A Model of Heat Conduction

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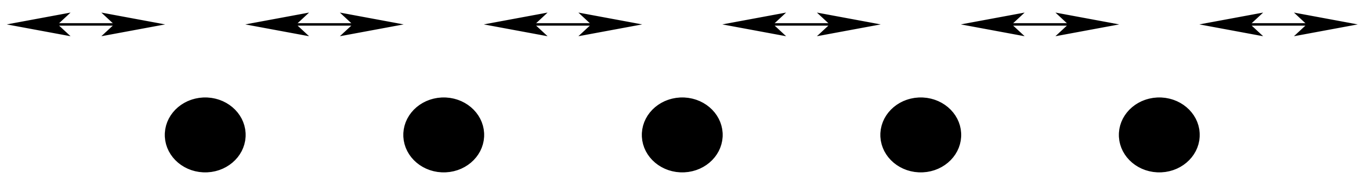
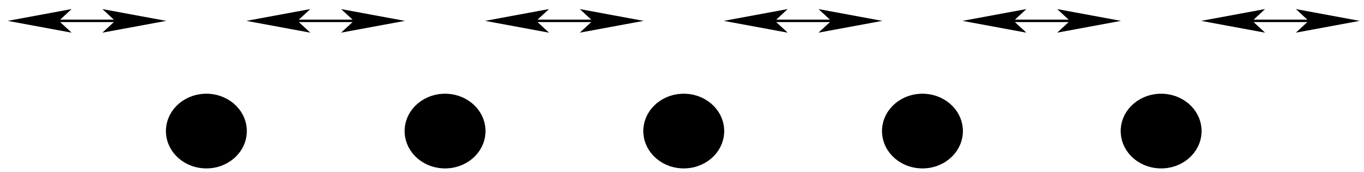
- (Non-rigorous) derivation of a Boltzmann equation from a particle model
- Mathematical results about Boltzmann equation
- Comparison of Boltzmann equation and particle model (numerical study)



The particle model is inspired by the scatterer model Lai-Sang Young and I developed, but with 1-dimensional dynamics

Discrete Space (Finite Number of Cells)

A varying number of particles of mass m and
N equidistant scatterers of mass M in a row.



The scattering rules for the momenta in 1D are elastic

$$S\begin{pmatrix} p \\ q \end{pmatrix} \to \begin{pmatrix} \tilde{p} \\ \tilde{q} \end{pmatrix} \begin{matrix} \text{(particle)} \\ \text{(scatterer)} \end{matrix}$$

$$S = \begin{pmatrix} -\sigma & 1-\sigma \\ 1+\sigma & \sigma \end{pmatrix}, \quad \sigma = (M-m)/(M+m)$$

The scatterers have finite mass M but they do NOT move
The particles move in direction of sign of momenta
They are injected (and leave) at the ends of the chain

The ``inertial'' mass of the scatterers is infinite...

We want to find time-stationary distributions when particles are injected from outside (out of equilibrium)

This will be done for a Boltzmann equation which is an approximation to the particle problem

To derive the Boltzmann equation, assume independence of probability distributions

At the end, check the quality of this approximation (numerically)

We arrange space in N cells (of length L each) and for each cell we have probability distributions:

$F_{L,i,in}(p)$: probability that particles with momentum $p > 0$ enter cell #i from the left (per second)

...

$g_i(q)$: probability that the i-th scatterer has momentum $q \in \mathbb{R}$ $\quad (\int g = 1)$

Important remark: (1D!!!) Expected time to stay in cell is $F(p)/|p|$ $\Rightarrow$ Expected number of particles in cell is infinite (when $F(0) \neq 0$)

The equations describing free-flight and scattering are of the form (omitting index of cell)

$$g(\tilde{q}) = \frac{1}{\lambda} \int_{\mathbb{R}} dp \; g(q) \; F(p)$$

where $F = F_{L,in} + F_{R,in}$ and $\lambda = \int_{\mathbb{R}} F \approx$ particle flux

What comes out of the cell?

$$F_{L,out}(\tilde{p}) = \int_{q \;:\; \tilde{p}<0} dq \, g(q) \, F(p)$$

$$F_{R,out}(\tilde{p}) = \int_{q \;:\; \tilde{p}>0} dq \, g(q) \, F(p)$$

And the cells are coupled by $F_{L,i,in} = F_{R,i-1,out}$

Continuum Limit

$N \to \infty$, $i/N = x \in [0,1]$, scattering probability $1/N$. After some gymnastics, using things like

$$F_{L,i,in}(p) - F_{R,i,out}(p) = F_{L,i,in}(p) - F_{L,i+1,in}(p) \approx N\partial_x F(p,x)$$

one gets the Boltzmann equations

$$m\partial_t F(t,p,x) + p\partial_x F(t,p,x) = |p| \int dq \left(F(t,\tilde{p},x)g(t,\tilde{q},x) - F(t,p,x)g(t,q,x) \right)$$

$$\partial_t g(t,q,x) = \int dp \left(F(t,\tilde{p},x)g(t,\tilde{q},x) - F(t,p,x)g(t,q,x) \right)$$

The closure assumptions are hidden in the independence of the F and g at different x (as well as in the product structure)

The stationary equation $x \in [0,1]$

$$\partial_x F(p,x) = \mathrm{sign}(p) \int dq \left(F(\tilde{p},x) g(\tilde{q},x) - F(p,x) g(q,x) \right)$$

$$0 = \int dp \left(F(\tilde{p},x) g(\tilde{q},x) - F(p,x) g(q,x) \right)$$

Remark:

$$F(p,x) = \lambda e^{-\beta(p-ma)^2} , \quad g(q,x) = e^{-\beta(m/M)(q-Ma)^2}$$

are solutions for all $\beta > 0$, $\lambda > 0$, and $a \in \mathbb{R}$

Want $\int dq\, g = 1$ (but not necessarily $\int dp\, F = 1$)

I omit the normalizing square roots

We would like to "bifurcate" from these equilibrium solutions by imposing $F(p, x = 0)$ for $p > 0$ and $F(p, x = 1)$ for $p < 0$

That is: We want to impose nonequilibrium INCOMING fluxes

Main result :

This problem has solutions

Several difficulties make the result less general than Pierre and I expected (but perhaps there are better tricks)

Continue with $m = 1$

We write $F(p,0) = \exp(-p^2)\cdot v(p)$ and define

$$C = \{v \ : v(p) \geqslant 0, v \not\equiv 0, \int |dv(p)| + \int e^{-p^2} |v(p)| < \infty$$

$$\text{and } 0 < \lim_{p\to\pm\infty} Z \cdot v(p) < 1\} \quad \text{with } Z = \sqrt{\pi} / \int dp\, F(p,0)$$

