Revised Version for TCAD 3015

Fast Positive-Real Balanced Truncation Via Quadratic Alternating Direction Implicit Iteration

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Response to the Associate Editor and Reviewers is attached at the end of the paper

Fast Positive-Real Balanced Truncation Via Quadratic Alternating Direction Implicit Iteration

Ngai Wong† and Venkataramanan Balakrishnan

***Abstract*— Balanced truncation (BT), as applied to date in model order reduction (MOR), is known for its superior accuracy and computable error bounds. Positive-real balanced truncation (PRBT) is a particular BT procedure that preserves passivity and stability, and imposes no structural constraints on the original state space. However, PRBT requires solving two algebraic Riccati equations (AREs), whose computational complexity limits its practical use in large-scale systems. This paper introduces a novel quadratic extension of the alternating direction implicit (ADI) iteration, called QADI, that efficiently solves an ARE. A Cholesky factor version of QADI, called CFQADI, exploits low-rank matrices and further accelerates PRBT.**

***Index Terms*— Model order reduction, positive-real balanced truncation, alternating direction implicit, ADI, Riccati equation**

I. INTRODUCTION

Simulation of interconnects after parasitic extraction, despite its computational load, is a critical post-layout verification step in deep submicron VLSI design. The high data volume and initial model orders, however, forbid direct computer manipulation. Model order reduction (MOR) comes into place whereby a high-order model is reduced to a (considerably) smaller one without much degradation in accuracy [1]. Moreover, stability and passivity[1] of the original model must be preserved to guarantee stable global simulation [1], [3], [4].

Projection-type MOR schemes such as PRIMA [3] and pole analysis via congruence transformations (PACT) [5], usually implemented with the computationally efficient Krylov subspace projection, preserve passivity. However, both algorithms assume special state space structures that are not always feasible [4]. Reduced models from these schemes show similar responses to the original systems, but there is neither direct error connection between the two nor optimality guarantee. On the other hand, balanced truncation (BT) schemes, such as standard BT and positive-real BT (PRBT)[2], offer superior accuracy in reduced-order models [4], [8]–[10] with deterministic error bounds [11], [12], but are largely restricted by the complexity of solving high-order matrix equations and factorizations. To quickly solve the Lyapunov equations (linear matrix equations) in standard BT, recent advances utilize the alternating direction implicit (ADI) iteration [13], [14] and Smith method [6], [15] (i.e., ADI with one shift) to exploit low-rank input/output matrices pertinent to physical models. A Cholesky factor (CF) variant of ADI, called CF-ADI [14], directly computes the factored solution. This avoids the matrix factorizations in standard BT and speeds it up to an extent comparable to the projection-based methods [14]–[16]. However, standard BT does not necessarily preserve passivity. PRBT guarantees stability and passivity and has no special structural requirements on the initial state space [4], [10], but faces even heavier computation due to the solution of algebraic Riccati equations (AREs) which are quadratic matrix equations. Conventional ways of solving an ARE include identifying the stable invariant subspace of a Hamiltonian matrix, or by the Newton method that solves a Lyapunov equation in each iteration, e.g., [6], [7], [15], [17]–[20]. Nonetheless, the Hamiltonian approach, like eigenvector/Schur-vector or matrix sign function methods etc., do not explicitly utilize sparse/low-rank matrices and are relatively slow. Using efficient iterative solver algorithms for Lyapunov equations, such as ADI and CF-ADI, the Newton method and its variants exploit matrix structures and have been successfully adapted to large-scale AREs. But then these schemes are based on linearization in each Newton step, and their outer (global) convergence is dependent on inner (local) convergence in each step.

The main contribution of this paper (an extension of [21]) is the formulation of a quadratic ADI algorithm, called *QADI*, that directly and efficiently solves a (large-size) ARE. Using a linear fractional transformation (LFT) framework which largely simplifies the otherwise intractable derivations, a CF version of QADI, called *CFQADI*, is introduced which further exploits low-rank matrices and produces a factored solution that accelerates PRBT. This work parallels and generalizes the results of [14], viz., on standard BT and CF-ADI, to their second-order counterparts, viz., on PRBT and CFQADI. It is shown that (CF)QADI enjoys similar convergence and computational efficiency to (CF-)ADI, and that the PRBT/CFQADI integration constitutes a powerful candidate to high-speed, large-scale, passivity-preserving MOR.

II. PRELIMINARIES

A. Basics of PRBT

Interconnect and package modelings generally make use of passive RLC components. Consider a large-scale RLC network

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[1]A passive system is one that does not generate energy internally, e.g. [2]. A strictly passive system is dissipative and is automatically stable. In linear systems, passivity is equivalent to positive realness.

[2]PRBT is the BT procedure wherein a pair of algebraic Riccati equations (AREs) are solved. It is also commonly called positive-real truncated balanced realization (PR-TBR) [4]. Ref. [6] uses balanced stochastic truncation (BST) to denote PRBT, though a more common perception of BST refers to the BT approach in which one Lyapunov equation and one ARE are solved [7].

cast into a state space

$$\dot{x} = A_0 x + B_0 u \quad , y = C_0 x + D_0 u, \tag{1}$$

where $A_0 \in \mathbb{R}^{n\times n}$, $B_0, C_0^T \in \mathbb{R}^{n\times m}$, $D_0 \in \mathbb{R}^{m\times m}$, B_0, C_0 are generally of low-ranks (i.e., $m \ll n$) and u and y are power-conjugate [6]. A_0 is stable or equivalently its spectrum is in the open left half plane, denoted by $spec(A_0) \subset \mathbb{C}_-$. Let $M > 0$ ($M \geq 0$) denote a positive definite (positive semidefinite) matrix M, we assume without loss of generality that $D_0 + D_0^T > 0$, otherwise [say, in modified nodal analysis (MNA) where $D_0 = 0$] the reduction technique in [22] is iteratively used to achieve this. Also, an impulse-free system in the *descriptor* form [1] with a singular E_0 before $\dot{x}$ can be put into the standard form in (1) [4]. Define the matrix root $DD^T = (D_0 + D_0^T)^{-1}$, $B = B_0 D$, $C = D^T C_0$, and $A = A_0 - BC$. In PRBT, the unique stabilizing solutions, $X, Q (\in \mathbb{R}^{n\times n}) \geq 0$, to the dual AREs,

$$A^T X + XA + XBB^T X + C^T C = 0, \tag{2a}$$

$$AQ + QA^T + QC^T CQ + BB^T = 0, \tag{2b}$$

are solved such that $spec(A + BB^T X) \subset \mathbb{C}_-$ and $spec(A^T + C^T CQ) \subset \mathbb{C}_-$. Let $X = ZZ^T$ and $Q = YY^T$ be any Cholesky factorizations, the "economic" singular value decomposition (SVD) of the following cross product is found:

$$Y^T Z = U\Sigma V^T,\ \Sigma = diag(\sigma_1, \sigma_2, \cdots, \sigma_k) \geq 0,\ k \leq n. \tag{3}$$

