Physics-Informed Solutions of Rarefied Gas Dynamics Problems via Theory of Functional Connections

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Contents

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Contents

Introduction: Overview

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- The *Rarefied Gas Dynamics*, or free molecular flow, describes the fluid dynamics of gas where the mean free path *(λ)* of the molecules is larger than the size *(d)* of the chamber under test: Knudsen number $\mathrm{Kn} = \frac{\lambda}{d} > 1.$

- The *Poiseuille Flow* is a laminar pressure-induced flow in a channel of length *l* and width *d,* with $l \gg d$.

- The *Thermal Creep Flow* is a flow of a slightly rarefied gas caused by the temperature gradient along a wall.

Introduction: Goal

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- To show the capability of *Theory of Functional Connections* (TFC) [1] in solving RGD problems with high accuracy.
- The problems studied are based on the BGK model of the integro-differential Boltzmann Transport Equation for particles.

[1] Mortari, D. (2017). The theory of connections: Connecting points. *Mathematics*, *5*(4), 57.

Contents

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Transport Theory for Rarefied Gas Dynamics

- Solving Boltzmann Transport Equations for Rarefied Gas Dynamics is generally hard and computationally expensive
  - No direct analytical solutions except in very limited cases
- Methods to solve Boltzmann Transport Equations generally are
  - **Semi-analytical**
    - High accuracy in limited cases
  - **Numerical**
    - Hard implementation

$$u\frac{\partial}{\partial\tau}Y(\tau,u)+Y(\tau,u)=\int_{-\infty}^{\infty}\Psi(u)Y(\tau,u)du$$

TFC approach to solve Linear ODEs

- TFC derives expressions, called *constrained expressions,* with an embedded set of *n* linear constraints

$$y(t) = g(t) + \sum_{k=1}^{n} \eta_k p_k(t) = g(t) + \boldsymbol{\eta}^T \boldsymbol{p}(t)$$

- According to the literature, to solve ODEs, the $g(t)$ used will be an expansion of orthogonal polynomials (Chebyshev): $g(t) = \boldsymbol{h}^T \boldsymbol{\xi}$
  - The solution of the problem is reduced to the calculation of the coefficients of the expansion of Chebyshev polynomials

Contents

Poiseuille Flow in a plane channel

BGK model is used to examine theoretically and numerically the flow of a rarefied gas between to parallel plates. According to Siewert [2]:

$$\frac{1}{2}k\theta + \theta c_x \frac{\partial}{\partial x} Z(x, c_x) + Z(x, c_x) = \pi^{-1/2} \int_{-\infty}^{\infty} e^{-u^2} Z(x, u) du$$

for $x \in \left(-\frac{d}{2}, \frac{d}{2}\right)$ and $c_x \in (-\infty, \infty)$, with the following reflecting boundary conditions:

$$\begin{cases} Z\left(-\frac{d}{2}, c_x\right) = (1-\alpha) Z\left(-\frac{d}{2}, -c_x\right) \\ Z\left(\frac{d}{2}, -c_x\right) = (1-\alpha) Z\left(\frac{d}{2}, c_x\right) \end{cases}$$

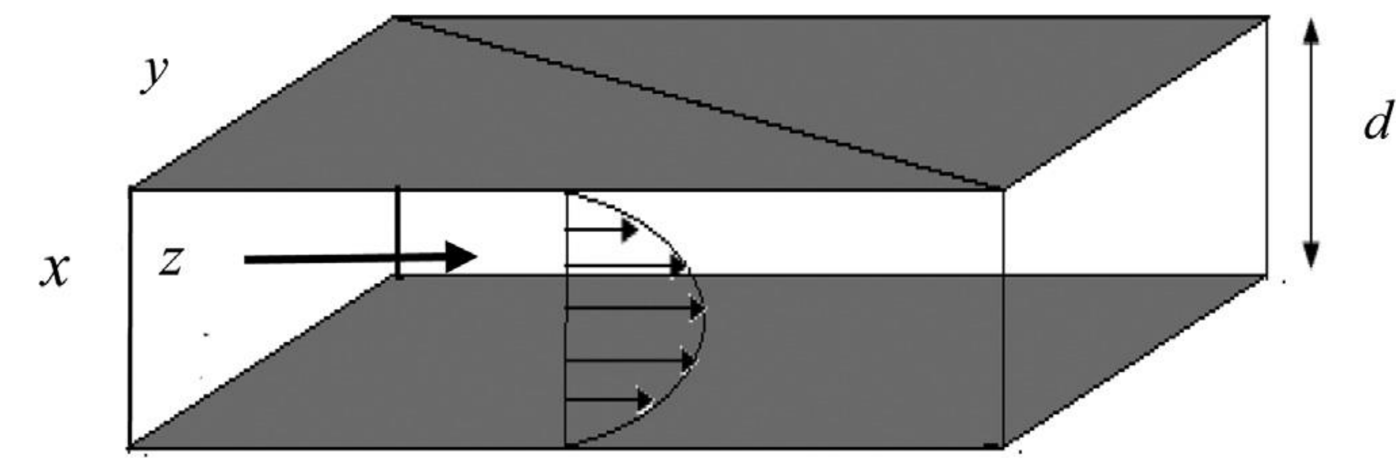

Image from [Ganapol 2019]

for $c_x \in (0, \infty)$. Here, *d* is the channel thickness, *k* is proportional to the *Δp* that causes the flow, *x* is the spatial variable, $\alpha \in (0,1]$ is the accomodation coefficient, θ is the mean-free time, and

$$Z(x, c_x) = \pi^{-1} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-(c_y^2 + c_z^2)^2} c_z h(x, c_x, c_y, c_z) dc_y dc_z$$

Where (c_x, c_y, c_z) are the three components of the molecular velocity and *h* is a perturbation from Maxwell distrtibution.

[2] Siewert, C. E., Garcia, R. D. M., & Grandjean, P. (1980). A concise and accurate solution for Poiseuille flow in a plane channel. Journal of Mathematical Physics, 21(12), 2760-2763.

