

Applications of Regime-switching in the Nonlinear Double-Diffusivity (D-D) Model

Amit K Chattopadhyay^{a)}

*Department of Applied Mathematics and Data Science,
College of Engineering and Physical Sciences, Aston University, Aston Triangle,
Birmingham B4 7ET, UK*

Elias C. Aifantis

*Laboratory of Mechanics and Materials, Aristotle University of Thessaloniki,
GR-54124 Thessaloniki, Greece^{b)}*

(Dated: today)

The linear double-diffusivity (D-D) model of Aifantis, comprising two coupled Fick-type partial differential equations and a mass exchange term connecting the diffusivities, is a paradigm in modeling mass transport in inhomogeneous media, e.g. fissures or fractures. Uncoupling of these equations led to a higher order [Partial Differential Equation \(PDE\)](#) that reproduced the non-classical transport terms, analyzed independently through Barenblatt's pseudoparabolic equation and the Cahn-Hilliard spinodal decomposition equation. In the present article, we study transport in a nonlinearly coupled D-D model and determine the regime-switching of the associated diffusive processes using a revised formulation of the celebrated Lux method that combines forward Fourier transform with a Laplace transform followed by an Inverse Fourier transform of the governing reaction-diffusion (R-D) equations. This new formulation has key application possibilities in a wide range of non-equilibrium biological and financial systems by approximating closed-form analytical solutions of nonlinear models.

Keywords: Double Diffusivity, Spatiotemporal correlation, Fourier transform, Laplace transform

^{a)}Electronic mail: a.k.chattopadhyay@aston.ac.uk

^{b)}Electronic mail: mom@mom.gen.auth.gr

I. INTRODUCTION

Diffusive mixing of multiple phases is a well-studied topic, particularly in the realm of microfluidics^{1,2}. While these studies invariably pointed to the dynamical evolution of an interface characterized by properties of the individual and correlated phases³, the precise dependence of parameters in this interface growth process had to wait until Aifantis produced a sequence of groundbreaking studies to analytically solve the double-diffusion problem^{4,5}. Their “trick” lay in unentangling the coupled diffusion of two phases, “diffusivity paths” in the material science parlance, thereby analyzing their relative growth through a study of the emergent interface dynamics^{6,7}. The problem has been revisited in recent times by Lux to understand the maximum likelihood probability of such events where the forward Kolmogorov model was analyzed using a combination of Fourier and Laplace transforms^{8,9}. While the Lux method employs the full arsenal of a dynamically evolving probability density function by numerically solving the Fokker-Planck model, it is largely limited to understanding linear diffusive mixing much like the original Aifantis models. The Lux method also lacks the simplicity of the Aifantis description that actually allows a detailed parameterization of the multi-diffusive process.

In a recent work¹⁰, a theoretical framework was established to approximate a closed-form solution of the ensemble-averaged density profiles and correlation statistics of coupled nonlinear double-diffusive processes, starting from the paradigmatic (linear) Aifantis double-diffusivity (D-D) model⁴⁻⁷, and extended to the nonlinear regime in analogy to the paradigmatic Walgraef-Aifantis model¹¹⁻¹⁴. Later studies focused on the stochastically driven versions of the D-D and W-A models¹⁵⁻¹⁷, which established the importance of understanding fluctuation effects in such dynamics.

Over the last few decades, the D-D model has become quite popular in both the applied mathematics and the material science communities due to its interesting mathematical properties of the former¹⁸⁻²⁰ that allow for robust interpretation of experimental observations for the latter²¹⁻²³. While there is no paucity of numerical estimation of nonlinear models, including those for double diffusion, from the perspective of theoretical modeling, analytical clarity had to give way to quantitative precision.

The present article is the first in line to provide a closed-form approximate solution of the nonlinear model resulting from a combination of the D-D and W-A type models. The

D-D:W-A motivated model leads to a coupled system of reaction-diffusion (R-D) equations where the diffusion terms resemble those contained in these models; the linear terms as in the D-D model; while the nonlinear terms resemble the W-A model (third order), but contain, in addition, cross-coupled terms (second order).

While examples of numerically analyzed reaction-diffusion models are available aplenty, there is little or no understanding of the parametric dependence of these processes and the nature of regime-switching transitions they may initiate. [While D-D models, both linear and nonlinear, have been extensively studied computationally, studies on dynamical phase transitions of these models are few and far between, barring exceptions⁹.](#) This is crucial for analyzing movements between states, as well as to comprehend how one (diffusive) state may affect others, an approach that we recently studied from a complementary perspective¹⁰.

There is another dimension to the present work. While the present article studies two nonlinearly cross-coupled diffusive processes and how the diffusivities can be extracted exactly from a combination of forward Fourier transform (FT), followed by Laplace transform (LT), and then an inverse Fourier transform (IFT), the mathematical foundation is generic enough to accommodate the more realistic case of forced (e.g. stochastic forcing) nonlinear D-D models as in Refs.^{15,16}. Broadly speaking, the framework will allow us to analyze diffusion equations with nonlinearity²⁴, both forced and equilibrium models. Also, free boundary problems such as the distribution of temperature in a homogeneous material during phase-transition²⁵ can be studied, i.e., the time evolution of the phase boundaries, the so-called Stefan problem.

The other application of this framework could be in traveling wave and pattern formation which can be mapped onto D-D models, such as the Fisher-Kolmogorov-Petrovsky-Piskunov (Fisher-KPP) model for the propagation of an advantageous gene in a population^{26,27}, Gray-Scott model for diffusion of chemical species^{27,28}. Similar studies can be found in the aforementioned W-A model of dislocation patterning in cyclically deforming metals which have been extensively studied numerically in the post-bifurcation regime^{12,13}. None of these was designed for closed-form analysis of nonlinearly coupled time-evolving diffusivity models, as is the target of this study.

