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Data science in the Cahn-Hilliard model

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Content

What is the model of Cahn-Hilliard, what does it model and what applications does it have?

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- ▶ The Cahn Hilliard model is a system of partial differential equations, which has fourth order derivatives and a Laplacian operator on the nonlinear term $f(\phi)$.

- ▶ models the creation, evolution and dissolution of a diffuse interface in a controlled diffuse field, under given initial and boundary conditions and is defined as follows:

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

- ▶ Where $\Omega \subset \mathbb{R}^d$ ($d = 2, 3$) is a bounded domain and where the two boundary conditions considered in $(1)_2$ 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

- ▶ Taking into account the formulation, a variational formulation associated with the model, we can introduce numerical schemes, for now discrete only in time, of first and second order.

- ▶ 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.

- ▶ During this process, the first one hundred thousand iterations thrown by the programming code associated with each scheme numeric.

▶ During this process, the first one 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.

▶ The data thrown by the numerical schemes are intended to show us a numerical approach to the solution of the problem and to be able to visualize and understand the behavior observed physically in order to compare the results with the mathematical theory.

▶ To carry out the respective numerical simulations and be able to obtain the data to perform the analysis and comparisons for each of the respective numerical schemes, it was necessary to use computer tools y software especializado. Which are:

(a) FreeFem++   (b) Mathlab   (c) Paraview

Figure: Tools for the analysis and development of results
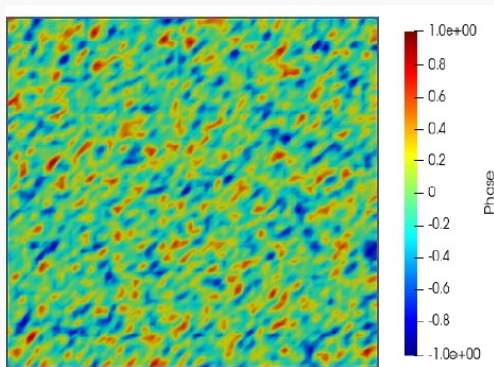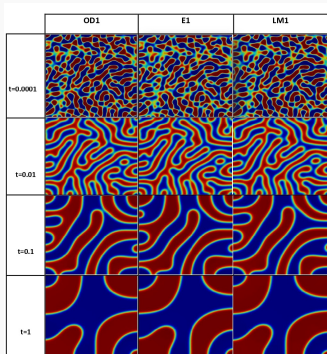
Figure: Spinodal decomposition
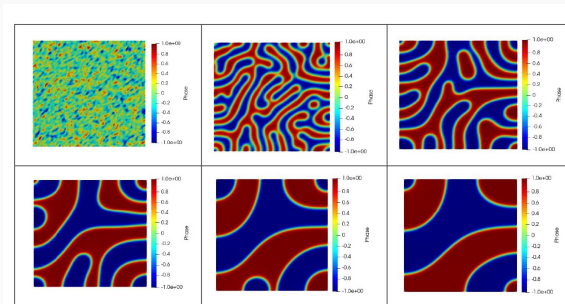
Figure: Comparison of the dynamics of numerical schemes.

	OD1	E1	LM1
t=0.0001			
t=0.01			
t=0.1			
t=1			

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

- ▶ The figures (3), (4) 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

- ▶ Para estas simulaciones se considera el dominio $\Omega = (0,1)^2$ utilizando una malla estructurada con $h = \frac{1}{90}$. En todas las simulaciones se toma $\gamma = 0.0001$, $\varepsilon = 0.01$ y se considera la condición inicial para ϕ correspondiente a un dato inicial aleatorio con valores entre -10^{-2} y 10^{-2}
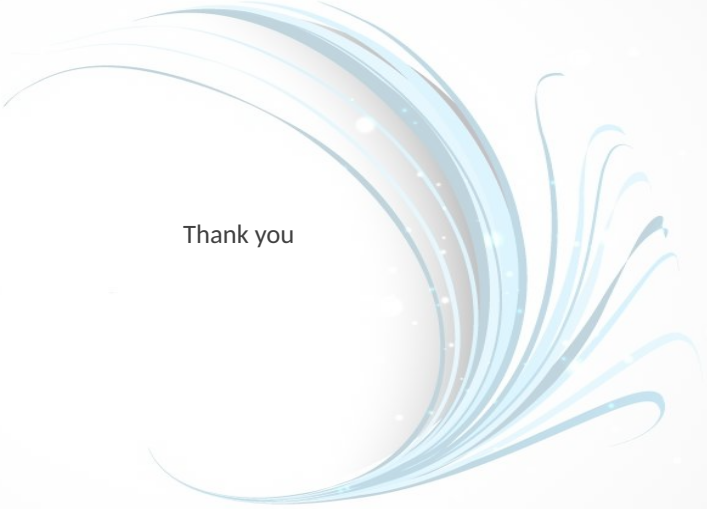
▶ All the previous process and the results obtained to be able to determine the approximations to the equilibrium solutions for the Cahn-Hilliard model, were possible through the analysis of the data obtained by the respective numerical simulations.

▶ The importance of data science in solving models described in partial differential equations and in general to problems where the use of numerical tools is necessary to reach an approximate solution is evident.

▶ In addition, it can be deduced that the entire data analysis process in the EDPs consists of four stages, as shown in the figure (5).

Figure: Structure of data science applied in EDPs
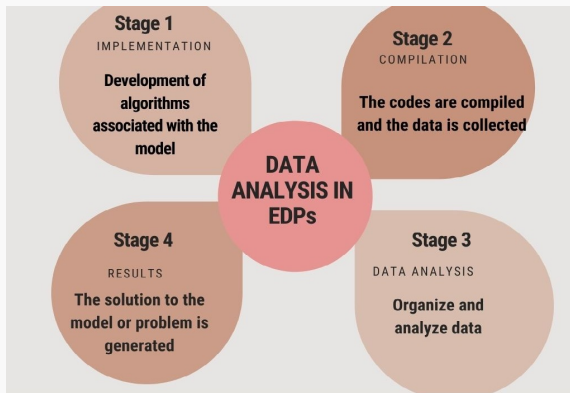
[1]   I. Moreno. *Numerical study for the Cahn-Hilliard equation*, 2021.

[2]   J. W. Cahn. *On spinodal decomposition*, Acta Metallurgica, 9 (1961), 795–801, 1961.

[3]   J. W. Cahn y J. E. Hilliard. *Free energy of a nonuniform system. I. Interfacial free energy*, The Journal of Chemical Physics, 28 (1958), 258–267.

[4]   G. Allaire. *Numerical analysis and optimization: an introduction to mathematical modeling and numerical simulation*. Oxford University Press, 2007.

[5]   F. Guillén-González y G.Tierra. *On linear schemes for a Cahn-Hilliard diffuse interface model*, Journal of Computational Physics, 234 (2013) 140–171.

Thank you