Model Order Reduction Methods for Multivariate Parameterized Dynamical Systems obtained by the Finite Integration Theory

Kynthia Stavrakakis[1], *Tilmann Wittig*[2], *Wolfgang Ackermann*[1], and *Thomas Weiland*[1]

[1] Institut für Theorie Elektromagnetischer Felder, Technische Universität Darmstadt, Schlossgartenstr. 8, 64289 Darmstadt, Germany

stavrakakis@temf.tu-darmstadt.de, ackermann@temf.tu-darmstadt.de, weiland@temf.tu-darmstadt.de

[2] Computer Simulation Technology AG, Bad Nauheimer Str. 19, 64289 Darmstadt, Germany

tilmann.wittig@cst.com

Abstract

In electrodynamic field computations the continuous Maxwell equations are typically discretized in the space variables, i. e the continuous space is mapped onto a finite set of discrete elements leading to a system of differential equations constituting the Maxwell grid equations. These dynamical systems can be very large. Due to limited computational, accuracy and storage capabilities, simplified models, obtained by means of model order reduction (MOR) methods, which capture the main features of the original model are then successfully used instead of the original models. Most commonly MOR via projection is used. Variation of model parameters like geometrical or material parameters give rise to multivariate dynamical systems. It is aimed that also the simplified models keep this parameter dependence. In this work, MOR methods are presented for multivariate systems based on the finite integration technique (FIT). The methods are applied to numerical examples with both geometrical and material variations.

1 Systems obtained by the Finite Integration Technique

Based on the Maxwell grid equations in FIT [1], we consider dynamical systems, denoted by $\mathbf{\Sigma}$, where in- and output vectors $\mathbf{i}$ and $\mathbf{u}$ respectively and an auxiliary vector $\mathbf{x}$ are defined. In the following, it is shown how different classes of dynamical systems are obtained in the univariate and multivariate case of the FIT equations in frequency domain:

$$2\mathbf{C}_{\mathrm{FIT}}\tilde{\mathbf{e}} = -s\,\mathbf{M}_{\mu}\hat{\mathbf{h}}, \quad \mathbf{S}\mathbf{M}_{\mu}\hat{\mathbf{h}} = 0, \quad \widetilde{\mathbf{C}}_{\mathrm{FIT}}\hat{\mathbf{h}} = (s\,\mathbf{M}_{\varepsilon} + \mathbf{M}_{\sigma})\tilde{\mathbf{e}} + \hat{\tilde{\mathbf{j}}}_{e}, \quad \widetilde{\mathbf{S}}\mathbf{M}_{\epsilon}\tilde{\mathbf{e}} = 0. \tag{1}$$

Here, $\mathbf{M}_{\varepsilon}, \mathbf{M}_{\sigma}, \mathbf{M}_{\mu}$ are diagonal matrices, which express the geometry and material property of each meshcell and are contained in the discrete equivalent of the material equations: $\hat{\tilde{\mathbf{d}}} = \mathbf{M}_{\varepsilon}\tilde{\mathbf{e}}$, $\hat{\tilde{\mathbf{j}}} = \mathbf{M}_{\sigma}\tilde{\mathbf{e}} + \hat{\tilde{\mathbf{j}}}_{e}$, $\hat{\mathbf{h}} = \mathbf{M}_{\mu}^{-1}\hat{\tilde{\mathbf{b}}}$. The matrices $\mathbf{S}$ and $\mathbf{C}_{\mathrm{FIT}}$ (as well as $\widetilde{\mathbf{S}}, \widetilde{\mathbf{C}}_{\mathrm{FIT}}$) are topology matrices representing the divergence and the curl operator, respectively. The in- and output matrices $\mathbf{B}$ and $\mathbf{C}$ can be defined by $\hat{\tilde{\mathbf{j}}}_{s} = \mathbf{R}\mathbf{i}$ and $\mathbf{u} = \mathbf{C}\tilde{\mathbf{e}}$, respectively. Elimination of $\hat{\mathbf{h}}$ leads to,