This is a convex Banach cone ensuring that

- v has limits (and is positive, F is a rate...)
- $F(p,0)$ is not Gaussian, since we require

$$\lim_{p\to\pm\infty} \frac{F(p)\, e^{p^2} \int e^{-s^2} ds}{\int F(s) ds} < 1$$

- In the cone, the "temperatures" (but not the distributions!) must be the same for $p > 0$ and $p < 0$
- The variation norm $\int |dv(p)|$ accounts for discontinuity of F at $p = 0$

Main Result : For any v_* in the interior of the cone C and for all initial conditions $v(\cdot, x = 0)$ near v_* the Boltzmann equation has a (unique) solution in C for $x \in [0, x_0]$ with $x_0 > 0$. The map $v(\cdot, x = 0) \mapsto v(x_0)$ is a diffeomorphism

Consequence : In the image of the neighborhood, I can choose $v(p, x_0)$ for $p < 0$. In other words, within the limits of applicability of the main result, I can choose $v(p>0, x=0)$ and $v(p<0, x_0)$, that is, I can prescribe the incoming (slightly different) momentum and particle flux profiles (at the ends $x = 0$, $x = x_0$) and obtain a unique non-equilibrium steady state

Remarks about the proof – which hopefully explains why we take these "funny" conditions on the cone

- It is not obvious that the density of $F(x,\cdot)$ remains a positive function
- The Boltzmann equation has two parts, for F with a space derivative, for g it is simpler. So we solve first for $g(x,\cdot)$, given $F(x,\cdot)$, and then integrate to find F

$$\partial_x F(p,x) = \mathrm{sign}(p) \int dq \left(F(\tilde{p},x) g(\tilde{q},x) - F(p,x) \right)$$

$$g(q,x) = \frac{\int dp\, F(\tilde{p},x) g(\tilde{q},x)}{\int dp\, F(p,x)}$$

We view the second equation as a fixed point problem. Solve, and substitute into the first equation and integrate. The difficult part is the second equation. To study it fix the integral of F to 1

Since x is a spectator in the g-equation, we consider instead

$$g(q) = \int dp\, F(\tilde{p})\, g(\tilde{q})$$

N.B. $\tilde{p} = -\sigma p \quad + (1-\sigma) q$
$\tilde{q} = (1+\sigma p) \quad + \sigma q$

This is a convolution operator, and we use spectral properties. The cone C guarantees that the r.h.s. is (for $F \in \operatorname{int} C$) a quasi-compact operator with isolated largest eigenvalue (equal to 1)

Conjecture: the essential spectral radius ends at the larger of the 2 limits of $v(p)$:
the numerical spectrum is $\{\sigma^n\}_{n=0}^{\infty}$

Let $\mu \equiv \frac{m}{M} = \frac{1-\sigma}{1+\sigma}$ and $g(q) = \exp(-\mu q^2)u(q)$ and define

$$\|u\|_1 = \int dq\, e^{-\mu q^2} |u(q)|$$

and

$$\|u\|_* = \|u\|_1 + \int |du(q)| \ .$$

The main estimate is then for any $v \in C$:

There exist a $\zeta < 1$ and an $R > 0$ (both depend on v continuously) such that the convolution operator
$K_v \Leftrightarrow g \mapsto \int dp F(\tilde{p}) g(\tilde{q})$
satisfies for any $\|u\|_* < \infty$ the bound

$$\int |dK_v(u)| \leqslant \zeta \int |du| + R\|u\|_1$$

Why can't we have $\beta \neq \beta'$?

$$F(p,0) = \begin{cases} \exp(-\beta p^2), & p > 0 \\ \exp(-\beta' p^2), & p < 0 \end{cases}$$

The problem is that convolution mixes contributions from positive and negative p. The reflection by the scatterer exchanges temperature information between the positive to the negative momentum side

This makes us lose compactness, and we don't know how to show existence and uniqueness of g without some information. Numerics shows it is much better... why?

The discontinuity of F at $p = 0$ is a realistic phenomenon and is the reason why we consider the variation norm $\int |dv(p)|$ instead of $\int dp\,|v'(p)|$.
With such norms the compactness of convolution is well known (one gains a derivative) and in fact the probability densities are smooth in p and q except at $p = 0$

Numerical study

Compare the Boltzmann model to the particle model from which it is derived

- One does not need the cone C
- The role of x_0 should become clear

Reconsider

$$\partial_x F(p,x) = \gamma \,\mathrm{sign}(p) \int dq \left(F(\tilde{p},x) g(\tilde{q},x) - F(p,x) g(q,x) \right)$$

$$0 = \int dp \left(F(\tilde{p},x) g(\tilde{q},x) - F(p,x) g(q,x) \right)$$

This Boltzmann limit was obtained by assuming in the particle model that

particles interact (in 1 cell) with probability γ/N and cross the cell without collision with probability $1-\gamma/N$

As $N \to \infty$, the cross-section of the scatterers is assumed to be γ/N.

Like the Grad limit: The number of scatterers increases with N

Boltzmann simulations

$$\partial_x F(p,x) = \mathrm{sign}(p) \int dq \left(F(\tilde{p},x) g(\tilde{q},x) - F(p,x) \right)$$

$$g(q,x) = \frac{\int dp\, F(\tilde{p},x) g(\tilde{q},x)}{\int dp\, F(p,x)}$$

We discretize the space of p and q and integrate from $x = 0$ to $x = 1$. The second equation is an eigenvalue problem with unknown eigenfunction $g = g_{F(\cdot,x)}$

Substitute the g:

$$\partial_x F(p,x) = \mathrm{sign}(p) \int dq \left(F(\tilde{p},x) \cdot g_{F(\cdot,x)}(\tilde{q},x) - F(p,x) \right)$$

