INDUSTRIAL UNIVERSITY OF SANTANDER

Data science in the Cahn-Hilliard model

Author:
Iván Moreno Villamil
Códe: 2228085

Teacher:
Fabio D. Lora Clavijo
Teacher. physics school

Industrial University of Santander
Faculty of Science
School of physics
Bucaramanga
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1 Introduction

Currently, the study of data science is of great importance for any problem or research project in the different areas of human knowledge. For this reason, it has become essential for us to learn to collect, store and manipulate the data obtained from our investigations, in order to extract meaning and knowledge, using the resources and tools that are available. That is why within the mathematical models used to describe some physical, economic or social phenomenon or any other, which is developed and modeled through the theory of partial differential equations (PDEs), it is necessary to use numerical analysis tools, with which numerical approximations are made to approximate a solution through the information obtained by the numerical implementation. In general, these numerical schemes associated with the models generate a large amount of data that depends on my established parameters, which makes it necessary to store them in order to later manipulate them and be able to carry out a previous analysis, in order to be able to give an approximate solution or comparisons with others. models, depending on the interest and study on the model and give answers to our hypothesis raised for the phenomenon and that allows us to validate and reproduce the set of observations considered. This report is carried out with the purpose of stand out the importance of data science in the models developed through EDPs, making a brief study of the model associated with the Cahn-Hilliard equation, which allows studying the behavior of a homogeneous mixture between two substances by using an order parameter ϕ, this behavior is known as the diffusion process.

2 Model of the Cahn-Hilliard

In order to understand the importance and relevance of data science in the study of EDP models, the associated model for the nonlinear Cahn-Hilliard equation is presented, which has fourth-order derivatives and a Laplacian operator on the term nonlinear $f(\phi)$, which models the creation, evolution and dissolution of a fuzzy interface in a controlled fuzzy field, under given initial and boundary conditions and is defined as follows:

$$\begin{cases} \phi_t = \gamma \Delta w \quad \text{in } \Omega \times (0,T), \\ w = -\Delta \phi + f(\phi) \quad \text{in } \Omega \times (0,T), \\ \frac{\partial \phi}{\partial n} = \frac{\partial w}{\partial n} = 0 \quad \text{on } \partial\Omega \times (0,T), \\ \phi|_{t=0} = \phi_0 \quad \text{in } \Omega. \end{cases} \tag{1}$$

Where $\Omega \subset \mathbb{R}^d$ $(d = 2, 3)$ is a bounded domain and where the two boundary conditions considered in $(1)_3$ imply that none of the mixture can pass through the walls of the container Ω, ϕ denotes the so-called phase field function which is used to locate the phases within the system, assuming different stable values for each phase (for example $\phi = 1$ in one phase and $\phi = -1$ in the other) and in the interfacial regions the function varies smoothly. This causes the phase parameter to vary constantly during the evolution of the model until reaching a state where the variation of the phases is uniform.

Furthermore, $f(\phi)$ is defined by the so-called Ginzburg-Landau double well function which is defined as:

$$F(\phi) = \frac{(\phi^2 - 1)^2}{4\varepsilon^2}, \tag{2}$$

with

$$f(\phi) = F'(\phi) = \frac{\left(\phi^2 - 1\right)\phi}{\varepsilon^2}, \tag{3}$$

where the parameter $\varepsilon > 0$ represents the width of the interfacial layer, and $\gamma > 0$ is a relaxation constant.

3 Application of data science to the Cahn-Hilliard model

To perform the numerical approximation associated with the model (1), we define a weak or (variational) formulation as follows:

Definición 3.1. We will say that a pair (ϕ, w) is a weak solution of the problem (1) if $\phi \in L^\infty(0,T; H^1(\Omega))$, $\phi_t \in L^2(0,T; (H^1(\Omega))')$, $w \in L^2(0,T; H^1(\Omega))$, and

the following variational formulation is satisfied:

$$\begin{cases} \langle \phi_t, \overline{w} \rangle + (\nabla w, \nabla \overline{w}) = 0, \quad \forall \overline{w} \in H^1(\Omega), \\ (w, \overline{\phi}) = (\nabla \phi, \nabla \overline{\phi}) + (f(\phi), \overline{\phi}), \quad \forall \overline{\phi} \in H^1(\Omega), \end{cases} \tag{4}$$

where $(f, g) = \int_\Omega f(x)g(x)dx$ denotes the dot product in the space $L^2(\Omega)$ and $\langle \phi_t, \overline{w} \rangle$ denotes the duality product between $(H^1(\Omega))'$ and $H^1(\Omega)$.

