A Probabilistic Model for Nanocell Reliability Evaluation in presence of Transient Errors

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A Probabilistic Model for Nanocell Reliability Evaluation in presence of Transient Errors

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Abstract

In this paper, we propose a novel extended continuous time birth-death model for reliability analysis of a nanocell device. A nanocell consists of conducting nanoparticles connected via randomly placed self-assembled monolayer of molecules. These molecules behave as a negative differential resistor. The mathematical expression for expected nanocell lifetime and its availability, in presence of transient errors is computed. On the basis of our model, an algorithm is developed and implemented in MATLAB, PERL and HSPICE, to automatically generate the proposed model representation for a given nanocell. It is used to estimate the $success\_ratio$ as well as the nanocell reliability, while considering the uncertainties induced by transient errors. The theoretical results for reliability are validated by simulating HSPICE model of nanocell in presence of varying defect rates. It is observed that the device reliability increases with increase in the number of nanoparticles and molecules. A lower and upper bounds for nanocell reliability are calculated in theory which is validated in simulations.

I. Introduction

Molecular Electronics is emerging as a promising alternative to present CMOS technology [1]. Such a device is fabricated by chemical self-assembly of a single or array, or layers of molecules to exhibit the behavior of a wire, a switch or a latch. The nitro-substituted Oligo (Phenylene Ethynylene) (OPE) molecules are a class of fully conjugated aromatic molecules, that are extensively used as molecular wires or molecular switches [2]. For example, $2'$-amino-4,$4'$di(ethynylphenyl)-$5'$-nitro-1-benzenethiol [2]–[5] is an OPE molecule that behaves as a Negative Differential Resistor (NDR) and a latch. Tour et *al.* [6], [7] proposed a molecular electronic device called nanocell. In contrast to other molecular devices, a nanocell consists of conducting gold nanoparticles connected via randomly placed OPE molecules. The nanocell is addressed by relatively small number of leads located at its edges. A self-assembled monolayer of alkanethiols coats each nanoparticle and thus prevents them from coalescing into a multi-particle array. The electrical contacts between adjacent nanoparticles and between nanoparticles and I/O leads is established via molecule-metal chemical bonding [2], [3]. The in-built defect tolerance, small size, postfabrication programmability through mortal training and the lack of requirement of precise molecular ordering features makes it a good choice for future nanoscale devices.

In nanoscale devices, the transient errors play a vital role [1]. The defect rate can be in the range 10^{-3} to 10^{-7} in nanoscale devices [9], [10]. These defects can occur due to hard errors or soft errors. The hard errors or structural defects are caused during the device fabrication and later due to aging effects. Noise, thermal perturbation, cosmic rays, etc. are the environmental factors that may cause a soft transient error to occur. As compared to other nanoscale devices, a nanocell is defect tolerant even in presence of high defect rate [6]–[8]. This is because of multiple redundant conducting paths present between input and output node of a nanocell. Thus, even if some of the molecules fail, the device functions correctly until no such path is present. As we know, effect of transient errors is for a short while, so the failed molecules may get repaired after sometime. Throughout this paper, by molecular failure, we mean to say that it has turned 'OFF'. This can happen because of (i) broken chemical bond (connection) between nanoparticle and molecule, or (ii) the transient errors cause a conformational change to the molecule and it switches to a low conducting state [4]. Similarly, repairing of a molecule denotes that it turns $'ON'$ and now it is functioning properly. The transition between high and low conductance states is driven by the interaction between external electric field and molecular dipole moment of middle phenylene ring in OPE molecule [2]–[5].

This failure and repair behavior of the molecules within the nanocell can be modeled as a continuous time birth-death process [11], [12]. A birth-death process is a Markov chain with states $\{0, 1, \ldots\}$ for which transitions from state S_n may go only to either state S_{n-1} or state S_{n+1}. That is, only one step transitions are allowed in a birth-death process. A novel extended continuous time birth-death model is proposed in this paper and it is used for reliability evaluation of a nanocell in presence of transient errors. Thus, the time-space probabilistic analysis of the nanocell is proposed in this paper. It is observed that the nanocell functions reliably as long as (i) the failure rate is less than the repair rate, (ii) at least one path is present between input and output.

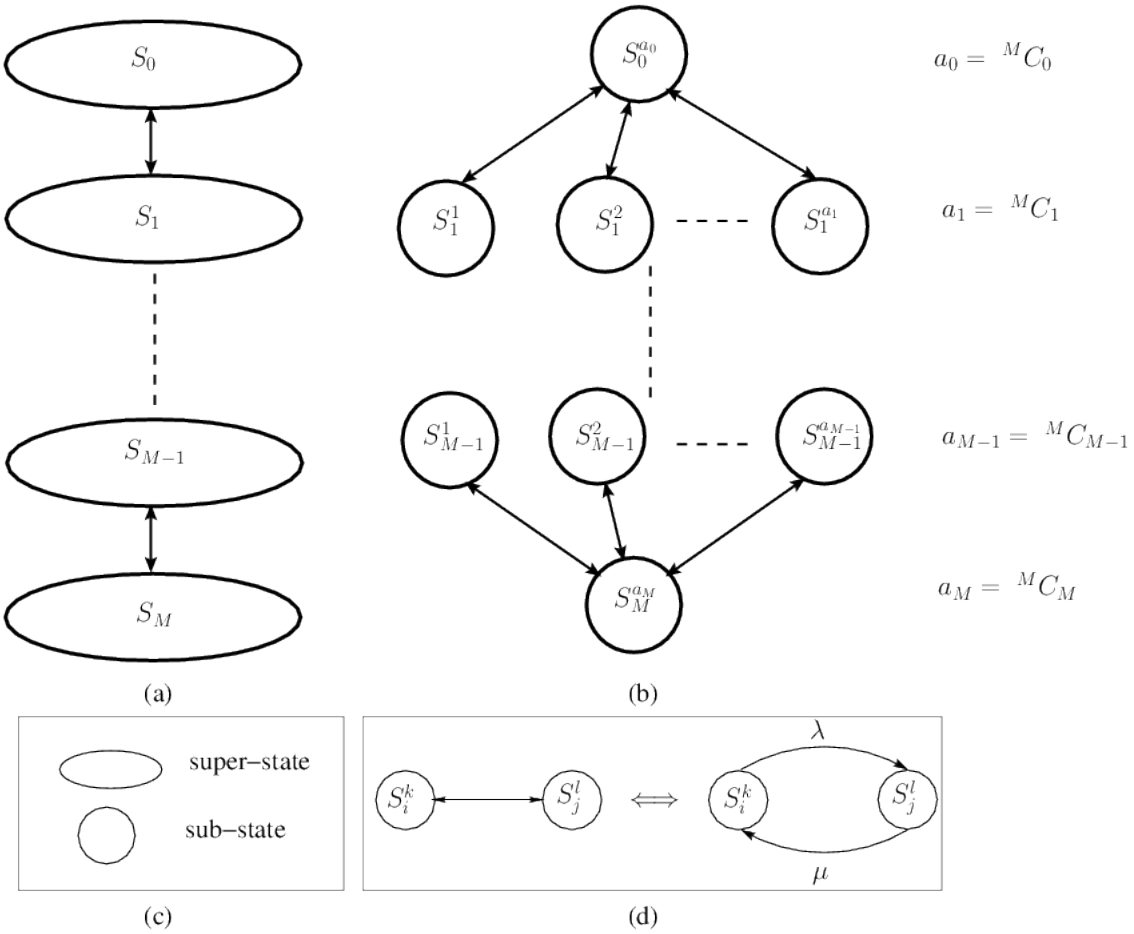

Fig. 1: Continuous time birth - death model for Nanocell (a) abstract model with only super-states (b) detailed model with sub-states (c) Here, each circle represents a sub-state and a set of sub-states at each level combine to form a super-state, which is represented by an ellipse (d) bidirectional arrows between these states represents two unidirectional arrows, one for failure and another for repair.