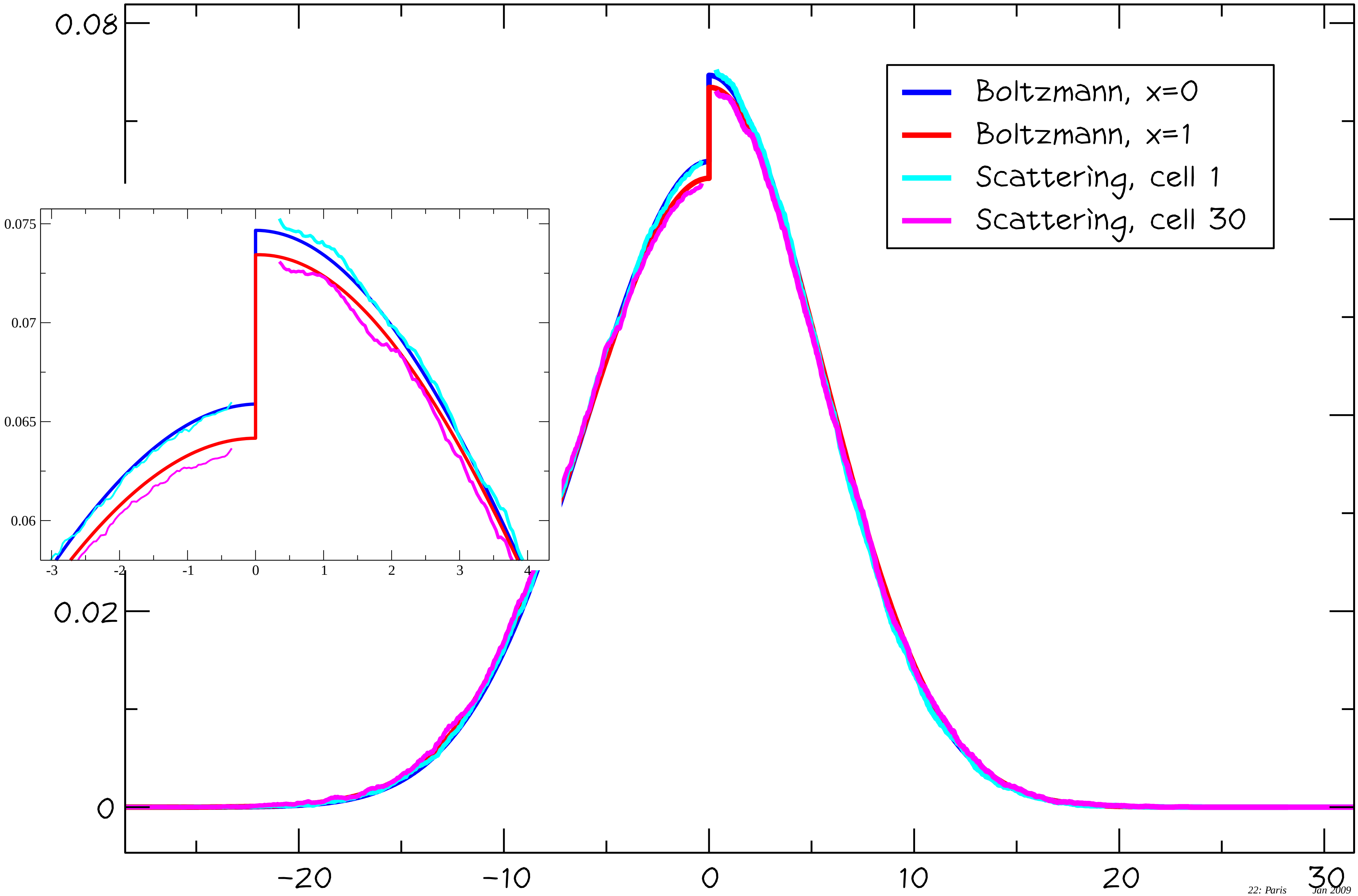
Take as initial condition

$$F_0(p,0) = \begin{cases} \lambda \exp(-\beta p^2), & p > 0 \\ \lambda' \exp(-\beta' p^2), & p < 0 \end{cases}$$

and see if $F(p, x = 1)$ for $p < 0$ is the desired incoming Gaussian $\lambda' \exp(-\beta' p^2)$. Iteratively correct $F_0 \to F_1 \to$

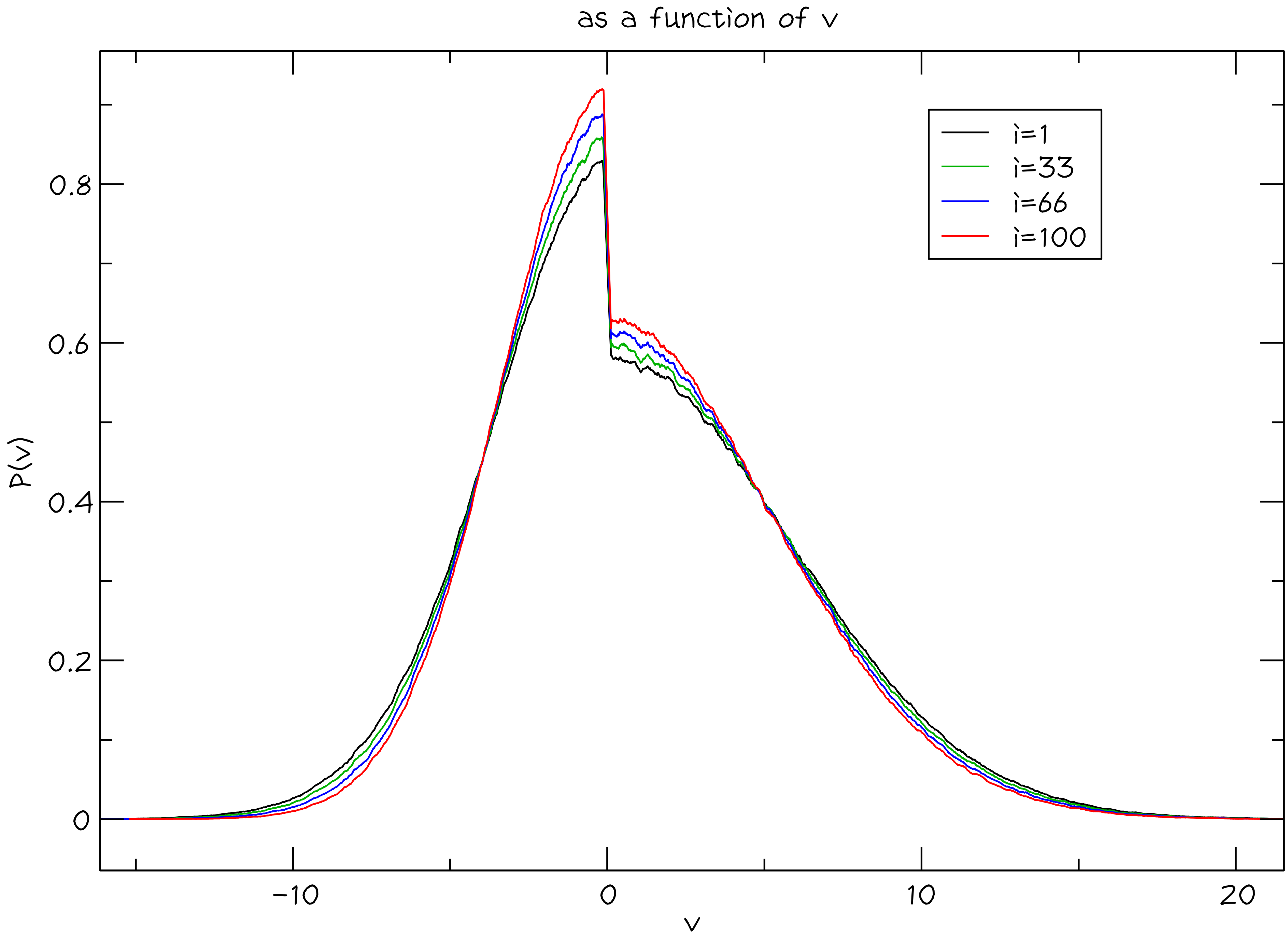
poor man's inverting the diffeomorphism of the Theorem (shooting)

