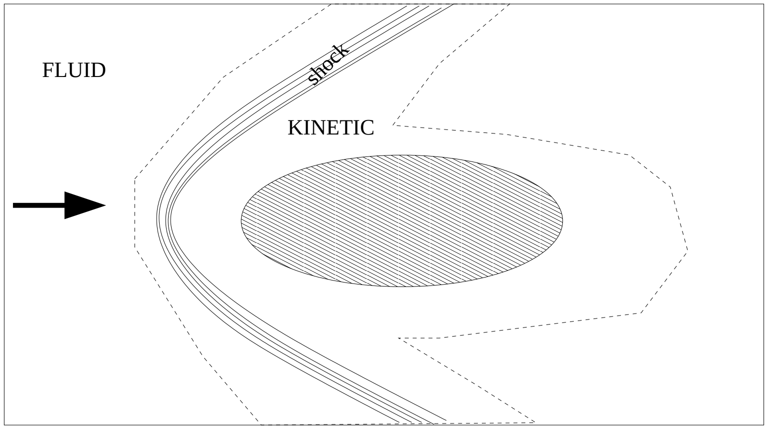
Fluid Models
with
Localized Kinetic Upscaling Effects

Jian-Guo Liu, U Maryland

P. Degond and Luc Mieussens (U Toulouse)

INTRODUCTION

- kinetic models: accurate description of particles but computationaly expensive
- if the particles are in an equilibrium state: simpler asymptotic models are available (fluid models)
- in many cases, the flow is in equilibrium in the major part of the domain, except is small zones where kinetic effects are important



- natural idea: to "couple" kinetic and fluid models

INTRODUCTION

- Heterogeneous Multiscale Method (HMM)
  - HMM, Weinan E & B Engquist 2003
  - Asymptotic preserving schemes, Shi Jin 1999
  - Implicit-yet explicitly implementable-schemes, Jin & Xin 1995, XiaoPing Wang & Weinan E 2001
  - Domain decomposition strategy, smooth transition, Degond, Jin, Mieussens 2005; DG, Weinan E, Chi-Wang Shu etc
  - A dynamic atomistic-continuum method, Weinan E and Z. Huang 2002; Minimizing boundary reflections in coupled-domain simulations, W. Cai, de Koning, Bulatov and S. Yip 2000; Molecular dynamics boundary conditions for regular crystal lattices, Wagner and Karpov and W.K. Liu 2004;
  - Spanning the coninuum to quantum length scales in a dynamic simulation of brittle fracture, Abraham etc 1999

- many works on this subject (rarefied gas dynamics, neutron transport, radiative transfert):

  → mainly decomposition domain techniques

  examples: rarefied gas dynamics

  - Bourgat-Le Tallec-Mallinger-Qiu-Tidriri (INRIA, 96, 97)
  - Neunzert-Struckmeier-Klar (Kaiserslautern 96, 98, 00)

problem of the interface:

- location ?
- interface boundary conditions for kinetic and fluid models ?
- dynamic coupling ?

- recently: automatic multiscale methods
  - for rarefied gas dynamics: Tiwari (98), Ohsawa-Ohwada (02), Ohwada (06)

INTRODUCTION

- this work: *macroscopic fluid models with localized kinetic upscaling effects*
  - fluid models are solved in the whole domain
  - a localized kinetic upscaling that corrects the fluid model wherever it is necessary
  - no interface boundary conditions are necessary
  - very general (works for various kinetic models)

OUTLINE

1. **kinetic and fluid models**
2. **fluid models with localized kinetic upscaling**
3. **numerical examples, hydrodynamical time scale**
4. **numerical examples, diffusion time scale**
5. **summary**

KINETIC AND FLUID MODELS

kinetic model (Boltzmann)

$$\partial_t f + v\partial_x f = \frac{1}{\varepsilon}Q(f) \tag{1}$$

where $f(t, x, v)$ is the distribution function

fluid model (Euler)

$$\partial_t \vec{\rho} + \partial_x F(\vec{\rho}) = 0, \tag{2}$$

where $\vec{\rho} = (\rho, \rho u, \frac{\rho u^2}{2} + \frac{\rho\theta}{2})$ is the vector of macroscopic quantities

KINETIC AND FLUID MODELS

passing from kinetic to fluid model

- moments of the kinetic equation:

$$\partial_t f + v \partial_x f = \frac{1}{\varepsilon} Q(f) \qquad \xrightarrow{\langle \vec{m} g \rangle = \int (1, v, \frac{v^2}{2}) g \, dv} \qquad \partial_t \vec{\rho} + \partial_x \langle \vec{m} v f \rangle = 0$$

  ("conservation laws")

- limit $\varepsilon \to 0$ in the kinetic equation:

$$Q(f) \to 0 \text{ then } f \to E[\vec{\rho}]$$

  ("equilibrium state")

- limit $\varepsilon \to 0$ in the conservation laws:

$$\partial_t \vec{\rho} + \partial_x \underbrace{\langle \vec{m} v E[\vec{\rho}] \rangle}_{F(\vec{\rho})} = 0$$

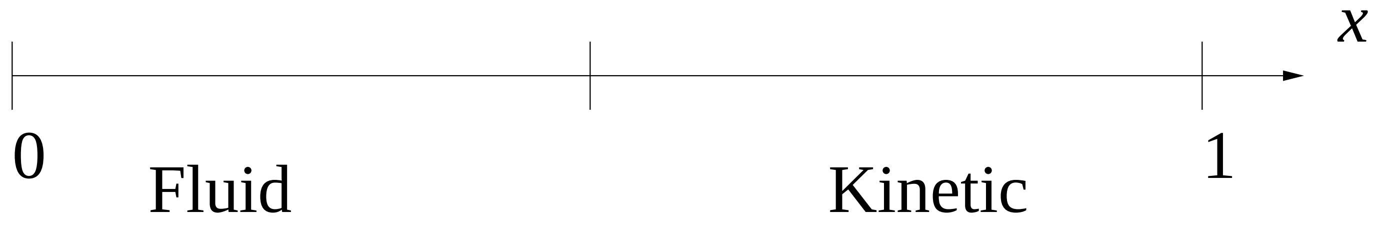
  (”asymptotic fluid model”)

KINETIC AND FLUID MODELS

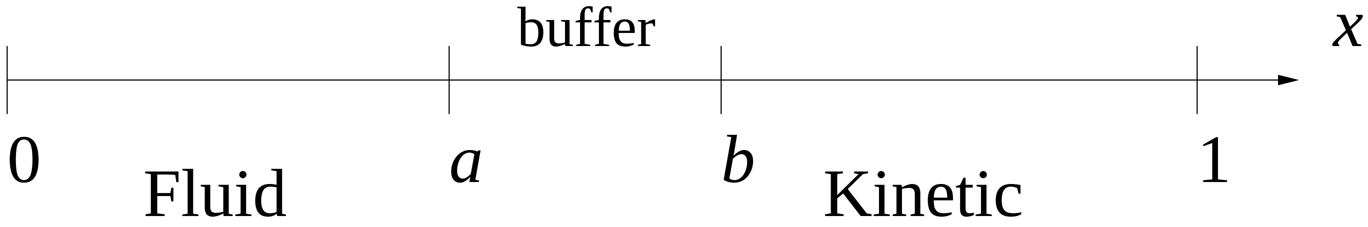
various asymptotic models available

- 0^{th}, 1^{st}, 2^{nd}, 3^{rd} order models
- linear/non-linear models
- hydrodynamic/diffusion asymptotics
- etc.

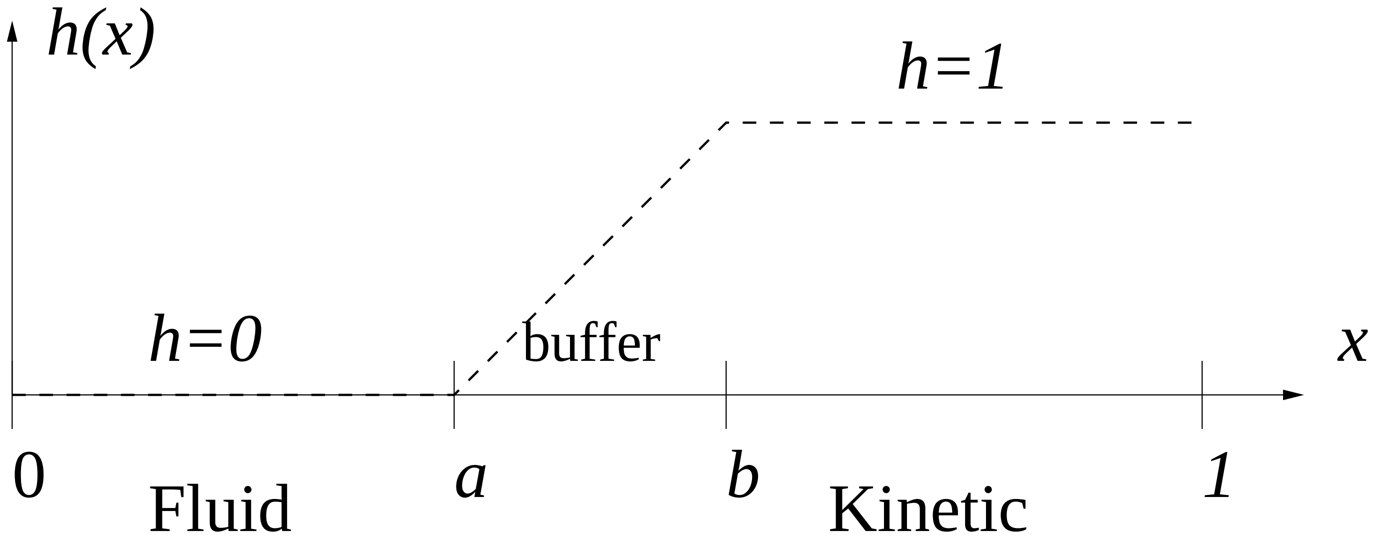
KINETIC/FLUID DOMAIN DECOMPOSITION



KINETIC/FLUID DOMAIN DECOMPOSITION



KINETIC/FLUID DOMAIN DECOMPOSITION

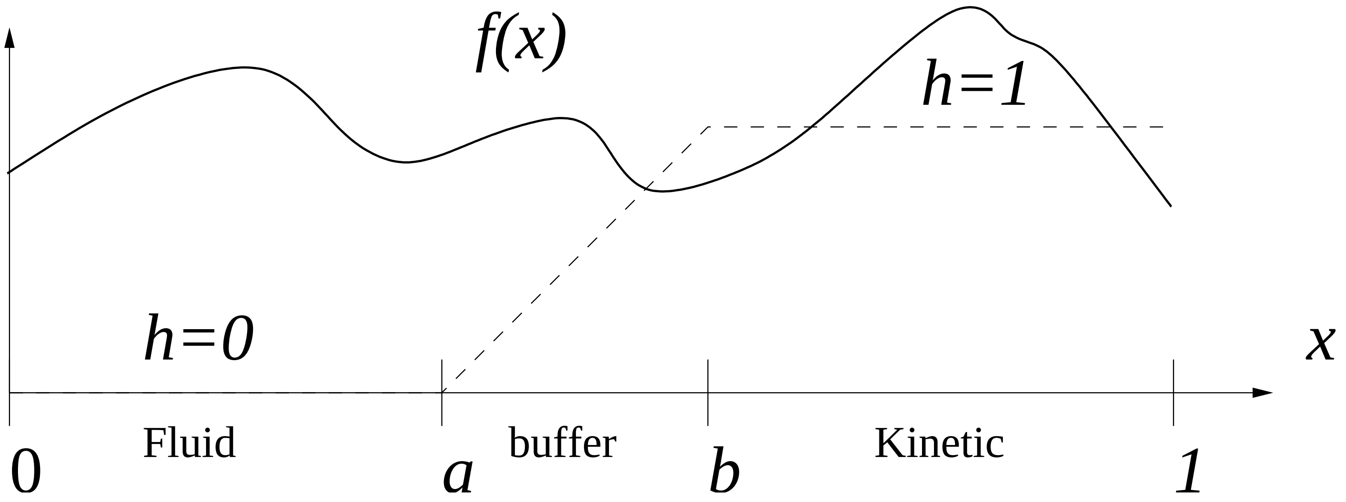


transition function

KINETIC/FLUID DOMAIN DECOMPOSITION

a) kinetic/kinetic coupling

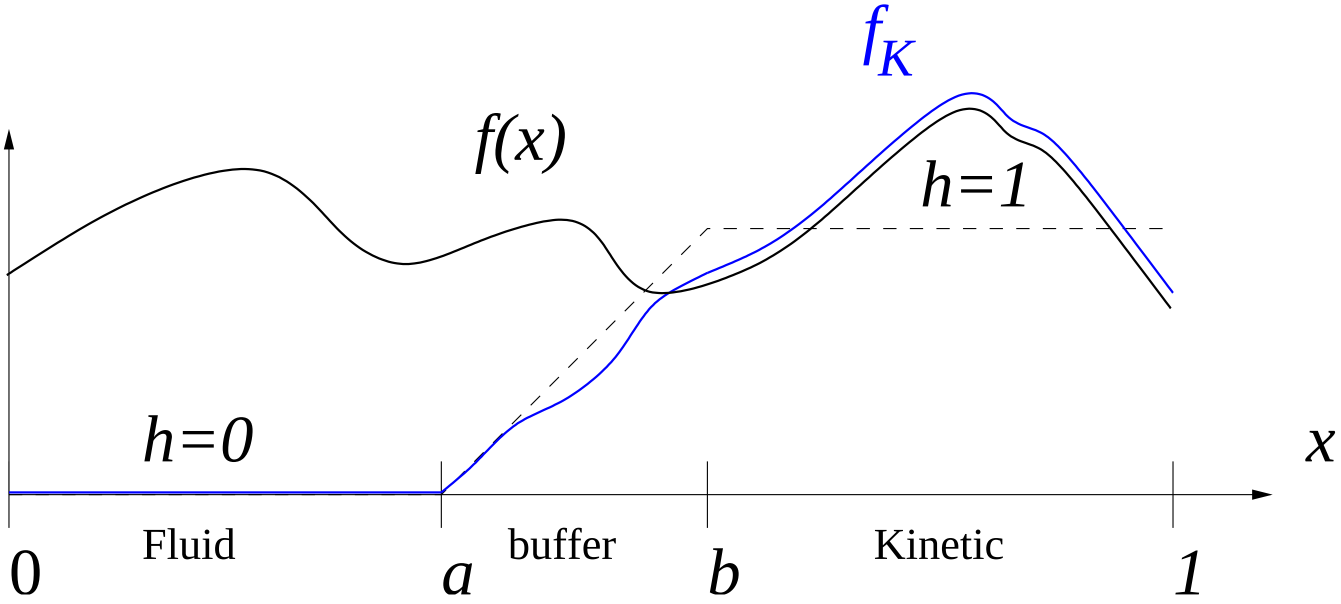
- $f(t,x,v)$ solution of $\partial_t f + v\partial_x f = \frac{1}{\varepsilon}Q(f)$ in $[0,1]$



KINETIC/FLUID DOMAIN DECOMPOSITION

a) kinetic/kinetic coupling

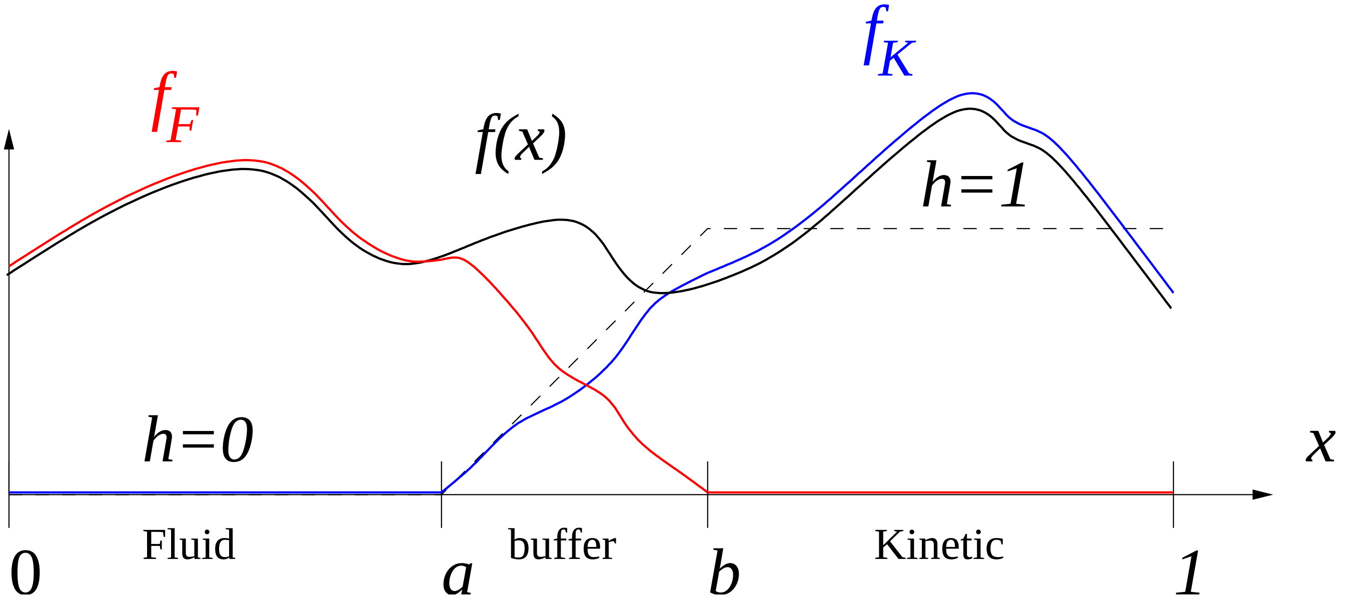
- $f(t,x,v)$ solution of $\partial_t f + v\partial_x f = \frac{1}{\varepsilon}Q(f)$ in $[0,1]$
- kinetic part: $f_K = h(x)f(t,x,v)$



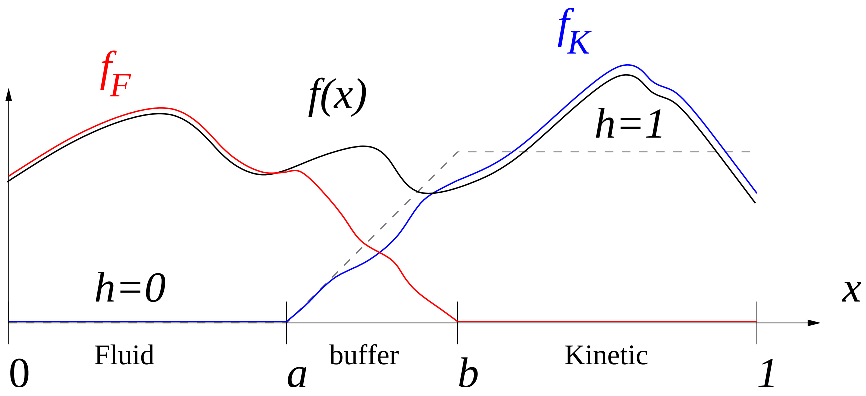
KINETIC/FLUID DOMAIN DECOMPOSITION

a) kinetic/kinetic coupling

- $f(t,x,v)$ solution of $\partial_t f + v\partial_x f = \frac{1}{\varepsilon}Q(f)$ in $[0,1]$
- kinetic part: $f_K = h(x)f(t,x,v)$
- "fluid" part: $f_F = (1-h(x))f(t,x,v)$



KINETIC/FLUID DOMAIN DECOMPOSITION



THEN

- f_K and f_F are defined everywhe in [0,1]
- we have $f = f_K + f_F$

- equation for f_K and f_F:

$$\partial_t f_K + hv\partial_x f_K + hv\partial_x f_F = \frac{1}{\varepsilon} hQ(f_K + f_F),$$

$$\partial_t f_F + (1-h)v\partial_x f_F + (1-h)v\partial_x f_K = \frac{1}{\varepsilon}(1-h)Q(f_K + f_F).$$

(no approximation)

KINETIC/FLUID DOMAIN DECOMPOSITION

therefore, the coupling model

$$\begin{aligned}
&\partial_t f_K + hv\partial_x f_K + hv\partial_x E[\vec{\rho}_F] = \frac{1}{\varepsilon} hQ(f_K + E[\vec{\rho}_F]) \\
&\partial_t \vec{\rho}_F + (1-h)\partial_x F(\vec{\rho}_F) + (1-h)\partial_x \langle v\vec{m} f_K\rangle = 0
\end{aligned}$$

is in fact

$$\partial_t \vec{\rho}_F + \partial_x F(\vec{\rho}_F) = 0 \quad \text{in the fluid zone}$$

$$\partial_t f_K + v\partial_x f_K = \frac{1}{\varepsilon} Q(f_K) \quad \text{in the kinetic zone}$$

$$\begin{cases}
\partial_t f_K + hv\partial_x f_K + hv\partial_x E[\vec{\rho}_F] = \frac{1}{\varepsilon} hQ(f_K + E[\vec{\rho}_F]) \\
\partial_t \vec{\rho}_F + (1-h)\partial_x F(\vec{\rho}_F) + (1-h)\partial_x \langle v\vec{m} f_K\rangle = 0
\end{cases} \quad \text{in the buffer}$$

KINETIC/FLUID DOMAIN DECOMPOSITION

moreover, the global kinetic solution f is approximated by

- $E[\vec{\rho}_F]$ in the fluid zone;
- f_K in the kinetic zone;
- $f_K + E[\vec{\rho}_F]$ in the buffer

→ first proposed for coupling linear transport model / diffusion equation by P. Degond and S. Jin (05)

→ extended to nonlinear kinetic models / hydrodynamic models by P. Degond, S. Jin and L. M. (05)

KINETIC/FLUID DOMAIN DECOMPOSITION

- not well balanced: uniform flows may be non-preserved
- Burgers equation

$$\partial_t \rho + \rho \partial_x \rho = \partial_t \rho + \partial_x \rho^2/2 = 0$$

- Jin-Xin relaxation model

$$\partial_t \rho + \partial_x j = 0, \qquad \partial_t j + \partial_x \rho = \frac{1}{\varepsilon}(\rho^2/2 - j),$$

- discrete-velocity model:

$$\partial_t f_1 + \partial_x f_1 = \frac{1}{\varepsilon}(M_1[\rho] - f_1), \qquad \partial_t f_2 - \partial_x f_2 = \frac{1}{\varepsilon}(M_2[\rho] - f_2).$$

- the equilibrium is $(M_1[\rho], M_2[\rho]) = \frac{1}{2}(\rho + \rho^2/2, \rho - \rho^2/2)$,
  not homogeneous w.r.t ρ.
- numerical test with a uniform initial data and with an initial discontinuity.