Poiseuille Flow in a plane channel

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Reformulation of the problem

According to Barichello and Siewert [3], we introduce some change of variables:

$$\tau = \frac{x}{\theta} \qquad ; \qquad \delta = \frac{d}{\theta} \qquad ; \qquad u = c_x$$

Our equation become:

$$\frac{1}{2}k\theta + \mu\frac{\partial}{\partial\tau}Z(\tau,u) + Z(\tau,u) = \pi^{-1/2}\int_{-\infty}^{\infty} e^{-u^2}Z(\tau,u)du$$

for $\tau \in \left(-\frac{\delta}{2},\frac{\delta}{2}\right)$, and $u \in (-\infty,\infty)$ with the following reflecting boundary conditions:

$$\begin{cases} Z\left(-\frac{d}{2},c_x\right) = (1-\alpha)Z\left(-\frac{d}{2},-c_x\right) \\ Z\left(\frac{d}{2},-c_x\right) = (1-\alpha)Z\left(\frac{d}{2},c_x\right) \end{cases} \qquad \text{for } u \in (0,\infty)$$

Now, in order to obtain a homogeneous version of the problem, we make use of a particular solution that accounts for the inhomogeneous term in that equation, and so we introduce

$$Z(\tau,u) = \frac{1}{2}k\theta[\tau^2 - 2\tau u + 2u^2 - a^2 - 2Y(\tau,u)]$$

[3] Barichello, L. B., & Siewert, C. E. (1999). A discrete-ordinates solution for Poiseuille flow in a plane channel. *Zeitschrift für angewandte Mathematik und Physik ZAMP*, *50*(6), 972-981.

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By plugging $Z(\tau, u)$ in the previous equations, we get the following problem:

$$u\frac{\partial}{\partial \tau}Y(\tau,u) + Y(\tau,u) = \int_{-\infty}^{\infty}\Psi(u)Y(\tau,u)du$$

Where $2a = \delta$, $\tau \in (-a, a)$, and $u \in (-\infty, \infty)$.

Subject to:

$$\begin{cases} Y(-a,u) = (1-\alpha)Y(-a,-u) + \alpha u^2 + au(2-\alpha) \\ Y(a,-u) = (1-\alpha)Y(a,u) + \alpha u^2 + au(2-\alpha) \end{cases}$$

for $u \in (0, \infty)$.

$\Psi(u)$ is a weight function defined by:

$$\Psi(u) = \pi^{-1/2}e^{-u^2}$$

Poiseuille Flow in a plane channel

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TFC Solution

In order to apply the TFC , we need a new variable *x* (instead of *τ*), that ranges in [-1,1], to use Chebyshev polynomials.

The new *x* variable has been defined as follows [4]:

$x = c(\tau - \tau_0) + x_0$ where c is a mapping coefficient: $c = \frac{x_f - x_0}{\tau_f - \tau_0}$

And thus,

$$x = c(\tau + a) - 1 \quad \text{and} \quad c = \frac{1}{a}$$

According to the change of variable we have:

$$Y(\tau, u) = Y(x, u)$$
$$\frac{d}{d\tau} Y(\tau, u) = c \frac{d}{dx} Y(x, u)$$

So, the problem becomes

$$cu \frac{\partial}{\partial x} Y(x, u) + Y(x, u) = \int_{-\infty}^{\infty} \Psi(u) Y(x, u) du$$

[4] Mortari, D. (2017). Least-squares solution of linear differential equations. Mathematics, 5(4), 48.

Poiseuille Flow in a plane channel

To use a Gauss-Legendre quadrature (which ranges in [-1,1]), we can use an other change of variable, $\mu \in (0,1)$.

$$u = -\log(\mu) \quad ; \quad du = -\frac{1}{\mu} d\mu \quad ; \quad \Psi(\mu) = \pi^{-1/2} e^{-(-\log(\mu))^2}$$

and rewrite:

$$-c \log(\mu) \frac{\partial}{\partial x} Y(x,\mu) + Y(x,\mu) = \int_{-1}^{1} \frac{1}{\mu} \Psi(\mu) Y(x,\mu) d\mu$$

We discretize the μ for N points:

$$\mu \quad \rightarrow \quad \boldsymbol{\mu} = \{\mu_i\}_{i=1}^{N} \; ; \qquad (\boldsymbol{\mu} \in (N \times 1))$$

The problem can be split for both positive and negative molecular velocity, and the integral can be solved with a Gauss-Legendre quadrature:

$$-c \log(\mu_i) \frac{\partial}{\partial x} Y(x,\mu_i) + Y(x,\mu_i) = \sum_{k=1}^{N} w_k \frac{1}{\mu_k} \Psi(\mu_k)[Y(x,\mu_k) + Y(x,-\mu_k)]$$

$$c \log(\mu_i) \frac{\partial}{\partial x} Y(x,-\mu_i) + Y(x,-\mu_i) = \sum_{k=1}^{N} w_k \frac{1}{\mu_k} \Psi(\mu_k)[Y(x,\mu_k) + Y(x,-\mu_k)]$$

s.t.

$$\begin{cases} Y(-a,\mu) = (1-\alpha) Y(-a,-\mu) + \alpha \cdot \log(\mu)^2 + a \cdot log(\mu)(2-\alpha) \\ Y(a,-\mu) = (1-\alpha) Y(a,\mu) + \alpha \cdot \log(\mu)^2 + a \cdot log(\mu)(2-\alpha) \end{cases}$$

Colors blue and red are used to represent the positive and negative flux, respectively.

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For the sake of simplicity, we can use a different notation:

$$-c\log(\mu_i)\frac{\partial}{\partial x}Y_i^+ + Y_i^+ = \sum_{k=1}^{N} w_k \frac{1}{\mu_k}\Psi(\mu_k)[Y_k^+ + Y_k^-]$$

$$c\log(\mu_i)\frac{\partial}{\partial x}Y_i^- + Y_i^- = \sum_{k=1}^{N} w_k \frac{1}{\mu_k}\Psi(\mu_k)[Y_k^+ + Y_k^-]$$

s.t.

$$\begin{cases} Y_0^+ = (1-\alpha)Y_0^- + \alpha\cdot\log(\mu_i)^2 + a\cdot log(\mu_i)(2-\alpha) \\ Y_f^- = (1-\alpha)Y_f^+ + \alpha\cdot\log(\mu_i)^2 + a\cdot log(\mu_i)(2-\alpha) \end{cases}$$

