CSC/DRI group retreat 2020

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BigBlueButton

Book of Abstracts

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A Greedy Update Method in Comparison With the GMREST Method for Nonsymmetric Problems

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In many applications such as parameter-dependent partial differential equations and control theory, matrix equations of the form

$$\sum_{k=1}^{K} A_k X B_k^T = C$$

are of interest. For k, N, $m \in \mathbb{N}$, the matrices involved are $A_k \in \mathbb{R}^{N \times N}$, $B_k \in \mathbb{R}^{m \times m}$, $C \in \mathbb{R}^{N \times m}$ and the unknown is $X \in \mathbb{R}^{N \times m}$. Often, the matrices A_k are not symmetric. The low-rank solver GMREST from [Weinhandl et al. '19] bases on the GMRES method. Its application is not restricted to positive definite problems and can be applied to such matrix equations. Algorithm 4 from [Kressner-Sirkovic '15], a greedy rank-1 update method, was also developed for matrix equations of this kind. In the talk, we will compare the greedy rank-1 update method with the GMREST method for different applications. We will point out, why the application of the greedy rank-1 update method to parameter-dependent fluid-structure interaction problems can be crucial while it clearly outperforms the GMREST method from [Weinhandl et al. '19] in most other cases where the matrices A_k are nonsymmetric for all $k \in \{1, ..., m\}$.

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Damping Optimization of Parameter-Dependent Mechanical Systems using the Reduced Basis Method

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Dampers are used for instance in structure engineering to stabilize constructions, e.g. buildings, bridges or dams. The dampers are externally included to avoid strong movements caused by external forces with frequencies close to the eigenfrequencies of the structure. We want to optimize these dampers in order to stabilize the constructions against external forces.

Our aim is to optimize parameter-dependent dampers that are incorporated into mechanical mass-spring-damper systems. Therefore, we evaluate the input response of the system, which can be computed by solving parameter-dependent Lyapunov equations. To accelerate the optimization process we want to solve the Lyapunov equations by applying the reduced basis method. There we solve the Lyapunov equations on a reduced space that approximates the solution space.
This space is spanned by the low-rank factors of the solutions of the Lyapunov equations, for some test parameters. If the numerical rank of the solutions is large, we face the problem of large reduced spaces.

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Computing Nonlinear Boundary via Exponential Support Tensor Machine

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The machine learning model for binary classification for tensor input data was proposed in my previous work. The main key point was to compute the kernel matrix for each pair of tensor input data, more efficiently. Along with it, we have explained TT-CP expansion and other theoretical aspects of this model which controls the stability and reliability aspects of it.

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In the paper named ``Exponential Machine'',  authors have used linear boundary classification

   I am interested in looking at combining both the results to compute nonlinear boundary (k
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Operator inference combined with neural network to learning nonlinear dynamical systems

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Recently, operator inference (OpInf) approaches have got a lot of attention. They aim at constructing reduced-order modeling directly from the data, without requiring a discretized full-order model. In a recent paper [Benner et. al '2020], the OpInf problem for nonlinear systems was considered, where analytic nonlinear functions of the governing equation are known. However, there are many scenarios, where the exact analytical nonlinear function is not known. The question is: can we learn the nonlinear term using a deep neural network, making the learning dynamical system approach completely black-box?

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How (Not) to Compare Model Order Reduction Algorithms

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Publications on model reduction research typically culminate in the numerical results section, which (supposedly) illustrates or justifies the previous theoretical findings. These numerical experiments generally show results supporting the proposed model reduction algorithm or modification thereof. However, an experimental design or an experiment itself involving model reduction is easily flawed. In this contribution, we will discuss common design pitfalls of computer-based model reduction experiments, recurring misrepresentation or misinterpretation of experimental results, good practices for scientific numerical evaluation of model order reduction algorithms, and review guidelines for model reduction numerics.

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Can we compute the matrix inertia of Kronecker-structured saddlepoint matrices?

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Nonlinear model predictive control schemes solving the step-wise local optimization problems via, e.g. ipopt lead to the necessity to solve large KKT systems in each step of the optimizer. The KKT system itself is a saddle point matrix and, due to the outer MPC approach, ideally has Kronecker structure.

