From the *pn* junction to the UFSD design

The role of numerical simulation

9.05.2019

Marco Mandurrino, INFN Torino



- I. Overview of semiconductor devices
 - The *pn* junction
 - Low Gain Avalanche Detectors (LGAD)
- II. Electronic device modeling
 - Analytical description
 - Numerical implementation

III. LGAD design using numerical simulations

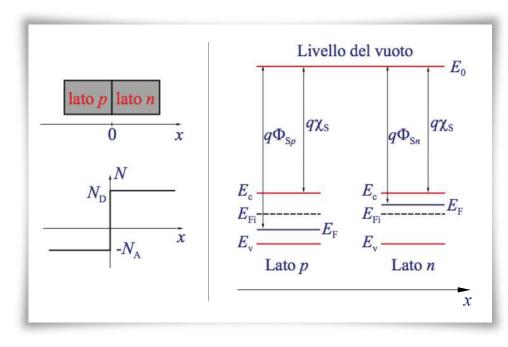


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- Definition: the *pn* junction is a semiconductor region where a *p*-type and an *n*-type doped materials are placed side by side.
- **Example:** the *abrupt junction* of two *uniformly doped* semiconductors.

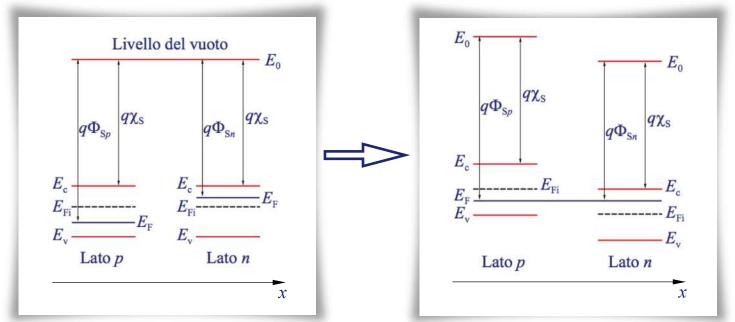


 $q\chi$ is the electronic affinity (~4.05 eV in Si) $q\Phi$ is the semiconductor work function

$$\begin{split} q\Phi_{\mathrm{S}p} &= q\chi_{\mathrm{S}} + E_{\mathrm{g}} - (E_{\mathrm{F}} - E_{\mathrm{v}}) = q\chi_{\mathrm{S}} + E_{\mathrm{g}} - k_{\mathrm{B}}T\ln\frac{N_{\mathrm{v}}}{N_{\mathrm{A}}} \\ q\Phi_{\mathrm{S}n} &= q\chi_{\mathrm{S}} + (E_{\mathrm{c}} - E_{\mathrm{F}}) = q\chi_{\mathrm{S}} + k_{\mathrm{B}}T\ln\frac{N_{\mathrm{c}}}{N_{\mathrm{D}}} \end{split}$$

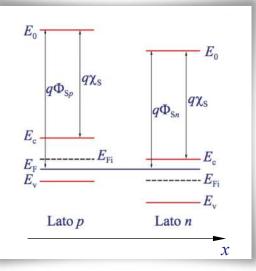
Golden-rules to compute the final band-diagram:

- 1. E_{g} and $q\chi$ are conserved by definition;
- 2. $E_{\rm F}$ must be **constant** across the junction;



3. E_0 and bands must be **continuous** functions (in space x).

- The gradient of carriers concentration produces a transient, in which electrons travel from the *n*-side to the *p*-side (the vice-versa holds for holes). This mechanism behaves as a diffusion-like dynamics
- The diffusion of free charges depletes a zone across the junction, called spacecharge region (SCR), where fixed charges (ionized atoms) are no more compensated by free charges (ρ≠0). Far from the junction, we still have compensation (neutral regions, ρ=0)

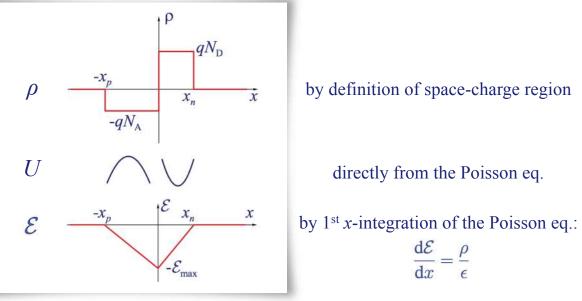


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Within the space-charge region (p≠0) the field is not a constant and bands are no more straight lines. In particular, due to the Poisson equation of semiconductors

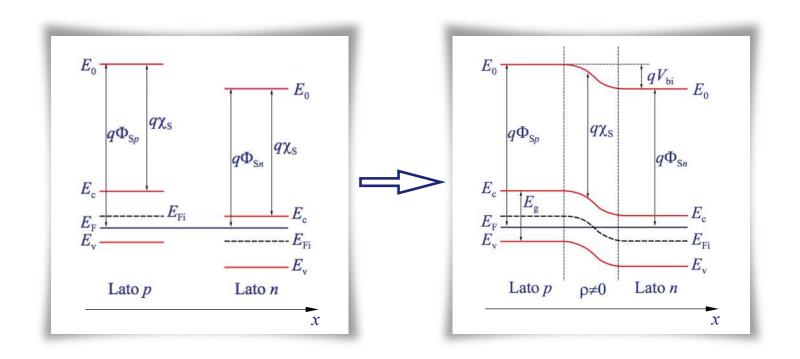
$$\frac{\mathrm{d}^2 U}{\mathrm{d}x^2} = q\frac{\rho}{\epsilon}$$

where $U = -q\varphi$ is the *potential energy* felt by free charges, we have

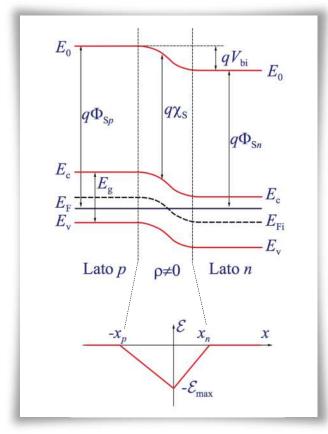


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• So, finally we have:



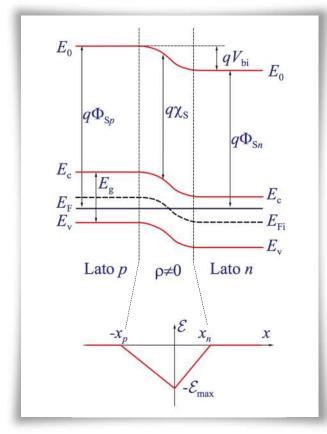
What we concluded has several important physical implications:



- 1. $\mathcal{E} \neq 0$ implies the onset of a **drift current** of carriers tending to **compensate the diffusion** of free charges such that J = 0;
- 2. A **built-in potential** qV_{bi} , created across the junction, represents an additional **barrier for the diffusion** of electrons towards the *p*-side (and holes in the *n*-side)

$$qV_{bi} = q\Phi_{Sp} - q\Phi_{Sn} = E_g - k_B T \ln \frac{N_v N_c}{N_A N_D}$$
$$= k_B T \ln \frac{N_v N_c}{n_i^2} - k_B T \ln \frac{N_v N_c}{N_A N_D}$$
$$= k_B T \ln \frac{N_A N_D}{n_i^2}$$

What we concluded has several important physical implications:



3. By integrating the Poisson equation, and thanks to the *neutrality law* $N_A x_p = N_D x_n$, one has

$$\mathcal{E}(x) = \begin{cases} -\frac{qN_{\mathrm{A}}}{\epsilon}(x+x_p) & -x_p \le x < 0\\ \frac{qN_{\mathrm{D}}}{\epsilon}(x-x_n) & 0 \le x < x_n \end{cases}$$

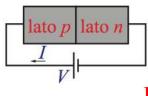
and

$$\mathcal{E}_{\max} = \frac{qN_{\mathsf{A}}}{\epsilon} x_p = \frac{qN_{\mathsf{D}}}{\epsilon} x_n$$

4. In the same way:

$$\varphi(x) = \begin{cases} \frac{qN_{\mathbf{A}}}{2\epsilon}(x+x_p)^2 & -x_p \le x < 0\\ -\frac{qN_{\mathbf{D}}}{2\epsilon}(x-x_n)^2 + \frac{qN_{\mathbf{A}}}{2\epsilon}x_p^2 + \frac{qN_{\mathbf{D}}}{2\epsilon}x_n^2 & 0 \le x < x_n \end{cases}$$

> What happens if the junction is no more at equilibrium?



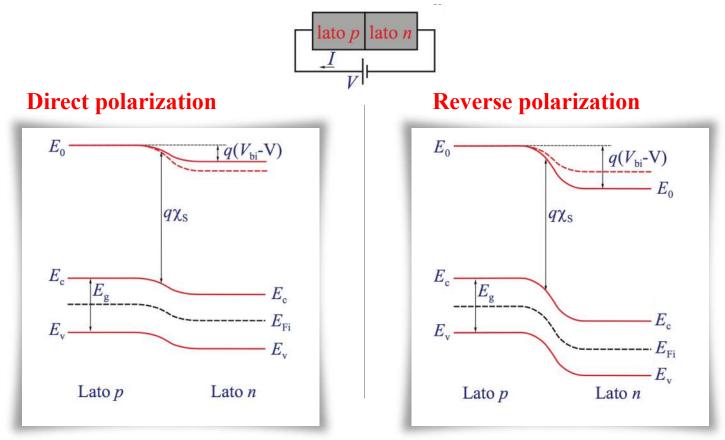
Direct polarization

- V > 0, I > 0
- J_{diff} dominates
- electrons from *n* to *p*-side
- holes from *p* to *n*-side
- $qV < qV_{bi}$

Reverse polarization

- *V* < 0, *I* < 0
- *J*_{drift} dominates
- electrons from *p* to *n*-side
- holes from *n* to *p*-side
- $qV > qV_{bi}$

> What happens if the junction is no more at equilibrium?

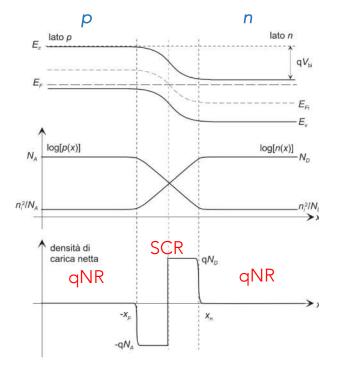


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• *pn* junction at **equilibrium**:

$$V_{\rm bi} = V_T \log \frac{N_{\rm A} N_{\rm D}}{n_{\rm i}^2}$$

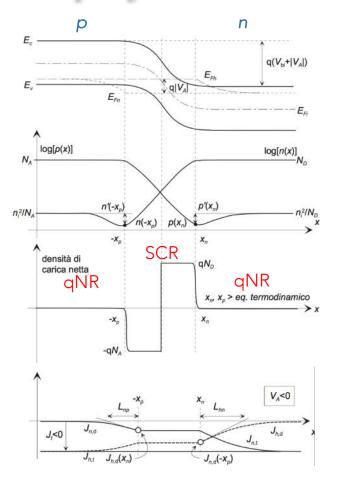
$$p_{p0}(-x_p) = N_{A}$$
 $p_{n0}(x_n) = n_i^2/N_{D}$
 $n_{n0}(x_n) = N_{D}$ $n_{p0}(-x_p) = n_i^2/N_{A}$



pn junction in reverse polarization:

$$n'_p = n_p - n_{p0}$$
 $p'_n = p_n - p_{n0}$ < 0

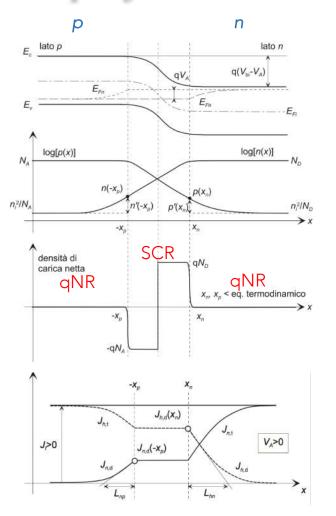
- V_{bias} < 0, I < 0
- *J*_{drift} dominates
- electrons from p- to n-side
- holes from n- to p-side
- $qV_{bias} > qV_{bi}$



• *pn* junction in **forward polarization**:

$$n'_p = n_p - n_{p0}$$
 $p'_n = p_n - p_{n0}$ > 0

- V_{bias} > 0, I > 0
- J_{diff} dominates
- electrons from n- to p-side
- holes from p- to n-side
- $qV_{bias} < qV_{bi}$





