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An efficient implementation of the direct parametrisation for invariant manifolds for nonlinear model order reduction of large dimensional finite element systems

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Résumé — The derivation of periodic orbits together with stability analysis of large dimensional finite element models of continuum structures represents and important goal during the design of structures operating at resonance as for instance MEMS resonators. However, the huge computational requirements involved for full-order simulations make model order reduction techniques essential to quantitatively estimate the nonlinear dynamic response of structures within useful time-spans. In this contribution we present a computational algorithm to derive reduced order models of nonlinear structure using the direct parametrisation for invariant manifolds. Implementation, computational performance, and examples of real structures analysed with the presented implementation are reported.
Mots clés — model order reduction, invariant manifold theory, software

1 Introduction

Most engineering structures must feature complex geometries to meet the design requirements. As a consequence analytic methods [1] are not applicable if the aim is to accurately estimate the structure response. In this setting, numerical methods prove essential. Indeed, the finite element method allows deriving quantitatively accurate information on the structure behaviour, together with information regarding the stability of the response [2]. However, when ones wants to compute for instance the steady-state response of a nonlinear vibrating structure, the computational burden of large dimensional finite element model makes their adoption during the design stage of mechanical components difficult to apply [3]. This is especially true when the structure under analysis cannot be simplified and the resulting finite element model is composed of millions of degrees of freedom, which is a fairly common in fields as the semiconductor industry, since devices as resonating MEMS gyroscopes are made by multiple proof-masses and elastic springs, the geometry of which is too complicated to be accurately described by simple structural models [4]. The difficulties associated to the computation of periodic orbits in models of this caliber has been evidenced in multiple works, where computational times of days or even weeks have been reported, to compute the full frequency response curve (FRC) of a system. As a result of the inadequacy of full order models for the design of nonlinear vibrating structures, model order reduction methods are necessary and compulsory methods to compute periodic orbits from finite element models [5].

Dimensionality reduction methods should be able to provide three essential features. First of all, they should identify a subspace that is invariant with respect to system motion [7]. Invariance refers to the property of a subset to develop trajectories fully enclosed within the defined subspace. While this property is a necessary condition for a proper reduced model, the identified subspace should also be able to recover the solution of the full order system [6]. At last, the identified subspace should be able to attract trajectories initiated within its neighborhood, that is the identified subspace should be a slow attractive manifold for the system [8]. Within the context of vibratory systems, linear projection methods only partially meet the above the properties [9]. This is a natural consequence of the lack of invariance of linear modal subspaces in presence of nonlinear coupling terms between modes [10]. As a consequence, the research on model order reduction for vibratory systems shifted from linear to nonlinear reduction methods to derive reduced models of smaller dimensions and with identified embeddings that satisfy the

above properties. This is possible in the damped scenario, but this class of methods can be applied also for undamped-unforced systems, where only the invariance property is retained [11, 12].

An appealing feature of vibratory systems is that the origin is either a stable or an asymptotically stable fixed point of the system. Furthermore, in absence of internal resonances it is possible to identify at least a two-dimensional invariant manifold tangent at the origin to its corresponding linear subspace [13]. These two properties lead to the natural consequence that parametrising the system motion along those manifold is an appealing model order reduction strategy. The method exploited to derive such reduced models is the parametrisation method for invariant manifolds introduced by by Cabré, Fontich and de la Llave [14, 15, 16]. The method does not only provide the topology of the invariant manifold over which the reduced model is built, but also the dynamics of the system along the embedding as well [17], the latter being called the reduced dynamics in our context of vibratory systems. The method has been successfully applied in a wide series of works, either using the normal form method [18], or as originally formulated as a proper parametrisation technique [19].