Suppose $\sigma_1 \geq \cdots \geq \sigma_r \gg \sigma_{r+1} \geq \cdots \geq \sigma_k$. Let I_m be an identity matrix of dimension m and $0_{m\times n}$ be an $m \times n$ zero matrix. Define the left and right projection matrices to be $T_L = \begin{bmatrix} I_r & 0_{r\times(k-r)} \end{bmatrix} \Sigma^{-\frac{1}{2}} V^T Z^T$ and $T_R = YU\Sigma^{-\frac{1}{2}} \begin{bmatrix} I_r & 0_{r\times(k-r)} \end{bmatrix}^T$, respectively, the system $(T_L A_0 T_R, T_L B_0, C_0 T_R, D_0)$ is the PR-balanced and truncated model whose states are aligned in descending involvement in the energy transfer process [4].

B. Basics of ADI

In general, *alternating direction implicit* (ADI) iteration [13], [14] solves the Lyapunov equation

$$A^T W + WA + C^T C = 0, \tag{4}$$

where the matrix dimensions are consistent with those in (2a). Here A is assumed stable so there exists a unique W ($\in \mathbb{R}^{n\times n}$) ≥ 0 that solves (4). The basic ADI consists of two iterative half-steps,

$$(A^T + p_j I) W_{j-\frac{1}{2}}^T = -C^T C - W_{j-1}^T (A - p_j I), \tag{5a}$$

$$(A^T + p_j I) W_j = -C^T C - W_{j-\frac{1}{2}} (A - p_j I), \tag{5b}$$

where $W_0 = 0$ and the shift parameters $p_j \in \mathbb{C}_-$ ($j = 1, 2, \cdots$) appear as real numbers or conjugate pairs. For compactness we define $S_j = (A + p_j I)^{-1}$ and $T_j = (A - p_j I)$. A useful fact is that for any integers m and n, the multiplication among S_m, T_n, and A are commutative, and similarly for S_m^T, T_n^T, and A^T. It can be verified that

$$W_j = -\sum_{i=1}^{j} 2p_i \left(\prod_{k=1}^{i-1} S_k^T T_k^T \right) S_i^T C^T C S_i \left(\prod_{k=1}^{i-1} T_k S_k \right). \tag{6}$$

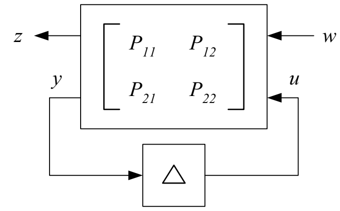

Fig. 1. A lower LFT system.

In [14] it is shown that the ordering of p_j's in (6) is immaterial. Combining (4) and (5), we get

$$W - W_j = \left(\prod_{k=1}^{j} S_k^T T_k^T \right) W \left(\prod_{k=1}^{j} T_k S_k \right). \tag{7}$$

Since A is stable, it is easily shown that $\rho(T_k S_k) < 1$ where $\rho(\circ)$ denotes the spectral radius. Convergence of this form is termed *superlinear* [14]. To achieve the fastest convergence in, say, L runs of (5), p_j's are chosen (or approximately chosen) according to the minimax problem

$$\min_{\{p_1, p_2, \cdots, p_L\}} \left(\max_{\lambda_i \in spec(A)} \left| \prod_{j=1}^{L} \frac{p_j - \lambda_i}{p_j + \lambda_i} \right| \right). \tag{8}$$

Solution of (8) is a well-studied topic and the reader is referred to, e.g., [14], [15] and the references therein. From (7) we can also derive a "residual error" expression for the Lyapunov operator, namely,

$$A^T W_j + W_j A + C^T C = \left(\prod_{k=1}^{j} S_k^T T_k^T \right) C^T C \left(\prod_{k=1}^{j} T_k S_k \right). \tag{9}$$

Because $\rho(T_k S_k) < 1$, the norm of the right hand side of (9) approaches zero when j tends to infinity.

III. Quadratic ADI

We focus on the following ARE which is a recap of (2a),

$$A^T X + XA + XBB^T X + C^T C = 0. \tag{10}$$

A is assumed stable and a stabilizing solution $X \geq 0$ exists such that $spec(A + BB^T X) \subset \mathbb{C}_-$. The bounded real lemma [18] states that such an X exists if and only if $sup\, \bar{\sigma}(C(j\omega - A)^{-1} B) < 1$, $\forall \omega \in \mathbb{R}$, where $\bar{\sigma}(\circ)$ denotes the maximum singular value. The following second-order generalization of ADI, called *quadratic ADI* or *QADI*, is proposed for solving (10),

$$(A^T + X_{j-1}^T BB^T + p_j I) X_{j-\frac{1}{2}}^T = -C^T C - X_{j-1}^T (A - p_j I), \tag{11a}$$

$$(A^T + X_{j-\frac{1}{2}} BB^T + p_j I) X_j = -C^T C - X_{j-\frac{1}{2}} (A - p_j I), \tag{11b}$$

where $X_0 = 0$ and $p_j \in \mathbb{C}_-$, $j = 1, 2, \cdots$, are either real or conjugate pairs. Apparently, (11) reduces to (5) when $B = 0$. For ease of illustration we will assume, for the rest of the paper, all p_j's are negative real. However, all qualitative results hold true for conjugate pairs if we combine two runs of (11) into one and in that case all quantities remain real. This seemingly simple modification of ADI, however, gives rise to complicated derivations due to its quadratic nature. An insight that greatly simplifies analyses of QADI is to recognize (11) as linear fractional transformations (LFTs) [18]. Referring to Fig. 1, with $P = \begin{bmatrix} P_{11} & P_{12} \\ P_{21} & P_{22} \end{bmatrix}$, we define the (lower) LFT, denoted by $F_l(P,\Delta)$, as the transfer matrix from w to z, i.e., $z = F_l(P,\Delta)w$, which is a mapping of Δ,

$$F_l(P,\Delta) = P_{11} + P_{12}\Delta\,(I - P_{22}\Delta)^{-1}\,P_{21},$$

where the matrix dimensions are implicitly assumed compatible and the matrix inverse well-defined. With the definitions $S_j = (A+p_jI)^{-1}$ and $T_j = (A-p_jI)$, it can be shown that

$$X_{j-\frac{1}{2}} = F_l(P_j, X_{j-1}) \quad \text{and} \quad X_j = F_l(P_j^T, X_{j-\frac{1}{2}}) \quad (12)$$

where $P_j = \begin{bmatrix} -C^TCS_j & -T_j^T + C^TCS_jBB^T \\ S_j & -S_jBB^T \end{bmatrix}$.

