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CROSS-GRAMIAN BASED MODEL REDUCTION FOR DATA-SPARSE SYSTEMS*

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Abstract. Model order reduction (MOR) is common in simulation, control and optimization of complex dynamical systems arising in modeling of physical processes, and in the spatial discretization of parabolic partial differential equations in two or more dimensions. Typically, after a semi-discretization of the differential operator by the finite or boundary element method, we have a large state-space dimension n. In order to accelerate the simulation time or to facilitate the control design, it is often desirable to employ an approximate reduced-order system of order r, with $r \ll n$, instead of the original large-scale system. We show how to compute a reduced-order system with a balancing-related model reduction method. The method is based on the computation of the cross-Gramian $\mathcal{X}$, which is the solution of a Sylvester equation. As standard algorithms for the solution of Sylvester equations are of limited use for large-scale (possibly dense) systems, we investigate approaches based on the iterative sign function method, using data-sparse matrix approximations (the hierarchical matrix format) and an approximate arithmetic. Furthermore, we use a modified iteration scheme for computing low-rank factors of the solution $\mathcal{X}$. The projection matrices for MOR are computed from the dominant invariant subspace of $\mathcal{X}$. We propose an efficient algorithm for the direct calculation of these projectors from the low-rank factors of $\mathcal{X}$. Numerical experiments demonstrate the performance of the new approach.

Key words. Model reduction, balanced truncation, cross-Gramian, hierarchical matrices, sign function method.

AMS subject classifications. 93B11, 93B40, 93C20, 37M05.

1. Introduction.

We consider linear time-invariant (LTI) systems of the following form

$$\Sigma : \begin{cases} \dot{x}(t) = Ax(t) + Bu(t), & t > 0, \quad x(0) = x^0, \\ y(t) = Cx(t) + Du(t), & t \geq 0, \end{cases} \tag{1.1}$$

with state matrix $A \in \mathbb{R}^{n\times n}$, and $B \in \mathbb{R}^{n\times m}$, $C \in \mathbb{R}^{p\times n}$, $D \in \mathbb{R}^{p\times m}$. The system (1.1), denoted by $\Sigma(A, B, C, D)$, is assumed to be square ($m = p$) and can be single-input/single-output (SISO) ($m = p = 1$) or multi-input/multi-output (MIMO) ($m = p > 1$). Furthermore, we assume stability of (1.1), i.e., all eigenvalues of the coefficient matrix A, denoted by $\Lambda(A)$, are assumed to be in the open left half plane $\mathbb{C}^-$. In practice, e.g., in the control of partial differential equations, the system matrix A often comes from the spatial discretization of some partial differential operator. In this case, n is typically large and the system matrices are sparse. On the other hand, boundary element discretizations of integral equations lead to large-scale *dense* matrices that often have a data-sparse representation [23, 32]. Hence, in general, we will not assume sparsity of A, but we will assume that a data-sparse representation of A exists. In this case we call (1.1) a *data-sparse* system.

Model order reduction (MOR) aims at approximating a given large-scale system (1.1) by a system of reduced order r, $r \ll n$. In system theory and control of ordinary differential equations, balanced truncation (BT) [29] and related methods are the methods of choice since they have some desirable properties: they preserve the stability of the system and provide a global computable error bound which allows an adaptive choice of the reduced order. The basic approach relies on balancing the controllability Gramian and the observability Gramian of $\Sigma(A, B, C, D)$. A variant of the classical BT method is based on the cross-Gramian [1,

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3, 18, 34]. The major part of the computational complexity of both MOR approaches stems from the solution of large-scale matrix equations, i.e., of two Lyapunov equations for BT or of one Sylvester equation for the cross-Gramian (CG) approach. In [1], the reduced-order system is computed from the eigenspaces associated with large eigenvalues of the $n \times n$ cross-Gramian. This is computationally very demanding and thus fails for the problems considered in this work. The approaches in [3, 18, 34] belong to the class of Krylov projection methods as they iteratively compute low-rank approximations to the cross-Gramian by an implicitly restarted Arnoldi method. An approximately balanced reduced-order system is obtained by a partial eigenvalue decomposition of this Gramian.

Here, we will discuss an alternative for large-scale, data-sparse systems, based on the sign function method for Sylvester equations [7, 12]. The derived CG approach is described in Section 2, which is divided into three parts. First, Section 2.1 gives the background for balancing-related MOR. Then, the efficient solution of Sylvester equations by a data-sparse sign function method [5] is reviewed in Section 2.2. Based on the computed approximate low-rank factors of the Gramian, we propose an effective computation of the projection matrices for MOR in Section 2.3. Several numerical simulations demonstrate the performance of the new method in Section 3 and concluding remarks follow in Section 4.

2. Approximate cross-Gramian approach.

In the following section we shortly review the main properties of BT and the close connection to the CG approach.

2.1. Background.

BT [29] eliminates the states corresponding to the $n - r$ smallest *Hankel singular values* (HSVs) from a balanced realization of $\Sigma(A, B, C, D)$ to obtain a system of order $r \ll n$ [36, Section 3.9], [2, Section 7.1]. The HSVs of (1.1) are given by the square roots of the eigenvalues of $\mathcal{P}\mathcal{Q}$, i.e.,

$$\Lambda(\mathcal{P}\mathcal{Q}) = \{\sigma_1^2, \ldots, \sigma_n^2\}, \quad \sigma_1 \geq \cdots \geq \sigma_n \geq 0,$$

where $\mathcal{P}$ denotes the controllability Gramian while $\mathcal{Q}$ is the observability Gramian of (1.1). The reduced-order model

$$\hat{\Sigma} : \begin{cases} \dot{\hat{x}}(t) = \hat{A}\hat{x}(t) + \hat{B}u(t), & t > 0, \quad \hat{x}(0) = \hat{x}^0, \\ \hat{y}(t) = \hat{C}\hat{x}(t) + \hat{D}u(t), & t \geq 0, \end{cases} \tag{2.1}$$

with $\hat{A} \in \mathbb{R}^{r \times r}$, $\hat{B} \in \mathbb{R}^{r \times m}$, $\hat{C} \in \mathbb{R}^{p \times r}$, $\hat{D} \in \mathbb{R}^{p \times m}$, is achieved by applying the blocks T_l, T_r of the balancing transformation matrix T ($T\mathcal{P}\mathcal{Q}T^{-1} = \mathrm{diag}(\sigma_1^2, \cdots, \sigma_n^2)$), defined by

$$T = \begin{bmatrix} T_l \\ * \end{bmatrix}, \quad T^{-1} = [\,T_r, \, *\,], \quad \text{with } T_l^T, T_r \in \mathbb{R}^{n \times r},$$

to (1.1) as follows

$$(\hat{A}, \hat{B}, \hat{C}, \hat{D}) = (T_l A T_r, T_l B, C T_r, D). \tag{2.2}$$