Taking into account the formulation (4), we can introduce numerical schemes, for now discrete only in time, of first and second order. For this we define $t_n = nk$, with $k > 0$ denoting the passage of time (time parameter), and we obtain the following general approximation scheme: Given $\phi^n \in H^1(\Omega)$, find $(\phi^{n+1}, w^{n+\frac{1}{\alpha}}) \in H^1(\Omega) \times H^1(\Omega)$ solution of:

$$\begin{cases} (\delta_t \phi^{n+1}, \overline{w}) + (\nabla w^{n+\frac{1}{\alpha}}, \nabla \overline{w}) = 0, \quad \forall \overline{w} \ \in H^1(\Omega), \\ (w^{n+\frac{1}{\alpha}}, \overline{\phi}) = (\nabla \phi^{n+\frac{1}{\alpha}}, \nabla \overline{\phi}) + (f_k(\phi^{n+1}, \phi^n), \overline{\phi}), \quad \forall \overline{\phi} \in H^1(\Omega), \end{cases} \tag{5}$$

where we will use different semi-implicit approximations of the potential defined in (3), which we express as $f_k(\phi(t_{n+1}), \phi(t_n))$, giving rise to various numerical schemes. Likewise, $\phi^{n+\frac{1}{\alpha}} = \phi^{n+1}$ if $(\alpha = 1)$ or $\phi^{n+\frac{1}{\alpha}} = \phi^{n+\frac{1}{2}} = \frac{\phi^{n+1}+\phi^n}{2}$ if $(\alpha = 2)$, and $\delta_t \phi^{n+1} = \dfrac{\phi^{n+1} - \phi^n}{k}$. The initialization of the scheme (5) is given by the initial conditions of the problem (1), that is, $\phi^0 = \phi(0) = \phi_0$ in Ω.

Finally, to obtain completely discrete numerical schemes, we will use the finite element method for the spatial approximation, and the finite difference method for the temporal approximation.

To obtain the results of the numerical calculations associated with the numerical models, a large amount of data was collected on a time and space scale. During this process, the first hundred thousand iterations thrown by the programming code associated with each numerical scheme were taken into account, where with each iteration the behavior of the fluid was simulated according to our parameters established for said simulation, that is, the values thrown for each numerical iteration it gives us the position of the fluid in time and space, with the aim of comparing the evolution of interface phases and the energy stability of each of these associated numerical schemes.

Therefore, the collection of the data of each value associated with the numerical simulation generates our information base, which allows us to obtain an approximation to the solution of the problem and to be able to visualize and understand the behavior observed physically in order to be able to compare the results with mathematical theory, so that we can ensure that indeed our mathematical model fits the real problem, through our numerical models. In addition, it also allowed us to define which model behaves more efficiently and approaches the solution of our problem in a more stable, precise and stable way.

4 Compilation and results obtained

To carry out the respective numerical simulations and to be able to obtain the data to carry out the analysis and comparisons for each of the respective numerical schemes, it was necessary to use specialized computing tools and software, such as FreeFem++, which is a programming language and software focused on solving partial differential equations using the finite element method, which is written in the C++ programming language.

The results obtained from the programming codes in FreeFem++ associated with each numerical model for each iteration were saved in a folder saved in the Mathlab software in VTK (Visualization Toolkit) format, which is a free software system, which does not allow carrying out 3D by computer. graphics, image processing and visualization.These data allow us to generate comparative graphs with respect to the energy levels of each of the numerical models associated with the Cahn-Hilliard problem. In addition, the ParaView tool was used with the acquired data, which is an open source multiplatform data visualization and analysis application. Paraview is known and used in many different communities to analyze and visualize scientific data sets. It is an application built on the libraries (VTK). With this application it was possible to visualize the evolution of the different phases in time of the different numerical schemes associated with the model, which is evidenced in the following figures:

Figure 1: Spinodal decomposition

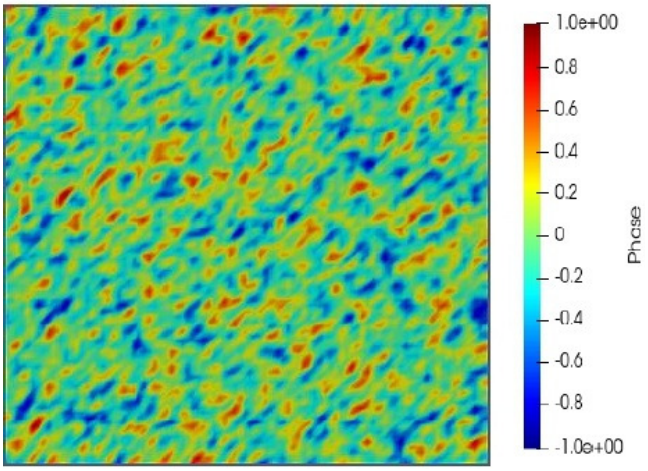


Figure 2: Comparison of the dynamics of numerical schemes.

