BPINN-EM: Fast Stochastic Analysis of Electromigration Damage using Bayesian Physics-Informed Neural Networks

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ABSTRACT

Electromigration (EM) induced aging and degradation in interconnect wires is inherently a stochastic process, with lifetime typically measured in terms of mean time to failure at both wire and circuit levels. However, existing approaches still incur high computing costs, as computing both means and variances is generally expensive. In this work, we propose a novel fast variational analysis framework to tackle the challenges of stochastic estimation of EM stress evolution in multi-segment interconnect wires. We utilize Bayesian networks in conjunction with the recently introduced hierarchical (two-step) physics-informed neural networks (PINN). The resulting method, termed BPINN-EM, enables rapid variational stress analysis of metal wires by leveraging the robust uncertainty quantification capability of Bayesian networks with expedited training over small dataset. Moreover, we devise BPINN-EM to incorporate Bayesian networks only in the first stage of the hierarchical PINN, thereby circumventing the need for sampling across the entire PINN level during training and significantly reducing training costs. Our results on several general multi-segment interconnect structure demonstrate that the proposed BPINN-EM approach is much more efficient than conventional baselines and state-of-the-art algorithms. Compared to a Monte Carlo simulator implemented in COMSOL, BPINN-EM offers a 240× speedup. Moreover, compared to the recently proposed EMSpice simulated by the Monte Carlo method, the new method provides more than an 85× speedup with almost no loss of accuracy.

KEYWORDS

Electromigration (EM), Physics informed neural network (PINN), Bayesian neural network (BNN)

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1 INTRODUCTION

Electromigration (EM) is the phenomenon introduced due to the migration of metal atoms inside the metal interconnects when they interact with high current carrying electrons. This migration of metal atoms increase compressive stress at the anode and tensile stress at the cathode. If the stress exceeds critical stress, a void is formed near the cathode or a hillock may get formed near the anode. The formation of void or hillock results in circuit failure. EM lifetime of interconnect wires typically is characterized by mean time to failure (MTTF) due to its inherently variational nature [1].

Traditionally the MTTF or mortality of an interconnect wire is related to the current density of the wire via the well-known Black and Blech-based EM models [2, 3]. But such single wire segment EM models however face growing criticism for being overly conservative as it consider one wire segment in isolation. Recent study shows that the stress evolution of wire segments in one EM tree (confined by the metal atom liner and barriers of interconnect wire) are highly correlated and needs to be considered together [4, 5]. As a result, many physics based analytical and numerical solutions have been proposed as alternative to the Black's model [6–20]. The crux of these methods is to solve physics based Korhonen's partial differential equation for the EM stress evolution [21]. However, solving Korhonen's equation and other PDEs using traditional numerical methods remains a challenge due to their inherent limitations. On top of this, stochastic physics-based EM analysis using Monte Carlo method becomes even more prohibitively expensive.

Recently, a machine learning based approach known as physics-informed neural networks (PINN) has emerged to address the learning and encoding of physics laws expressed by nonlinear partial differential equations (PDE) in complex physical, biological, or engineering systems [22, 23]. PINN based approach has been applied to solve Korhonen's equation recently [24–26]. In PINN, the physics laws, boundary conditions, and initial conditions of the PDEs are explicitly enforced via loss functions in neural networks, demonstrating promising results for small-scale PDE problems with a limited number of variables.

Recently, the Physics-Informed Neural Network (PINN) approach has been employed to solve Korhonen's equation, demonstrating promising results [24–27]. Additionally, a hierarchical PINN scheme has been proposed for fast EM analysis [25, 27]. In these approaches, the stress evolution in multi-segment interconnects is addressed in two stages. Firstly, parameterized surrogate models of stress evolution in single wire segments are obtained either using neural networks or analytical solutions. Subsequently, in the second stage, the PINN scheme is applied to ensure that stress continuity and atomic flux conservation physics are satisfied for all segments in a multi-segment interconnect wire. This approach significantly reduces the number of variables in the second PINN training, leading to training efficiency. However, none of these PINN-based approaches have addressed the variability of EM effects.

On the other hand, Bayesian Neural Networks (BNNs) becomes an important deep neural networks due to their powerful uncertainty quantification capability, handling scarce dateset and preventing overfitting [28]. In this paper we leverage variance quantification capability of the BNN for fast estimation of the variance in EM stress

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distribution on multi-segment interconnect structure. Our novel contributions in this work are:

- We propose a new PINN architecture, which combine recently proposed hierarchical PINN and Bayesian network for variational analysis. To the best of the authors' knowledge, this is the first study incorporating Bayesian Physics Informed Neural Network to varational EM stress analysis.
- Moreover, we devise BPINN-EM to incorporate Bayesian networks only in the first stage of the hierarchical PINN, thereby circumventing the need for sampling across the entire PINN level during training and significantly reducing training costs, which can be very cost-efficient for training. In the first stage, the BNN is trained to estimate the variance in EM stress for a single segment by taking time varying current as input along with other physical properties.
- In the second stage, we utilize a PINN to enforce the stress continuity and atomic flux conservation to obtain the variance stress predictions for any multi-segment structures. In this way, we only need to do one training (sample) for the PINN network for the whole variational analysis and modeling, which is very cost-efficient.
- BPINN-EM demonstrates superior simulation efficient over traditional Monte Carlo method. Once the models have been built, it can deliver more than 240× speedup Monte Carlo with marginal errors. Moreover, compared to the recently proposed EMspice [18] simulated by the Monte Carlo method, the new method provides more than an 85× speedup with almost no loss of accuracy.

The paper is organized as follows: Section 2 reviews existing works on physics-based EM model and its analysis techniques and recently proposed stochastic EM analysis methods. The theoretical concepts used in our method are explained in Section 3. Section 4 proposes the *BPINN-EM* with detailed description of two levels inside the framework. Experimental results are presented in Section 5. Finally, section 6 concludes this paper.

