Spline quasi-interpolation as a tool for resistive RAM reset voltage determination

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a joint work with

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Outline

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Motivation

An in-depth description of bipolar resistive switching in Cu/HfO_x/Pt devices, a 3D Kinetic Monte Carlo simulation approach

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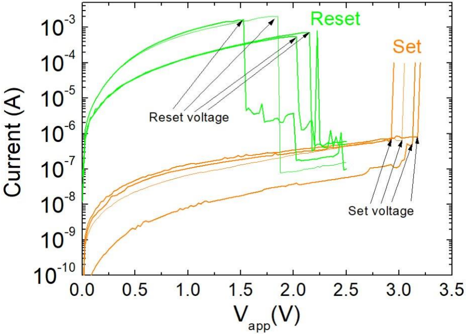
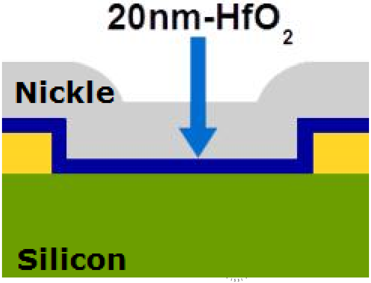
Motivation

Main problem: Estimation of the reset voltage, i.e. the voltage at which the filament is destroyed, producing a sudden drop in the current.
We will use the experimental measurements of the devices fabricated by F. Campabadal and M. B. González from the IMBCNM (CSIC) in Barcelona.





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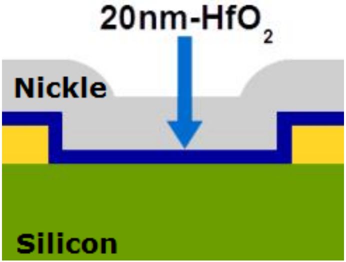
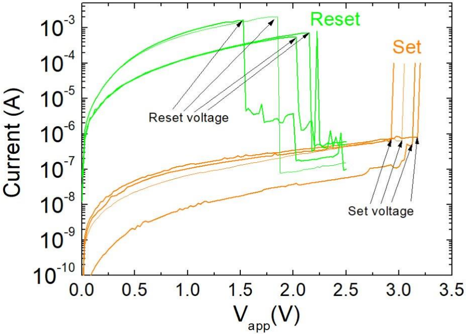


The device is based on a $Ni/HfO_2/Si-n^+$ structure.

It is composed by two layers of metal (nickel and silicon) and a layer of Hafnium oxide, that acts as dielectric.

Motivation



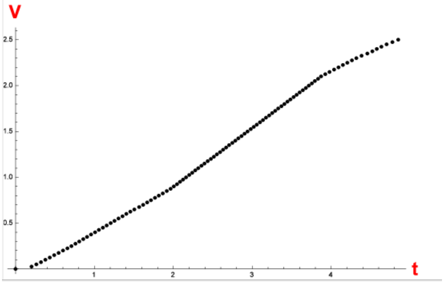
The plot shows experimental current versus applied voltage for several set/reset transitions in a long Reset-Set series for the device above.

Working in the charge-flux domain

The sudden decrease of the current from the reset voltage implies that its integral against time will stabilize from that value. Therefore, instead of working with variables V and I we will use new variables ϕ (the flux) and Q (the charge) defined as follows:

$$\phi(t) = \int_{t_0}^{t} V(\tau)\, d\tau \qquad \text{and} \qquad Q(t) = \int_{t_0}^{t} I(\tau)\, d\tau$$

A typical case:



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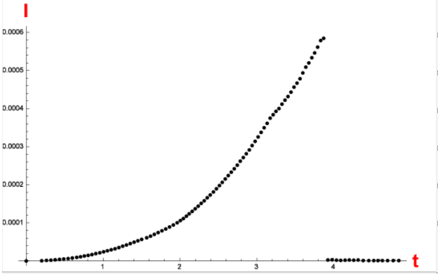

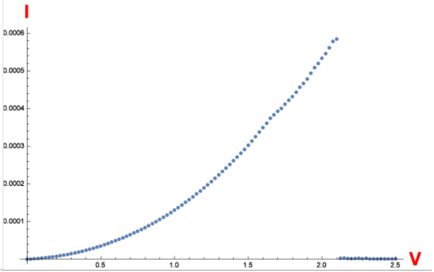

Only the variables V and I can be measured in the laboratory.

How to obtain the values of ϕ and Q at times t_i from $V(t_i)$ and $I(t_i)$?

