Quantum vs classical thermal model for resistive random access memories

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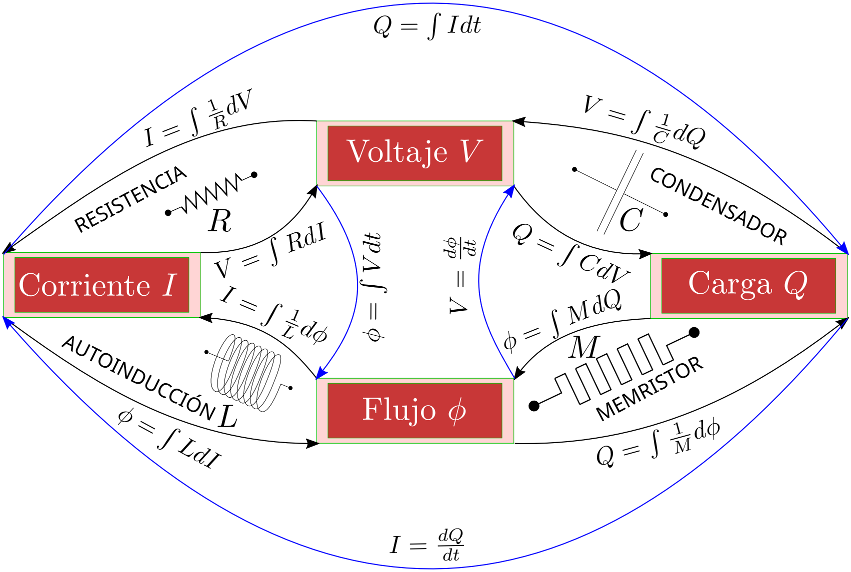
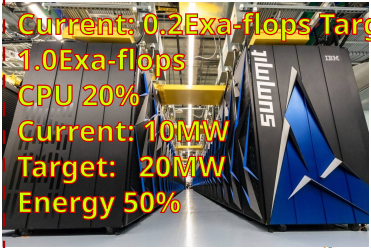
Overview

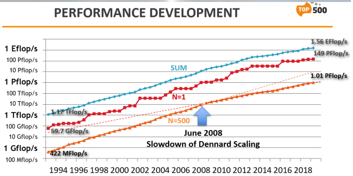


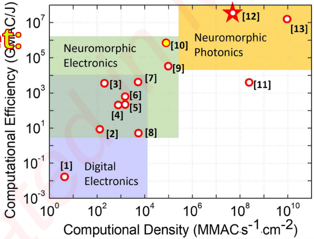
$Q = \int I dt$
$I = \int \frac{1}{R} dV$
$V = \int \frac{1}{C} dQ$
Voltaje V
RESISTENCIA
R
CONDENSADOR
C
Corriente I
Carga Q
$V = \int R dI$
$I = \int \frac{1}{L} d\phi$
$\phi = \int V dt$
$V = \frac{d\phi}{dt}$
$Q = \int C dV$
$\phi = \int M dQ$
M
MEMRISTOR
AUTOINDUCCIÓN L
Flujo ϕ
$\phi = \int L dI$
$Q = \int \frac{1}{M} d\phi$
$I = \frac{dQ}{dt}$

Density vs Efficiency vs Cost



Current: 0.2Exa-flops Target: 1.0Exa-flops
CPU 20%
Current: 10MW
Target: 20MW
Energy 50%





