An Algorithm with Global Error Control for the Numerical Solution of the Generalized Density Profile Equation

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Outline of the talk

1. **Introduction**
2. **Existence and uniqueness of solution**
3. **The singularities of the problem and the associated one-parameter families of solutions**
4. **Shooting method based on asymptotic expansions**
5. **Numerical algorithm**
6. **Numerical results**
7. **Conclusions and future work**

INTRODUCTION

Physical interpretation: The behavior of mixtures of fluids (for example: liquid-gas) is described by the *Cahn-Hillard* theory.
Free volume energy:

$$E(\rho, |\nabla \rho|^2) = E_0(\rho) + \frac{\gamma}{2}|\nabla \rho|^2, \;\; \gamma > 0,$$

where ρ- density of the fluid.
$E_0(\rho)$ - classical volume free energy
γ - surface tension coefficient (independent from $|\nabla \rho|$).

Generalized Model

If we allow that the surface tension depends on $\nabla\rho$, the free volume energy takes the form

$$E(\rho, |\nabla\rho|) = E_0(\rho) + \frac{c}{p}|\nabla\rho|^p, \ \ \gamma > 0, p > 1;$$

in this case we obtain the following PDE:

$$c\, \text{div}(|\nabla\rho|^{p-2}\nabla\rho) = \mu(\rho) - \mu_0;$$

The operator in the left-hand side is the p-laplacian, where $p > 1$ (if $p = 2$ we obtain the classical laplacian).
In the case of spherical bubbles, we obtain the radial ODE:

$$r^{1-N}\left(r^{N-1}|\rho'(r)|^{p-2}\rho'(r)\right)' = f_p(\rho), \qquad (0 < r < \infty),$$

where f_p is a function with three real roots, whose specific form depends on p.

Right-Hand Side

In the classical laplacian case ($p = 2$), f_2 is a third degree polynomial

$$f_2(\rho) = 4\lambda^2(\rho - \xi)(\rho + 1)\rho,$$

where ξ is a real parameter;
In the degenerate laplacian case ($p \neq 2$), f_p has the form

$$f_p(\rho) = 2p\lambda^2(\rho - \xi)(\rho + 1)\rho|\rho - \xi|^\alpha|\rho + 1|^\alpha,$$

where $\alpha = 0$ in the case $p = 2$; for $p \neq 2$ the value of α will be discussed later.

Boundary Conditions

$$\left| \lim_{r \to 0+} \rho(r) \right| < \infty, \quad \lim_{r \to 0+} r\rho'(r) = 0,$$

$$\lim_{r \to \infty} \rho(r) = \xi, \quad \lim_{r \to \infty} \rho'(r) = 0.$$

In the bubble case (if $\xi > 0$) , we search for a strictly increasing solution.
In the droplet case (if $\xi < -1$), we search for a strictly decreasing solution.

References

F.dell'Isola, H.Gouin and P.Seppecher, "Radius and Surface Tension of Microscopic Bubbles by Second Gradient Theory", C.R.Acad. Sci. Paris, **320**(Serie IIb), 211–216 (1995).

F.dell'Isola, H.Gouin and G.Rotoli, "Nucleation of Spherical Shell–Like Interfaces by Second Gradient Theory: Numerical Simulations", Eur. J. Mech. B / Fluids **15**, 545–568 (1996).

H.Gouin and G.Rotoli, "An Analytical Approximation of Density Profile and Surface Tension of Microscopic Bubbles for Van der Waals Fluids", Mechanics Research Communications **24**, 255–260 (1997).

N. Kim, L. Consiglieri and J.F.Rodrigues, On non-newtonian incompressible fluids with phase transitions, Mathematical Methods in Applied Sciences, **29** 1523–1541 .

Existence and Uniqueness of Solution

Existence and uniqueness results for problems of this type can be found in:

B. Franchi, E. Lanconelli, and J. Serrin, Existence and uniqueness of nonnegative solutions of quasilinear equations in R., Adv. Math., 118, 177-243 (1996)

From this work, it follows that, when $p \leq 2$, for $0 < \xi < 1$, the considered problem (choosing $\alpha = 0$) has a unique bubble-type solution.

For $p > 2$,existence and uniqueness of solution is guaranteed only if we choose $\alpha = p - 2$ in the right hand side function.
This topic was investigated in detail in a separate work:
G. Hastermann, P. Lima, L. Morgado, E. Weinmüller, Density Profile Equation with p-Laplacian: Analysis and Numerical Simulation, Applied Mathematics and Computation 225 (2013) 550–561.