The worst output error between (1.1) and (2.1) is bounded [19] (if $x(0) = 0$) by

$$\|y - \hat{y}\|_2 \leq 2\left(\sum_{j=r+1}^{n} \sigma_j\right) \|u\|_2, \tag{2.3}$$

with $\|\cdot\|_2$ denoting the $\mathcal{L}_2$-norm for square-integrable functions on $[0, \infty)$. This error bound provides a reasonable way to adapt the selection of the reduced order r. In addition, the reduced-order system remains stable and balanced with the same HSVs $\{\sigma_1,\ldots,\sigma_r\}$ of the original system.

In 1983, a new system Gramian was defined for stable SISO systems,

$$\mathcal{X} := \int_0^\infty e^{At} BC\, e^{At} dt, \tag{2.4}$$

which contains information on controllability of the system as well as on observability [16]. Therefore, $\mathcal{X} \in \mathbb{R}^{n\times n}$ is called the *cross-Gramian* of the system (1.1). The definition was extended to symmetric MIMO systems [17, 28]. Note that a realization $\Sigma(A,B,C,D)$ is called symmetric if the corresponding transfer function matrix (TFM) $G(s) = C(sI-A)^{-1}B+D$ is symmetric. This is trivially the case for systems with $A = A^T$, $B = C^T$, $D = 0$. In [17, 28], properties of the cross-Gramian were derived which underline the usefulness of $\mathcal{X}$ for the purpose of model order reduction. It was shown [16, 17, 28] that for SISO and for symmetric MIMO systems, the cross-Gramian satisfies

$$\mathcal{X}^2 = \mathcal{P}\mathcal{Q}. \tag{2.5}$$

By this identity, the HSVs of $\Sigma(A,B,C,D)$ are analogously given by the magnitude of the eigenvalues of $\mathcal{X}$,

$$\sigma_i = |\lambda_i(\mathcal{X})|, \quad \text{for } i = 1,\ldots,n.$$

It is possible to compute a reduced-order system directly from the cross-Gramian $\mathcal{X}$. Note that under state-space transformations, the eigenvalues of $\mathcal{X}$ are invariant

$$\tilde{\mathcal{X}} = \int_0^\infty e^{TAT^{-1}t} TBCT^{-1} e^{TAT^{-1}t} dt = T\mathcal{X}T^{-1}.$$

If $\mathcal{X}$ is diagonalizable and T is a balancing transformation, then

$$\tilde{\mathcal{X}} = \mathrm{diag}(\lambda_1,\cdots,\lambda_n), \quad \text{with } |\lambda_1| \geq \cdots \geq |\lambda_n|,$$

and the reduced-order system is simply given by the first r states of the balanced realization. For SISO and symmetric MIMO systems, the system dynamics are projected onto the eigenspaces associated with the largest eigenvalues of $\mathcal{X}$. The computed reduced-order model has the same properties as in BT model reduction, i.e., stability is preserved and a computable global error bound exists. Note that this can also be done for non-symmetric, square MIMO systems (with $m = p$), but without the theoretical background provided for the symmetric case, and therefore without any guarantee for the quality of the reduced-order system. In Section 3 it is shown for a numerical example that such a reduced-order system can be a reasonable approximation to a non-symmetric MIMO system as well. An alternative is proposed in [34] where a non-symmetric, possibly non-square MIMO system is embedded into a symmetric, square system of the same order but with more inputs and outputs.

In the following we describe an efficient implementation for MOR by a CG approach, using an approximate sign function solver for the solution of the Sylvester equation, and a low-rank product QR algorithm for the computation of the projection matrices. This CG approach yields an alternative for the widely used BT method at approximately the same costs. A further motivation for this approach is given in [34] by the following consistency argument. In usual BT implementations, suitable for large-scale systems, the basis sets T_l and T_r for projection are computed from approximations to the exact controllability and observability Gramians. Since both Gramians are approximated separately it can not be ensured

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that the same basis sets would have been computed by the full system Gramians. In other words, there might be a gap between the approximation errors of $\mathcal{P}$ and $\mathcal{Q}$, which influences the computed reduced-order system in some way. This problem does not occur if we compute projection matrices from an approximation to the cross-Gramian. Moreover, the examples in Section 3 indeed demonstrate that the CG approach sometimes has advantageous properties compared to BT.

2.2. Efficient solution of large-scale Sylvester equations. The cross-Gramian (2.4) is equivalently given by the solution of the Sylvester equation [27]

$$A\mathcal{X} + \mathcal{X}A + BC = 0. \tag{2.6}$$

For the numerical solution of large-scale Sylvester equations we consider the modified sign function method as described in [5]. This method combines the iteration scheme with the hierarchical ($\mathcal{H}$) matrix format [23, 24] and the corresponding approximate arithmetic [20, 22], and computes low-rank factors of $\mathcal{X}$. The overall procedure is shown in Algorithm 1 below, for more details (including scaling strategies) we refer to [5]. In the following, we describe some of the important steps of the algorithm.

The matrix sign function gives an expression for the solution $\mathcal{X}$ of the Sylvester equation (2.6) [31] by

$$\operatorname{sign}\begin{bmatrix} A & BC \\ 0 & -A \end{bmatrix} = \begin{bmatrix} -I & 2\mathcal{X} \\ 0 & I \end{bmatrix}.$$

