Two phase solutions for a forward-backward equation

Corrado Mascia

Dipartimento di Matematica “G. Castelnuovo”

Joint works with P. Lafitte (Lille), A. Terracina (Roma 1), A. Tesei (Roma 1)

Laboratoire Jacques-Louis Lions
Université Pierre et Marie Curie

Seminar on Compressible Fluids – March 30th, 2011
Two-phase Entropy Solutions of a Forward–Backward Parabolic Equation

CORRADO MASCIA, ANDREA TERRACINA & ALBERTO TESI

Abstract

This article deals with the Cauchy problem for a forward–backward parabolic equation, which is of interest in physical and biological models. Considering such an equation as the singular limit of an appropriate pseudoparabolic third-order regularization, we consider the framework of entropy solutions, namely weak solutions satisfying an additional entropy inequality inherited by the higher order equation. Moreover, we restrict the attention to two-phase solutions, that is solutions taking values in the intervals where the parabolic equation is well-posed, proving existence and uniqueness of such solutions.

1. Introduction

In this paper we study the forward–backward parabolic equation in one space dimension

\[ u_t = (\phi(u))_{xx} \quad \text{in } \mathbb{R} \times (0, T] =: S_T, \quad (1) \]

subject to the initial condition

\[ u(x, 0) = u_0(x) \quad \text{for } x \in \mathbb{R}. \quad (2) \]

We suppose that the function \( \phi \) is nonmonotone and piecewise linear, namely (see Fig. 1):

\[ \phi(u) = \begin{cases} \phi_-(u) & \text{for } u \leq b, \\ \phi_0(u) & \text{for } b < u < c, \\ \phi_+(u) & \text{for } u \geq a. \end{cases} \]

where

\[ \phi_\pm(u) := a_\pm u + \beta_\pm, \quad \phi_0(u) := \frac{A(a - b) - B(u - c)}{c - b}. \]

NUMERICAL EXPLORATION OF A FORWARD–BACKWARD DIFFUSION EQUATION

P. LAFITTE

EPFL SIMPAF - INRIA Lille Nord Europe Research Centre
Parc de la Haute Borne, 46, avenue Halley
F-59650 Villeneuve d’Ascq cedex, France

and

Laboratoire Paul Painlevé, UMR 8524, C.N.R.S.
Université de Sciences et Technologies de Lille, Cité Scientifique
F-59655 Villeneuve d’Ascq cedex, France

lafitte@math.univ-lille1.fr

C. MASCIA

Dipartimento di Matematica “G. Castelnuovo”
Sapienza, Università di Roma, P.le Aldo Moro, 2
00185 Rome, Italy
mascia@mat.uniroma1.it

Received (Day Month Year)
Revised (Day Month Year)
Communicated by (xxxxxxxxx)

We analyze numerically a forward-backward diffusion equation with a cubic-like diffusion function, emerging in the framework of phase transitions modeling and its “entropy” formulation determined by considering it as the singular limit of a third-order pseudo-parabolic equation. Precisely, we propose schemes for both the second and the third order equations, we discuss the analytical properties of their semi-discrete counterparts and we compare the numerical results in the case of initial data of Riemann type, showing strengths and flaws of the two approaches, the main emphasis being given to the propagation of transition interfaces.

Keywords: Phase transitions, pseudo-parabolic equations, numerical approximation, finite differences.

AMS Subject Classification: 65M30 (80A22, 47J40, 35K70).

