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Special SEE Session:

The MuElec extension for
microdosimetry in silicon

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Geant4 Space Users Workshop, Barcelona - 03/05/2013

Context and motivation

Brief description of the theory

Implementation in Geant4: The MuElec extension

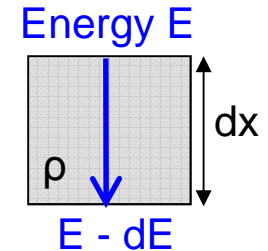
Some validation/verification results

Proton track simulation in Geant4

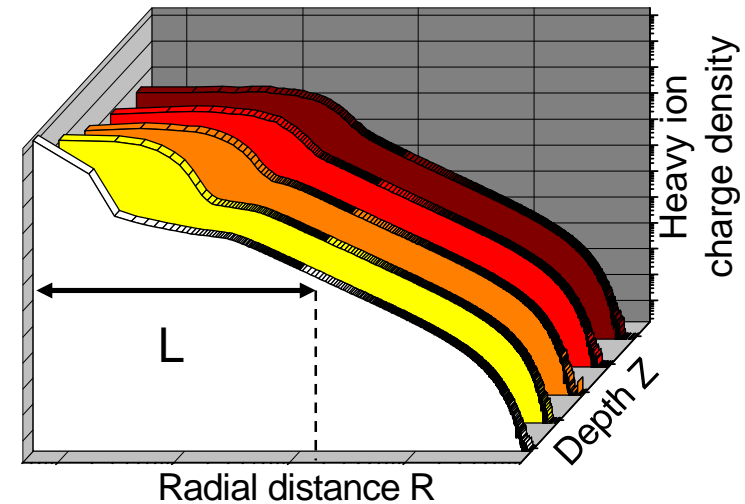
Conclusion and Perspectives

CONTEXT: Need to take into account radial dimension of the ion track

- Test for SEE sensitivity: measure of the SEE cross section vs. LET
- LET = Linear Energy Transfer $LET = -\frac{1}{\rho} \frac{dE}{dx}$
- ⇒ Assume same LET = same effect.



- Vary with depth Z, penetration into matter
⇒ Energy deposition = f(Z).
- But also radial dimension R of ion track
⇒ Energy deposition = f(Z,R).
- Decreasing size of components L
⇒ $L < 0.25 \mu\text{m} \Rightarrow L \sim R$ or $L < R$

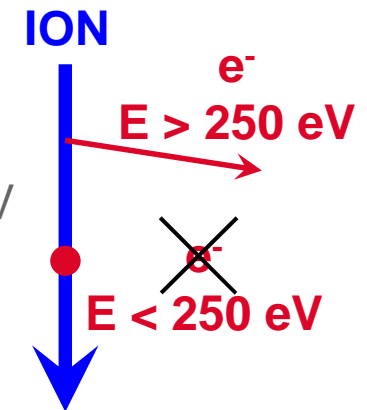


⇒ Heavy-ion induced SEE simulation in advanced devices requires the accurate description of radial ionization profiles.

- Heavy-ion induced SEE simulation in advanced devices requires the accurate description of radial ionization profiles.
- Geant4 = adequate tool to simulate ion tracks
 - Successfully used in combination with TCAD [1] or SEE prediction tool [2]
 - Down to the 32 nm node.

- Inherent limits in Geant4 ionization models (Livermore):
 - Recommended secondary production threshold at 250 eV
 - Limits the accuracy of ion track below 10 nm in radius

⇒ **Need for more accurate Geant4 ionization models !**



- Since 2010, development of the “**MuElec**” (μ -electronics) extension in Geant4 for microdosimetry in silicon

⇒ **Part of Geant4 since release 9.6 beta (June 2012).**

[1] Raine *et al.*, IEEE TNS, vol. 57, 2010.

[2] Raine *et al.*, IEEE TNS, vol. 58, 2011.

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BRIEF DESCRIPTION OF THE THEORY

- Calculation of **ionizing cross-section** for the **generation of electrons by incident electrons, protons and heavy ions**:

- Based on the Complex Dielectric Function Theory (CDFT).
- Using the procedure described by Akkerman *et al.* [1].

- **CDFT basic quantity: Energy Loss Function**

$$\text{ELF}(\hbar\omega, \vec{q}) = \text{Im} \left[\frac{-1}{\varepsilon(\omega, \vec{q})} \right]$$

- Differential Cross Section:

$$\frac{d\sigma}{d(\hbar\omega)}(E, \hbar\omega) = \frac{1}{\pi N a_0 E} \int_{q_-}^{q_+} \text{ELF}(\hbar\omega, \vec{q}) \frac{dq}{q}$$

- Total Cross Section:

$$\sigma(E) = \int_0^{\frac{E+E_b}{2}} \frac{d\sigma}{d(\hbar\omega)} d(\hbar\omega)$$

Different q_{\pm} depending on incident particle: e^- or proton/heavy ion

- Stopping power:

$$S(E) = N \int_0^{E/2} \hbar\omega \frac{d\sigma}{d(\hbar\omega)} d(\hbar\omega)$$

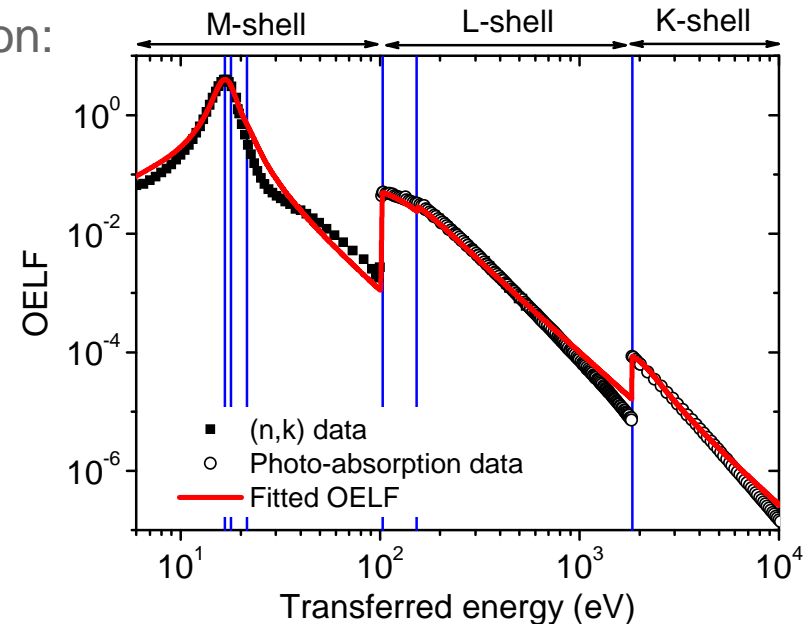
[1] Akkerman *et al.*, NIM B, vol. 227, 2005.

BRIEF DESCRIPTION OF THE THEORY

■ Determination of the Energy Loss Function:

- Optical ELF (OELF): ELF at $q = 0$.
- Determined from optical exp. data
- Fitted with a sum of Drude functions

- Extension at $q \neq 0$: $E_j(q) = E_j + \frac{\hbar^2 q^2}{2m_e}$



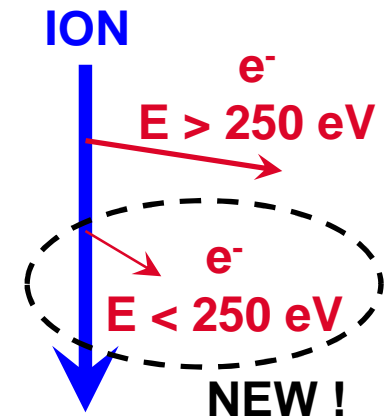
■ 6 cross-sections, allowing to distinguish 6 different ionizing interactions:

- Plasmon excitation,
- Ejection of an electron from the 5 Si electronic shells:

M1 (3s), M2 (3p), L1 (2s), L2 (2p) and K (1s) shells.