$$\mathbf{M}_{\varepsilon}s^{2}\tilde{\mathbf{e}} + \mathbf{M}_{\sigma}s\tilde{\mathbf{e}} + \mathbf{C}_{\mathrm{FIT}}^{\mathrm{T}}\mathbf{M}_{\mu}^{-1}\mathbf{C}_{\mathrm{FIT}}\tilde{\mathbf{e}} = s\mathbf{B}\mathbf{i}, \quad \mathbf{u} = \mathbf{C}\tilde{\mathbf{e}}. \tag{2}$$

which is a second-order linear system in $\tilde{\mathbf{e}}, (\mathbf{x} = \tilde{\mathbf{e}})$. Higher order systems, are obtained from the grid equations for more complex material relations [4] and the relation between $\mathbf{x}$ and $\mathbf{i}$ changes to: $\sum_{k=0}^{\mathrm{N_A}} \mathbf{A}_k\, s^k\mathbf{x} = \sum_{k=0}^{\mathrm{N_B}} \mathbf{B}_k\, s^k\mathbf{i}$.

For the multivariate systems, we observe that whereas in (2) the frequency parameter s appears explicitly, other parameters, e.g. the material parameters ε, μ and σ, or geometry parameters are implicitly included in $\mathbf{M}_{\varepsilon}, \mathbf{M}_{\mu}$ and $\mathbf{M}_{\sigma}$ in a nonlinear dependence. Some MOR techniques, though, which will be used in the following, require an explicit dependence on the parameters. For geometrical variations in $x-$, $y-$ and $z-$ direction, denoted by $\boldsymbol{\nu} = (\nu_x, \nu_y, \nu_z)$, with $\nu_u, \in [0, 1], u = x, y, z$, we consider the mesh being stretched rectilinearly according to the geometry variation, so that the mesh topology is maintained. The mesh modifications result in a variation of the geometry dependent material matrices $\mathbf{M}_{\varepsilon}, \mathbf{M}_{\mu}$ and $\mathbf{M}_{\sigma}$. Their substitution in (2) leads to an expression with explicit dependence on s, ν_x, ν_y and ν_z, where the system matrix of the resulting system is a polynomial of time-invariant matrices. Analogous results hold for material variations, take representatively ε, which are easier to consider, though, as no series expansion is required. Let $\mathbf{D}_{\varepsilon_1}, \mathbf{D}_{\varepsilon_2}$ be the material matrices corresponding to the parameters $\varepsilon_1, \varepsilon_2$, respectively. The matrix corresponding

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to any ε is then: $\mathbf{D}_\varepsilon = \mathbf{D}_{\varepsilon,1} + (\mathbf{D}_{\varepsilon,2} - \mathbf{D}_{\varepsilon,1})\nu_\varepsilon,\ \ \nu_\varepsilon \in [0 \dots 1]$. Thus, from (2), an explicit dependence on both s and ε follows. The systems obtained from material and geometrical variations can be generalized with the help of systems which are set up by multivariate matrix polynomials of degree $|\boldsymbol{\alpha}|_{\max}$ and r scalar variables $s_1, s_2, \dots, s_r \in \mathbb{C}$.

$$\left(\sum_{|\boldsymbol{\alpha}|=0}^{|\boldsymbol{\alpha}|\le|\boldsymbol{\alpha}|_{\max}} \mathbf{s}^{\boldsymbol{\alpha}}\mathbf{A}_{\boldsymbol{\alpha}}\right)\mathbf{x}(\mathbf{s}) = \left(\sum_{|\boldsymbol{\alpha}|=0}^{|\boldsymbol{\alpha}|\le|\boldsymbol{\alpha}|_{\max}} \mathbf{s}^{\boldsymbol{\alpha}}\mathbf{b}_{\boldsymbol{\alpha}}\right)\mathbf{i}(\mathbf{s}), \quad \mathbf{u}(\mathbf{s}) = \left(\sum_{|\boldsymbol{\alpha}|=0}^{|\boldsymbol{\alpha}|\le|\boldsymbol{\alpha}|_{\max}} \mathbf{s}^{\boldsymbol{\alpha}}\mathbf{c}_{\boldsymbol{\alpha}}^{*}\right)\mathbf{x}(\mathbf{s}). \tag{3}$$