2 REVIEW OF RELEVANT WORK

2.1 Numerical solutions based on deep neural networks

Many numerical solutions to solve the PDE of Korhonen's equations in the past such as finite difference methods [18, 29, 30], finite element method (FEM) [15] and some analysis or semi-analysis solutions [17, 19, 31], which typically come with some assumptions/restriction about the topology of the interconnect trees.

On the other hand, machine learning based approaches have been proposed to address the challenges of fast EM analysis. Recently, EM analysis based on generative adversarial networks (GANs) was introduced for fast transient hydrostatic stress analysis [32]. It outperformed analytic-based EM solvers in speed while maintaining accuracy, but its applicability is limited to a fixed region due to producing fixed-size images. This restriction hinders its practical use in real chip scenarios and doesn't represent multisegment interconnects well. To overcome these limitations, Jin et al. proposed an enhanced graph neural network (GNN)-based EM solver [33]. GNNs capture more natural relationships among design objectives, making the knowledge transferable across designs. However, both methods rely on supervised learning, requiring extensive training from numerical solvers or empirical data.

To overcome this limitation, recent advancements in unsupervised learning have introduced frameworks known as *physics-informed neural networks (PINN)* or *physics-constrained neural networks* [34–36]. These frameworks reframe the process of solving partial differential equations (PDEs) as a nonlinear optimization task handled by deep neural networks (DNNs). These networks are equipped with loss functions designed to enforce the principles of physics as represented by the PDE and its boundary conditions. However, while some progress has been made in applying these frameworks to relatively simple PDE problems [37–39], their effectiveness has been limited, with only modest advancements in addressing more complex aerodynamics simulations [40].

Several PINN-based EM solvers have been proposed recently. In [24], PINN was used directly to solve for the stress evolution in confined metal for simple straight interconnects. Recently, Hou *et al.* further proposed the incorporation of analytic formulae into the final loss functions of the PINN method [26]. Jin *et al.* recently developed a hierarchical PINN method in which two training stages are used to address training and convergence issues encountered with plain PINN [25]. In this method, the first stage DNN model for a single wire was built using a supervised learning method. Lamichhane further extended the two-stage PINN to solve the EM stress evolution in post-voiding phase [27]. However, all of those methods did not explicitly consider the stochastic or variational natures of EM damages, which will be addressed in this work.

2.2 Existing work for stochastic EM Analysis and assessment

Variational or stochastic EM impacts on wire lifetime have been studied in the past. Study in [41] shows that as technology scales, both mean time to failure and failure time distributions degrades, which remains challenging for advanced interconnects. Work in [1] proposed earlier work to consider variability in the EM analysis. This method still consider one wire segment in isolation with both analytic and numerical solutions to calculate time to failure. It considers two types of variations: circuit-level where resistance of wires are random variable (RV) and wire geometry-level where non ideal wire geometries (like bump and necking) are RV due to lithography variations. Work in [42] considers both global/local process variations for power grid and Hermite polynomial chaos based method is applied for both variational EM analysis and final lifetime analysis using on Black's EM model. In [43], the whole power grid are analyzed to consider the inherent redundancy of the grids by solving the Korhonen's PDE using finite difference methods. EM diffusivity is considered as RV and Monte Carlo based method is applied for variational analysis with some ad-hoc acceleration techniques. Method in [44] mainly focuses on the variability in the input currents where stochastic current models are used to consider current models in functional blocks and variance or covariance are explicitly computed via matrix solving of whole power grids, which is still very expensive.

Recently Yang *et al.* proposed a Bayesian PINN framework in order to quantify noise in the observations and avoid the overfitting problem inherent in regular PINN [45]. They illustrate the efficiency of their method on common and relatively simple problems. Their method however applies Bayesian based sampling for the whole PINN for the training, which can be very time expensive for large domains like multi-segment interconnect structures.

In this work, we also mainly consider the variational impacts from the currents. But our method is orthogonal to any variaitonal sources as the Bayesian networks are trained through Monte Carlo like sampling and it will be as general and flexible as Monte Carlo method.

3 PRELIMINARIES

3.1 EM stress modeling

Electromigration (EM) involves the movement of metal atoms from the cathode to the anode within confined metal interconnect wires. This migration occurs due to the exchange of momentum between conducting electrons and metal atoms [2]. As EM progresses, the hydrostatic stress gradually builds up. Once the stress surpasses a critical threshold, void formation begins at the cathode, while hillocks emerge at the anode of the interconnects. Ultimately, these phenomena can result in open circuits or short circuits, posing a reliability issue induced by EM in modern VLSI circuits.

Black's formula predicts the time-to-failure (TTF) caused by electromigration (EM) based on empirical or statistical data fitting, but it's only applicable to a specific single wire [2]. Blech's limit, another method used to check for immortality, fails to estimate transient hydrostatic stress and has faced criticism for leading to unnecessary overdesign [3]. To address this issue, the Korhonen equations, a physics-based EM model, are utilized to depict the evolution of hydrostatic stress in general multi-segment interconnects [46].

The general multi-segment interconnect comprises n nodes, with p interior junction nodes denoted as $x_r \in x_{r1}, x_{r2}, \cdots, x_{rp}$ and q block terminals denoted as $x_b \in x_{b1}, x_{b2}, \cdots, x_{bq}$, along with several branches. Korhonen's physics-based partial differential equation (PDE) for this general structure during the nucleation phase is expressed as follows [17, 31]:

$$\begin{aligned}
&\frac{\partial \sigma_{ij}(x,t)}{\partial t} = \frac{\partial}{\partial x}\left[\kappa_{ij}\left(\frac{\partial \sigma_{ij}(x,t)}{\partial x} + G_{ij}\right)\right], t > 0\\
&BC: \sigma_{ij_1}(x_i,t) = \sigma_{ij_2}(x_i,t), t > 0\\
&BC: \sum_{ij} \kappa_{ij}\left(\left.\frac{\partial \sigma_{ij}(x,t)}{\partial x}\right|_{x=x_r} + G_{ij}\right) \cdot n_r = 0, t > 0\\
&BC: \kappa_{ij}\left(\left.\frac{\partial \sigma_{ij}(x,t)}{\partial x}\right|_{x=x_b} + G_{ij}\right) = 0, t > 0\\
&IC: \sigma_{ij}(x,0) = \sigma_{ij,T}
\end{aligned} \tag{1}$$