The plan of the paper is as follows: Section II summarizes the model equation and provides a physical explanation of the mechanisms involved. Section III represents the non-dimensionalized representation of the model, the relevant non-dimensional governing equa-

tions and their linear stability analysis. Section IV first reinvents the Lux maximal-likelihood definition of regime-switching diffusions^{8,9}; then superimposes the D-D methodology⁷ onto the Lux maximum-likelihood approach, and finally, uses this hypothesis to solve for the densities of the phases around the stable fixed point as eigenvalue solutions. Section V summarizes the outcomes of the Chattopadhyay-Aifantis-Lux (CAL) model and discusses its wider implications.

II. THE MODEL

The starting point of this work is the nonlinear double diffusion (D-D) model that was recently analyzed to calculate the transition between two diffusive states, the so-called “transmissibility” model. In Ref.¹⁰, the emphasis was on arriving at an approximate formulation of the overlap strength of diffusive state “1” on that of diffusive state “2”, estimated from the correlation strength of the dynamical process that was analyzed from a mapping of the technique used to calculate Reproduction number R_0 in epidemic models²⁹⁻³¹. While being able to capture the cross-correlation of one diffusive process with the other, the approach had a key limitation in that it could not provide a measure of the regime-switching processes between the two diffusive systems. The present work attempts to understand this mechanism using a modified Fourier Transform method in the light of the Lux formalism⁹.

We consider $\tilde{\rho}_1$ and $\tilde{\rho}_2$ as the concentrations/densities for the two distinct D-D species along two different paths whose governing equations are given by

$$\frac{\partial \tilde{\rho}_1}{\partial \tilde{t}} = D_1 \frac{\partial^2 \tilde{\rho}_1}{\partial \tilde{x}^2} - k_1 \tilde{\rho}_1 + k_2 \tilde{\rho}_2 + \lambda_1 \tilde{\rho}_1 \tilde{\rho}_2 + \sigma_1 \tilde{\rho}_1^2 \tilde{\rho}_2 \quad (1a)$$

$$\frac{\partial \tilde{\rho}_2}{\partial \tilde{t}} = D_2 \frac{\partial^2 \tilde{\rho}_2}{\partial \tilde{x}^2} + k_1 \tilde{\rho}_1 - k_2 \tilde{\rho}_2 + \lambda_2 \tilde{\rho}_1 \tilde{\rho}_2 + \sigma_2 \tilde{\rho}_1 \tilde{\rho}_2^2 \quad (1b)$$

where D_1 and D_2 are diffusion coefficients, k_1 and k_2 are the rate mass exchange between different paths. The nonlinear terms represent the interactions between different species (interstitials, vacancies, and other point or line defects such as dislocations) when the density of one species influences the creation or annihilation of the other.

III. NON-DIMENSIONALIZATION OF THE DOUBLE DIFFUSING WALGRAEF-AIFANTIS MODEL

Let $\tilde{x} = ax$, $\tilde{t} = bt$, $\tilde{\rho}_1 = c_1\rho_1$, $\tilde{\rho}_2 = c_2\rho_2$. Substituting in Eqs. (1a-1b), then assuming that the diffusion coefficients remain unchanged after scaling, and choosing coefficients of nonlinear product terms as unity after scaling, for $\sigma_1 = \sigma_2 = \sigma$, we have

$$\frac{\partial \rho_1}{\partial t} = D_1 \frac{\partial^2 \rho_1}{\partial x^2} - \left(\frac{k_1 \sigma}{\lambda_1 \lambda_2} \right) \rho_1 + \left(\frac{k_2 \sigma}{\lambda_1^2} \right) \rho_2 + \rho_1 \rho_2 + \rho_1^2 \rho_2 \quad (2a)$$

$$\frac{\partial \rho_2}{\partial t} = D_2 \frac{\partial^2 \rho_2}{\partial x^2} + \left(\frac{k_1 \sigma}{\lambda_2^2} \right) \rho_1 - \left(\frac{k_2 \sigma}{\lambda_1 \lambda_2} \right) \rho_2 + \rho_1 \rho_2 + \rho_1 \rho_2^2. \quad (2b)$$

Note, the variables ρ_1 and ρ_2 , representing Eqs. (2a,2b), are non-dimensional. The numerical model uses this system of a non-dimensional dynamical system.

A. Linear Stability Analysis

Perturbing Eqs (2a,2b) around the fixed points (ρ_1^*, ρ_2^*) , *i. e.* $\rho_i = \hat{\rho}_i + \rho_i^*$ ($i = 1, 2$), we get the linearly stabilized representation as follows

$$\frac{\partial \hat{\rho}_1}{\partial t} = D_1 \frac{\partial^2 \hat{\rho}_1}{\partial x^2} + F_1(\hat{\rho}_1, \hat{\rho}_2) \quad (3a)$$

$$\frac{\partial \hat{\rho}_2}{\partial t} = D_2 \frac{\partial^2 \hat{\rho}_2}{\partial x^2} + F_2(\hat{\rho}_1, \hat{\rho}_2), \quad (3b)$$

where $F_1(\hat{\rho}_1, \hat{\rho}_2) = - \left(\frac{k_1 \sigma}{\lambda_1 \lambda_2} - \rho_2^* - 2\rho_1^* \rho_2^* \right) \hat{\rho}_1 + \left(\frac{k_2 \sigma}{\lambda_1^2} + \rho_1^* + \rho_1^{*2} \right) \hat{\rho}_2$, and $F_2(\hat{\rho}_1, \hat{\rho}_2) = \left(\frac{k_1 \sigma}{\lambda_2^2} + \rho_2^* + 2\rho_1^* \rho_2^* \right) \hat{\rho}_1 - \left(\frac{k_2 \sigma}{\lambda_1 \lambda_2} - \rho_1^* - \rho_2^{*2} \right) \hat{\rho}_2$. The homogeneous equilibrium (HE) state or the uniform steady state $(\rho_1^*, \rho_2^*)^{11, 14}$, is thus defined as $F_i(\rho_1^*, \rho_2^*) = 0$ ($i = 1, 2$).

Near the HE states, the linearized version of the Eqs (3a-3b) is given by

$$\frac{\partial \bar{\rho}}{\partial t} = \begin{bmatrix} D_1 & 0 \\ 0 & D_2 \end{bmatrix} \frac{\partial^2 \bar{\rho}}{\partial x^2} + Q \bar{\rho}, \quad (4)$$

where $\bar{\rho} = \begin{bmatrix} \hat{\rho}_1 \\ \hat{\rho}_2 \end{bmatrix}$, and Q is the Jacobian of $\begin{bmatrix} F_1(\hat{\rho}_1, \hat{\rho}_2) \\ F_2(\hat{\rho}_1, \hat{\rho}_2) \end{bmatrix}$ at the equilibrium states (ρ_1^*, ρ_2^*) . In defining Eqn (4), we have assumed a one-dimensional representation that can be generalized

to higher dimensions without any loss of generality. We consider $\bar{\rho} = \begin{bmatrix} \phi_1(t) \\ \phi_2(t) \end{bmatrix} e^{i\omega x}$ for real ω and get

$$\begin{bmatrix} \frac{d\phi_1}{dt} \\ \frac{d\phi_2}{dt} \end{bmatrix} = (Q - \omega^2 D) \begin{bmatrix} \phi_1(t) \\ \phi_2(t) \end{bmatrix}, \quad (5)$$

where $D = \begin{bmatrix} D_1 & 0 \\ 0 & D_2 \end{bmatrix}$. For stability, $\text{Det}(Q - \omega^2 D) > 0$ and $\text{Tr}(Q - \omega^2 D) < 0$ for all real values of the frequency ω .

We define the regime-switching process between the two diffusive states by “1” and “2”, respectively with variances $\sigma^2(s_1) = m_1$ and $\sigma^2(s_2) = m_2$. The state variable ρ_t of this diffusion will then obey $d\rho_t = \sigma(s_t) dW_t$ with W_t denoting the random (Brownian) motion where the hidden state process s_t is characterized by the *intensity matrix*,

$$Q = \begin{bmatrix} -\left(\frac{k_1\sigma}{\lambda_2^2} - \rho_2^* - 2\rho_1^*\rho_2^*\right) & \left(\frac{k_2\sigma}{\lambda_1^2} + \rho_1^* + \rho_1^{*2}\right) \\ \left(\frac{k_1\sigma}{\lambda_2^2} + \rho_2^* + 2\rho_1^*\rho_2^*\right) & -\left(\frac{k_2\sigma}{\lambda_1\lambda_2} - \rho_1^* - \rho_2^{*2}\right) \end{bmatrix}. \quad (6)$$

The eigenvalues of this intensity matrix Q determine the conversion rates (switch rates) between the two diffusive regimes^{8,9}. We note that for a Markovian process, the Q for Continuous Time Markov Chains (CTMCs) can be generally represented as

$$Q = \begin{bmatrix} -\sum_{i=2}^n \lambda_{1 \rightarrow i} & \lambda_{1 \rightarrow 2} & \dots & \lambda_{1 \rightarrow n} \\ \lambda_{2 \rightarrow 1} & -\sum_{i=1, i \neq 2}^n \lambda_{2 \rightarrow i} & \dots & \lambda_{2 \rightarrow n} \\ \dots & \dots & \dots & \dots \\ \lambda_{n \rightarrow 1} & \lambda_{n \rightarrow 2} & \dots & \lambda_{n \rightarrow n} \end{bmatrix}$$

Following the prescription in Ref.⁸, we can calculate the probability of transition between states 1 and 2 close to the steady state within the intensity matrix (Q) framework.

The linearly stable fixed points (ρ_1^*, ρ_2^*) can be obtained from Eqns (3a,3b), defined as $\frac{\partial \hat{\rho}_1}{\partial t} = \frac{\partial \hat{\rho}_2}{\partial t} = 0$ that, in the Fourier transformed $k - t$ space can be solved from the coupled

equations

$$\begin{aligned} \left(D_1 k^2 + \frac{k_1 \sigma}{\lambda_1 \lambda_2} - \rho_2^* - 2\rho_1^* \rho_2^* \right) \rho_1^* &= \left(\frac{k_2 \sigma}{\lambda_1^2} + \rho_1^* \rho_1^{*2} \right) \rho_2^* \\ \left(\frac{k_1 \sigma}{\lambda_2^2} + \rho_2^* + 2\rho_1^* \rho_2^* \right) \rho_1^* &= \left(D_2 k^2 + \frac{k_2 \sigma}{\lambda_1 \lambda_2} - \rho_1^* - \rho_2^{*2} \right) \rho_2^* \end{aligned} \quad (7)$$

Clearly, $(\rho_1^*, \rho_2^*) = (0, 0)$ is a trivial fixed point although there can be nontrivial fixed points too which would have to be numerically evaluated for specific parameter values.

IV. REGIME SWITCHING NONLINEAR DOUBLE-DIFFUSION

Rewriting Eqns (3a,3b) as a linearly perturbed dynamical system around the steady state(s), we get

$$\frac{\partial \hat{\rho}_1}{\partial t} = D_1 \frac{\partial^2 \hat{\rho}_1}{\partial x^2} - \alpha_1 \hat{\rho}_1 + \alpha_2 \hat{\rho}_2 \quad (8a)$$

$$\frac{\partial \hat{\rho}_2}{\partial t} = D_2 \frac{\partial^2 \hat{\rho}_2}{\partial x^2} + \alpha_3 \hat{\rho}_1 - \alpha_4 \hat{\rho}_2, \quad (8b)$$

where $\alpha_1 = \frac{k_1 \sigma}{\lambda_1 \lambda_2} - \rho_2^* - 2\rho_1^* \rho_2^*$, $\alpha_2 = \frac{k_2 \sigma}{\lambda_1^2} + \rho_1^* + \rho_1^{*2}$, $\alpha_3 = \frac{k_1 \sigma}{\lambda_2^2} + \rho_2^* + 2\rho_1^* \rho_2^*$ and $\alpha_4 = \frac{k_2 \sigma}{\lambda_1 \lambda_2} - \rho_1^* - \rho_1^{*2}$. We will use a combination of Fourier Transform (FT) and Laplace Transform (LT) sequentially to arrive at the regime-switching transition probabilities. The following notations will be used ($i = 1, 2$):

$$\hat{\rho}_i(x, t) \xrightarrow{\text{FT}} \bar{\rho}_i(\omega, t),$$

$$\hat{\rho}_i(x, t) \xrightarrow{\text{LT}} \tilde{\rho}_i(x, s).$$

We assume initial conditions $\hat{\rho}_1(x, 0) = \beta_1 \delta(x)$ and $\hat{\rho}_2(x, 0) = \beta_2 \delta(x)$. Fourier Transform of Eqns (8a,8b) gives

$$\frac{\partial \bar{\rho}_1}{\partial t} = -D_1 \omega^2 \bar{\rho}_1 - \alpha_1 \bar{\rho}_1 + \alpha_2 \bar{\rho}_2, \quad (9a)$$

$$\frac{\partial \bar{\rho}_2}{\partial t} = -D_2 \omega^2 \bar{\rho}_2 + \alpha_3 \bar{\rho}_1 - \alpha_4 \bar{\rho}_2. \quad (9b)$$

The FT above is followed by Laplace Transform of Eqns (9a,9b) leading to

$$\mathcal{L}[\rho_1'](s) = s\mathcal{L}[\bar{\rho}_1](s) - \beta_1 = -(D_1 \omega^2 + \alpha_1) \mathcal{L}[\bar{\rho}_1](s) + \alpha_2 \mathcal{L}[\bar{\rho}_2](s), \quad (10a)$$

$$\mathcal{L}[\rho_2'](s) = s\mathcal{L}[\bar{\rho}_2](s) - \beta_2 = \alpha_3 \mathcal{L}[\bar{\rho}_1](s) - (D_2 \omega^2 + \alpha_4) \mathcal{L}[\bar{\rho}_2](s). \quad (10b)$$

Eqns(10a,10b) can be reduced to obtain

$$\mathcal{L}[\bar{\rho}_1](s) = \frac{\beta_2\alpha_2 + \beta_1(s + D_2\omega^2 + \alpha_4)}{(s + D_1\omega^2\alpha_1)(s + D_2\omega^2\alpha_4) - \alpha_2\alpha_3}, \quad (11a)$$

$$\mathcal{L}[\bar{\rho}_2](s) = \frac{\beta_1\alpha_3 + \beta_2(s + D_1\omega^2 + \alpha_1)}{(s + D_1\omega^2\alpha_1)(s + D_2\omega^2\alpha_4) - \alpha_2\alpha_3}. \quad (11b)$$

For both Eqns(11a,11b), the poles s_0 are defined by the equation

$$(s_0 + D_1\omega^2\alpha_1)(s_0 + D_2\omega^2\alpha_4) = \alpha_2\alpha_3, \quad (12)$$

producing

$$s_{0\pm} = \frac{-(D_1 + D_2)\omega^2 - \alpha_1 - \alpha_4 \pm \sqrt{\Delta}}{2}, \quad (13)$$

where $\Delta = [(D_1 + D_2)\omega^2 + \alpha_1 + \alpha_4]^2 - 4[(D_1\omega^2 + \alpha_1)(D_2\omega^2 + \alpha_4) - \alpha_2\alpha_3] = [(D_1\omega^2 + \alpha_1) - (D_2\omega^2 + \alpha_4)]^2 - 4\alpha_2\alpha_3$. These results eventually lead to the Inverse Fourier Transforms as follows

$$\begin{aligned} \bar{\rho}_1(\omega, t) = & \frac{1}{\sqrt{\Delta}} \left[\{\beta_2\alpha_2 + \beta_1(s_{0+} + D_2\omega^2 + \alpha_4)\} e^{s_+t} \right. \\ & \left. - \{\beta_2\alpha_2 + \beta_1(s_{0-} + D_2\omega^2 + \alpha_4)\} e^{s_-t} \right], \end{aligned} \quad (14a)$$

$$\begin{aligned} \bar{\rho}_2(\omega, t) = & \frac{1}{\sqrt{\Delta}} \left[\{\beta_1\alpha_3 + \beta_2(s_{0+} + D_1\omega^2 + \alpha_1)\} e^{s_+t} \right. \\ & \left. - \{\beta_1\alpha_3 + \beta_2(s_{0-} + D_1\omega^2 + \alpha_1)\} e^{s_-t} \right], \end{aligned} \quad (14b)$$

where $\Delta = (s_{0+} - s_{0-})^2$.

The relevant Inverse Fourier Transform (IFT) of the function $\rho_i(x, t)$ will be then given by

$$\hat{\rho}_i(x, t) = \int_{-\infty}^{\infty} \bar{\rho}_i(\omega, t) e^{ix\omega} d\omega.$$

Clearly, the above integration cannot be done in its present form. Hence, we resort to a different construction.

The poles from Eqn. (13) can be represented as

$$s_{0\pm} = -\frac{1}{2} \left[\{(D_1 + D_2)\omega^2 + (\alpha_1 + \alpha_4)\} \pm \sqrt{((D_1 - D_2)\omega^2 + (\alpha_1 - \alpha_4))^2 + 4\alpha_2\alpha_3} \right] \quad (15)$$

Substituting $\lambda(\omega) = \frac{1}{2}\{(D_1 + D_2)\omega^2 + (\alpha_1 + \alpha_4)\}$ and $\mu(\omega) = \frac{1}{2}\{(D_1 - D_2)\omega^2 + (\alpha_1 - \alpha_4)\}$, Eqn. (15) can be rewritten as

$$s0_{\pm} = - \left[\lambda(\omega) \pm \sqrt{\mu^2(\omega) + \alpha_2\alpha_3} \right] \quad (16)$$

Starting from Eqns.(11a,11b) and defining $R_i(s) = \mathcal{L}[\bar{\rho}_i](s)$, the next step in the Lux formulation⁹ is the evaluation of $\bar{\rho}_i(\omega, t)$ which can be obtained from an Inverse Laplace Transform:

$$\bar{\rho}_1(\omega, t) = \mathcal{L}^{-1}[R_1] = \mathcal{L}^{-1} \left[\frac{\beta_2\alpha_2 + \beta_1(s + D_2\omega^2 + \alpha_4)}{(s - s0_+)(s - s0_-)} \right]. \quad (17)$$

Revisiting Eqn (11a), we can write

$$\begin{aligned} R_1 &= \left(\frac{1}{s0_+ - s0_-} \right) \left[\left(\frac{1}{s - s0_+} \right) - \left(\frac{1}{s - s0_-} \right) \right] [\beta_2\alpha_2 + \beta_1s + \beta_1(D_2\omega^2 + \alpha_4)] \\ &= \frac{1}{2\sqrt{\mu^2 + \alpha_2\alpha_3}} \left[\{\beta_1s0_+ + \beta_2\alpha_2 + \beta_1(D_2\omega^2 + \alpha_4)\} \left(\frac{1}{s - s0_+} \right) \right. \\ &\quad \left. - \{\beta_1s0_- + \beta_2\alpha_2 + \beta_1(D_2\omega^2 + \alpha_4)\} \left(\frac{1}{s - s0_-} \right) \right] \end{aligned} \quad (18)$$

Eqn (18) leads to

$$\begin{aligned} \bar{\rho}_1(\omega, t) &= \mathcal{L}[R_1^{-1}](t) \\ &= \frac{1}{2\sqrt{\mu^2 + \alpha_2\alpha_3}} \left[\{\beta_1s0_+ + \beta_2\alpha_2 + \beta_1(D_2\omega^2 + \alpha_4)\} e^{s0_+t} \right. \\ &\quad \left. - \{\beta_1s0_- + \beta_2\alpha_2 + \beta_1(D_2\omega^2 + \alpha_4)\} e^{s0_-t} \right] \end{aligned} \quad (19)$$

Rearranging the kernel in Eqn (19), we can write

$$\begin{aligned} \bar{\rho}_1(\omega, t) &= e^{-\lambda t} \left[\beta_1 \cosh \left(\sqrt{\mu^2 + \alpha_2\alpha_3} t \right) \right. \\ &\quad \left. - \frac{\beta_1\mu - \beta_2\alpha_2}{\sqrt{\mu^2 + \alpha_2\alpha_3}} \sinh \left(\sqrt{\mu^2 + \alpha_2\alpha_3} t \right) \right]. \end{aligned} \quad (20)$$

Similarly, we get

$$\begin{aligned} \bar{\rho}_2(\omega, t) &= e^{-\lambda t} \left[\beta_2 \cosh \left(\sqrt{\mu^2 + \alpha_2\alpha_3} t \right) \right. \\ &\quad \left. - \frac{\beta_1\alpha_3 + \beta_2\mu}{\sqrt{\mu^2 + \alpha_2\alpha_3}} \sinh \left(\sqrt{\mu^2 + \alpha_2\alpha_3} t \right) \right]. \end{aligned} \quad (21)$$

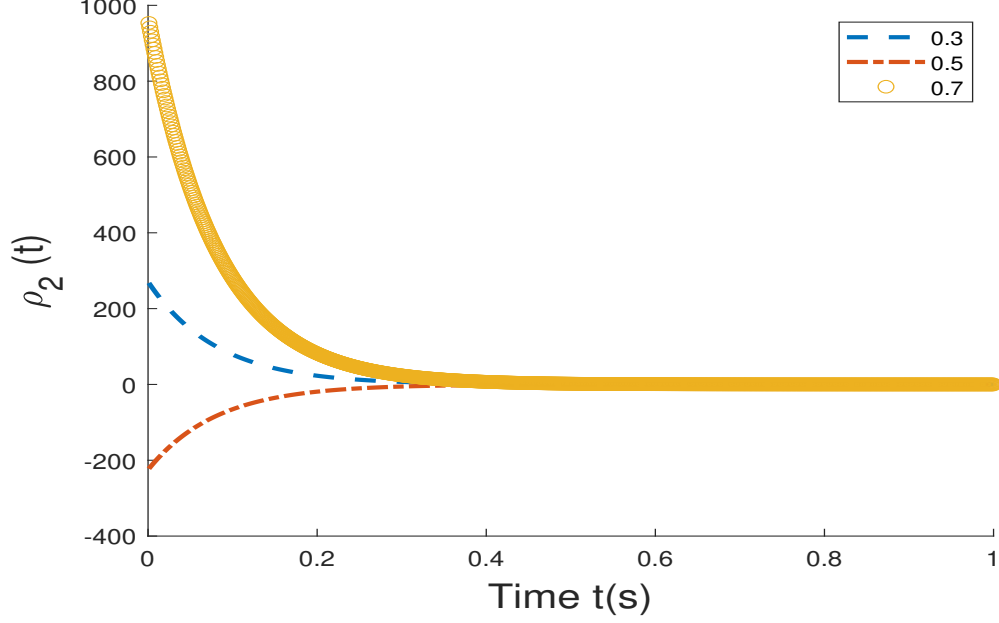


FIG. 1: $\rho_1(x, t)$ versus time t at spatial locations $x = 0.3$ (dashed), $x = 0.5$ (dot-dashed) and $x = 0.7$ (circles) for the steady state $\rho_1^* = \rho_2^* = 0$.

Now substituting $\bar{p}_1(\omega, t) = e^{-\lambda t} \frac{\sinh(\sqrt{\mu^2 + \alpha_2 \alpha_3 t})}{\sqrt{\mu^2 + \alpha_2 \alpha_3}}$ and $\bar{p}_2(\omega, t) = \omega^2 \bar{p}_1(\omega, t)$, we get the desired expressions as follows

$$\bar{p}_1(\omega, t) = \beta_1 \left(\frac{\partial \bar{p}_1}{\partial t} + D_2 \bar{p}_2 \right) + (\beta_2 \alpha_2 + \beta_1 \alpha_4) \bar{p}_1, \quad (22a)$$

$$\bar{p}_2(\omega, t) = \beta_2 \left(\frac{\partial \bar{p}_1}{\partial t} + D_1 \bar{p}_2 \right) + (\beta_1 \alpha_3 + \beta_2 \alpha_1) \bar{p}_1. \quad (22b)$$

The diffusion variables can now be obtained from a Fast Fourier Transform (FFT) of the equations

$$\hat{\rho}_i(x, t) = \frac{1}{\pi} \int_0^\infty \bar{\rho}_i(\omega, t) \cos(\omega x) d\omega, \quad (23)$$

where $i = 1, 2$. To solve for the densities $\hat{\rho}_i(x, t)$, we need to solve Eqn (23) around the stable fixed points as outlined in Eqn (7).

The approach adopted in this Chattopadhyay-Aifantis-Lux (CAL) method has advantages over the one from Lux and the original W-A model. First, the solution presented in this article applies to the nonlinear D-D model close to the stable fixed points of the linear D-D model that is already beyond the Lux prescription which is tailored for the linear model.

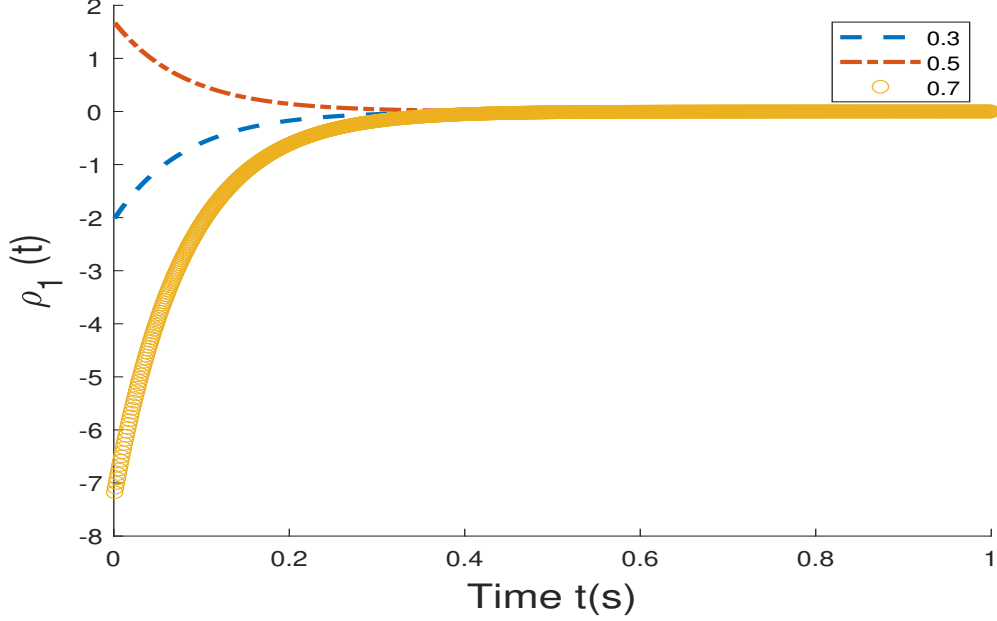


FIG. 2: $\rho_2(x, t)$ versus time t at spatial locations $x = 0.3$ (dashed), $x = 0.5$ (dot-dashed) and $x = 0.7$ (circles) for the steady state $\rho_1^* = \rho_2^* = 0$.

Secondly, the nonlinearity considered here is more general than in the W-A model as it contains all forms of (non-conserved) cross-couplings up to the third order. The highest (cubic) nonlinearity considered here generalizes the Ginzburg-Landau (G-L) formulation for phase transition. Thus our model accommodates not only amplitude instabilities (as in G-L) but also phase instabilities. Moreover, combining Eqns. (20,21) with Eqn. (23), we have a complete solution of the densities as functions of space and time, together with an ODE-based formulation as shown in Eqn. (22a,22b). This needs to be numerically evaluated as shown in Figures 1 and 2. The plots have been drawn for the steady state $\rho_1^* = \rho_2^* = 0$ using some values from²¹: $D_1 = 10^{-16}$, $D_2 = 5.510^{-19}$, $k_1 = 510^{-3}$, $k_2 = 610^{-5}$. Values of the cross-coupling parameters have been dimensionally matched against linear parameters and typically considered at 2 orders of magnitude lower than the linear parameter: $\lambda_1 = 210^{-8}$, $\lambda_2 = 10^{-8}$, $\sigma_1 = \sigma_2 = \sigma = 10^{-12}$. The initial conditions too have been value matched against linear solutions: $\beta_1 = 210^{-3}$ and $\beta_2 = 10^{-3}$. The solutions are highly dependent on initial conditions and especially on the nonlinearity parameters λ_1 , λ_2 , σ . The solution in Eqn (23) can also be used to evaluate the spatial evolution of the density functions in the large time (steady state) limit.

The Lux method⁸ offers similar solutions in terms of the Bessel function for a specific

choice of initial conditions. Ours is a more generic formulation that applies to cross-coupled diffusivity models.

V. CONCLUSIONS

The model and results presented here have been drawn from a unique amalgam of the original approaches by Aifantis^{4,5} and Lux^{8,9}. Multiple diffusion of species is not a new topic and is key to understanding the dynamics of interacting active systems, both in continuum systems with excluded-volume effects included³² as also in discrete molecular systems³³. The challenge though is solving such models with nonlinear interactions included. This is where our novel technique can be a major savior. This combination ensures a methodological novelty whereby the Maximum likelihood description can be extended to accommodate nonlinearly coupled diffusive systems, potentially including reaction-diffusion systems. This has key implications for a variety of inhomogeneous fields where mass transport is a governing process. Since the motivation of our model comes from inhomogeneous diffusion in materials¹⁶ and disease spreading^{10,31} in epidemiology, the discussion here will be directed towards the financial sector. But before expanding on that topic, we first provide some concluding remarks on the mathematical precept and comparisons between analytical with numerical solutions from the perspective of evolutionary biology and epidemiology.

Clearly, a comparison of the dynamical variable $R_0(t)$, motivated by the epidemiological literature, with the autocorrelation function reveals the richness of the dynamics of a reaction-diffusion system which offers an option of interpolating the results from the epidemic model into the double-diffusion domain, in the process providing a closed-form solution of the latter that has remained elusive thus far. Comparing the time evolution of R_0 with the autocorrelation function gives information of the origin of the observed abundance of different species in a reaction-diffusion system; for this, we need to numerically solve coupled equations Eqns. (20,21) and Eqn. (23) typically at the point of symmetry ($x = 0.5$).

Therefore, the introduction of the epidemiologically motivated quantity $R_0(t)$ into the studies of the reaction-diffusion systems can play a crucial role in understanding such systems in more depth. Since this interpolation between two unrelated disciplines only uses the mathematical similarity between two (or multiple) reaction-diffusion species, expressed as double-diffusion in material science, as compared to infection rate growth in epidemiology,

the approach is generic enough to be applied to all coupled reaction-diffusion models. At the point of symmetry ($x = 0.5$ in our model), both quantities (R_0 and autocorrelation) will asymptotically match their values with evolving time allowing for a closed form mapped (from mathematical biology) solution of the R-D model. As a comparison with the numerical solution confirms close convergence with the approximate mapped solution (based on the $R_0(t)$ formula as a descriptor of the correlation strength of the diffusing variables), the solution provides a handle to studies analyzing higher-order perturbations and relevant bifurcations, also including stochastic terms. Future studies involving spatially forced multi-diffusion and reaction-diffusion models will be considered, particularly with reference to econometric systems⁹.

ACKNOWLEDGMENT

The authors gratefully acknowledge partial financial support from the H2020-MSCA-RISE-2016 program, grant no. 734485, entitled “Fracture Across Scales and Materials, Processes and Disciplines (FRAMED). AKC acknowledges insightful comments from A Konstantinidis.”.

REFERENCES

- ¹J. D. Martin and S. D. Hudson, *Mass transfer and interfacial properties in two-phase microchannel flows*, New J. Phys. **11**, 115005 (2009).
- ²T. M. Squires and S. R. Quake, *Microfluidics: Fluid physics at the nanoliter scale*, Rev. Mod. Phys. **77**, 977 (2005).
- ³A. -L. Barabasi and H. E. Stanley, *Fractal Concepts in Surface Growth*, Cambridge University Press (1991).
- ⁴E. C. Aifantis, *A new interpretation of diffusion in high-diffusivity paths—a continuum approach*, Acta Metallurgica **27**(4), 683-691 (1979).
- ⁵E. C. Aifantis, *Continuum basis for diffusion in regions with multiple diffusivity*, Journal of Applied Physics **50**, 1334 (1979).
- ⁶E. C. Aifantis, *On the problem of diffusion in solids*, Acta Mechanica **37**, 265-296 (1980).

- ⁷E. C. Aifantis, *Gradient nanomechanics: Applications to deformation, fracture, and diffusion in nanopolycrystals*, Metall. Mater. Trans. A **42**, 2985 (2011).
- ⁸T. Lux, *The Markov-Switching Multifractal Model of Asset Returns*, Journal of Business & Economic Statistics **26**, Issue 2 (2008).
- ⁹T. Lux, *Inference for Nonlinear State Space Models: A Comparison of Different Methods applied to Markov-Switching Multifractal Models*, Econometrics and Statistics **21**, 69 (2022), <http://hdl.handle.net/10419/181491>.
- ¹⁰A. K. Chattopadhyay, B. Kundu, S. K. Nath and E. C. Aifantis, *Transmissibility in Interactive Nanocomposite Diffusion: The Nonlinear Double-Diffusion Mode*, Frontiers Appl. Maths. Stat. **8** (2022): <https://doi.org/10.3389/fams.2022.852040>.
- ¹¹D. Walgraef and E. C. Aifantis, *Dislocation patterning in fatigued metals as a result of dynamical instabilities*, Journal of Applied Physics **58**, 688 (1985).
- ¹²E. C. Aifantis, *On the dynamical origin of dislocation patterns*, Materials Science and Engineering **81**, 563-574 (1986).
- ¹³J. Pontes, D. Walgraef, and E. C. Aifantis, *On dislocation patterning: Multiple slip effects in the rate equation approach*, Intl. J. Plasticity **22**, 1486 (2006).
- ¹⁴K. Spillotis, L. Russo and E. C. Aifantis, *Analytical and numerical bifurcation analysis of dislocation pattern formation of the Walgraef–Aifantis model*, International Journal of Non-Linear Mechanics **102**, 41-52 (2018).
- ¹⁵A. K. Chattopadhyay and E. C. Aifantis, *Double diffusivity model under stochastic forcing*, Physical Review E **95**, 052134 (2017).
- ¹⁶A. K. Chattopadhyay and E. C. Aifantis, *On stochastic resonance in a model of double diffusion*, Materials Science and Technology, **34**:13, 1606-1613 (2018).
- ¹⁷A. -A. Tsambali, A. Konstantinidis and E. C. Aifantis, *modeling double diffusion in soils and materials*, Journal of the Mechanical Behavior of Materials; <https://doi.org/10.1515/jmbm-2018-2003>.
- ¹⁸E. C. Aifantis and J. M. Hill, *On the theory of diffusion in media with double diffusivity I—Basic mathematical results*, J. Mech. Appl.Math. **33**, 1 (1980).
- ¹⁹E. C. Aifantis and J. M. Hill, *On the theory of diffusion in media with double diffusivity II—Basic mathematical results*, Q. J. Mech. Appl.Math. **33**, 1 (1980).
- ²⁰, K. Kuttler and E. C. Aifantis, *Existence and uniqueness in nonclassical diffusion*, Quarterly of Applied Mathematics **45**(3), 549-560 (1987).

- ²¹D. A. Konstantinidis, I. E. Eleftheriadis and E. C. Aifantis, *On the Experimental Validation of the Double Diffusivity Model*, Scripta Materialia **38**, 573-580 (1998).
- ²²D. A. Konstantinidis and E. C. Aifantis, *Further Experimental Evidence of the Double Diffusivity Model*, Scripta Materialia **40**, 1235-1241 (1999).
- ²³D. Konstantinidis, I. Eleftheriadis and E. C. Aifantis, *Application of double diffusivity model to superconductors*, Journal of Materials Processing Technology **108**(2):185-187 (2001).
- ²⁴J. L. Vasquez, A de Pablo, F. Quirós and A. Rodríguez, *Classical solutions and higher regularity for nonlinear fractional diffusion equations*, JEMS **19**(7), 1949–1975 (2017).
- ²⁵L. I. Rubinstein, *The Stefan Problem*, Translations of Mathematical Monographs **27** (2010), [American Mathematical Society; First Edition \(December 31, 1971\)](#).
- ²⁶M. El-Hachem, S. W. McCue, W. Jin, Y. Du and M. J. Simpson, *Revisiting the Fisher–Kolmogorov–Petrovsky–Piskunov equation to interpret the spreading–extinction dichotomy*, Proc. of Roy. Soc. A **275**(2299); <https://doi.org/10.1098/rspa.2019.0378>.
- ²⁷J. D. Murray, *Mathematical Biology (Biomathematics Series)*, 1994 Edition, (2nd, Corr. Ed) Publisher: Springer-Verlag New York Inc.
- ²⁸J. E. Pearson, *Complex Patterns in a Simple System*, Science **261**(5118), 189-192 (1993).
- ²⁹H Nishiura, *Correcting the Actual Reproduction Number: A Simple Method to Estimate R_0 from Early Epidemic Growth Data*, International Journal of Environmental Research in Public Health **7**(1): 291–302 (2010).
- ³⁰A Cori, N M Ferguson, C Fraser, S Cauchemez, *A New Framework and Software to Estimate Time-Varying Reproduction Numbers During Epidemics*, American Journal of Epidemiology **178**(9): 1505–1512 (2013)..
- ³¹A. K. Chattopadhyay, D. Choudhury, G. Ghosh, B. Kundu and S. K. Nath, *Infection kinetics of Covid-19 and containment strategy*, Scientific Reports volume 11, Article number: 11606 (2021).
- ³²M. Bruna and S. J. Chapman, *Diffusion of multiple species with excluded-volume effects*, J. Chem. Phys. **137**, 204116 (2012).
- ³³X. Yan, et al. *A collaborative diffusion mechanism of multiple atoms during Cu-Ag bimetal surface reconstruction*, Phys. Chem. Chem. Phys. **25**, 10405-10416 (2023).