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LDRD PROJECT TITLE: Numerical Continuation Methods for Intrusive Uncertainty Quantification Studies

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Abstract
Rigorous modeling of engineering systems relies on efficient propagation of uncertainty from input parameters to model outputs. In recent years, there has been substantial development of probabilistic polynomial chaos (PC) Uncertainty Quantification (UQ) methods, enabling studies in expensive computa- tional models. One approach, termed "intrusive", involving reformulation of the governing equations, has been found to have superior computational performance compared to non-intrusive sampling-based methods in relevant large-scale problems, particularly in the context of emerging architectures. However, the utility of intrusive methods has been severely limited due to detrimental numerical instabilities associated with strong nonlinear physics. Previous methods for stabilizing these constructions tend to add unacceptably high computational costs, particularly in problems with many uncertain parameters. In order to address these challenges, we propose to adapt and improve numerical continuation methods for the robust time integration of intrusive PC system dynamics. We propose adaptive methods, starting with a small uncertainty for which the model has stable behavior and gradually moving to larger uncertainty where the instabilities are rampant, in a manner that provides a suitable solution.

1 Introduction

Typically, UQ methods can be separated in two categories, intrusive and non-intrusive. While non-intrusive PC methods leave computational models unchanged, they are unfeasible for large dimen- sional inputs due to the large number of required samples. Intrusive PC approaches rely on re- formulating the model equations and their main advantage is that the new model needs to be solved only once, thus providing the PC expansion on outputs of interest.

The intrusive approach relies on Galerkin projection of the governing equations to arrive at a new set of equations for the PC modes [8, 6]. The intrusive formulation requires re-writing computational codes and introducing new numerical solution approaches. Time integration algorithms need par- ticular attention since these intrusive systems can become unstable in problems of practical interest.

Reagan *et al* [15] examined the development of non-negligible values for the probability of negative state variables in an ODE model for chemical ignition, and the impact on the stability of the numerical model. Stability and accuracy concerns with long time horizons, were remediated by the use of multi- element local PC methods [11, 10, 16, 12]. However, the resulting constructions require spatial refinement everywhere in the stochastic space [12, 13], rather than only in the vicinity of non-linear solutions. As a result, this is an ineffective resolution of the problem except in very low-dimensional contexts. The approach proposed for this project is not limited by dimensionality and can be, in principle, applied to global intrusive Galerkin PC in ODE systems.

2 Problem Description

We propose a new approach to stabilize of the Galerkin ODE system. For proof-of concept we will use a two-equation ODE system corresponding to a simple chemical model that exhibits explosively growing modes in an ignition configuration [4]

$$\begin{aligned} \frac{\mathrm{d}x}{\mathrm{d}t} = -x\,(1+y)\,, \qquad & \frac{\mathrm{d}y}{\mathrm{d}t} = \frac{1}{\epsilon}\,(x-\gamma y+\beta xy) \\ x_{t=0} = x^0, \qquad & y_{t=0} = y^0. \end{aligned} \tag{1}$$

Here, variables x, y are the non-dimensional concentration for two chemical species, with initial values x^0 and y^0, and β, γ, and ϵ are model parameters. We represent the uncertain solution as PC expansions [8]

$$\begin{aligned} x(t,\boldsymbol{\xi}) &= \sum_i x_i(t)\Psi_i(\boldsymbol{\xi}) \\ y(t,\boldsymbol{\xi}) &= \sum_i y_i(t)\Psi_i(\boldsymbol{\xi}). \end{aligned} \tag{2}$$

Substituting for x, y in Eqs. (1), and applying Galerkin projection, we get, for $k = 0, \ldots, P$,

$$\dot{x}_k = -x_k - \sum_i \sum_j x_i y_j C_{ijk} \tag{3}$$

$$\dot{y}_k = \frac{1}{\epsilon}\left(x_k - \gamma y_k + \sum_i \sum_j x_i y_j \beta C_{ijk}\right), \tag{4}$$

where C_{ijk} are deterministic coefficients that can be computed off-line:

$$C_{ijk} \equiv \frac{\langle \Psi_i \Psi_j \Psi_k \rangle}{\langle \Psi_k^2 \rangle}$$

