An inverse problem for a model of cell motion and chemotaxis

Christian Klingenberg

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An inverse problem for a model of cell motion and chemotaxis

Christian Klingenberg

Mathematics Dept., Würzburg University, Germany

jointly with:

Kathrin Hellmuth	Würzburg University, Germany
Ru-yu Lai	Univ. of Minnesota, Minneapolis, USA
Qin Li	Univ. of Wisc. in Madison, USA
Marlies Pirner	Würzburg University, Germany
Min Tang	Shanghai Jiao Tong Univ., China

and others

I will now describing the context of this topic

there are various ways to model phenomena in nature

time scale

1 sec

10^{-6} sec

10^{-10} sec

interacting molecules

microscopic description

10^{-9} m

10^{-6} m

10^{-2} m

length scale

kinetic equations

Boltzmann-type equations

mesoscopic description

interacting molecules

microscopic description

fluid equations

e.g. Euler equations, Navier-Stokes, …

macroscopic description

kinetic equations

Boltzmann-type equations

mesoscopic description

interacting molecules

microscopic description

today’s lecture will focus kinetic equations

fluid equations
e.g. Euler equations, Navier-Stokes, …
macroscopic description

kinetic equations
Boltzmann-type equations
mesoscopic description

interacting molecules
microscopic description

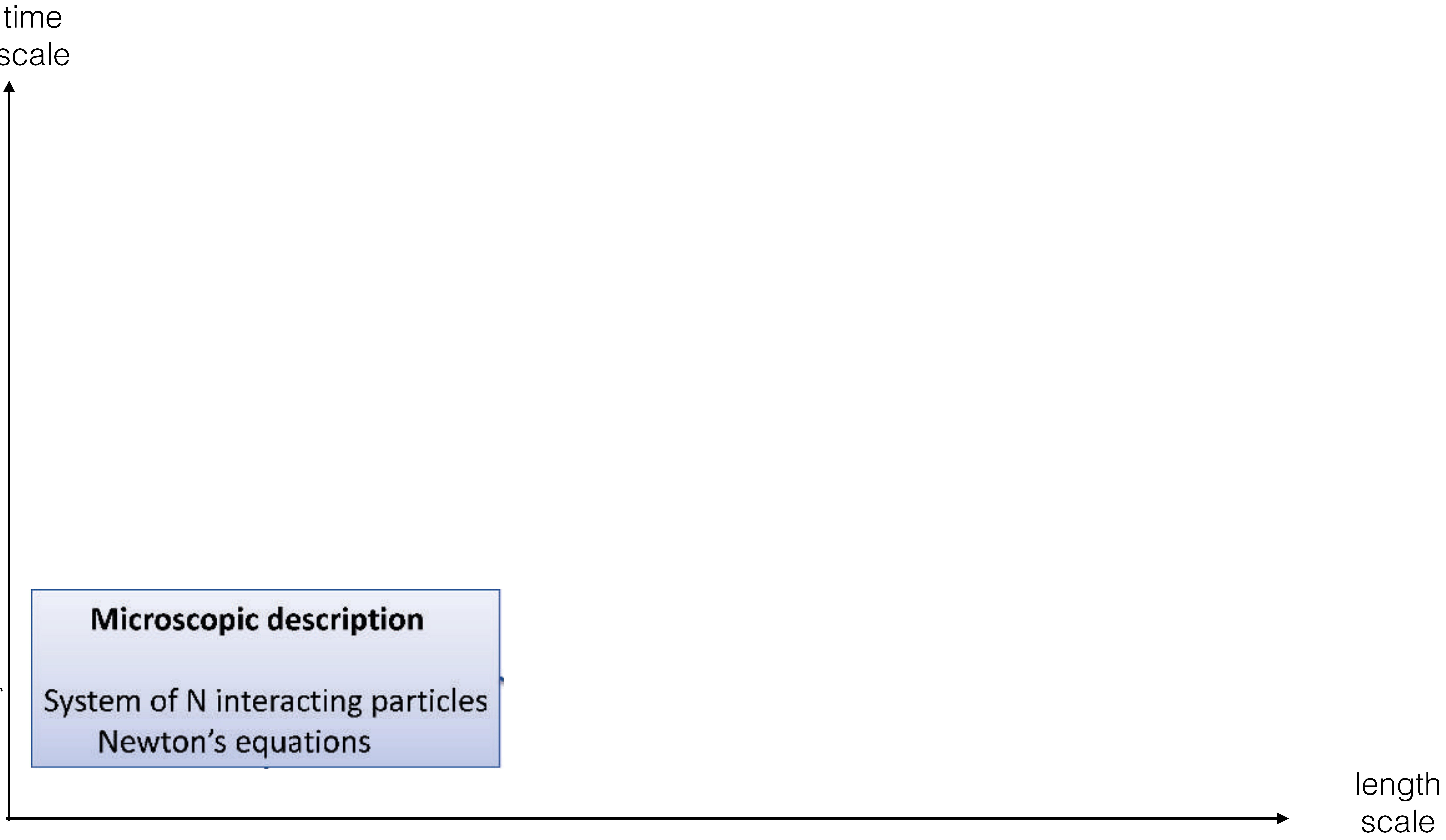
today’s lecture will focus kinetic equations and its fluid limits

fluid equations
e.g. Euler equations, Navier-Stokes, …
macroscopic description

kinetic equations
Boltzmann-type equations
mesoscopic description

interacting molecules
microscopic description

one needs to rescale time and space to go from one description to the next

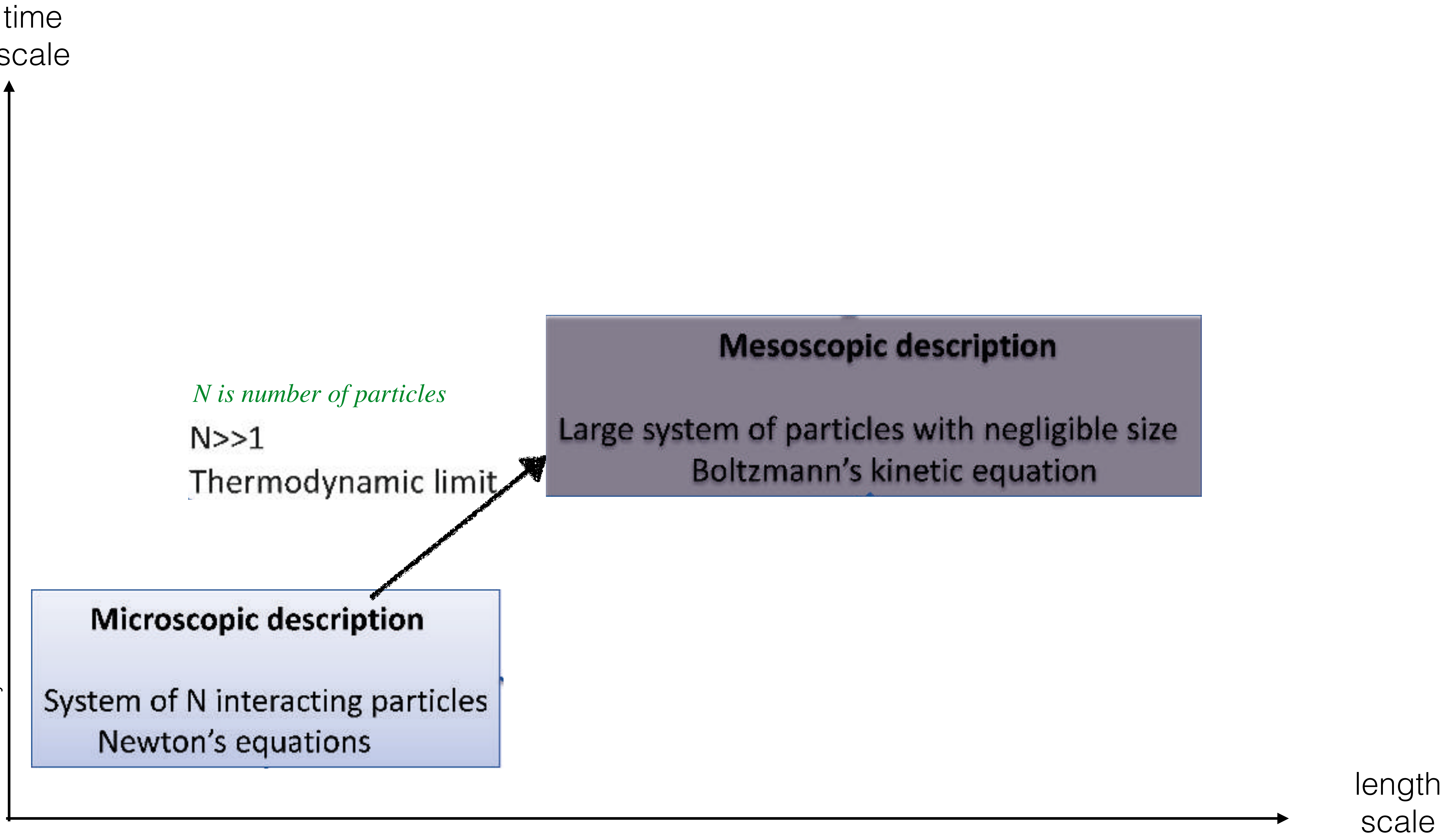


Microscopic description

System of N interacting particles
Newton's equations

Laure Saint-Raymond

one needs to rescale time and space to go from one description to the next



N is number of particles

N>>1

Thermodynamic limit

Microscopic description

System of N interacting particles
Newton's equations

Mesoscopic description

Large system of particles with negligible size
Boltzmann's kinetic equation

Laure Saint-Raymond

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Newton’s equations

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N>>1
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Large system of particles with negligible size
Boltzmann’s kinetic equation

$T_{\text{collision}} << T_{\text{observation}}$
Fast relaxation limit

Macroscopic description

Continuous fluid
Equations of hydrodynamics
(Euler, Navier-Stokes…)

length scale

Laure Saint-Raymond

one needs to rescale time and space to go from one description to the next

time scale

Euler limit $(\tilde{x}, \tilde{t}) = (\epsilon x, \epsilon t)$

Macroscopic description

Continuous fluid
Equations of hydrodynamics
(Euler, Navier-Stokes...)

$T_{collision} << T_{observation}$

Fast relaxation limit

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Large system of particles with negligible size
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Thermodynamic limit

Microscopic description

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Newton's equations

length scale

Laure Saint-Raymond

one needs to rescale time and space to go from one description to the next

time scale

Euler limit $(\tilde{x}, \tilde{t}) = (\epsilon x, \epsilon t)$

diffusive limit $(\tilde{x}, \tilde{t}) = (\epsilon x, \epsilon^2 t)$

Macroscopic description

Continuous fluid
Equations of hydrodynamics
(Euler, Navier-Stokes...)