- All calculation details in:
 - A. Valentin, *et al.*, "Geant4 physics processes for microdosimetry simulation: very low energy electromagnetic models for electrons in silicon", NIM B, vol. 288, pp. 66 - 73, 2012.
 - A. Valentin, *et al.*, "Geant4 physics processes for microdosimetry simulation: very low energy electromagnetic models for protons and heavy ions in silicon", NIM B, vol. 287, pp. 124 - 129, 2012.

- **No secondary production threshold energy.**
- **Discrete approach on the entire energy range:** explicit simulation of all interactions on a step-by-step basis.



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IMPLEMENTATION IN GEANT4: THE MUELEC EXTENSION

DESCRIPTION OF THE MUELEC EXTENSION

- Based on the existing Geant4-DNA framework (see previous presentation), which uses the same initial theory (CDFT) in liquid water.
- MuElec extension:
 - In \$G4INSTALL/source/processes/electromagnetic/lowenergy
 - 4 classes (2 processes, one model each)

Process	Interaction	Particle	Energy range
G4MuElecInelastic	Ionization	e ⁻	16.7 eV - 100 MeV
		Proton Heavy ion	50 keV/amu - 1 GeV/amu
G4MuElecElastic	Elastic scattering	e ⁻	16.7 eV - 100 MeV

- 2 additional classes: G4MuElecCrossSectionDataSet
G4MuElecSiStructure
- Tabulated total and differential cross sections in data files G4EMLOW6.32

[1] Akkerman *et al.*, NIM B, vol. 227, 2005.

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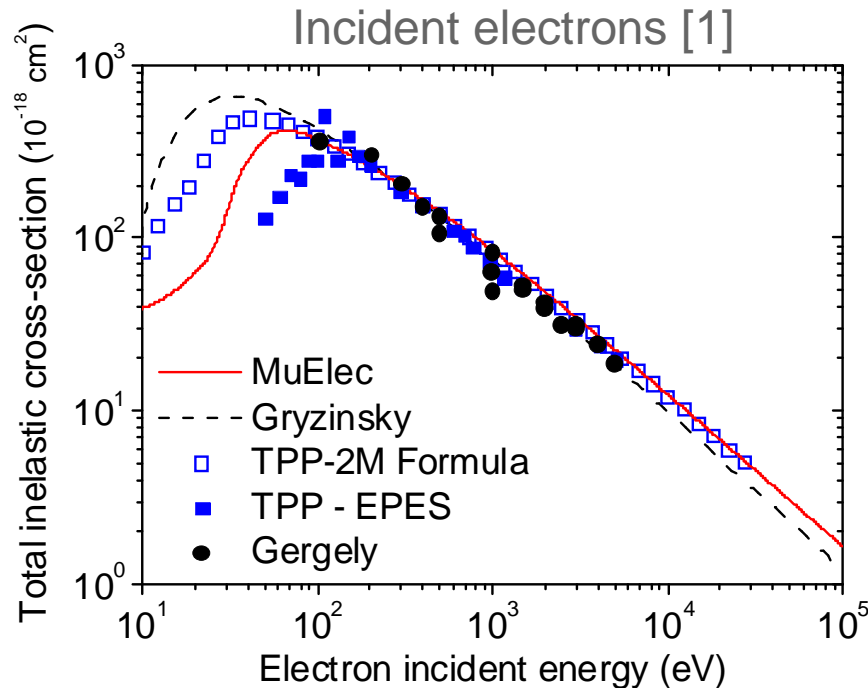
➤ **Some validation results**