Additionally, if model parameters are uncertain, their functional form can be represented through PCEs under certain conditions. For the tests presented in this resport we consider parameter β to be uncertain, represented as a PC expansion as

$$\beta(\boldsymbol{\xi}) = \sum_i \beta_i \Psi_i(\boldsymbol{\xi}). \tag{5}$$

This PCE can be subsituted in Eq. (1) along with the expansions in Eq. (2) leading to a Galerkin system with a larger number of nested sums

$$\dot{y}_k = \frac{1}{\epsilon}\left(x_k - \gamma y_k + \sum_i \sum_j \sum_l x_i y_j \beta_l C_{ijlk}\right), \tag{6}$$

The expressions for the PC modes of x remain the same as in Eq. (3), and C_{ijlk} are deterministic coefficients that can be computed off-line:

$$C_{ij\ell k} \equiv \frac{\langle \Psi_i \Psi_j \Psi_\ell \Psi_k \rangle}{\langle \Psi_k^2 \rangle}.$$

For large initial uncertainties in the species concentrations and model parameters, the intrusive system exhibits unstable behavior. Standard time integration techniques fail to converge as the system develops non-negligible probabilities for unphysical states. In order to prevent this behavior we propose to develop time integration algorithms enhanced with techniques adapted from the numerical continuation community [1, 9].

Specifically we propose to start with stable solutions over the entire time range, and then use arclength continuation techniques [5] to provide the initial guess for the solution in the regime where non-linear effects are dominant. In the next section we will discuss an approach to augment the intrusive ODE approach with a constrain for the solution at long time horizon. This constrain can potentially prevent the solution to diverge while in the unstable regime.

2.1 Numerical Approach

Let $\mathbf{u} = \{x_0, x_1, \ldots, x_{P-1}, y_0, y_1, \ldots, y_{P-1}\}$. We compute a solution corresponding to initial condition u^0 for the Galerkin system (3) and (6).

$$\dot{\mathbf{u}}(s) = T\mathbf{g}(\mathbf{u}(s)),\ t \to s = \frac{t}{T} \tag{7}$$

where $\mathbf{g}$ is the vector constructed with the right hand sides (rhs) corresponding to each PCE mode in Eqs. (3) and (6). The time coordinate is normalized by the time horizon, T over which Eq. (7) is integrated.

The initial value problem (IVP) is discretized using a first-order backward differentiation formula (BDF) [2]

$$\mathbf{u}_i - \mathbf{u}_{i-1} = \Delta t_i\, T\, g(\mathbf{u}_i) \tag{8}$$

Here $u_i = \{x_{0,i}, x_{1,i}, \ldots, x_{P-1,i}, y_{0,i}, y_{1,i}, \ldots, y_{P-1,i}\}$ is the solution at s_i. This system can be integrated step by step starting from the IC $u = u^0$. We rewrite Eq. (8) as

$$f(\mathbf{u}_i) = \mathbf{u}_i - \mathbf{u}_{i-1} - \Delta t_i\, T\, g(\mathbf{u}_i) = 0 \tag{9}$$

and solve for $\mathbf{u}_i$ via Newton iteration

$$\mathbf{u}_i^m = \mathbf{u}_i^{m-1} - J_{m-1}^{-1} f(\mathbf{u}_i^{m-1}) \tag{10}$$

where $J_i = \partial f(\mathbf{u}_i)/\partial \mathbf{u}_i$ is a square Jacobian matrix with $(2P)^2$ elements. Typically, 5-10 iterations are necessary to drive the norm of the residual $||J_{m-1}^{-1} f(\mathbf{u}_i^{m-1})||$ down to machine precision.

We continue the derivation by constructing a system of equations simulaneously for all time locations s_i. Let $\tilde{u} = \{\mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_N\}$ be the vector holding all PC modes at all times, $s_1 = \Delta t_1$, $s_2 = s_1 + \Delta t_2$, $\ldots$, $s_N = s_{N-1} + \Delta t_N = 1$. The system of equations can be then written as

$$F(\tilde{u}) = 0, \tag{11}$$

where $F_i = f(\mathbf{u}_i)$ is the sub-vector of equation corresponding to thr PC modes at s_i. The Jacobian matrix $\partial F/\partial \tilde{u}$ is block-diagonal, with each block containing Jacobian matrices J_i. It also contains sub-diagonal blocks corresponding to $\partial f(\mathbf{u}_i)/\partial \mathbf{u}_{i-1}$.

