Lifshitz-Slyozov with collisions, asymptotic behavior: numerical methods.

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Model

We consider the Lifshitz-Slyozov (model for grain formation):

$$\begin{cases} \partial_t f + \partial_x (V f) = 0, \quad t \geq 0,\ x \geq 0, \\ V(t,x) = a(x)c(t) - b(x), \\ c(t) + \int_0^\infty x f(t,x) dx = \rho, \quad t \geq 0, \end{cases}$$

with initial data $f^0 \geq 0$ and $c^0 \geq 0$.

- $f(t,x)$ number density of *macro*-particles of size x at time t;
- c *monomers* concentration;
- $\int_0^\infty x f(t,x) dx$ proportional to the mass of macro-particles;
- $a(x) = x^{1/3}$ et $b(x) = 1$ are classically considered (as in this talk); in this case, $V(t,0) < 0$;
- this problem is known to be well-posed: there exists a unique solution $(c,f) \in \mathcal{C}^0([0,T]) \times L^\infty(0,T,L^1(\mathbb{R}_+^*,(1+x)dx)$ (cf. Niethammer-Pego, Collet-Goudon, Laurençot...).

Problem

Model proposed in 1961. The asymptotic in time behavior is interesting in the chemical view point... And from the mathematical point of vue. Lifshitz and Slyozov conjectured that

- $c(t)$ tends to 0 as $K_{LS}e^{-t/3}$;
- $\int_0^\infty f(t,x)dx$ tends to 0 as $C_{LS}(K_{LS},\rho)e^{-t}$;
- $\int_0^\infty x^{1/3}f(t,x)dx / \int_0^\infty f(t,x)dx$ behaves as $t^{1/3}/K_{LS}$;
- $f^{rescaled}(t,x)$ tends to a certain asymptotic profile; the correct scaling is

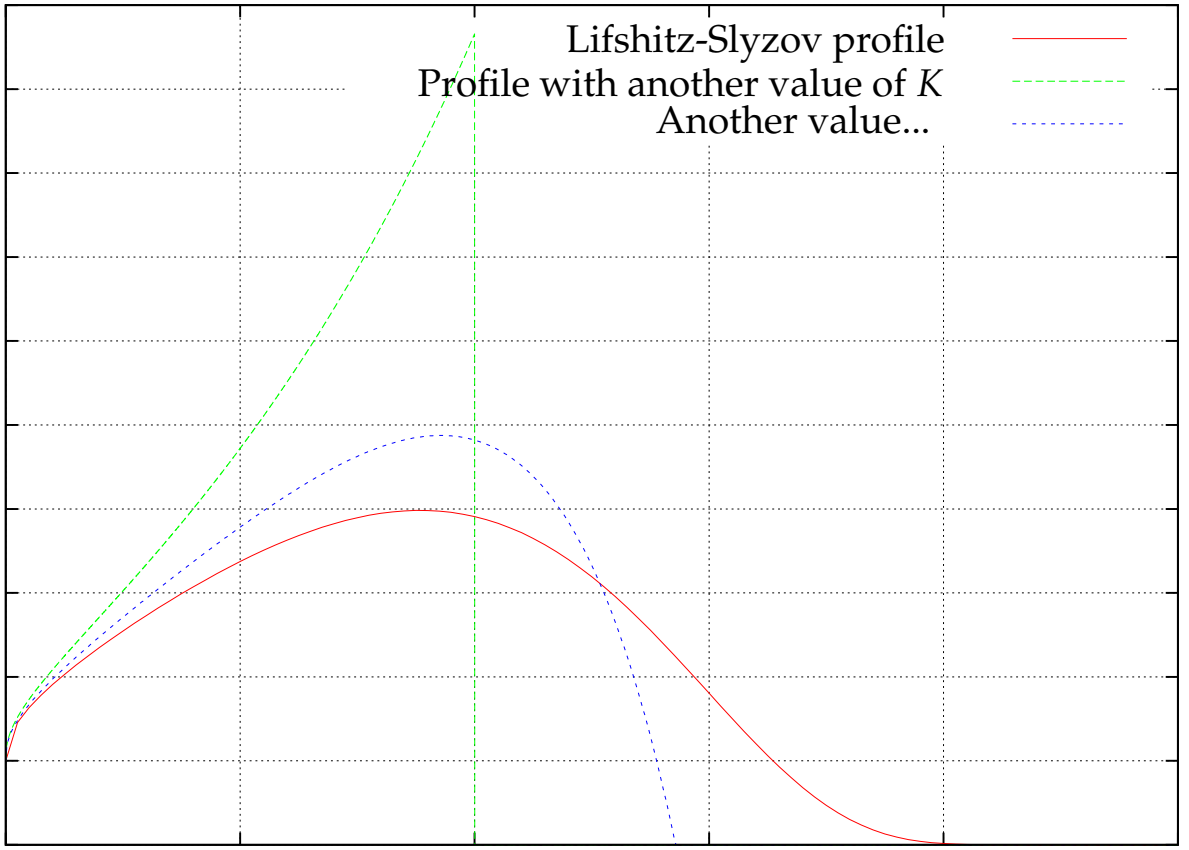
$$\begin{cases} f(t,x) = \frac{1}{(1+t)^2} g\left(\ln(1+t), \dfrac{x}{1+t}\right), \\ \tau = \ln(1+t), \quad y = \frac{x}{1+t}, \quad d(\tau) = (1+t)^{1/3}c(t), \end{cases}$$

and the system becomes

$$\begin{cases} \partial_\tau g + \partial_y(Wg) = g, \quad \tau \geq 0,\ y \geq 0, \\ W(\tau,y) = y^{1/3}d(\tau) - 1 - y, \\ d(\tau)e^{-\tau/3} + \int_0^\infty y g(\tau,y)dy = \rho, \quad \tau \geq 0. \end{cases}$$

Stationnary states of the rescled system

There exists a stationnary profile for any value $K > K_{LS}$ of d.



K_{LS} is the smallest admissible value for d, and the only one associated to a $\mathcal{C}^\infty$ profile. The greater K is, the less smooth the profile is.

Numerical exploration

We want to explore numerically the asymptotic behavior (and the L-S conjecture).
A finite volume scheme:

$$\frac{f_j^{n+1} - f_j^n}{\Delta t} + \frac{V_{j+1/2}^n f_{j+1/2}^n - V_{j-1/2}^n f_{j-1/2}^n}{\Delta x} = 0, \quad n \in \mathbb{N}, j \in \mathbb{N}.$$

where $V_{j+1/2}^n = V(n\Delta t, x_{j+1/2})$, with $x_{j+1/2} = (j+1)\Delta x$
(c^n, approximation of c at time $n\Delta t$, is assumed to be known).
Problem: numerical diffusion of usual stable transport schemes can be predominant in large time.
$\longrightarrow$ Use of a non-dissipative algorithm [Després-L.].
It is an algorithme dedicated to the computation of approximate to Cauchy problems for $\partial_t u + a\partial_x u = 0$.
This algo is stable, convergent, first order, and not dissipative:
it has infinitely many asymptotic profiles that are stationary on characteristic curves.

Brief overview on the limited downwind scheme

$\partial_t u + a\partial_x u = 0$ with $a > 0$,
$u_j^{n+1} = u_j^n - a\lambda(u_{j+1/2}^n - u_{j-1/2}^n)$, où $\lambda = \Delta t/\Delta x$.
Let $m_{j+1/2}^n = \min(u_j^n, u_{j+1}^n)$
and $M_{j+1/2}^n = \max(u_j^n, u_{j+1}^n)$,
then $b_{j+1/2}^n = \max\left(m_{j+1/2}^n, (u_j^n - M_{j-1/2}^n)/(a\lambda) + M_{j-1/2}^n\right)$
and $B_{j+1/2}^n = \min\left(M_{j+1/2}^n, (u_j^n - m_{j-1/2}^n)/(a\lambda) + m_{j-1/2}^n\right)$.
Then, under the CFL condition $a\lambda \leq 1$, $b_{j+1/2}^n \leq B_{j+1/2}^n$, and if $u_{j+1/2}^n \in [b_{j+1/2}^n, B_{j+1/2}^n]$, the scheme is TVD and satisfies a local maximum principle.
Limited downwind scheme: minimization of $|u_{j+1/2}^n - u_{j+1}^n|$ under the (upwind) constraint $u_{j+1/2}^n \in [b_{j+1/2}^n, B_{j+1/2}^n]$.
(In the case of constant velocity, this scheme is equivalent to Ultrabee limiter, and, in the case of a Heaviside initial datum, it is equivalent to the SLIC interface reconstruction algorithm).

Application to the *conservative* transport equation

Here we are interested in $\partial_t f + \partial_x (Vf) = 0$ with the scheme

$$f_j^{n+1} = f_j^n - \lambda \left(V_{j+1/2}^n f_{j+1/2}^n - V_{j-1/2}^n f_{j-1/2}^n \right).$$

We write it in the form $f_j^{n+1} =$

$$f_j^n - V_j^n \lambda \left(f_{j+1/2}^n - f_{j-1/2}^n \right) - \lambda \left(f_{j+1/2}^n (V_{j+1/2}^n - V_j^n) + f_{j-1/2}^n (V_j^n - V_{j-1/2}^n) \right),$$

where $V_j^n = V(n\Delta t, x_j)$ with $x_j = (j + 1/2)\Delta x$,

and look at the stability for part $f_j^{n+1/2} = f_j^n - V_j^n \lambda \left(f_{j+1/2}^n - f_{j-1/2}^n \right)$ of the algo.

One can use the limited downwind (in the *conservative* scheme). But this does not guarantee positivity.