We propose to use spline quasi-interpolation on non-uniform partitions to approximate V and I in order to obtain approximations to ϕ and Q.

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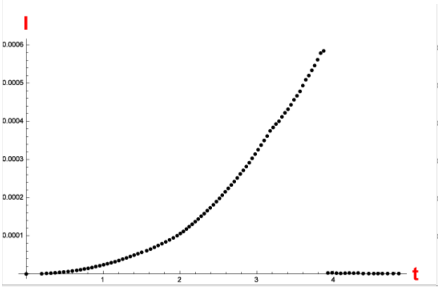

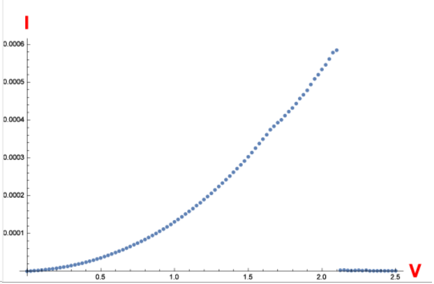

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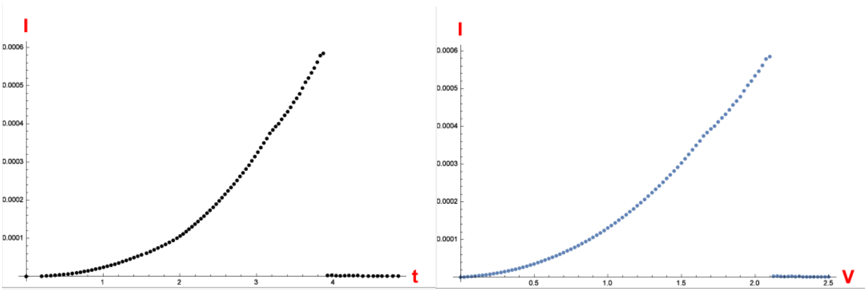

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Spline quasi-interpolation

Given a continuous function f defined on the interval $I := [a, b]$, let us suppose we know its values at the simple knots of the partition Δ given by

$$a := t_0 < t_1 < t_2 < \cdots < t_{n-1} < t_n := b.$$

For constructing approximations to f, for every integer $d \geq 2$ let us consider the $n + d-$dimensional linear space

$$\mathcal{S}_{d+1}(\Delta) := \left\{ s \in C^{d-1}(I) : s_{|[t_i, t_{i+1}]} \in \mathbb{P}_d \right\}$$

of spline functions of order $d + 1$ associated with Δ, with $\mathbb{P}_d$ denoting the space of polynomials of degree less than or equal to d. To define an appropriate basis to this space we consider the extended partition with multiple extremal point given by

$$t_{-d} = \cdots = t_{-1} = t_0 < t_1 < t_2 < \cdots < t_{n-1} < t_n = t_{n+1} = \cdots = t_{n+d}.$$

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Spline quasi-interpolation

With $[z_1, z_2, \ldots, z_m]\, g$ denoting the divided difference of g at the indicated knots and $(\cdot)_+^k$ representing the truncated power of degree k given by

$$z_+^k := \begin{cases} z^k, & z \geq 0, \\ 0, & z < 0, \end{cases}$$

for every $i \in \{-d, \ldots, n-1\}$, let

$$B_{i,d+1}(t) := (t_i - t_{i-d-1})\,[t_{i-d-1} \ldots t_i]\,(\cdot - t)_+^d$$

be the B-spline of order $d+1$ with knots $t_{i-d-1}, \ldots, t_i$. It is a function in $\mathcal{S}_{d+1}(\Delta)$ supported on $[t_{i-d-1}, t_i]$. The B-spline sequence $(B_i)_{1 \leq i \leq n+d}$ is a basis for $\mathcal{S}_{d+1}(\Delta)$. Every B-spline is compactly supported and positive in the interior of its support, and they form a partition of unity. Moreover, they can be computed by recurrence.

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Spline quasi-interpolation

For a given function $f \in C(I)$, from the values $f(\Delta) := (f(t_i))_{0 \le i \le n}$ it is possible to define the quasi-interpolant

$$Af(t) := \sum_{i=1}^{n+d} \mu_{i,d+1}(f) B_{i,d+1}(t), \; t \in I,$$

where every coefficient $\mu_{i,d+1}(f)$ is an appropriate linear combination of values of f at points t_i in the support of $B_{i,d+1}$. It is possible to define coefficients to produce an operator

$$\begin{array}{rccc} \mathcal{A}: & C(I) & \longrightarrow & \mathcal{S}_{d+1}(\Delta) \\ & f & \longmapsto & \mathcal{A}(f) = Af \end{array}$$

exact on the space of polynomials of degree less than or equal to d.

