A Fast Method for Steady-State **Memristor Crossbar Array Circuit** Simulation

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Abstract-In this work we propose an effective preconditioning technique to accelerate the steady-state simulation of large-scale memristor crossbar arrays (MCAs). We exploit the structural regularity of MCAs to develop a specially-crafted preconditioner that can be efficiently evaluated utilizing tensor products and block matrix inversion. Numerical experiments demonstrate the efficacy of the proposed technique compared to mainstream preconditioners.

Index Terms-Memristor, Neural Network, Crossbar Circuits, Preconditioner, GMRES

I. INTRODUCTION

MCAs (Memristor Crossbar Arrays) [1] has gained substantial ① attention recent years because of its potential application in M high-performance AI hardware and neuromorphic computing [2], calling for efficient circuit simulation tools. However, efficient simulation of MCAs has become increasingly challenging. The expected size of MCA is growing rapidly to accommodate the millions of weights involved in state-of-the-a works [3]. Furthermore, a large amount of simulation for statistical characterization or if the training/ini-dures are to be studied at circuit simulation level. Existing steady-state simulation of MCA circuits the millions of weights involved in state-of-the-art neural networks [3]. Furthermore, a large amount of simulations are needed for statistical characterization or if the training/inference proce-

 Existing steady-state simulation of MCA circuits is often done by SPICE, in which a sparse linear system resulted from the modified nodal analysis (MNA) must be solved in each Newton iteration. The matrix size can be huge, e.g., a 1024 × 1024 MCA leads to a matrix size > 10⁶, resulting in severe bottlenecks in time and memory consumption if direct solvers are used. Iterative solvers can improve the scalability, but existing general-purpose preconditioners [4] are often not adequately efficient for large-scale MCA circuits. In this work, we leverage the special topology of MCAs to develop an efficient preconditioning technique to accelerate the steady-state simulation of MCAs. Specifically, the preconditioner has the following features:
 1) It takes advantages of the topological regularity of MCAs to generate special block structures;
 2) Its inverse and application to vectors can be efficiently evaluated by Kronecker product and block matrix inversion Existing steady-state simulation of MCA circuits is often done

- evaluated by Kronecker product and block matrix inversion formula.

II. BACKGROUND

A voltage-controlled MCA is illustrated by Fig 3. It can be divided into three parts: the top metal layer, the middle vertical memristor devices and the bottom metal layer, as shown in Fig. 1(a), Fig. 1(b) and Fig. 1(c). The top and the bottom metal layers are assumed to be two uniform grids, with equal conductance for each grid segment (but the conductance per segment can be different for the two layers). The memristor devices lie between the corresponding points of the two grids.

The steady-state MNA equation is given in (1), where G_t and G_b are the conductance matrices for the top and the bottom layers.

 V_t and V_b are the corresponding nodal voltage unknowns. I_t and I_b are the nonlinear functions of V_t and V_b relating the steadystate memristor currents to the applied voltages. Additionally, Y_t and Y_b are the boundary conditions. All of them combine to form the matrix equation (9). The whole nonlinear equation is solved by the Newton's method (3) with the Jacobian matrix given in (4).



(a) The middle layer of (b) The top metal layer (c) The bottom metal with conductance repre-layer with conductance memristors. sented as G_{t} . represented as G_b .

Fig. 1: A division of MCA crossbar

$$G_t * V_t + I_t(V_t, V_b) - Y_t = 0$$
(1a)

$$G_b * V_b - I_b(V_t, V_b) - Y_b = 0$$
 (1b)

$$G_t = I \otimes G \tag{2a}$$

$$G_b = G \otimes I \tag{2b}$$

$$J\left(\vec{V_n}\right) * \left(\vec{V_{n+1}} - \vec{V_n}\right) = \left(-F\left(\vec{V_n}\right)\right)$$
(3)

$$I = F' = \begin{bmatrix} G_t & 0\\ 0 & G_b \end{bmatrix} + \begin{bmatrix} \frac{\partial I_t}{\partial V_t} & \frac{\partial I_t}{\partial V_b}\\ \frac{-\partial I_b}{\partial V_t} & \frac{-\partial I_b}{\partial V_b} \end{bmatrix}$$
(4)