Positivity is guaranteed modifying the constraint on the flux, replacing $B_{j+1/2}^n$ with $\tilde{B}_{j+1/2}^n = \min \left(B_{j+1/2}^n, m_{j-1/2}^n V_{j-1/2}^n / V_{j+1/2}^n + f_j^n / (\lambda V_{j+1/2}^n) \right)$ (in the case where the velocity is locally positive).

Application to the conservative transport equation

In the case where the velocity is locally negative, the same can be done.
When the velocity changes sign, the upwind scheme is used.

Prop. Uner the CFL condition $\lambda||V(n\Delta t)||_\infty \leq 1$, one has $b^n_{j+1/2} \leq \tilde{B}^n_{j+1/2}$ for every j, and if $f^n_{j+1/2} \in [b^n_{j+1/2}, \tilde{B}^n_{j+1/2}]$ for any j,

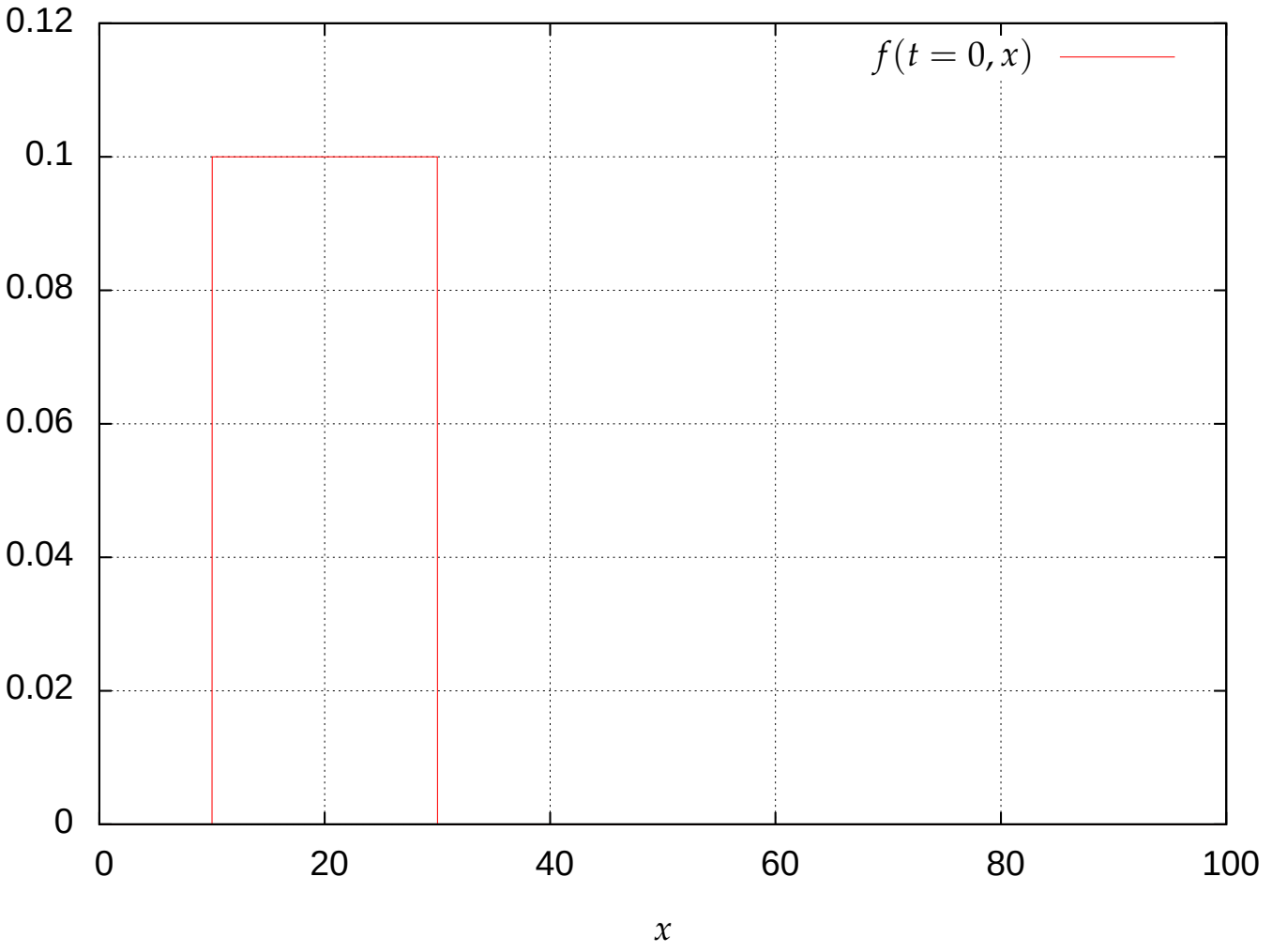
- $f^{n+1/2}_j = f^n_j - \lambda V^n_j \left(f^n_{j+1/2} - f^n_{j-1/2}\right)$ satisfies a local maximum principle;
- if $f^n_j \geq 0$ for any j, $f^{n+1}_j \geq 0$ for any j.

After this conservative transport step, we compute the new value of the monomers concentration:

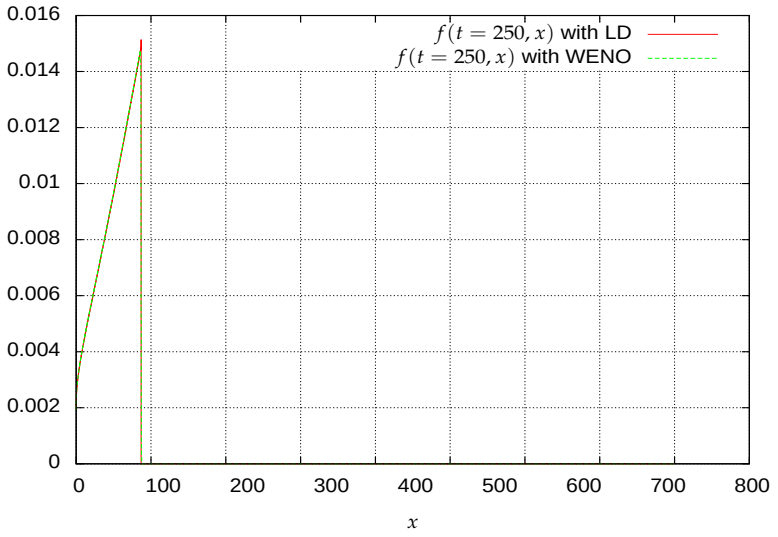
$$c^{n+1} = \rho - \Delta x \sum_{j \geq 0} x_j f^{n+1}_j.$$