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Spline quasi-interpolation

If the coefficient has the form

$$\mu_{i,d+1}(f) := \begin{cases} \sum_{j=0}^{d} \alpha_{i,j} f(t_j), & 1 \leq i \leq d, \\ \sum_{j=0}^{d} \alpha_{i,j} f(t_{i+j-d-1}), & d+1 \leq i \leq n, \\ \sum_{j=0}^{d} \alpha_{i,j} f(t_{n-d+j}), & n+1 \leq i \leq n+d, \end{cases}$$

then the values of the coefficientes $\alpha_{i,j}$ are determined by solving some Vandermonde systems of linear equations.

Spline quasi-interpolation

For every $1 \le i \le n$ it holds

$$\|f - \mathcal{A}(f)\|_{\infty,[t_{i-1},t_i]} \le (1 + \|\mathcal{A}\|_\infty)\, \mathrm{d}_{\infty,[t_{i-1},t_i]}(f, \mathbb{P}_d),$$

with

$$\mathrm{d}_{\infty,[t_{i-1},t_i]}(f, \mathbb{P}_d) := \inf \left\{ \|f - p\|_{\infty,[t_{i-1},t_i]} : p \in \mathbb{P}_d \right\}$$

and

$$\|f - p\|_{\infty,[t_{i-1},t_i]} := \max_{t \in [t_{i-1},t_i]} |f(t) - p(t)|.$$

In particular, for $f \in C^{d+1}(I)$, we get

$$\|f - \mathcal{A}(f)\|_{\infty,I} = \mathcal{O}\left(h^{d+1}\right),$$

with $h := \max\{h_i, 1 \le i \le n\}$ and $h_i := t_i - t_{i-1}$.

Spline quasi-interpolation

The quasi-interpolant Af can be evaluated in a stable way by using the recurrence relation for B-splines. Moreover, since the problem of interest needs to compute $\int_{t_0}^{t} Af(\tau)\,d\tau$ when f is the voltage or the current, this can be done by using the expressions

$$\int_{-\infty}^{t} B_{i,d+1}(\tau)\,d\tau = \frac{t_i - t_{i-d-1}}{d+1} \sum_{j=i-d-1}^{\infty} B_{j,d+2}(t),$$

as well as the recurrence relations for B-splines.

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Discrete Orthogonal Polynomials on nonuniform sequences of knots

Consider the scalar product

$$\langle f, g\rangle := \sum_{i=1}^{M} f(x_i)\, g(x_i),$$

where the nodes x_i, $i = 1, \ldots, M$, do not need to be equispaced.
A sequence of polynomials $\{p_n, n = 0, \ldots, M\}$ such that the degree of p_n is equal to n is said to be orthogonal with respect to the scalar product if

$$\langle p_n, p_m\rangle = 0,\ \ n \neq m.$$

If the leading coefficients of p_n are equal to 1, then the polynomials are called monic

$$p_n(x) = x^n + a_{n-1}^{(n)} x^{n-1} + \cdots + a_0^{(n)},$$

and we will denote them as $\bar{p}_n$.
We have

$$\mathbb{P}_M = \operatorname{span}\{\bar{p}_0, \bar{p}_1, \ldots, \bar{p}_M\}.$$

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Discrete Orthogonal Polynomials

The norm of the monic polynomials is obtained from the scalar product taking into account that

$$\langle \bar{p}_n, \bar{p}_m \rangle = \sum_{i=1}^{M} \bar{p}_n(x_i)\, \bar{p}_m(x_i) = d_n^2(M)\, \delta_{nm}.$$