Note that we are slightly abusing the LFT notion as it normally denotes a transfer matrix rather than matrix operation. However, all algebras in LFT are applicable as long as the matrix operands are compatibly dimensioned. The chief property of LFTs is that their interconnection again results in an LFT. In particular, the nested connection $X_j = F_l(P_j^T, F_l(P_j, X_{j-1}))$, called a *Redheffer Star Product* [18], is an LFT. This enables the combination of the two half-steps in (11) into one, namely,

$$X_j = M_{11}^{(j)} + M_{12}^{(j)} X_{j-1}(I - M_{22}^{(j)}X_{j-1})^{-1}(M_{12}^{(j)})^T, \quad (13)$$

$$M_{11}^{(j)} = -2p_jS_j^TC^T(I - CS_jBB^TS_j^TC^T)^{-1}CS_j, \quad (14a)$$

$$M_{22}^{(j)} = -2p_jS_jB(I - B^TS_j^TC^TCS_jB)^{-1}B^TS_j^T, \quad (14b)$$

$$\begin{aligned} M_{12}^{(j)} &= I - 2p_jS_j^T(I - C^TCS_jBB^TS_j^T)^{-1} \\ &= I - 2p_jS_j^T + S_j^TC^TCM_{22}^{(j)}. \end{aligned} \quad (14c)$$

It can be seen that a symmetric X_{j-1} implies a symmetric X_j. Since $X_0 = 0$, all X_j's are symmetric.

A. Well-Posedness

The matrix inverses in (14a)-(14c) are always well-defined because the passivity assumption ensures the existence of a stabilizing solution, which in turn guarantees $\bar{\sigma}(CS_jB) < 1$ due to the bounded real lemma. It remains to show that the inverse $(I - M_{22}^{(j)}X_{j-1})^{-1}$ in (13) is always well-defined, and in fact $X_{j-1}(I - M_{22}^{(j)}X_{j-1})^{-1} \geq 0$, thereby verifying the well-posedness of QADI. To begin with, we state two lemmas useful for the proof. As noted, p_j's are assumed to be negative real for ease of illustration.

Lemma 1: Assume (10) has a stabilizing solution X. Define $\tilde{A} = A + BB^TX$ so that $spec(\tilde{A}) \subset \mathbb{C}_-$. Let $\tilde{S}_j = (\tilde{A} + p_jI)^{-1}$ and $\tilde{T}_j = (\tilde{A} - p_jI)$, we have

$$X - X_j = F_l\left(\begin{bmatrix} 0 & \tilde{S}_j^T\tilde{T}_j^T \\ \tilde{T}_j\tilde{S}_j & 2p_j\tilde{S}_jBB^T\tilde{S}_j^T \end{bmatrix}, X - X_{j-1}\right), \quad (15)$$

and it follows that $X - X_{j-1} \geq 0$ implies $X - X_j \geq 0$.

Proof: We first rewrite (11a) and (11b) by the knowledge of (10). Let $\tilde{P}_j = \begin{bmatrix} 0 & -\tilde{T}_j^T \\ \tilde{S}_j & \tilde{S}_jBB^T \end{bmatrix}$, we have

$$X - X_{j-\frac{1}{2}} = F_l(\tilde{P}_j, X - X_{j-1}), \quad (16a)$$

$$X - X_j = F_l(\tilde{P}_j^T, X - X_{j-\frac{1}{2}}). \quad (16b)$$

Applying the star product we get (15). ∎

Lemma 2: Assume (10) has a stabilizing solution X. Let $S_j = (A + p_jI)^{-1}$ and $T_j = (A - p_jI)$, we have $\bar{\sigma}(B^TS_j^T(C^TC - 2p_jX)S_jB) < 1$.

Proof: Rearranging (10), we get

$$\begin{aligned} &(A+p_jI)^TX + X(A+p_jI) + XBB^TX \\ &\quad + \begin{bmatrix} C \\ \sqrt{-2p_j}Z^T \end{bmatrix}^T \begin{bmatrix} C \\ \sqrt{-2p_j}Z^T \end{bmatrix} = 0, \end{aligned} \quad (17)$$

where $X = ZZ^T$. Obviously, X is also a stabilizing solution to (17). The bounded real lemma implies

$$\bar{\sigma}\left(\begin{bmatrix} C \\ \sqrt{-2p_j}Z^T \end{bmatrix}(A+p_jI)^{-1}B\right) = \bar{\sigma}\left(\begin{bmatrix} C \\ \sqrt{-2p_j}Z^T \end{bmatrix}S_jB\right) < 1,$$

and the proof follows. ∎

The next lemma then proves the well-posedness.

Lemma 3: Assume (10) has a stabilizing solution X. Then in each QADI iteration, $X_{j-1}(I - M_{22}^{(j)}X_{j-1})^{-1}$ is well-defined and is positive semidefinite.

Proof: First, we note that

$$M_{22}^{(j)} = -2p_jS_jB(I - B^TS_j^TC^TCS_jB)^{-1}B^TS_j^T \geq 0.$$

Expanding $X_{j-1}(I - M_{22}^{(j)}X_{j-1})^{-1}$ we get (18) on the top of next page. In going from the second to the third line of (18) we have used the matrix inversion lemma. Clearly, Lemma 3 holds if $\bar{\sigma}(B^TS_j^T(C^TC - 2p_jX_{j-1})S_jB) < 1$ and $X_{j-1} \geq 0$ for $j = 1, 2, \cdots$, which we will prove inductively.