where $\boldsymbol{\alpha} = (\alpha_1, \dots, \alpha_r)$ is a multiindex, [6], and $\mathbf{A}_{\boldsymbol{\alpha}} \in \mathbb{C}^{n\times n}, \mathbf{x}, \mathbf{b}_{\boldsymbol{\alpha}}, \mathbf{c}_{\boldsymbol{\alpha}} \in \mathbb{C}^{n\times 1}$. For simplicity reasons we consider single-input-single-output systems and therefore use $\mathbf{b}_{\boldsymbol{\alpha}}, \mathbf{c}_{\boldsymbol{\alpha}}$ instead of matrices $\mathbf{B}$ and $\mathbf{C}$.

2 MOR-Techniques for univariate and multivariate dynamical systems

For the systems $\boldsymbol{\Sigma}$ defined above, e. g. (2) and (3), a reduced order system $\hat{\boldsymbol{\Sigma}}$ is defined as a system having exactly the same form as $\boldsymbol{\Sigma}$ but with a much smaller dimension. The systems are uniquely determined by their transfer function $\mathbf{H}$, which is defined by $\mathbf{u} = \mathbf{H}\mathbf{i}$, and are given by rational functions [2]. One way to approximate the original system by a reduced order system $\hat{\boldsymbol{\Sigma}}$ is to approximate its transfer function by a rational function of lower degree, e.g. by matching the k lowest moments $\mathbf{H}_i, i = 1 \dots k$ of its Taylor series expansion with the corresponding moments $\hat{\mathbf{H}}_i, i = 1 \dots k$ of $\hat{\mathbf{H}}$. The direct calculation of the moments is an ill-conditioned problem [2]. Thus, implicit methods which iteratively build up the matrix $\mathbf{V} = \text{span}\,(\mathbf{H}_i), i = 1 \dots k$ are preferred. This procedure corresponds to projecting the system on an appropriate subspace and truncation, i. e. with $\mathbf{V}$ a new auxiliary vector $\bar{\mathbf{x}}$ is defined by $\bar{\mathbf{x}} = \mathbf{V}\mathbf{x}$ and then, the system equation is multiplied with a matrix $\mathbf{W}^{\mathrm{T}}$, which we set $\mathbf{W} = \mathbf{V}$, as through this choice stability and passivity are preserved in the reduced model [4]. The implicit iteration used is the Arnoldi algorithm, which produces $\mathbf{V}$, such that $\text{colsp}\{\mathbf{V}\} \supseteq \mathcal{K}_q(\mathbf{A}, \mathbf{x})$, where $\text{colsp}\{\mathbf{V}\}$ denotes the column space of $\mathbf{V}$ and $\mathcal{K}_q(\mathbf{A}, \mathbf{x})$ is the Krylov subspace related to $\mathbf{A}$ with dimension q. In this way, the original system $\boldsymbol{\Sigma}$ is reduced to the system $\hat{\boldsymbol{\Sigma}}$. For powers of $s > 2$, as e. g. in $\sum_{k=0}^{\mathrm{N_A}} \mathbf{A}_k\ s^k\mathbf{x} = \sum_{k=0}^{\mathrm{N_B}} \mathbf{B}_k\ s^k\mathbf{i}$, the classical Arnoldi is not applicable and the well conditioned asymptotic waveform evaluation (WCAWE), [3, 4], is used instead.

For the multivariate case, we consider the multivariate Taylor series expansion of $\mathbf{x}(\mathbf{s})$ and $\mathbf{H}(\mathbf{s})$ around the expansion point $\mathbf{s}_0$ along with their iteratively determined moments $\mathbf{x}_{\boldsymbol{\beta}}$ and $\mathbf{H}_{\boldsymbol{\beta}}$ [5, 6]:

$$\mathbf{x}(\mathbf{s}) = \sum_{|\boldsymbol{\beta}|=0}^{\infty} \mathbf{x}_{\boldsymbol{\beta}}(\mathbf{s}_0)(\mathbf{s}-\mathbf{s}_0)^{\boldsymbol{\beta}}, \quad \mathbf{H}(\mathbf{s}) = \sum_{|\boldsymbol{\beta}|=0}^{\infty} \mathbf{H}_{\boldsymbol{\beta}}(\mathbf{s}_0)(\mathbf{s}-\mathbf{s}_0)^{\boldsymbol{\beta}}, \quad \mathbf{x}_{\boldsymbol{\beta}} = \mathbf{A}_{\mathbf{0}}^{-1}\,(\mathbf{b}_{\boldsymbol{\beta}} - \sum_{|\boldsymbol{\alpha}|=1}^{|\boldsymbol{\alpha}|\le|\boldsymbol{\alpha}|_{\max}} \mathbf{A}_{\boldsymbol{\alpha}}\mathbf{x}_{\boldsymbol{\beta}-\boldsymbol{\alpha}}), \quad |\boldsymbol{\beta}| \le q. \tag{4}$$

Analogous results hold for the reduced order model, with $\hat{\mathbf{A}}_{\boldsymbol{\alpha}}, \hat{\mathbf{b}}_{\boldsymbol{\alpha}}, \hat{\mathbf{c}}_{\boldsymbol{\alpha}}$ and $\hat{\mathbf{x}}$. If we choose $\mathbf{V}$ such that

$$\det(\mathbf{W}^{\mathrm{T}}\mathbf{A}_{\mathbf{0}}\mathbf{V}) \neq 0, \quad \text{span}\left\{\bigcup_{|\boldsymbol{\beta}|=0}^{|\boldsymbol{\beta}|\le q} \mathbf{x}_{\boldsymbol{\alpha}}\right\} \subseteq \text{colsp}\mathbf{V}, \tag{5}$$

then the first moments of the multivariate Taylor series expansion of $\mathbf{x}(\mathbf{s})$ around an expansion point $\mathbf{s}_0$ match those of $\hat{\mathbf{x}}(\mathbf{s})$, [5,6]. The direct calculation of the moments is an ill-conditioned problem and is therefore replaced by numerically stable and efficient algorithms, e. g. the multivariate Arnoldi and the contraction method presented below.

For the first method, let the first k moments $\mathbf{x}_{\boldsymbol{\beta}}$ be numbered by $i = 1, \dots, k$, i. e. $\mathbf{x}_{\boldsymbol{\beta}_i}$ and let $\mathbf{v}_1, \dots, \mathbf{v}_k$ be an orthonormal basis of span $\{\mathbf{x}_{\boldsymbol{\beta}_1}, \dots, \mathbf{x}_{\boldsymbol{\beta}_k}\}$ which we wish to extend by $\mathbf{v}_{k+1}$ with the help of the moment $\mathbf{x}_{\boldsymbol{\beta}}$. With the reduced QR-factorization of $[\mathbf{x}_{\boldsymbol{\beta}_1} \dots \mathbf{x}_{\boldsymbol{\beta}_k}]$ we can write for each i: $\mathbf{x}_{\boldsymbol{\beta}_i} = \mathbf{V}_k\mathbf{h}_{\boldsymbol{\beta}_i}$, where $\mathbf{h}_{\boldsymbol{\beta}_i}$ are the coordinate vectors. Thus, from (4) we obtain (6), which is then separated in terms of $\mathbf{h}_k$ and $\mathbf{r}_k$ into horizontal and perpendicular components of span($\mathbf{V}$) by summing up the horizontal and perpendicular parts of all $\mathbf{A}_{\mathbf{0}}^{-1}\mathbf{A}_{\boldsymbol{\alpha}}\ \mathbf{V}_k, \forall\boldsymbol{\alpha}, |\boldsymbol{\alpha}| \le |\boldsymbol{\alpha}|_{max}$ with respect to colspan $(\mathbf{V}_k)$.

