

$$\boldsymbol{M}_n^l B(\boldsymbol{x},t)\equiv\int_0^{t/\tau+\varepsilon}\mathrm{d}s\,[1+\tau^{-1}\delta(t-\tau s)]\,s^n\mathrm{e}^{-s}\exp\left(\frac{1}{2}s^2\lambda^2\nabla^2\right)B(\boldsymbol{x},t-\tau s) \tag{54}$$

instead of (48), for the study of evolution of a system that was initially at equilibrium at $t=0$. Obviously, operators (53) and (54) reduce to operators (21) and (48), respectively, when $t\to\infty$.

As a specific application of such an initial value problem, we consider the time evolution of a diffusing cloud of colour in a no-flow, isothermal arbitrary Knudsen number medium. This is achieved by setting $\boldsymbol{u}=0$ and $\rho,\theta=\text{const.}$ in (37) or (47). This case, which can be analysed in detail, corresponds to a variety of physical situations such as the initial marking of a number of molecules by some flow-insignificant (radioactive) tracer and observing how its concentration disperses in time. The initial value scalar equation as in (47) for the no-flow case reduces to

$$\partial_t A(\boldsymbol{x},t)=\eta\int_0^{t/\tau+\varepsilon}\mathrm{d}s[1+\tau^{-1}\delta(t-\tau s)]s\mathrm{e}^{-s}\exp\left[\frac{s^2\lambda^2\nabla^2}{2}\right]\nabla^2 A(\boldsymbol{x},t-\tau s). \tag{55}$$

Equation (55) coincides in form with (19) from our previous work (Part 1), even though the latter defines a macroscopic dynamics of fluid velocity of unidirectional flow, the only difference being the substitution (52) that is responsible for finite time effects. It is important to emphasize that (55) is not an approximation but a real solution of (24) and (25) corresponding to a process with $\boldsymbol{u}=0$ and ρ, $\theta=\text{const.}$, namely diffusion in quiescent media (or in a solid). Observe in that regard that (55) is a finite mean free path generalization of the common low-Kn no-flow diffusion/heat equation $\partial_t A=\eta\nabla^2 A$, to which (55) obviously reduces when $\tau\to 0$, $\lambda\to 0$.

Now we proceed to obtaining solutions of (55) with the initial distribution $A(\boldsymbol{x}, t=0)=A_0(\boldsymbol{x})$ that has finite support in space. At time t, this distribution is intuitively expected to have a 'front' $X(t)$ that obeys a diffusion law $X(t)\approx\sqrt{\eta t}$ at large times $t\gg\tau$ and a ballistic law, $X(t)\approx c_s t$ (where the sound speed $c_s\equiv\sqrt{\theta}\equiv\sqrt{\eta/\tau}$) at very early times $t\ll\tau$. Let us now see how this intuition is confirmed by direct calculation. It follows from (55) that $\partial_t\langle A\rangle=0$, so that $\langle A\rangle\equiv\int \mathrm{d}\boldsymbol{x}\, A(\boldsymbol{x}, t)=\int \mathrm{d}\boldsymbol{x}\, A(\boldsymbol{x}, 0)$ is constant in time, which means global conservation of average colour. Next, we rewrite (55) as

$$\left.\begin{aligned}\partial_t A(\boldsymbol{x}, t) = \eta\nabla^2\boldsymbol{M}(t, \nabla^2)A,\\ \boldsymbol{M}(t, \nabla^2)B(\boldsymbol{x}, t)\equiv\int_0^{t/\tau+\varepsilon}\mathrm{d}s[1+\tau^{-1}\delta(t-\tau s)]s\,\exp\left(-s+\frac{s^2\lambda^2\nabla^2}{2}\right)B(\boldsymbol{x}, t-\tau s).\end{aligned}\right\}\tag{56}$$

The $2n$th moments of $A(\boldsymbol{x}, t)$ are defined as

$$X^{2n}(t)\equiv\int \mathrm{d}\boldsymbol{x}\,\boldsymbol{x}^{2n}A(\boldsymbol{x}, t)\equiv\left\langle\boldsymbol{x}^{2n}A\right\rangle.$$