The major drawback of the parametrisation method for invariant manifolds in its original formulation is that it requires diagonalising the linear operator of the system, which is unfeasible for large dimensional finite element models. Only recently, the method has been recast for vibratory systems in its direct form in the seminal works reported by different research groups in [20, 21, 22, 23]. The direct formulation leverages a nonlinear coordinate change from physical to normal coordinates without the necessity to compute the full eigenspectum of the system, hence providing a mean to apply this method to truly large finite element structural models. This represents a a major breakthrough in the context of nonlinear model order reduction techniques since the resulting reduced models are independent from the size of the original finite element model, being the dimension of the reduced model proportional only to the size of the manifold over which the dynamics of the system is parametrised.

In the present contribution, we present a numerical package that implements to the most efficient formulation of the method, following the results reported in [23]. Numerical examples on large scales models are shown with considerations on the potential further development for the method.

The remainder of the paper is organised as follows. In Section 2, we report the main considerations on the equations of motion and on the direct parametrisation method for invariant manifold. In Section 3, we detail the main features that make the formulation proposed in [23] so efficient, highlighting how the governing equations, the symmetric structure of the problem, and the weak form associated to the nonlinearity tensors can be exploited to enhance the performance of the technique. At last, in Section 4, final considerations and remarks for future developments are reported.

2 The direct parametrisation method for invariant manifolds

Let us consider the system of differential equations obtained through finite element discretisation of the conservation of linear momentum for a vibratory system in a finite elasticity framework and modeled with a Saint Venant-Kirchhoff constitutive model.

$$\mathbf{M}\ddot{\mathbf{U}} + \mathbf{C}\dot{\mathbf{U}} + \mathbf{K}\mathbf{U} + \mathbf{G}(\mathbf{U},\mathbf{U}) + \mathbf{H}(\mathbf{U},\mathbf{U},\mathbf{U}) = \mathbf{0}, \tag{1}$$

with $\mathbf{M}$ mass matrix, $\mathbf{C}$ damping matrix, $\mathbf{K}$ stiffness matrix, $\ddot{\mathbf{U}}$ nodal accelerations, $\dot{\mathbf{U}}$ nodal velocities, $\mathbf{U}$ displacement field, $\mathbf{G}(\mathbf{U},\mathbf{U})$ quadratic nonlinearity tensor, and $\mathbf{H}(\mathbf{U},\mathbf{U},\mathbf{U})$ cubic nonlinearity tensor. For vibratory systems nonlinear terms stem naturally from the decomposition of the internal power in its linear, quadratic, and cubic components. As a result, the polynomial structure of Eq. (1) stems naturally from the governing differential equations. Without loss of generality, damping is modeled as Rayleigh damping, i.e. $\mathbf{C} = \alpha\mathbf{M} + \beta\mathbf{K}$, with α and β non negative scalar coefficients. Equation (1) is rewritten in first order formulation by introducing the velocity $\mathbf{V} = \dot{\mathbf{U}}$.

$$\mathbf{M}\dot{\mathbf{V}} + \mathbf{C}\mathbf{V} + \mathbf{K}\mathbf{U} + \mathbf{G}(\mathbf{U},\mathbf{U}) + \mathbf{H}(\mathbf{U},\mathbf{U},\mathbf{U}) = \mathbf{0}, \tag{2a}$$

$$\mathbf{M}\dot{\mathbf{U}} - \mathbf{M}\mathbf{V} = \mathbf{0}, \tag{2b}$$

where the second equation has been pre-multiplied by the mass matrix. For $\mathbf{C} = \mathbf{0}$ the origin represents a marginally stable fixed point since the linearisation of Eq. (2) at the origin is characterised by a purely imaginary eigenspectrum. On the other hand, for $\mathbf{C} \neq \mathbf{0}$ the origin is an asymptotically stable fixed point since all eigenvalues are characterised by a negative real part. We define the eigenmodes of the structure ϕ_j as the eigenvectors obtained from the generalised eigenvalue problem associated to the linearised Eq. (1). To each ϕ_j we associate an eigenfrequency ω_j and for each eigenmode we can identify at least an invariant manifold tangent at the origin to the plane spanned by modal displacement and velocity associated to ϕ_j in phase space. Parametrisation on the system along such manifold is obtained by introducing a nonlinear change of coordinates between physical variables and the normal coordinates $\mathbf{z}$, the latter corresponding to the set of coordinates defined over the embedding spanned by the manifold :