$T_{\text{collision}} << T_{\text{observation}}$
Fast relaxation limit

Mesoscopic description

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Boltzmann's kinetic equation

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N>>1
Thermodynamic limit

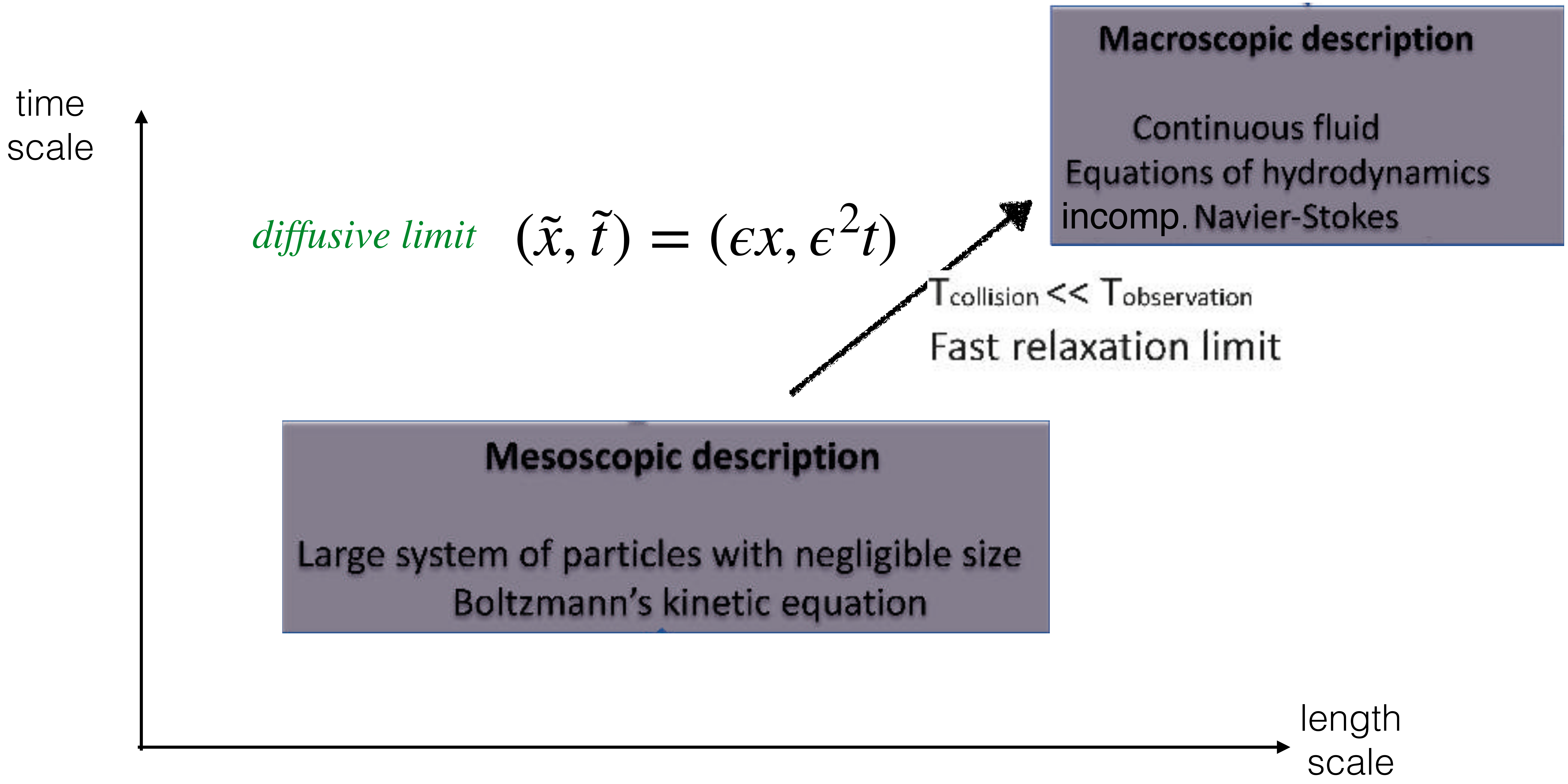
Microscopic description

System of N interacting particles
Newton's equations

length scale

Laure Saint-Raymond

we shall focus on



Laure Saint-Raymond

example

kinetic neutron transport equation:

$$\partial_t f + \frac{1}{\varepsilon} v \cdot \nabla_x f = \frac{\sigma_T}{\varepsilon^2} (\frac{1}{2} \int_{-1}^{1} f dv' - f)$$

example

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$$\Big\downarrow \; \epsilon \to 0$$

macroscopic diffusion equation:

$$\rho_t = \partial_x\left(\frac{1}{3\sigma_T}\partial_x \rho\right)$$

with $\rho(t,x) = \frac{1}{2}\int_{-1}^{1} f(v')\, dv'$

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given a PDE model at the *mesoscopic* level with given initial and boundary data

one would like to prove well-posedness of this solution f_ϵ

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$$\partial_t f + \frac{1}{\varepsilon} v \cdot \nabla_x f = \frac{\sigma_T}{\varepsilon^2}(\frac{1}{2}\int_{-1}^{1} f dv' - f)$$

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given the corresponding PDE model at the *macroscopic* level with given initial and boundary data

one would like to prove well-posedness of this solution ρ

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given the corresponding PDE model at the *macroscopic* level with given initial and boundary data

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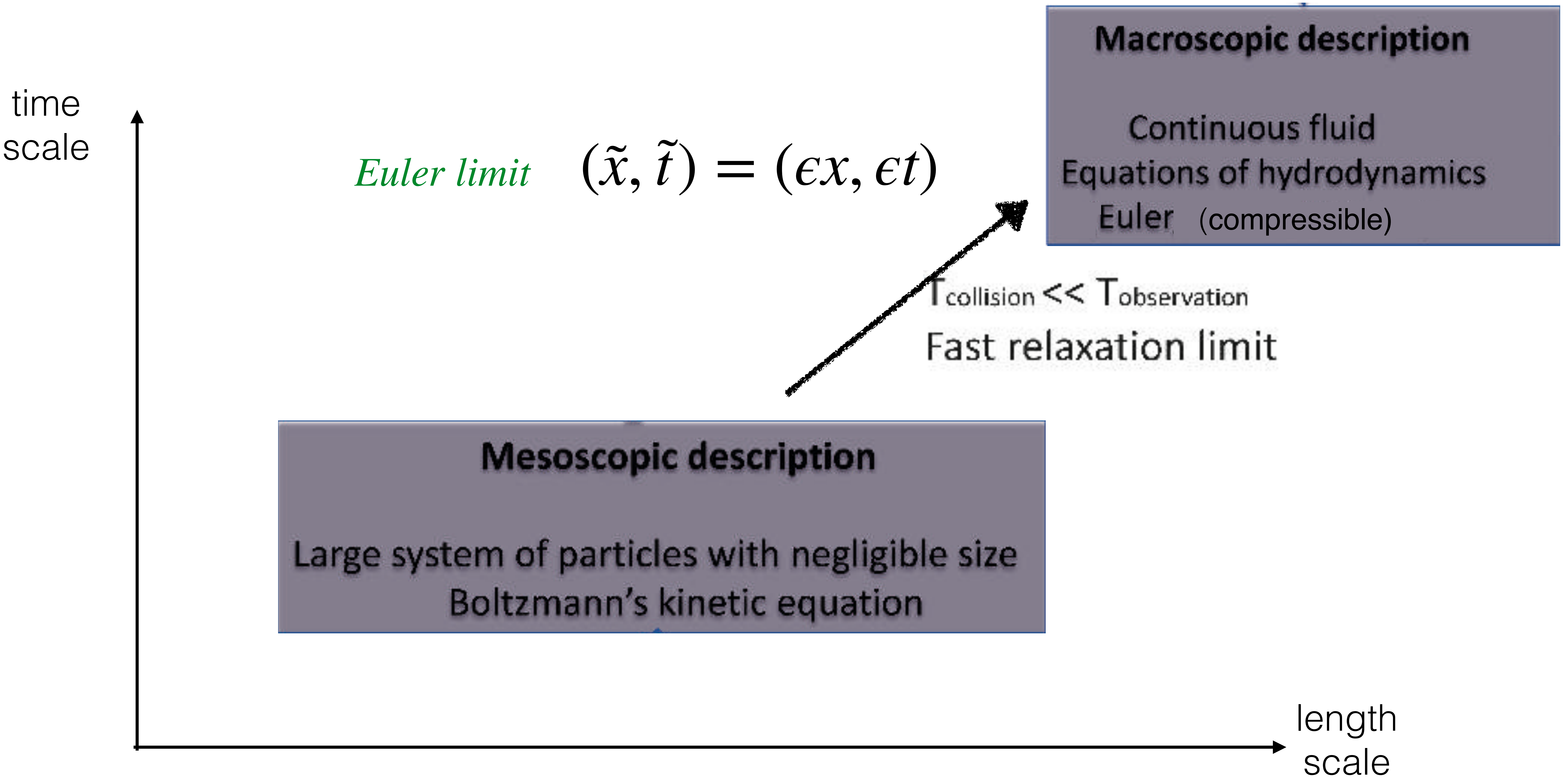
finally one would like to prove convergence under the appropriate scaling ($\int f_\epsilon dv \to \rho$)

rigorous proof of this limit is difficult



time scale

Euler limit $(\tilde{x}, \tilde{t}) = (\epsilon x, \epsilon t)$

Macroscopic description

Continuous fluid
Equations of hydrodynamics
Euler (compressible)

$T_{\text{collision}} << T_{\text{observation}}$

Fast relaxation limit

Mesoscopic description

Large system of particles with negligible size
Boltzmann's kinetic equation

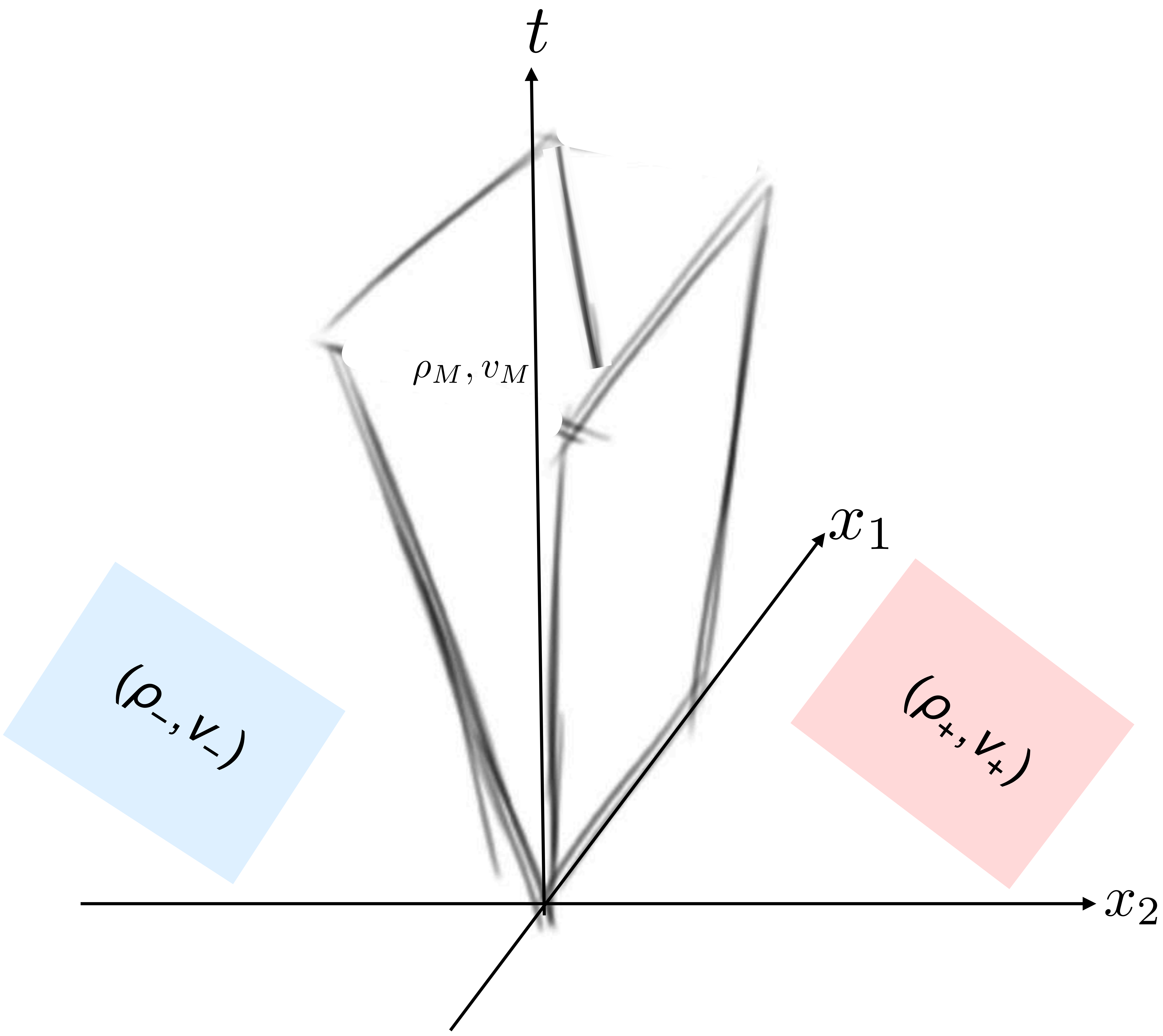
length scale

Laure Saint-Raymond

there are huge difficulties in showing well-posedness of the 2-d compressible Euler equations

$$\begin{aligned} \partial_t \varrho + \mathrm{div}_x(\varrho\, v) &= 0 \\ \partial_t(\varrho\, v) + \mathrm{div}_x(\varrho\, v \otimes v) + \nabla_x\, [p(\varrho)] &= 0 \end{aligned}$$