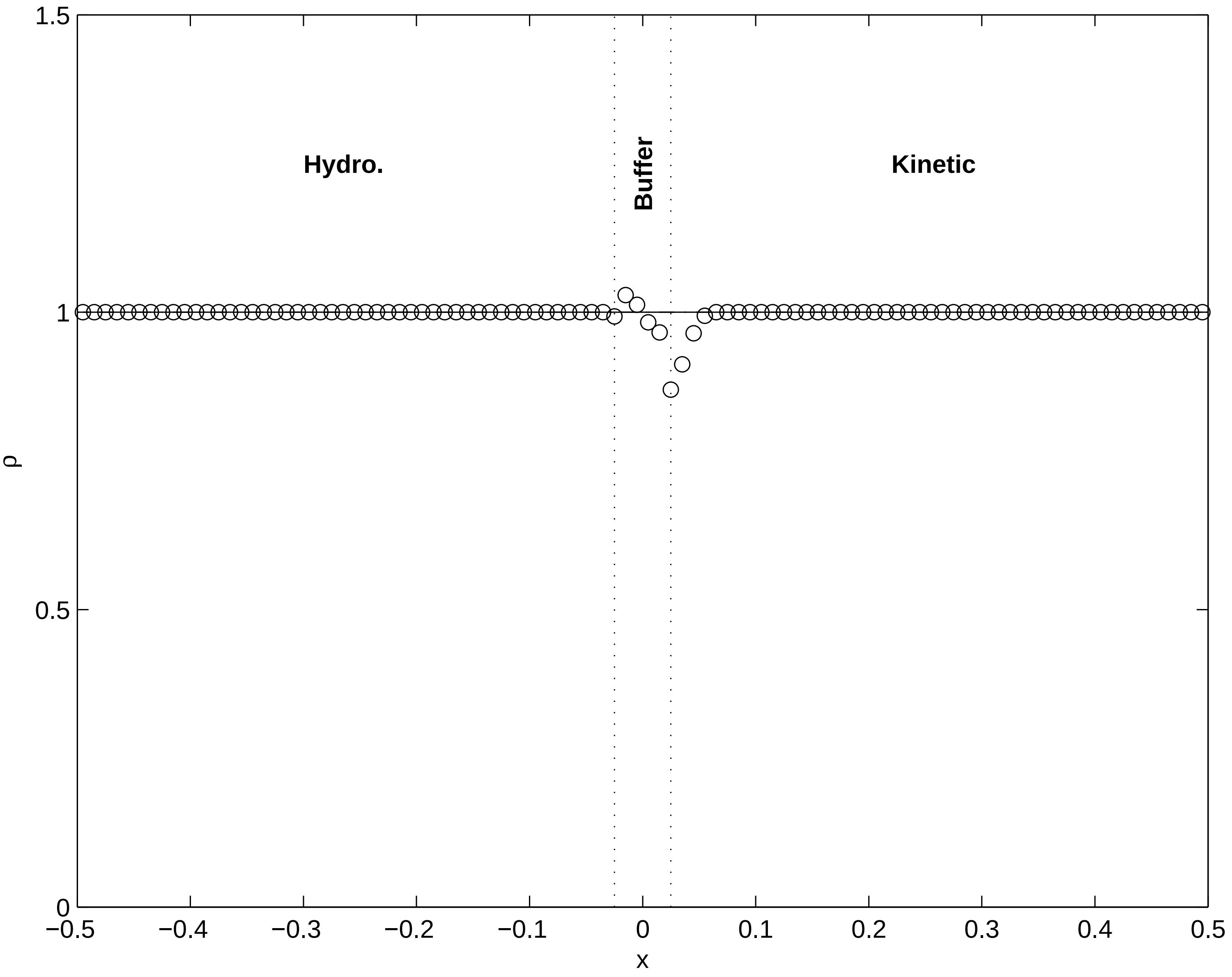


Figure 1: The numerical solution of $\vec{\rho}$ for the Jin-Xin relaxation model at $t = 0.025$ for the uniform initial condition. The solid line is the (constant) solution of the full kinetic model, while 'o' is the numerical solution of the coupling model with 100 grid points.

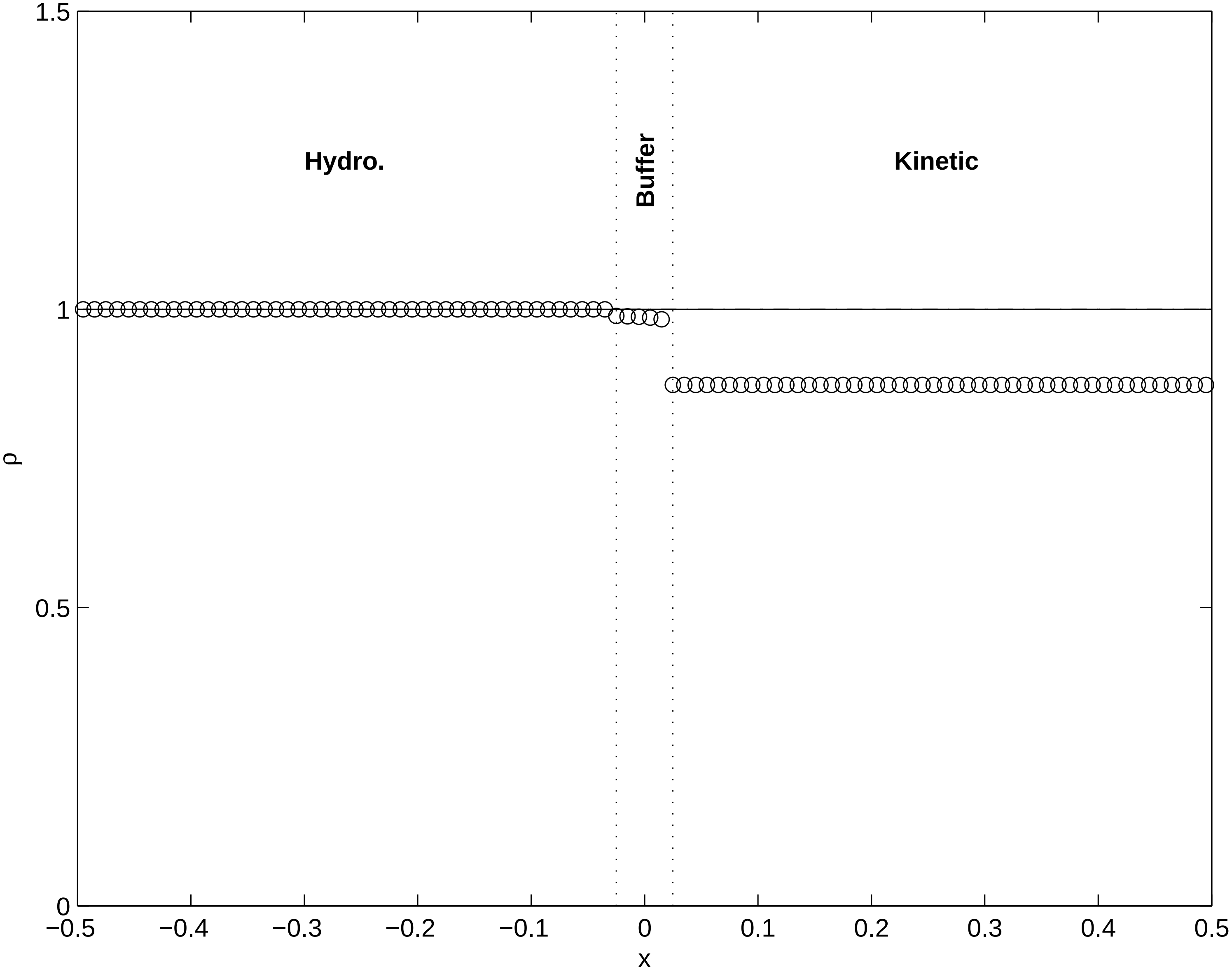


Figure 2: The numerical solution of $\vec{\rho}$ for the Jin-Xin relaxation model at steady state for the uniform initial condition. The solid line is the (constant) solution of the full kinetic model, while 'o' is the numerical solution of the coupling model with 100 grid points.

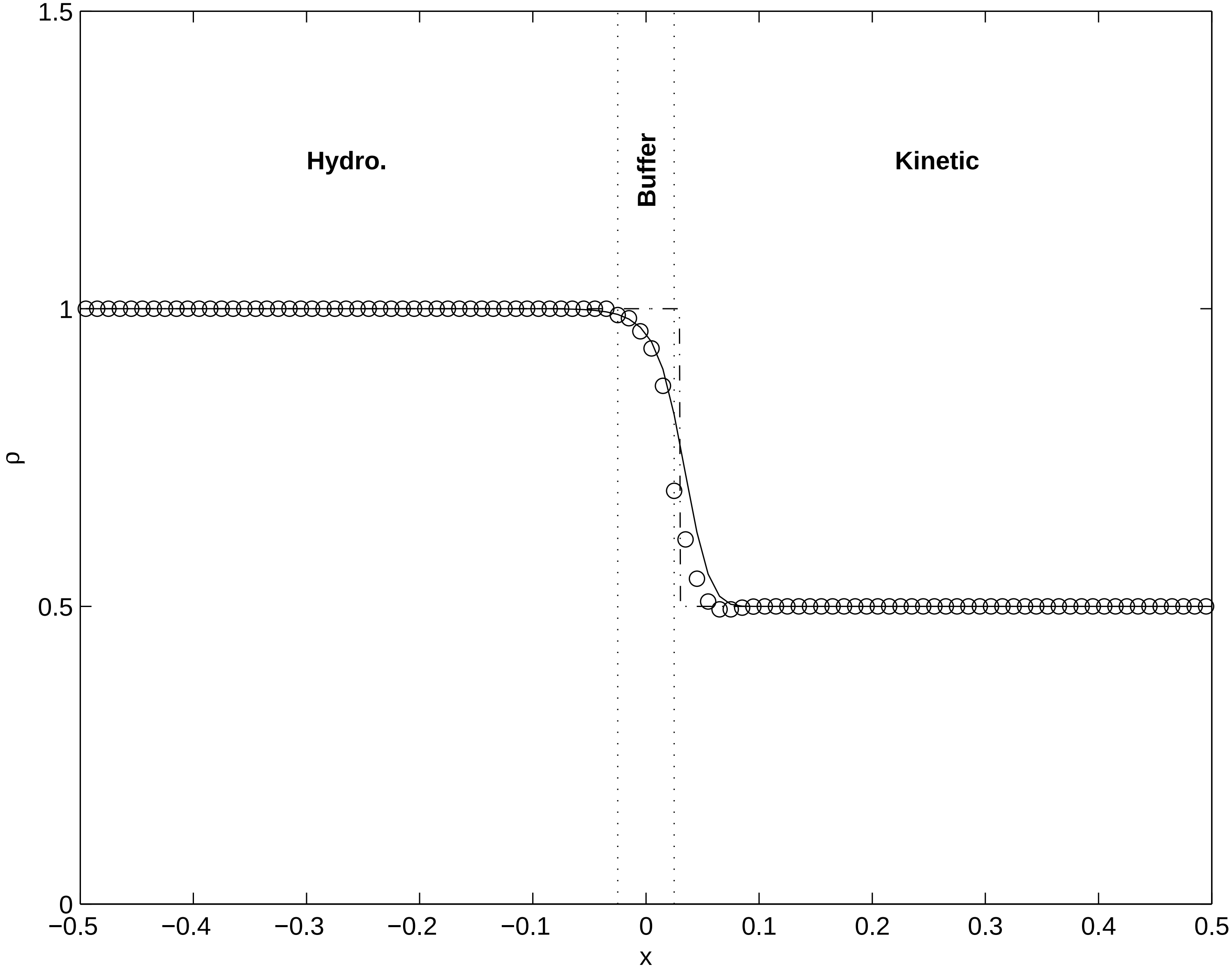


Figure 3: The numerical solution of $\vec{\rho}$ for the Jin-Xin relaxation model at $t = 0.0450$ for the shock initial condition, with narrow (top) and large (bottom) buffer zone. The solid line is the numerical solution of the full kinetic model, while 'o' is the numerical solution of the coupling model (100 grid points), and '.-' is the exact solution for the Burgers equation (full hydrodynamic limit).

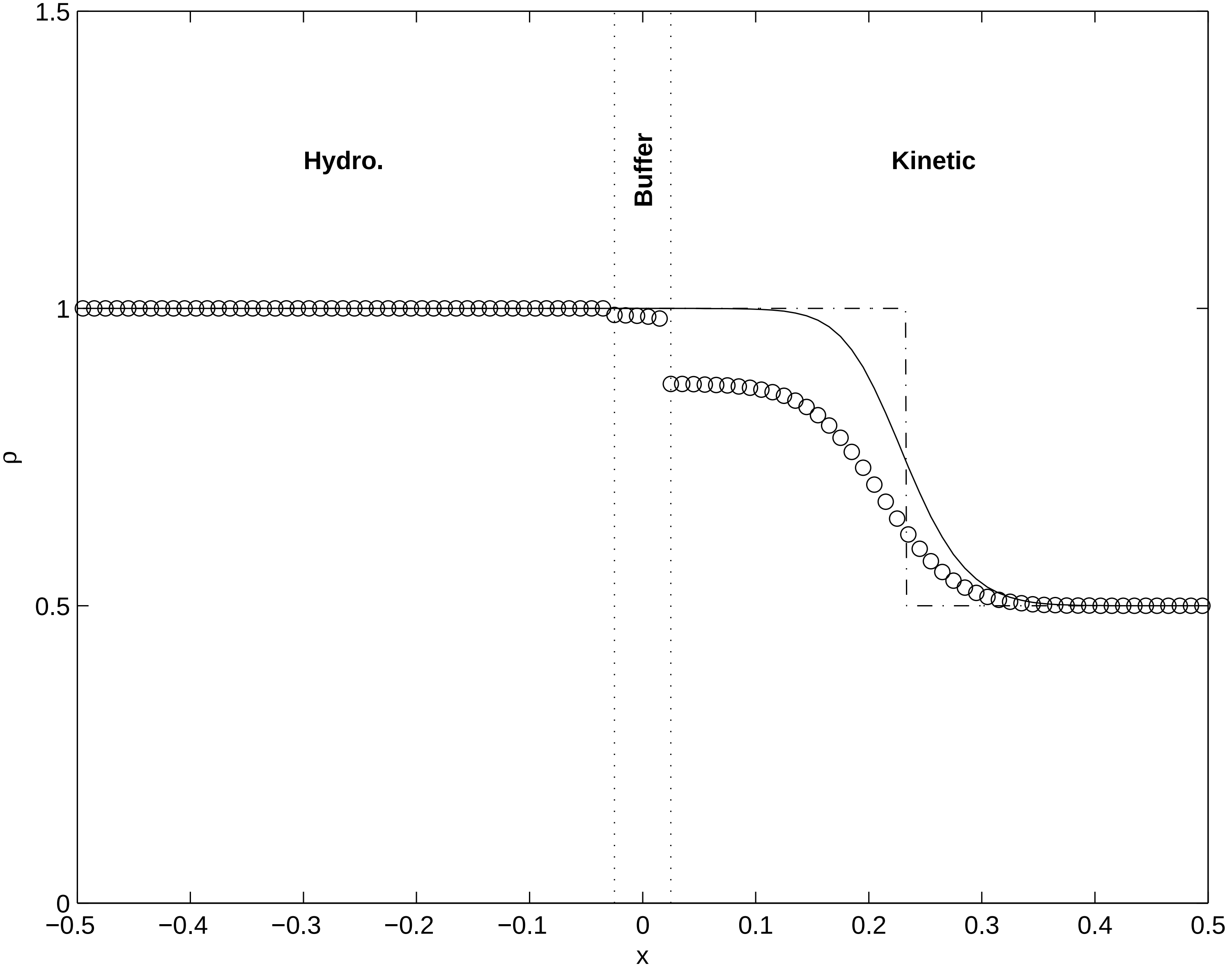


Figure 4: The numerical solution of $\vec{\rho}$ for the Jin-Xin relaxation model at $t = 0.3150$ for the shock initial condition, with narrow (top) and large (bottom) buffer zone. The solid line is the numerical solution of the full kinetic model, while 'o' is the numerical solution of the coupling model (100 grid points), and '.-' is the exact solution for the Burgers equation (full hydrodynamic limit).

KINETIC/FLUID DOMAIN DECOMPOSITION

Explanation:

- uniform flows should be preserved : if $\vec{\rho}$ is a constant (in space and time), then
  - $f = E[\vec{\rho}]$ is a constant solution of the full kinetic model
  - $f_K = hE[\vec{\rho}]$ and $\vec{\rho}_F = (1-h)\vec{\rho}$ are solution of the coupling model
  - but f is approximated by

$$f_K + E[\vec{\rho}_F] = hE[\vec{\rho}] + E[(1-h)\vec{\rho}]$$

  - this is equal to

$$hE[\vec{\rho}] + (1-h)E[\vec{\rho}] = E[\vec{\rho}] = f$$

but only if

$$E[\lambda\vec{\rho}] = \lambda E[\vec{\rho}] \text{ for every } \lambda \text{ (homogeneity property)}$$

→ true for linear models

→ true for Maxwellian equilibrium (rarefied gas dynamics)

→ wrong for other statistics (Fermi-Dirac, Bose-Einstein), or some toy models

FLUID MODELS WITH LOCALIZED KINETIC UPSCALING

kinetic model

$$\partial_t f + v \partial_x f = \frac{1}{\varepsilon} Q(f)$$

micro-macro decomposition

$$f = E[\vec{\rho}] + g$$

equivalent model for $(\vec{\rho}, g)$:

$$\begin{aligned}
&\partial_t \vec{\rho} + \partial_x F(\vec{\rho}) + \partial_x \langle v \vec{m} g \rangle = 0 \\
&\partial_t g + v \partial_x g = Q(E[\vec{\rho}] + g) - (\partial_t + v \partial_x) E[\vec{\rho}]
\end{aligned}$$

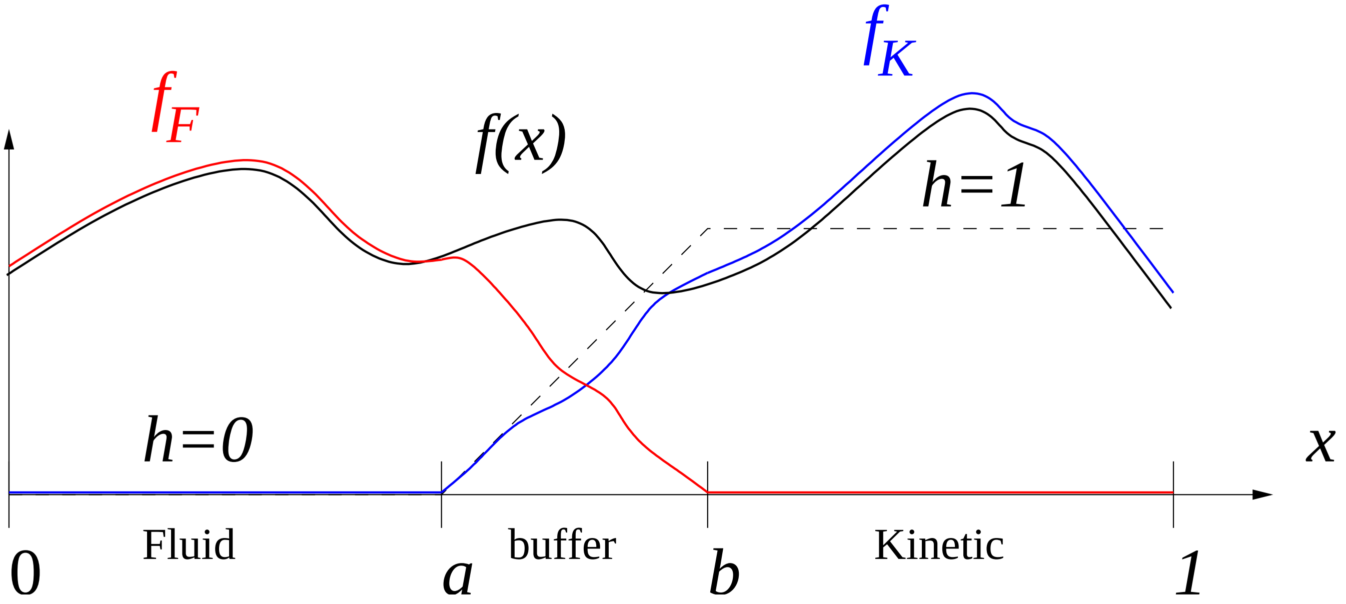
FLUID MODELS WITH LOCALIZED KINETIC UPSCALING

a) localized kinetic upscaling

$$\partial_t \vec{\rho} + \partial_x F(\vec{\rho}) + \partial_x \langle v \vec{m} g \rangle = 0$$

$$\partial_t g + v \partial_x g = Q(E[\vec{\rho}] + g) - (\partial_t + v \partial_x) E[\vec{\rho}]$$

kinetic part: $g_K = h(x) g(t,x,v)$, “fluid” part: $g_F = (1 - h(x)) g(t,x,v)$



FLUID MODELS WITH LOCALIZED KINETIC UPSCALING

- $(\vec{\rho}, g)$ solution of the micro-macro formulation
- the transition function h is used to split g **only**
- kinetic part: $g_K = h(x)g(t,x,v)$
- “fluid” part: $g_F = (1-h(x))g(t,x,v)$
- as $\varepsilon \to 0$, $g_F \to 0$
- we obtain the micro-Macro model (for hydrodynamic scale)

$$\partial_t \vec{\rho} + \partial_x F(\vec{\rho}) + \partial_x \langle v\vec{m} g_K \rangle = 0,$$

$$\partial_t g_K + hv\partial_x g_K = \frac{h}{\varepsilon} Q(E[\vec{\rho}] + g_K) - h(\partial_t + v\partial_x)E[\vec{\rho}],$$

FLUID MODELS WITH LOCALIZED KINETIC UPSCALING

$$\partial_t \vec{\rho} + \partial_x F(\vec{\rho}) + \partial_x \langle v \vec{m} g_K \rangle = 0,$$

$$\partial_t g_K + h v \partial_x g_K = \frac{h}{\varepsilon} Q(E[\vec{\rho}] + g_K) - h(\partial_t + v\partial_x) E[\vec{\rho}],$$

can be written as the following fluid model

$$\partial_t \vec{\rho} + \partial_x F(\vec{\rho}) + U(g_K) = 0$$

where

- the upscaling term $U(g_K)$ is 0 in the fluid zone ($h = 0$, major part of the domain)
- elsewhere ($h \neq 0$), $U(g_K)$ is computed by solving the kinetic equation

  $$\partial_t g_K + h v \partial_x g_K = \frac{h}{\varepsilon} Q(E[\vec{\rho}] + g_K) - hD(\vec{\rho})$$

  related to the fluid equation through the downscaling term $D(\vec{\rho})$
- in kinetic zones ($h = 1$) the full kinetic equation is recovered

