PARABOLIC PDES AND THEIR NUMERICAL APPROXIMATION ON LARGE DOMAINS IN THE PRESENCE OF NOISE
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1 Background

Partial differential equations of parabolic type arise frequently in modelling fluid and continuum mechanics as well as in mathematical biology. Their description as infinite-dimensional dynamical system has been a very active field of research in recent years. This approach has improved the theoretical understanding of these models and provided many useful tools for computational and experimental purposes. The purpose of the grant was to examine the long-time behaviour of parabolic partial differential equations (PDEs) and their numerical approximation both with and without stochastic forcing. We considered these equations posed on large or unbounded domains Ω. Taking a large (or unbounded) domain is equivalent to looking at the small (or zero) viscosity limit. From a modelling view it may be though of looking at the case where there are no boundary effects.

Recently these has been much activity in studying models that include stochastic terms. A number of authors have considered noise which is smooth in space and white noise in time, for example [1, 19, 16] consider the 2D Navier-Stokes equation and obtain regularity results with smooth forcing and [2] considers Gevrey regularity of attractors for stochastic reaction-diffusion equations. There has been less work on the numerical analysis of the approximation of these stochastic PDEs (SPDEs).

As specific examples we took a parabolic PDE with a Ginzburg–Landau type nonlinearity and the Kuramoto–Sivashinsky (KS) equation. The complex Ginzburg–Landau (CGL) equation arises in a number of different areas in mathematical physics: it describes phase transitions in superconductivity and the evolution of the amplitude of perturbations to steady states at the onset of instability in a number of areas in fluid dynamics. The KS equation arises as another amplitude modulation equation, however this is fourth order in space.

We examined the long time behaviour of these systems and considered the global attractor $\mathcal{A}(\Omega)$. In particular we were interested in measuring the complexity of $\mathcal{A}(\Omega)$ as a set in a function space. One possible measure of this is the (box counting) dimension d (see [21]). However, it has been shown that d scales with the domain size [8] and estimation of this number requires a large number of high-precision computations. A seemingly more accessible quantity, called the ε–entropy has been described in [5, 4, 6, 3]. Drawing on ideas from information theory [10], the (Kolmogorov) ε–entropy is defined as

$$H_\varepsilon = \lim_{\ell\to\infty} \frac{\log \mathcal{N}(\varepsilon,\ell)}{2\ell} , \tag{1.1}$$

where $\mathcal{N}(\varepsilon,\ell)$ is the minimum number of balls of radius ε in the topology of $L^\infty([-\ell,\ell])$ that are needed to cover the attractor $\mathcal{A} = \mathcal{A}(\infty)$. The idea of ε–entropy is to describe the local complexity (in space) by introducing a localised metric on $\mathcal{A}(\Omega)$. It also only requires computing the solutions of Eq.(2.1) to a low accuracy (the parameter ε). Moreover, the resulting number is (asymptotically) independent of the size of the domain Ω.

In [5], Collet and Eckmann consider the CGL equation posed on an infinite domain ($L = \infty$). They show that the limit Eq.(1.1) exists and is bounded from above and below by $\mathcal{O}(\log(1/\varepsilon))$. This suggests that

$$d_{\text{up}} = \limsup_{\varepsilon \to 0} \frac{H_\varepsilon}{\log(1/\varepsilon)} \tag{1.2}$$

should be positive and finite. The number d_{up} can be interpreted as a spatial density of dimension (see[5, 4]). To obtain these results the Gevrey regularity of the solutions is exploited.

For the deterministic case work on this grant represents the first work investigating ε–entropy for a numerical scheme, obtaining upper and lower bounds [14]. We have also made the first attempts at estimating this quantity numerically for PDEs [12].

For the stochastically forced case the work in [18] has the first result of existence of an invariant measure on an unbounded domain, this is for the non-trivial dynamics of the complex Ginzburg–Landau equation. This work also introduces and obtains bounds on the entropy and dimensions for the stochastically forced case. In [13] strong approximations of SPDEs is considered and it is shown that solutions of a new scheme are in a discrete Gevrey space. This is exploited to improve a strong error estimate.

Dr J. Rougemont (now at Luminy Marseille) was employed on the grant.

Related to the stochastics area on this grant Lord, Lythe and Shardlow have obtained EPSRC funding for a workshop *SDEs and SPDEs : Numerical methods and applications* GR/R91106/01.

