Force-driven rarefied flows between diffuse-reflecting boundaries

V. E. Ambruș[1,2], V. Sofonea[1], R. Fournier[3], S. Blanco[3]

[1] Centre for Fundamental and Advanced Technical Research, Romanian Academy
Bd. Mihai Viteazul 24, RO 300223 Timișoara, Romania

[2] Department of Physics, West University of Timișoara
Bd. Vasile Parvan 4, RO 300223 Timișoara, Romania

[3] LAPLACE, Université de Toulouse, CNRS, INPT, UPS, France.

ICMMES 2017, Nantes
20/07/2017

Outline

Setup: one-dimensional flow in the gravitational field

Boltzmann equation

- The aim is to solve

$$\partial_t f + \frac{p}{m}\partial_x f - mg\partial_p f = -\frac{1}{\tau}[f - f^{(\mathrm{eq})}], \qquad \tau = \frac{\mathrm{Kn}}{n}. \tag{1}$$

  subject to diffuse reflection boundary conditions:

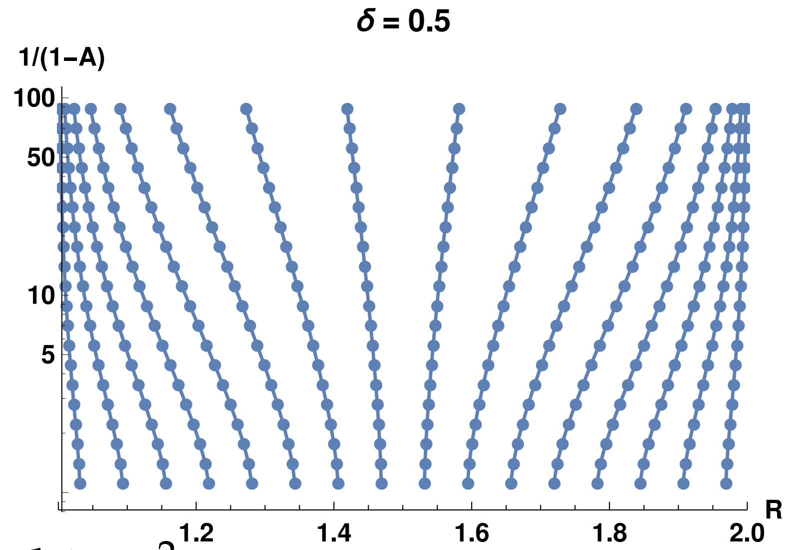
$$\begin{gathered} f(p > 0, x = -L/2) = f_+^{(\mathrm{eq})}, \qquad f(p < 0, x = L/2) = f_-^{(\mathrm{eq})}, \\ f_\pm^{(\mathrm{eq})} = \frac{n_\pm}{\sqrt{2\pi m T_\pm}} e^{-p^2/2mT_\pm} \end{gathered} \tag{2}$$

- $n_\pm$ are fixed by imposing a vanishing mass flux at the wall:

$$n_+ = -\frac{\int_{-\infty}^0 dp\, f\, p}{\int_0^\infty dp\, p\,[f_+^{(\mathrm{eq})}/n_+]}, \qquad n_- = -\frac{\int_0^\infty dp\, f\, p}{\int_{-\infty}^0 dp\, p\,[f_-^{(\mathrm{eq})}/n_-]}. \tag{3}$$

- The recovery of the above half-range integrals requires half-range quadratures!

Numerical scheme



- Let us write the Boltzmann equation in the following form:

$$\frac{\partial f}{\partial t} + \frac{p}{m}\frac{\partial f}{\partial z} = -\frac{1}{\tau}[f - f^{(\mathrm{eq})}] + mg\partial_p f.$$

- The time-stepping is implemented using the TVD RK-3 scheme.[1]
- We employ the following coordinate stretching:[2]

$$x(\eta) = \frac{L}{2A}\tanh\eta. \tag{4}$$

- Writing the advection term as:

$$\frac{p}{m}\partial_x f = \frac{\mathcal{F}_{s+1/2} - \mathcal{F}_{s-1/2}}{x(\eta_{s+1/2}) - x(\eta_{s-1/2})}, \tag{5}$$

the fluxes $\mathcal{F}_{s+1/2}$ are implemented using WENO-5.[3]

[1] C.-W. Shu, S. Osher, J. Comput. Phys. **77** (1988) 439.
[2] R. Mei and W. Shyy, JCP **143** (1998) 426; Z. Guo and T. S. Zhao, PRE **67** (2003) 066709.
[3] L. Rezzolla, O. Zanotti, *Relativistic hydrodynamics* (Oxford University Press, Oxford, UK, 2013).