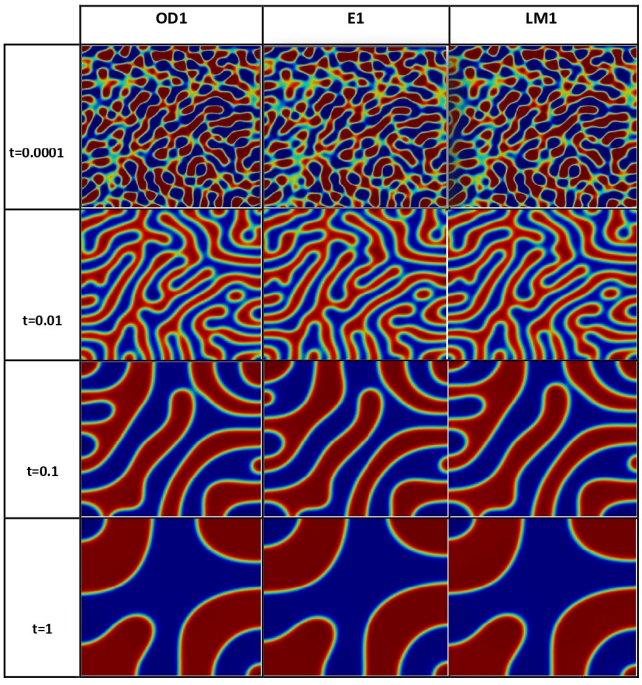
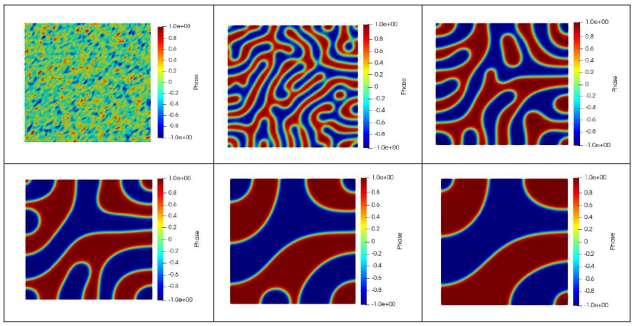


Figure 3: Evolution of the semi-implicit Cahn-Hilliard model in 2D.

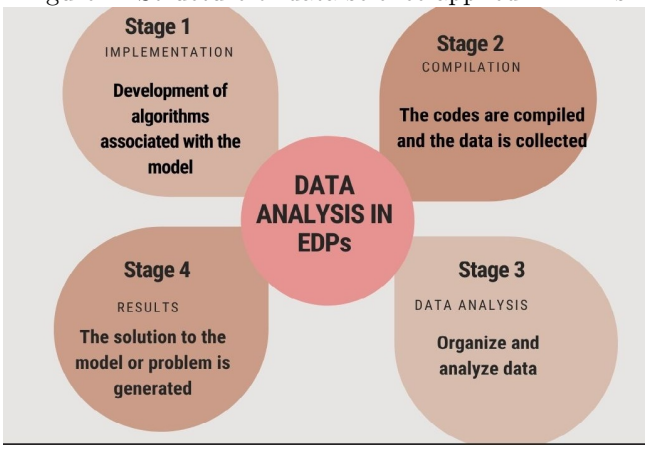


The figures (2), (3) show the dynamic comparison of each of the schemes studied, and where the behaviors assumed by each of the phases of each of the fluids. For these simulations, the domain $\Omega = (0,1)^2$ is considered using a structured mesh with $h = \frac{1}{90}$. In all the simulations $\gamma = 0.0001$, $\varepsilon = 0.01$ is taken and the initial condition for ϕ corresponding to a random initial data with values between -10^{-2} and 10^{-2}, with the aim of simulating a spinodal decomposition, that is, it shows the mixture of two fluids at the moment ϕ_0, as shown shown in the figure (1) at the first moment.

5 Conclusions

All the previous process and the results obtained to be able to determine the approximations to the equilibrium solutions for the Cahn-Hilliard model, were possible through the analysis of the data obtained by the respective numerical simulations, without this compilation and respective analysis through the tools of software it would not have been possible to try to approximate a solution to our proposed model, in order to make the comparison charts between the different schemes associated with our model. What has been described above shows the relevance and importance of data science in scientific research, specifically applied to the resolution of models described in partial differential equations and in general to problems where the use of numerical tools is necessary to be able to reach an approximate solution. In addition, it can be deduced that the entire data analysis process in the EDPs consists of four stages, as shown in the figure (4).

Figure 4: Structure of data science applied in EDPs



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