Here, BC and IC denote boundary and initial conditions, respectively. ij represents a branch connected to nodes i and j, while n_r indicates the unit inward normal direction of the interior junction node r on branch ij. $\sigma(x,t)$ denotes the hydrostatic stress, $G = \frac{Eq*}{\Omega}$ signifies the electromigration driving force, and $\kappa = \frac{D_a B \Omega}{k_B T}$ represents the diffusivity of stress. In these equations, E stands for the electric field, $q*$ represents the effective charge, $D_a = D_0 \exp\left(\frac{-E_a}{k_B T}\right)$ denotes the effective atomic diffusion coefficient, where D_0 is the pre-exponential factor, B is the effective bulk elasticity modulus, Ω represents the atomic lattice volume, k_B signifies Boltzmann's constant, T is the absolute temperature, and E_a indicates the activation energy for electromigration. σ_T stands for the initial thermal-induced residual stress. For this work, we assume the initial stress to be zero.

3.2 Variations in EM stress

Conventionally, we solve Eq (1) to get the transient stress distribution on the general multisegment interconnects. We then compare the obtained solution with the critical stress and then estimate the failure time using the void nucleation time t_{nuc}. This type of deterministic analysis using DC average of the input current fails to consider the variations in EM stress due to input current variations, process variations, temperature variations, diffusivity variations etc. Hence failure time estimation using the deterministic approach using DC average current models gives us very optimistic and less realistic lifetime [44].

If we define $\mathbf{x}$ as the vector representing electrical and physical parameters involved in EM stress evolution, and v as the errors due to variations. Due to the uncertainty on the parameters and the noise values, they can be considered as random variables in the corresponding spaces i.e. $\mathbf{x} \in \mathbb{X}$ and $v \in \mathbb{V}$. We assume that the solutions of EM stress are independently Gaussian distributed and centered at hidden real values:

$$\bar{\sigma} = \mathcal{F}(\mathbf{x}) + v \tag{2}$$

here, $\bar{\sigma}$ is the EM stress solutions computed using parameters $\mathbf{x}$ plus the noise v due to variations. $\mathcal{F}(.)$ can be any solver used to solve Eq (1) e.g. FEM based method COMSOL [47], FDM based method EMSpice [18]. The random variation noise is usually considered independent following standard Gaussian distributions, with zero mean and variance of Var_σ. A conventional method to quantify the mean and variance in EM stress calculation represented by Eq (2) is to use direct Monte Carlo simulation. However, Monte Carlo simulations require Eq (1) to be simulated for multi-segment interconnects repeatedly. This can be very expensive especially as the number of segments in the interconnect structure increases.

3.3 Bayesian networks for variational analysis

Using Bayesian framework, EM stress σ is represented with a surrogate model $\tilde{\sigma}(\mathbf{x};\omega)$:

$$\sigma \approx \tilde{\sigma}(\mathbf{x};\omega) \tag{3}$$

here ω is the vector of parameters of surrogate Bayesian model with a prior distribution $P(\omega)$. The dataset $\mathcal{D}$, used to train the surrogate model can be represented as:

$$\begin{aligned}
&\mathcal{D} = \{(\mathbf{x}^{(i)}, \bar{\sigma}^{(i)})\}_{i=1}^{N}\\
&\{\bar{\sigma}^{(i)}\}_{i=1}^{N} = \left\{\mathcal{F}\left(\mathbf{x}^{(i)}\right) + v^{(i)}\right\}_{i=1}^{N}
\end{aligned} \tag{4}$$

here N is the training data size, v is the noise in simulation which can be assumed to be random samples from a independent Gaussian distribution with zero mean and variance Var_σ. Given the dataset $\mathcal{D}$, and the prior knowledge $P(\omega)$, likelihood of the observation can be calculated as:

$$\begin{aligned}
P(\mathcal{D}|\omega) = &\prod_{i=1}^{N} \frac{1}{\sqrt{2\pi Var_\sigma^{(i)}}}\\
&\times exp\left[-\frac{\left(\tilde{\sigma}\left(\mathbf{x}^{(i)};w\right) - \bar{\sigma}^{(i)}\right)^2}{2Var_\sigma^{(i)}}\right]
\end{aligned} \tag{5}$$

the posterior likelihood can be obtained using Bayes's theorem:

$$P(\omega|\mathcal{D}) = \frac{P(\mathcal{D}|\omega)P(\omega)}{P(\mathcal{D})} \propto P(\mathcal{D}|\omega)P(\omega) \tag{6}$$

here, ∝ symbol means 'equality up to a constant' is the probability of dataset $P(D)$ is not easily solvable analytically. Hence in practice we only get an un-normalized expression $P(\omega|\mathcal{D})$. Therefore, to get a posterior EM stress σ for given parameter vector $\mathbf{x}$, we get samples $\{\omega^{(i)}\}_{i=1}^{M}$ from $P(\omega|\mathcal{D})$ and get the variational stress statistics (mean and variance) from samples $\{\tilde{\sigma}(\mathbf{x};\omega^{(i)})\}_{i=1}^{M}$.