The new basis vector and the corresponding coordinate vector follow immediately

$$\mathbf{x}_\beta = \mathbf{A_0}^{-1}\left(\mathbf{b}_\beta - \sum_{|\alpha|=1}^{|\alpha|\le r} \mathbf{A}_\alpha \mathbf{V}_k \mathbf{h}_{\beta-\alpha}\right) = \mathbf{V}_k \mathbf{h}_k + \mathbf{r}_k, \quad \mathbf{v}_{k+1} = \frac{\mathbf{r}_k}{\|\mathbf{r}_k\|}, \text{ and } \mathbf{h}_{\beta_{k+1}} = \begin{pmatrix} \mathbf{h}_k & \|\mathbf{r}_k\| \end{pmatrix}'. \tag{6}$$

The contraction method starts from relating the Taylor series expansion of $\mathbf{x}$ in (4) with the resolution of (3),

$$\mathbf{x}(\mathbf{s}) = \sum_{k=0}^{\infty} \sum_{|\beta|=k} \mathbf{x}_\beta(\mathbf{s}_0)(\mathbf{s}-\mathbf{s}_0)^\beta = \sum_{k=0}^{\infty} \mathbf{A_0}^{-1} \left(\sum_{|\alpha|=0}^{|\alpha|\le|\alpha|_{\max}} \mathbf{s}^\alpha \mathbf{A}_\alpha \right)^k \left(\sum_{|\alpha|=0}^{|\alpha|\le|\alpha|_{\max}} \mathbf{s}^\alpha \mathbf{b}_\alpha \right) \mathbf{i}(\mathbf{s})). \tag{7}$$

in which $\sum_{\beta_k} \mathbf{x}_\beta(\mathbf{s}_0)(\mathbf{s}-\mathbf{s}_0)^\beta$ is a homogenous polynomial in r variables with degree k. Let $\mathbf{p} = \mathbf{s} - \mathbf{s}_0$ and consider sets $\mathcal{S}_0 \subset \ldots \mathcal{S}_k \subset \ldots \mathcal{S}_q \subset \mathbb{R}^r$ in which $\mathcal{S}_k, k = 0 \ldots q$ is unisolvent in homogenous polynomials of degree k in r variables, i. e. any polynomial with r variables and degree k is completely determined by its values at the points of $\mathcal{S}_k$ [5]. For example, $\mathcal{S}_k$ can be given by $\mathcal{S}_k = \{(\boldsymbol{\gamma}, q-|\boldsymbol{\gamma}|,\ |\boldsymbol{\gamma}| \le k)\},\ k = 0 \ldots q$ in which $\boldsymbol{\gamma}$ is a multiindex of dimension $r-1$. For $|\boldsymbol{\beta}| \le q$ the determination of the moments of the multivariate problem is reduced to the calculation of Krylov subspaces of univariate models at the points $\mathbf{p} \in \mathcal{S}_k$, which as mentioned before, can be reduced by using the WCAWE:

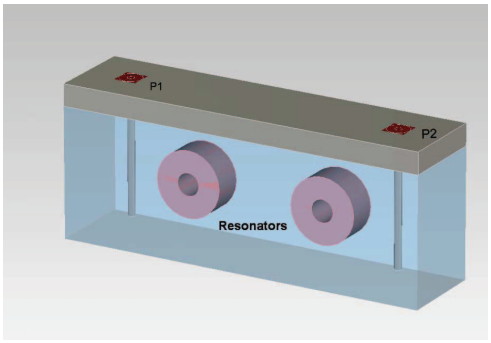
$$\bigcup_{|\boldsymbol{\beta}|\le q} \text{colspan}\,\{\mathbf{x}_\beta(\mathbf{s}_0)\} = \bigcup_{\mathbf{p}\in\mathcal{S}} \mathcal{K}_{q+1} \left\{ \mathbf{A_0}^{-1} \left(\sum_{|\alpha|=0}^{|\alpha|\le|\alpha|_{\max}} \mathbf{s}^\alpha \mathbf{A}_\alpha \right), \left(\sum_{|\alpha|=0}^{|\alpha|\le|\alpha|_{\max}} \mathbf{s}^\alpha \mathbf{b}_\alpha \right) \mathbf{i}(\mathbf{s}) \right\}. \tag{8}$$

Both methods introduced above require an explicit dependence on the parameters, as in (3), which is naturally not given for FIT systems in (2). The curl-curl equation (2) can only be linearized as described in section 1 when the mesh topology is fixed for all parameter changes. Obviously, this is a strong limiting factor for geometrical variations, as the systems often result from FIT-models with automatically created meshes, which are not necessarily the same. For material parameters, though, these methods are appropriate, as will be shown in the example section.