FLUID MODELS WITH LOCALIZED KINETIC UPSCALING

example 1: discrete-velocity model

kinetic model:

$$\partial_t f_1 + \partial_x f_1 = \frac{1}{\varepsilon}(M_1[\rho] - f_1), \qquad \partial_t f_2 - \partial_x f_2 = \frac{1}{\varepsilon}(M_2[\rho] - f_2).$$

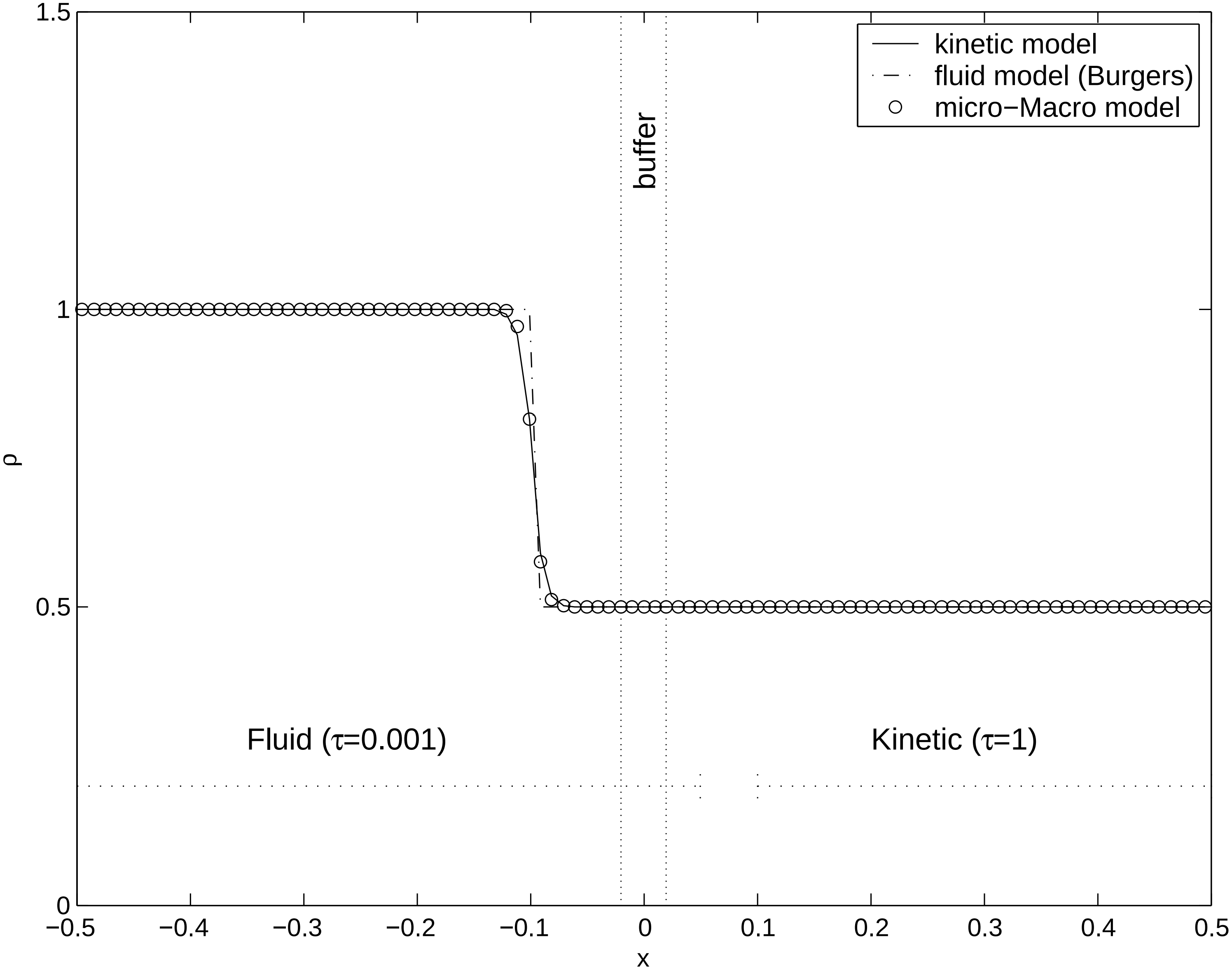
fluid model (Burgers):

$$\partial_t \rho + \partial_x \rho^2/2 = 0$$

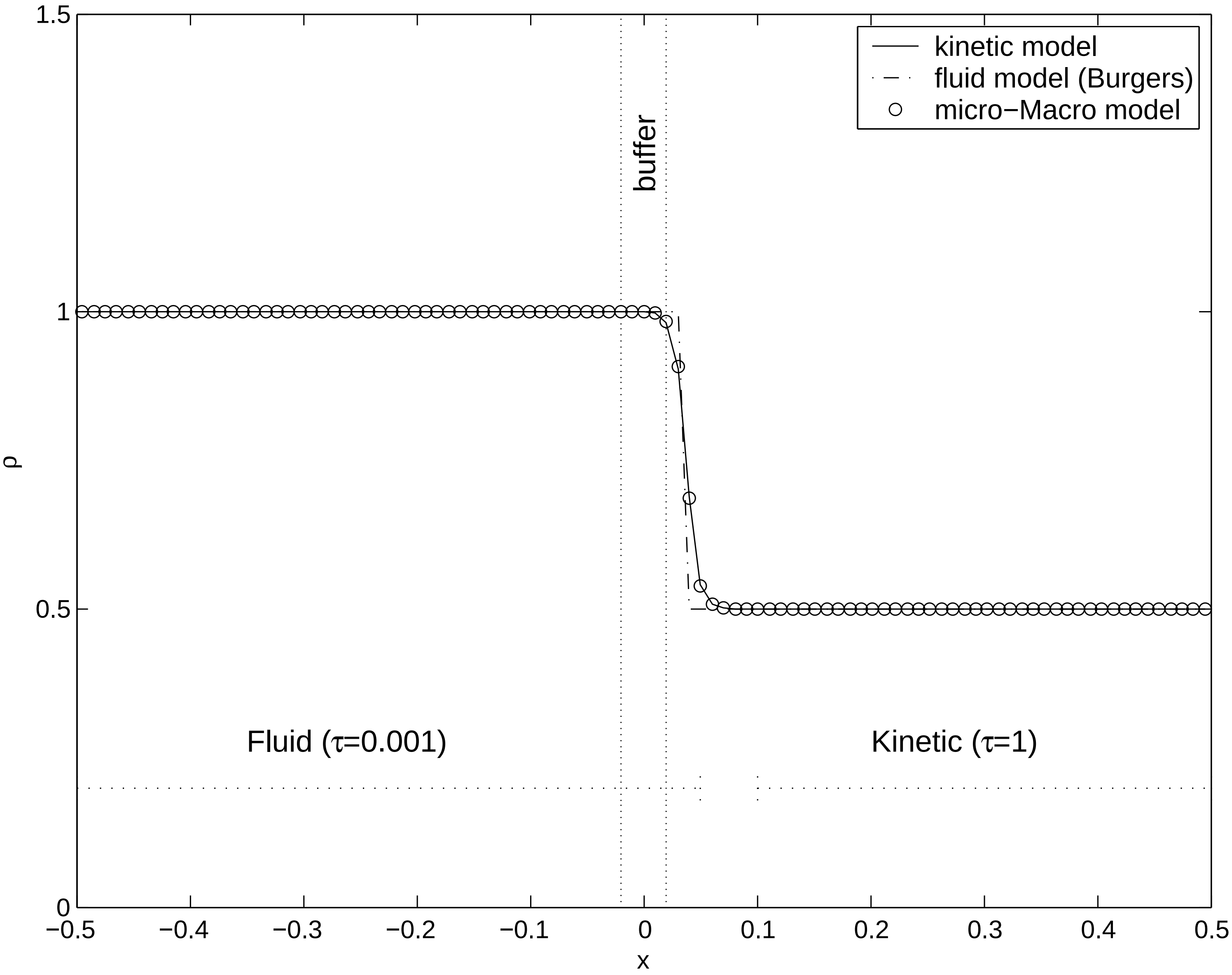
micro-Macro model:

$$\partial_t \rho + \partial_x \rho^2/2 + \partial_x (g_K^1 - g_K^2) = 0,$$

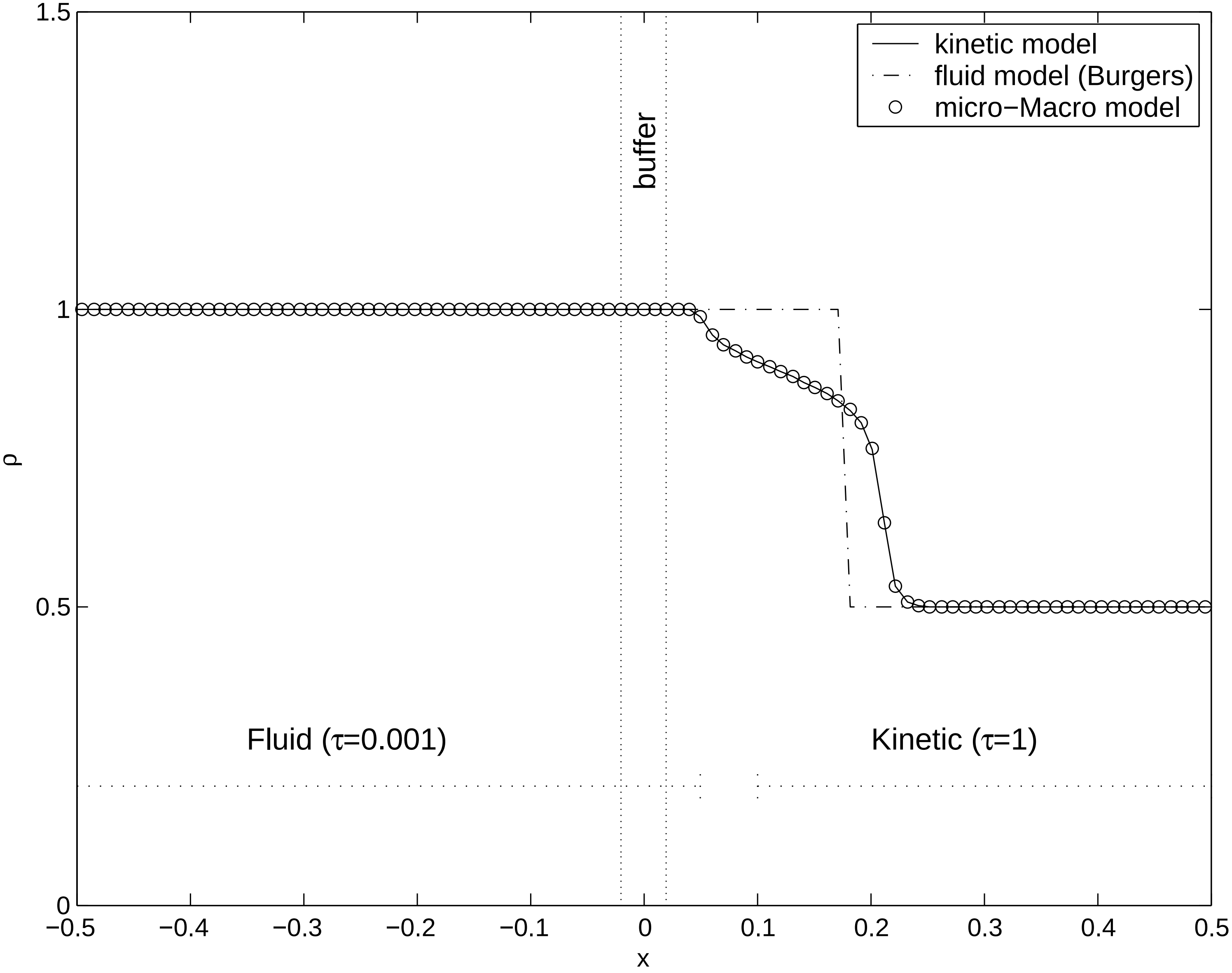
$$\partial_t \begin{pmatrix} g_K^1 \\ g_K^2 \end{pmatrix} + h\partial_x \begin{pmatrix} g_K^1 \\ -g_K^2 \end{pmatrix} = -\frac{1}{\varepsilon} \begin{pmatrix} g_K^1 \\ g_K^2 \end{pmatrix} - h(\partial_t \begin{pmatrix} M_1 \\ M_2 \end{pmatrix} + \partial_x \begin{pmatrix} M_1 \\ -M_2 \end{pmatrix})$$



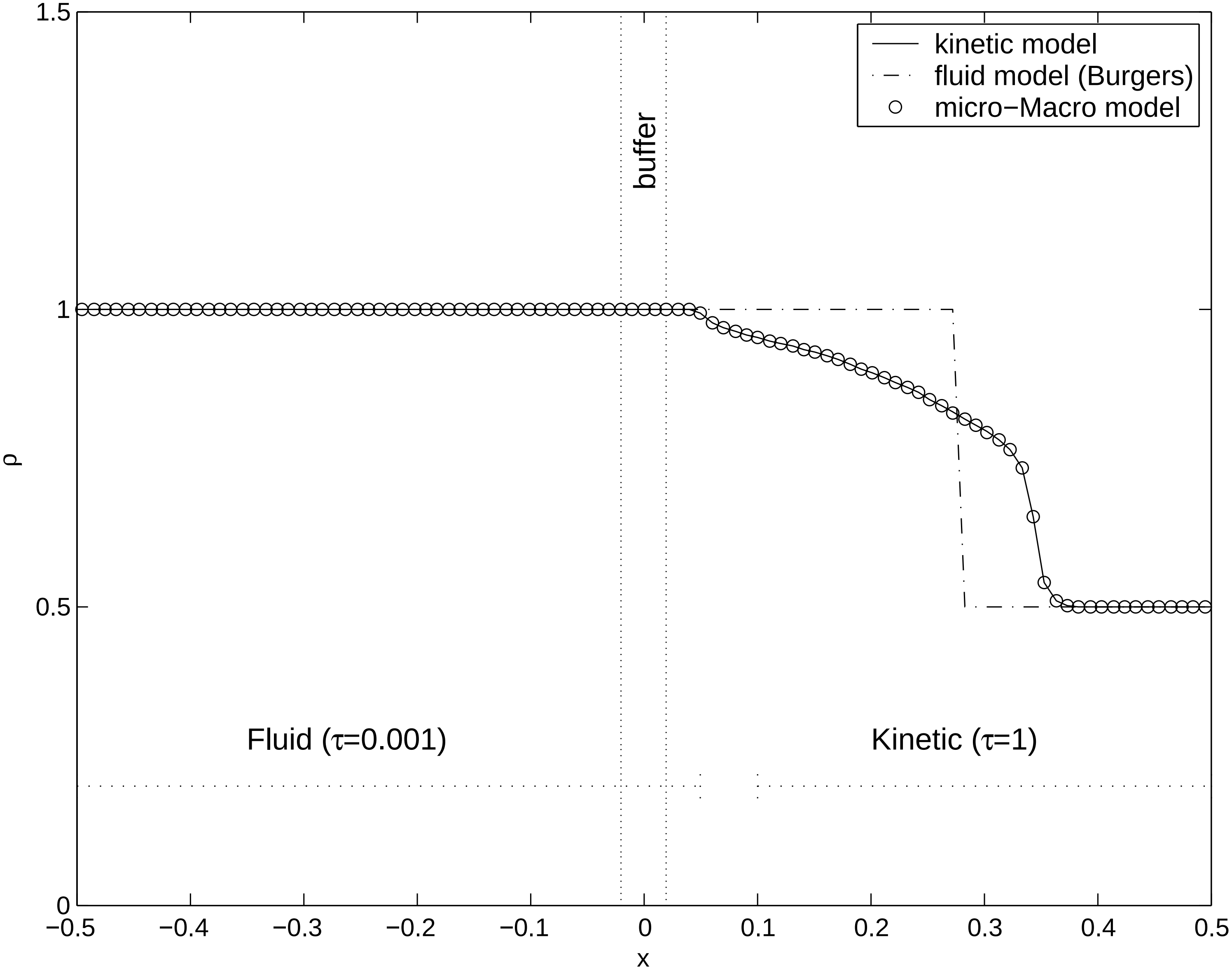
The numerical solution of $\vec{\rho}$ for the Jin-Xin relaxation model with a space dependent relaxation time (from 0.001 to 1) at $t = 0.0909$.



The numerical solution of $\vec{\rho}$ for the Jin-Xin relaxation model with a space dependent relaxation time (from 0.001 to 1) at $t = 0.2773$.



The numerical solution of $\vec{\rho}$ for the Jin-Xin relaxation model with a space dependent relaxation time (from 0.001 to 1) at $t = 0.4773$.



The numerical solution of $\vec{\rho}$ for the Jin-Xin relaxation model with a space dependent relaxation time (from 0.001 to 1) $t = 0.5909$.

FLUID MODELS WITH LOCALIZED KINETIC UPSCALING

example 2: BGK equation of Rarefied Gas Dynamics

kinetic model:

$$\partial_t f + v \partial_x f = Q(f) = \frac{\nu}{\varepsilon}(E[\vec{\rho}] - f),$$

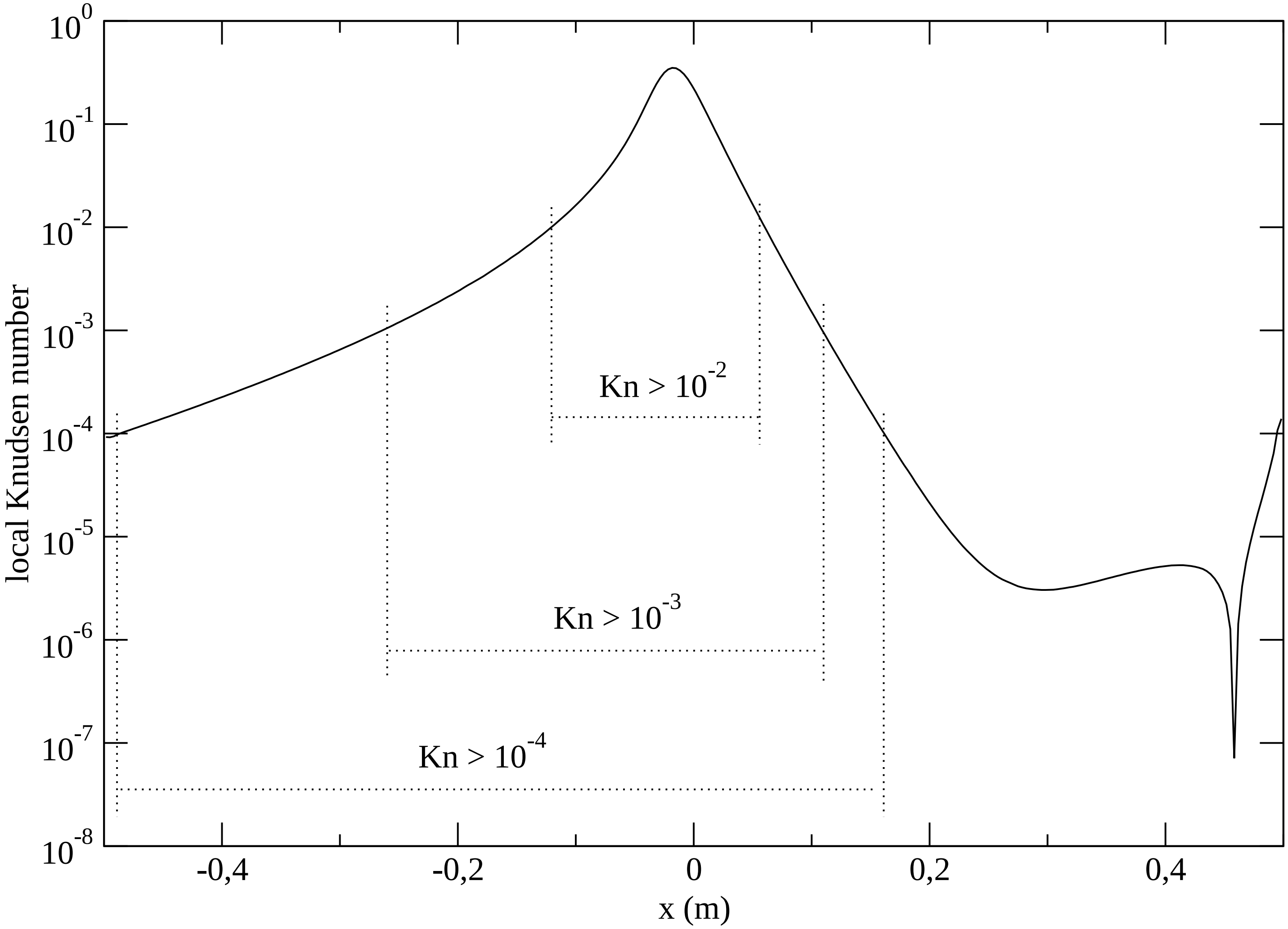
fluid model (Euler):

$$\partial_t \vec{\rho} + \partial_x F(\vec{\rho}) = 0,$$

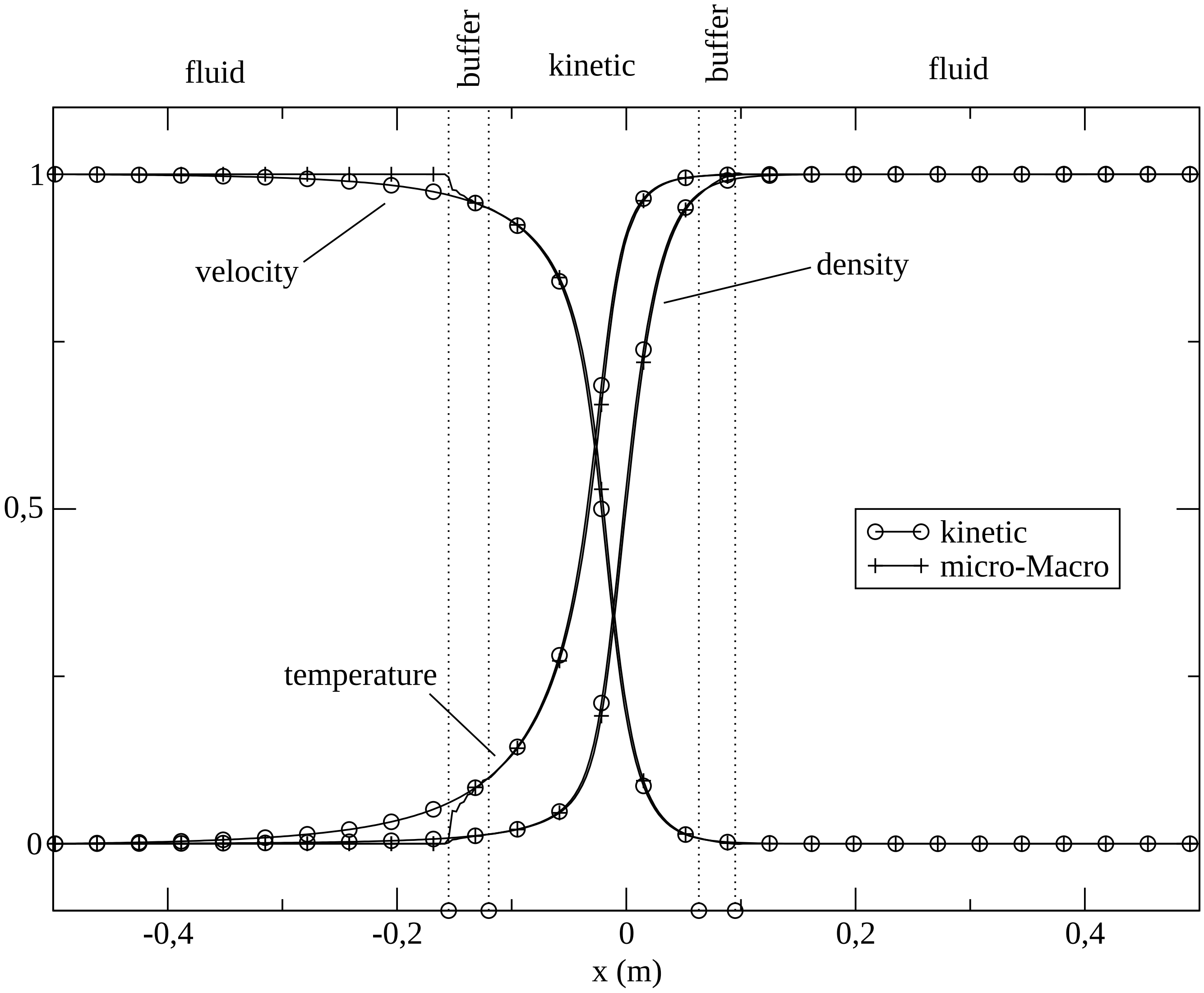
coupled model:

$$\partial_t \vec{\rho} + \partial_x F(\vec{\rho}) + \partial_x \langle v \vec{m} g_K \rangle = 0,$$