$$\mathbf{U} = \boldsymbol{\Psi}(\mathbf{z}), \quad \mathbf{V} = \boldsymbol{\Upsilon}(\mathbf{z}), \tag{3}$$

with $\boldsymbol{\Psi}(\mathbf{z})$ and $\boldsymbol{\Upsilon}(\mathbf{z})$ nonlinear functions of the normal coordinates. The motion of the system along the embedding is then defined as :

$$\dot{\mathbf{z}} = \mathbf{f}(\mathbf{z}), \tag{4}$$

with $\mathbf{f}(\mathbf{z})$ the reduced dynamics. Following this definition, time derivatives of displacement and velocity are then computed from the gradient of the mappings with respect to the normal coordinates :

$$\dot{\mathbf{U}} = \nabla_{\mathbf{z}}\boldsymbol{\Psi}(\mathbf{z})\mathbf{f}(\mathbf{z}), \quad \dot{\mathbf{V}} = \nabla_{\mathbf{z}}\boldsymbol{\Upsilon}(\mathbf{z})\mathbf{f}(\mathbf{z}). \tag{5}$$

Substitution of mappings and their derivatives in Eq. (2), yields the so-called invariance equation [17], which can be solved to retrieve the expressions of mappings and reduced dynamics :

$$\mathbf{M}\nabla_{\mathbf{z}}\boldsymbol{\Upsilon}(\mathbf{z})\mathbf{f}(\mathbf{z}) + \mathbf{C}\boldsymbol{\Upsilon}(\mathbf{z}) + \mathbf{K}\boldsymbol{\Psi}(\mathbf{z}) + \mathbf{G}(\boldsymbol{\Psi}(\mathbf{z}),\boldsymbol{\Psi}(\mathbf{z})) + \mathbf{H}(\boldsymbol{\Psi}(\mathbf{z}),\boldsymbol{\Psi}(\mathbf{z}),\boldsymbol{\Psi}(\mathbf{z})) = \mathbf{0}, \tag{6a}$$

$$\mathbf{M}\nabla_{\mathbf{z}}\boldsymbol{\Psi}(\mathbf{z})\mathbf{f}(\mathbf{z}) - \mathbf{M}\boldsymbol{\Psi}(\mathbf{z}) = \mathbf{0}. \tag{6b}$$

The solution of the invariance equation is generally performed order by order, following the general guidelines proposed for example in [17]. However, if the method is applied in its general form without leveraging the symmetries of the resulting formulation together with specificities related to FE formulation and vibratory systems, high memory requirements and long computational times required to extract nonlinearity tensors are required. In the remainder of this paper, the key aspects of the implementation as detailed in [23] are highlighted, and we show how the method can be improved in such a way that it can properly model large dimensional finite element systems.

3 Method and Computational performance

Let us expand the mappings as polynomial functions of the normal coordinates and in such a way that identity tangency with a given modal subspace is verified :

$$\boldsymbol{\Psi}(\mathbf{z}) = \boldsymbol{\Phi}\mathbf{z} + \sum_{p=2}^{o} [\boldsymbol{\Psi}(\mathbf{z})]_p, \tag{7a}$$

$$\boldsymbol{\Upsilon}(\mathbf{z}) = \boldsymbol{\Phi}\boldsymbol{\Lambda}\mathbf{z} + \sum_{p=2}^{o} [\boldsymbol{\Upsilon}(\mathbf{z})]_p, \tag{7b}$$

with $[\boldsymbol{\Psi}(\mathbf{z})]_p$ and $[\boldsymbol{\Upsilon}(\mathbf{z})]_p$ collection of polynomials terms of $\mathbf{z}$ of equal order p :