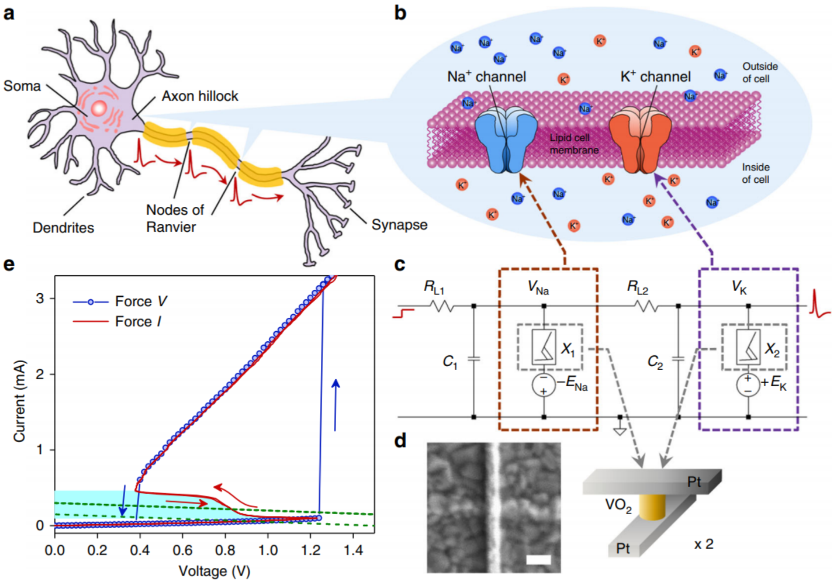
[1] SinNNaker
[2] NeuroGrid
[3] TrueNorth
[4] Nvidia
[5] TPUv3
[6] Graphcore
[7] Groq
[8] HICANN
[9] Silicon Photonics
[10] Memristors
[11] Hybrid Si/III-V SNN PIC
[12] Nanophotonics
[13] Subwavelength
[14] Subwavelenth photonis

1.6% >3% (420TWh) ~23%

2014 2016 2025

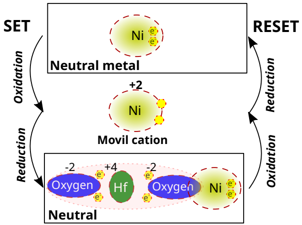
Energy in DataCenters (% of global power)

Beyond the Von Neumann algebra

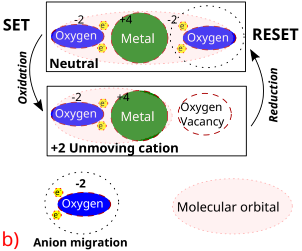


Migrations and characterization

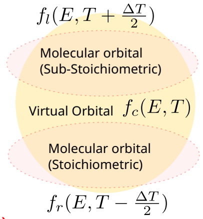
Conductive bridging RAM | Valence change memories | Virtual orbital



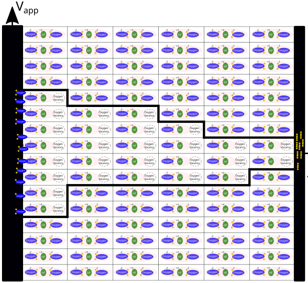
a)

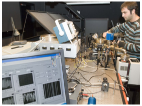


b)



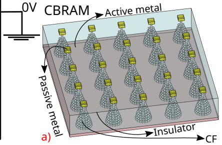
c)

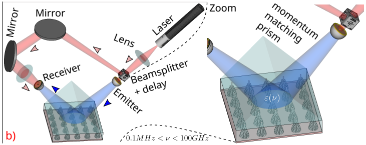




$$\rho\left(T(\vec{r})\right) C_P\left(T(\vec{r})\right) \vec{u}(\vec{r}) \cdot \nabla T(\vec{r}) + \nabla \cdot \vec{q}(\vec{r}) = Q_h(\vec{r})$$

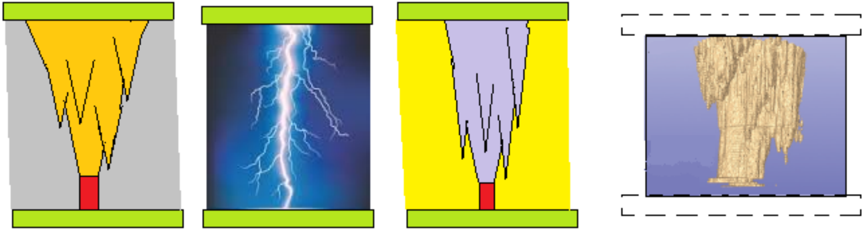
$$\vec{u}(\vec{r}) \simeq \vec{0} \qquad \nabla \cdot \vec{q}(\vec{r}) = Q_h(\vec{r})$$





Geometry

Something in Common



HfO Metallic filament RRAM/ReRAM

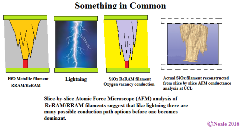
Lightning

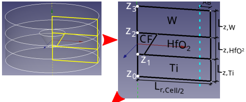
SiOx ReRAM filament Oxygen vacancy conduction

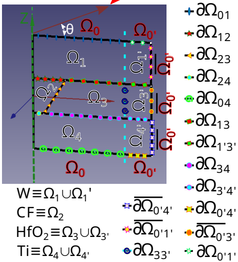
Actual SiOx filament reconstructed from slice by slice AFM conductance analysis at UCL

Slice-by-slice Atomic Force Microscope (AFM) analysis of ReRAM/RRAM filaments suggest that like lightning there are many possible conduction path options before one becomes dominant.