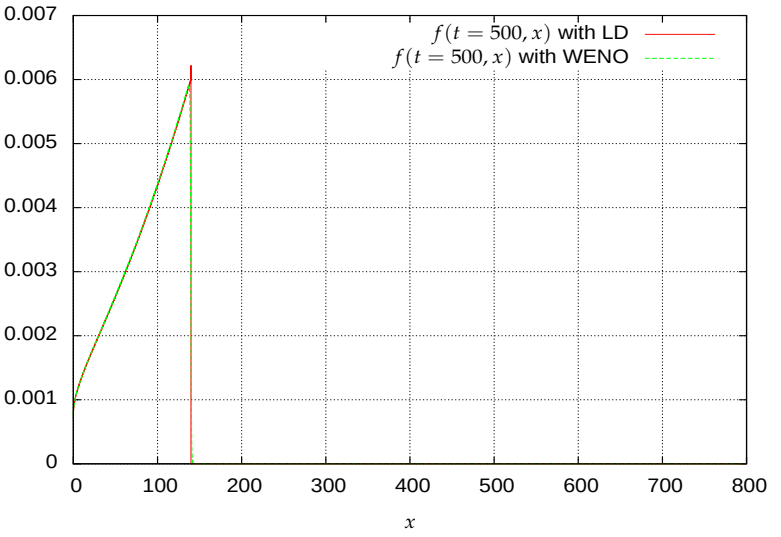
Numerical results

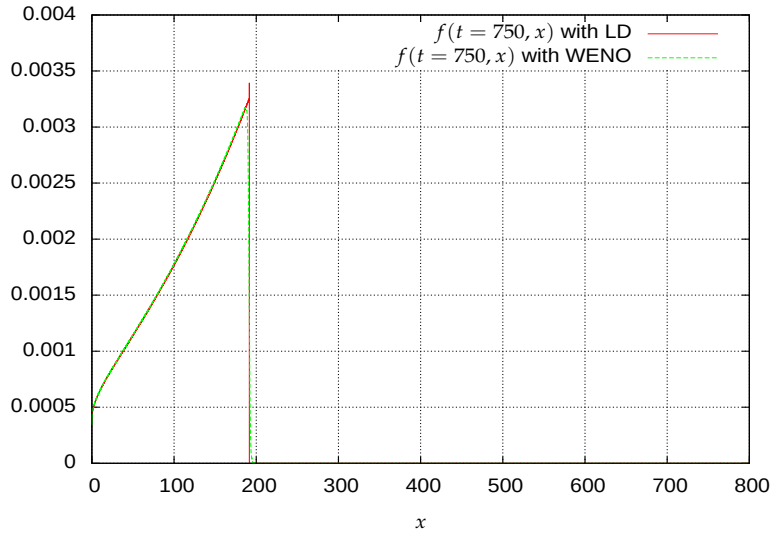
Initial data: $c^0 = 1$ and

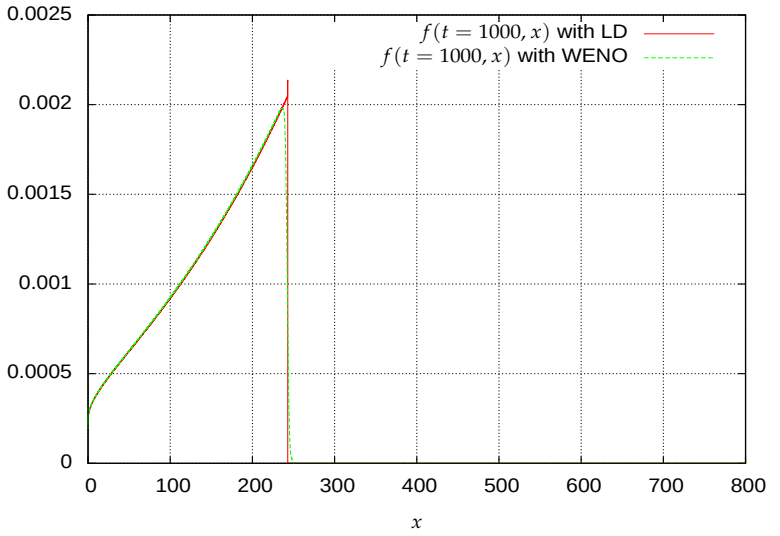


Numerical results









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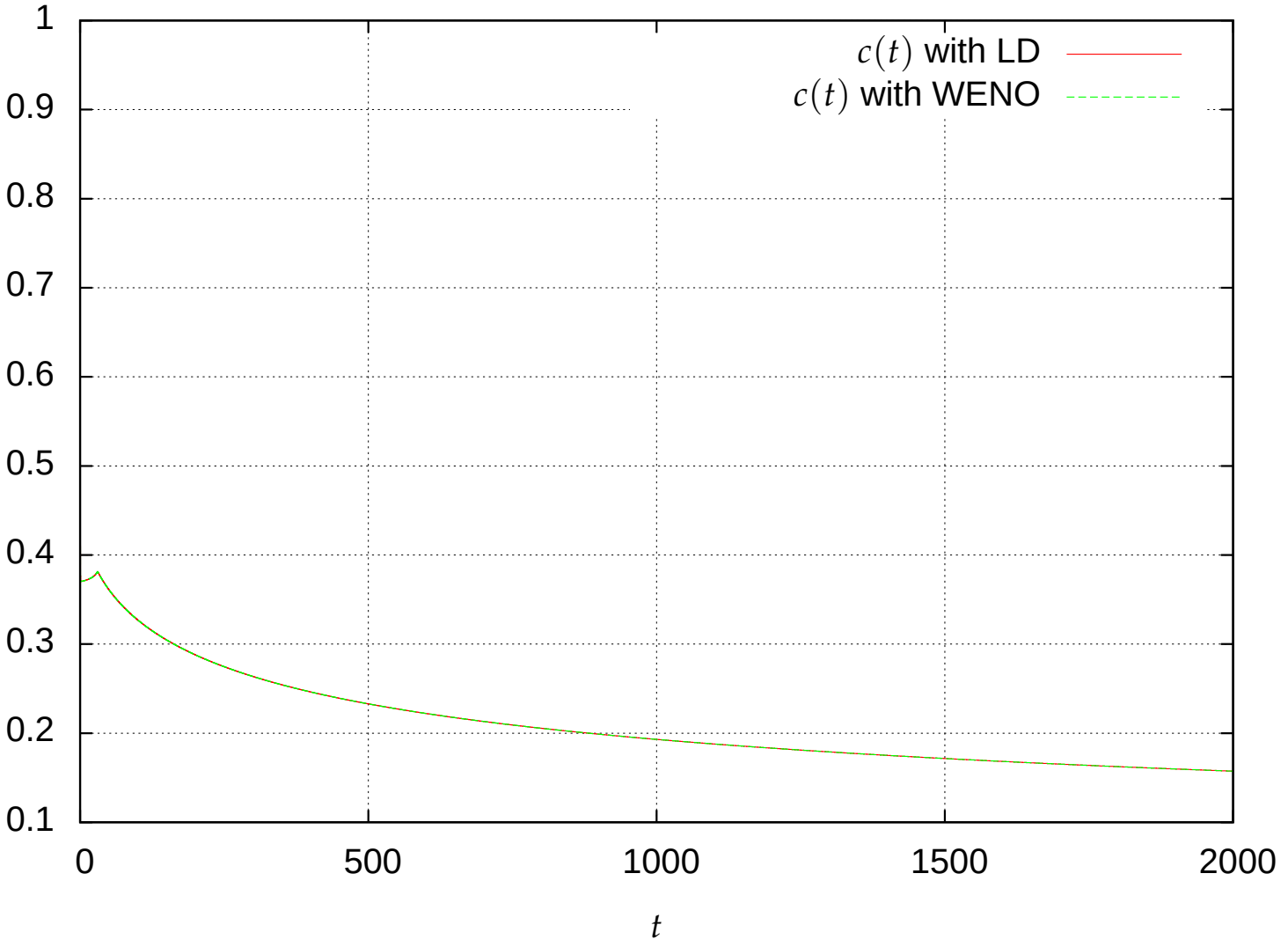

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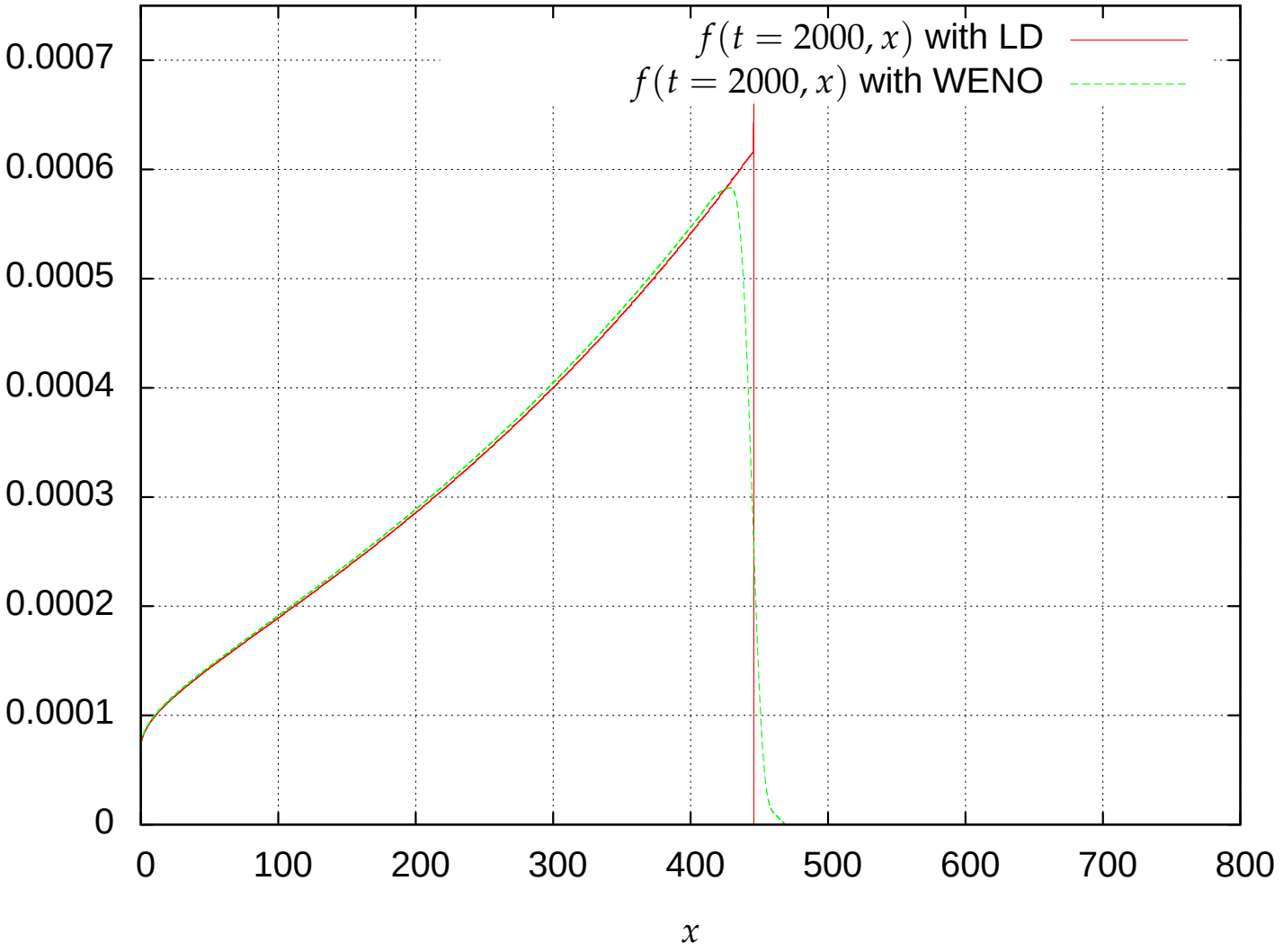
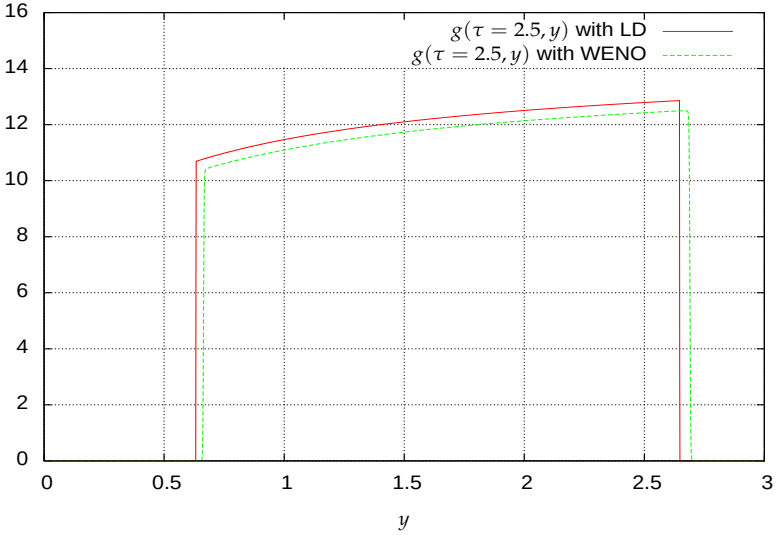
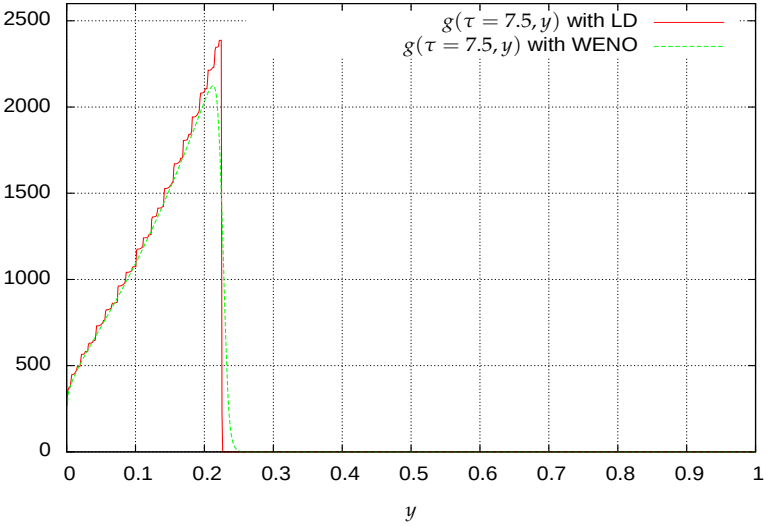
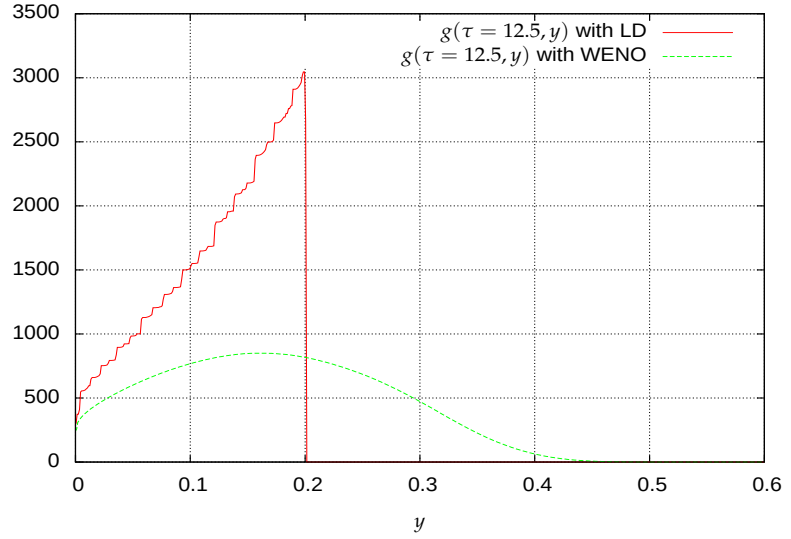