$$\begin{aligned}
[\boldsymbol{\Psi}(\mathbf{z})]_p &= \sum_{i_1=1}^{2n}\sum_{i_2=1}^{2n}\dots\sum_{i_p=1}^{2n} \boldsymbol{\Psi}^{(p)}_{i_1 i_2 \dots i_p} z_{i_1} z_{i_2} \dots z_{i_p} = \sum_I \boldsymbol{\Psi}^{(p)}_I \boldsymbol{\pi}^{(p)}_I, \\
[\boldsymbol{\Upsilon}(\mathbf{z})]_p &= \sum_{i_1=1}^{2n}\sum_{i_2=1}^{2n}\dots\sum_{i_p=1}^{2n} \boldsymbol{\Upsilon}^{(p)}_{i_1 i_2 \dots i_p} z_{i_1} z_{i_2} \dots z_{i_p} = \sum_I \boldsymbol{\Upsilon}^{(p)}_I \boldsymbol{\pi}^{(p)}_I.
\end{aligned} \tag{8a}$$

where normal coordinates monomials are collected in the symbol π_I, with I set of indexes of the combination. n is the number of master modes embedded in the reduced model and it is equal to half of the dimension of the manifold being parametrised. $\mathbf{\Phi}$ is the eigenfunctions matrix of the associated master modes, and $\mathbf{\Lambda}$ the diagonal matrix that stores the eigenvalues of the master modes :

$$\mathbf{\Phi} = [\phi_1, \phi_2, \ldots, \phi_n, \phi_1, \phi_2, \ldots, \phi_n], \tag{9a}$$

$$\mathbf{\Lambda} = \text{diag}\left[\lambda_1, \ldots, \lambda_n, \bar{\lambda}_1, \ldots \bar{\lambda}_n\right]. \tag{9b}$$

with λ_j eigenvalues of the first-order problem and $\bar{(\cdot)}$ complex conjugate operation. Similar structure is provided also to the reduced dynamics :

$$\boldsymbol{f}(\mathbf{z}) = \mathbf{\Lambda}\mathbf{z} + \sum_{p=2}^{o} [\boldsymbol{f}(\mathbf{z})]_p, \tag{10}$$

with :

$$[\boldsymbol{f}(\mathbf{z})]_p = \sum_{i_1=1}^{2n} \sum_{i_2=1}^{2n} \ldots \sum_{i_p=1}^{2n} \mathbf{f}^{(p)}_{i_1 i_2 \ldots i_p} z_{i_1} z_{i_2} \ldots z_{i_p} = \sum_I \mathbf{f}^{(p)}_I \boldsymbol{\pi}^{(p)}_I, \tag{11}$$

Substitution of such expansions in the invariance equation provides the following set of homological equations :

$$\forall\, I \in \mathcal{H}^{(p)}, \forall\, p = 1, ..., o,$$

$$\mathbf{M}\mathbf{\Upsilon}^{(p)}_I \boldsymbol{\sigma}_I + \sum_{s=1}^{2n} \left(\mathbf{M}\boldsymbol{\phi}_s \lambda_s f^{(p)}_{sI}\right) + \mathbf{M}\boldsymbol{\nu}^{(p)}_I + \mathbf{C}\mathbf{\Upsilon}^{(p)}_I + \mathbf{K}\mathbf{\Psi}^{(p)}_I + \check{\mathbf{G}}^{(p)}_I + \check{\mathbf{H}}^{(p)}_I = \mathbf{0}, \tag{12a}$$

$$\mathbf{M}\mathbf{\Psi}^{(p)}_I \boldsymbol{\sigma}_I + \sum_{s=1}^{2n} \left(\mathbf{M}\boldsymbol{\phi}_s f^{(p)}_{sI}\right) + \mathbf{M}\boldsymbol{\mu}^{(p)}_I - \mathbf{M}\mathbf{\Upsilon}^{(p)}_I = \mathbf{0}. \tag{12b}$$

