To this end, taken from current mechanical engineering practice, there are two popular methods, and both are incorporated in some commercial software simulation tools: modal reduction [4] and dynamic conden- sation [5]. The idea behind modal reduction is to approximate a dynamic system response through a linear combination of several, often low-frequency, natural eigenmodes of the system. The second approach is based on the Guyan method [6], and is just an intuitive engineering extension of the Shur complement method from a stationary to a time-dependent formulation. The main problem with all of the above order reduction methods is that their success primarily depends on engineering intuition, since they are not based on a solid mathematical background. Hence, they could	the most striking examples here being car crash simulations (see, for example, Ref. [2]). Nevertheless, this typically requires parallel computations (see the benchmark report in Ref. [3]) which increases the cost of simulation drastically, and as a result, limits simulation applicability considerably. In order to facilitate computations, engineers often simplify the original rigorously derived governing equations or, instead, use simple empirical models: we use the term "quick-and-dirty" (QAD) calculations. Another approach, the topic of the present article, is to perform model reduction, that is, to formally reduce the dimension of a system of ODEs derived from a rigorous approach before integrating it in time.	 www.imtek.uni-freiburg.de/simulation korvink@inttek.uni-freiburg.de preprint submitted to Sensors Update, Feb. 2002 1. Introduction The goal of MEMS computer-aided design and simulation is to accurately and efficiently represent the behavior of the system in question. This allows technologists to develop a better understanding of the sys- tem, and as a result, to quickly choose an optimal design. A hugely successful example of the application of computer-aided design (CAD) is in the simulation of electrical integrated circuits, for which the simulator's output is almost the same as that produced by a real circuit prototype. This drives MEMS-designers to cre- ate similar techniques for MEMS simulations. It so happens that electrical circuit and MEMS simulations are quite different in nature (see, for example, the discussion in Ref. [1]). A circuit is rather accurately described by lumped elements such as discrete resistors, capacitors, inductors, transistors and so on. The transient response of the circuit can be immedi- ately written as a system of ordnary differential equations (ODEs) with the system's dimension of the order of the number of nodes connecting lumped elements in the circuit. On the other hand, the governing partial differential equations (PDEs) for MEMS-devices do not always lend themselves to intuitive lumping as ODEs, and hence are solved numerically by first spatially semi-discretising them by means of finite ele- ment, boundary element and similar methods. This also leads to a system of ODEs, but its dimension depends on the quality of discretization, and it could routinely lead to ODE system sizes of between ten thousand and a million equations, especially in the case of 3D simulations. The relation between differen- tial equations, models are shown in Fig. 1. 	Kevrew: Automatic Model Keduction for Transient Simulation of MEMS-based Devices Evgenii B. Rudnyi and Jan G. Korvink IMTEK—Institute for Microsystem Technology Albert Ludwig University Freiburg
In principle, a system of ODEs can also be solved faster if it is possible to increase the efficiency of the time integrator. Recently, there have been some promising results in this direction based on matrix exponential approximations [10], but so far there are no engineering examples, and hence this will be outside of the scope of our review. We start our review with a statement of the mathematical problem for model reduction, where we introduce terms and give them the equivalents used in the MEMS community. Then we consider low-dimensional linear systems of ODEs. It is safe to state that, for this case, the problem of automatic model reduction is almost completely solved. It appears that almost all modern model reduction methods for large-scale systems are based, in one way or another, on Krylov subspace methods [11], and therefore a	Nevertheless, the classification in this review is made on the basis of a mathematical perspective and therefore follows the structure of Ref. [7]. What we have found is that, even though different engineering communities are facing quite different challenges, many solution techniques are related. At a first glance, the simulation of groundwater flow in discretely fractured porous media has nothing to do with MEMS-devices. It is therefore not surprising that these two engineering communities do not follow each other's work. However, the model reduction problem they are trying to solve is absolutely the same if we consider it from a mathematical viewpoint.	PDEs & Geometry Discretization Mesh Reduced Order Fig. 1 Some of the routes leading from a device description to a reduced order system of ODEs. The arrows represent translations between descriptions: 1) Lumping is done by hand, either as a circuit equivalent, or as an algebraic expression; 2) Adaptive meshing determines the size of the subse- quent model; 3) Circuit equivalents or algebraic model reducer take a large system of ODEs. The anesh result in a set of ODEs; 5) An algebraic model reducer take a large system of ODEs and pro- duces a smaller (and hence reduced order) yet equivalent system of ODEs. be referred to as non-automatic model reduction methods, and there appears to be no way to improve this situation. Certainly, without experience and intuition, we do not recommend their use. On the other hand, model reduction has received a great deal of attention from mathematicians, who have developed a number of methods with which to approximate large-scale dynamics systems (for a mathemat- ical review, see Ref. [7]), and which to improve the sautomatic model reduced by several orders of magnitude, almost without sacrificing precision, see e.g. [8] and [9]. However, there still remains a certain gap between these ideas and common MEMS engineering practice, and the aim of the present review is to start to fill this gap. Our review complements Ref. [7] (where automatic model reduction is considered mathematically) on the	Device Description I Pirect Translation I Discrete System of ODEs