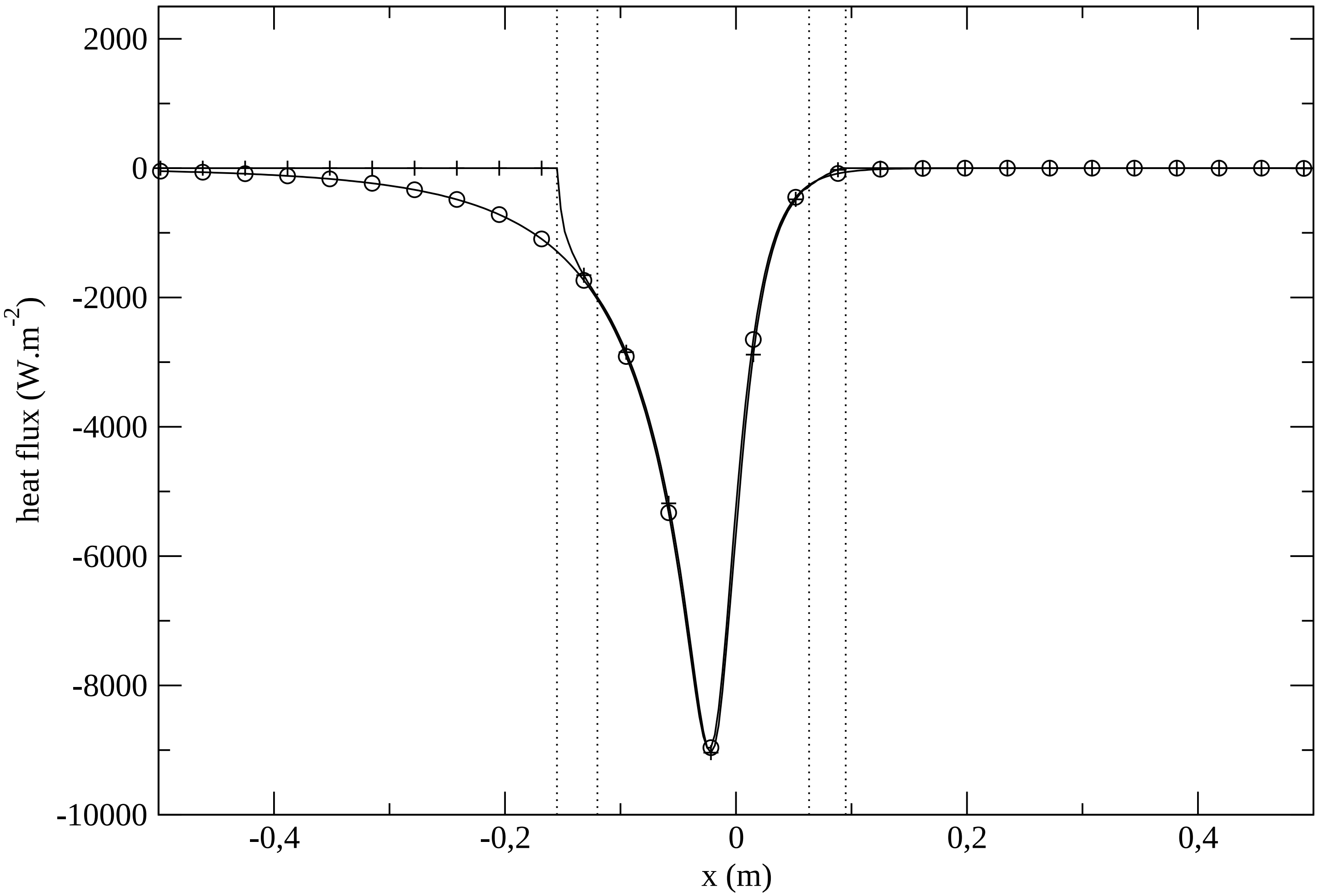
$$\partial_t g_K + h v \partial_x g_K = -\frac{1}{\varepsilon} \nu g_K - h(\partial_t + v \partial_x) E[\vec{\rho}],$$



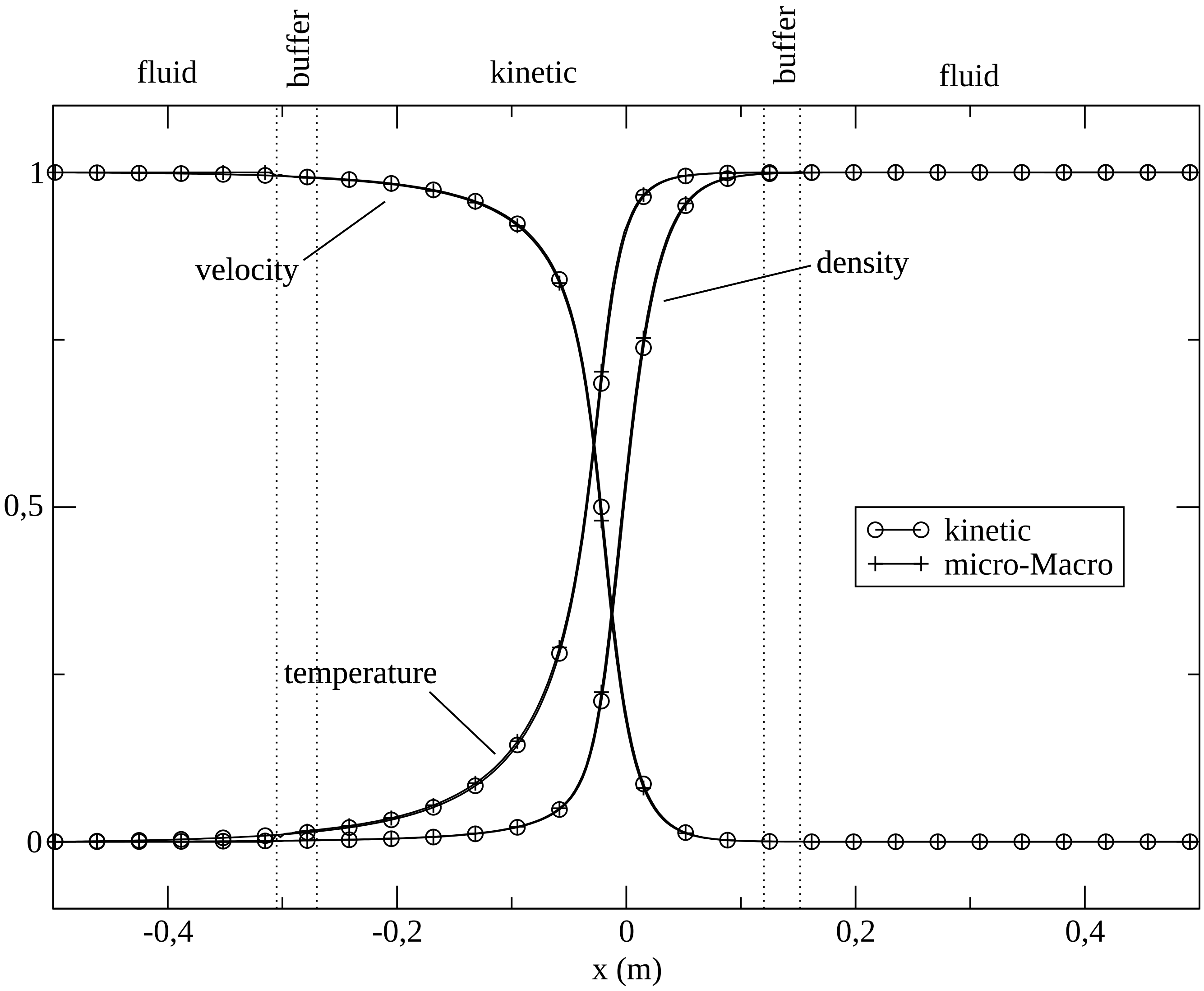
Local Knudsen number for the stationary normal shock wave (in log scale). The three zones where the kinetic upscaling will be used are represented by dotted lines



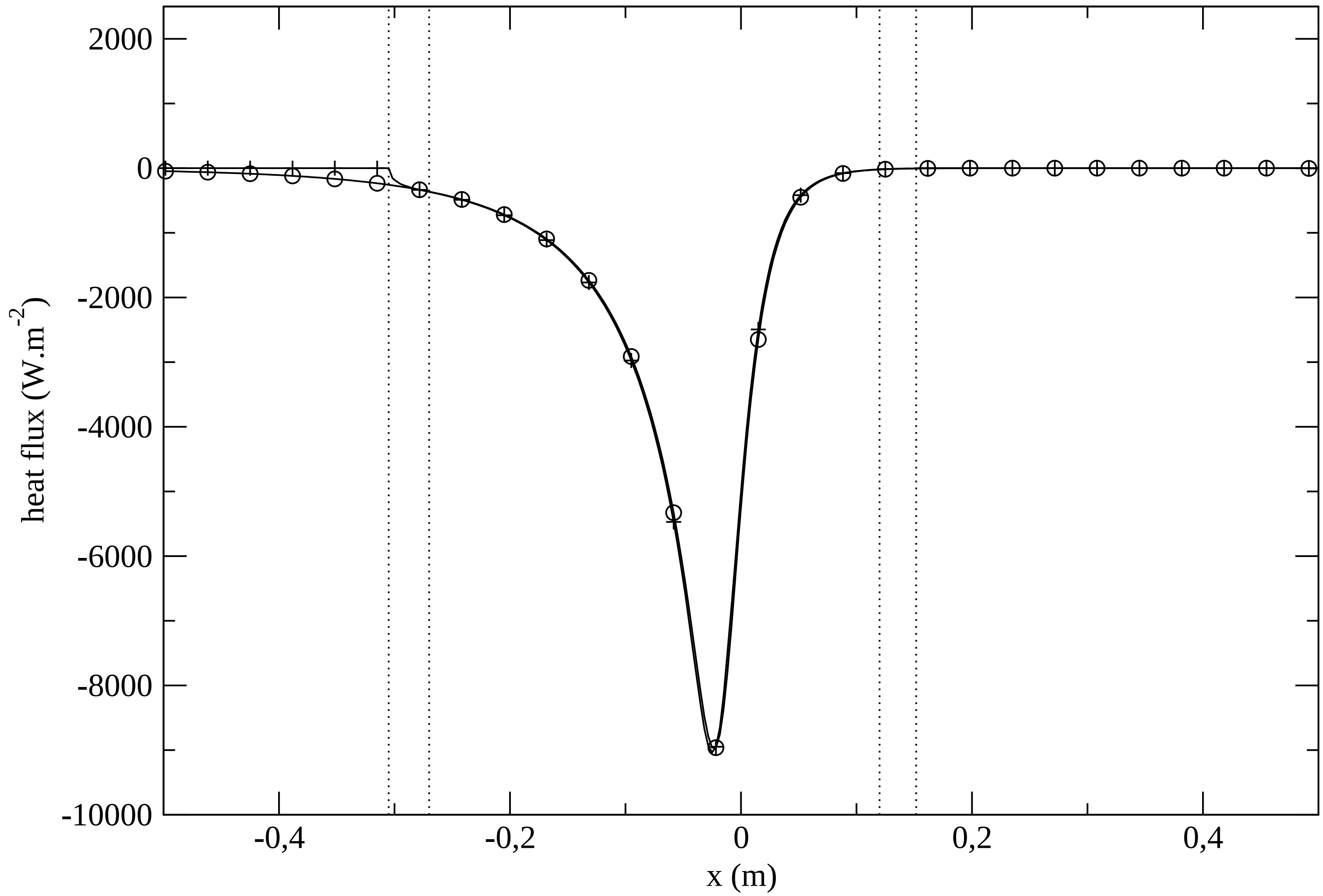
Density, velocity and temperature for the stationary normal shock wave. Comparison of the full kinetic BGK equation to the micro-Macro model with a kinetic zone defined by a local Knudsen number greater than 10^{-2}.



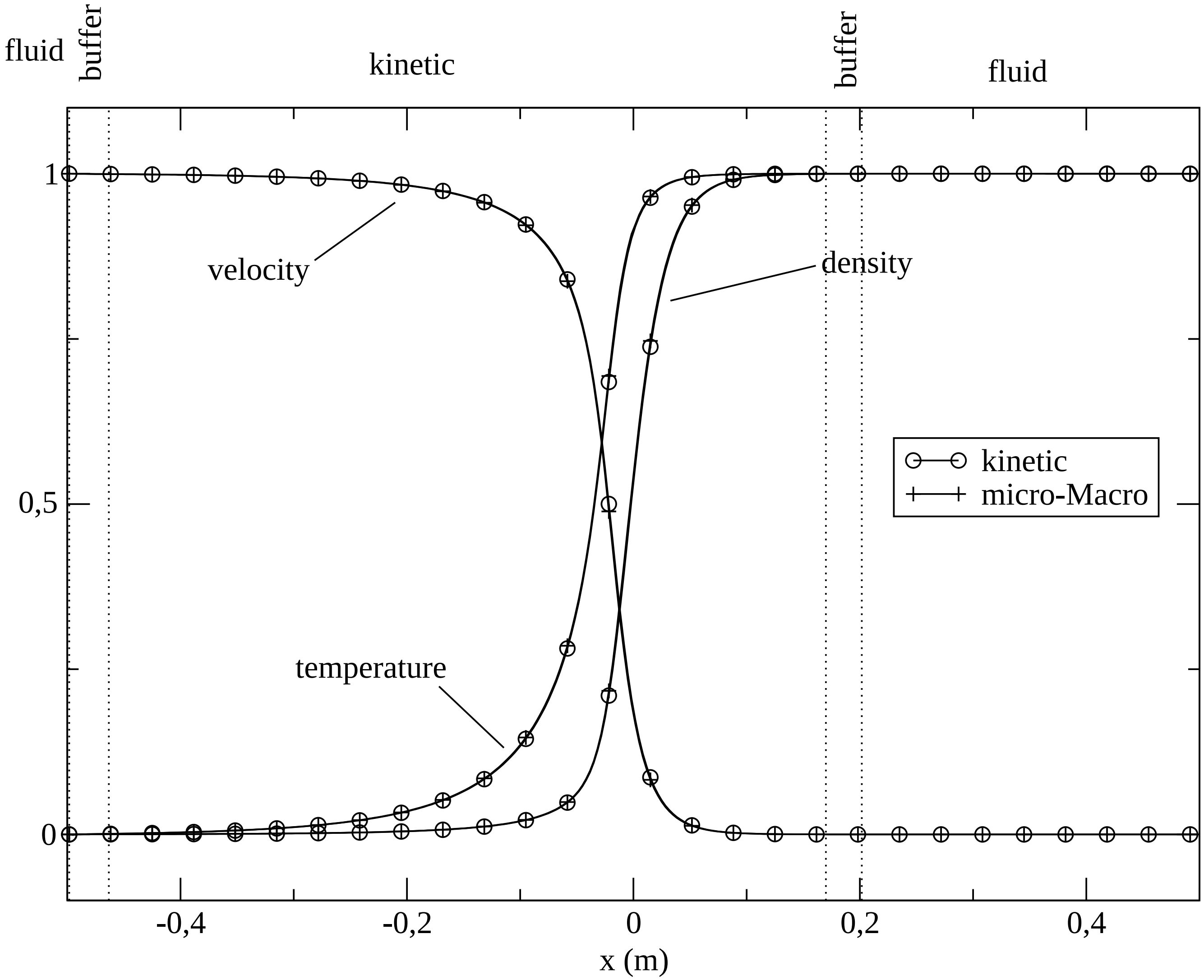
heat flux (bottom) for the stationary normal shock wave. Comparison of the full kinetic BGK equation to the micro-Macro model with a kinetic zone defined by a local Knudsen number greater than 10^{-2}.



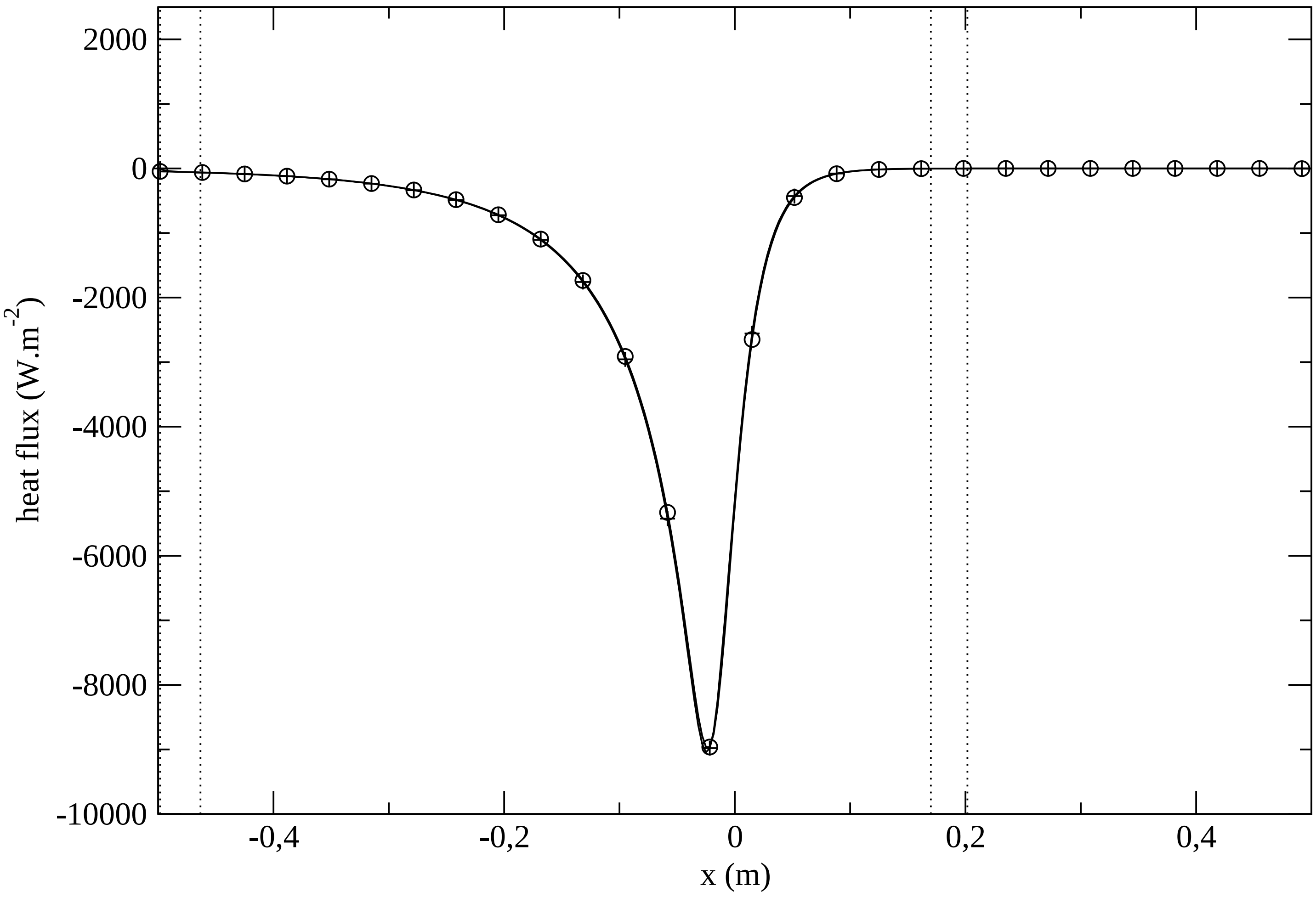
Density, velocity and temperature for the stationary normal shock wave. Comparison of the full kinetic BGK equation to the micro-Macro model with a kinetic zone defined by a local Knudsen number greater than 10^{-3}.



