# Pulse shape simulation for germanium detectors - SolidStateDetectors.jl

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#### **Example Detector Simulation Setup**

13:00	https://indico.cern.ch/event/1142628/timetable/#20220622		
	Digital processing of HPGe signals		
14:00			
		13:30 - 15:00	
15:00			
	HPGe detector pulse shape simulation	Felix Hagemann @	
16:00			
		15:30 - 17:00	









#### **Example Detector Simulation Setup**



#### SolidStateDetectors.jl



- Open-source simulation software package, written in **julia**
- 3D calculation of electric potentials and electric fields
- Can simulate arbitrary geometries, e.g. segmented detectors
- Documentation: <u>https://juliaphysics.github.io/SolidStateDetectors.jl/stable/</u>
- Fast field calculation: SIMD on CPU, also supports GPU calculation
- Calculation of capacitance matrix
- Simulation of fields in undepleted detectors  $\Rightarrow$  C-V curves
- Experimental features: diffusion and self-repulsion of charge clouds





### **Pulse Shape Simulation Chain**





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- 1. Maxwell equation:
  - $abla \cdot \mathbf{D}(\mathbf{r}) = 
    ho(\mathbf{r})$

$$\mathbf{D}(\mathbf{r}) = \epsilon_0 \epsilon_r(\mathbf{r}) \mathbf{E}(\mathbf{r})$$

$${f E}({f r})=-
abla \Phi({f r})$$

Required input:

- . charge density  $ho({f r})$ ,
- dielectric distribution  $\,\epsilon_r({f r})$
- boundary conditions for  $\Phi({f r})$

density Bias voltage

Impurity

Detector geometry

$$\nabla \cdot (\epsilon_r(\mathbf{r}) \cdot \nabla \Phi(\mathbf{r})) = -\frac{\rho(\mathbf{r})}{\epsilon_0}$$

Electric potential

SSD solves this numerically

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- Successive Over-Relaxation (SOR) algorithm
- Red-Black division of the grid  $\rightarrow$  parallelization (CPU vectorization, GPU support)
- Adaptive grid







Numerical approach: Divide your world (detector + surroundings) into small parts and calculate for each part (grid point) its

PACTED Filegrid:Start with a coarse grid (10 x 10 x 10 points)<br/>and become finer (eg. 200 x 200 x 200 points)





How to calculate the potential of a single grid point?

$$\nabla \cdot (\epsilon_r(\mathbf{r}) \cdot \nabla \Phi(\mathbf{r})) = -\frac{\rho(\mathbf{r})}{\epsilon_0}$$

Integral form:

$$\iiint_V \nabla \cdot (\epsilon_r(\mathbf{r}) \cdot \nabla \Phi(\mathbf{r})) \ dV = \iiint_V -\frac{\rho(\mathbf{r})}{\epsilon_0} \ dV$$

Divergence theorem:

$$\oint_{S} \left( \epsilon_{r}(\mathbf{r}) \cdot \nabla \Phi(\mathbf{r}) \right) \cdot d\mathbf{S} = - \iiint_{V} \frac{\rho(\mathbf{r})}{\epsilon_{0}} \, dV$$

































- $\Phi = A \cdot \Phi + Q$  System of N linear equations
- $\mathbf{\Phi}^{k+1} = \mathbf{A} \cdot \mathbf{\Phi}^k + \mathbf{Q}$  Gauss-Seidel method Set initial state:  $\mathbf{\Phi}^0$

Solve this equation several times, until an equilibrium is reached (until it "converges", i.e. the potential does not change any more).

The Successive Over-Relaxation (SOR) method is based on the Gauss-Seidel method, but normally converge much faster to its equilibrium.



#### **Red-Black Algorithm**



$$\mathbf{\Phi}^{k+1} = \mathbf{A} \cdot \mathbf{\Phi}^k + \mathbf{Q}$$
 N equations

Red-Black algorithm (Even / Odd)

$$\Phi_R^{k+1} = \mathbf{A}_R \cdot \Phi_B^k + \mathbf{Q}_R \qquad | N/2 \text{ equations} \\ \Phi_B^{k+1} = \mathbf{A}_B \cdot \Phi_R^k + \mathbf{Q}_B \qquad | N/2 \text{ equations}$$

Red (black) points do not depend on values of other red (black) points, so they can be updated simultaneously







julia > calculate\_electric\_potential!(sim)