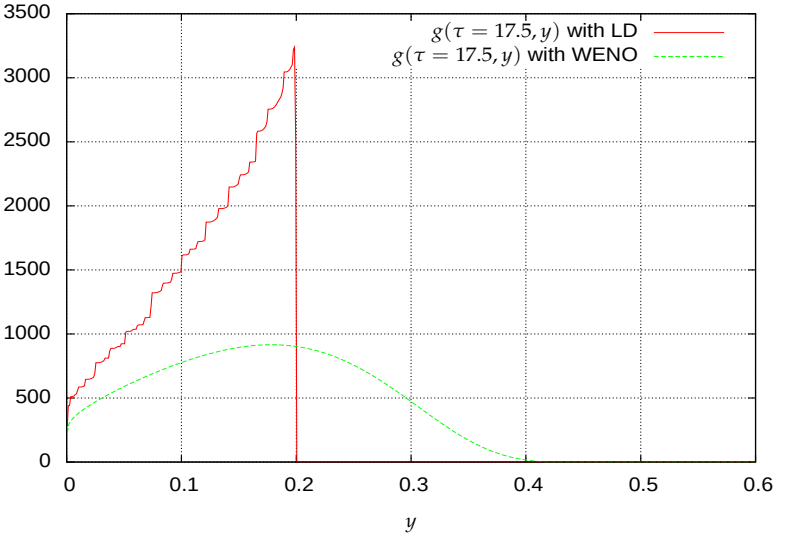
Numerical results for the rescaled equation

(Same inital data.)









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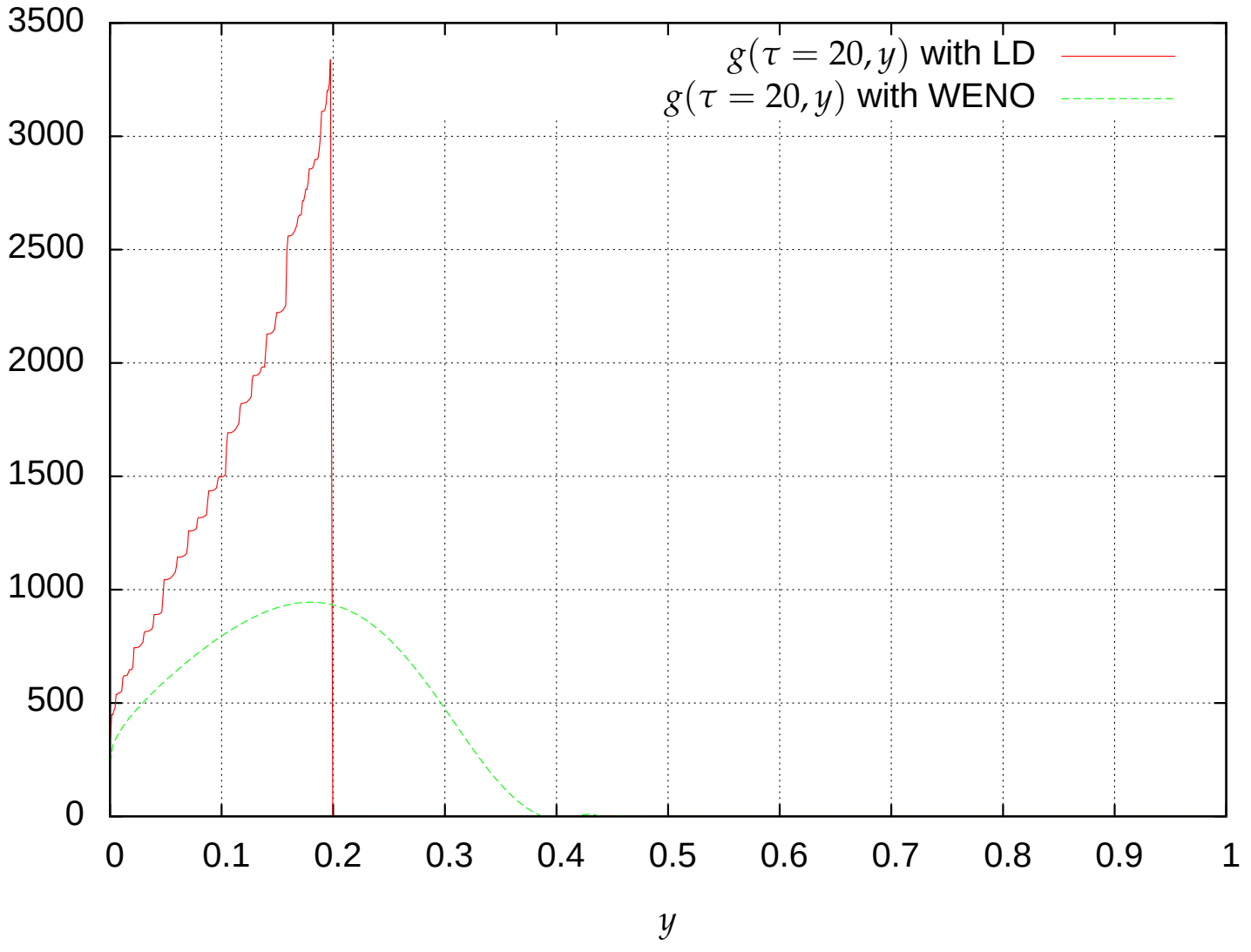