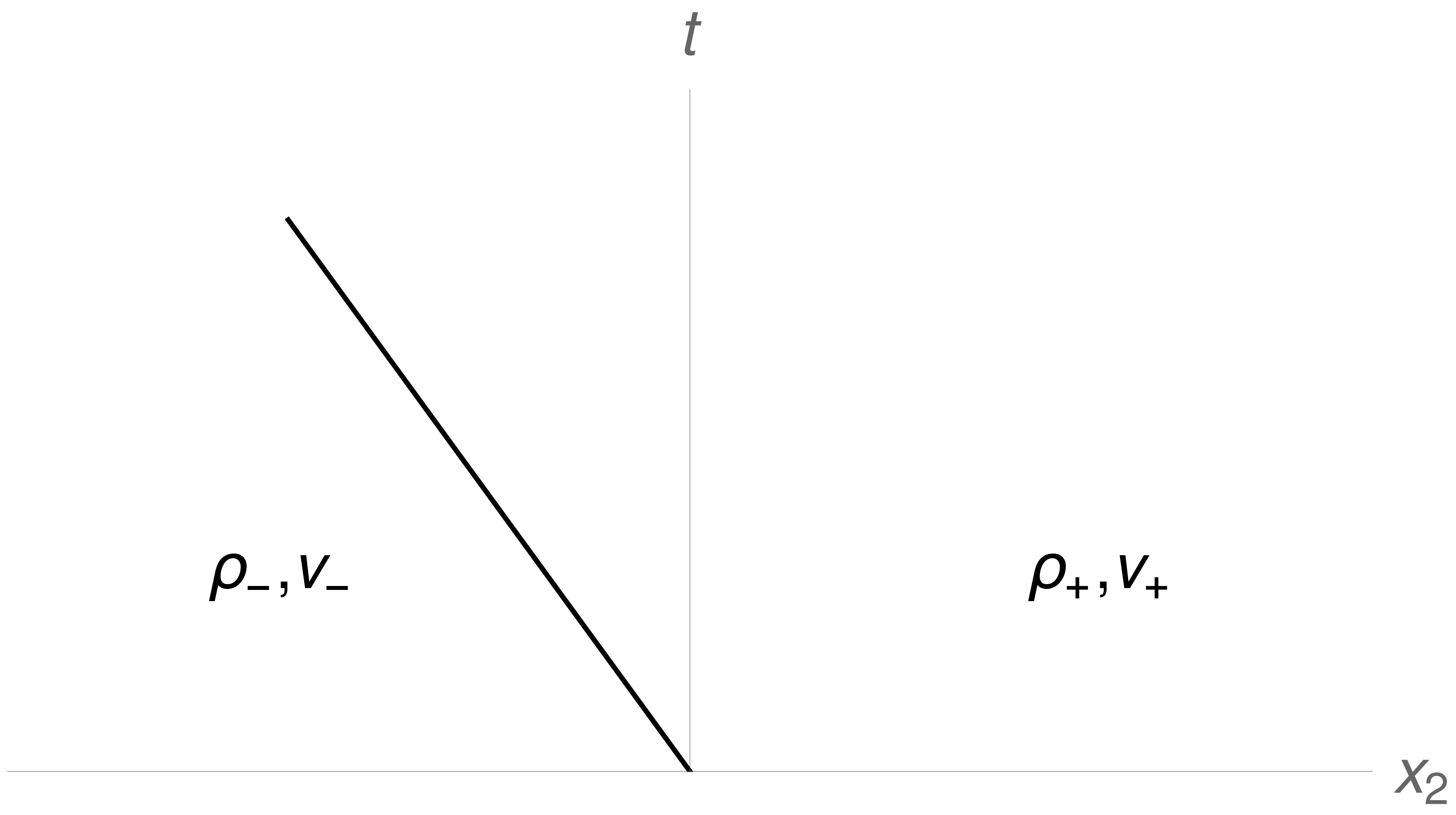
consider this initial value problem in 2 space dimensions



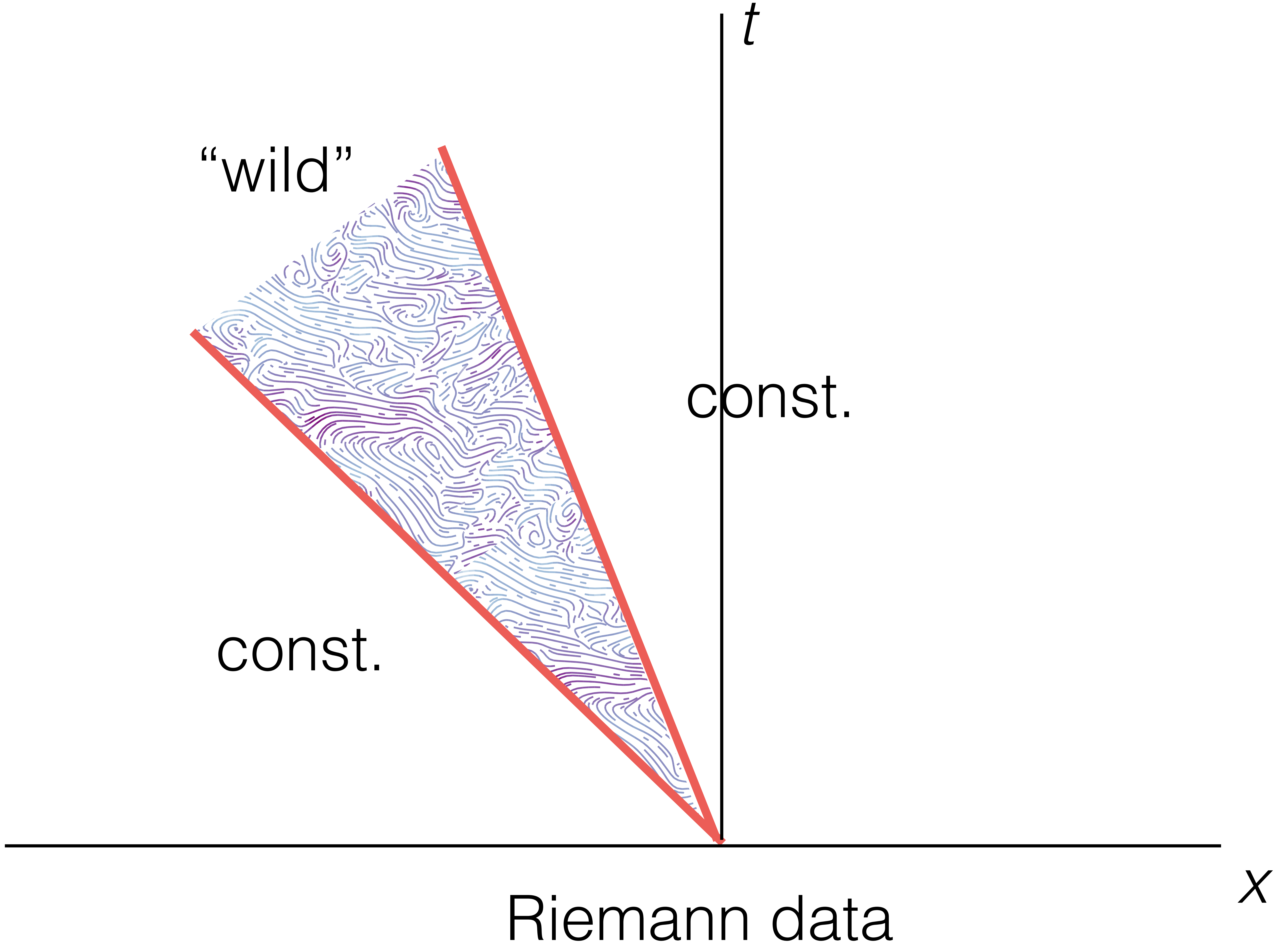
Two shocks

for example:

Standard solution consists of just one shock

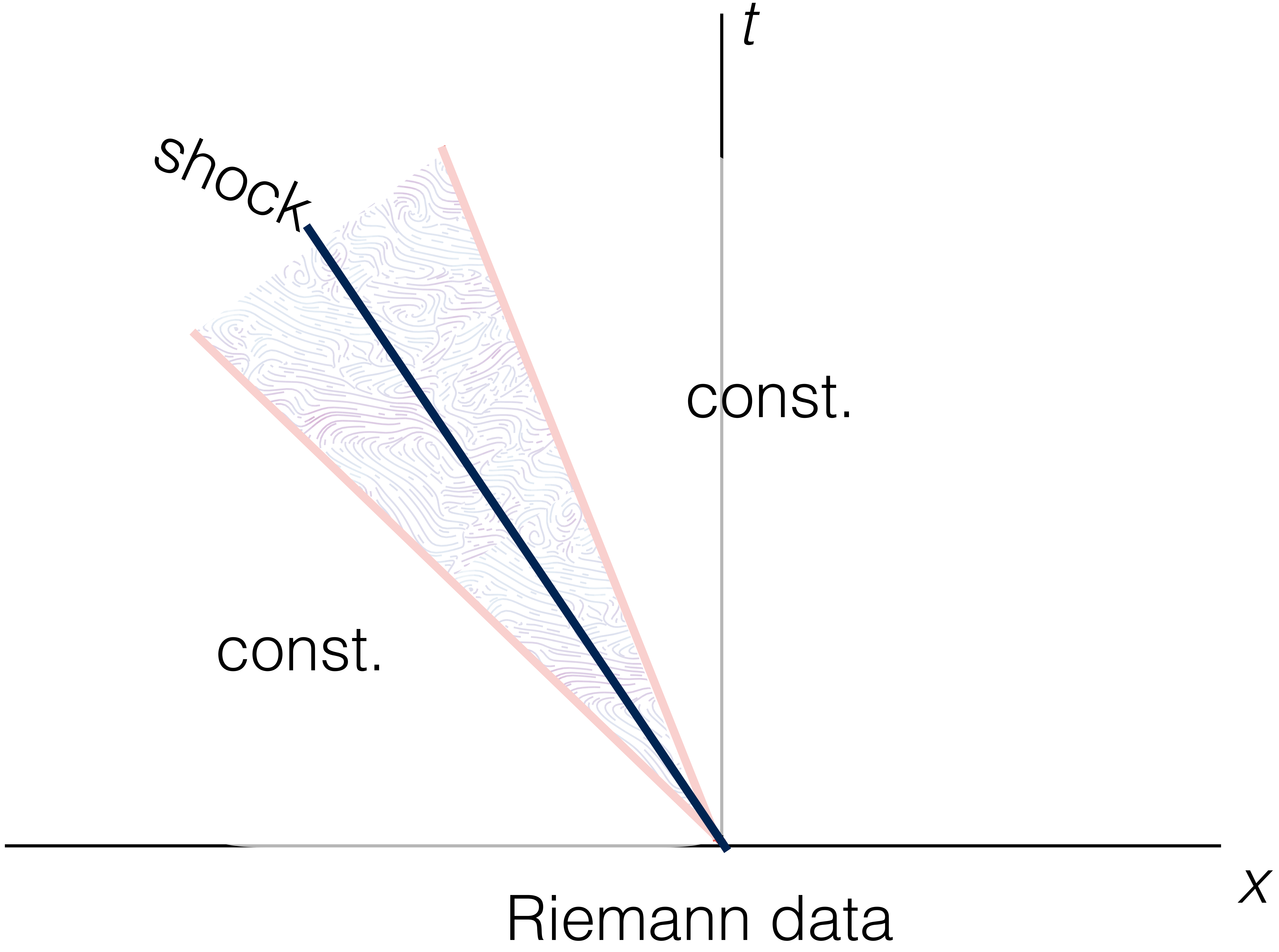


in addition to the standard solution there are many “wild solutions”

