Practical issues of Model Order Reduction with Krylov-subspace methods

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Abstract
Model Order Reduction plays an increasingly important role in electronic simulations. The actual implementation of the methods however, leads to many practical problems. In this paper orthogonalisation in Krylov subspace methods and realization of reduced models are discussed. Validation of the methods is done in an existing layout simulator.

Introduction
The continuing trend towards higher frequencies and smaller feature sizes forces the designer of electronic circuits to take into account the electromagnetic effects caused by the interconnect structures. Straightforward coupling of circuit simulators with Maxwell solvers is prohibitive because of the large computational effort associated with this. Also, it seems unnecessary to use a detailed simulation of the electromagnetic effects for current problems. Therefore, one often attempts to capture the main electromagnetic effects into a compact model for the interconnect structure, and couples this to the circuit simulation programme.
In this process, Model Order Reduction methods play an increasingly important role. Especially Krylov-subspace methods have shown themselves to be very accurate and suited for this area of application [1,2]. These Krylov-subspace methods are well-known and used in many different applications. Not only linear time invariant (LTI) systems can be subject of these methods, also weakly non-linear or quadratic models are treated in the same way as LTI systems [3]. Many of these methods guarantee preservation of passivity, which makes them even more interesting.
The actual implementation of Model Order Reduction methods leads to many practical problems. Several issues will be discussed in this paper. The paper is built up as follows. First the basic idea of Model Order Reduction via Krylov-subspaces is explained. Then, in the following section, we take a closer look to orthogonalisation of the Krylov space. Accuracy and efficiency of the methods can be influenced after taking care of the orthogonalisation of the Krylov space. Further, the realization of the reduced model is addressed. We are convinced that being able to translate the reduced system into a circuit, which can be treated by a circuit simulator, has tremendous advantages.
Finally, in this paper we will show an example of the application of our methods to the modelling of a large 2D PCB problem. The models of this PCB are formulated as an n-port. The ports of the model are preserved during reduction and to these ports, other components or models can be attached. If the number of internal nodes is much larger than the number of ports, a significant reduction both in size of the model and in computational time is obtained and transient results are available.

Model Order Reduction
In general the systems considered in this paper have the form:

$$\begin{pmatrix} \mathbf{C} & \mathbf{0} \\ \mathbf{0} & -\mathbf{L} \end{pmatrix} \tfrac{d}{dt}\mathbf{x}(t) + \begin{pmatrix} \mathbf{G} & \mathbf{P}^T \\ \mathbf{P} & -\mathbf{R} \end{pmatrix} \mathbf{x}(t) = \mathbf{B}_i \mathbf{u}(t)$$

$$\mathbf{y} = \mathbf{B}_o^T \mathbf{x}(t)$$

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Many methods for modelling passive electronic components or circuits can be formulated in this way. A nice example of this statement is the Partial Element Equivalent Circuit method (PEEC) by Ruehli [5]. In [4] a similar method is derived. Adding some extra conditions, these equations can be translated into an RLC-circuit. In that case, the state space vector **x** consists of voltages and currents. If the system has more than one input, then $\mathbf{B}_i$ has more then one column.
A common way to find a solution for these systems is to transform the system into the frequency domain, applying a Laplace transform. The derivative $\frac{d}{dt}\mathbf{x}(t)$ is then transformed to $s\mathbf{X}(s)$. The complex variable s can be interpreted as a complex frequency. By eliminating the state space vector a transfer function can be formulated, which gives a direct relation between input and output in the frequency domain:

$$\mathbf{H}(s) = \mathbf{B}_o^T(\mathbf{G} + s\mathbf{C})^{-1}\mathbf{B}_\mathbf{i}$$

There are many methods to replace this large and expensive model by a smaller model, which approximates the behaviour of the original system. In general, a frequency range in which the approximation must be reasonable, is predefined. Krylov subspace methods do this by generating a Krylov space $\mathcal{K}(\mathbf{B},\mathbf{A}) = [\mathbf{B}_i, \mathbf{A}\mathbf{B}_i, \mathbf{A}^2\mathbf{B}_i, ...]$ and then projecting the original system onto this space. If the number of columns of this space is smaller then the size of the original system, the system is reduced. The transfer function of the reduced system can be formulated as:

$$\tilde{\mathbf{H}}(s) = \tilde{\mathbf{B}}_o^T(\tilde{\mathbf{G}} + s\tilde{\mathbf{C}})^{-1}\tilde{\mathbf{B}}_\mathbf{i}$$