II. Probabilistic Modeling of the Nanocell

Consider a nanocell having N nanoparticles connected via M molecular switches. Let $\chi(t)$ denote the number of $'ON'$ molecules at time t. The functional behavior of the nanocell depends on $\chi(t)$ as well as on the combinations in which these molecules are connected. This is also called spatial connectivity of the molecules. Let at any time t, $\chi(t) = m$, where $m \leq M$. Then, there are ${}^MC_m$ ways in which m out of M molecules are $'ON'$ at time t.

Further, assume that at any time t, the nanocell is in super-state S_j if $(M-j)$ molecules are $'ON'$ (or j molecules are $'OFF'$) and $S_j^k, \forall k = 1, 2, \ldots, a_j$ are a set of sub-states of this super-state. In other words, the sub-states of super-state S_j denote the combinations in which these $(M-j)$ molecules are $'ON'$ and there can be $a_j = {}^MC_j = {}^MC_{M-j}$ possible combinations. The transient errors can occur at any instant of time, because of which the system can transit from a given state to another state. In this way, the nanocell can be modeled as a continuous time birth - death process. Let the state space of this process be $I = \{0, 1, 2, \ldots M\}$ and $T = \{t | 0 \leq t < \infty\}$ be its parameter space. Thus, as shown in Fig. 1(b), at any time t, one of the sub-states S_j^k, $k = 1$ *to* a_j of a super-state S_j, can make:

1) a *down* transition to one of the $(M-j)$ out of ${}^MC_{j+1}$ sub-states of S_{j+1} super-state, with failure rate λ_j.
2) an *up* transition to one of the j out of ${}^MC_{j-1}$ sub-states of S_{j-1} super-state, with repair rate μ_j.

So, $(M-j)+(j) = M$ edges are connected to each sub-state. As shown in Fig. 1(d), each bidirectional arrow between sub-states represents two unidirectional arrows, one for failure and another for repair. Hence, the total in-degree and out-degree for each sub-state is 2xM. Also, each sub-state of S_j has j parent sub-states and $(M-j)$ child sub-states. The total number of super-states are $M+1$ and sub-states are $\sum_{j=0}^{M} {}^MC_j = 2^M$. The Fig. 4 in Section IV shows the state transition model for an example nanocell consisting of 5 molecules and Fig. 2 depicts this example nanocell.

Let the repair rate for all the states be equal and be denoted by μ. Also, let the failure rate for all states be equal and be

denoted by λ. We here define a non-negative continuous function $q_j(t)$ defined by:

$$\begin{aligned} q_j(t) &= -\frac{\partial}{\partial t} p_{jj}(v,t)|_{v=t} \\ &= \lim_{h\to 0} \frac{p_{jj}(t,t) - p_{jj}(t,t+h)}{h} \\ &= \lim_{h\to 0} \frac{1 - p_{jj}(t,t+h)}{h}, \qquad \text{since } p_{jj}(t,t) = 1 \end{aligned} \tag{1}$$

Here, p_{jj} is defined as the conditional probability of being in same state j. Similarly, for each j, ($j \neq k$) there is a non-negative continuous function $q_{jk}(t)$ defined by:

$$\begin{aligned} q_{jk}(t) &= \frac{\partial}{\partial t} p_{jk}(v,t)|_{v=t} \\ &= \lim_{h\to 0} \frac{p_{jk}(t,t+h) - p_{jk}(t,t)}{h} \\ &= \lim_{h\to 0} \frac{p_{jk}(t,t+h)}{h}, \qquad \text{since } p_{jk}(t,t) = 0 \end{aligned} \tag{2}$$

The $q_{jk}(t)$ is also known as transition rate and p_{jk} denote the conditional transition probability from state j to k. Then, the transition rate and the transition probabilities are related by:

$$p_{jk}(t,t+h) = q_{jk}(t)\cdot h + o(h), \qquad j \neq k; \tag{3}$$

$$p_{jj}(t,t+h) = 1 - q_j(t)\cdot h + o(h), \qquad j = k; \tag{4}$$

Here, $o(h)$ denote the probability that two or more transitions occur in time $(t, t+h]$. Also, for this birth-death model, the transition rates for each sub-state are related to their failure and repair rates by following equations:

$$q_j = \lambda + \mu \tag{5}$$

$$q_{j,j-1} = \mu \tag{6}$$

$$q_{j,j+1} = \lambda \tag{7}$$

Now, consider that at time t, the system is in sub-state k of super-state j (i.e., S_j^k). Then, using equations (4) and (5) conditional probability that the system will remain in same sub-state at time (t+h] is:

$$p_{jj}(t,t+h) = 1 - (j\mu + (M-j)\lambda)\cdot h + o(h) \tag{8}$$

Similarly, using equations (3), (6) and (7), the conditional probability that system makes *up* or *down* transitions to S_j^k in the interval (t+h] is given by:

$$p_{j+1,j}(t,t+h) = (M-j)\mu\cdot h + o(h) \tag{9}$$

$$p_{j-1,j}(t,t+h) = j\lambda\cdot h + o(h) \tag{10}$$

Then, using equations (8), (9) and (10), the total probability that the nanocell is in sub-state S_j^k at time (t+h] is computed as:

$$\begin{aligned} P(\chi(t+h)=j) &= P_j(t+h) \\ &= P_j(t)p_{jj}(t,t+h) + P_{j-1}(t)p_{j-1,j}(t+h) + P_{j+1}(t)p_{j+1,j}(t+h) + o(h) \\ &= P_j(t)[1 - (j\mu + (M-j)\lambda).h + o(h)] + P_{j-1}(t)[j\lambda.h + o(h)] + \\ &\quad P_{j+1}(t)[(M-j)\mu + o(h)] + o(h) \end{aligned} \tag{11}$$

Dividing both sides of equation (11) by h and taking $\lim_{h\to 0}$, we obtain:

$$\frac{d}{dt}P_j(t+h) = -(j\mu + (M-j)\lambda)P_j(t) + j\lambda P_{j-1}(t) + (M-j)\mu P_{j+1}(t) \tag{12}$$

Thus, we can write differential equation for initial and final state as:

$$\frac{d}{dt}P_0(t) = -M\lambda P_0(t) + M\mu P_1(t) \tag{13}$$

$$\frac{d}{dt}P_M(t) = -M\mu P_M(t) + M\lambda P_{M-1}(t) \tag{14}$$

A. Computing the steady state probability of a nanocell

Let the derivative $dP_j(t)/dt = 0$, then the steady-state probability that the system is in state k, is denoted by p_k, where

$$p_k = \lim_{t\to\infty} P_k(t) \tag{15}$$

Substituting this steady-state probability in differential-difference equation (13), we obtain:

$$0 = -M\lambda p_0 + M\mu p_1 \tag{16}$$

$$p_1 = \frac{\lambda}{\mu} p_0 \tag{17}$$

Similarly, from equation (14),

$$p_M = \frac{\lambda}{\mu} p_{M-1} \tag{18}$$

Then, the steady-state probability expression obtained from equation (12) can be rewritten as:

$$\begin{aligned}(M-j)\lambda p_j - (M-j)\mu p_{j+1} &= j\lambda p_{j-1} - j\mu p_j \\ \dots &= \lambda p_0 - \mu p_1\end{aligned}$$

As we know, $\lambda p_0 - \mu p_1 = 0$ (from equation (17)), we can write:

$$\begin{aligned}j\lambda p_{j-1} &= j\mu p_j \\ p_j &= \frac{\lambda}{\mu} p_{j-1} \\ p_j &= \left(\frac{\lambda}{\mu}\right)\left(\frac{\lambda}{\mu}\right) p_{j-2} \\ p_j &= \left(\frac{\lambda}{\mu}\right)\left(\frac{\lambda}{\mu}\right)\left(\frac{\lambda}{\mu}\right) p_{j-3}\end{aligned}$$