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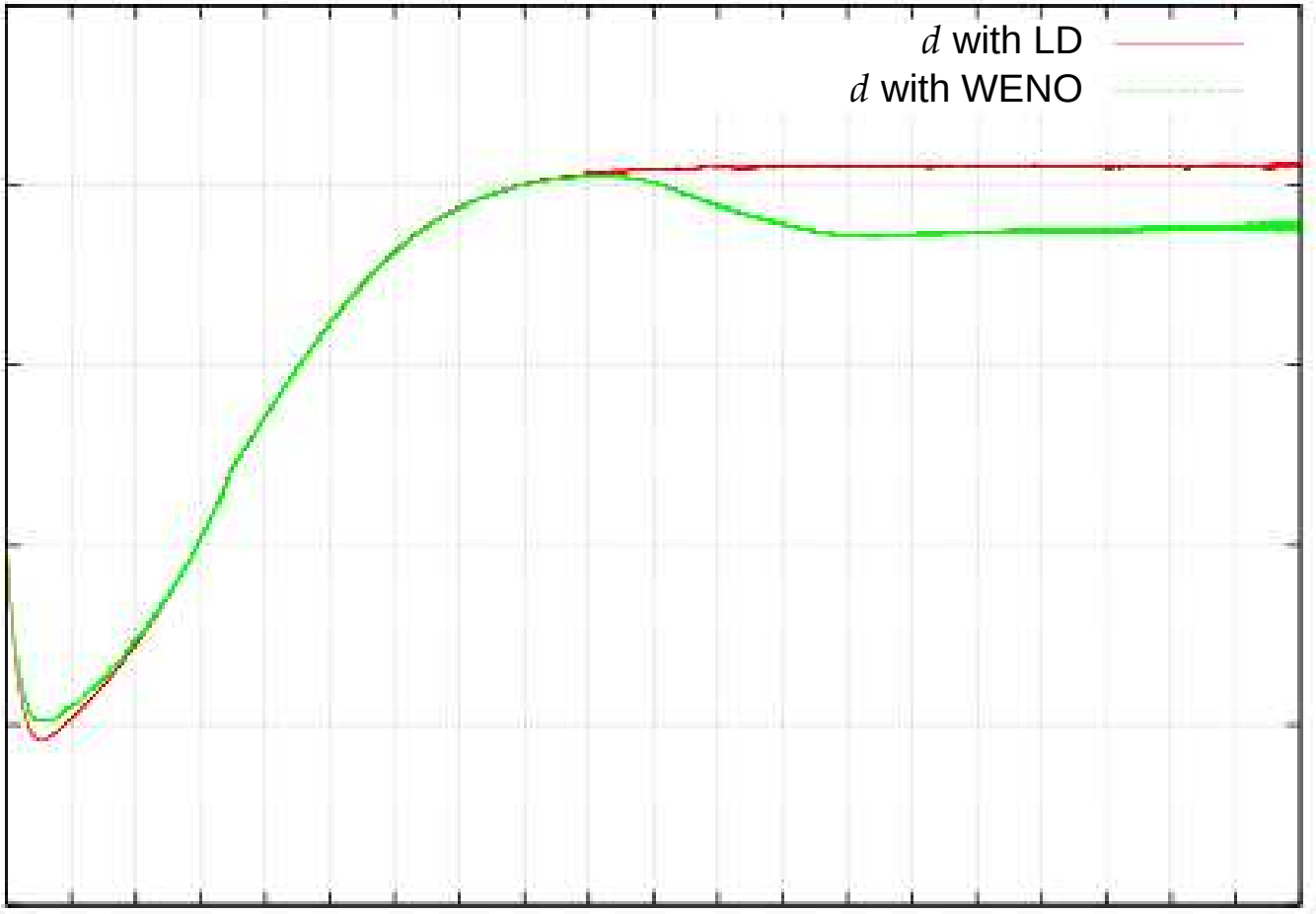
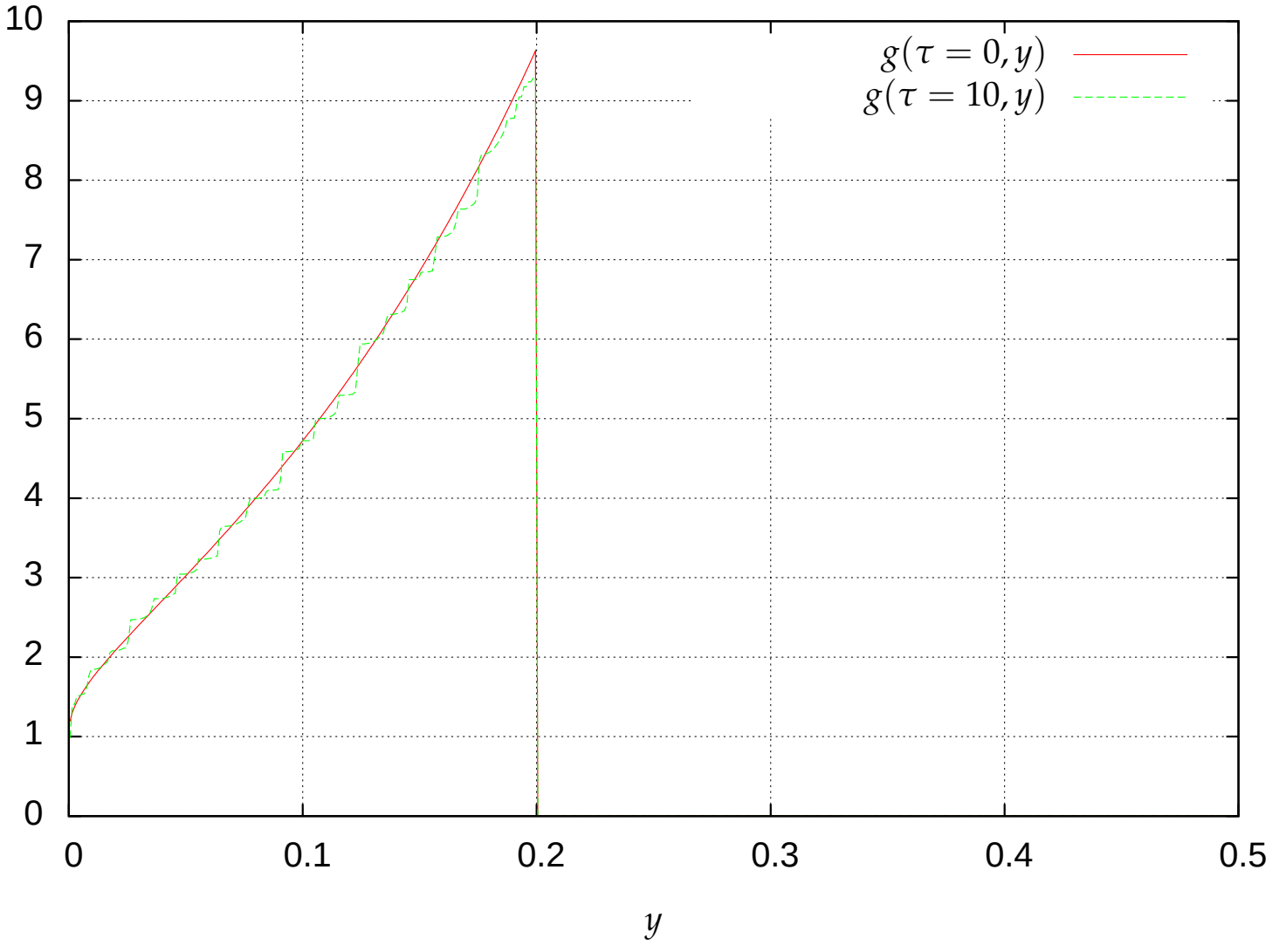


Numerical results for the rescaled equation: equilibrium initla datum



Lifshitz-Slyozov WITH coagulation-fragmentation

$$\begin{cases} \partial_t f + \partial_x (Vf) = Q(f), \quad t \geq 0,\ x \geq 0, \\ V(t,x) = c(t) x^{1/3} - 1, \\ c(t) + \int_0^\infty x f(t,x) dx = \rho, \quad t \geq 0, \end{cases}$$

with

$$Q(f)(t,x) = Q^+(f)(t,x) - Q^-(f)(t,x)$$
$$= 1/2 \int_0^x f(t,x-y) f(t,y) dy - \int_0^\infty f(t,x) f(t,y) dy.$$

Properties of this coagulation operator:

- $\int_0^\infty Q(f)(t,x) dx = 0$: mass conservation;
- $\int_0^\infty Q(f)(t,x) dx \leq 0$: decreasing of the number of macro-particles.

Algo for Lifshitz-Slyozov + coagulation-fragmentation

A splitting is used:

1. $n \to n+1/2$: resolution of $\partial_t f + \partial_x V f = 0$ with the limited downwind scheme;
2. $n+1/2 \to n+1$: resolution of $\partial_t f = Q(f)$;
3. computation of c.

For the second step, (at least) two methods are possible. the first one, naive, consists in evaluating directly the integrals. A semi-implicit scheme is used to solve $\partial_t f + fL(f) = Q^+(f)$: this equation is written in the form

$$\partial_t \left(f e^{\left(\int_0^t L(f)(s,x)ds\right)} \right) = e^{\left(\int_0^t L(f)(s,x)ds\right)} Q^+(f).$$

This leads to

$$f_j^{n+1} = e^{-\Delta t L^{n+1/2}} f_j^{n+1/2} + Q^+{}_j^{n+1/2}.$$

Major drawback: because of the convolutions, the support of the solutions is $\mathbb{R}_+$. We thus have to troncate them. Thus the discrete convolution is not conservative (not good for large time observations).