Set $j = 1$ in (13). By noting $X_0 = 0$ and $M_{11}^{(j)} \geq 0$ for all j's, X_1 is well-defined and positive semidefinite. By Lemma 1 we have $X \geq X_1$, also from Lemma 2 we have

$$\bar{\sigma}(B^TS_2^T(C^TC - 2p_2X_1)S_2B) \leq \bar{\sigma}(B^TS_2^T(C^TC - 2p_2X)S_2B) < 1.$$

Set $j = 2$ in (13). From the results above, X_2 is well-defined and positive semidefinite. By Lemma 1 we have $X \geq X_2$, also from Lemma 2 we have

$$\bar{\sigma}(B^TS_3^T(C^TC - 2p_3X_2)S_3B) \leq \bar{\sigma}(B^TS_3^T(C^TC - 2p_3X)S_3B) < 1.$$

The argument extends to all j's similarly. ∎

B. Convergence

Analogous to ADI, QADI exhibits superlinear convergence. To show this, we apply (15) recursively to itself. Since $X_0 = 0$,

$$X - X_j = \Pi_j^TX(I + \Omega_jX)^{-1}\Pi_j \quad (19)$$

with $\Pi_j = \left(\prod_{k=1}^{j}\tilde{T}_k\tilde{S}_k\right)$,

$$\Omega_j = -\sum_{i=1}^{j} 2p_i\left(\prod_{k=1}^{i-1}\tilde{S}_k\tilde{T}_k\right)\tilde{S}_iBB^T\tilde{S}_i^T\left(\prod_{k=1}^{i-1}\tilde{T}_k^T\tilde{S}_k^T\right).$$

An interesting observation is that Ω_j is exactly the jth iterate of the ADI solution to the Lyapunov equation [cf. (6)]

$$\tilde{A}\Omega + \Omega\tilde{A}^T + BB^T = 0. \quad (20)$$

So we have $\Omega_j \to \Omega$ as $j \to \infty$. Also, it is easily proved that $X \geq X(I + \Omega_jX)^{-1}$, which renders $X - X_j \leq \Pi_j^TX\Pi_j$. Comparing this to (7), the error bound from ADI may be borrowed: to achieve the fastest convergence in, say, L runs of

$$\begin{aligned}&X_{j-1}\left(I-(-2p_j)S_jB(I-B^TS_j^TC^TCS_jB)^{-1}B^TS_j^TX_{j-1}\right)^{-1}\\&=X_{j-1}\left(I-\sqrt{-2p_j}S_jB(I-B^TS_j^TC^TCS_jB)^{-\frac{1}{2}}\sqrt{-2p_j}(I-B^TS_j^TC^TCS_jB)^{-\frac{1}{2}}B^TS_j^TX_{j-1}\right)^{-1}\\&=X_{j-1}+(-2p_j)X_{j-1}S_jB\left(I-B^TS_j^T(C^TC-2p_jX_{j-1})S_jB\right)^{-1}B^TS_j^TX_{j-1}.\end{aligned}\tag{18}$$

QADI, p_j's are chosen (or approximately chosen) according to the minimax problem,

$$\min_{\{p_1,p_2,\cdots,p_L\}}\left(\max_{\lambda_i\in spec(\tilde{A})}\left|\prod_{j=1}^{L}\frac{p_j-\lambda_i}{p_j+\lambda_i}\right|\right),\tag{21}$$

which is effectively a minimax problem on the spectral radius of Π_j. This shows the superlinear convergence of QADI with the difference that the shifts p_j's are now determined from the spectrum of $\tilde{A}$ instead of that of A. Fortunately, though $\tilde{A}=A+BB^TX$ is self-referential to X, its spectrum is known *a priori* (e.g., [18], [23]). Specifically,

$$spec(\tilde{A})=spec(H)\cap\mathbb{C}_-,\ \text{where } H=\begin{bmatrix}A & BB^T\\ -C^TC & -A^T\end{bmatrix}\tag{22}$$

is the *Hamiltonian* matrix associated with (10).

C. Cholesky Factor Variant

Analogous to CF-ADI [14], when low-rank B and C are present, it is desirable for QADI to work with the Cholesky factor (CF) iterate Z_j where $X_j=Z_jZ_j^T$. Utilizing (13) and (14), we formulate a CF variant of QADI called *CFQADI*. In particular, setting $Z_0=0$, for $j=1,2,\cdots$,

1. $(M_{11}^{(j)})^{\frac{1}{2}}=\sqrt{-2p_j}S_j^TC^T(I-CS_jBB^TS_j^TC^T)^{-\frac{1}{2}}$ (23a)
2. $M_{22}^{(j)}=-2p_jS_jB(I-B^TS_j^TC^TCS_jB)^{-1}B^TS_j^T$ (23b)
3. $M_{12}^{(j)}=I-2p_jS_j^T+S_j^TC^TCM_{22}^{(j)}$ (23c)
4. $Z_j=[(M_{11}^{(j)})^{\frac{1}{2}}\quad M_{12}^{(j)}Z_{j-1}(I-Z_{j-1}^TM_{22}^{(j)}Z_{j-1})^{-\frac{1}{2}}]$ (23d)

Each sweep of (23) increases the number of columns in Z_j by that in C^T. Low-rank B and C also allow the use of matrix inversion lemma in (23a)-(23c) to reduce arithmetics. All properties of QADI carry over to CFQADI since they are mathematically equivalent. Consequently, for low-rank input/output matrices, CFQADI provides significant computational and memory savings as only low-rank factors are stored. Symmetry of X_j is perfectly preserved by reconstruction from Z_j. Moreover, the converged factor Z, where $X=ZZ^T$, can readily be adapted to PRBT.

IV. Numerical examples

We study the CPU times of different PRBT implementations. Characterization of QADI and CFQADI as standalone ARE solvers may be found in [21]. On the one hand, PRBT is realized in the conventional way whereby two AREs are solved, followed by CF and SVD computation (cf. Section II-A). The ARE solvers used include the Matlab subroutine `aresolv` with the `schur` and `eigen` flags chosen in turn. The former implements the Schur-vector method, while the latter uses the eigenvector method [17]. Two other Fortran 77 subroutines, `slcares` (Schur-vector method) and `slcaregs` (generalized Schur-vector method), are invoked from the SLICOT library [20] via a Matlab gateway. On the other hand, fast PRBT implementations utilizing CF iterates are deployed using CFQADI and the recently proposed NSCARE algorithm [6]. In line with the approach in [7], [15], NSCARE is a Newton method variant for solving an (especially large-scale) ARE. It uses Smith method and constructs a CF solution to the Lyapunov equation in each Newton step, thereby indirectly forming a concatenated CF solution to an ARE. Both CFQADI and NSCARE are coded in Matlab m-script (text) files. [In solving AREs of the form (2), we do not assume nor exploit any structure, such as bands or sparsity, in A.] All experiments were done in the Matlab R14 (SP2) environment on a 3GHz PC with 3G RAM. Both NSCARE and CFQADI are non-Hamiltonian solvers, while others are based on identifying the stable invariant subspace of a Hamiltonian matrix. Fig. 2 plots the metric $\|X_j-X\|_F/\|X\|_F$, $\|\circ\|_F$ being the Frobenius norm, in typical ARE solutions by QADI (or equivalently CFQADI) at several ARE orders. Superlinear convergence of (CF)QADI can be observed from these almost straight lines.