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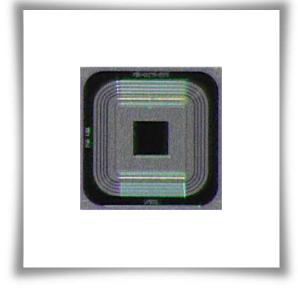
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Towards a technological step...

first *n-p-n* "tip"-transistor

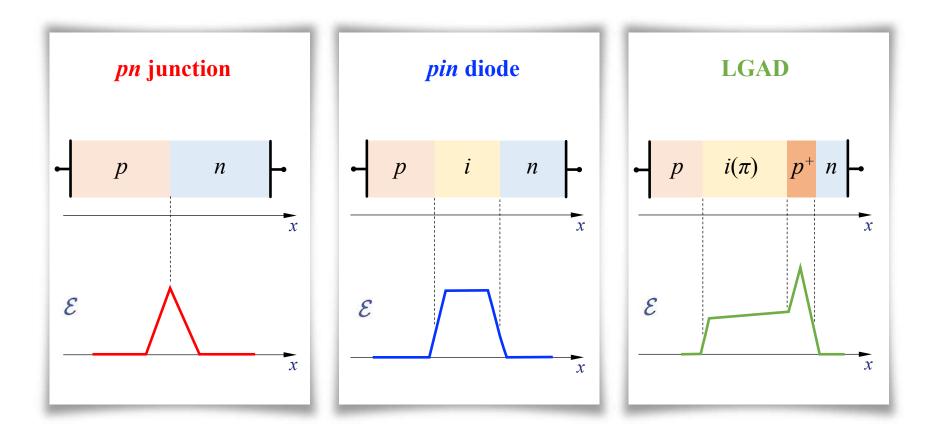


Ultra Fast Silicon Detector

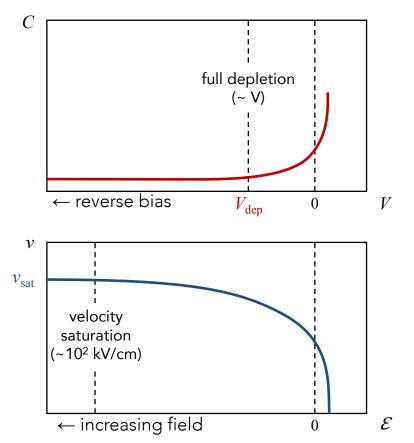


J. Bardeen, W. Brattain, W. Shockley Bell Labs. - NJ (1948) UFSD Group INFN Torino and FBK Trento (2018)

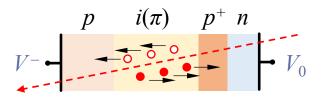
Extending our application domain to other systems



• How large the **external biasing voltage** has to be?



What is charge multiplication in LGAD?



- Primary charges (electron/hole pairs) are produced by ionization, while the particle is crossing the sensor;
- Due to the reverse field, electrons drift towards the *n*-side and holes towards the *p*-side;
- When electrons travel along the *p*⁺ region (the *gain* or *multiplication*-layer) they experience an high field;
- This field is responsible for the impact ionization, which produces an avalanche multiplication of secondary charges;
- Now the **total current** is due to the **additional avalanche contribution**.

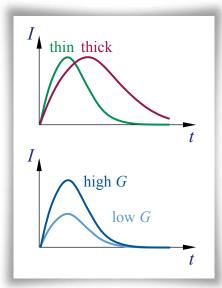
> Why using LGAD to detect particles at CERN?

I. We need charge multiplication:

- 1. LGAD exploit the so-called **avalanche multiplication**, a process which belongs to the class of **generation/recombination (GR) mechanisms**;
- 2. Charge multiplication allows to obtain large and fast signals:
 - the **thinner** the sensor, the **faster** the signal;
 - the higher the gain, the larger the signal.

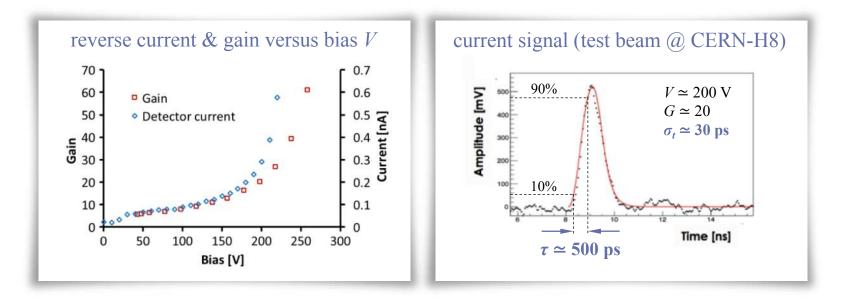
II. We need a good S/N:

- 1. Also the noise related to the current signal is proportional to the gain
- 2. The gain G has to be kept as low as required by electronics ($G \sim 10-20$)



► Why using LGAD to detect particles at CERN?

Examples of 50 µm LGAD performance:



Can we predict the avalanche contribution to the total current?

Let's introduce a bit of physical-mathematics...

- 1. The avalanche process is modeled via its ionization coefficient α , i.e. the inverse of the electron/hole mean free path (cm⁻¹);
- 2. In the literature, several expressions of α are available. In general, all of them are based on the Chynoweth's theory (1958), according to which:

$$lpha_{n,p}(\mathcal{E}) = \gamma A_{n,p} \exp\left(-\gamma rac{B_{n,p}}{\mathcal{E}}
ight)$$

3. Once the coefficient has been obtained, one has to evaluate the **net** avalanche generation rate U_{aval} , i.e. the number of multiplied e⁻/h⁺ pairs per volume (cm⁻³) per unit time (s⁻¹), as:

$$U_{\text{aval}} = rac{\mathrm{d}n}{\mathrm{d}t} = rac{\mathrm{d}p}{\mathrm{d}t} = lpha_n n v_n + lpha_p p v_p$$

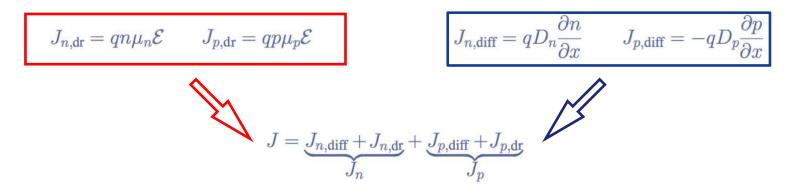
... Now we need a complete description of the system!



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- We recall the **twofold nature of the current** in a semiconductor device:
 - *a.* **Drift current**, driven by the *electric field*;
 - b. Diffusion current, due to the density gradient of *free charges*.