In the time domain the reduced model will be formulated as:

$$\tilde{\mathbf{C}}\frac{d}{dt}\tilde{\mathbf{x}}(t) + \tilde{\mathbf{G}}\tilde{\mathbf{x}}(t) = \tilde{\mathbf{B}}_i\mathbf{u}(t)$$

$$\hat{\mathbf{y}} = \tilde{\mathbf{B}}_o^T\tilde{\mathbf{x}}(t)$$

The advantage of Krylov subspace methods is that they are cheap and generally applicable.

There are several properties of the original transfer function which have to be preserved during reduction, to be able to speak of a good approximation. To start with, obviously the behaviour of the system should be approximated well. Because we have a closed relation in the frequency domain for this behaviour, the main goal of many Model Order Reduction methods is to approximate the behaviour in the frequency domain. However, finding a good approximation, does not guarantee stability. Stability, the property that in time domain the signal stays bounded, is a very important property. In frequency domain stability is defined as: all poles of the system are in the closed half plane of the complex plane. Poles are defined as follows: all s for which the inverse of **(G+***s***C)** does not exist. PVL, proposed by Freund and Feldmann in [6] is an example of a MOR method, which approximates the frequency behaviour of a system well, but does not always preserve stability. For the methods proposed in [1] and [2] it can be proven that stability is preserved during reduction.
Next to being stable, an RLC circuit is also passive. Passivity is defined as the inability to generate energy. Passivity is stronger than stability. A passive circuit is stable if it is combined with any feedback loop. Passivity should also be preserved by a MOR method.

Orthogonalisation

One of the issues one has to deal with in implementing Krylov-subspace methods is the orthogonalisation of the Krylov-space.
In a Krylov space the vector or block of vectors $\mathbf{B}_i$ is repetitively multiplied by the matrix **A**. Because of this repetitive multiplication the columns of the space tend to the dominant eigenvector(s) of **A** and the difference between two successive columns becomes very small. Numerically this will lead to severe round-off errors. For accuracy reasons we therefore propose to do the orthogonalisation of the Krylov columns during their generation. So, before a new block is generated, the previous block is orthogonalized with respect to all previous blocks. This improves the numerical properties of the space and avoids the need of an expensive orthogonalisation afterwards, with for instance a Singular Value Decomposition.

In the case where a Krylov space is built up for several right-hand sides simultaneously the orthogonalisation must be done carefully and in the right order. Although in theory the ordering of the columns does not change the span of the Krylov space, in practice one should bare in mind that we deal here with a numerical process. The columns of the Krylov space can be almost dependent. If, in that case, orthogonalisation is not done carefully and in the right order, essential information can be lost and spurious information might be created. In practice we saw some very dramatic examples of this event. A block Arnoldi orthogonalisation as done in [2] provides us with a good order in which the columns of the Krylov space are generated and orthogonalized.

Applying a Block Arnoldi orthogonalisation solely does not ensure accurate approximation. Especially in time-domain simulations one can see significant errors if Block Arnoldi is applied straightforwardly. We used Modified Gram-Schmidt to orthogonalize the separate blocks. But it is known that (Modified) Gram-Schmidt must be applied with care. In practice we saw that some columns in the Block Krylov space, which were orthogonalized, still had inner products of the order 10^{-9} or even bigger, instead of 0, which introduces significant errors. This was already seen with a fairly small amount of columns. As a remedy we did the orthogonalisation a second time, to ensure that the columns in the space are orthogonal up to machine precision. In all our tested cases, applying this re-orthogonalisation once was enough to avoid these problems [7].

In our latest research, the theory of the underlying Krylov spaces provided us an efficient implementation of the algorithms, which orthogonalizes the Krylov subspace during generation in an accurate way. These algorithms were tested and compared to the original implementation and behaved considerably better.

Improvements on the Krylov space

Another important property of the reduced model is, that it should be as small as possible. Therefore we need to have a closer look at the generation of the Krylov space.

