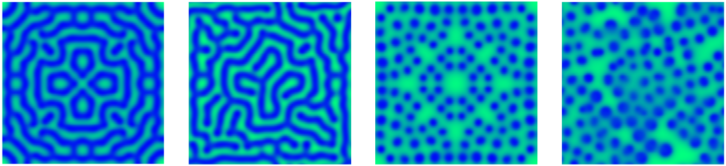
Theoretical study and numerical simulation of pattern formation in reaction-diffusion systems



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Nonlinear Stochastic Evolution Equations:
Analysis, Numerics and Applications
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Main reference

Main reference.

Erika Hausenblas, Tsiry Randrianasolo, M. Th.
Theoretical study and numerical simulation of pattern formation in the deterministic and stochastic Gray–Scott equations.
Submitted for publication (2018).

References (Deterministic evolution equations).

M. Th., Jochen Abhau
A numerical study of adaptive space and time discretisations for Gross–Pitaevskii equations.
J. Comp. Phys. 231/20 (2012) 6665–6681.

Sergio Blanes, Fernando Casas, M. Th.
Splitting and composition methods with embedded error estimators.
In preparation.

Scope

Scope (Deterministic and stochastic partial differential equations).

- Mathematical models based on reaction-diffusion systems provide fundamental tools for description and investigation of processes in biology, biochemistry, and chemistry.

  In specific situations, spatial-temporal patterns are formed.

- Gray–Scott equations constitute elementary two-component system describing autocatalytic reaction processes.

  Choice of decisive parameters determines form of complex patterns.

- Derivation of macroscopic models from physical principles neglects certain aspects of microscopic dynamics. Suitable approach that accounts for significant microscopic effects relies on incorporation of stochastic processes and consideration of SPDEs.

Objectives and questions

Objectives and questions.

- **Modelling.**

  Study stochastic Gray–Scott equations driven by independent spatially time-homogeneous Wiener processes.

  Additive versus multiplicative noise?

  Itô versus Stratonovich integral?

- **Theoretical study.**

  Deduce existence and uniqueness result.

  Appropriate regularity assumptions on prescribed initial states and Wiener processes?

- **Numerical simulation.**

  Apply high-order time-adaptive operator splitting method combined with fast Fourier transform for deterministic Gray–Scott equations.

  Suitable low-order modification for stochastic Gray–Scott equations?

Reaction-diffusion systems

Chemical reactions
Pattern formation
Deterministic models
Stochastic models

Chemical reactions

Chemical reactions. Consider elementary model for reaction of chemical substances.

- Activator U stimulates own production and production of inhibitor V.
- Inhibitor V represses production of activator U and converts to third substance.

$$\begin{cases} U + 2V \longrightarrow 3V \\ V \longrightarrow P \end{cases}$$

Reaction equations. Study system of reaction equations for associated time-dependent concentrations $u, v : [0, T] \to \mathbb{R}$ (reaction rates $\alpha_v > \alpha_u > 0$)

$$\begin{cases} u'(t) = \alpha_u - \alpha_u\, u(t) - u(t)\,\big(v(t)\big)^2\,, \\ v'(t) = -\,\alpha_v\, v(t) + u(t)\,\big(v(t)\big)^2\,. \end{cases}$$

Reaction-diffusion equations. Incorporation of additional diffusion terms leads to reaction-diffusion system, which serves as elementary model for isothermal autocatalytic reaction processes.

Gray–Scott equations

Gray–Scott equations. Gray–Scott equations constitute elementary two-component reaction-diffusion system for space-time-dependent functions $u, v : I \times [0, T] \to \mathbb{R}$ (diffusion coefficients $D_u, D_v > 0$)

$$\begin{cases} \partial_t u(x,t) = D_u \, \Delta u(x,t) + \alpha_u - \alpha_u \, u(x,t) - u(x,t) \big(v(x,t) \big)^2 , \\ \partial_t v(x,t) = D_v \, \Delta v(x,t) - \alpha_v \, v(x,t) + u(x,t) \big(v(x,t) \big)^2 . \end{cases}$$

Reference. Gray, Scott. *Chemical oscillations and instabilities* (1994).

Patterns. Numerical simulation of Gray–Scott equations in different parameter regimes reveals rich variety of spatio-temporal patterns not observed in other reaction-diffusions systems.

Reference. Pearson. *Complex patterns in a simple system* (1993).

Pattern formation – A glance at history ...