Our constrained expressions are:

$$Y_i^+ = \boldsymbol{h}\cdot\boldsymbol{\xi_i^+} + \eta_i^+ \quad ; \quad Y_i^- = \boldsymbol{h}\cdot\boldsymbol{\xi_i^-} + \eta_i^-$$

And according to the boundary conditions:

$$Y_0^+ = \boldsymbol{h_0}\cdot\boldsymbol{\xi_i^+} + \eta_i^+ \qquad Y_f^- = \boldsymbol{h_f}\cdot\boldsymbol{\xi_i^-} + \eta_i^-$$

$$Y_f^+ = \boldsymbol{h_f}\cdot\boldsymbol{\xi_i^+} + \eta_i^+ \qquad Y_0^- = \boldsymbol{h_0}\cdot\boldsymbol{\xi_i^-} + \eta_i^-$$

Replacing them in the previous system of equations, we obtain:

$$\begin{cases} \boldsymbol{h_0}\cdot\boldsymbol{\xi_i^+} + \eta_i^+ = (1-\alpha)\boldsymbol{h_0}\cdot\boldsymbol{\xi_i^-} + \eta_i^- + \alpha\cdot\log(\mu_i)^2 + a\cdot log(\mu_i)(2-\alpha) \\ \boldsymbol{h_f}\cdot\boldsymbol{\xi_i^-} + \eta_i^- = (1-\alpha)\boldsymbol{h_f}\cdot\boldsymbol{\xi_i^+} + \eta_i^+ + \alpha\cdot\log(\mu_i)^2 + a\cdot log(\mu_i)(2-\alpha) \end{cases}$$

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Let's call new parameters:

$K_i = \alpha \cdot \log(\mu_i)^2 + a \cdot log(\mu_i)(2-\alpha)$ and $\beta = (1-\alpha)$

and rewrite

$$\begin{cases} \boldsymbol{h_0} \cdot \boldsymbol{\xi_i^+} + \eta_i^+ = \beta \cdot \boldsymbol{h_0} \cdot \boldsymbol{\xi_i^-} + \eta_i^- + K_i \\ \boldsymbol{h_f} \cdot \boldsymbol{\xi_i^-} + \eta_i^- = \beta \cdot \boldsymbol{h_f} \cdot \boldsymbol{\xi_i^+} + \eta_i^+ + K_i \end{cases} \Rightarrow \begin{cases} \eta_i^+ - \beta\eta_i^- = \beta \cdot \boldsymbol{h_0} \cdot \boldsymbol{\xi_i^-} - \boldsymbol{h_0} \cdot \boldsymbol{\xi_i^+} + K_i \\ -\beta\eta_i^- + \eta_i^- = \beta \cdot \boldsymbol{h_f} \cdot \boldsymbol{\xi_i^+} - \boldsymbol{h_f} \cdot \boldsymbol{\xi_i^-} + K_i \end{cases}$$

$$\begin{bmatrix} 1 & -\beta \\ -\beta & 1 \end{bmatrix} \cdot \begin{bmatrix} \eta_i^+ \\ \eta_i^- \end{bmatrix} = \begin{bmatrix} \beta \cdot \boldsymbol{h_0} \cdot \boldsymbol{\xi_i^-} - \boldsymbol{h_0} \cdot \boldsymbol{\xi_i^+} + K_i \\ \beta \cdot \boldsymbol{h_f} \cdot \boldsymbol{\xi_i^+} - \boldsymbol{h_f} \cdot \boldsymbol{\xi_i^-} + K_i \end{bmatrix} \Rightarrow \begin{bmatrix} \eta_i^+ \\ \eta_i^- \end{bmatrix} = \frac{1}{1-\beta^2} \cdot \begin{bmatrix} 1 & \beta \\ \beta & 1 \end{bmatrix} \cdot \begin{bmatrix} \beta \cdot \boldsymbol{h_0} \cdot \boldsymbol{\xi_i^-} - \boldsymbol{h_0} \cdot \boldsymbol{\xi_i^+} + K_i \\ \beta \cdot \boldsymbol{h_f} \cdot \boldsymbol{\xi_i^+} - \boldsymbol{h_f} \cdot \boldsymbol{\xi_i^-} + K_i \end{bmatrix}$$

Introducing a new parameter: $\gamma = \frac{1}{1-\beta^2}$

$$\begin{bmatrix} \eta_i^+ \\ \eta_i^- \end{bmatrix} = \begin{bmatrix} \gamma & \gamma\beta \\ \gamma\beta & \gamma \end{bmatrix} \cdot \begin{bmatrix} \beta \cdot \boldsymbol{h_0} \cdot \boldsymbol{\xi_i^-} - \boldsymbol{h_0} \cdot \boldsymbol{\xi_i^+} + K_i \\ \beta \cdot \boldsymbol{h_f} \cdot \boldsymbol{\xi_i^+} - \boldsymbol{h_f} \cdot \boldsymbol{\xi_i^-} + K_i \end{bmatrix}$$

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$$\begin{cases} \eta_i^+ = \gamma\left(\beta^2 \boldsymbol{h_f} - \boldsymbol{h_0}\right) \cdot \boldsymbol{\xi_i^+} + \gamma\beta\left(\boldsymbol{h_0} - \boldsymbol{h_f}\right) \cdot \boldsymbol{\xi_i^-} + \gamma K_i(\beta + 1) \\ \eta_i^- = \gamma\beta\left(\boldsymbol{h_f} - \boldsymbol{h_0}\right) \cdot \boldsymbol{\xi_i^+} + \gamma\left(\beta^2 \boldsymbol{h_0} - \boldsymbol{h_f}\right) \cdot \boldsymbol{\xi_i^-} + \gamma K_i(\beta + 1) \end{cases}$$

Calling $\theta = \gamma(\beta + 1)$

$$\begin{cases} \eta_i^+ = \gamma\left(\beta^2 \boldsymbol{h_f} - \boldsymbol{h_0}\right) \cdot \boldsymbol{\xi_i^+} + \gamma\beta\left(\boldsymbol{h_0} - \boldsymbol{h_f}\right) \cdot \boldsymbol{\xi_i^-} + \theta K_i \\ \eta_i^- = \gamma\beta\left(\boldsymbol{h_f} - \boldsymbol{h_0}\right) \cdot \boldsymbol{\xi_i^+} + \gamma\left(\beta^2 \boldsymbol{h_0} - \boldsymbol{h_f}\right) \cdot \boldsymbol{\xi_i^-} + \theta K_i \end{cases}$$