Finally, we augment the system of equations 11 with a constrain at $t = T$.

$$||\mathbf{u}_N|| - \delta = 0 \tag{12}$$

where δ is a small number. This constrain is based on the property of the ODE system employed in this work that $x, y \to 0$ as $T \to \infty$. This constrain is used to replace the set of equations $f(\mathbf{u}_N) = 0$ in Eq. (11). Further, the solution at $s_N = 1$ is constructed as

$$\mathbf{u}_N = \mathbf{u}_{N-1} + \Delta t_N\, T\, g(\mathbf{u}_{N-1}) \tag{13}$$

The new system (11)-(12) is now a boundary value problem (BVP) with unknowns $\mathbf{u}$ and T.

3 Results and Discussion

In this section we present results for the numerical continuation studies applied to several model problems. First, we will tackle the Bratu problem [3], which is a classical problem exhibiting bifurcations and for which the solution is well-known. We continue the numerical experiments with the deterministic ODE system, followed by the intrusive ODE system constructed by Galerkin projection.

3.1 Bratu Problem

The classical Bratu problem [3] is a elliptic partial differential equation which comes from a simplification of the solid fuel ignition model in thermal combustion theory [7]. In a 1D configuration, the equation is written as:

$$\frac{\partial^2 u}{\partial x^2} + c\exp(u) = 0, \quad u(0) = u(1) = 0 \tag{14}$$

Discretization We assume an equally spaced grid for $x = 0 \ldots 1$, with grid space Δ. A centered finite discretization of Eq. (14) is given by

$$\frac{u_{i-1} - 2u_i + u_{i+1}}{\Delta^2} + c\exp(u_i) = 0, \quad i = 2, 3, \ldots, n-1 \tag{15}$$

with $\Delta = 1/(n-1)$ and $u_1 = u_n = 0$. In matrix form:

$$Au + c\exp(u) = 0 \tag{16}$$

where A is a tri-diagonal matrix with $A_{i,i-1} = A_{i,i+1} = \Delta^{-2}$, and $A_{i,i} = -2\Delta^{-2}$. The exponential term is a short notation for $c\exp(u) = \{c\exp(u_1), \ldots, c\exp(u_n)\}^T$.

Newton method Eq. (16) is cast as $F(u) = 0$ with $F_i(u)$ being given by the left hand side (lhs) of Eq. (15). The Newton solution approach is written as

$$u^{(k+1)} = u^{(k)} - J(u^{(k)})^{-1} F(u^{(k)}) \tag{17}$$

The Jacobian matrix is tridiagonal, and its entries are the same as for the matrix A described above.

3.1.1 Arclength Continuation

Eq. (14) has a solution only for $c \leq 3.514$. For $c < 3.514$ there are two solutions for each c, one stable and one unstable. For $c \approx 3.514$ the Bratu problem has only one solution.

In order to determine all solutions, we start from the stable branch and, then gradually moving in the parameter space toward the unstable branch, using a pseudo-arclength continuation approach. In this framework, the system of equations (16) is augmented with a constraint, i.e.

$$Au_j + c_j \exp(u_j) = 0 \tag{18}$$

$$||u_j - u_{j-1}|| - \Delta s = 0 \tag{19}$$

Here, subscript j identifies the solution to the Bratu problem corresponding to c_j. In the finite difference discretization $u_{j,i}$ refers to the u_j value at grid point i.

In this new formulation, both c_j and the corresponding solution u_j are unknowns and to be determined based on the additional constraint that distance between solutions to Bratu problem for successive constant values should be equal to an imposed threshold Δs.