Thus, steady state or limiting probability of super-state S_j is given as:

$$p_j = \left(\frac{\lambda}{\mu}\right)^j p_0 \tag{19}$$

Since $\sum_{k\geq 0}^{M} p_k = 1$,

$$\begin{aligned}\left(\frac{\lambda}{\mu}\right)^0 p_0 + \left(\frac{\lambda}{\mu}\right)^1 p_0 + \left(\frac{\lambda}{\mu}\right)^2 p_0 + \ldots + \left(\frac{\lambda}{\mu}\right)^M p_0 &= 1 \\ \left[\sum_{j\geq 0}^{M} \left(\frac{\lambda}{\mu}\right)^j p_0\right] &= 1 \\ p_0 = \frac{1}{\sum_{j\geq 0}^{M}\left(\frac{\lambda}{\mu}\right)^j} &= \frac{1-\rho}{1-\rho^{M+1}}\end{aligned} \tag{20}$$

where $\rho = \frac{\lambda}{\mu}$ and $\rho \neq 1$. If $\rho = 1$, then $p_0 = \frac{1}{M+1}$. Hence, we have derived the expression for steady state probability.
Using the properties of modified geometric distribution, mean and variance of number of molecules present in the nanocell is given as [11], [12]:

$$E[\chi] = \frac{\rho}{1-\rho} \tag{21}$$

$$VAR[\chi] = \frac{\rho}{(1-\rho)^2} \tag{22}$$

For system to be stable, $\rho < 1$, that is, or mean time to repair should be less than mean time to failure ($\lambda < \mu$).

B. Computing total probability that a nanocell is in a given sub-state

Let initial state of the system is S_0, then $P_0(0) = 1$ and $P_k(0) = 0$ for $k \geq 1$. Taking Laplace Transform of equations (13) and (14), [12] we get:

$$\begin{aligned} s\bar{P}_0(s) - P_0(0) &= -M\lambda\bar{P}_0(s) + M\mu\bar{P}_1(s) \\ (s + M\lambda)\bar{P}_0(s) &= 1 + M\mu\bar{P}_1(s) \\ \bar{P}_0(s) &= \frac{1}{s + M\lambda} + \frac{M\mu}{s + M\lambda}\bar{P}_1(s) \end{aligned} \tag{23}$$

Similarly,

$$\begin{aligned} s\bar{P}_M(s) - P_M(0) &= -M\mu\bar{P}_M(s) + M\lambda\bar{P}_{M-1}(s) \\ (s + M\mu)\bar{P}_0(s) &= M\lambda\bar{P}_{M-1}(s) \\ \bar{P}_M(s) &= \frac{M\lambda}{s + M\mu}\bar{P}_{M-1}(s) \end{aligned} \tag{24}$$

In this way, by taking Laplace Transform of equation (12), we get the generalized equation as

$$\bar{P}_j(s) = \frac{j\lambda}{s + j\mu + (M-j)\lambda}\bar{P}_{j-1}(s) + \frac{(M-j)\mu}{s + j\mu + (M-j)\lambda}\bar{P}_{j+1}(s) \tag{25}$$

This equation can be solved to determine the time domain expression for probability. For example, consider that in a nanocell only two nanoparticles ($N = 2$) are present connected by one molecule ($M = 1$). So, there are only two super-states and $2^1 = 2$ sub-states, namely S_0^1 and S_1^1. The state diagram for this case can be represented by Fig. 1(d), by substituting $j = k = l = 1,\ i = 0.$ Substituting $M = 1$ in equations (23), (24) and (25), we can derive the following expression:

$$\bar{P}_0(s) = \left(\frac{\mu}{\lambda + \mu}\right)\frac{1}{s} + \left(\frac{\lambda}{\lambda + \mu}\right)\frac{1}{s + \lambda + \mu} \tag{26}$$

Then, on inverting the transform to the time domain, we obtain:

$$P_0(t) = \left(\frac{\mu}{\lambda + \mu}\right) + \left(\frac{\lambda}{\lambda + \mu}\right)e^{-(\lambda+\mu)t} \tag{27}$$

since $P_0 + P_1 = 1$, we get

$$P_1(t) = \left(\frac{\lambda}{\lambda + \mu}\right) + \left(\frac{\lambda}{\lambda + \mu}\right)e^{-(\lambda+\mu)t} \tag{28}$$

In this way, we can derive the expression for total probability of a nanocell, being in a given state, for any value of M. We know that, the nanocell will function reliably as long as one path is present between input and output nodes. For this, we have to find the sub-states at which at least one path is available and compute the probability that nanocell is in one of these states at time t. Then, their joint probability is to be calculated to derive the expression for reliability at time t.
In contrast to this, we can also compute the probabilities of being $'ON'$ and $'OFF'$ of a single molecule (computed by equation (27) and (28)) and based on their spatial connectivity, we can derive the expression for upper and lower bounds on reliability, expected nanocell lifetime and nanocell availability. The mathematical framework for this approach is discussed in the next section.

III. Lifetime Analysis of Nanocell

A. Expected System Lifetime of a Nanocell

The system lifetime is defined as the time up to which the system is correctly functional [11], [12]. A system is comprised of one or more components and its lifetime is dependent on the lifetime of each of these individual components as well as on their spatial connectivity. For example, in our case, the nanocell will function correctly as long as one of the conducting path is present between its input and output node. Thus, it depends on (i) the lifetime of the individual molecule and (ii) their spatial arrangement. Let $F_i(t)$, $i = 1, 2, \ldots, M$ denote the lifetime distribution of the molecule m_i and $\bar{F}_i(t) = 1 - F_i(t)$. Here, individual molecule can be modeled as a two-state continuous time birth-death model as shown in Fig. 1(d), by substituting $j = k = l = 1,\ i = 0$. The lifetime of the molecule m_i is the duration up to which it is in state S_0^1. We represent this for molecule m_i by probability P_0^i . Then, from equation (27), we write:

$$F_i(t) = P_0^i(t) = \left(\frac{\mu}{\lambda + \mu}\right) + \left(\frac{\lambda}{\lambda + \mu}\right)e^{-(\lambda+\mu)t} \tag{29}$$

Then, the reliability of the nanocell can be expressed by the molecule's lifetime, as:

$$R(\bar{F}(t)) = P(Nanocell > t) \tag{30}$$

where $\bar{F}(t) = \{\bar{F_1}(t), \bar{F_2}(t), \ldots, \bar{F_M}(t)\}$. Then, by definition, the expected lifetime of a nanocell is:

$$E(Nanocell) = \int_0^\infty R(\bar{F}(t))dt \tag{31}$$

Let $\{path_1, path_2, \ldots, path_s\}$ denote minimal path sets connecting input node to the output node and we define $E_i, \forall\, i = 1 \ldots s$ as E_i = {at least one molecular connection on path $path_i$ has failed}. If at least one of the molecules in the minimal path set has failed, the system will fail eventually. Mathematically, it is denoted as:

$$\begin{aligned} 1 - R(\bar{F}(t)) &= P(E_1 E_2 \ldots E_s) \\ &= P(E_1)P(E_2|E_1)\ldots P(E_s|E_1 E_2 \ldots E_{s-1}) \end{aligned}$$

Henceforth, it can be easily derived that failure of at least one molecule in the minimal path $path_i$ can increase the probability of failure of at least one molecule in the path $path_j$. This would be the case if both the paths $path_i$ and $path_j$ overlap. So,

$$P(E_j|E_i) \geq P(E_j)$$

Similarly,

$$P(E_i|E_1 E_2 \ldots E_{i-1}) \geq P(E_i)$$

Substituting in equations stated above we get,

$$1 - R(\bar{F}(t)) \geq \prod_i P(E_i)$$

or,

$$R(\bar{F}(t)) \leq R_{UB}(\bar{F}(t)) = 1 - \prod_i \left[1 - \prod_{j \in path_i} P_0^j\right] \tag{32}$$

In this way, we have derived the expression of upper bound on reliability of nanocell.
Let $\{cut_1, cut_2, \ldots cut_r\}$ denote the minimal cut sets. We define the events $C_1, C_2, \ldots, C_r$ by C_i = {at least one molecular device in cut_i is functioning}. Since, the nanocell will function iff all of the events C_i occur, we say,

$$\begin{aligned} R(\bar{F}(t)) &= P(C_1, C_2 \ldots C_r) \\ &= P(C_1)P(C_2|C_1)\ldots P(C_r|C_1 \ldots C_{r-1}) \\ &\geq \prod_i P(C_i) \end{aligned}$$

Hence,

$$R(\bar{F}(t)) \geq R_{LB}(\bar{F}(t)) = \prod_i \left[1 - \prod_{j \in cut_i} (1 - P_0^j)\right] \tag{33}$$

As we know, the nanocell will work as long as at least one of the conducting paths is present between input and output node.