The total number of combinations for an order p is collected in the set $\mathcal{H}^{(p)}$. All the remaining quantities are defined as :

$$\boldsymbol{\sigma}_I = \lambda_{i_1} + \lambda_{i_2} + \ldots + \lambda_{i_p}, \tag{13a}$$

$$\boldsymbol{\mu}^{(p)}_I = \sum_{s=1}^{2n} \sum_{k=2}^{p-1} \sum_{l=0}^{p-k} \mathbf{\Psi}^{(p-k+1)}_{i_1 \ldots i_l s i_{l+k+1} \ldots i_p} f^{(k)}_{s i_{l+1} \ldots i_{l+k}}, \tag{13b}$$

$$\boldsymbol{\nu}^{(p)}_I = \sum_{s=1}^{2n} \sum_{k=2}^{p-1} \sum_{l=0}^{p-k} \mathbf{\Upsilon}^{(p-k+1)}_{i_1 \ldots i_l s i_{l+k+1} \ldots i_p} f^{(k)}_{s i_{l+1} \ldots i_{l+k}}, \tag{13c}$$

$$\check{\mathbf{G}}^{(p)}_I = \sum_{k=1}^{p-1} \mathbf{G}\left(\mathbf{\Psi}^{(k)}_{i_1 \ldots i_k}, \mathbf{\Psi}^{(p-k)}_{i_{k+1} \ldots i_p}\right), \tag{13d}$$

$$\check{\mathbf{H}}^{(p)}_I = \sum_{k=1}^{p-2} \sum_{l=1}^{p-k-1} \mathbf{H}\left(\mathbf{\Psi}^{(k)}_{i_1 \ldots i_k}, \mathbf{\Psi}^{(l)}_{i_{k+1} \ldots i_{k+1}}, \mathbf{\Psi}^{(p-k-l)}_{i_{k+1+1} \ldots i_p}\right). \tag{13e}$$

Equation (12) can be solved to retrieve mappings and reduced dynamics coefficients. However, if the method is solved with the above formulation severe limitations are met since the number of monomials increases with the number of index permutations and the resulting linear system is large. Furthermore, it appears that all monomials need to be computed, while explicit symmetry of the system structure can be obtain to reduce the number of homological equations that are solved.

A first improvement from Eq. (12) is obtained by noticing that Eq. (12b) is an algebraic relation between velocity and displacement mappings, which can be substituted in Eq. (12a) to halve the dimension of the linear system, leading to the following homological equation :

$$\left(\sigma_I^2 \mathbf{M} + \sigma_I \mathbf{C} + \mathbf{K}\right) \mathbf{\Psi}^{(p)}_I + \sum_{j=1}^{2n} \left(\left(\sigma_I + \lambda_j\right)\mathbf{M} + \mathbf{C}\right) \phi_j f^{(p)}_{jI} = -\check{\mathbf{G}}^{(p)}_I - \check{\mathbf{H}}^{(p)}_I - \mathbf{M}\boldsymbol{\nu}^{(p)}_I - \left(\sigma_I \mathbf{M} + \mathbf{C}\right)\boldsymbol{\mu}^{(p)}_I. \tag{14}$$

A second improvement on the solution of the homological equations, stems from the symmetry of the associated monomials. To this aim, let us introduce the following shift operation for the indexes of the monomials :

$$i_k^* = \begin{cases} i_k + n & \text{if } i_k \leq n, \\ i_k - n & \text{if } i_k > n. \end{cases} \tag{15}$$

Since the resulting displacement and velocity must be real valued, the following symmetries hold between the expansion monomials :

$$\bar{\boldsymbol{\Psi}}^{(p)}_{I^*} = \boldsymbol{\Psi}^{(p)}_{I}, \tag{16a}$$

$$\bar{\boldsymbol{\Upsilon}}^{(p)}_{I^*} = \boldsymbol{\Upsilon}^{(p)}_{I}, \tag{16b}$$

$$\bar{f}^{(p)}_{s^* I^*} = f^{(p)}_{sI}. \tag{16c}$$

The immediate benefit of this property is that the number of homological equations that need to be solved is halved compared to the method formulated for generic dynamic systems.

