Orthogonalisation in Krylov subspace methods for model order reduction

References

[1] M. Kamon and N. Marques and Y. Massoud and L. Silveira and J. White, *Interconnect Analysis: From 3-D Structures to Circuit Models*, Proceedings of DAC (1999)
[2] Luca Daniel and Joel Philip, Model *Order Reduction for Strictly Passive and Causal Distributed Systems*, Proceedings of DAC (2002), 46-51.
[3] H. Yu and L. He, *Vector Potential Equivalent Circuit Based on PEEC Inversion*, Proceedings of DAC (2004).

Orthogonalisation in Krylov subspace methods for model order reduction

P.J. Heres[1] and W.H.A. Schilders[2]

[1] Eindhoven University of Technology, Department of Mathematics and Computer Science, p.j.heres@tue.nl
[2] Philips Research Laboratories Eindhoven

Abstract. Modelling of electronic structures nowadays involves a broad frequency range and coupling of analog and digital behaviour. Much research and increasing computational resources enables the designers to simulate complicated and large structures. One of the approaches to make this modelling feasible is Model Order Reduction. A wide range of different techniques has been investigated in the last few decades. Especially Krylov-subspace methods have proved themselves to be very suitable for this area of application (eg. [2], [3], [5] and [6]). Many of these methods guarantee preservation of passivity, which makes them even more interesting. However, implementing the methods straight-forwardly is not enough to make them applicable for real-life applications. In order to make the methods accurate, efficient and suitable for large systems extra attention and mathematical knowledge is needed. In this paper we will focus on the orthogonalisation of the Krylov space, which is seen to be of importance. Special attention is paid to the orthogonalisation of a Block Krylov space. Also some directions to cheaply avoid some of the redundancy in the Krylov space methods are pointed out in this paper.

Krylov subspace methods. Modelling of an electronic structure leads to the following Differential Algebraic Equation (DAE):

$$\left(\mathbf{C}\frac{d}{dt}+\mathbf{G}\right)x(t)=\mathbf{Bu}(t)$$

$$y(t)=\mathbf{L}^{\mathbf{T}}x(t) \qquad (1)$$

This model can be derived in several ways. It can for instance be a transmission line model, a PEEC model or an FDTD model with spatial discretizations. This system of equations can be transformed to the frequency domain with a Laplace transform:

$$(s\mathbf{C}+\mathbf{G})\mathbf{X}(s)=\mathbf{BU}(s)$$

$$\mathbf{Y}(s)=\mathbf{L}^{\mathbf{T}}\mathbf{X}(s) \qquad (2)$$

When the state space vector in frequency domain *X(s)* is eliminated, a transfer function is obtained. This transfer function gives a direct relation between input and output of the system. A Krylov-subspace method generates a Krylov subspace based on the input matrix *B* and a generating matrix *A*. For the matrix continuing columns forming a basis for the Krylov space the following basic property holds:

$$\mathbf{AV}_m = \mathbf{V}_{m+1}\mathbf{H} \quad \text{for all } m \, , \tag{3}$$

for some matrix *H*. The actual definition of *B* and *A* depends on the method of choice. In a next step the system matrices are explicitly or implicitly projected onto an orthonormal basis of the Krylov space. If the dimensions of the space are smaller than the dimensions of the original system, an order reduction is achieved. Details can be found in [2], [3], [5] and [6].

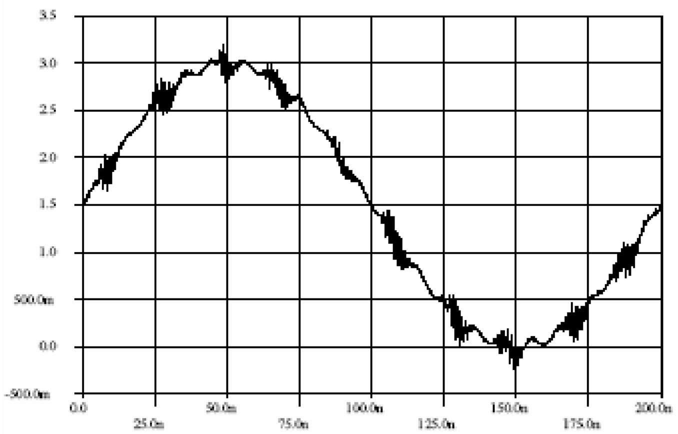
Orthogonalisation. In the mentioned methods an orthonormal basis of the Krylov space must be generated. The orthogonalisation can be done during the generation of the columns or afterwards. The latter occurs in the Laguerre-SVD method [3]. We advocate here the orthogonalisation during the generation of the columns. Then more directions than only the dominant eigenvector can be calculated accurately and severe numerical artefacts are avoided. We therefore propose to orthogonalize a newly generated block of vectors immediately after generation. We used Modified Gram-Schmidt for this and we orthogonalize against all previously generated vectors. Also the vectors in a block are orthogonalized. After the newly generated columns are made orthogonal with respect to all previously generated columns, they are normalized. This procedure costs some computation time, but the accuracy of the method is dramatically increased in all directions. Also numerical artefacts are avoided.
We also propose to apply a second refinement on the orthogonalisation, in order to ensure orthogonality up to the machine precision. This is needed to ensure stability, especially during time domain simulations of the reduced model.