Pattern formation. In 1950s, BORIS BELOUSOV succeeded in stimulating reactions of chemical substances that led to periodic changes of their concentrations, visible as oscillations in colour. Belousov–Zhabotinsky reaction is (most) famous example of non-equilibrium thermodynamics.

> *I performed this reaction as an assignment after it was referenced in Ilya Prigogine's book "The End of Certainty" as an example of a chemical reaction that gained new properties when far from equilibrium. I used various recipes from Wolfgang Jahnke and Arthur T. Winfree's 1991 paper in the Journal of Chemical Education, "Recipes for Belousov–Zhabotinsky Reagents." The later half of the video is a time-lapse of a 34 min. reaction, showing it in about 3 min.*
>
> See https://www.youtube.com/watch?v=IBa4kgXI4Cg (time 0:50)

Turing patterns. ALAN TURING suggested that main mechanisms of morphogenesis are captured by mathematical models for systems of chemical substances, which react together and diffuse through tissue. In TURING (1952), he studies reaction-diffusion systems and explains development of patterns.

Reaction-diffusion systems. Brusselator corresponds to system of reaction-diffusion equations and serves as elementary model for nonlinear chemical oscillators

$$\begin{cases} \partial_t u(x,t) = D_u \, \Delta u(x,t) + f_u\big(u(x,t), v(x,t)\big)\,, \\ \partial_t v(x,t) = D_v \, \Delta v(x,t) + f_v\big(u(x,t), v(x,t)\big)\,, \end{cases}$$

see PRIGOGINE, LEFEVER (1968).

Our deterministic model

Deterministic models

Deterministic models. Consider systems of coupled reaction-diffusion equations for space-time-dependent functions $u, v : I \times [0,T] \subset \mathbb{R}^d \times \mathbb{R} \to \mathbb{R}$

$$\begin{cases} \partial_t u(x,t) = D_u \Delta u(x,t) + f_u\big(u(x,t), v(x,t)\big), \\ \partial_t v(x,t) = D_v \Delta v(x,t) + f_v\big(u(x,t), v(x,t)\big). \end{cases}$$

For suitable choices of constants $D_u, D_v > 0$ (diffusion coefficients) and nonlinear functions $f_u, f_v : \mathbb{R}^2 \to \mathbb{R}$ (reactions), observe formation of spatio-temporal patterns.

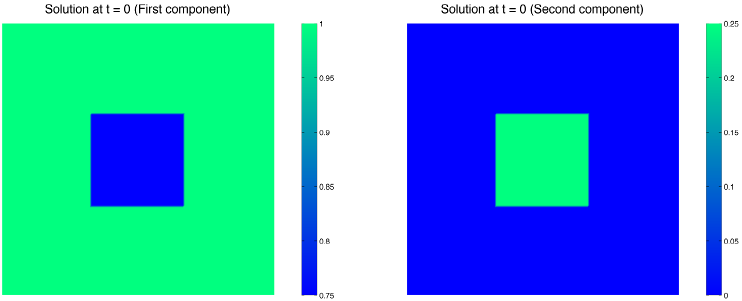
Gray–Scott equations. Focus on study of Gray–Scott equations involving cubic reaction terms ($\alpha_v > \alpha_u > 0$)

$$f_u(u,v) = \alpha_u (1-u) - g(u,v), \quad f_v(u,v) = -\alpha_v v + g(u,v),$$
$$g(u,v) = u v^2.$$

Illustration. Choice of decisive parameters determine shape of patterns (stripes, spots)

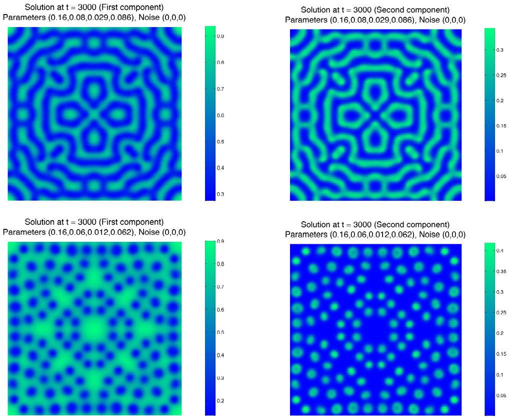
$$D_u = 0.16, \quad D_v = 0.08, \quad \alpha_u = 0.029, \quad \alpha_v = 0.086,$$
$$D_u = 0.16, \quad D_v = 0.06, \quad \alpha_u = 0.012, \quad \alpha_v = 0.062.$$

Illustration (Initial states)



Prescribed initial states for deterministic Gray–Scott equations.