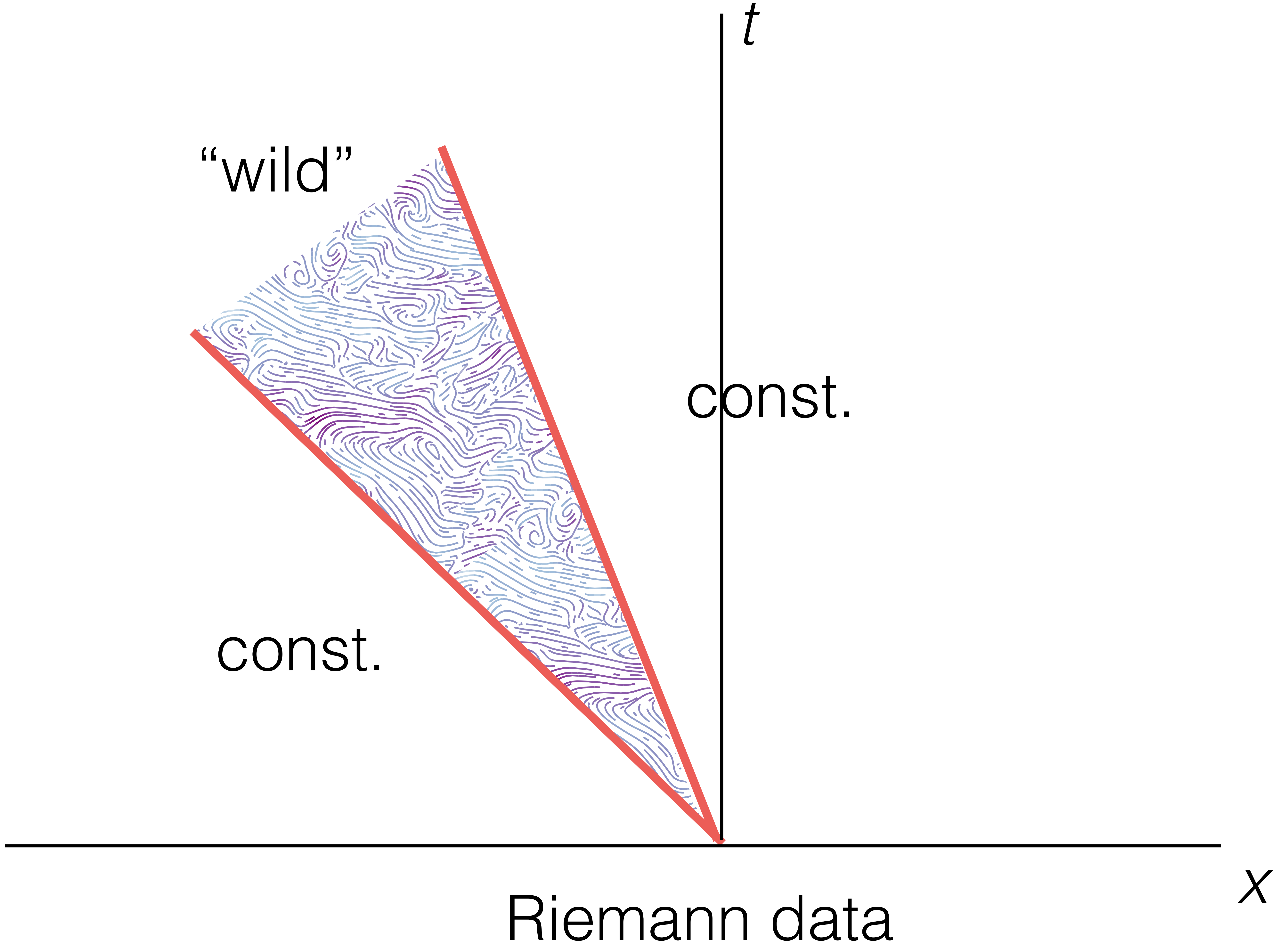


Klingenberg, Simon Markfelder: “*The Riemann problem for the multidimensional isentropic system of gas dynamics is ill-posed if it contains a shock*”
Archive for Rational Mechanics and Analysis (2018)

this is the standard solution



this is one of many “wild solutions”



all of these many solutions are entropy solutions

E. Feireisl; C. Klingenberg; S. Markfelder, “On the density of ‘wild’ initial data for the compressible Euler system”, Calculus of Variations (2020) as long as we don’t know well-posedness of the limit of Boltzmann for $\epsilon \to 0$ in the hyperbolic scaling (namely the Euler equations) it is difficult to prove this limit

example of a well-posedness proof for a kinetic equation

a ***multi-species*** kinetic model

force

$$\partial_t f_1 + v \cdot \nabla_x f_1 + \frac{F_1}{m_1} \cdot \nabla_v f_1 = Q_{11}(f_1, f_1) + Q_{12}(f_1, f_2)$$

$$\partial_t f_2 + v \cdot \nabla_x f_2 + \frac{F_2}{m_2} \cdot \nabla_v f_2 = Q_{22}(f_2, f_2) + Q_{21}(f_2, f_1)$$

force

modeled by ***two*** *interaction terms*

we use the BGK approximation

$$\partial_t f_1 + \nabla_x \cdot (v f_1) + \frac{F_1}{m_1} \nabla_v f_1 = \nu_{11} n_1 (M_1 - f_1) + \nu_{12} n_2 (M_{12} - f_1)$$

$$\partial_t f_2 + \nabla_x \cdot (v f_2) + \frac{F_2}{m_2} \nabla_v f_2 = \nu_{22} n_2 (M_2 - f_2) + \nu_{21} n_1 (M_{21} - f_2)$$

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$$M_1(x,v,t) = \frac{\boxed{n_1}}{\sqrt{2\pi \frac{\boxed{T_1}}{m_1}}^3} \exp(-\frac{|v - \boxed{u_1}|^2}{2\frac{T_1}{m_1}})$$

$$M_{12}(x,v,t) = \frac{\boxed{n_{12}}}{\sqrt{2\pi \frac{\boxed{T_{12}}}{m_1}}^3} \exp(-\frac{|v - \boxed{u_{12}}|^2}{2\frac{T_{12}}{m_1}})$$

$$M_2(x,v,t) = \frac{\boxed{n_2}}{\sqrt{2\pi \frac{\boxed{T_2}}{m_2}}^3} \exp(-\frac{|v - \boxed{u_2}|^2}{2\frac{T_2}{m_2}})$$

$$M_{21}(x,v,t) = \frac{\boxed{n_{21}}}{\sqrt{2\pi \frac{\boxed{T_{21}}}{m_2}}^3} \exp(-\frac{|v - \boxed{u_{21}}|^2}{2\frac{T_{21}}{m_2}}$$

we use the BGK approximation

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can determine these coefficients such that conservation properties, H-theorem holds

- Klingenberg, C., **Pirner**, M., Puppo, G.: "A consistent kinetic model for a two component mixture with an application to plasma", Kinetic and Related Models Vol. 10, No. 2, pp. 445–465 (2017)

we can show well-posedness of this model

- Klingenberg, C. & **Pirner**, M.: “Existence, Uniqueness and Positivity of solutions for BGK models for mixtures”, Journal of Differential Equations, 264, pp. 207-227 (2019)

$$\partial_t f_1 + \nabla_x \cdot (v f_1) + \frac{F_1}{m_1} \nabla_v f_1 = \nu_{11} n_1 (M_1 - f_1) + \nu_{12} n_2 (M_{12} - f_1)$$

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next we consider uncertainties in the kinetic context

examples:

- when deriving the collision kernel from measurements there might be uncertainties (with variable z):

$$\epsilon\partial_t f(v) + v\partial_x f(v) = \frac{\sigma(x, \overset{\substack{\text{stochastic variable}\\ \downarrow}}{z})}{\epsilon}\left[\frac{1}{2}\int_{-1}^{1} f(v')\,dv' - f(v)\right]$$

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- the measurements of the initial and boundary data might be uncertain

there could also be uncertainties in the fluid context

examples:

- the diffusivity coefficient my be known only with uncertainty

$$\rho_t = \partial_x \left[\frac{1}{3\sigma(x, \underset{\uparrow}{z})} \partial_x \rho \right]$$

stochastic variable

there could also be uncertainties in the fluid context

examples:

- the diffusivity coefficient my be known only with uncertainty

$$\rho_t = \partial_x \left[\frac{1}{3\sigma(x,z)} \partial_x \rho \right]$$

- the measurements of the initial and boundary data might be uncertain *numerics of uncertainties in the kinetic context*

generalized polynomial chaos stochastic Galerkin method (gPC) *the generalized polynomial chaos method (gPC)*

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- we consider a set of orthonormal basis function $\{\phi_j(z)\}$ for the space of random functions

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- we expand the functions into a Fourier series w.r.t. this basis

$$f(z) = \Sigma f_j \phi_j(z)$$

the generalized polynomial chaos method (gPC)

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- we expand the functions into a Fourier series w.r.t. this basis

$$f(z) = \Sigma f_j \phi_j(z)$$

- truncate this series

- substitute into the stochastic system to obtain a deterministic system for the first N gPC coefficients

one would like to show accuracy of the gPC method

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for this one checks the boundedness or the decay in time of the derivatives

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this can be deduced from *hypocoercivity*

consider the (single species) BGK equation

$$\partial_t f + v\partial_x f = \sigma(\underset{\substack{\uparrow \\ \text{stochastic variable}}}{z})\big(\mathcal{M} - f\big)$$

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one attempts to prove decay in time for f and its derivatives

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for the linearized BGK equation decay in f has been done in

Li, Q., & Wang, L.. Uniform regularity for linear kinetic equations with random input based on hypocoercivity.
SIAM/ASA Journal on Uncertainty Quantification, 5(1), (2017)

consider the (single species) BGK equation

$$\partial_t f + v\partial_x f = \sigma(z)\big(\mathcal{M} - f\big)$$

stochastic variable

one attempts to prove decay in time for f and its derivatives

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Li, Q., & Wang, L.. Uniform regularity for linear kinetic equations with random input based on hypocoercivity. *SIAM/ASA Journal on Uncertainty Quantification*, *5*(1), (2017)

we generalize this result and show decay for all derivatives in z by using Liapunov techniques from

