A Parallel FFT Accelerated Transient Field-Circuit Simulator

Ali E. Yılmaz, Jian-Ming Jin, and Eric Michielssen

Abstract—A novel fast electromagnetic field-circuit simulator that permits the full-wave modeling of transients in nonlinear microwave circuits is proposed. This time-domain simulator is composed of two components: (i) A full-wave solver that models interactions of electromagnetic fields with conducting surfaces and finite dielectric volumes by solving time-domain surface and volume electric field integral equations, respectively; (ii) A circuit solver that models field interactions with lumped circuits, which are potentially active and nonlinear, by solving Kirchhoff's equations through modified nodal analysis. These field and circuit analysis components are consistently interfaced and the resulting coupled set of nonlinear equations is evolved in time by a multidimensional Newton-Raphson scheme. The solution procedure is accelerated by allocating field- and circuit-related computations across the processors of a distributed-memory cluster, which communicate using the message-passing interface standard. Furthermore, the electromagnetic field solver, whose demand for computational resources far outpaces that of the circuit solver, is accelerated by an FFT based algorithm, viz. the time-domain adaptive integral method. The resulting parallel FFT accelerated transient field-circuit simulator is applied to the analysis of various active and nonlinear microwave circuits, including power-combining arrays.

Index Terms—Parallel processing, microwave circuits, nonlinear circuits, time-domain integral equations, transient analysis.

I. INTRODUCTION

As operating frequencies increase, accurate and efficient hybrid full-wave field-circuit simulation tools are becoming increasingly indispensable in the design of microwave circuits as well as in the assessment of their vulnerability to unintentional coupling, crosstalk, packaging effects, and intentional electromagnetic interference. Microwave circuits can be analyzed using either frequency- or time-domain simulators; however, when the circuit under study contains nonlinear components, time-domain methods enjoy the advantage of allowing for the direct analysis of field-circuit interactions without resorting to harmonic balance or port extraction methods [1]. Although early efforts at formulating hybrid time-domain field-circuit simulators relied on integral-equation schemes – the goal often consisted in the analysis of electromagnetic interactions with nonlinearly loaded wires [2]-[4] – most of the ensuing simulators invoked time-domain differential-equation methods. By now, various extensions to both the finite-difference time-domain (FDTD) [5]-[11] and finite-element time-domain (FETD) [12], [13] methods aimed at incorporating device physics/behavior into electromagnetic analysis environments have been proposed. The most rigorous of these schemes permit the simultaneous solution of the Maxwell and semiconductor carrier transport equations by casting them as a strongly coupled nonlinear system of differential equations on the same grid [14], [15]. To minimize computational cost, whenever possible, these differential equation solvers account for device and circuit behavior (as opposed to physics) through their description in terms of equivalent lumped elements and macromodels [16]. However, lumped loads and circuits, be they passive or active, linear or nonlinear, static or time-varying, can be quite easily accounted for in time-domain integral-equation solvers as well [1]-[4].

Indeed, the recent development of stable [17]-[19], accurate [20], and fast [21]-[29] marching on in time based integral-equation solvers for analyzing large-scale transient scattering and radiation phenomena calls for a study into the applicability of these solvers to the analysis of microwave circuits. Modern-day fast time-domain integral-equation solvers are either accelerated by plane wave time domain (PWTD) [22] or by fast Fourier transform (FFT) [23]-[29] based algorithms. Use of either algorithm permits the analysis of transient electromagnetic phenomena with far more degrees of freedom than possible by classical time-domain integral-equation approaches. Recently, a PWTD accelerated electromagnetic field solver was coupled to a SPICE-like circuit simulator and applied to the analysis of transients on microwave circuits with nonlinear loads [30]. Here, we report, instead, on the hybridization (formulation and implementation) of an FFT accelerated solver with a modified nodal analysis based circuit simulator; an initial implementation of this scheme was described in [31]. The main reason for pursuing FFT accelerated field-circuit analysis tools is as follows. Just like their frequency-domain
counterparts, PWTD accelerated time-domain integral-equation solvers are asymptotically superior to FFT accelerated ones when analyzing electromagnetic transients on arbitrarily shaped three-dimensional (3D) surfaces. FFT accelerated solvers, however, generally outperform PWTD accelerated ones when analyzing transients on quasi-planar, volumetric, or densely-packed structures, which are often encountered in microwave circuits. This paper supports this trend. Furthermore, the availability of parallel FFT algorithms [32] and the relative ease of load balancing parallel FFT accelerated time-marching solvers render the FFT route even more appealing. The specific FFT based algorithm used in this paper is the time-domain adaptive integral method (TD-AIM) [29], which allows the efficient analysis of electromagnetic field interactions with nonuniformly discretized microwave structures/circuits.

The hybridization of this FFT accelerated field solver with a modified nodal analysis based circuit solver results in a coupled nonlinear system of equations, which is solved by a Newton-Raphson algorithm to compute the time evolution of the fields, currents, and voltages on the microwave circuit. In this paper, the hybrid field-circuit simulator is implemented on a distributed-memory computer cluster that communicates through the message-passing interface. The computational work is divided among multiple processors using a simple but effective parallelization paradigm: field and circuit unknowns and associated operations are assigned to separate groups of processors. It is shown that this strategy allows for the separate development and optimization of field and circuit solvers and results in near-optimal parallel scalability for the hybrid solver. The proposed scheme is described in Section II and applied to the analysis of microwave circuits in Section III, which is followed by a section outlining the conclusions of this study.

II. FORMULATION

This section details the proposed parallel FFT accelerated transient field-circuit simulator. Subsections II.A and II.B formulate the field and circuit equations, respectively. These two subsections introduce notation that enables the description of the field and circuit solvers’ hybridization (including DC analysis), the method for solving the coupled system of equations (including complexity analysis), and the acceleration of the hybrid simulator (including parallelization); these topics are covered in subsections II.C, II.D, and II.E.