1. Introduction

The aim of the present article is to investigate numerically the solutions to a nonlinear diffusion equation of the form

\[ \frac{\partial u}{\partial t} = \frac{\partial^2 \phi(u)}{\partial x^2}, \quad (x, t) \in \mathbb{R} \times (0, +\infty) \quad (1.1) \]
1. Forward-backward diffusion
   - An ill-posed problem
   - Transitions dynamics

2. Origin of the model
   - Phase transitions
   - Memory effects

3. The pseudo-parabolic regularization
   - Piecewise smooth solutions
   - Numerical experiments

4. Links to hyperbolic equations
   - The van der Waals fluids
   - Which synthesis?
Plan

1. Forward-backward diffusion
   - An ill-posed problem
   - Transitions dynamics

2. Origin of the model
   - Phase transitions
   - Memory effects

3. The pseudo-parabolic regularization
   - Piecewise smooth solutions
   - Numerical experiments

4. Links to hyperbolic equations
   - The van der Waals fluids
   - Which synthesis?
Model equation

Nonlinear diffusion equation:

\[
\frac{\partial u}{\partial t} = \Delta \phi(u)
\]

If \( \phi' \geq \nu > 0 \), the equation is parabolic;
if \( \phi' \geq 0 \), the equation is degenerate parabolic,
if \( \phi' \) changes sign, the equation is forward-backward.

Typical examples: \( J \) given bounded interval

Cahn–Hilliard: \( \phi \uparrow\downarrow\uparrow \) (phase transitions)

\[
\phi'(u) < 0 \quad \iff \quad u \in J;
\]

Perona–Malik: \( \phi \downarrow\uparrow\downarrow \) (image processing).

\[
\phi'(u) > 0 \quad \iff \quad u \in J.
\]

See also Barenblatt, Bertsch, Dal Passo, Ughi (1993), turbulent flows
Padrón (1993), aggregating populations.
An ill-posed problem

Here: diffusion function $\phi$ with an “increasing” cubic-like shape

$$\frac{\partial u}{\partial t} = \Delta \phi(u)$$

spinodal region: interval $J = (b, a)$

$\leadsto$ the Cauchy problem is ill-posed.

Passing to weak formulation, solutions to the Cauchy problem may become infinite.

Höllig (1983): $\phi$ piecewise linear, $x \in \mathbb{R}^1$: for (smooth) initial data $u_0$ such that

$$u_0(\pm \infty) < b < \sup_{x \in \mathbb{R}} u_0(x)$$

the problem has infinite solutions.

Generalization in: Zhang (2006) general $\phi$, $x \in \mathbb{R}^1$

(via differential inclusions).
Infinitely many evolutions

Starting from an initial datum with values in the spinodal region

\[ \text{stable} \]

\[ \text{unstable} \]

\[ a \]

\[ b \]

it is possible to build (infinitely many) solutions assuming the initial datum in \( L^1 \) as \( t \to 0^+ \) given by (infinitely many) transitions from one stable phase to the other

(Precisely, Höllig considers \( v \) such that \( \partial v / \partial x = u \).)
Transitions dynamics

1. Transitions formation
   how is the initial transition pattern determined?

2. Transitions evolution
   which are the rules governing the dynamics of the transition between stable phases?

3 unknowns
   \( u^\pm \) (right/left limits)
   \( \xi \) (jump position)

2 conditions
   \[
   [\phi(u)] = 0 \\
   \xi' [u] + [\partial_x \phi(u)] = 0 \quad (R-H)
   \]

[\( f \)] jump of function \( f \)
Two possible versions

Two possible versions to assign the missing condition:

1. **Steady transition** (given boundary)

   \[ \left[ \frac{\partial \phi(u)}{\partial x} \right] = 0 \]

   From R–H, it follows \( \xi' \equiv 0 \); \( \phi(u^{\pm}) \) varies in time.

2. **Moving transition** (free boundary)

   \[ \phi(u^-) = \phi(u^+) = C \]

   From R–H, it follows \( \xi' = -\frac{\partial_x \phi(u)}{[u]} \)
Plan

1. Forward-backward diffusion
   - An ill-posed problem
   - Transitions dynamics

2. Origin of the model
   - Phase transitions
   - Memory effects

3. The pseudo-parabolic regularization
   - Piecewise smooth solutions
   - Numerical experiments

4. Links to hyperbolic equations
   - The van der Waals fluids
   - Which synthesis?
Phase transitions

**Phase:** a distinct and homogeneous form of matter separated by its surface from other forms.

**Transition:** the process of changing from one state to another.

Here, spinodal decomposition:

mechanism generating a separation in a compound in regions with different chemical and physical properties.