Franz Achleitner, Anton Arnold, and Eric A. Carlen. On multi-dimensional hypocoerciv BGK models. Kinetic & Related Models, 11(4), (2018)

write $f = \mathcal{M} + \epsilon h$

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substituting gives

$$\partial_t h + v\partial_x h = \sigma(z)(\mathcal{M} - h)$$

$$h = h(t, x, v, z)$$

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substituting gives

$$\partial_t h + v\partial_x h = \sigma(z)(\mathcal{M} - h)$$

$$h = h(t, x, v, z)$$

we can show

$$||\partial_z^l h|| \leq Ce^{-\lambda t} \qquad l \in \mathcal{N}$$

Herzing, T., Klingenberg, C., Pirner, M.: "Hypocoercivity of the linearized BGK-equation with stochastic coefficients", submitted (2021)

numerics of uncertainties in the fluid context

numerics of uncertainties in the fluid context

Black-Scholes equation:

$$\frac{\partial V(S,t)}{\partial t}+\frac{1}{2}\sigma^2 S^2\frac{\partial^2 V(S,t)}{\partial S^2}+rS\frac{\partial V(S,t)}{\partial S}-rV(S,t)=0$$

numerics of uncertainties in the fluid context

(time inverted) Black-Scholes equation:

$$\frac{\partial V(S,t)}{\partial t} - \frac{1}{2}\sigma^2 S^2 \frac{\partial^2 V(S,t)}{\partial S^2} + rS\frac{\partial V(S,t)}{\partial S} - rV(S,t) = 0$$

deterministic diffusion coefficient (volatility)

numerics of uncertainties in the fluid context

(time inverted) Black-Scholes equation:

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deterministic diffusion coefficient (volatility)

$$\frac{\partial V(S,t,\Theta)}{\partial t} - \frac{1}{2}\Sigma(\Theta)^2 S^2 \frac{\partial^2 V(S,t,\Theta)}{\partial S^2} + rS\frac{\partial V(S,t,\Theta)}{\partial S} - rV(S,t,\Theta) = 0$$

stochastic diffusion coefficient (volatility)

in financial applications the diffusion coefficient depends on finitely many stochastic variables

$$\Sigma(\Theta_1, ..., \Theta_L)$$

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the stochastic Galerkin approach is computationally costly

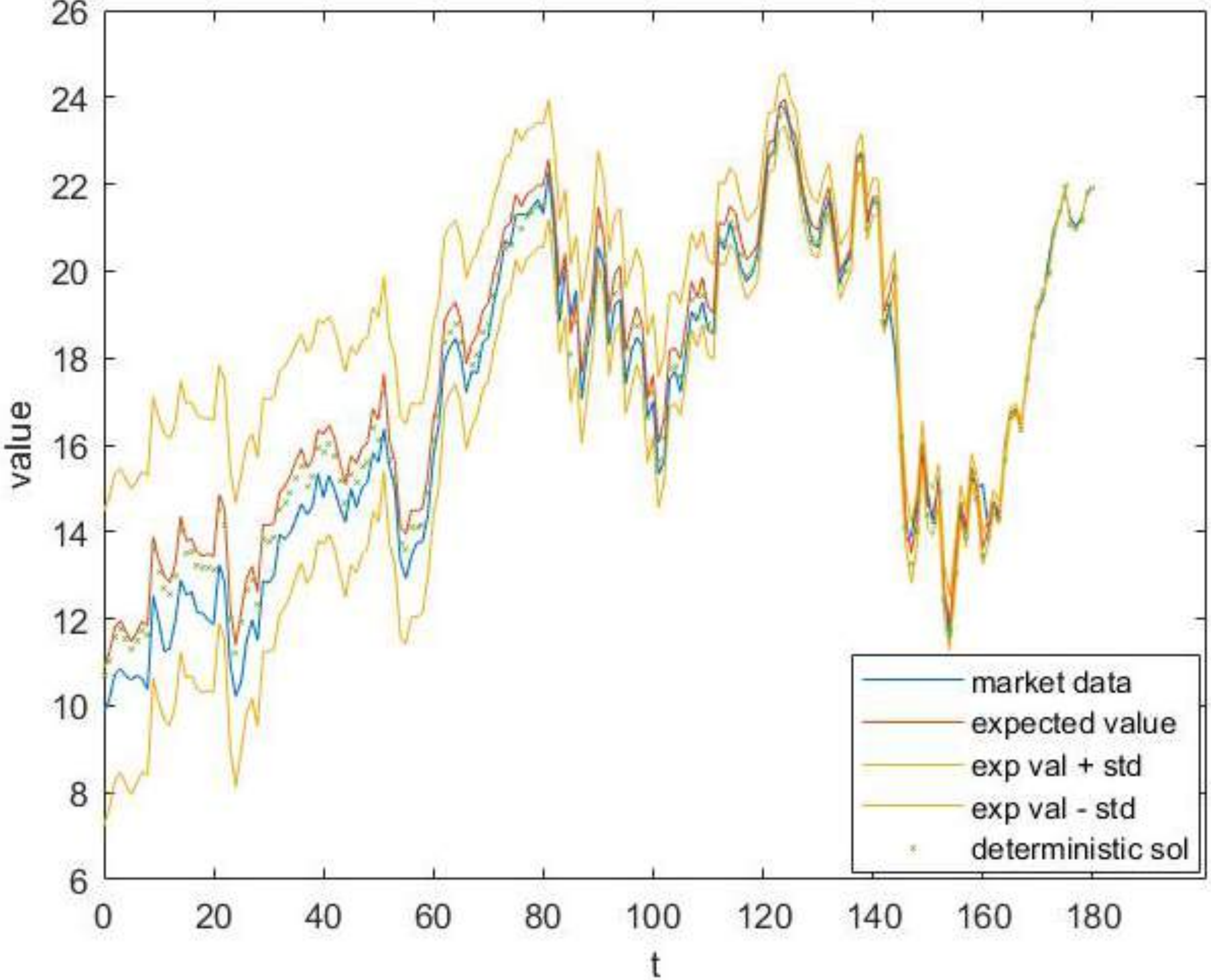
in financial applications the diffusion coefficient depends on finitely many stochastic variables

$$\Sigma(\Theta_1, ..., \Theta_L)$$

the stochastic Galerkin approach is computationally costly

hence we improve computational efficiency using a machine learning (bi-fidelity) approach

L. Liu and X. Zhu, A bi-fidelity method for the multiscale Boltzmann equation with random parameters, Journal of Computational Physics 402 (2020)



Comparing the stochastic Black-Scholes model to real market data

Hellmuth, K., Klingenberg, C.: “Computing Black Scholes with uncertain volatility - a machine learning approach, manuscript (2021)

back to the kinetic problem

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in the forward problem we are given a collision kernel and study the effect of this on the solution

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given (parts of) the solution to the kinetic problem, find the coefficients

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this is the inverse problem for kinetic equations we shall illustrate this

radiative transfer equation

$$\partial_t u + \theta \cdot \nabla_x u = -\mu u + \int_{\mathbb{S}^{n-1}} \Phi(\theta', \theta) u(t, x, \theta')\, d\theta' + \sigma T^4$$
$$\partial_t T = \Delta_x T - \sigma T^4 + \mu \frac{1}{|\mathbb{S}^{n-1}|} \int_{\mathbb{S}^{n-1}} u(t, x, \theta)\, d\theta\,,$$

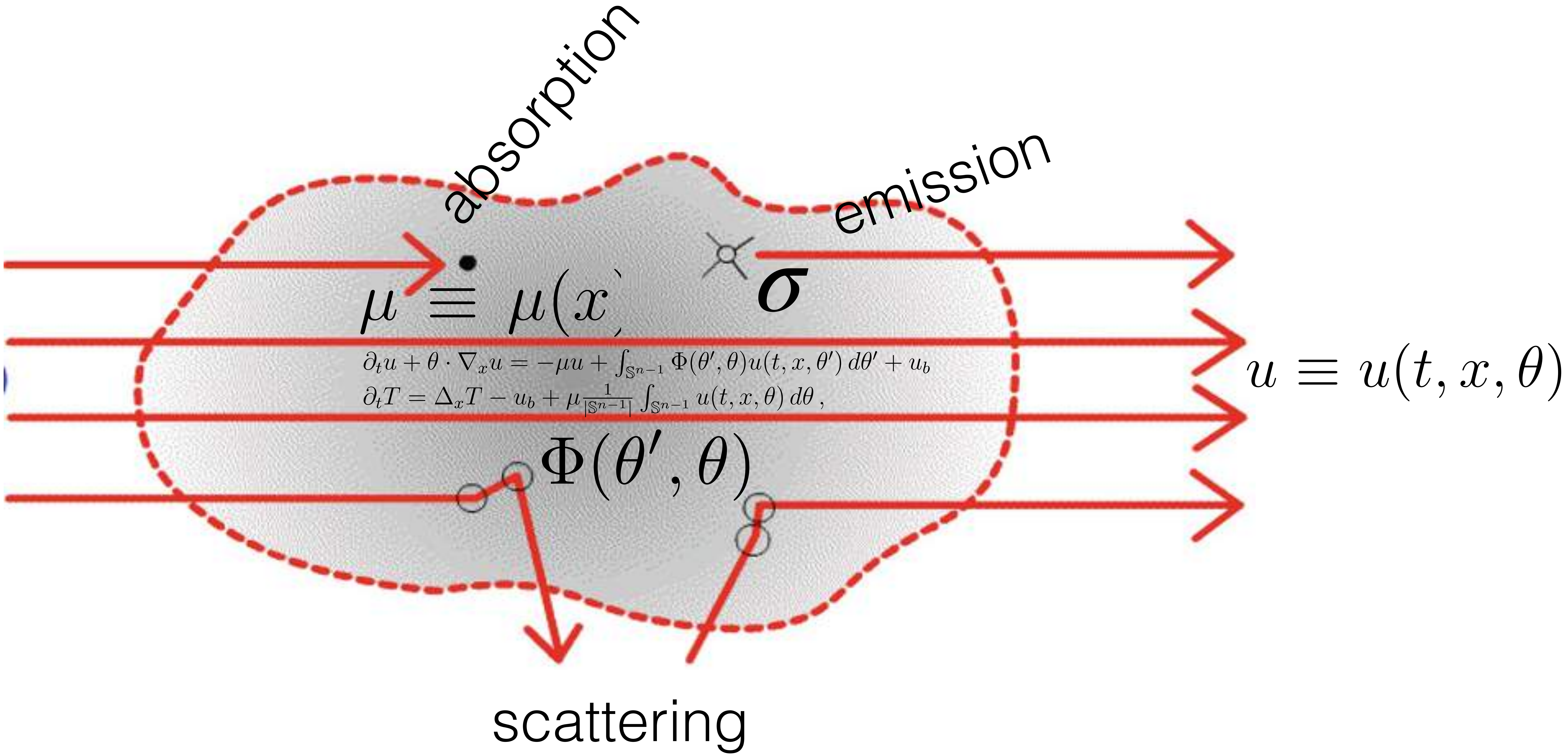
$u \equiv u(t, x, \theta)$ describes the radiation intensity