If $\mathbf{B}_i$ has more than one column, the Krylov space consists of blocks. The system matrices are projected on an orthonormal basis of this space. If a system has more than one input, a Krylov space is generated which contains the moments of the expansion of the transfer function for every port. If the number of ports is large, the size of our reduction can grow significantly, because every input needs at least a couple of moments in the space. Therefore we want to be as careful as possible with adding extra columns to the space. If a Krylov space is build up in a Block fashion too much information for an efficient Model Order Reduction scheme can be generated. This is because of the fact that while one column in the block has already converged, others could still have to iterate a bit further, to be approximated satisfactory. We would like to stop iterating one column, if this column has converged, without violating the properties of a Krylov space. In our research we found a fairly simple way to implement this wish.

But even with this last improvement, which enabled us to limit the size of the Krylov space associated to different ports, there is still a chance that we generate unwanted information. For instance, if the iterative method finds poles far outside of our spectrum, or poles with a small residue, this information enlarges the model, while it does not add significantly to the accuracy to the model. Using a method similar to Implicit Restart by Sorensen in [8] we are able to remove unwanted poles, from the spectrum of our reduced model.

Realization

The need for a realization of the reduced circuit is obvious, because of the coupling between the Maxwell solver and the circuit simulator, mentioned in the introduction. We would rather not calculate expensive time-domain results via the frequency domain results. We also would like the model to be usable in different settings and for different input signals. We want to represent the reduced n-port model in terms of a circuit, understandable for a circuit simulation.

Note that the state space vector of a general RLC-circuit consists of both voltages and current. In general, projecting the state space vectors, mixes the voltages and current and therefore the reduced system has lost its physical meaning. We propose therefore to define the reduced state space vector consisting entirely of voltage unknowns. The separate rows of the reduced model can then be interpreted as current relations. With a combination of resistances, capacitors and current sources these rows in the reduced matrices can be realized.

Because the number of ports is preserved during reduction, we are still able to couple the ports of the reduced system to the rest of the circuit. With these circuits we were able to do stable transient simulations.

Results

To verify their abilities we applied the proposed MOR techniques in an already existing layout-simulator, Fasterix. Fasterix can handle layered 2D-structures. Firstly, the simulator generates a large RLC-circuit in a PEEC-like fashion [4]. Then, a build-in reduction method, called the super-node algorithm, reduces the system, while keeping a good fit with the original behaviour of the system in frequency domain. The disadvantage of this reduction method, is that is does not guarantee stability for general input of geometry and excitation signal. In order to be able to do time-domain simulations, we applied our proposed Krylov-space method on the large RLC-circuit. In a second step, the reduced system is translated into an equivalent circuit as proposed in a previous section. The time-domain results of this circuit are stable and give a good approximation of the original behaviour (see figure 1(b)).

In [9], which is also presented at this conference, we take a closer look at the actual implications of MOR in Fasterix.

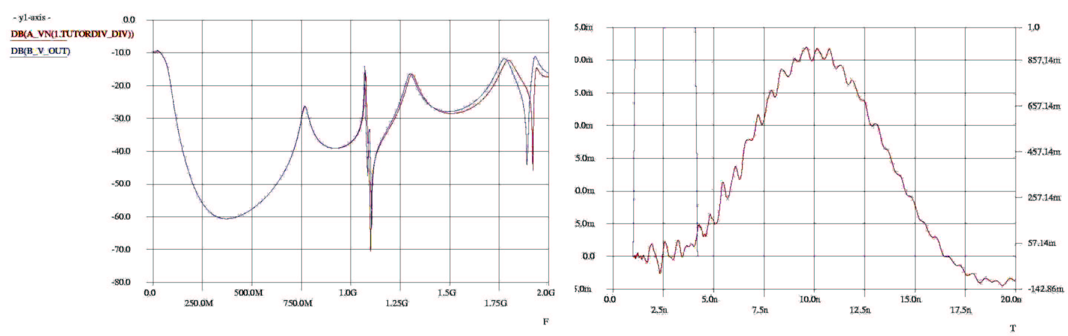

Figure 1: (a) The behaviour in frequency domain can be approximated very well (b) Because of the proven passivity of the realized circuit, transient analysis is possible.

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