Proton track simulation

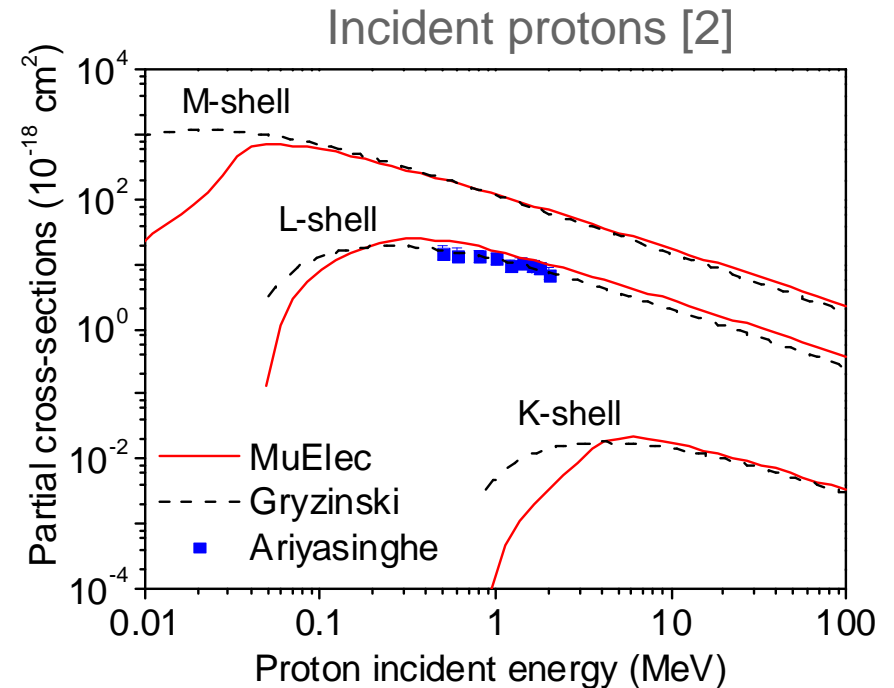
Conclusion and Perspectives

SOME VALIDATION RESULTS

■ Inelastic cross-section



⇒ Satisfying agreement with data from literature > **50 eV**

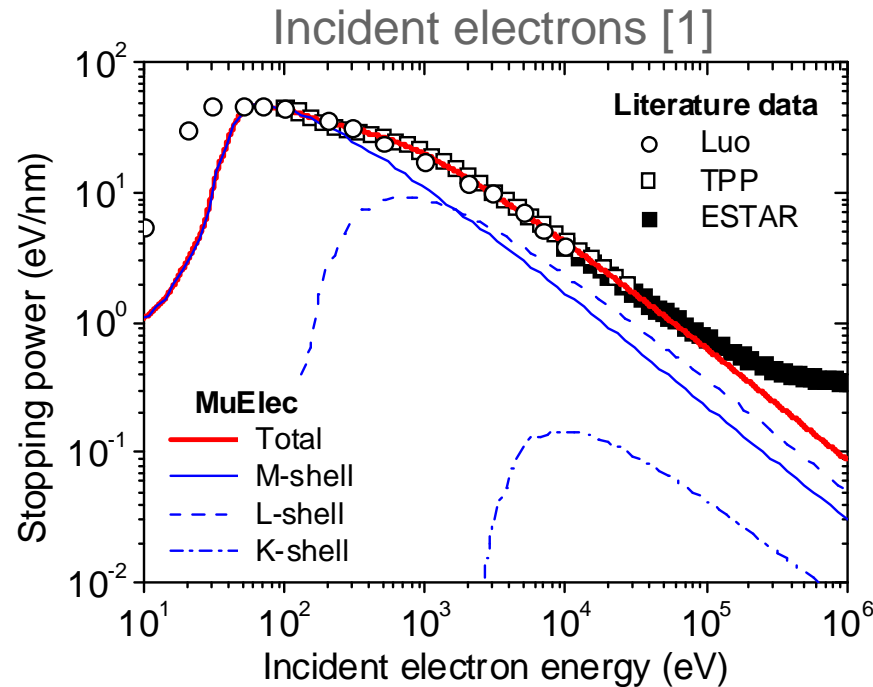


⇒ Satisfying agreement with data from literature > **50 keV**

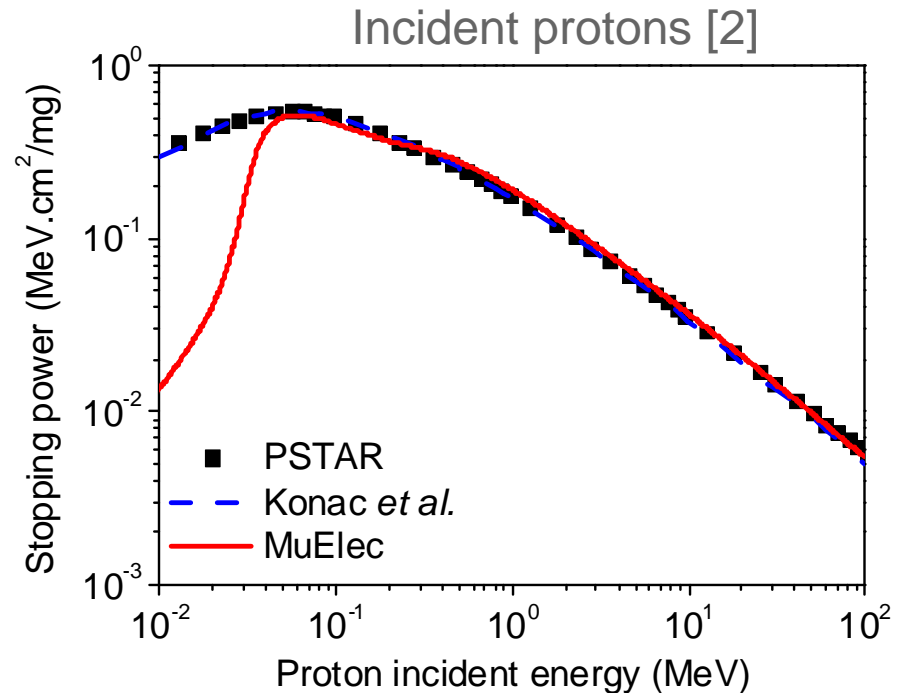
For more detailed discussion and validations: [1] A. Valentin, *et al.*, NIM B, vol. 288, pp. 66 - 73, 2012.

[2] A. Valentin, *et al.*, NIM B, vol. 287, pp. 124 - 129, 2012.

Stopping power



⇒ Satisfying agreement with data from literature > 50 eV and < 50 keV

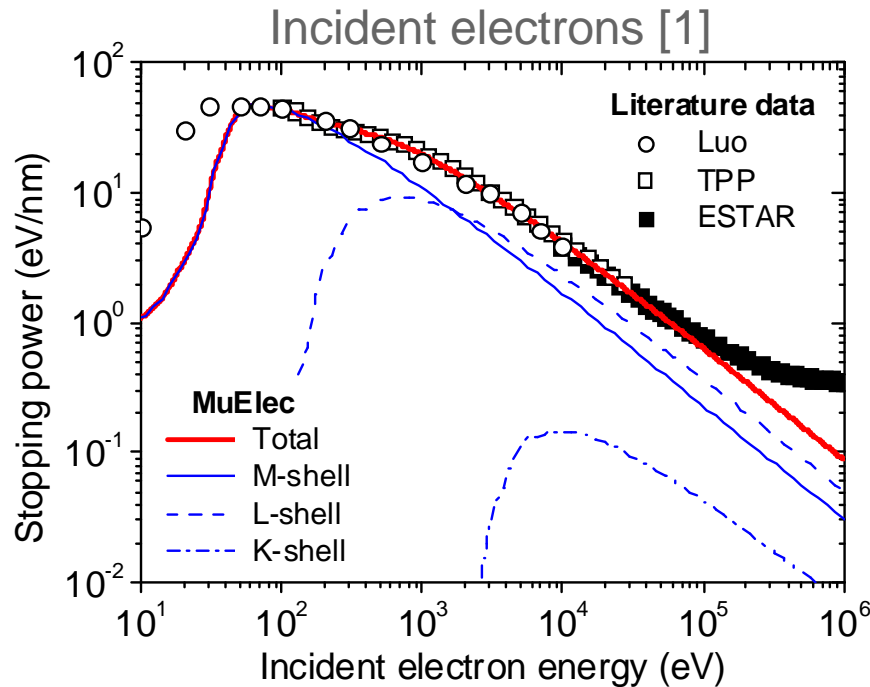


⇒ Satisfying agreement with data from literature > 50 keV

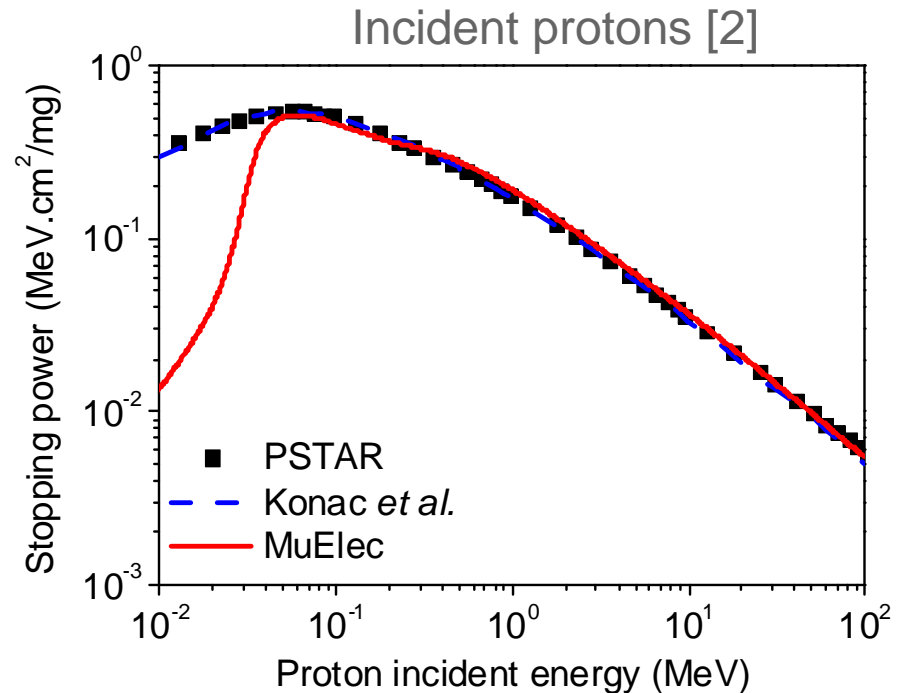
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Stopping power



