# Singular behavior of a rarefied gas on a planar boundary

Shigeru Takata (髙田 滋)

Department of Mechanical Engineering and Science
Kyoto University, Japan

takata.shigeru.4a@kyoto-u.ac.jp

*Joint work with Hitoshi Funagane*

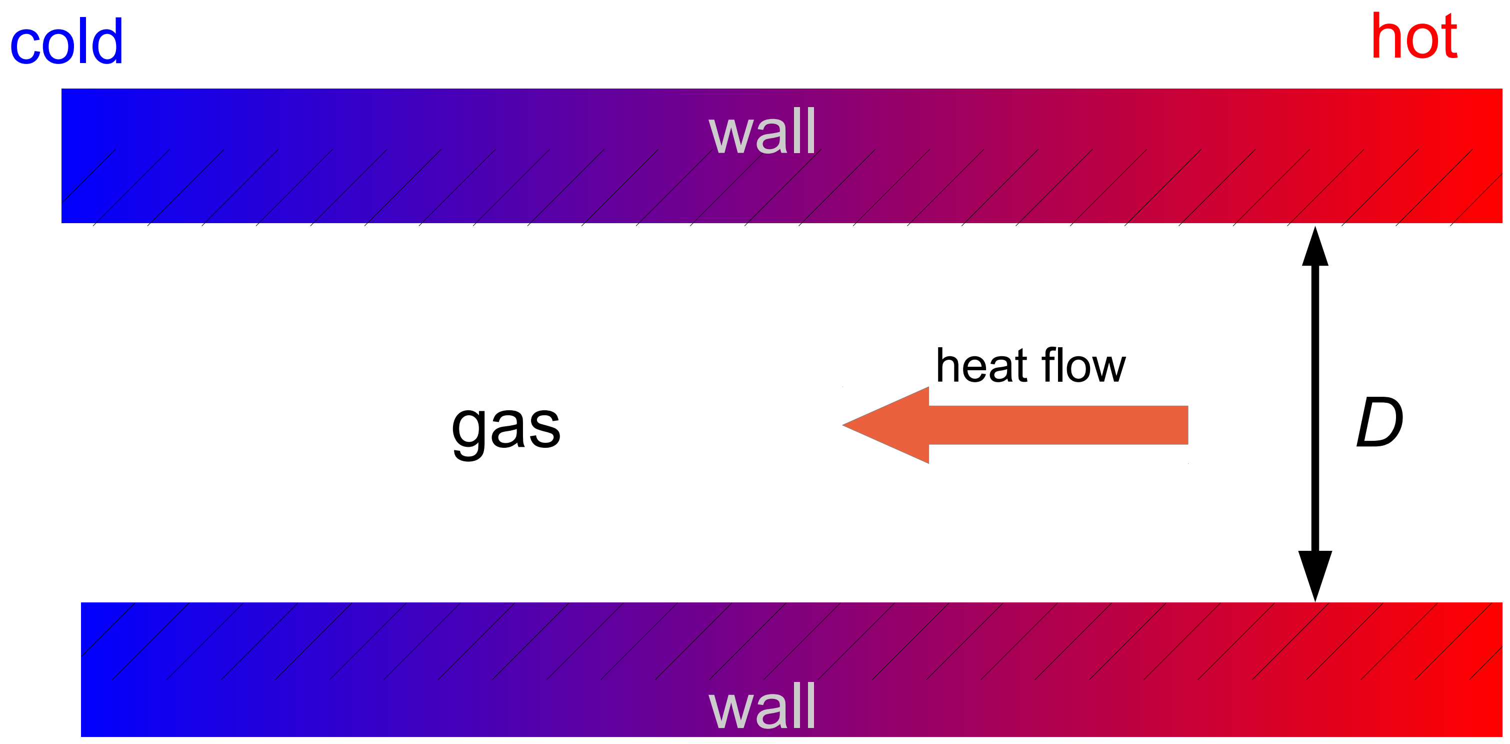
*Also appreciation for helpful discussions to*
*Kazuo Aoki, Masashi Oishi (Kyoto Univ., Japan)*
*Tai-Ping Liu, I-Kun Chen (Academia Sinica, Taipei)*

# Contents

- Introduction
- Setting of a specific problem
- Macroscopic singularity in physical space
- Microscopic singularity in molecular velocity
- Damping model and the source of macroscopic singularity
- Conclusion