A. Electromagnetic Field Equations

Let $S$ and $V$ denote the conducting surfaces and potentially inhomogeneous dielectric volumes, respectively, that comprise the microwave structure under study. In the following, all conductors are assumed perfect and all dielectrics are assumed linear, isotropic, nonmagnetic, nondispersive, lossless, and of permittivity $\varepsilon(\mathbf{r})$. Extensions to lossy conductors and dielectrics are possible, see [26], [33]-[35]. The microwave structure resides in free space with permittivity $\varepsilon_0$. The permeability of the structure and the surrounding free space is denoted by $\mu_0$. A known transient electromagnetic field excites $S \cup V$; it is assumed that this field’s spectrum essentially vanishes for frequencies $f > f_{\text{max}}$ and that the field is nearly zero $\forall \mathbf{r} \in S \cup V$ for $t \leq 0$. The incident field induces surface currents $\mathbf{J}^s(\mathbf{r}, t)$ on $S$ and volume (polarization) currents $\mathbf{J}^p(\mathbf{r}, t)$ in $V$. These currents, in turn, generate the scattered electric field

$$E_{\text{sc}}(\mathbf{r}, t, \mathbf{r}', \mathbf{J}^s) = -\partial_t A(\mathbf{r}, t, \mathbf{r}', \mathbf{J}^s) - \nabla \Phi(\mathbf{r}, t, \mathbf{r}', \mathbf{J}^p), \quad (1)$$

where $\partial_t$ represents the time derivative and $A$ and $\Phi$ are the vector and scalar potentials:

$$A(\mathbf{r}, t, \mathbf{r}', \mathbf{J}^s) = \iint_S \frac{\mu_0 J^s(\mathbf{r}', t - R / c_0)}{4\pi R} \, ds' + \iiint_V \frac{\mu_0 J^p(\mathbf{r}', t - R / c_0)}{4\pi R} \, dv', \quad (2)$$

$$\Phi(\mathbf{r}, t, \mathbf{r}', \mathbf{J}^p) = -\int_0^{t-R/c_0} \nabla \cdot J^s(\mathbf{r}', t') \, dt' ds' - \int_0^{t-R/c_0} \nabla \cdot J^p(\mathbf{r}', t') \, dt' dv'. \quad (3)$$

Here, $R = |\mathbf{r} - \mathbf{r}'|$ is the distance between source point $\mathbf{r}'$ and observation point $\mathbf{r}$ and $c_0 = 1 / \sqrt{\varepsilon_0 \mu_0}$ is the free-space speed of light. The volume current density relates to the electric flux density $D^\text{vol}(\mathbf{r}, t) = \varepsilon(\mathbf{r}) E^\text{vol}(\mathbf{r}, t)$ as $\mathbf{J}^p(\mathbf{r}, t) = \kappa(\mathbf{r}) \nabla \cdot \mathbf{E}^\text{vol}(\mathbf{r}, t)$, where $\kappa(\mathbf{r}) = 1 - \varepsilon_0 / \varepsilon(\mathbf{r})$ is the contrast ratio [36], [37]. Integral equations for the surface and volume currents (or better, the flux – see below) are arrived at by (i) forcing the temporal derivative of the sum of the incident and scattered electric fields tangential to $S$ to vanish and (ii) by expressing the temporal derivative of the total field as the sum of the temporal derivatives of the incident and scattered fields throughout $V$:

$$\partial_t E_{\text{sc}}(\mathbf{r}, t)_{\text{lm}} = -\partial_t E_{\text{sc}}(\mathbf{r}, t, \mathbf{r}', \mathbf{J}^s)_{\text{lm}} \quad \forall \mathbf{r} \in S,$$

$$\partial_t E_{\text{vol}}(\mathbf{r}, t) = \partial_t E_{\text{sc}}(\mathbf{r}, t, \mathbf{r}', \mathbf{J}^s) - \partial_t E_{\text{sc}}(\mathbf{r}, t, \mathbf{r}', \mathbf{J}^p) \quad \forall \mathbf{r} \in V. \quad (4)$$

Upon expressing $E_{\text{sc}}(\mathbf{r}, t, \mathbf{r}', \mathbf{J}^s)$ in (3) using (1)-(2), as well as the above stated relationships linking $\mathbf{J}^s(\mathbf{r}, t)$, $\mathbf{D}^\text{vol}(\mathbf{r}, t)$, and $\mathbf{E}^\text{vol}(\mathbf{r}, t)$, a coupled set of surface-volume time-domain integral equations in $\mathbf{J}^s(\mathbf{r}, t)$ and $\mathbf{J}^p(\mathbf{r}, t)$ is obtained. These integral equations are solved numerically by discretizing $\mathbf{J}^s(\mathbf{r}, t)$ and $\mathbf{D}^\text{vol}(\mathbf{r}, t)$ using $N_i N_t$ and $N_i N_t$ space-time basis functions, respectively, as

$$\mathbf{J}^s(\mathbf{r}, t) = \sum_{i=1}^{N_i} \sum_{l=1}^{N_t} I_{i,l}^s S_{i,l}(\mathbf{r}) T(t - l' \Delta t),$$

$$\mathbf{D}^\text{vol}(\mathbf{r}, t) = \sum_{i=1}^{N_i} \sum_{l=1}^{N_t} I_{i,l}^p V_{i,l}(\mathbf{r}) T(t - l' \Delta t). \quad (4)$$
Here, \( P_{k,f} \) and \( P_{k,f'} \) are unknown expansion coefficients (electromagnetic unknowns) and \( \Delta t = \beta / f_{\text{max}} \) is the time-step size; typically \( 0.04 \leq \beta \leq 0.1 \). In this paper, the surface basis functions \( \mathbf{S}_i(\mathbf{r}) \) are Rao-Wilton-Glisson (RWG) functions [38] defined on pairs of triangular patches that approximate \( S \). The volume basis functions \( \mathbf{V}_k(\mathbf{r}) \) are zeroth-order divergence conforming functions [36] defined over tetrahedral elements, which approximate the dielectric volumes \( V \), and over each of which \( \kappa(\mathbf{r}) \) (hence \( \kappa(\mathbf{r}) \)) is assumed constant; this implies that \( \mathbf{J}(\mathbf{r},t) \equiv \sum_{k=1}^{N_v} \sum_{l=1}^{N_e} P_{k,f} \kappa_k(\mathbf{r}) \mathbf{V}_k(\mathbf{r}) \partial_\mathbf{r} T(t - l' \Delta t) \).