• Then we introduce (all) the **GR mechanisms** through their **net rates** *U*:

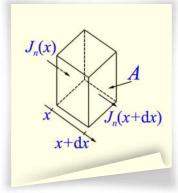
$$U_n = R_n - G_n \qquad \qquad U_p = R_p - G_p$$

$$\approx \frac{n - n_0}{\tau_n} = \frac{n'}{\tau_n} \qquad \qquad \approx \frac{p - p_0}{\tau_p} = \frac{p'}{\tau_p}$$

- To derive the **global current density** (field + charge + GR):
 - 1. in a volume dV = Adx the time variation of the electron density (similarly for holes) is

field + charge GR

$$\frac{\partial n}{\partial t}Adx = \frac{J_n(x)}{-q}A - \frac{J_n(x+dx)}{-q}A + G_nAdx - R_nAdx$$



2. by using the 1st-order Taylor series expansion

$$J_n(x + \mathrm{d}x) \approx J_n(x) + \frac{\partial J_n}{\partial x} \,\mathrm{d}x$$

and assuming $dx \rightarrow 0$, we obtain the **continuity equations**:

$$\frac{\partial n}{\partial t} = -\frac{1}{q} \frac{\partial J_n}{\partial x} - U_n \qquad \frac{\partial p}{\partial t} = -\frac{1}{q} \frac{\partial J_p}{\partial x} - U_p$$

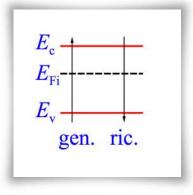
Since the drift component depends on the electric field, we need a third equation to close the system, the Poisson equation, which connects the *field* to the *charge densities*.

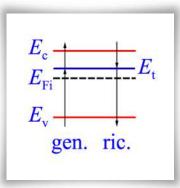
The final (1D) mathematical framework is:

continuity eqs.
$$-\int \begin{cases} \frac{\partial n}{\partial t} = \frac{1}{q} \frac{\partial J_n}{\partial x} - U_n \\ \frac{\partial p}{\partial t} = -\frac{1}{q} \frac{\partial J_p}{\partial x} - U_p \\ \frac{\partial \mathcal{E}}{\partial x} = \frac{\rho}{\epsilon} \end{cases}$$

$$\frac{\partial \mathcal{E}}{\partial x} = \frac{q\mu_n n\mathcal{E}}{\rho} + \frac{qD_n \frac{\partial n}{\partial x}}{\rho}, \quad J_p = \frac{q\mu_p p\mathcal{E}}{\rho} - \frac{qD_p \frac{\partial p}{\partial x}}{\rho} \qquad \text{TRANSPORT EQS.}$$
and $\mathcal{E} = -\frac{\partial \varphi}{\partial x}, \quad \rho = q \left(p - n + N_{\rm D}^+ - N_{\rm A}^-\right).$

- Avalanche generation is not the only GR mechanism occurring in silicon devices. In general, we have to account for two different families:
 - A. Band-to-band generation/recombination
 - Auger direct tunnelin



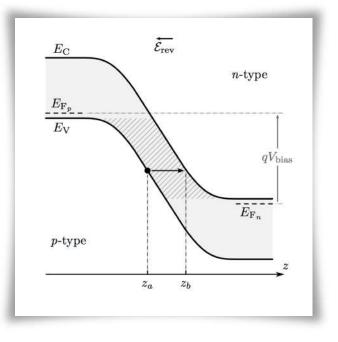


B. Defect-assisted generation/recombination

- Shockley-Read-Hall (SRH)
- o trap-assisted tunneling
- 0 ...

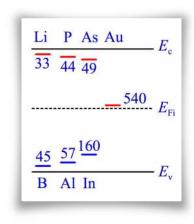
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 - A. Band-to-band generation/recombination
 - Auger
 - *direct tunneling* ...

- B. Defect-assisted generation/recombination
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- Avalanche generation is not the only GR mechanism occurring in silicon devices. In general, we have to account for two different families:
 - A. Band-to-band generation/recombination
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 - 0 ...

- B. Defect-assisted generation/recombination
 - o Shockley-Read-Hall (SRH)
 - *trap-assisted tunneling*
 - 0 ...



• SRH processes are determined by such a net rate statistics

$$U_{\rm SRH} = \frac{np - n_i^2}{\tau_p \left(n + n_i \,\mathrm{e}^{\frac{E_{\rm trap} - E_{\rm F_i}}{k_{\rm B}T}} \right) + \tau_n \left(p + n_i \,\mathrm{e}^{\frac{E_{\rm F_i} - E_{\rm trap}}{k_{\rm B}T}} \right)}$$

where $\tau_{n,p}$ are proper **electron/hole lifetimes**, i.e. the average time interval (~10⁻⁷-10⁻⁹ s) between two consecutive scattering processes originating (or annihilating) e⁻/h⁺ pairs.

Moreover, band-to-band tunneling is modeled with the usual Kane expression (1961)

 $U_{\rm tunn} = A \, \mathcal{E}^2 \cdot \exp\left(-B/\mathcal{E}\right)$

with A and B (V/cm) material-dependent parameters.



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We need a method to compute the DD model

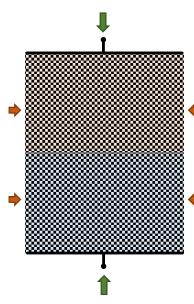
$$\overline{\begin{cases} \frac{\partial n}{\partial t} = \frac{1}{q} \frac{\partial J_n}{\partial x} - U_n \\ \frac{\partial p}{\partial t} = -\frac{1}{q} \frac{\partial J_p}{\partial x} - U_p \\ \frac{\partial \mathcal{E}}{\partial x} = \frac{\rho}{\epsilon} \end{cases}}$$

where φ is the input function, *n*, *p* and \mathcal{E} are the unknowns of the continuity equations and where the Poisson equation closes the system.

We have to solve a set of *non-linear*, *secondary-order* PDEs, in *space* and *time*, for the whole device!