Alternate coagulations computation

Second method, by Filbet and Laurençot: write the equation under form

$$\partial_t(xf)(t,x) = xQ(f)(t,x) = -\partial_x J(f)(t,x)$$

with

$$J(f)(t,x) = \int_0^x \int_{x-u}^{\infty} uf(t,u)f(t,v)dvdu,$$

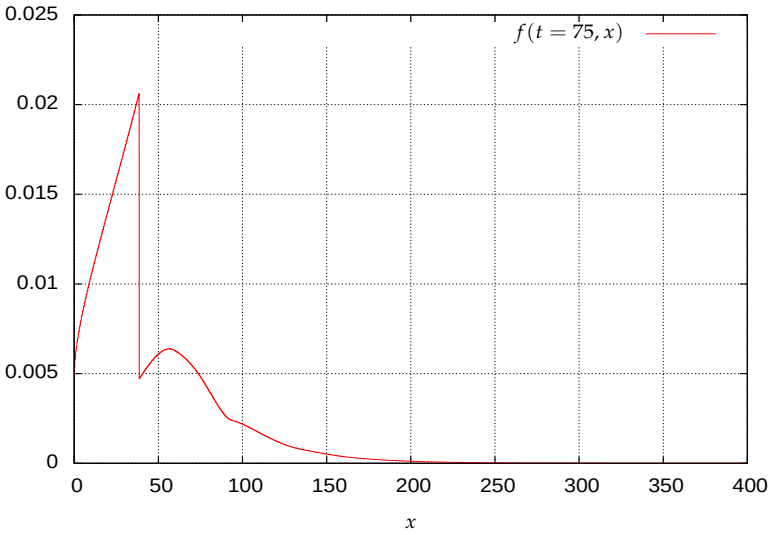
then troncate the integration, posing

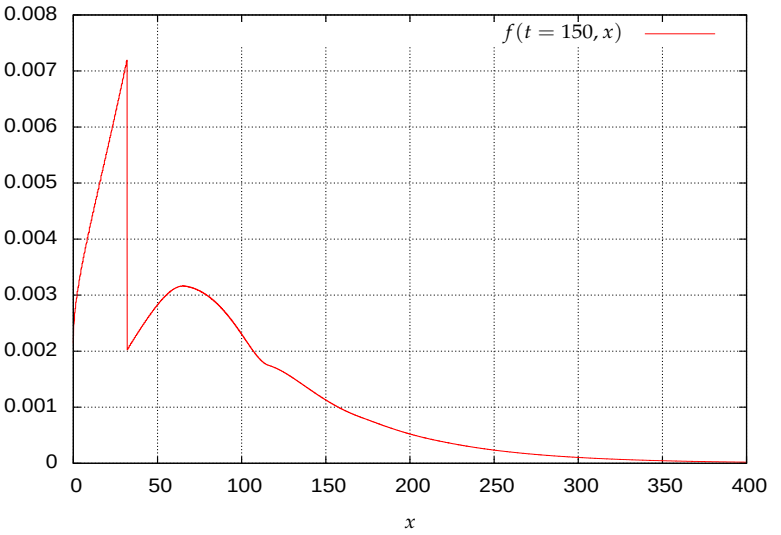
$$J_R(f)(t,x) = \int_0^x \int_{x-u}^{R-u} uf(t,u)f(t,v)dvdu,$$

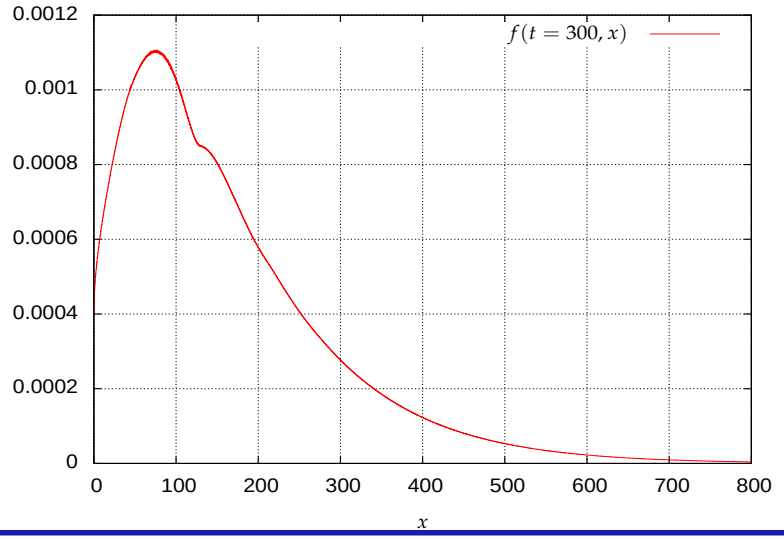
that satisfies $J_R(f)(t,0) = J_R(f)(t,R) = 0$ and thus ensures conservation of the mass $\int_0^R xf(t,x)dx$.
(Analysis of the convergence of this method as $R \longrightarrow +\infty$: see Filbet-Laurençot 2004.)

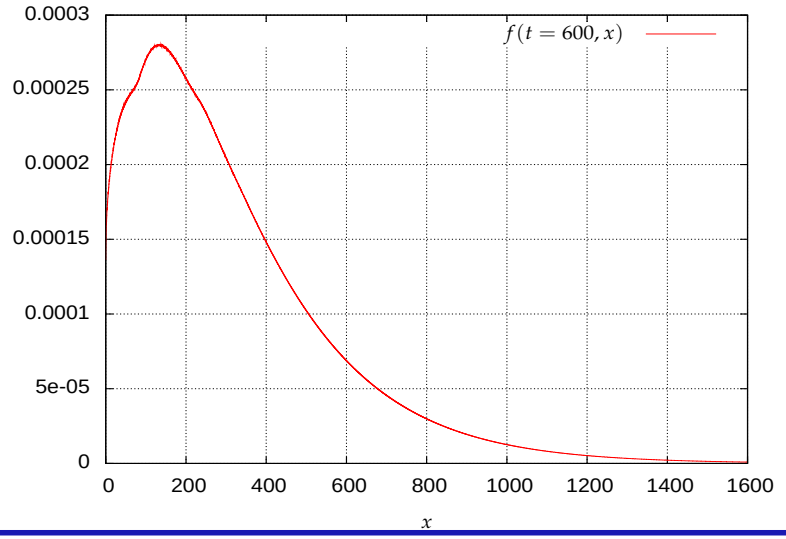
Numerical results

Actually we put a coefficient ε in front of the collision operator. Same initial data, $\varepsilon = 1/100$...