Bayesian model in this work uses fully connected neural network with $L \geq 1$ hidden layers as surrogate model. For a fully connected Bayesian network (interchangebly addressed as BNN throughout this paper), the model parameters ω are the concatenation of the weights and biases matrices of all the layers used in the network. It is a common practice in BNN to use an independent Gaussian distribution with a zero mean as a prior for ω so that the fully connected layers with L number of layers, the weights w_l and biases b_l for each layer $l = 0, 1, ..., L$ have the variances $\mathrm{Var}_{w,l}$ and $\mathrm{Var}_{b,l}$ [48]. From this it can be inferred that the output of the neural network using these layers is actually a Gaussian process as the width of the layers goes to infinity [48]. The optimal values of ω are the values that maximize the posterior likelihood $P(\omega|D)$ and usually denoted as ω^*. The likelihood can be maximized by numerically optimizing the logarithm of Eq (6). The optimal samples of posterior can be obtained to get samples of $\tilde{\sigma}(\mathbf{x},\omega^*)$ using Monte Carlo methods. The mean and variance of these samples are then used to approximate the variations in EM stress σ.

4 PROPOSED BPINN-EM FOR FAST STOCHASTIC EM STRESS ANALYSIS

The proposed *BPINN-EM* utilizes the hierarchical two stage approach to estimate the variations in stochastic EM stress on general multi-segment structure. Fig. 1 shows the overall algorithm flow of the proposed BPINN-EM framework.

To prepare our framework to perform variational stress analysis on multisegment interconnect structure, first we get posteriors of BNN model using sampling technique for a single wire segment. BNN model is then used to approximate the stochastic EM stress at boundary nodes of all the segments in second stage. In the second-stage, a PINN is trained using these boundary stress values to enforce the atomic flux conservation and stress continuity on the entire multisegment interconnect structure. Once trained, the combination of BNN and PINN can then be used to estimate the variations in stochastic stress on the multisegment interconnect structure. We initially sample the posterior samples of Bayesian network using Hamiltonian Monte Carlo (HMC) method with the dataset generated from simulations. Additionally, to train our PINN, we utilize Bayesian network to approximate EM stress at boundary nodes of the segments only and not on the entire interconnect structure. This results in very time efficient training of the PINN. Furthermore, after the training of PINN is completed, it can be used to quantify variations in variational stress across the whole multisegment interconncet structure, eliminating the need for retraining.

4.1 Estimation of variations in EM stress using Bayesian network and Hamiltonian Monte Carlo sampling

In this section we further explain the proposed *BPINN-EM* in detail. *BPINN-EM* utilizes the variance quantification property of Bayesian Neural Networks (BNN) to obtain the stochastic stress distribution on multi-segment interconnect structures. The posteriors of the BNN surrogate model are sampled using variational EM stress simulation data generated with COMSOL [47]. In our approach, the BNN model is employed to infer variational EM stress on each segment of the multi-segment structure separately [25, 27]. In the second phase, PINN is responsible for ensuring that the generated stress at each segment satisfies stress continuity and atomic flux conservation at each inter-segment junction of the multi-segment interconnect structure.

To generate the training dataset $\mathcal{D}$ for Bayesian Neural Networks (BNN), we conduct direct Monte Carlo simulations in COMSOL. To account for variations in input current, each Monte Carlo simulation involves sampling branch currents for interconnect structures from a Gaussian distribution such that $J \in \mathcal{N}(\mu_j, \mathrm{Var}_j)$, where J represents the current density distribution, μ_j is the mean, and Var_j is the variance of the distribution. We note that the Monte Carlo simulation can capture other potential variations in electromigration (EM) stress [44]. Using samples from the Monte Carlo simulations, we obtain variations in the distribution of stress, characterized by the stress mean μ_σ and stress variance Var_σ. The time-varying stochastic EM stress targets $\bar{\sigma}$ for BNN training are then sampled from the distribution $\mathcal{N}(\mu_\sigma, \mathrm{Var}_\sigma)$.

As depicted in Fig. 1, the physical and electrical parameters of each segment within a general multi-segment interconnect structure are considered to prepare input parameters for the Bayesian Neural Network (BNN) surrogate model. The BNN network takes inputs $\mathbf{x} = \{X, T, L, W, J(t), F_1(t), F_2(t)\}$. Here, X is the position vector, T is the time vector, L is the length of the wire under consideration, and W is the width of the wire. $J(t)$ represents the branch current density, which varies over time according to $J \sim \mathcal{N}(\mu_j, \mathrm{Var}_j)$. $F_1(t)$ and $F_2(t)$ denote the atomic flux at the left node for horizontal wires and the bottom node for vertical wires, respectively, in the multi-segment interconnect structure. Similarly, $F_2(t)$ is the atomic flux at the right node for horizontal wires and the upper node for vertical wires. For single wires with stopping boundaries, $F_1 = F_2 = 0$. However, their values are not zero for single wires extracted from multi-segment interconnect structures. The values of F_1 and F_2 will be determined in the second stage PINN by enforcing the necessary electromigration (EM) physics conditions.

BPINN-EM uses Hamiltonian Monte Carlo(HMC) approach to explore the parameter space of our BNN model. HMC is a gradient based Markov Chain Monte Carlo(MCMC) approach that uses Hamiltonian dynamics to explore the parameter space. HMC approach we use first simulates the Hamiltonian dynamics using numerical integration method and then corrected by using Metropolis-Hastings acceptance step. Given a dataset $\mathcal{D}$, we assume target posterior distribution for ω as:

$$P(\omega|\mathcal{D}) \simeq exp(-U(\omega)) \tag{7}$$

where $U(\omega) = -log(P(\mathcal{D}|\omega)) - log(P(\omega))$ In order to sample from posterior, HMC uses an auxiliary momentum variable r to construct a Hamiltonian system:

$$H(\omega, r) = U(\omega) + \frac{1}{2} r^T \mathrm{M}^{-1} r \tag{8}$$

here, M is a mass matrix usually set to be identity matrix, I. HMC then generates samples from joint distribution of (ω, r) as:

$$\pi(\omega, r) \sim exp(-U(\omega) - \frac{1}{2} r^T \mathrm{M}^{-1} r) \tag{9}$$