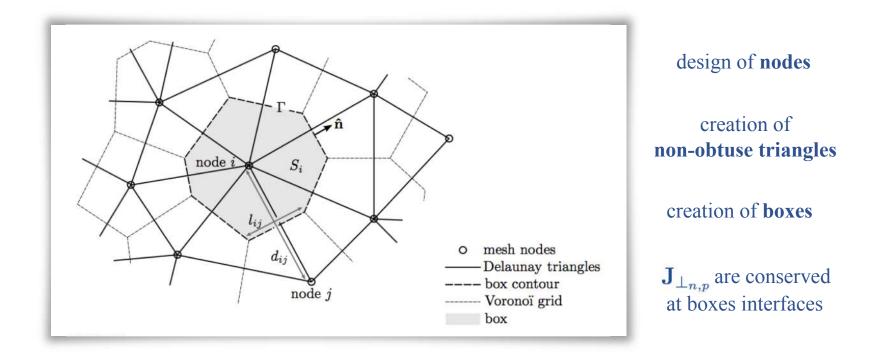
The strategy

- Dynamics (bias ramps, transients, ...) is treated as a sequence of *small* increments between stationary states at equilibrium: the **quasi-stationary process**;
- At each quasi-stationary step the mathematics has to be simplified through proper approximations and algorithms:

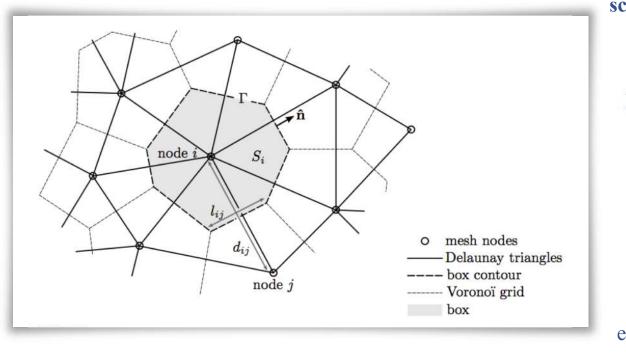


- 1. the geometry is discretized (e.g.: Delaunay-Voronoï procedure)
- 2. DD system is rewritten and adapted to the mesh grid
- 3. PDEs are linearized and transformed into ODEs (FD schemes)
- 4. I.C. and B.C. are defined
- 5. the *new* DD model is solved via **iterative methods** (Newton) in all mesh nodes

1. The geometry is discretized (e.g.: Delaunay-Voronoï procedure)



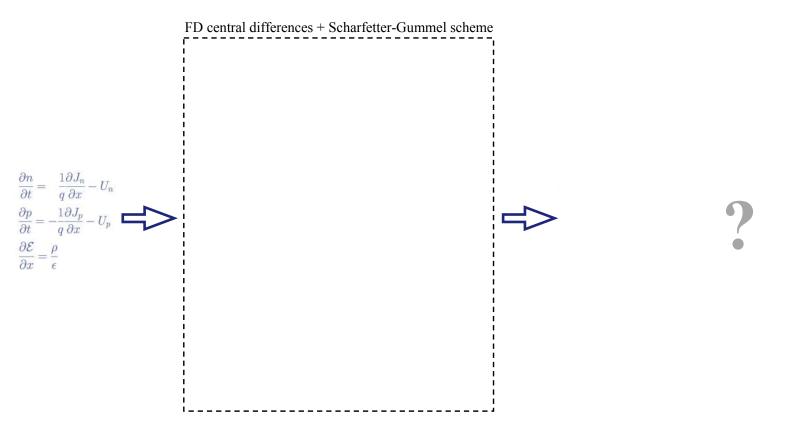
2. Drift-Diffusion system is rewritten and adapted to the mesh grid



scalar/vector operators and constants are transformed: $\frac{\partial}{\partial t} \int_{S} x \, ds \Rightarrow \frac{\partial x_i}{\partial t} S_i$ $\oint_{\Gamma} \mathbf{F}_{\perp} \, d\gamma \Rightarrow \sum_{j} l_{ij} \, \langle \mathbf{F}_{\perp} \rangle_{ij}$ $\int_{S} c \, ds \Rightarrow c_i S_i$

by **averaging** the **in/out quantities** at each box side, they are computed at **nodes**

3. PDEs are linearized and transformed into ODEs (FD schemes)

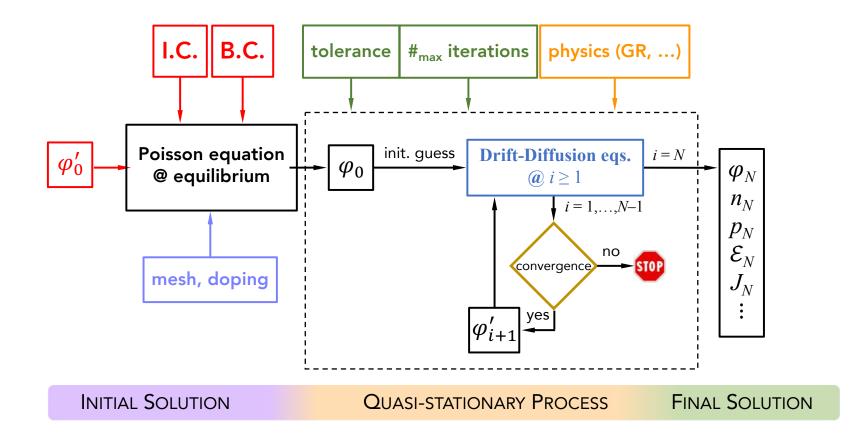


4. I.C. and B.C. are defined

Initial Conditions: starting polarization at contacts Boundary Conditions:

$$\begin{split} \frac{\partial n(\mathbf{r},t)}{\partial \hat{\mathbf{n}}} &= 0, \quad \frac{\partial p(\mathbf{r},t)}{\partial \hat{\mathbf{n}}} = 0 \quad \text{and} \quad \frac{\partial \phi(\mathbf{r},t)}{\partial \hat{\mathbf{n}}} = 0 \\ & \mathbf{Neumann} \text{ homogeneous (insulators, external edges,...)} \\ \begin{cases} n(\mathbf{r},t) \mu_n \frac{\partial \phi(\mathbf{r},t)}{\partial \hat{\mathbf{n}}} &= D_n \frac{\partial n(\mathbf{r},t)}{\partial \hat{\mathbf{n}}} \\ p(\mathbf{r},t) \mu_p \frac{\partial \phi(\mathbf{r},t)}{\partial \hat{\mathbf{n}}} &= -D_p \frac{\partial p(\mathbf{r},t)}{\partial \hat{\mathbf{n}}} \\ \epsilon_s \frac{\partial \phi(\mathbf{r},t)}{\partial \hat{\mathbf{n}}} \Big|_s &= \epsilon_{\text{diel}} \frac{\partial \phi(\mathbf{r},t)}{\partial \hat{\mathbf{n}}} \Big|_{\text{diel}} \end{cases} \quad \mathbf{Neumann non-homogeneous (dielectrics)} \\ \begin{cases} n(\mathbf{r},t) = \frac{1}{2} \left(\sqrt{\sum_k C_k^{\pm 2}(\mathbf{r},t) + 4n_i^2} + \sum_k C_k^{\pm}(\mathbf{r},t) \right) \\ p(\mathbf{r},t) &= \frac{1}{2} \left(\sqrt{\sum_k C_k^{\pm 2}(\mathbf{r},t) + 4n_i^2} - \sum_k C_k^{\pm}(\mathbf{r},t) \right) \\ \phi(t) &= V_{\text{bias}}(t) + \text{const.} \end{split} \quad \mathbf{Dirichlet non-homogeneous (contacts)} \end{split}$$