In large-scale computations it is of particular interest to compute low-rank solution factors if $\mathcal{X}$ has low rank ($\operatorname{rank}(\mathcal{X}) \ll n$) or, at least, low numerical rank. The latter case is of particular relevance; in many large-scale applications it can be observed that the eigenvalues of $\mathcal{X}$ decay rapidly, see e.g., [4, 21, 30]. Then, the memory requirements can be considerably reduced by computing low-rank approximations to the full-rank factors directly. Thus, $\mathcal{X} \approx \tilde{Y}\tilde{Z}$, with $\tilde{Y} \in \mathbb{R}^{n \times n_\tau(\mathcal{X})}$, $\tilde{Z} \in \mathbb{R}^{n_\tau(\mathcal{X}) \times n}$, exploiting the expected low numerical rank of $\mathcal{X}$: $n_\tau(\mathcal{X}) \ll n$. The sign function can be modified for the direct calculation of such low-rank factors [7, 12]. The numerical rank $n_\tau(\mathcal{X})$ is determined during the iteration by a given threshold τ, applying rank-revealing QR factorizations in the corresponding steps of Algorithm 1 below. Note that Q_C in step 12 of Algorithm 1 can be directly accumulated in B_{k+1} and needs not be generated explicitly. However, the computational complexity of the method grows cubically and storage requirements grow quadratically with n. To avoid this effect, the large-scale matrix A and the iterates A_k are approximated in the data-sparse $\mathcal{H}$-matrix format (denoted by $A_{\mathcal{H}}$) during the sign function iteration. The hierarchical matrix arithmetic ($\oplus$, $LU_{\mathcal{H}}$, $\mathcal{H}$-forward/backward substitution) is used to reduce the computational cost in these iteration parts. The approximate operations are of linear-polylogarithmic complexity, $\mathcal{O}(n\log^2(n)k(\epsilon)^2)$, where $k(\epsilon)$ denotes the blockwise ranks in an $\mathcal{H}$-matrix approximation, which are determined by a parameter ϵ to obtain a relative error $\mathcal{O}(\epsilon)$. For detailed descriptions of the $\mathcal{H}$-matrix format and arithmetic, see, e.g., [14, 20, 22, 24]. Thus, the overall complexity of the data-sparse sign function iteration, as summarized in Algorithm 1, is linear-polylogarithmic.

The described algorithm is especially suitable for large-scale systems obtained by the spatial discretization of parabolic partial differential equations which might have fully populated system matrices. Note that, in principle, all methods which compute low-rank factors of $\mathcal{X}$, e.g., [7, 8, 12], can be used in the CG approach for MOR as described in the next section.

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ALGORITHM 1 (Calculate approximate factors $\tilde{Y}$, $\tilde{Z}$ of $\mathcal{X}$ for $A\mathcal{X} + \mathcal{X}A + BC = 0$).

INPUT: $A \in \mathbb{R}^{n\times n}$, $B \in \mathbb{R}^{n\times m}$, $C \in \mathbb{R}^{m\times n}$, convergence tolerance tol, rank drop tolerance τ.
OUTPUT: Approximations $\tilde{Y}$ and $\tilde{Z}$ to full-rank factors of the solution $\mathcal{X}$.

$A_0 \leftarrow A_{\mathcal{H}}$
$B_0 \leftarrow B$
$C_0 \leftarrow C$
$k = 0$
while $\|A_k + I_n\| >$ tol **do**
  $[L, U] \leftarrow LU_{\mathcal{H}}(A_k)$
  Solve $LW = (I_n)_{\mathcal{H}}$ by $\mathcal{H}$-forward substitution.
  Solve $UV = W$ by $\mathcal{H}$-backward substitution.
  $A_{k+1} \leftarrow \frac{1}{2}(A_k \oplus V)$
  $B_{k+1} \leftarrow \frac{1}{\sqrt{2}} \begin{bmatrix} B_k & VB_k \end{bmatrix}$
  $C_{k+1} \leftarrow \frac{1}{\sqrt{2}} \begin{bmatrix} C_k \\ C_k V \end{bmatrix}$
  Compute a rank-revealing QR factorization

$$C_{k+1} = Q_C \begin{bmatrix} R_{11} & R_{12} \\ 0 & R_{22} \end{bmatrix} \Pi_C$$

  with $\|R_{22}\|_2 < \tau \|C_{k+1}\|_2$ and $R_{11} \in \mathbb{R}^{s\times s}$.
  Compress rows of C_{k+1} to size s:

$$C_{k+1} \leftarrow [\, R_{11},\ R_{12}\,]\, \Pi_G.$$

  Compute a rank-revealing LQ factorization

$$B_{k+1} Q_C = \Pi_B \begin{bmatrix} L_{11} & 0 \\ L_{21} & L_{22} \end{bmatrix} Q_B$$

  with $\|L_{22}\|_2 < \tau \|B_{k+1}\|_2$ and $L_{11} \in \mathbb{R}^{t\times t}$, $(Q_B)_{11} := Q_B(1:t, 1:s)$.
  Compress columns of $B_{k+1}Q_C$ to size t:

$$B_{k+1} \leftarrow \Pi_B \begin{bmatrix} L_{11} \\ L_{21} \end{bmatrix}.$$

  if $t < s$ **then**
    Multiply C_{k+1} from the left by $(Q_B)_{11} \in \mathbb{R}^{t\times s}$: $C_{k+1} \leftarrow (Q_B)_{11} C_{k+1}$.
  else
    Multiply B_{k+1} by $(Q_B)_{11} \in \mathbb{R}^{t\times s}$: $B_{k+1} \leftarrow B_{k+1} (Q_B)_{11}$.
  end if
  $k = k + 1$
end while
$\tilde{Y} \leftarrow \frac{1}{\sqrt{2}} B_k$, $\tilde{Z} \leftarrow \frac{1}{\sqrt{2}} C_k$

2.3. Computation of the projection matrices. We compute the projection matrices T_l and T_r for MOR as the left and right dominant invariant subspaces of $\mathcal{X}$ by particular Schur decompositions of $\tilde{Y}\tilde{Z}$. We propose a numerically efficient and accurate algorithm for the computation of these dominant invariant subspaces. First, a basis for the right invariant subspace of $\tilde{Y}\tilde{Z}$ corresponding to the r largest eigenvalues is computed,

$$(\tilde{Y}\tilde{Z})\, V_r = V_r\Lambda_1,$$

where $\Lambda_1 = \operatorname{diag}(\lambda_1, \ldots, \lambda_r)$ so that $|\lambda_r| \geq |\lambda_{r+1}|$ and the eigenvalues are in non increasing magnitude order. The remaining $n-r$ eigenvalues of $\tilde{Y}\tilde{Z}$ are smaller in magnitude. The columns of $V_r \in \mathbb{R}^{n\times r}$ span the dominant right invariant subspace of $\tilde{Y}\tilde{Z}$. In practice, we compute a Schur decomposition of the "small" matrix product $\tilde{Z}\tilde{Y} \in \mathbb{R}^{n_\tau(\mathcal{X})\times n_\tau(\mathcal{X})}$. The Schur decomposition will be done without explicitly computing the product of the two factors $\tilde{Z}$ and $\tilde{Y}$ using the following *low-rank* version of the so-called *product QR algorithm*.