This choice of basis functions enforces the continuity of the normal component of the surface current density across patches and the electric flux density across tetrahedrons, respectively. The temporal basis functions \( T(t) \) are shifted Lagrange interpolants [18]. It is important to note that the composite basis functions in (4) are localized in space-time. Upon substituting (4) into (3) and testing the resulting equation at times \( l \Delta t \) with the spatial functions \( \mathbf{S}_i(\mathbf{r}), \ldots, \mathbf{S}_{N_s}(\mathbf{r}) \) and \( \kappa_1(\mathbf{r}) \mathbf{V}_1(\mathbf{r}), \ldots, \kappa_{N_t}(\mathbf{r}) \mathbf{V}_{N_t}(\mathbf{r}) \), a total of \( N_{\text{EM}} N_t = (N_s + N_v) N_t \) equations for \( N_{\text{EM}} N_t \) expansion coefficients result:

\[
\mathbf{V}_{\text{EM}} = \sum_{l=1}^{N_t} \mathbf{Z}_{l,N_l} \mathbf{I}_{\text{EM}}^l \text{ for } l = 1, 2, \ldots, N_t. \tag{5}
\]

Here, \( N_t \) denotes the longest transit time of a free-space propagating electromagnetic field across \( S \cup V \), expressed in terms of time steps [29]. Expressions for the entries of the vectors \( \mathbf{V}_{\text{EM}} \) and \( \mathbf{I}_{\text{EM}}^l \) and matrices \( \mathbf{Z}_{l,N_l} \) are provided in the Appendix. The system of equations (5) is recast into the following form and solved by forward substitution (i.e., by marching on in time):

\[
\mathbf{Z}_0 \mathbf{I}_{\text{EM}}^l = \mathbf{V}_{\text{EM}}^l - \sum_{l'=\max(1,l-N_t)}^{l-1} \mathbf{Z}_{l'-N_t} \mathbf{I}_{\text{EM}}^{l'} \text{ for } l = 1, 2, \ldots, N_t. \tag{6}
\]

The matrix \( \mathbf{Z}_0 \), which represents immediate electromagnetic interactions, is a sparse but non-diagonal impedance matrix of size \( N_{\text{EM}} \times N_{\text{EM}} \), with typically \( O(N_{\text{EM}}) \) nonzero elements. The vectors \( \mathbf{I}_{\text{EM}}^l \) hold the unknown current and flux coefficients and the known tested incident field values at time \( l \Delta t \), respectively. The dominant computational cost of the field solver involves the evaluation of the space-time convolution appearing on the right-hand side of (6), viz. the computation of the scattered electromagnetic fields, which requires \( O\left(N_{\text{EM}}^2\right) \) operations per time step [29].

B. Circuit Equations

The proposed solver allows the microwave structure described above to contain an arbitrary number of lumped circuits with independent reference/ground nodes. Equations governing circuit behaviors are formulated, starting from the circuit topologies and Kirchoff’s laws, via modified nodal analysis using the SPICE2 approach [39] as detailed next; specific details of how the circuits are coupled to the electromagnetic system are further discussed in subsection II.C. The circuit unknowns are node voltages and voltage-source currents; hence, the total number of circuit unknowns, denoted as \( N_{\text{CKT}} \), is equal to the total number of non-ground nodes and voltage sources in the circuits. A total of \( N_{\text{CKT}} \) equations in terms of these unknowns are obtained by imposing Kirchoff’s voltage law at the voltage-defined elements and current law at all nodes except the grounds. Branch equations relating currents to voltages are obtained from element stamps and companion models that are formulated using the trapezoidal integration rule. The circuit unknowns are evolved in time using the same time step size as the field solver, \( \Delta t \), which is assumed constant throughout the simulation. While contemporary circuit solvers employ variable time stepping schemes, the fixed but small \( \Delta t \) dictated by the field solver was found to be sufficiently accurate for the applications considered in this paper. When analyzing circuits composed of linear and nonlinear resistors, capacitors, inductors, as well as dependent and independent voltage and current sources for \( N_t \) time steps, this procedure yields \( N_{\text{CKT}} N_t \) equations for \( N_{\text{CKT}} N_t \) unknowns:

\[
\mathbf{Y}_{\text{CKT}} \mathbf{V}_{\text{CKT}}^{\text{CKT}} + \mathbf{I}_{\text{CKT},\text{nl}}^{\text{CKT}} \mathbf{V}_{\text{CKT}}^{\text{CKT}} = \mathbf{I}_{\text{CKT}}^{\text{CKT}} \text{ for } l = 1, 2, \ldots, N_t. \tag{7}
\]

The matrix \( \mathbf{Y} \), which represents branch equations of linear and time-invariant circuit elements, is a sparse admittance matrix of size \( N_{\text{CKT}} \times N_{\text{CKT}} \) with typically \( O(N_{\text{CKT}}) \) nonzero elements. The vectors \( \mathbf{V}_{\text{CKT}}^{\text{CKT}} \) and \( \mathbf{I}_{\text{CKT}}^{\text{CKT}} \) hold the circuit unknowns and source currents and voltages, respectively, and the vector \( \mathbf{V}_{\text{CKT},\text{nl}}^{\text{CKT}} \) represents the branch equations of nonlinear and time-varying elements at time \( l \Delta t \).

![Fig. 1. Coupling of electromagnetic and circuit systems. (a) The surface unknown \( k \) of edge-length \( d \) is connected to a one-port circuit at terminals \( a \) and \( 0 \). (b) Coupling from circuit system point of view. (c) Coupling from electromagnetic system point of view.](image-url)
C. Coupled System of Equations

The lumped circuits are connected to the conducting surfaces $S$ through electromagnetic surface unknowns and are modeled as local voltage sources. To illustrate this procedure, assume that electromagnetic surface unknown $k$ is loaded by a one-port circuit whose terminals are at nodes $a$ and $0$ (Fig. 1(a)). The field solver requires as one of its inputs the time-derivative of the voltage difference between the two terminals $\partial_t V_{\text{EM}}^k(a)$ and the circuit solver requires the port current $I_{\text{EM}}^l(k) d$, where $d$ is the length of the edge. Thus, the following coupled system of equations results when the two solvers are interfaced:

$$f(x_l) = \begin{bmatrix} Z_0 C' & I_{\text{EM}}^l \\ C & Y_l \end{bmatrix} \begin{bmatrix} V_{\text{EM}}^l \\ \mathbf{v}^l_{\text{CKT}} \end{bmatrix} + \begin{bmatrix} 0 \\ J_{\text{CKT},nl} \end{bmatrix} \begin{bmatrix} \mathbf{v}^l_{\text{CKT}} \end{bmatrix} = b_l. \quad (8)$$

