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50. Internationales Wissenschaftliches Kolloquium
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New Parametric Variational Techniques for MEMS Simulation Based on Finite Element Method

ABSTRACT

The article is focused on new finite element technologies which account for parameter variations in a single finite element run. The key idea of the new approach is to compute not only the governing system matrices of the FE problem but also n high order partial derivatives with regard to design parameters by means of Automatic Differentiation (AD). As result, Taylor vectors of the system's response can be expanded in the vicinity of the initial position capturing dimensions and physical parameter. Essential speed-up can be achieved for shape optimization, sensitivity analyses and data sampling needed for reduced order modeling of MEMS.

INTRODUCTION

Finite element techniques have become state of the art for component design of MEMS. Physical effects related with electromagnetic, mechanical, fluid and thermal fields in complex devices are accurately described for static, harmonic and transient load situations. In the past, time consuming finite element models could automatically be reduced in its model size by matrix condensation or projection techniques. Results are low-order black-box models which allow for both, time efficient analyses within finite element tools or export to electronic circuit or system design environment [1]. Drawback of existing finite element techniques is that those algorithms can only analyze a single model configuration with specified dimensions and physical parameters. In practice, designers want to know the influence of parameter variations on the structural response in order to optimize the entire system and to assess the effect of tolerances (sensitivity analyses [2]) or changed material properties. In fact, designers long for parametric model results in the same way as known from analytical methods.

Currently, parametric models of complex devices are extracted by numerical data sampling and subsequent function fit algorithms. Each sample point must be obtained by a separate finite element run whereby the change of geometrical dimensions is realized by mesh morphing or remesh functionality. Usually one needs between several ten to some hundreds of sample data in order to capture the influence of design parameters accurately which is cumbersome for practical use [3]. Variational technologies have been applied for thickness optimization of shell structures in mechanical engineering [4]. This article extends the approach [5] to design of coupled domain microsystems where strain energy and capacitance functions relate interactions between electrostatic and structural domains. Benefits of variational technologies compared to ordinary data sampling procedures become obvious for multi-parameter problems.

THEORETICAL BACKGROUND

Taylor series expansion is a common engineering approach to estimate the system response at changed parameters. A static system depending on a set of parameters p can be described by

$$u(p) = K(p)^{-1} F(p), \qquad (1)$$

where K is the governing system matrix, F the load vector and u the unknown solution vector. The first derivative of u with respect to p at the evaluation point p_0 is given by

$$u(p_0)' = K(p_0)^{-1}\left(F(p_0)' - K(p_0)' u(p_0)\right), \qquad (2)$$

and higher order derivatives can be computed from the following recursive formula:

$$u(p_0)^{(n)} = K(p_0)^{-1}\left(F(p_0)^{(n)} - \sum_{i=1}^{n} C_n^i \, K(p_0)^{(n)} u(p_0)^{(n-i)} \right), \qquad (3)$$

where C is the binomial coefficient. Finally the Taylor series expansion becomes

$$u(p) = u(p_0) + \sum_{i=1}^{n} \frac{1}{i!} u(p_0)^{(i)} \Delta p^i \qquad (4)$$

Obviously, Taylor vectors must only be computed at a single model configuration referred as p_0. The entire variational approach requires just one matrix inverse, all other operations are time efficient matrix-vector products.

In contrast to ordinary FEM, one needs a parametric solid model what captures the influence of design variables on geometric dimensions and material properties Fig. 1. The next step will be to create a parametric finite element mesh Fig. 2. In the general case, the mesh have been generated by some kind of mesh generator which do not contain analytical descriptions of the mesh representation. Parametric means that the nodal table does not only contain a single value for each spatial direction, rather each coordinate will be described by a function (commonly polynomial) with regard to global parameter p. In order to build a parametric mesh, one first select nodes associated with parameters and build a perturbation of the boundary. Next one have to extend the perturbation inside the mesh. A convenient way to transform global parameter to polynomial nodal coordinates (Fig. 2) is a Laplacian algorithm known from mesh morphing of FEM [6].