T is the temperature

$\Phi(\theta', \theta)$ given kernel, describing scattering of photons

$\mu \equiv \mu(x)$ is a given absorption coefficient

$\boldsymbol{\sigma}$ given emission coefficient

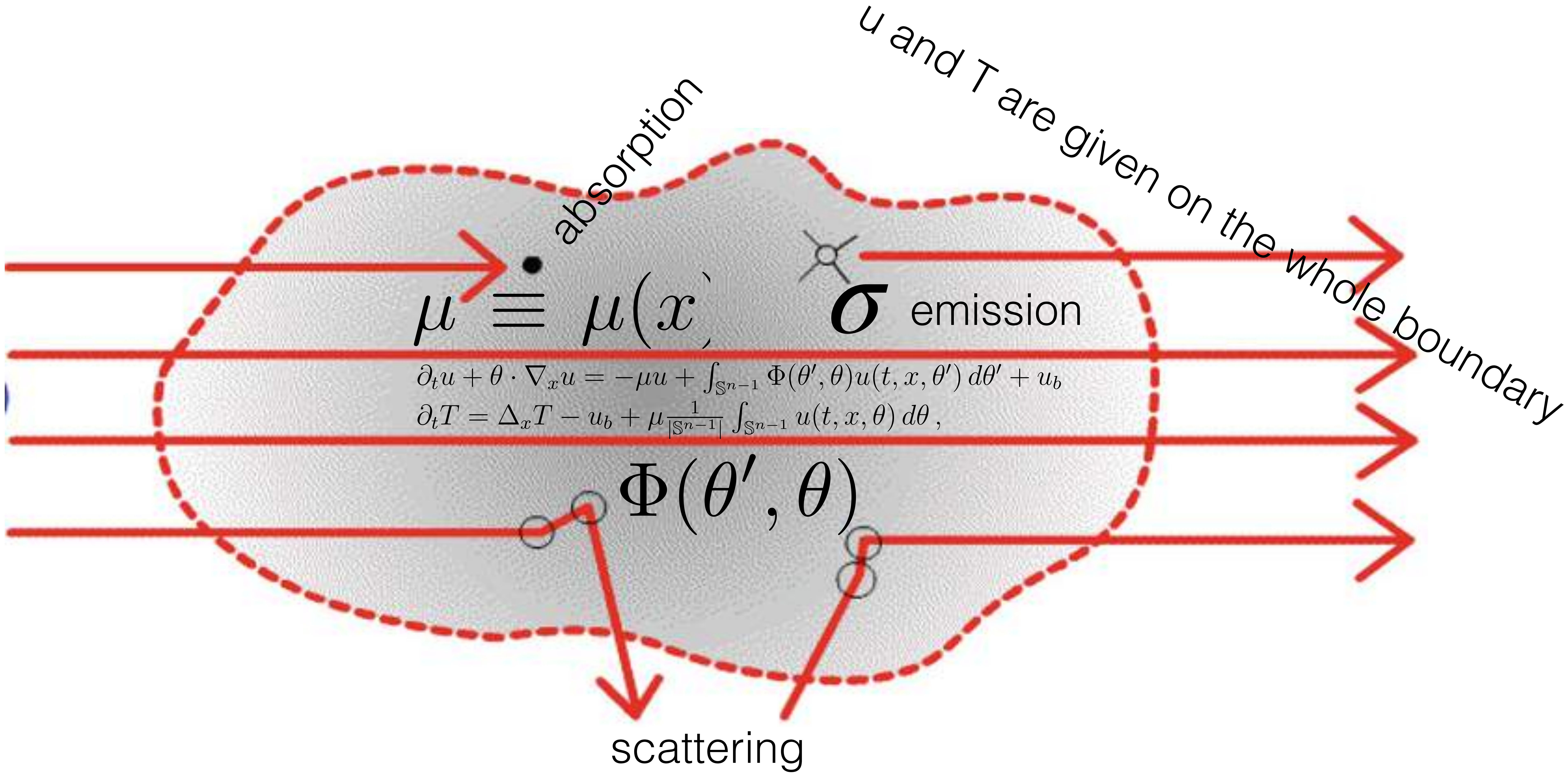


$$\partial_t u + \theta \cdot \nabla_x u = -\mu u + \int_{\mathbb{S}^{n-1}} \Phi(\theta', \theta) u(t, x, \theta')\, d\theta' + u_b$$
$$\partial_t T = \Delta_x T - u_b + \mu \frac{1}{|\mathbb{S}^{n-1}|} \int_{\mathbb{S}^{n-1}} u(t, x, \theta)\, d\theta\,,$$

forward problem

solve u and T inside the body

- with given values u and T on the boundary,
- the kernel $\Phi(\theta', \theta)$, emission $\boldsymbol{\sigma}$ and absorbtion $\boldsymbol{\mu}$ are known



$$\partial_t u + \theta \cdot \nabla_x u = -\mu u + \int_{\mathbb{S}^{n-1}} \Phi(\theta', \theta) u(t, x, \theta')\, d\theta' + u_b$$

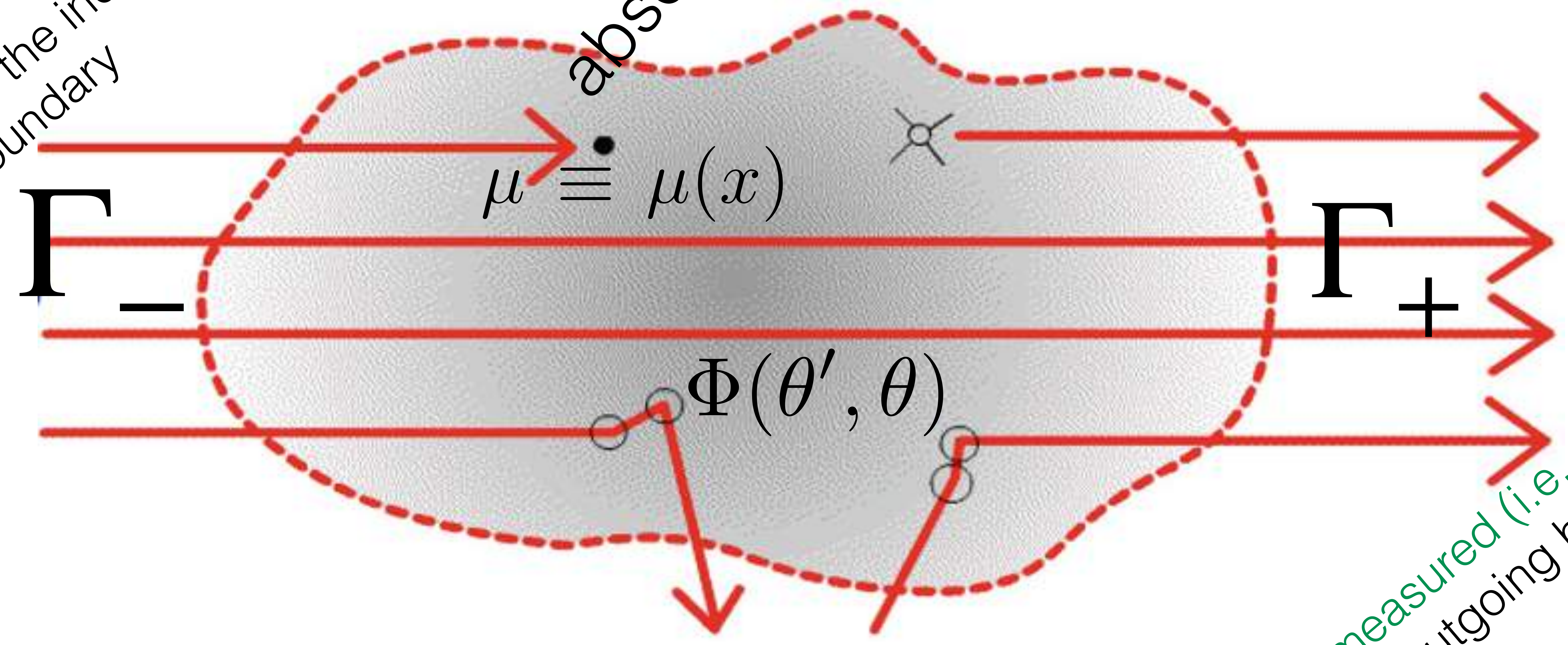
$$\partial_t T = \Delta_x T - u_b + \mu \frac{1}{|\mathbb{S}^{n-1}|} \int_{\mathbb{S}^{n-1}} u(t, x, \theta)\, d\theta\,,$$

inverse problem

reconstruct emission coefficient σ

- given the kernel $\Phi(\theta', \theta)$, and absorption μ
- temperature **T** is given on the whole boundary
- given the incoming data $u_{|\Gamma_-}$
- given the outgoing measurement $u_{|\Gamma_+}$

inverse problem



u is *given* on the incoming boundary

Γ_-

given

absorption

$\mu \equiv \mu(x)$

determine

emission $\boldsymbol{\sigma}$

Γ_+

$\Phi(\theta', \theta)$

scattering

given

u is measured (i.e. given) on the outgoing boundary

stationary case, set scattering $\mathbf{\Phi}$ *= 0*

$$
\begin{aligned}
&\theta \cdot \nabla_x u + \overset{\text{given}}{\mu} u = \sigma T^4 && \text{in } \Omega \times \mathbb{S}^{n-1} \\
&\Delta_x T - \sigma T^4 = -\underset{\text{given}}{\mu} \langle u \rangle && \text{in } \Omega\,, \\
&u = u_B && \text{on } \Gamma_-\,, \\
&T = T_B && \text{on } \partial\Omega\,,
\end{aligned}
$$

$$\langle u \rangle(x) := \frac{1}{|\mathbb{S}^{n-1}|} \int_{\mathbb{S}^{n-1}} u(x,\theta)\, d\theta$$

we prove that the emission coefficient $\boldsymbol{\sigma}$

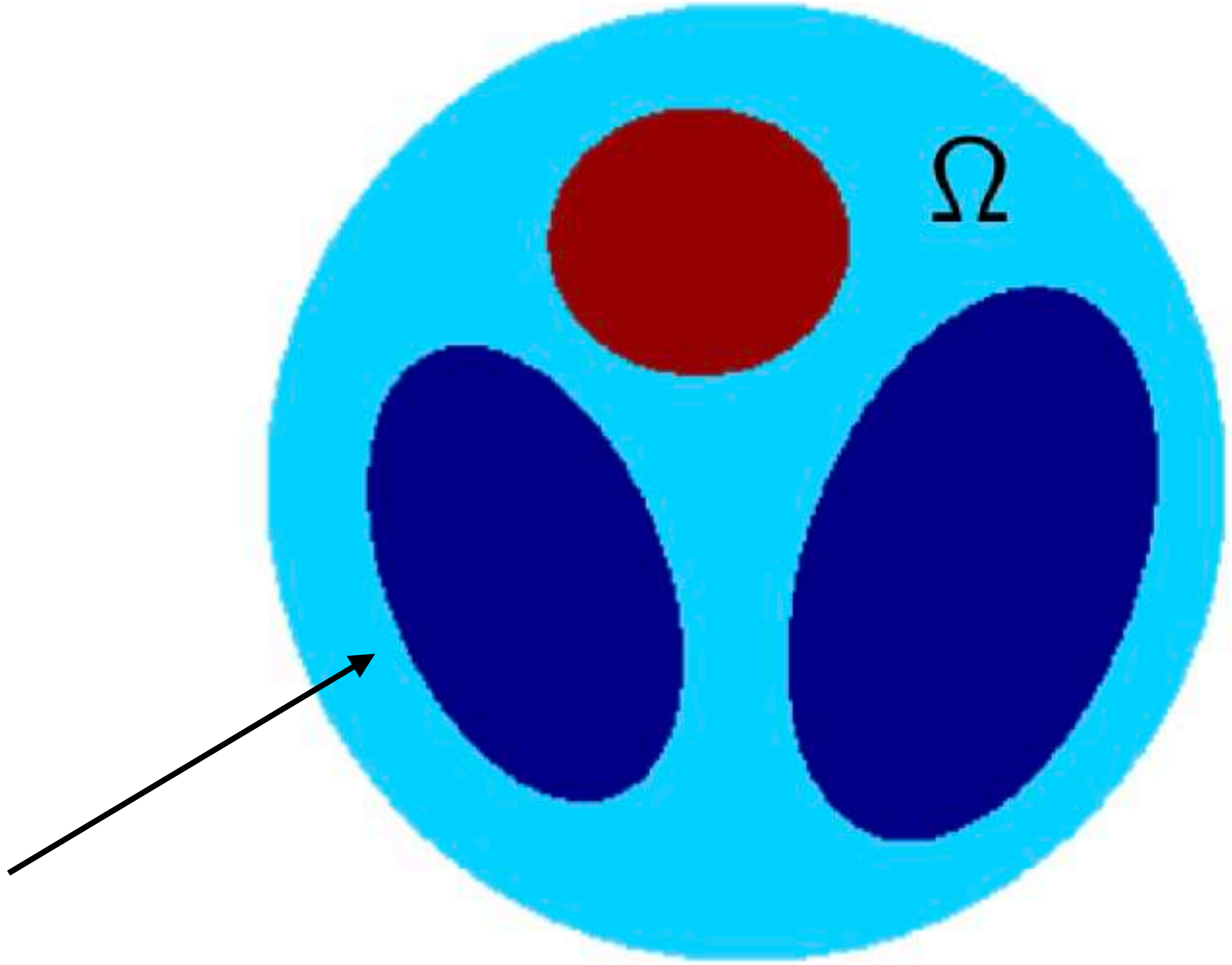
- exists
- is unique
- depends continuously on the data