ы system of algebraic-differential equations (ADEs). From a computational point of view the operations in tion is possible in principle. If matrix E is degenerate then we do not have a system of ODEs, but rather a Mathematically this implies that matrix E is not degenerate (i.e., it is invertible) and that this transformawhere together with the new variables z = dy/dt, becomes ond order in time. It is a simple matter to convert them to the form of Eq (1) by increasing number of systems in motion, as well as general electrical circuits, are usually described by systems of ODEs of secficients depend on time explicitly in which case it is termed a linear time-varying system [12]). Mechanical wise we will call it nonlinear. (Strictly speaking this is not correct. There is an intermediate case when coefcases, our citations should actually be read as "see, for example, Ref ... ". eral results. Some algorithms for model reduction exist but, in contrast to linear systems, unfortunately, it non-linear systems of ODEs. Here success depends on a particular problem, and there are almost no genis known but the challenge remains as to how to compute it in reasonable time. Finally, we take a look at do not scale to large systems. Here one can say that, in principle, the answer to automatic model reduction power. Computationally speaking, the algorithms for model reduction appropriate for small linear systems system of ODEs depends on the problem dimension (the number of equations in the system) to the cubic of ODEs. The challenge faced here is that the computational time required for a model reduction of a linear short introduction to Krylov subspace methods is given. After that, we switch to large-scale linear systems tion step, we rewrite Eq (1) from an implicit to an explicit system of ODEs plines, but we hope that this does not pose an insurmountable problem. In order to perform a model reducsecond order systems of ODE directly. which is again in the form of Eq (1). In some cases the methods treated in the review can be generalized to unknowns and equations by a factor of two, e.g., by treating the first derivatives in time as unknown. Thus the system load. If the matrices contain constant coefficients then the system of ODEs is linear, and other- $F \in \mathfrak{R}^n \times \mathfrak{R}^n$ are system matrices, typically sparse and often symmetric, and the vector $f \in \mathfrak{R}^n$ describes where the unknown vector $\mathbf{x}(t) \in \mathfrak{R}^n$ contains unknowns functions in time, $E \in \mathfrak{R}^n \times \mathfrak{R}^n$ and seems that human intervention is inevitable. It is necessary to stress that Eq (5) should be read in a mathematical, and not in a computational sense. The naming of system matrices as well as the notation is quite different for different engineering disci-In the present review we limit our consideration to a system of first order ODEs, written in the form It should be noted that we have not tried to reflect the priority of research groups in this field. In many **Mathematical Statement for Model Reduction** $A = E^{-1} \cdot F, A \in \mathfrak{R}^n \times \mathfrak{R}^n$ and $\boldsymbol{b} = E^{-1} \cdot f, \boldsymbol{b} \in \mathfrak{R}^n$ $\begin{bmatrix} M & 0 \\ 0 & I \end{bmatrix} \cdot \frac{d}{dt} \begin{bmatrix} z \\ y \end{bmatrix} = - \begin{bmatrix} C & K \\ -I & 0 \end{bmatrix} \cdot \begin{bmatrix} z \\ y \end{bmatrix} + \begin{bmatrix} f \\ 0 \end{bmatrix}$ $M \cdot \frac{d^2 \mathbf{y}}{dt^2} + C \cdot \frac{d \mathbf{y}}{dt} + K \cdot \mathbf{y} = \mathbf{f}$ $E \cdot \frac{dx}{dt} = F \cdot x + f$ $\frac{dx}{dt} = A \cdot x + b$ ઝ 4 6 Ξ 3 follows ODEs. described according to some norm

they destroy the sparsity of the original matrices. In other words, computationally it is necessary to work with the two original sparse matrices. The question on how to effectively compute Eq (5) for the case of Krylov subspace methods is discussed in Section 4.2.

The main problem with Eq (4) is the high dimensionality of the vector x, which is typically equal to the product of the number of unknowns in a system of PDEs to be solved by the number of nodes introduced during the discretization process. This in turn leads to the high dimension of system matrices and finally to the huge computational cost to solve the system's response.

In performing model reduction on Eq (4), the hope is that, for many systems of ODEs of practical importance, the behavior of vector x in time, x(t), is effectively described by some low-dimensional subspace as follows

$$\boldsymbol{x} = \boldsymbol{X} \cdot \boldsymbol{z} + \boldsymbol{\varepsilon}, \ \boldsymbol{z} \in \mathfrak{R}^{k}, \ \boldsymbol{k} < \boldsymbol{n}$$
(6)

Eq (6) states that, with the exception of a small error described by vector $\mathbf{\varepsilon} \in \Re^n$, the possible movement of the *n*-dimensional vector \mathbf{x} belongs, for all times, to a *k*-dimensional subspace, with *k* much smaller than *n*, and is determined by an $n \times k$ transformation matrix *X*. The matrix *X* is composed from *k n*-dimensional vectors that form a basis for the reduced subspace, and the *k*-dimensional vector \mathbf{z} represents a new low order set of coordinates for the given basis.

The task of model reduction is to find such a subspace for which the error difference in Eq (6) is minimal coording to some norm

$$\min \|\mathbf{\varepsilon}(t)\| = \min \|\mathbf{x}(t) - X \cdot \mathbf{z}(t)\| \tag{7}$$

Note that in Eq (7), we have functions in time, so that the norm in this case is represented by some integral over time [13]. When the subspace is found, Eq (4) should be projected onto it, and this projection process produces a system of ODEs of reduced order k

(8)
$$\hat{q} = \hat{y} + \hat{y} + \hat{y} + \hat{y}$$

which can then be used later on, perhaps in another simulation package

The physical background for model reduction so far is that the discretization grid used to solve the original PDEs is far from an optimal basis to represent the solution of the PDEs. From this point of view, the model reduction according to Eq (7) is, in a sense, similar to adaptive grid generation [14]. However, the opportunities of model reduction to minimize the problem dimensionality are much greater, because adaptive grid generation still deals with local shape functions (with local support), and the basis for the lowdimensional subspace in Eq (6) is formed from global domain functions, that is, each vector includes a contribution from the entire geometrical domain (much as eigenvectors do). Form this point of view, model reduction complements adaptive grid generation, or makes an alternative in a sense as will now be described.

An adaptive grid generation process starts with some initial grid, and then the grid in different parts of the computational domain gets refined or coarsened based on a priori or a posteriori local error estimators [15]. A model reduction strategy requires a fine initial grid, for which it produces an effective global low-dimensional basis, based on global error estimators. Then, in order to choose the best computational strategy, it is necessary to compare the time taken for model reduction of a system of ODEs built on the fine grid with the sum of times for adaptive grid generation and the subsequent model reduction of the refined grid system of ODEs.