Based on the parametric finite element model one can utilize automatic differentiation algorithms to the governing equations of the FE problem in order to calculate n high order derivatives. The general algorithm to extract a finite element matrix and its derivatives is illustrated in Fig. 3 for an twenty node solid element.

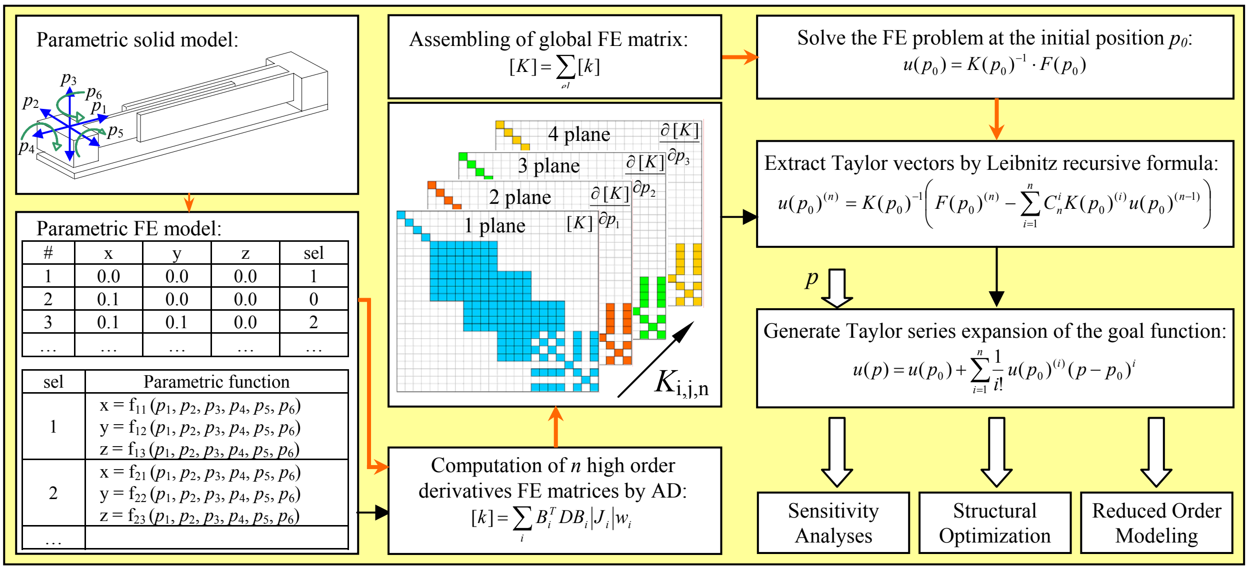

Fig. 1: Flow chart of parametric variational FE techniques.

Differentiation rules describe how to combine partial derivatives and binomial coefficients in order to form elementary mathematical operations. The beauty of the approach is that higher order derivatives follow from a recursive combination of existing derivatives with binomial coefficients Fig. 4. Automatic differentiation rules are only required for a few basic arithmetic operations such as product and quotient of two differential planes. Other more complicated operations as matrix inverse or determinant are substituted by elementary functions or differential matrix calculus. Remarkable is that automatic differentiation rules give an exact representation of high order derivatives [7].

A specialized data structure is commonly applied to process and store partial derivatives with given order. Partial derivatives have been arranged in successive planes of matrices in a third dimension whereby the index corresponds to a notation given in [7].

EXTRACTION OF CAPACITANCE FUNCTIONS

Capacitance stroke functions are directly extracted from the electrostatic field solution based on Laplacian partial differential equation. The governing FE equation system is given by

$$K(p)\,\varphi(p) = Q(p), \tag{5}$$

where K is the dielectric conductivity matrix, φ the voltage potential and Q the charge accumulated on the conductors. All terms depend on a set of parameter p which might be transversal shift in spatial directions. A typical example of interest is a comb cell shown in Fig. 1.