Here, $x_l = \begin{bmatrix} I_{\text{EM}}^{lT} & V_{\text{CKT}}^{lT} \end{bmatrix}$ is the vector of unknowns at time $l\Delta t$. The matrix $C'$, which represents field to circuit coupling, is formed according to Fig. 1(b) and is used to compute currents observed at the circuit terminals. The matrix $\mathbf{C}$ and the vector $\mathbf{K}_l$, which represent circuit to field coupling, are used to compute the numerical derivatives of terminal voltages and are formed according to Fig. 1(c). For circuits with three or more terminals, the entries of $C'$, $C''$, and $K_l$ can be found through a straightforward extension of the procedure in Fig. 1 [30]. In general, if there are $N_{\text{PORT}}$ ports, $C'$ and $C''$ will have a total of $2N_{\text{PORT}}$ nonzero elements. Other coupling schemes that introduce additional unknowns at the circuit terminals (contacts) exist [40]. Regardless of the scheme used, however, the off-diagonal matrix blocks representing coupling between the circuit and field formulations/solvers are sparse.

Notice that, while the circuit solver can incorporate initial conditions (typically computed from a DC analysis) for the circuit unknowns (i.e., $V_{\text{CKT}}^l = V_{\text{EM}}^l$ and $I_{\text{DC}}^l = I_{\text{EM}}^l$ for $l = 0$), the field solver assumes zero initial conditions (i.e., $I_{\text{EM}}^l = 0$ and $V_{\text{EM}}^l = 0$ for $l \leq 0$). In this paper, microwave circuits with DC sources are analyzed in two ways: (i) Zero initial conditions are assumed everywhere; the DC sources are turned on gradually (in order not to violate the finite bandwidth assumption), and the transient analysis is performed only after the system reaches steady state. Depending on the specifics of the simulation being conducted, this procedure may require too many time steps and lead to low-frequency stability problems, which are avoided by the second scheme. (ii) The DC and transient responses are separated, similar to [10], [11], using the linearity of the electromagnetic system as follows. On the one hand, the total electromagnetic response at time $l\Delta t$ is represented as $V_{\text{EM}}^l + I_{\text{EM}}^l$ and the field solver models only the transient response $I_{\text{EM}}^l$. On the other hand, the total circuit response at time $l\Delta t$ is represented as $V_{\text{CKT}}^l$ and the circuit solver models both the DC response and the transient response (by enforcing the DC solution as initial conditions through $V_{\text{CKT}}^l$ and $I_{\text{DC}}^l$). To maintain consistency, DC voltages and currents are introduced at the interface (Fig. 1(b)). Hence, the hybrid field-circuit solver uses the (pre-computed) vectors $V_{\text{EM}}^l$, $I_{\text{EM}}^l$, $I_{\text{DC}}^l$, and the entries of $I_{\text{EM}}^l$ at the circuit ports to account for the DC conditions in the second scheme. These values can be computed through a DC analysis of the circuits with the microwave structure characterized either explicitly, e.g., through fast electrostatic solvers [41], or approximately, e.g., as a small resistor modeling the DC resistance of the conductors between circuits [11].

D. Solution Algorithm/Computational Complexity Analysis

At each time step $l = 1, 2, \ldots, N_t$, the following five-stage Newton-Raphson algorithm is used to solve the coupled nonlinear system of equations (8):

Stage (i): Compute the right-hand-side vector $b_l$. Then for each Newton iteration $p = 1, 2, \ldots$

Stage (ii): Evaluate the residual vector $r_{l,p-1} = f(x_{l,p-1}) - b_l$, where $x_{l,p-1} = \begin{bmatrix} I_{\text{EM}}^{lT} & V_{\text{CKT}}^{lT} \end{bmatrix}$ is the solution vector from the previous Newton step and the initial guess is $x_{l,0} = x_{l,-1}$, i.e., the solution at the previous time step.

Stage (iii): If $\|r_{l,p-1}\| < tol \times \|b_l\|$ then stop; the solution at time $l\Delta t$ is $x_{l,p-1}$.

Stage (iv): Compute the Jacobian sub-matrix $J_{l,p}^{pl} = \frac{\partial I_{\text{EM}}^l}{\partial V_{\text{CKT}}^l}$.

Stage (v): Iteratively solve

$$J_{l,p}s_p = \begin{bmatrix} Z_0 & C' \\ C & Y_l + J_{l,p}^{pl} \end{bmatrix} s_p = r_{l,p-1} \quad (9)$$

for the Newton step $s_p$ and find the next solution vector $x_{l,p} = x_{l,p-1} - s_p$.

Note that, in general all four submatrices of the Jacobian matrix $J_{l,p}$ in (9) are sparse and the algorithm needs only one Newton iteration per time step if there are no nonlinear circuit elements. It should be emphasized that the above solution algorithm is different from that of [30]. While the algorithm in [30] solves a smaller system of equations and therefore might potentially require fewer Newton iterations, here the Jacobian matrix is computed significantly faster. This is because, unlike [30], the above algorithm does not require a matrix solution to compute the entries of $J_{l,p}$; indeed they can be computed analytically. Furthermore, the algorithm here is more amenable to the parallelization framework discussed in subsection II.E. The computational complexity of the above algorithm is analyzed next.

The algorithm evaluates and stores $b_l$, which is independent of the Newton iteration, in $O(N_{\text{EM}}^2 + N_{\text{CKT}})$ operations. Then, at each Newton iteration $p$, the algorithm
requires $O(N_{EM} + N_{CKT})$ operations to evaluate the vectors $f(x_{p-1})$ and $r_{p-1}$, $O(N_{tx})$ operations to update $A^{t}_{i,j,p}$, and $O(N_{1} (N_{EM} + N_{CKT}))$ operations to solve for the Newton step. Here, $N_{tx}$ is the number of nonzero entries of $A^{t}_{i,j,p}$, and $N_{1}$ is the average number of iterations needed to solve (9). In general, $N_{EM} \gg N_{CKT}$ and $N_{EM} \gg N_{tx}$. Thus, the (two) dominant computational operations are the evaluation of the scattered electromagnetic fields in stage (i) and the iterative solution of the Newton step $b_{p}$ in stage (v). For each time step, the computations involved in stages (i) and (v) require $O(N_{EM}^{2} + N_{CKT})$ and $O(N_{p}N_{1} (N_{EM} + N_{CKT}))$ operations, respectively, where $N_{p}$ denotes the average number of Newton iterations. In our experience, the dominant computational operation for typical microwave circuits is incurring in stage (i), the calculation of $b_{i}$.