2 Key Advances and Supporting Methodology

2.1 Deterministic case

In [14] we consider semi-discrete and fully discrete approximations of nonlinear parabolic equations of the form

$$\partial_t u = \nu \Delta u + \gamma u + F(u) , \qquad x \in [-L\pi, L\pi]^d , \qquad t \geq 0 , \tag{2.1}$$

for a complex valued function $u = u(x,t)$ and bounded continuous initial condition $u(x,0) = u_0(x)$. We define (see (1.1),(1.2)) the spatial density of ε-entropy, topological entropy and dimension for the attractors and show that these quantities are bounded. Since we are interested in the large volume limit L^∞ is the natural topology to work in. There are a number of technical issues to consider. In the definitions of our norms we need to weight the norms appropriately to be able to obtain bounds that are independent of the domain size. Our approach is different to the approach of [17] in that we never explicitly work in Fourier space. We note also that the norms used in [17] grow with the domain size (due to the embedding constant), a problem we avoid here by using a suitable cutoff.

Key to obtaining bounds is a classical sampling formula (see [7] or [10] where it is called the Cartwright formula) which relies on the solutions to the PDEs being in a Gevrey class of regularity. Gevrey regularity for solutions of numerical schemes has only been considered by a few authors [15, 20]. Here we modified the approach of [20] and examined semi-discrete and fully discrete approximations of (2.1). In terms of the Fourier coefficients the fully discrete scheme is given by

$$u_m^N((n+1)h) = e^{h\lambda_m} u_m^N(nh) + \left(\int_0^h e^{(h-s)\lambda_m} \, ds \right) \mathrm{P}^N \mathcal{T} F\big(\mathcal{T}^{-1} u^N(nh)\big)_m \tag{2.2}$$

where λ_m are the eigenvalues of the linear operator, $\mathcal{T}$ is the Fourier transform and P^N is a projection like operator onto a finite number of modes (not a true projection to get bounds independent of the domain in the limit). We were then able to prove novel results on the Gevrey regularity of solutions for the scheme and upper and lower bounds for the dimension of the attractor valid in the limit as the domain size tends to infinity.

In [12] we report on numerical experiments with the ε-entropy for the complex Ginzburg–Landau equation and the Kuramoto–Sivashinsky equation. These are non-trivial computations as a rough order of magnitude calculation shows that using

$$\mathcal{N}(\varepsilon,\ell)\;\approx\;e^{C\ell\log(1/\varepsilon)}\;,$$

assuming $C=1$, $\ell=20$, and $\varepsilon=1/2$, gives an estimate of $\mathcal{N}\approx 10^7$, that is approximately 10^7 balls of radius $1/2$. There were a number of issues to consider. Firstly we needed to compute a good sample of the global attractor for both the CGL and KS equation, for which we found that computing many different trajectories gave better results, then to increase the sample size we exploited the spatial periodicity. Secondly we needed to compute a cover in an efficient manner, for this we essentially implemented the box assisted sorting algorithm of [9]. These numerical results for the deterministic equation illustrate the practical limitation due to memory size in the estimation of the ε-entropy. The results indicate that resolving ε–entropy is at the limit of computational power at present.

Main publications on deterministic case:
[14] G. J. LORD AND J. ROUGEMONT, *Topological and ε-entropy for large volume limits of discretised parabolic equations*, SIAM J. Num. Anal., (2002).

[12] ——, *Numerical computation of the ε–entropy for parabolic equations*, In Preperation, Department of Mathematics, Heriot-Watt, 2002.

2.2 Stochastic Forcing

We considered the stochastic PDEs of the following type

$$\partial_t u(t)\;=\;\Delta u(t)+F\big(u(t)\big)+\mathcal{Q}\dot{W}(t)\;. \tag{2.3}$$

The corresponding integral equation is given by

$$u(t)\;=\;e^{t\Delta}u(0)+\int_0^t e^{(t-s)\Delta}F\big(u(s)\big)\underset{\cdot}{s}+\int_0^t e^{(t-s)\Delta}\mathcal{Q}\underset{\cdot}{\mathrm{W}}(s)\;, \tag{2.4}$$

where the stochastic integral is taken in Itô's sense.