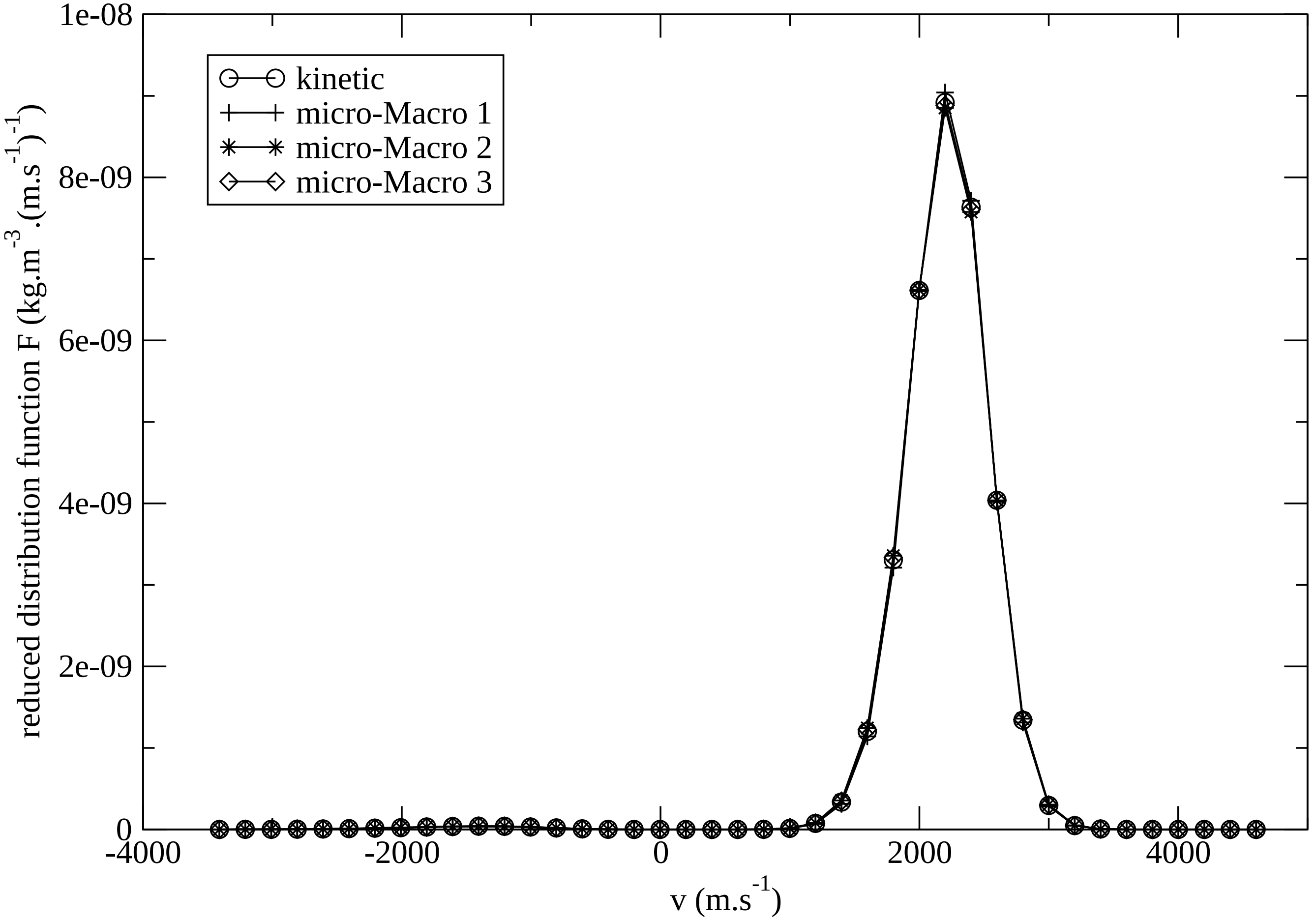
heat flux (bottom) for the stationary normal shock wave. Comparison of the full kinetic BGK equation to the micro-Macro model with a kinetic zone defined by a local Knudsen number greater than 10^{-3}.



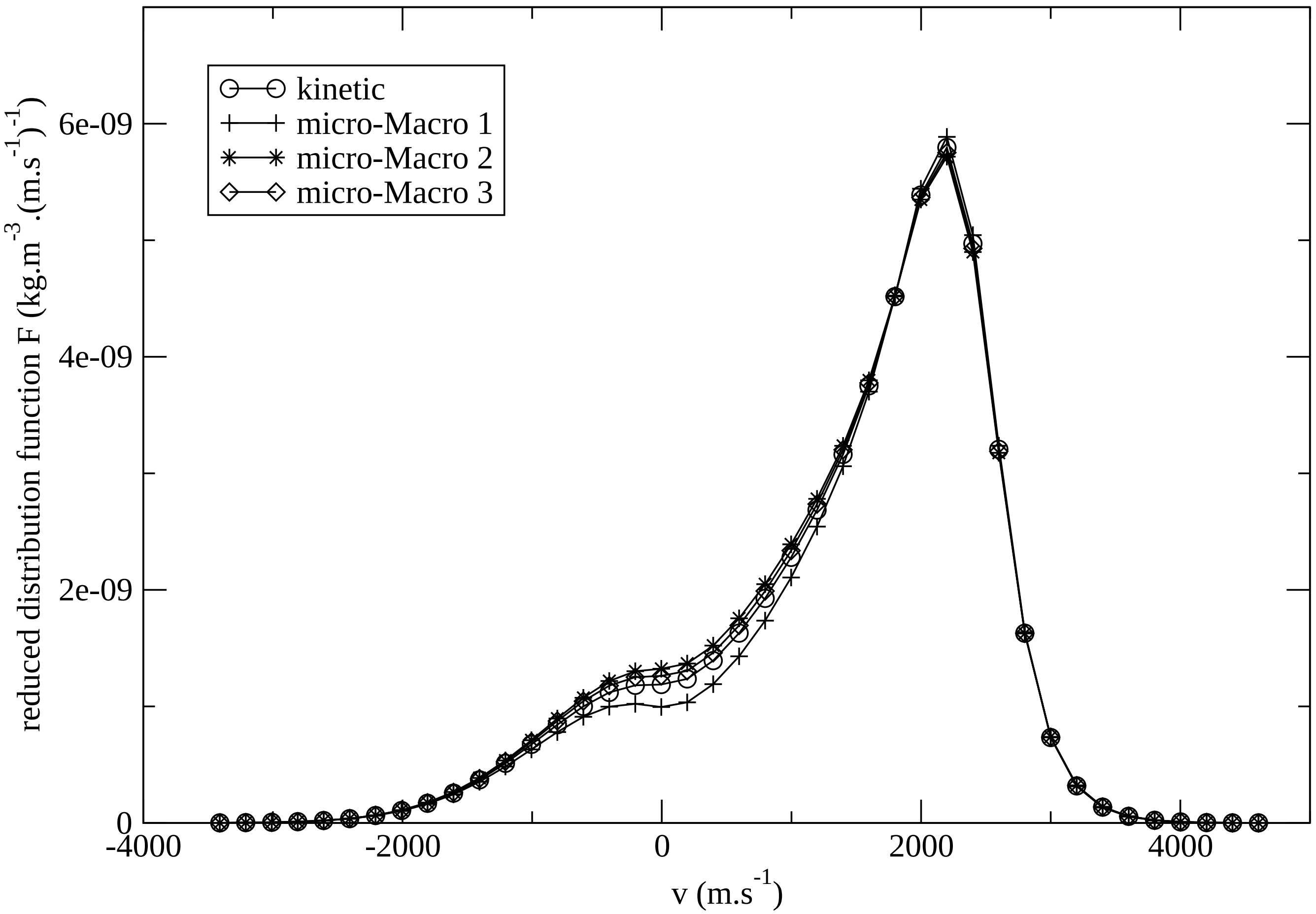
Density, velocity and temperature for the stationary normal shock wave. Comparison of the full kinetic BGK equation to the micro-Macro model with a kinetic zone defined by a local Knudsen number greater than 10^{-4}.



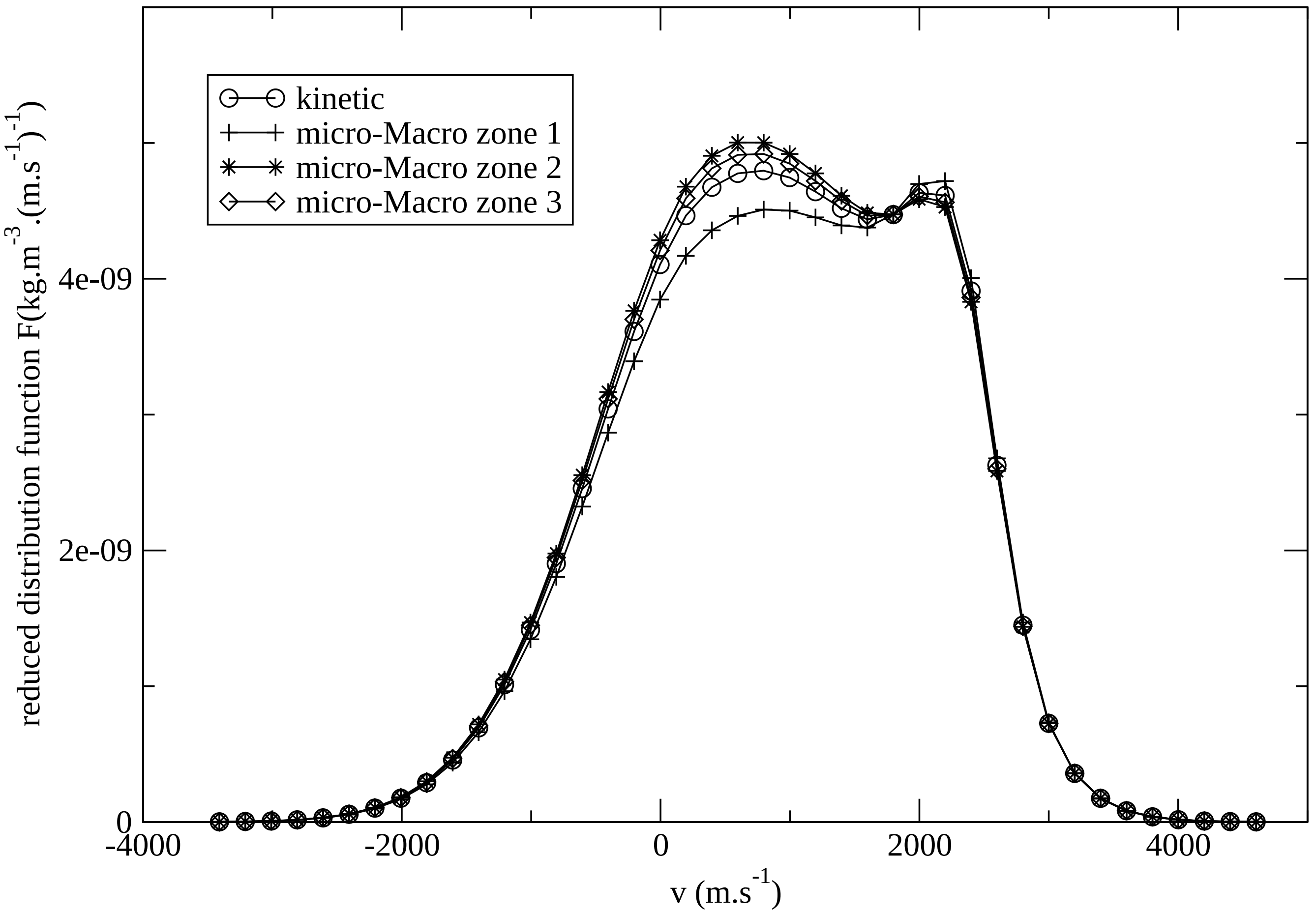
heat flux (bottom) for the stationary normal shock wave. Comparison of the full kinetic BGK equation to the micro-Macro model with a kinetic zone defined by a local Knudsen number greater than 10^{-4}.



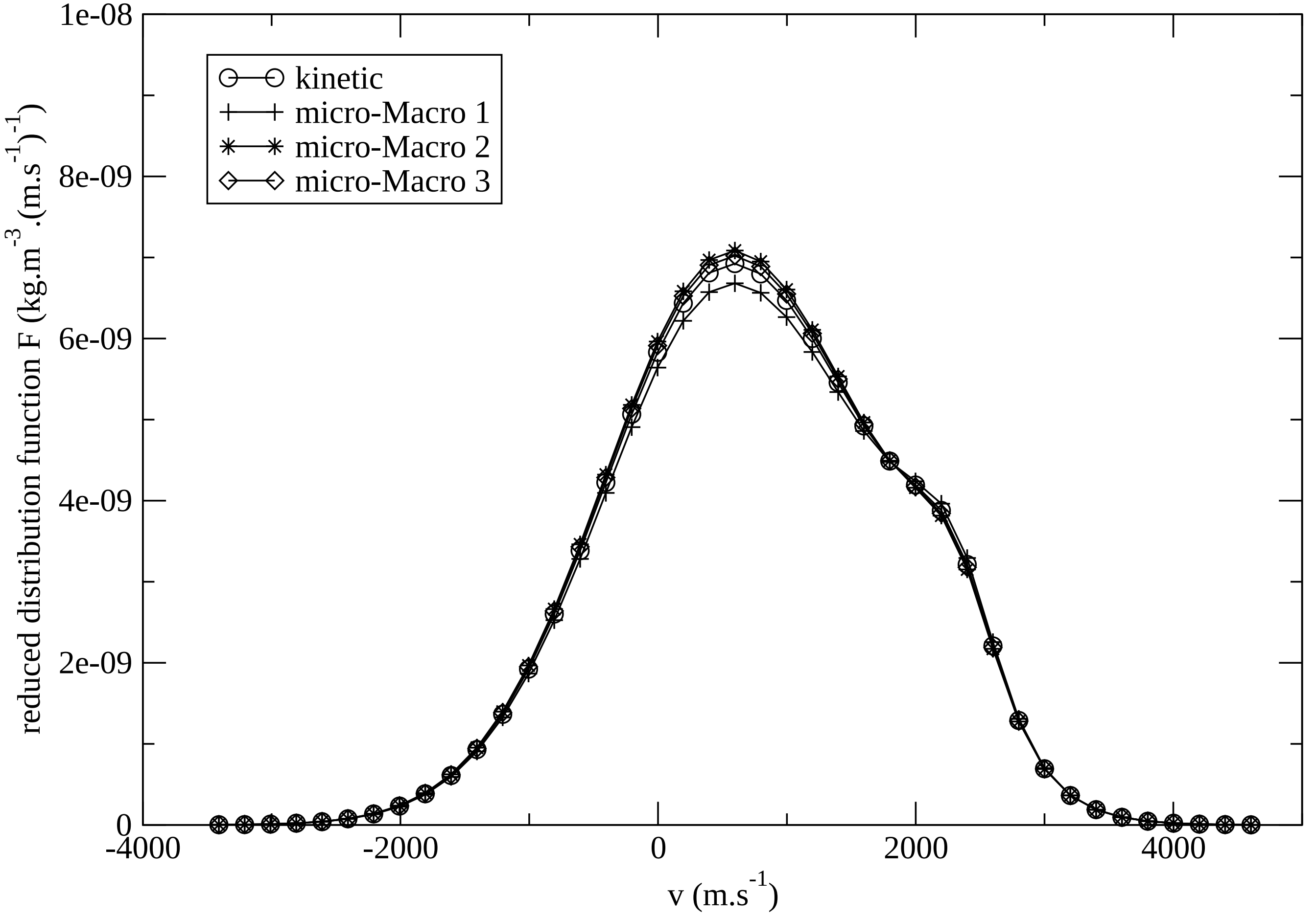
Stationary normal shock wave problem: reduced distribution function $F(x, v)$ at $x = -0.1383$ m (upstream) for BGK and micro-Macro model used with three different kinetic zones (1: $Kn > 10^{-2}$, 2: $Kn > 10^{-2}$, 3: $Kn > 10^{-2}$).



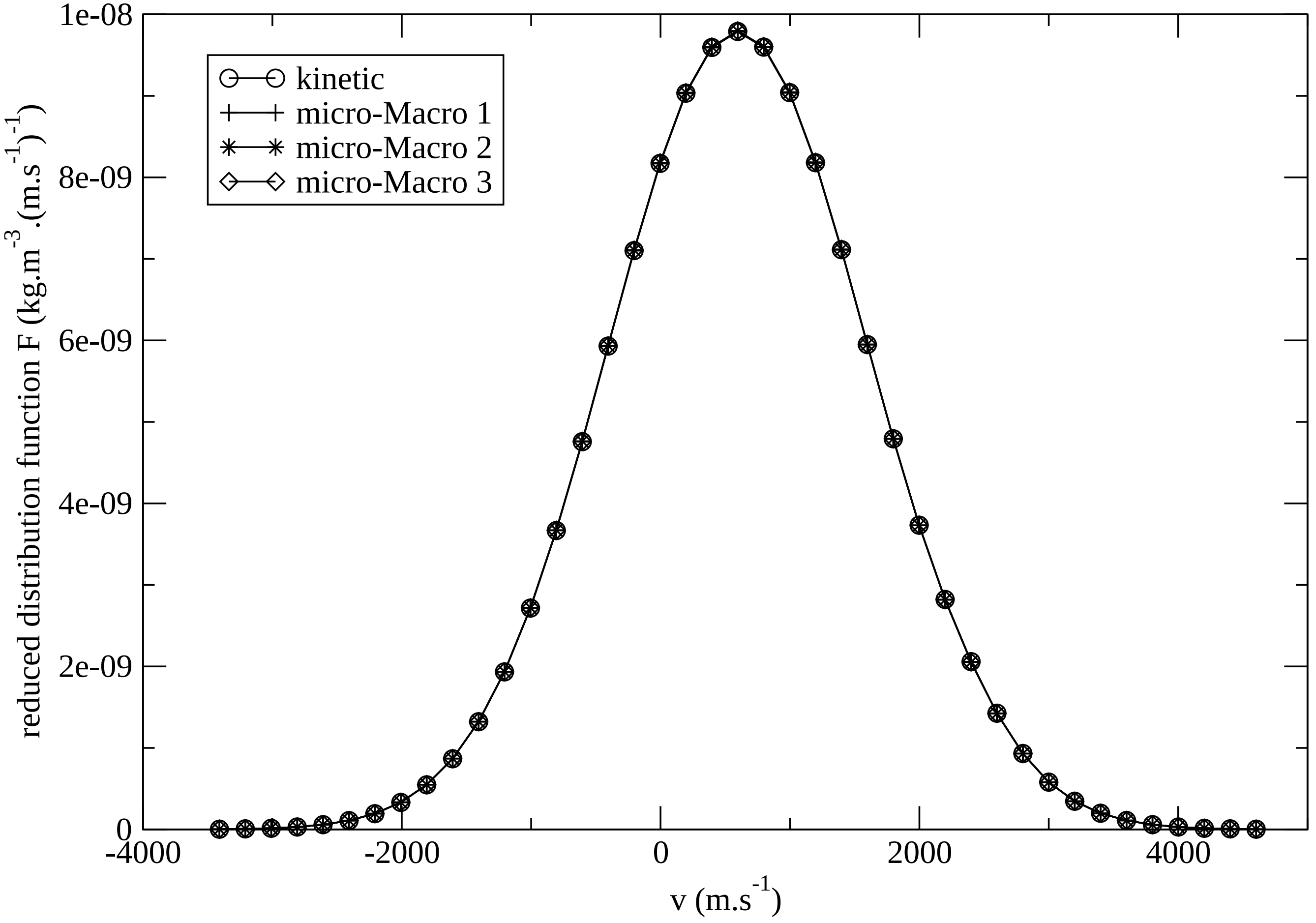
Stationary normal shock wave problem: reduced distribution function $F(x, v)$ at $x = -0.0217$ m (left part of the shock) for BGK and micro-Macro model used with three different kinetic zones (1: $Kn > 10^{-2}$, 2: $Kn > 10^{-2}$, 3: $Kn > 10^{-2}$).



Stationary normal shock wave problem: reduced distribution function $F(x, v)$ at $x = 0$ m (in the shock) for BGK and micro-Macro model used with three different kinetic zones (1: $Kn > 10^{-2}$, 2: $Kn > 10^{-2}$, 3: $Kn > 10^{-2}$).



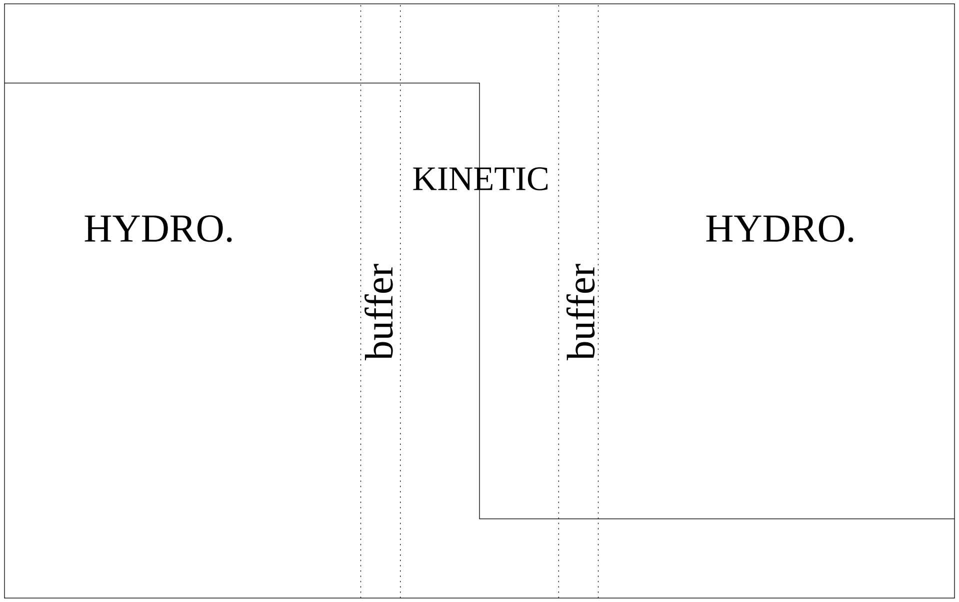
Stationary normal shock wave problem: reduced distribution function $F(x, v)$ at $x = 0.0117$ m (right part of the shock) for BGK and micro-Macro model used with three different kinetic zones (1: $Kn > 10^{-2}$, 2: $Kn > 10^{-2}$, 3: $Kn > 10^{-2}$).