Classical approach







$$\nabla \cdot \vec{J}_e(\vec{r}) = \sum_j Q_{j,v}(\vec{r})$$

$$\vec{J}_e(\vec{r}) = \sigma(\vec{r})\vec{E}(\vec{r})$$

$$\vec{E}(\vec{r}) = -\nabla V(\vec{r})$$

$$V(\vec{r}) = \begin{cases} 0V & if \quad \vec{r} \in \partial\Omega_{01} \cup \partial\Omega_{0'1'} \\ 1V & if \quad \vec{r} \in \partial\Omega_{04} \cup \partial\Omega_{0'4'} \end{cases}$$

$$\frac{\partial V(\vec{r})}{\partial \hat{n}} \Rightarrow \vec{J}(\vec{r}) \cdot \hat{n} = 0 \text{ if } \vec{r} \in \overline{\partial\Omega_{0'1'}} \cup \overline{\partial\Omega_{0'3'}} \cup \overline{\partial\Omega_{0'4'}}$$

$$+$$

$$\nabla \cdot \vec{q}(\vec{r}) = Q_h(\vec{r})$$

$$\vec{q}(\vec{r}) = -k(\vec{r}) \cdot \nabla T(\vec{r}) \qquad \frac{\partial T(\vec{r})}{\partial \hat{n}} \Rightarrow -\vec{q}(\vec{r}) \cdot \hat{n} = q_0 \text{ if } \vec{r} \in \overline{\partial\Omega_{0'1'}} \cup \overline{\partial\Omega_{0'3'}} \cup \overline{\partial\Omega_{0'4'}}$$

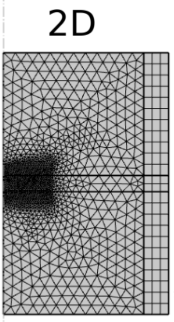
$$Q_h(\vec{r}) = \vec{J}_e(\vec{r}) \cdot \vec{E}(\vec{r})$$

$$q_0 = \hat{r} \cdot \begin{pmatrix} k_{rr} & k_{r\theta} & k_{rz} \\ k_{\theta r} & k_{\theta\theta} & k_{\theta z} \\ k_{zr} & k_{z\theta} & k_{zz} \end{pmatrix} \nabla T(\vec{r}) = k_{rr} \nabla_r T(\vec{r})$$

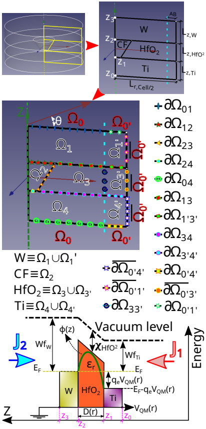
$$Q_h(\vec{r}) = \begin{cases} \sigma_W(\vec{r})||\nabla V(\vec{r})||^2 & if \quad \vec{r} \in \Omega_1 \cup \Omega_1' \\ \frac{\sigma_{CF}||\nabla V(\vec{r})||^2}{1+\alpha_T(T(\vec{r})-T_0)} & if \quad \vec{r} \in \Omega_2 \\ \sigma_{HfO_2}(\vec{r})||\nabla V(\vec{r})||^2 & if \quad \vec{r} \in \Omega_3 \cup \Omega_3' \\ \sigma_{Ti}(\vec{r})||\nabla V(\vec{r})||^2 & if \quad \vec{r} \in \Omega_4 \cup \Omega_4' \end{cases}$$

$$T(\vec{r}) = \begin{cases} T_0 & if \quad \vec{r} \in \partial\Omega_{01} \cup \partial\Omega_{0'1'} \\ T_0 & if \quad \vec{r} \in \partial\Omega_{04} \cup \partial\Omega_{0'4'} \end{cases}$$