We now take the next step and put the model reduction problem into a more general form. Often, engineers are not interested in the solution of Eq (4) over the entire computational domain, that is, for values at

Eq (5) are highly disadvantageous: first, they are prohibitively expensive for large-scale systems, second

all nodes, but rather in only a few of their combinations. Control theorists [16] take this into account and convert Eq (4) to

$$\begin{cases} \frac{dx}{dt} = A \cdot x + B \cdot u \\ v = C \cdot x \end{cases}$$

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Equation (9) treats the system as a "black box", which would the case when a system's high-dimensional internal state vector \boldsymbol{x} , governed by ODEs, is not directly accessible to an external observer. The observer can influence the system state by some input functions, specified by the vector $\boldsymbol{u} \in \mathfrak{R}^m$, and which are distributed to the internal nodes in accordance to the *scatter* matrix $B \in \mathfrak{R}^n \times \mathfrak{R}^m$. The number of input signal, the observer is interested in only a few outputs, specified by vector $\boldsymbol{y} \in \mathfrak{R}^p$ with the dimension $p \ll n$. The relationship between required outputs and the system state is given by the *gather* matrix $C \in \mathfrak{R}^p \times \mathfrak{R}^n$. As a result, we have a high-dimensional system of ODEs in relation to vector \boldsymbol{x} , the system state vector, which is governed by a small number of external inputs, and from the viewpoint of an external observer; contains a small number of relevant outputs. We will not describe here the well-known system-theoretic results of this equation, such as zero state and zero input, but refer the curious reader to the control theory literature [16].

Eq (9) is a generalization of Eq (4). If matrix *B* in Eq (9) represents a single vector, equal to vector **b** of Eq (1), then vector **u** will contain only one element, a single input, and we can equate it to a step function. Now let us say that matrix *C* is an identity matrix, that is, y = x, then we have a special case w.r. t. the original system of ODEs, which we call "single input - *complete* output" or SICO.

The multiple input case holds when matrix B has several columns corresponding to multi-load simulations, or when the system is consecutively subject to a variety of loads distributed to different nodes. In this case, each function in vector u has a "step" shape limited by the application time of the load (see Fig. 2).

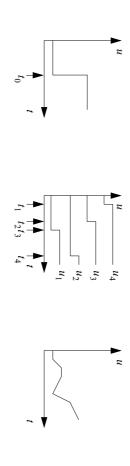


Fig. 2 Different input functions, often provided in engineering simulation programs. a) A step function activating at t_0 . b) A vector of step functions, each activating at a different time. c) A piecewise lin-

ear function

Matrix C is usually formed by picking only those rows from the unit matrix which correspond to chosen nodes. In this case, vector y is just a small subset of the state vector x.

The problem of model reduction in the case of Eq (9) consists in the reduction of the dimension of the state vector to order $k \ll n$, while retaining the same number of inputs and outputs

$$\begin{cases} \frac{d\mathbf{z}}{dt} = \hat{A} \cdot \mathbf{z} + \hat{B} \cdot \mathbf{u} \\ \hat{\mathbf{y}} = \hat{C} \cdot \mathbf{z} \end{cases}$$
(10)

The input vector u in Eq (10) is exactly the same as in Eq (9), but the output vector $y \in \mathfrak{R}^k$ is just some approximation of the original vector $y \in \mathfrak{R}^k$. This transformation is sketched in Fig. 3.

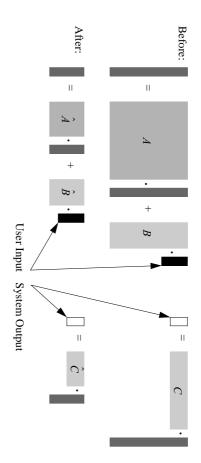


Fig. 3 Sketch of the model reduction equations (9) before and (10) after the model reduction step. The dimensions of the system matrices A, B and C and the internal state vectors z and z are significantly smaller after model reduction. The input vector $\boldsymbol{u} \in \Re^m$ and output vector $\boldsymbol{y} \in \Re^k$ remain the same size.

The quality of the model reduction step of Eq (10) is determined by a norm

$$\min \| \mathbf{y}(t) - \mathbf{y}(t) \| = \min \| \mathbf{y}(t) - \hat{C} \cdot \mathbf{z}(t) \|$$
(11)

which ideally should hold for any input vector $\boldsymbol{u} \in \Re^m$. The difference between Eq (11) and Eq (7) is that now we search for a reduced subspace given by Eq (6) to minimize the difference between given outputs only, and not for the whole state vector. Certainly, if we have found a subspace that minimizes Eq (7), then Eq (11) will be satisfied automatically. However, we expect that a subspace minimizing Eq (11) will have a much lower dimension than a subspace minimizing Eq (7).

If matrices B and C both consist of a single column and row respectively then the system is termed Single-Input-Single-Output (SISO), otherwise it is referred to as Multiple-Input-Multiple-Output (MIMO).

A dynamic system is often considered in the frequency domain, when the Laplace transform operator $L\{.\}$ is applied to the input and output vectors [13]

$$L\{y(t)\} = Y(s), L\{u(t)\} = U(s)$$
(12)

and where the relationship between input and output is described by the transfer function

$$Y(s) = G(s) \cdot U(s) \tag{13}$$

Most of the results in model reduction obtained so far concern the case of a linear system of ODEs and where all the matrices of Eqs (4) and (9) are composed of constant numbers. In this case, the transfer function is readily expressed via the system matrices as