Force in full-range models

Expansion with respect to full-range polynomials

- f can be expanded as:

$$f = \frac{e^{-p^2/2}}{\sqrt{2\pi}} \sum_{\ell=0}^{\infty} \frac{1}{\ell!} \mathcal{F}_\ell H_\ell(p), \qquad \mathcal{F}_\ell = \int_{-\infty}^{\infty} dp\, f\, H_\ell(p). \tag{6}$$

- $\partial_p f$ can be obtained using $\partial_p[H_\ell(p) e^{-p^2/2}] = -e^{-p^2/2} H_{\ell+1}(p)$:[4]

$$\partial_p f = -\frac{e^{-p^2/2}}{\sqrt{2\pi}} \sum_{\ell=0}^{\infty} \frac{1}{\ell!} \mathcal{F}_\ell H_{\ell+1}(p). \tag{7}$$

- Eq. (6) can be used to eliminate $\mathcal{F}_\ell$:

$$\partial_p f = \int_{-\infty}^{\infty} dp'\, \mathcal{K}(p,p') f(p'), \qquad \mathcal{K}(p,p') = -\frac{e^{-p^2/2}}{\sqrt{2\pi}} \sum_{\ell=0}^{\infty} H_{\ell+1}(p) H_\ell(p'). \tag{8}$$

[4] V. E. Ambruș, V. Sofonea, J. Comput. Sci. **17** (2016) 403.

Discretisation of momentum space[5]

- The full range moments of f can be recovered using the full-range Gauss-Hermite quadrature:

$$\int_{-\infty}^{\infty} dp\, f\, p^s \simeq \sum_{k=1}^{Q} f_k p_k^s, \tag{9}$$

where the equality is exact if $Q > s$ and the series expansion of f is truncated at $\ell = Q - 1$.

- The discrete populations f_k are:

$$f_k = \frac{w_k}{e^{-p^2/2}/\sqrt{2\pi}} f(p_k), \qquad w_k = \frac{Q!}{[H_{Q+1}(p_k)]^2}, \tag{10}$$

while $\{p_k, k = 1, 2, \dots\}$ is the set of roots of $H_Q(p)$.

- The kernel $\mathcal{K}(p, p') \to \mathcal{K}_{k,k'}$:

$$\mathcal{K}_{k,k'} = -w_k \sum_{\ell=0}^{Q-1} H_{\ell+1}(p_k) H_\ell(p_{k'}). \tag{11}$$

[5] V. E. Ambruș, V. Sofonea, J. Comput. Phys. **316** (2016) 1.

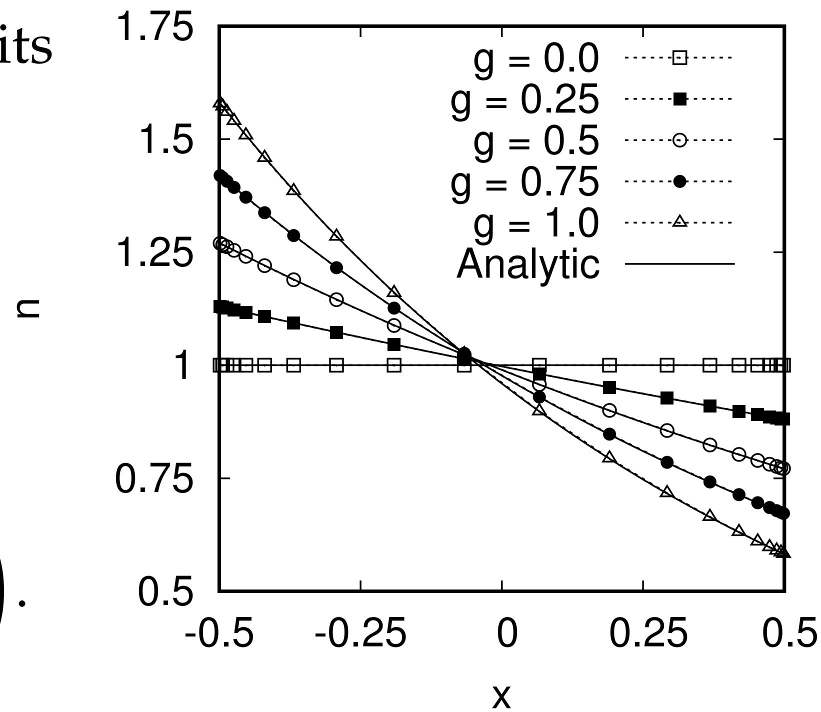
The good: equilibrium flow

- The particular case $T_+ = T_- = T_w$ admits an isothermal equilibrium solution:

$$f = \frac{n(x)}{\sqrt{2\pi m T_w}} e^{-p^2/2mT_w},$$

where $n(x)$ is the barometric profile:

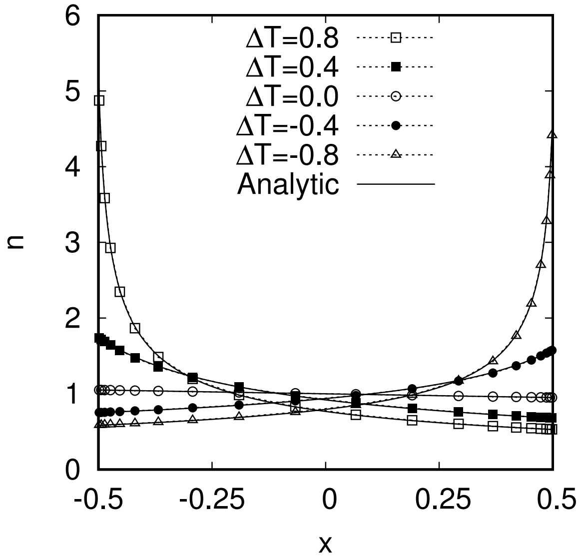
$$n(x) = \frac{mg\mathcal{N}}{2T_w \sinh(mgL/2T_w)} \exp\left(-\frac{mgx}{T_w}\right).$$



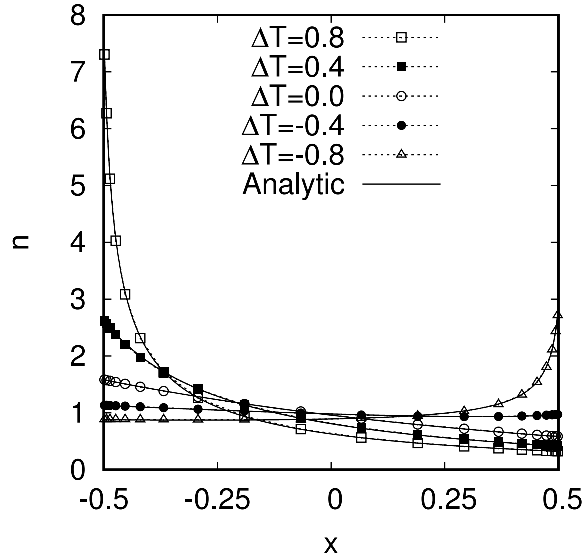
,

- The above solution is valid for all values of τ.
- The results were obtained with HLB(5) at Kn = 0.5 ($N_x = 20$ nodes).