2D



Semi-Classical approach



$$\nabla \cdot \vec{J}_e(\vec{r}) = \sum_j Q_{j,v}(\vec{r})$$

$$\vec{J}_e(\vec{r}) = \sigma(\vec{r})\vec{E}(\vec{r})$$

$$\vec{E}(\vec{r}) = -\nabla V(\vec{r})$$

$$\hat{n}\cdot\left(\vec{J}_1(\vec{r}_s) - \vec{J}_2(\vec{r}_s)\right) = \sum_j Q_{j,s}(\vec{r}_s)$$

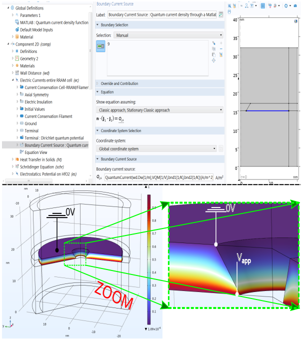
$$\Phi(r,z) = E_F + Wf_W - \chi_{HfO_2} + \frac{(Wf_{Ti} - Wf_W)\,z}{D(r,z)} + \Phi_{image}(r,z) + q_e V_{QM}(r,z) + \Upsilon_{zc}(r,z)$$

$$\varphi(E',r) = e^{\frac{-2}{\hbar}\int_{z_1}^{z_2}\sqrt{2m(\Phi(r,z)-E')}dz}$$

$$N_1(E',r,z_1)dE' = \Theta_1(r,z_1)\,ln\left(1+e^{-\frac{E'+q_eV_{QM}(r,z_1)-E_F}{k_BT(r,z_1)}}\right)$$

$$N_2(E',r,z_2)dE' = \Theta_2(r,z_2)\,ln\left(1+e^{-\frac{E'-E_F}{k_BT(r,z_2)}}\right)$$

$$\Theta_1(r,z_1) = \frac{mk_BT(r,z_1)}{2\pi^2\hbar^3}\quad \Theta_2(r,z_2) = \frac{mk_BT(r,z_2)}{2\pi^2\hbar^3}$$



$\Upsilon_{zc}(r,z) \ll q_e V_{QM}(r,z) + \Phi_{image}(r,z) \Rightarrow$ new map $(r,z) \to r$

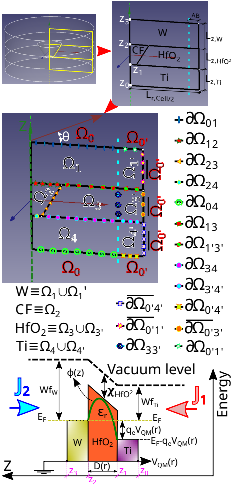
r_1, $r_2 \to \vec{J}_{QM}(r) \Rightarrow \vec{J}_{QM}(V_{QM}, D, T_1, T_2)$

Surjective! z_1 and z_2 from $\Phi(r,z) - E' = 0 \Rightarrow$
$D = z_2 - z_1$ and $V_{app} = V_{QM}(z1) - V_{QM}(z2)$

$$\nabla G(\vec{r})\cdot\nabla G(\vec{r}) + \sigma_\omega G(\vec{r})\left(\nabla\cdot\nabla G(\vec{r})\right) = (1+2\sigma_\omega)\,G^4(\vec{r})$$

$$D(\vec{r}) = 1/G(\vec{r}) - 1/G_0$$

Full quantum approach



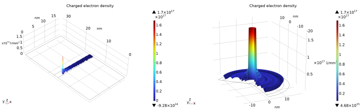
$$\nabla\cdot\vec{J}_e(\vec{r}) = \sum_j Q_{j,v}(\vec{r})$$

$$\vec{J}_e(\vec{r}) = \sigma(\vec{r})\vec{E}(\vec{r})$$

$$\vec{E}(\vec{r}) = -\nabla V(\vec{r})$$

$$\hat{n}\cdot\left(\vec{J}_1(\vec{r}_s)-\vec{J}_2(\vec{r}_s)\right) = \sum_j Q_{j,s}(\vec{r}_s)$$