# Contents

# Introduction
## (with a specific example: *thermal transpiration*)

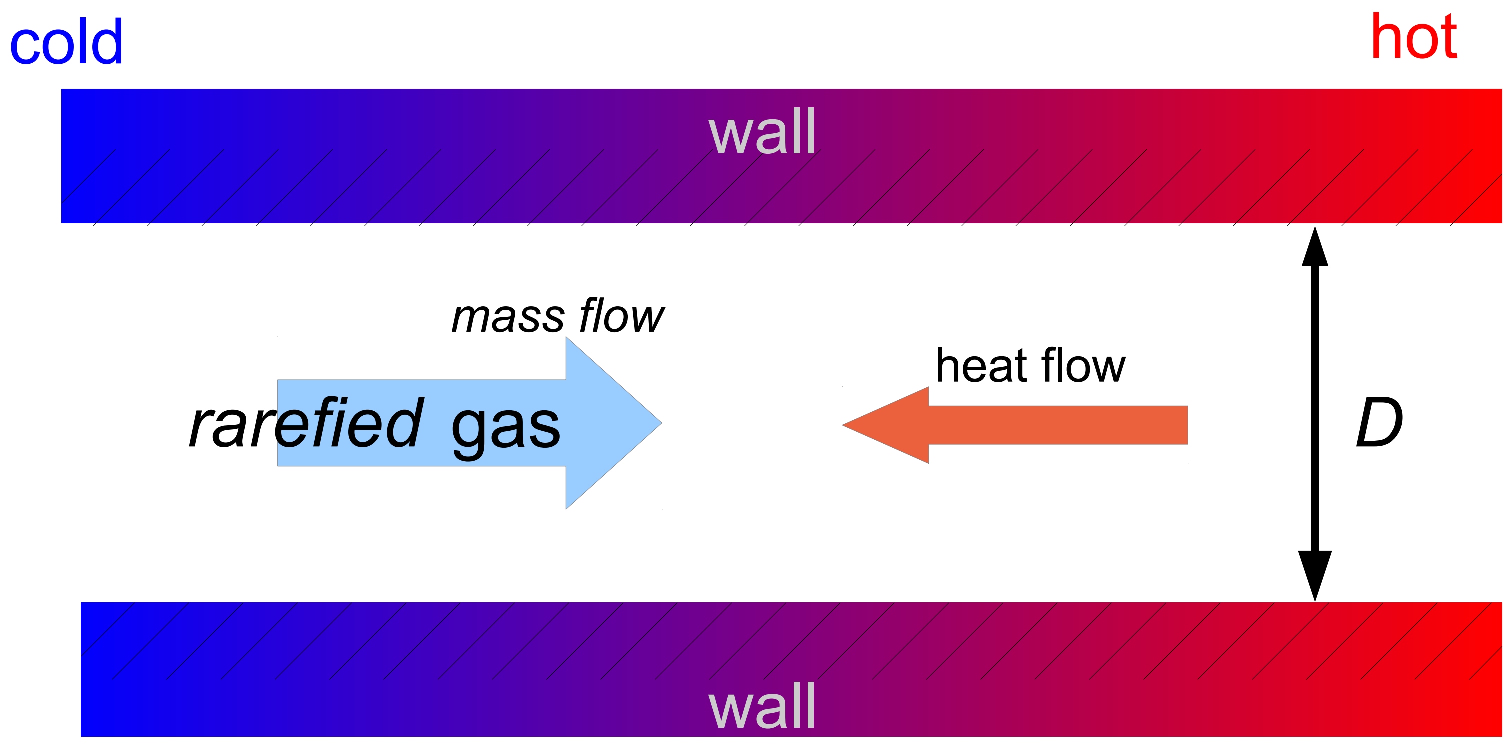



$$\text{rarefied gas: mean free path } \ell \sim D$$

$$k = \frac{\sqrt{\pi}}{2}\frac{\ell}{D}: \text{ “Knudsen number”}$$

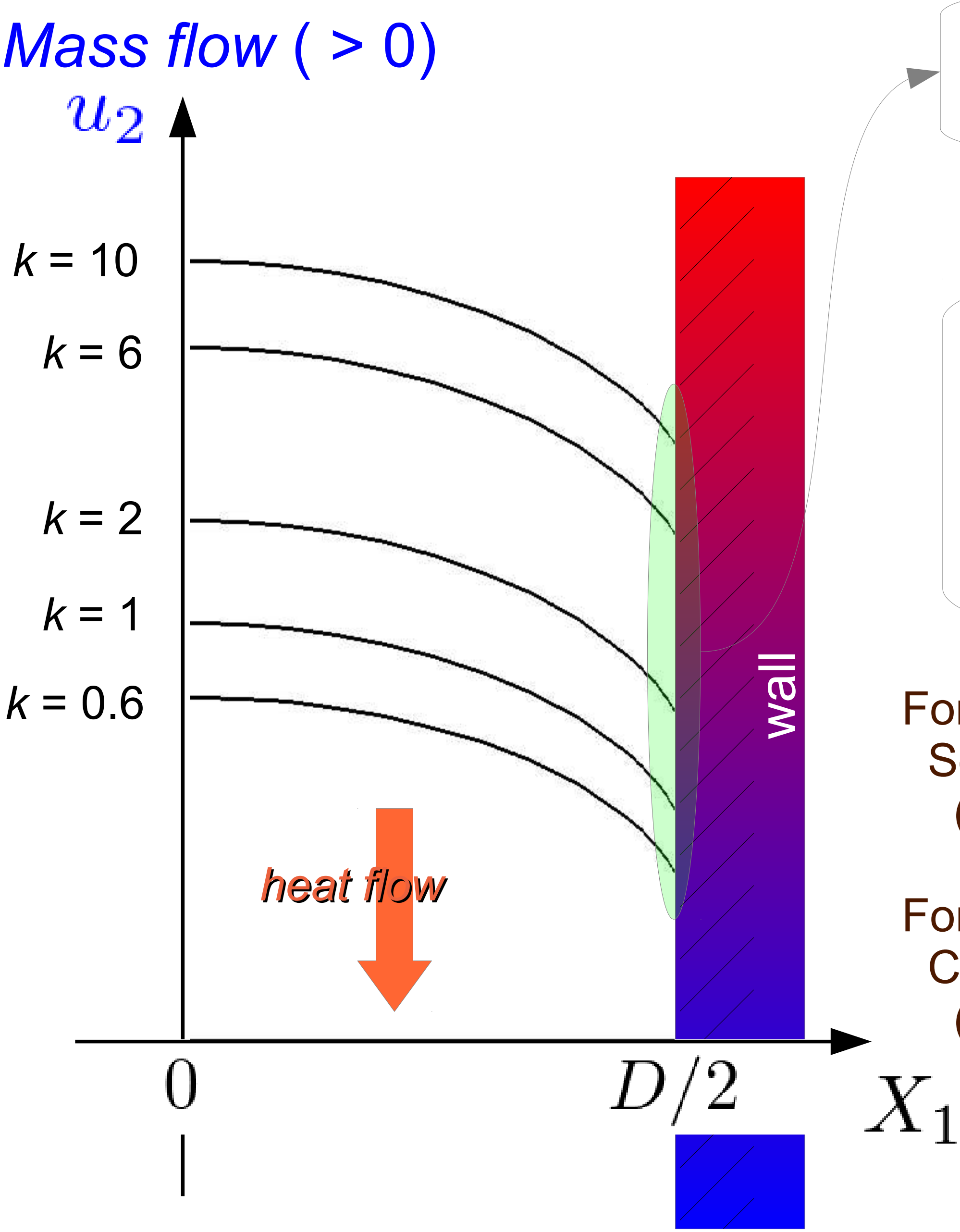
# Introduction

## (with a specific example: *thermal transpiration*)




$$\text{rarefied gas: mean free path } \ell \sim D$$

$$k = \frac{\sqrt{\pi}}{2}\frac{\ell}{D}: \text{ "Knudsen number"}$$




Present concern

$y$: distance from the wall

$$u_2(y) - u_2(0) \propto y \ln y$$

$$\Leftrightarrow \quad \frac{du_2}{dy} \propto \ln y \ (\to \infty \text{ as } y \to 0)$$

For small *k* (near continuum limit)
Sone (1969, 2007)
(structure of the Knudsen layer
in the generalized slip-flow theory; BKW or BGK)
For large *k* (near free molecular limit)
Chen-Liu-T. (preprint)
(math. proof for the hard-sphere gas)

***Logarithmic divergence is expected, irrespective of the Knudsen number***

cf) *Lilly & Sader* (2007, 2008)
empirical arguments by a power-law
fitting to numerical data

# Purpose of research

*to confirm*

- the same logarithmic gradient divergence occurs *irrespective of the Knudsen number*

*to show*

- the above spatial singularity of weighted average of VDF induces *another logarithmic gradient divergence in molecular velocity* on the boundary

*to identify*

- *the origin of the above singularities, proposing a simple damping model*

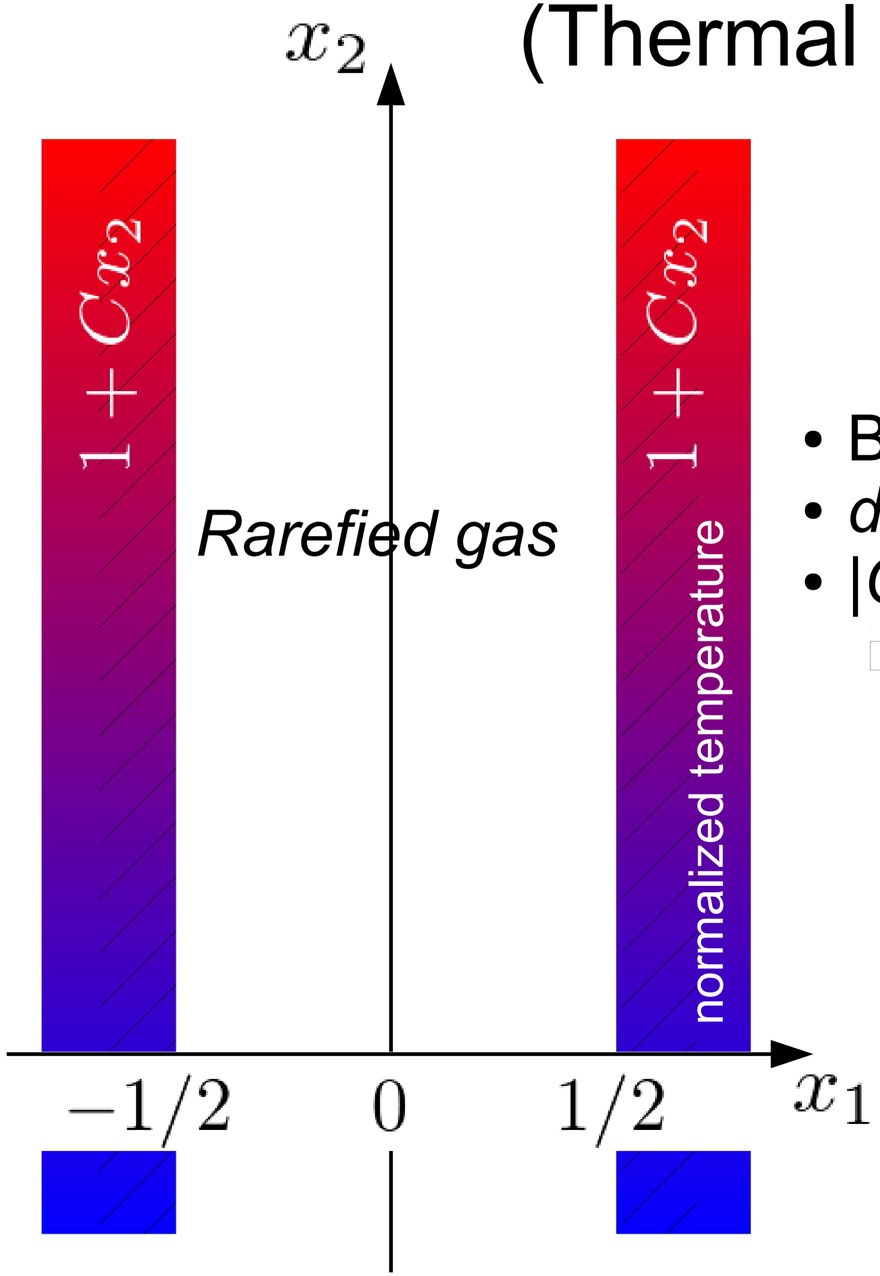
*Method: analysis + numerics*

These features should be observed *generally* *on a planar boundary,* though we deal with only the thermal transpiration here.

# Contents

- Introduction
- Setting of a specific problem
- Macroscopic singularity in physical space
- Microscopic singularity in molecular velocity
- Damping model and the source of macroscopic singularity
- Conclusion

# Setting of a specific problem
## (Thermal transpiration)

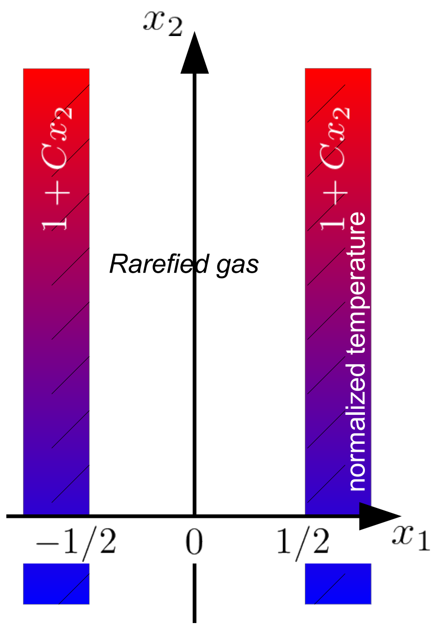



Assumptions

- Boltzmann equation (*hard-sphere gas*)
- *diffuse reflection* boundary condition
- $|C| << 1$

  ⇨ Linearization around a reference absolute Maxwellian

*Then formulate the problem for the perturbation from a local Maxwellain with the wall temperature and the uniform reference pressure*




$$\zeta_1 \frac{\partial \phi}{\partial x_1} = -\frac{1}{k}\nu(|\boldsymbol{\zeta}|)\phi + \frac{1}{k}K[\phi] - \zeta_2(|\boldsymbol{\zeta}|^2 - \frac{5}{2}),$$

$$\text{b.c.} \quad \phi = 0, \quad \zeta_1 \lessgtr 0, \ x_1 = \pm\frac{1}{2}.$$

$\phi(x_1, \boldsymbol{\zeta})$: perturbation of VDF (divided by $C$)