III. THE PROPOSED PRECONDITIONING TECHNIQUE

In this work we focus on using the iterative solution method of GMRES (Generalized minimal residual method) to solve the sparse total Jacobian matrix in (4). J consists of two parts: the linear conductance matrix from the interconnect and the nonlinear Jacobian from the I-V functions of the memristor devices.

A. Preconditioner Formulation

Firstly, we choose a particular indexing scheme to give J a special sparsity structure. The top and the bottom layers both use natural indexing, but the directions are perpendicular to each other, as illustrated in Fig. 1. There are two reasons for this choice: 1) the four blocks in the nonlinear Jacobian matrix are now all diagonal; 2) by assuming equal conductances for all segments at the same layer, we can rewrite the top and the bottom linear conductance matrices $G_t, G_b \in \mathcal{R}^{n^2 \times n^2}$ into Kronecker products (2a) and (2b), where $G \in \mathcal{R}^{n \times n}$ is the conductance matrix of single row or column (8).

$$P = \begin{bmatrix} G_t + a_1 I & -a_1 I \\ -a_2 I & G_b + a_2 I \end{bmatrix}$$
(5)

Next, we develop a special preconditioner of the form in (5) with the same block structure. The a_1 and a_2 are the mean of the diagonal elements of $\frac{\partial I_t}{\partial V_b}$ and $\frac{-\partial I_b}{\partial V_b}$, which can be considered as the average conductance of the memristor devices. Notice that $\frac{\partial I_t}{\partial V_t}$ and $\frac{\partial I_t}{\partial V_b}$ are opposite, as well as $\frac{-\partial I_b}{\partial V_t}$ and $\frac{-\partial I_b}{\partial V_b}$, since V_b and V_t are the voltages across the memristors.

B. Fast Evaluation of Preconditioner

$$\begin{bmatrix} A & B \\ C & D \end{bmatrix}^{-1} = \begin{bmatrix} -M^{-1}DB^{-1} & M^{-1} \\ B^{-1} + B^{-1}AM^{-1}DB^{-1} & -B^{-1}AM^{-1} \end{bmatrix}_{(6)}$$

$$M = (C - DB^{-1}A)$$

$$= (-a_2I - (G_b + a_2I)(-a_1I)^{-1}(G_t + a_1I))$$

$$= (-a_2I + \frac{1}{a_1}(G \otimes I + a_2I)(I \otimes G + a_1I))$$

$$= (-a_2I + \frac{1}{a_1}(G_2 \otimes I)(I \otimes G_1))$$

$$= (-a_2I + \frac{1}{a_1}(G_2 \otimes G_1))$$
(7)

It is important to have a fast scheme to evaluate $P^{-1}v$. We first apply the Woodbury block matrix inversion identity (6). Note that the off-diagonal blocks B and C are just identity matrices whose inverse is trivial. The core operation is to obtain $M^{-1}v = (C - DB^{-1}A)^{-1}v$.

To this end, we rewrite M into (7), with G_1 and G_2 given in (10a) and (10b). In typical MCAs, the memristor conductance is generally much smaller than that of interconnects. Therefore, one can drop the first term on the right hand side of (11) and approximate M as in (15) and (14). To compute (16), where $\hat{g}_{i,j}^2$ is the element of \widehat{G}_2 . Vector v can be rearranged by (17), \widehat{V}_j represent the j^{th} column of \widehat{V} . Consider the j^{th} row in (18). Finally, we can deduce original equation to (19).