$$G(s) = C \cdot (sI - A)^{-1} \cdot B \tag{14}$$

 1000 to 2000. 4. Introduction to Krylov Subspaces It happens that, in many cases, very good candidates for the required low-order subspace of Eq (6) are Krylov subspaces, and almost all modern model reduction methods for large-scale systems are based on 	The border between small and large systems depends on the computer power available and of course it steadily grows. According to Ref [20], the model reduction of a randomly generated linear system of order 512 takes 76 seconds on a 400 MHz Pentium II processor PC. Since processors now promise 1.2 GHz clock speed, this enables us to define current small systems as those with state vector dimensions in the range of	The time required to solve the Lyapunov equations as well as to perform a singular value decomposition grows as the cubic power in the number of equations, or is $O(n^3)$. Hence, if the system order increases twice, the time required to solve a new problem will increase about eight times. In other words, even though the results described above are valid all linear dynamic systems, practically we can use them for another words.	The SLICOT library implements three methods, a Balanced Truncation Approximation, a Singular Pertur- bation Approximation and the Hankel-Norm Approximation, as well as including a special benchmark problem [20][21]. All three methods and their variations are extensively used in control theory and there are numerous examples of their applications. However, they are out of the scope of the present review, since, due to computational reasons, they are limited to relatively small systems.	Another practical consequence of this result is that the success of model reduction depends only on the decay rate of the Hankel values. Fig. 4 shows examples of the behavior of Hankel values for a few typical applications. If we can estimate this decay rate for a particular application, this would give us a complete answer as to the extent to which we could reduce the original system [18][19].	provided that the Hankel singular values have been sorted in descending order. Note that this equation is valid for arbitrary input functions. This means that model reduction based on these methods can be made fully automatic. A user just sets an error bound and then, by means of Eq (18), the algorithm finds the smallest possible dimension of the reduced system, k , which satisfies that bound. Alternatively, a user specifies the dimension of the reduced system and the algorithm estimates the error bound for the reduced system.	$\sigma_{i} = \sqrt{\lambda_{i}(P \cdot Q)} $ (17) Once these values are known, there are a number of model reduction methods with guaranteed error bounds for the difference between the transfer function of an original <i>n</i> -dimensional system and its reduced <i>k</i> -dimensional system, as follows $\ G - \hat{G}\ _{\infty} \leq 2(\sigma_{k+1} + \dots + \sigma_{n}) $ (18)	$A \cdot P + P \cdot A^{T} = -B \cdot B^{T} $ (15) $A^{T} \cdot Q + Q \cdot A = -C^{T} \cdot C $ (16) for the controllability grammian <i>P</i> and observability grammian <i>Q</i> . Then the Hankel singular values of the original dynamic system are equal to the square root of the eigenvalues of the product of the controllability and observability grammians	3. Small Linear Systems Control theory has a very strong theoretical result for stable systems, <i>i. e.</i> , those systems for which the real parts of all the eigenvalues of the system matrix A in Eq (9) are negative. Each linear dynamic system (9) has <i>n</i> so-called Hankel singular values, σ_i (see Ref. [17] for mathematical details), which can be computed if one solves two Lyapunov equations
The main disadvantage of the Arnoldi method is that each new Arnoldi vector should be orthogonal to all previously generated vectors. This means that the computational cost grows disproportionately with the dimension of the subspace. The current alternative is to use a Lanczos algorithm, where the subspace (19) is considered as a right Krylov subspace. In addition to it, and in parallel, the left Krylov subspace	$X^*AX = H_A$ (20) The Hessenberg matrix for the Arnoldi process is made of an upper tridiagonal matrix plus one diagonal below the main diagonal. It can be considered as an orthogonal projection of the matrix A onto the given Krylov subspace.	4.1 Arnoldi and Lanczos algorithms to build the Krylov subspace A numerically stable procedure for building a Krylov subspace (19) is an Arnoldi process [11][22][23]. It generates an orthonormal basis $X \in \Re^n \times \Re^k$ for the Krylov subspace and a Hessenberg matrix, $H_A \in \Re^k \times \Re^k$, related to the original matrix as follows	tter, tiv	ce of k-th dimension of the matrix $A \in \Re^n \times \Re^n$ and vector $v \in \Re^n$ is defined as a the original vector v and the vectors produced by consecutive multiplication of ector up to $k-1$ times, or $k-1$	 Fig. 4 Decay of normalized Hankel singular values for four typical applications (from Ref. [7]). We expect these curves to also be typical for MEMS. them, one way or another. It should be noted that those iterative methods for solving a system of linear equations that are based on Krylov subspaces have been included in the list of the ten top algorithms of the 20th century [11]. 	-14- -16 -10 -10 -10 -10 -10 -10 -10 -10 -10 -10	-10- -12-	Normalited singular values of Oroso Oranmian X

$${}^{l}_{k}(A^{*}, \mathbf{w}) = span\{\mathbf{w}, A^{*}, \mathbf{w}, \dots, (A^{*})^{k-1}, \mathbf{w}\}$$
(21)

is also generated, where the vector w can be equal or not to vector v, depending on the applications, and A is the conjugate transpose of the matrix A

matrices X and Y such that The Lanczos algorithm produces a pair of biorthogonal bases for subspaces (19) and (21) contained in the

$$X = I \tag{22}$$

 \mathbb{Y}_*

it is necessary to deal with just two previously generated vectors. The Lanczos Hessenberg matrix is related to the original matrix as and a Hessenberg matrix H_L that is in tridiagonal form. This means that, for any iteration of the algorithm,

$$\cdot A \cdot X = H_L \tag{23}$$

∀.

ular to subspace (21). Fig. 5 illustrates the orthogonal and oblique projections of a vector. Because the and can be considered to be an oblique projection of A onto the subspace (19) while remaining perpendic-

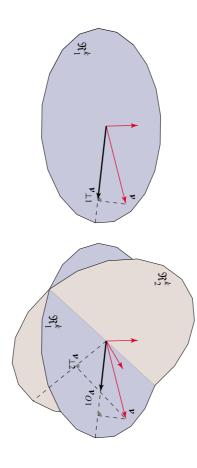


Fig. 5 Example of an orthogonal and an oblique projection of a vector. The disks represent subspaces $\mathfrak{R}_i^t \subset \mathfrak{R}^n$ of the real linear space \mathfrak{R}^n of a model reduction problem. A general vector $\mathbf{v} \in \mathfrak{R}^n$ is on the right demonstrates an oblique projection $v_{01} \in \Re_1^k$ determined by the "shadow" cast by an orthogonal projection of v onto a second subspace $v_{\perp 2} \in \Re_2^*$. projected onto a subspace. The left figure illustrates an orthogonal projection $v_{\perp 1} \in \mathfrak{R}_1^{\kappa}$. The figure

ally less stable than the Arnoldi process: a typical trade-off of accuracy vs. efficiency. The Lanczos and and w are same, in other words, when the Krylov subspaces (19) and (21) are equivalent. Arnoldi algorithms are mathematically equivalent if the matrix A is symmetric and the starting vectors vLanczos algorithm is based on three-term recurrences, it is faster for large k. However, it is computation-

block-Lanzcos algorithms [24][25]. Here we define the appropriate right and left Krylov subspaces as This leads to a generalization of the Arnoldi and Lanzcos algorithms to the so-called block-Arnoldi and Instead of just one starting vector v, one can take a number of starting vectors expressed by the matrix B.