- TCAD procedure for each node:
 - a) Choose a maximum number of iterations $\#_{max}$ and a tolerance ε
 - b) Impose proper I.C. and B.C.
 - c) Start from an initial guess φ'_0 for the electrostatic potential
 - d) The equilibrium solution φ_0 is obtained by solving only the Poisson equation with the I.C. and B.C.
- If we have to perform a **voltage ramp** or a **transient**:
 - d) each step *i* of the ramp (with i = 1,...,N) is treated as a **quasi-stationary state**. The potential resulting from the Poisson solution at equilibrium φ_0 is used as initial guess for solving the **DD equations** at steps $i \ge 1$
- If the solution is found within the maximum number of iterations #_{max} and with an error smaller than the tolerance ε, then the system converges and the scheme go further, otherwise:
 - The pitch of the steps Δi is decreased
 - The tolerance *\varepsilon* is increased
 - If the alternatives above fails, then the method is **aborted**



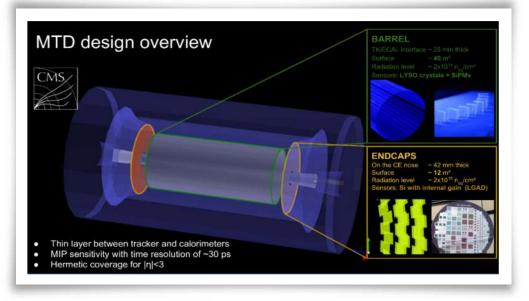


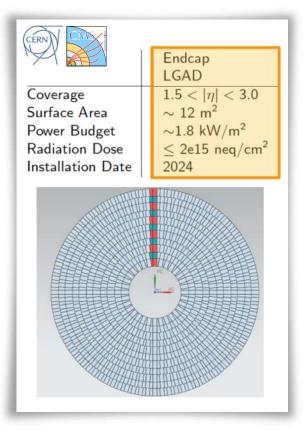
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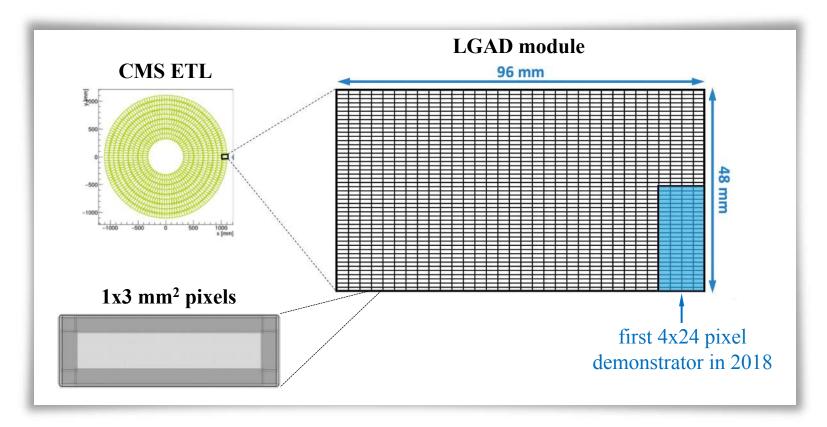
► Why LGAD are so innovative?

- Large signals coupled with low Gain \implies high S/N
- Fast signals ⇒ high time resolution
- Simple design ⇒ low production cost
- Huge ongoing R&D ⇒ radiation hardness

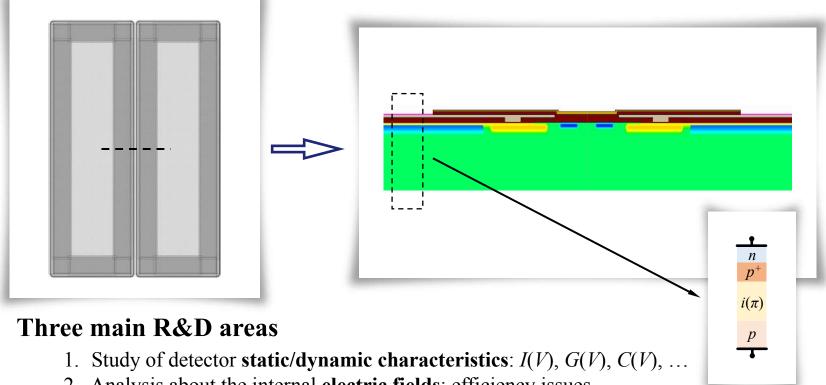




► How a real LGAD module is made?

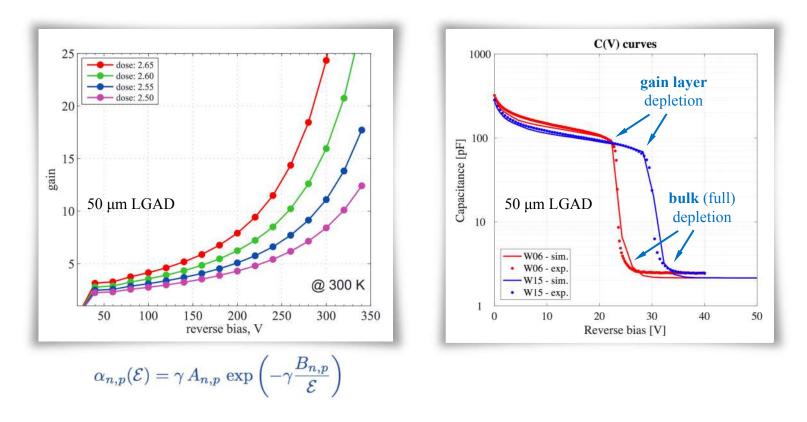


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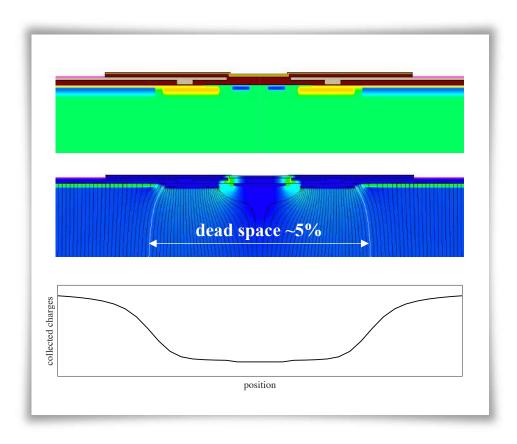