For the tests described here, the infinity norm was used for Eq. (19). For solutions to Bratu problem, this is equivalent to

$$|u_{j,n/2} - u_{j-1,n/2}| = \Delta s$$

To simplify the derivations for the Jacobian matrix of the extended non-linear system, we use the square of the above constraint:

$$\left(u_{j,n/2} - u_{j-1,n/2}\right)^2 = \Delta s^2$$

The Jacobian matrix corresponding to Eqs. (18)-(19) is a $(n+1)\times(n+1)$ square matrix, where n is the number of grid points discretizing the 1D $[0,1]$ range for the Bratu problem solutions.

$$\begin{aligned} &J_{i,i-1} = J_{i,i+1} = \Delta^{-2},\ J_{i,i} = -2\Delta^{-2},\ J_{i,n+1} = \exp(u_{j,i}), \quad i = 1,2,\ldots,n \\ &J_{n+1,i} = 2(u_{j,i} - u_{j-1,i}), \quad i = 1,2,\ldots,n \end{aligned} \tag{20}$$

Algorithm 1 describes the numerical continuation methodology for the Bratu problem. In this pseudo-code, the Jacobian is constructed according to Eq. (20) and $F(c_j^{k-1}, u_j^{k-1})$ is given by the lhs of Eqs. (18)-(19). For $j = 2$, the initial conditions are set as $c_2^1 = c_1 + 10^{-3}$, $u_2^1 = u_1$.

Algorithm 1: Numerical continuation algorithm for Bratu problem.

Input: c_1, Δs

Output: History of solutions for several c values

Solve Eq. (14) for u_1 **foreach** $j = 2, \ldots, N_{sol}$ **do**

  Set initial condition: $c_j^1 = 2c_{j-1} - c_{j-2}$, and $u_j^1 = 2u_{j-1} - u_{j-2}$

  Iterate $\{c_j^k, u_j^k\}^T = \{c_j^{k-1}, u_j^{k-1}\}^T - J^{-1}F(c_j^{k-1}, u_j^{k-1})$ until convergence

end

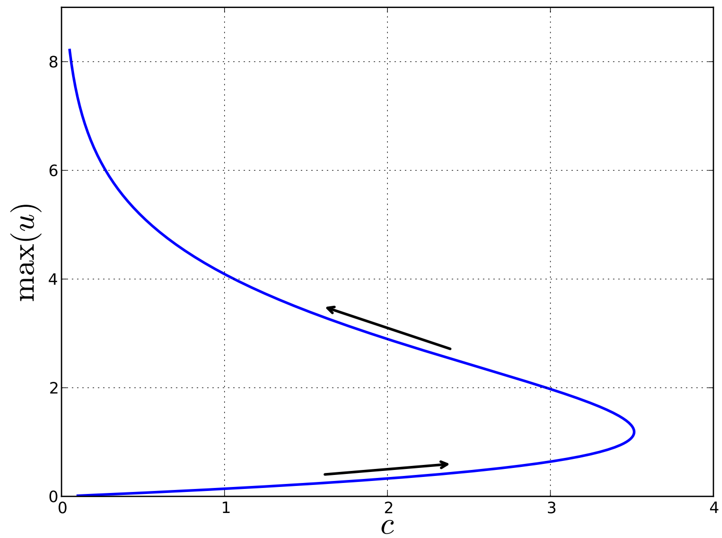

Figure 1: Lower and upper branch for solutions to Bratu problem for a range of feasible c values. The arrows indicate the progression of the numerical continuation approach.