$\boldsymbol{\zeta}$: dimensionless molecular velocity

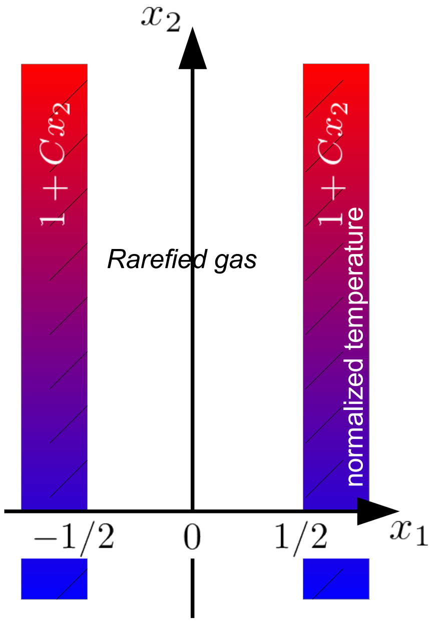
$E(|\boldsymbol{\zeta}|) = \pi^{-3/2}\exp(-|\boldsymbol{\zeta}|^2)$: normalized reference absolute Maxwellian

Hard-sphere gas

$$\nu(|\boldsymbol{\zeta}|) = \frac{1}{2\sqrt{2}}\left(\exp(-|\boldsymbol{\zeta}|^2) + (2|\boldsymbol{\zeta}| + \frac{1}{|\boldsymbol{\zeta}|})\int_0^{|\boldsymbol{\zeta}|}\exp(-t^2)dt\right),$$

$$K[\Phi] = \int \kappa(\boldsymbol{\xi}, \boldsymbol{\zeta})\Phi(\boldsymbol{\xi})E(|\boldsymbol{\xi}|)d\boldsymbol{\xi},$$

$$\kappa(\boldsymbol{\xi}, \boldsymbol{\zeta}) = \frac{\sqrt{\pi}}{\sqrt{2}}\frac{1}{|\boldsymbol{\xi} - \boldsymbol{\zeta}|}\exp\left(\frac{|\boldsymbol{\xi} \times \boldsymbol{\zeta}|^2}{|\boldsymbol{\xi} - \boldsymbol{\zeta}|^2}\right) - \frac{\sqrt{\pi}}{2\sqrt{2}}|\boldsymbol{\xi} - \boldsymbol{\zeta}|,$$




$$\zeta_1 \frac{\partial \phi}{\partial x_1} = -\frac{1}{k}\nu(|\boldsymbol{\zeta}|)\phi + \frac{1}{k}K[\phi] - \zeta_2(|\boldsymbol{\zeta}|^2 - \frac{5}{2}),$$

$$\text{b.c.} \quad \phi = 0, \quad \zeta_1 \lessgtr 0, \ x_1 = \pm\frac{1}{2}.$$

NOTE 1

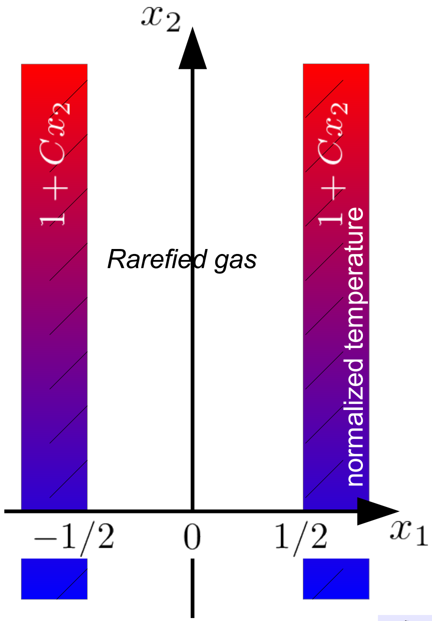
This problem can be solved formally as

$$\phi = \int_{\mp 1/2}^{x_1} \frac{1}{k\zeta_1} \exp\left(-\frac{\nu(|\boldsymbol{\zeta}|)}{k|\zeta_1|}|x_1 - s|\right) K[\phi](s, \boldsymbol{\zeta}) ds + \phi_0, \quad \zeta_1 \gtrless 0,$$

where

$$\phi_0 = -\frac{k}{\nu(|\boldsymbol{\zeta}|)}[1 - \exp\left(-\frac{\nu(|\boldsymbol{\zeta}|)}{k\zeta_1}(x_1 \pm \frac{1}{2})\right)]I, \quad \zeta_1 \gtrless 0,$$

$$I = \zeta_2(|\boldsymbol{\zeta}|^2 - \frac{5}{2}).$$




$$\zeta_1 \frac{\partial \phi}{\partial x_1} = -\frac{1}{k}\nu(|\boldsymbol{\zeta}|)\phi + \frac{1}{k}K[\phi] - \zeta_2(|\boldsymbol{\zeta}|^2 - \frac{5}{2}),$$

$$\text{b.c.} \quad \phi = 0, \quad \zeta_1 \lessgtr 0, \ x_1 = \pm\frac{1}{2}.$$

## NOTE 2

$\phi/\zeta_2$ can be sought as a function of three variables $(x_1, \zeta_1, |\boldsymbol{\zeta}|)$ or $(x_1, \mu, \zeta)$ by using new coordinates

$$\zeta = |\boldsymbol{\zeta}|, \ \mu = \zeta_1/\zeta, \ \tan\varphi = \zeta_3/\zeta_2.$$

All the moments of $\phi$ up to the second order vanish except for the mass flow $u_2$ in the $x_2$-direction

$$u_2[\phi] = \int \zeta_2 \phi E(|\boldsymbol{\zeta}|) d\boldsymbol{\zeta}$$

$$E(|\boldsymbol{\zeta}|) = \pi^{-3/2}\exp(-|\boldsymbol{\zeta}|^2)$$

# Contents

- Introduction
- Setting of a specific problem
- Macroscopic singularity in physical space
- Microscopic singularity in molecular velocity
- Damping model and the source of macroscopic singularity
- Conclusion

# Gradient divergence of $u_2$: Basic structure

$$\zeta_1 \frac{\partial \phi}{\partial x_1} = -\frac{1}{k}\nu(|\boldsymbol{\zeta}|)\phi + \frac{1}{k}K[\phi] - \zeta_2(|\boldsymbol{\zeta}|^2 - \frac{5}{2}),$$

$$\text{b.c.} \quad \phi = 0, \quad \zeta_1 \lesseqgtr 0, \ x_1 = \pm\frac{1}{2}.$$

This problem can be solved formally as

$$\phi = \int_{\mp 1/2}^{x_1} \frac{1}{k\zeta_1} \exp\left(-\frac{\nu(|\boldsymbol{\zeta}|)}{k|\zeta_1|}|x_1 - s|\right) K[\phi](s, \boldsymbol{\zeta})ds + \phi_0, \quad \zeta_1 \gtrless 0,$$

where

$$\phi_0 = -\frac{k}{\nu(|\boldsymbol{\zeta}|)}[1 - \exp\left(-\frac{\nu(|\boldsymbol{\zeta}|)}{k\zeta_1}(x_1 \pm \frac{1}{2})\right)]I, \quad \zeta_1 \gtrless 0,$$

$$I = \zeta_2(|\boldsymbol{\zeta}|^2 - \frac{5}{2}).$$

# Gradient divergence of $u_2$: Basic structure

$$\zeta_1 \frac{\partial \phi}{\partial x_1} = -\frac{1}{k}\nu(|\boldsymbol{\zeta}|)\phi + \frac{1}{k}K[\phi] - \zeta_2(|\boldsymbol{\zeta}|^2 - \frac{5}{2}),$$

$$\text{b.c.} \quad \phi = 0, \quad \zeta_1 \lessgtr 0, \ x_1 = \pm\frac{1}{2}.$$

This problem can be solved formally as

$$\phi = \int_{\mp 1/2}^{x_1} \frac{1}{k\zeta_1} \exp\left(-\frac{\nu(|\boldsymbol{\zeta}|)}{k|\zeta_1|}|x_1 - s|\right) K[\phi](s, \boldsymbol{\zeta}) ds + \phi_0, \quad \zeta_1 \gtrless 0,$$

where

$$\phi_0 = -\frac{k}{\nu(|\boldsymbol{\zeta}|)}[1 - \exp\left(-\frac{\nu(|\boldsymbol{\zeta}|)}{k\zeta_1}(x_1 \pm \frac{1}{2})\right)]I, \quad \zeta_1 \gtrless 0,$$

$$I = \zeta_2(|\boldsymbol{\zeta}|^2 - \frac{5}{2}).$$

$$u_2[\phi_0] = \int \zeta_2 \phi_0 E d\boldsymbol{\zeta}$$

$$(x_1 \pm 1/2) \ln |x_1 \pm 1/2|$$

$$= \frac{k}{6\sqrt{\pi}} \sum_{i=+,-} \int_0^\infty \frac{\zeta^4}{\nu(\zeta)} (\zeta^2 - \frac{5}{2})(a_i^2 - 6) a_i \mathrm{Ei}(1, a_i) \exp(-\zeta^2) d\zeta$$

$$+ \frac{k}{6\sqrt{\pi}} \sum_{i=+,-} \int_0^\infty \frac{\zeta^4}{\nu(\zeta)} (\zeta^2 - \frac{5}{2})(4 + a_i - a_i^2) \exp(-a_i - \zeta^2) d\zeta$$

$$- \frac{4k}{3\sqrt{\pi}} \int_0^\infty \frac{\zeta^4}{\nu(\zeta)} (\zeta^2 - \frac{5}{2}) \exp(-\zeta^2) d\zeta,$$

where

$$a_\pm = \frac{\nu(\zeta)}{k\zeta} |x_1 \pm \frac{1}{2}|, \quad \mathrm{Ei}(1, a > 0) = \int_1^\infty \frac{1}{x} \exp(-ax) dx.$$

$$\mathrm{Ei}(1, a > 0) = -\gamma - \ln a + e^{-a} \sum_{n=1}^\infty \frac{1}{n!} \left( \sum_{r=1}^\infty \frac{1}{r} \right) a^n, \quad (\gamma\text{: Euler's constant}),$$