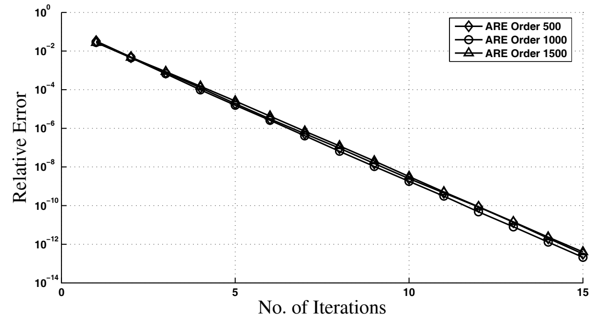

Fig. 2. (CF)QADI: convergence of X_j to the stabilizing X at several orders.

TABLE I
CPU times (sec) of various PRBT implementations and PRIMA.

MOR Schemes	Spiral Inductor	RLC Ladder
PRBT/aresolv(schur)	†(98.4+28.1) 126.5	(2286.6+136.0) 2422.6
PRBT/aresolv(eigen)	(53.3+26.1) 79.4	(403.3+125.9) 529.2
PRBT/slcares	(46.0+4.2) 50.2	(390.0+17.4) 407.4
PRBT/slcaregs	(85.2+3.9) 89.1	(904.2+17.8) 922.0
PRBT/NSCARE	(7.19+0.97) 8.16	(20.56+0.80) 21.36
PRBT/CFQADI	(2.84+0.02) 2.86	(2.67+0.02) 2.69
PRIMA	0.67	2.53

† PRBT time breakdown: (Two AREs + Matrix Factorizations) Total

PRBT is performed on two benchmarks: a spiral inductor model of order 500 and an RLC ladder circuit of order 800 [6]. CFQADI has been used since its CF iterates can

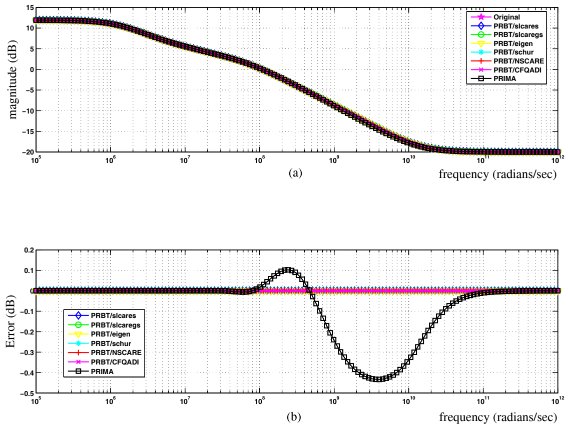

Fig. 3. (a) Frequency responses of the spiral inductor model (order=500) and the reduced-order models (order=9). (b) Approximation errors.

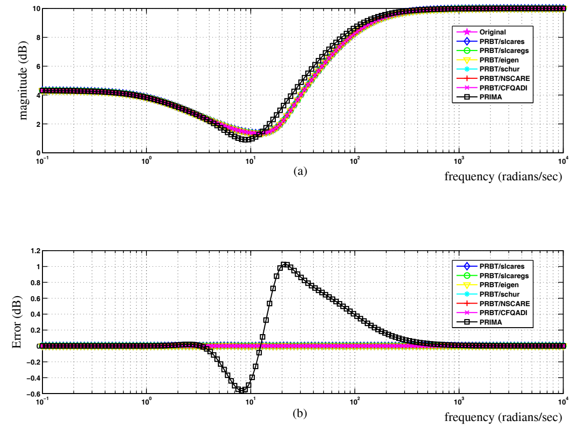

Fig. 4. (a) Frequency responses of the RLC ladder model (order=800) and the reduced-order models (order=6). (b) Approximation errors.

take advantage of low-rank input/output matrices to reduce computation and memory space. Table I tabulates the CPU times of various PRBT implementations and also that by the projection-based PRIMA [3] algorithm. All reduced-order models are passive. Figs. 3(a) and 4(a) show the frequency responses of the original and reduced-order models, while Figs. 3(b) and 4(b) plot the approximation errors. It is seen that the PRBT curves by different solvers virtually overlap because they all solve the same set of AREs, while the PRIMA curves exhibit relatively larger errors. This is expected as reduced-order models from PRBT tend to have excellent global accuracy [4], [6]. Moreover, PRBT avoids the selection of expansion points and final model order as in PRIMA. Solutions from CFQADI and NSCARE are computed to the same or better accuracy than those by other PRBT algorithms. Specifically, for these CF-iterate approaches in which Z_j and Y_j ($X_j = Z_j Z_j^T$, $Q_j = Y_j Y_j^T$) are progressively computed, the cross-product stopping criterion [16], which monitors the Frobenius norm update in $Y_j^T Z_j$ [cf. (3)], has been used. And it can be further shown that the set of singular values of $Y_j^T Z_j$ thus obtained, $\{\hat{\sigma}_i\}$, approaches that in $Y^T Z$, $\{\sigma_i\}$, exponentially [16].

Moreover, among all PRBT implementations, NSCARE and CFQADI exhibit superior speed and scalability over others, with CFQADI being the fastest. This is even more obvious in high-order examples, including some not reported here, where CFQADI approaches the speed of PRIMA. Despite the comparable speed of NSCARE to CFQADI, the final CF solution from CFQADI always have much fewer columns and thus lower ranks. For example, in the spiral inductor case, the size of the terminating Z_j and Y_j by NSCARE is about 500×380, and only about 500×100 for CFQADI. In the ladder circuit case, they are about 800×450 and 800×25, respectively. This can be attributed to the strength of PRBT/CFQADI in capturing the fast decaying singular values of the cross product, and also explains the remarkable speed of CFQADI. On the other hand, NSCARE builds the CF solution to an ARE progressively from intermediate Lyapunov equations. Subsequently, convergence of NSCARE is dependent on the convergence in respective Lyapunov equations, while that of CFQADI is reliant on the spectrum of the Hamiltonian matrix (which determines the shifts) formed directly from the original ARE matrices. Another major merit of these CF-type algorithms, as seen from the breakdowns in Table I, is the avoidance of the (large-scale) CF factorizations and SVD. Although [6] has shown that PRBT time by Hamiltonian-based solvers can almost be halved by complete subspace separation, the speed improvement by CFQADI is much more than double, e.g., PRBT/CFQADI is more than $150\times$ faster than PRBT/`slcares` in the second benchmark.