They satisfy a three term recurrence relation:

$$\bar{p}_0(x) := 1,$$

$$\bar{p}_1(x) := x - \alpha_0 = x - \frac{\langle x, 1 \rangle}{\langle 1, 1 \rangle} = x - \frac{1}{M} \sum_{i=1}^{M} x_i,$$

$$\bar{p}_{n+1}(x) := (x - \alpha_n)\, \bar{p}_n(x) - \beta_n \bar{p}_{n-1}(x), \; n = 1, 2, \ldots, M$$

where the coefficients can be computed as follows:

$$\alpha_n := \frac{\langle x\bar{p}_n(\cdot), \bar{p}_n(\cdot) \rangle}{\langle \bar{p}_n(\cdot), \bar{p}_n(\cdot) \rangle} = \frac{\langle x\bar{p}_n(\cdot), \bar{p}_n(\cdot) \rangle}{d_n^2(M)},$$

$$\beta_n := \frac{\langle x\bar{p}_n(\cdot), \bar{p}_{n-1}(\cdot) \rangle}{\langle \bar{p}_{n-1}(\cdot), \bar{p}_{n-1}(\cdot) \rangle} = \frac{\langle \bar{p}_n(\cdot), \bar{p}_n(\cdot) \rangle}{d_{n-1}^2(M)} = \frac{d_n^2(M)}{d_{n-1}^2(M)}.$$

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The main objective

Given a set of discrete data $\{x_i, y_i\}$, $i = 1, \ldots N$, with abscissae x_i not necessarily equispaced, our goal is to determine subsets of data $\{x_i, y_i\}$, $i = i_1, \ldots, i_M$, that form a polynomial curve up to degree $\delta_{\text{máx}}$.
The procedure can be divided in two parts:

1. Given a subset of data, determine if these data form a polynomial curve.
2. Once we have determined that a given data subset forms a polynomial curve, find the maximal subset, containing this given data subset, that forms a polynomial curve of the same degree.

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Checking of polynomial curves

Let's take a subset of data $\{x_i, y_i\}$, $i = i_1, \ldots, i_M$, and consider the scalar products

$$r_n := \langle y, \bar{p}_n(\cdot)\rangle = \sum_{j=1}^{M} y_{j+i_1-1}\bar{p}_n(x_j)$$

Since the polynomials $\bar{p}_j$ are linearly independent, the data y_i can be expressed as a linear combination of $\bar{p}_j(x_i)$:

$$y_i = \sum_{j=1}^{M} c_j\bar{p}_j(x_i, M).$$

Using the orthogonality relation, we find that

$$r_n = \langle \bar{p}_n(\cdot), \bar{p}_n(\cdot)\rangle c_n = d_n^2(M)c_n.$$

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Checking of polynomial curves

So, if the data y_i come from a polynomial of degree δ, we will have that all the scalar products r_n will be 0, for $n > \delta$.
In practice, we will consider that a coefficient r_n vanish if $|r_n| < \epsilon$, being ϵ a given threshold.

Determination of polynomial subsets

Once we know how to check if a given set of data forms a polynomial curve, we have to determine the polynomial subsets of data in the whole data set. To do this we follow the following steps:

- Choose a node x_m. We will check if a subset of points starting or ending at x_m forms a polynomial curve of degree δ, with $\delta = 0, 1, \ldots, \delta_{\text{máx}}$. We start with $\delta = 0$ and take the first $\delta + 2$ points; i.e., $i_1 = m$ and $i_M = m + \delta + 1$ (the subset starts at x_m) or $i_1 = m - \delta - 1$ and $i_M = m$ (the subset ends at x_m). We now check if this subset of data forms a polynomial curve of degree δ using the previous procedure. If if doesn't, we increase δ by 1, and start again checking if the points form a polynomial curve of degree $\delta + 1$. We end this part when $\delta = \delta_{\text{máx}}$.
- If we have found that the initial $\delta + 2$ data points form a polynomial curve of degree δ, we begin a binary search for larger subsets of polynomial data. If the initial data start at x_m, the binary search will be found between $i_M = m + \delta + 1$ and N. Otherwise, the binary search will be between $i_M = 1$ and $m - \delta - 1$. The search ends when it detects the maximal subset of data that forms a polynomial subset of degree δ.

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Determination of polynomial subsets

- Once we have found the maximal subset that forms a polynomial subset of degree δ, we restart the procedure to search polynomial subsets on the rest of the data, not including during the procedure any point that belongs to any previous polynomial subset found.
- If the initial minimal data points doesn't form a polynomial curve we start the procedure again taking as new initial point i_{m+1} or i_{m-1}.
- We stop the whole process when there are not enough data to consider.

When we have a subset that forms a polynomial curve of degree δ, we compute the polynomial itself, as

$$p(x) = \sum_{i=0}^{\delta} c_i \bar{p}_i(x).$$

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Algorithm

Once we know how to construct a spline quasi-interpolant to a given function and to determine straight lines associated to portions of data, we can propose the algorithm to estimate the reset voltage. The stabilization of the charge as function of the flux guarantees the existence of a straight segment.