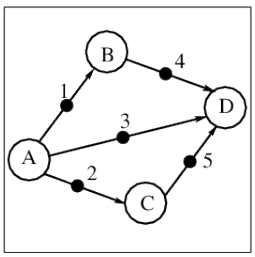

Fig. 2: An example nanocell consisting of four nanoparticles and five molecular switches. Here, the unfilled (white) circles represent the nanoparticles and the filled (black) circles with arrows represent the molecular switches. The direction of the arrows denotes the current flow. The nanoparticles A and D are the input and output nodes, respectively.

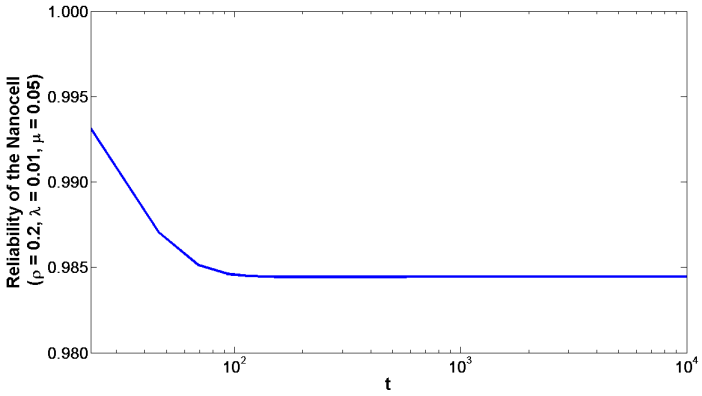

Fig. 3: Upper bound on reliability (R_{UB}), from $t = 0$ to $t = 10000$ units, for the example nanocell

Thus, we can rewrite the expression of expected lifetime of nanocell as:

$$E_{UB}(\text{Nanocell}) = \int_0^\infty \left[1 - \prod_i \left\{1 - \prod_{j \in path_i} F_j(t)\right\}\right] dt \tag{34}$$

$$E_{LB}(\text{Nanocell}) = \int_0^\infty \prod_i \left[1 - \prod_{j \in cut_i} (1 - F_j(t))\right] dt \tag{35}$$

Thus, we get the lower and upper bounds on expected system lifetime for an example nanocell as shown in Fig. 2, we get

$$\begin{aligned} E_{UB}(\text{Nanocell}) &= \int_0^\infty \left[1 - \{1 - P_0^1(t)P_0^4(t)\}\{1 - P_0^3(t)\}\{1 - P_0^2(t)P_0^5(t)\}\right] dt \\ E_{LB}(\text{Nanocell}) &= \int_0^\infty \left[1 - \{1 - P_0^1(t)\}\{1 - P_0^3(t)\}\{1 - P_0^2(t)\}\right] \left[1 - \{1 - P_0^1(t)\}\right. \\ &\quad \left.\{1 - P_0^3(t)\}\{1 - P_0^5(t)\}\right] \left[1 - \{1 - P_0^4(t)\}\{1 - P_0^3(t)\}\{1 - P_0^5(t)\}\right] \\ &\quad \left[1 - \{1 - P_0^4(t)\}\{1 - P_0^3(t)\}\{1 - P_0^2(t)\}\right] dt \end{aligned}$$

On substituting P_0^i by equation (29), for all $i = 1, \ldots, 5$, and $\rho = 0.2$, we have plotted the R_{UB} for the example nanocell in the Fig. 3.

B. Availability of a Nanocell

The nanocell availability, at any time t, can be defined as the probability that it is functioning properly at t and it is denoted as:

$$A(t) = P\{\text{nanocell is working at } t\} \tag{36}$$

Since, all molecules act independently, $A(t)$ can be expressed in terms of reliability function as follows:

$$A(t) = R(A_1(t), \ldots, A_n(t)) \tag{37}$$

where,

$$A_i(t) = P\{\text{molecule } i \text{ is } 'ON' \text{ at } t\} \tag{38}$$

$$= \left(\frac{\mu_i}{\lambda_i + \mu_i}\right) + \left(\frac{\lambda_i}{\lambda_i + \mu_i}\right) e^{-(\lambda_i + \mu_i)t} \qquad \text{(from equation (27))} \tag{39}$$

Assuming constant failure and repair rates for all molecules, i.e., $\lambda_i = \lambda$ and $\mu_i = \mu$ for $i = 1, 2, 3, \ldots$. Thus

$$A_i(t) = \frac{\mu}{\lambda + \mu} + \frac{\lambda}{\lambda + \mu} e^{-(\lambda + \mu)t} \tag{40}$$

Then, limiting or steady-state availability for each molecule is

$$A_i = \lim_{t \to \infty} A_i(t) = r\left(\frac{\mu}{\lambda + \mu}\right) \tag{41}$$

Using the equations (32) and (33), we can determine the upper and lower bounds on nanocell availability as

$$\begin{aligned} A_{UB}(t) &= 1 - \prod_i \left[1 - \prod_{j \in path_i} P_0^j(t) \right] \\ &= 1 - \prod_i \left[1 - \prod_{j \in path_i} \left\{ \frac{\mu_j}{\lambda_j + \mu_j} + \frac{\lambda_j}{\lambda_j + \mu_j} e^{-(\lambda_j + \mu_j)t} \right\} \right] \end{aligned}$$

and

$$\begin{aligned} A_{LB}(t) &= \prod_i \left[1 - \prod_{j \in cut_i} (1 - P_0^j(t)) \right] \\ &= \prod_i \left[1 - \prod_{j \in cut_i} \left\{ \frac{\lambda_j}{\lambda_j + \mu_j} (1 - e^{-(\lambda_j + \mu_j)t}) \right\} \right] \end{aligned}$$

The bounds on the steady state availability of the Nanocell are given as

$$A_{UB} = 1 - \prod_i \left[1 - \prod_{j \in path_i} \left\{ \frac{\mu_j}{\lambda_j + \mu_j} \right\} \right] \quad (42)$$

$$A_{LB} = \prod_i \left[1 - \prod_{j \in cut_i} \left\{ \frac{\lambda_j}{\lambda_j + \mu_j} \right\} \right] \quad (43)$$

IV. Experimental setup for reliability analysis of nanocell

To exemplify the proposed model, consider a small nanocell which contains four nanoparticles (A, B, C, D) connected via five molecular switches (1, 2, 3, 4, 5), as shown in Fig. 2. There are three conducting paths which connects input node A to output node D, namely (i) $A-1-B-4-D$, (ii) $A-2-C-5-D$, and (iii) $A-3-D$. Let at $t=0$, all five molecules are functioning. This means, the nanocell is in the initial state of the proposed model and this state is denoted by S_0^1. At next level, one of the five molecules may fail, due to some soft transient error. As stated earlier, the rate of failure is denoted by λ and rate of repair by μ. When nanocell is in super-state S_1, it is actually in one of the ${}^5C_1 = 5$ different sub-states. Similarly, at S_2, ${}^5C_2 = 10$ sub-states are possible, and so on. In all, there are six super-states and $\sum_{j=0}^{5} {}^5C_j = 2^5 = 32$ sub-states. Each of the super-states can make one-step up or $down$ transition, but one-step transition among the sub-states at same level is not possible. However, initial and final states can make only $down$ and up transitions, respectively. Thus, in general, with every sub-state, a set of parent and child sub-states are associated, and it can transit to only these states. This scenario for the example nanocell is depicted from the Fig. 4. As shown in this figure, there are nine sub-states for which no path is present between input and output node of the nanocell. The light filled circles represent these sub-states and we will call these states as the $nanocell - failure - states$. The remaining 23 states are called $nanocell - functioning - states$. The steady state probability that the nanocell is in one of the super-state can be calculated by equations (19) and (20) derived in previous section.