- 2. Analysis about the internal **electric fields**: efficiency issues, ...
- 3. Radiation tolerance

1. Study of detector static/dynamic characteristics: I(V), G(V), C(V), ...

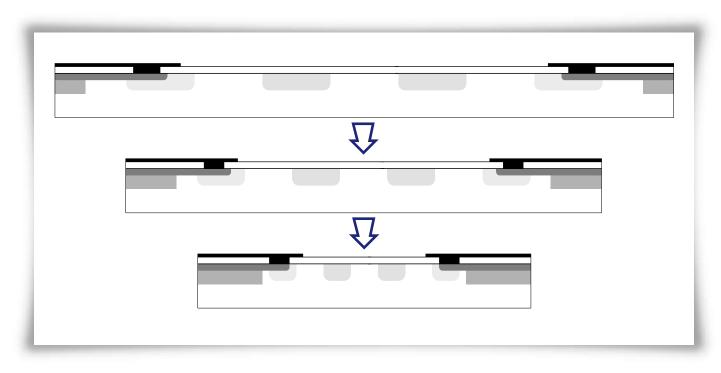


2. Analysis about the internal electric fields: efficiency issues, ...

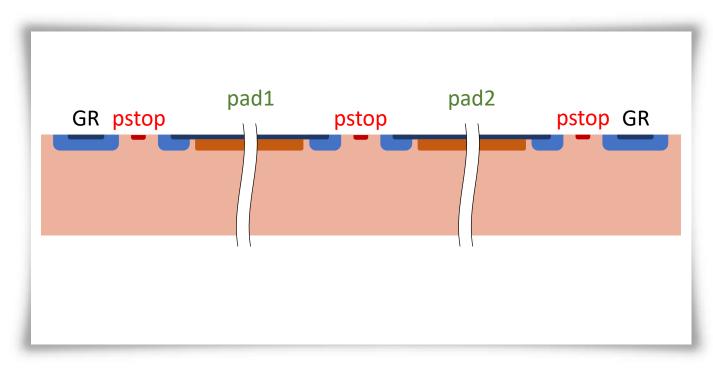


- 2. Analysis about the internal electric fields: efficiency issues, ...
- Two main strategies:

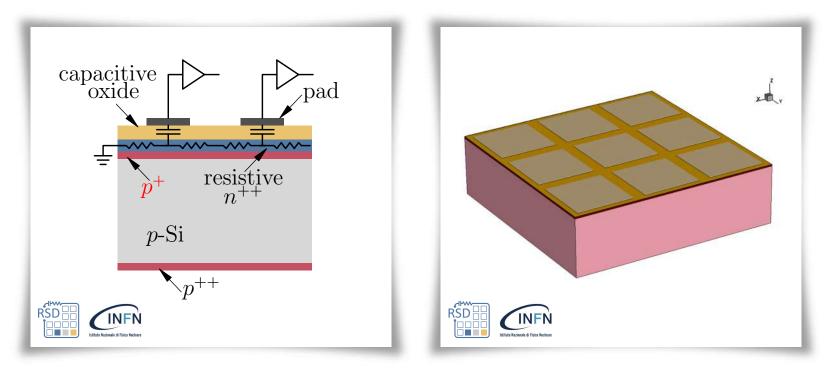
a. layout scaling



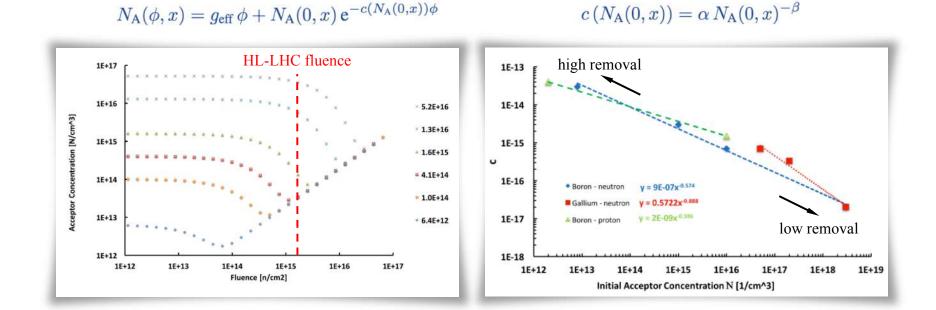
- 2. Analysis about the internal electric fields: efficiency issues, ...
- Two main strategies:
 - a. layout scaling



- 2. Analysis about the internal electric fields: efficiency issues, ...
- Two main strategies:
 - b. implement a new readout approach



3. Radiation tolerance



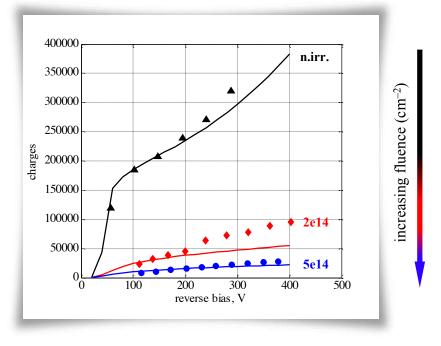
empirical acceptor removal/creation law

3. Radiation tolerance

empirical acceptor removal/creation law

 $N_{\rm A}(\phi, x) = g_{\rm eff} \phi + N_{\rm A}(0, x) \, {\rm e}^{-c(N_{\rm A}(0, x))\phi}$