⇒ Satisfying agreement with data from literature > 50 eV and **< 50 keV**



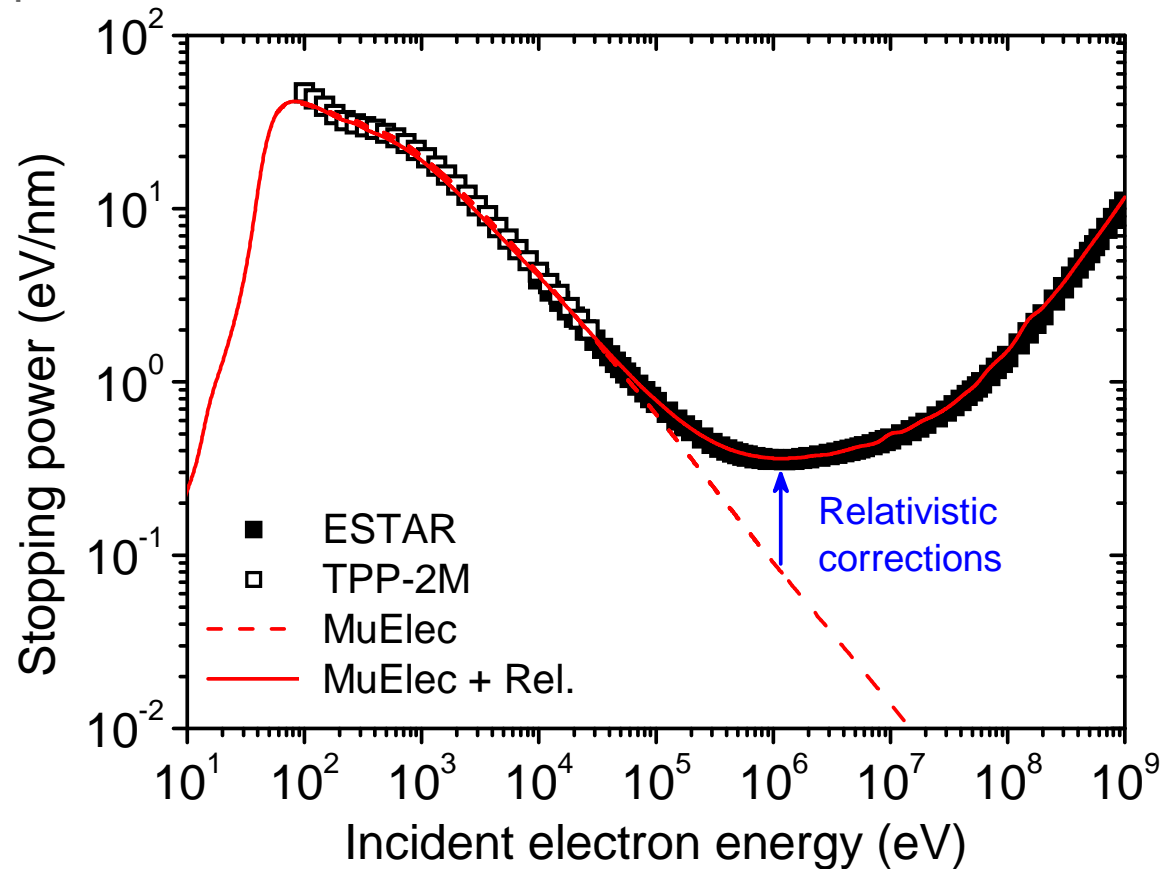
⇒ Satisfying agreement with data from literature > 50 keV

< 23 MeV

For more detailed discussion and validations: [1] A. Valentin, *et al.*, NIM B, vol. 288, pp. 68 - 75, 2012.

[2] A. Valentin, *et al.*, NIM B, vol. 287, pp. 124 - 129, 2012.

- Including relativistic corrections:
 - Up to 1 GeV/amu for protons and heavy ions
 - Up to 100 MeV for electrons



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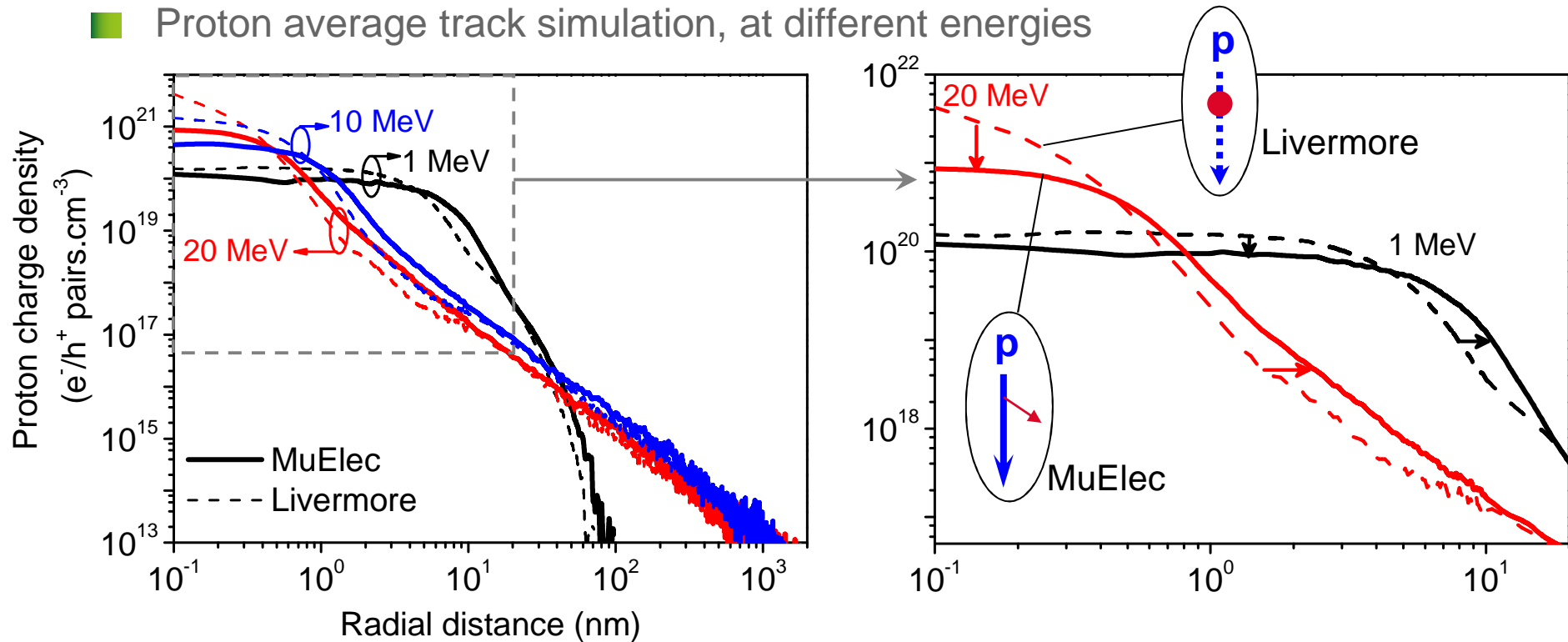
Some validation results