One last important peculiarity of the method formulated for dynamical systems stemming from PDE discretisation is that nonlinearity terms can be computed directly from the weak form of the problem without computing the full nonlinearity tensors $\mathbf{G}(\mathbf{U},\mathbf{U})$ and $\mathbf{H}(\mathbf{U},\mathbf{U},\mathbf{U})$. Indeed, from the decomposition of the internal power term into linear, quadratic, and cubic terms the following expressions can be obtained :

$$\begin{aligned} \check{\mathbf{G}}^{(p)}_I = \sum_{k=1}^{p-1} \int_\Omega & \frac{1}{2}\gamma(\boldsymbol{\Psi}^{(k)}_{i_1\dots i_k}, \boldsymbol{\Psi}^{(p-k)}_{i_{k+1}\dots i_p}) : \mathcal{A} : \varepsilon(\mathbf{w}_h) + \frac{1}{2}\varepsilon(\boldsymbol{\Psi}^{(k)}_{i_1\dots i_k}) : \mathcal{A} : \gamma(\boldsymbol{\Psi}^{(p-k)}_{i_{k+1}\dots i_p}, \mathbf{w}_h) + \\ & \frac{1}{2}\varepsilon(\boldsymbol{\Psi}^{(p-k)}_{i_{k+1}\dots i_p}) : \mathcal{A} : \gamma(\boldsymbol{\Psi}^{(k)}_{i_1\dots i_k}, \mathbf{w}_h)\, d\Omega, \end{aligned} \tag{17a}$$

$$\begin{aligned} \check{\mathbf{H}}^{(p)}_I = \sum_{k=1}^{p-2} \sum_{l=1}^{p-k-1} \int_\Omega & \frac{1}{6}\gamma(\boldsymbol{\Psi}^{(k)}_{i_1\dots i_k}, \boldsymbol{\Psi}^{(l)}_{i_{k+1}\dots i_{k+1}}) : \mathcal{A} : \gamma(\boldsymbol{\Psi}^{(p-k-l)}_{i_{k+1+1}\dots i_p}, \mathbf{w}_h) + \\ & \frac{1}{6}\gamma(\boldsymbol{\Psi}^{(p-k-l)}_{i_{k+1+1}\dots i_p}, \boldsymbol{\Psi}^{(k)}_{i_1\dots i_k}) : \mathcal{A} : \gamma(\boldsymbol{\Psi}^{(l)}_{i_{k+1}\dots i_{k+1}}, \mathbf{w}_h) + \\ & \frac{1}{6}\gamma(\boldsymbol{\Psi}^{(l)}_{i_{k+1}\dots i_{k+1}}, \boldsymbol{\Psi}^{(p-k-l)}_{i_{k+1+1}\dots i_p}) : \mathcal{A} : \gamma(\boldsymbol{\Psi}^{(k)}_{i_1\dots i_k}, \mathbf{w}_h)\, d\Omega, \end{aligned} \tag{17b}$$

where Ω is the domain of integration, $\mathcal{A}$ is the fourth-order elasticity tensor, and the following operators have been introduced to lighten the notation :

$$\varepsilon(\mathbf{a}) = \frac{1}{2}\left(\nabla\mathbf{a} + \nabla^T\mathbf{a}\right), \qquad \gamma(\mathbf{a},\mathbf{b}) = \frac{1}{2}\left(\nabla^T\mathbf{a}\cdot\nabla\mathbf{b} + \nabla^T\mathbf{b}\cdot\nabla\mathbf{a}\right), \tag{18}$$

with $\mathbf{a}$ and $\mathbf{b}$ generic vector fields. Equations (17) can be computed through Gaussian quadrature over the domain and this approach allows avoiding storing the full nonlinearity tensors.