IV. NUMERICAL RESULTS

In the following tests, the top and bottom wire conductance g per segment are normalized to 1. We adopt the Yakopcic model [5] as the RRAM model. Since the proposed method is expected to handle RRAM devices of various states, we obtain the conductance matrix of RRAM by randomly setting the internal state variable of their model, with a maximum conductance being 0.4 to meet the approximation condition (12). The GMRES solver from Scipy is used with a uniform relative tolerance of 10^{-6} .

Fig. 2 shows the residual history of GMRES with and without the proposed preconditioner. The test case is a 128×128 crossbar with the matrix dimension of 32768×32768 . It can be seen that the proposed preconditioner drastically accelerates the convergence of GMRES.

Fig. 4 compares the iteration number for MCAs of five difference sizes $(32 \times 32, 64 \times 64, 128 \times 128, 256 \times 256 \text{ and } 512 \times 512)$. The matrix sizes are labeled on the lines and the corresponding iteration numbers summarized in the table. It is clear that the computational saving from the proposed preconditioner grows rapidly as the matrix size increases.

Table I compares the proposed preconditioner against other mainstream preconditioners such as the Jacobi and the ILU pre-



Fig. 2: Residual of preconditioned GMRES (PGMRES) and baseline GMRES for 128×128 crossbar .

TABLE I. Comparison of Total CPU Time Consumption and Iteration Steps to Coverage

	Before Preconditioned		Jacobi Preconditioner		ILU Preconditioner		Our Preconditioner	
Crossbar Dimension (n)	Steps	CPU time consumption/s	Steps	CPU time consumption/s	Steps	CPU time consumption/s	Steps	CPU time consumption/s
16*16	67	0.01596	60	0.00897	3	0.00598	11	0.00299
32*32	227	0.05785	203	0.03092	15	0.01396	11	0.02194
64*64	678	0.30377	551	0.14319	111	0.14561	13	0.09275
128*128	1645	1.97858	1610	0.95511	308	1.24064	13	0.57907
256*256	7526	28.51413	5361	23.41768	589	11.05555	13	4.77912
512*512	22801	331.31852	19273	324.20583	3120	309.91122	17	225.12859

conditioner. The iteration number and the total CPU runtime are recorded for MCAs of different sizes. For small cases, the three types of preconditioners perform comparably well. For larger cases, the proposed preconditioner requires much fewer iterations than the other two preconditioners. The runtime reduction is less significant due to the evaluation of preconditioner not being fully optimized. Future efforts will be devoted to speed up this part.

V. CONCLUSION

We have devised an efficient preconditioner for fast iterative solution of the Jacobian matrices appearing in steady-state MCA simulation. The preconditioner leverages the special sparsity pattern in the Jacobian matrices resulted from a deliberately crafted indexing scheme. Tensor product and block matrix inversion techniques are utilized to significantly accelerate the preconditioner evaluations during the iterative solutions. Numerical results have demonstrated the efficacy of the proposed preconditioner.

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$$G = \begin{bmatrix} 2g & -g & \cdots & 0 \\ -g & 2g & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & 2g & -g \\ 0 & \cdots & -g & 2g \end{bmatrix}$$
(8)

$$F = \begin{bmatrix} G_t & 0\\ 0 & G_b \end{bmatrix} * \begin{bmatrix} V_t\\ V_b \end{bmatrix} + \begin{bmatrix} I_t\\ -I_b \end{bmatrix} - \begin{bmatrix} Y_t\\ Y_b \end{bmatrix} = 0$$
(9)

$$G_{1} = \begin{bmatrix} 2g + a_{1} & -g & \cdots & 0 \\ -g & 2g + a_{1} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & 2g + a_{1} & -g \\ 0 & \cdots & -g & 2g + a_{1} \end{bmatrix}_{n*n}$$
(10a)

$$G_{2} = \begin{bmatrix} 2g + a_{2} & -g & \cdots & 0 \\ -g & 2g + a_{2} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & 2g + a_{2} & -g \\ 0 & \cdots & -g & 2g + a_{2} \end{bmatrix}_{n*n}$$
(10b)