E. Parallelization and TD-AIM Acceleration

The solution of (8) is accelerated by parallel processing. One parallelization approach might be to simultaneously distribute all $N_{EM} + N_{CKT}$ unknowns among the $P$ available processors without separating electromagnetic and circuit unknowns. This approach, however, forces all processors handling both types of unknowns to run both electromagnetic and circuit solvers; this, in turn, leads to load balancing problems. Furthermore, it is not clear how to retrofit existing parallel field and circuit solvers to operate in unison inside such a framework. In this work, the parallelization strategy is to distribute electromagnetic and circuit-related unknowns and operations to separate sets of processors. Of the $R_{EM} + R_{CKT}$ available processors, $R_{EM}$ processors are dedicated to computations governing the updates of the $N_{EM}$ field unknowns and $R_{CKT}$ processors are used for operations related to updating the $N_{CKT}$ circuit unknowns. The two sets of processors communicate only when evaluating $r_{p-1}$ and its norm and while iteratively solving (9) in the Newton-Raphson algorithm of subsection II.D. Moreover, the two systems interact only at the loading ports and hence the two sets of processors exchange only $2N_{PORT}$ numbers when they communicate. Thus, the total amount of communication between the two sets of processors is $O(N_{p}N_{1}N_{PORT})$ bytes at each time step and is negligible compared to other communication and computation costs. This strategy allows for the separate development of field and circuit solvers and enables hybridization of already developed and optimized parallel field and circuit solvers in the Newton-Raphson framework without loss of their load-balancing features. Indeed, in this paper the circuit solver is hybridized with a highly scalable parallel FFT based field solver [29] as described next.

The FFT-acceleration is employed to reduce the $O(N_{EM}^{2})$ cost of computing the first $N_{EM}$ entries of $b_{i}$ at each time step, which quickly overwhelms the $R_{EM}$ processors. FFT based algorithms for accelerating electromagnetic analysis originated with the $k$-space method [42, 43] and were initially used for frequency-domain analysis involving uniformly discretized structures. They were later extended to incorporate nonuniformly discretized structures through the introduction of auxiliary uniform grids [41, 44] and parallelized [44]-[46] to allow large-scale static and time-harmonic analysis. Recently, FFT based algorithms have been adopted to permit the parallel analysis of electromagnetic transients on large arbitrarily shaped structures [23]-[29]. Here, the TD-AIM algorithm [29] is used.

The TD-AIM scheme embeds the microwave structure in an auxiliary 3D Cartesian grid with $N_{c} = N_{cx} \times N_{cy} \times N_{cz}$ nodes that are separated by $\Delta x$, $\Delta y$, and $\Delta z$ in the three orthogonal directions. Each of the impedance matrices is approximated as $Z_{x\rightarrow y} \approx Z^{near}_{x\rightarrow y} + Z^{FFT}_{x\rightarrow y}$ by using these auxiliary grid points. The matrices $Z^{near}_{x\rightarrow y}$ help preserve accuracy by reproducing the original entries of $Z_{x\rightarrow y}$; their entries are nonzero for only near-field interactions, for which they are equal to $Z_{x\rightarrow y} - Z^{FFT}_{x\rightarrow y}$. The matrices $Z^{FFT}_{x\rightarrow y}$, on the other hand, are approximations of the original matrices that are efficiently multiplied with the vectors $\Phi_{l}$ using multidimensional FFTs. The TD-AIM algorithm computes the first $N_{EM}$ entries of $b_{i}$ in four steps: (I) At each time step $l$, all current-coefficients $\Phi_{l}$ are locally projected onto the auxiliary grid, such that sources that reside on the auxiliary grid accurately approximate the transient fields radiated by the original sources outside a near-field region. In order to use only one auxiliary grid and the same propagation operators for both, the projection step for surface and volume sources is not identical. Because the fields radiated by volume sources require an additional temporal derivative (see (12) in Appendix), a finite difference scheme is used to compute the numerical derivatives of the volume coefficients, which are then projected onto the auxiliary grid. (II) Present and future transient fields produced by the sources on the auxiliary grid are computed on the same grid using vector- and scalar-potential propagators as described in [29] in a multilevel approach via global space-time FFTs. (III) The fields at time step $l$ are locally interpolated from the vector- and scalar-potential values on the auxiliary grid onto the primary mesh. (IV) The errors in the near-field region are corrected by computing $\sum_{l'=max(l-l_{N}),l_{N}}^{l+1} Z^{near}_{x\rightarrow y} \Phi_{l'}$ and adding it to the fields computed via steps (I)-(III). In this paper, the projection and interpolation operators of steps (I) and (III) are found by matching the multipole moments of point sources on the auxiliary grid to those of $\hat{x}$, $\hat{y}$, and $\hat{z}$ components and the gradients of the functions $S_{l}(r)$ and $\kappa(r)V_{l}(r)$ [29, 44]. Hence, four projection matrices are used for surface and volume basis functions. Because the projection operations and the correction matrices $Z^{near}_{x\rightarrow y}$ are localized in space and time, the dominant computational burden of the TD-AIM scheme is...
the computation of 4D space-time FFTs in step (II). Using a multilevel algorithm and employing parallel FFTs (e.g., via the FFTW library [32]), the space-time FFTs are computed in $O(N_\text{EM} \log N_\text{EM} + N_\text{EM}^2/R_{\text{EM}})$ operations per processor per time step. A detailed description of the parallel FFTs in this context is given in [29]. For volumetric or quasi-planar structures $N_\text{c} = N_\text{EM}$, whereas $N_\text{g} = N_\text{EM}^{1/3}$ (for volumetric) or $N_\text{g} = N_\text{EM}^{2/3}$ (for quasi-planar) [29].

To sum up, the two computationally dominant stages of the proposed algorithm, stages (i) and (v), are both accelerated by parallelization while stage (i) is further accelerated by the TD-AIM algorithm. For typical microwave circuits, neglecting the communication costs, the time spent in stages (i) and (v) at each time step scales as $O(N_\text{EM} \log N_\text{EM} / R_{\text{EM}} + N_{\text{CKT}} / R_{\text{CKT}})$ and $O(N_\text{EM}^2 + N_{\text{EM}} / N_{\text{CKT}} / R_{\text{CKT}})$ per processor, respectively. Ignoring the circuit processors and operations, the processors exchange, at each time step, a total of $O(N_\text{EM})$ bytes while computing FFTs in stage (i) and depending on the numbering and distribution of the unknowns amongst them $O(N_\text{EM})$ to $O(N_\text{EM}^2)$ bytes in stage (v). Hence, communication costs, which are subdominant to computation costs for stage (i), may become the bottleneck for stage (v) as the number of processors is increased.