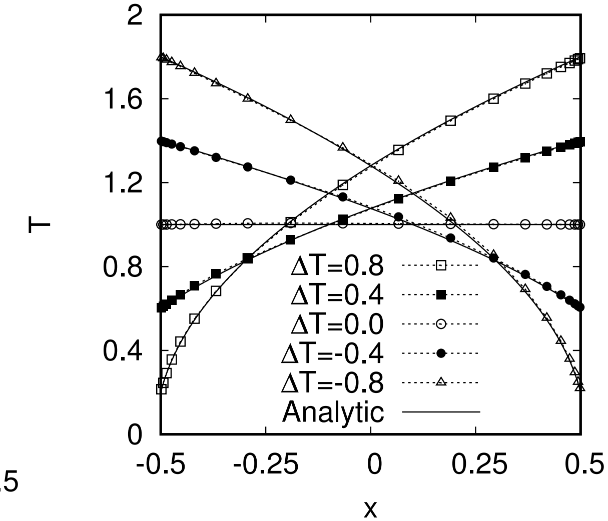
The good: Navier-Stokes



$g = 0.1$



$g = 1.0$



Independent of g

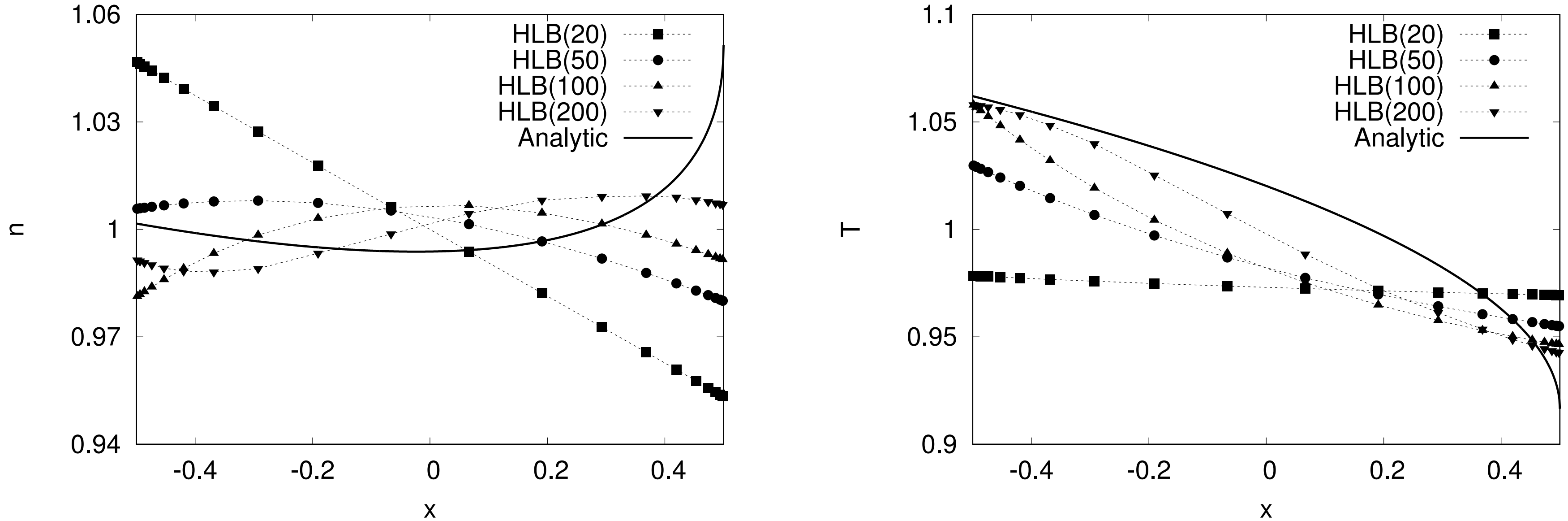
- The NS solution is:

$$n(x) = \frac{mg\mathcal{N}}{2T(x)\sinh\frac{mgL}{T_+ + T_-}} \exp\left[-\frac{mgL}{T_-^2 - T_+^2}[2T(x) - T_- - T_+]\right],$$

$$T(x) = \sqrt{Ax + B}, \qquad A = \frac{T_-^2 - T_+^2}{L}, \qquad B = \frac{T_-^2 + T_+^2}{2}.$$

- Excellent agreement using HLB(5) at Kn $= 0.001$ using $N_x = 100$ nodes.

The bad: free molecular flow



$$g = 0.1,\ T_+ = 1.4,\ T_- = 0.6$$

- Ballistic regime analytic solution:

$$n(x) = mg\mathcal{N}\,\frac{\frac{1}{\sqrt{T_+}}e^{\frac{mg(L-2x)}{2T_+}}\operatorname{erfc}\left(-\sqrt{\frac{mg(L-2x)}{2T_+}}\right) + \frac{1}{\sqrt{T_-}}e^{\frac{mg(L-2x)}{2T_-}}\operatorname{erfc}\left(\sqrt{\frac{mg(L-2x)}{2T_-}}\right)}{\sqrt{T_+}\left[e^{mgL/T_+}\operatorname{erfc}\left(-\sqrt{\frac{mgL}{T_+}}\right)-1\right] + \sqrt{T_-}\left[e^{mgL/T_-}\operatorname{erfc}\left(\sqrt{\frac{mgL}{T_-}}\right)-1\right]},$$

$$T(x) = \frac{\sqrt{T_+}e^{\frac{mg(L-2x)}{2T_+}}\operatorname{erfc}\left(-\sqrt{\frac{mg(L-2x)}{2T_+}}\right) + \sqrt{T_-}e^{\frac{mg(L-2x)}{2T_-}}\operatorname{erfc}\sqrt{\frac{mg(L-2x)}{2T_-}}}{\frac{1}{\sqrt{T_+}}e^{\frac{mg(L-2x)}{2T_+}}\operatorname{erfc}\left(-\sqrt{\frac{mg(L-2x)}{2T_+}}\right) + \frac{1}{\sqrt{T_-}}e^{\frac{mg(L-2x)}{2T_-}}\operatorname{erfc}\sqrt{\frac{mg(L-2x)}{2T_-}}}.$$