# Gradient divergence of $u_2$: Basic structure

$$\zeta_1 \frac{\partial \phi}{\partial x_1} = -\frac{1}{k}\nu(|\boldsymbol{\zeta}|)\phi + \frac{1}{k}K[\phi] - \zeta_2(|\boldsymbol{\zeta}|^2 - \frac{5}{2}),$$

$$\text{b.c.} \quad \phi = 0, \quad \zeta_1 \lessgtr 0, \; x_1 = \pm\frac{1}{2}.$$

This problem can be solved formally as

$$\phi = \int_{\mp 1/2}^{x_1} \frac{1}{k\zeta_1} \exp\left(-\frac{\nu(|\boldsymbol{\zeta}|)}{k|\zeta_1|}|x_1 - s|\right) K[\phi](s,\boldsymbol{\zeta}) ds + \phi_0, \quad \zeta_1 \gtrless 0,$$

where

$$\phi_0 = -\frac{k}{\nu(|\boldsymbol{\zeta}|)}[1 - \exp\left(-\frac{\nu(|\boldsymbol{\zeta}|)}{k\zeta_1}(x_1 \pm \frac{1}{2})\right)]I, \quad \zeta_1 \gtrless 0,$$

$$I = \zeta_2(|\boldsymbol{\zeta}|^2 - \frac{5}{2}).$$

# Gradient divergence of $u_2$: Basic structure

$$\zeta_1 \frac{\partial \phi}{\partial x_1} = -\frac{1}{k}\nu(|\boldsymbol{\zeta}|)\phi + \frac{1}{k}K[\phi] - \zeta_2(|\boldsymbol{\zeta}|^2 - \frac{5}{2}),$$

$$\text{b.c.} \quad \phi = 0, \quad \zeta_1 \lessgtr 0, \ x_1 = \pm\frac{1}{2}.$$

$$\phi_0 = \int_{\mp\frac{1}{2}}^{x_1} \frac{1}{\zeta_1} \exp\left(-\frac{\nu}{k|\zeta_1|}|x_1 - s|\right) I ds$$

This problem can be solved f

$$\phi = \int_{\mp 1/2}^{x_1} \frac{1}{k\zeta_1} \exp\left(-\frac{\nu(|\boldsymbol{\zeta}|)}{k|\zeta_1|}|x_1 - s|\right) K[\phi](s, \boldsymbol{\zeta}) ds + \phi_0, \quad \zeta_1 \gtrless 0,$$

where

$$\phi_0 = -\frac{k}{\nu(|\boldsymbol{\zeta}|)}[1 - \exp\left(-\frac{\nu(|\boldsymbol{\zeta}|)}{k\zeta_1}(x_1 \pm \frac{1}{2})\right)]I, \quad \zeta_1 \gtrless 0,$$

$$I = \zeta_2(|\boldsymbol{\zeta}|^2 - \frac{5}{2}).$$

# Gradient divergence of $u_2$: Basic structure

$$\zeta_1 \frac{\partial \phi}{\partial x_1} = -\frac{1}{k}\nu(|\boldsymbol{\zeta}|)\phi + \frac{1}{k}K[\phi] - \zeta_2(|\boldsymbol{\zeta}|^2 - \frac{5}{2}),$$

$$\text{b.c.} \quad \phi = 0, \quad \zeta_1 \lessgtr 0, \; x_1 = \pm\frac{1}{2}.$$

$$\phi_0 = \int_{\mp\frac{1}{2}}^{x_1} \frac{1}{\zeta_1} \exp\left(-\frac{\nu}{k|\zeta_1|}|x_1 - s|\right) I ds$$

This problem can be solved f

$$\phi = \int_{\mp 1/2}^{x_1} \frac{1}{k\zeta_1} \exp\left(-\frac{\nu(|\boldsymbol{\zeta}|)}{k|\zeta_1|}|x_1 - s|\right) K[\phi](s, \boldsymbol{\zeta}) ds + \phi_0, \quad \zeta_1 \gtrless 0,$$

where

$$\phi_0 = -\frac{k}{\nu(|\boldsymbol{\zeta}|)}[1 - \exp\left(-\frac{\nu(|\boldsymbol{\zeta}|)}{k\zeta_1}(x_1 \pm \frac{1}{2})\right)]I, \quad \zeta_1 \gtrless 0,$$

$$I = \zeta_2(|\boldsymbol{\zeta}|^2 - \frac{5}{2}).$$

# Gradient divergence of $u_2$: Basic structure

$$\zeta_1 \frac{\partial \phi}{\partial x_1} = -\frac{1}{k}\nu(|\boldsymbol{\zeta}|)\phi + \frac{1}{k}K[\phi] - \underline{\zeta_2(|\boldsymbol{\zeta}|^2 - \frac{5}{2})},$$

$$\text{b.c.} \quad \phi = 0, \quad \zeta_1 \lessgtr 0, \ x_1 = \pm\frac{1}{2}.$$

This problem can be solved f

$$\phi_0 = \int_{\mp\frac{1}{2}}^{x_1} \frac{1}{\zeta_1} \exp\Big(-\frac{\nu}{k|\zeta_1|}|x_1 - s|\Big) I ds$$

$$\phi = \int_{\mp 1/2}^{x_1} \frac{1}{k\zeta_1} \exp\left(-\frac{\nu(|\boldsymbol{\zeta}|)}{k|\zeta_1|}|x_1 - s|\right) K[\phi](s, \boldsymbol{\zeta}) ds + \phi_0, \quad \zeta_1 \gtrless 0,$$

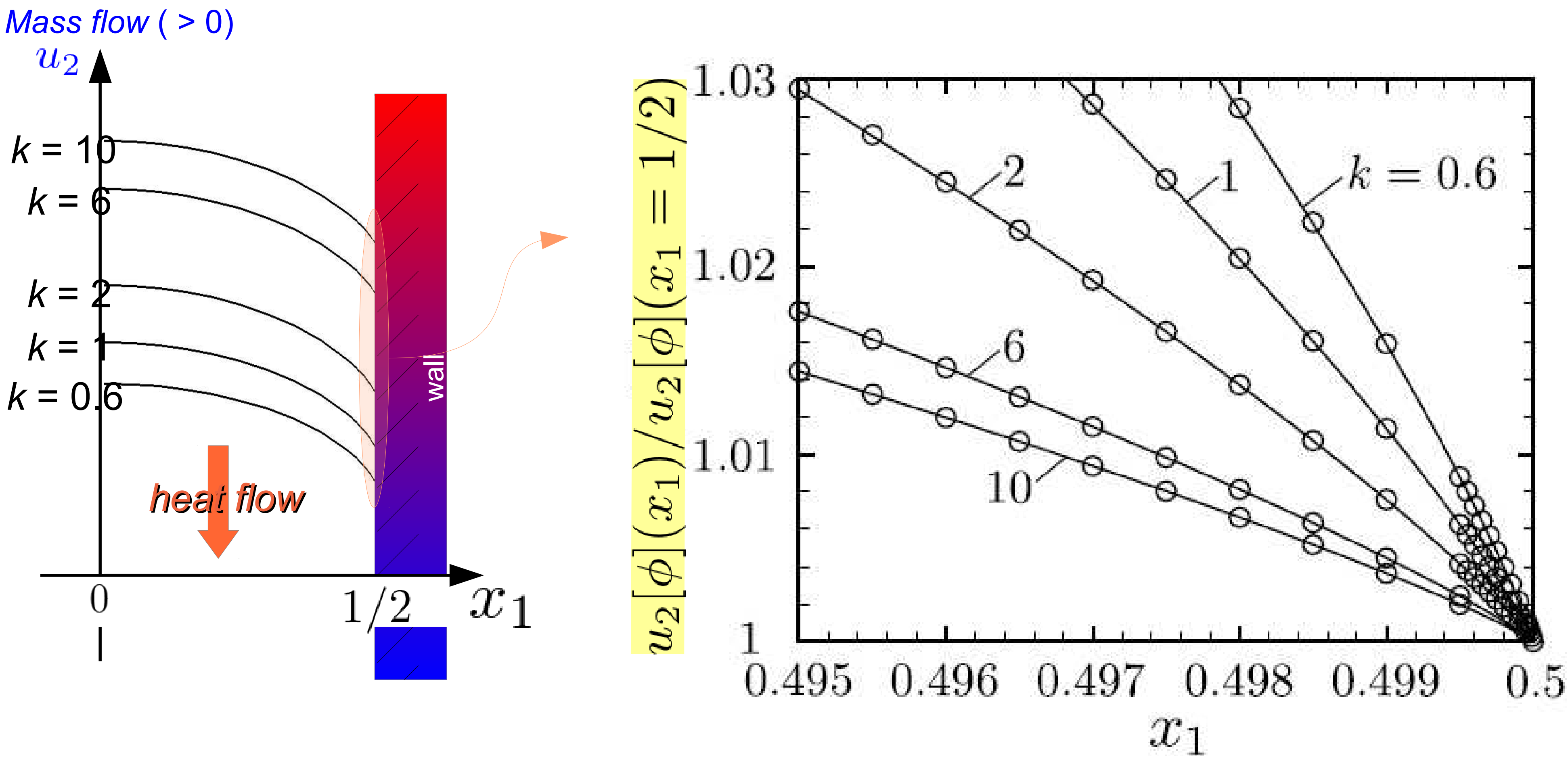
where

$$\underline{\phi_0 = -\frac{k}{\nu(|\boldsymbol{\zeta}|)}[1 - \exp\left(-\frac{\nu(|\boldsymbol{\zeta}|)}{k\zeta_1}(x_1 \pm \frac{1}{2})\right)]I}, \quad \zeta_1 \gtrless 0,$$

$$I = \zeta_2(|\boldsymbol{\zeta}|^2 - \frac{5}{2}).$$

Since *the structure is the same*, the same singular nature is expected from the *K* part (as far as the *K* behaves well).