First, this nanocell is modeled and it is simulated in HSPICE. The high ($V_{high} = 2.0V$) and low ($V_{low} = 0.5V$) voltages are applied to the input node A and received at the output node D with acceptable noise margin. That is, output voltage for read $'1'$ is 1.9927 V and for read $'0'$ is 0.4927 V. Thirty-two instances of this nanocell are generated, each depicting the behavior of one of these 32 sub-states. On simulating the nanocell instances corresponding to the nine $nanocell - failure - states$ sub-states, zero voltage value is received at the output node.

Let at t_0, the nanocell is in S_0^1 sub-state, i.e., all molecules are $'ON'$ initially. Then, corresponding nanocell instance is simulated in HSPICE. After some time t_1, due to soft errors it may move to one of its child sub-state, say S_1^2, with probability of failure p_f. Again at t_2, it may move to either its parent state with repair rate μ or to one of its child state (say S_3^4) with failure rate λ. This transition path is represented by pattern filled circles in the Fig. 4. The repair probability is represented by p_r and $p_s = 1 - (p_f + p_r)$, where p_s is probability that it will continue to be in same state. Here, p_f and p_r are exponentially distributed with mean λ and μ, respectively and let $p_s = 0$. The p_f is explored for eleven different values between 0 to 1 and 10000 Monte Carlo Simulations are done in each case. The sequence of states and corresponding output voltages for read $'1'$ and $'0'$ are saved for each run. It is observed that, if $p_f < p_r$ or $\lambda < \mu$, then the nanocell is in $nanocell - functioning - states$ for most of the time. For these states, the acceptable output voltage is always received. We here define $success\_ratio$ as the ratio of correct read '1' and '0' to the number of simulation. Hence, for $\rho < 1$, $success\_ratio$ is close to unity. This is depicted

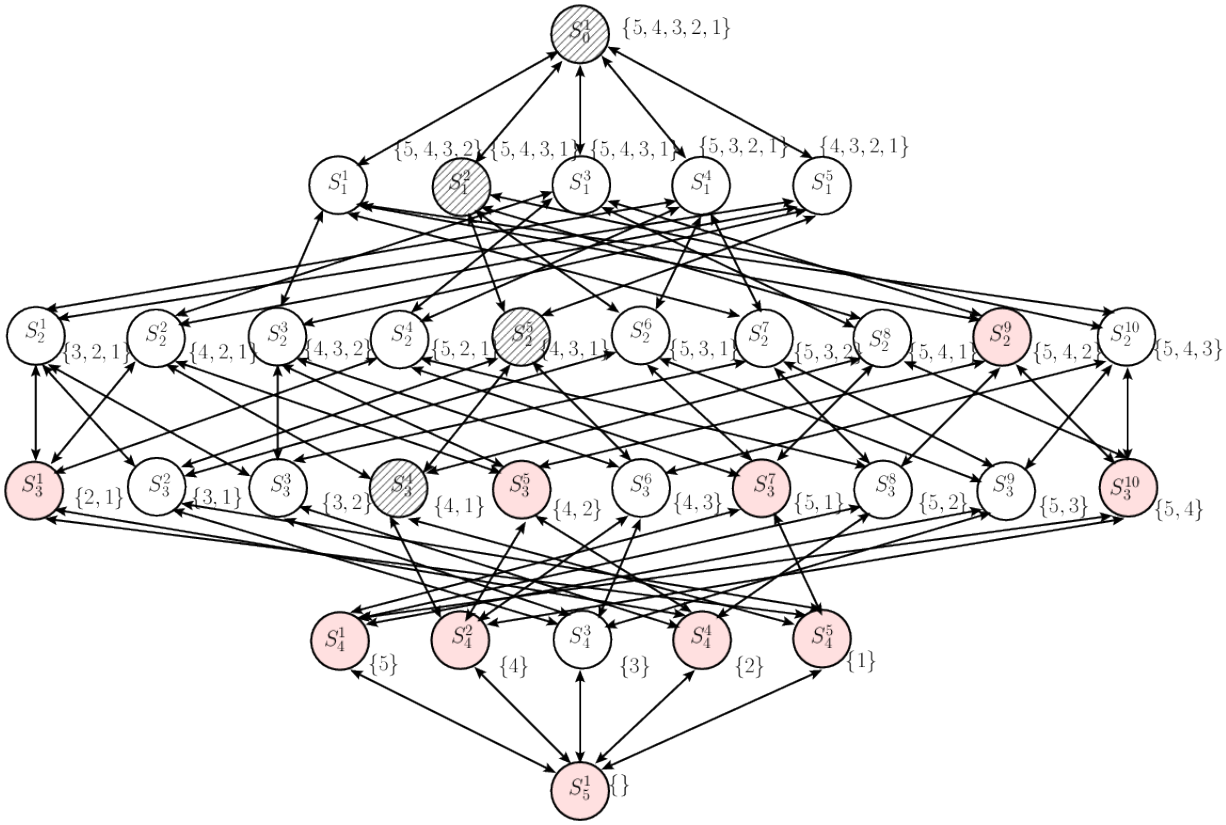

Fig. 4: Representation of the example nanocell in the proposed model. Here, the circles represent the sub-states and the set $\{i, j, \ldots\}$ corresponding to each sub-state, represents the set of $'ON'$ molecules in that state. The filled sub-states are the $nanocell - failure - states$ and remaining sub-states are the $nanocell - functioning - states$. The patterned filled circles represent one of the possible sequence in which the nanocell may make transition.

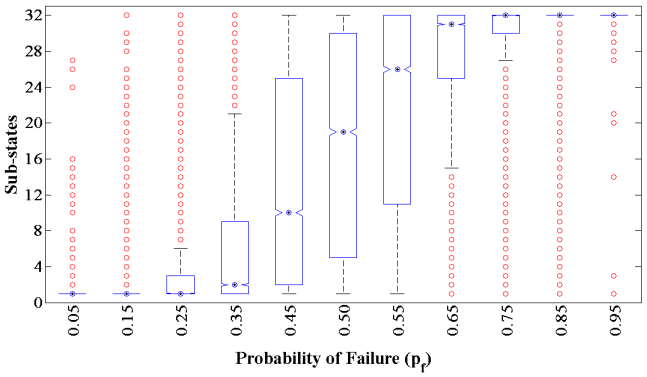

Fig. 5: Simulation results for the sequence of sub-states of the example nanocell with constant λ and μ in each vase. The p_f is exponentially distributed and it is explored for different values between 0 to 1. One thousand Monte Carlo simulations are done for each case. Here, (i) the central mark is the median (ii) the edges of the box are 25^{th} and 75^{th} percentiles (iii) the whisker extend to the most data points which are not considered as outliers (iv) the unfilled dots represent the outliers.