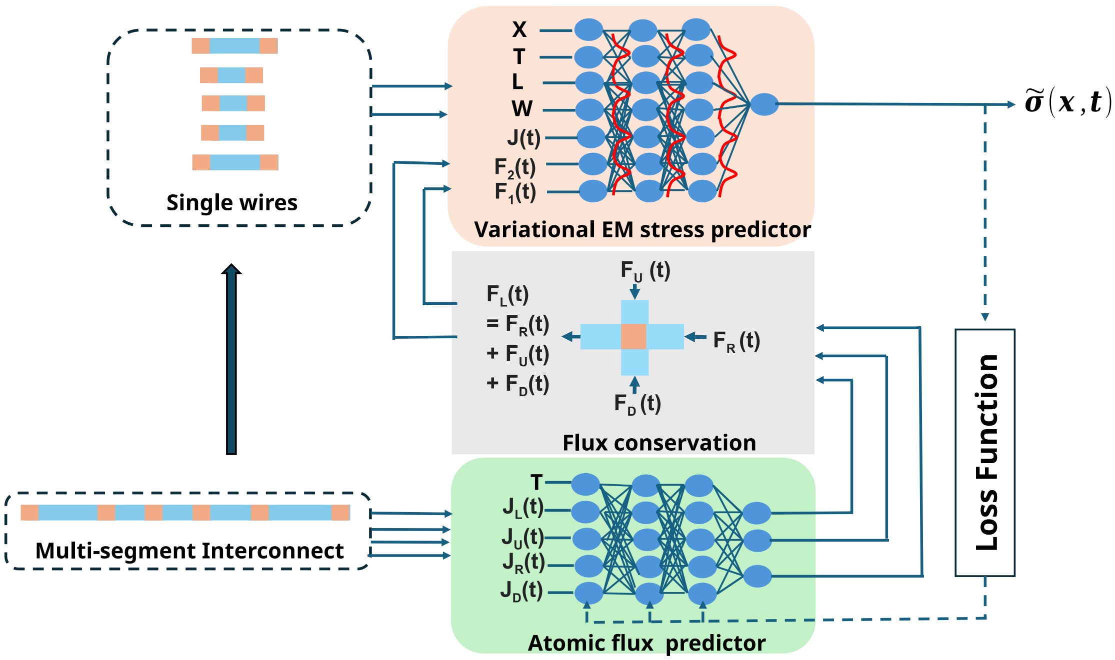

Figure 1: Framework of proposed BPINN-EM variational EM stress simulator and surrogate model

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Algorithm 1 Sampling variational EM stress using BNN and Hamiltonian Monte Carlo Sampler

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Require: initial states for ω^{t_0} and time step size δt

  for $k = 1$ to N **do**

    Sample $r^{t_{k-1}}$ from $\mathcal{N}(0, M)$,

    $(\omega_0, r_0) \leftarrow (\omega^{t_{k-1}}, r^{t_{k-1}})$

    for $i = 0$ to $(L - 1)$ **do**

      $r_i \leftarrow r_i - \frac{\delta t}{2} \nabla U(\omega_i)$

      $\omega_{i+1} \leftarrow \omega_i + \delta t M^{-1} r_i$

      $r_{i+1} \leftarrow r_i - \frac{\delta t}{2} \nabla U(\omega_{i+1})$

    end for

    Metropolis-Hastings step:

    Sample p from Uniform$[0, 1]$

    $\alpha \leftarrow \min\{1, \exp(H(\omega_L, r_L) - H(\omega^{t_{k-1}}, r^{t_{k-1}}))\}$

    if p $\geq \alpha$ **then**

      $\omega^{t_k} \leftarrow \omega_L$

    else

      $\omega^{t_k} \leftarrow \omega^{t_{k-1}}$

    end if

  end for

  Calculate $\{\tilde{\sigma}(\mathbf{x}, \omega^{t_{N+1-j}})\}_{j=1}^{M}$ as samples of $\sigma(x)$

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here, the ω samples have marginal distribution as we eliminate the r samples. The samples are generated from the following Hamiltonian dynamics

$$\begin{aligned} d\omega &= \mathrm{M}^{-1} r dt, \\ dr &= -\nabla U(\omega) dt \end{aligned} \tag{10}$$

Eq (10) is discretized using leapfrog method and Metropolis-Hastings step is used to reduce the discretization error. Algorithm 1 illustrates the details of HMC to get variational EM stress samples $\{\tilde{\sigma}(\mathbf{x}; \omega^{(i)})\}_{i=1}^{M}$ [45].

In our framework, we initially sample the posteriors of the Bayesian network, which are subsequently used for inference. Employing a BNN surrogate model for estimating stochastic electromigration (EM) stress offers several advantages. BNNs have demonstrated efficiency in quantifying errors and handling sparse datasets by mitigating overfitting [28]. This implies that BNNs can be trained or sampled using relatively smaller datasets compared to Deep Neural Networks (DNNs). Consequently, this reduces the simulation time required for data generation, enhancing practicality and scalability. Furthermore, utilizing smaller datasets results in shorter training times. For example, in our experiment, we observed a training time of approximately 6.5 hours with 40,000 data points for variational analysis. In contrast, a similar approach [25] for estimating deterministic EM stress using fully connected DNNs required more than 20 hours for 80,000 data points.

4.2 Enforcing stress continuity and atomic flux conservation using PINN

The BNN surrogate model used in the first stage of *BPINN-EM* accurately provides samples of variational EM stress for each segment within multi-segment interconnect structures when provided with the correct input set $\mathbf{x} = \{X, T, L, W, J(t), F_1(t), F_2(t)\}$ for that wire. For single segments with blocking boundary nodes, the BNN alone is sufficient to estimate the stochastic EM for these wires, as the atomic fluxes at their terminals are $F_1 = F_2 = 0$. However, in reality, interconnects are often multi-segment wires or trees. Therefore, for the single wires within these interconnects, two conditions must be addressed: stress continuity and atomic flux conservation at the junctions of the segments, as depicted in Eq (1). To satisfy these conditions and obtain F_1 and F_2, we employ PINN, which enforces stress continuity and atomic flux conservation at the segment junctions [25, 27].