**Paradigm:** Emergence of oscillations starting from an (almost) homogeneous configuration may be generated by the presence of negative diffusion:

- Region $\phi' < 0$: spinodal region or unstable phase;
- Region $\phi' > 0$: stable phase.
Cahn–Hilliard equation

Generalized diffusion equation for the concentration $u$

$$\frac{\partial u}{\partial t} = -D \text{div} (-\text{grad } v) = D \Delta v \quad (D > 0)$$

($\text{div}$: divergence theorem, $\text{grad}$: Fick’s law),

where $v$ denotes the (chemical) potential.

Cahn, Hilliard (1958): the potential $v$ coincides with the static potential

$$v_s := \frac{\delta F}{\delta u} \quad \text{where} \quad F[u] := \int \left\{ \Phi(u) + \frac{1}{2} \gamma |\text{grad } u|^2 \right\} \, dx.$$ 

Thus

$$\frac{\partial u}{\partial t} = D \Delta \left( \phi(u) - \gamma \Delta u \right) \quad \text{con} \quad \phi := \Phi'.$$

Usually, the function $\Phi$ has a double-well form.
Jäckle, Frisch (1985): the potential $v$ is given by

$$v = v_s + v_m$$

where $v_m$ denotes the memory potential

$$v_m := \psi(u)(x, t) + \int_{-\infty}^{t} \theta'(t - s) \psi(u)(x, s) \, ds$$

$$= \int_{-\infty}^{t} \theta'(t - s) (\psi(u)(x, s) - \psi(u)(x, t)) \, ds$$

with $\theta$ (decreasing) such that $\theta(0) = 1$ and $\theta(+\infty) = 0$.

The term $v_m$ vanishes:
- at the equilibrium, $u = u(x)$;
- or, in absence of memory, $\theta' = -\delta_0$.

The form of the term $v_m$ is inspired by the Boltzmann superposition principle used in viscoelasticity.
An exponential decaying memory

Given $\tau > 0$, let us choose

$$\theta(t) := \exp\left(-\frac{t}{\tau}\right) \Rightarrow \frac{\partial}{\partial t}\left(v_m - \psi(u)\right) = -\frac{1}{\tau} v_m$$

Coupling with the diffusion equation

$$\frac{\partial u}{\partial t} = D \Delta(v_s + v_m)$$

we get

$$\tau \frac{\partial^2 u}{\partial t^2} + \frac{\partial u}{\partial t} = D \Delta\left(v_s + \tau \frac{\partial}{\partial t}\left(v_s + \psi(u)\right)\right)$$

that gives, setting $\psi := \tau(\phi + \psi)$, the fifth order equation

$$\tau \frac{\partial^2 u}{\partial t^2} + \frac{\partial u}{\partial t} = D \Delta\left(\phi(u) + \frac{\partial \psi(u)}{\partial t} - \gamma \Delta u - \gamma \tau \Delta \frac{\partial u}{\partial t}\right)$$
An intricated equation

The complete equation is rather complicate

$$\tau \frac{\partial^2 u}{\partial t^2} + \frac{\partial u}{\partial t} = D \Delta \left( \phi(u) + \frac{\partial \psi(u)}{\partial t} - \gamma \Delta u - \gamma \tau \Delta \frac{\partial u}{\partial t} \right)$$

A natural approach is to consider some simplifications

- $\tau = 0 : \quad \frac{\partial u}{\partial t} = D \Delta \left( \phi(u) - \gamma \Delta u \right) \quad \text{(Cahn–Hilliard)}$
- $\gamma = 0 : \quad \tau \frac{\partial^2 u}{\partial t^2} + \frac{\partial u}{\partial t} = D \Delta \left( \phi(u) + \frac{\partial \psi(u)}{\partial t} \right)$

Which are the differences (if any) in the dynamics dictated by the different reductions?
Plan