In particular, the second moment $X^2(t)$ is naturally identified with the evolving front:

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}X^2(t)&\equiv\left\langle\boldsymbol{x}^2\nabla^2\boldsymbol{M}(t, \nabla^2)\eta A\right\rangle=2d\left\langle\boldsymbol{M}(t, \nabla^2)\eta A\right\rangle=2d\left\langle\boldsymbol{M}(t, 0)\eta A\right\rangle\\ &=2d\eta\int_0^{t+\varepsilon}\mathrm{d}s\;[1+\tau^{-1}\delta(t-\tau s)]\;\exp(-s)\int\mathrm{d}\boldsymbol{x}\,A(\boldsymbol{x}, t)\\ &=2d\eta\left\langle A\right\rangle\int_0^{t+\varepsilon}\mathrm{d}s\;[1+\tau^{-1}\delta(t-\tau s)]\;\exp(-s)=2d\eta\left\langle A\right\rangle(1-\mathrm{e}^{-t/\tau}).\end{aligned}\tag{57}$$

The first equality in (57) is obtained by using the divergence theorem and noting that $\nabla^2\boldsymbol{x}^2=2d$. Notice that the dimension of $\boldsymbol{x}$-space d is commonly, but not always, equal to the phase space dimensionality D. The second equality is based on the observation that each nonzero term in the expansion of $\boldsymbol{M}$ in powers of the Laplace operator vanishes at ∞ because A vanishes.

It is noteworthy that the time behaviour of $X^2(t)$ defined by (57) is the same as for the well-known telegraphers equation (Bender & Orszag 1999)

$$\tau\,\partial_{tt}A(\boldsymbol{x}, t)+\partial_t A(\boldsymbol{x}, t)=\eta\nabla^2A(\boldsymbol{x}, t),\tag{58}$$

recently derived in the context of nanofluidics in Yakhot & Colosqui (2007) and applied to nanoresonator problems in Karabacak, Yakhot & Ekinci (2007). Indeed, take the second moment of (58):

$$\tau\frac{\mathrm{d}^2}{\mathrm{d}t^2}X^2(t)+\frac{\mathrm{d}}{\mathrm{d}t}X^2(t)=\eta\int\mathrm{d}\boldsymbol{x}\,\boldsymbol{x}^2\nabla^2A(\boldsymbol{x}, t)=2d\eta\left\langle A\right\rangle.\tag{59}$$

The solution of the differential equation (59) satisfying $(\mathrm{d}/\mathrm{d}t)X^2(t=0)=0$ is

$$X^2(t)-X^2(0)=2d\eta\left\langle A\right\rangle\left[t+\tau(\mathrm{e}^{-t/\tau}-1)\right],\tag{60}$$

which is identical to (57) at all times. However this is only an, albeit non-trivial, coincidence, as higher spatial moments of (59) should be different from those of (55) because otherwise the respective full solutions would coincide. By the way, solution of (55) need not to invoke an initial condition for $(\mathrm{d}/\mathrm{d}t)X^2(t=0)=0$. Expression (60) confirms our intuitive picture presented above. Indeed, at $t\gg\tau$, (60) yields $X^2(t)\approx 2d\left\langle A\right\rangle\eta t$, a typical diffusion behaviour. On the other hand, when $t\ll\tau$, (60) gives a ballistic law, $X^2(t) \approx d \langle A \rangle c_s^2 t^2$, agreeing with the correct physical behaviour for scalar evolution at very early times as follows from the classical Langevin equation (cf. Reif 1985).