As depicted in Fig 1, our atom flux estimation framework employs a Multilayer Perceptron (MLP). This MLP is fed with time-varying current densities from the segments connected to each inter-segment junction of a multi-segment interconnect structure. For each inter-segment junction, since there can be a maximum of four segments connected to it, the MLP receives $J_L(t)$, $J_U(t)$, $J_R(t)$, and $J_D(t)$, representing the current densities at segments on the left, up, right, and down, respectively. It's important to note that these current densities vary over time for each segment and are modeled as random samples from Gaussian distributions, denoted as $J_s \sim \mathcal{N}(\mu_{js}, \mathrm{Var}_{js})$ for $s \in L, U, R, D$. Additionally, the time vector T is included as an input to the MLP since both its inputs and outputs vary with time. As illustrated in Fig 1, the MLP outputs time-varying atomic fluxes through the nodes of segments connected to each inter-segment junction in three directions, such as up, right, and down, denoted by $F_U(t)$, $F_R(t)$, and $F_D(t)$, respectively. The atomic flux at the segment node connected to the left, i.e., $F_L(t)$, is then computed by conserving the total atomic flux, as suggested by Eq (1). Consequently, we obtain the atomic fluxes ($F_1(t)$, $F_2(t)$) through both ends of all segments in the multi-segment interconnects.

Another crucial consideration for the predicted atomic fluxes ($F_1(t)$, $F_2(t)$) in forecasting the stochastic EM stress distribution across multi-segment interconnect structures is ensuring stress continuity at the inter-segment junctions. To enforce stress continuity at these junctions, it's imperative to align the variational EM stress at the nodes of all segments connected to the inter-segment junctions, ensuring their overlap. This alignment is achieved through the utilization of the loss function given by Eq (11). The role of this loss function is to minimize the discrepancy between the variational EM stress at the boundary nodes of all segments connected to the inter-segment junctions within the multi-segment interconnect structure.

$$L = \frac{1}{N_I} \sum_{i=1}^{N_I} \sum_{k=2}^{K_i} ((\tilde{\sigma}_k(t)) - (\tilde{\sigma}_{k-1}(t)))^2 \tag{11}$$

Here, $\tilde{\sigma}_k(t)$ represents the variational EM stress at the boundary of the k^{th} segment connected at the inter-segment junction i. K_i denotes the number of segments connected to the inter-segment junction i, and N_I signifies the total number of inter-segment junctions in the general multi-segment structure.

The loss function, defined in Eq (11), serves to optimize the parameters of the atomic flux predictor MLP. As this loss converges, the MLP becomes adept at predicting the optimal atomic fluxes at the nodes of the segments connected to each inter-segment junction within a multi-segment interconnect structure. These predicted atomic fluxes are termed 'optimal' as they adhere to the conditions of atomic flux conservation and stress continuity. Consequently, optimal atomic fluxes ($F_1(t)$ and $F_2(t)$) are predicted for both ends of all segments within the multi-segment interconnect structure. Upon the completion of PINN training, the combined framework of PINN and Bayesian networks can be effectively employed to estimate variations in EM stress across the entire interconnect structure, utilizing EM stress samples.

5 EXPERIMENTAL RESULTS AND DISCUSSION

All modules utilized in *BPINN-EM* are developed using Python 3.9.18 with PyTorch 2.2.1. The training and testing procedures are conducted on a Linux server equipped with two Intel 22-core E5-2699 CPUs, 320 GB of memory, and an Nvidia TITAN RTX GPU. In the subsequent section, we present the experimental results pertaining to data preparation and variational stress estimation.

5.1 Data generation and preparation

To prepare the dataset for the BNN model, we leverage the Finite Element Method (FEM) using COMSOL. For both training and testing, we generated a total of 50,000 single wires. Among these, 40,000 wires are allocated for training the BNN model, while 10,000 are reserved for testing its accuracy and performance. These wires originate from multi-segment interconnects with the number of segments ranging from 5 to 250. The lengths of segments within these multi-segment interconnects vary from 10 μm to 50 μm. To maintain simplicity, we standardize the width of all wires to 1 μm. EM stress calculations are conducted over a time period from 0 to 1×10^8 seconds. To introduce variations in the input current, branch currents are sampled from a random normal distribution in each iteration of the Monte Carlo process. We employ four different $\frac{\mu}{\sqrt{\mathrm{Var}}}$ ratios: 0.10, 0.15, 0.20, and 0.25, to diversify the input current variations. Additionally, to account for other sources of variation, we conduct Monte Carlo simulations in COMSOL and generate our dataset. Specifically, we utilize 30 iterations of Monte Carlo simulations to construct the training dataset for this study.

5.2 Accuracy and performance of Bayesian network

Our BNN is implemented using the Hamiltorch package [49], employing the algorithm described in Section 4.1. PyTorch tensors are utilized for handling inputs, model parameters, and outputs. Hamiltorch overcomes the large data handling limitations of traditional Hamiltonian Monte Carlo methods by splitting datasets. Our BNN model consists of three hidden layers, each with 128 units. We utilize 100 Hamiltonian Monte Carlo (HMC) samples for training the BNN model. With a training dataset size of 40,000, the runtime for Hamiltorch is approximately 6.5 hours.

HMC is utilized to obtain posterior samples from the BNN, which are then employed to derive samples of variational EM stress for calculating mean and standard deviation of the variations. To ensure a fair performance comparison with Monte Carlo simulations, we infer 30 samples of variational EM stress from the BNN model for our illustrations. Mean ($\mu_{\tilde{\sigma}}$) and variance ($\mathrm{Var}_{\tilde{\sigma}}$) are computed from these samples for comparison with targets.