Boltzmann vs Particle Model (30 cells)

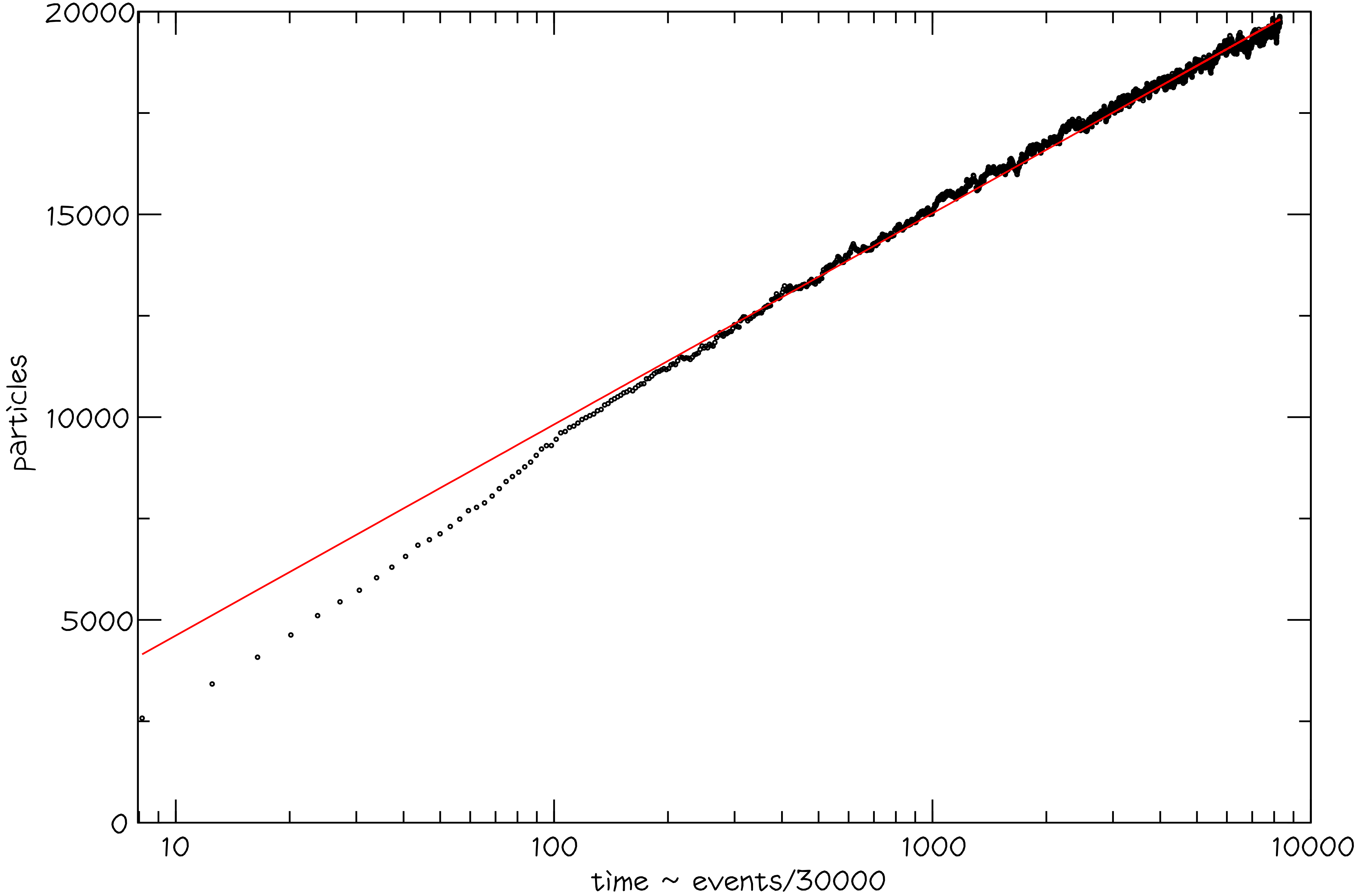


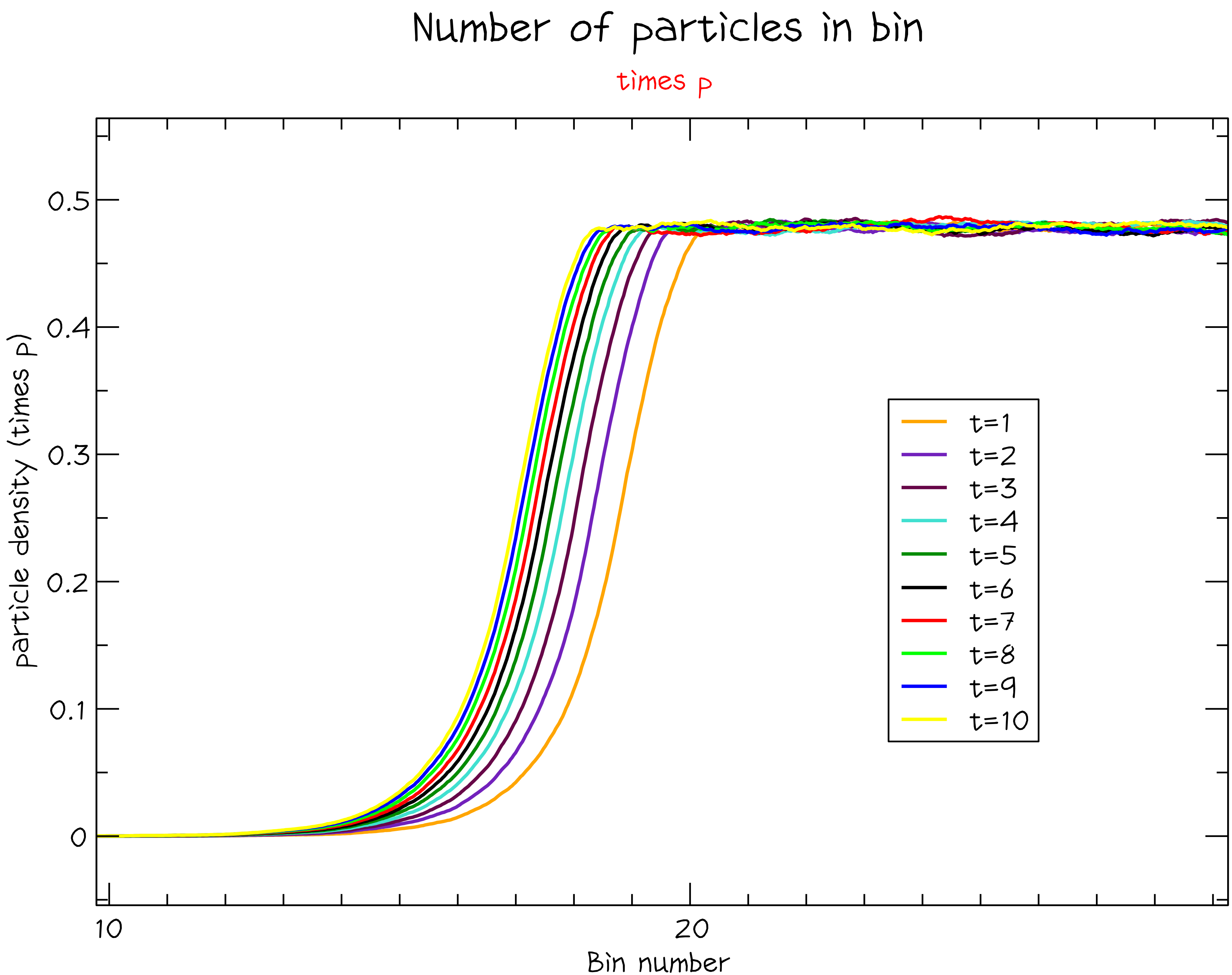
Particle simulations: $T_L = 3T_R$, $j_L = j_R$ Will take $\gamma = 1$.

Distribution of velocity



of particles as function of time





Number of particles in bin
times p
particle density (times p)
0.5
0.4
0.3
0.2
0.1
0
10
20
Bin number