1. Define in the space $\mathcal{S}_{d+1}(\Delta)$ with knots t_i the C^{d-1} quasi-interpolants

$$V_{\text{app}}(t) := \sum_{i=1}^{n+d} \mu_{i,d+1}(V) B_{i,d+1}(t)$$

$$I_{\text{app}}(t) := \sum_{i=1}^{n+d} \mu_{i,d+1}(I) B_{i,d+1}(t)$$

to V and I, respectively. The coefficients $\mu_{i,d+1}(V)$ and $\mu_{i,d+1}(I)$ involve the values of V and I at the knots t_i.

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Algorithm

2 Define approximations ϕ_{app} and Q_{app} to ϕ and Q, respectively, as follows:

$$\phi_{app}(t) := \int_{t_0}^{t} V_{app}(\tau)\, d\tau \qquad \text{and} \qquad Q_{app}(t) := \int_{t_0}^{t} I_{app}(\tau)\, d\tau.$$

They are in $\mathcal{S}_{d+2}(\Delta)$.

3 Given a threshold ε, compute the subset providing a straight segment to the data $(\phi_{app}(t_i), Q_{app}(t_i))$, $i = 0, \ldots, n$, and let J_ε be the initial abscissae of such a segment.

4 Let the reset charge Q_{reset} be equal to $Q_{app}(t_{J_\varepsilon})$.

5 Fit a model $Q = Q(\phi)$ to data $Q_{app}(t_j)$, $j = 0, \ldots, k$, for a enough large $k \leq J_\varepsilon$ (typically, a quadratic polynomial).

6 Let the estimated reset flux ϕ_{reset} be the solution in I of the equation $Q_{app}(\phi) = Q_{reset}$.

7 Let t_{reset} be the solution in I of the equation $\phi_{app}(t) = \phi_{reset}$.

8 Let the reset voltage V_{reset} be equal to $V_{app}(t_{reset})$.

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Algorithm

We will use C^1-quadratic quasi-interpolation to illustrate the performance of the proposed method. It provides cubic convergence. The coefficients of the quasi-interpolant $Q_3 f$ are given by the following expressions:

$$\mu_{1,3}(f) = f(t_0),$$

$$\mu_{2,3}(f) = \frac{h_2}{2(h_1+h_2)} f(t_0) + \frac{h_1+h_2}{2h_2} f(t_1) - \frac{h_1^2}{2h_2(h_1+h_2)} f(t_2),$$

$$\mu_{i,3}(f) = \frac{h_i}{2(h_{i-1}+h_i)} f(t_{i-2}) - \frac{h_{i-1}+h_{i-2}}{2h_{i-1}} f(t_{i-1}) - \frac{h_{i-2}}{(h_{i-1}+h_{i-2})h_{i-1}} f(t_i),$$

$$\mu_{n+1,3}(f) = -\frac{h_n^2}{2h_{n-1}(h_{n-1}+h_n)} f(t_{n-2}) + \frac{h_{n-1}+h_n}{2h_{n-1}} f(t_{n-1}) + \frac{h_{n-1}}{2(h_{n-1}+h_n)} f(t_n),$$

$$\mu_{n+2,3}(f) = f(t_n).$$

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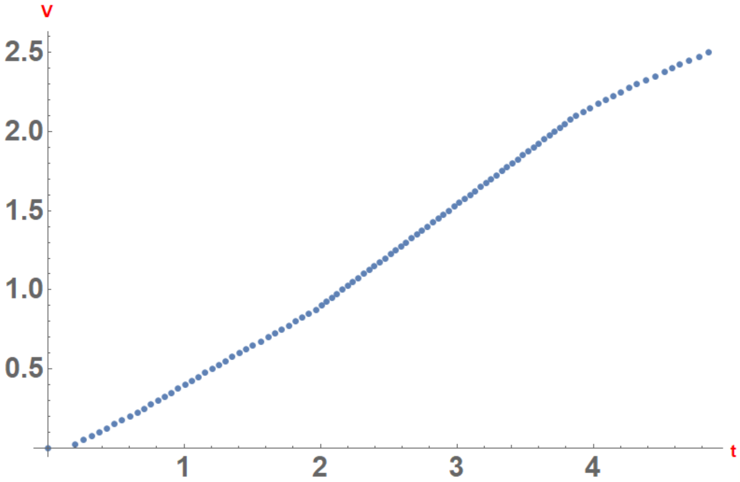
Examples