V. Remarks

(CF)QADI is a new (large-scale) ARE solver algorithm with simple codings. To our knowledge, CFQADI is the first algorithm that directly computes the CF solution to an ARE through CF iterates, instead of the concatenated CF solution from Newton method [6], [15]. With low-rank input/output matrices, the CF solution thus obtained is usually of low-rank, thereby avoiding large-size matrix factorizations and SVD in the original PRBT procedure. The low-rank factor also reduces memory requirement and improves scalability. The runtimes of QADI and CFQADI are dominated by the number of shifts. The most expensive step is the matrix inversion in finding S_j for each p_j, which takes roughly $3n^3$ flops in the most general case when A is dense. If the number of shifts is L (which equals one in our experiments), the work of both algorithms is proportional to $3Ln^3$. All other operations in CFQADI are of $O(n^2)$ due to exploitation of low-rank matrices. In contrast, the complexities of the Schur-vector and eigenvector methods are roughly $50n^3 \sim 150n^3$ flops. Therefore, work of (CF)QADI increases in a cubic manner, but much more slowly than that in conventional solvers. If matrix inversion can be done in $O(n^2)$ work, e.g., when A is sparse or banded, then (CF)QADI will reduce to an $O(n^2)$ algorithm. Regarding memory, CFQADI requires $O(nm)$ space (usually $m \ll n$) due to its storage of CF iterates. Most conventional algorithms require $O(n^2)$ space due to the storage of square matrices.

For simplicity and demonstration, only a single shift has been used in CFQADI, which is analogous to the Smith method as a special case of ADI [6], [15]. Referring to (22), we have chosen $p = -\sqrt{\rho(\tilde{A})/\rho(\tilde{A}^{-1})}$ [6]. Owing to the symmetry in the spectrum of H, we also have $p = -\sqrt{\rho(H)/\rho(H^{-1})}$, which is then estimated through simple power iterations. Some useful facts are in order: in solving the dual AREs in (2) via CFQADI, the following Hamiltonian matrices are set up for finding shifts, namely,

$$H = \begin{bmatrix} A & BB^T \\ -C^TC & -A^T \end{bmatrix} \text{ and } H' = \begin{bmatrix} A^T & C^TC \\ -BB^T & -A \end{bmatrix},$$

corresponding to (2a) and (2b), respectively. With some care, it can be shown that $spec(H) = -spec(H') = spec(H')$. Therefore, the same set of shifts p_j's for (2a) can be reused in (2b). Also, the efficient implicitly-restarted shift-and-invert Arnoldi algorithm in [23], called SHIRA, is particularly suitable for the computation of extremal eigenvalues of H.

When CFQADI is terminated before convergence (due to slow convergence or time constraint), the PRBT/CFQADI-reduced model may only be near-passive and passivity enforcement is needed. This can be done by, e.g., the algorithm in [2]. Fortunately, the reduced models are of low orders (a few tens), rendering such enforcement computationally fast. Generally, (CF)QADI performs better in damped systems than in lightly-damped systems where the spectral radius $\rho(\tilde{T}_k\tilde{S}_k)$, and so that of Π_j [cf. (19)], is near unity. Such problem can be mitigated by choosing multiple p_j's to accelerate the convergence of (CF)QADI or by using parallel computing, despite a bigger overhead in finding p_j's and more explicit inversions. However, these topics are beyond the scope of this paper and will not be elaborated.

VI. Conclusion

This paper has presented a highly efficient positive-real balanced truncation (PRBT) implementation based on the fast algebraic Riccati equation (ARE) solver called quadratic alternating direction implicit (QADI) iteration. Well-posedness and convergence of QADI have been analytically proved. QADI facilitates a Cholesky factor variant, called CFQADI, that exploits low-rank matrices and avoids large-scale matrix factorizations, thereby resulting in fast PRBT computation and significant memory savings. Numerical examples have verified the remarkable efficacy of the PRBT/CFQADI integration over conventional PRBT realizations.

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Response to the Associate Editor and Reviewers

Comments are in italic fonts and our response is in normal fonts.

Associate Editor's comments and our response:

The review process for your submission has been concluded. Enclosed you can find the reviewer's scores and comments. As you can see from the comments, the reviewers are not entirely in agreement as to the relevance of the paper. However, they all agree that there are several issues that would need to be addressed before the submission could be considered for publication.

Given the strength of some of the comments I cannot recommend this submission for publication at this point. After careful consideration of all the arguments, I have decided to follow the recommendation of one of the reviewers that the manuscript be shortened to a Transactions Brief paper and re-submitted. With this in mind, I urge you to revise your manuscript to retain the major results of the work, and possibly incorporate the reviewers' comments within the constraint of the manuscript length, and resubmit the revised version.

We would like to thank the Associate Editor and the four reviewers for their precious time and comments. The comments and suggestions received have indeed led to a great improvement on the quality of the paper. We have tried to address every comment/suggestion carefully and have made some important changes to the paper (see below and the response to reviewers). In particular:

1) We have followed the decision by the Editor and Associate Editor and have made our best effort to shorten the paper. The revised version now stands at six pages. We understand that beginning with June 2006, TCAD transactions briefs are limited to five pages. However, we appeal to the Editors to permit us to submit this six-page brief owing to two reasons: First, the review of the original paper (9 pages) actually started in March 2006; second, we sincerely believe that any further reduction will seriously impair the presentation of the major results of the paper, and our ability to satisfactorily address the new issues raised by the reviewers.
2) We have changed the paper title from "Fast Positive Real Balanced Truncation Via A Quadratic Extension of the Alternating Direction Implicit Iteration" to "Fast Positive-Real Balanced Truncation Via Quadratic Alternating Direction Implicit Iteration". As can be seen, the two titles are practically the same, but the latter would allow us to save some space and keep the paper's length to a minimum. Again, we hope that this title change can be granted.

I caution you, as pointed out by a couple of the reviewers, that the new submission must show substantial additional work with respect to previously published or submitted work, including Ref. 17 in this paper, as well as your ICCAD 2005 paper.

When you submit the revised paper, please include a page or two describing your responses to the reviewers' comments and detailing the changes that you have made. This information should be included at the end of your manuscript.

First, the current paper (and also its old version) is completely different from our recent TCAD 2006 paper (Ref. [6] of the current paper, Ref. [17] of the old paper). Specifically, the current paper is on the fast solution of algebraic Riccati equations (AREs) and the fast implementation of positive-real balanced truncation (PRBT) using a second-order extension of the alternating direction implicit (ADI) iteration. The TCAD 2006 paper, on the other hand, focuses on the traditional Newton-method solution of AREs, using a proposed NSCARE algorithm, and another projection-based reduction method working on Hamiltonian matrices. The significant speed improvement and memory savings in PRBT/CFQADI over PRBT/NSCARE has been contrasted in the current paper.