# Mass flow profile near the boundary

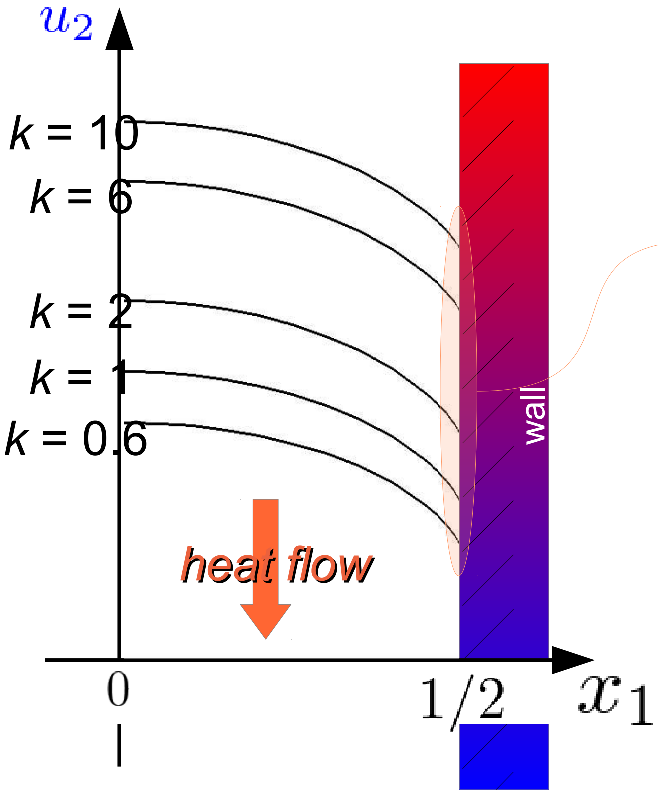


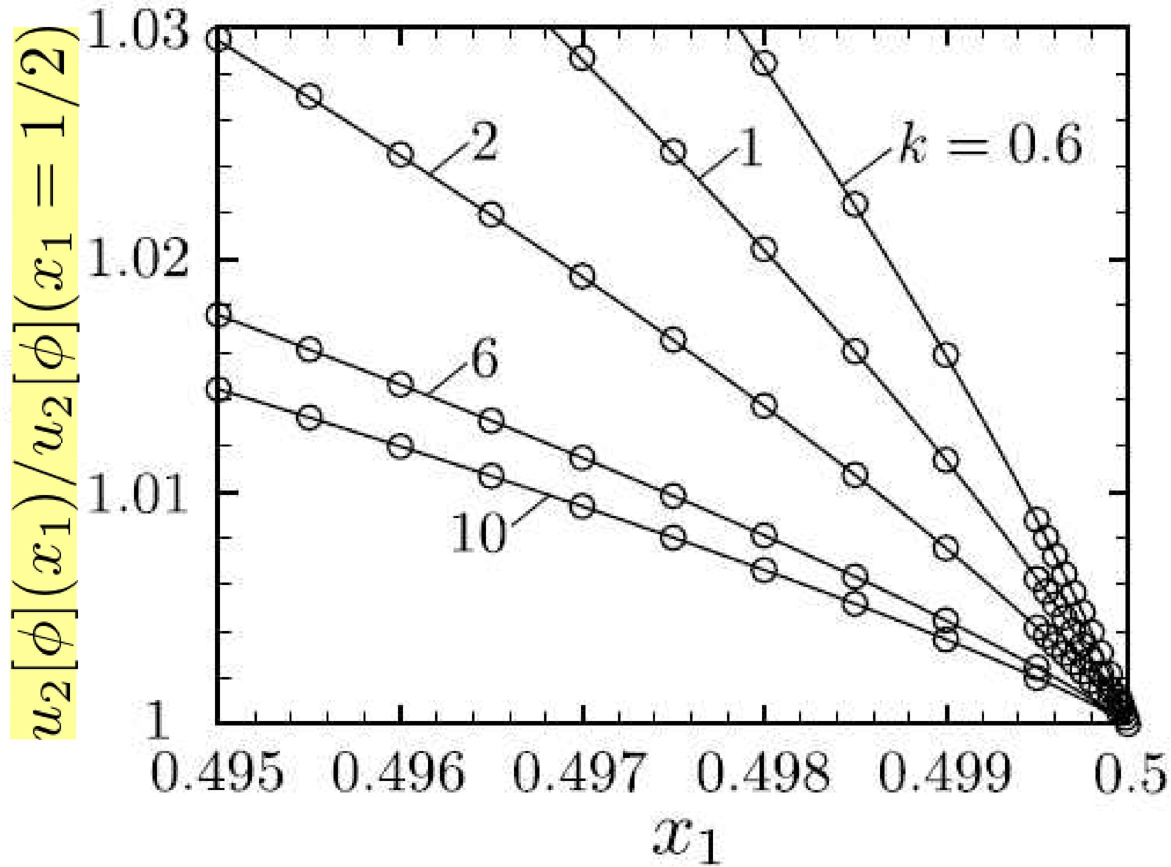

open circle: present numerical result

solid line: least mean square approx.

$$a + b(1/2 - x_1)\ln(1/2 - x_1) + c(1/2 - x_1)$$

# Mass flow profile near the boundary




| $k$ | $a$ | $b$ | $c$ |
|---|---|---|---|
| 10 | 0.3468 | -0.1640 | 0.1304 |
| 6 | 0.2940 | -0.1728 | 0.1196 |
| 2 | 0.1907 | -0.2003 | 0.0603 |
| 1 | 0.1337 | -0.2221 | -0.0159 |
| 0.6 | 0.0969 | -0.2378 | -0.106 |

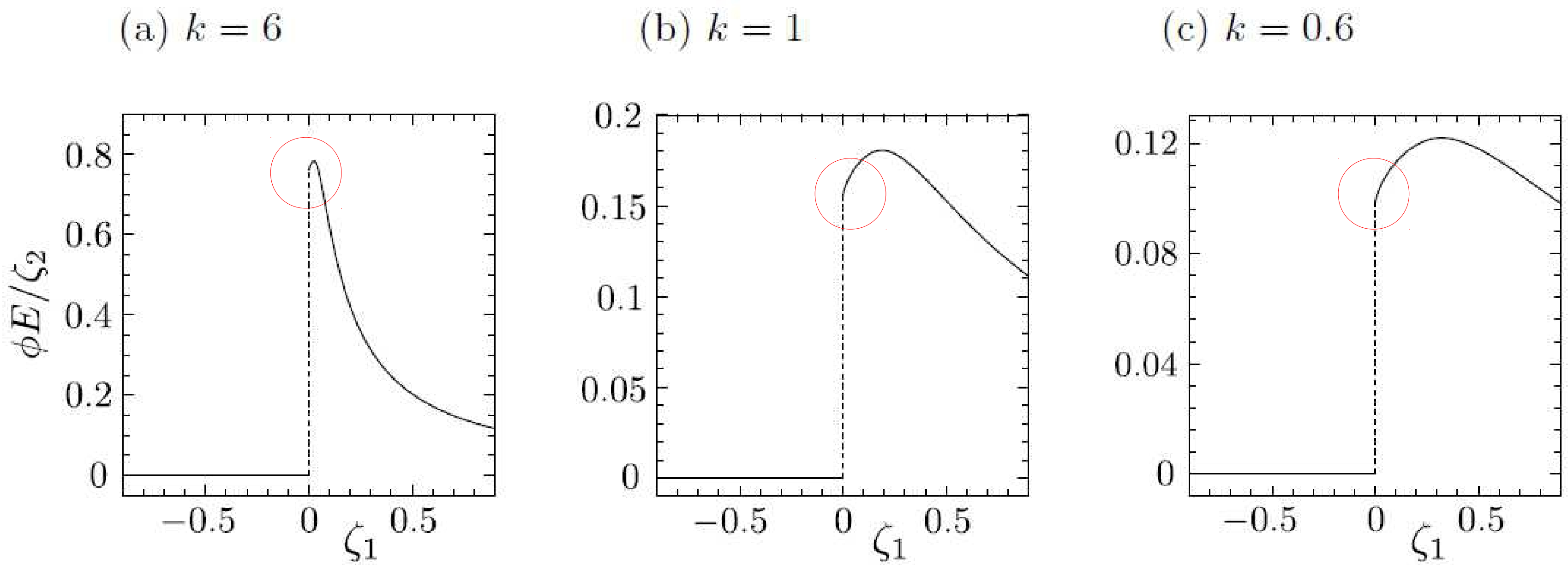
open circle: present numerical result

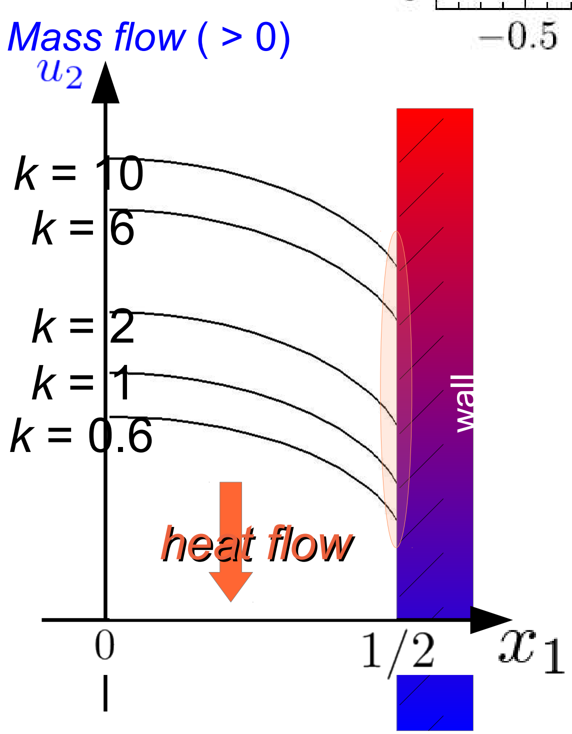
solid line: least mean square approx.