Ipopt uses the matrix inertia of the KKT system to accelerate computations. Classic LU-based solvers use the matrix factorization to derive the inertia as a side product. Due to the Kronecker structure, we want to use structured linear algebra solvers tackling Sylvester-type equations rather than the LU of the large Kronecker matrix. For optimal performance of ipopt, this, however, requires a way to compute or estimate the inertia of the Kronecker matrix from the small block data.

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Choosing Outputs for "good" Riccati Feedback Control of the Stefan Problem

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Our goal is the feedback stabilization of a two-dimensional
two-phase Stefan problem, which can model solidification and melting of pure materials.
The solid and liquid phases are separated by an interface.
We want to control and stabilize the interface position.

After linearization and discretization, the stabilization problem results in a
non-autonomous differential Riccati equation (DRE).
To compute a feedback control, we derive from the solution of the DRE a feedback-gain matrix, which we can apply to the
state-deviation in a perturbed Stefan problem.

The performance of the feedback-control strongly depends on the in- and outputs of the system.
Especially the choice of the outputs is not straightforward.
With different output variants that we tested, the feedback control succesfully stabilizes the interface position.
However, the time-period until a pertubed interface is stabilized back to the desired position is not satisfactory yet.

5

Structured Transfer Functions of Quadratic-Bilinear Systems

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As structured interpolation of transfer functions has been proven to be effective in the setting of structured linear and bilinear systems, we are aiming for a similar structure-preserving model order reduction approach for quadratic-bilinear systems, e.g., for quadratic-bilinear mechanical systems \begin{align} \begin{aligned} 0 & = M\ddot{q}(t) + D\dot{q} + Kq(t)\\ & \quad{}+{} H_{\mathrm{vv}}(\dot{q}(t) \otimes \dot{q}(t)) + H_{\mathrm{vp}}(\dot{q}(t) \otimes q(t)) + H_{\mathrm{pv}}(q(t) \otimes \dot{q}(t)) + H_{\mathrm{pp}}(q(t) \otimes q(t))\\ & \quad{}-{} \sum_{j = 1}^{m} N_{\mathrm{p}, j}q(t)u(t) - \sum_{j = 1}^{m} N_{\mathrm{v}, j}\dot{q}(t)u(t) - B_{\mathrm{u}}u(t),\\ y(t) & = C_{\mathrm{p}}q(t) + C_{\mathrm{v}}\dot{q}(t), \end{aligned} \end{align} with appropriately sized matrices.

So far, there are quite different frameworks for interpolation of unstructured systems in the literature, e.g., based on symmetric or regular transfer functions. We will develop reasonable generalizations of those transfer functions to the structured system case, which can then be used in a structure-preserving interpolation framework.

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Describing Functions (DF) framework for modeling non-linearities

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The main contribution of this work is to provide new insights for capturing the behavior of hard non-linearities beyond the classical weakly nonlinear *Volterra input-output map* (VIOMAP). The VIOMAP approach is a special polynomial map unable to capture hard non-linearities due to the ill-conditioned high polynomial terms. On the other hand, the *describing functions* (DF) framework allows more general map constructions such as rational, which makes the hard non-linear behavior more stable for approximation. Data-driven methods as the *Loewner framework* (LF) can benefit from that concept.

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Extending Reduced Basis Method to Systems Solved by Black-Box ODE Solvers

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The Reduced Basis Method has been quite successful for reducing fully-discretized system of parametric partial differential equations. However, not much is known in terms of applying it to a semi-discretized system of ordinary differential equations, solved by standard black-box solvers,

like `ode45,ode15s`, etc. We intend to investigate the question of how *a posteriori* error estimation can be achieved for such systems.

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Model reduction of the P2D-PSD battery model

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With the numerous applications of batteries ranging from digital devices to electric cars, accurate modelling of batteries has become an essential part of designing efficient and reliable batteries. Up to now, when modelling batteries, people have been assuming constant particle size of the active materials which does not replicate exactly what is happening in reality. However, with the newly introduced, pseudo-two-dimensional particle size distribution (P2D-PSD), a more accurate model of the batteries can be obtained. This introduces more complexity in the system and thus involves more computation time. Our objective is to find a reduced order model that would reduce the computation time while still having an accurate model.

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Robustness comparison of two error estimators

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In a recent research, we have proposed two different error estimators for the reduced transfer functions of parametric linear systems. One is based on the dual-residual system; the other is based on the primal-residual system. Theoretically, they should have similar accuracy. Numerically, we find the primal-residual based estimator is more accurate. Same conclusions are drawn for three different examples. At present, there is no theoretical explanation for the numerical phenomena.