Second, the current paper represents an extended and evolutionary work of our ICCAD 2005 paper (Ref. [21] of the current paper, Ref. [18] of the old paper), and contains substantially more technical details and some latest results. These are itemized in our reply to reviewer 4. Overall, motivated by the reviewers' comments, the current paper has seen some major difference from the old version:

1) The introduction has been shortened, and non-critical content removed.
2) Some references of the previous version have been deleted and some new ones added to the current version.
3) Many equations have been reformatted to save space.
4) The numerical section has been re-written to omit known results from our ICCAD 2005 paper (namely, the random circuit examples and the lowest-order benchmark have been removed to save space). Now the numerical examples give a deeper exposition of PRBT/CFQADI performance which is also the main contribution of the paper. Due to a computer upgrade, the numerical examples have been re-run and the new results logged.
5) The stopping criterion regarding CFQADI iteration has been elaborated on and its implications for PRBT/CFQADI have been discussed.
6) Several typos have been corrected.

First reviewer's comments and our response:

This interesting paper presents a quadratic version ADI algorithm to efficiently solve a passive balanced-truncation-based model-order reduction. There are some concerns that should be taken into account in the revision.

- Introduction section:

The authors start to give an overview of the balanced truncation by saying that the method has recently been advocated, yet, they miss several key references that introduce the method to the EDA community, for example:

1) *"Efficient frequency-domain modeling and circuit simulation of transmission lines," Silveira, L.M.; Elfadel, I.M.; White, J.K.; Chilukuri, M.; Kundert, K.S.; Components, Packaging, and Manufacturing Technology, Part B: Advanced Packaging, IEEE Transactions on [see also Components, Hybrids, and Manufacturing Technology, IEEE Transactions on] Volume 17, Issue 4, Nov. 1994 Page(s):505 - 513*
2) *"Model order reduction of large circuits using balanced truncation Rabiei," P.; Pedram, M.; Design Automation Conference, 1999. Proceedings of the ASP-DAC '99. Asia and South Pacific 18-21 Jan. 1999 Page(s):237 - 240 vol.1*

and some recently published work on balanced truncation, for example:

"Model-order reduction using variational balanced truncation with spectral shaping," Heydari, P.; Pedram, M.; Circuits and Systems I: Regular Papers, IEEE Transactions on [see also Circuits and Systems I: Fundamental Theory and Applications, IEEE Transactions on] Volume 53, Issue 4, April 2006 Page(s):879 - 891

- A pre-print version of reference 17 should be provided to reviewers, if it has not yet appeared in the Transactions.

Thank you very much for pointing out these important references. The introduction section has been largely rewritten and the suggested papers have been included. The pre-print of Ref. [6] (Ref. [17] of the old paper) is now available at the TCAD website with paper ID 2646 in the Oct 2006 issue (http://tcad.polito.it/list06.html).

Second reviewer's comments and our response:

The article is clear and well-organized. It describes an algorithm for positive real balanced truncation which takes advantage of the fact that the solution of the AREs can be factored. The English (missing 'the's, word choice) needs to be checked again.

Thank you very much for the positive comments. We have carefully shortened the paper and checked the wordings. It is hoped that this new version would read better than before.

Third reviewer's comments and our response:

This paper has made the following original contributions:

1) *A formulation of quadratic ADI.*

2) *Rigorous theoretical treatment on the well-posedness and convergence.*
3) *A framework based on Linear Fractional Transformation (LFT), which greatly simplifies the algebra.*
4) *Solid numerical examples and model order reduction results.*

This paper is well-written and well-organized.

We thank the reviewer for the positive comments. We have managed to preserve these contributions in this shortened version of the paper.

A few comments for the authors to improve the paper:

1) Although the convergence of QADI is established in this paper, the convergence is largely dependent on the choice of the parameters p, whose computation is mostly non-trivial. In practice, an algorithm like QADI usually will not run until convergence. In that case, how reliable (in the sense of accuracy) is the algorithm comparing to other heuristics such as in [R1]?

In the remarks before conclusion, we have pointed out how p may be obtained efficiently using properties of the Hamiltonian matrices. In QADI, the superlinear convergence usually gives excellent accuracy after several tens of iterations (e.g., see Fig. 2 in the current paper). For the heuristics in [R1] (this reference also appears in Ref. [6] of the current paper), one major problem is that convergence, and consequently also accuracy, is not necessarily guaranteed. Furthermore, the heuristics in [R1] requires an initial orthonormal basis V whose choice is not obvious, and that they all assume $A + A^T < 0$ which may not be readily achievable.

The current paper focuses on PRBT/CFQADI which is compared to other PRBT implementations. In our numerical examples, we have adapted the cross-product stopping criterion in Ref. [16] of the current paper. So instead of waiting for each of the two Cholesky factors Z_j and Y_j (corresponding to the two AREs) to converge, CFQADI is stopped whenever the update in $Y_j^T Z_j$ is smaller than a preset tolerance. This is physically meaningful since for real-world systems the singular values of the cross-product usually decay fast, which means that the significant state activities of the original model usually take place in only low-dimensional subspaces. Thus the initial system can be approximated well with low-rank projectors associated with the larger set of singular values.

In fact, in all our experiments including those not reported in the paper, such cross-product monitoring consistently results in just a few tens of CFQADI iterations, which is also borne out by the low-rank converged Cholesky factors during PRBT/CFQADI. And then the accuracy of the projected (PR-reduced) model is as if each ARE is solved to machine accuracy with standard solvers in the conventional PRBT flow. This can also be told from the virtually overlapped frequency responses of various PRBT reduced models.

Compared to the old paper, these points are clearly discussed in the revised paper.

2) Error bound etc. is not discussed in the paper. The solid point of Balanced Truncation is that it has a nice error bound and stability guarantee. Now in the iterative setting, the computation has to be terminated at some step. Then what's the approximation error?

3) Especially, in the model order reduction playground, you will not iterate for too many times (as it quickly increases the order of the reduced order model). Then, how is the passivity (or even stability) is guaranteed if the iteration is terminated early?

[R1] A. Hodel and K. Poolla, "Heuristic approaches to the solution of very large sparse Lyapunov and Algebraic Riccati equation," in Proc. 27th IEEE Conf. Decision & Control, Austin, TX, 1988, pp. 2217-2222.

This is a very good question. We refer the reviewer to Ref. [16] of the current paper wherein it has been shown that the BT approximant by ADI-type approach actually converges to the exact BT approximant exponentially (though the results in Ref. [16] are for standard BT and ADI-type solve of Lyapunov equations, the results hold true for the QADI framework due to its inheritance of ADI properties). Such exponential convergence also extends to the singular values with which the standard BT or PRBT error bound is formulated. As mentioned above, since our PR-reduced models by CFQADI are computed to the same accuracy as those from exact PRBT flow, the error bound (Ref. [12] of the current paper) is still valid. Moreover, passivity and thus stability are always preserved in our examples.