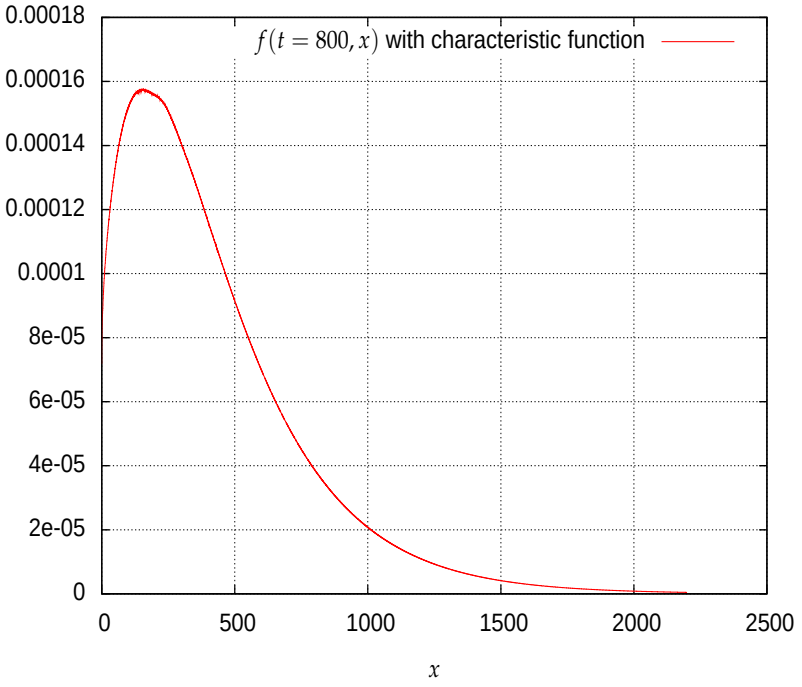


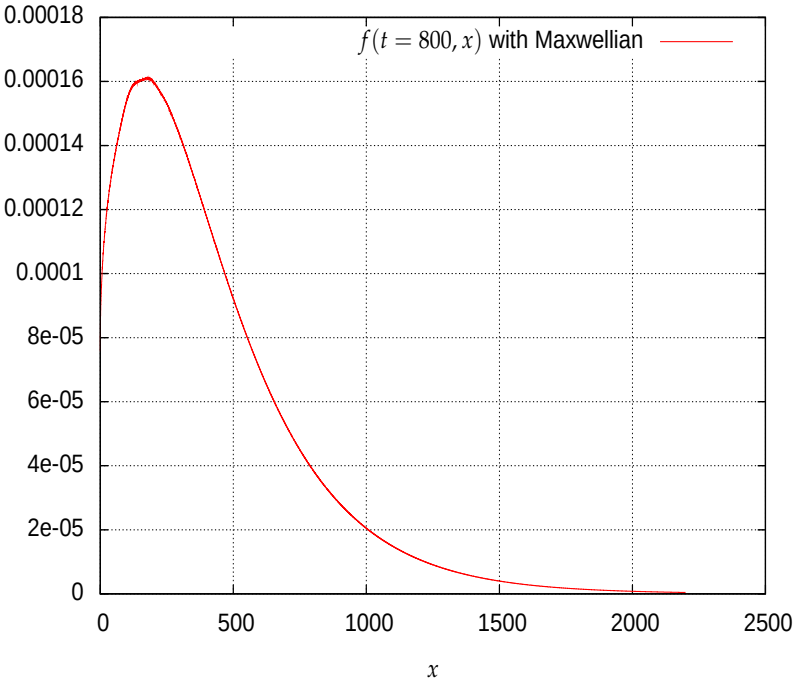




Numerical results: comparison with another initial datum

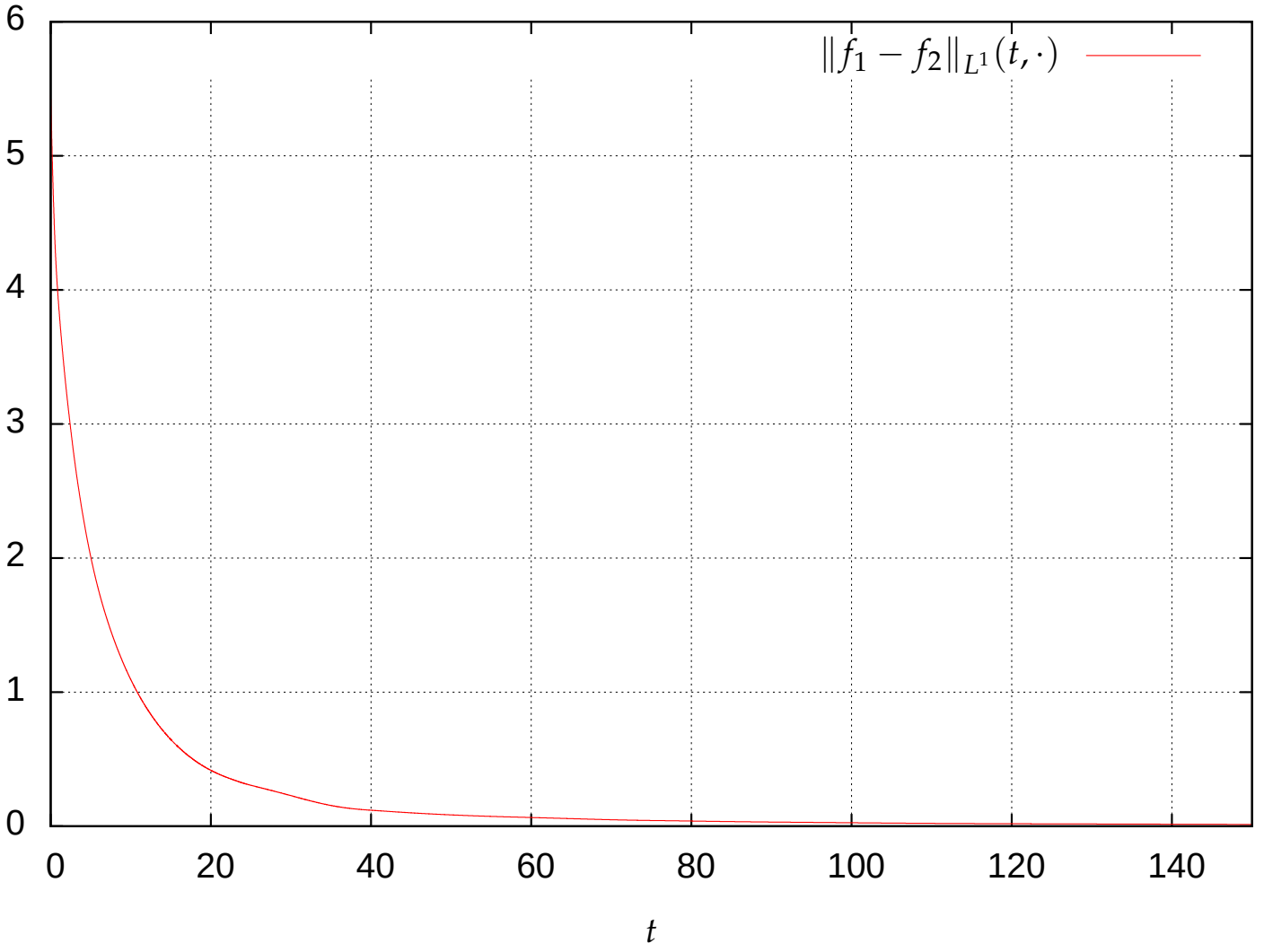
Results are compared to those with a Maxwellian initial datum (which, without collisions, leads to the Lifshitz-Slyozov predicted asymptotic solution). $\varepsilon = 1/100$.





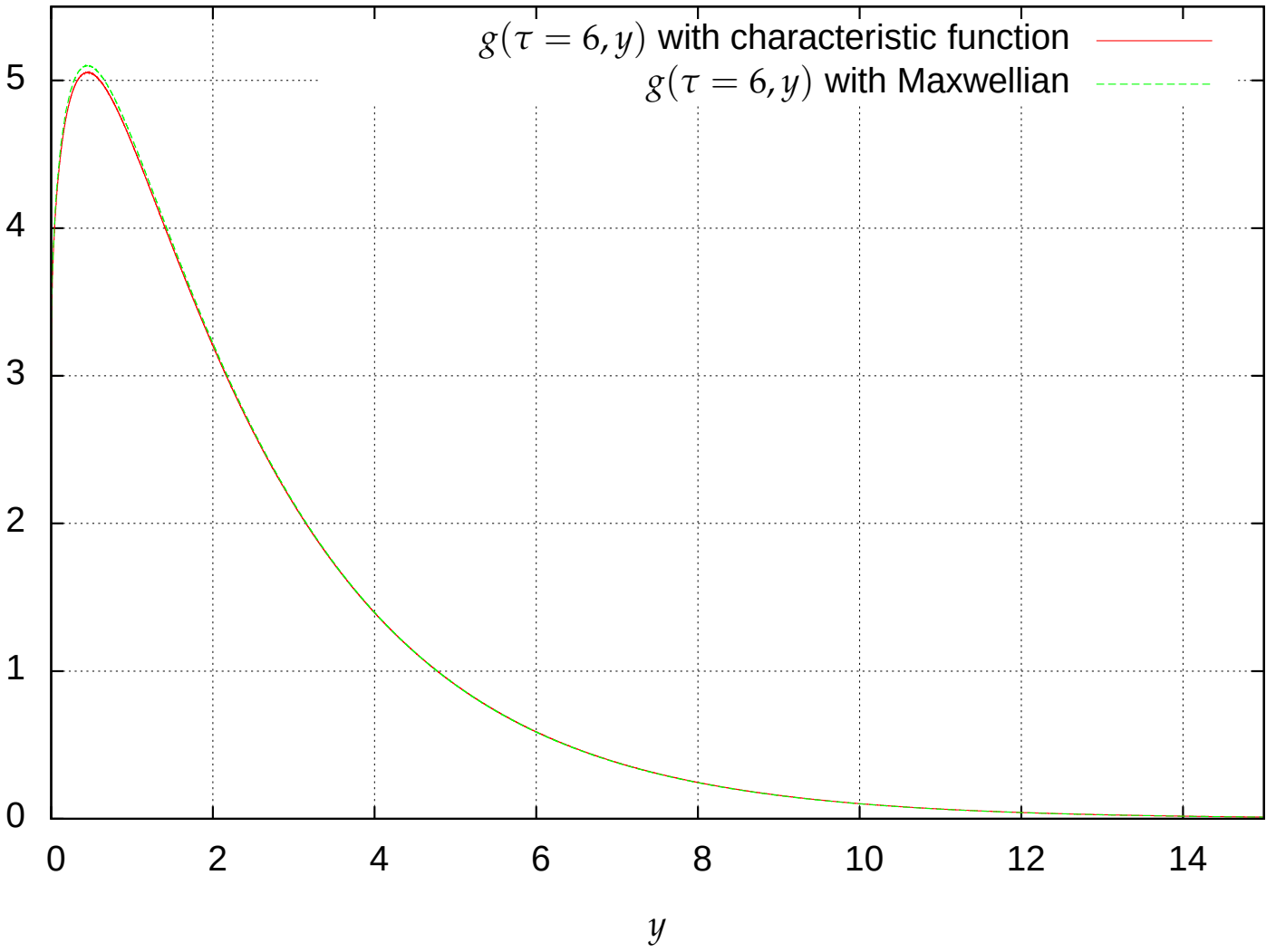
Numerical results: comparison with another initial datum

Evolution of the difference between the two solutions, $\varepsilon = 1/10$.



Numerical results for the rescaled equation

$\varepsilon = 1/10.$



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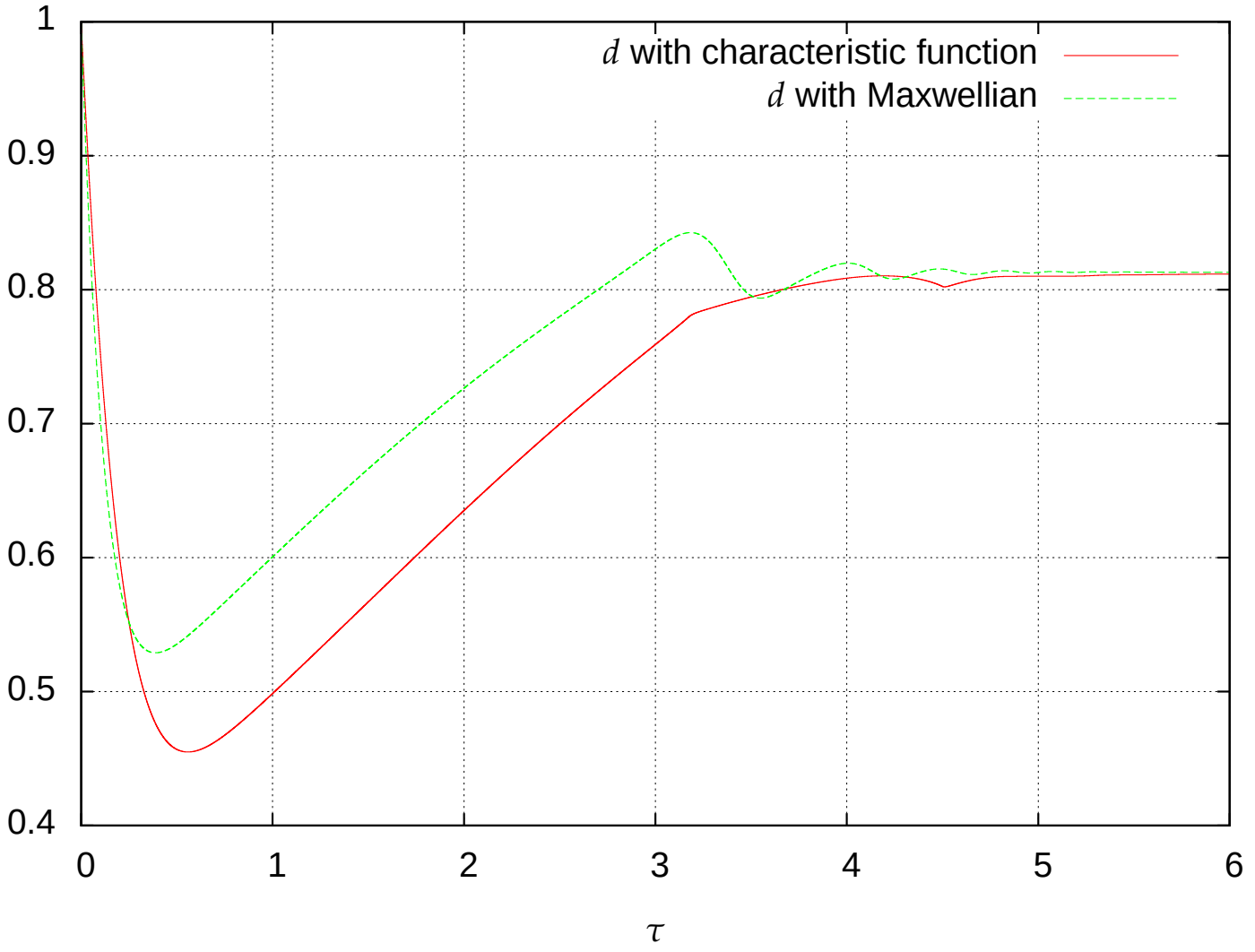