The Singularity at $r = 0$

Initial conditions:

$$\lim_{r \to 0+} \rho(r) = \rho_0 \quad \lim_{r \to 0+} r\rho'(r) = 0. \tag{1}$$

We assume that in the neighborhood of $r = 0$ the solution can be represented as

$$\rho(r) = \rho_0 + Cr^k(1 + o(1)), \quad \text{as} \quad r \to 0^+, \tag{2}$$

Asymptotic approximation close to the origin

Proposition 3.1. Let $N > 1$ and $p > 1$. For each ρ_0, the considered singular Cauhy problem has, in the neighborhood of $r = 0$, a unique holomorphic solution that can be represented by

$$\rho\left(x,\rho_0\right) = \rho_0 + \frac{p-1}{p}\left(\frac{f_p(\rho_0)}{N}\right)^{\frac{1}{p-1}} r^{\frac{p}{p-1}}\left[1 + y_1 r^{\frac{p}{p-1}} + o\left(x^{\frac{p}{p-1}}\right)\right], \quad (3)$$

where y_1 can be determined analytically.

Singularity at Infinity

As $r \to \infty$ we introduce the variable substitution

$$\rho(r) = \xi + r^{\frac{1-N}{(p-1)2}} z(r). \quad (4)$$

In the new variable z we obtain an asymptotically autonomous equation. In order to analyse the asymptotic behavior of the solutions, we can consider the autonomous equation:

$$(p-1) z''_{\infty}(r) = 2p\lambda^2 \frac{z_{\infty}(r)^{p-1} \xi^{p-1} (\xi + 1)}{z'_{\infty}(r)^{p-2}}. \quad (5)$$

We search for a solution of (5) in the form

$$z_{\infty}(r) = c \exp(\tau r), \quad (6)$$

where c and τ are constants.

Asymptotic Expansion at Infinity

Subsituting in the equation, we obtain:

$$z_\infty(r) = c\,\exp\left(-\sqrt[p]{2p\lambda^2\frac{(1+\xi)\xi^{p-1}}{p-1}r}\right). \tag{7}$$

Then, the solution of the non-autonomous equation can be expressed in the form of a Lyapunov series:

$$z(r) = \sum_{k=1}^{\infty} b^k C_k(r) e^{-\tau k r}, \tag{8}$$

where the functions C_k can be determined by solving a set of linear ODEs.

Asymptotic Expansion at Infinity

We have obtained an asypmptotic expression of the solutions which satisfy the condition

$$\lim_{r\to\infty} z(r) = \lim_{r\to\infty} z'(r) = 0. \tag{9}$$

In the old variable ρ, we obtain the asymptotic expression

$$\rho(r) = \xi - bC_1(r)r^a e^{-\tau r}(1 + o(1)), \qquad r \to \infty. \tag{10}$$

We must compute the value of b for which the solution satisfies the prescribed boundary condition close to 0.

Numerical Approximation - Shooting Method

R - bubble radius ($\rho(R) = 0$).
r_0 - initial approximation of R.

First Auxiliary Problem $\rho_-(r)$ - monotone solution on $[\delta, r_0]$, which satisfies the boundary conditions

$$\rho_-(\delta) = \rho_0 + \frac{p-1}{p}\left(\frac{f_p(\rho_0)}{N}\right)^{\frac{1}{p-1}} \delta^{\frac{p}{p-1}}\left[1 + y_1 \delta^{\frac{p}{p-1}}\right], \tag{11}$$

$$\rho_-(r_0) = 0. \tag{12}$$

Second Auxiliary Problem $\rho_+(r)$ - monotone solution on $[r_0, r_\infty]$, which satisfies the boundary conditions

$$\rho_+(r_0) = 0, \qquad \rho_+(r_\infty) = \xi - b r_\infty^a C_1(r_\infty) e^{-\tau r_\infty}. \tag{13}$$

Numerical Approximation - Shooting Method

For a given value of r_0, each of the auxiliary problems can be solved numerically. Then we construct the global solution:

$$\rho(r) = \begin{cases} \rho_-(r), & \text{if } \delta \le r \le r_0; \\ \rho_+(r), & \text{if } r_0 \le r \le r_\infty. \end{cases} \tag{14}$$

Let $\Delta(r_0) = \rho'_+(r_0) - \rho'_-(r_0)$.
The true value of r_0 is computed from the condition that $\Delta(r_0) = 0$.