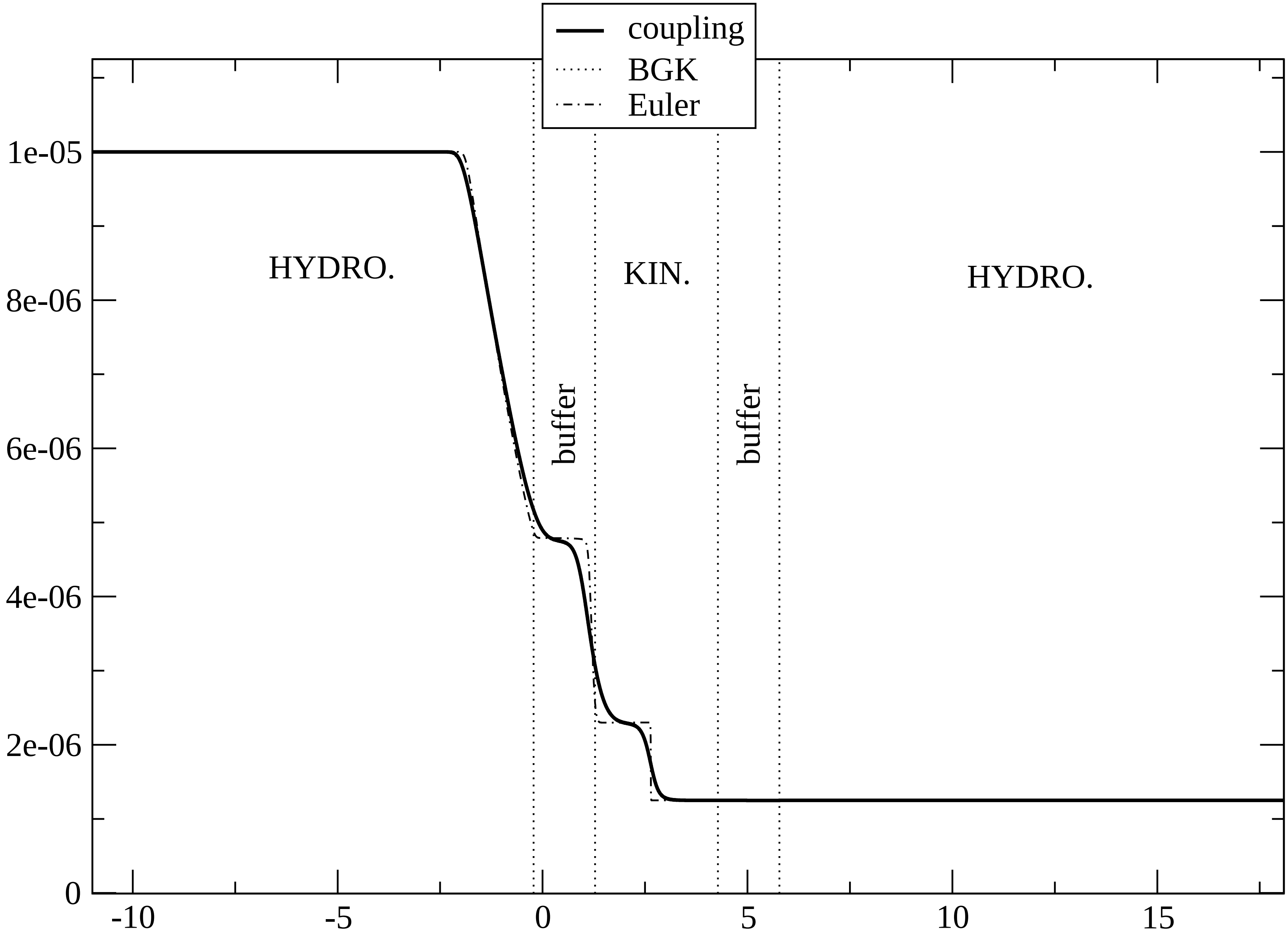


Stationary normal shock wave problem: reduced distribution function $F(x, v)$ at $x = 0.0717$ m (downstream) for BGK and micro-Macro model used with three different kinetic zones (1: $Kn > 10^{-2}$, 2: $Kn > 10^{-2}$, 3: $Kn > 10^{-2}$).

NUMERICAL RESULTS

- Sod problem:
- The interface moves at the shock speed
- two buffer zones
- 10.000 cells in space, 100 in velocity




coupling
BGK
Euler
HYDRO.
KIN.
HYDRO.
buffer
buffer
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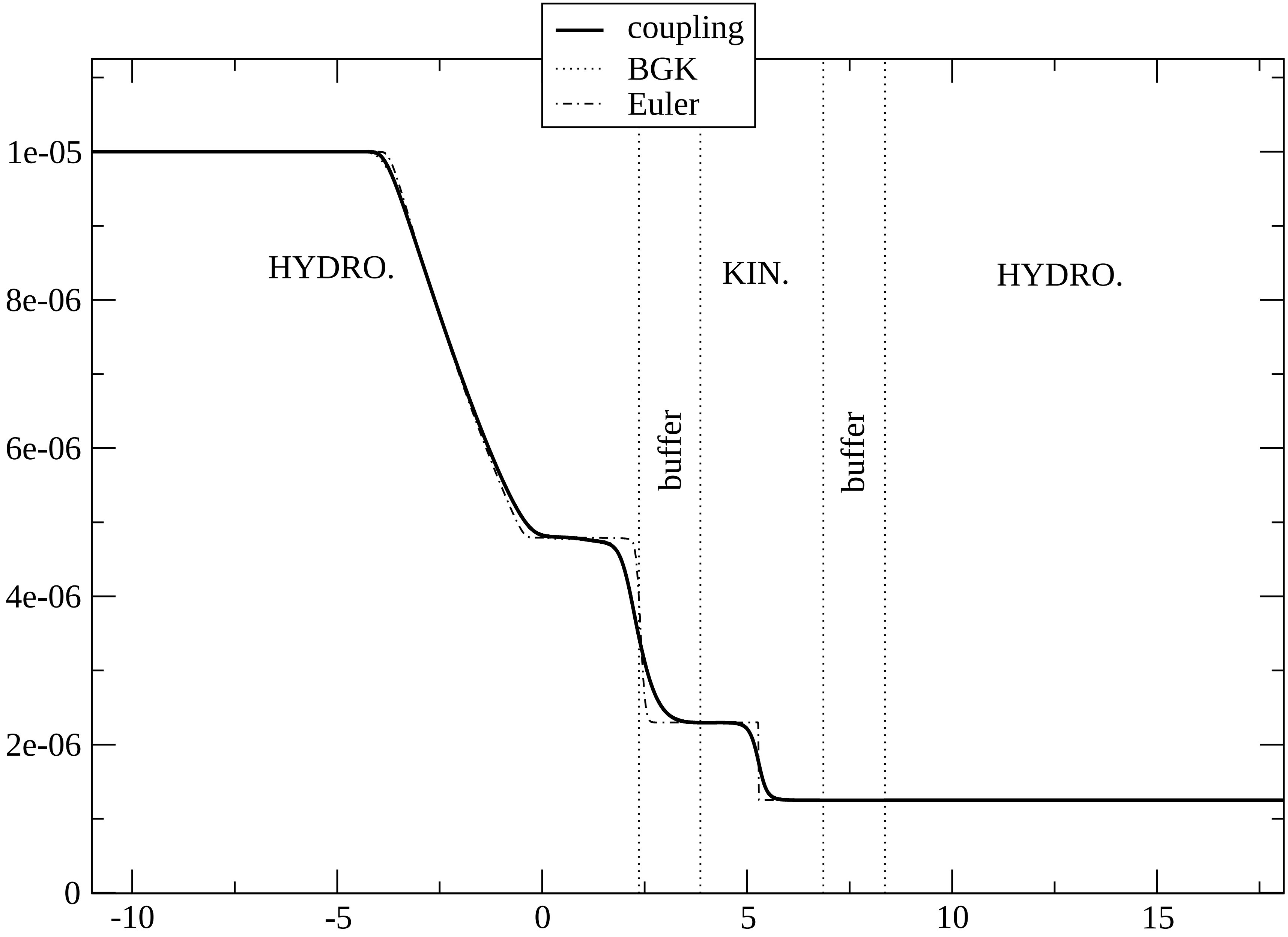
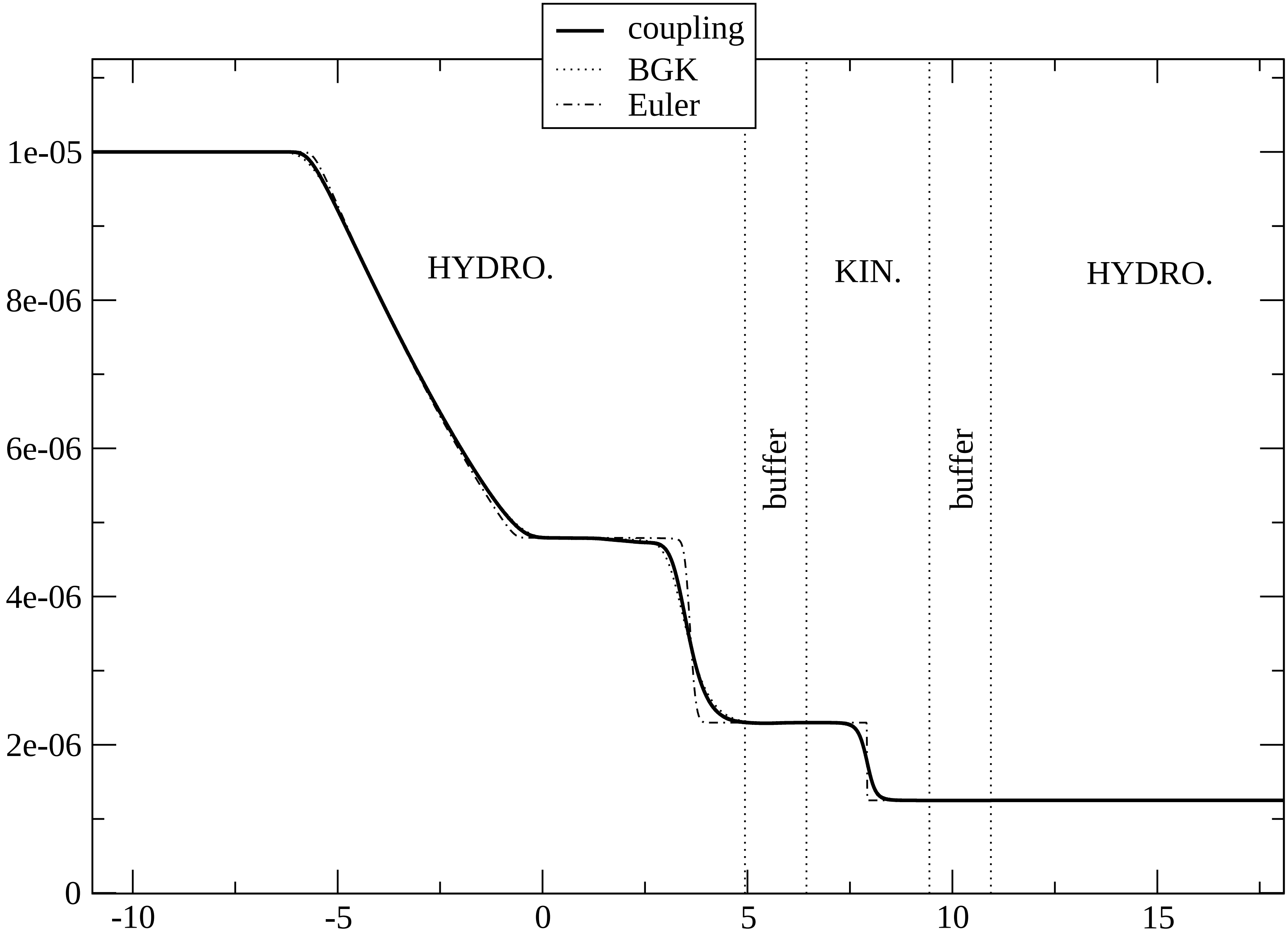
8e-06
6e-06
4e-06
2e-06
0
-10
-5
0
5
10
15


coupling
BGK
Euler
1e-05
8e-06
6e-06
4e-06
2e-06
0
-10
-5
0
5
10
15
HYDRO.
KIN.
HYDRO.
buffer
buffer


coupling
BGK
Euler
HYDRO.
KIN.
HYDRO.
buffer
buffer
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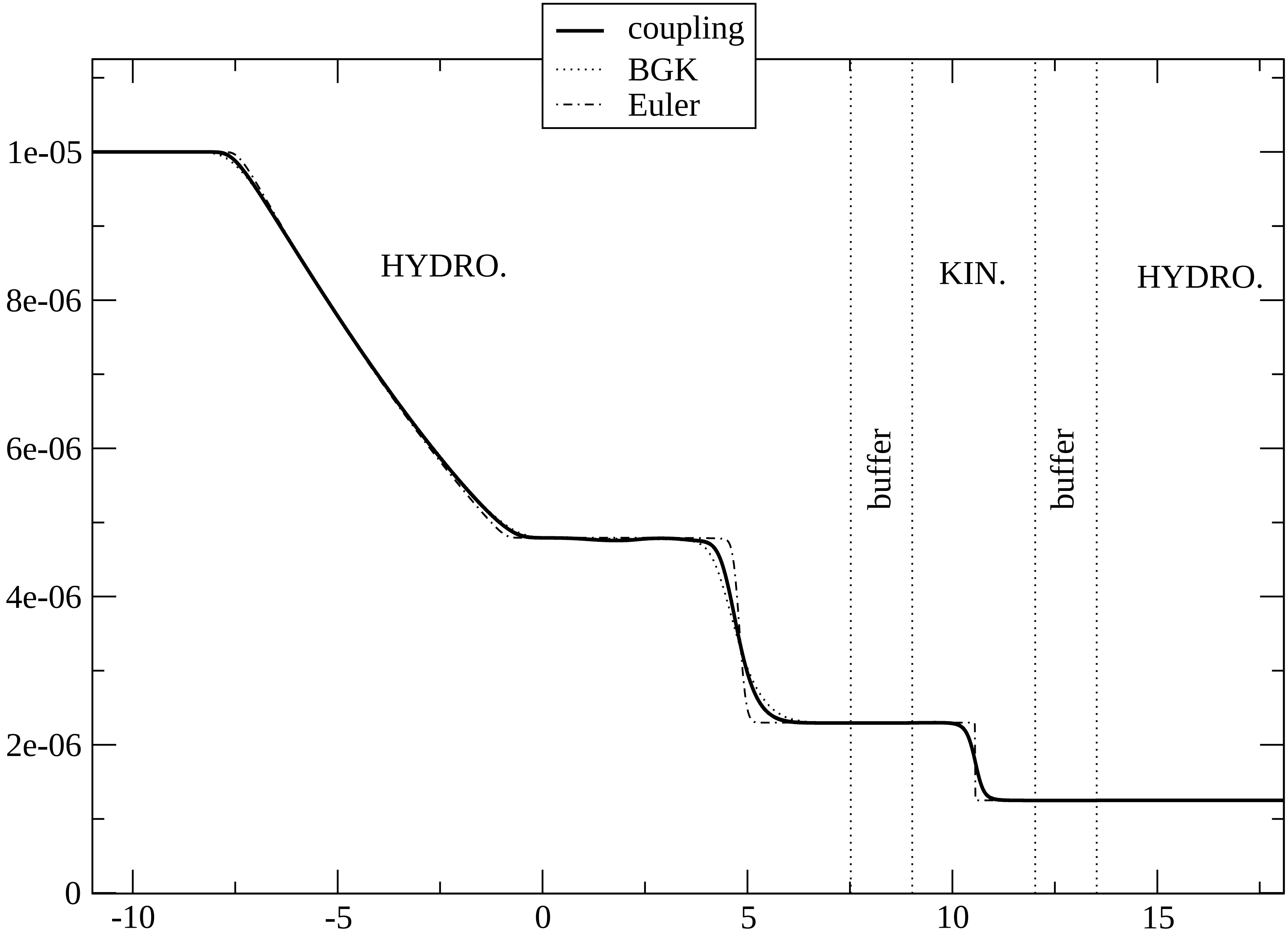
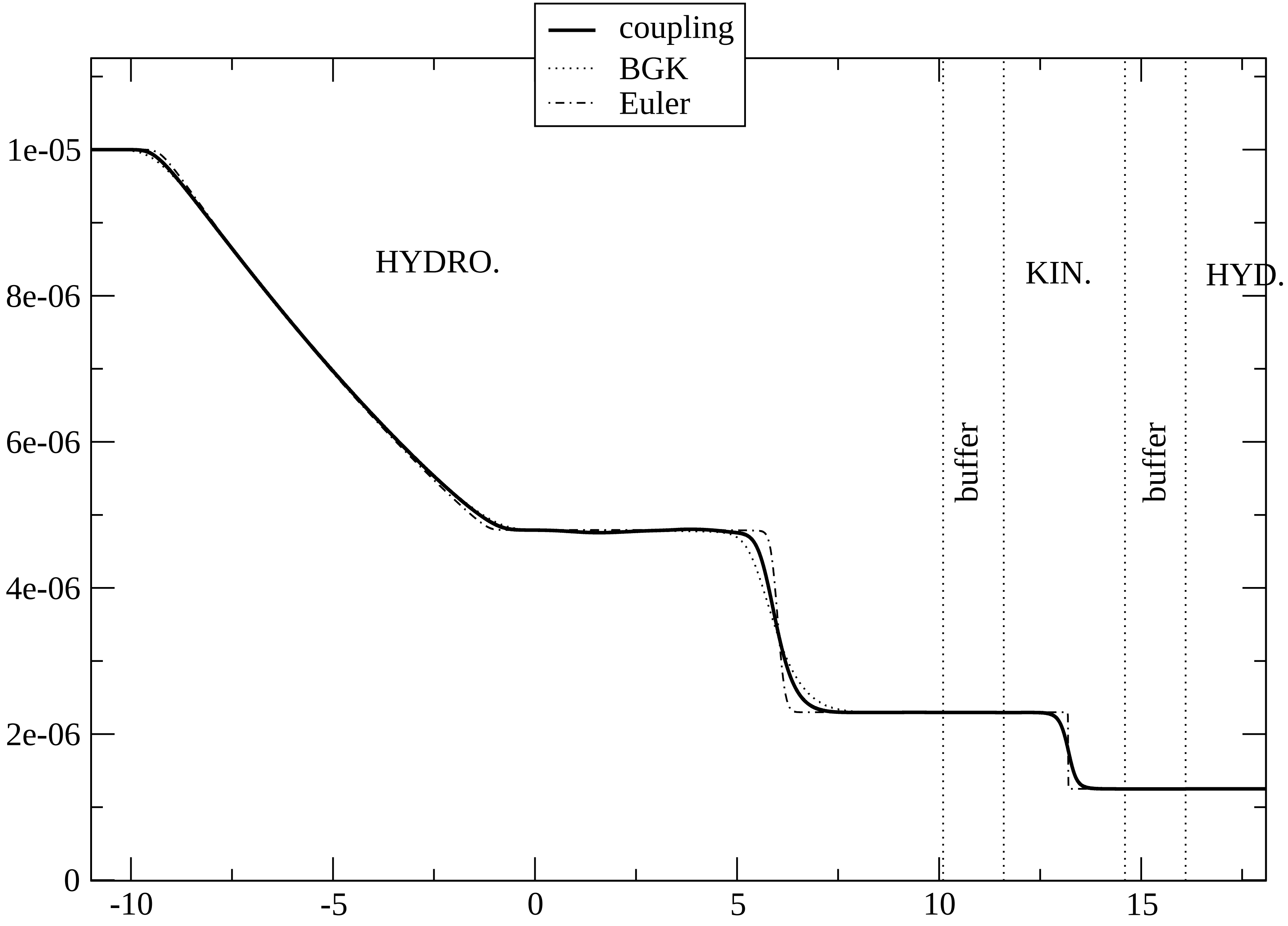
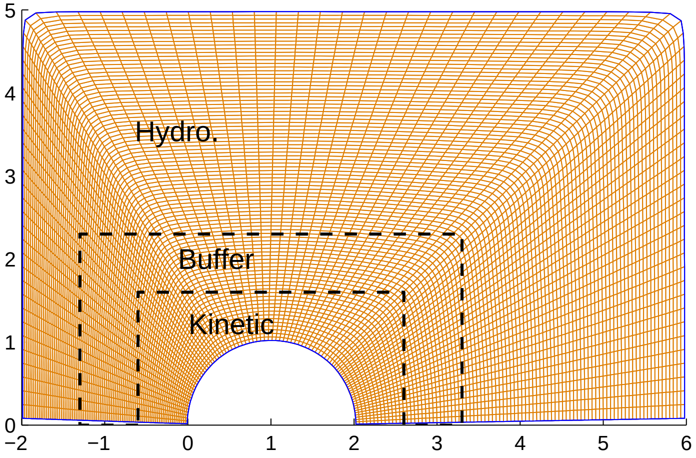
8e-06
6e-06
4e-06
2e-06
0
-10
-5
0
5
10
15

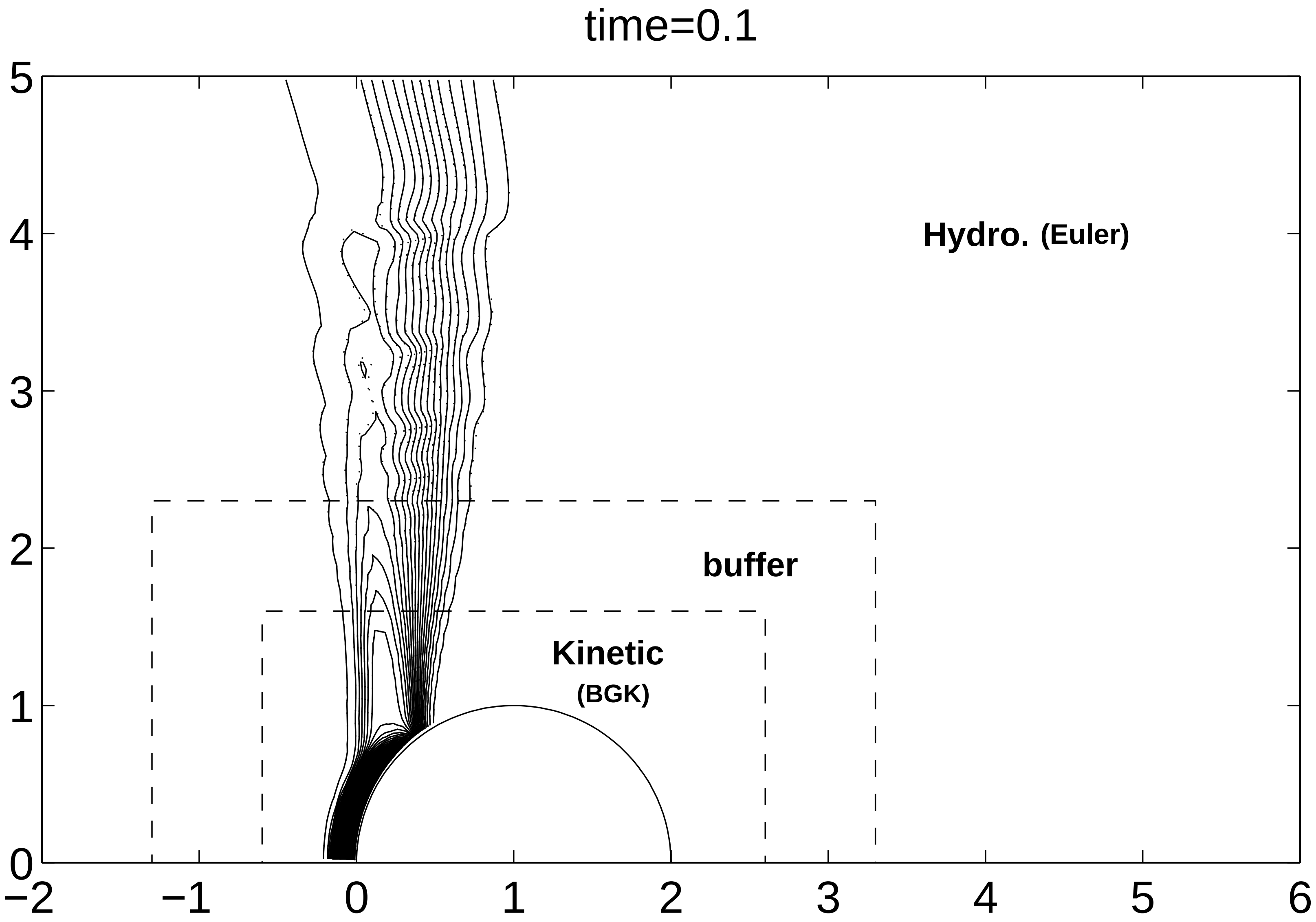

coupling
BGK
Euler
HYDRO.
buffer
KIN.
buffer
HYDRO.
1e-05
8e-06
6e-06
4e-06
2e-06
0
-10
-5
0
5
10
15