Force in half-range models

Expansion with respect to half-range polynomials (naïve)

- In order to allow $f(p)$ to become discontinuous at $p = 0$, the following split is assumed:

$$f(p) = \begin{cases} f^+(p), & p > 0, \\ f^-(p), & p < 0, \end{cases} \qquad f^\pm = \frac{e^{-p^2/2}}{\sqrt{2\pi}} \sum_{\ell=0}^{\infty} \mathcal{F}_\ell^\pm \mathfrak{h}_\ell(|p|),$$

$$\mathcal{F}_\ell^+ = \int_0^\infty dp\, f(p)\, \mathfrak{h}_\ell(p), \qquad \mathcal{F}_\ell^- = \int_{-\infty}^0 dp\, f(p)\, \mathfrak{h}_\ell(-p). \tag{12}$$

- The derivatives of $f^\pm$ can be computed analytically:

$$\frac{\partial f^\pm}{\partial p} = \mp \frac{e^{-p^2/2}}{\sqrt{2\pi}} \sum_{\ell=0}^{\infty} \mathcal{F}_\ell^\pm \left[\frac{\mathfrak{h}_{\ell,\ell}}{\mathfrak{h}_{\ell+1,\ell+1}} \mathfrak{h}_{\ell+1}(|p|) + \sum_{s=0}^{\ell} \frac{\mathfrak{h}_{\ell,0}\mathfrak{h}_{s,0}}{\sqrt{2\pi}} \mathfrak{h}_s(|p|) \right]. \tag{13}$$

- The first order moment of $\partial_p f$ evaluates to:

$$\int_{-\infty}^{\infty} dp\, \partial_p f = -\sum_{\ell=0}^{\infty} \frac{\mathfrak{h}_{\ell,0}}{\sqrt{2\pi}} (\mathcal{F}_\ell^+ - \mathcal{F}_\ell^-) = -[f^+(0) - f^-(0)]. \tag{14}$$

- When a discontinuity is present at $p = 0$, $f^+(0) \neq f^-(0)$.
- The LHS of Eq. (14) always evaluates to 0!

Expansion with respect to half-range polynomials: distributions

- The error is due to a missing term when taking the derivative of f.
- This term is due to the implicit split at $p = 0$:

$$f(p) = \theta(p) f^+(p) + \theta(-p) f^-(p). \tag{15}$$

- The derivative also acts on $\theta(\pm p)$:

$$\partial_p f = \theta(p)\partial_p f^+ + \theta(-p)\partial_p f^-(p) + \delta(p)[f^+(0) - f^-(0)]. \tag{16}$$

- The δ term is sufficient to ensure $\int dp\, \partial_p f = 0$.
- The projection of $\delta(p)[f^+(p) - f^-(p)] = \delta(p)[f^+(0) - f^-(0)]$ is:

$$[\delta(p)]^\pm [f^+(p) - f^-(p)] = \frac{e^{-p^2/2}}{4\pi} \left[\sum_{s=0}^{\infty} \mathfrak{h}_{s,0}(\mathcal{F}_s^+ - \mathcal{F}_s^-)\right] \left[\sum_{\ell=0}^{\infty} \mathfrak{h}_{\ell,0}\mathfrak{h}_\ell(|p|)\right]. \tag{17}$$

Discretisation of the momentum space[6]

- The half range moments of f can be recovered using the half-range Gauss-Hermite quadrature:

$$\int_0^\infty dp\, f\, p^s \simeq \sum_{k=1}^{Q} f_k p_k^s, \qquad \int_{-\infty}^0 dp\, f\, p^s \simeq \sum_{k=1}^{Q} f_{Q+k}(-p_k)^s, \tag{18}$$

  where the equality is exact if $Q > s$ and the series expansion of $f^\pm$ is truncated at $\ell = Q - 1$.