1. Compute an economy-size QR decomposition of $\tilde{Y}$ with column pivoting:
$$\tilde{Y} = Q_1R_1\Pi^T, \qquad Q_1 \in \mathbb{R}^{n\times n_\tau(\mathcal{X})},\ R_1 \in \mathbb{R}^{n_\tau(\mathcal{X})\times n_\tau(\mathcal{X})},$$
where Q_1 has orthonormal columns, R_1 is upper triangular and Π is a permutation.
2. Multiply and permute
$$\begin{aligned}\hat{Z} &\leftarrow \tilde{Z}Q_1 \in \mathbb{R}^{n_\tau(\mathcal{X})\times n_\tau(\mathcal{X})},\\ \hat{Y} &\leftarrow R_1\Pi^T \in \mathbb{R}^{n_\tau(\mathcal{X})\times n_\tau(\mathcal{X})}.\end{aligned}$$
3. Compute the product Hessenberg form of $\hat{Z}\hat{Y}$
$$H_1H_2 \leftarrow U_1^T\hat{Z}U_2U_2^T\hat{Y}U_1,$$
where H_1 is upper Hessenberg, H_2 upper triangular, U_1 and U_2 are orthogonal [26, Section 4.2.3].
4. Compute the product Schur decomposition
$$S_1S_2 \leftarrow W_1^TH_1W_2W_2^TH_2W_1,$$
where S_1 is in real Schur form, S_2 is upper triangular, W_1 and W_2 are orthogonal [26, Section 4.2.1]. The eigenvalues are ordered by descending magnitude.

The low-rank product QR algorithm yields the invariant subspace of $\tilde{Z}\tilde{Y}$ by the column span of U_1W_1,

$$\tilde{Z}\,\tilde{Y}\,U_1W_1 = U_1W_1\,S_1S_2.$$

By ordering the eigenvalues, the dominant right invariant subspace of the approximate cross-Gramian $\tilde{Y}\tilde{Z}$ corresponding to the r largest (in magnitude) eigenvalues can be derived using the first r columns of U_1W_1 (denoted by the MATLAB colon notation $U_1W_1(:,1:r)$) setting $V_r := \tilde{Y}\,(U_1W_1(:,1:r)) \in \mathbb{R}^{n\times r}$. Note that the size r of the reduced-order system can be easily determined by a given error tolerance using the criterion

$$\min\left\{r \in \mathbb{N}\ \middle|\ 2\sum_{j=r+1}^{n}|\tilde{\lambda}_j(\tilde{Y}\tilde{Z})| \leq \text{tol}\right\}.$$

The left dominant invariant subspace of $\tilde{Y}\tilde{Z}$ is given by the column span $W_l \in \mathbb{R}^{n\times r}$ satisfying

$$W_l^T(\tilde{Y}\tilde{Z}) = \Lambda_1W_l^T.$$

We can compute W_l analogously to V_r via the low-rank product QR algorithm applied to $\tilde{Y}^T\tilde{Z}^T$. The projection matrices for MOR are obtained similarly to the *balancing-free SR method* [35] by an orthogonalization of V_r and W_l. For this purpose we compute two economy-size QR decompositions

$$V_r = Q_r R_r \quad \text{and} \quad W_l = Q_l R_l, \quad Q_r, Q_l \in \mathbb{R}^{n\times r},$$

setting $T_r = Q_r, T_l = (Q_l^T Q_r)^{-1}Q_l^T$, and obtain a reduced-order system by projection (2.2). All steps of the cross-Gramian approach are summarized in Algorithm 2.

ALGORITHM 2 (Approximate Cross-Gramian approach for LTI systems (1.1)).

INPUT: $A_{\mathcal{H}} \in \mathbb{R}^{n\times n}$, $B \in \mathbb{R}^{n\times m}$, $C \in \mathbb{R}^{m\times n}$, $D \in \mathbb{R}^{m\times m}$, tol, τ, ϵ.
OUTPUT: $\hat{A} \in \mathbb{R}^{r\times r}$, $\hat{B} \in \mathbb{R}^{r\times m}$, $\hat{C} \in \mathbb{R}^{m\times r}$, $\hat{D} \in \mathbb{R}^{m\times m}$; reduced order r, error bound δ.

1: Compute low-rank factors $\tilde{Y} \in \mathbb{R}^{n\times n_\tau(\mathcal{X})}$, $\tilde{Z} \in \mathbb{R}^{n_\tau(\mathcal{X})\times n}$ of the cross-Gramian $\mathcal{X}$ by Algorithm 1.
2: Compute right invariant subspace U_1W_1 of $\tilde{Z}\tilde{Y}$ by the low-rank product QR algorithm with eigenvalues in non increasing order $|\tilde{\lambda}_1| \geq \cdots \geq |\tilde{\lambda}_{n_\tau(X)}|$.
3: Adaptive choice of r by tol: $\delta = 2\sum_{j=r+1}^{n_\tau(\mathcal{X})} |\tilde{\lambda}_j| \leq$ tol.
4: Compute right dominant invariant subspace $V_r \in \mathbb{R}^{n\times r}$ of $\tilde{Y}\tilde{Z}$:
$$V_r = \tilde{Y}(U_1W_1(:, 1:r)).$$
5: Compute right invariant subspace U_1W_1 of $\tilde{Y}^T\tilde{Z}^T$ by the low-rank product QR algorithm.
6: Compute left dominant invariant subspace $W_l \in \mathbb{R}^{n\times r}$ of $\tilde{Y}\tilde{Z}$:
$$W_l = \tilde{Z}^T(U_1W_1(:, 1:r)).$$
7: Compute QR decompositions $V_r = Q_rR_r$, $W_l = Q_lR_l$ and projection matrices
$$T_r = Q_r, \quad T_l = (Q_l^TQ_r)^{-1}Q_l^T.$$
8: Compute reduced-order model:
$$\hat{A} = T_lA_{\mathcal{H}}T_r,\ \hat{B} = T_lB,\ \hat{C} = CT_r,\ \hat{D} = D.$$

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3. Numerical results. All numerical experiments were performed on an SGI Altix 3700 (32 Itanium II processors, 1300 MHz, 64 GBytes shared memory, only one processor is used). We make use of the LAPACK and BLAS libraries for performing the standard dense matrix operations and include the routine DGEQPX of the RRQR library [13] for computing the rank-revealing QR factorization. For the $\mathcal{H}$-matrix approximation we employ HLib 1.2 [15]. The parameter ϵ which determines the desired accuracy in each matrix block (see at the end of Section 2.2) is chosen in dependency on the rank drop tolerance τ, by $\tau = \epsilon = 10^{-6}$. This is inspired by preliminary work for an approximate BT method also using the $\mathcal{H}$-matrix format for the solution of the arising large-scale Lyapunov equations [6]. It is shown in [6] by a rough error analysis that the choice $\tau = \epsilon$ leads to an error of size ϵ in the computed Hankel singular values as well as in the projection matrices, and thus in the reduced-order model. The results obtained by the CG method are compared with results from this approximate BT method.