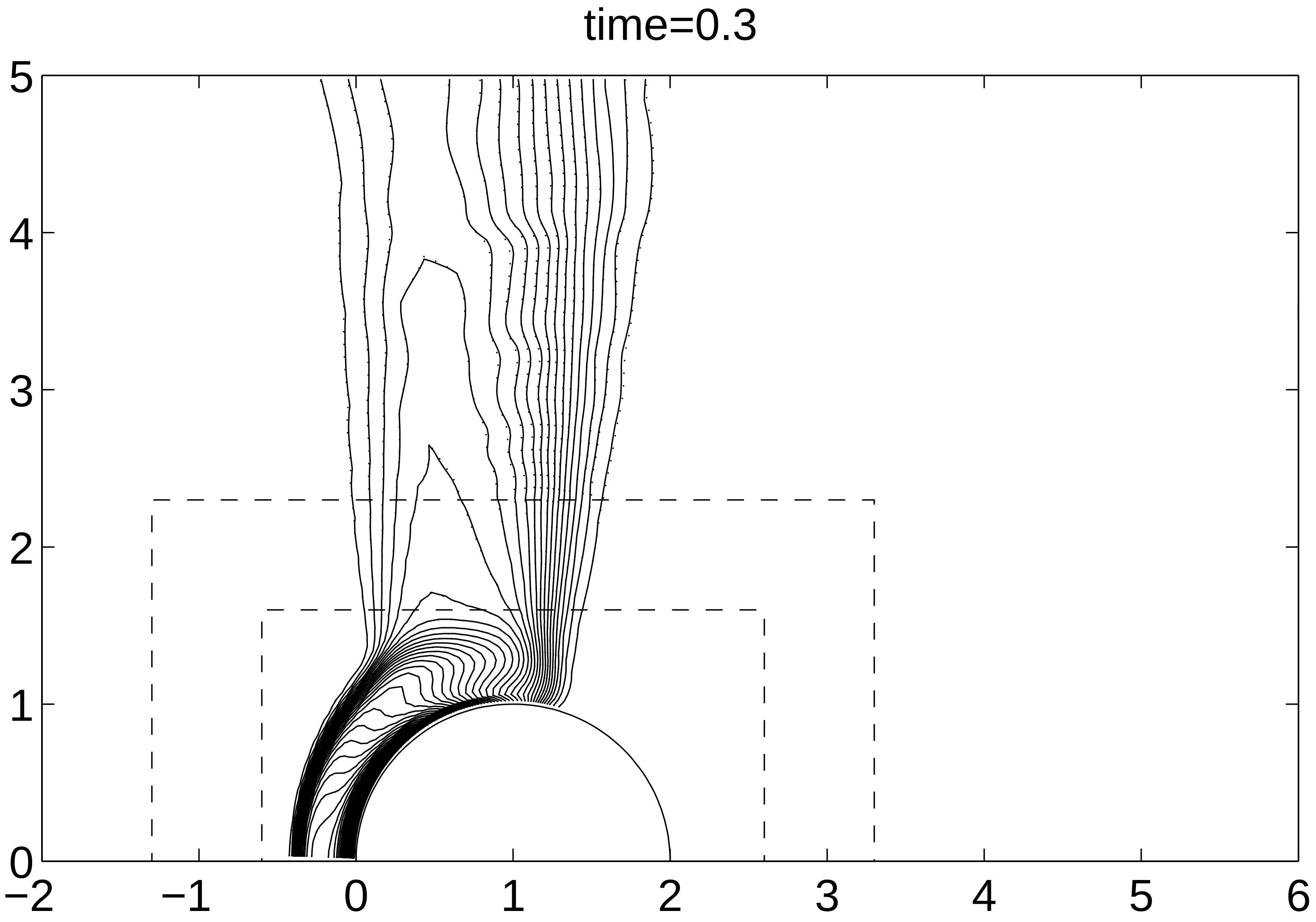

coupling
BGK
Euler
1e-05
8e-06
6e-06
4e-06
2e-06
0
-10
-5
0
5
10
15
HYDRO.
KIN.
HYD.
buffer
buffer

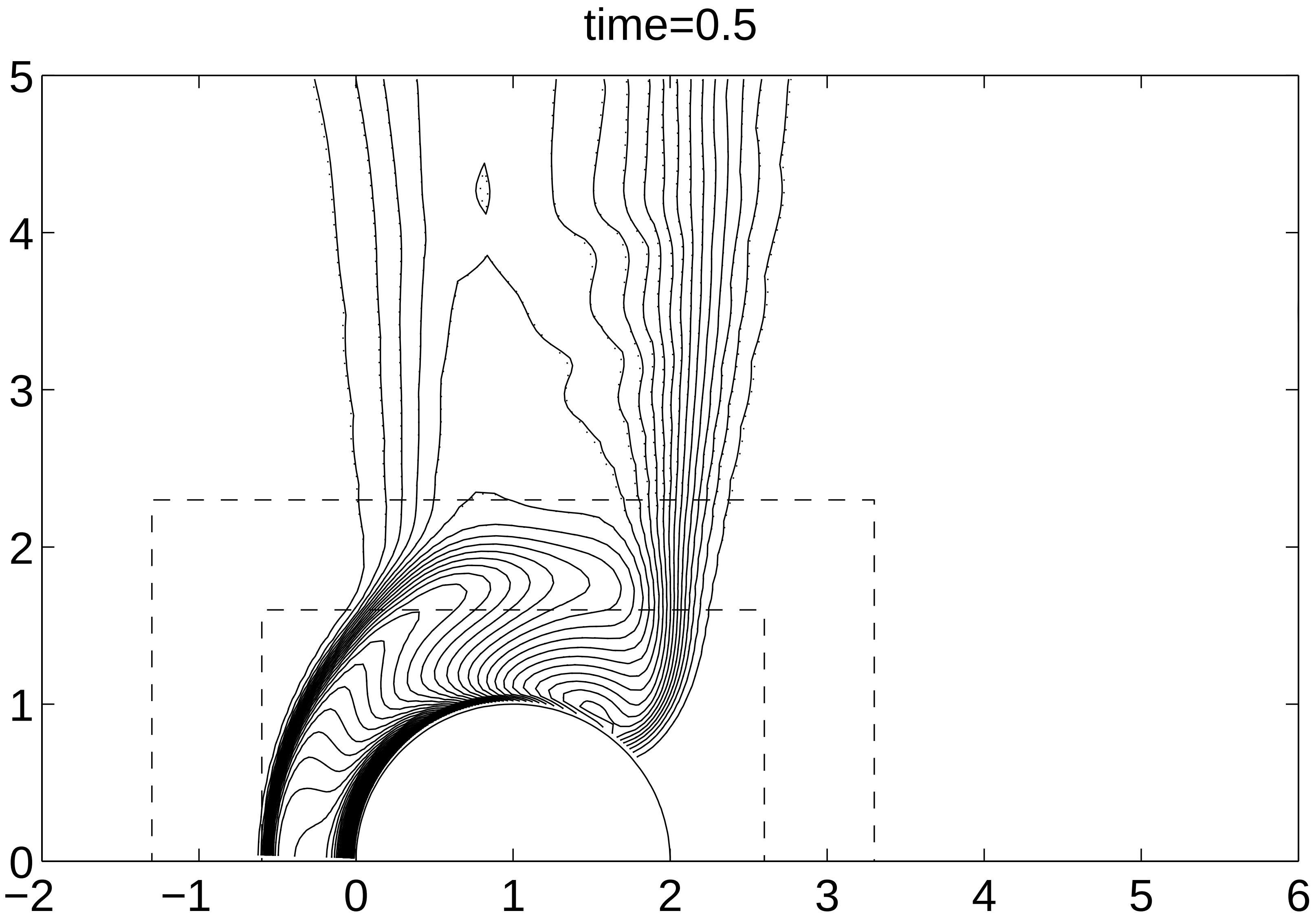
NUMERICAL RESULTS

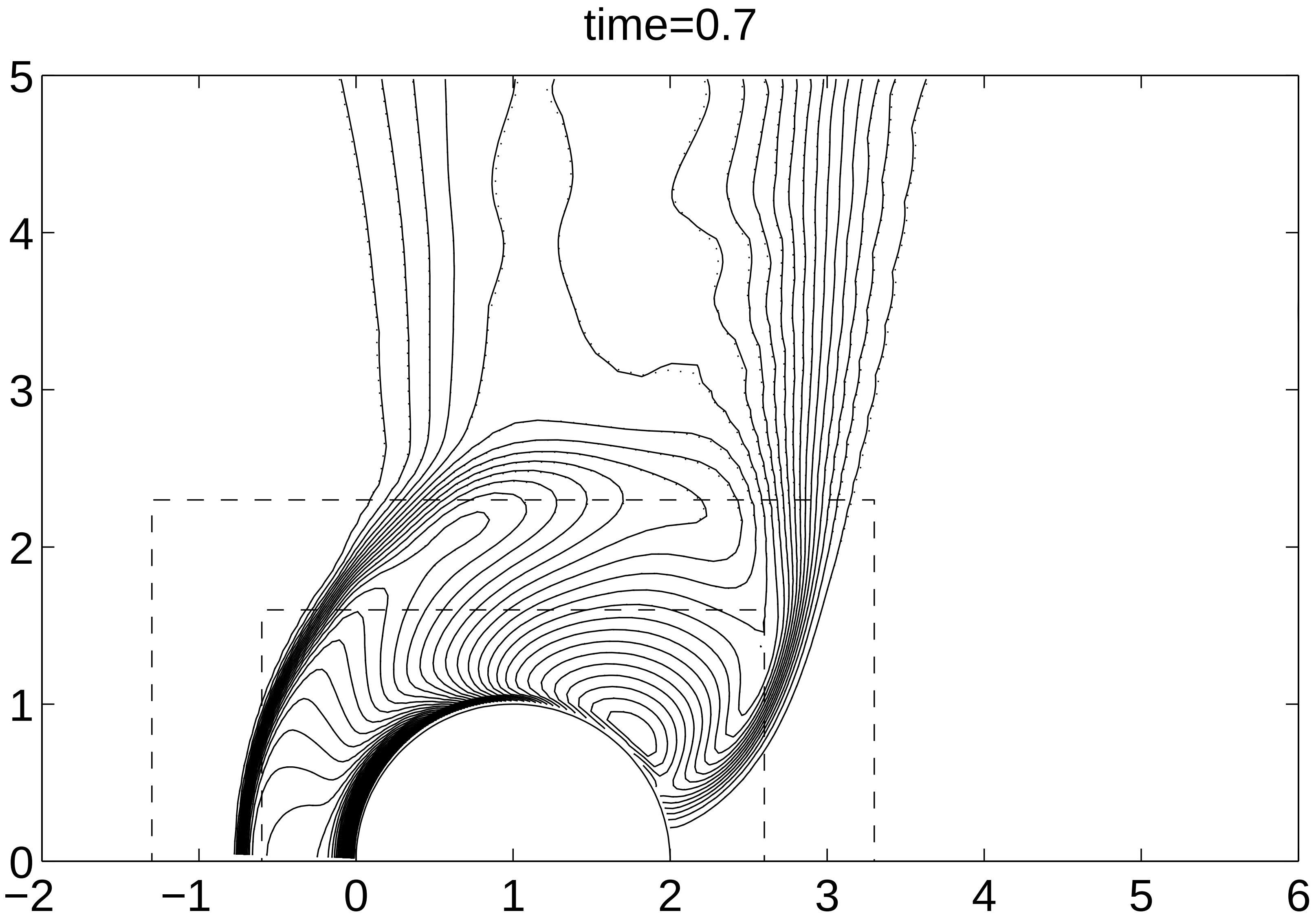
- 2D problem: static coupling BGK/Euler
- idea: boundary layer resolved by the kinetic model
- interface not aligned with the mesh
- coarse mesh (90 × 90 cells, 20 × 20 velocities): too much numerical diffusion to make fair comparisons
- Knudsen=0.005 and Mach shock=2.81.

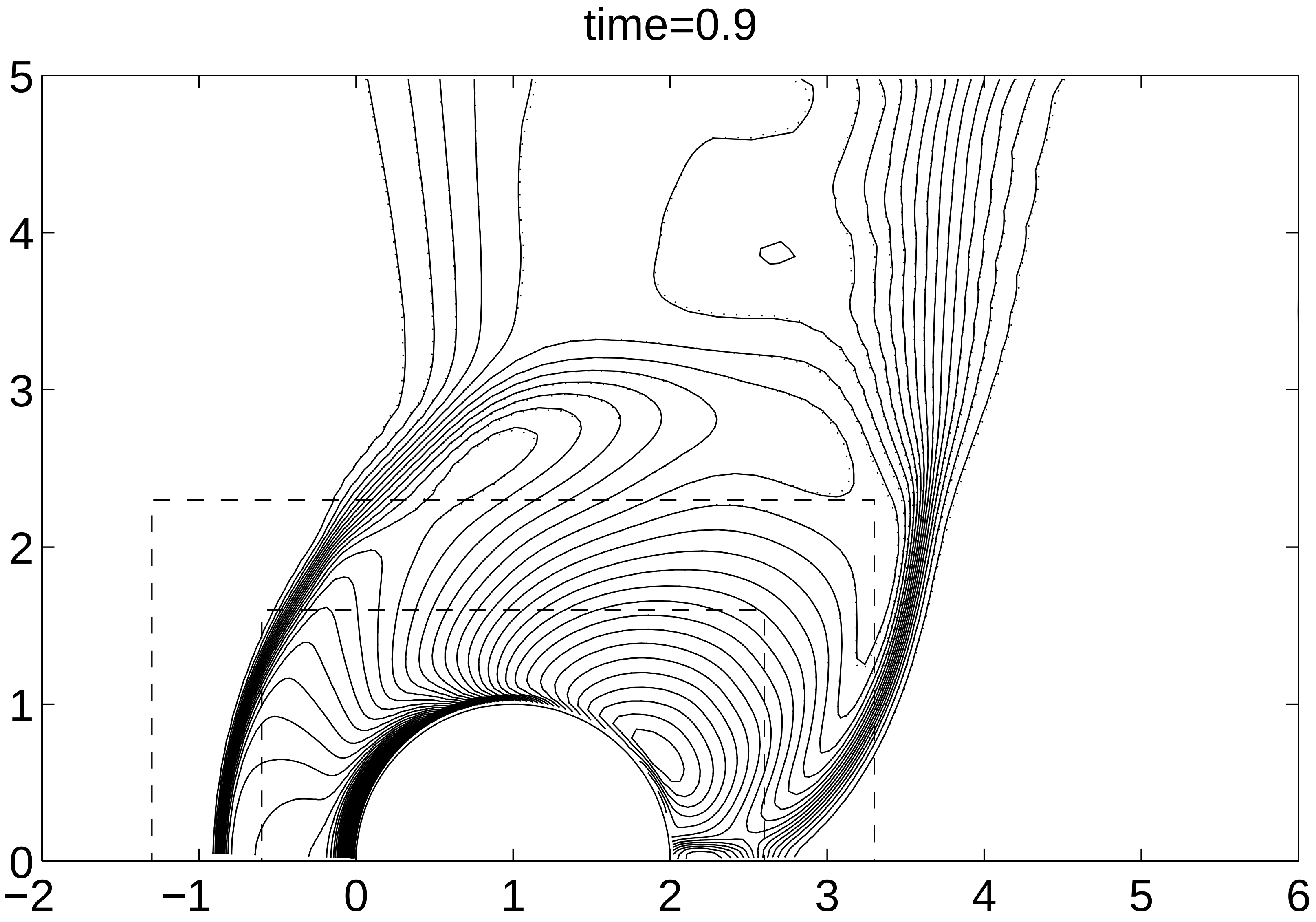



time=0.1
Hydro. (Euler)
buffer
Kinetic
(BGK)
5
4
3
2
1
0
−2
−1
0
1
2
3
4
5
6


time=0.3
5
4
3
2
1
0
−2
−1
0
1
2
3
4
5
6


time=0.5
5
4
3
2
1
0
−2
−1
0
1
2
3
4
5
6


time=0.7
5
4
3
2
1
0
−2
−1
0
1
2
3
4
5
6


time=0.9
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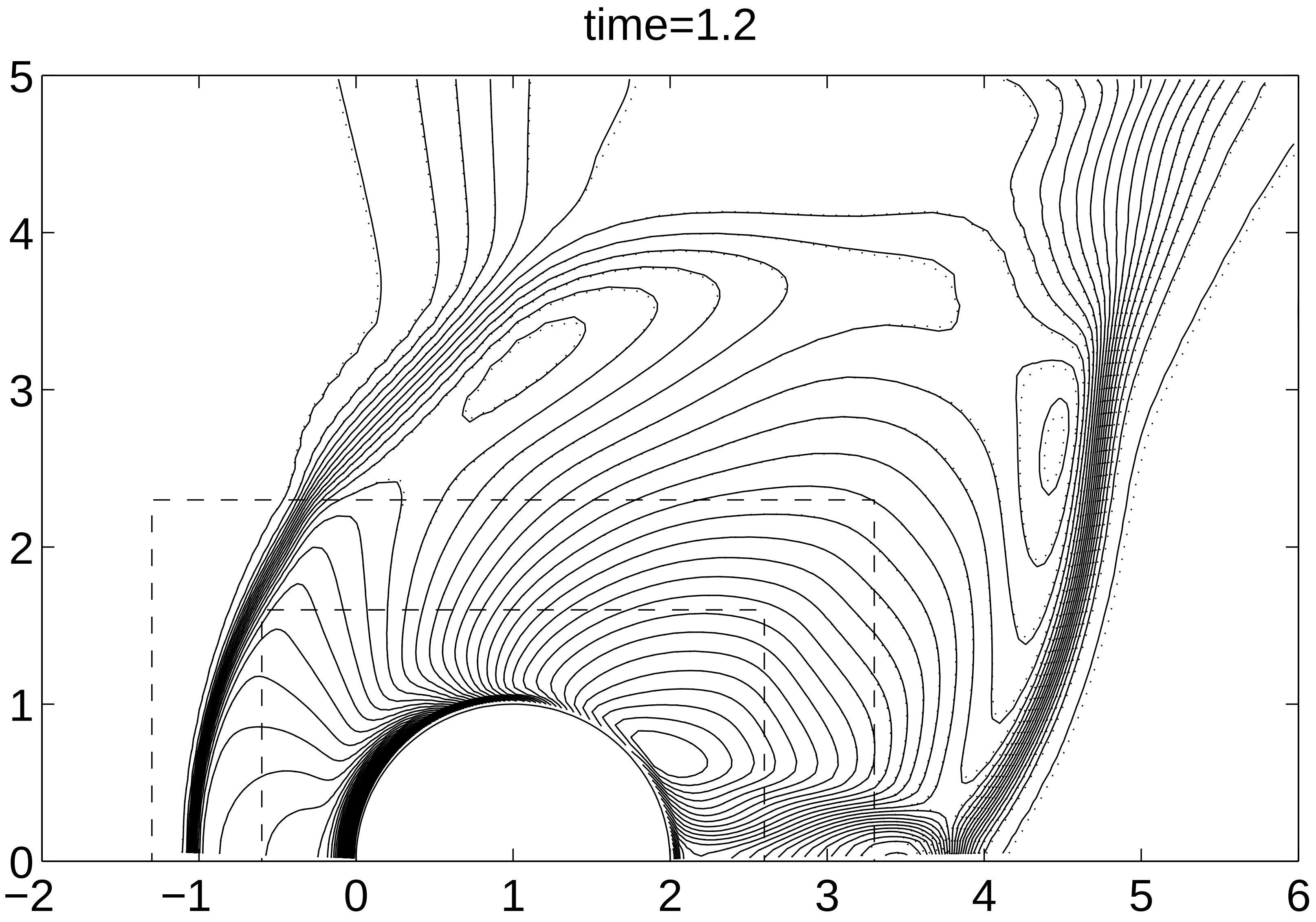
4
3
2
1
0
−2
−1
0
1
2
3
4
5
6


time=1.2
5
4
3
2
1
0
−2
−1
0
1
2
3
4
5
6

FLUID MODELS WITH LOCALIZED KINETIC UPSCALING

example 3: radiative heat transfer

kinetic model:

$$\partial_t T - \partial_{xx} T = -\sigma(B(T) - [I])/\varepsilon^2$$

$$\varepsilon \partial_t I + \mu \partial_x I = \frac{1}{\varepsilon}\sigma(B(T) - I)$$

fluid model:

$$\partial_t (T + B(T)) - \partial_x(\partial_x T + \frac{1}{3\sigma}\partial_x B(T)) = 0.$$

energy conservation equation

$$\partial_t (T + [I]) + \partial_x(-\partial_x T + [\mu I]/\varepsilon) = 0. \tag{3}$$