Illustration (Patterns in Gray–Scott equations)



Deterministic Gray–Scott equations with different choices of parameters $(D_u, D_v, \alpha_u, \alpha_v)$.
Components of numerical solution at certain time. Movies available at

http://techmath.uibk.ac.at/mecht/MyHomepage/Research/StochasticGrayScottEquations/MovieMyCase1.mov
http://techmath.uibk.ac.at/mecht/MyHomepage/Research/StochasticGrayScottEquations/MovieMyCase2.mov

Evolution equation

Evolution equation. Introduce convenient abbreviations

$$A_u = D_u \Delta - \alpha_u I, \quad A_v = D_v \Delta - \alpha_v I, \quad g(u,v) = u\, v^2 .$$

Rewrite Gray–Scott equations as system of evolution equations

$$\begin{cases} u'(t) = A_u\, u(t) + \alpha_u - g\big(u(t), v(t)\big), \\ v'(t) = A_v\, v(t) + g\big(u(t), v(t)\big). \end{cases}$$

Remark. With regard to specification and analysis of time-adaptive high-order operator splitting methods, employ compact reformulation

$$U'(t) = F\big(U(t)\big) = A_U\, U(t) + G\big(U(t)\big),$$

$$U(t) = \begin{pmatrix} u(t) \\ v(t) \end{pmatrix}, \quad A_U = \begin{pmatrix} A_u & 0 \\ 0 & A_v \end{pmatrix}, \quad G\big(U(t)\big) = \begin{pmatrix} \alpha_u - g\big(u(t), v(t)\big) \\ g\big(u(t), v(t)\big) \end{pmatrix}.$$

Our stochastic model

Stochastic Gray–Scott equations

Stochastic Gray–Scott equations. Focus on study of initial value problem for stochastic Gray–Scott equations driven by independent spatially time-homogeneous Wiener processes (multiplicative noise, Itô integral)

$$\begin{cases} \mathrm{d}u(t) = \Big(A_u\, u(t) + \alpha_u - g\big(u(t), v(t)\big)\Big)\,\mathrm{d}t + \sigma_u\, u(t)\,\mathrm{d}W_u(t)\,, \\ \mathrm{d}v(t) = \Big(A_v\, v(t) + g\big(u(t), v(t)\big)\Big)\,\mathrm{d}t + \sigma_v\, v(t)\,\mathrm{d}W_v(t)\,, \\ u(0) = u_0\,, \quad v(0) = v_0\,, \quad t \in (0, T)\,. \end{cases}$$

Remark. With regard to specification of Lie–Trotter splitting method, consider compact reformulation

$$\begin{cases} \mathrm{d}U(t) = \Big(A_U\, U(t) + G\big(U(t)\big)\Big)\,\mathrm{d}t + \Sigma\big(U(t)\big)\,\mathrm{d}W_U(t)\,, \quad t \in (0, T)\,, \\ U(0) = U_0\,. \end{cases}$$

Theoretical study

Analytical framework
Main result
Sketch of proof

Objective

Objective. Provide theoretical study of stochastic Gray–Scott equations that is, under suitable regularity requirements on independent spatially time-homogeneous Wiener processes (W_u, W_v) and certain regularity as well as positivity assumptions on initial states (u_0, v_0), prove existence, uniqueness, regularity as well as positivity of solution processes (u, v).

Analytical framework

Space domains

Space domains. With regard to modelling of pattern formation, natural to study simple geometries and to impose homogeneous Neumann or periodic boundary conditions. Use that focus on space domains of form

$$I = [-a_1, a_1] \times \cdots \times [-a_d, a_d] \subset \mathbb{R}^d, \quad d \in \{1, 2, 3\},$$

permits explicit characterisations and calculations.

- Representation of space-dependent functions by Fourier series.
- Eigenvalue decomposition associated with Laplace operator (diffusion terms, fractional Gaussian fields).

Numerical simulation. Numerical simulation based on operator splitting methods benefits from straightforward implementation of components.

Wiener processes – Approach

Approach. Study class of Wiener processes with values in space of tempered distributions (on unbounded space domain)

$$\mathscr{W} : \Omega \times [0,T] \longrightarrow \mathscr{S}'\big(\mathbb{R}^d, \mathbb{R}\big).$$

Employ construction that permits interpretation as Wiener processes with values in certain Hilbert spaces

$$W : \Omega \times [0,T] \longrightarrow \mathscr{H}.$$

Reference. Peszat, Zabczyk. *Stochastic evolution equations with a spatially homogeneous Wiener process* (1997).