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Optimization of Passive Systems

Author: Tim Mitchell[None]

Co-author: Paul Van Dooren

We present algorithms to compute the extremal value of a real parameter for which a given rational transfer function of a linear time-invariant system remains passive. This quantity is linked to finding a realization of a rational transfer function such that its passivity radius is maximized. We begin by adapting the Hybrid Expansion-Contraction (HEC) algorithm, originally proposed for approximating the H-infinity norm of large-scale systems, to a generic setting which we call a root-max problem. By then showing how our passivity optimization problem is also a root-max problem, we use the HEC algorithm to develop new globally convergent algorithms with faster local convergence and higher reliability than earlier techniques.

8

Clustering-based model order reduction

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We will discuss open problems in our approach to structure-preserving model order reduction using clustering and projection. The first is developing more general a priori error bounds. The second is guaranteeing synchronization-preservation for nonlinear multi-agent systems. Finally, we will discuss potential relation to hyper-reduction.

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Newman's bound and the Loewner framework

Author: Thanos Antoulas[None]

Newman's bound in rational interpolation and its relation with the Loewner framework will be explored.

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Preliminary studies on reduced-order modeling of fluid dynamic problems

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We present some approaches for obtaining the reduced-order model of incompressible Navier-Stokes equations from the existing literature. The focus of our work is ultimately going to be towards the development of non-intrusive model reduction techniques which would be useful when one has no information about the discretized system. The talk will be given keeping this in mind and potential procedures in that direction would be discussed. We choose two-dimensional Taylor-Green vortex as the test problem during our studies.

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Fast, matrix-free matrix-vector product with the Loewner matrix

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The Loewner framework is one of the most successful data-driven model order reduction techniques. Given k right interpolation data and h left interpolation data, the standard layout of this approach is composed of two stages.

First, the $kh \times kh$ Loewner matrix $\mathbb{L}$ and shifted Loewner matrix $\mathbb{L}_s$ are constructed. Then, an SVD of $\mathbb{L}_s - \gamma\mathbb{L}$, $\gamma \in \mathbb{C}$ belonging to one of the data sets, provides the projection matrices used to compute the sought reduced model.

These two steps become numerically challenging for large k and h in terms of both computational time and storage demand.

We show how the structure of $\mathbb{L}$ and $\mathbb{L}_s$ can be exploited to reduce the cost of performing $(\mathbb{L}_s - \gamma\mathbb{L})x$ while avoiding the explicit allocation of $\mathbb{L}$ and $\mathbb{L}_s$.

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Complex unitary QR and symplectic orthogonal QR decompositions

Author: Carolin Penke[None]

The QR decomposition is certainly among the most useful tools in the arsenal of numerical linear algebra, both in real as well as in complex arithmetic. Symplectic orthogonal QR decompositions follow a similar idea. They are less ubiquitous but find use in the context of Hamiltonian eigenvalue problems. We point out that an orthogonal symplectic QR decomposition is in fact the very same thing as a complex unitary QR decomposition.

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Convergence Issues while Computing the Generalized Matrix Sign Function

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The Generalized Matrix Sign Function (GMSF) of a Matrix pair (A, B) is typically computed using Newton's method. The naive implementation of the iteration step $A_{k+1} = \frac{1}{2}(A + BA_k^{-1}B)$ takes at least $4\frac{2}{3}m^3$ flops, which makes it a computational tough task. With the help of a preprocessing step, the complexity can be reduced down to $2m^3$ flops. Typical ways to achieve this are, on the one hand, the QR decomposition of B. This makes B upper triangular matrix and thus a matrix-matrix product with B gets cheaper. On the other hand, B can be transformed to a bi-diagonal matrix or upper band matrix using orthogonal transformations. In this case, we can perform a matrix-matrix product within $\mathcal{O}(m)$ flops. Although all variants should lead to the same result, some of them yield strange convergence behaviors in rare case, while other variants converge without any problems. At the moment a classification of the matrix pairs is missing identifying when a variant of the GMSF will fail or stagnate.