Replacing them in the constrained expressions, we have:

$$Y_i^+ = \left(\boldsymbol{h} - \gamma \boldsymbol{h_0} + \gamma\beta^2 \boldsymbol{h_f}\right) \cdot \boldsymbol{\xi_i^+} + \gamma\beta\left(\boldsymbol{h_0} - \boldsymbol{h_f}\right) \cdot \boldsymbol{\xi_i^-} + \theta K_i$$

$$Y_i^- = \gamma\beta\left(\boldsymbol{h_f} - \boldsymbol{h_0}\right) \cdot \boldsymbol{\xi_i^+} + \left(\boldsymbol{h} - \gamma \boldsymbol{h_f} + \gamma\beta^2 \boldsymbol{h_0}\right) \cdot \boldsymbol{\xi_i^-} + \theta K_i$$

Poiseuille Flow in a plane channel

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And replacing the constrained expressions in the equations of our problem, we have:

$$\left(-c\log(\mu_i)\,\boldsymbol{h}' + \boldsymbol{h} - \gamma \boldsymbol{h_0} + \gamma\beta^2 \boldsymbol{h_f}\right)\cdot \boldsymbol{\xi}_i^+ + \gamma\beta\left(\boldsymbol{h_0}-\boldsymbol{h_f}\right)\cdot\boldsymbol{\xi}_i^- - \sum_{k=1}^{N} w_k \frac{1}{\mu_k}\Psi(\mu_k)\left[\left(\boldsymbol{h}-\theta\boldsymbol{h_0}+\theta\beta\boldsymbol{h_f}\right)\cdot\boldsymbol{\xi}_k^+ + \left(\boldsymbol{h}-\theta\boldsymbol{h_f}+\theta\beta\boldsymbol{h_0}\right)\cdot\boldsymbol{\xi}_i^-\right] = -\theta K_i + \sum_{k=1}^{N} 2\theta K_k$$

$$\gamma\beta\left(\boldsymbol{h_f}-\boldsymbol{h_0}\right)\cdot\boldsymbol{\xi}_i^+ + \left(c\log(\mu_i)\,\boldsymbol{h}' + \boldsymbol{h} - \gamma \boldsymbol{h_f} + \gamma\beta^2 \boldsymbol{h_0}\right)\cdot \boldsymbol{\xi}_i^- - \sum_{k=1}^{N} w_k \frac{1}{\mu_k}\Psi(\mu_k)\left[\left(\boldsymbol{h}-\theta\boldsymbol{h_0}+\theta\beta\boldsymbol{h_f}\right)\cdot\boldsymbol{\xi}_k^+ + \left(\boldsymbol{h}-\theta\boldsymbol{h_f}+\theta\beta\boldsymbol{h_0}\right)\cdot\boldsymbol{\xi}_i^-\right] = -\theta K_i + \sum_{k=1}^{N} 2\theta K_k$$

For the sake of simplicity, we write the inhomogeneous term as:

$b_i^+ = -\theta K_i + \sum_{k=1}^{N} 2\theta K_k$ and $b_i^- = -\theta K_i + \sum_{k=1}^{N} 2\theta K_k$

Expanding the summations, we get the following matrix form:

$$\begin{bmatrix} -c\log(\mu_i)\,\boldsymbol{h}' + \boldsymbol{h} - \gamma \boldsymbol{h_0} + \gamma\beta^2 \boldsymbol{h_f} - w_k\frac{1}{\mu_k}\Psi(\mu_k)\left(\boldsymbol{h}-\theta\boldsymbol{h_0}+\theta\beta\boldsymbol{h_f}\right) & \gamma\beta\left(\boldsymbol{h_0}-\boldsymbol{h_f}\right) - w_k\frac{1}{\mu_k}\Psi(\mu_k)\left(\boldsymbol{h}-\theta\boldsymbol{h_f}+\theta\beta\boldsymbol{h_0}\right) \\ \gamma\beta\left(\boldsymbol{h_f}-\boldsymbol{h_0}\right) - w_k\frac{1}{\mu_k}\Psi(\mu_k)\left(\boldsymbol{h}-\theta\boldsymbol{h_0}+\theta\beta\boldsymbol{h_f}\right) & c\log(\mu_i)\,\boldsymbol{h}' + \boldsymbol{h} - \gamma \boldsymbol{h_f} + \gamma\beta^2 \boldsymbol{h_0} - w_k\frac{1}{\mu_k}\Psi(\mu_k)\left(\boldsymbol{h}-\theta\boldsymbol{h_f}+\theta\beta\boldsymbol{h_0}\right) \end{bmatrix}\cdot\begin{bmatrix}\boldsymbol{\xi}_i^+ \\ \boldsymbol{\xi}_i^-\end{bmatrix} = \begin{bmatrix} b_i^+ \\ b_i^- \end{bmatrix}$$

For the sake of simplicity we write the following terms as:

$$\blacksquare_i = -c\log(\mu_i)\,\boldsymbol{h'}^{\boldsymbol{T}} + \boldsymbol{h}^{\boldsymbol{T}} - \gamma\boldsymbol{h}_{\boldsymbol{0}}^{\boldsymbol{T}} + \gamma\beta^2\boldsymbol{h}_{\boldsymbol{f}}^{\boldsymbol{T}} \qquad \bullet_i = c\log(\mu_i)\,\boldsymbol{h'}^{\boldsymbol{T}} + \boldsymbol{h}^{\boldsymbol{T}} - \gamma\boldsymbol{h}_{\boldsymbol{f}}^{\boldsymbol{T}} + \gamma\beta^2\boldsymbol{h}_{\boldsymbol{0}}^{\boldsymbol{T}}$$

$$\blacksquare_k = -w_k\frac{1}{\mu_k}\Psi(\mu_k)\left(\boldsymbol{h}-\theta\boldsymbol{h_0}+\theta\beta\boldsymbol{h_f}\right)^T \qquad \clubsuit_k = \gamma\beta\left(\boldsymbol{h_0}-\boldsymbol{h_f}\right)^T$$

$$\bullet_k = -w_k\frac{1}{\mu_k}\Psi(\mu_k)\left(\boldsymbol{h}-\theta\boldsymbol{h_f}+\theta\beta\boldsymbol{h_0}\right)^T \qquad \spadesuit_k = \gamma\beta\left(\boldsymbol{h_f}-\boldsymbol{h_0}\right)$$