$${}_{k}^{r}(A,B) = \operatorname{span}\{B, A \cdot B, ..., A^{q} \cdot B\}$$
(24)

$$K_{k}^{l}(A^{*}, C) = \operatorname{span}\{C, A^{*} \cdot C, ..., (A^{*})^{q} \cdot C\}$$
(25)

$$(A^*, C) = \operatorname{span}\{C, A^* \cdot C, ..., (A^*)^q \cdot C\}$$
(25)

cations in Eq (24) and (25) in order to generate a k-dimensional subspace. Typically, q is equal to the quoof linearly dependent vectors in (24) and (25). tient of k by the number of columns of the matrices B or C, but the exact answer depends on the existence One difficulty with the block-Krylov subspaces is that it is more difficult to predict the number of multipli-

4.2 Computing the inverse of the system matrix

puter system. the sparse form of the matrices, and to create fast application-specific implementations for the required them a user only needs to provide consecutive matrix by vector multiplications. This allows us to exploit $A \cdot \nu$ product. The driver algorithms do not have to know the details how matrix A is stored in the com-One computational advantage of all Krylov subspace methods is in their iterative nature, *i.e.*, to perform

compute the product matrix A. Recalling Eq (5), this means that for both the Arnoldi and Lanzcos processes it is necessary to For model reduction problems, the Krylov subspace (19) is actually based on the inverse of the system

$$F^{-1} \cdot E \cdot \mathbf{v} \tag{26}$$

spo We now discuss, using this example, the advantage of the iterative structure of the Krylov subspace meth-

computational cost to compute this product is very high due to the presence of the matrix inverse. Hence its direct computation is unwise. It is much more efficient to compute the product $F^{-1} \cdot E \cdot v$. First, before the itive definite matrix, see [23]), which can take into account the sparse structure of F: procedure, one performs an LU-decomposition of F (or equivalently, a Cholesky decomposition for a pos-F and E are large-dimensional sparse matrices, but the product $F^{-1} \cdot E$ might be a dense matrix, and the

$$F = L \cdot U \tag{27}$$

where L and U are lower and upper triangular matrices, respectively. This is costly, but we will require Land U many times. Then, each multiplication $F^{-1} \cdot E \cdot v$ is performed in three steps:

- E is multiplied by \mathbf{v} , $\mathbf{a} = E \cdot \mathbf{v}$. E is sparse and so this is a potentially a fast operation
- a) The linear equations $L \cdot b = a$ are forward solved, so that $b = L^{-1} \cdot E \cdot v$. Since L is lower triangular this is again a fast operation.

2

b) The backward solution of the linear equations $U \cdot c = b$ then gives us the desired product $U^{-1} \cdot L^{-1} \cdot E \cdot v$. Again, since U is upper triangular, this is a fast operation.

access to the full matrix A^{-1} ; otherwise we would have no option but to compute it. Once again, the above speedup is possible only because higher level algorithms do not need to have

much time. Hence, the second step above changes to When the dimension of A grows large enough LU-decomposition is no longer useful because it takes too

ative method can be reasonably fast for a particular F matrix. The linear equations $F \cdot b = a$ are solved by an iterative method, $b = F^{-1} \cdot E \cdot v$. If lucky, an iter-

2

it is important not to confuse them with those reviewed in the present paper. The modified step above matrix P, which transforms the original linear system to an equivalent $P \cdot F \cdot b = P \cdot a$, but which has It should be noted that the success of iterative Krylov methods for a linear solve step depends on the structemplate-oriented review of Krylov-based methods for the solution of linear systems can be found in [26] tions to solve the linear system of equations. In addition to books [22] and [23], an excellent object oriented implies that, for any computation of the subsequent Krylov vector, it is necessary to use second level iterature of the matrix, and for the general case, their effective use requires finding a preconditioner, another Iterative methods for the solution of a system of linear equations are also based on Krylov subspaces, and