III. APPLICATIONS

The accuracy and efficiency of the proposed scheme are demonstrated by analyzing various microwave systems and circuits. First an active antenna and a microwave amplifier are analyzed and the results obtained are compared to measurement and simulation data available in the literature. Next a grid amplifier is simulated and the results compared with both frequency-domain simulations and measurements available in the literature. In all simulations, the TD-AIM kernel matches up to third-order moments when projecting sources onto the auxiliary grid, and defines the near-field region of a basis function as the space extending 4 (auxiliary grid) cells in each direction away from it (that is, $\gamma$ as defined in [29], is 4). Bandwidths of Gaussian pulses are specified as two-sided and quantify the frequency range over which spectral power densities are no less than 45 dB below their peak values. The results in this section are obtained using a cluster of 1 GHz Pentium III processors with $R_{\text{CKT}} = 1$. In each and every case, the parallel efficiency of the scheme is examined by observing its run time and memory requirements. While a direct performance comparison with other simulators is not performed, the below applications clearly demonstrate the viability of the solver for analyzing large and detailed microwave systems and circuits.

A. Active Patch Antennas

The first microwave system analyzed consists of an array of two (nonlinear) Gunn diode loaded patch antennas. The antennas reside on a 0.789 mm thick dielectric substrate of permittivity $\varepsilon = 2.33\varepsilon_0$ that measures $41.4 \times 37.21$ mm; the substrate is backed by an equally sized ground plane (Fig. 2(a)). The construction and experimental characterization of this antenna were reported in [5], [47]; prior efforts at analyzing it relied on FDTD [5] and FETD [12] methods. In our model, the Gunn diodes connect across the centers of strips bonding the patches to the ground plane (Fig. 2(b)). Each diode is modeled by an equivalent circuit identical to that used in [5], [12] and detailed in Fig. 3, leading to $N_{\text{CKT}} = 4$ circuit unknowns. The field solver processes a mesh of the array comprised of triangles and tetrahedrons with average edge length of approximately 1 mm, leading to

![Fig. 2. Active patch antenna. Dimensions of the structure are in millimeters. The geometry dimensions and diode locations are shown in (a) top view and (b) side view.](image)

![Fig. 3. The $i - V$ characteristics of the Gunn diodes and their circuit model, which is identical to [5,12].](image)
$N_s = 6,222$ surface and $N_v = 24,947$ volume unknowns. The analysis is carried out for $N_t = 1,000$ time steps, with $\Delta t = 5$ ps and $N_c = 40$. The TD-AIM accelerator uses an auxiliary grid with spacings $\Delta x = 1$ mm, $\Delta y = 0.9$ mm, and $\Delta z = 0.2$ mm, resulting in $N_c = 45 \times 45 \times 8$ auxiliary grid points.

The array is excited by a normally incident $\hat{x}$-polarized Gaussian plane wave pulse, with $0.1$ mV/m peak-amplitude, $12$ GHz center frequency, and $8$ GHz bandwidth. The oscillations due to this low-power broadband plane wave are allowed to build up (Fig. 4(a)) and the resulting steady-state voltages across the diodes are plotted in Fig. 4(b). The oscillations across the two diodes are out of phase, as was observed in [5,12]. The fundamental frequency of the oscillations computed by the simulator is $12$ GHz (Fig. 4(c)), which agrees well with the values of $12.2$ GHz and $12.08$ GHz computed via differential-equation based schemes of [5,12] and the measured value of $11.8$ GHz. Figure 4(e) compares the normalized $\hat{y}$ polarized electric-field pattern of the antenna in the $x-z$ ($H$-) plane computed by the proposed method at $12$ GHz to measurements at $11.8$ GHz [47]. Good agreement is observed.

B. Microwave Amplifier

To further verify the accuracy of the simulator, a nonlinear microwave amplifier circuit is analyzed next. Microstrip matching networks are connected to a packaged transistor, which resides on a $0.7874$ mm thick dielectric substrate of permittivity $\varepsilon(r) = 2.33\varepsilon_0$ that measures $17.526 \times 16.256$ mm; the substrate is backed by an equally sized ground plane (Fig. 5(a)). This circuit was previously analyzed by FDTD based [8], FETD based [13], and PWTD accelerated integral-equation based [30] methods. Here, the circuit solver models the MESFET using the nonlinear large signal circuit model in Fig. 5(b), which is similar to those in [8], [13], [30]; a total of $N_{CKT} = 9$ circuit unknowns result. The field solver processes a mesh of the microwave amplifier comprised of triangles and
tetrahedrons with average edge length of approximately 1 mm, leading to \( N_s = 951 \) surface and \( N_v = 4,318 \) volume unknowns. The TD-AIM auxiliary grid spacings are \( \Delta x = 0.6 \, \text{mm}, \Delta y = 0.6 \, \text{mm}, \) and \( \Delta z = 0.2 \, \text{mm}, \) resulting in \( N_c = 30 \times 30 \times 8 \) auxiliary grid points.

First, the nonlinear behavior of the amplifier is studied. The input (1) and output (2) ports are driven by DC sources with internal impedance and amplitudes \( V_{GG} \) and \( V_{DD} \), respectively. For this analysis, the DC sources are turned on from zero, according to the first scheme described in subsection II.C, using a three-derivative smooth window function [48]:

\[
V_{GG}(t) = -0.81 f(t,1 \, \text{ns}) \, \text{V}, \quad V_{DD}(t) = 18.96 f(t,1 \, \text{ns}) \, \text{V},
\]

\[
f(t, \tau) = \begin{cases} 
0 & t \leq 0 \\
10(t/\tau)^3 - 15(t/\tau)^4 + 6(t/\tau)^5 & 0 < t < \tau \\
1 & t \geq \tau.
\end{cases}
\]  

(10)

After 3 ns, when a steady state is reached, the transient source \( V_s \) is activated at the input:

\[
V_s(t) = v_i g(t-3 \, \text{ns},6 \, \text{GHz}) \, \text{V},
\]

\[
g(t,f_c) = f(t,S/f_c) \sin(2\pi f_c t).
\]  

(11)

The analysis is carried out for \( N_t = 2000 \) time steps, with \( \Delta t = 5.2 \, \text{ps} \) and \( N_f = 18 \). Figure 6(a) shows the transient input and output voltage waveforms at the transistor terminals when the amplifier is driven by the 6 GHz single-tone excitation of (11) at an input power level of 5.95 dBm (i.e., \( v_i = 1.34 \, \text{V} \)). The power dissipated in the loading resistor is calculated from the Fourier transform of the steady-state current minus the DC current at the output port. The output power is observed at the harmonic frequencies of 6 GHz as shown in Fig. 6(b) for various different input power levels. Figures 7(a)-(c) compare the power levels of the first three harmonics with those simulated by the FDTD scheme of [8] and FETD scheme of [13]. Good agreement is observed.

