Numerical Solution of the Density Profile Equation Using an Integral Method

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March 16, 2015

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Outline of the talk

1. **Introduction**
2. **Existence and uniqueness of solution**
3. **Integral formulation**
4. **Numerical algorithm**
5. **Numerical results**
6. **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 $|\nabla\rho|$).

Using principles of classical mechanics,the following system of partial differential equations for v and ρ:

$$\rho_t + div(\rho\vec{v}) = 0,$$

$$\frac{d\vec{v}}{dt} + \nabla(\mu(\rho) - \gamma\triangle\rho) = 0,$$

where μ - chemical potential $(\mu(\rho) = E_0'(\rho))$.
If we consider the case without motion of the fluid, then we obtain a single equation:

$$\gamma\triangle\rho = \mu(\rho) - \mu_0,$$

Spherical Symmetry

If we consider the case of spherical bubbles and introduce polar coordinates, we obtain the following equation:

$$\gamma\left(\rho'' + \frac{N-1}{r}\rho'\right) = \mu(\rho) - \mu_0, \qquad r \in (0,\infty). \tag{1}$$

We search for a soluttion which satisfies the boundary conditions

$$\rho'(0) = 0 \tag{2}$$

(following from spherical symmetry) and

$$\lim_{r\to\infty} \rho(r) = \rho_l > 0, \tag{3}$$

In the bubble case ρ_l is the density of the liquid and we search for a strictly increasing solution.
In the droplet case ρ_l is the density of the gas and we search for a strictly decreasing solution.

The chemical potential μ is a third degree polynomial, such that the difference $\mu - \mu_0$ has 3 real roots. Then the right-hand side of our equation may be written in the form

$$\mu(\rho) - \mu_0 = 4\alpha(\rho - \wp_1)(\rho - \wp_2)(\rho - \rho_l), \qquad 0 < \wp_1 < \wp_2 < \rho_l, \;\; \alpha > 0. \tag{4}$$

New variable:

$$x = \frac{\rho - \wp_2}{\wp_2 - \wp_1},$$

Let us define the positive constant $\lambda = \sqrt{\frac{\alpha}{\gamma}(\wp_2 - \wp_1)}$, and denote $\xi = \frac{\rho_l - \wp_2}{\wp_2 - \wp_1} > 0$. Then, we can investigate the boundary value problem

$$x''(r) + \frac{N-1}{r}x'(r) = 4\lambda^2(x(r)+1)\rho(r)(x(r) - \xi), \tag{5}$$

$$x'(0) = 0, \quad x(\infty) = \xi, \tag{6}$$

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).

Existence and Uniqueness of Solution

In Limaetal.2006, it was shown (using a variational approach developed in Derrick1965), that a solution of this problem can exist only if ξ satisfies $0 < \xi < 1$.
Furthermore, based on the results of gazzolaetal2000, it is possible to show that this restriction on ξ is also a sufficient condition for the existence of such a solution.
References:

- Limaetal.2006 P.M. Lima, N.V. Chemetov, N.B. Konyukhova, and A.I. Sukov, *Analytical-numerical investigation of bubble-type solutions of nonlinear singular problems*, J. Comput. Appl. Math. **189** (2006), 260-273.
- Derrick1965 *Comments on nonlinear wave equations as models for elementary particles*, J. Math. Phys. **5** (1965), 1252–1254.
- Gazzolaetal.2000 F. Gazzola, J. Serrin, and M. Tang, *Existence of ground states and free boundary problems for quasilinear elliptic operators*, Adv. Differential Equations **5** (2000), 1–30.

Singularities of the Problem

$$x''(r) + \frac{N-1}{r}x'(r) = 4\lambda^2(x(r)+1)\rho(r)(x(r)-\xi), \tag{7}$$

$$x'(0) = 0, \quad x(\infty) = \xi, \tag{8}$$

The problem is singular at $x = 0$ and as $x \to \infty$.

Different approaches: Shooting method, collocation methods

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- N.B. Konyukhova, P.M. Lima, M.L. Morgado and M.B. Soloviev, *B*ubbles and droplets in nonlinear physics models: analysis and numerical simulation of singular nonlinear boundary value problems, Comp. Maths. Math. Phys. **48**, N.11 (2008)2018-2058.
- G.Yu. Kulikov, P.M.Lima and M.L. Morgado,*A*nalysis and numerical approximation of singular boundary value problems with the p-Laplacian in fluid mechanis, Journal of Computational and Applied Mathematics,**262** (2014) 87-104.