1. Forward-backward diffusion
   - An ill-posed problem
   - Transitions dynamics

2. Origin of the model
   - Phase transitions
   - Memory effects

3. The pseudo-parabolic regularization
   - Piecewise smooth solutions
   - Numerical experiments

4. Links to hyperbolic equations
   - The van der Waals fluids
   - Which synthesis?
The regularized equation \((\varepsilon > 0)\)

Following Novick-Cohen, Pego (1991), let us consider

\[ \psi(u) = \varepsilon u, \quad \gamma = 0, \quad \tau = 0. \]

so that we end up with a pseudoparabolic (or Sobolev type) equation

\[ \frac{\partial u}{\partial t} = D \Delta \left( \phi(u) + \varepsilon \frac{\partial u}{\partial t} \right) \]

The same third order term appears also in Benjamin, Bona, Mahony (1973).

1. **Well posed-ness.** the Cauchy problem (zero-flux boundary conditions) with initial datum \(u_0 \in L^\infty\) has a unique global solution in \(C^1([0, \infty), L^\infty)\).

2. **Equilibrium stability.** If \(U\) is such that \(\phi(U) = C \in \mathbb{R}, C \in (A, B)\),

\[ \int_{\Omega} (u_0 - U) \, dx = 0 \quad \Rightarrow \quad |u(\cdot, t) - U|_{L^\infty} \leq c e^{-\nu t} |u_0 - U|_{L^\infty} \]

for \(|u_0 - U|_{L^\infty}\) small, \(\nu > 0\).
The singular limit $\varepsilon \to 0^+$

Plotnikov (1994) analyze the limit $\varepsilon \to 0^+$ by means of Young measures (see Slemrod (1991), Demoulini (1996), . . . , Horstmann, Schweizer (2008)).

A fundamental rôle is played by the entropy inequality:

given $v^\varepsilon := \phi(u^\varepsilon) + \varepsilon \partial_t u^\varepsilon$, for $g \in C^1$, $g' > 0$, setting

$$G(u) := \int_{u_0}^{u} g(\phi(s)) ds;$$

there holds

$$\frac{\partial G(u^\varepsilon)}{\partial t} - \text{div} \left( g(v^\varepsilon) \nabla v^\varepsilon \right) + g'(v^\varepsilon) |\nabla v^\varepsilon|^2$$

$$= - \frac{1}{\varepsilon} \left[ g(\phi(u^\varepsilon)) - g(v^\varepsilon) \right] \left( \phi(u^\varepsilon) - v^\varepsilon \right) \leq 0$$

giving a corresponding inequality in the limit $\varepsilon \to 0^+$.

The term entropy is chosen for the analogy with the case of conservation laws.
Piecewise smooth solution for $\varepsilon = 0$

Evans, Portilheiro (2004): solutions with pure stable phases, i.e. the space $\Omega \times [0, T]$ is divided into two regions $V_1, V_2$ such that

$$u \leq b \text{ in } V_1, \quad u \geq a \text{ in } V_2,$$

If $u$ is a weak entropy solution, smooth in the interior of $V_1, V_2$, with smooth boundary $\Gamma := \overline{V_1} \cap \overline{V_2}$, (normal vector $(\nu_x, \nu_t)$),

1. $u$ is a classical solution at the interior of $V_1$ and of $V_2$;
2. at any point of $\Gamma$, the function $\phi(u)$ is continuous and

$$\nu_t [u] = \nu_x \cdot [\nabla \phi(u)] \quad \text{(Rankine–Hugoniot)};$$

3. finally, along $\Gamma$, there holds

$$\begin{cases} 
\nu_t = 0 & \phi(u) \neq A, B, \\
\nu_t \geq 0 & \phi(u) = A, \\
\nu_t \leq 0 & \phi(u) = B.
\end{cases}$$
Transition rules, 1/2

Steady transition: if
\[ \phi(u) \in (A, B), \] then \[ \xi' \equiv 0 \]