➤ **Proton track simulation in Geant4**

Conclusion and Perspectives

PROTON TRACK SIMULATION IN GEANT4

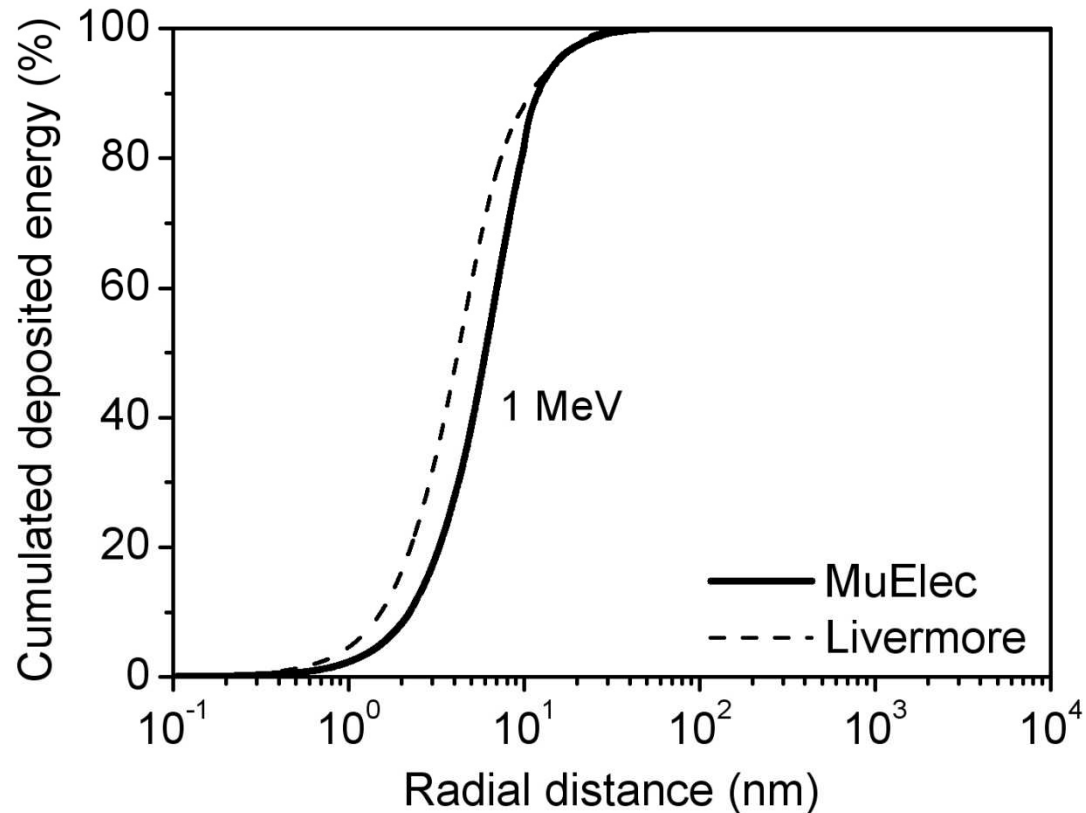
- Comparison between the **MuElec** extension and existing Geant4 models (**G4EmLivermorePhysics** physics list).
- Proton average track simulation, at different energies



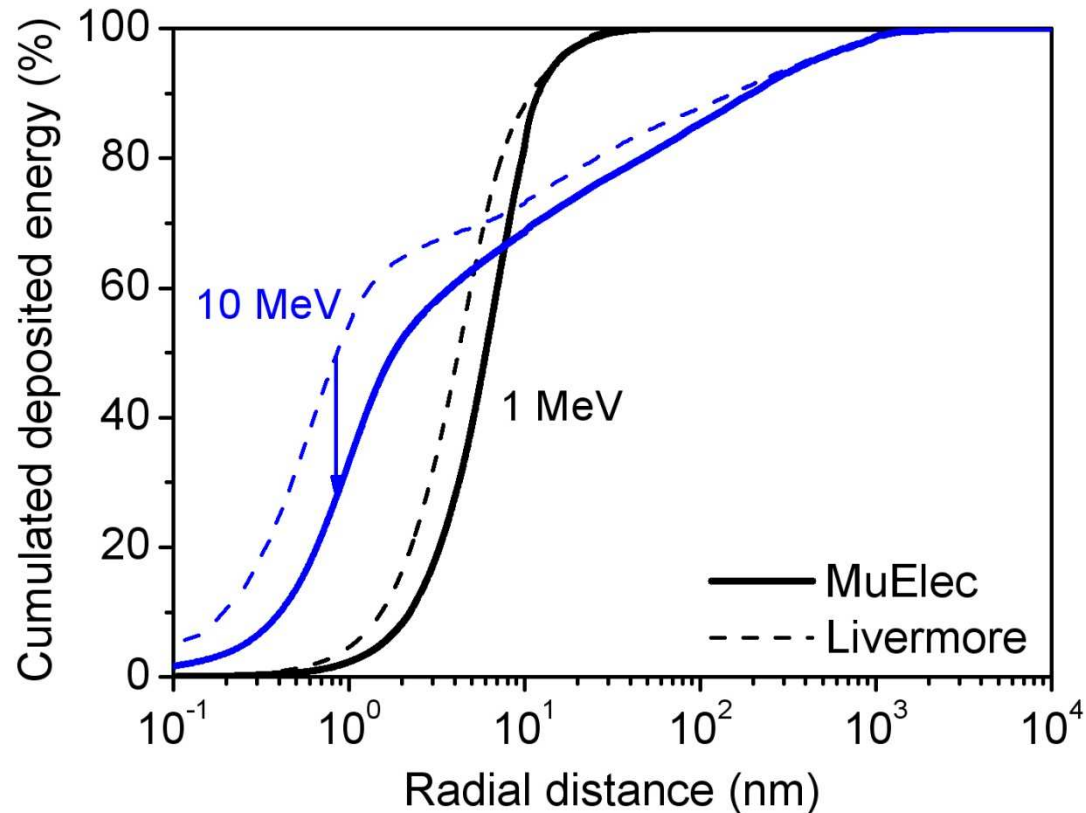
- As expected, main differences between models in the first 10 nm.

PROTON AND ION TRACK SIMULATION IN GEANT4

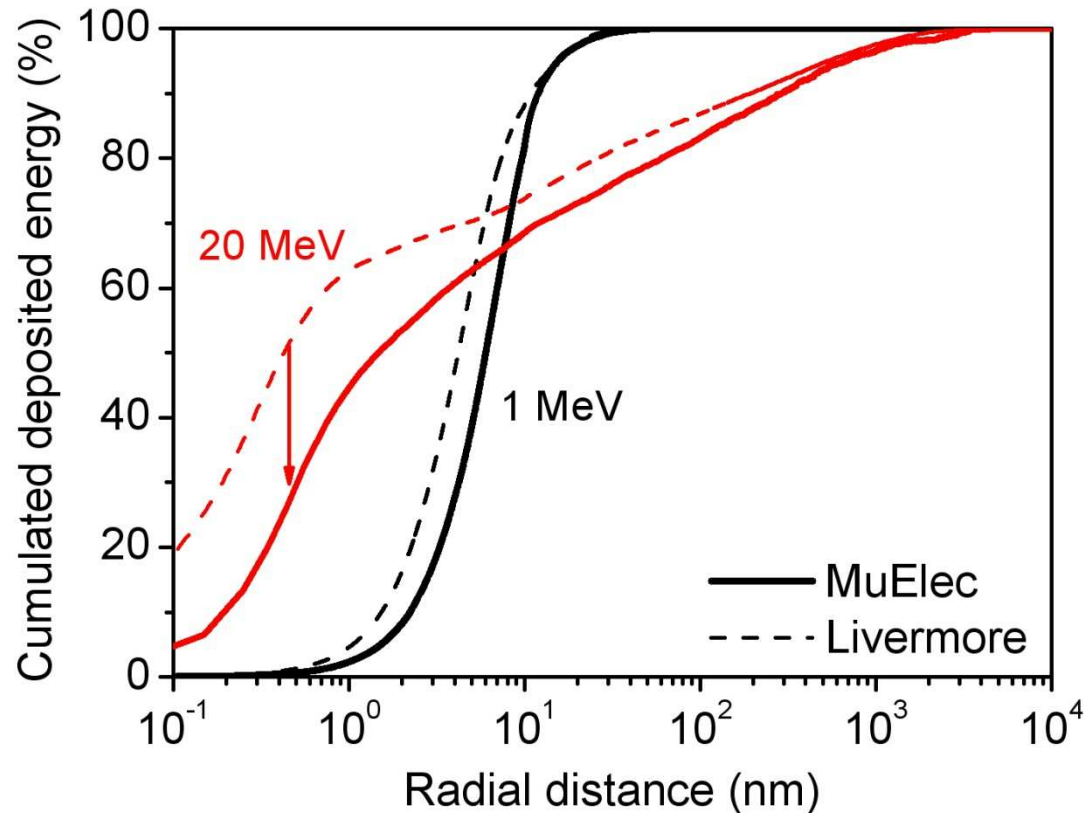
- As expected, main differences between models in the first 10 nm.
- Cumulated deposited energy:



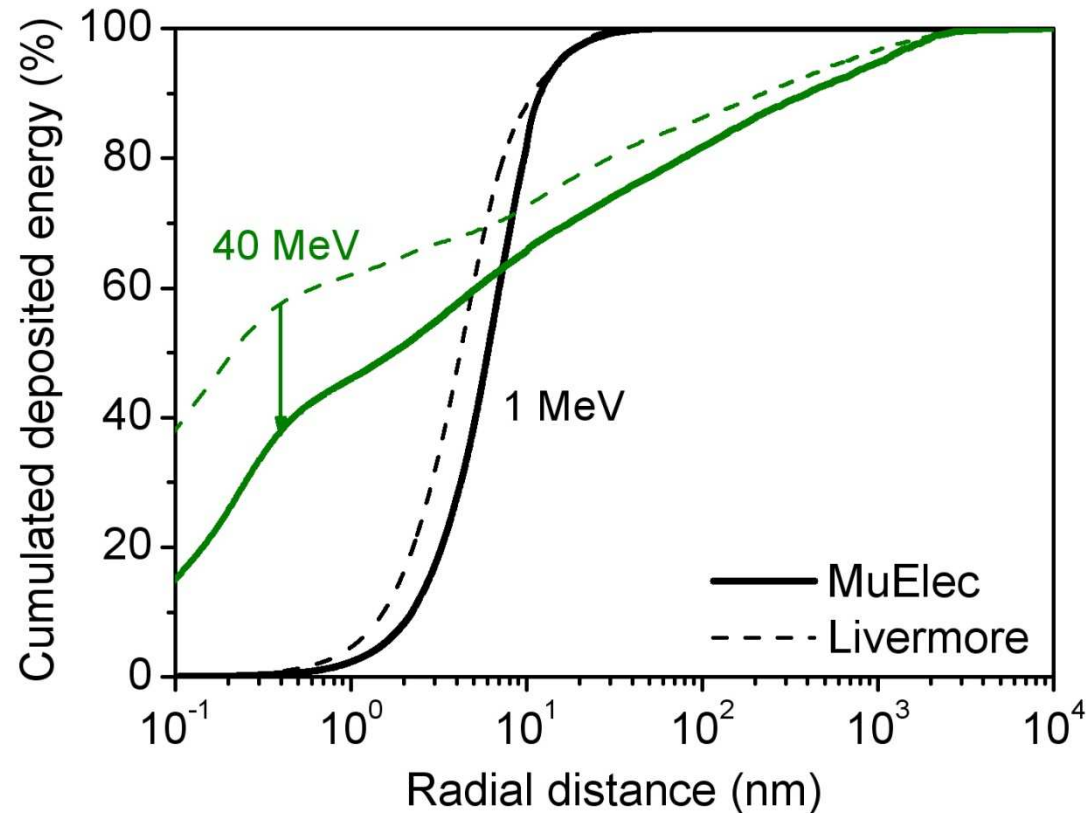
- As expected, main differences between models in the first 10 nm.
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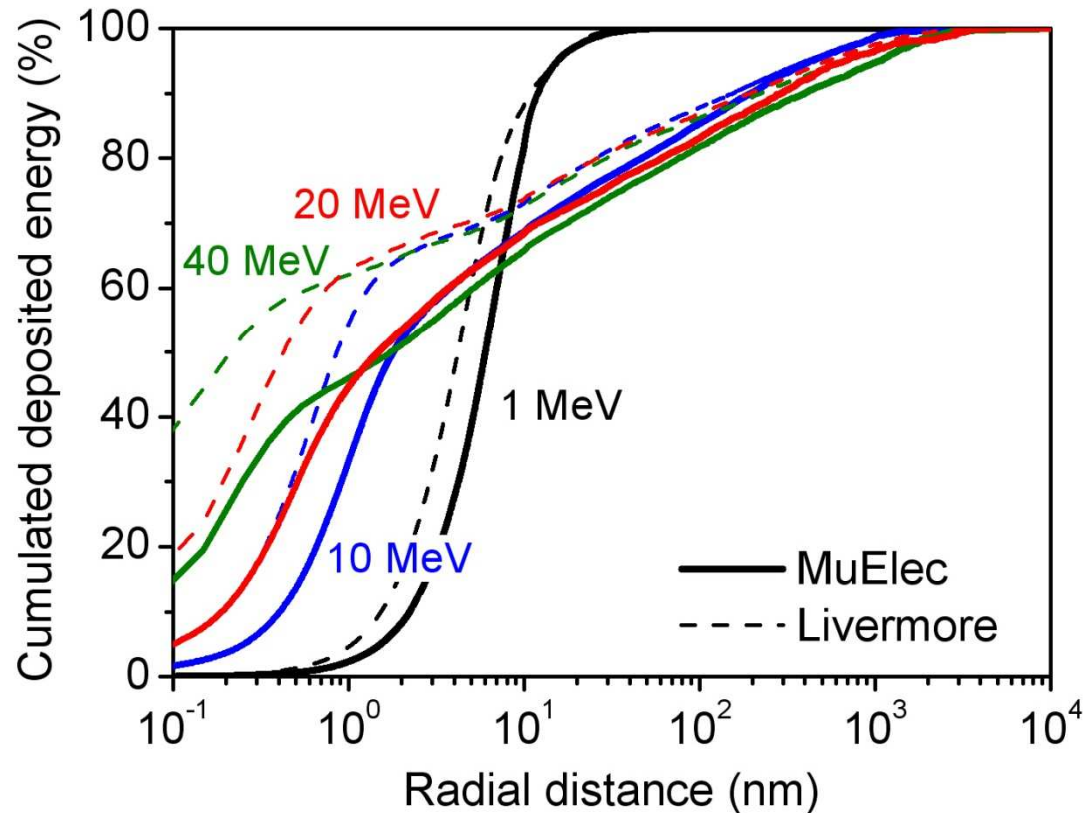
- As expected, main differences between models in the first 10 nm.
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- As expected, main differences between models in the first 10 nm.
- Cumulated deposited energy:



- As expected, main differences between models in the first 10 nm.
- Cumulated deposited energy:



- Increasing difference with increasing energy, located in the first 2-3 nm.
- ⇒ **First application results presented at NSREC (July 2012).**

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CONCLUSION AND PERSPECTIVES

- New Geant4 ionization models: “**MuElec**” extension.
- Explicit **generation of very low energy electrons**, down to 16.7 eV.