Klingenberg, C., Lai, R., Li, Q.: "Reconstruction of the emission coefficient in the nonlinear radiative transfer equation", SIAM Journal on Applied Mathematics, Vol. 81, 1 (2021) now consider the limit to the macroscopic equation

this (stationary) kinetic model in the parabolic scaling leads to an elliptic problem

the related problem for the corresponding macroscopic fluid equation is ill-posed,
similar to the Calderon problem

$$\begin{aligned} \nabla \cdot \sigma \nabla u &= 0 \text{ in } \Omega, \\ u\big|_{\partial\Omega} &= f. \end{aligned}$$



conductivity (in the kinetic case emission) $\boldsymbol{\sigma}$

Calderon problem: recover $\boldsymbol{\sigma}$ from knowledge of solution on the boundary

the ill posed Calderon problem is typically numerically solved by a so called Tychonov regularization.

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we will illustrate this for chemotaxis

consider another kinetic model: chemotaxis

bacteria move by either “running” in a straight line and at random times rotating and the moving on

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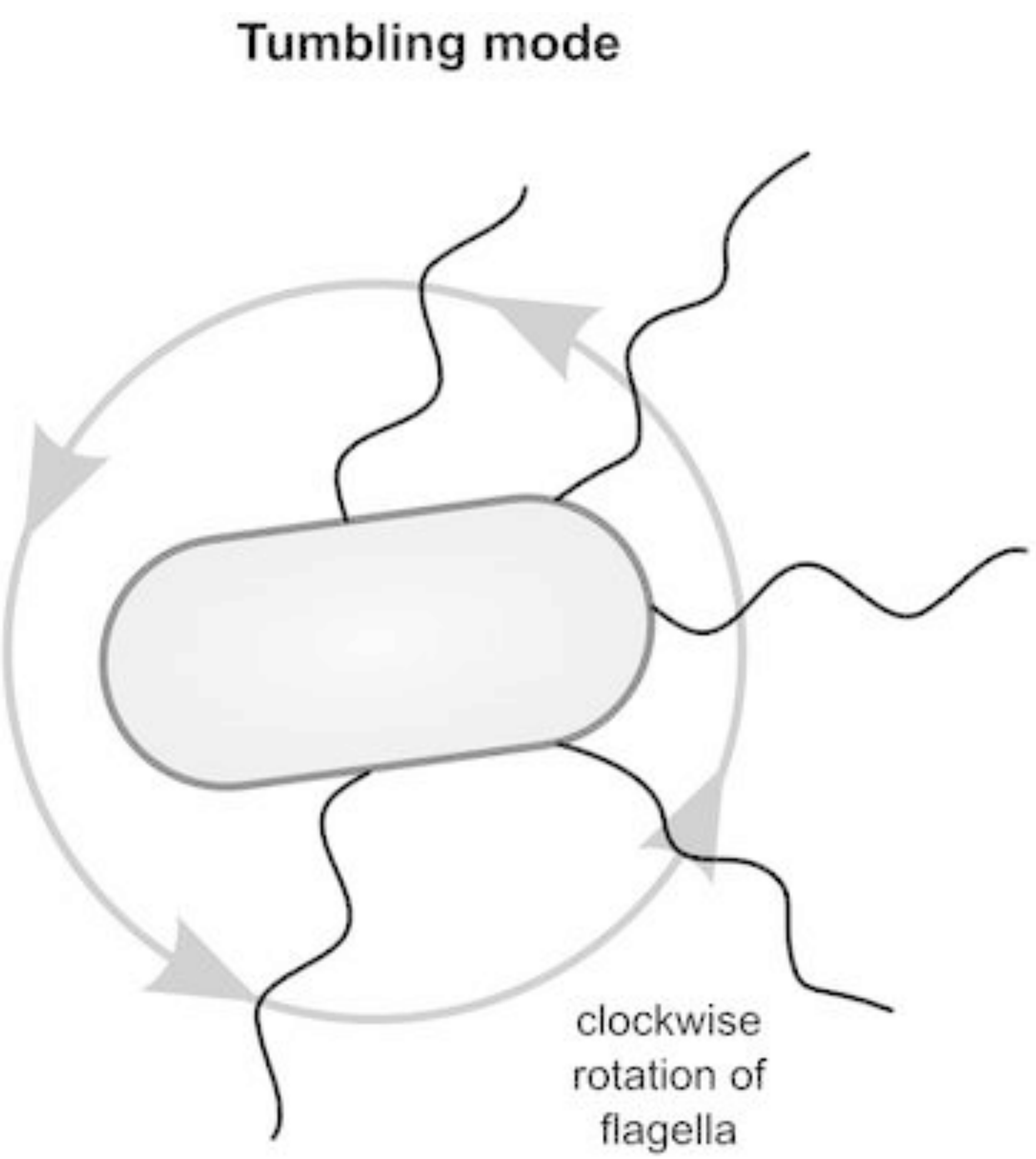
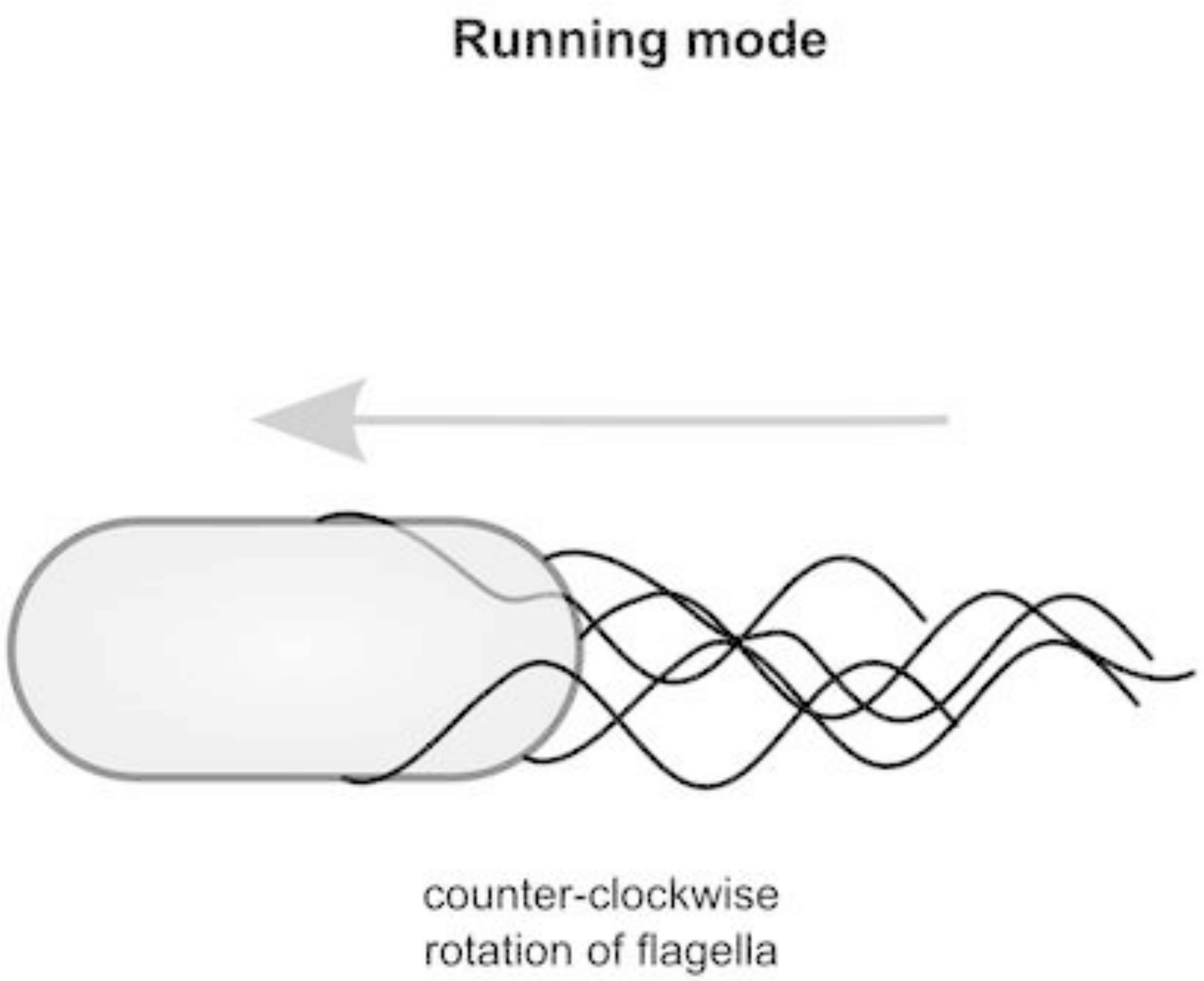