This leaves the question of what happens with early termination. As far as we are aware, this question remains with *every* numerical implementation of iterative algorithms for standard BT or PRBT. (Indeed, even with "non-iterative" algorithms such as subspace-based methods, there are inner iterations which may terminate early in case of ill-conditioned data, resulting in potential problems.) This is why passivity check, and enforcement if necessary, is still required in practical implementations. That is, given that PRBT would normally produce a passive reduced-order models, usually only the checking is required. For an "early-terminated" PRBT, the reduced model is usually close-to-passive, and passivity enforcement is still relatively simple. Fortunately, the reduced models are usually of low orders (a few tens), rendering the check and enforcement easy and computationally fast. For this task we may use the algorithm in S. Grivet-Talocia, "Passivity enforcement via perturbation of Hamiltonian matrices," TCAS1, vol. 51, no. 9, pp. 1755-1769, 2004. This reference has also been incorporated into the revised paper.

Fourth reviewer's comments and our response:

After a recapitulating summary of established methods of model order reduction, the authors mention various numerical methods for their computation. Many unnecessary abbreviations are used which confuse the reader.

After that, the basics of positive real balanced truncation are presented. As a motivating example for positive real systems, electrical circuits are mentioned. It was claimed that electrical circuits modeled by the modified nodal analysis can be always transformed into a control system in standard form, that is $\dot{x} = Ax + Bu$, $y = Cx + Du$. *However, this is in general not true since such a system may differentiate the input and thus it has in general an improper transfer. For instance, criteria for the improperness may be found in "D. Est éz Schwarz and C. Tischendorf. Structural analysis for electric circuits and consequences for MNA. Int. J. Circ. Theor. Appl., 28, pp. 131-162, 2000".*

We thank the reviewer for directing us to this reference on the index or properness of differential algebraic equations (DAEs) regarding modified nodal analysis (MNA)-formatted circuits. We would like to point out that the scope of our paper is on passivity-preserving model order reduction of linear passive circuits that arise usually from the RLC parasitics extraction for interconnect/package simulation. According to the literature, such MNA circuits (which are essentially RLC circuits without controlled sources, and thus with no CV loops or LI cutsets) are of index 1 and that the DAE simulation should be well-conditioned (which is generally true for index $\leq$2).

The difficulties of high-index-order DAEs from MNA lie mainly in their simulation exercise, e.g., extremely small step sizes and poor numerical conditionings in integration/differentiation routines. But then these issues may be handled before the model order reduction (MOR) process. For example, in Ref. [1] of the current paper (Bai, Dewilde and Freund, "Reduced-order modeling," 2002), it is mentioned that a DAE may be linearized or decoupled into linear and nonlinear parts for MOR. Of course, a more general state-space format is the descriptor system, $E\dot{x} = Ax + Bu$, $y = Cx + Du$ where E can be singular. But then it has been pointed out in Ref. [4] of the current paper (Phillips, Luca Daniel and Miguel Silveira, "Guaranteed passive balancing transformations for model order reduction," 2003) that an initial projection step can make E nonsingular, thus putting the state space into the regular form $\dot{x} = Ax + Bu$, $y = Cx + Du$. Another way of looking at it is that a descriptor system can always be decoupled into an impulsive part and a regular part upon which MOR is carried out (Wong and Chu, "A fast passivity test for descriptor systems via structure-preserving transformations of skew-Hamiltonian/Hamiltonian matrix pencils," DAC 2006). In fact, in MOR practice, especially in the context of balanced truncation, it is not uncommon to assume a regular state space. Examples include Refs. [1], [4], [6]-[9], [14]-[16] in the revised paper.

Thereafter, the ADI method (original references are given) for the iterative solution of continuous-time Lyapunov equations is introduced. Based on the idea of the ADI method, the quadratic ADI for iteratively solving Riccati equations is introduced and its feasibility and convergence is proven. The section concludes with a more efficient version of QADI which is based on Cholesky factorization. Before several concluding remarks are given, Section IV discusses and compares QADI with several other methods in practical example. The authors mention that randomly generated SISO RLC circuits are considered. For a better recapitulation, it would be nice to see which particular circuit is considered since it is really unclear what "randomly generated RLC circuit" means.

Those randomly generated RLC circuits in the old paper are similar to the RLC ladder example in it, but with the values of the RLC elements randomized. In the current paper, this part has been eliminated due to space limitation. We have instead referred the reader to Ref. [21] of the current paper (i.e., the ICCAD 2005 paper) which contains similar results and characterizations.

Summarizing, the main contribution of this paper is the more detailed explanation of the QADI method which is already published by the same authors in "IEEE/ACM International Conference on Computer-Aided Design, 2005. ICCAD-2005. 6-10 Nov. 2005 Page(s):801 - 805" and it therefore presents no novel research.

Moreover, the title of the submitted suggests that positive real balanced truncation (which is only one possible application of numerics of AREs) are mainly considered. The referee thinks that it is bold to publish one result about numerics of AREs in two papers each presenting one application area of AREs. Additionally, there are several factual inconsistencies in the work especially when considering electrical circuits and remarks about the actual state of research which are utterly wrong.

Therefore, I propose to reject this paper.

We recognize the IEEE practice that whenever a journal paper is submitted as an extension or an evolutionary work of a published conference paper, it must be substantially revised to contain more technical content. We submit that this is the case here:

1) The linear fractional transformation (LFT) framework is used to greatly simplify the otherwise intractable algebras and derivations of QADI and CFQADI. This is entirely new as compared to the ICCAD 2005 paper.
2) The proof for well-posedness and convergence in the ICCAD paper were essentially incomplete sketches. In this journal version, a complete and rigorous proof is shown in detail.
3) In the numerical section, comparison of CFQADI is further made with a recently proposed NSCARE algorithm which also seeks to obtain Cholesky factor solution to Riccati equations. This is absent from the ICCAD paper.
4) The performance of CFQADI against other solvers is analyzed in greater depth than in the ICCAD paper (e.g., time breakdowns for solving Riccati equations and matrix factorizations are given).
5) The stopping criterion governing PRBT/CFQADI and its implications are discussed in much greater detail. The ICCAD paper contains only a minor note about this.
6) Techniques for the computation of shifts in CFQADI and the use of the same shift in solving the dual Riccati equations in PRBT (see Section V) represent content that is absent from the ICCAD paper.

In view of these observations, we are hopeful that this reviewer will consider this revised paper more favorably.