For the accuracy and performance analysis of the surrogate BNN model, we tested 10,000 single wires extracted from multi-segment interconnect structures, ensuring they have non-zero atomic fluxes at their boundaries. We employed COMSOL and EMSpice for accuracy and performance evaluation, with COMSOL chosen for its status as a standard commercial tool and EMSpice, as verified in [18], demonstrating accuracy and performance analysis against standard tools with openly available implementation details. While the related method in [44] demonstrates satisfactory performance in variance calculation, it falls short in comparison with standard tools and also lacks comprehensive implementation details. Therefore, we obtained variational EM stress for the test wires using COMSOL and EMSpice for comparison with our proposed *BPINN-EM*.

Monte Carlo simulations were conducted for 30 iterations to estimate variations in EM stress for both COMSOL and EMSpice. Similarly, 30 posterior samples from HMC were used in *BPINN-EM* to infer variational EM stress samples, thus approximating variations.

Fig 2a shows an example of variational current density used to derive variational EM stress, as illustrated in Fig 2b. The figure demonstrates a close agreement between the mean and standard deviations of variational EM stress at a terminal node of a single wire with those obtained from COMSOL and EMSpice. When tested with the 10,000 wires, the stress range spans from -3.2 $\times 10^9$ Pa to 4.5 $\times 10^9$ Pa. We employ root mean square error (RMSE) to gauge accuracy, computed collectively as $RMSE = (RMSE_{mean} + RMSE_{std})/2$. Here, $RMSE_{mean}$ represents the error in means and $RMSE_{std}$ represents the error in standard deviation. The average RMSE for the test wires against COMSOL (also our targets) is 2.72 $\times 10^6$ Pa, translating to a relative error of approximately 0.036%. Against EMSpice, the average RMSE is 1.1 $\times 10^6$ Pa, resulting in a relative error of about 0.014%.

COMSOL, being a FEM-based method, is relatively slow in simulation. The average runtime for the test wires using COMSOL is approximately 86 seconds, whereas with EMSpice, it is about 12 seconds. The average inference time for the BNN is approximately 0.015 seconds. These observations indicate that for a single wire, the BNN can provide a speedup of more than 5700× over COMSOL with the correct parameters. Compared to EMSpice, the BNN surrogate model can lead to an 800× speedup.

The BNN surrogate model itself proves to be fast and accurate in estimating variations in stochastic EM stress for single wires. Moreover, this surrogate model requires training or sampling only once with a relatively smaller dataset, facilitating a relatively short training/sampling time.

5.3 Overall accuracy and performance analysis

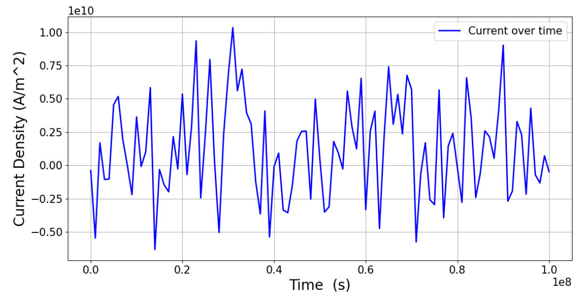
The PINN utilized in the second phase of *BPINN-EM* is also implemented using PyTorch. The MLP in the PINN employs layer sizes of [5,100,100,100,100,3]. We employ the Adam Optimizer [50] with a learning rate of 0.001 for optimization through backpropagation.

To evaluate the performance and accuracy of *BPINN-EM* on multi-segment interconnect structures, we utilize 1000 such structures with segment numbers ranging from 50 to 250. These structures are analyzed to obtain variational EM stress using COMSOL, EMSpice, and *BPINN-EM*. In all three approaches, 30 samples are used to estimate variations in stochastic EM stress. Table 1 presents accuracy and performance results for multi-segment interconnect structures with various segment numbers. For these structures, the range of EM stress spans from -3.51$\times 10^9$ to 4.54$\times 10^9$. We employ RMSE for accuracy comparison, calculated as $RMSE = (RMSE_{mean} + RMSE_{std})/2$. For the 1000 multi-segment interconnect structures, the average RMSE against COMSOL is 2.51$\times 10^7$, corresponding to approximately 0.31% error. Compared to EMSpice, an average RMSE of 1.9$\times 10^6$ is observed, which translates to around 0.024% error.

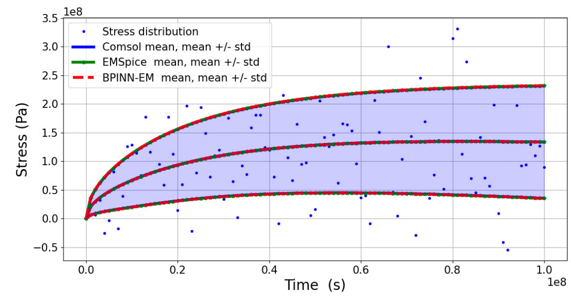
Fig 3 illustrates the variations in EM stress represented by mean and standard deviation (std.) for a five-segment interconnect structure with physical and electrical properties as depicted in Fig 3a. In this figure, EM stress variations at inter-segment junctions of this interconnect structure are depicted in figures 3b, 3c, 3d, and 3e. Here, we observe that *BPINN-EM* accurately estimates the variations in EM stress, showing good agreement with COMSOL and EMSpice.

The variances in stochastic EM stress for multi-segment interconnect structures are approximated using Monte Carlo simulation for 30 iterations in the case of COMSOL and EMSpice. The average runtime for this process in COMSOL is approximately 2900 seconds, while for EMSpice, it is around 1025 seconds. In *BPINN-EM*, variations in stochastic EM stress are approximated using samples from the BNN, sampled using HMC. However, the BNN surrogate model must first obtain the optimal atomic flux at the ends of each segment within the multi-segment interconnect structures from PINN. Therefore, the training time of PINN is also considered along with the inference time of BNN for runtime comparison. For the multi-segment interconnects under study, the average runtime for our method, *BPINN-EM*, is observed to be around 20 seconds. Hence, on average, our method can provide estimates of variational EM stress 145× faster than COMSOL and around 52× faster than EMSpice.