Next, the broadband behavior of the amplifier is analyzed using the large signal circuit model of Fig. 5(b) under small signal operation. The input port is driven by a unit amplitude Gaussian pulse modulated at 7 GHz with 12 GHz bandwidth. For this analysis, the bias conditions are modeled with DC sources at the ports and initial conditions at the circuits, according to the second scheme described in subsection II.C.
In this case, only $N_t = 500$ time steps are needed, with $\Delta t = 4.0$ ps and $N_R = 22$. The input and output voltage waveforms at the ports shown in Fig. 5(a) are plotted in Figure 8(a). The $S$-parameters of the amplifier are extracted at the ports over the frequency range of 2-10 GHz and compared with those obtained using the differential-equation based schemes of [8] and [13] in Fig. 8(b). The results obtained using the TD-AIM scheme are in good agreement with those obtained using the differential equation algorithms. Good agreement is observed.

C. Reflection-Grid Amplifier

Lastly, a quasi-optical grid amplifier is analyzed [49], [50]. During the past decade, various grid amplifiers that employ up to hundreds of transistors have been demonstrated [51]. While most grid amplifiers use a transmission architecture, here, a grid-amplifier with an “active mirror” architecture that aids in heat-sinking [52], [53] is analyzed. The grid amplifier, which is modeled after those reported in [52], [53], is composed of sixteen 6-terminal differential amplifiers that are connected by...
a microstrip network mounted on a 0.8 mm thick dielectric substrate of permittivity $\varepsilon (r) = 2.33\varepsilon_0$ that measures $39.47 \times 27.46$ mm; the substrate is backed by an equally sized ground plane, whose distance from the bottom of the dielectric varies in between 1.6 mm and 31.6 mm in the cases analyzed. (Figs. 9(a)-(c)). The amplifier chips measure $0.4 \times 0.4$ mm and are modeled using the nonlinear large signal circuit model of Fig. 10(a), which is identical to that specified in [53], resulting in $N_{\text{CKT}} = 192$ circuit unknowns.

Note that, because the detailed circuit models for the transistors used in [53], which were custom built, were not available, here the transistors are modeled using the simple Ebers-Moll model of Fig. 10(b) [39]. The field solver processes a mesh of the reflection-grid amplifier using triangles and tetrahedrons with average edge length of approximately 0.8 mm, leading to $N_s = 8,487$ surface and $N_v = 42,592$ volume unknowns. The simulations are carried out for $N_t = 512$ to $N_t = 1,536$ time steps depending on the incident field angle and the ground plane position, the time step size is $\Delta t = 4$ ps, and $N_{\text{grid}}$ varies between 43 and 51 depending on the ground plane position. The TD-AIM auxiliary grid spacings are $\Delta x_l = 0.75$ mm, $\Delta y_l = 0.75$ mm, and $\Delta z_l = 0.375$ mm, resulting in $N_s = 56 \times 40 \times 8$ to $N_s = 56 \times 40 \times 96$ auxiliary grid points depending on the ground plane position.

As shown in Fig. 10(a), the amplifier bias conditions are

| TABLE I
| EBERS-MOLL MODEL PARAMETERS |
|---|---|---|---|---|
| $I_s$ | 2 fA | $C_{JE0}$ | 13 fF | $M_{JE}$ | 0.33 |
| $\beta_F$ | 28.32 | $C_{JC0}$ | 6 fF | $M_{JC}$ | 0.33 |
| $\beta_R$ | 3 | $V_{JE}$ | 0.6 V | $\tau_R$ | 0.5 ps |
| $\tau_F$ | 0.5 ps | $V_{JC}$ | 0.6 V | $FC$ | 0.8 |

Note that, because the detailed circuit models for the transistors used in [53], which were custom built, were not available, here the transistors are modeled using the simple Ebers-Moll model of Fig. 10(b) [39]. The field solver processes a mesh of the reflection-grid amplifier using triangles and tetrahedrons with average edge length of approximately 0.8 mm, leading to $N_s = 8,487$ surface and $N_v = 42,592$ volume unknowns. The simulations are carried out for $N_t = 512$ to $N_t = 1,536$ time steps depending on the incident field angle and the ground plane position, the time step size is $\Delta t = 4$ ps, and $N_{\text{grid}}$ varies between 43 and 51 depending on the ground plane position. The TD-AIM auxiliary grid spacings are $\Delta x_l = 0.75$ mm, $\Delta y_l = 0.75$ mm, and $\Delta z_l = 0.375$ mm, resulting in $N_s = 56 \times 40 \times 8$ to $N_s = 56 \times 40 \times 96$ auxiliary grid points depending on the ground plane position.