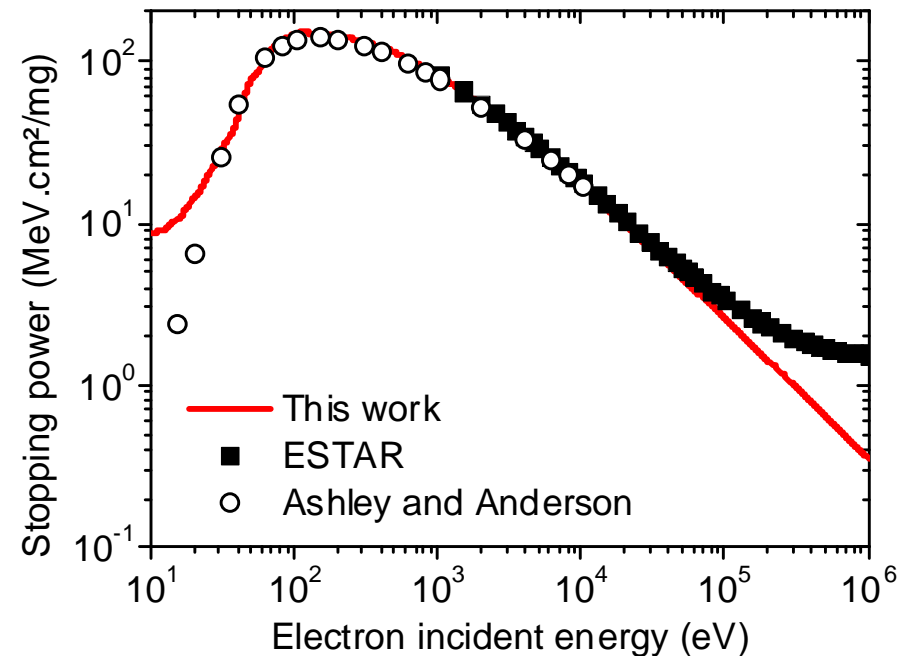
- Validated in comparison with data from literature:
 - e⁻: 50 eV - 100 MeV
 - Proton/heavy ions: 50 keV/amu - 1 GeV/amu

- Two published articles describing theory, Geant4 implementation, validation/verification results
- One application article in IEEE TNS, Dec. 2012.

- MuElec web page: Accessible from the web page of the LowE EM WG
<https://twiki.cern.ch/twiki/bin/view/Geant4/LoweMuElec>

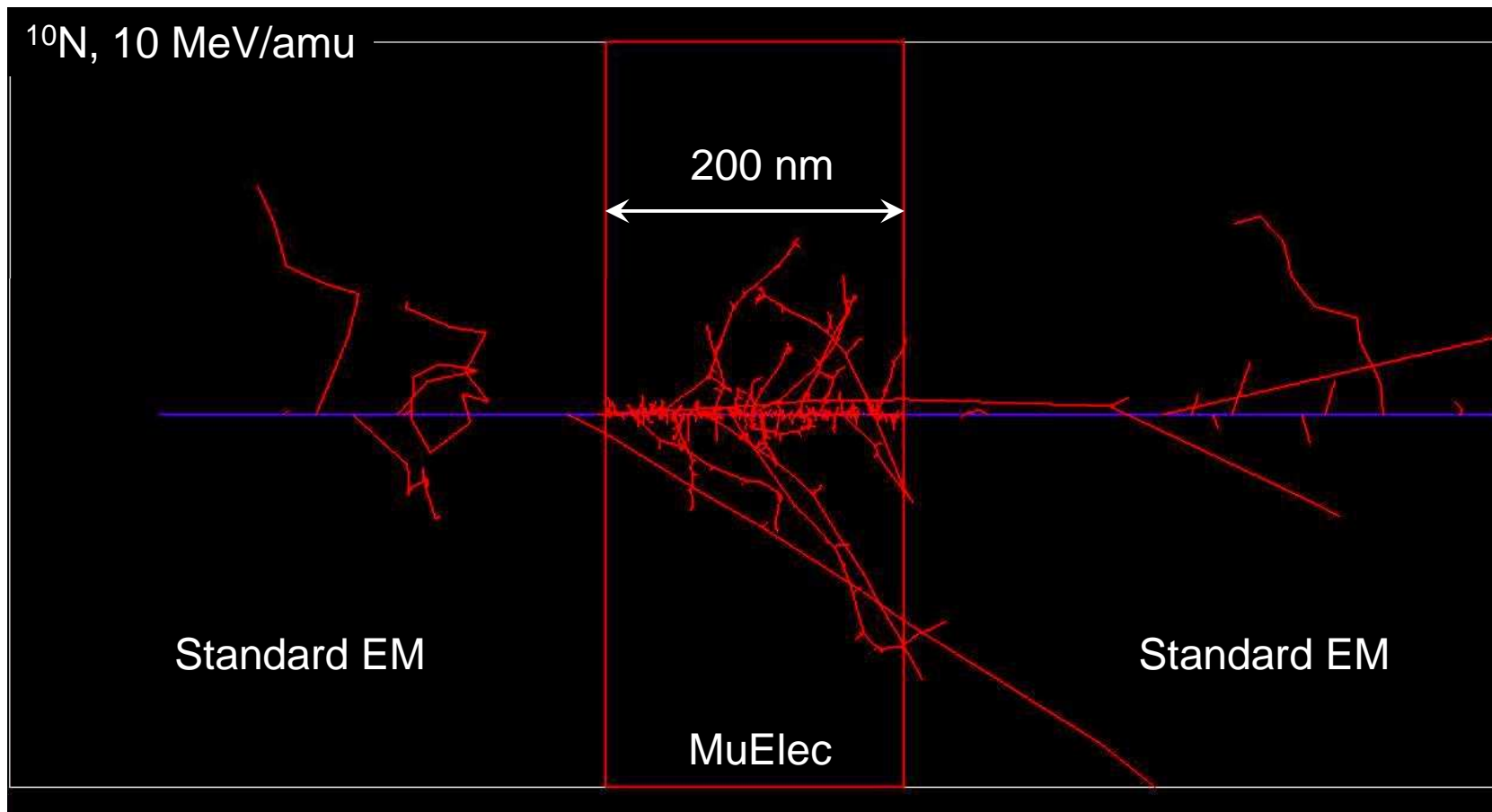
PERSPECTIVES: Extension to other materials

- SiO_2 in progress
 - Preliminary calculations performed



- Need for additional validation
 - To be implemented in Geant4
- In contact with other teams to develop MuElec for additional materials: dielectrics (ONERA), gold (MGH)

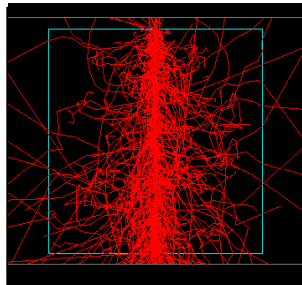
- Release of a user example and a dedicated physics constructor to show how to combine Standard EM or Low Energy EM processes with MuElec Physics processes (similar to **microdosimetry** example)



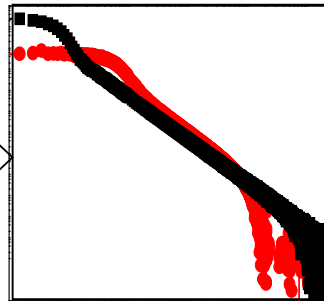


MuElec and G4EmLivermorePhysics tracks in TCAD simulations

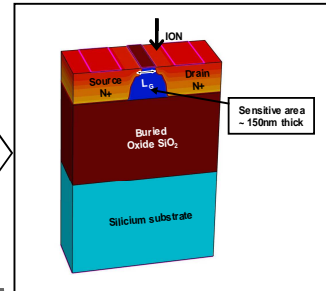
Geant4
Simulation
(Monte Carlo)