Integral Formulation of the Problem

Rewrite the ODE in the form

$$r^{1-N}(r^{N-1}x'(r))' = f(x(r)), \quad (9)$$

where

$$f(x) = 4\lambda^2(x-\xi)x(x+1).$$

Then, dividing both sides of (9) by r^{1-n} and integrating on $[0, \infty[$, we obtain

$$x'(r) = \int_0^r \frac{\tau^{N-1}}{r^{N-1}} f(x(\tau))d\tau, \quad r > 0. \quad (10)$$

We obtain an integro-differential equation (IDE) of the first kind with a weakly singular kernel. We search for a solution which satisfies the boundary conditions

$$x'(0) = 0, \qquad \lim_{r\to\infty} x(r) = \xi$$

The first boundary condition is satisfied by any solution of the IDE.

Qualitative Properties of Solutions

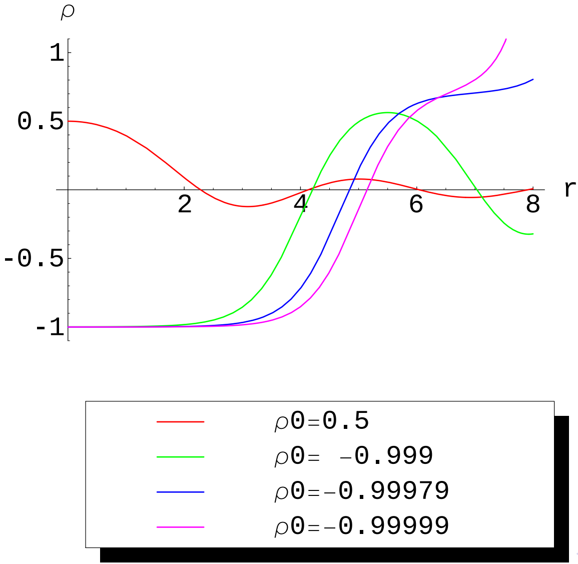
In order to implement a numerical algorithm, we must take into account that the considered equation has 3 types of solutions:

1. If $x(0) < x^*$, then the solution $x(r)$ blows up at a finite r;
2. If $x(0) > x^*$, then the solution $x(r)$ is oscillatory and $\lim_{t\to\infty} x(r) = 0$;
3. If $x(0) = x^*$, then the solution $x(r)$ is monotonic and $\lim_{t\to\infty} x(r) = \xi$;

Here x^* is not known a priori. In our algorithms we compute x^* by the shooting method.

Different Types of Solutions

Case of $\xi = 0.7$. Graphs of solutions with different initial values.



Bissection Method

To determine x^* we start with a certain interval $[a, b] \subset [-1, 0]$, such that

a) if $x(0) = a$, then the solution $x(r)$ (approximated by the implicit Euler method) is of the first type; this is recognized because at a certain $r_i < R$ we have $x(r_i) \geq \xi$;

b) if $x(0) = b$, then the solution $x(r)$ is of the second type (we know that this happens if, for a certain $r_i < R$, we obtain $x(r_{i+1}) \leq x(r_i)$);

this means that there exists a unique value $x^* \in]a, b[$ such that if $x(0) = x^*$, then we obtain a solution of the third type.

We construct a sequence of intervals $[a_k, b_k]$, $k = 1, 2, \dots$ such that $[a_k, b_k] \subset [a_{k-1}, b_{k-1}]$, $b_k - a_k = (b_{k-1} - a_{k-1})/2$ and $x^* \in [a_k, b_k]$. The iteration process stops when $b_k - a_k < \epsilon$, for a given ϵ.

Numerical Methods

This kind of equations can be efficiently solved by product integration methods.

We introduce a uniform grid on a certain interval $[0, R]$ and denote $r_i = ih$, where h-stepsize, $i = 0, 1, \ldots, n$. Then we approximate the solution of the IDE by avector

$$x_h = (x_0, x_1, \ldots, x_n), \qquad x_i \approx x(r_i).$$

According to the (Implicit Euler Method) the components of this vector must satisfy the equation:

$$x_{i+1} - x_i = \frac{h^2}{r_{i+1}^{N-1}} \sum_{j=1}^{i+1} (r_j)^{N-1} f(x_j), \quad i = 1, ..., n-1. \tag{11}$$

With this scheme, we don't need to compute the kernel at $r = 0$.

The nonlinear equation at each step is solved by the fixed point method, which converges fast, for a sufficiently small stepsize.