$$a + b(1/2 - x_1)\ln(1/2 - x_1) + c(1/2 - x_1)$$

# Contents

# Velocity distribution function on the boundary for $|\zeta| = 1$




*Common feature for impinging molecules to the boundary, almost parallel to it*

At $x_1 = 1/2$

$$\phi = \begin{cases} \int_{-1/2}^{1/2} \frac{1}{k\zeta_1} \exp\left(-\frac{\nu}{k\zeta_1}(\frac{1}{2} - s)\right) K[\phi](s, \boldsymbol{\zeta})ds + \phi_0, & \zeta_1 > 0, \\ 0, \quad \zeta_1 < 0. \end{cases}$$

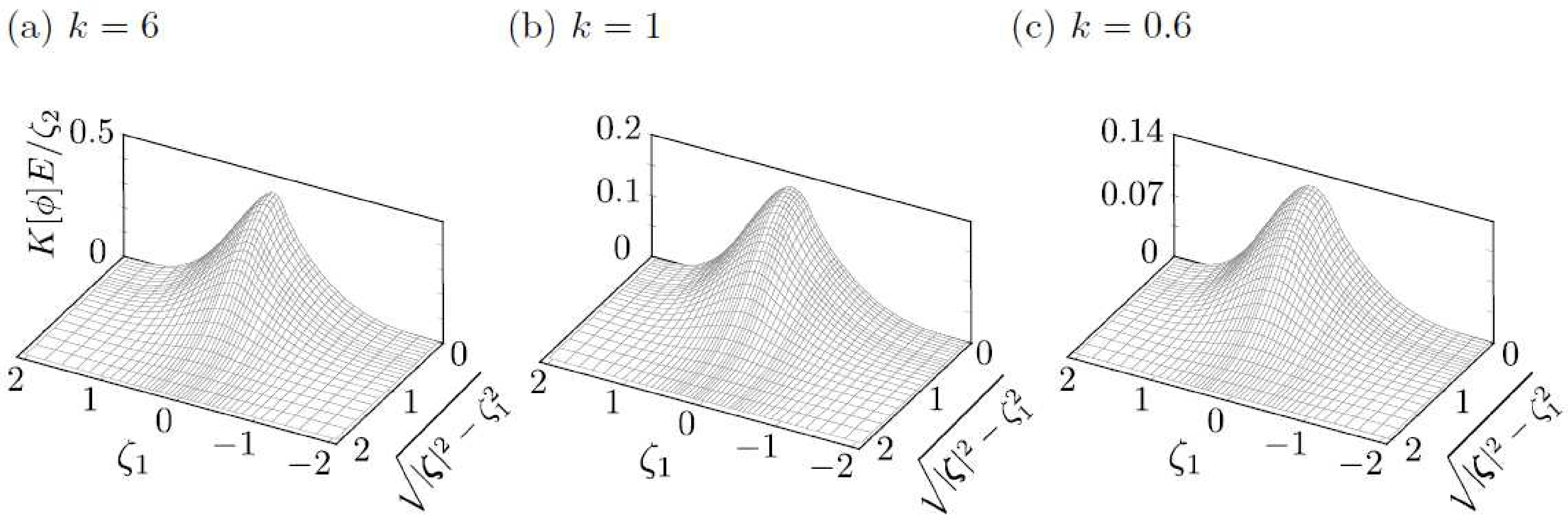
$$\phi_0 = -(k/\nu)[1 - \exp(-\nu/k\zeta_1)]I \text{ for } \zeta_1 > 0,$$

BGK (or BKW) model: $K[\phi] = 2\zeta_2 u_2[\phi]$

$K[\phi](s)$ is singular in $s$ at $s = \pm\frac{1}{2}$ as $(s \mp \frac{1}{2}) \ln|s \mp \frac{1}{2}|$ because of $u_2[\phi](s)$ but is regular in $|\boldsymbol{\zeta}|$

We expect the same property for the Boltzmann collision kernel

## ***Evidence*** $K[\phi](s=\frac{1}{2},\boldsymbol{\zeta})$ on the boundary

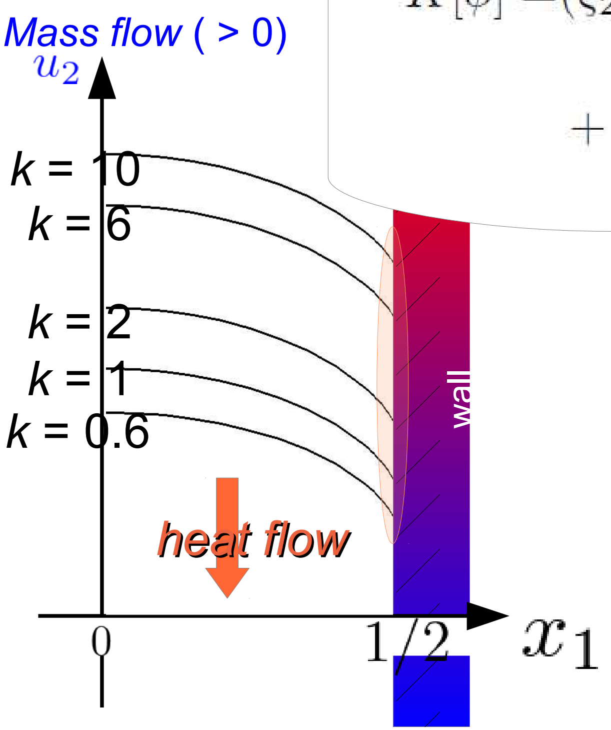



$$K[\phi] =(\zeta_2/|\boldsymbol{\zeta}|)[f_-(\zeta_1,|\boldsymbol{\zeta}|)(s-\frac{1}{2})\ln|s-\frac{1}{2}| + f_+(\zeta_1,|\boldsymbol{\zeta}|)(s+\frac{1}{2})\ln(s+\frac{1}{2})$$
$$+ f_0(\zeta_1,|\boldsymbol{\zeta}|) + \sum_{m=1}^{\infty} s^m f_m(\zeta_1,|\boldsymbol{\zeta}|)].$$

At $x_1 = 1/2$

$$\phi = \begin{cases} \int_{-1/2}^{1/2} \frac{1}{k\zeta_1} \exp\left(-\frac{\nu}{k\zeta_1}(\frac{1}{2}-s)\right) K[\phi](s,\boldsymbol{\zeta})ds + \phi_0, & \zeta_1 > 0, \\ 0, & \zeta_1 < 0. \end{cases}$$

$$K[\phi] = (\zeta_2/|\boldsymbol{\zeta}|)\Big[f_-(\zeta_1,|\boldsymbol{\zeta}|)(s-\frac{1}{2})\ln|s-\frac{1}{2}| + f_+(\zeta_1,|\boldsymbol{\zeta}|)(s+\frac{1}{2})\ln(s+\frac{1}{2}) + f_0(\zeta_1,|\boldsymbol{\zeta}|) + \sum_{m=1}^{\infty} s^m f_m(\zeta_1,|\boldsymbol{\zeta}|)\Big].$$




$\phi \sim \zeta_1 \ln \zeta_1$ for small $\zeta_1 > 0$ and thus its gradient diverges logarithmically as $\zeta_1 \to 0_+$

# Numerical validation

$$\phi = \int_{\mp 1/2}^{x_1} \frac{1}{k\zeta_1} \exp\left(-\frac{\nu(|\boldsymbol{\zeta}|)}{k|\zeta_1|}|x_1 - s|\right) K[\phi](s, \boldsymbol{\zeta}) ds + \phi_0, \quad \zeta_1 \gtrless 0,$$

Two methods have been tested for numerical integration

*Method 1. Piecewise quadratic interpolation in s*

*Method 2. Piecewise quadratic +* $s \ln s$ *interpolation in s*

for $K[\phi]$ from its discretized data

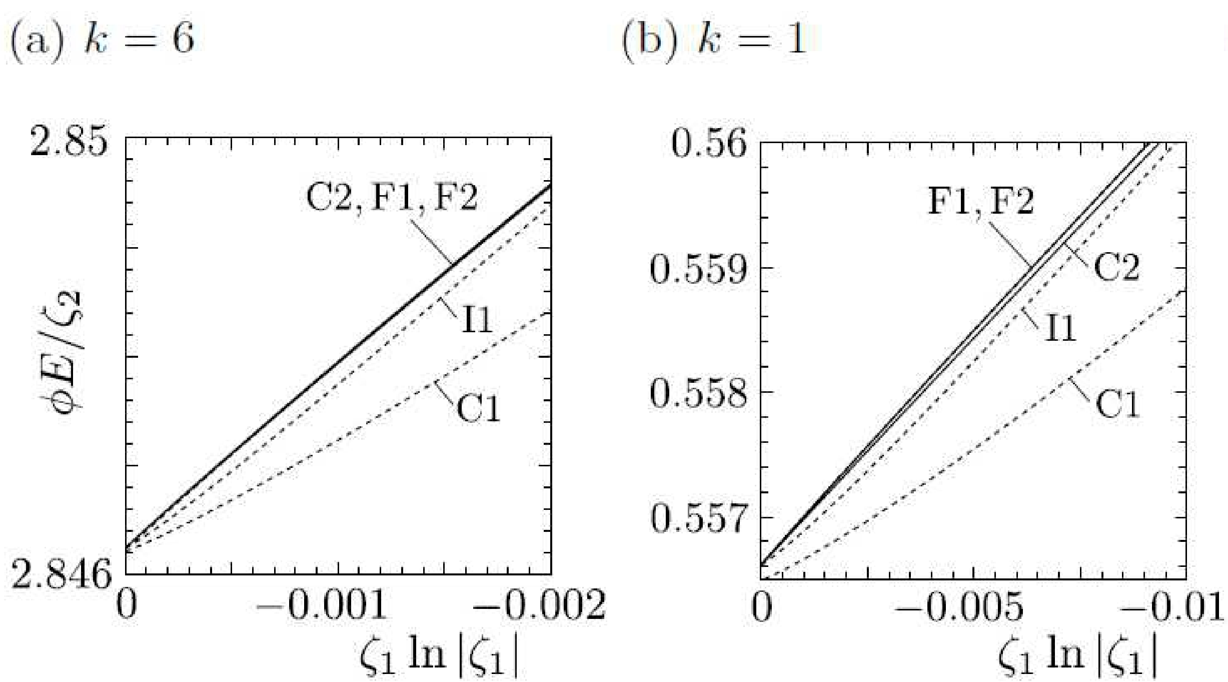
$$K[\phi] = (\zeta_2/|\boldsymbol{\zeta}|)[\underline{f_-(\zeta_1, |\boldsymbol{\zeta}|)(s - \tfrac{1}{2}) \ln|s - \tfrac{1}{2}| + f_+(\zeta_1, |\boldsymbol{\zeta}|)(s + \tfrac{1}{2}) \ln(s + \tfrac{1}{2})}$$
$$+ f_0(\zeta_1, |\boldsymbol{\zeta}|) + \sum_{m=1}^{\infty} s^m f_m(\zeta_1, |\boldsymbol{\zeta}|)].$$