Specification. Focus on fractional Gaussian fields, use characterisation by fractional Laplacian as well as fractional Sobolev spaces, and restrict Euclidean space to cartesian product of bounded intervals

$$W : \Omega \times [0,T] \longrightarrow H^{\gamma}(I,\mathbb{R}), \quad I = [-a_1,a_1] \times \cdots \times [-a_d,a_d] \subset \mathbb{R}^d.$$

Wiener processes – Specifications

Specifications. Focus on fractional Gaussian fields with covariance operators related to inner product of fractional Sobolev spaces and hence to fractional Laplace operators (exponent $\gamma \geq 0$, weights $\alpha, D > 0$)

$$\mathcal{Q} : \mathscr{S}\big(\mathbb{R}^d, \mathbb{R}\big) \times \mathscr{S}\big(\mathbb{R}^d, \mathbb{R}\big) \longrightarrow \mathbb{R},$$
$$\mathcal{Q}(\phi_1, \phi_2) = \big(\phi_1 | \phi_2\big)_{H^{-\gamma}(\mathbb{R}^d, \mathbb{R})} = \big((\alpha - D\,\Delta)^{-\gamma}\,\phi_1 | \phi_2\big)_{L_2(\mathbb{R}^d, \mathbb{R})},$$
$$\phi_1, \phi_2 \in \mathscr{S}\big(\mathbb{R}^d, \mathbb{R}\big) \subset H^{-\gamma}(\mathbb{R}^d, \mathbb{R}).$$

Use that completion of space of Schwartz functions with respect to norm defined by covariance operator coincides with fractional Sobolev space

$$\sqrt{\mathcal{Q}(\phi, \phi)} = \|\phi\|_{H^{-\gamma}(\mathbb{R}^d, \mathbb{R})} = \|(\alpha - D\,\Delta)^{-\frac{\gamma}{2}}\,\phi\|_{L_2(\mathbb{R}^d, \mathbb{R})},$$
$$\mathscr{S}_{\mathcal{Q}} = H^{-\gamma}\big(\mathbb{R}^d, \mathbb{R}\big),$$

and that fundamental space employed in construction of Wiener processes with values in Hilbert spaces given by dual space

$$W : \Omega \times [0, T] \longrightarrow \mathscr{H} = \mathscr{S}_{\mathcal{Q}}' = H^{\gamma}\big(\mathbb{R}^d, \mathbb{R}\big).$$

Wiener processes – Explicit representations

Explicit representations. Use that focus on bounded space domains of simple structure

$$I = [-a_1, a_1] \times \cdots \times [-a_d, a_d] \subset \mathbb{R}^d\,, \quad d \in \{1,2,3\}\,,$$

permits explicit representations.

- Complex-valued Fourier functions form complete orthonormal system in Lebesgue space $L_2(I,\mathbb{R})$ and satisfy eigenvalue relation

$$d = 1\,, \quad I = [-a,a]\,, \quad \psi_m^{(\mathbb{C})} : I \longrightarrow \mathbb{C} : x \longrightarrow \frac{1}{\sqrt{2a}}\, \mathrm{e}^{\mathrm{i}\pi \frac{m}{a} (x+a)}\,,$$

$$\partial_{xx} \psi_m^{(\mathbb{C})} = \lambda_m \psi_m^{(\mathbb{C})}\,, \quad \lambda_m = -\frac{\pi^2}{a^2}\, m^2\,, \quad m \in \mathbb{Z}\,.$$

- Scaled real-valued Fourier functions yield complete orthonormal systems of underlying fractional Sobolev spaces

$$H^\gamma(I,\mathbb{R}) = \overline{{}_{\mathbb{R}}\left\langle \psi_m^{(\mathbb{R},\gamma)}, m \in \mathbb{N}^d \right\rangle},$$

$$d = 1\,, \quad \psi_m^{(\mathbb{R},\gamma)} = (\alpha - D\,\lambda_m)^{-\frac{\gamma}{2}}\, \psi_m^{(\mathbb{R})}\,, \quad m \in \mathbb{Z}\,.$$

Main result

Regularity requirements

Regularity requirements.