Poiseuille Flow in a plane channel

It becomes:

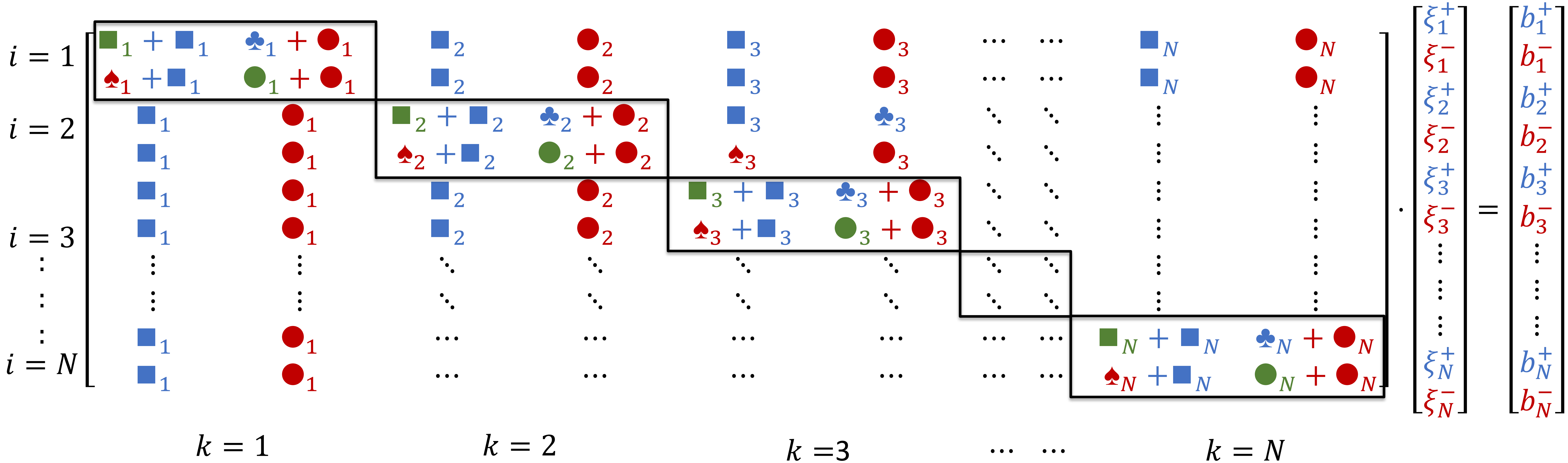
$$\begin{bmatrix} {\color{green}\blacksquare}_i + {\color{blue}\blacksquare}_k & {\color{blue}\clubsuit}_k + {\color{red}\bullet}_k \\ {\color{red}\spadesuit}_k + {\color{blue}\blacksquare}_k & {\color{green}\bullet}_i + {\color{red}\bullet}_k \end{bmatrix} \cdot \begin{bmatrix} \xi_i^+ \\ \xi_i^- \end{bmatrix} = \begin{bmatrix} b_i^+ \\ b_i^- \end{bmatrix}$$

$${\color{green}\blacksquare}_i = -c\log(\mu_i)\,\boldsymbol{h'}^{\boldsymbol{T}} + \boldsymbol{h}^{\boldsymbol{T}} - \gamma \boldsymbol{h}_{\boldsymbol{0}}^{\boldsymbol{T}} + \gamma\beta^2 \boldsymbol{h}_{\boldsymbol{f}}^{\boldsymbol{T}} \qquad {\color{green}\bullet}_i = c\log(\mu_i)\,\boldsymbol{h'}^{\boldsymbol{T}} + \boldsymbol{h}^{\boldsymbol{T}} - \gamma \boldsymbol{h}_{\boldsymbol{f}}^{\boldsymbol{T}} + \gamma\beta^2 \boldsymbol{h}_{\boldsymbol{0}}^{\boldsymbol{T}}$$

$${\color{blue}\blacksquare}_k = -w_k \frac{1}{\mu_k}\Psi(\mu_k)\left(\boldsymbol{h} - \theta \boldsymbol{h}_{\boldsymbol{0}} + \theta\beta \boldsymbol{h}_{\boldsymbol{f}}\right)^T \qquad {\color{blue}\clubsuit}_k = \gamma\beta\left(\boldsymbol{h}_{\boldsymbol{0}} - \boldsymbol{h}_{\boldsymbol{f}}\right)^T$$

$${\color{red}\bullet}_k = -w_k \frac{1}{\mu_k}\Psi(\mu_k)\left(\boldsymbol{h} - \theta \boldsymbol{h}_{\boldsymbol{f}} + \theta\beta \boldsymbol{h}_{\boldsymbol{0}}\right)^T \qquad {\color{red}\spadesuit}_k = \gamma\beta\left(\boldsymbol{h}_{\boldsymbol{f}} - \boldsymbol{h}_{\boldsymbol{0}}\right)$$

And we can obtain the following system:



Poiseuille Flow in a plane channel

To find the vector of unknowns

$$\boldsymbol{\xi} = [\xi_{\boldsymbol{1}}^{+}\,;\xi_{\boldsymbol{1}}^{-};\xi_{\boldsymbol{2}}^{+}\,;\xi_{\boldsymbol{2}}^{-};\dots\dots\dots;\xi_{\boldsymbol{N}}^{+}\,;\xi_{\boldsymbol{N}}^{-}]$$

we need to solve the following linear system via Least-Squares :

$$\boldsymbol{A}\cdot\boldsymbol{\xi} = \boldsymbol{B}$$

where:

$$\xi_i^{\pm} = (m \times 1) \qquad \boldsymbol{\xi} = (2\cdot m\cdot N \;\times\; 1) \qquad b_i^{\pm} = (M \times 1) \qquad \boldsymbol{B} = (2\cdot M\cdot N \;\times\; 1)$$

$$\blacksquare_i, \bullet_i, \blacksquare_k, \clubsuit_k, \spadesuit_k, \bullet_k = (M \times m) \qquad \boldsymbol{A} = (2\cdot M\cdot N \;\times\; 2\cdot m\cdot N)$$