Besides the data-sparse solver for Sylvester equations in Algorithm 1, all computational steps of the cross-Gramian approach (Algorithm 2) are computed in dense arithmetic. For the product QR algorithm, we employ the routine MB03VD from the SLICOT Library [9, 33] to compute the product Hessenberg form of a product of matrices without evaluating any part of the product. The matrix product is transformed further to product real Schur canonical form by the HAPACK [25, 26] routine DHGPQR, and reordered by DTGSRT such that the magnitudes of the eigenvalues appear in non increasing order.

Note that, in order to measure the accuracy of the computed reduced-order systems, we have to analyze the influence of the $\mathcal{H}$-matrix error introduced by the approximation of the original coefficient matrix A in $\mathcal{H}$-matrix format. Thus, the data-sparse MOR methods are actually applied to

$$G_{\mathcal{H}}(s) := C(sI - A_{\mathcal{H}})^{-1}B + D.$$

We split the approximation error into two parts using the triangle inequality:

$$\|G - \hat{G}\|_\infty \leq \|G - G_{\mathcal{H}}\|_\infty + \|G_{\mathcal{H}} - \hat{G}\|_\infty, \tag{3.1}$$

where $\|\cdot\|_\infty$ denotes the $\mathcal{H}_\infty$-norm of a rational transfer function. For the approximate BT method, error bounds are derived in [6]. We recall the bound for the specific case of systems with symmetric, negative definite matrix A (and $A_{\mathcal{H}}$, respectively). With $\hat{G}$ as TFM associated to the reduced-order system (2.1), obtained by applying BT to $G_{\mathcal{H}}$, and some assumptions [6, Theorem 4.4], the approximation error (3.1) is bounded by

$$\|G - \hat{G}\|_\infty \leq \frac{1}{\lambda_1(A)^2}\|C\|_2\|B\|_2\mathcal{O}(\epsilon) + 2\left(\sum_{j=r+1}^{n}\tilde{\sigma}_j\right), \tag{3.2}$$

where λ_1 is the largest eigenvalue of A and $\tilde{\sigma}_j$ are the HSVs of $\Sigma(A_{\mathcal{H}}, B, C, D)$. Note that $|\sigma_j - \tilde{\sigma}_j| \sim \epsilon$ by choosing the tolerances accordingly, i.e., $\tau = \epsilon$ and $\tilde{\sigma}_j = |\tilde{\lambda}_j|$. If all the involved quantities are computed with an approximation error of order $\mathcal{O}(\epsilon)$, this bound is also valid for SISO and symmetric MIMO systems reduced by the CG approach, due to the theoretical equivalence to BT.

As a basis for our test examples, we consider a convection-diffusion equation in the unit square $\Omega = (0,1)^2$ with a heat source in some subdomain Ω_u:

$$\frac{\partial \mathbf{x}}{\partial t}(t,\xi) = \nabla^T(a(\xi)\cdot\nabla\mathbf{x}(t,\xi)) + c\cdot\nabla\mathbf{x}(t,\xi) + b(\xi)u(t), \quad \xi\in\Omega,\ t\in(0,\infty), \tag{3.3}$$

where $b(\cdot) = \mathcal{X}_{\Omega_u}$ and $\mathcal{X}_{\Omega_u}$ is the characteristic function of the control domain. The diffusion coefficient a is a material-specific quantity depending on the heat conductivity, the density and the heat capacity. The convective term is described by $c \in \mathbb{R}^2$. We impose homogeneous Dirichlet boundary conditions and discretize with linear finite elements $\varphi_1, \ldots, \varphi_n$ and n inner grid points ξ_i. In the weak form of the partial differential equation we use a classical

Galerkin approach: $\mathbf{x}(t,\xi) \approx \sum_{i=1}^{n} \tilde{x}_i(t)\varphi_i(\xi)$. For the n unknowns $\tilde{x}_i$ we obtain a system of linear differential equations

$$E\dot{\tilde{x}}(t) = -\tilde{A}\tilde{x}(t) + \tilde{B}u(t), \tag{3.4}$$

with matrices E, $\tilde{A}$, $\tilde{B}$ defined by the entries

$$E_{ij} = \int_\Omega \varphi_i(\xi)\varphi_j(\xi)\,d\xi, \qquad \tilde{A}_{ij} = \int_\Omega a(\xi)\,\langle\nabla\varphi_i(\xi), \nabla\varphi_j(\xi)\rangle + \langle c, \nabla\varphi_j(\xi)\rangle\varphi_i(\xi)\,d\xi,$$

$$\tilde{B}_{i1} = \int_\Omega b(\xi)\varphi_i(\xi)\,d\xi, \qquad \text{for } i,j = 1,\dots,n.$$

The output equation is given by a measurement of the temperature in a small subdomain Ω_o:

$$y(t) = \tilde{C}\tilde{x}(t), \qquad \text{where} \quad \tilde{C}_{1j} = \begin{cases} 1, & \xi_j \in \Omega_o, \\ 0, & \text{otherwise}, \end{cases} \qquad \text{for } j = 1,\dots,n.$$

The number of basis function of the finite element ansatz space is chosen as $n = 16,384$. We approximate the $n \times n$ mass matrix E in $\mathcal{H}$-matrix format and transform the equation to standard form using a formatted Cholesky decomposition $E = LL^T$ such that $x := L^T\tilde{x}$. The resulting state matrix $A = -L^{-1}\tilde{A}L^{-T}$ is also stored as $\mathcal{H}$-matrix. Thus, we have a large-scale stable LTI system as introduced in (1.1), with $B = L^{-1}\tilde{B} \in \mathbb{R}^{n\times 1}$ and $C = \tilde{C}L^{-T} \in \mathbb{R}^{1\times n}$, i.e., a SISO system.