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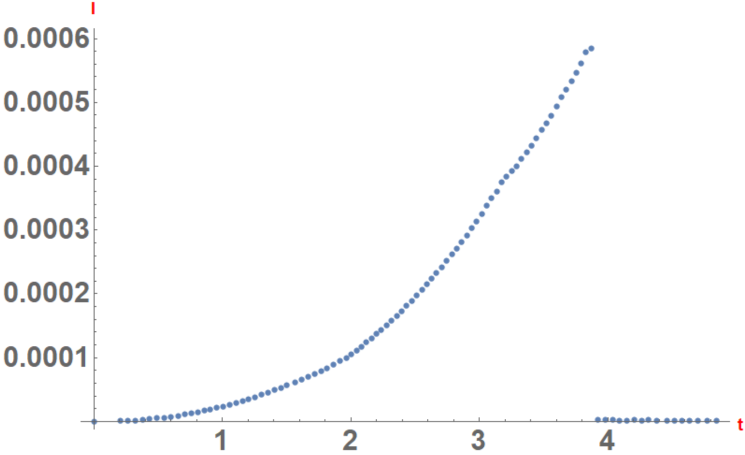

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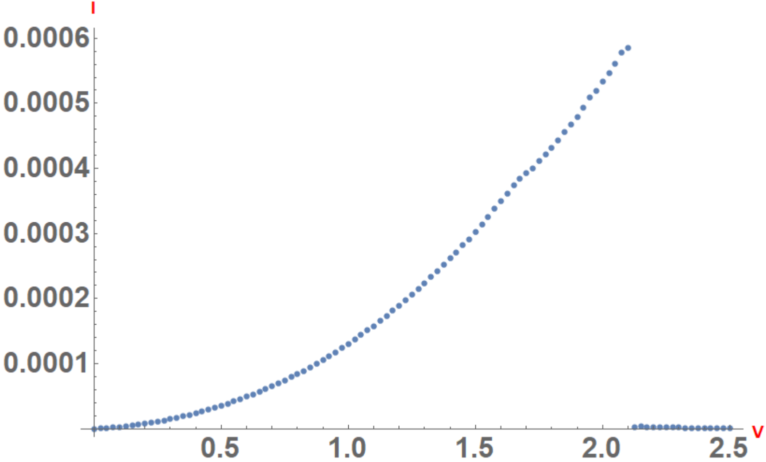

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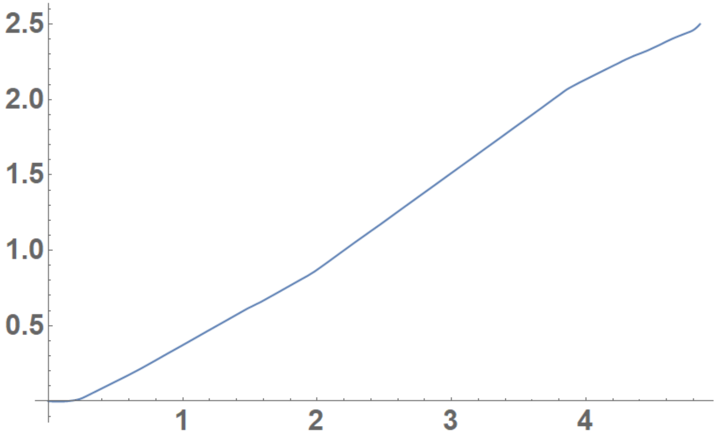

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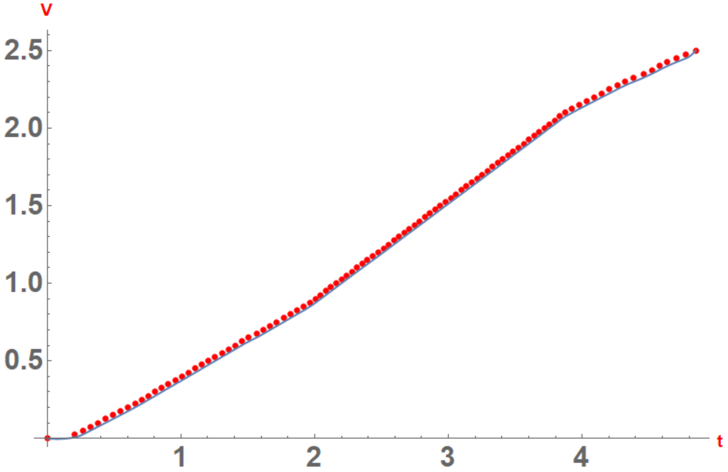