Algorithm 1 Reliability Evaluation Algorithm for Nanocell (REAN)

inputs
N := Number of Nanoparticles in the nanocell,
M := Number of molecules in the nanocell,
IP := Primary Input Node,
OP := Primary Output Node,
MAX_RUNS := Maximum number of simulation runs;
outputs
$success\_ratio$:= Number of times correct output is received for Max_Num simulations;
$STATE\_SEQUENCE$:= Array of sequence of sub-states visited by nanocell in MAX_RUNS simulations;
do
Generate an instance of a nanocell consisting of N nanoparticles connected by M molecular switches;
num= 0;
for i = 0 to M **do**
for j = 1 to ${}^{M}C_i$ **do**
$SUBSTATE(num)$ = Generate a sub-state when $(M - i)$ out of M molecules are present in 'ON' state;
$NANOCELL(num)$ = Create an instance of nanocell corresponding to $SUBSTATE(i)$;
num = num + 1;
end for
end for
for i = 1 to 2^M **do**
$PARENT(i)$ = Compute set of parents for $SUBSTATE(i)$;
$CHILD(i)$ = Compute set of children for $SUBSTATE(i)$;
end for
Initially, in the nanocell, all M molecules are 'ON' and $STATE\_SEQUENCE(1)$ = $SUBSTATE(1)$;
$present\_state$=1;
for k = 1 to MAX_RUNS **do**
Simulate the nanocell instance $NANOCELL(SUBSTATE(present\_state))$;
$DATAOUT(k)$ = output voltage of nanocell instance $NANOCELL(SUBSTATE(t))$;
$STATE\_SEQUENCE(k)$ = $present\_state$;
Generate the value of p_f and p_r by exponential distribution using inverse transform method;
Compute $p_s = 1 - p_f - p_r$;
if $p_f + p_r \leq 1$ **then**
if $p_s > p_r$ and $p_s > p_f$ **then**
Remain in same state;
else if $p_r > p_f$ **then**
$present\_state$ = PARENT($present\_state$), that is make an UP transition to any one of the parents sub-state;
else
$present\_state$ = CHILD($present\_state$), that is make an $DOWN$ transition to any one of the children sub-state;
end if
else
GOTO step 31;
end if
end for
$success\_ratio$ = Compute number of times correct output is received using array $DATAOUT(1:10000)$;
return ($success\_ratio$, $STATE\_SEQUENCE$)

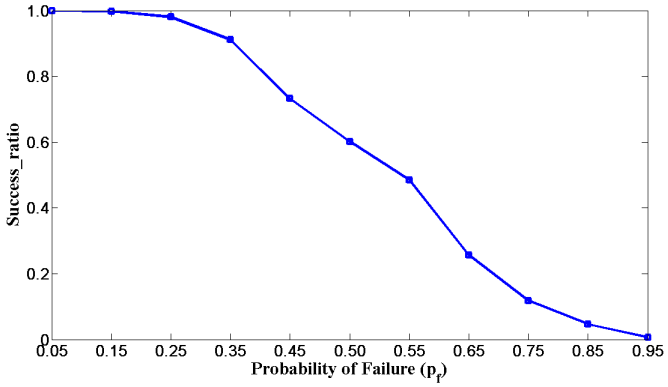

Fig. 6: Simulation results for $success\_ratio$ for different values of failure probability (p_f).

TABLE I: Simulation results for the example nanocell for different values of failure probability p_f. The $success\_ratio$ represents the ratio of number of successful read $'1'$ and $'0'$ out of 10000 simulations. Upper and lower bounds on reliability are represented by R_{UB} and R_{LB}, respectively.

p_f	$\rho = \frac{\lambda}{\mu}$	$success\_ratio$	R_{UB}	R_{LB}
0.05	0.02	0.9998	0.9999	0.9999
0.15	0.09	0.9973	0.9979	0.9978
0.25	0.21	0.9826	0.9843	0.9816
0.35	0.41	0.9109	0.9315	0.9099
0.45	0.75	0.7318	0.8051	0.7204
0.55	1.34	0.4851	0.6153	0.4352
0.65	2.44	0.2565	0.4052	0.1711
0.75	4.82	0.1178	0.2159	0.0348
0.85	11.67	0.0464	0.0891	0.0023
0.95	58.40	0.0064	0.0152	0.00001

from the Fig. 5 and Fig. 6.

This simulation procedure is discussed in Reliability Evaluation Algorithm for Nanocell (REAN) as shown in Algorithm 1. The Algorithm 1 used for Monte Carlo simulation, is implemented in MATLAB, HSPICE and PERL. Table I shows the $success\_ratio$ obtained for each value of p_f. Also using the equations (32) and (33), the upper and lower bounds on reliability are computed in MATLAB, for $t = 0$ to $t = 10000$ units. It is observed that, $success\_ratio$ obtained by using the proposed model lies within the range [R_{UB}, R_{LB}]. So, our proposed model computes the nanocell reliability efficiently. Also, any of the two methods, discussed here, can be used for estimating the nanocell lifetime.

Again, consider the same example nanocell. Assume that p_f and p_r are distributed exponentially and for each simulation run the values of λ and μ change. Also, let the probability $p_s = 1 - p_f - p_r$ and $\rho < 1$. Then, starting from the initial state, we perform simulations ten different times, each for 10000 runs. Then, as shown in the Fig. 7, for each of the 10 cases, the median lies in the range $(12, 20)$. The sub-states for this range are $nanocell - functioning - states$. Further, as the number of nanoparticles (N) and molecules (M) will increase, the number of connected paths between input and output node will increase exponentially. Also, total number of sub-states and number of $nanocell - functioning - states$ sub-states will increase. This will result in large state-space for the nanocell. Thus, with increase in number of molecules, the probability of transiting to $nanocell - failure - state$ will decrease. For example if $M = 20$, total number of sub-states are $2^{20} = 1048576$, which are extremely large number of states. For such a system, the probability that at least one path is present between input to output is close to unity (pg. 592 of [11]). So, the number of successful read $'1'$ and $'0'$ increases exponentially. Hence, the nanocell reliability increases with increase in number of molecules. Hence, we can conclude that, under high variability and uncertainties, the nanocell will remain reliable and defect tolerant as long as $\rho < 1$.

V. Conclusions and Future Work

In this paper, a novel extended continuous time birth-death model is proposed to evaluate the reliability of a nanocell, in presence of transient errors. For this mathematical framework, the steady state probability and probability of being in each sub-state is computed. The proposed approach is extended to compute the expected lifetime and availability of the nanocell using the birth-death model of molecules and their spatial connectivity. On the basis of our model, an algorithm is developed and implemented in MATLAB, PERL and HSPICE, to automatically generate the proposed model representation for a given

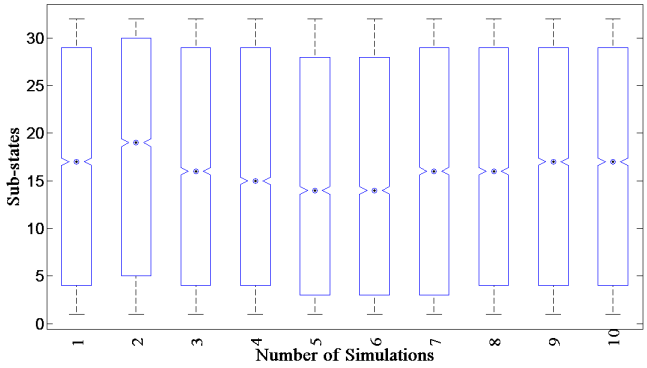

Fig. 7: Simulation results for example nanocell for 10 different cases. For each case, simulations are done for 10000 times, with varying λ and μ.

nanocell. It is used to estimate the $success\_ratio$ as well as the nanocell reliability, while considering the uncertainties induced by transient errors. It is observed that as long as, molecular failure rate is less than its repair rate, the nanocell functions correctly. Also, with increase in number of molecules, the nanocell reliability increases. Thus, we can conclude that, a nanocell device remains defect tolerant and it works reliably in presence of transient errors as long as (i) at least one path is present between input and output node, (ii) the failure rate of molecules is less than their repair rate. To satisfy the first condition, the number of nanoparticles must be greater than 20. Hence, we can argue that, at nano-scale, the nanocell device can function reliably and can withstand high defect rates due to transient errors. The extension of this model which considers the aging effects is under progress and is part of future work. Such a model can be used for estimating the data retention time of the nanocell memory. Also, in future, we plan to validate the mathematical framework by fabricated nanocell, in presence of environmental uncertainties and aging effects.