First we choose the diffusion constant as $a(\cdot) \equiv 1.0$ and set $c = (0,0)^T$, thus equation (3.3) simplifies to the non stationary heat equation. We compare the frequency response errors $\|G_{\mathcal{H}} - \hat{G}\|_\infty$, obtained by the cross-Gramian approach, with those of the approximate BT method [6]. The $\mathcal{H}_\infty$-norm error between $G_{\mathcal{H}}$ and $\hat{G}$ is estimated by the pointwise absolute values computed at 20 fixed frequencies $\omega_k = 10^{-4},\dots,10^6$ in logarithmic scale, as described in [6].

With $\mathrm{tol} = 10^{-4}$, the reduced order is determined as $r = 4$ and the approximate error bound is computed to be $\delta = 4.3 \times 10^{-5}$. Note that using $\tilde{Y}$ and $\tilde{Z}$ in Algorithm 2 reduces the computable part of the original BT error bound (2.3) to

$$\delta = 2 \sum_{j=r+1}^{n_\tau(\mathcal{X})} |\tilde{\lambda}_j|,$$

since only the largest $n_\tau(\mathcal{X})$ eigenvalues of the cross-Gramian $\tilde{Y}\tilde{Z}$ are computed by the low-rank product QR algorithm. Thus, δ may under-estimate the error (2.3) if $n_\tau(\mathcal{X}) < n$. In practise, the estimate usually gives an accurate error measure. The frequency response errors for the $\mathcal{H}$-matrix based BT and CG method are shown in the upper plot of Figure 3.1. We observe that both curves as well as the computed error bounds δ nearly coincide. We also depict the errors between the original (without $\mathcal{H}$-matrix approximation) and the CG reduced-order system $\|G - \hat{G}\|_\infty$ in the lower plot of Figure 3.1 to demonstrate the reliability of our approach. Note that there is no visible difference between the corresponding error plots and that all curves satisfy the approximate error bound δ. Thus, other error sources using the $\mathcal{H}$-matrix format in the CG approach seem to be negligible.

Next we vary $a(\cdot)$ over the domain:

$$a(\xi) = \begin{cases} 10, & \xi \in [-1,1] \times [-\frac{1}{3}, \frac{1}{3}], \\ 10^{-4}, & \xi \in [-\frac{1}{3}, \frac{1}{3}] \times \left([-1, -\frac{1}{3}) \cup (\frac{1}{3}, 1]\right), \\ 1, & \text{otherwise}. \end{cases}$$

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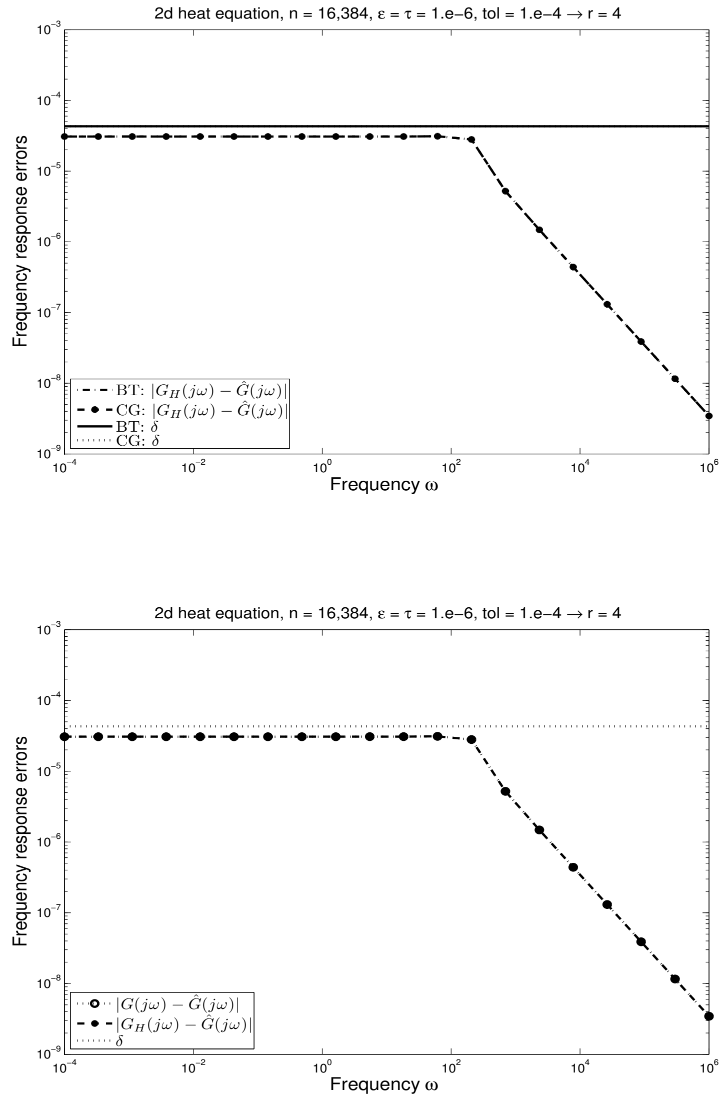

FIGURE 3.1. *Frequency response errors for the two-dimensional heat equation using the cross-Gramian approach as described in Algorithm 2.*

By the given tolerance of 10^{-4}, the reduced order is determined by $r = 3$. The frequency response errors for BT and CG reduced-order models are not distinguishable in the upper plot of Figure 3.2. We observe a good approximation of the reduced systems particularly for larger frequencies. The differences between $\|G - G_{\mathcal{H}}\|_\infty$ and $\|G_{\mathcal{H}} - \hat{G}\|_\infty$ for the CG approach are again negligible, see the lower plot in Figure 3.2. This means that using approximate Gramians does not contribute much to the errors between the original and the reduced-order system. The results fulfill the approximate error bound of $\delta = 8.7 \times 10^{-5}$.