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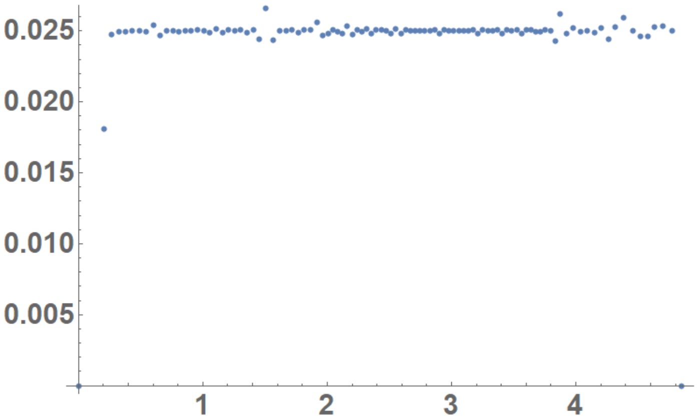

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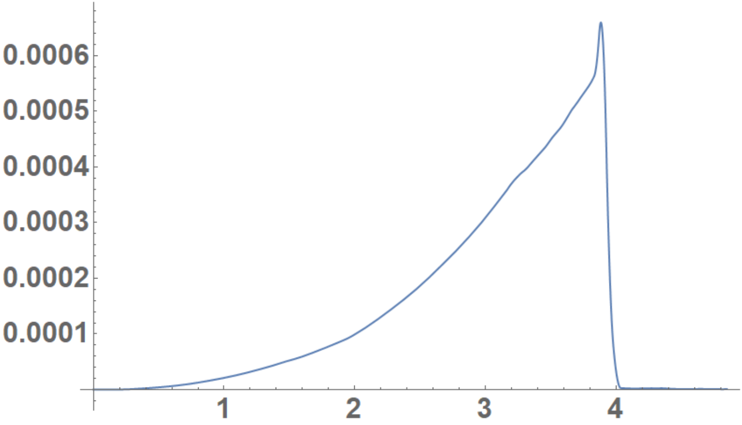

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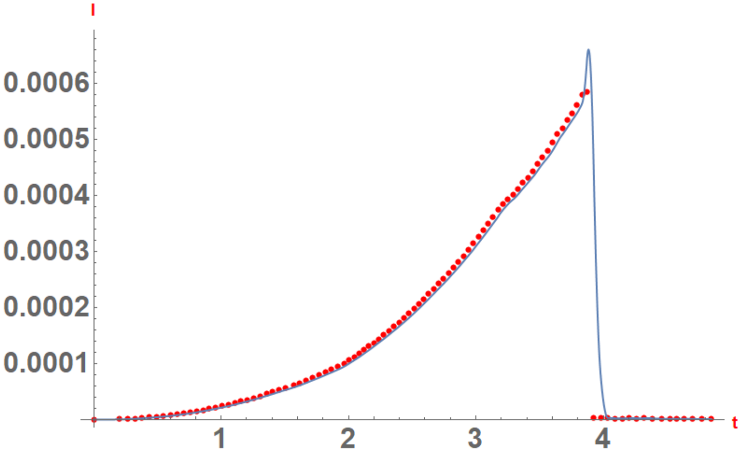

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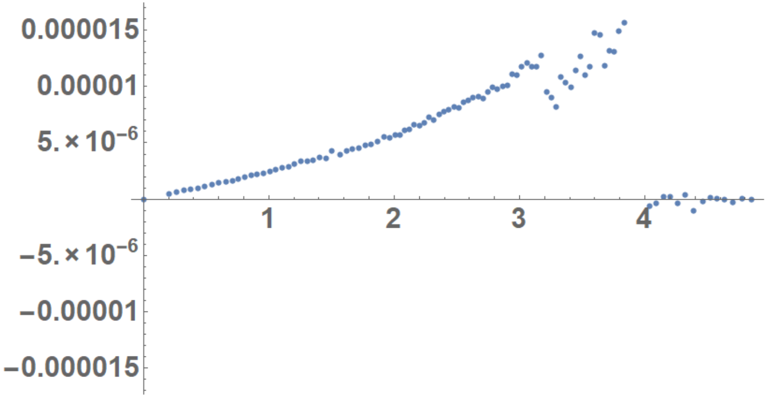