- The discrete populations $\{f_1, f_2, \dots f_{2Q}\}$ are $(1 \le k \le Q)$:

$$\begin{pmatrix} f_k \\ f_{Q+k} \end{pmatrix} = \frac{w_k}{e^{-p^2/2}/\sqrt{2\pi}} \begin{pmatrix} f(p_k) \\ f(-p_k) \end{pmatrix}, \qquad w_k = \frac{p_k a_Q^2}{\mathfrak{h}_{Q+1}^2(p_k)\left[p_k + \mathfrak{h}_{Q,0}^2/\sqrt{2\pi}\right]}, \tag{19}$$

  while $\{p_k, k = 1, 2, \dots Q\}$ is the set of roots of $\mathfrak{h}_Q(p)$ and $p_{Q+k} = -p_k$.

[6] V. E. Ambruș, V. Sofonea, J. Comput. Phys. **316** (2016) 1.

The ugly: kernel for force term

- We are now looking for a recipe to calculate the momentum space derivative of f:

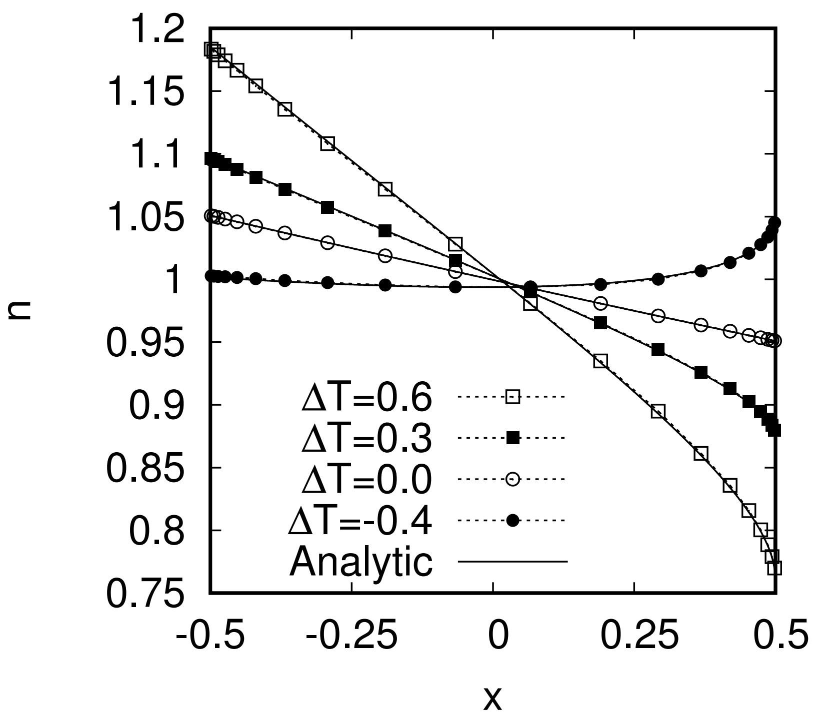
$$(\partial_p f)_k = \sum_{k'=1}^{2Q} \mathcal{K}_{k,k'} f_{k'} . \tag{20}$$

- The $2Q \times 2Q$ matrix $\mathcal{K}_{k,k'}$ has the following elements:

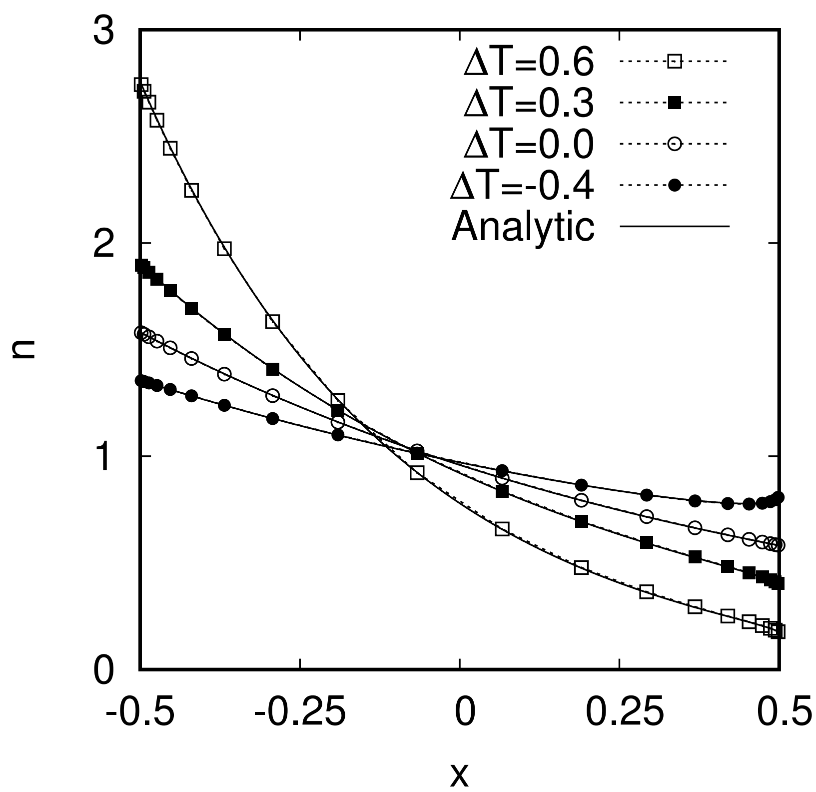
$$\mathcal{K}^{\mathfrak{h}}_{k,k'} = \frac{w_k \sigma_k}{p_0} \left\{ \frac{1 + \sigma_k \sigma_{k'}}{2} \sum_{\ell=0}^{Q-2} \mathfrak{h}_\ell(|p_{k'}|) \left[\sum_{s=\ell+1}^{Q-1} \frac{\mathfrak{h}_{\ell,0} \mathfrak{h}_{s,0}}{\sqrt{2\pi}} \mathfrak{h}_s(|\overline{p}_k|) - \frac{\mathfrak{h}_{\ell+1}(|\overline{p}_k|)}{a_\ell} \right] \right.$$
$$\left. - \frac{1}{2\sqrt{2\pi}} \left[\sum_{s=0}^{Q-1} \mathfrak{h}_{s,0} \mathfrak{h}_s(|p_k|) \right] \times \left[\sum_{\ell=0}^{Q-1} \mathfrak{h}_{\ell,0} \mathfrak{h}_\ell(|p_{k'}|) \right] \right\} . \tag{21}$$