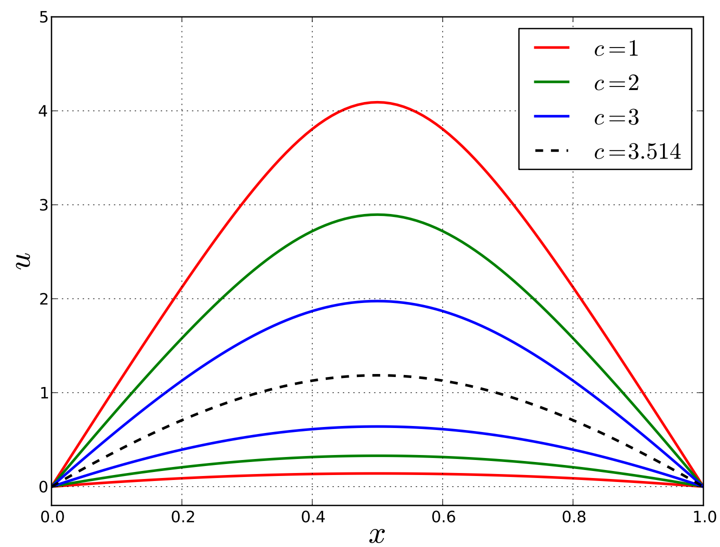

Figure 2: Solutions to Bratu problem for several c values. The dashed profile correspond to the turning point, $c \approx 3.514$. Solution below this profile corresponds to the lower, stable branch, while profiles larger than the dashed profile correspond to the upper, unstable branch.

3.2 Numerical Continuation for a Two-Equation ODE

We first start to apply a numerical continuation approach for the two-species model by tackling the deterministic ODE system in Eq. (1), augmented with the constrain in Eq. (12). For the deterministic model, this constrain is written as

$$\sqrt{x_N^2 + y_N^2} - \delta = 0 \tag{21}$$

For this series of tests, we start with the IVP solution corresponding to $u^0 = \{x^0, 0\}$, with $x^0 = 1$. We then gradually increase the magnitude of x^0, while simulaneously imposing the constrain above. For this series of tests, $\delta = 10^{-19}$, $\beta = 1$, and $\epsilon = 0.01$.

Figures 3 and 4 show the (x, y) phase plots for family of solutions corresponding to increasing values of x^0, from 1 to 6. It is interesting to note that the time horizon T, shown in Fig. 5 adjusts itself with changing boundary conditions for x.

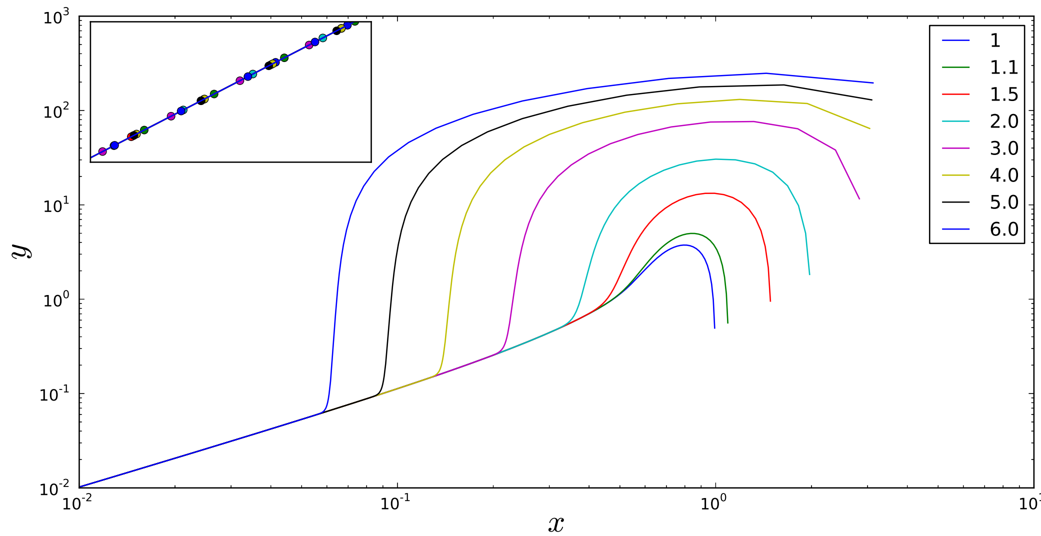

Figure 3: Phase plot for the solution of Eqs. (1) and (21). The inset frame is a detail of the lower left corner and extends 2×10^{-4} in both x and y.

3.3 Numerical Continuation for the ODE corresponding to the PC modes

Next we proceed to explore the solution for the intrusive formulation of the ODE system. For this set of tests we employ the same setting for the model parameters as in [14]. Specifically, we employ a log-normal distribution for β, $\log \beta \sim N(-0.02, 0.2^2)$, leading to a mean and standard deviation, $\mu_\beta = 1$ and $\sigma_\beta = 0.202$, respectively.