6. Discussion

In this paper, we extended our earlier formulation (Chen *et al.* 2007) of a theory that is entirely macroscopic (in the sense of dealing with a few fields evolving in physical space, *viz.* $\rho(\boldsymbol{x}, t)$, $\boldsymbol{u}(\boldsymbol{x}, t)$ and $\theta(\boldsymbol{x}, t)$), starting from the kinetic Boltzmann–BGK model (defined in (1) and (2)) that is defined in the phase space $(\boldsymbol{x}, \boldsymbol{v}, t)$. Such macroscopic descriptions are usually derived from kinetic theory as expansions in low Kn. Following that path, closed-form equations for mass, momentum and energy of (compressible) hydrodynamics are available asymptotically as $Kn \rightarrow 0$. Putting mathematical well-posedness issues aside, generalized hydrodynamics may be constructed in closed form in this way that is accurate up to a desired order in $Kn \approx 1$. In our non-perturbative approach, equations (20), (23) and (37) are derived from (1), (2) and (24), (25) without any approximation in Knudsen (or Mach or Reynolds) number. Therefore, their well-posedness follows from that for the underlying BGK system (cf. also Part 1). Equations (20), (23) and (37) describe physical systems under precisely the same limitations as those of the underlying BGK dynamics, such as the assumption of a hierarchy of relaxation times, self-consistent description based on single-point distribution function, single relaxation time approximation, etc. In this paper we accomplished, without approximation, the projection (or coarse graining) of the constant τ BGK kinetic system from phase space $(\boldsymbol{x}, \boldsymbol{v}, t)$ to physical space $(\boldsymbol{x}, t)$.

The non-locality in time and infinite order in spatial derivatives presented in (20), (23), (37), (46), (47) and (49) are a clear signature of their kinetic theory origins. Note in this regard that the presence of infinite derivatives makes these equations effectively equivalent to closed-form macroscopic formulation in terms of integral equations (13)–(16) from Part 1 that are not rewritten here. Therefore, (20), (23), (37), (46), (47) and (49) only require boundary conditions to set the values of all fields at the domain boundary, as opposed to a large number of boundary conditions for high-order derivatives or moments (cf. Struchtrup & Torrilon 2007). We mention only that the macroscopic equations derived here ‘remember’ their origin in kinetic theory in such a way that bounce-back conditions on the distribution function imply $U(x) = -U(-x)$, if the boundary is at $x = 0$. For example, in Part 1 this enables solution for channel flows using antisymmetric Fourier series. The same approach applies to more general flow with bounce-back conditions at walls of arbitrary shape. Future work will extend the treatment to complex finite boundaries. The key idea is to introduce appropriate spatial delta functions following the treatment of finite time effects in § 5.

Even though (20), (23) and (37) contain the same information as their integral-in-space counterparts, they present a more revealing form for the macroscopic flow structures, and might be technically more useful for studying arbitrary Kn (and non-isothermal/compressible) flow problems in a d-dimensional space. Such studies may include direct generalization of the study of the Knudsen minimum in a plane channel from Part 1 or shear wave decay from equilibrium (Colosqui *et al.* 2009). As other diverse applications, one can study the internal structure of shock waves.

The low Ma/incompressible description (46), (47) and (49) presented in § 4 is perhaps the only result that is based on approximation. Indeed, throughout that section we assume that ρ and θ are constant, except in the $B^{00}_{\alpha\beta}$ term in (41) where the product $\rho\theta$ is allowed to vary in order to shorten the derivation. Note (as an excuse and not as a justification) that this expansion is not in powers of Kn but rather of Ma, so that one would follow exactly the same procedure for derivation of incompressible, $Kn = 0$ classical hydrodynamics from (1). Furthermore, as discussed in Part 1, the exact results derived here can also include various other approximations to model broader and/or more realistic situations.

Recently (Chen *et al.* 2004), Boltzmann–BGK kinetics (see (1)–(2)) was suggested as a useful framework for understanding turbulence and building turbulence models, especially nonlinear models. Contributions to turbulent stress that are second order in the ratio of turbulent and mean flow times (which is the effective Knudsen number of this framework) were shown by Chen *et al.* (2004) to be in a good quantitative agreement with the results that other authors obtain from entirely different considerations. From this perspective, (20), (23) and (37), and perhaps the incompressible version (46), (47) and (49), may be useful for extending turbulent models of highly anisotropic/non-equilibrium turbulent flow beyond second order. In that case, transport coefficients such as ν and η are to be identified with eddy viscosity/diffusion coefficients that depend on mean flow and turbulence properties.