Block Arnoldi Orthogonalisation. When B_i has more than one column, a Block Krylov space is built. Orthogonalisation and normalization in a Block Krylov can be done in several orders. We state that in this case it is important to preserve the basic property of a Krylov space (3). If this property is violated, strange things can happen. We saw already for very small Krylov spaces of 8 columns, that the transfer function did not resemble the original function at all. The order of orthogonalisation in Block Arnoldi Orthogonalisation, as proposed in PRIMA [5] is seen as a right order to orthogonalize a Block Krylov subspace. Here also we applied a second orthogonalisation step, to ensure exact orthogonality.

Further improvements. Krylov-subspace methods are known for their redundancy. The method is relatively cheap, but it can still contain a lot of information which is not really needed for an accurate approximation. Many authors proposed therefore a combination of a Krylov-subspace method with another method, to form a two-step method. First a course approximation is calculated with a cheap Krylov-subspace method. In a second step the order of this approximation is decreased by a more expensive but more controllable method like a Truncated Balanced Realization method [4] or by Proper Orthogonal Decomposition [1]. In our research we discovered that a lot can already be done, very cheaply, during the first run of the Krylov- subspace method.
If a Block Krylov-subspace method is used, it can occur that one of the columns in a new block is almost zero or almost completely spanned by the other columns in the block. In that case we want to stop iterating with this columns, while proceeding with the others. Simply removing information from the space we project on, can lead to the same problems we saw with careless orthogonalisation. With a modified way to calculate a QR-decomposition in the Block Arnoldi Algorithm we are now able to stop iterating with any wanted column, at any wanted time, be-

cause still the basic property of Krylov spaces holds for this algorithm.
Apart from the removal of columns, we also propose a way to remove unwanted poles from the system, without distroying the Krylov space property. This can be done in a way comparable to the Implicit Restarted Arnoldi by Sorensen [7].

Results. All proposed improvements make Krylov-subspace methods suitable for application on real problems. The methods were compared and validated on PCB problems generated by the 2.5D EM similator Fasterix, using a PEEC-like algorithm. Time domain simulations results of a 5000x5000 sized problems, with 57 ports, showed the use of Krylov-subspace methods in an industrial context. The figure below shows the comparison of a 228 sized reduced model with the output of the layout-simulator.



References

[1] G. Berkooz, P. Holmes, and J.L. Lumley. Turbulence, coherent structures, dynamical systems and symmetry. Technical report, Cambrigde Monographs on Mechanics, 1996.
[2] Peter Feldmann and Roland W. Freund. Efficient linear circuit analysis by padé approximation via the lanczos process. IEEE Trans. Computer-Aided Design, 14:137-158, 1993.
[3] Luc Knockaert and Daniel De Zutter. Passive reduced order multiport modeling: The padé-arnoldi-svd connection. Int. J. Electronics and Communications, 53:254-260, 1999.
[4] Bruce. C. Moore. Principal component analysis in linear systems: Controllability, observability, and model reduction. IEEE Trans. Automatic Control, AC-26(1):17-31, 1981.
[5] A. Odabasioglu and M. Celik. Prima: Passive reduced-order interconnect macromodeling algorithm. IEEE. Trans. Computer-Aided Design, 17(8):645-654, August 1998.
[6] D. Skoogh. A rational krylov method for model order reduction. Technical Report 1998-47, Department of Mathematics, Chalmers Unversity of Technology and the university of Goteborg, Goteborg, 41296, Sweden, 1998.
[7] D.C. Sorensen. Implicit application of polynomial filters in a k-step arnoldi method. SIAM J. Matrix Analysis and Applications, 13(1):357-385, January 1992.