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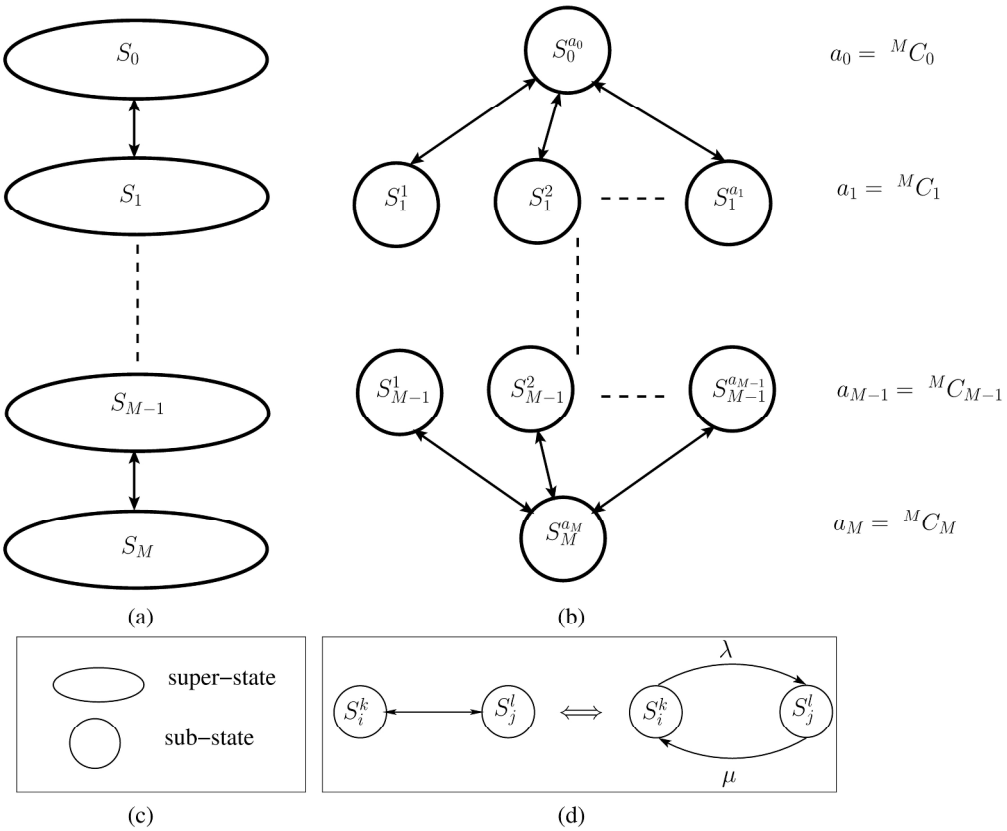

Fig. 1: Continuous time birth - death model for Nanocell (a) abstract model with only super-states (b) detailed model with
sub-states (c) Here, each circle represents a sub-state and a set of sub-states at each level combine to form a super-state, which
is represented by an ellipse (d) bidirectional arrows between these states represents two unidirectional arrows, one for failure
and another for repair.
245x202mm (300 x 300 DPI)

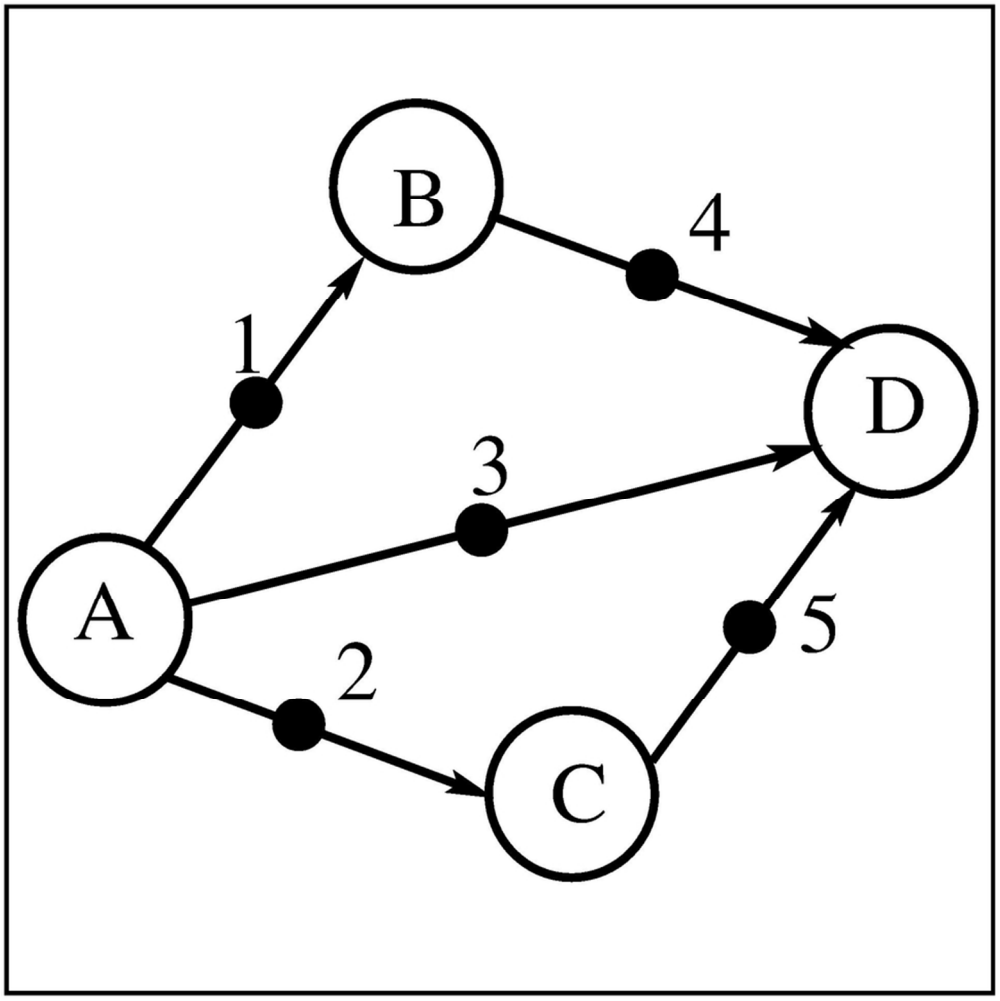

Fig. 2: An example nanocell consisting of four nanoparticles and five molecular switches. Here, the unfilled (white) circles
represent the nanoparticles and the filled (black) circles with arrows represent the molecular switches. The direction of the
arrows denotes the current flow. The nanoparticles A and D are the input and output nodes, respectively.
82x82mm (300 x 300 DPI)

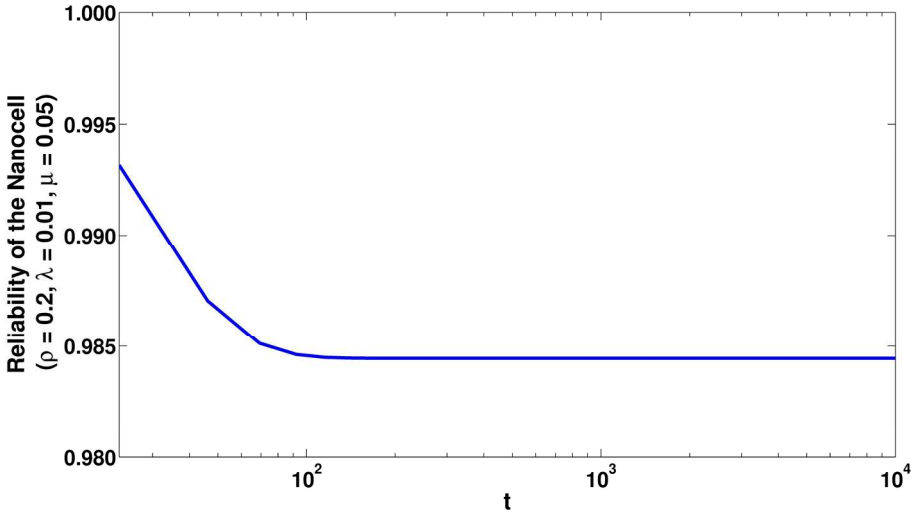

Fig. 3: Upper bound on reliability (R_{UB}), from t = 0 to t = 10000 units, for the example nanocell 184x100mm (300 x 300 DPI)