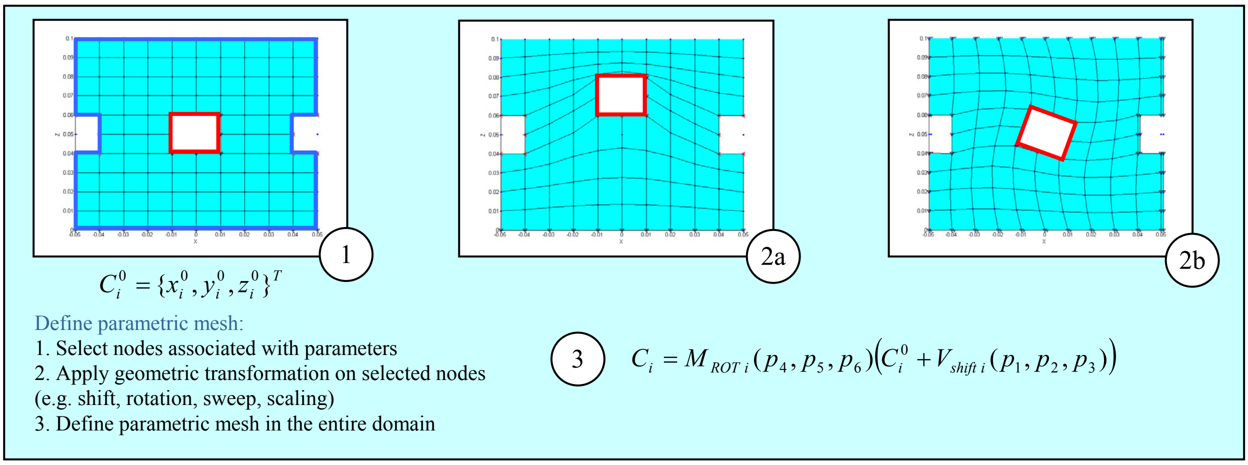

Fig. 2: Parametric finite element mesh.