Once the linear system is solved, the solutions for positive and negative flux can be found as:

$$Y^{+} = \left(\boldsymbol{h} - \gamma\boldsymbol{h_0} + \gamma\beta^2\boldsymbol{h_f}\right)\cdot\boldsymbol{\xi}^{+} + \gamma\beta\left(\boldsymbol{h_0} - \boldsymbol{h_f}\right)\cdot\boldsymbol{\xi}^{-} + \theta K$$

$$Y^{-} = \gamma\beta\left(\boldsymbol{h_f} - \boldsymbol{h_0}\right)\cdot\boldsymbol{\xi}^{+} + \left(\boldsymbol{h} - \gamma\boldsymbol{h_f} + \gamma\beta^2\boldsymbol{h_0}\right)\cdot\boldsymbol{\xi}^{-} + \theta K$$

Poiseuille Flow Results

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Code Analysis and Benchmarking

To demonstrate the precision of the TFC in solving the problem, we report the macroscopic velocity profile, that according to [5] is given by:

$$q(\tau) = \frac{1}{k\theta}\int_{-\infty}^{\infty}\Psi(u)Z(\tau,u)du$$

By replacing the expression of $Z(\tau,u)$ into $q(\tau)$ we get

$$q(\tau) = \frac{1}{2}(1 - a^2 + \tau^2) - Y_0(\tau)$$

where

$$Y_0(\tau) = \int_{-\infty}^{\infty}\Psi(u)Y(\tau,u)du$$

Which it can be computed making use of a Gaussian-Legendre quadrature

$$Y_0(\tau) = \int_{-1}^{1}\frac{1}{\mu}\Psi(\mu)Y(\tau,\mu)d\mu = \sum_{k=1}^{N} w_k \frac{1}{\mu_k}\Psi(\mu_k)[Y_i^+ - Y_i^-]$$

[5] Loyalka, S. K., Petrellis, N., & Storvick, T. S. (1979). Some exact numerical results for the BGK model: Couette, Poiseuille and thermal creep flow between parallel plates. *Zeitschrift für angewandte Mathematik und Physik ZAMP*, *30*(3), 514-521.

Poiseuille Flow Results

Microscopic velocity profile $q(\tau)$

TABLE 1. The macroscopic velocity profile $q(\tau)$ for a plan channel of half width $a = 1$, with $m = 50 \pm 2$, $M = 200$, and $N = 22$. All the digits match the benchmark published by Barichello et al. [3]

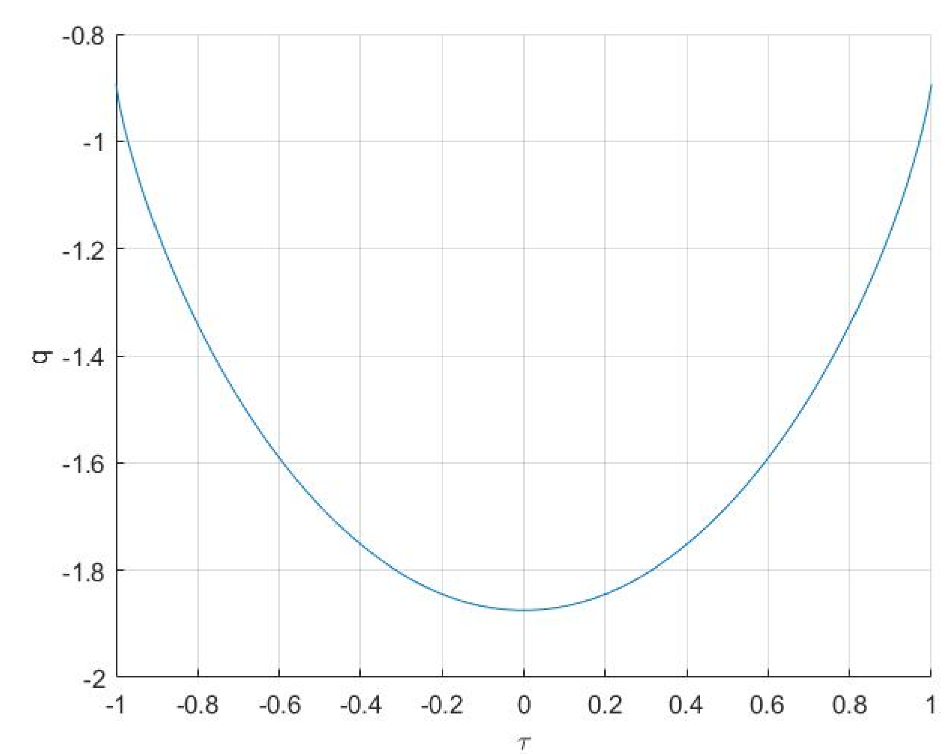
τ	$\alpha = 0.50$	$\alpha = 0.80$	$\alpha = 0.88$	$\alpha = 0.96$	$\alpha = 1.00$
0.0	-3.65222	-2.31962	-2.11741	-1.94880	-1.87458
0.1	-3.64484	-2.31215	-2.10992	-1.94129	-1.86706
0.2	-3.62258	-2.28964	-2.08735	-1.91866	-1.84440
0.3	-3.58512	-2.25176	-2.04937	-1.88058	-1.80627
0.4	-3.53185	-2.19790	-1.99537	-1.82644	-1.75206
0.5	-3.46179	-2.12707	-1.92435	-1.75524	-1.68078
0.6	-3.37332	-2.03767	-1.83472	-1.66539	-1.59082
0.7	-3.26373	-1.92699	-1.72378	-1.55421	-1.47952
0.8	-3.12792	-1.79004	-1.58657	-1.41674	-1.34193
0.9	-2.95402	-1.61528	-1.41163	-1.24164	-1.16676
1.0	-2.67641	-1.34037	-1.13753	-9.68381e-1	-8.93925e-1

RGD via TFC
N = 22

vs.

