A kernel Proper Orthogonal Decomposition (kPOD) for nonlinear dimensionality reduction of parametric problems

Alba Muixí[1,*], Pedro Díez[1,2], Sergio Zlotnik[1,2] and Alberto García-González[2]

[1] International Center for Numerical Methods in Engineering (CIMNE)
Universitat Politècnica de Catalunya
Campus Nord UPC, 08034 Barcelona, Spain
*e-mail: alba.muixi@upc.edu

[2] Laboratori de Càlcul Numèric (LaCàN)
Universitat Politècnica de Catalunya
Campus Nord UPC, 08034 Barcelona, Spain

ABSTRACT

Reduced-order models (ROM) are essential to solve parametric problems in applications that require multiple queries to the model, for instance, in optimization or uncertainty quantification. The family of parametric solutions lies in a manifold of low dimension (equal to the number of independent parameters), that is embedded in a space of large dimension, given by the degrees of freedom in the numerical discretization. In this framework, a posteriori ROM are based on a family of solutions of the full-order problem (snapshots), that are used to construct a reduced basis for the following queries to the system. For instance, the well-known Proper Orthogonal Decomposition (POD) reduces the problem into a linear subspace of lower dimension, which is identified by applying Principal Component Analysis (PCA) on the set of snapshots. However, the manifold of solutions is often nonlinear, and the PCA linear subspace has a dimension much larger than the intrinsic dimension of the manifold.

The new strategy presented here is to use a nonlinear dimensionality reduction technique, the kPCA [1], to find a nonlinear manifold approximating the manifold of parametric solutions, and to solve the problem in this manifold. The nonlinear manifold discovered with kPCA is expected to be of much lower dimension than the linear manifold from PCA. The novelties in the approach include: 1) the use of local approximations, defined by neighbouring snaphots, 2) the enrichment of the approximation space with quadratic terms, 3) the construction of the kernel using physical properties of the problems, and 4) the solution of the reduced system with a novel algorithm that explores the space within a Delaunay tessellation of the snapshots. The performance of the proposed strategy is assessed for different numerical tests. The results show a significant improvement in the numerical accuracy with respect to the standard POD.

REFERENCES

[1] García-González, A., Huerta, A., Zlotnik, S. and Díez, P. A kernel principal component analysis (kPCA) digest with a new backward mapping (pre-image reconstruction) strategy, 2021.