- Presence of cubic nonlinearity in Gray–Scott equations explains desired Sobolev regularity of solution processes and imposed regularity requirement on initial states

$$(u_0, v_0) \in W_4^1(I, \mathbb{R}) .$$

- Elementary integral criterium for infinite series explains regularity requirement on Wiener processes

$$S(\gamma) = \sum_{m \in \mathbb{Z}^d} (\alpha - D\,\lambda_m)^{-\gamma} < \infty \quad \text{if} \quad \gamma > \tfrac{d}{2} .$$

Space-dependent constraint on exponent ensures for instance that embedding defines Hilbert–Schmidt operator

$$\begin{aligned} \|I\|^2_{L_{\mathrm{HS}}(H^\gamma(I,\mathbb{R}), L_2(I,\mathbb{R}))} &= \sum_{m \in \mathbb{Z}^d} \left\| \psi_m^{(\mathbb{R},\gamma)} \right\|^2_{L_2(I,\mathbb{R})} \\ &= \sum_{m \in \mathbb{Z}^d} \left\| (\alpha - D\,\Delta)^{-\frac{\gamma}{2}}\, \psi_m^{(\mathbb{R},\gamma)} \right\|^2_{H^\gamma(I,\mathbb{R})} = S(\gamma) < \infty . \end{aligned}$$

Main result

Main result (in essence). Assume that the prescribed initial states are positive and satisfy the regularity requirement

$$u_0, v_0 \in W_4^1(I,\mathbb{R}), \quad u_0, v_0 \geq 0.$$

Suppose further that the stochastic processes defining the Gray–Scott equations are cylindrical Wiener processes on a Hilbert space that is continuously embedded in the fractional Sobolev space

$$H^\gamma(I,\mathbb{R}), \quad \gamma > \tfrac{d}{2}.$$

Then, there exists a uniquely determined pair of positive solution processes to the stochastic Gray–Scott equations (a.s.)

$$u(t), v(t) \in W_4^1(I,\mathbb{R}), \quad u(t), v(t) \geq 0, \quad t \in [0,T].$$

Proof. Consequent use of standard means.

Numerical simulation

Operator splitting methods for deterministic equations
Suitable modification for stochastic equations

Analysis and numerics go hand in hand

Analysis and numerics go hand in hand.

- Theoretical analysis of stochastic Gray–Scott equations suggests use of Fourier spectral method in numerical simulation.
  - Space discretisation based on suitable approximation in underlying Sobolev space (truncation of infinite sum, quadrature approximation by trapezoidal rule)

$$f = \sum_{m \in \mathcal{M}} f_m \mathscr{F}_m \,.$$

  - Realisation of fractional Gaussian fields by generation of normally distributed numbers and application of inverse Laplacian (eigenvalue decomposition)

$$(I - \Delta)^{-\gamma} f = \sum_{m \in \mathbb{Z}^d} f_m \, (1 - \lambda_m)^{-\gamma} \mathscr{F}_m \,.$$

Considerations before implementation

Our considerations before we started with the implementation.

- Reliable and efficient implementation of deterministic Gray–Scott equations desirable as basis for stochastic case.
- Implementation of Fourier spectral method based on fast Fourier transform (FFT) in general outperforms other approaches.

  Numerical comparison of FFT versus FEM space discretisations for nonlinear Schrödinger equations in semi-classical regime, see THALHAMMER, ABHAU (2012).
- Special form of components suggests use of Fourier spectral method and realisation by FFT.

  Geometry (space domain given by cartesian product of intervals).

  Boundary condition (periodic or homogeneous Neumann bc).

  Diffusions term (space-time independent coefficients).

  Stochastic noise (fractional Gaussian fields).

Choice of compatible time discretisation?

Considerations before implementation

Our considerations before we started with the implementation.

- Time discretisation by operator splitting methods complements space discretisation based on Fourier spectral method (FFT).

  Various works on deterministic nonlinear Schrödinger equations confirm reliable and efficient behaviour of time-adaptive high-order splitting methods combined with spectral space discretisations, see THALHAMMER (2012), THALHAMMER, ABHAU (2012).

  Superior performance of Fourier spectral method even though constrained to uniform meshes compared to locally adaptive finite element method. Spectral convergence rate and efficiency of FFT predominates.

  Similar conclusions expected to hold for deterministic reaction-diffusion equations with pattern formation (high resolution in space and time required).

Deterministic versus stochastic case

Deterministic versus stochastic case.