rithms for the right (31) and left Krylov subspaces type approximant of the original transfer function (14). On the other hand, if one performs Lanczos algoproduces such matrices H_A and X such that the reduced system that is, number s_o (in most applications $s_o = 0$), k, G(s), which retains the essential behavior of the large-dimensional original rational function. This is of the form of Eq (28) tiple-Output (MIMO) case a transfer matrix is of dimension p by m, each element of which being a function always be expressed in the factored form as of a single column and row accordingly, the transfer matrix (14) is a scalar rational function which can 5.1 and we briefly review them in the second part of this section. ally effective strategies in order to apply methods based on Hankel singular values to large-scale systems start the present section with them. These methods are computationally feasible but, on the other hand, they trol theory algorithms for large-scale systems. As a result, most of the practical work in model reduction of 'n systems that are generated through the discretization of PDEs by the finite element method, refer to Ref implicitly matches the first k moments in Eq (29), that is, the Arnoldi process implicitly produces a Padétem, where all moments will be $p \times m$ matrices. match first q < 2k moments. This is easily generalized to the multiple input - multiple output (MIMO) sys-Padé approximants match the maximum number of moments, q = 2k, while Padé-type approximants formulated in terms of moment matching in the expansion of the transfer functions around some given where z_i and p_i are zeros and poles of the transfer function and a is a constant. In the Multiple-Input-Muldo not provide a global error estimate. Recently, there have been considerable efforts to find computationlarge linear dynamic systems have been tied to Padé approximants of the transfer function (14), and we [27]. superior convergence properties. For a discussion on the importance of preconditioning for solving linear It happens that the Arnoldi process for the right Krylov subspace The idea of Padé [28] and Padé-type [29] approximants is to find a rational function of smaller dimension For the case of Single-Input-Single-Output (SISO) systems, when matrices A and C both are composed As was already mentioned, algorithm time complexity limitations do not allow us to directly employ con-Approximating a Transfer Function by Padé and Padé-type Approximants Large Linear Systems $\hat{A} = H_A^{-1} \cdot (I + s_o H_A), \ \hat{B} = H_A^{-1} \cdot X^* \cdot (A - s_o I)^{-1} \cdot B, \ \hat{C} = C \cdot X$ $K_{k}^{r}\{(A-s_{o}I)^{-1}, (A-s_{o}I)^{-1} \cdot B\}$ $G(s) = \frac{a(s-z_1)...(s-z_{n-1})}{(s-p_1)...(s-p_n)}$ $m_i = \hat{m}_i \text{ for } i = 0, ..., q$ $G(s) = \sum_{i=0}^{\infty} m_i (s - s_o)^i$ (32) (31) (29) (30) (28)greatly simplify for the case of an expansion about $s_0 = 0$, and that there are computationally more effective formulas for producing the reduced matrices B and C. (31) with $s_o = 0$ is a very good choice for the lower dimensional subspace in Eq (6) [8][9][37]-[43]. In reduced model, this does not mean that its computer implementation will really produce a passive model in reduced model. It is also worth noting that, even though when some algorithm provably produces a passive many moments as possible so as to obtain the most accurate representation for the same dimension r of the cess. They seem to prefer, while preserving the properties of the original dynamic system, to match as maticians still bet on the Lanczos algorithms [24][25][35][36], because, as was mentioned above, it takes attention should be paid to preserve the properties of the original dynamical system. It happens that the nately, both the "out-of-the-box" Arnoldi and Lanczos algorithms do not guarantee this, and special position for each value of s_i . zos algorithms were applied to the union of the Krylov subspaces (31) and (33) for different values of s_i . general, they make a good approximation of the transfer function (14) near the expansion point s_o only. by the Arnoldi process does not take into account matrix C at all, while model reduction by means of the because it is possible to recover the solution for all of the original unknowns by means of Eq (6). This work during the discretization of a diffusion-convection partial differential equation, then the Krylov subspace practice, mainly because of the inevitable numerical rounding errors [24] into account the observability matrix C and it matches twice the number of moments of the Arnoldi protion method "block Arnoldi plus congruent transform" or (PRIMA) of Ref. [34]. On the other hand, mathethe coordinate transformed Arnoldi [33] for stable model reduction, and the provably passive model reducprocess and algorithms, respectively). Probably for this reason, engineers often choose the Arnoldi process: Arnoldi process is mathematically more simple than Lanczos algorithm (this is stressed by their names especially in electrical circuit simulations, that the reduced system also possesses these properties. Unfortuinverse of the system matrices (see Section 4.2), then in this case it is necessary to perform an LU-decomhow many are needed. Computationally this adds an additional load. If one uses LU-decomposition for the The main methodological challenge here is to decide how to choose the expansion points, and to determine This idea was implemented in the so-called Rational Krylov method [31][32], where the Arnoldi or Lancpoints s_i and requiring the reduced transfer function to match the first moments at all expansion points account the left Krylov subspace (33). Lanczos algorithm is made by an oblique projection on the right Krylov subspace (31) that takes into moments matched here is twice that of the Arnoldi process. This has a simple explanation. Model reduction which will match 2k moments of the original dynamic system [24][25][30][31]. Note that Eqs (32) and (34) matrices H_L , X and Y produce the reduce system this case, the model reduction step (8) can be viewed as an approximate solution of the original system (4) viewpoint we term it Single-Input-Complete-Output or SICO. It so happens that if system (4) is obtained (bounded), and passive, which is to say, the system does not generate energy. If so, then it is important, This can be improved by multi-point expansion, i.e., expanding the transfer function (14) about several Still, both approaches are based on moment matching and they are by nature local, in the sense that, in Now let us return to the original case of model reduction for systems (4) to (8). From a control theory The Lanczos algorithm produces a reduced system closer to the original one, because the number of The original dynamic system can be stable, that is, when time goes to infinity the values of x remain finite $\hat{A} = H_L^{-1} \cdot (I + s_o H_L), \ \hat{B} = H_L^{-1} \cdot Y \cdot (A - s_o I)^{-1} \cdot B, \ \hat{C} = C \cdot X$ $K_{k}^{l} \Big\{ \left[(A - s_{o}I)^{-1} \right]^{*}, \left[(A - s_{o}I)^{-1} \right]^{*} \cdot C^{*} \Big\}$

(33)

(34)