Numerical Solution of Initial Value Problems

The above described algorithm has been implemented in the form of a MATLAB code.
All the arising initial value problems (IVP) were solved by means of a ODE solver with the following properties :

- Nested implicit Runge-Kutta method of order 4;
- Automatic stepsize selection based on local error estimation (embedded Runge-Kutta pair approach).
- Cheap global error estimation.

References:

- G. Yu. Kulikov, Cheap global error estimation in some Runge-Kutta pairs, IMA J. Numer. Anal., 33 (2013), pp. 136–163.
- G. Yu. Kulikov, S. K. Shindin, Adaptive nested implicit Runge-Kutta formulas of Gauss type, Appl. Numer. Math., 59 (2009), pp. 707–722.

Variational Formulation- Energy Integral

The considered BVP can be considered as a variational problem. In this case, we consider the minimization of the energy integral:

$$J := J(\rho) := \int_0^{\infty} \left(p^{-1}\rho'(r)^p + f_p(\rho(r))\right) r^{N-1} dr \qquad (15)$$

The convergence of this integral is a necessary condition for the solvability of the considered BVP.
$J(\rho)$ was computed numericallly, along with the solution, and the obtained approximations are displayed in the next slides.

Numerical Results - Density

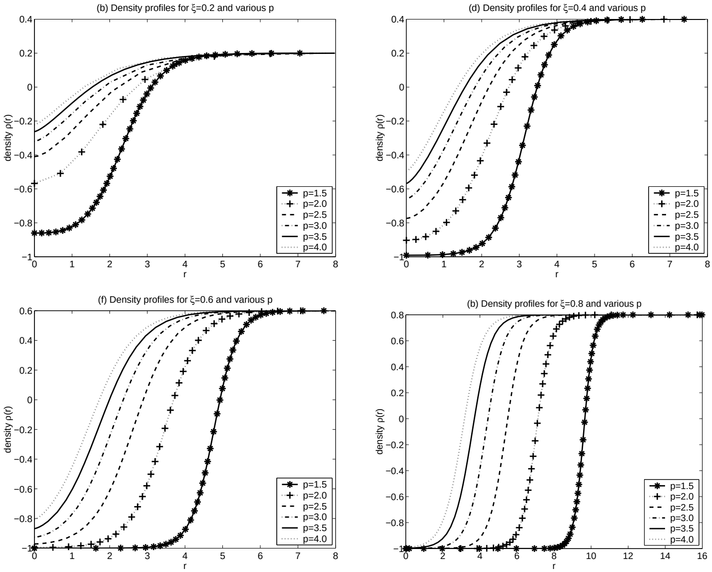

Figure: Density profiles for $\xi = 0.2, 0.4, 0.6, 0.8$ and various p.

Numerical Results - Energy Integral

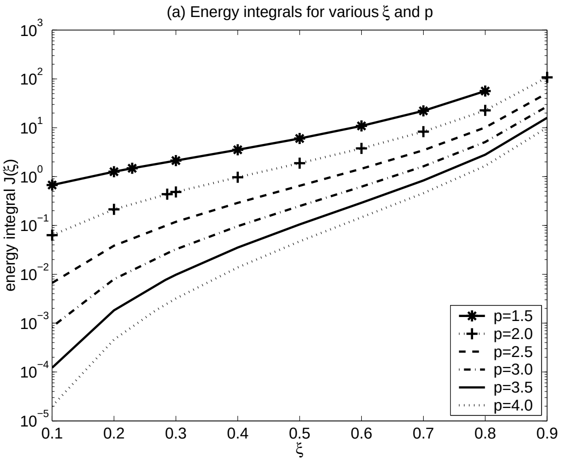

Figure: Energy Integral for various ξ and p.

Numerical Results - Interface Thickness

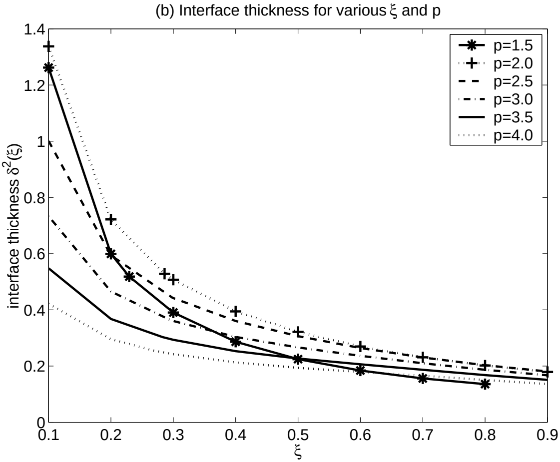

Figure: Inferface Thickness for various ξ and p.