Overall, these three main features yield an efficient implementation of the method that overcomes limitations of similar applications of the method. An example of computational performance achieved with the presented derivation is reported in Fig. 1, where performance obtained for deriving reduced models starting from the finite element model of a MEMS micromirror is reported. In (a) we report computational times and memory requirements used to parametrise the finite element model for different values of mesh refinements. Data are reported for an asymptotic expansion of order 5. In (b) we show the convergence of the undamped response of the system obtained for a model of 5'034'996 degrees of freedom using a single master mode reduction. Overall, the obtained performance of the method highlight how it can be efficiently applied to predict the nonlinear dynamic response of complex structures characterised by millions of degrees of freedom.

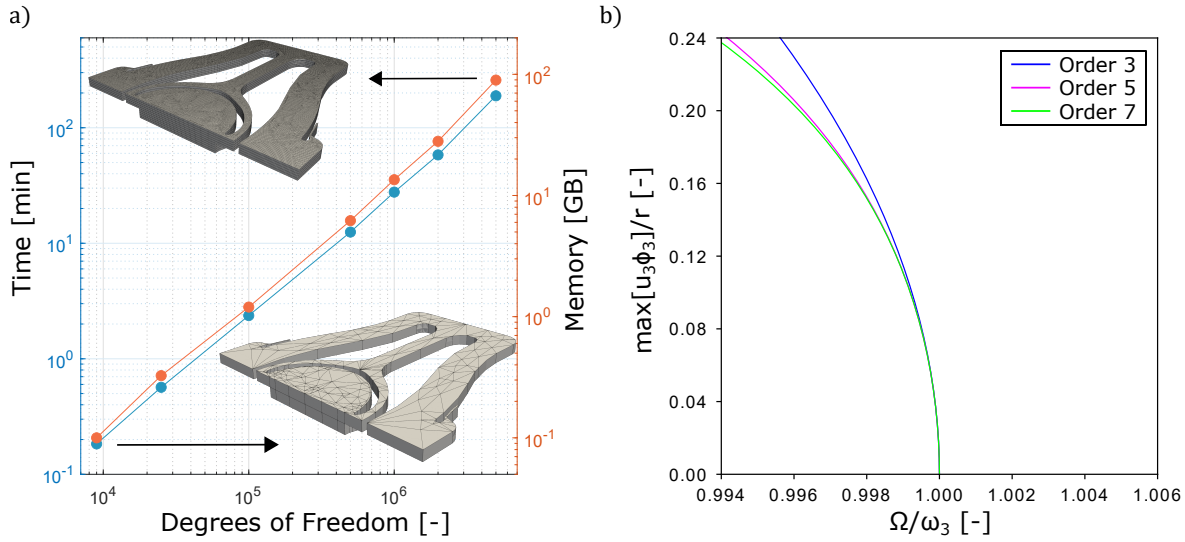

FIGURE 1 – (a) computational performance obtain to derive reduced models on finite element systems of increasing number of degrees of freedom. Data are reported for single master mode reduction and for an asymptotic expansion of order 5. Performance are reported for a FORTRAN implementation of the method and analyses were run on a computer that features an AMD® Ryzen 9 5950X and 128GB RAM. (b) convergence of the undamped response with the order of the asymptotic expansion. Undamped responses are obtained using a real normal form style parametrisation and for a model of 5'034'996 degrees of freedom.

4 Conclusions

In the present contribution, a novel implementation of the direct parametrisation method for invariant manifolds, especially tailored for mechanical systems and in general for real-valued dynamic systems stemming from finite element discretisation of partial differential equations, has been presented. The benefits of adopting the method for model order reduction purpose, are highlighted on a reference system that contains up to 5 millions degrees of freedom, underlining how the reached performance make the presented method ideal for designing structures subjected to geometric nonlinearities in a fast and accurate manner.

5 Code Availability

A Julia implementation of the method will be available through the package MORFEInvariantManifold. The package can be downloaded at https://github.com/aopreni/MORFEInvariantManifold.jl, while a series of example structures reduced with the same package can be downloaded at https://github.com/aopreni/MORFEInvariantManifold_examples.

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