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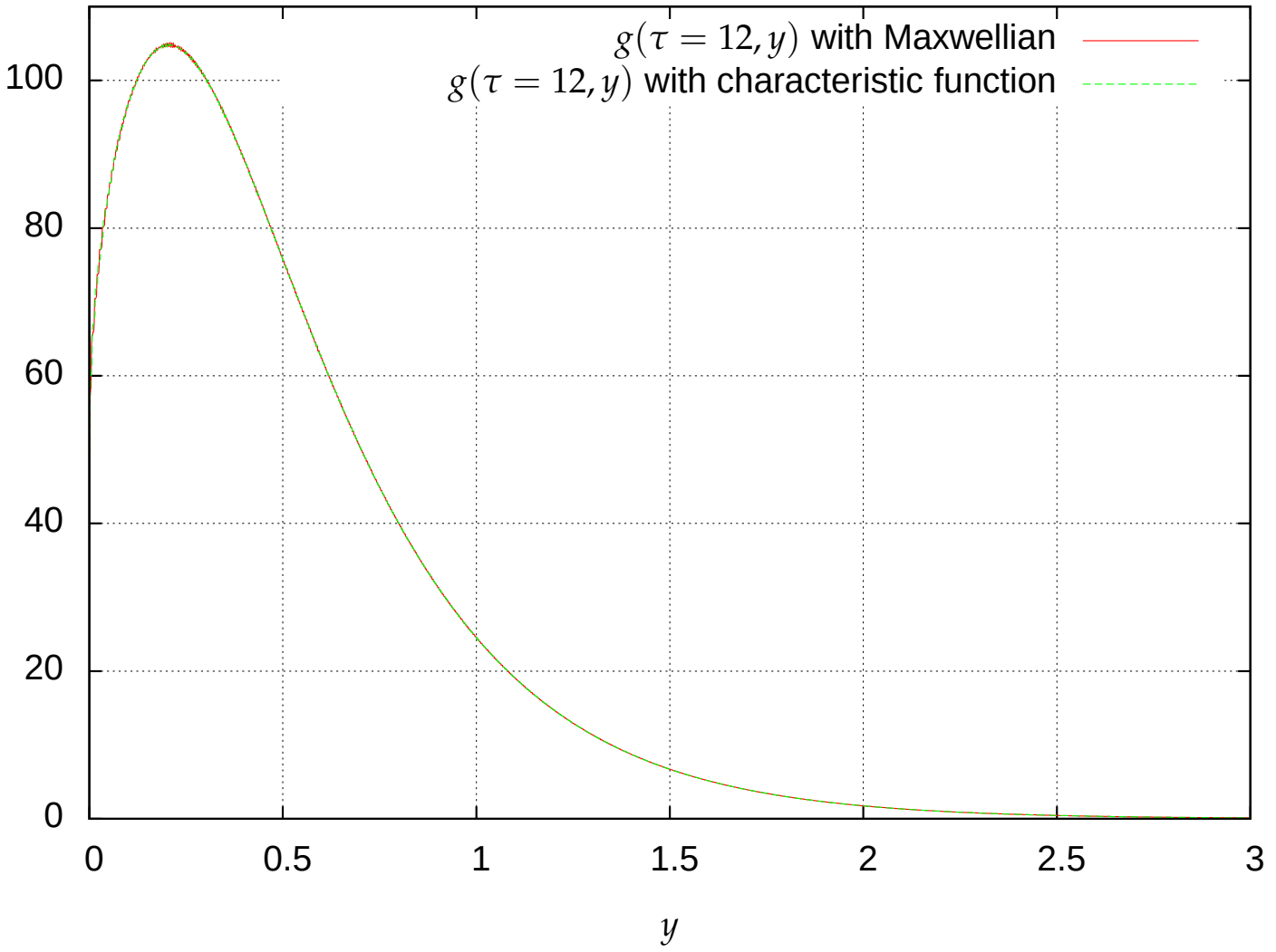

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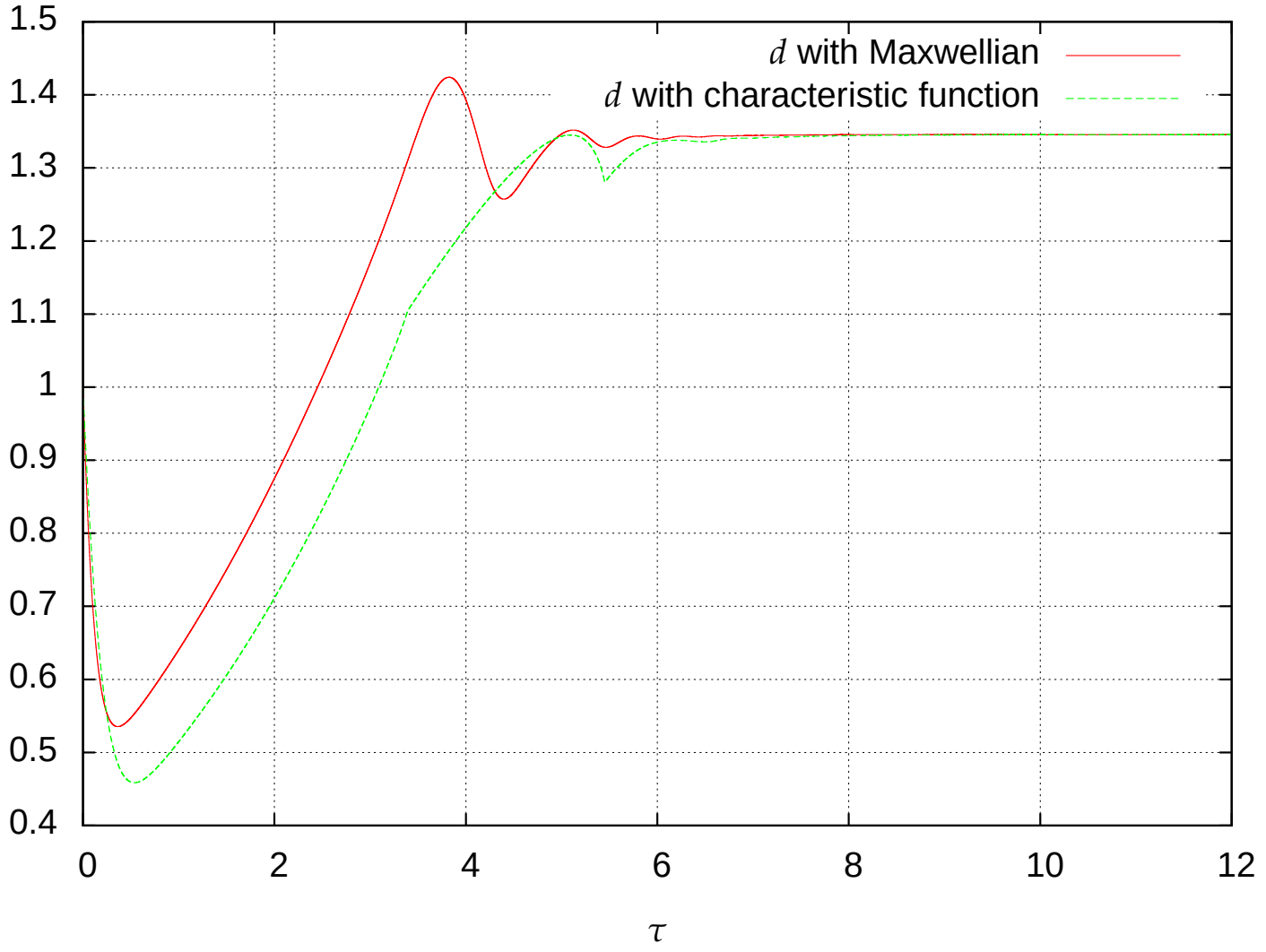

Conclusion

- The different stationary profiles of the rescaled Lifshitz-Slyozov system seem to be asymptotically in time reachable, with suitable initial data (the behavior at the end of the support of the data seem to determine the large time asymptotics);
- With a coagulation term, the asymptotic solution seems not to depend on the initial data;
- when ε tends to 0, the asymptotic in time solution seems to tend toward the unique profile conjectured by Lifshitz and Slyozov.