$$diag(M) = \left(-a_2 + \frac{1}{a_1}(2g + a_2)(2g + a_1)\right) \tag{11}$$

$$20a_2 < \frac{1}{a_1}(2g+a_2)(2g+a_1) \tag{12}$$

$$M \cong \hat{M} = \widehat{G_2} \otimes G_1 \tag{13}$$

$$\widehat{G}_{2} = \begin{bmatrix} \frac{2g+a_{2}}{a_{1}} & -g & \cdots & 0\\ -g & \frac{2g+a_{2}}{a_{1}} & \cdots & 0\\ \vdots & \ddots & \vdots\\ 0 & \cdots & \frac{2g+a_{2}}{a_{1}} & -g\\ 0 & \cdots & -g & \frac{2g+a_{2}}{a_{1}} \end{bmatrix}_{n*n}$$

$$M^{-1} \cong \widehat{M}^{-1} = \widehat{G}_{2}^{-1} \otimes G_{1}^{-1}$$
(15)

$$\left(\widehat{G_{2}}^{-1} \otimes G_{1}^{-1}\right) v$$

$$= \left(\widehat{G_{2}}^{-1} \otimes G_{1}^{-1}\right) \begin{bmatrix} v_{1,1} \\ v_{1,2} \\ \vdots \\ v_{1,n-1} \\ v_{2,1} \\ \vdots \\ v_{2,n} \\ \vdots \\ v_{n,n} \end{bmatrix}$$
(10)

$$= \begin{bmatrix} \frac{1}{\hat{g}_{1,1}^{2}} * G_{1}^{-1} & \cdots & \frac{1}{\hat{g}_{1,n}^{2}} * G_{1}^{-1} \\ \vdots & \ddots & \vdots \\ \frac{1}{\hat{g}_{n,1}^{2}} * G_{1}^{-1} & \cdots & \frac{1}{\hat{g}_{n,n}^{2}} * G_{1}^{-1} \end{bmatrix} \begin{bmatrix} v_{1,2} \\ \vdots \\ v_{1,n-1} \\ v_{1,n} \\ v_{2,1} \\ \vdots \\ v_{2,n} \\ \vdots \\ v_{n,n} \end{bmatrix}$$

$$\hat{V} = \begin{bmatrix} v_{1,1} & \cdots & v_{1,n} \\ \vdots & \ddots & \vdots \\ v_{n,n} & \cdots & v_{n,n} \end{bmatrix}_{n*n} = \begin{bmatrix} \widehat{V_1} & \cdots & \widehat{V_n} \end{bmatrix}$$
(17)

$$\frac{1}{\hat{g}_{j,1}^{2}} * G_{1}^{-1} \widehat{V}_{1} + \frac{1}{\hat{g}_{j,2}^{2}} * G_{1}^{-1} \widehat{V}_{2} + \ldots + \frac{1}{\hat{g}_{j,n}^{2}} * G_{1}^{-1} \widehat{V}_{n} \\
= \left[G_{1}^{-1} \widehat{V}_{1} \quad \ldots \quad G_{1}^{-1} \widehat{V}_{n} \right] \left[\begin{array}{c} \frac{1}{\hat{g}_{j,1}^{2}} \\ \vdots \\ \vdots \\ \frac{1}{\hat{g}_{j,n}^{2}} \end{array} \right] \\
\left(\widehat{G}_{2}^{-1} \otimes G_{1}^{-1} \right) v = G_{1}^{-1} \widehat{V} G_{2}^{-1} \quad (19)$$



Fig. 3: A general MCA is shown with BL (bit line) and WL (word line).



Fig. 4: Iteration number to coverage of dimension of crossbar $32 \times 32, 64 \times 64, 128 \times 128, 256 \times 256$ and 512×512 .