Now we include convection by setting $c = (0, 1)^T$, which leads to a nonsymmetric stiffness matrix $\tilde{A}$ in (3.4). To make the convective term dominant, the diffusion coefficient is reduced to $a(\cdot) \equiv 10^{-4}$ over the whole domain Ω. In this example the eigenvalues of A are

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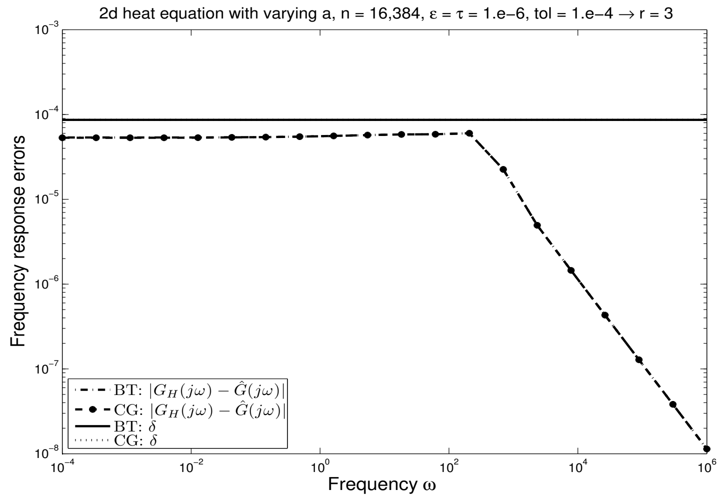

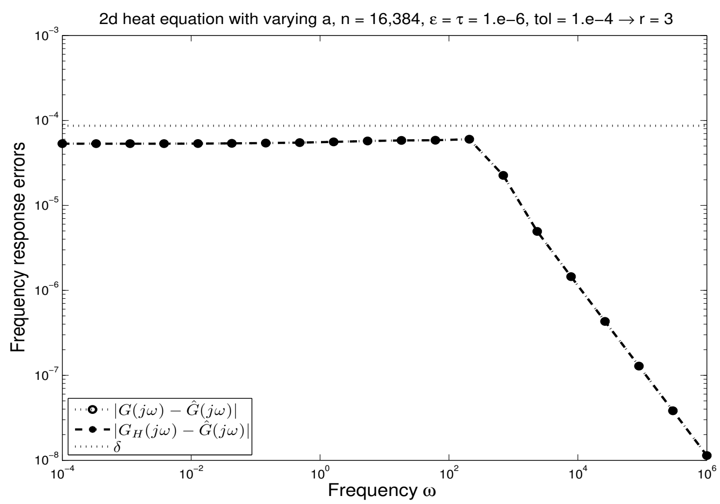

FIGURE 3.2. *Frequency response errors for the two-dimensional heat equation with varying diffusion using the cross-Gramian approach as described in Algorithm 2.*

close to the imaginary axis, i.e., $\min_{i=1,\dots,n} |\mathrm{Re}(\lambda_i(A))| \approx 2 \times 10^{-3}$, so that the sign function iteration suffers from numerical problems when using an approximate arithmetic with error tolerance greater than 4×10^{-6}; see the discussion in [11, Remark 1.3.5]. For this example it is advised to set $\epsilon = 10^{-8}$ to avoid error amplification introduced, amongst others, by the reciprocal of the square of the real part of the critical eigenvalue λ_1 (compare with the bound for the symmetric case (3.2)); for details see [6]. The reduced order for the tolerance 10^{-4} is determined to be $r = 9$. The error in the CG reduced-order model satisfies the computed error estimate $\delta = 3.3 \times 10^{-5}$, and is nearly the same as for the BT reduced-order system; see Figure 3.3. Furthermore, the CG error curves for $\|G - \hat{G}\|_\infty$ and $\|G_{\mathcal{H}} - \hat{G}\|_\infty$ are very close.

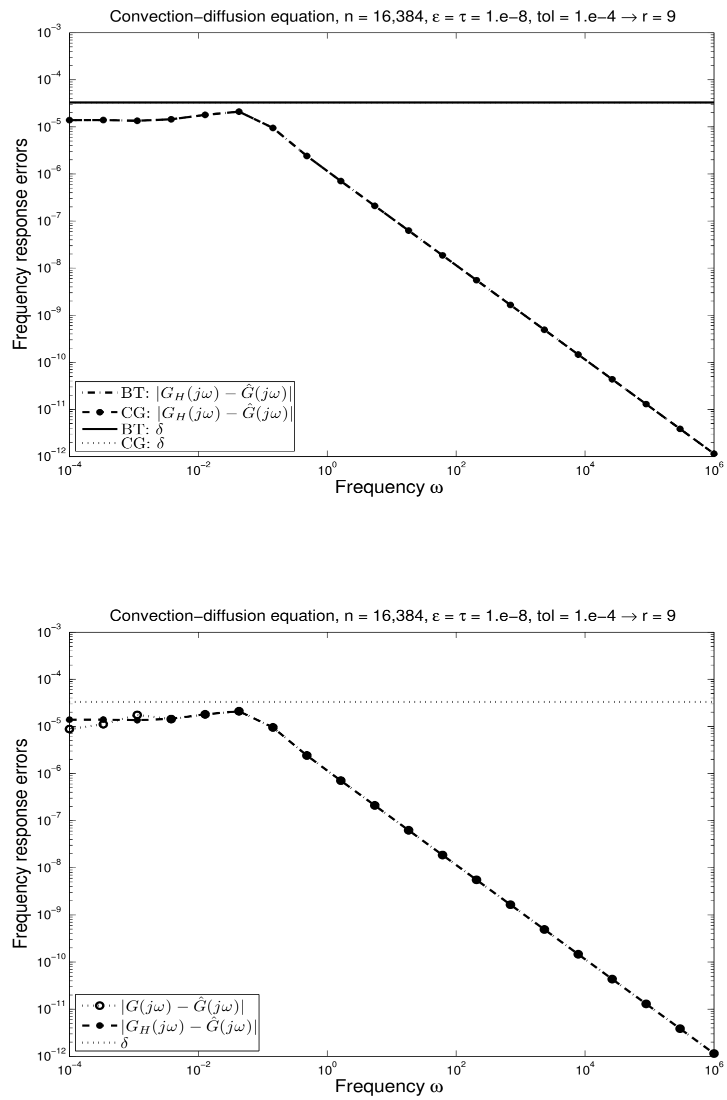

FIGURE 3.3. *Frequency response errors for the convection-diffusion equation using the cross-Gramian approach as described in Algorithm 2.*

Next we apply Algorithm 2 to a symmetric MIMO system as obtained by the spatial discretization of (3.3) with $a(\cdot) \equiv 1.0$, $c = (0,0)^T$, using again $n = 16,384$ grid points. The dimension of the input space is enlarged to $m = 8$, additionally setting $C = B^T$. The reduced order determined by the CG approach for tol $= 10^{-4}$ is $r = 11$. In Figure 3.4 the error plots for several of the 64 input/output channels of the system are depicted. All graphs satisfy the computed error estimate $\delta = 8.1 \times 10^{-5}$.