The results of § 5 can be viewed as supporting the soundness of (20), (23), (37) (and their non-flow version (55)). Note that regular hydrodynamics may have infinite signal propagation speed V for the heat equation. In particular, for diffusion from a point source, $V(t)$ is naturally identified with $\mathrm{d}(X^2(t))^{1/2}/\mathrm{d}t$ that diverges as $1/\sqrt{t}$ as $t \to 0$. This type of classical physics has been studied since Einstein, and is acceptable for coarse grained dynamics at space–time scales larger than mean free path since it does not account for the fact that individual particles cannot propagate faster than ballistically. The system (20), (23) and (37), which is obtained non-perturbatively and pretends to be exact at all scales must be intrinsically free of such a divergence in propagation speed, without appealing to the argument that ‘some kinetic or other microscopic theory will regularize it’. Indeed, from (57), $V(t) = c_s$ for times smaller than τ.

In statistical physics, the general pattern is that while the description of a given system at a more microscopic level contains more information, a more macroscopic description conveys better insight about the general patterns of the system’s coarse-grained behaviour. For a fluid system, a macroscopic description usually has a narrower range of physics applicability than its microscopic parent, due to various coarse-graining approximations used. Therefore, a macroscopic description without approximation of its underlying microscopic physics origin may be of some theoretical interest, as it gives exact, undistorted information relating the detailed microscopic dynamics and its macroscopic consequences.

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Appendix. The left-ordering operator $\boldsymbol{P}$

The left-ordering operator $\boldsymbol{P}$ (see (18)) used extensively in §§ 2 and 3 above is essential for development of the equations for arbitrary Knudsen number flows. It is, therefore, helpful to consider in more detail here some of its properties.

Consider a ring R consisting of indexed elements z_α and x_β such that all z-elements commute and all x-elements commute but z-elements and x-elements do not commute with each other. For a given field K, this induces a (graded) algebra $\boldsymbol{W}$ whose elements E are sums of words $W = zzx\ldots z..$ scaled by coefficients λ in the field K. We define an operator $\boldsymbol{P}$ as left ordering with respect to z if it acts on each element E by moving all the z-elements to the left side of each word W of E (where they of course commute). The action of $\boldsymbol{P}$ is compatible with the underlying structure of $\boldsymbol{W}$ (e.g. $(\boldsymbol{P}(A+B))C=(\boldsymbol{P}A)C+(\boldsymbol{P}B)C$, $\boldsymbol{P}(\alpha A+\beta B)=\alpha\boldsymbol{P}A+\beta\boldsymbol{P}B,\ldots$ and so on). Note also that $\boldsymbol{P}\boldsymbol{P}=\boldsymbol{P}$, $\boldsymbol{P}A\boldsymbol{P}B=\boldsymbol{P}AB$, and a useful property that the commutator is always zero under the action of $\boldsymbol{P}$:

$$\boldsymbol{P}[A,B]=\boldsymbol{P}(AB-BA)=\boldsymbol{P}AB-\boldsymbol{P}BA=0, \tag{A 1}$$

even when $[A,B]$ is not 0.

Our intended interpretation is that R is a ring of differential operators ($z_\alpha=\partial/\partial x_\alpha$) and functions of x, K is the real or complex field, and that words W are generated by power series expansion of formal expressions F that contain differential operators. While functions F are assumed to be infinitely differentiable in z in a formal way, the issue of how would such power series converge is outside the scope of defining rules of this formal calculus. To demonstrate that using left-ordered operators is actually easier that the usual differential operator calculus, consider a gas dynamics example involving an algorithmic sequence of events needed to produce an expansion term that is, say, order n in Ma and order m in Kn:

Using a (hypothetically existing) theory involving regular differentiation:

(i) Formally expand in order to collect all powers n in U and powers m in τ (or λ), being careful about relative placement of differential operators according to conventional rules;

(ii) Let each differential operator act on everything to the right of it.

Using left ordering of differential operators:

(i) Formally expand to order n in U and order m in τ (or λ) while treating all the differential operators as formal symbols that commute with everything else, thanks to (A 1). Combine terms as desired for clarity or ease of manipulation;

(ii) Apply $\boldsymbol{P}$ sending all the differential operators to the left in an arbitrary order.

(iii) Let differential operators act upon the right side according to conventional rules. This of course can be also done in an arbitrary order.

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