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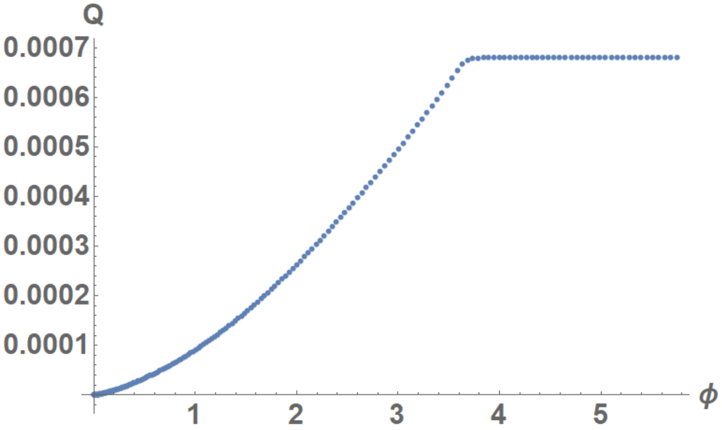

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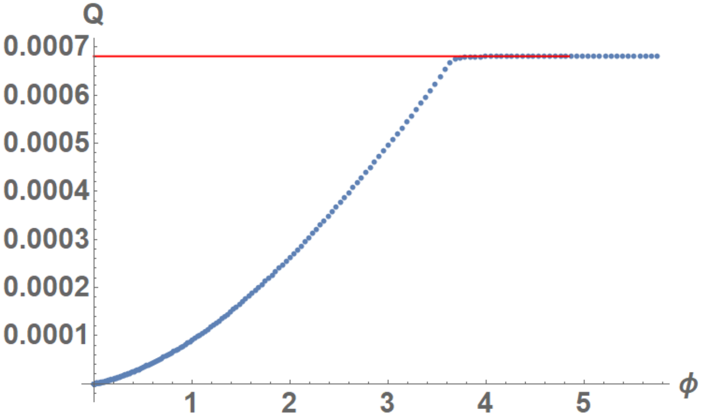

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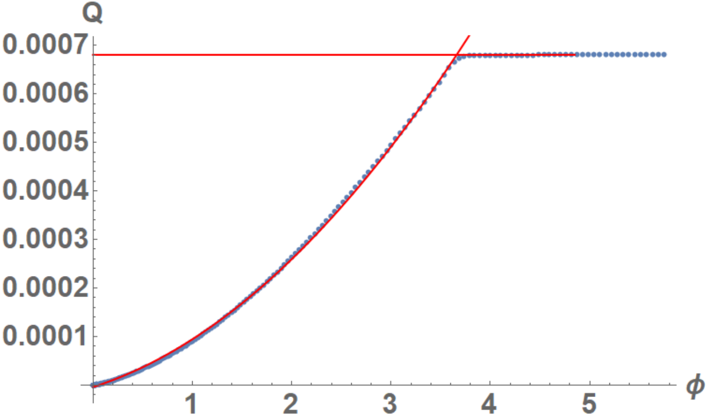

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Examples

Once isolated the stable region, the algorithm gives an estimated reset flux equal to 3,61924 Vs, and an estimated reset voltage of 2,09777 V, in good agreement with the experimental data.

The method based on quasi-interpolation and numerical differentiation (QI&ND) overestimates the real value yielding a reset voltage equal to 2,1066 V.

In order to compare both methods at this level of detail, we have added noise to the original RRAM current versus voltage curves. More precisely, we have defined the current values as follows,

$$I_{new,a} = I + a * r * I,$$

where the parameter a takes the values 0,01, 0,03, 0,05, 0,1, and r is a random number in $[0, 1]$.

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In order to compare both methods at this level of detail, we have added noise to the original RRAM current versus voltage curves. More precisely, we have defined the current values as follows,

$$I_{\mathrm{new},a} = I + a * r * I,$$

where the parameter a takes the values 0,01, 0,03, 0,05, 0,1, and r is a random number in $[0, 1]$.

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Examples

	QI&DOP		QI&ND	
a	ϕ_{reset}	V_{reset}	ϕ_{reset}	V_{reset}
0,01	3,61970	2,09787	3,65933	2,10667
0,03	3,61903	2,09772	3,65919	2,10664
0,05	3,61903	2,09833	3,66088	2,10701
0,10	3,61903	2,10074	3,66787	2,10854

Thank you for your attention