$$V(\vec{r}) = V_{QM}(\vec{r})$$



+

$$\nabla\cdot\vec{D}(\vec{r}) = \rho_v(\vec{r})$$

$$\vec{D}(\vec{r}) = \varepsilon_r\varepsilon_0\vec{E}_{QM}(\vec{r})$$

$$\vec{E}_{QM}(\vec{r}) = -\nabla V_{QM}(\vec{r})$$

$$H\psi(\vec{r}) = E\psi(\vec{r}) \qquad \vec{r}\in\Omega_3$$

$$n_\rho(\vec{r}) = \sum_m\sum_i \frac{2g_{i,m}\left|\Psi_{i,m}(\vec{r})\right|^2}{1+e^{\frac{E_{i,m}-E_F}{k_BT}}}$$

$$\rho_v(\vec{r}) = q_e n_\rho(\vec{r}) e^{e^{-\alpha\frac{-q_e(V_{QM}(\vec{r})-V_{QM,old}(\vec{r}))}{k_BT(\vec{r})}}}$$

$$V_{QM}(\vec{r}) = V(\vec{r}) \text{ if } \vec{r}\in\partial\Omega_{13}\cup\partial\Omega_{23}\cup\partial\Omega_{34}$$

$$\hat{n}\cdot\vec{D}(\vec{r}) = \hat{n}\cdot\vec{D}_0(\vec{r}) \text{ if } \vec{r}\in\partial\Omega_{33'}$$

$$\hat{n}\cdot\nabla\psi(\vec{r}) = 0 \text{ if } \vec{r}\in\partial\Omega_{34}\cup\partial\Omega_{23}\cup\partial\Omega_{13}$$

$$\hat{n}\cdot\nabla\psi(\vec{r}) = j\left(\frac{1}{\hbar}\sqrt{\frac{2(E-V)}{\hat{n}\cdot m_{eff}^{-1}\cdot\hat{n}}}\right)\psi(\vec{r}) \text{ if } \vec{r}\in\partial\Omega_{33'}$$

Physics and studies

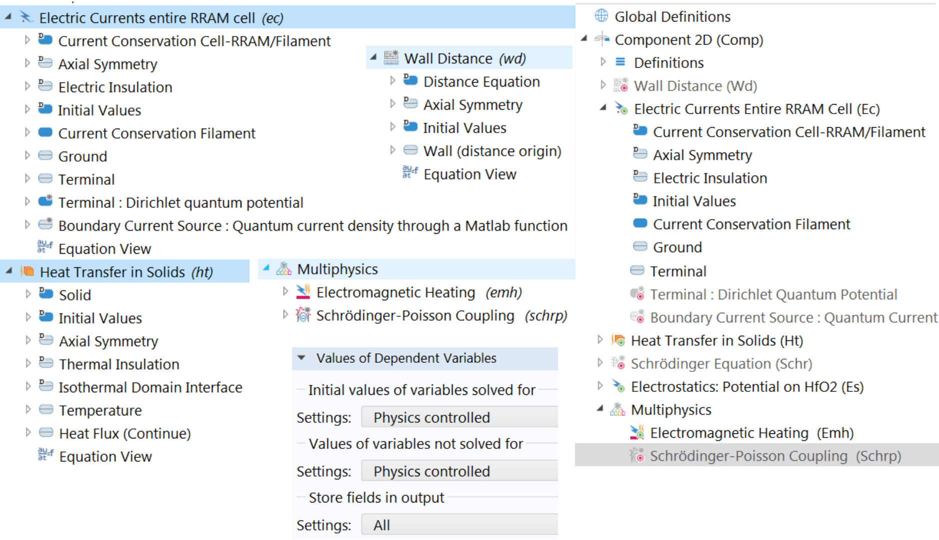
- Global Definitions
  - Parameters 1
  - MATLAB : Quantum current density function
  - Default Model Inputs
  - Material
- Component 2D *(comp)*
  - Definitions
  - Geometry 2
  - Materials
  - Wall Distance *(wd)*
  - Electric Currents entire RRAM cell *(ec)*
  - Heat Transfer in Solids *(ht)*
  - Schrödinger Equation *(schr)*
  - Electrostatics: Potential on HfO2 *(es)*
  - Multiphysics
  - Mesh 2
- Classic approach
- Semi-Classic approach
- Full quantum approach (High-Precision and slow, Matlab function)
- Results

COMSOL Multiphysics
Semiconductor Module
AC/DC Module
Heat Transfer Module
LiveLink™ for MATLAB®