t=1
t=2
t=3
t=4
t=5
t=6
t=7
t=8
t=9
t=10

This is typical for non-normalizable measures. The number of particles is proportional to $F(p)/|p|$ which is non-integrable in 1 dimension.

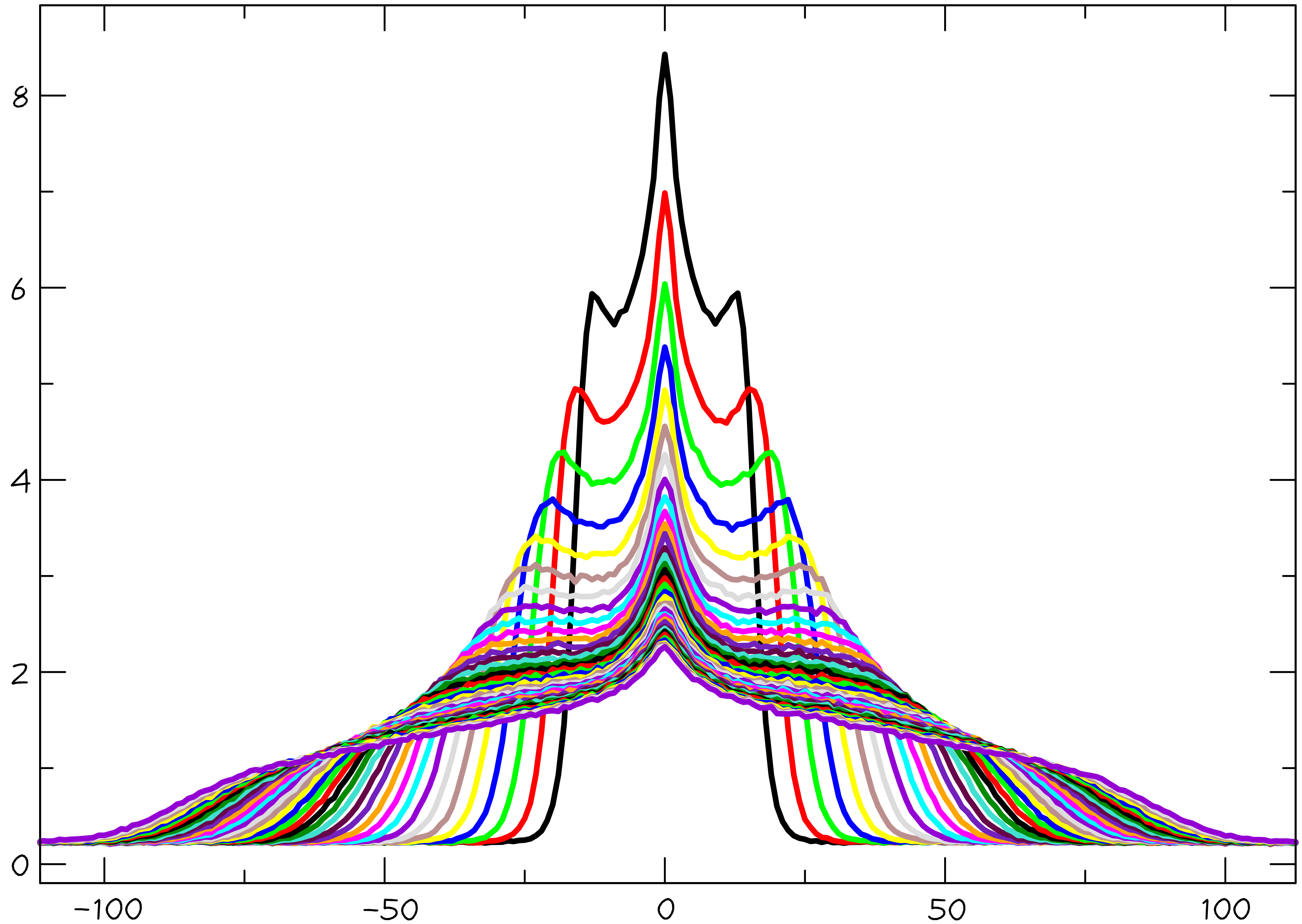
Similar to tangents in 1-d maps: Collet-Ferrero; Annales de l'Institut Henri Poincaré (A) Physique théorique, 52 (1990), p. 283-301