A general idea to decrease the computational time is to change the exact grammians to their low-rank approximations. It happens that it is possible if the number of inputs and outputs are much less than the dimension of the state vector, $m \ll n$ and $p \ll n$, and this is the case for the most important practical applications. As a result, it is possible to solve Lyapunov equations for low-rank grammian approximations much faster than for exact grammians [64][65][66][67]. For the case of a dense matrix A , the computational time is already proportional to the square of the system dimension n , and it may be linearly proportional to n for the case of a sparse matrix A . Also, the advantage of these methods is that they can be formulated in terms of matrix-vector products only, as for the Krylov subspace methods. The second step, balancing, with	 but mathematically this is identical with a Padé-type approximant (32) when the matrix <i>C</i> is just discarded. We next list examples of the papers in which Padé and Padé-type approximants via Kyptor subspace methods have been used for the model reduction of a linear system (9). The papers come from several distinct communities: The largest community comes from electrical engineering where model reduction is mostly employed to deal with the so-called microchip interconnect problem [44], 45], 480 interconnect and packaging based on an alternate Partial Element Equivalent Circuit (PEEC) formulation [46], Compled losy transmission lines [50], Magetoquasistatic analysis for packaging parasities with skin effect [51], PEEC model of an electronagnetic analyses [54], and Electronagnetic wave propagation by the finite difference method [57]. Acceltatic analysis of packaging parasities with skin effect [51], PEEC model of an electronagnetic analyses [54], and Electronagnetic wave propagation by the finite difference model reduction so model reduction for an electronagnetic maximum on model reduction for the model reduction of a generic nodel reduction is at the beginning stage if we compare the number of papers in which model reduction for an exist on optical tomography problem [44]. Radionuclide decay chain transport in horous media [43]. Gonundwater flow [37]] 88, Mass transport in hydrogeologic environments [39], Photon diffusion optical tomography problem [44]. Radionuclide decay chain transport in dual-poresity media [43], community which has just recently started to exploit the model model for a micromitrific so in work protein method second of the MEMS community which has just recently started to exploit the moden opportunities of devecton-diffusion PDEs, even though this body of work is much closer to typical MEMS simulations. 5.2 Approximating Lypenton Equations 40 molel for a micromitry appears to devecting the solution of the production for as stemestor to typical MEMS community whi	has been superseded by the use of a Krylov subspace (31) to approximate the matrix exponential [10][23],
6.1 Proper Orthogonal Decomposition For systems with strong nonlinear effects, linearization is impossible because a linearized system cannot capture the complexity of the original phenomena. We remind ourselves that nonlinear systems may show instabilities such as snap-through, and bifurcations, and ultimately the onset of chaotic behaviour, all of which should be represented in the reduced system. In this case, in order to find an appropriate low-dimensional subspace (6), one can use results of the full order simulation of the original dynamic system (4), and this is implemented within the proper orthogonal decomposition (POD; another popular name is Karhunen-	into account [62][67]. A very simple case of model reduction arises when the inputs are the same as the outputs, and matrix <i>A</i> is symmetric. Note, that if matrices <i>E</i> and <i>F</i> in Eq (1) are symmetric matrix <i>A</i> [33]. In this case, the grammians are equal to each other because Eqs (15) and (16) become the same: then it is necessary to solve just a single Lyapunov equations (15) and (16), the Sylvester equation [68] (3) find the so-called cross-grammian <i>R</i> . It happens that in the case of a linear dynamic system with a sym- metric transfer function, the Hankel singular values are equal to the eigenvalues of the cross-grammian, and here there is also no need for balancing. This is always true for any SIGO system, because in this case, to convert any linear dynamic system to one with a symmetric transfer function. Some methods for model reduction based on solving large dimensional Lyapunov equations of order more than 12000 were solved by LYPACK within a few hours on a regular workstation. 6. Nonlinear Systems Mow let us allow the elements of the system matrices to depend on the state vector <i>x</i> and on the time. If they depend explicitly on time only, then we have a special case of a time-varying system, and there are examples of extending Krylov subspace model reduction methods to this case [54][70]. Note that, even when system matrices to depend on the state vector <i>x</i> and on the time. If they depend explicitly on time only then we have a special case of a general non-linear system order to make model reduction is to split the whole system into nonlinear and linear parts and then to aphy the model reduction is to split the whole system into nonlinear and linear parts and then to make model reduction of the fresulting linear system. Definitely, the answer as to whether the is possible dependent of the model reduction of nonlinear system sample in Refs [71][72], where, the sequent to aphy the model reduction for the resulting linear is systems applicable to small-dimensional prob- lems (71	the use of low-rank grammians, is also much faster because there are special algorithms that can take this

and, for the general case of Eq (36) , the reduced model becomes	$\hat{A} = X^* \cdot A \cdot X$ and $\hat{b} = X^* \cdot b$ (42)	The final step is to project original non-linear equation onto the low-dimensional basis. For Eq (4), when the elements of A and b depend on x , we can write	depends on the quality of the generated "snapshots", that is, whether they are representative or not.	and Eq (39) actually reduces this norm to a minimum. The problem is that it is difficult to predict, a priori, whether this error estimate can be used for the transition from Eq (4) to (8), because this already strongly	$\ W - \hat{W}\ \tag{41}$	The transition from Eq (37) to (39) can be made completely automatic because according to SVD-theory there is an error estimate based on singular values with the norm	$X = \hat{U} \tag{40}$	where the reduced matrices are formed from the full matrix by leaving only k dominant vectors. Eq (39) shows that all observations are effectively described by a small number of vectors \mathbf{u}_i , which gives a reduced basis on which to project the original differential equation:	$w = \bigcup \cdot \Sigma \cdot v = \sum_{i=1}^{N} o_i (\boldsymbol{u}_i \cdot \boldsymbol{v}_i) $ (39)		where $\Sigma = diag\{\sigma_i\}$ is a diagonal matrix of singular values, $U = \{u_i\}$ is a matrix of left singular vectors, and $V = \{v_i\}$ is a matrix of right singular vectors. Provided the singular values of W rapidly decay we can take only a small number singular vectors, $k \ll s$, corresponding to the largest singular values, and this gives us a low-rank approximation of matrix W of the form	$W = U \cdot \Sigma \cdot V^{T} = \sum_{i=1}^{s} \sigma_{i} (\boldsymbol{u}_{i} \cdot \boldsymbol{v}_{i}^{T}), \ \Sigma \in \Re^{n} \times \Re^{s}, \ U \in \Re^{n} \times \Re^{n}, \ S \in \Re^{s} \times \Re^{s} $ (38)	Nevertheless, the following POD steps are completely formal. For a given "snapshot" matrix W it is formally possible to find a low rank approximation within a given error margin by means of a Singular Value Decomposition (SVD) [7][23]	be taken. Hence, POD is more of an "art", and typically, for any new nonlinear system, it is necessary to make a special investigation in this respect.	choose the most typical input functions, and to perform simulations with them. Unfortunately, there exist almost no formal rules as to how to choose the number "snapshots" to collect and at what times they should	possible to perform model reduction for any input functions, for non-linear systems it is necessary to	generated low-dimensional basis will lead to a poor quality of approximation. If, for linear systems, it was	Eq (4). This is the most crucial step during POD because the reduced basis will be obtained from matrix W only and if it does not give a good representation of the whole ensemble of possible values of \mathbf{x} then the	where matrix W is composed from s state vectors x_i , corresponding to different times of simulations of	$W = \{\mathbf{x}_i\}, \ W \in \mathfrak{R}^n \times \mathfrak{R}^s $ (37)	Let us consider a slightly simplified procedure for a finite-dimensional system. The first step is to perform one or more simulations and to collect a series of so-called "snapshots"	process can be based on the system matrices without performing a full order simulation.	Loève decomposition) [77]. This is the main difference w. r. t. linear systems, where the model reduction
Another problem is that Padé and Padé-type approximants are local by their nature, and they might be not optimal if one would like to obtain a good approximation of the transfer function over a wide range of s ,	approximation does, but for most engineering purposes this should be good enough.	then to use the local error estimate on the border of this range as a monitor as to when to stop the model reduction process, because the approximation error typically increases faster the further on is from the expension point. This procedure still does not give a clobal error estimate as the balanced transation	the transfer function is required. It is possible to set s_0 to an expansion point in the middle of this range and	provided in Ref. [52], where a local error estimate has been suggested for model reduction based on the Lanczos algorithm. First, it is necessary to estimate a range of frequencies in which the approximation of	A typical question with moment matching techniques is: when to stop model reduction. A good strategy is	moments and thus provides a better approximation of the original system. As a result, the Arnoldi process is the best choice for those who would like to implement moment matching methods fast and from scratch,	implement it much easier than the Lanczos algorithm. On the other hand, the latter can match more	tor large-scale linear dynamic time-invariant systems. The moment matching methods for model reduction based on the Arnoldi and Lanczos algorithms are in a mature state. They scale well with the size of the system, their behavior is fairly predictable, and they are easily implemented in almost any computational environment. As was already mentioned, the Arnoldi process is more computationally stable and one can	Let us summarize the current status of automatic model order reduction. The situation is reasonably good	7. Conclusion	outputs, and this limits its applicability in system simulation. Recently, the method has been generalized [98][99] in order to take into account ideas from the linear control theory. The generalization is based on the introduction of "empirical grammians" which are computed based on "empirical snapshots". This opens new perspectives for applications of POD to nonlinear model reduction and hopefully in the future we will see further development of these ideas.	the full SVD decomposition [96][97] and thus keeping computational time within reasonable limits. The original POD procedure does not take into account the information about required evotem inputs and	The SVD decomposition of a matrix is a computationally demanding method: the time grows as the cube of the matrix dimension. This means that when the dimension of matrix W grows we might not have enough computational resources in order to make the decomposition (38). It happens that again iterative methods based on the Krylov subspaces can help to find the dominant singular vectors without performing	linear PDE [88]-[90], and various Mechanical engineering problems [78],[91]-[93]. The MEMS community has also started to employ this technique [71][94][95].	Control of a solid fuel ignition [80], Chemical vapor deposition [81][82] and other Distributed reacting systems [83]-[86], Cascading failures in power systems [87], Feedback control of systems governed by a non-	employed in a variety of disciplines tied with nonlinear dynamics: Rapid thermal processing systems [79],		reduced from 21540 to 15 (about 1500 times) but, because of the above reason, the time of the simulation was reduced only by a factor of six.	then constitutes the main computational cost. For example, in Ref. [78], the size of the state vector has been	computed by means of symbolic manipulations. This is practically unfeasible. In the general case one may only compute the right sides in (42) for each time step during the simulation of the reduced model and this	There is a hidden computational problem with Eq (42), momentarily ignoring Eq (43), which is, how to compute the reduced system matrices. Matrix A contains some functions of x and hence Eq (42) should be		$\frac{dz}{dz} = X^* \cdot f(X \cdot z(t), u(t)) $ (43)