This part is missing in Method 1

## *Evidence*

Velocity distribution func. on the boundary

$x_1 = \frac{1}{2}$, $|\boldsymbol{\zeta}| = 0.5$




| | grid | | | Note |
|---|---|---|---|---|
| | coarse | intermediate | fine | |
| Method 1 | C1 | I1 | F1 | Slow convergence |
| Method 2 | C2 | - | F2 | Satisfactory convergence |



Validate the logarithmic singularity of VDF on the boundary

# Contents

# Contribution to macroscopic singularity

$$\phi = \int_{\mp 1/2}^{x_1} \frac{1}{k\zeta_1} \exp\left(-\frac{\nu(|\boldsymbol{\zeta}|)}{k|\zeta_1|}|x_1 - s|\right) K[\phi](s,\boldsymbol{\zeta})ds + \phi_0, \quad \zeta_1 \gtrless 0,$$

$$K[\phi] = (\zeta_2/|\boldsymbol{\zeta}|)[f_-(\zeta_1,|\boldsymbol{\zeta}|)(s-\frac{1}{2})\ln|s-\frac{1}{2}| + f_+(\zeta_1,|\boldsymbol{\zeta}|)(s+\frac{1}{2})\ln(s+\frac{1}{2}) + \underline{f_0(\zeta_1,|\boldsymbol{\zeta}|)} + \sum_{m=1}^{\infty} s^m f_m(\zeta_1,|\boldsymbol{\zeta}|)].$$

1. No contribution from $\zeta_1 > 0$ (impinging side)
2. Contribution only from $f_0(\zeta_1 = 0, |\boldsymbol{\zeta}|)$ for $\zeta_1 < 0$ (reflected side)

$\Rightarrow$ same as the contribution from

$$\phi_0 = \int_{\mp\frac{1}{2}}^{x_1} \frac{1}{\zeta_1} \exp\left(-\frac{\nu}{k|\zeta_1|}|x_1 - s|\right) I ds$$

Keeping in mind the item 2 in the previous slide, we define

$$f := \int_{\mp\frac{1}{2}}^{x_1} \frac{1}{\zeta_1} \exp\Big(-\frac{\nu}{k|\zeta_1|}|x_1 - s|\Big) I ds$$
$$+ \int_{\mp\frac{1}{2}}^{x_1} \frac{1}{k\zeta_1} \exp\Big(-\frac{\nu}{k|\zeta_1|}|x_1 - s|\Big) \frac{1}{k} K[\phi]|_{\zeta_1=0, x_1=\pm\frac{1}{2}} ds, \quad \zeta_1 \lessgtr 0$$

Note: $\phi = \int_{\mp 1/2}^{x_1} \frac{1}{k\zeta_1} \exp\left(-\frac{\nu(|\boldsymbol{\zeta}|)}{k|\zeta_1|}|x_1 - s|\right) K[\phi](s, \boldsymbol{\zeta}) ds + \phi_0, \quad \zeta_1 \gtrless 0,$

$$f = -\frac{k}{\nu}(\frac{1}{k}K[\phi] - I)|_{\zeta_1=0,\ x_1=\pm 1/2} \exp\left(-\frac{\nu}{k\zeta_1}(x_1 \mp \frac{1}{2})\right), \quad \zeta_1 \lessgtr 0. \qquad (5.1)$$

The singularity of $u_2[\phi]$ should be reproduced by the corresponding moment $u_2[f]$ of $f$

Equation (5.1) is the solution of a simple damping model

$$\zeta_1 \frac{\partial f}{\partial x_1} = -\frac{\nu}{k} f, \qquad (5.2a)$$
$$f = -\frac{k}{\nu}(\frac{1}{k}K[\phi] - I)|_{\zeta_1=0,\ x_1=\pm 1/2}, \quad \zeta_1 \lessgtr 0,\ x_1 = \pm 1/2. \qquad (5.2b)$$

Keeping in mind the item 2 in the previous slide, we define

$$f := \int_{\mp\frac{1}{2}}^{x_1} \frac{1}{\zeta_1} \exp\Big(-\frac{\nu}{k|\zeta_1|}|x_1 - s|\Big) I ds$$
$$+ \int_{\mp\frac{1}{2}}^{x_1} \frac{1}{k\zeta_1} \exp\Big(-\frac{\nu}{k|\zeta_1|}|x_1 - s|\Big) \frac{1}{k} K[\phi]|_{\zeta_1=0, x_1=\pm\frac{1}{2}} ds, \quad \zeta_1 \lessgtr 0$$

Note: $\phi = \int_{\mp 1/2}^{x_1} \frac{1}{k\zeta_1} \exp\left(-\frac{\nu(|\boldsymbol{\zeta}|)}{k|\zeta_1|}|x_1 - s|\right) K[\phi](s, \boldsymbol{\zeta}) ds + \phi_0, \quad \zeta_1 \gtrless 0,$

$$f = -\frac{k}{\nu}\Big(\frac{1}{k}K[\phi] - I\Big)|_{\zeta_1=0,\ x_1=\pm 1/2} \exp\left(-\frac{\nu}{k\zeta_1}\Big(x_1 \mp \frac{1}{2}\Big)\right), \quad \zeta_1 \lessgtr 0. \tag{5.1}$$

The singularity of $u_2[\phi]$ should be reproduced by the corresponding moment $u_2[f]$ of $f$

Equation (5.1) is the solution of a simple damping model

$$\zeta_1 \frac{\partial f}{\partial x_1} = -\frac{\nu}{k} f, \tag{5.2a}$$

$$f = -\frac{k}{\nu}\Big(\frac{1}{k}K[\phi] - I\Big)|_{\zeta_1=0,\ x_1=\pm 1/2}, \quad \zeta_1 \lessgtr 0,\ x_1 = \pm 1/2. \tag{5.2b}$$

Keeping in mind the item 2 in the previous slide, we define

$$f := \int_{\mp\frac{1}{2}}^{x_1} \frac{1}{\zeta_1} \exp\Big( - \frac{\nu}{k|\zeta_1|}|x_1 - s|\Big) I ds$$

$$+ \int_{\mp\frac{1}{2}}^{x_1} \frac{1}{k\zeta_1} \exp\Big( - \frac{\nu}{k|\zeta_1|}|x_1 - s|\Big) \frac{1}{k} K[\phi]|_{\zeta_1=0, x_1=\pm\frac{1}{2}} ds, \quad \zeta_1 \lessgtr 0$$

Note: $\phi = \int_{\mp 1/2}^{x_1} \frac{1}{k\zeta_1} \exp\left( -\frac{\nu(|\boldsymbol{\zeta}|)}{k|\zeta_1|}|x_1 - s| \right) K[\phi](s, \boldsymbol{\zeta}) ds + \phi_0, \quad \zeta_1 \gtrless 0,$

$$f = -\frac{k}{\nu}(\frac{1}{k}K[\phi] - I)|_{\zeta_1=0,\ x_1=\pm 1/2} \exp\left( -\frac{\nu}{k\zeta_1}(x_1 \mp \frac{1}{2}) \right), \quad \zeta_1 \lessgtr 0. \qquad (5.1)$$

The singularity of $u_2[\phi]$ should be reproduced by the corresponding moment $u_2[f]$ of $f$

Equation (5.1) is the solution of a simple damping model

$$\zeta_1 \frac{\partial f}{\partial x_1} = -\frac{\nu}{k} f, \qquad (5.2a)$$

$$f = -\frac{k}{\nu}(\frac{1}{k}K[\phi] - I)|_{\zeta_1=0,\ x_1=\pm 1/2}, \quad \zeta_1 \lessgtr 0,\ x_1 = \pm 1/2. \qquad (5.2b)$$

Keeping in mind the item 2 in the previous slide, we define

$$f := \underline{\int_{\mp\frac{1}{2}}^{x_1} \frac{1}{\zeta_1} \exp\left( - \frac{\nu}{k|\zeta_1|} |x_1 - s| \right) I ds}$$
$$+ \int_{\mp\frac{1}{2}}^{x_1} \frac{1}{k\zeta_1} \exp\left( - \frac{\nu}{k|\zeta_1|} |x_1 - s| \right) \frac{1}{k} K[\phi]|_{\zeta_1=0, x_1=\pm\frac{1}{2}} ds, \quad \zeta_1 \lessgtr 0$$