Studies

- Classic approach
  - Step 1: Stationary Classic approach
  - Solver Configurations
  - Job Configurations
- Semi-Classic approach
  - Step 1: Stationary-Semi-Classic approach
  - Solver Configurations
  - Job Configurations
- Full quantum approach (High-Precision and slow, Matlab
  - Step 1: Stationary
  - Step 2: Schrödinger-Poisson
  - Solver Configurations
  - Job Configurations

Study I: Classical approach



Study II: Semi-Classical approach

- Electric Currents entire RRAM cell *(ec)*
  - Current Conservation Cell-RRAM/Filament
  - Axial Symmetry
  - Electric Insulation
  - Initial Values
  - Current Conservation Filament
  - Ground
  - Terminal
  - Terminal : Dirichlet quantum potential
  - Boundary Current Source : Quantum current density through a Matlab function
  - Equation View
- Wall Distance *(wd)*
  - Distance Equation
  - Axial Symmetry
  - Initial Values
  - Wall (distance origin)
  - Equation View
- Heat Transfer in Solids *(ht)*
  - Solid
  - Initial Values
  - Axial Symmetry
  - Thermal Insulation
  - Isothermal Domain Interface
  - Temperature
  - Heat Flux (Continue)
  - Equation View
- Multiphysics
  - Electromagnetic Heating *(emh)*
  - Schrödinger-Poisson Coupling *(schrp)*

Values of Dependent Variables

Initial values of variables solved for

Settings: Physics controlled

Values of variables not solved for

Settings: User controlled

Method: Solution

Study: Classic approach, Stationary Classic approach

Selection: Automatic (single solution)

Store fields in output

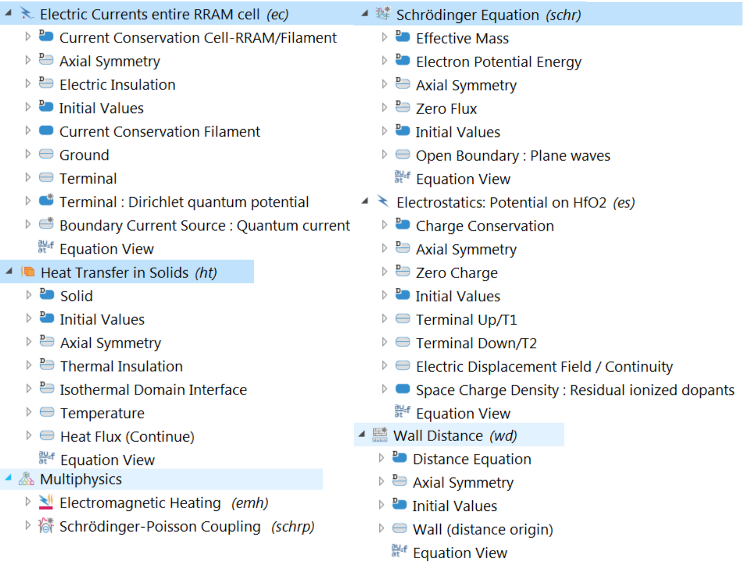
Settings: All

Physics and Variables Selection

☑ Modify model configuration for study step

- Definitions
- Wall Distance (Wd)
- Electric Currents Entire RRAM Cell (Ec)
  - Current Conservation Cell-RRAM/Filament
  - Axial Symmetry
  - Electric Insulation
  - Initial Values
  - Current Conservation Filament
  - Ground
  - Terminal
  - Terminal : Dirichlet Quantum Potential
  - Boundary Current Source : Quantum Current Density
- Heat Transfer in Solids (Ht)
- Schrödinger Equation (Schr)
- Electrostatics: Potential on HfO2 (Es)
- Multiphysics
  - Electromagnetic Heating (Emh)
  - Schrödinger-Poisson Coupling (Schrp)

Study III-1: Full quantum approach



Study III-2: Full quantum approach

- Full quantum approach (High-Precision and slow, Matlab function)
  - Step 1: Stationary
  - Step 2: Schrödinger-Poisson

Physics interface	Solve for	Equation form
Wall Distance (wd)	☑	Automatic (Stationary)
Electric Currents entire RRAM cell (ec)	☑	Automatic (Stationary)
Heat Transfer in Solids (ht)	☑	Automatic (Stationary)
Schrödinger Equation (schr)	☐	Automatic (Stationary)
Electrostatics: Potential on HfO2 (es)	☑	Automatic (Stationary)