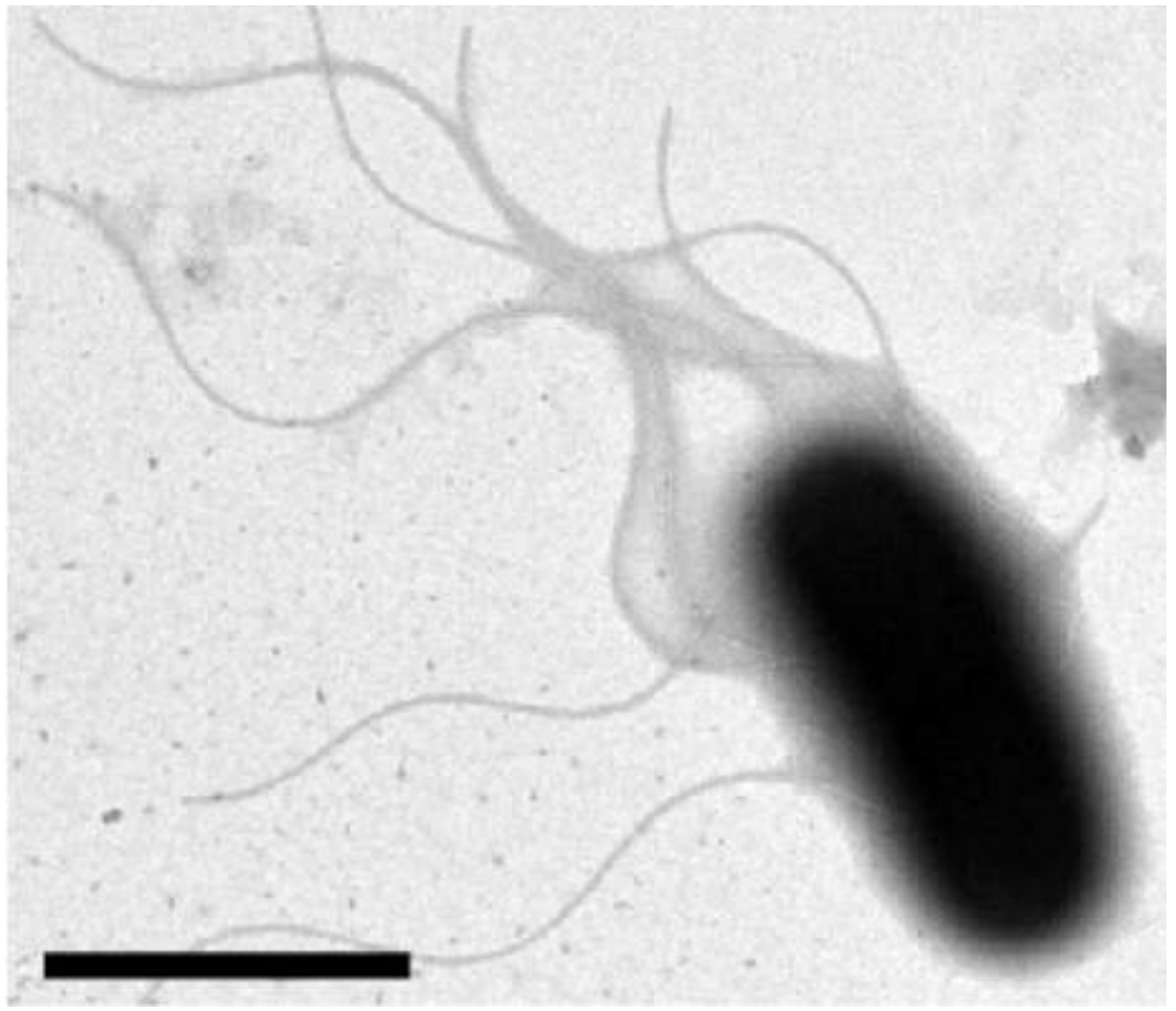
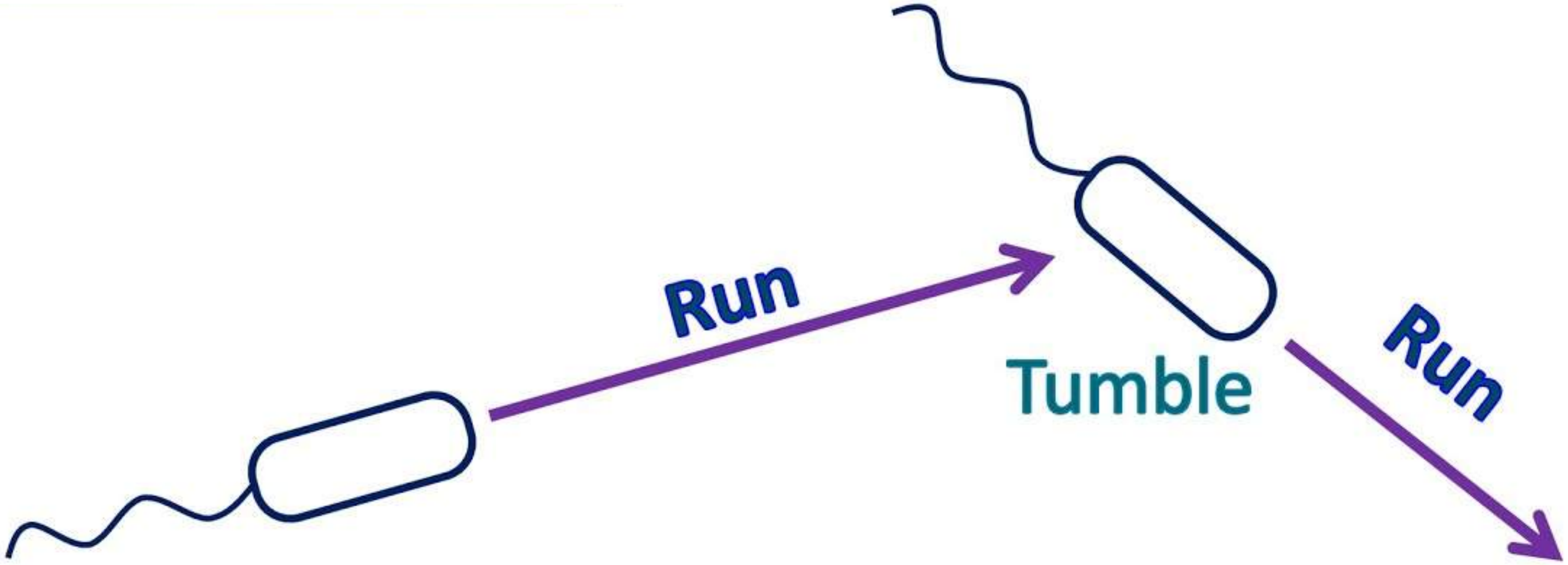
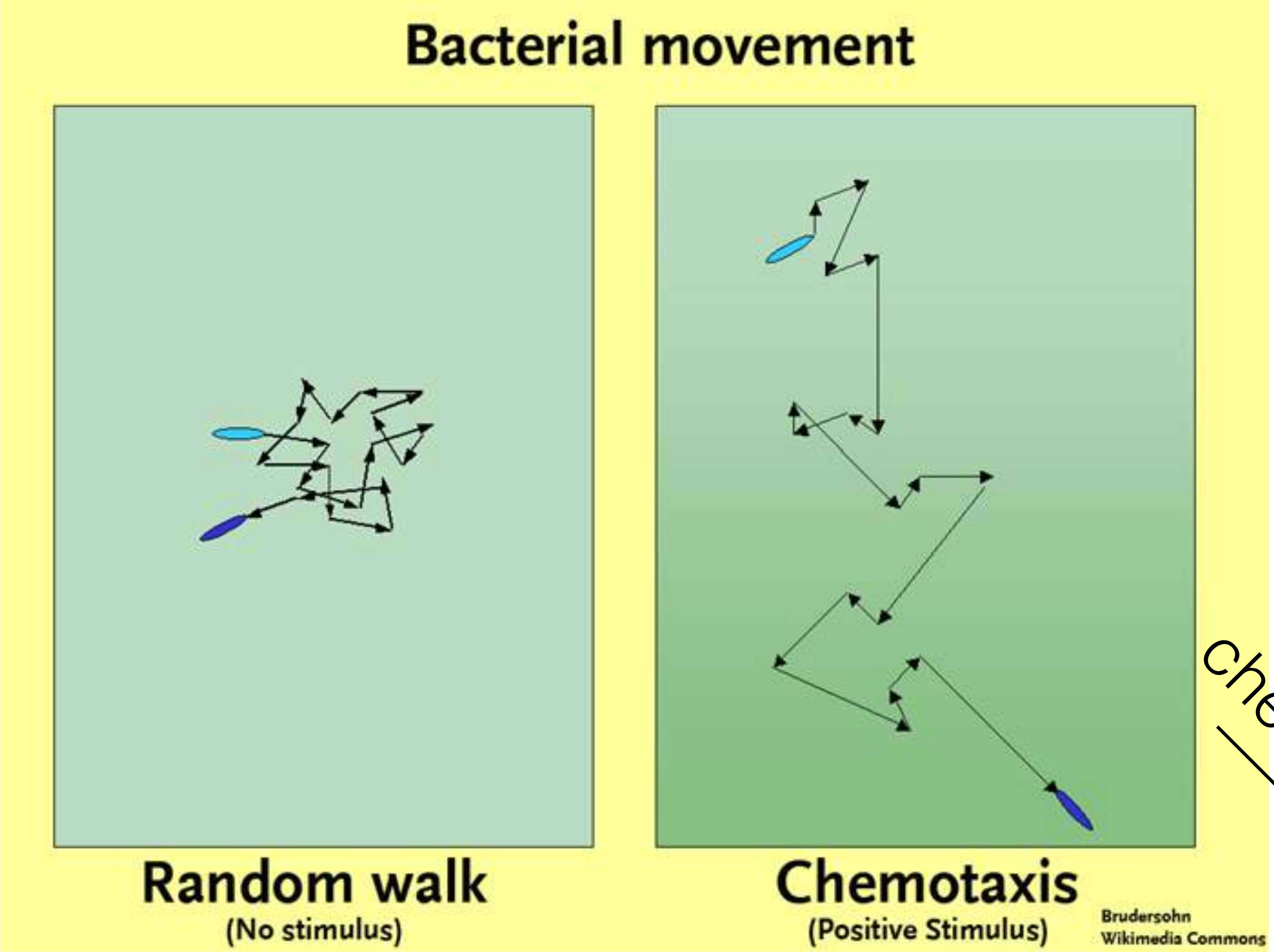


photo taken with an electron microscope

Chemotaxis



these bacteria like to move in the direction of a chemical attractant



Brudersohn
Wikimedia Commons

no chemical attractant

chemical attractant

chemotaxis

$$\varepsilon^2 \frac{\partial f_\varepsilon}{\partial t} + \varepsilon v \cdot \nabla_x f_\varepsilon = - \int_V (T_\varepsilon^*[S]f - T_\varepsilon[S]f')dv'$$

$$-\Delta S_\varepsilon = \rho_\varepsilon = \int_V f_\varepsilon \, dv$$

$$\uparrow$$

$$S_\varepsilon(x,t) = \frac{1}{4\pi} \int_{\mathbb{R}^3} \frac{\rho_\varepsilon(y,t)}{|x-y|} \, dy$$

Chalub, F. A., Markowich, P. A., Perthame, B., & Schmeiser, C.: Kinetic models for chemotaxis and their drift-diffusion limits. In *Nonlinear Differential Equation Models, (2004)*

B. Perthame, M. Tang, N. Vauchelet, Derivation of the bacterial run-and-tumble kinetic equation from a model with biochemical pathway Journal of Mathematical Biology, Vol. 73, No. 5, (2016) one can consider the limit of this mesoscopic model to a macroscopic model, called Keller-Segel model

$$\frac{\partial}{\partial t}\varrho - \Delta\varrho + \mathrm{div}(\varrho\chi\nabla c) = 0, \quad t \geq 0,\ x \in \mathbb{R}^d,$$

$$\nabla c = -\lambda_d\ \frac{x}{|x|^d} \star \varrho,$$

in

Chalub, F. A., Markowich, P. A., Perthame, B., & Schmeiser, C.: Kinetic models for chemotaxis and their drift-diffusion limits. In *Nonlinear Differential Equation Models, (2004)*

it is proven

solution of the kinetic chemotaxis problem

$\rightarrow$ (as $\epsilon \rightarrow 0)$

to solution of macroscopic Keller-Segel model

so solutions of the forward problems converge (kinetic -> macroscopic) given a situation where the solution to the inverse problem for the kinetic equation is well-posed

the solution to the inverse problem for the macroscopic equation is ill posed for the inverse problem

the *well-posed* solution to the inverse problem of the kinetic chemotaxis equation

$$\overset{\textbf{?}}{\to} \quad (\text{as} \quad \epsilon \to 0)$$

to an *ill posed* solution of the inverse problem to the Keller-Segel model

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thus we use the probabilistic setting

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we consider the solution of the inverse problem both in the kinetic and macroscopic setting

we consider the convergence of one to the other in a norm suitable to this context we prove convergence in the Bayesian setting, in an appropriate norm

Helmuth, K., Klingenberg, C., Li, Q., Tank, M.: “Multiscale convergence of the inverse problem for chemotaxis in the Bayesian setting", manuscript (2021)

Conclusion

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in future work we plan to devise efficient machine learning algorithms for these inverse problems

Thank you for your attention !