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Treating the incompressibility constraint in model reduction and optimal control of flow problems with free boundaries

Author: Jan Heiland[None]

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In the Eulerian formulation, a flow with a free boundary is posed on a domain that changes over time. This time dependency transfers to a time dependency of the discrete operators in a spatially discretized model. In particular, the discrete incompressibility constraint and, thus, the state space for the velocity will depend on time.

Following up on recent developments of POD for adaptive grids, we investigate how a time dependent incompressibility constraint can be incorporated in model reduction and optimal control.

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Sparse Recovery based Quadrature for Integration of Solutions to Hyperbolic Problems

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Let $f : \Omega \times D \to R$ be some parameterized function with the parameter domain D. We develop a sparse empirical quadrature to compute $I(\mu) = \int_\Omega f(x, \mu)dx$. To this end, we compute $I(\mu)$ for a set of training parameters and compute the weights of the quadrature using sparse recovery. At least computationally, we observe that the number of non-zero weights in such a quadrature are bounded by the rank of a snapshot matrix. Since the snapshot matrix of solutions to hyperbolic problems do not have a low rank, we could not preserve the sparsity of the empirical quadrature. Therefore, to retain sparsity, we discuss the possibility of taking the samples of $I(\mu)$ from a calibrated snapshot matrix, which has a low rank.

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(Interpolatory) parametric model order reduction

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I will try to give an overview over PMOR methods for linear systems developed within the group but also outside, not claiming completeness. I will also present an interpolator parametric model order reduction method and its extension to MIMO systems.

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Variational data assimilation for POD based MPC

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For many problem settings, the underlying dynamics can be described by (systems of) ordinary or partial differential equations based on physical laws and equations. However, many practical applications require highly sophisticated models, which are often impractical for numerical computations due to their complexity. For this reason, model simplifications are often carried out leading to model errors. Moreover, in many practical settings, there are unknown quantities (e.g. parameters, boundary conditions etc.) which leads to a further source of errors (model uncertainty).

Apart from the physical model of the considered problem setting, a different source of knowledge of the dynamical behavior is measurement data. However, measurement data is often limited, because it is usually expensive to take or only partially (or even not) available.

The concept of variational data assimilation aims to find a best compromise between the physical model and the measurement data. The advantage of this approach is that the resulting numerical solution not only complies with the physics of the system but also is close to the measurements.

In this talk, we develop a variational data assimilation approach for POD based model predictive control (MPC). In particular, we are concerned with an optimal control problem with a very large (or even infinitely large) time horizon, which is tackled within MPC by splitting the time domain into a sequence of smaller time horizon problems and solving open-loop problems. Since the solution of the open-loop MPC subproblems can be an expensive task, we solve POD surrogates instead. After each MPC iteration, we incorporate measurement data into the POD reduced-order model using ideas of variational data assimilation in order to get closer to the reality.

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On Preconditioning and Recycling Subspaces Strategies for Multilinear Systems

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Iterative linear solvers and strategies for accelerating their convergence have been extensively studied by researchers for many decades. Recently, two classes of iterative solvers for tensor-represented systems have proven their effectiveness in solving high dimensional problems. These are low rank Krylov-based solvers and alternating-least-squares-based solvers. Nonetheless, rounding the tensors, even with high accuracy, combined with the typical nature of badly conditioned operators seem to hinder their convergence. Hence, preconditioners and convergence acceleration techniques such as recycling subspaces are instrumental to have efficient solvers. Extending these strategies from the linear case to the multilinear case is not straightforward. In this talk, I will discuss the related difficulties and give solutions to some of them and perspectives to what might be the way to tackle the others.

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Computation of the flat output for a class of underactuated Lagrangian systems

Author: Alexander Zuyev[None]

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The flatness-based approach is a powerful method for solving a variety of control theoretic problems such as motion planning, trajectory tracking, and stabilization of nonlinear systems. This method is limited to control systems with endogenous linearizing feedback, and the idea of parameterizing the

trajectories and inputs of such systems in terms of the flat output and its derivatives goes back to the works of Hilbert and Cartan on under-determined differential equations. In general, the problem of checking flatness remains open, although many important classes of mathematical models, including fully-actuated Lagrangian systems, are known to be flat.

In this talk, we consider a nonlinear Lagrangian mechanical system with a scalar input. We are interested in computing a flat output in a neighborhood of unstable equilibrium of this system. An analytic solution of the system of partial differential equations that defines the flat output is presented. The leading terms of the obtained flat output are compared with the Brunovsky output for the linearized problem, for which an efficient computation algorithm is available.