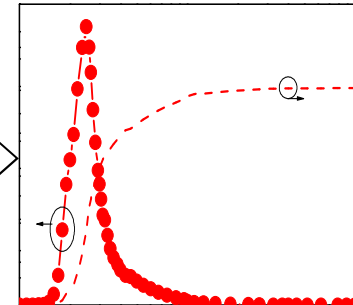
Track structure



Synopsys
Simulation



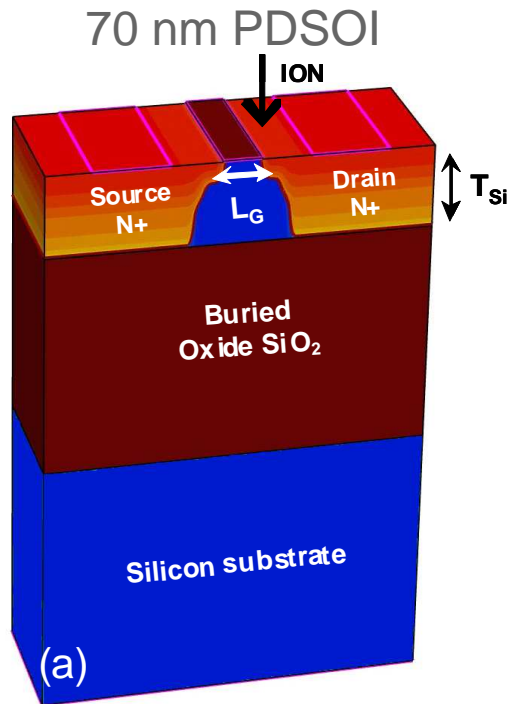
Response of the
transistor
(isolated device)



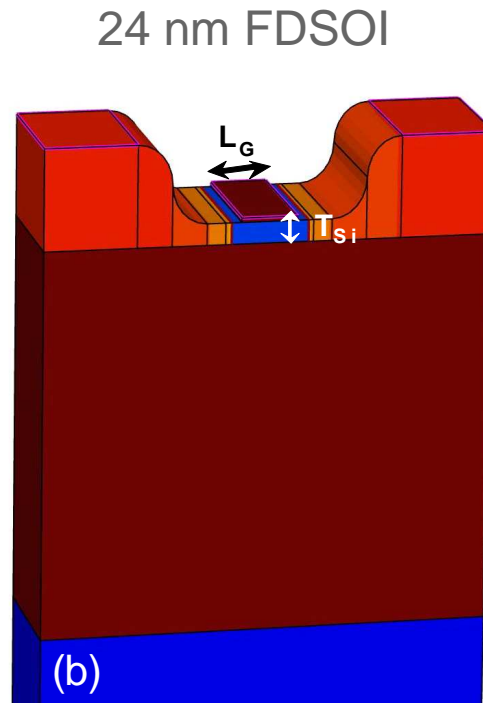
Particle-matter interaction

TCAD Simulation

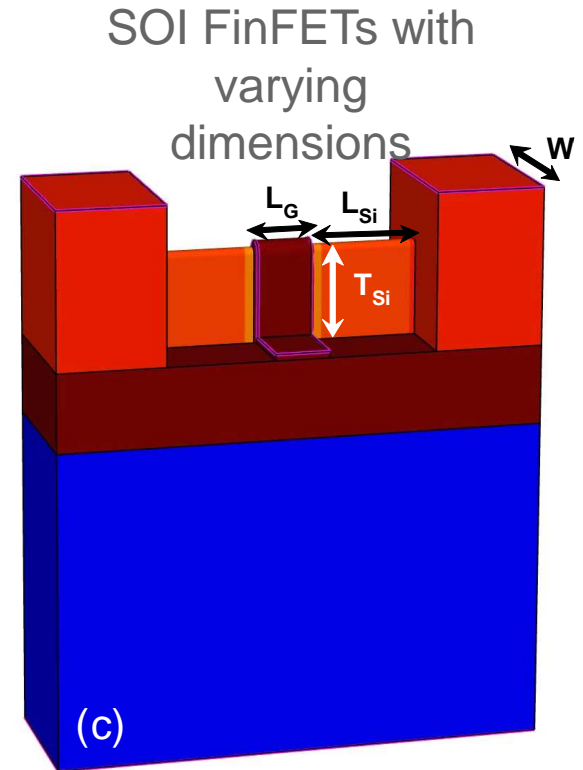
- ^{78}Kr ions, different energies: 5, 10, 15 and 23 MeV/amu + 40 MeV/amu
- Different transistor structures



$L_G = 70 \text{ nm}$
 $T_{Si} = 150 \text{ nm}$

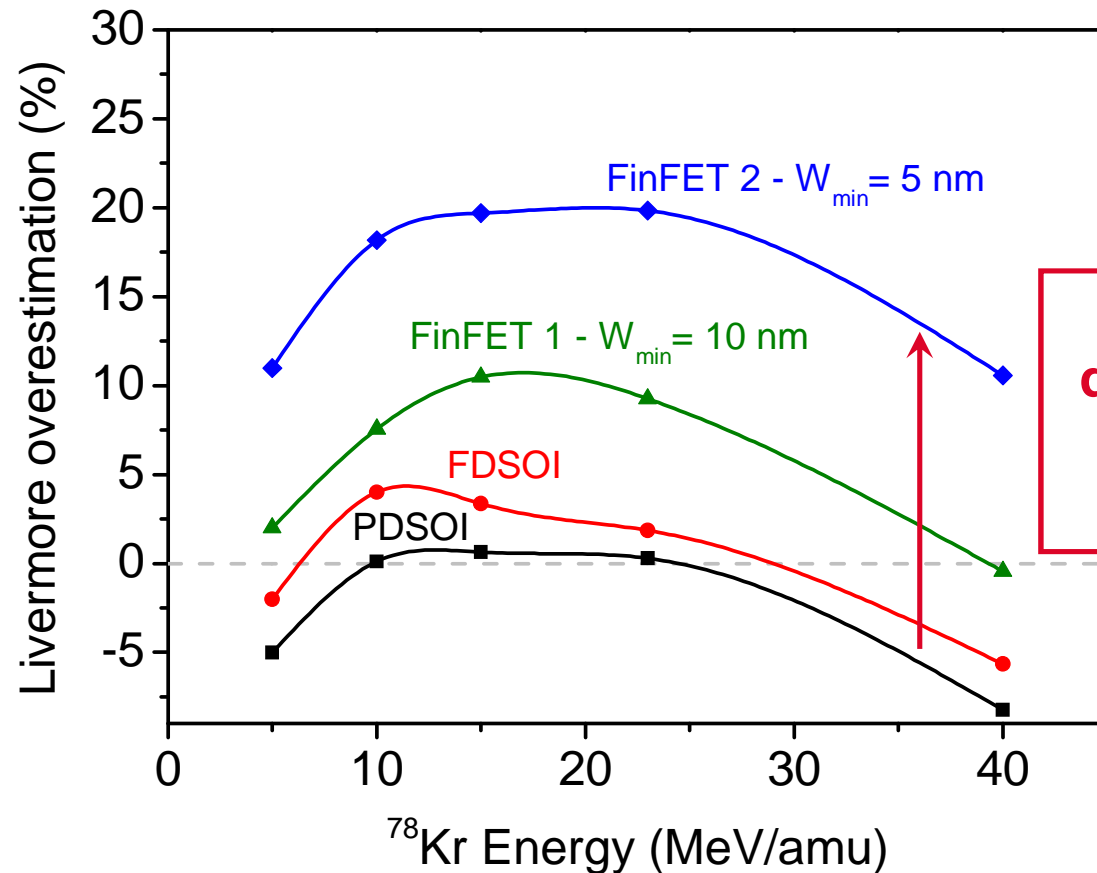


$L_G = 24 \text{ nm}$
 $T_{Si} = 8 \text{ nm}$



$L_G = 20 \text{ nm}$
 $L_{Si} = 100; 40 \text{ nm}$
 $W_{Si} = 10; 5 \text{ nm}$
 $T_{Si} = 50; 30; 12 \text{ nm}$

- MuElec and G4EmLivermorePhysics tracks in TCAD simulations
- Results as percentage difference between the two approaches:



- MuElec and G4EmLivermorePhysics tracks in TCAD simulations
- Results as percentage difference between the two approaches:

