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Reaction-diffusion systems in natural sciences and new technology transfer

Abstract: Diffusion mechanisms in natural sciences and innovation management involve partial differential equations (PDEs). This is due to their spatio-temporal dimensions. Functional semi-discretized PDEs (with lattice spatial structures or time delays) may be even more adapted to real world problems. In the modeling process, PDEs can also formalize behaviors, such as the logistic growth of populations with migration, and the adopters' dynamics of new products in innovation models. In biology, these events are related to variations in the environment, population densities and overcrowding, migration and spreading of humans, animals, plants and other cells and organisms. In chemical reactions, molecules of different species interact locally and diffuse. In the management of new technologies, the diffusion processes of innovations in the marketplace (e.g., the mobile phone) are a major subject. These innovation diffusion models refer mainly to epidemic models. This contribution introduces that modeling process by using PDEs and reviews the essential features of the dynamics and control in biological, chemical and new technology transfer. This paper is essentially user-oriented with basic nonlinear evolution equations, delay PDEs, several analytical and numerical methods for solving, different solutions, and with the use of mathematical packages, notebooks and codes. The computations are carried out by using the software Wolfram Mathematica®7, and C++ codes.

Keywords: difference-differential equation; diffusion process; partial differential equations; reaction-diffusion equation; soliton; stochastic control; traveling wave solution.

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1 Introduction

This introductive paper[1] is devoted to diffusion processes as they occur in population dynamics studies of biological and ecological domains[2], and in adopter's dynamics of new products in the marketing area[3]. The importance of this subject is reflected in a vast literature since the seminal article of Skellam in 1951 [Skellam JG. *Biometrika* 1951, 38, 196–218] on the random population dispersal in a linear and two-dimensional habitat. This paper consists of three main parts about the wave propagation phenomena, the diffusion process and the illustrative application to domains, such as population dynamics, chemical kinetics and the spatio-temporal diffusion of technological innovations.

2 Wave propagation phenomena

The propagation phenomena embody the dispersive and diffusive aspects of wave phenomena. This introductive presentation is on the nonlinear wave propagation in different areas of applications. Firstly, we present the different types of waves, the basic concepts of wave motion, the dispersion relation for simple wave equations, the wave equation and d'Alembert's solution. A second aspect of this introduction concerns the traveling waves and soliton solutions for which the tanh-function method is preconized, among numerous analytical and numerical techniques for solving PDEs. A third aspect introduces the adaptation of the tanh-function method to semi-discretized differential systems such as systems with lattice spatial structures.

2.1 Nonlinear wave propagation

Nonlinear wave phenomena occur in many areas of natural sciences, such as fluid dynamics, chemistry

1 This paper is based on a Plenary Lecture [1], held at the WSEAS International Conference System in 2012.
2 A brief history of mathematical diffusion in ecology is presented in [2].
3 The basic deterministic and stochastic innovation diffusion models are introduced in [3].

(e.g., chemical kinetics involving reactions), mathematical biology (e.g., population dynamics) and solid state physics (lattice vibration). In physics, a wave describes a disturbance that is propagating through space and time with energy transfer. Waves may be illustrated by mechanical waves (i.e., waves on strings, acoustic waves, water waves, seismic waves, etc.), quantum mechanical waves, electromagnetic waves and also gravitational waves. There are different types of waves: mechanical waves and electromagnetic waves requiring or not requiring a medium, respectively, and transverse or longitudinal waves depending on the direction of their oscillations. Transverse waves have perpendicular oscillations to the direction of propagation (the direction of energy transfer). On the contrary, longitudinal waves have parallel oscillations. Mechanical waves can possess these two properties, whereas all electromagnetic waves are transverse.

2.1.1 Wave motion

The simplest propagating and unchanging one-dimensional (1D) wave is the sine wave, which elevation is given by $u(x,t)=A\ \sin(\theta(x,t))$ with $\theta=2\pi\left(\frac{x}{\lambda}-\frac{t}{T}\right)=kx-\omega t$, where A denotes the amplitude[4], $\theta(x,t)$ the phase function (in radians), λ the wavelength (in meters), T the period, i.e., the time for a complete oscillation (in seconds), $k(=2\pi/\lambda)$ the wave number (in radian per meter) and ω the angular frequency (in radians per second). Both measurements k and ω evaluate the wave oscillation in space and time, respectively. The phase function may also be written as $\theta=\frac{2\pi}{\lambda}(x-vt)$, where v is the phase velocity, i.e., the speed at which the wave is travelling. A generalized modulated wave takes the form $u(x,t)=A(x,t)\sin(kx-\omega t+\phi)$, where $A(x,t)$ denotes an amplitude envelope of the wave and ϕ the phase.

2.1.2 Dispersion relation

The simplest wave equation for propagating to the right is the first order linear PDE $u_t=-cu_x$ with propagation speed c (in units per second) and without changing its form. Supposing a sinuosidal solution, the dispersion relation (i.e., how the frequency depends on the wave number) is simply $\omega=ck$. The phase velocity is determined[5] by $v_p=\omega/k$.

Suppose that the traveling wave pulse can be broken into two simpler component waves of the form $u_i=A\ \sin(k_ix-\omega_it)$, $i=1,2$. By adding the wave components, we find the wave packet $u=A\ \sin(k_ax-\omega_at)\sin(k_mx-\omega_mt)$. In the first part of the expression, k_a and ω_a denote the average wave number and frequencies, respectively. In the second part, $k_m=\frac{k_1-k_2}{2}$ is half the difference of the wave numbers, and $\omega_m=\frac{\omega_1-\omega_2}{2}$ is the modulation frequency[6]. We deduce the group velocity v_g, i.e., the speed at which the wave packet is traveling $v_g=\lim_{\Delta k\to 0}\frac{\Delta\omega}{\Delta k}=\frac{d\omega}{dk}$.

Suppose that the simplest wave equation is now $u_t=\beta u_{xxx}-cu_x$. Assuming sinusoidal solutions of the form $u=A\ \sin(kx-\omega t)$, substituting into the PDE and rearranging terms, we easily find the dispersion relation $\omega=\beta k^3+ck$, the phase velocity $v_p=\beta k^2+c$ and the group velocity is $v_g=3\beta k^2+c$.

More generally, the dispersion relation for the frequency ω of 1D waves of wave number k is expressed by $\omega=\omega(k)$. Thus, in the dispersive case, waves of different frequencies have different velocities (e.g., electromagnetic wave in medium), whereas in the non-dispersive case, waves of different frequency have the same velocity (e.g., electromagnetic waves in vacuum). The phase speed being expressed by $v=\frac{\omega(k)}{k}$, v is independent of k for all k, only if $\omega(k)=C$. Non-dispersive waves imply that all disturbances propagate without deformation.

2.1.3 Wave equation[7]

The most familiar hyperbolic wave equation is:

$$u_{tt}=c^2\Delta u, \tag{1}$$

where Δ denotes the Laplace operator. A wave equation describes the propagation of a disturbance (e.g., the vibration of a string). The wave operator (or d'Alembertian operator) can be expressed by: $\partial_t^2-c^2\nabla^2\equiv\Box_c$.

4 The unit of the amplitude depends on the type of waves: transverse mechanical waves in meters, longitudinal sound waves in pressure units, electromagnetic waves in volts/meter.

5 The phase velocity is deduced algebraically from the formulas: $\lambda=2\pi/k$, $T=2\pi/\omega$ and $\lambda=vT$.

6 This property is deduced from the identity [4]: $\sin(\alpha)+\sin(\beta)=\sin\left(\frac{\alpha+\beta}{2}\right)+\sin\left(\frac{\alpha-\beta}{2}\right)$.

7 Inspired from [5], pp. 94–97, with different notations.

Factoring the wave operator as $(\partial_t - c\partial_x)(\partial_t + c\partial_x)$, suggests the transformation to the characteristic coordinates ξ,η for which $\xi = x - ct$ and $\eta = x + ct$. The wave equation becomes $\partial^2_{\xi\eta} u = 0$, for which the general solution is $u(\xi,\eta) = F(\xi) + G(\eta)$. Back-transforming to the coordinates x,t, the general solution is: $u(x,t) = F(x-ct) + G(x+ct)$.

Suppose that there exist boundary conditions on the initial displacement (shape) $u(x,0) = f(x)$ and on the initial velocity $u_t(x,0) = g(x)$. The boundary conditions (BCs) imply the system:

$$F(x)+G(x)=f(x), \tag{2}$$

and

$$cG'(x)-cF'(x)=g(x). \tag{3}$$

Integrating (3), we obtain:

$$G(x)-F(x)=G(x_0)-F(x_0)+\frac{1}{c}\int_{x_0}^{x} g(s)\,ds. \tag{4}$$

The expressions for $F(x)$ and $G(x)$ are obtained by solving the system (2) to (4). Substituting their respective arguments $x-ct$ and $x+ct$ into F and G yields the system:

$$\left.\begin{array}{l} F(x-ct) = -\frac{1}{2}G(x_0)+\frac{1}{2}F(x_0)+\frac{1}{2}f(x-ct)-\frac{1}{2c}\int_{x_0}^{x-ct} g(s)ds \\ G(x+ct) = -\frac{1}{2}F(x_0)+\frac{1}{2}G(x_0)+\frac{1}{2}f(x+ct)+\frac{1}{2c}\int_{x_0}^{x+ct} g(s)ds \end{array}\right]$$

Combining the two integrals into a single term, the general d'Alembert's solution for the wave equation takes the form:

$$u(x,t)=\frac{1}{2}(f(x-ct)+f(x+ct))+\frac{1}{2c}\int_{x-ct}^{x+ct} g(s)\,ds.$$

The value of the solution at position x and time t depends on the initial values of f at $x-ct$ and $x+ct$, and on the values of g between these points. This represents the sum of two simple waves and reflects the superposition principle for the linear equations. These two waves are propagating in opposite directions with a constant phase speed $|c|$. Because the phase speed is independent of the wave number, these waves are non-dispersive. The solutions of the Cauchy boundary initial value problem (BIVP) are shown in Figure 1. The phase speed is unity. The BCs are the initial displacement $f(x)=e^{-x^2}$ and the initial velocity $g(x)=0$, as in [5], p. 95.

2.2 Traveling wave and soliton solutions

The traveling wave is a solution by which waves propagate by right or left translations at a constant velocity. The tanh-function method finds these solutions for most nonlinear evolution equations and systems. Cnoidal waves are progressing periodic waves that are appropriate to a wide range of periodical problems. The soliton is a solitary wave maintaining its shape and traveling at a constant phase speed.

2.2.1 Traveling waves [6, 7]

A traveling wave is a function of the form:

$$u(x,t)=f(x-vt),\ f:\mathbb{R}\mapsto\mathcal{R},$$

where $\mathcal{R}$ is a vector space $\mathbb{R}$ or $\mathbb{C}$. A traveling wave propagates by right translations with velocity v. Let a polynomial PDE P of u and its derivatives

$$P(u,u_x,u_t,u_{xx},u_{xxx},\ldots)=0. \tag{5}$$

Now, consider

$$u(x,t)=U(\xi),\ \xi=k(x-vt).$$

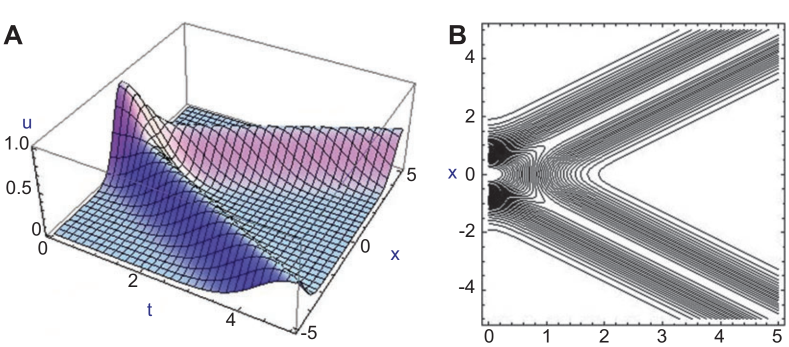

Figure 1 3D plot (A) and contours (B) of solutions of d'Alembert's solution for the wave equation.

The following changes $\frac{\partial}{\partial t}=-kv\frac{d}{d\xi}$, $\frac{\partial}{\partial x}=k\frac{d}{d\xi}$, $\frac{\partial^2}{\partial x^2}=k^2\frac{d}{d\xi}$,… transform the polynomial PDE into an ordinary differential equation (ODE) in $U(\xi)$

$$Q(U,U',U'',U^{(3)},\ldots)=0.$$

This equation should be successively integrated as long as the equation contains derivatives. Supposing the BCs $U(\xi)\to 0$ and $U^{(n)}(\xi)\to 0$, $n=1,2,\ldots$ for $\xi\to\pm\infty$, the integration constants should be zero.

2.2.2 Tanh-function method[8]

There is no unified method to find all the solutions of nonlinear wave equations. However, there are numerous analytical and numerical techniques, such as separation approach, inverse scattering, Backlund and Darboux transformation, Hirota's bilinear forms and hyperbolic tangent.

This tanh-method for exact solutions of nonlinear evolution equations is restricted to the search of traveling wave solutions for a large class of nonlinear PDEs [20]. Let a system of K polynomial differential equations

$$\mathbf{P}(\mathbf{u}(\mathbf{x}), \mathbf{u}'(\mathbf{x}), \mathbf{u}''(\mathbf{x}),\ldots \mathbf{u}^{(m)}(\mathbf{x}))=0, \tag{6}$$

where the dependent variable $\mathbf{u}$ has K components and the independent variable $\mathbf{x}$, N components. The traveling frame of reference is $\xi=\sum_{j=1}^{N}c_j x_j+\delta$, where the components c_j of the wave vector $\mathbf{x}$ and the phase δ are constant. The method is based on the *a priori* assumption that the traveling solution can be expressed in terms of the tanh-function, such as $Y=\tanh\,\xi$. Applying the chain rule repeatedly, the operators $\frac{\partial}{\partial x_j}=\frac{\partial\xi}{\partial x_j}\frac{dY}{\partial\xi}\frac{d}{dY}=c_j\left(1-Y^2\right)\frac{d}{dY}$ transform the system (6) into a coupled system of nonlinear ODEs $\mathbf{Q}(Y, \mathbf{U}(Y), \mathbf{U}'(Y), \mathbf{U}''(Y),\ldots)=\mathbf{0}$.

Suppose, a scalar polynomial PDE, as in [16]

$$P(u,u_t,u_x,u_{xx},\ldots)=0, \tag{7}$$

where $\xi=k(x-vt)$, so that $u(x,t)=U(\xi)$.

We use the following changes iteratively $\frac{\partial}{\partial t}=-kv\frac{d}{d\xi}$, $\frac{\partial}{\partial x}=k\frac{d}{d\xi}$, $\frac{\partial^2}{\partial x^2}=k^2\frac{d^2}{d\xi^2}$.

Eq. (7) is then transformed into the reduced ODE:

$$Q(U,U',U'',\ldots)=0. \tag{8}$$

The first derivative $\tanh'\xi=1-\tanh^2\xi$ and all higher-order derivatives are polynomials[9] in Y. We deduce the following change of variables:

$$\frac{d}{d\xi}=\left(1-Y^2\right)\frac{d}{dY}, \tag{9}$$

$$\frac{d^2}{d\xi^2}=-2Y\left(1-Y^2\right)\frac{d}{dY}+\left(1-Y^2\right)^2\frac{d^2}{dY^2}, \tag{10}$$

$$\frac{d^3}{d\xi^3}=2\left(1-Y^2\right)\left(3Y^2-1\right)\frac{d}{dY}-6Y\left(1-Y^2\right)^2\frac{d^2}{dY^2}+\left(1-Y^2\right)^3\frac{d^3}{dY^3}. \tag{11}$$

Next, we conjecture a solution of the polynomial form:

$$u\left(x,t\right)=U\left(\xi\right)=\sum_{i=1}^{M}a_i Y^i, \tag{12}$$

where the degree M must be determined. This parameter can be found by balancing the highest order derivative terms with the highest power nonlinear terms in the reduced ODE. Substituting Eq. (12) into Eq. (8), we obtain a set of algebraic equations. In fact, all the parameterized coefficients of Y^i must vanish. The resulting nonlinear algebraic equations for $k,v,a_0,a_1,\ldots,a_M$ determines these parameters. Then, using Eq. (12), we obtain an analytic solution for $u(x,t)$ in a closed form.

2.2.3 Cnoidal waves and soliton [21–24]

Cnoidal waves are progressing periodic waves. They are applied to a wide range of problems in fluid (e.g., surface water waves propagating in a canal) and solid mechanics, in plasma physics [25] and astrophysics [26]. The formula

8 The basic method in [8] is presented in Appendix A. The different steps of the tanh-method algorithm are illustrated by the nonlinear Boussinesq system in Appendix B. Numerous solutions of PDEs are in [9, 10]. Numerical methods for the solutions of PDEs are notably in [11–13]. Handbooks of solutions are in [14] for linear PDEs and in [15] for nonlinear PDEs. In [16], nonlinear wave equations are integrated by using He's variational iteration method, the tanh-function method, and the ansatz method. Various extensions of the tanh-function method are also available, such as the extended tanh-function method proposed in [17, 18], by using the properties of a Ricatti differential equation. In [19] a trial function method is also proposed, with application to the Burgers and Korteweg-de Vries equations, and their generalization.

9 Owing to the identity [4] $\cosh^2\xi-\sinh^2\xi=1$, the first three derivatives are: $\tanh'\xi=1-\tanh^2\xi=1-Y^2$, $\tanh''\xi=-2\,\mathrm{sech}^2\xi\tanh\xi=-2Y+2Y^3$ and $\tanh''\xi=-2\,\mathrm{sech}^4\xi+4\,\mathrm{sech}^2\xi\tanh^2\xi=-2+8Y-6Y^4$.

for this profile involves the Jacobian elliptic function. Let the Korteweg-de Vries (KdV) evolution equation[10] [27]:

$$2u_t+3uu_x+\frac{1}{3}u_{xxx}=0. \quad (13)$$

This dispersive equation describes unidirectional propagation of weakly nonlinear and long waves. Assume the traveling wave solution without change of form $u(x,t)=u(\xi)$, with traveling wave coordinate $\xi=x\text{-}Vt$ where $V>0$ denotes the phase speed of waves, traveling to the right. The traveling-wave solutions are obtained by using the following steps for the two types of waves, the cnoidal waves and the solitary waves[11]. Substituting $u(\xi)$ in Eq. (13) yields the ODE:

$$-2Vu'_\xi+3uu'_\xi+\frac{1}{3}u'''_\xi=0.$$

Integrating twice yields:

$$\frac{1}{6}\left(u'_\xi\right)^2=C_2+C_1u+Vu^2-\frac{1}{2}u^3\equiv f(u)>0, \quad (14)$$

where C_1 and C_2 are integration constants. It can be proved that $f(u)$ requires three real-valued stationary points r_1,r_2,r_3 such as $r_1\le r_2\le r_3$ to obtain periodic solutions. We have:

$$f(u)=-\frac{1}{2}(u-r_1)(u-r_2)(u-r_3). \quad (15)$$

Comparing Eq. (14) and the expansion of Eq. (15), we deduce[12] notably that $V=(r_1+r_2+r_3)/2$. Defining $v=\frac{u}{r_3}$, $s_j=\frac{r_j}{r_3}$, $j=1,2$, a crest is at $\xi=0$ and $v(0)=0$. Replacing in Eq. (15), we get:

$$\left(v'_\xi\right)^2=3r_3(v-s_1)(v-s_2)(1-v). \quad (16)$$

A further variable is $y(\xi)$ through:

$$v=1+(s_2-1)\sin^2(y). \quad (17)$$

Plugging Eq. (17) into Eq. (16) yields:

$$\left(y'_\xi\right)^2=\frac{3}{4}r_3(1-s_1)\left(1+\frac{1-s_2}{1-s_1}\sin^2(y)\right).$$

Then,

$$\frac{dy}{d\xi}=\sqrt{k\left(1-m^2\sin^2 y\right)}, \quad (18)$$

where $k=\frac{3}{4}r_3(1-s_1)$ and $m^2=\frac{1-s_2}{1-s_1}$ with $k>0$ and $m^2\in[0,1]$. We may solve Eq. (18) implicitly to obtain:

$$F(y|m)=\int_0^{y(\xi)}\frac{d\theta}{\sqrt{k\left(1-m^2\sin^2\theta\right)}}. \quad (19)$$

The left hand side (LHS) of Eq. (19) is defined, for fixed m, in terms of the inverse of the mapping $y\mapsto F(y|m)$. Hence, $\sin(y)=\mathrm{sn}\left(\sqrt{k}\,\xi|m\right)$. Therefore, we find $v(x,t)=1+(s_2-1)\mathrm{sn}^2\left(\sqrt{k}\,\xi|m\right)$. Then, the final result is of the form[13]

$$u(x,t)=r_2+(r_3-r_2)\mathrm{cn}^2\left(\sqrt{\frac{3}{4}(r_3-r_1)}\,\xi|m\right),$$

where $\xi=x-\frac{1}{2}(r_1+r_2+r_3)$ and $m=\sqrt{\frac{r_3-r_2}{r_3-r_1}}$. Figure 2 on LHS shows a 3D plot of the progressive waves of the KdV equation.

2.2.4 Soliton

A soliton is a solitary wave, maintaining its shape and traveling at a constant phase speed. Lets impose the BCs $u,u'_\xi,u''_\xi\to 0$ as $\xi\to\pm\infty$. Then the arbitrary constants C_1, C_2 in Eq. (14) are zero. When $r_1\to r_2$ and is taken to be zero, we obtain the soliton (see [21], pp. 21–22 and [28]):

$$u(x,t)=2V\,\mathrm{sech}^2\left(\sqrt{\frac{3}{4}V}\,(x-Vt)\right) \quad (20)$$

Proof Eq. (14) becomes:

$$\left(u'_\xi\right)^2=3u^2(-u+2V) \quad (21)$$

A real solution exists only if $-u+2V\ge 0$. Eq. (21) can be integrated as:

$$\int\frac{du}{u\sqrt{-3u+6V}}=\pm\int d\xi. \quad (22)$$

Using the substitution $u=2V\,\mathrm{sech}^2(\theta)$ yields Eq. (20)[14] Q.E.D. ■

10 The original equation as it was used for water waves in dimensional form was defined by $\eta_t+\sqrt{gh}\,\eta_x+\frac{3}{2}\sqrt{\frac{g}{h}}\eta\eta_x+\frac{1}{6}h^2\eta_{xxx}=0$, where $\eta(x,t)$ denotes the surface elevation at the horizontal coordinate x and time t, g is gravitational acceleration and h is mean water depth.

11 The complete determination of the cnoidal solutions is available at http://www.wikiwaves.org/wiki/index.php? title=KdV_Cnoidal_Waves_Solutions&oldid=12515 for a standard KdV $u_t+6uu_x+u_{xxx}=0$.

12 We have $2f(u)=r_1r_2r_3-(r_1r_2+r_1r_3+r_2r_3)u+(r_1+r_2+r_3)u^2-u^3$. Comparing with Eq. (14), we deduce $V=(r_1+r_2+r_3)/2$, $C_1=-(r_1r_2+r_1r_3+r_2r_3)/2$ and $C_2=r_1r_2r_3/2$.

13 The elliptic parameter m determines the shape of the cnoidal wave: the cnoidal becomes a cosine function for $m=0$ and gets peaked crests and flat through for $m\approx 1$.

14 When integrating Eq. (22), the constant of integration x_0 may be ignored. This is the phase shift that indicates the position of the peak at $t=0$.

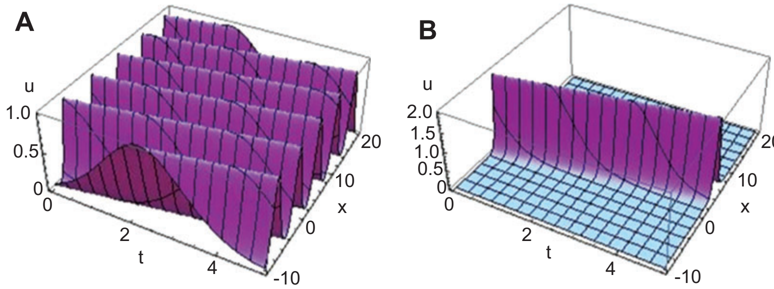

Figure 2 Cnoidal (A) and soliton (B) progressive waves of the KdV equation.

Figure 2 on right hand side (RHS) shows a 3D plot of the soliton of the KdV equation.

2.3 Hyperbolic tangent solutions of difference-differential equation systems[15]

The tanh-function method also solves semi-discretized differential systems, where the spatial variable is discrete and the time variable is kept continuous. We show how the algorithm for PDEs is modified to take into account the properties of difference-differential equations (DDEs) due to shift elements. This approach is illustrated by the Toda lattice equation, for which the solutions are computed automatically.

2.3.1 Difference-differential systems

The tanh-method must be adapted to solve the particular DDEs and systems. In such semi-discretized systems, the spatial variables are discrete while the time variable is still continuous. Their solution may describe particles motions in lattice, current in electrical networks, pulses in biological chains, etc. [20]. The Mathematica® package by [20] computes exact traveling wave solutions of nonlinear polynomial DDEs. Let the system of DDEs:

$$\Phi\Big(\mathbf{u}_{\mathrm{n}+\Delta_1}(\mathbf{x}),\ldots,\mathbf{u}_{\mathrm{n}+\Delta_k}(\mathbf{x}),\mathbf{u}'_{\mathrm{n}+\Delta_1}(\mathbf{x}),\ldots,\mathbf{u}'_{\mathrm{n}+\Delta_k}(\mathbf{x}),\ldots,\mathbf{u}^{(r)}_{\mathrm{n}+\Delta_1}(\mathbf{x}),\ldots,\mathbf{u}^{(r)}_{\mathrm{n}+\Delta_k}(\mathbf{x})\Big)=0, \tag{23}$$

where $\mathbf{u}$ is an M-dimensional dependent variable, $\mathbf{n}$ an Q-dimensional vector of discrete independent variables, $\mathbf{x}$ an N-dimensional vector of continuous variables, with the shift elements $\Delta_i \in \mathbb{Z}^Q$, $i=1,k$. We look for solutions in the traveling frame of reference:

$$\xi_{\mathbf{n}}=\sum\nolimits_{i=1}^{Q} d_i n_i+\sum\nolimits_{j=1}^{N} c_j x_j+\delta.$$

2.3.2 Tanh-method for DDEs

The five steps of the algorithm of the tanh-method for DDEs are the same steps as for PDEs with necessary adaptations.

In step 1, a DDE is transformed into a nonlinear DDE in $T_n=\tanh(\xi_n)$, by repeatedly using the chain rule:

$$\frac{d}{dx_j}=\frac{\partial \xi_{\mathbf{n}}}{\partial x_j}\frac{dT_{\mathbf{n}}}{d\xi_{\mathbf{n}}}\frac{d}{dT_{\mathbf{n}}}=c_i\left(1\text{-}T_{\mathbf{n}}^2\right)\frac{d}{dT_{\mathbf{n}}} \tag{24}$$

We have[16]:

$$T_{\mathbf{n}+\Delta_s}=\frac{T_{\mathbf{n}}+\tanh(\phi_s)}{1+T_{\mathbf{n}}\tanh(\phi_s)} \tag{25}$$

where $\phi_s=\Delta_{s1}d_1+\cdots+\Delta_{sQ}d_Q$. The system (23) is transformed into:

$$\Psi\Big(\mathbf{U}_{\mathrm{n}+\Delta_1}(T_{\mathbf{n}}),\ldots,\mathbf{U}_{\mathrm{n}+\Delta_k}(T_{\mathbf{n}}),\mathbf{U}'_{\mathrm{n}+\Delta_1}(T_{\mathbf{n}}),\ldots,\mathbf{U}'_{\mathrm{n}+\Delta_k}(T_{\mathbf{n}}),\ldots,\mathbf{U}^{(\mathbf{r})}_{\mathrm{n}+\Delta_1}(T_{\mathbf{n}}),\ldots,\mathbf{U}^{(\mathbf{r})}_{\mathrm{n}+\Delta_k}(T_{\mathbf{n}})\Big)=0. \tag{26}$$

In step 2, we determine the degree of the polynomial solution of the form $U_{i,\mathbf{n}}(T_{\mathbf{n}})=\sum\nolimits_{j=0}^{M_i} a_{ij}T_{\mathbf{n}}^j$. The leading exponents M_i are determined by substituting $U_{i,\mathbf{n}+\Delta_s}(T_{\mathbf{n}})=T_{\mathbf{n}+\Delta_s}^{M_i}$, defined by Eq. (25). In step 3, we form the algebraic system for the coefficients a_{ij}, by substituting:

$$U_{i,\mathbf{n}+\Delta_s}(T_{\mathbf{n}})=\sum\nolimits_{j=0}^{M_i} a_{ij}T_{\mathbf{n}+\Delta_s}^j \tag{27}$$

into Eq. (26) and using Eq. (25). In step 4, the nonlinear system of coefficients is solved. In step 5, the solitary

15 This section is inspired and adapted from [20], with some different notations. The Mathematica® package DDE Special Solutions. m has been implemented for this study, and is running Mathematica®7.

16 We are using the addition theorem [4]: $\tanh(x\pm y)=\dfrac{\tanh(x)\pm\tanh(y)}{1\pm\tanh(x)\tanh(y)}$.

wave solutions are formed and tested numerically and symbolically.

Example The following example is the scalar Toda lattice taken from [20]. The polynomial DDE is of the form[17]:

$$u_{n;xt}=(1\text{-}u_{n;t})(u_{n-1}\text{-}2u_n+u_{n+1}), \qquad (28)$$

where $u_n=u_n(x,t)$. The DDE (28) is with one discrete independent variable (n) and two continuous independent variables (x) and (t). The traveling frame of reference for this example is $\xi_n=d_1n+c_1x+c_2t+\delta$.

Repeatedly applying the chain rule (24), we obtain:

$$c_1c_2\left(1\text{-}T_n^2\right)\left(2T_nU_n'\text{-}\left(1\text{-}T_n^2\right)U_n''\right) \\ +\left(1+c_2\left(1\text{-}T_n^2\right)U_n'\right)\left(U_{n-1}\text{-}2U_n+U_{n+1}\right)=0, \qquad (29)$$

where $T_n=\tanh(\xi_n)$. The vector of shifts is $\Delta=(-1,0,+1)^T$. To determine the degree of the polynomial solution, we have to balance terms with the shifts. If we have to balance terms with shift Δ_l, we substitute into Eq. (29): $U_{i,n+\Delta_s}=\chi_iT_i^{M_i}$ for $s=l$ or $U_{i,n+\Delta_s}=\chi_i$ for $s\neq l$. Pulling off the highest degrees, we find only one term $\{M_1\}$ for shifts Δ_1 and Δ_3, but more contributing terms $\{M_1, M_1+1, M_1+2, 2M_1+1\}$ for Δ_2. Equating the two highest terms $M_1+2=2M_1+1$, we find $M_1=1$. Substituting Eq. (27) for M_1 with Eq. (25) into Eq. (29), simplifying and setting the coefficients of the power terms in T_n to zero, yields the algebraic system:

$$\left.\begin{aligned} a_{11}\text{-}c_1&=0 \\ c_1c_2\text{-}\tanh^2(d_1)\text{-}a_{11}c_2\tanh^2(d_1)&=0 \\ c_1c_2\text{-}\tanh^2(d_1)\text{-}2a_{11}c_2\tanh^2(d_1)+c_1c_2\tanh^2(d_1)&=0 \end{aligned}\right]$$

Assuming that the coefficient a_{10} is arbitrary and that a_{11}, c_1, d_1 are nonzero coefficients, we obtain $a_{11}=c_1=\dfrac{\sinh^2(d_1)}{c_2}$.

Therefore, the exact close form solution for the scalar Toda lattice is:

$$u_n(x,t)=a_{10}+\frac{\sinh^2(d_1)}{c_2}\tanh\left(d_1n+\frac{\sinh^2(d_1)}{c_2}x+c_2t+\delta\right).$$

17 The original Toda lattice equation in [20] is of the form $y_{n;xt}=e^{y_{n-1}\text{-}y_n}\text{-}e^{y_n\text{-}y_{n+1}}$. The variable $y_n(x,t)$ states for the displacement from the equilibrium of the n-th unit mass, under an exponential decaying interaction force between nearest neighbors. To obtain a polynomial DDE, we must have the changing variable $u_{n;t}=e^{y_{n-1}\text{-}y_n}\text{-}1$. The demonstration of how to obtain Eq. (28) is shown in [20].

3 Analysis and control of diffusion processes

This section introduces the analysis and control of diffusion processes for the following three aspects: the stochastic nature of the diffusion processes, the mechanisms by which differential systems are controlled and the particular reaction-diffusion equations with extensions and time delays.

Firstly, the stochastic nature of a diffusion process is often verified by considering a collection of particles moving along the real line in both directions. This motion is confirmed to obey a forward Kolmogorov differential equation, with drift and diffusion terms. The Itô stochastic differential equation (SDE) is an equivalent representation of the process. Secondly, the control of a diffusion process may be realized through different mechanisms, such as: an internal feedback for autoregulating the system or an external action by which the determination of optimal control variables is required in order to put the system at the desired position at a finite or infinite horizon. Thirdly, the reaction-diffusion (RD) equation is presented with extensions and time delays.

3.1 Diffusion process

In the following section, it is established that random moves of particles along the real line correspond to a forward Kolmogorov equation with drift and diffusion elements. Moreover, the Itô SDE affirms an equivalent representation of the phenomena.

3.1.1 Kolmogorov differential equation

A collection of particles moves randomly on the real line $\mathbb{R}$, with steps Δx every time unit τ (see [29], pp. 404–406 and [30], pp. 362–365). The time domain $[0,\infty)$ is divided into intervals of equal length Δt. The probabilities of moving to the right or to the left are, respectively, p and q so that $p+q=1$. The problem is to determine the equation that describes the change in the number of particles at position x. Let $X(t)$ be the discrete-time Markov chain (DTMC) for the random walk, where $X(t)\in\{0,\pm\Delta x,\pm2\Delta x,\ldots\}$ for $t\in\{0,\Delta t,2\Delta t,\ldots\}$. Let $\text{Prob}\{X(t)=x\}=u(x,t)$. From the analysis of the DTMCs, we obtain:

$$u(x,t+\Delta t)=pu(x\text{-}\Delta x,t)+qu(x+\Delta x,t). \qquad (30)$$

Using a Taylor series expansion for the RHS of Eq. (30) and collecting the terms yields:

$$u(x,t+\Delta t)=u(x,t)+(q-p)u_x(-\Delta x)+\frac{1}{2}u_{xx}(\Delta x)^2+\mathcal{O}\left((\Delta x)^3\right). \quad (31)$$

Subtracting $u(x,t)$ and dividing both sides of Eq. (31), we have:

$$\frac{u(x,t+\Delta t)-u(x,t)}{\Delta t}=(q-p)u_x\frac{\Delta x}{\Delta t}+\frac{1}{2}u_{xx}\frac{(\Delta x)^2}{\Delta t}+\mathcal{O}\left(\frac{(\Delta x)^3}{\Delta t}\right).$$

Assuming $\lim_{\Delta x,\Delta t\to 0}(p-q)\frac{\Delta x}{\Delta t}=c$, $\lim_{\Delta x,\Delta t\to 0}\frac{(\Delta x)^2}{\Delta t}=\mathcal{D}$, and $\lim_{\Delta x,\Delta t\to 0}\frac{(\Delta x)^3}{\Delta t}=0$, we may write the diffusion equation with drift

$$u_t=-cu_x+\frac{\mathcal{D}}{2}u_{xx},\quad x\in\mathbb{R}, \quad (32)$$

where $\mathcal{D}$ denotes the diffusion term and the drift constant c. This equation is the forward Kolmogorov differential equation. Supposing an unbiased and symmetric movement, for which we have the equiprobability $p=q=0.5$. The limiting stochastic process is $u_t=\frac{\mathcal{D}}{2}u_{xx}$, $x\in\mathbb{R}$ and represents the Brownian motion (no drift).

3.1.2 Cauchy problem for a Brownian motion

Let the Cauchy problem (see [31], pp. 312–313):

$$u_t=\mathcal{D}\,u_{xx},\ t\in(0,\infty) \quad (33)$$

for which the initial condition is $u(x,0)=u_0(x)$, $x\in\mathbb{R}$. A Fourier transform of $u(x,t)$ in x is defined by:

$$\mathcal{F}[u]\equiv\mathcal{U}(s,t)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}u(x,t)\,e^{isx}dx.$$

Applying Fourier transforms to (33) yields[18] $\mathcal{U}_t(s,t)=-\mathcal{D}s^2\mathcal{U}(s,t)$, $s\in\mathbb{R}$ for which the transformed Dirichlet initial condition is $\mathcal{U}_0(s)$. The inverse Fourier transform $\mathcal{F}^{-1}[\mathcal{U}(s,t)]$ and the convolution theorem of Fourier[19] yield the solution:

$$u(x,t)=\frac{1}{2\sqrt{\mathcal{D}\pi t}}\int_{-\infty}^{\infty}u_0(v)e^{-\frac{(x-v)^2}{4\mathcal{D}t}}dv.$$

Lets suppose that the initial density is concentrated at x_0, that is the Dirac delta function $u(x,0)=u_0\delta(x-x_0)$, the solution of the initial value problem (IVP) is a normal density function with mean x_0 and variance $\mathcal{D}t$.

3.1.3 Itô stochastic differential equation

Definition A stochastic process $\{X(t):t\in[0,\infty)\}$ satisfying an Itô SDE is such that:

$$dX(t)=a(X(t),t)dt+b(X(t),t)dW(t). \quad (34)$$

It can be shown (see [30], pp. 380–387) that an Itô solution of Eq. (34) satisfying conditions is a solution of the Kolmogorov equation with drift coefficient $a(x,t)$ and diffusion coefficient $b^2(x,t)$, that is:

$$p_t=-(a(x,t)p)_x+\frac{1}{2}\left(b^2(x,t)p\right)_{xx}.$$

The SDE corresponding to forward Kolmogorov diffusion equation, Eq. (32), is:

$$dX(t)=cdt+\sqrt{\mathcal{D}}dW(t),\quad X(0)=x_0,$$

where $p(x,t)$ is the probability density function of $X(t)$. so that:

$$X(t)\sim\mathcal{N}(x_0+ct,\mathcal{D}t).$$

3.2 Controlled diffusion process[20]

Many dynamical systems show periodic increases that require some feedback control mechanisms. The stochastic control for a system, in a noisy environment, is another approach, by which we seek to minimize a cost quadratic function subject to the dynamics of the system.

3.2.1 Feedback control

In numerous cell cultures, some enzymes show periodic increases in their activity during division. Murray [36], pp. 143–148, recalls the regulatory mechanisms. In cellular physiology, models may be capable of self-regulation and control (e.g., metabolites repressing the enzymes which are necessary for their own synthesis).

18 The Fourier transform is obtained by using the properties $\mathcal{F}[\partial u/\partial x]=-is\mathcal{U}(s,t)$ and $\mathcal{F}[\partial^2u/\partial x^2]=-s^2\mathcal{U}(s,t)$, assuming that $u(x,t)\to 0$ and $\partial u(x,t)/\partial x\to 0$ as $x\to\pm\infty$.

19 The convolution theorem of Fourier states that $\mathcal{F}^{-1}[\mathcal{A}(s)\mathcal{B}(s)]=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}A(v)B(x-v)dv$.

20 See [32] for a precise overview on controlled diffusion processes, regarding the existence of optimal controls and their characterization. Numerous studies on this domain deal with control problems of linear systems with a quadratic performance criterion [33, 34]. The control theory for PDEs is studied in [35].

One simple schematic feedback control system is illustrated in [36], p. 144, for the production of an enzyme. This representation is a generalization of the early Goodwin oscillator with damping in 1965 [37]. The effect is generally nonlinear and may activate or inhibit the reactions (see [36], pp. 122–130 on autocatalysis[21], activation and inhibition).

3.2.2 Basic enzyme reaction[22]

Enzyme reactions involving proteins (or enzymes) take place in living organisms (Figure 3). Enzymes react selectively on a compound (substrates) (e.g., hemoglobin in red blood cells is an enzyme and oxygen a substrate). The enzymes then have an important role in regulating biological processes as activators or inhibitors in a reaction. The basic enzyme reaction model was proposed by Michaelis and Menten [39] in 1913, who studied the kinetics of an enzymatic reaction mechanism. The model involves a substrate S reacting with an enzyme E to form the complex SE, which is converted into a product P and the enzyme. The enzyme reaction is represented in Figure 3.

In this model, a reversible reaction is followed by a one-way reaction, where constant parameters k_1, k_{-1}, k_2 are associated with the rates of reaction. The mechanism is such that the substrate S is converted into a product P, via the catalyst E: one molecule of S combines with one molecule of E to get SE, which may produce one molecule of P and one molecule of E. According to the law of mass action, the rate of reaction is proportional to the product of the concentrations of the reactions. Let the concentrations $[S]\equiv s$, $[E]\equiv e$, $[SE]\equiv c$ and $[P]\equiv p$. We obtain the following nonlinear system of reaction equations [38]:

$$\left.\begin{aligned} s_t' &= -k_1 es + k_{-1}c \\ e_t' &= -k_1 es + (k_{-1}+k_2)c \\ c_t' &= k_1 es - (k_{-1}+k_2)c \\ p_t' &= k_2 c \end{aligned}\right]$$

Thus, according to the first equation, the rate of change of the concentration $[S]$ consists of a loss rate proportional to $[S][E]$ and of a gain rate proportional to concentration $[SE]$. Given the initial conditions $s(0)=s_0$, $e(0)=e_0$ and $c(0)=p(0)=0$, the solutions give the concentrations and

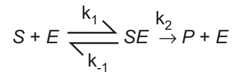

Figure 3 Basic enzyme reaction mechanism by Michaelis and Menten [39].

the rates of the reactions as functions of time (See [38], pp. 175–178).

3.2.3 Stochastic control

The state of a system $X(t)$ is described by an Itô process or linear SDE and we suppose a quadratic cost J^u depending on the states (x) and on control variables (u). The problem is to choose a control trajectory that minimizes the quadratic objective J^u subject to the dynamics of the system. According to a theorem, a set of controls is an optimal solution to the control problem, if there exist continuous differentiable functions satisfying the Hamilton-Jacobi-Bellman PDE. This technique is presented with one example in Appendix C.

3.3 Reaction-diffusion equations

RD equations are parabolic PDEs that notably express population growth with simple random diffusion. Such equations may have extensions such as with an additional advection term. This corresponds, for example, to chemical species that react locally, can diffuse in the solvent and is transported by a bulk movement of the solvent. RD equations with time delays (even constant) enhance the realism of the specifications for real life problems.

3.3.1 RD equations [40, 41]

PDEs that model population growth with a simple random diffusion are RD equations. The vector form of RD systems is:

$$\mathbf{u}_t = \mathbf{f}(\mathbf{u}) + \mathcal{D}\,\Delta\mathbf{u},$$

where $\mathbf{u}=\mathbf{u}(x,t)$ are the dependent variables, $\mathbf{f}$ the reaction functions and $\mathcal{D}$ the diffusion matrix [40].

Let $N(x,t)$ be the density of population at time $t\in[0,\infty)$ and position $x\in\Omega$. A scalar RD is[23] (see [31], pp. 309–316):

21 The autocatalysis is the process whereby a chemical is involved in its own production (e.g., a molecule of X combines with one of A to form two molecules of X).

22 This introduction to basic chemical reactions is inspired from [38], pp. 175–178.

23 An extension to the local population density $N(x,y,t)$ with spreading in a 2D uniform space is of the form $N_t=f(N)+\mathcal{D}(N_{xx}+N_{yy})$.

$$N_t=f(N)+\mathcal{D}N_{xx},$$

where $f(N)$ denotes the reaction rate and $\mathcal{D}N_{xx}$ the diffusion rate. For one-species population growth[24], we may have an exponential growth with $f(N)=rN$ (Malthusian populations), a logistic growth[25] with $f(N)=rN(1\text{-}N/K)$, the negative logistic for population decay by Skellam [43] $f(N)=\text{-}g^2N(1\text{-}N/K)$ or the asymmetric Gompertz $f(N)=rN\ln(K/N)$.

Suppose the RD equation with exponential growth (See [31], pp. 314–315):

$$N_t=rN+\mathcal{D}N_{xx},\quad x\in(L,0),$$

with the initial condition $N(x,0)=\varphi(x)$ $x\in[L,0]$ and the BCs $N(0,t)=N(L,t)=0$. The change of variable $P(x,t)=N(x,t)e^{-rt}$ leads to the following IBVP:

$$P_t=\mathcal{D}P_{xx}$$

with the conditions $P(x,0)=\varphi(x)$, $x\in[L,0]$ and $P(0,t)=P(L,t)=0$.

The solution to $N(x,t)$ is the solution to $P(x,t)$ multiplied by e^{rt}. Hence, we have:

$$N(x,t)=\sum_{n=1}^{\infty}B_n\sin\left(\frac{n\pi x}{L}\right)e^{\left\{r\text{-}\mathcal{D}\left(\frac{n\pi}{L}\right)^2\right\}t} \tag{35}$$

where

$$B_n=\frac{2}{L}\int_0^L N_0(x)\sin\frac{n\pi x}{L}dx,\quad x\in[L,0].$$

In this model, the additional growth term increases the density locally and speeds up the spatial spread in the population.

3.3.2 Extended RD equations

In [44], pp. 240–243, molecular reaction-diffusion arises in chemical domains. Let a single autocatalytic process $A+2B\rightarrow 3B$ with rate k_1ab^2. The RD equation describes how the local concentration varies in an infinitesimal volume. The reaction kinetics takes the form:

$$a_t=\mathcal{D}_A\,\Delta a\text{-}k_1ab^2.$$

The first term on the RHS denotes the net diffusive inflow of species A into the volume element.

The FitzHugh-Nagumo equation arises in population genetics and models the transmission of nerve impulses (see [15], pp. 179–181). It is of the form:

$$u_t=u_{xx}\text{-}u(1\text{-}u)(a\text{-}u).$$

There are three stationary solutions. The solutions $u=a$, $u=1$ are stable and $u=0$ is unstable if $a\in[-1,0)$. The solutions $u=0$, $u=1$ are stable and $u=a$ is unstable if $a\in(0,1)$. A stationary nonhomogeneous solution in implicit form (with arbitrary constants C_1 and C_2) is:

$$\int\frac{du}{\sqrt{\frac{1}{4}u^4\text{-}\frac{1}{3}(1+a)u^3+\frac{1}{2}au^2+C_1}}=\pm x+C_2.$$

In the reaction-diffusion-advection equation, a chemical species reacts, can diffuse in the solvent and is transported by the bulk movement of the solvent. We have:

$$u_t+\nabla(\mathbf{v}u\text{-}\mathcal{D}\nabla u)=f,$$

where $u(\mathbf{x},t)$ denotes the concentration of species, $\mathbf{x}\in\mathbb{R}^n$ the chemical species, $\mathcal{D}$ the diffusion coefficient, $\mathbf{v}\in\mathbb{R}^n$ the bulk velocity and f the reaction term.

3.3.3 Delayed RD equation [45]

The RD equation of KPP-Fisher type is a natural extension of a logistic growth model. It takes the form:

$$u_t=r\,u\left(1\text{-}\frac{u}{K}\right)+\Delta u, \tag{36}$$

with $u\equiv u(x,t)$, where $r,\mathcal{D}$ are positive parameters. A simpler normalized form is obtained by rescaling the variables [46] such as with $\bar{x}=\sqrt{\frac{r}{\mathcal{D}}}x$ and $\bar{t}=rt$. The normalized form of Eq. (36) is:

$$u_t=u(1\text{-}u)+u_{xx} \tag{37}$$

Incorporating a single discrete time delay[26] into Eq. (37), we notably obtain[27] the Hutchinson equation [51], that is:

$$u_t=u(x,t)(1\text{-}u(x,t\text{-}\tau))+u_{xx} \tag{38}$$

24 Other specifications of the population growth rate and two-species population are given in [42], pp. 310–311.

25 Biological applications for the deterministic and stochastic logistic growth are in [30], pp. 421–424.

26 Schaaf [47] first studied, in 1987, traveling wave solutions for a scalar RD equation with a discrete delay, by using the phase-plane technique. In [48] the existence and stability of delayed PDEs are studied. In [49] the existence of traveling wave solutions in delayed RD systems is demonstrated.

27 Another way to incorporate a time delay is derived from [50], that is $u_t=u(x,t\text{-}\tau)\,(1\text{-}u(x,t))+u_{xx}$.

The traveling front of Eq. (37) means a solution of the form $u(x,t)=U(\xi)$, $\xi=x+ct$. Plugging into Eq. (38), we obtain a DDE in U, that is:

$$cU'_{\xi}=U(\xi)\left(1\text{-}U(\xi\text{-}c\tau)\right)+U''_{\xi} \tag{39}$$

subject to the asymptotic BCs:

$$\lim_{\xi\to-\infty} U(\xi)=0 \text{ and } \lim_{\xi\to+\infty} U(\xi)=1.$$

Theorem (Zou [46]):

(i) For every $c\geq 2$, Eq. (39) with BCs has a monotone solution, regardless of the value of the delay $\tau>0$.

(ii) For every $c\in(0,2)$, Eq. (39) with BCs also has a monotone solution, if $\tau\geq\left(\frac{2}{c}\right)^2 \ln\frac{2}{c}$.

Proof (see [46]) Different methods may be used to solve the resulting DDEs, such as: the method of steps algorithm, the Laplace transform, the differential transform method, etc. [52, 53]. The Mathematica® implementation for DDEs only support constant positive or negative delays is using the primitive ND Solve. The example shown in Figure 4 is:

$$x''(t)+x(t\text{-}1)=0, \quad t\in(0,10]. \quad \blacksquare$$

with $x(t)=t^2$, $t\in[-1,0]$.

Delay partial differential equations (DPDEs) may better fit to the real world modeling of the population dynamics[28]. The parabolic DPDE is:

$$u_t=a(t)u_{xx}\text{-}q(t)u(x,t\text{-}\tau)$$

where τ denotes a constant positive delay.

The temporal Wazewska-Czyzeska and Lasota equation describes the survival of red blood cells in animals. This equation may be extended by incorporating a spatial component as in [56], p. VII. The spatiotemporal delay RD equation becomes:

$$p_t=dp_{xx}\text{-}\delta p(x,t)+qe^{-ap(x,t-\tau)}$$

where $\Omega\subset\mathbb{R}$ is a bounded domain and $(x,t)\in\Omega\times(0,\infty)$. The state variable $p(x,t)$ denotes the number of red blood cells located at x at time t. The constant time delay $\tau>0$ denotes the time needed to produce blood cells. The parameter δ is the death rate of red blood cells. The parameters q and a are related to the generation of red blood.

28 The dynamics and control of time delay differential systems are notably studied in [53], with applications to economics. Time lags in physical and biological models are notably in [54, 55].

```
In[1]:= sol = NDSolve[{x''[t] + x[t - 1] == 0,
         x[t /; t ≤ 0] == t^2}, x, {t, -1, 10}]
Out[1]= {{x → InterpolatingFunction[{{-1., 10.}}, <>]}}
```

Figure 4 Mathematica® implementation of DDEs with constant delays.

4 Applications of evolution equations

Migrations in population dynamics and innovation diffusion of new products can be modeled by using the same diffusion equation. Advection and diffusion are two different (PDE-based) transport mechanisms[29]. The advection equation describes the bulk movement of particles in a transporting environment (e.g., a swarm of insects in the air or pollutants in a river).

The 1D advection equation[30] takes the form:

$$a_t=\text{-}ca_x$$

It describes the advection of a scalar field $a(x,t)$ carried along by a flow of constant speed[31]. The solution is $a(x,t)=f(x\text{-}ct)$, where f is deduced from the initial condition $a(x,0)=f(x)$. The diffusion equation is a parabolic PDE[32] for describing the random motion of particles. A physical propagation problem (diffusion) is an IVP. The IVP may be a parabolic PDE of the form[33]:

$$u_t=\alpha u_{xx}, \quad x\in(0,L)$$

with the initial condition $u(x,0)=f(x)$, $f\in C^1$.

4.1 Population biology dispersal model

An RD equation such as Fisher-KPP equation[34] for population models acknowledges two main properties: firstly,

29 A convection combines these two types of transport.

30 This equation is closely related to the hyperbolic wave equation $u_{tt}=c^2u_{xx}$, where u is the displacement and c the wave speed. Such a PDE is derived from a fundamental conservation law.

31 This equation may be rewritten as $a_t/a_x=\text{-}c, a_x\neq 0$ so that the level curves $a(x,t)$ are straight lines of slope c and so that the general solution takes the form $\varphi(ct\text{-}x)$ for an arbitrary C^1 function φ.

32 Recall that a parabolic PDE is one instance, in addition to 'hyperbolic' and 'elliptic' PDEs, of a discriminant-based classification for PDEs in two independent variables. For more independent variables, the same instances proceed from an eigenvalue-based classification.

33 Additional BCs such as $u(0,t)=u(L,t)=0$, $t>0$ transform the model into an IBVP. This physical problem represents the heat conduction in a rod for which the ends are at a zero temperature while the initial temperature at any other point is given by $f(x)$ (see [12], p. 127).

34 Fisher's equation was simultaneously introduced by Fisher [57] in 1937 and Kolmogorov et al. [58] for phase transition problems in combustion, physiology, ecology, etc.

the solution is traveling through the spatial domain at a finite rate of speed, and secondly conditions on the spatial domain are determined for population persistence. These two problems are known as 'the traveling wave solutions' and 'the critical patch size'.

4.1.1 Fisher-KPP equation

The Fisher-KPP equation is the parabolic PDE[35]:

$$N_t = rN(1\text{-}N) + \mathcal{D}N_{xx}, \quad x \in \Omega \subset \mathbb{R} \tag{40}$$

where $N(x,t)$ denotes population density at spatial position x at time $t>0$ with $N(x,0)=N(x)$. The reaction term is the logistic term $rN(1\text{-}N)$ and the diffusion rate or random motion is $\mathcal{D}N_{xx}$.

4.1.2 Traveling wave solutions

Definition A traveling wave solution of (40) is a solution that can be expressed in terms of the scalar $\xi = x\text{-}vt$ where the constant v is the wave speed. We may write $N(\xi)=N(x\text{-}vt)$.

Let $N_\xi' = \text{-}P$, we obtain the system of first-order ODEs:

$$\begin{cases} N_\xi' = \text{-}P \\ P_\xi' = \text{-}\dfrac{v}{\mathcal{D}}P + \dfrac{r}{\mathcal{D}}N(1\text{-}N) \end{cases} \tag{41}$$

We also impose the following restrictions to the solution $N(\xi)$: $N(\xi) \in [0,1]$, $N(\xi) \to 1$ as $\xi \to \text{-}\infty$ and $N(\xi) \to 0$ as $\xi \to \infty$. The phase plane dynamics[36] is illustrated in Figure 5, for $r=v=\mathcal{D}=1$. The equilibrium point $E(0,0)$ is locally asymptotically stable[37].

Traveling wave solutions at this point suppose that the characteristic equation has a negative discriminant, i.e., $\delta = v^2/\mathcal{D}^2 - 4r/\mathcal{D} < 0$. The minimal wave speed for the existence of traveling wave solutions is then $2\sqrt{r\mathcal{D}}$. The other equilibrium point at [1,0] is unstable.

4.1.3 Critical patch size

What is the minimal size of the spatial domain needed for a population survival? This problem has been studied in [60] for an RD equation with exponential growth[38]. The IBVP is:

$$N_t = rN + \mathcal{D}N_{xx}, \quad x \in (0,L)$$

with the homogeneous Dirichlet BCs: $N(0,t)=N(L,t)=0$ and $N(x,0)=N_0(x)$. The conditions on the spatial domain so that the solutions (35) approaches zero is $r < \mathcal{D}\left(\dfrac{\pi}{L}\right)^2$ (see [31], pp. 319–321). The reversed inequality then defines the minimal patch size for the population to survive. Solving the equality for L yields the critical patch size $L_c = \pi\sqrt{\dfrac{\mathcal{D}}{r}}$. Thus, the population size increases if $L>L_c$ and decreases to zero if $L<L_c$.

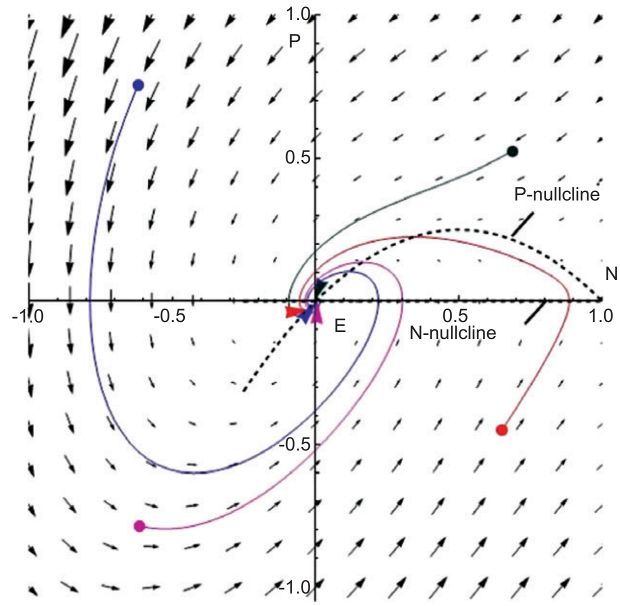

Figure 5 Phase plane dynamics of system (41) of ODEs with parameter values $r=v=\mathcal{D}=1$.

4.2 Chemical reaction and diffusion [42]

A SDE is developed for chemical reactions between molecules[39]. A fixed volume contains a uniform mixture of chemical species, interacting through chemical reactions. Two different assumptions are made for interacting reactions and for spontaneous reactions. In the first situation, the reaction rates are proportional to the rates of the participating molecules. In the latter situation, the reaction rate is proportional to the rate of the particular species.

35 The generalization of Fisher's equation in [59] is $u_t = \mathcal{D}u_{xx} + u - u^k$, for which an exact analytical solution is proposed for traveling waves.
36 For more cases and details, see Allen [31], pp. 321–324.
37 Figure 5 has been produced by using the Mathematica graphical interface 'Equation Trekker' for specifying initial conditions and plotting the resulting numerical solution to the system of ODEs.
38 The application of this study is the growth of phytoplankton (the bottom of the marine food chain). The conditions for population persistence and extinction have also been demonstrated for a diffusive logistic equation and different types of domains.
39 This model is taken from Allen [42], pp. 166–169.

The problem is: given the initial numbers of molecules of some different chemical species, what will be the molecular population levels at a finite horizon?

4.2.1 Modeling chemical reactions

Suppose there are three chemical species S_1, S_2, S_3 whose constant number of molecules and reaction rates are, respectively, $X=(X_1, X_2, X_3)^T$ and μ_1, μ_2, μ_3. Then, the three chemical species interact through molecular collisions or spontaneously in four different ways, as shown[40] in Table 1.

4.2.2 Mean change and covariance matrix

The mean is given by:

$$E[\Delta\mathbf{X}]=\sum_{i=1}^{4} p_i(\Delta\mathbf{X})_i.$$

We find

$$\begin{pmatrix} -\mu_1X_1X_2+\mu_2X_3+\mu_3(X_2)^2X_3-\mu_4(X_1)^2 \\ -\mu_1X_1X_2+\mu_2X_3-\mu_3(X_2)^2X_3+\mu_4(X_1)^2 \\ \mu_1X_1X_2-\mu_2X_3-\mu_3\dfrac{(X_2)^2}{2}X_3+\mu_4\dfrac{(X_1)^2}{2} \end{pmatrix}\equiv\mathbf{f}(X_1,X_2,X_3)\Delta t.$$

The variance-covariance matrix is given by

$$E\left[(\Delta\mathbf{X})(\Delta\mathbf{X})^T\right]=\sum_{i=1}^{4} p_i(\Delta\mathbf{X})_i(\Delta\mathbf{X})_i^T.$$

We have[41]

$$E\left[(\Delta\mathbf{X})(\Delta\mathbf{X})^T\right]=\begin{pmatrix} a+4b & a-4b & -a-2b \\ a-4b & a+4b & -a+2b \\ -a-2b & -a+2b & a+b \end{pmatrix}\equiv g(X_1,X_2,X_3)\Delta t,$$

where $a\equiv\mu_1X_1X_2+\mu_2X_3$ and $b\equiv\mu_3(X_2)^2X_3/2+\mu_4(X_1)^2/2$.

4.2.3 Stochastic differential equation

The Itô SDE is of the form:

$$d\mathbf{X}(t)=\mathbf{f}(X_1,X_2,X_3)dt+\sqrt{g(X_1,X_2,X_3)}d\mathbf{W}(t), \quad (42)$$

with $\mathbf{X}(0)=\mathbf{X}_0$ and where $\mathbf{W}(t)$ denotes a vector of three independent Wiener processes.

Chemical reaction	Possible change	Probability
$S_1+S_2\rightarrow S_3$	$(\Delta\mathbf{X})_1=(-1,-1,+1)^T$	$p_1=\mu_1X_1X_2\Delta t$
$S_3\rightarrow S_1+S_2$	$(\Delta\mathbf{X})_2=(+1,+1,-1)^T$	$p_2=\mu_2X_3\Delta t$
$2S_2+S_3\rightarrow 2S_1$	$(\Delta\mathbf{X})_3=(+2,-2,-1)^T$	$p_3=\mu_3X_3\dfrac{(X_2)^2}{2}\Delta t$
$2S_1\rightarrow 2S_2+S_3$	$(\Delta\mathbf{X})_4=(-2,+2,+1)^T$	$p_4=\mu_4\dfrac{(X_1)^2}{2}\Delta t$

Table 1 Possible molecular population changes in Δt and probabilities.

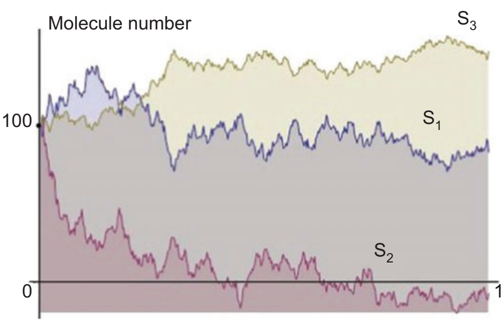

Figure 6 Molecular population numbers for one simple path.

4.2.4 Molecular population migration

The diffusion of molecular population levels for one sample path is shown in Figure 6 by solving[42] the SDE, Eq. (42), for particular values of the constant reaction rates as $\mu_1=0.02$, $\mu_2=0.4$, $\mu_3=0.001$, $\mu_4=0.03$ and initial number of molecules assumed to be $X_1(0)=X_2(0)=X_3(0)=100$.

4.3 Innovation diffusion model

Innovation diffusion models describe the process by which innovation products (or new ideas or practices) are communicated over time through certain channels and expand through a population of adopters[43]. The typical time path of the cumulative adopter distribution (e.g., for

40 In the third chemical reaction, the rate depends on a collision involving two molecules of X_2 and two molecules of X_3. Because there are $C_{X_2}^2=X_2(X_2-1)/2$ ways to select the molecule X_2, the rate of reaction depends approximately on $(X_2)^2/2$.

41 In practice, the entries v_{ij} of the variance-covariance matrix have been determined by using $v_{kl}=\sum_{i=1}^{4}p_i\delta_i(k,l), k,l=1,3$ where $\delta_i=(\Delta X)_i\otimes(\Delta X)_i$.

42 The computations are using the Fortran codes proposed by Allen [42], pp. 208–213. For this study, the Fortran code has been translated into C++ codes by using f2c (version 19980831 for lcc-win32). The output for a new program is the input data file for one Mathematica®7 notebook. A notebook produces the plots and statistics for the problem.

43 Further applications of the PDEs to economics and finance are in [61].

a mobile phone) is a sigmoidal S-shaped time curve: few adopters at the beginning (mainly professionals), then more and more adopters and finally diffusion to public at large. The market is saturated at the upper limit. Modeling the innovations has an extensive literature in marketing. Analogies are with models of epidemics.

4.3.1 Dynamics of new products [62]

A general model of new product acceptance is composed of $M(t)$ participants to the market, of $N(t)$ adopters of the new product and m the maximum of potential customers [63]. There are three distinct segments of the market: the current market $N(t)$, the potential market m-$N(t)$ and the untapped market $M(t)$-m. The typical expansion model of new adopters is:

$$\frac{dN}{dt}=g(t)(m-N(t)), \quad (43)$$

where $N(t)$ is the cumulative numbers of prior adopters, m-$N(t)$ the potential adopters and $g(t)$ the expansion coefficient or probability of adoption[44]. The marketing problem is: how many of the potential adopters will buy the new product at time t?

4.3.2 Bass logistic model

The Bass dynamics model [64] is governed by the ratio of two control parameters p and q, respectively, the innovation and the imitation rates. The evolution of the adopters may be the nonlinear ODE (43). Suppose that $g(t)$ takes the linear specification[45] $g(t)=p+q\frac{N(t)}{m}$ and define $X(t)=\frac{N(t)}{m}$, the Bass model is the logistic equation:

$$\frac{dX}{dt}=(p+qX(t))(1-X(t)). \quad (44)$$

Integrating (44) by parts, the time path is:

$$X(t)=\frac{1-e^{-(p+q)t}}{1+(q/p)e^{-(p+q)t}}$$

The maximum expansion rate is obtained for $d^2X/dt^2=0$ (at the inflexion point of the time path), where $\hat{X}=\frac{1}{2}-\frac{p}{2q}$. To find the time $\hat{t}$, when $X(\hat{t})$ is a maximum penetration rate, we solve:

$X(t)=\hat{X}$ in time t and obtain $\hat{t}=-\frac{\ln(p/q)}{p+q}$.

4.3.3 Stochastic innovation diffusion

The innovation diffusion process may be disturbed by random impacts from the environment (e.g., socioeconomic factors) as well from the system itself. Uncertainties are inherent in the marketing approach due to changing consumer tastes, technology conditions, etc. These uncertainties can be modeled by using normally distributed parameters [66] or by formulating an adapted Itô SDE[46]. The stochastic Bass' innovation model in [68] is reformulated as[47]:

$$dN=\left(p(m-N)+\frac{q}{m}(m-N)N\right)dt+c\left(\frac{p}{q}+\frac{N}{m}\right)dW$$

where W is a Wiener process and c the noise parameter. The mean value (first moment) of the solution is[48]:

$$E[N]=\frac{m\,e^{(p+q)t}}{\frac{1}{\frac{p}{q}+\frac{N_0}{m}}+\frac{q}{p+q}\left(e^{(p+q)t}-1\right)}-\frac{mp}{q}$$

4.3.4 Spatial innovation diffusion

How innovations are diffusing in different geographical spaces? The space and time dimensions in the diffusion process are integrated in [70]. The Bass model becomes the PDE:

$$N_t=(p(x)+q(x)N)(m(x)-N),$$

where $N(x,t)$ denotes the cumulative number of adopters in domain x at time t. The innovation dynamics shows a characteristic wave-like set of S-shaped curves.

Recently, spatially-dependent imitation processes are introduced into the classical imitation-innovation

44 In that case, the rate of diffusion at time t equals the expected number of adopters.

45 The dynamics of the external (innovation) and internal (imitation) effects is analyzed in [65], pp. 12–26. The generalized von Bertalanffy model is also shown to have flexible properties with regards to the symmetry and point of inflexion of the integral diffusion curves.

46 Population biology models with time delay in a noisy environment are studied in [67]. The population-dependent diffusion model in [3] incorporates a stochastic component.

47 Different notations are used in [68].

48 The model is solved by reducing the nonlinear SDE to a linear form [68] .The same method is used in [69] to solve a stochastic logistic innovation diffusion model for Greece and USA.

Bass dynamics in [71]. The resulting multi-agent imitation model generates spatio-temporal patterns. A microscopic approach is adopted by Hashemi et al [71]. In this innovation-imitation model, the imitation process depends on the spatial proximity of a multitude of interacting agents. The agents observe their neighborhood and reevaluate their decisions. The mean-field technique of the statistical Physics is used to replace the large number of micro-interactions by one efficient interaction. A system of Fokker-Planck PDEs is then obtained for probability densities.

The nonlinear field dynamics is exactly solvable. However, the solution process requires successive transformations that lead to a solvable evolution equation. These transformations are, notably: a Taylor expansion of the imitation function (for infinitesimal interacting neighborhoods), a Galileo transformation of coordinates (to get dimensionless coordinates), and a Hopf-Cole logarithmic transformation of the Boltzmann PDEs (to linearize). The resulting system is reduced to a Telegraphist equation for which a general solution can be found.

5 Conclusion

This presentation introduces the dynamics of population dispersal in biology, in chemistry and spatial diffusion of new products in marketing. The importance of RD equations has been shown with a variety of population growth specifications. Basic 1D diffusion models have been considered. The dynamics of such models have mainly been on traveling wave solutions and on critical patch size. Appendices A to C allow to develop some technical practices of the modeling process: the Mathematica® implementation for PDEs and DDEs special solutions, the tanh-function method applied to the Boussinesq system and the stochastic control technique with an example, for which the complete solution is given.

Further developments and applications may extend this introductive presentation. The models can be generalized to multi-agent models and to multiple species. The space dimension may be extended. Other specifications of the population growth may be chosen as an alternative (e.g., a predator-prey specification for multiple species, such as with the diffusional Lotka-Volterra system [40], pp. 21–23). Other domains include population biology, ecology and economics. Constant and variable time delays may be introduced more systematically.

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Appendix A. Mathematica implementation for PDE Special Solutions

Using the Wolfram Mathematica® package [72] for solving a PDE (see [15], pp. 1687–1734 and [5]), one has three possibilities: the Mathematica® function DSolve, the PDE Special Solutions.m Mathematica® and DDE Special Solutions package. A short description with demonstrations is proposed for each package.

A.1 DSolve[...] Mathematica® function

This Mathematica® primitive DSolve[...] for finding exact solutions in closed form of ODEs may also solve PDEs. DSolve can find general solutions for linear and weakly nonlinear PDEs. The primitive NDSolve[...] solves PDEs numerically. The syntax of such primitives for one unknown function with two arguments is:

DSolve [{*PDE*, *boundary conditions*}, *u*[*x*,*t*], {*x*,*t*}, *option*].

DSolve generates arbitrary functions, whereas NDSolve yields an interpolating function. The following primitives are for the hyperbolic wave equation:

$$u_{tt}-c^2u_{xx}=0.$$

In Figure 7, C_1 and C_2 are arbitrary functions. The characteristics for which the solution is constant are the two families of straight lines $x=k\pm\frac{t}{|c|}$, where k is an arbitrary constant. The following primitives consider the BIVP with Cauchy boundary conditions: $u(x,0)=e^{-x^2}$, $u_t(x,0)=0$ and $u(x_0,t)=u(x_1,t)$.

In Figure 8, the boundary Cauchy problem is solved numerically. The 3D plot and the contours for this solution are represented in Figure 1.

```
In[1]:= waveEquation = D[u[x, t], {x, 2}] == c^2 D[u[x, t], {t, 2}]
Out[1]= u(2,0) [x, t] == c² u(0,2) [x, t]

sol = DSolve[waveEquation, u[x, t], {x, t},
   GeneratedParameters → (Subscript[c, #] &)] // Simplify
Out[2]= {{u[x, t] → c1[t - √c² x] + c2[t + √c² x]}}
```

Figure 7 Mathematica® primitives for solving the wave equation.

```
• Cauchy boudary conditions:
In[5]:= f[x_] := Exp[-x^2] (* initial displacement *)
In[6]:= g[x_] := 0 (* initial velocity *)
• Solution of the BIVP for the wave equation:
NDSolve[{waveEquation /. c → 1, u[x, 0] == f[x],
  Derivative[0, 1][u][x, 0] == 0, u[-5, t] == u[5, t]}, u, {x, -5, 5}, {t, 0, 5}]
Out[8]= {{u → InterpolatingFunction[{{-5., 5.}, {0., 5.}}, <>]}}
• Plotting Figure 1:
Show[GraphicsArray[{Plot3D[Evaluate[u[x, t] /. First[%]], {t, 0, 5}, {x, -5, 5},
    PlotPoints → 150, Mesh → 30, ImageSize → 350], ContourPlot[Evaluate[u[x, t]
     /. First[%]], {t, 0, 5}, {x, -5, 5}, PlotPoints → 150, ContourShading → None,
     ContourStyle → Black, Contours → 35, ImageSize → 300]}]]
```

Figure 8 Mathematica® primitives for solving the wave equation BIVP.

A.2 ATFM.m Mathematica® package

A.2.1 Algorithm

ATFM denotes automated tanh-function method. This Mathematica® package in [73] can handle numerous nonlinear evolution equations. It automates the tanh-polynomial method, for which traveling wave solutions are found by taking $u(x,t)=U(\xi)$, where $\xi=x\text{-}ct\text{-}\delta$. The substitution into the initial PDE yields an ODE for $U(\xi)=\sum_{i=0}^{M} a_i T^i$, where $T=\tanh(k\xi)$. The positive integer M to be determined by balancing the highest order of the linear and nonlinear term(s). The a_i $(i=0,\ldots,M)$ are real constant with $a_M\neq 0$.

A.2.2 Procedure

The Mathematica® function is:

$$\text{ATFM}[eqn\_, U\_, T\_, M\_, param\_\_],$$

in which *eqn* is the ODE in U to be solved, M the degree of the tanh-polynomial, and *param* the sequence of parameters, if any.

Examples.

Two examples are the KdV equation and the Kawahara equation [25]. The ODE in T for the KdV equation is:

$$\text{kdv}=\text{-}cU_T'+UU_T'+U_T'''=0.$$

with $T=\tanh(k(x\text{-}ct\text{-}\delta))$ where c is the phase speed, k the wave number, δ the phase shift. The ODE in T for the Kawahara equation[49] is:

$$\text{kawahara}=\text{-}cU_T'+UU_T'+U_T'''\text{-}U_T^{(5)}=0.$$

The solution given by ATFM for the KdV equation is:

$$u(x,t)=c+4k^2\,(2\text{-}3\tanh^2(k(x\text{-}ct\text{-}\delta)))$$

The solution by AFTM for the Kawahara equation is:

$$u(x,t)=\frac{105}{169}\operatorname{sech}^4\left(\frac{1}{2\sqrt{3}}\left(x\text{-}\frac{36}{169}t\text{-}\delta\right)\right)$$

The ATFM listing for these two examples is in Figure 9.

A.3 PDE Special Solutions.m Mathematica® package for PDEs [74]

The Mathematica® package[50] PDE Special Solutions.m in [75, 76] computes traveling wave solutions as polynomials in either $T=\tanh\xi$, $S=\operatorname{sech}\xi$, CN=cn(ξ:m) or SN=sn(ξ:m) with $\xi=\sum_{j=0}^{N} c_j x_j+\delta$, where the coefficients of the spatial

49 This equation takes place in the theory of shallow water waves with surface tension, in the theory of magneto-acoustic waves in plasmas.
50 The package has been implemented on PC in a Mathematica®7 environment, for this study.

```
In[1]:= << Calculus`ATFM`

In[2]:= kdv = -c der[U[T], T, 1] + U[T] der[U[T], T, 1] + der[U[T], T, 3];
        ATFM[kdv, U, T, 2, c]
```

$$\{c + 4 k^2 (2 - 3 T^2),\ k,\ c\}$$

```
In[4]:= sol = %; sol[[1, 1]] /. T -> Tanh[k (x - c t + x0)] // Simplify
```

$$\text{Out[4]= } c + 4 k^2 \left(2 - 3\,\mathrm{Tanh}[k (-c t + x + x0)]^2\right)$$

```
In[5]:= kawahara = -c der[U[T], T, 1] + U[T] der[U[T], T, 1] + der[U[T], T, 3] - der[U[T], T, 5];
        ATFM[kawahara, U, T, 4, c]; s = %; sol[[1, 1]] /. T -> Tanh[k (x - c t + x0)] // Simplify;
        s2 = sol[[1, 1]] /. T -> Tanh[k (x - c t - x0)];
```

$$\left\{\frac{1}{169}(69 + 169 c - 210 T^2 + 105 T^4),\ -\frac{1}{2\sqrt{13}},\ c\right\}$$

$$\left\{\frac{1}{169}(69 + 169 c - 210 T^2 + 105 T^4),\ \frac{1}{2\sqrt{13}},\ c\right\}$$

$$\left\{\frac{33800 c + 3\left(-1798 + 546 i\sqrt{31} + \left(-8680 - 3640 i\sqrt{31}\right) T^2 + 1085\left(11 + 3 i\sqrt{31}\right) T^4\right)}{33800},\ -\frac{1}{4}\sqrt{\frac{1}{65}\left(-31 - 3 i\sqrt{31}\right)},\ c\right\}$$

$$\left\{\frac{33800 c + 3\left(-1798 + 546 i\sqrt{31} + \left(-8680 - 3640 i\sqrt{31}\right) T^2 + 1085\left(11 + 3 i\sqrt{31}\right) T^4\right)}{33800},\ \frac{1}{4}\sqrt{\frac{1}{65}\left(-31 - 3 i\sqrt{31}\right)},\ c\right\}$$

$$\left\{\frac{33800 c + 3\left(-1798 - 546 i\sqrt{31} + 280 i\left(31 i + 13\sqrt{31}\right) T^2 + 1085\left(11 - 3 i\sqrt{31}\right) T^4\right)}{33800},\ -\frac{1}{4}\sqrt{\frac{1}{65}\left(-31 + 3 i\sqrt{31}\right)},\ c\right\}$$

$$\left\{\frac{33800 c + 3\left(-1798 - 546 i\sqrt{31} + 280 i\left(31 i + 13\sqrt{31}\right) T^2 + 1085\left(11 - 3 i\sqrt{31}\right) T^4\right)}{33800},\ \frac{1}{4}\sqrt{\frac{1}{65}\left(-31 + 3 i\sqrt{31}\right)},\ c\right\}$$

```
In[7]:= sol = s2 /. {k → 1/(2 √13), c → 36/169} // Simplify
```

$$\text{Out[7]= } \frac{1}{169}\left(62 - 39\,\mathrm{Tanh}\left[\frac{-\frac{36 t}{169} + x - x0}{2\sqrt{13}}\right]^2\right)$$

Figure 9 KdV and Kawahara PDE solutions by using the ATFM Mathematica® package.

coordinates are the components of the wave vector, with a constant phase δ. This package leads to closed-form solutions of nonlinear PDEs.

The main function is:
PDESpecialSolutions[{equations},{functions},{variables},{parameters}, options]

The options are (the default options are underlined): Form→Tanh|Sech|SecTanh|JacobiCN|JacobiSN (i.e., how the solutions are expressed), Input Form→True|False (i.e., the standard Mathematica output form), Degree Of the Polynomial→{m[1]→Integer, m[2]→Integer...}, Symbolic Test→True|False (i.e., the solutions are tested truly symbolically), Numeric Test→True|False (i.e., the solutions are accepted if they pass one or more tests; the 13 tests consist of random numbers ranging from 0 to 1 for all parameters).

One example is the Boussinesq equation with real parameter α

$$u_{tt}\text{-}u_{xx}+3uu_{xx}+3(u_x)^2+\alpha u_{xxxx}=0.$$

This equation has been proposed to describe water waves in shallow water. The first steps of the tanh-method by using this Mathematica package for this example are shown in Figure 10.

The first steps of the algorithm are in Figure 10, that is: *Step 1* – transform the nonlinear PDE into a nonlinear ODE in T=tanh; *Step 2* – determine the maximum degree of the polynomial solution; *Step 3* – determine the nonlinear algebraic system for the coefficients. The next steps to get the solution in tanh are in Figure 11; *Step 4* – solution of the algebraic system; *Step 5* – expressions of the wave solution for given expressions of ξ.

We obtain the solution:

$$u(x,t)=\frac{1}{3}\left(1+8\alpha c_1^2\text{-}\frac{c_2^2}{c_1^2}\right)\text{-}4\alpha c_1^2\tanh^2\xi,$$

where $\xi=c_1x+c_2t$. For one another wave vector ($c_1=k$, $c_2=\text{-}kv$), we obtain the solution: $u(x,t)=\frac{1}{3}(1\text{-}v^2+8\alpha k^2)\text{-}4\alpha k^2\tanh^2\xi$ where $\xi=k(x\text{-}vt)$.

The 3D plot and contours are shown in Figure 12, for all the parameters taking the unit value.

A.4 DDE special solutions.m Mathematica® package for DDEs

The Mathematica package®[51] DDE Special Solutions.m in [20] computes traveling wave solutions as polynomials in T_n=tanh ξ_n, for one discrete independent variable (n) and N continuous independent variables. The traveling frame of reference is $\xi_n=d_1n+\sum_{j=0}^{N}c_jx_j+\delta$, where the coefficients

51 The package has been implemented on a PC in a Mathematica®7 environment for this study.

```
In[1]:= << Calculus`PDESpecialSolutions`
   Package PDESpecialSolutions.m was succesfully loaded.
Out[1]= •

In[2]:= PDESpecialSolutions[
     D[u[x, t], {t, 2}] - D[u[x, t], {x, 2}] + 3 * u[x, t] * D[u[x, t], {x, 2}] +
       3 * (D[u[x, t], x])^2 + α * D[u[x, t], {x, 4}] == 0, u[x, t], {x, t}, {α},
        Verbose → True, Form → Tanh, SymbolicTest → False, NumericTest → False]
   The given system of differential equations is:
   3 (u_x)^2 + u_tt - u_xx + 3 u (u_xx) + α (u_xxxx) == 0
   Transform the differential equation(s) into a nonlinear ODE in T=Tanh
   {2 T c[1]^2 u[1]'[T] + 16 T α c[1]^4 u[1]'[T] - 24 T^3 α c[1]^4 u[1]'[T] - 2 T c[2]^2 u[1]'[T] - 6 T c[1]^2 u[1][T] u[1]'[T] + 3 c[1]^2 u[1]'[T]^2 - 3 T^2 c[1]^2 u[1]'[T]^2 - c[1]^2 u[1]''[T] +
     T^2 c[1]^2 u[1]''[T] - 8 α c[1]^4 u[1]''[T] + 44 T^2 α c[1]^4 u[1]''[T] - 36 T^4 α c[1]^4 u[1]''[T] + c[2]^2 u[1]''[T] - T^2 c[2]^2 u[1]''[T] + 3 c[1]^2 u[1][T] u[1]''[T] - 3 T^2 c[1]^2 u[1][T] u[1]''[T] -
     12 T α c[1]^4 u[1]^(3)[T] + 24 T^3 α c[1]^4 u[1]^(3)[T] - 12 T^5 α c[1]^4 u[1]^(3)[T] + α c[1]^4 u[1]^(4)[T] - 3 T^2 α c[1]^4 u[1]^(4)[T] + 3 T^4 α c[1]^4 u[1]^(4)[T] - T^6 α c[1]^4 u[1]^(4)[T]}
   Time Used:0.078
   Determine the maximal degree of the polynomial solutions.
   {{m[1] → 2}}
   Time Used:0.078
   Derive the nonlinear algebraic system for the coefficients.
   Seeking polynomial solutions of the form
   {{u[1][T] → a[1, 0] + T a[1, 1] + T^2 a[1, 2]}}
   The nonlinear algebraic system is
   {{{-12 a[1, 1] c[1]^2 (3 a[1, 2] + 2 α c[1]^2) == 0, -30 a[1, 2] c[1]^2 (a[1, 2] + 4 α c[1]^2) == 0,
      2 a[1, 1] (c[1]^2 - 3 a[1, 0] c[1]^2 + 9 a[1, 2] c[1]^2 + 8 α c[1]^4 - c[2]^2) == 0, 3 a[1, 1]^2 c[1]^2 - 2 a[1, 2] c[1]^2 + 6 a[1, 0] a[1, 2] c[1]^2 - 16 α a[1, 2] c[1]^4 + 2 a[1, 2] c[2]^2 == 0,
      -3 (3 a[1, 1]^2 c[1]^2 - 2 a[1, 2] c[1]^2 + 6 a[1, 0] a[1, 2] c[1]^2 - 6 a[1, 2]^2 c[1]^2 - 40 α a[1, 2] c[1]^4 + 2 a[1, 2] c[2]^2) == 0},
     {a[1, 0], a[1, 1], a[1, 2]}, {c[1], c[2]}, {α}, {α, a[1, 2], c[1], c[2]}}}
   Time Used:0.016
```

Figure 10 Boussinesq wave equation by using Mathematica®: first steps of the tanh-method.

● **Solve the nonlinear algebraic system.**

```
In[3]:= Clear[s]; s = Solve[{
       -12 a[1, 1] c[1]^2 (3 a[1, 2] + 2 α c[1]^2) == 0, -30 a[1, 2] c[1]^2 (a[1, 2] + 4 α c[1]^2) == 0,
       2 a[1, 1] (c[1]^2 - 3 a[1, 0] c[1]^2 + 9 a[1, 2] c[1]^2 + 8 α c[1]^4 - c[2]^2) == 0,
       3 a[1, 1]^2 c[1]^2 - 2 a[1, 2] c[1]^2 + 6 a[1, 0] a[1, 2] c[1]^2 - 16 α a[1, 2] c[1]^4 + 2 a[1, 2] c[2]^2 == 0,
       -3 (3 a[1, 1]^2 c[1]^2 - 2 a[1, 2] c[1]^2 + 6 a[1, 0] a[1, 2] c[1]^2 - 6 a[1, 2]^2 c[1]^2 - 40 α a[1, 2] c[1]^4 + 2 a[1, 2] c[2]^2) == 0
      }, {a[1, 0], a[1, 1], a[1, 2]}] // Simplify
   Solve::svars : Equations may not give solutions for all "solve" variables. >>
Out[3]= {{a[1, 1] → 0, a[1, 2] → 0}, {a[1, 0] → 1/3 (1 + 8 α c[1]^2 - c[2]^2/c[1]^2), a[1, 1] → 0, a[1, 2] → -4 α c[1]^2}}
```

● **Solitary wave solution**

```
In[4]:= Clear[soliton]; soliton = a[1, 0] + T a[1, 1] + T^2 a[1, 2] /.
      {a[1, 0] → s[[2, 1, 2]], a[1, 1] → s[[2, 2, 2]], a[1, 2] → s[[2, 3, 2]], T → tanh[ξ]} // Simplify
Out[4]= 1/3 (1 + 8 α c[1]^2 - c[2]^2/c[1]^2) - 4 α c[1]^2 tanh[ξ]^2

In[5]:= soliton2 = soliton /. {c[1] → k, c[2] → -v k, ξ → k (x - v t)} // Simplify
Out[5]= 1/3 (1 - v^2 + 8 k^2 α - 12 k^2 α tanh[k (-t v + x)]^2)
```

Figure 11 Boussinesq wave equation by using Mathematica®: wave solution in tanh.

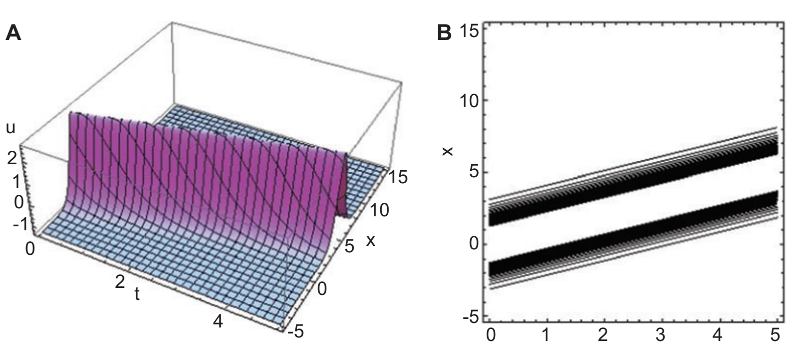
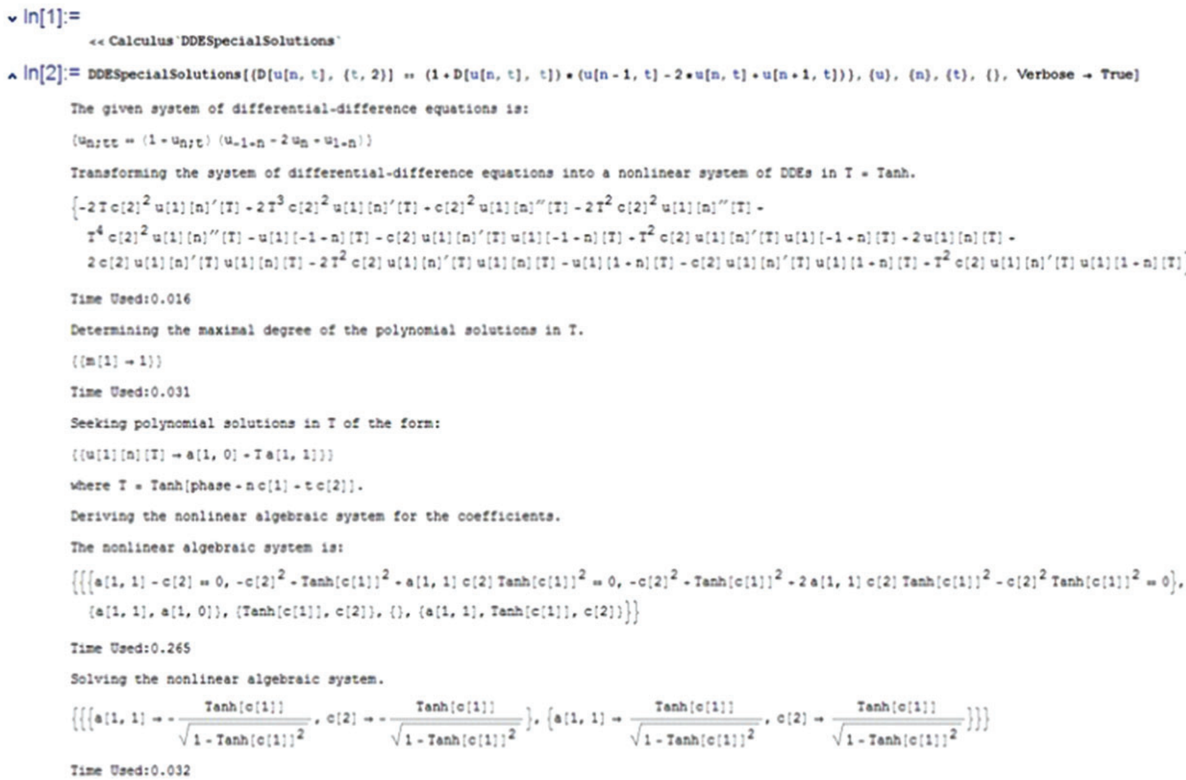


Figure 12 Boussinesq wave equation by using Mathematica®: 3D plot (A) and contours (B) for k=v=α=1.



```
In[1]:=
    << Calculus`DDESpecialSolutions`
In[2]:= DDESpecialSolutions[{D[u[n, t], {t, 2}] == (1 + D[u[n, t], t]) * (u[n - 1, t] - 2 * u[n, t] + u[n + 1, t])}, {u}, {n}, {t}, {}, Verbose → True]
  The given system of differential-difference equations is:
  {u_{n;tt} == (1 + u_{n;t}) (u_{-1+n} - 2 u_n + u_{1+n})}
  Transforming the system of differential-difference equations into a nonlinear system of DDEs in T = Tanh.
  {-2 T c[2]^2 u[1][n]'[T] + 2 T^3 c[2]^2 u[1][n]'[T] + c[2]^2 u[1][n]''[T] - 2 T^2 c[2]^2 u[1][n]''[T] +
   T^4 c[2]^2 u[1][n]''[T] - u[1][-1 + n][T] - c[2] u[1][n]'[T] u[1][-1 + n][T] + T^2 c[2] u[1][n]'[T] u[1][-1 + n][T] + 2 u[1][n][T] +
   2 c[2] u[1][n]'[T] u[1][n][T] - 2 T^2 c[2] u[1][n]'[T] u[1][n][T] - u[1][1 + n][T] - c[2] u[1][n]'[T] u[1][1 + n][T] + T^2 c[2] u[1][n]'[T] u[1][1 + n][T]}
  Time Used:0.016
  Determining the maximal degree of the polynomial solutions in T.
  {{m[1] → 1}}
  Time Used:0.031
  Seeking polynomial solutions in T of the form:
  {{u[1][n][T] → a[1, 0] + T a[1, 1]}}
  where T = Tanh[phase + n c[1] + t c[2]].
  Deriving the nonlinear algebraic system for the coefficients.
  The nonlinear algebraic system is:
  {{{a[1, 1] - c[2] == 0, -c[2]^2 + Tanh[c[1]]^2 + a[1, 1] c[2] Tanh[c[1]]^2 == 0, -c[2]^2 + Tanh[c[1]]^2 + 2 a[1, 1] c[2] Tanh[c[1]]^2 - c[2]^2 Tanh[c[1]]^2 == 0},
   {a[1, 1], a[1, 0]}, {Tanh[c[1]], c[2]}, {}, {a[1, 1], Tanh[c[1]], c[2]}}}
  Time Used:0.265
  Solving the nonlinear algebraic system.
  {{{a[1, 1] → -Tanh[c[1]]/Sqrt[1 - Tanh[c[1]]^2], c[2] → -Tanh[c[1]]/Sqrt[1 - Tanh[c[1]]^2]}, {a[1, 1] → Tanh[c[1]]/Sqrt[1 - Tanh[c[1]]^2], c[2] → Tanh[c[1]]/Sqrt[1 - Tanh[c[1]]^2]}}}
  Time Used:0.032
```

Figure 13 Single Toda lattice DDE equation by using Mathematica®: first steps of the tanh-method.

of the spatial coordinates are the components of the wave vector, with a constant phase δ. This package leads to closed-form solutions of nonlinear DDEs.

The main function is:

DDESpecialSolutions[{equations},{functions},{variables},{parameters}, options]

The options are (the default options are underlined): Verbose→True|<u>False</u>, Input Form→<u>True</u>|False (i.e., the standard Mathematica output form), Degree Of the Polynomial→{m[1]→Integer, m[2] →Integer...}, Min Degree Of The Polynomial→1, Max Degree Of The Polynomial→3, Solve Algebraic System→<u>True</u>|False (i.e., the algebraic system is generated but not automatically solved), Symbolic Test→<u>True</u>|False (i.e., the solutions are tested truly symbolically), Numeric Test→<u>True</u>|False (i.e., the solutions are accepted if they pass one or more tests; the 13 tests consist of random numbers ranging from 0 to 1 for all parameters).

Another example, taken from [20], is the scalar Toda equation with one discrete variable (n) and one continuous variable[52] (t), that is:

$$u_{n;tt}=(1+u_{n;t})\,(u_{n-1}-2u_n+u_{n+1}). \tag{45}$$

where $u_n \equiv u_n(t)$. The first steps of the tanh-method by using this Mathematica package for this example are shown in Figure 13. Applying the chain rule $\frac{\partial}{\partial x_j}=\frac{\partial \xi_n}{\partial x_j}\frac{dT_n}{d\xi_n}\frac{d}{dT_n}$ to Eq. (45), yields[53]:

$$\begin{aligned}
&-2T_n(c_2)^2U_n'+2T_n^3(c_2)^2U_n'+(c_2)^2U_n''-2T_n^2(c_2)^2U_n''\\
&\quad+T_n^4(c_2)^2U_n''-U_{n-1}-c_2U_n'U_{n-1}+T_n^2c_2U_n'U_{n-1}\\
&\quad+2U_n+2c_2U_n'U_n-2T_n^2c_2U_n'U_n-U_{n+1}\\
&\quad-c_2U_n'U_{n+1}+T_n^2c_2U_n'U_{n+1}.
\end{aligned} \tag{46}$$

The maximal degree of the polynomial solution in T_n is 1. Then, we have the polynomial solution $U_n=a_0+a_1T_n$. The nonlinear algebraic system of the coefficients is:

$$\left.\begin{aligned}
a_1-c_2&=0\\
-(c_2)^2+\tanh^2(c_1)+a_1c_2\tanh^2(c_1)&=0\\
-(c_2)^2+\tanh^2(c_1)+2a_1c_2\tanh^2(c_1)-(c_2)^2\tanh^2(c_1)&=0
\end{aligned}\right]$$

We find $a_1=c_2=\mp\dfrac{\tanh(c_1)}{\sqrt{1-\tanh^2(c_1)}}$.

52 The previous scalar Toda equation in subsection 1.3 was with two continuous variables (x,t).

53 The first five terms of Eq. (46) correspond to the transformation of $u_{n;tt}\equiv\partial^2u_n/\partial t^2$.

```
Building and (numerically and/or symbolically) testing the travelling wave solutions.
The possible non-trivial solutions (before any testing):
{{{u[n, t] → a[1, 0] - Sinh[c[1]] Tanh[phase + n c[1] - t Sinh[c[1]]]}, {u[n, t] → a[1, 0] + Sinh[c[1]] Tanh[phase + n c[1] + t Sinh[c[1]]]}}}
Numerically testing the solutions.
The following solutions will be numerically tested:
{{{u[n, t] → a[1, 0] - Sinh[c[1]] Tanh[phase + n c[1] - t Sinh[c[1]]]}, {u[n, t] → a[1, 0] + Sinh[c[1]] Tanh[phase + n c[1] + t Sinh[c[1]]]}}}
The following solutions passed the numerical test:
{{{u[n, t] → a[1, 0] - Sinh[c[1]] Tanh[phase + n c[1] - t Sinh[c[1]]]}, {u[n, t] → a[1, 0] + Sinh[c[1]] Tanh[phase + n c[1] + t Sinh[c[1]]]}}}
Symbolically testing the solutions.
WARNING: the symbolic test of solutions may be slow.
Be patient! To skip the symbolic test, set the option SymbolicTest to False.
Only the solutions that passed the numeric test will be tested symbolically.
To test all solutions, set the option NumericTest to False.
The following solutions will be tested symbolically:
{{{u[n, t] → a[1, 0] - Sinh[c[1]] Tanh[phase + n c[1] - t Sinh[c[1]]]}, {u[n, t] → a[1, 0] + Sinh[c[1]] Tanh[phase + n c[1] + t Sinh[c[1]]]}}}
The following solutions (in factored form) passed the symbolic test:
{{{u[n, t] → a[1, 0] - Sinh[c[1]] Tanh[n c[1] - t Sinh[c[1]]]}, {u[n, t] → a[1, 0] + Sinh[c[1]] Tanh[n c[1] + t Sinh[c[1]]]}}}
Time Used:0.702
The final solutions were tested both numerically and symbolically.
Out[2]= {{{u[n, t] → a[1, 0] - Sinh[c[1]] Tanh[n c[1] - t Sinh[c[1]]]},
    {u[n, t] → a[1, 0] + Sinh[c[1]] Tanh[n c[1] + t Sinh[c[1]]]}}}
```

Figure 14 Single Toda lattice DDE equation by using Mathematica®: wave solution in tanh.

Finally, the numerically and symbolically tested solutions of the scalar Toda lattice DDE equation are (Figure 14):

$$u_n(t)=a_0 \mp \sinh(c_1)\tanh\left(c_1 n \mp \sinh(c_1)t\right).$$

Appendix B. Tanh-method application to the Boussinesq system

The different steps of the tanh-method's algorithm are illustrated by the nonlinear Boussinesq system[54]:

$$\left.\begin{aligned} u_t+v_x+uu_x&=0\\ v_t+(vu)_x+u_{xxx}&=0\end{aligned}\right]$$

The Boussinesq system is solved manually and automatically by using the Mathematica® package PDE Special Solutions.m.

B.1 Solutions by hand

The different steps of the tanh-method algorithm are:

Step 1 – transform the nonlinear PDE into a nonlinear ODE in T=tanh; *Step 2* – determine the maximum degree of the polynomial solution; *Step 3* – determine the nonlinear algebraic system for the coefficients; *Step 4* – solution of the algebraic system; *Step 5* – expressions of the wave solution for given expressions of ξ.

For this example, we have:

– *Step 1*: *Use the traveling wave transformations*. Using the traveling wave transformations $u(x,t)=U(\xi)$ and $v(x,t)=V(\xi)$, $\xi=k(x\text{-}vt)$, we obtain the reduced system of ODEs:

$$\left.\begin{aligned} -kvU'_\xi+kV'_\xi+kUU'_\xi&=0\\ -kvV'_\xi+kVU'_\xi+kUV'_\xi+k^3U^{(3)}_\xi&=0\end{aligned}\right]$$

– *Step 2*: *Postulate the tanh-series and use transformations*. We expect that $U(\xi)=\sum_{i=0}^{M} a_i Y^i$ and $V(\xi)=\sum_{j=0}^{N} b_j Y^j$, where Y=tanh ξ. The use of the transformations in Eq. (9) to Eq. (11) reduces to:

$$\left.\begin{aligned} -kv\left(1\text{-}Y^2\right)U'_Y+k\left(1\text{-}Y^2\right)V'_Y+k\left(1\text{-}Y^2\right)UU'_Y&=0\\ -kv\left(1\text{-}Y^2\right)V'_Y+k\left(1\text{-}Y^2\right)VU'_Y+k\left(1\text{-}Y^2\right)UV'_Y&\\ +2k^3\left(1\text{-}Y^2\right)\left(3Y^2\text{-}1\right)U'_Y\text{-}6k^3Y\left(1\text{-}Y^2\right)U''_Y+k^3\left(1\text{-}Y^2\right)^3U^{(3)}_Y&=0\end{aligned}\right] \tag{47}$$

– *Step 3*: *Determine the maximum exponents M and N*. In the first Eq. (47), the linear term of highest order V'_Y is balanced with the highest order nonlinear term UU'_Y to get $2+(N\text{-}1)=2+M+(M\text{-}1)$ then $N=2M$. In the

54 In addition to this example, a system of coupled modified Korteweg-de Vries (KdV) nonlinear equations is taken [16].

second Eq. (47), $U_Y^{(3)}$ is balanced with UV_Y' to have $6+(M\text{-}3)=2+M+(M\text{-}1)$, then we deduce $N=2$, $M=1$. The two finite expansions are $u(x,t)=U(Y)=a_0+a_1Y$, $a_1\neq 0$ and $v(x,t)=V(Y)=b_0+b_1Y+b_2Y^2$, $b_2\neq 0$.

– *Step 4*: *Determine and solve the algebraic nonlinear system of parameters*. This system is obtained by substituting $U,U_Y',U_Y'',U_Y^{(3)}$ and V,V_Y' in Eq. (47), by expanding and collecting for Y and then equating all the coefficients of Y^i to 0. The algebraic system is:

$$\left.\begin{array}{r} -va_1+b_1+a_0a_1=0 \\ 2b_2+a_1^2=0 \\ -2k^2a_1\text{-}vb_1+a_0b_1+a_1b_0=0 \\ -2vb_2+2a_0b_2+2a_1b_1=0 \\ 8k^2a_1+vb_1\text{-}a_0b_1\text{-}a_1b_0+3a_1b_2=0 \end{array}\right]$$

Solving the system, we retain the solution $a_0=v$, $a_1=2k$, $b_0=2k^2$, $b_1=0$, $b_2=-2k^2$.

– *Step 5*: *Solution of the nonlinear Boussinesq equation in closed form*. The solution in terms of tanh is $u(x,t)=v+2k\tanh(k(x\text{-}vt))$ and $v(x,t)=2k^2\,\text{sech}^2(k(x\text{-}vt))$.

B.2 Automated solutions

The first steps of the tanh-method by using this Mathematica® package for this example are shown in Figure 15:

Step 1 – transform the nonlinear PDE into a nonlinear ODE in $T=\tanh(\xi)$; *Step 2* – determine the maximum degree of the polynomial solution; *Step 3* – determine the nonlinear algebraic system for the coefficients.

The next steps to get the solution in tanh are in Figure 16: *Step 4* – solution of the algebraic system; *Step 5* – expressions of the wave solution for given expressions of ξ. We obtain the solutions: $u(x,t)=-\frac{c_2}{c_1}\pm 2c_1\tanh\xi$, where $\xi=\delta+c_1x+c_2t$ and $v(x,t)=2c_1^2\,\text{sech}^2\,\xi$. For another wave vector ($c_1=k$, $c_2=-kv$), we obtain the solutions: $u(x,t)=v\pm 2k\tanh\xi$ and $v(x,t)=2k^2\,\text{sech}^2\,\xi$ where $\xi=k(x\text{-}vt)$ (Figure 16).

Appendix C. Stochastic control problem[55]

The technique of stochastic control was developed by Fleming [78] in 1969. Introductions to this technique with applications are notably in [79, 80].

55 This presentation is inspired and extended from [77] with different notations.

C.1 Control problem

A finite-horizon stochastic problem consists of a value function which arguments are time t, the state variables $\mathbf{x}(t)\in X\subset\mathbb{R}^m$ and controls $\mathbf{u}\in U$, subject to a vector SDE. The problem may be written:

$$\underset{u}{\text{maximize}}\;E_0\left[\int_0^T g^i(x,u,t)+q\big(x,(T)\big)\right] \tag{48}$$

subject to

$$d\mathbf{x}=f(\mathbf{x},u,t)dt+\sigma(\mathbf{x},t)d\mathbf{W}. \tag{49}$$

and

$$\mathbf{x}(0)=\mathbf{x}_0 \tag{50}$$

where E_0 is the expectation operator at time 0, $\boldsymbol{\sigma}[\mathbf{x},t]$ an $\Theta\times m$ matrix, and $\mathbf{W}(t)$ a Θ-dimensional Wiener process. Let the covariance matrix be $\Omega[x(t),t]=\sigma[x(t),t]\,\sigma[x(t),t]^T$ with its elements Ω_{hs} in raw h and column s.

C.2 Theorem

A set of controls $u^*(t)=\phi(\mathbf{x},t)$ forms an optimal solution to the control problem (48)–(50), if there exist continuous differentiable functions $V(\mathbf{x},t):\mathbb{R}^m\times[0,T]\mapsto\mathbb{R}$, satisfying the Hamilton-Jacobi-Bellman equation

$$-V_t(\boldsymbol{x},t)\text{-}\frac{1}{2}\sum_{h,s=1}^{m}\Omega_{hs}(\boldsymbol{x},t)V_{x_hx_s}(\boldsymbol{x},t)$$
$$=\underset{u}{\text{maximize}}\left\{g^i(\boldsymbol{x},u,t)+V_x(\boldsymbol{x},t)f(\boldsymbol{x},u,t)\right\},$$

and

$$V(\mathbf{x},T)=q(\mathbf{x}).$$

Proof. See [77], pp. 16–18.

C.3 Example

Let the stochastic control problem

$$\underset{u}{\text{maximize}}\,E_0\left[\int_0^T\left(\sqrt{u}\text{-}\frac{c}{\sqrt{x}}\right)e^{-rt}dt+e^{-rT}q\sqrt{x(T)}\right]$$

subject to

$$dx=\left(a\sqrt{x}\text{-}b\,x\text{-}u\right)dt+\sigma\,x\,dW,$$

and $x(0)=x_0\in X$, where a,b,c,σ are positive parameters. Using the theorem, we have the two equations

$$-V_t\text{-}\frac{1}{2}\sigma^2x^2V_{xx}=\underset{u}{\text{maximize}}\left\{\left(\sqrt{u}\text{-}\frac{c}{\sqrt{x}}u\right)e^{-rt}+V_x\left(a\sqrt{x}\text{-}b\,x\text{-}u\right)\right\}, \tag{51}$$

```
PDESpecialSolutions[{
  D[u[x, t], t] + D[v[x, t], x] + u[x, t] * D[u[x, t], x] == 0,
  D[v[x, t], t] + D[(u[x, t] * v[x, t]), x] + D[u[x, t], {x, 3}] == 0
 }, {u[x, t], v[x, t]}, {x, t}, {}, Verbose → True, SymbolicTest → True, NumericTest → False]
The given system of differential equations is:
u_t + u (u_x) + v_x == 0
v (u_x) + u_xxx + v_t + u (v_x) == 0
Transform the differential equation(s) into a nonlinear ODE in T=Tanh
{c[2] u[1]'[T] + c[1] u[1][T] u[1]'[T] + c[1] u[2]'[T], -2 c[1]^3 u[1]'[T] + 6 T^2 c[1]^3 u[1]'[T] + c[1] u[2][T] u[1]'[T] +
 c[2] u[2]'[T] + c[1] u[1][T] u[2]'[T] - 6 T c[1]^3 u[1]''[T] + 6 T^3 c[1]^3 u[1]''[T] + c[1]^3 u[1]^(3)[T] - 2 T^2 c[1]^3 u[1]^(3)[T] + T^4 c[1]^3 u[1]^(3)[T]}
Time Used:0.016
Determine the maximal degree of the polynomial solutions.
{{m[1] → 1, m[2] → 2}, {m[1] → 2, m[2] → 4}}
Time Used:0.046
Derive the nonlinear algebraic system for the coefficients.
Seeking polynomial solutions of the form
{{u[1][T] → a[1, 0] + T a[1, 1], u[2][T] → a[2, 0] + T a[2, 1] + T^2 a[2, 2]}, {u[1][T] → a[1, 0] + T a[1, 1] + T^2 a[1, 2], u[2][T] → a[2, 0] + T a[2, 1] + T^2 a[2, 2] + T^3 a[2, 3] + T^4 a[2, 4]}}
The nonlinear algebraic system is
{{{{(a[1, 1]^2 + 2 a[2, 2]) c[1] == 0, a[1, 0] a[1, 1] c[1] + a[2, 1] c[1] + a[1, 1] c[2] == 0, 3 a[1, 1] c[1] (a[2, 2] + 2 c[1]^2) == 0, 2 (a[1, 1] a[2, 1] c[1] + a[1, 0] a[2, 2] c[1] + a[2, 2] c[2]) == 0,
   a[1, 1] a[2, 0] c[1] + a[1, 0] a[2, 1] c[1] - 2 a[1, 1] c[1]^3 + a[2, 1] c[2] == 0}, {a[1, 0], a[1, 1], a[2, 0], a[2, 1], a[2, 2]}, {c[1], c[2]}, {}, {a[1, 1], a[2, 2], c[1], c[2]}},
 {{3 (a[1, 1] a[1, 2] + a[2, 3]) c[1] == 0, 2 (a[1, 2]^2 + 2 a[2, 4]) c[1] == 0, a[1, 0] a[1, 1] c[1] + a[2, 1] c[1] + a[1, 1] c[2] == 0,
   a[1, 1]^2 c[1] + 2 a[1, 0] a[1, 2] c[1] + 2 a[2, 2] c[1] + 2 a[1, 2] c[2] == 0, 5 (a[1, 2] a[2, 3] + a[1, 1] a[2, 4]) c[1] == 0, 6 a[1, 2] a[2, 4] c[1] == 0,
   a[1, 1] a[2, 0] c[1] + a[1, 0] a[2, 1] c[1] - 2 a[1, 1] c[1]^3 + a[2, 1] c[2] == 0, 2 (a[1, 2] a[2, 0] c[1] + a[1, 1] a[2, 1] c[1] + a[1, 0] a[2, 2] c[1] - 8 a[1, 2] c[1]^3 + a[2, 2] c[2]) == 0,
   3 (a[1, 2] a[2, 1] c[1] + a[1, 1] a[2, 2] c[1] + a[1, 0] a[2, 3] c[1] + 2 a[1, 1] c[1]^3 + a[2, 3] c[2]) == 0,
   4 (a[1, 2] a[2, 2] c[1] + a[1, 1] a[2, 3] c[1] + a[1, 0] a[2, 4] c[1] + 6 a[1, 2] c[1]^3 + a[2, 4] c[2]) == 0},
  {a[1, 0], a[1, 1], a[1, 2], a[2, 0], a[2, 1], a[2, 2], a[2, 3], a[2, 4]}, {c[1], c[2]}, {}, {a[1, 2], a[2, 4], c[1], c[2]}}}
Time Used:0.032
```

Figure 15 Boussinesq wave system by using Mathematica®: first steps of the tanh-method.

```
Solve the nonlinear algebraic system.
{{{a[1, 0] → -c[2]/c[1], a[1, 1] → -2 c[1], a[2, 0] → 2 c[1]^2, a[2, 1] → 0, a[2, 2] → -2 c[1]^2},
  {a[1, 0] → -c[2]/c[1], a[1, 1] → 2 c[1], a[2, 0] → 2 c[1]^2, a[2, 1] → 0, a[2, 2] → -2 c[1]^2}}, {}}
Time Used:0.015
Build and (numerically and/or symbolically) test the solutions.
The possible non-trivial solutions (before any testing) are:
{{{u[x, t] → -c[2]/c[1] - 2 c[1] Tanh[phase + x c[1] + t c[2]], v[x, t] → 2 c[1]^2 - 2 c[1]^2 Tanh[phase + x c[1] + t c[2]]^2},
  {u[x, t] → -c[2]/c[1] + 2 c[1] Tanh[phase + x c[1] + t c[2]], v[x, t] → 2 c[1]^2 - 2 c[1]^2 Tanh[phase + x c[1] + t c[2]]^2}}, {}}
Time Used:0.624

The (numerically and/or symbolically) tested final solutions:
Out[20]= {{{u[x, t] → (-c[2] + 2 c[1]^2 Tanh[phase + x c[1] + t c[2]])/c[1],
    v[x, t] → -2 c[1]^2 (-1 + Tanh[phase + x c[1] + t c[2]]) (1 + Tanh[phase + x c[1] + t c[2]])}},
  {{u[x, t] → -(c[2] + 2 c[1]^2 Tanh[phase + x c[1] + t c[2]])/c[1],
    v[x, t] → -2 c[1]^2 (-1 + Tanh[phase + x c[1] + t c[2]]) (1 + Tanh[phase + x c[1] + t c[2]])}}}
```

Figure 16 Boussinesq wave system by using Mathematica®: wave solution in tanh.

and

$$V(x,T)=e^{-rT}q\sqrt{x}. \tag{52}$$

Performing maximization in Eq. (51) and solving in the control u yields:

$$u^*=\frac{x}{4\left(c+V_x\sqrt{x}\,e^{rt}\right)^2}=\phi^*(x,t). \tag{53}$$

By substituting $\phi^*(x,t)$ into Eq. (51), we get the PDE

$$-V_t=\frac{1}{2}\sigma^2x^2V_{xx}+\frac{\sqrt{x}e^{-rt}}{2\left(c+V_x\sqrt{x}\,e^{rt}\right)}\times\left(1-\frac{c}{2\left(c+V_x\sqrt{x}\,e^{rt}\right)}\right)+V_x\left(a\sqrt{x}-bx-\frac{x}{4\left(c+V_x\sqrt{x}\,e^{rt}\right)^2}\right) \tag{54}$$

For finding a closed form, we assume a solution of the following polynomial $V(x,t)=\sum_{k=0}^{M}a_k(t)\sqrt{x^k}$ where the highest power M must be determined by balancing the

LHS and the RHS highest power of Eq. (54). We find that the polynomial solution is only valid for M=1. We then have:

$$V(x,t)=a_0+a_1\sqrt{x}.$$

Letting $a_0=B(t)e^{-rt}$ and $a_1=A(t)e^{-rt}$, we retain:

$$V(x,t)=\left(B(t)+A(t)\sqrt{x}\right)e^{-rt}. \tag{55}$$

Substituting this optimal value function into Eq. (54) and collecting terms yields the two conditions that $A(t)$ and $B(t)$ must satisfy:

$$A'=\left(r+\frac{b}{2}+\frac{1}{8}\sigma^2\right)A-\frac{1}{2\left(c+\frac{A}{2}\right)}+\frac{c}{4\left(c+\frac{A}{2}\right)^2}+\frac{A}{8\left(c+\frac{A}{2}\right)^2}$$

and

$$B'=rB-\frac{a}{2}A.$$

Substituting Eq. (55) into the boundary condition (52), we find that $A(T)=q$ and $B(T)=0$. By using (53), the optimal control for this stochastic problem is:

$$\phi^*(x,t)=\frac{x}{4\left(c+\frac{A}{2}\right)^2}.$$

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