Second Order Method

In this case we approximate the integro-differential equation by the second order multistep scheme

$$\frac{3x_{i+2} - 4x_{i+1} + x_i}{2h} = \frac{1}{r_{i+2}^{N-1}} \frac{h}{2} \left(2 \sum_{j=1}^{i+1} (r_j)^{N-1} f(x_j) + r_{i+2}^{N-1} f(x_{i+2}) \right), \quad i = 0, \tag{12}$$

In order to compute x_1 we use the approximate formula

$$x_1 = x_0 + \frac{h^2}{2N} f(x_0); \tag{13}$$

We use the following second-order formula to approximate the derivative of x:

$$x'(r_{i+2}) = \frac{3x_{i+2} - 4x_{i+1} - x_i}{2h} + O(h^2),$$

and the integral is approximated by the trapezoidal rule.

Numerical Results

$x_0 = x(0)$ - gas density at the center of the bubble

ξ	$x(0)$(1st order)	$x(0)$(2nd order)
0.1	-0.2999	-0.3046
0.15	-0.4358	-0.4427
0.2	-0.5597	-0.5679
0.28	-0.7280	-0.7356
0.3	-0.7636	-0.7708
0.4	-0.8990	-0.9031
0.5	-0.9696	-0.9712
0.6	-0.9950	-0.9953
0.7	-0.9998	-0.9998
0.8	-0.99992178	-0.99992178

Convergence order

Implicit Euler Method, with $\xi = 0.5$

h	$x^h(0)$	$x^{2h} - x^h$
0.01	-0.96958965	
0.005	-0.97036934	$7.8E-4$
0.0025	-0.97075918	$3.9E-4$
0.00125	-0.97095410	$1.95E-4$

Trapezoidal Method, with $\xi = 0.5$

h	$x^h(0)$	$x^{2h} - x^h$
0.01	-0.97113484	
0.005	-0.97112361	$1.12E-5$
0.0025	-0.97112057	$3.04E-6$
0.00125	-0.97111961	$9.60E-7$

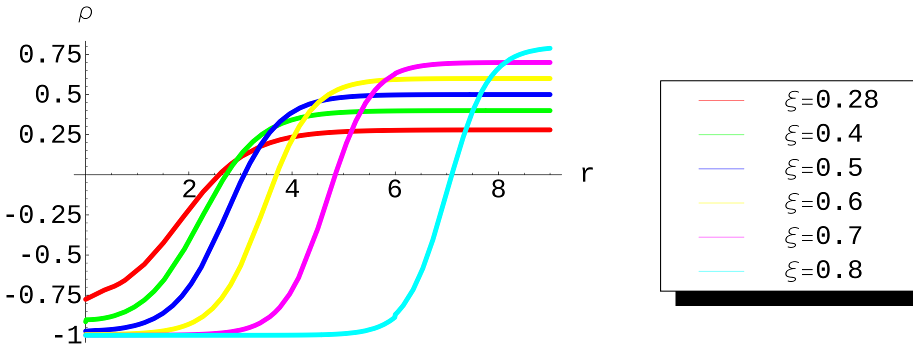
Bubble Radius

If $x(R) = 0$, then R- bubble radius.

ξ	$x(0)$	R
0.1	-0.2999	3.15
0.2	-0.5597	2.58
0.3	-0.7636	2.43
0.4	-0.8990	2.66
0.5	-0.9696	2.98
0.6	-0.9950	3.51
0.7	-0.9998	4.92
0.8	-0.99992178	7.61

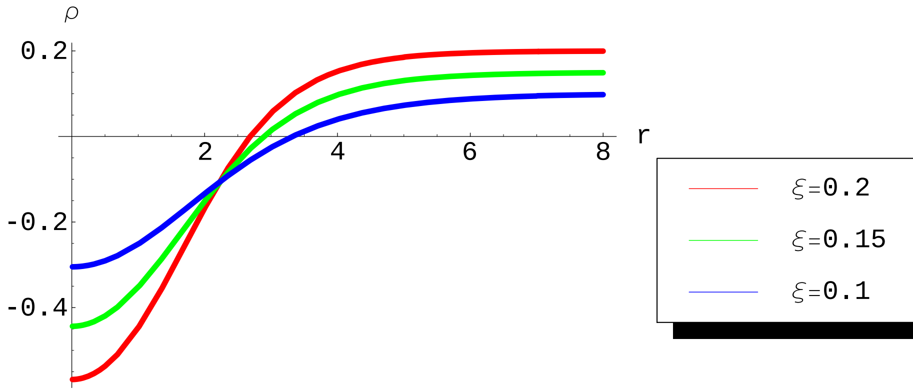
Solution Graphs

Density profiles for $\xi \geq 0.28$



Solution Graphs

Density profiles for $\xi < 0.28$



Conclusions and Future Work

- The integral formulation provides an alternative approach to analyze the problem and obtain numerical approximations.
- So far, we have applied **low-order methods** to the solution of the Volterra Integral equation which results in simple and stable algorithms.
- In the future, we intend to apply the integral formulation to the case of the degenerate laplacian .