Note: $\phi = \int_{\mp 1/2}^{x_1} \frac{1}{k\zeta_1} \exp\left( - \frac{\nu(|\boldsymbol{\zeta}|)}{k|\zeta_1|} |x_1 - s| \right) K[\phi](s, \boldsymbol{\zeta}) ds + \underline{\phi_0}, \quad \zeta_1 \gtrless 0,$

$$f = -\frac{k}{\nu}\left(\frac{1}{k} K[\phi] - I\right)|_{\zeta_1=0,\ x_1=\pm 1/2} \exp\left( - \frac{\nu}{k\zeta_1}\left(x_1 \mp \frac{1}{2}\right)\right), \quad \zeta_1 \lessgtr 0. \tag{5.1}$$

Note: The singularity of $u_2[\phi]$ should be reproduced by the corresponding moment $u_2[f]$ of $f$

Equation (5.1) is the solution of a simple damping model

$$\zeta_1 \frac{\partial f}{\partial x_1} = -\frac{\nu}{k} f, \tag{5.2a}$$

$$f = -\frac{k}{\nu}\left(\frac{1}{k} K[\phi] - I\right)|_{\zeta_1=0,\ x_1=\pm 1/2}, \quad \zeta_1 \lessgtr 0,\ x_1 = \pm 1/2. \tag{5.2b}$$

Keeping in mind the item 2 in the previous slide, we define

$$f := \int_{\mp\frac{1}{2}}^{x_1} \frac{1}{\zeta_1} \exp\Big(-\frac{\nu}{k|\zeta_1|}|x_1 - s|\Big) I ds$$
$$+ \int_{\mp\frac{1}{2}}^{x_1} \frac{1}{k\zeta_1} \exp\Big(-\frac{\nu}{k|\zeta_1|}|x_1 - s|\Big) \frac{1}{k} K[\phi]|_{\zeta_1=0, x_1=\pm\frac{1}{2}} ds, \quad \zeta_1 \lessgtr 0$$

Note: $\phi = \int_{\mp 1/2}^{x_1} \frac{1}{k\zeta_1} \exp\left(-\frac{\nu(|\boldsymbol{\zeta}|)}{k|\zeta_1|}|x_1 - s|\right) K[\phi](s, \boldsymbol{\zeta}) ds + \phi_0, \quad \zeta_1 \gtrless 0,$

$$f = -\frac{k}{\nu}(\frac{1}{k}K[\phi] - I)|_{\zeta_1=0,\ x_1=\pm 1/2} \exp\left(-\frac{\nu}{k\zeta_1}(x_1 \mp \frac{1}{2})\right), \quad \zeta_1 \lessgtr 0. \qquad (5.1)$$

Note: The singularity of $u_2[\phi]$ should be reproduced by the corresponding moment $u_2[f]$ of $f$

Equation (5.1) is the solution of a simple damping model

$$\zeta_1 \frac{\partial f}{\partial x_1} = -\frac{\nu}{k} f, \qquad (5.2a)$$

What does it mean physically?

$$f = -\frac{k}{\nu}(\frac{1}{k}K[\phi] - I)|_{\zeta_1=0,\ x_1=\pm 1/2}, \quad \zeta_1 \lessgtr 0,\ x_1 = \pm 1/2. \qquad (5.2b)$$

# What is it?

*Origin of the spatial singularity*

$$f = -\frac{k}{\nu}(\frac{1}{k}K[\phi] - I)|_{\zeta_1=0,\ x_1=\pm 1/2}, \quad \zeta_1 \lessgtr 0,\ x_1 = \pm 1/2.$$

*Let us go back to the original problem...*

$$\zeta_1 \frac{\partial \phi}{\partial x_1} = -\frac{1}{k}\nu(|\boldsymbol{\zeta}|)\phi + \frac{1}{k}K[\phi] - \underbrace{\zeta_2(|\boldsymbol{\zeta}|^2 - \frac{5}{2})}_{I}, \tag{2.3a}$$

$$\text{b.c.} \quad \phi = 0, \quad \zeta_1 \lessgtr 0,\ x_1 = \pm\frac{1}{2}. \tag{2.3b}$$

Since $\phi$ is a solution of $(2.3a)$, we have

$$\phi(x_1, \zeta_1 = 0) = \frac{k}{\nu}(\frac{1}{k}K[\phi] - I)|_{\zeta_1=0} \quad \text{for } -1/2 < x_1 < 1/2.$$

This expression gives the limiting value of $\phi$ for $\zeta_1 = 0_\pm$ and $x_1 \to \pm 1/2$, and thus we have the following relation on the boundary

*Impinging side limit*

*[note: reflected side =0]*

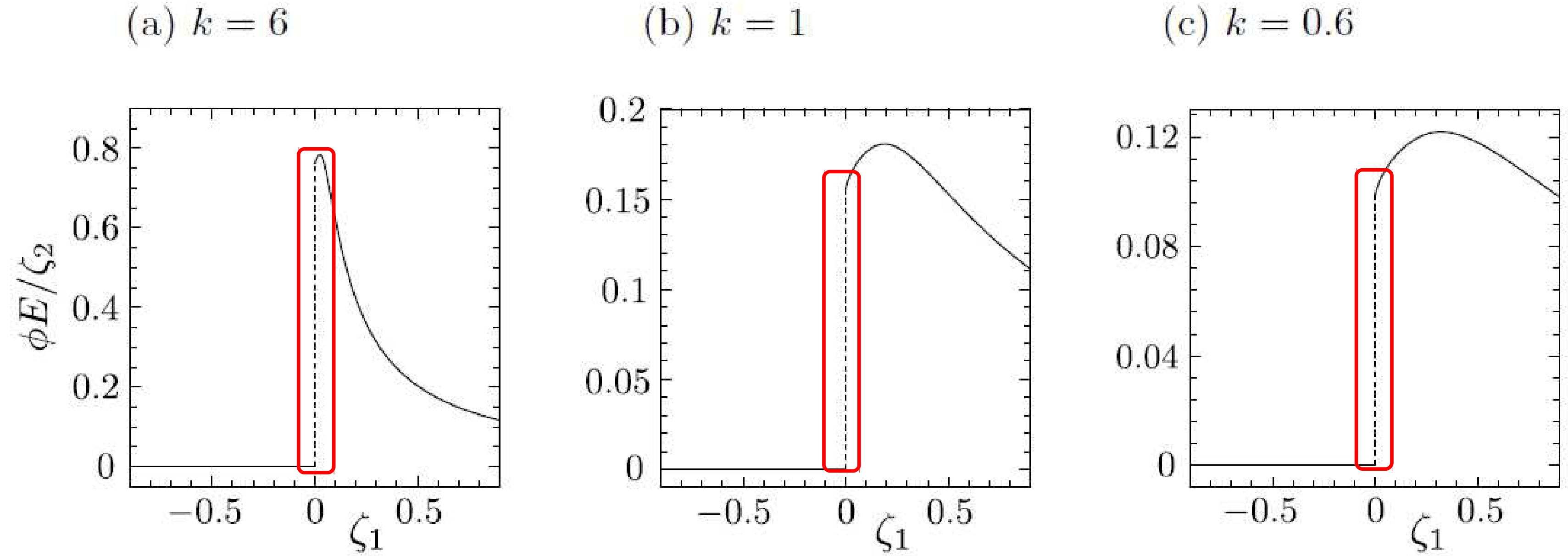
$$-\frac{k}{\nu}(\frac{1}{k}K[\phi] - I)|_{\zeta_1=0,\ x_1=\pm 1/2} = \phi(x_1 = \pm 1/2, \zeta_1 = 0_\mp) - \phi(x_1 = \pm 1/2, \zeta_1 = 0_\pm).$$

Equation (5.1) is the solution of a simple damping model

$$\zeta_1 \frac{\partial f}{\partial x_1} = -\frac{\nu}{k} f, \tag{5.2a}$$

$$f = -\frac{k}{\nu}\left(\frac{1}{k}K[\phi] - I\right)\Big|_{\zeta_1=0,\ x_1=\pm 1/2}, \quad \zeta_1 \lessgtr 0,\ x_1 = \pm 1/2. \tag{5.2b}$$

Discontinuity of VDF on the boundary at $\zeta_1 = 0$




Spatial singularity $(x_1 \pm \frac{1}{2}) \ln |x_1 \pm \frac{1}{2}|$ of $u_2[\phi]$ is the trace of the discontinuity of $\phi$ on the boundary at $\zeta_1 = 0$. It is produced by the damping of discontinuity through the collision frequency $\nu$.

# Comparison of the coefficient *b* of $x \ln x$
# *Original problem* vs. *Dumping model*

$$a + b(1/2 - x_1)\ln(1/2 - x_1) + c(1/2 - x_1)$$

| | $b$ | |
|---|---|---|
| $k$ | $u_2[\phi]$ | $u_2[f]$ |
| 10 | -0.1640 | -0.1641 |
| 6 | -0.1728 | -0.1730 |
| 2 | -0.2003 | -0.2005 |
| 1 | -0.2221 | -0.2223 |
| 0.6 | -0.2378 | -0.2379 |

↳ Numerically validated

# Conclusion

- The logarithmic gradient divergence of macroscopic quantity is confirmed *irrespective of the Knudsen number.*
- The spatial singularity of weighted average of VDF induces *another logarithmic gradient divergence in molecular velocity* on the boundary.
- The origin of the above singularities are *the discontinuity of VDF on the boundary and can be expressed by its damping through the collision frequency*

# Conclusion (# comments)

Our argument applies to

- Cut-off potential models, for which the splitting of the collision integral can be made
- More general boundary condition such as the Maxwell boundary condition (specular+diffuse) and other non-diffuse conditions