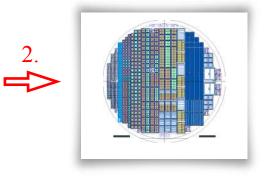


1. Study of detector static/dynamic characteristics: I(V), G(V), C(V), ...

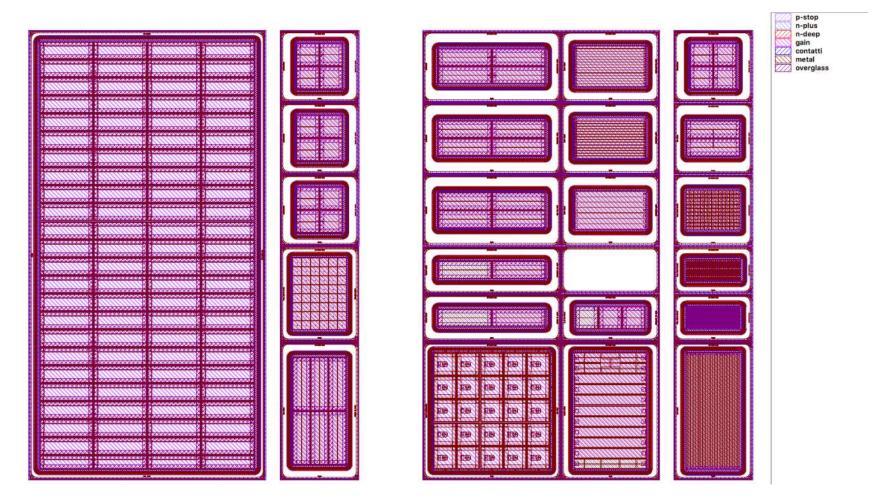
2. Analysis about the internal electric fields: efficiency issues, ...

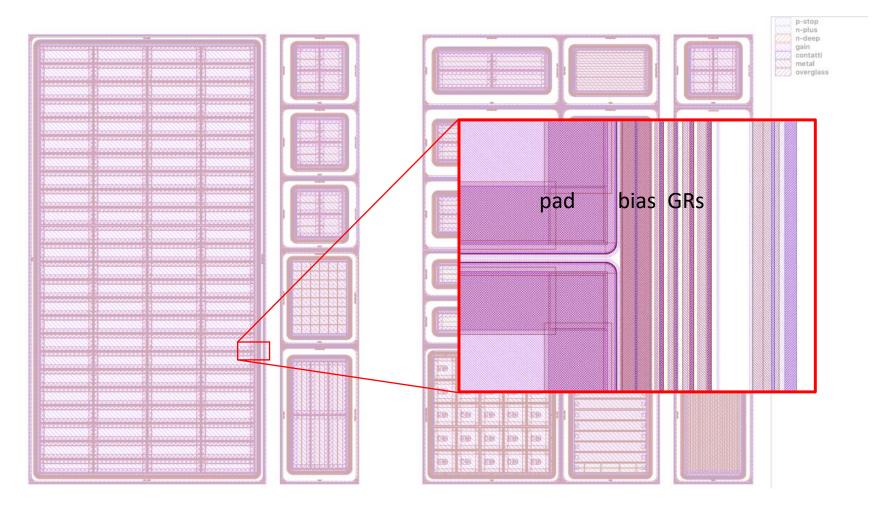
Wafer #	Dopant	Gain dose	Carbon
1	Boron	0.98	
2	Boron	1.00	
3	Boron	1.00	
4	Boron	1.00	low
5	Boron	1.00	High
6	Boron	1.02	low
7	Boron	1.02	High
8	Boron	1.02	
9	Boron	1.02	
10	Boron	1.04	
11	Gallium	1.00	
14	Gallium	1.04	
15	Gallium	1.04	low
16	Gallium	1.04	High
18	Gallium	1.08	

3. Radiation tolerance



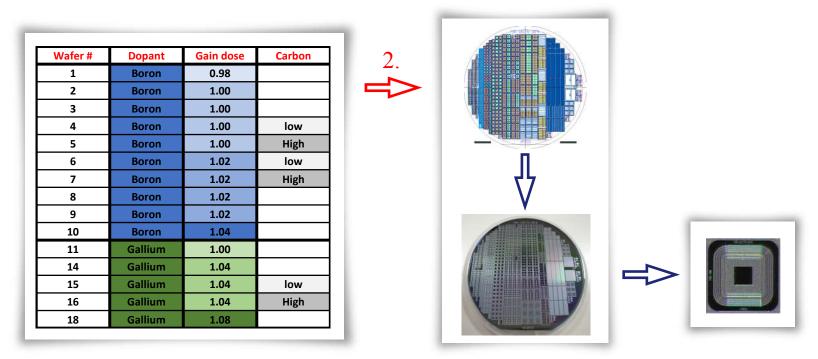
1. + 3.





1. Study of detector static/dynamic characteristics: I(V), G(V), C(V), ...

2. Analysis about the internal electric fields: efficiency issues, ...

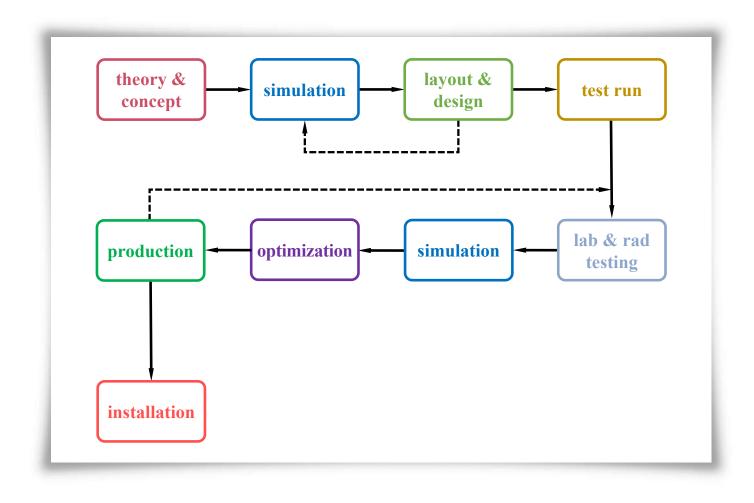


3. Radiation tolerance

1. + 3.

"From the pn junction to the UFSD design", Torino – 9.05.19

LGAD production: the complete workflow!



Contacts and Info

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 \Rightarrow To download this presentation and for more info about simulation: <u>http://personalpages.to.infn.it/~mandurri/teaching.html</u>

- \Rightarrow About the RSD experiment: <u>http://personalpages.to.infn.it/~mandurri/rsdproject.html</u>
- ⇒ Master Thesis Proposal: <u>http://personalpages.to.infn.it/~mandurri/teaching/Proposta_di_Tesi_LM_RSD.pdf</u>