Numerical Results - Bubble Radius

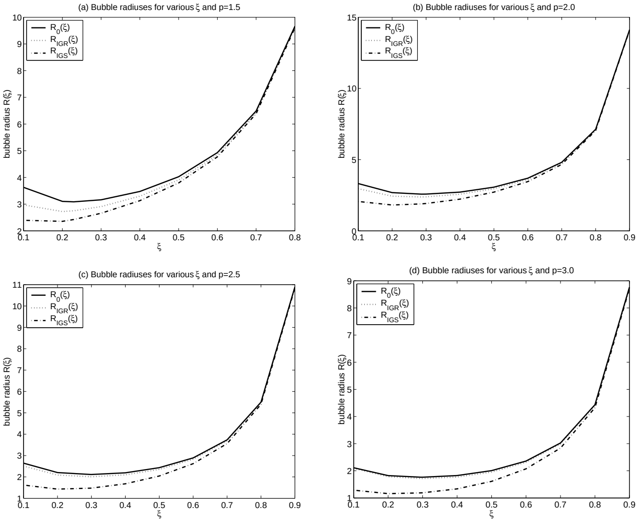

Figure: Bubble Radius (by different definitions) for $p = 1.5, 2, 2.5, 3$ and various ξ.

Numerical Results - Surface Tension

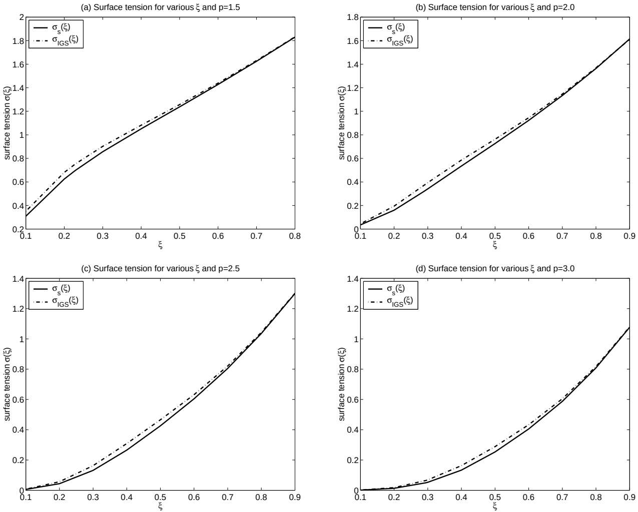

Figure: Surface tension (by different definitions) for $p = 1.5, 2, 2.5, 3$ and various ξ.

Conclusions about the Problem

- **By analysing the associate singular Cauchy problems we were able to describe the behavior of the solutions near the singularities.**
- **The results obtained for the p-laplacian confirm that many of the properties of the original model can be extended to the general one.**
- **In particular, for each value of p there is a minimal bubble radius, which is attained for a certain value of ξ.**
- **The density of the gas at the bubble centre (ρ_0) tends to -1 as ξ tends to 1 .**

Conclusions about the Numerical Methods

- **Numerical algorithms based on the shooting method are simple and work efficiently for $0.1 \leq \xi \leq 0.9$ and $1.5 \leq p \leq 4$.**
- **For values of ξ, close to 0 or to 1, it is difficult to find a good initial guess for the parameter ρ_0 (small variations of this parameter may lead to nonmonotone or blow-up solutions).**
- **Comparing with collocation methods, an advantage of this method is that avoids solving large systems of equations, where strong ill-conditioning may arise.**
- **The present method has a good potential for solving many important problems not only in fluid mechanics, but also in other areas of application where similar differential equations may arise.**

Integral Formulation of the Problem

$$\rho(r) = \int_0^r \frac{\tau^{n-1}}{r^{n-1}} f_2(\rho(\tau))d\tau;$$

$$f_2(\rho) = (\rho - \xi)\rho(\rho + 1).$$

Problem : find such $\rho(0)$, that $\lim_{r\to\infty} \rho(r) = \xi$;
The integral equation can be solved by the implicit Euler method or trapezoidal method.