Return to Equilibrium (Correlation Functions)

One can ask in this model how the system reacts to local perturbations. For example: take equilibrium steady state and put a large number of particles in the center of the system (with Maxwell distribution)

Evolution of particle number

as function of position



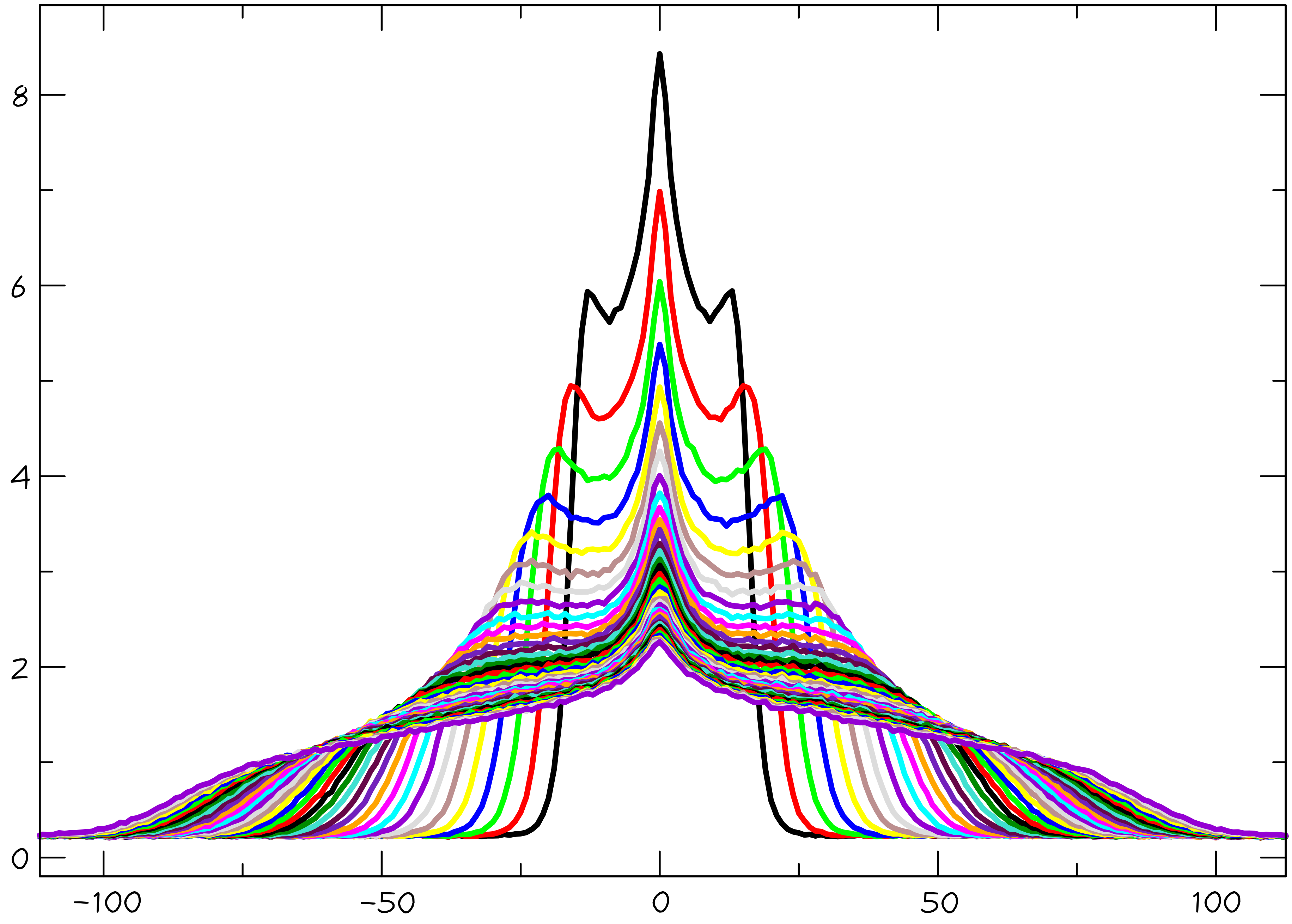
In fact, the particle number density φ in the large N limit is governed by the telegraph equation (neglecting the momentum exchange with the discs)

$$\left(\partial_t^2 + c\gamma\partial_t - \partial_x^2\right)\varphi(x,t) = 0$$

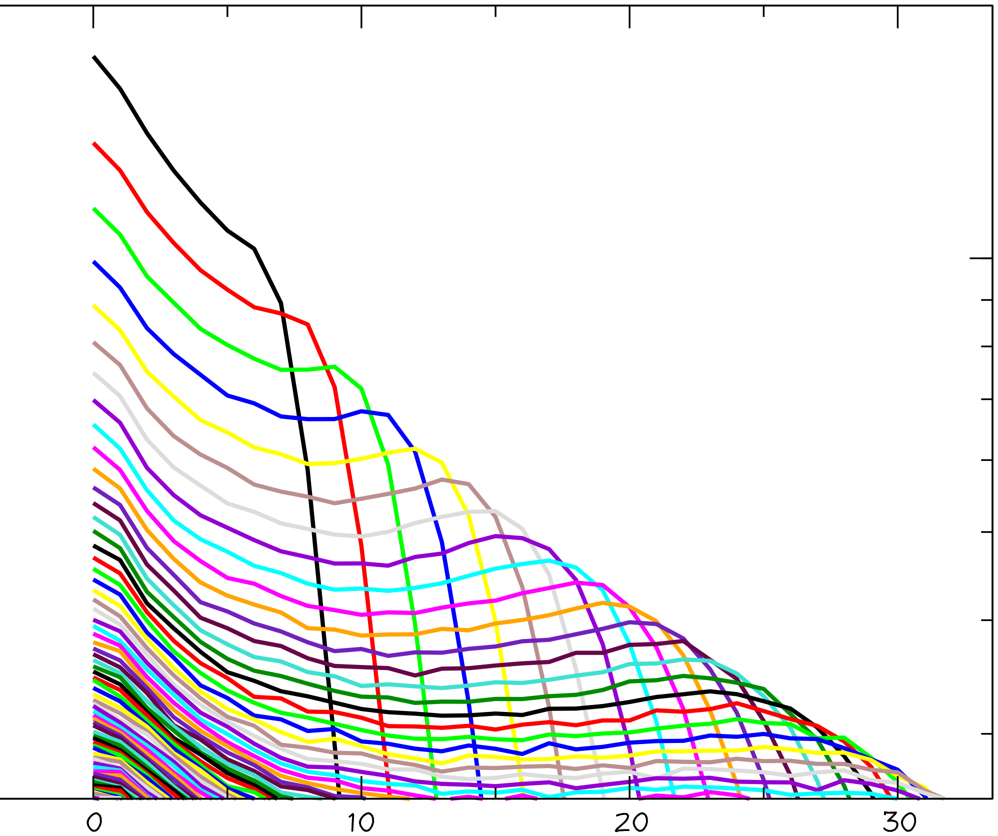
The solution can be explicitly written in terms of Bessel functions and one obtains a leading edge which moves with finite speed and is exponentially decaying, superposed with a diffusive term