In the last example we reduce the dimension of a non-symmetric system resulting from the finite element semi-discretization of a two-dimensional heat equation similar to (3.4). The number of grid points is $n = 5177$ and Neumann boundary conditions describing different inputs are applied at 6 parts of the boundary, thus $m = 6$. The output matrix C is defined

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to minimize the temperature difference between certain grid points with $p = 6$. BT and the CG approach are applied to reduce the dimension of the systems using a tolerance threshold of 10^{-4}. The results for two input/output channels are shown in Figure 3.5. It is observed that the CG reduced-order system is of smaller dimension $r = 14$ than the system computed by BT ($r = 18$). The corresponding error curves are quite close (in the lower plot, the CG error is even smaller) and the CG reduced-order system satisfies the error estimate, though no theoretical background exists for the CG approach applied to non-symmetric MIMO systems. This example shows that there exist situations where the CG approach is preferable to BT, although this is not supported by theory so far.

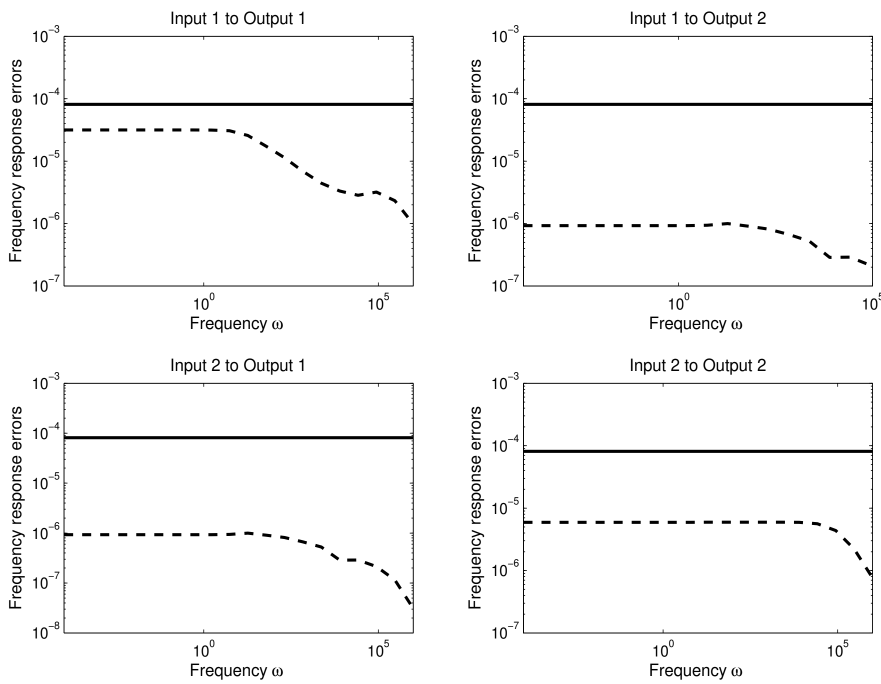

FIGURE 3.4. *Frequency response errors for the two-dimensional heat equation with $m = p = 8$, using the cross-Gramian approach as described in Algorithm 2.*

4. Conclusions. We have shown that a balancing-related cross-Gramian approach can be used for MOR of large-scale linear systems resulting from (semi-) discretizations of parabolic control systems. For SISO and for symmetric MIMO systems, the computed reduced-order models have the same desirable properties as obtained by the usual BT method. Furthermore, it is shown that the method can be applied to general systems, provided that $m = p$. Employing formatted arithmetic in a sign function-based Sylvester solver, approximate low-rank factors of the cross-Gramian can be computed with linear-polylogarithmic complexity. From these low-rank factors, the projection matrices for MOR are derived directly, using a low-rank product QR algorithm. The approximation quality of the reduced-order system depends on the parameter ϵ for the blockwise accuracy in the $\mathcal{H}$-matrix arithmetic. This is confirmed by several numerical experiments which demonstrate the usefulness of the CG approach.

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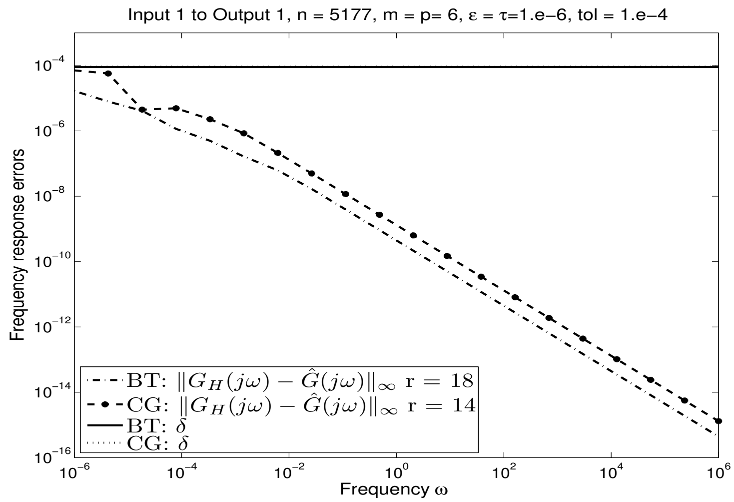

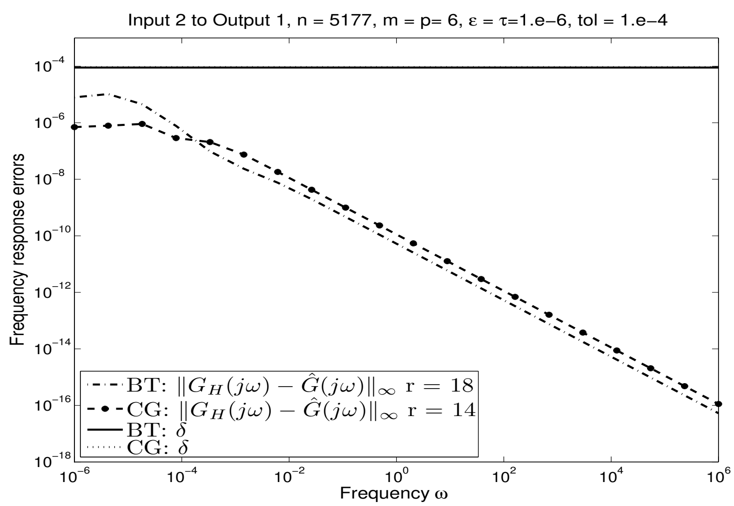

FIGURE 3.5. *Frequency response errors for the two-dimensional heat equation with $m = p = 6$, non-symmetric, using the cross-Gramian approach as described in Algorithm 2.*

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