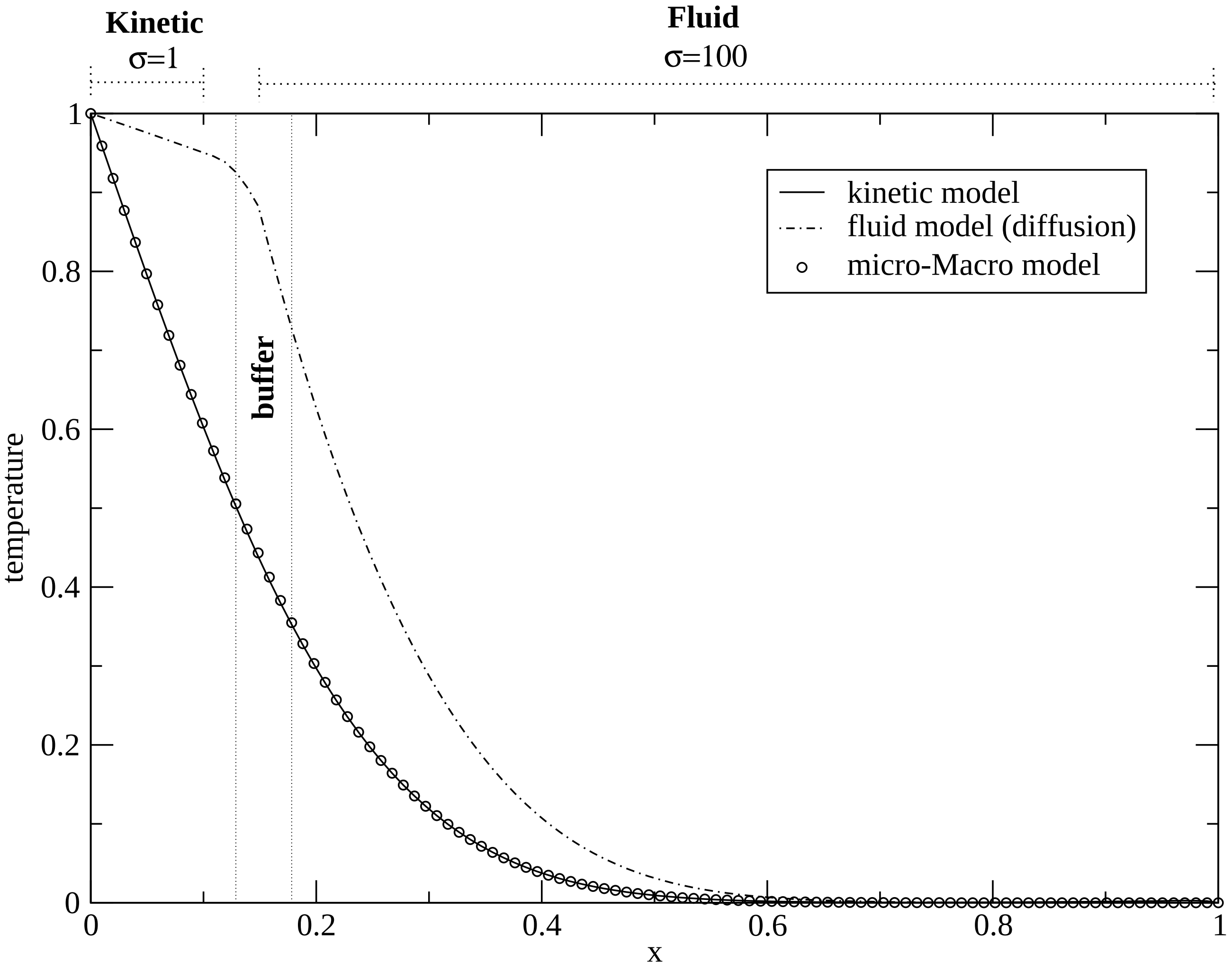
$$I = B(T) - \frac{\varepsilon}{\sigma}\mu \partial_x B(T) + \varepsilon g,$$

$$[I] = B(T) + \varepsilon[g], \quad [\mu I] = \varepsilon([\mu g] - \frac{1}{3\sigma}\partial_x B(T))$$

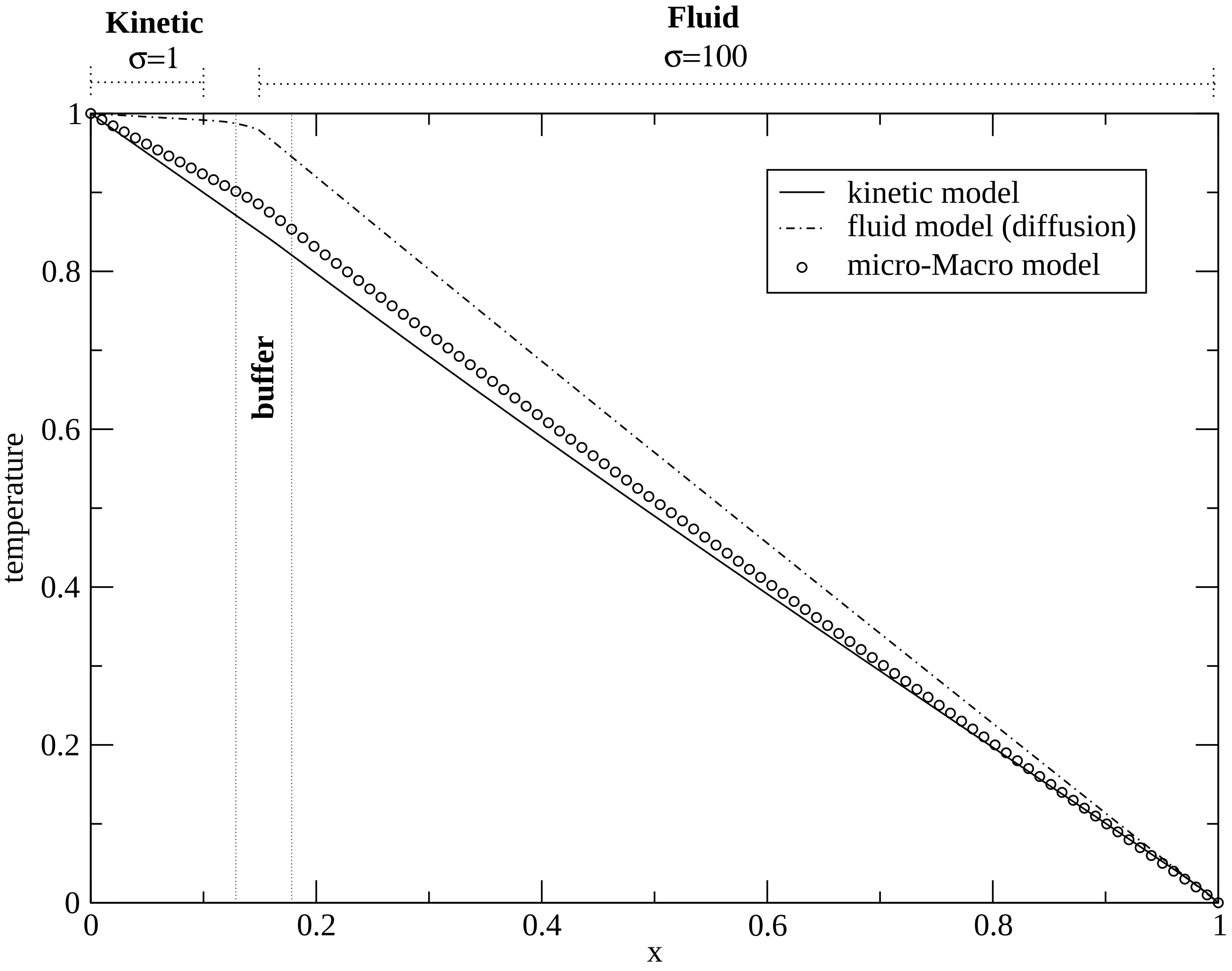
micro-Macro model:

$$\partial_t(T+B(T))+\varepsilon\partial_t[g_K]+\partial_x[\mu g_K]=\partial_{xx}T+\partial_x\left(\frac{1}{3\sigma}\partial_x B(T)\right), \tag{4}$$

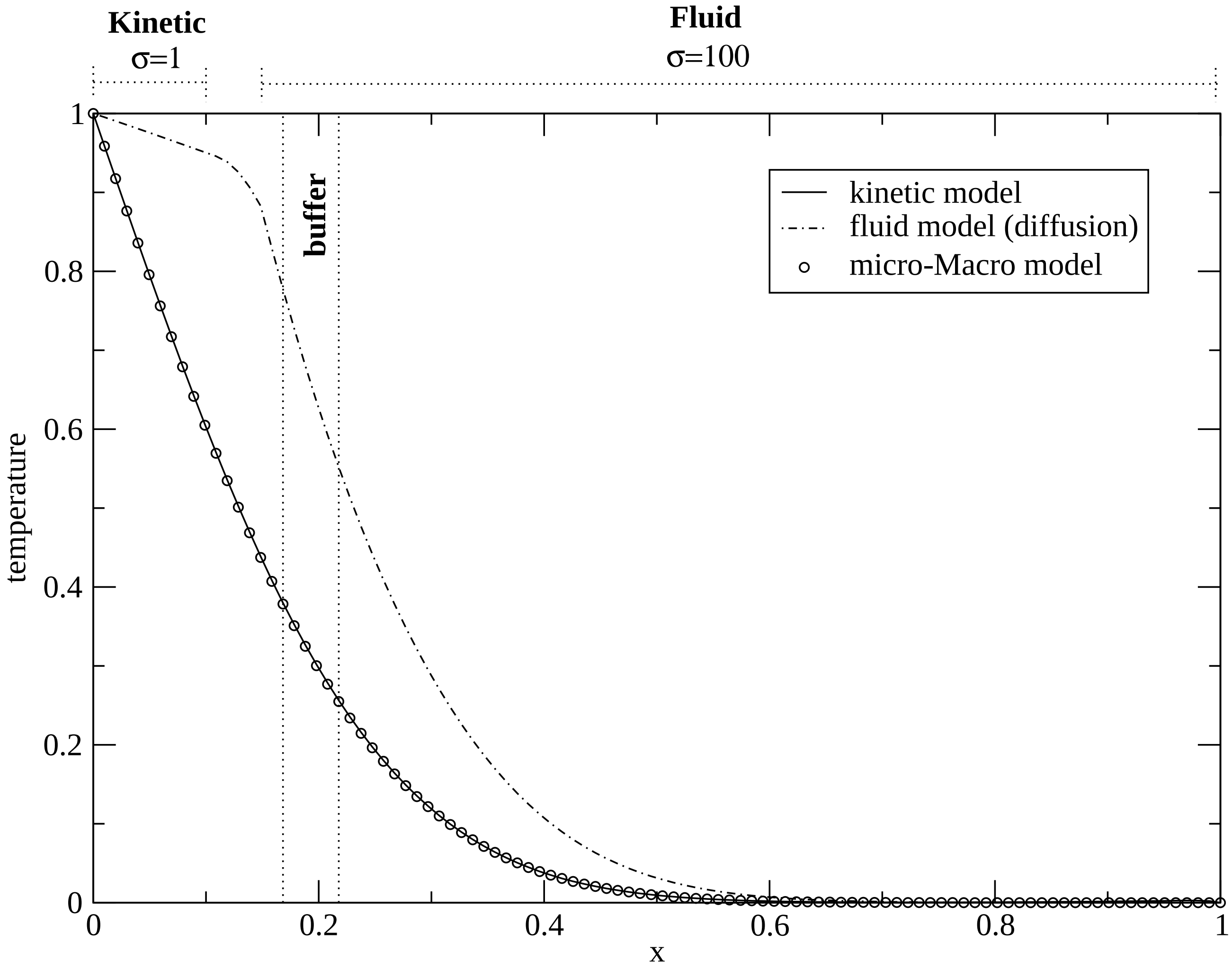
$$\varepsilon\partial_t g_K+h\mu\partial_x g_K=-\frac{\sigma}{\varepsilon}g_K-h\left(\partial_t B(T)-\mu^2\partial_x\left(\frac{1}{\sigma}\partial_x B(T)\right)\right)+\frac{\varepsilon\mu h}{\sigma}\partial_t\partial_x B(T), \tag{5}$$



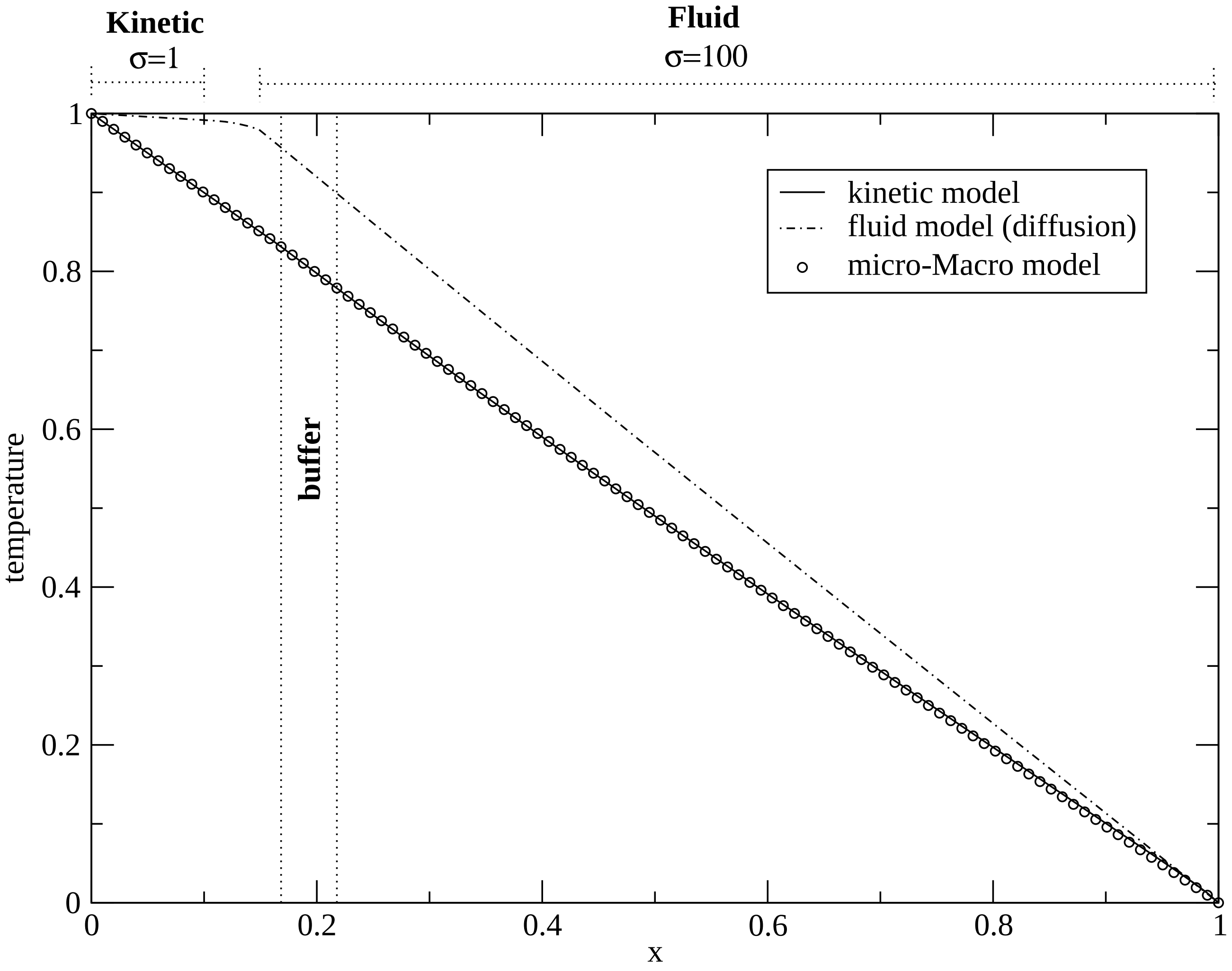
The numerical solution of the temperature for the radiative-heat transfer model with at $t = 0.0185$, with a buffer partially outside the fluid zone.



The numerical solution of the temperature for the radiative-heat transfer model at steady state, with a buffer partially outside the fluid zone.



The numerical solution of the temperature for the radiative-heat transfer model with at $t = 0.0185$, with a buffer inside the fluid zone.



The numerical solution of the temperature for the radiative-heat transfer model at steady state, with a buffer inside the fluid zone.

example 4: Semi-conductor model

Boltzmann-Poisson equation: for $x \in [0, L]$,

$$\partial_t f + \xi \partial_x f + \tfrac{q}{m} \partial_x \Phi \partial_\xi f = \tfrac{1}{\tau}(nM - f)$$
$$\epsilon \partial_{xx} \Phi = q(n - n_d)$$

where the lattice Maxwellian $M = \frac{1}{\sqrt{2\pi\theta}} e^{-\frac{\xi^2}{2\theta}}$ and the density $n = \int f(t, x, \xi) d\xi$. The boundary condition for $\Phi(0) = 0, \Phi(L) = Vbias$.

The notations:

$$\theta = \frac{k_b}{m} T_0, \quad \tau = \frac{m\mu}{q}$$

Scaling:

$$x = L * \hat{x},\ \xi = \sqrt{\theta}\hat{\xi},\ t = T * \hat{t}, T = \frac{L^2}{\tau\theta}, f = F * \hat{f},$$

$$M = \frac{1}{\sqrt{\theta}}\hat{M},\ n = F\sqrt{\theta}\hat{n}, n_d = F\sqrt{\theta}\hat{n}_d,\ \Phi = Vbias\ \hat{\Phi},$$

Set

$$\varepsilon = \frac{\tau\sqrt{\theta}}{L}, \alpha = \frac{q \cdot Vbias}{m\theta}, \beta^2 = \frac{\epsilon \cdot Vbias}{L^2 qF\sqrt{\theta}}$$

drop the hat, we get the dimensionless Boltzmann-Poisson equation:

$$\varepsilon\partial_t f + \xi\partial_x f + \alpha\partial_x\Phi\partial_\xi f = \frac{1}{\varepsilon}(nM - f)$$

$$\beta^2\partial_{xx}\Phi = (n - n_d)$$

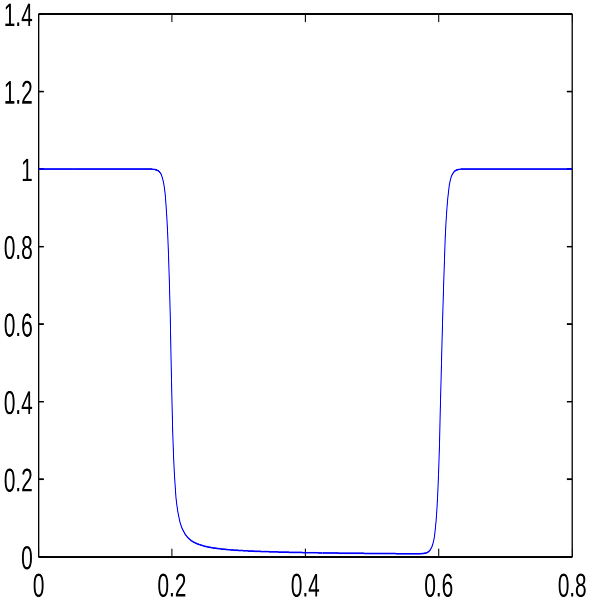
Example of simple diode model:

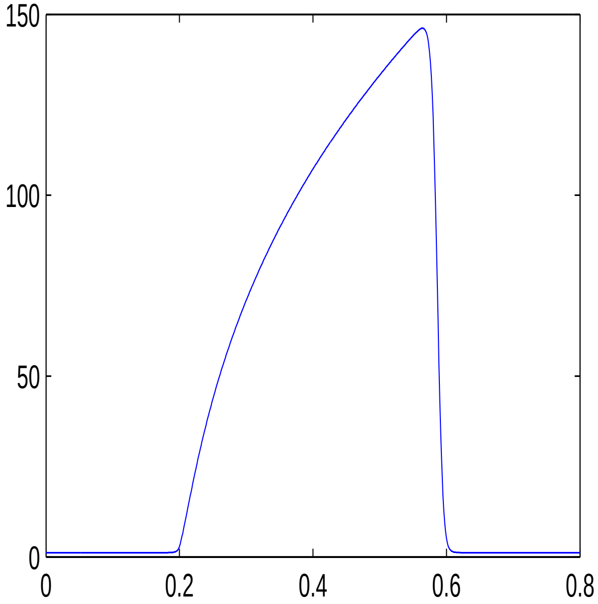
1. $\varepsilon = 1.7106 \times 10^{-3}$,

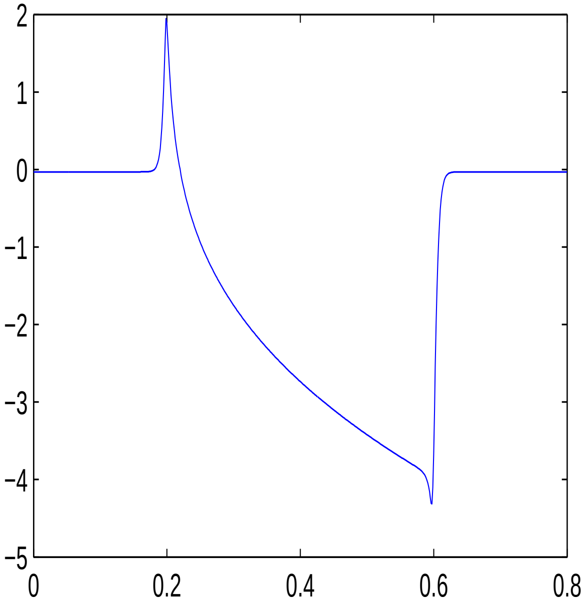
2. $T = \frac{L^2}{\tau\theta} = 1.768 \times 10^{-9}s = 1768\ ps$.

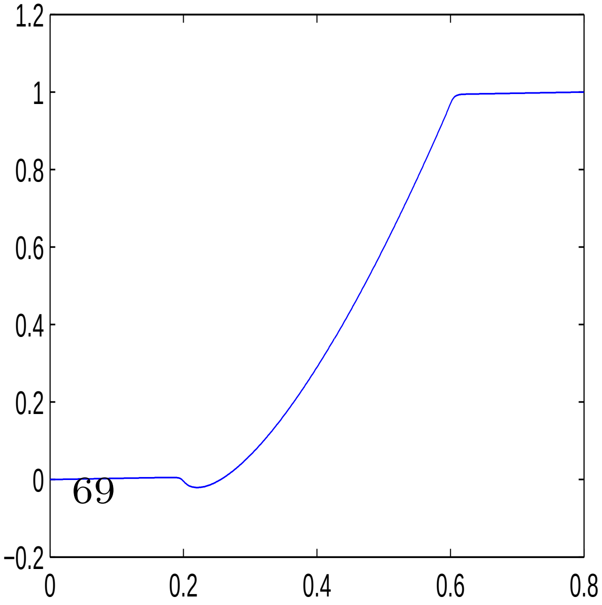
3. $\alpha = 38.683$.

4. $\beta = 0.03376$.


1.4
1.2
1
0.8
0.6
0.4
0.2
0
0
0.2
0.4
0.6
0.8


150
100
50
0
0
0.2
0.4
0.6
0.8


2
1
0
−1
−2
−3
−4
−5
0
0.2
0.4
0.6
0.8


1.2
1
0.8
0.6
0.4
0.2
0
−0.2
0
0.2
0.4
0.6
0.8

SUMMARY

- new methods to couple kinetic and fluid models
- easy to use:
  - complex shape interfaces are possible
  - no interface boundary conditions
- can be applied to various kinetic models
- more intensive comparisons are needed to validate the method
- extension to dynamic coupling in progress:
  - ok if the velocity of the interface is known
  - if this velocity depends on the solution itself: under development