Multiphysics couplings	Solve for	Equation form
Electromagnetic Heating (emh)	☑	Automatic (Stationary)
Schrödinger-Poisson Coupling (sc...	☐	Automatic (Stationary)

Values of Dependent Variables

Initial values of variables solved for

Settings: Physics controlled

Values of variables not solved for

Settings: User controlled

Method: Initial expression

Study: Semi-Classic approach, Stationary-Semi-Classic approach

Selection: Automatic (single solution)

Store fields in output

Settings: All

Iterations

Termination method: Fixed number of iterations

Number of iterations: 5

- Full quantum approach (High-Precision and slow, Matlab function)
  - Step 1: Stationary
  - Step 2: Schrödinger-Poisson

Label: Schrödinger-Poisson

Study Settings

Eigenvalue solver: ARPACK

Eigenvalue search method: Manual

Desired number of eigenvalues: ☑ 6

Unit: rad/s

Search for eigenvalues around: ☑ 0 rad/s

Eigenvalue search method around shift: Closest in absolute value

Use real symmetric eigenvalue solver: Automatic

☐ Real symmetric eigenvalue solver consistency check

Values of Dependent Variables

Initial values of variables solved for

Settings: Physics controlled

Values of variables not solved for

Settings: Physics controlled

Store fields in output

Settings: All

Results While Solving

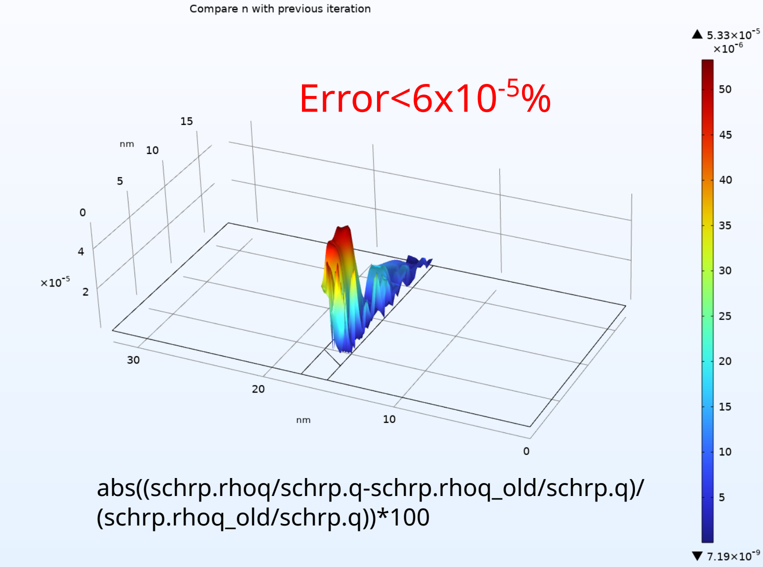
Physics and Variables Selection

☐ Modify model configuration for study step

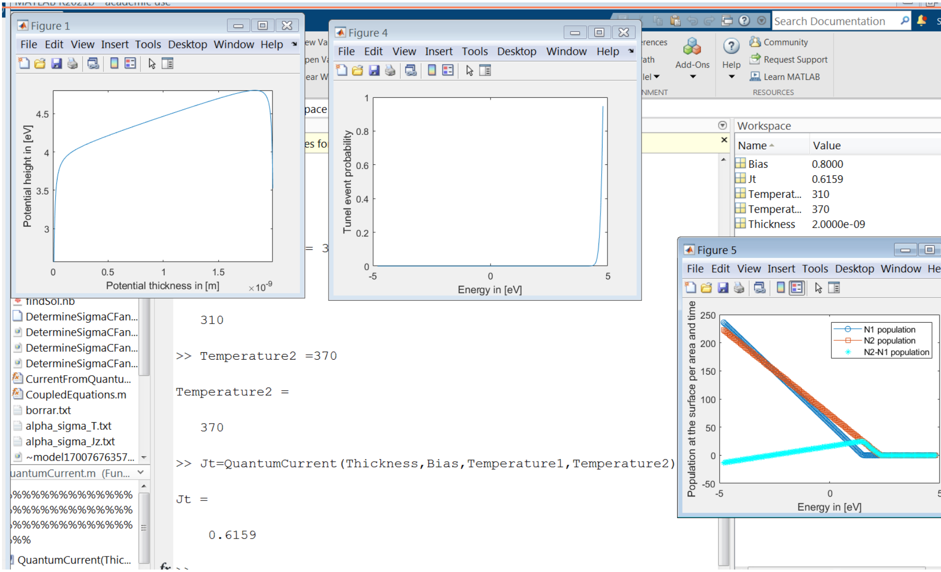
Physics interface	Solve for	Equation form
Wall Distance (wd)	☐	Automatic (Stationary)
Electric Currents entire RRAM cell (ec)	☑	Automatic (Schrödinger-Poisson)
Heat Transfer in Solids (ht)	☑	Automatic (Schrödinger-Poisson)
Schrödinger Equation (schr)	☑	Automatic (Schrödinger-Poisson)
Electrostatics: Potential on HfO2 (es)	☑	Automatic (Schrödinger-Poisson)