The paper [18] considers a randomly forced Ginzburg-Landau equation on an unbounded domain. The forcing is smooth and homogeneous in space and white noise in time. Dr Rougemont proved existence and smoothness of solutions, existence of an invariant measure for the corresponding Markov process and defined the spatial densities of topological entropy, of measure-theoretic entropy, and of upper box-counting dimension and proved inequalities relating these different quantities. The proof of existence of an invariant measure uses the compact embedding of some space of uniformly smooth functions into the space of locally square-integrable functions and a priori bounds on the semi-flow in these spaces. The bounds on the entropy follow from spatially localised estimates on the rate of divergence of nearby orbits and on the smoothing effect of the evolution.

In [13] we considered strong approximations to parabolic stochastic PDEs of the form (2.3). We proposed a scheme closely related to the scheme [20] which is more accurate and less stiff than traditional algorithms. For that we exploited the assumption that the noise lies in a Gevrey space of analytic functions. We show that our numerical scheme has solutions in a discrete equivalent of this space. As far as we are aware this is the only Gevrey regularity result for the numerical approximation of a SPDE. Finally in the paper we present numerical results for a SPDE with a Ginzburg-Landau nonlinearity and compare to the standard implicit Euler-Maruyama scheme.

Key publications on stochastic case:
[18] J. ROUGEMONT, *Space-time invariant measures, entropy, and dimension for stochastic Ginzburg-Landau equations*, Commun. Math. Phys., (2002).

[13] G. J. LORD AND J. ROUGEMONT,*A numerical scheme for stochastic pdes with Gevrey regularity*, tech. rep., Department of Mathematics, Heriot-Watt, 2002. Submitted.

3 Project Plan Review

We only made minor changes to the original plan. On the suggestion of one of the referees of the original grant proposal we considered general systems of PDEs rather than develop the analysis directly for Ginzburg–Landau nonlinearity.

The numerical results we obtained in [12] indicated that the ε-entropy is on the limit of being estimated for deterministic systems. Given this we decided to examine convergence and regularity of numerical solutions of SPDEs with smooth forcing, in particular as the Gevrey regularity was key to proving results on the deterministic case.

Since the first part of project [14] was technically challenging there was no time to investigate aspects of the Lyapunov spectrum or invariant measures for the numerical schemes as originally proposed.

4 Research Impact and Benefits to Society

This work has been presented to audiences from a mix of scientific backgrounds (see Dissemination activities). There have been expressions of interest in the work from co-workers and others concerned with the modeling of physical phenomena, in particular using spatially smooth noise. From industry L. Wright from NPL has expressed an interest in our results and how these might be used in some modelling.

Some of the basic stochastic differential equations material has been used in teaching at Heriot-Watt with graduate students from BAE systems.

5 Explanation of Expenditure

A laptop and desktop machine were purchased with the equipment money. The laptop has been used to present numerical results at meetings. We were particularly keen to obtain a machine with large memory to perform the computations on ε-entropy.

Dr Lord attended an EPSRC sponsored workshop at the University of Bristol on "Numerical Methods for Nonlinear Dynamics and Bifurcations" and presented as part of this software to compute solutions of stochastic PDEs with forcing Gevrey smooth in space and white noise in time.

6 Further Research or Dissemination Activities

Further dissemination will take place at future meetings such as the EPSRC supported workshop on *SDEs and SPDEs : Numerical methods and applications* GR/R91106/01 for which Dr Lord is PI, with G. Lythe and T. Shardlow as co-investigators.

Further research is planned in this area, in particular in the modelling of neural behaviour and it is proposed to investigate the effect of Gevrey noise on traveling waves and spiral waves in the Baer-Rinzel [11] and the FitzHugh-Nagumo models respectively. Discussion is also in progress to look at a model of cubic autocatalysis on an infinite strip.

Both Dr Rougemont and Dr Lord have been invited to speak on the work carried out under the grant at a number of institutions.

Dr Jacques Rougemont: has spoken at the University of Geneva, University of Durham

Dr Gabriel Lord: has spoken at Edinburgh University, University of Leeds, University of Bath and the CWI (Centrum voor Wiskunde en Informatica). He has presented work at the Dundee Numerical analysis conference and Numerical Methods for Nonlinear Dynamics & Bifurcations at the University of Bristol (July 02).

In addition, Dr G Lord has been invited to present at
- Nonlinear Stochastic Systems and Their Numerics : Oberwolfach (July 02)
- Workshop on Stochastic Computations: Foundations of Computational Mathematics at the IMA Minnesota (Aug 02)

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