RGD via ADO
N = 100

CPU time for the Least-Squares $\cong 0.24$ seconds



[3] Barichello, L. B., & Siewert, C. E. (1999). A discrete-ordinates solution for Poiseuille flow in a plane channel. *Zeitschrift für angewandte Mathematik und Physik ZAMP*, *50*(6), 972-981.

Poiseuille Flow Results

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Flow rate $\mathbf{Q}(a)$

Furthermore, we computed the flow rate

$$Q = -\frac{1}{2a^2}\int_{-a}^{a} q(\tau)d\tau$$

And by replacing the expression of $q(\tau)$ into $Q(\tau)$ we get

$$Q = \frac{1}{2a^2}\int_{-a}^{a} Y_0(\tau)d\tau - \frac{1}{2a}\left(1-\frac{2}{3}a^2\right)$$

- M=40 and m=24, for **2a=0.05**, with computational time = 0.04 s.
- M=300 and m=90, for **2a=9**, with computational time = 1.6 s.

TABLE 2. The flow rate $Q(a)$ for Barichello and Siewert digits [3]

$2a$	$\alpha = 0.50$	$\alpha = 0.80$	$\alpha = 0.88$	$\alpha = 0.96$	$\alpha = 1.00$
0.05	5.22330	3.08971	2.73834	2.43735	2.30226
0.10	4.55641	2.70774	2.40605	2.14824	2.03271
0.30	3.77847	2.24477	2.00107	1.79451	1.70247
0.50	3.54437	2.10227	1.87662	1.68634	1.60187
0.70	3.43767	2.03877	1.82201	1.63985	1.55919
0.90	3.38389	2.00924	1.79764	1.62022	1.54180
1.00	3.36822	2.00187	1.79206	1.61631	1.53868
2.00	3.37657	2.04139	1.83856	1.66937	1.59486
5.00	3.77440	2.43823	2.23506	2.06548	1.99077
7.00	4.08811	2.74611	2.54144	2.37038	2.29493
9.00	4.41019	3.06346	2.85756	2.68530	2.60925

All the results are obtained with a velocity discretization of N=30.

[3] Barichello, L. B., & Siewert, C. E. (1999). A discrete-ordinates solution for Poiseuille flow in a plane channel. *Zeitschrift für angewandte Mathematik und Physik ZAMP*, *50*(6), 972-981.

Poiseuille Flow Results

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Flow rate $Q(a)$

Finally, we pushed the code increasing the discretization of space, velocity, and number of Chebyshev Polynomials to reach the 7 digits benchmarks published by Ganapol [6].

Parameters used to compute the flow rate $Q(a)$ for each channel width.

$2a$	N	M	m	comp. time [s]
0.05	69	100	34	1.35
0.10	59	120	54	2.39
0.30	35	140	60	0.78
0.50	30	140	60	0.51
0.70	30	140	60	0.52
0.90	30	200	67	0.81
1.00	30	200	74	0.99
2.00	24	400	90	1.30
5.00	24	700	130	4.31
7.00	24	900	150	6.92
9.00	24	1400	150	10.12

TABLE 3. The flow rate $Q(a)$ for Ganapol digits [6]

$2a$	$\alpha = 0.50$	$\alpha = 0.80$	$\alpha = 0.88$	$\alpha = 0.96$	$\alpha = 1.00$
0.05	5.2232964	3.0897113	2.7383403	2.4373544	2.3022564
0.10	4.5564062	2.7077408	2.4060457	2.1482414	2.0327143
0.30	3.7784723	2.2447708	2.0010675	1.7945088	1.7024740
0.50	3.5443709	2.1022657	1.8766202	1.6863424	1.6018742
0.70	3.4376693	2.0387670	1.8220109	1.6398495	1.5591860
0.90	3.3838869	2.0092408	1.7976360	1.6202230	1.5417996
1.00	3.3682182	2.0018669	1.7920590	1.6163124	1.5386785
2.00	3.3765738	2.0413852	1.8385632	1.6693655	1.5948569
5.00	3.7744018	2.4382339	2.2350591	2.0654781	1.9907674
7.00	4.0881078	2.7461124	2.5414362	2.3703751	2.2949322
9.00	4.4101902	3.0634644	2.8575645	2.6852950	2.6092536

[6] Ganapol, B. D. (2016, November). Poiseuille channel flow by adding and doubling. In *AIP Conference Proceedings* (Vol. 1786, No. 1, p. 070009). AIP Publishing LLC.

Contents

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Thermal Creep Flow in a plane channel

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Following the formulation proposed by Ganapol [7], and taking some moments of the linearized BGK equation, the problem to be solved is the following:

$$c_x K_0 + \frac{1}{2} R_z + \frac{1}{2} K_z \left(c^2 + \frac{3}{2} \right) + c_x \frac{\partial}{\partial x} Z(x, c_x) + \lambda_0 Z(x, c_x) = \lambda_0 \pi^{-1/2} \int_{-\infty}^{\infty} e^{-c_x^2} Z(x, c_x) dc_x$$

for $x \in \left(-\frac{d}{2}, \frac{d}{2}\right)$ and $c_x \in (-\infty, \infty)$, with the following reflecting boundary conditions:

$$\begin{cases} Z\left(-\frac{d}{2}, c_x\right) = \alpha u_w + (1-\alpha) Z\left(-\frac{d}{2}, -c_x\right) \\ Z\left(\frac{d}{2}, -c_x\right) = \alpha u_w + (1-\alpha) Z\left(\frac{d}{2}, c_x\right) \end{cases}$$

for $c_x \in (0, \infty)$. Here, *d* is the channel thickness, u_w is the wall velocity, R_z and K_z are gradients in the flow direction z, K is the scattering kernel, K_0 is proportional to K, λ_0 is proportional to the frequency of collisions between the atoms, *x* is the spatial variable, $\alpha \in (0,1]$ is the accomodation coefficient, and the moment $Z(x, c_x)$ is:

$$Z(x, c_x) = \pi^{-1} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-\left(c_y^2 + c_z^2\right)^2} c_z h\left(x, c_x, c_y, c_z\right) dc_y dc_z$$

Where $\left(c_x, c_y, c_z\right)$ are the three components of the molecular velocity and *h* is a perturbation from Maxwell distribution.