Multiphysics couplings	Solve for	Equation form
Electromagnetic Heating (emh)	☑	Automatic (Schrödinger-Poisson)
Schrödinger-Poisson Coupling (schrp)	☑	Automatic (Schrödinger-Poisson)

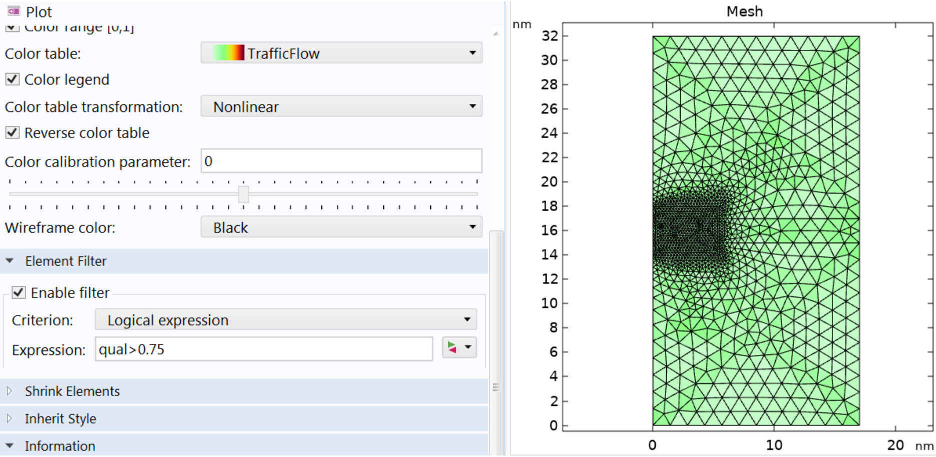
Convergence error (n-Full quantum approach)



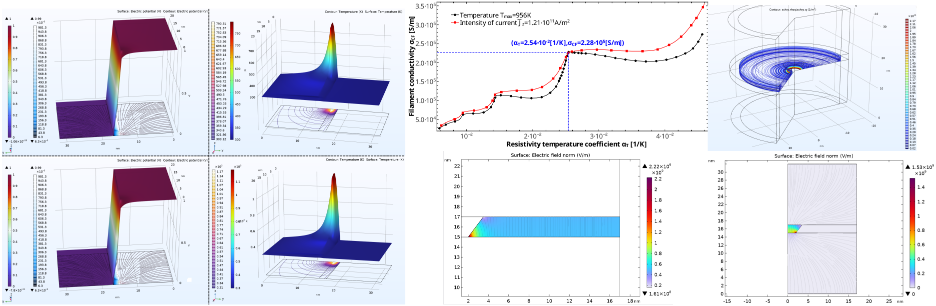
Full quantum approach: MATLAB function



Mesh quality: minimum element quality > 0.75



RESULTs & CONCLUSIONs



There are important differences in temperatures

In a nano-sized device, we should not expect high accuracy from a classical descriptor.

Simulations allow characterization

Fundamental parameters of a RRAM memory filament can be obtained from the combination of experimental data and simulation results.

THANK YOU ALL

People

- Infinite thanks to my very dear wife Galya for her generosity given the time this master has stolen from her.
- I want to thank my colleagues Miloslav and Lukas for their understanding and the time they have allowed me to dedicate to this Master.
- I would also like to thank the commendable work of my doctoral student Cristina, from the UGR in collecting data on materials.

MUCOM 2021/2022

Thank you for your attention!

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