trical engineering $s_o = 0$ seems to be a satisfying choice) and then to employ a truncated balanced approxorder model by means of moment matching techniques around a chosen s_o (for many cases outside of eleclov approximation or to employ a two-step strategy suggested in Ref. [51]. First one computes a medium imation to reduce the intermediate model as much as possible that is, the dimension of the reduced model might then be too large. Here one can think of a Rational Kry-

of the absolute error, but not that well if we consider the relative error. approximation could describe the transfer function behavior quite well if we consider it from the viewpoint range, and if the transfer function changes by many orders of magnitude, then the balanced truncation with the example from Ref. [100]. The norm (18) measures the absolute error over the whole frequency tems right now, provided the minimum over the norm (18) is enough for the application. Let us stress this neers. This will bring us truly automatic model reduction, just as we have for the case of small linear systhis area, and as the experience of mathematicians grows one can expect more practical outcomes for engifor a large linear system. It is quite evident that in the few next years we will see more practical examples in The development of model reduction based on the solution of Lyapunov equations is the next logical step

be inevitable here. First, it is necessary to see if a problem in question can be handled by The situation with nonlinear systems is quite different, and human intervention in some form appears to

- linearization,
- splitting to linear and non-linear subparts,
- some special effective case for a particular nonlinear dynamic system

a special investigation in order to learn the special behaviour and requirements of the system. Nevertheless, erated, and how often. Alternatives here are to follow the example of a similar nonlinear system, or to make when the governing equations can be directly projected to the reduced basis. sible to state that human intervention here is limited to decision making. After a researcher has decided on the POD suggests quite an appropriate framework for general nonlinear model reduction because it is pos-If not then the choice is clearly POD, where the main questions are: how many "snapshots" should be genfor those applications where it is possible to obtain a reduced system matrix (42) in a closed form, that is, how to obtain matrix (37), all other POD steps can be made fully automatic. POD is especially attractive

ç **On-line resources**

slide shows on model reduction with illustrations and examples [101][102]. Below there are homepages of scientists involved in model reduction, in which one can find additional resources: The advent of the internet has made accessible a wide variety of informational resources. There are good

- A. C. Antoulas http://www-ece.rice.edu/~aca/
- P. Benner http://www.math.uni-bremen.de/~benner/
- D. Boley http://www-users.cs.umn.edu/~boley/
- R. W. Freund http://cm.bell-labs.com/who/freund/
- B. B. King http://www.math.vt.edu/people/bbking/ . E. Marsden - http://www.cds.caltech.edu/~marsden/
- S. Lall http://element.stanford.edu/~lall/
- ? Penzl http://www.mathematik.tu-chemnitz.de/in_memoriam/penzl/
- Y. Saad http://www-users.cs.umn.edu/~saad/
- P. Van Dooren http://www.auto.ucl.ac.be/~vdooren/
- A. Varga http://www-er.df.op.dlr.de/staff/varga/

model reduction [106][107], SVD-Krylov model reduction [108], and POD [109][110] ular field: Adaptive meshing [103], Krylov subspaces [104], Control theory [105], Moment matching Also, there are a number of theses, available on the internet, which provide a good introduction in a partic-

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