- Common approach

  Operator splitting in combination with FFT

  Fine uniform space grid to ensure high resolution (inital choice)

- Deterministic case (regularity of problem data)

  Enhance reliability and efficiency

  Apply high-order splitting methods

  Employ local error control in time

- Stochastic case (low regularity of problem data)

  Reduce computational effort and enhance reliability

  Apply first-order splitting method

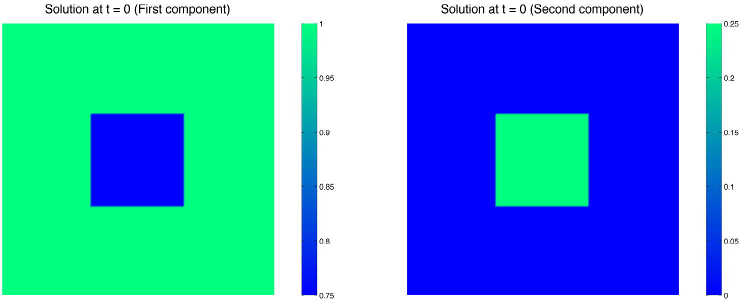
  Prevent failure due to large realisations of Wiener processes by incoporating possibility to decrease time stepsize accordingly.

Illustrations

Objective

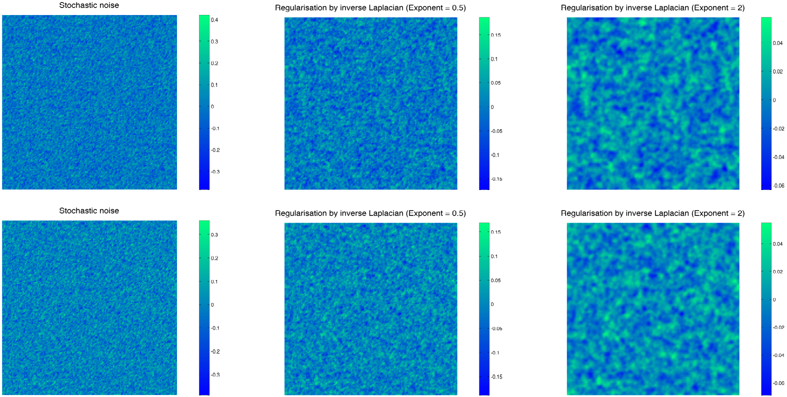
Objective. Illustrate formation of patterns in deterministic case and variation under influence of stochastic noise.

Initial states



Prescribed initial states for deterministic and stochastic Gray–Scott equations.

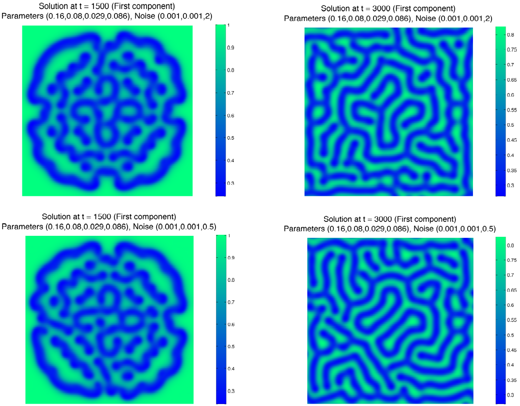
Stochastic noise



Two realisations of stochastic noise and regularisations by powers of inverse Laplacian

$$(1-\Delta)^{-\gamma}, \qquad \gamma \in \left\{\tfrac{1}{2}, 2\right\}.$$

Stochastic Gray–Scott equations (First case)



Stochastic Gray–Scott equations with first choice of $(D_u, D_v, \alpha_u, \alpha_v)$ and different choices of $(\sigma_u, \sigma_v, \gamma)$. First component of numerical solution at different times. Movies available at

http://techmath.uibk.ac.at/mecht/MyHomepage/Research/StochasticGrayScottEquations/MovieMyCase11.mov
http://techmath.uibk.ac.at/mecht/MyHomepage/Research/StochasticGrayScottEquations/MovieMyCase111.mov

Conclusions and future work

Summary.

- Existence, uniqueness, and regularity result for stochastic Gray–Scott equations.
- Efficient and reliable time integration of deterministic and stochastic Gray–Scott equations by adaptive operator splitting methods and Fast Fourier techniques.

Relevant open questions.

- Investigation of long-term dynamics.
- Study of more involved models.
- Numerical analysis.

Thank you!