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Symplectic Integrators for Differential Riccati Equations

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Let $A, S, X_0 \in \mathbb{R}^{n \times n}$ and $B \in \mathbb{R}^{n \times b}$ be. Moreover assume that S, X_0 are symmetric positive semidefinite.
We consider
\begin{align}
\dot{X}(t) &= A^T X (t) + X(t) A - X(t) S X(t) + C^T C, \\\\
X(0)&=X_0.
\end{align}
It is well known that the solution X can be obtained from the Hamiltonian system
\begin{align}
\begin{bmatrix} \dot{U}(t) \\\\ \dot{V}(t) \end{bmatrix}
&=
-H \begin{bmatrix} U(t) \\\\ V(t) \end{bmatrix}
=
-\begin{bmatrix} A & -S \\\\ -C^T C & -A^T \end{bmatrix}
\begin{bmatrix} U(t) \\\\ V(t) \end{bmatrix}, \\\\
\begin{bmatrix} U(0) \\\\ V(0) \end{bmatrix}
&=
\begin{bmatrix} I_n \\\\ X_0 \end{bmatrix},
\end{align}
by the formula $X(t) = V(t)U(t)^{-1}$.
The solution of the Hamiltonian system can be expressed in terms of the matrix exponential of the Hamiltonian $-H$, which is symplectic.
This motivates to approximate the flow by numerical schemes, which uses symplectic transformations.

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The AAA algorithm - some ideas, extensions, and challenges

Author: Ion Victor Gosea[None]

The scope of this contribution is to address some theoretical and numerical aspects concerning the AAA (Adaptive Antoulas-Anderson) algorithm for rational approximation. This method was introduced in 2018 by Nakatsukasa, Sete, and Trefethen and it is based on an interpolation scheme proposed by Antoulas and Anderson in 1986. The AAA algorithm can be viewed as a data-driven iterative procedure for fitting rational functions to a set of measurements. At the same time, it can be used as a MOR technique (the to-be fitted rational function is the transfer function of the ROM). In

this talk, we address such issues as pole sensitivity for the AAA models, connections to the Loewner framework (introduced by Mayo and Antoulas in 2007), and possible extensions for the special case for which derivative information is also available. For the latter, we present ways of adapting AAA to cope with Hermite interpolation.

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Steady states of reduced quadratic models obtained by lifting non-linear second-order models

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In recent work, we have reduced nonlinear second-order power grid models using balanced truncation techniques for quadratic systems. In order to do that, we 1) transform the original system to a first-order system and 2) use lifting to quadratize the first-order system. However, although the original quadratized system reaches steady state, the reduced quadratic system may only reach a partial steady state where a subset of the state variables continue to grow at a constant rate. In order to address this issue, it would be useful to know, given a reduced quadratic system, 1) if there exists steady states and 2) if they are stable. In this presentation, we look into the cause of the problem and preliminary attempts at answering the two questions.

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Identification of Second-Order Systems from Frequency Response Data

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In this talk, we present a data-driven approach to identify second-order systems of the form
\begin{equation}
\begin{array}{rcl}
\mathbf{M}\ddot{\mathbf{x}}(t) + \mathbf{D}\dot{\mathbf{x}}(t)+ \mathbf{K}\mathbf{x}(t) &=& \mathbf{B}\mathbf{u}(t),\qquad
\mathbf{x}(0) = 0,~\dot{\mathbf{x}}(0) = 0, \\
\mathbf{y}(t) &=& \mathbf{C}\mathbf{x}(t).
\end{array}
\end{equation}
These systems typically appear in order to perform various engineering studies, e.g., vibration analysis. The frequency response of the system can be given by the following rational structured function:

$H(s) = C \left(s^2\mathbf{M} + s\mathbf{D} + \mathbf{K}\right)^{-1}\mathbf{B}, which is also known as the transfer function. The frequency response of a system can be me$
$= \alpha\mathbf{M} + \beta\mathbf{K}$. As a consequence, the identification problem is solved analytically using the frequency data. In the second approach, the Rayleigh damping hypothesis is no longer assumed, and the problem is solved finding low-rank matrices that best fit the given data ensuring the second order structure. Finally, the efficiency of the proposed methods is demonstrated by means of various numerical benchmarks.