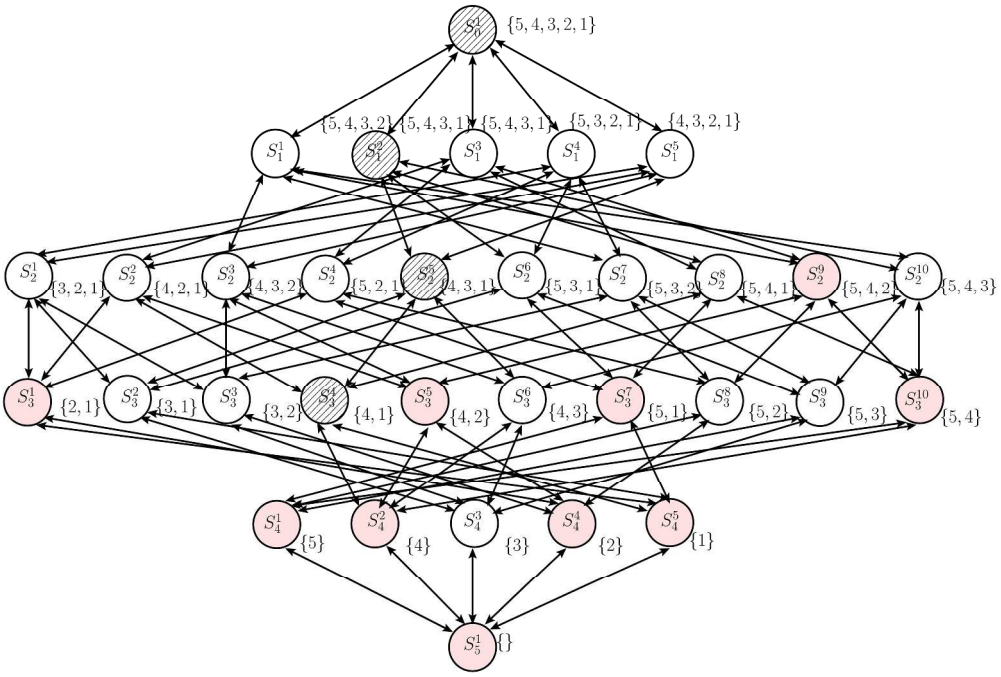

Fig. 4: Representation of the example nanocell in the proposed model. Here, the circles represent the sub-states and the set
{I, j, ...} corresponding to each sub-state, represents the set of 0ON0 molecules in that state. The filled sub-states are the
nanocell_failure_states and remaining sub-states are the nanocell_functioning _states. The patterned filled circles
represent one of the possible sequence in which the nanocell may make transition.
270x181mm (300 x 300 DPI)

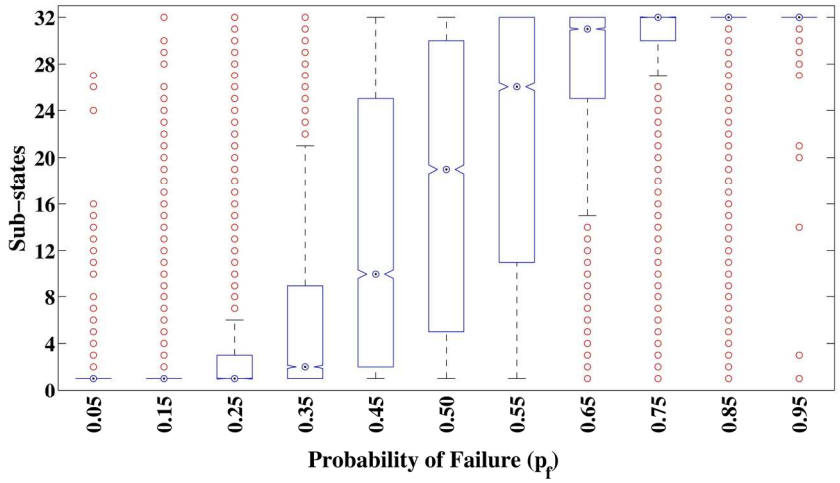

Fig. 5: Simulation results for the sequence of sub-states of the example nanocell with constant $^{\perp}$ and $_{\top}$ in each vase. The pf
is exponentially distributed and it is explored for different values between 0 to 1. One thousand Monte Carlo simulations are
done for each case. Here, (i) the central mark is the median (ii) the edges of the box are 25th and 75th percentiles (iii) the
whisker extend to the most data points which are not considered as outliers (iv) the unfilled dots represent the outliers.
179x95mm (300 x 300 DPI)

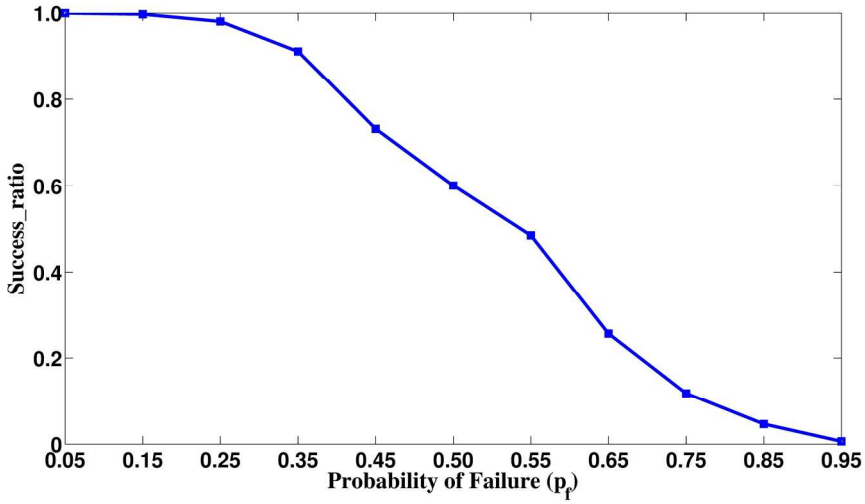

Fig. 6: Simulation results for success_ratio for different values of failure probability (pf).
179x95mm (300 x 300 DPI)

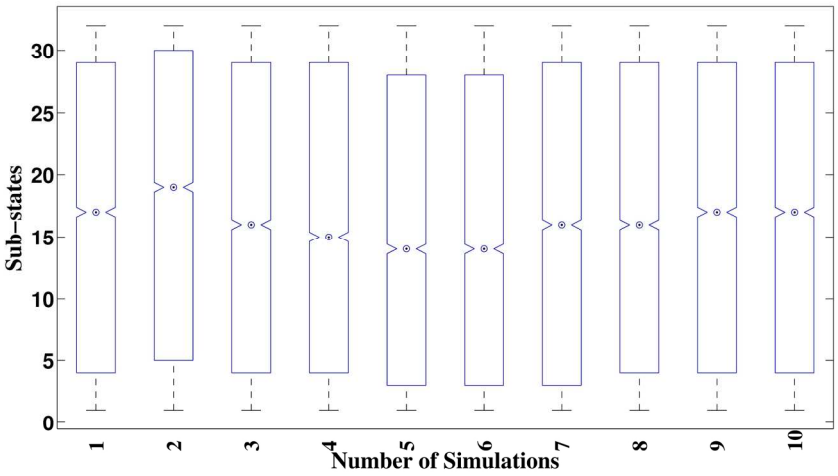

Fig. 7: Simulation results for example nanocell for 10 different cases. For each case, simulations are done for 10000 times,
with varying $^{\perp}$ λ and μ.
184x100mm (300 x 300 DPI)