The profiles of \( u \) and \( \phi(u) \): initial time (blue), evolution (red).
Transition rules, 2/2

Moving transition: if
\[ \phi(u) = B, \text{ then } \xi' \leq 0 \]

The profiles of \( u \) and \( \phi(u) \): initial time (blue), evolution (red).
Combined motion

Such rules guarantee uniqueness of the solution to the Cauchy problem (at least in the case of a single transition layer).
Uniqueness of two phase solutions

Two phase solution: a triple \((\xi, u, v)\) such that
\[
\frac{\partial u}{\partial t} = \frac{\partial^2 v}{\partial x^2}
\]
for \(x \neq \xi(t)\);
\[
u = \beta_{\pm}(v) \quad \text{for} \pm x > \xi(t)
\]
\(\beta_{\pm}: \) inverses of \(\phi\) in \((-\infty, b)\) and \((a, +\infty)\).

Mascia, Terracina, Tesei (2009): The jump conditions guarantee uniqueness of the two phase solution for the Cauchy problem
\[
\frac{\partial u}{\partial t} = \frac{\partial^2 \phi(u)}{\partial x^2} \quad u(x, 0) = u_0(x)
\]
with \(\phi(u_0) \in BC(\mathbb{R})\) such that
\[
u_0 \leq b \quad \text{in} \ (-\infty, 0), \quad \nu_0 \geq a \quad \text{in} \ (0, \infty).
\]
The proof is essentially based on a \(L^1\) stability argument.
Existence of two phase solutions

Local existence.
Consider separately the cases of moving/steady transition layer.

*moving boundary*: two-phase Stefan type problem
  (free boundary, iteration/fixed point arguments);
*steady boundary*: transmission problem
  (two diffusion equations connected so that $\phi(u)$ is $C^1$ at $x = 0$)

...piecewise linear case ✓
...general nonlinear case ❌

Global existence.
Glue together the two cases.

*delicate point*: to show that when one type of evolution leads
to a non-entropic evolution, the other type is admissible

...see Terracina (2011)
Numerical experiments

Lafitte, Mascia (2010): comparison of two approaches

1. first, fixed $\varepsilon > 0$, space discretization; then, pass to the limit $\varepsilon \to 0$.

$$
\frac{d U}{dt} = - \left( h^2 I + \varepsilon A \right)^{-1} A \phi(U) \quad \rightsquigarrow 
\frac{d U}{dt} = - h^{-2} A \phi(U)
$$

where $A$ is the matrix of the discrete Laplace operator.

2. first, pass to the limit $\varepsilon \to 0$; then, space discretization.

two main ingredients:

i. diffusion equation to be solved in the region of the stable phases;

ii. description of the interface motion $\xi$, based on entropy condition.

Framework:

– space interval $I = (0, 1)$;
– homogenous Neumann boundary conditions;
– test for the Riemann problem (self-similar solutions available).
Comparison of the two approaches, 1/3

- both of order 1 in \( h \) (space discretization);
- the interface \( \xi \) is better approximated by the two phase scheme.
Comparison of the two approaches, $2/3$

Evolution of the relative error of interface $\xi$ for data $(u^-, u^+) = (-2, 4)$:
- explicit scheme for the pseudo-parabolic equation (blue),
- two phase scheme (red).
Comparison of the two approaches, 3/3

Two phase solutions do not take values in the spinodal region \((b, a)\), while the movement of the boundary for solutions to

\[
\frac{dU}{dt} = -h^{-2} \bigtriangleup \phi(U)
\]

is due to a transition of a point from on stable phase to the other, by passing all along through the unstable region \((b, a)\).