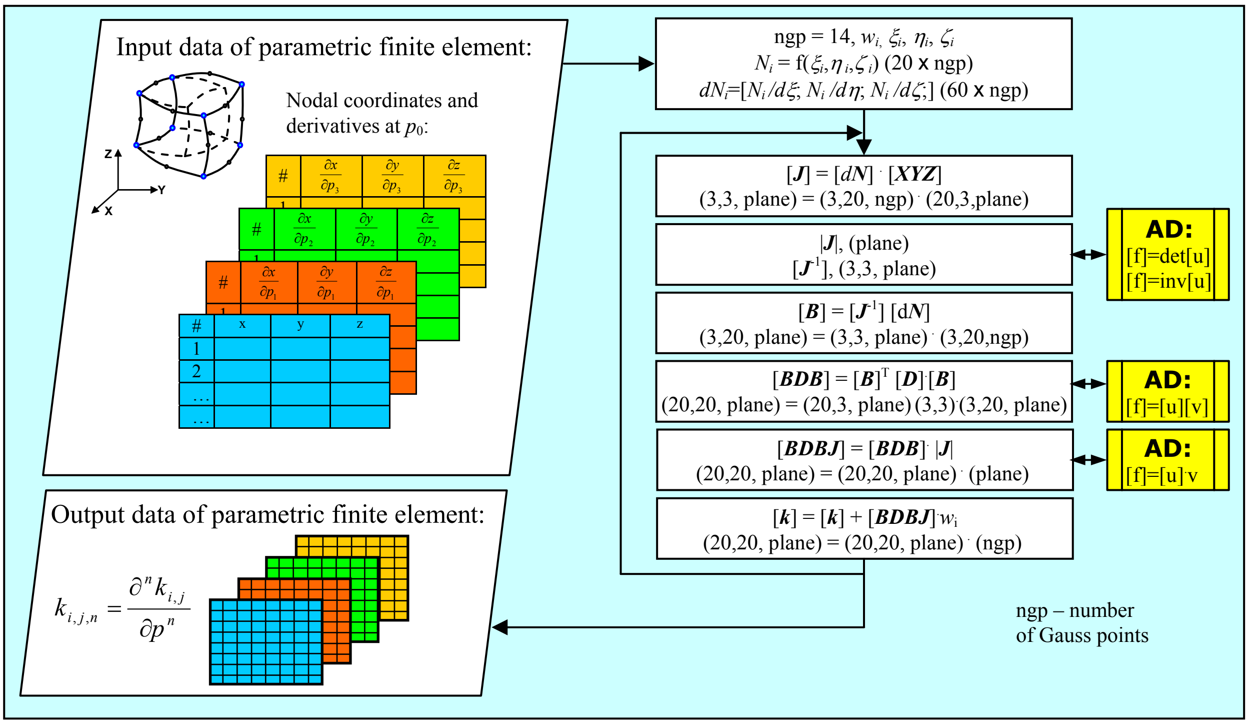

Fig. 3: Computing high order derivatives of FE matrices.

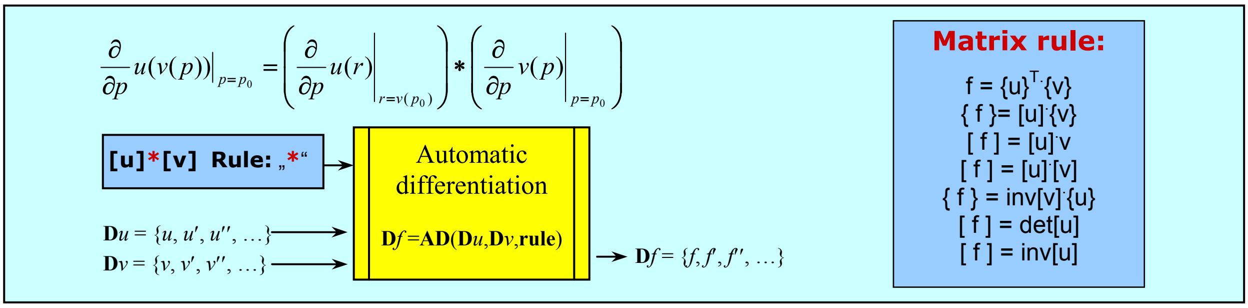

Fig. 4: Automatic differentiation.

The finite element equation system can be subdivided into nodes laying on conductor surfaces and nodes in the dielectric region. For capacitance computation, the voltage potential of conductor nodes is entirely constrained and charges on all other nodes become zero. The finite element equation system can be written as

$$\begin{bmatrix} K_{c,c} & K_{c,e} \\ K_{e,c} & K_{e,e} \end{bmatrix} \begin{bmatrix} V_c \\ \varphi(p)_e \end{bmatrix} = \begin{bmatrix} Q(p)_c \\ 0 \end{bmatrix}, \quad (6)$$

where the index ***c*** represents conductor nodes and e nodes of the electrostatic region (e.g. air). The solution procedure starts with a first step where all unknown voltage potentials are computed

$$\varphi(p)_e = K_{e,e}(p)^{-1}\left(-K_{e,c}(p)\, V_c\right), \quad (7)$$

and is followed by a second step

$$Q(p)_c = K_{c,c}(p)\, V_c + K_{c,e}(p)\, \varphi(p)_e, \quad (8)$$

where the charges on conductor nodes are determined. Note, all vectors and matrices depending on parameters are differential plane arrays.

In a next step, the Taylor series of charges with regard to shift of the movable finger is calculated by

$$Q(p)_c = Q(p_0)_c + \sum_{i=1}^{n} \frac{1}{i!} Q(p_0)_c^{(i)} \Delta p^i, \quad (9)$$

Finally, capacitances are extracted from the accumulated charge on conductor surfaces at unit voltage potential V

$$C(p) = \frac{\sum_{cond} Q(p)_c}{V}, \quad (10)$$

Fig. 5a illustrates the capacitance relationship depending on six parameters, shift and rotation in x-, y-, z-directions.