These findings affirm the viability of the proposed method, *BPINN-EM*, for expediting the estimation of variance in stochastic EM stress resulting from variations in EM parameters. Leveraging Bayesian networks in the initial stage also bolsters the scalability of our approach, as Bayesian models can be trained with relatively small datasets, mitigating the need for costly simulations to generate extensive datasets. Furthermore, the PINN can be swiftly trained, as it doesn't entail posterior sampling during training and solely requires EM stress data at boundary nodes. Once the PINN is trained, variations in stochastic EM stress at any node within a multi-segment interconnect structure can be approximated in terms of mean and variance using samples of EM stress obtained from the Bayesian network.



(a) Example of time-varying current distribution.

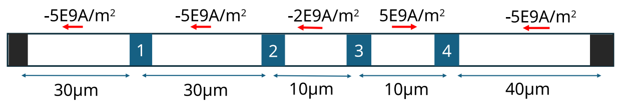


(b) Comparison of variation estimation between the proposed method, COMSOL, and EMSpice for a single segment.

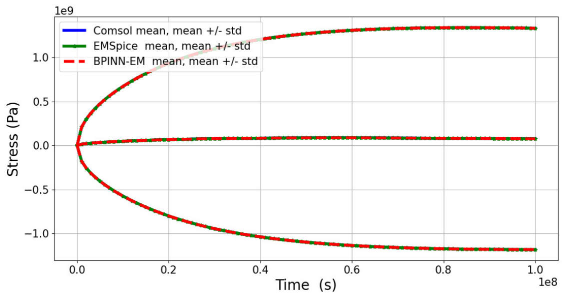
Figure 2: Illustration of time-varying current samples used in simulation and the corresponding stress variations obtained by employing currents from the same distribution. The depicted result showcases the time-varying stress at a node of a single segment with non-zero atomic flux, extracted from a multisegment interconnect.

6 CONCLUSION

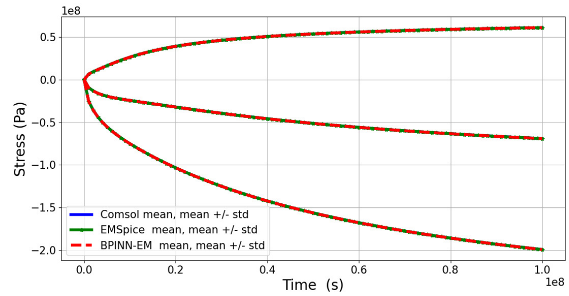
In this paper, we proposed a learning-based approach that leverages the powerful uncertainty quantification capability of Bayesian



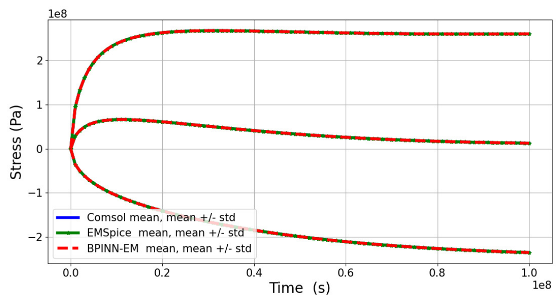
(a) Representation of a five-segment multi-segment interconnect structure. The depicted current densities are the mean values of the current densities used during simulation.



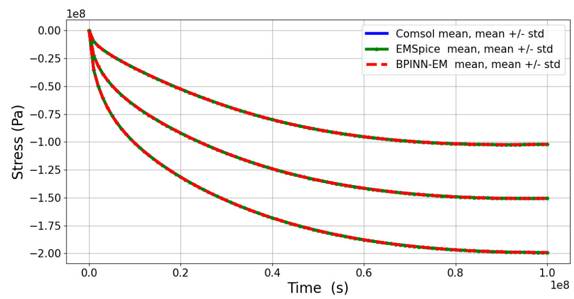
(b) Comparison of variations estimation between the proposed method, COMSOL, and EMSpice at inter-segment junction 1 of the depicted five-segment interconnect.



(c) Comparison of variations estimation between the proposed method, COMSOL, and EMSpice at inter-segment junction 2 of the depicted five-segment interconnect.



(d) Comparison of variations estimation between the proposed method, COMSOL, and EMSpice at inter-segment junction 3 of the depicted five-segment interconnect.



(e) Comparison of variations estimation between the proposed method, COMSOL, and EMSpice at inter-segment junction 4 of the depicted five-segment interconnect.

Figure 3: Illustration of stress variations at internal junctions of a multi-segment interconnect.

Table 1: Performance and accuracy comparisons with existing methods

# of wires	COMSOL	EMspice	*BPINN-EM*					
	Runtime (s)	Runtime (s)	Error(%) vs. Comsol	Error(%) vs. EMSpice	Inference time(s)	Training time(s)	Speedup vs. COMSOL	Speedup vs. EMSpice
50	1298	456	0.081	0.021	0.25	5.1	243x	86x
100	2239	764	0.092	0.028	0.43	9.6	223x	77x
150	2973	1032	0.12	0.031	0.39	16.0	181x	63x
200	3617	1334	0.31	0.036	0.61	28.4	124x	46x
250	4128	1521	0.98	0.044	0.80	41.5	98x	36x

Neural Networks (BNNs) and the unsupervised learning capability of Physics-Informed Neural Networks (PINNs) to learn from the variational effects of EM aging processes. The resulting method, termed BPINN-EM, can build the variational surrogate EM model with small number of dateset, which enables rapid variational stress analysis of multi-segment metal wires. Experimental results on general multi-segment interconnect structures demonstrate that our proposed method, BPINN-EM, is over 240 times faster than Monte Carlo simulations in FEM-based COMSOL and more than 85 times faster in FDM-based EMSpice, with negligible loss in accuracy

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