We start with the solution for the IVP corresponding to $\log x^0 \sim N(-0.02, 0.2^2)$. For this IVP we set the time horizon to $T = 12$. The results in Figs. 6 and 7 show the phase

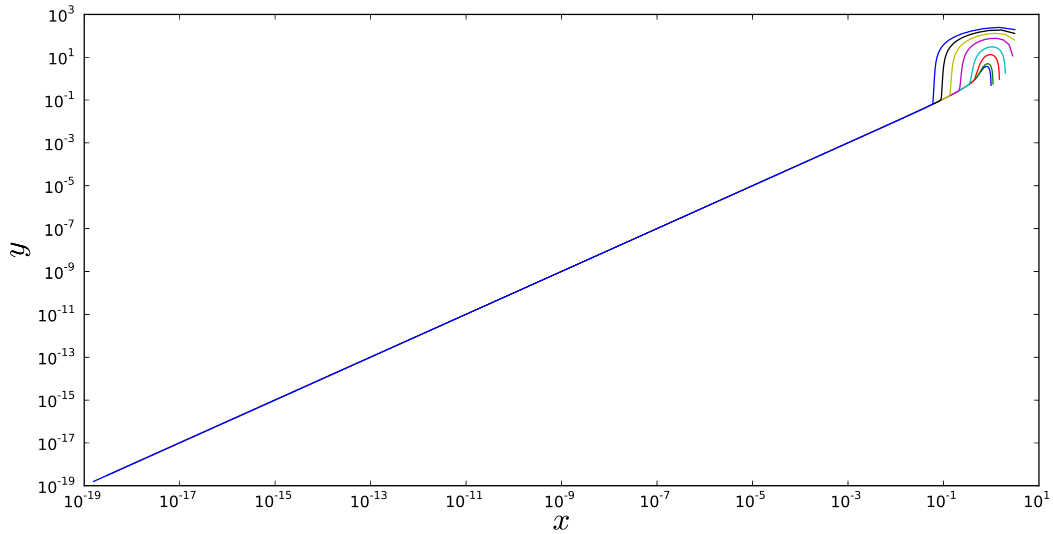

Figure 4: Same as Fig. 3, now showing the entire solution.

plot for the mean values of x and y and the time evolution of the first few modes in the 4-th order PCEs of both x and y. We then employed the IVP solution at $T = 12$ to compute the threshold value δ for the constrain in Eq. (12).

The IVP solution above together with the threshold value δ are then used to start the numerical continuation approach for the uncertain ODE system. We find that, in its current form, the system converges slowly, requiring a very large damping factor. While the damping Newton update keeps the solution from going out-of-bounds, the convergence properties of the system degrade significantly to the point the solution is now longer conrging.

4 Summary

In this report we investigate numerical algorithms aimed at providing robust solutions to initial value problem ODEs that are unstable for certain model parameters. For this study we employed a 2-equation ODE system that models an ignition process. We outline a numerical continuation approach augmented with a solution constrain at long time horizons, designed to prevent the solution from 'blowing-up'. We proceeded to test the numerical continuation algorithm on a model elliptic problem, followed by the determinsitic version of the ODE system. While these tests were successful, applying the same approach to the uncertain ODE system proved to be more difficult. Currently, the implicit approach requires significant damping, resulting in very poor convergence properties for the numerical continuation approach. Future work will tackle this problem to identify the algorithmic advances necessary to overcome the poor convergence properties.

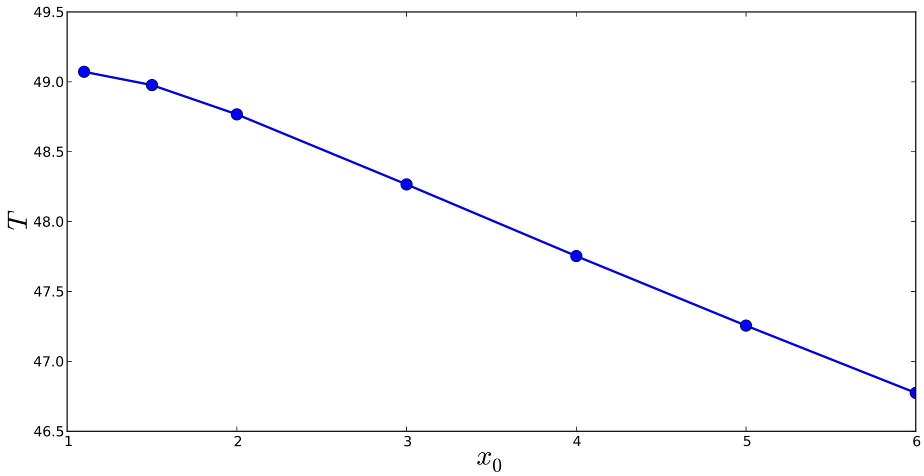

Figure 5: Final time T at which the ODE solution reaches $||\mathbf{u}_N|| = \delta$.

5 Anticipated Impact

This work represents a preliminary study on numerical methodologies for intrusive approaches for uncertain ODE systems. We explored avenues aimed to make the solution approaches robust to unstable regimes. Current results, while promising, suggest that more algorithmic work is necessary to improve the convergence properties and remove some of the limitations we currently encounter. With follow-up funding we plan to further investigate the algorithms proposed in this report.

The successful development of new algorithms will enable pervasive intrusive UQ in a number of computationally expensive applications at Sandia. Comprehensive studies for NW and ASC programs such as maneuverability during reentry and structural mechanics under thermal insult are not feasible with current algorithms due to high-dimensional input spaces.

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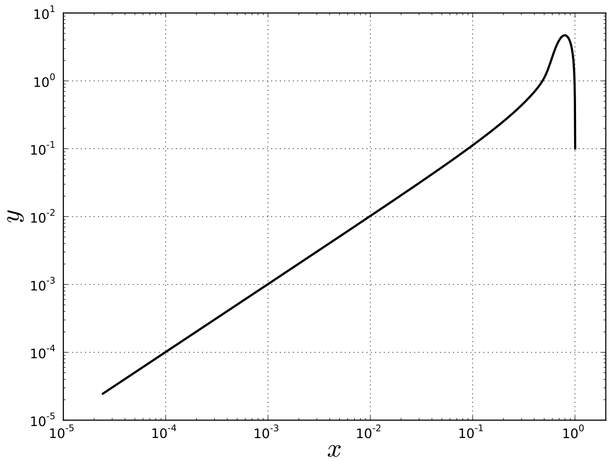

Figure 6: Phase plot for the mean modes corresponding to Eqs. (3) and (6), for $T = 12$.

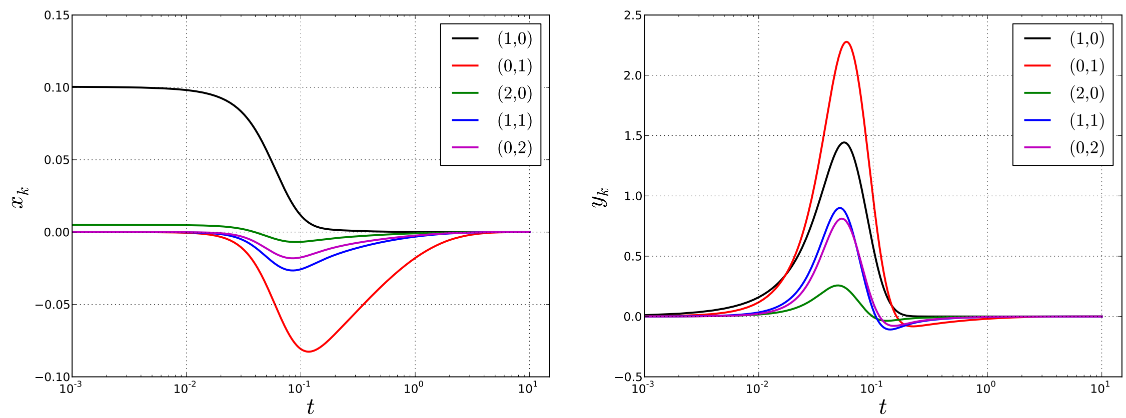

Figure 7: Time evolution of the first few PC modes of x (left frame) and y (right frame). The legend labels show the corresponding multi-indices.

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