Dynamical low rank approximation of time dependent PDEs with random data

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Abstract: Mathematical models, often based on partial differential equations, are widely used to describe and predict the behaviour of physical and engineering systems. However, in many situations, some parameters entering the model can not be exactly quantified. This uncertainty on the data may reflect, on the one side, our ignorance or inability to properly characterize all input parameters of the mathematical model; on the other side, it may describe an intrinsic variability of the physical system. A convenient framework to include uncertainty in the mathematical model is offered by probability theory, where all uncertain input parameters are treated as random variables or random fields. The aim in this case, is to quantify the effects of the uncertainty on the predicted quantities of interest relevant for the applications at hand. We focus on possibly non-linear time dependent partial differential equations of diffusion reaction type with stochastic parameters where the randomness can appear in the initial data, in the coefficients of the differential operator, in the forcing term, etc.

In the last decades, differential equations with random data received a lot of attention in the field of scientific computing and numerical analysis. Since the number of the stochastic variables that are involved in a single phenomenon is often of the order of tens/hundreds or even more, the numerical approximation of these differential problems remains a challenging task. A great effort has been devoted to develop methods that are more efficient than classical Monte Carlo approaches. Alternatively to sampling methods, one could consider generalized Polynomial Chaos (gPC) approximations of the solution with respect to a finite number of random variables parameterizing the probability space. At this step practical approximations can be obtained by different numerical techniques such as Galerkin projection or stochastic collocation method. However this approach could still be affected by the so called 'curse of dimensionality', especially when the solution features a complex dependence on the input parameters. This can be an issue in evolution problems, as the dependence of the solution on the random parameters can significantly vary in time . Then the approximation of the solution by means of fixed polynomial basis functions require during the evolution an increasing number of terms to maintain a proper level of accuracy, which possibly implies a too high computational effort.

We propose here a low rank method based on the Dynamically Orthogonal Field (DOF) approach, according to which the solution is approximated as a linear combination of a small number of deterministic orthogonal basis functions multiplied by random coefficients, both of them evolving in time in order to keep the dimensionality of the approximate problem as low as possible. To fix the idea we briefly introduce the mathematical settings. We consider the following time dependent stochastic PDE:

$$\begin{cases} \frac{\partial u(x,t,\omega)}{\partial t} = \mathcal{L}[u(x,t,\omega),\omega], & x \in D,\ t \in [0,T],\ \omega \in \Omega \\ \mathcal{B}[u(\xi,t,\omega)] = h(\xi,t), & \xi \in \partial D,\ t \in [0,T], \\ u(x,t=0,\omega) = u_0(x,\omega), & x \in D,\ \omega \in \Omega, \end{cases} \tag{1}$$

where D is the physical domain, ω is a random elementary event in a complete probability space $(\Omega, \mathcal{A}, \mathcal{P})$ and $\mathcal{L}$ is a general (linear or non-linear) differential operator. Now we look for an approximate solution

of rank S of the form:

$$u_S(x,t,\omega) = \bar{u}(x,t) + \sum_{i=1}^{S} u_i(x,t) y_i(t,\omega). \tag{2}$$

where $\bar{u} \simeq \mathbf{E}[u]$, $u_1, ...u_S$ are $L^2(D)-$orthogonal deterministic basis functions and $y_1, ..., y_S$ are zero mean stochastic variables. From a variational point of view, if $\mathcal{M}_S$ denotes the manifold of all the functions of rank S, the DO approximate solution u_S is obtained by projecting the residual of the governing equation onto the tangent space to $\mathcal{M}_S$ at $u_S(t)$ at each time, i.e.

$$\mathbb{E}\left[\left\langle \frac{\partial u_S(\cdot,t,\,\omega)}{\partial t} \;-\; \mathcal{L}(u_S(\cdot,t,\,\omega);\,\omega),\, v(\cdot,\,\omega)\right\rangle\right] = 0, \quad \forall v \in \mathcal{T}_{u_S(t)}\mathcal{M}_{\mathcal{S}} \tag{3}$$

The approximate solution is therefore forced to belong to a S dimensional manifold but at the same time the stochastic coefficients and the deterministic basis functions adapt to the structure of the solution at each time, in order to be as close as possible to the best rank S approximation, which is given by the truncated $S-$terms Karhunen-Lòeve expansion.
Our goal is to find a good balance between computational saving and effectiveness of the approximation. Indeed even if the DO expansion does not necessarily coincide with the Karhunen-Lòeve decomposition, the DO approach allows us to derive directly from the governing equation a coupled system of $S+1$ deterministic and S stochastic equations that completely characterize our approximate solution u_S at each time. An analogous approach in the deterministic framework, based on the Dirac-Frenkel variational principle, is present in the literature [1]-[3] and it is adopted in the field of the quantum dynamics.

By investigating the nature of the manifold of the solution we analyze the effectiveness of the DO approximate solution. In particular we provide an error analysis of the DO approximation of stochastic parabolic equation. we exploit the curvature bounds of the manifold given in [3] to show that, under suitable assumptions, the DO error can be bounded in terms of the best rank S approximation error. Specifically we show that Moreover, we show that in the case of deterministic linear operator, with an $S-$ dimensional stochastic initial datum, the DO approximate solution coincides with the exact solution.

Finally we propose a numerical method, able to handle the problem of the over approximation. In that case the number of modes S is bigger then the effective dimension of the exact solution and the covariance matrix of the stochastic coefficients is singular. This point has a great importance since it might happen that the exact solution has a rank smaller then the one used in the DO approximation at some time instant. This is typically the case when starting the algorithm from a deterministic initial condition or when looking at a system of equations converging asymptotically to a deterministic equilibrium, in which case the rank tends asymptotically to zero. The strategy we adopt consists in diagonalizing the covariance matrix, or rather re-orthogonalizing the random coefficients at each time step. Then only the modes associated to stochastic variables with variance bigger then zero will evolve while the other remain constant. From the numerical point of view, the DO system is decoupled in deterministic and stochastic equations, for the former we use Finite Element Methods and for the latter the Stochastic Collocation. The DO method and its convergence properties are assessed with several numerical examples.

[1] Othmar Koch and Christian Lubich, Dynamically low-rank approximation, SIAM J. Matrix Anal.Appl., Vol.29, No.2(2007), pp.434-454.
[2] Themistoklis P. Sapsis and Pierre F.J. Lermusiaux, Dynamically orthogonal field equations for continuous stochastic dynamical systems, Physica D, 238 (2009) 2347-2360,
[3] Dajana Conte and Christian Lubich, An error analysis of the multi-configuration time-dependent Hartree method of quantum dynamics, ESAIM: M2AN. Vol.44, 2010, pp.759-780.

Short biography – Undergraduate Studies: (*2005 - 2008*) Bachelor Degree in Applied Mathematics, Università degli Studi di Perugia, Italy; (*2009 - 2010*) curriculum Integrations of Engineering Mathematics (single courses), Politecnico di Milano; (*2010 - 2012*) Master Degree in Engineering Mathematics, Politecnico di Milano, Italy. Actual Position: PhD Student at the first year. The PhD project focuses on dynamical low rank approximations of PDEs with random parameters and it is financially supported by FNS.