[7] Barry D. Ganapol, 1D thermal creep channel flow in the BGK approximation by adding and doubling, Annals of Nuclear Energy, 2019

Thermal Creep Flow Results

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Microscopic velocity profile $q(\tau)$

Table 1: The macroscopic velocity profile $q(a, \alpha)$ for $\tau = 0$. All the digits match the benchmark published by Ganapol

$2a$	$\alpha = 0.50$	$\alpha = 0.80$	$\alpha = 0.88$	$\alpha = 0.96$	$\alpha = 1.00$
0.05	4.2225003e-02	2.8228521e-02	2.5723898e-02	2.3529621e-02	2.2529767e-02
0.1	6.5095538e-02	4.5719362e-02	4.2146466e-02	3.8989742e-02	3.7543105e-02
0.3	1.1876639e-01	9.2674511e-02	8.7524944e-02	8.2887055e-02	8.0734083e-02
0.5	1.5048508e-01	1.2482013e-01	1.1954218e-01	1.1473143e-01	1.1248014e-01
0.7	1.7295120e-01	1.4982556e-01	1.4492927e-01	1.4042737e-01	1.3830819e-01
0.9	1.9016554e-01	1.7032627e-01	1.6603492e-01	1.6206351e-01	1.6018580e-01
1.0	1.9742092e-01	1.7932563e-01	1.7537848e-01	1.7171628e-01	1.6998179e-01
2.0	2.4390839e-01	2.4205320e-01	2.4170175e-01	2.4139906e-01	2.4126448e-01
5.0	2.9311382e-01	3.1685309e-01	3.2293936e-01	3.2892781e-01	3.3188614e-01
7.0	3.0479340e-01	3.3544233e-01	3.4335590e-01	3.5116476e-01	3.5503062e-01
9.0	3.1086362e-01	3.4515054e-01	3.5403270e-01	3.6280930e-01	3.6715870e-01

Table 2: The macroscopic velocity profile $q(a, \alpha)$ for $\tau = a$. All the digits match the benchmark published by Ganapol

$2a$	$\alpha = 0.50$	$\alpha = 0.80$	$\alpha = 0.88$	$\alpha = 0.96$	$\alpha = 1.00$
0.05	3.9116032e-02	2.3909939e-02	2.1108934e-02	1.8626644e-02	1.7485627e-02
0.1	5.8802435e-02	3.7008351e-02	3.2848608e-02	2.9123484e-02	2.7398906e-02
0.3	1.0041326e-01	6.7026531e-02	6.0133956e-02	5.3818715e-02	5.0849454e-02
0.5	1.2148165e-01	8.3735395e-02	7.5575613e-02	6.7996314e-02	6.4399698e-02
0.7	1.3456419e-01	9.4790899e-02	8.5911823e-02	7.7583115e-02	7.3604566e-02
0.9	1.4345748e-01	1.0267633e-01	9.3351726e-02	8.4539468e-02	8.0308472e-02
1.0	1.4689594e-01	1.0581901e-01	9.6334414e-02	8.7343031e-02	8.3016855e-02
2.0	1.6430194e-01	1.2275654e-01	1.1261926e-01	1.0283132e-01	9.8061828e-02
5.0	1.7374607e-01	1.3300605e-01	1.2271306e-01	1.1264794e-01	1.0769889e-01
7.0	1.7467018e-01	1.3408240e-01	1.2379106e-01	1.1371337e-01	1.0875303e-01
9.0	1.7495630e-01	1.3442089e-01	1.2413143e-01	1.1405110e-01	1.0908783e-01

Flow rate $Q(a, \alpha)$

Table 3: The flow rate $Q(a, \alpha)$. All the digits match the benchmark published by Ganapol

$2a$	$\alpha = 0.50$	$\alpha = 0.80$	$\alpha = 0.88$	$\alpha = 0.96$	$\alpha = 1.00$
0.05	-1.6536888	-1.0808651	-9.7755253e-01	-8.8675895e-01	-8.4528926e-01
0.1	-1.2664416	-8.6598047e-01	-7.9142819e-01	-7.2531232e-01	-6.9492716e-01
0.3	-7.5808236e-01	-5.7120721e-01	-5.3382143e-01	-4.9997357e-01	-4.8419925e-01
0.5	-5.7057229e-01	-4.5516639e-01	-4.3103829e-01	-4.0890573e-01	-3.9849928e-01
0.7	-4.6496656e-01	-3.8645813e-01	-3.6950994e-01	-3.5380980e-01	-3.4637809e-01
0.9	-3.9538369e-01	-3.3924285e-01	-3.2681934e-01	-3.1522021e-01	-3.0970011e-01
1.0	-3.6854346e-01	-3.2050490e-01	-3.0976296e-01	-2.9970005e-01	-2.9489992e-01
2.0	-2.2450462e-01	-2.1292032e-01	-2.1016135e-01	-2.0752116e-01	-2.0624288e-01
5.0	-1.0753220e-01	-1.1165695e-01	-1.1271161e-01	-1.1374814e-01	-1.1425975e-01
7.0	-8.0362907e-02	-8.5334804e-02	-8.6615422e-02	-8.7877804e-02	-8.8502282e-02
9.0	-6.4219081e-02	-6.9077203e-02	-7.0332976e-02	-7.1572696e-02	-7.2186641e-02

$2a$	N	M	m	comp. time [s]
0.05	69	100	34	1.35
0.10	59	120	54	2.39
0.30	35	140	60	0.78
0.50	30	140	60	0.51
0.70	30	140	60	0.52
0.90	30	200	67	0.81
1.00	30	200	74	0.99
2.00	24	400	90	1.30
5.00	24	700	130	4.31
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9.00	24	1400	150	10.12

Parameters used to compute the flow rate $Q(a)$ for each channel width.

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Conclusions and Outlooks

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- The RGD problems are solved via TFC
  - The accuracy of the results is compared with the published benchmarks
  - Straightforward implementation

- TFC has also been applied to Radiative Transfer Equations (RTE)
  - Isotropic problems
  - Anisotropic Problems

- Future developments (via X-TFC)
  - To solve the 3D time-dependent RGD problems
  - To solve the 3D time-dependent RTE
  - To solve Neutron Transport Equations

Thanks for the attention

Questions time

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