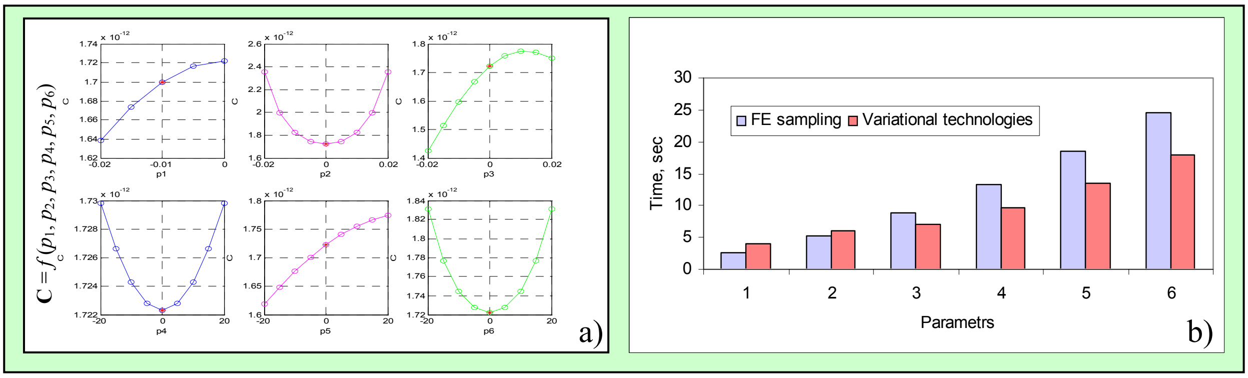

Fig. 5. Response curves of a capacitance stroke function with regard to six degrees of freedom of the movable finger and efficiency of ordinary FE sampling compared to variational FE

technologies.

Fig. 5a shows that the levitation effect of comb cells could be captured well. Response functions provide not only capacitance data but also the first and second derivatives needed for Maxwell force and electrostatic softening computations [6]. Sampling and function fit procedures are powerful if a low number of design variables have to be taken into account. Fig. 5b shows that computing time for two design parameters was still lower compared to new variational FE technologies. On the other hand, data acquisition time of sample methods grow exponentially the more variables must be processed.

CONCLUSION

Variational finite element technologies have been implemented in MATLAB for twenty node solid elements. The algorithms support linear static analyses of structural, thermal and electrostatic domains. Special emphasis was put on strain energy and capacitance extraction for reduced order modeling of MEMS. Solid modeling, mesh generation and visualization of results data has been realized within ANSYS/Multiphysics.

The number of differential planes is comparable with the number of samples required for function fit methods. Fortunately, automatic differentiation of additional planes is usually less expensive compared to further FE solution runs needed for sampling. Hence, the extra time taken for parametric modeling and mesh at the beginning of variational techniques disappears rapidly.

The accuracy of variational results depends mainly on mesh perturbations caused by mapping of global parameter to the nodal table. Generally internal finite element nodes must move smoothly with respect to dimensional modifications, especially in case of large displacements or complicated shape (e.g. perforation holes, sharp notches). Similar problems are widely known from mesh morphing of coupled domain analyses.

It could be shown that variational technologies are a promising alternative to existing data sampling and function fit procedures utilized for component and system design of MEMS. Especially for case studies of different geometrical dimensions, sensitivity analyses of manufacturing tolerances and model export for electronic design automation one needs fast and accurate models which capture the parameter relationship.

Further work will be focused on dynamic systems capturing inertial and damping effects. The ultimate goal will be to replace the time consuming FE data sampling process of reduced order modeling tools and to support parametric models in terms of geometrical dimensions and material properties.

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