Finally, in the last approach presented here, the neighbouring subspace method, the topology preservation assumption is circumvented by using univariate MOR methods on several expansion points within the parameter range. We pick several expansion points $\mathbf{s}_i, i = 1 \ldots N$ from (2) and build up the matrix $[\mathbf{V}_1 \mathbf{V}_2 \ldots \mathbf{V}_N]$. A singular value decomposition (SVD) [2] is applied in order to sort the directions by relative importance. The necessary condition for this method is the size of the system matrices to remain the same during the parameter variations. This can be achieved by freezing the mesh for one parameter and discretizing the whole structure on this fixed mesh, e. g. for the nominal value of the parameter while taking advantage of the perfect boundary approximation (PBA) feature in FIT. The PBA uses partially filled cells which allow an exact discretization of curvilinear boundaries of structures. Locally, it acts as a modified mesh cell, with the important difference that only one mesh cell is affected with no impact on the rest of the mesh. This fact can be used for handling geometry variations, even radial, in multivariate MOR.

3 Numerical Example

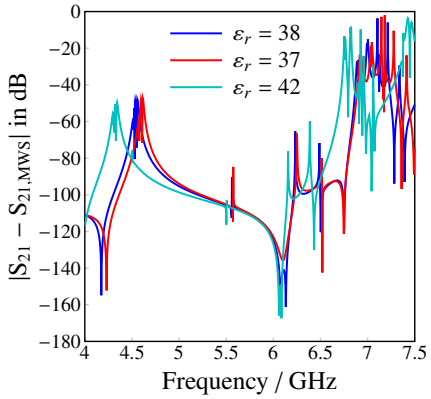
The Langer filter depicted in Fig. 1 is used for testing the contraction for a variation of the permittivity ε ot the cylindrical inclusions and the neighbouring subspace method for a variation of the radius of the inclusions. The parameter range for both methods are shown in Fig. 1. For both methods the transmission factors S_{21} are compared with respective FIT full-wave comparison solutions and the logarithmic error is shown in Fig. 2a and Fig. 2b, respectively.



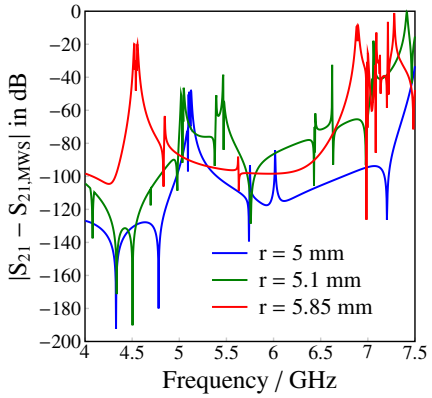
Contraction Method Parameter Range	
frequency s	4 . . . 7.5 GHz
permittivity ε_r	34 . . . 43 (38)

Neigbouring Subspace Method Parameter Range	
frequency s	4 . . . 7.5 GHz
radius r	5 . . . 6.4 (5.85mm)

Figure 1: Langer filter modeled with the FIT method. The nominal values of ε and r are placed in brackets.



(a) The error of S_{21} in dB in the frequency range 4 to 7.5 GHz for different arbitrary permittivity values ε_r. The projection matrix had 90 columns. The order q was 8 and the order of the WCAWE was $q_{\mathrm{WCAWE}} = 18$. The calculation time for $\mathbf{V}$ was approx. 47 min. The time for calculating the S_{21} of the reduced model was 12 s.



(b) The absolute logarithmic error of S_{21} in the frequency range 4 to 7.5 GHz for different radii r. The used projection matrix had 54 columns, 3 expansion points have been used, with 20 vetors each. The calculation time of $\mathbf{V}$ was approx. 15 min.

Figure 2: Logarithmic error of S_{21} with respect to the MWS comparison solution of the Langer filter using the contraction (left) and the neighbouring subspace method combined with the partially filled mesh feature of MWS (right).

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