(...movie...)
Plan

1. Forward-backward diffusion
   - An ill-posed problem
   - Transitions dynamics

2. Origin of the model
   - Phase transitions
   - Memory effects

3. The pseudo-parabolic regularization
   - Piecewise smooth solutions
   - Numerical experiments

4. Links to hyperbolic equations
   - The van der Waals fluids
   - Which synthesis?
Coming back to the fifth-order equation and neglecting the term $v_s$ relative to the cost of the transitions, for $\psi(u) = \varepsilon u$ and $D = 1$, we get the equation

$$\tau \frac{\partial^2 u}{\partial t^2} + \frac{\partial u}{\partial t} = \Delta \left( \phi(u) + \varepsilon \frac{\partial u}{\partial t} \right)$$

equivalent to the hyperbolic-parabolic system:

$$\begin{cases}
\frac{\partial u}{\partial t} + \text{div } J = 0 \\
\tau \frac{\partial J}{\partial t} + \text{grad } \phi(u) = \varepsilon \Delta J - J
\end{cases}$$

As $\varepsilon \to 0^+$, the system becomes hyperbolic-elliptic, with ellipticity region given by the values $u$ such that $\phi'(u) < 0$. 
The van der Waals fluids

J.D. van der Waals (1873): taking into account the volume of fluid particles, we get a non-monotone state equation for the pressure (\(\sim\) Nobel prize 1910)

The equations for isentropic fluids become

\[
\begin{align*}
\frac{\partial u}{\partial t} + \text{div } J &= 0 \\
\frac{\partial J}{\partial t} + \text{grad } \phi(u) &= 0
\end{align*}
\]

where the pressure \(\phi\) as changing monotonicity.

The system is hyperbolic-elliptic and possesses a natural entropy

\[\eta(u, J) = \phi(u) + \frac{1}{2} |J|^2,\]

that is not convex in the region where \(\phi\) is decreasing.
Selection criteria for transitions

One-dimensional case with \((*)\) to be made precise

\[
\begin{aligned}
\frac{\partial u}{\partial t} + \frac{\partial J}{\partial x} &= 0 \\
\frac{\partial J}{\partial t} + \frac{\partial \phi(u)}{\partial x} &= \frac{\partial^2 (*)}{\partial x^2}
\end{aligned}
\]

Slemrod (1983): A phase transition is admissible for the system with \((*) = 0\) if it can be obtained as limit of traveling wave \((U, J)(x - c t)\) of the system with \((*) \neq 0\).

In the context of van der Waals fluids, two (physical) selection criteria:

- viscosity: \((*) = \varepsilon J;\)
- visco-capillarity: \((*) = \varepsilon J + \gamma \frac{\partial u}{\partial x}.\)

In the theory of nonlinear elasticity, James (1980) considers an analogous problem, examining only the viscosity criterium.
Viscosity and visco-capillarity

Slemrod shows that the two criteria, viscosity and visco-capillarity, give rise to different admissibility conditions.

The choice of the "right" criterium is dictated by the specific problem.

...wide progeny with keywords:
non-classical shocks, kinetic relations...

Note that

\[
\frac{\partial^2 u}{\partial t^2} = \frac{\partial^2}{\partial x^2} \left( \phi(u) + \varepsilon \frac{\partial u}{\partial t} \right)
\]

\[
\frac{\partial^2 u}{\partial t^2} = \frac{\partial^2}{\partial x^2} \left( \phi(u) + \varepsilon \frac{\partial u}{\partial t} - \gamma \frac{\partial^2 u}{\partial x^2} \right)
\]

With respect to the case previously discussed, at the right-hand side there is a second order time derivative in place of the first order one.
Which synthesis?

Parabolic and hyperbolic versions have different rescaling properties

self-similar solution (scaling $x/\sqrt{t}$) vs. traveling waves

consequence of the presence of different time-scales.

...are they different “stories”?

Going back to the derivation of the equation, as $\varepsilon \to 0$, we obtain a hyperbolic-elliptic system with damping

\[
\begin{align*}
\frac{\partial u}{\partial t} + \text{div } J &= 0 \\
\tau \frac{\partial J}{\partial t} + \text{grad } \phi(u) &= -J
\end{align*}
\]

Is the parabolic dynamics the time-asymptotics of the hyperbolic one? (relation between heat and telegraph equation)

Rôle of the other higher order terms?