Evolution of particle number

as function of position

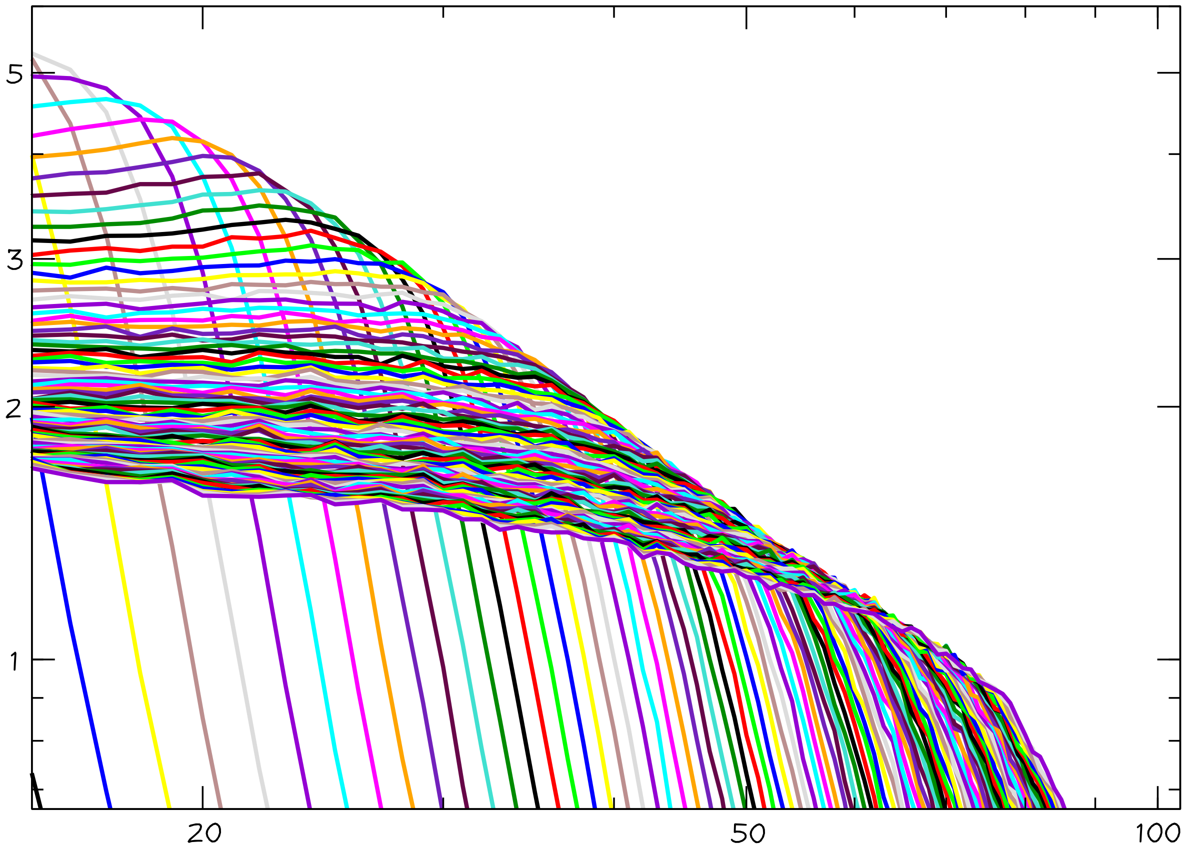


The leading telegraph edge



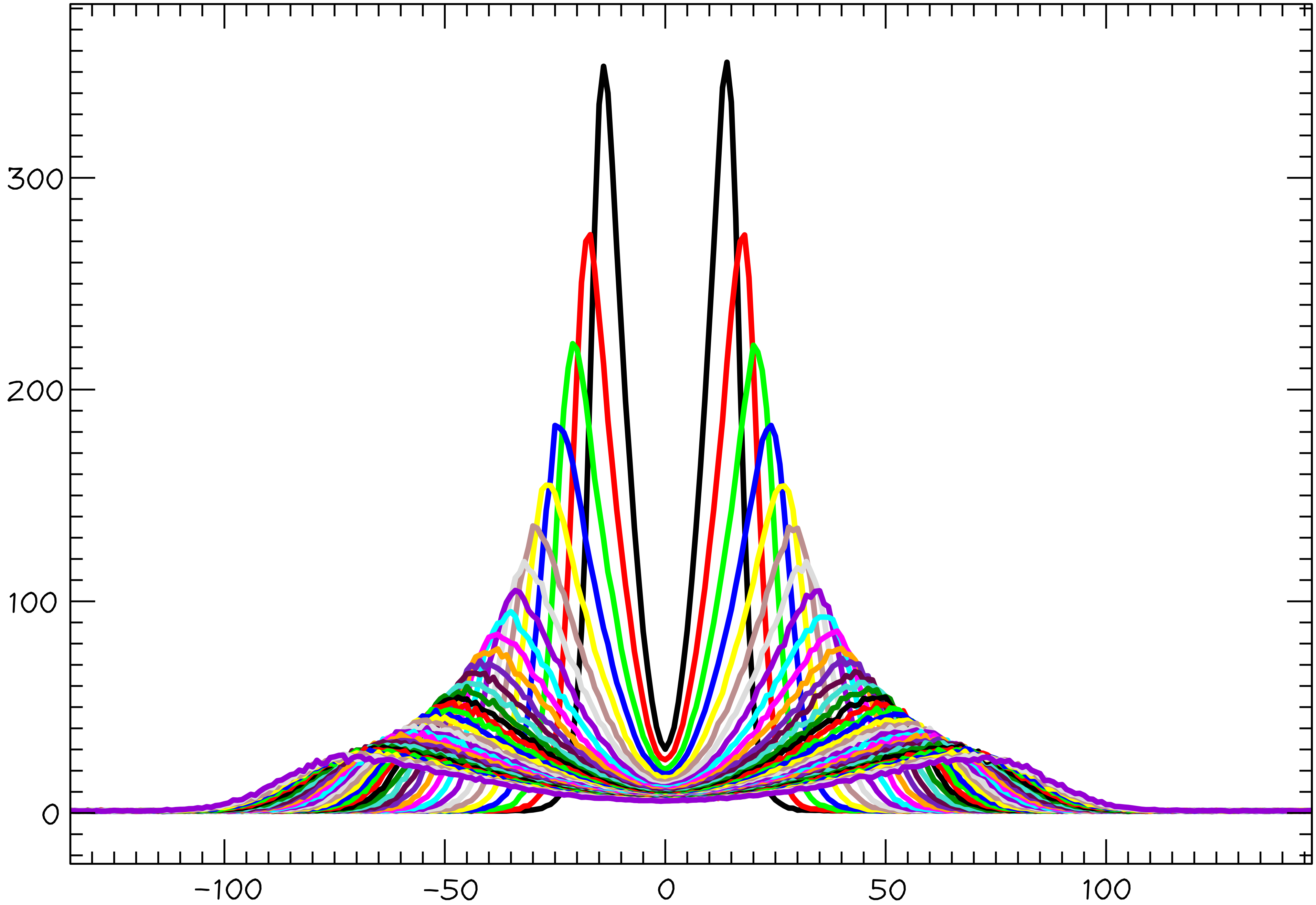
x: lin y:log

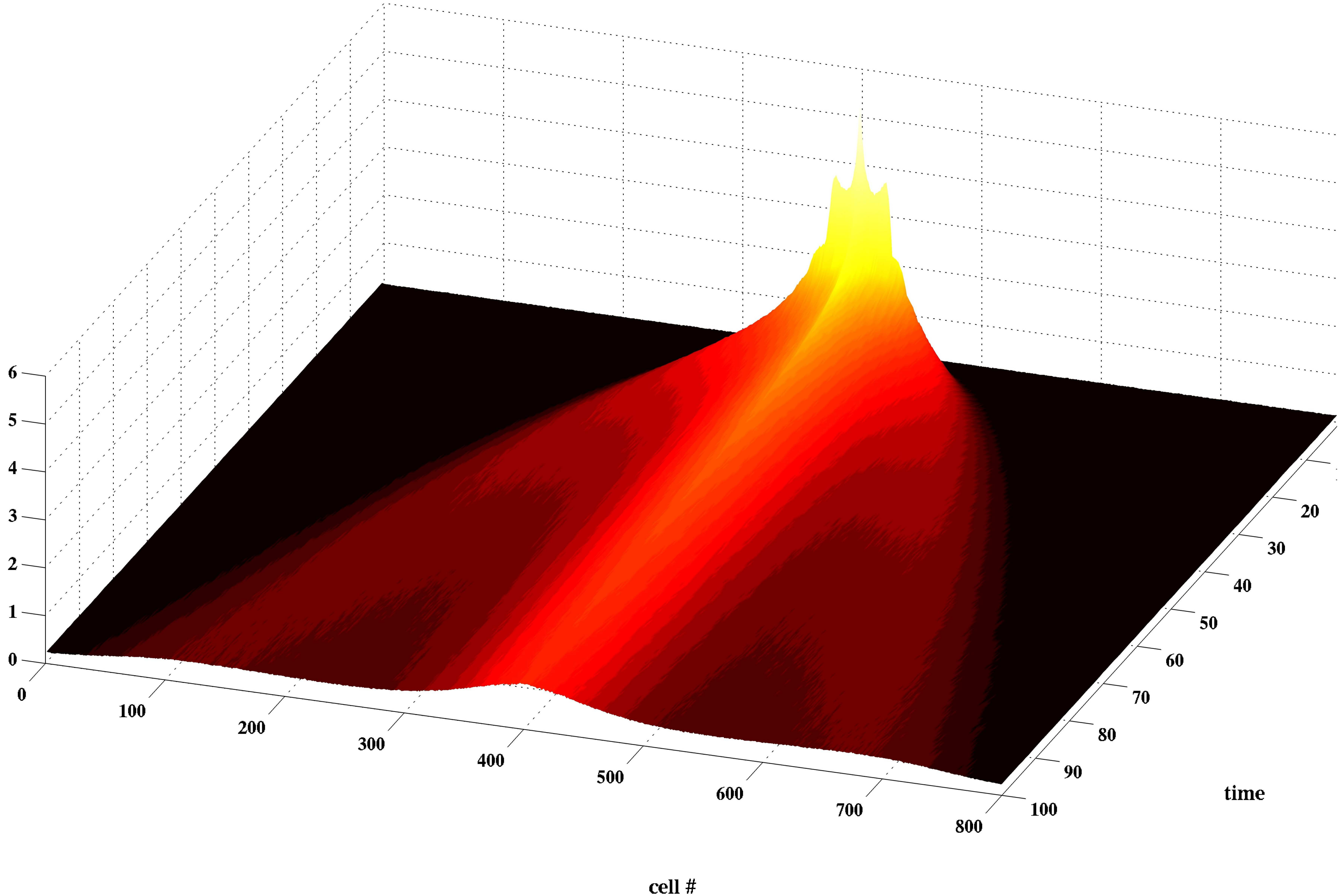
The leading diffusive edge



x: log y:log

Energy distribution as function of time





6
5
4
3
2
1
0
0
100
200
300
400
500
600
700
800
cell #
20
30
40
50
60
70
80
90
100
time

Conclusion

Back to Boltzmann: We found the solution by iterating the initial distribution until the other end was what we wanted. $F_0 \to F_1 \to \cdots$

Interesting problem: What if in this problem $F_n(p,0)$ ceases to be positive after n iterations when $p < 0$?

Cannot extract arbitrary energy profiles for $p < 0$ at $x = 0$ by injecting something at $x = 1$. (This is why we had x_0 in the theorem)

QUESTION: What ARE the possible exit distributions?