Validation

Ballistic regime: density profile



$g = 0.1$

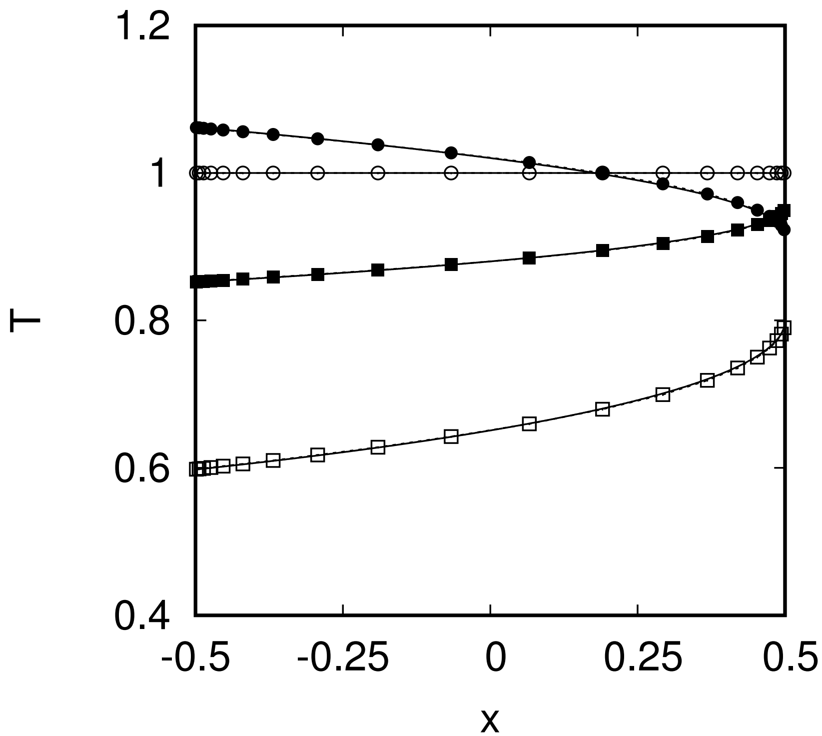


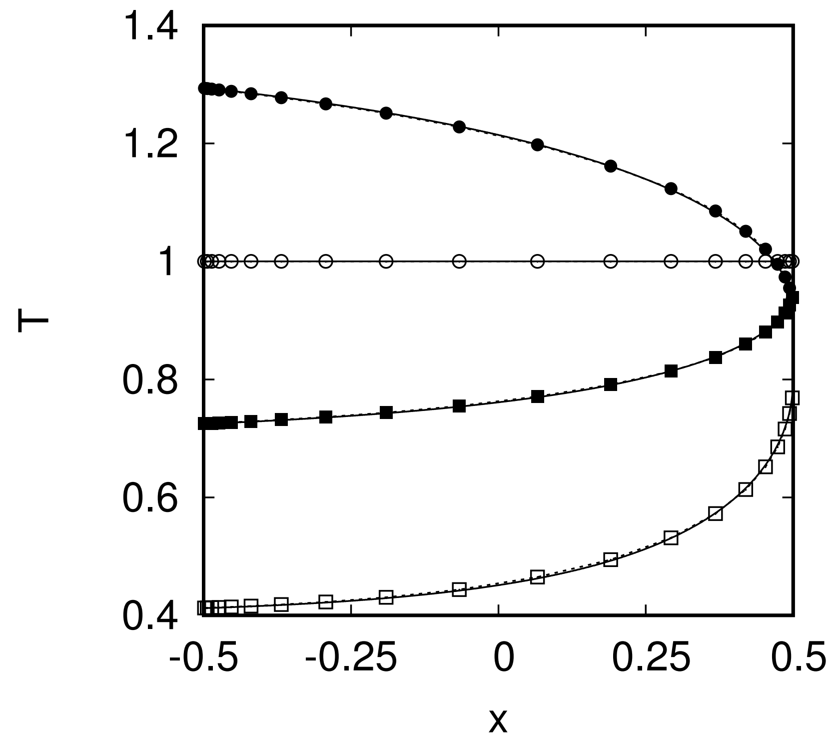
$g = 1.0$

$$n(x) = mg\mathcal{N}\frac{\frac{1}{\sqrt{T_+}}e^{\frac{mg(L-2x)}{2T_+}}\operatorname{erfc}\left(-\sqrt{\frac{mg(L-2x)}{2T_+}}\right) + \frac{1}{\sqrt{T_-}}e^{\frac{mg(L-2x)}{2T_-}}\operatorname{erfc}\left(\sqrt{\frac{mg(L-2x)}{2T_-}}\right)}{\sqrt{T_+}\left[e^{mgL/T_+}\operatorname{erfc}\left(-\sqrt{\frac{mgL}{T_+}}\right)-1\right] + \sqrt{T_-}\left[e^{mgL/T_-}\operatorname{erfc}\left(\sqrt{\frac{mgL}{T_-}}\right)-1\right]}.$$

Excellent agreement using HHLB(200), $N_x = 20$ nodes and $A = 0.99$.

Ballistic regime: temperature





$g = 0.1$ $\qquad$ $g = 1.0$

$$T(x) = \frac{\sqrt{T_+}e^{\frac{mg(L-2x)}{2T_+}}\,\mathrm{erfc}\left(-\sqrt{\frac{mg(L-2x)}{2T_+}}\right) + \sqrt{T_-}e^{\frac{mg(L-2x)}{2T_-}}\,\mathrm{erfc}\sqrt{\frac{mg(L-2x)}{2T_-}}}{\frac{1}{\sqrt{T_+}}e^{\frac{mg(L-2x)}{2T_+}}\,\mathrm{erfc}\left(-\sqrt{\frac{mg(L-2x)}{2T_+}}\right) + \frac{1}{\sqrt{T_-}}e^{\frac{mg(L-2x)}{2T_-}}\,\mathrm{erfc}\sqrt{\frac{mg(L-2x)}{2T_-}}}.$$

Excellent agreement using HHLB(200), $N_x = 20$ nodes and $A = 0.99$.

Conclusion

Conclusion

- The simulation of bounded flows in the rarefied regime requires the use of half-range quadratures.
- Implementing $\partial_p f$ using half-range quadratures requires the theory of distributions.
- Applications include:
  - Heat transfer between coaxial cylinders and concentric spheres;[7]
  - Circular Couette flow; circular lid-driven cavity;[8]
  - Other force-driven flows or flows in curved geometries in the rarefied regime.
- This work is supported by the grants from the Romanian National Authority for Scientific Research, CNCS-UEFISCDI having project numbers PN-II-RU-TE-2014-4-2910 and PN-II-ID-JRP-2011-2-0060.

[7] Presentation by Sergiu Busuioc on Tuesday.
[8] Presentation by Victor Sofonea on Wednesday.