As shown in Fig. 10(a), the amplifier bias conditions are
modeled by DC sources at the ports. After the DC conditions at the circuits are established via the second scheme described in subsection II.C, the grid is illuminated by a $\cos \theta - \sin \theta$ polarized Gaussian plane wave, with 1 V/m peak-amplitude, 10 GHz center frequency, and 10 GHz bandwidth. In the following simulations, the plane wave is incident from the $\sin \theta + \cos \theta$ direction and the gain of the grid is defined as the $\hat{y}$ (cross) polarized radar cross section of the structure at the specular angle ($\sin \theta + \cos \theta$ direction) divided by the top-surface area of the grid ($237.47 \times 25.46$ mm$^2$); this replicates the gain definitions of the measurement setup in [51-53]. First, for verification purposes, the gain of the grid under normal illumination computed by the proposed scheme is compared to that computed by a frequency-domain hybrid simulator. The frequency-domain simulator’s circuit-solver replaces the transistors with their small-signal models at the operating point, whereas its field-solver uses a (frequency-domain) AIM accelerated integral-equation scheme [43], which uses the same surface mesh, volume mesh, auxiliary grid, and moment-matching order as the time-domain solver. Figure 11(a) shows the grid gain computed by the frequency- and time-domain simulators, with the transistors either unbiased or biased at 3.5 V. In both cases, good agreement between the results obtained using both schemes is observed. When the transistors are biased, approximately 15 dB gain is observed around 8.4 GHz, which is in good agreement with the measurement of 15 dB at 8.4 GHz reported in [53]. Next, the effects of changes in various design parameters on the reflection-grid amplifier’s performance are studied. Figure 11(b) plots the grid gain with respect to the ground-plane position for various frequencies under normal illumination. Fig 11(c) shows the performance of the amplifier for off-normal illuminations at various frequencies and compares the gain with the $\cos^2 \theta$ obliquity factor. The data presented in both figures support the predicted and measured trends reported in [52]. Lastly, the measurement setup of [53] is
replicated by illuminating the array from $\theta = 20^\circ$ direction and the computed and measured gains are compared as a function of frequency in Fig. 11 (d). The disagreement between the measured and simulated results at higher frequencies may be attributed to a variety of differences between the measured and modeled structures, such as the thickness of the substrate, the ground-plane position and size, the details of chip connections to the grid, and transistor characteristics. Nevertheless, the correlation between the simulation results obtained using the proposed solver and the measured data of [52, 53] is evident. Finally, Fig. 12 illustrates the parallel performance of the field-circuit solver in the above simulations. Figure 12(a) shows that in all of the above applications most of the computation time is spent in stages (i) and (v) of the Newton-Raphson algorithm of subsection II.D, as expected. Figure 12(b) shows the memory requirement of the algorithm and its distribution among the processors. The memory scalability of the algorithm is limited for the microwave amplifier, which has the smallest number of unknowns among the three cases. This is mainly due to operating system overheads and data replication among processors, such as geometry description. These factors, however, scale at most linearly with number of unknowns and hence become subdominant for problems with more unknowns. In short, Fig. 12 verifies that both the computation time and the memory requirement of the proposed scheme show good parallel scalability for all three simulations presented.

IV. CONCLUSION

This paper outlined a parallel FFT accelerated hybrid field-circuit simulator and highlighted its application to the analysis of various nonlinear microwave systems. The proposed simulator models fields on distributed passives by time-domain integral equations and currents and voltages in devices approximated in terms of lumped elements by modified nodal analysis equations. The resulting nonlinear hybrid system of equations in field and circuit unknowns is solved using a Newton-Raphson algorithm, which is accelerated by distributing the computational work across multiple processors and by employing the TD-AIM algorithm to expedite field computations. The simulator can characterize a broad variety of microwave circuits accurately, as was demonstrated through comparison of data derived from it with independent measurements and simulations of a nonlinearly loaded patch antenna, a microwave amplifier, and a reflection-grid amplifier. Furthermore, as demonstrated in Section III, the distributed-memory parallelization of the algorithm shows near-ideal scalability, allowing the simulator to efficiently characterize nonlinear components on electrically large platforms.

The versatility of the proposed simulator can be increased through various extensions that are currently being developed. These include the incorporation of variable time-stepping and reduced-order macromodeling algorithms, as well as accurate lossy- and layered-media formulations for the time-domain integral equations.

APPENDIX

The entries of the vectors $V^{EM}_{f}$ and $I^{EM}_{f}$, which are of length $N_{EM}$, are

$$V^{EM}_{f}(k) = \begin{cases} \int_S S_i(r) \cdot \hat{E}^{inc}(r,t) ds & \text{for } k \leq N_s \\ \int_0^{\Delta t} \int_T V_s(r) \cdot \hat{E}^{inc}(r,t) dv & \text{else} \end{cases}$$

$$I^{EM}_{f}(k') = \begin{cases} I_{k'} & \text{for } k' \leq N_s \\ I_{k'} & \text{else} \end{cases}$$

The entries of the impedance matrices $Z_{l-l'}$, for $0 \leq l-l' \leq N_g$, each of which are of size $N_{EM} \times N_{EM}$, are
\[ Z_{t-f}(k,k') = \int_{S} \left[ \sum_{r} \phi_{k}^{2}(r,\tau) \right] \cdot S_{k}(r) \, ds \]
\[ + \int_{S} \left[ \sum_{v} \phi_{k}^{2}(r,\tau) \right] \, ds \quad \text{for} \quad k' \leq N_{s}, k \leq N_{s} \]
\[ \int_{S} \left[ \sum_{r} \phi_{k}^{2}(r,\tau) \right] \, ds \quad \text{for} \quad k' > N_{s}, k \leq N_{s} \]
\[ = \int_{V} \left[ \sum_{k} \phi_{k}^{2}(r,\tau) \right] \, dv \]
\[ + \int_{V} \left[ \sum_{v} \phi_{k}^{2}(r,\tau) \right] \, dv \quad \text{for} \quad k' \leq N_{s}, k > N_{s} \]
\[ \int_{V} \left[ \sum_{v} \phi_{k}^{2}(r,\tau) \right] \, dv \quad \text{for} \quad k' > N_{s}, k > N_{s} \]  

\[ (13) \]

Notice that the first and second conditions in (3) are enforced on conductor surfaces and dielectric volumes by testing them with surface and volume functions, respectively. In (13), the entries of \( Z_{t-f} \) are defined in terms of the first and second time derivatives of scalar and vector potentials due to each spatial basis function, respectively:

\[ \partial_{t} \phi_{k}^{2}(r,\tau) = \int_{S} \frac{T(t-R/c_{0})}{4\pi R} \nabla S_{k}(r') \, ds', \]
\[ \partial_{t} \phi_{k}(r,\tau) = \int_{S} \frac{T(t-R/c_{0})}{4\pi R} \mu_{0} S_{k}(r') \, ds', \]
\[ \partial_{t} \phi_{v}(r,\tau) = \int_{V} \frac{T(t-R/c_{0})}{4\pi R} \nabla' \phi_{k}(r') \, dv', \]
\[ \partial_{t} \phi_{v}(r,\tau) = \int_{V} \frac{T(t-R/c_{0})}{4\pi R} \mu_{0} \phi_{k}(r') \, dv', \]  

\[ (14) \]

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