#### Electric potential

#### julia > calculate\_electric\_potential!(sim)

#### Keywords

- convergence\_limit::Real: convergence\_limit times the bias voltage sets the convergence limit of the
  relaxation. The convergence value is the absolute maximum difference of the potential between two
  iterations of all grid points. Default of convergence\_limit is 1e-7 (times bias voltage).
- refinement\_limits: Defines the maximum relative (to applied bias voltage) allowed differences of the
  potential value of neighbored grid points in each dimension for each refinement.
  - rl::Real -> One refinement with rl equal in all 3 dimensions.
  - o rl::Tuple{<:Real,<:Real,<:Real} -> One refinement with rl set individual for each dimension.
  - o rl::Vector{<:Real} -> length(l) refinements with rl[i] being the limit for the i-th refinement.
  - rl::Vector{<:Real,<:Real,<:Real}} -> length(rl) refinements with rl[i] being the limits for the i-th refinement.
- min\_tick\_distance::Tuple{<:Quantity, <:Quantity, <:Quantity}: Tuple of the minimum allowed distance between two grid ticks for each dimension. It prevents the refinement to make the grid too fine. Default is 1e-5 for linear axes and 1e-5 / (0.25 \* r\_max) for the polar axis in case of a cylindrical grid.
- max\_tick\_distance::Tuple{<:Quantity, <:Quantity, <:Quantity}: Tuple of the maximum allowed distance between two grid ticks for each dimension used in the initialization of the grid. Default is 1/4 of size of the world of the respective dimension.
- max\_distance\_ratio::Real: Maximum allowed ratio between the two distances in any dimension to the two neighbouring grid points. If the ratio is too large, additional ticks are generated such that the new ratios are smaller than max\_distance\_ratio. Default is 5.
- grid::Grid: Initial grid used to start the simulation. Default is Grid(sim).

#### Documentation on GitHub

https://juliaphysics.github.io/SolidStateDetectors.jl/stable/



- use\_nthreads::Union{Int, Vector{Int}}: If <:Int, use\_nthreads defines the maximum number of threads to be used in the computation. Fewer threads might be used depending on the current grid size due to threading overhead. Default is Base.Threads.nthreads(). If <:Vector{Int}, use\_nthreads[1] defines the number of threads used for each grid (refinement) stage of the field simulation. The environment variable JULIA\_NUM\_THREADS must be set appropriately before the Julia session was started (e.g. export JULIA\_NUM\_THREADS=8 in case of bash).
- sor\_consts::Union{<:Real, NTuple{2, <:Real}}: Two element tuple in case of cylindrical coordinates.</li>
   First element contains the SOR constant for r = 0. Second contains the constant at the outer most grid point in r. A linear scaling is applied in between. First element should be smaller than the second one and both should be ∈ [1.0, 2.0]. Default is [1.4, 1.85]. In case of Cartesian coordinates, only one value is taken.
- max\_n\_iterations::Int: Set the maximum number of iterations which are performed after each grid refinement. Default is 10000. If set to -1 there will be no limit.
- not\_only\_paint\_contacts::Bool = true: Whether to only use the painting algorithm of the surfaces of Contact without checking if points are actually inside them. Setting it to false should improve the performance but the points inside of Contact are not fixed anymore.
- paint\_contacts::Bool = true: Enable or disable the painting of the surfaces of the Contact onto the grid.
- verbose::Bool=true: Boolean whether info output is produced or not.







### **Pulse Shape Simulation Chain**





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#### **Electric Field Calculation**

 $\Phi_{i,j,k}$ 

 $\mathbf{E}(\mathbf{r})$ 

Electric potential

Mean of finite difference:

$$\mathbf{E}_{i,j,k} = \begin{pmatrix} \mathbf{E}_{r}^{i,j,k}, E_{\varphi}^{i,j,k}, E_{z}^{i,j,k} \end{pmatrix} \qquad E_{r}^{i,j,k} = \frac{1}{2} \begin{pmatrix} \frac{\Phi_{i+1,j,k} - \Phi_{i,j,k}}{r_{i+1} - r_{i}} + \frac{\Phi_{i,j,k} - \Phi_{i-1,j,k}}{r_{i} - r_{i-1}} \end{pmatrix} \\ E_{i,j,k} = \begin{pmatrix} E_{r}^{i,j,k}, E_{\varphi}^{i,j,k}, E_{z}^{i,j,k} \end{pmatrix} \qquad E_{\varphi}^{i,j,k} = \frac{1}{2} \begin{pmatrix} \frac{\Phi_{i,j+1,k} - \Phi_{i,j,k}}{\varphi_{j+1} - \varphi_{j}} + \frac{\Phi_{i,j,k} - \Phi_{i,j-1,k}}{\varphi_{j} - \varphi_{j-1}} \end{pmatrix} \\ E_{z}^{i,j,k} = \frac{1}{2} \begin{pmatrix} \frac{\Phi_{i,j,k+1} - \Phi_{i,j,k}}{z_{k+1} - z_{k}} + \frac{\Phi_{i,j,k} - \Phi_{i,j,k-1}}{z_{k} - z_{k-1}} \end{pmatrix}$$

Electric field

Electric field at any point **r** (through linear interpolation)







#### **Electric Field Calculation**

julia > calculate\_electric\_field!(sim)





### **Pulse Shape Simulation Chain**





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#### one electron-hole pair per 2.96eV





#### Charge Drift Models

Charge carriers in germanium move in the presence of an electric field  ${f E}({f r})$ 

Drift velocity of electrons and holes:  $\mathbf{v}_{e,h}(\mathbf{r}) = \mu_{e,h} \, \mathbf{E}(\mathbf{r})$ 

 $\mu_{e,h}$  is the mobility tensor:

- saturates for high electric field strengths
- anisotropic in germanium
- temperature dependent

There are models for  $\mu_{e,h}$ :

L. Mihailescu *et al.*, Nucl. Instr. and Meth. A **447** (2000) 350, doi: <u>10.1016/S0168-9002(99)01286-3</u> B. Bruyneel *et al.*, Nucl. Instr. and Meth. A **569** (2006) 764, doi: <u>10.1016/j.nima.2006.08.130</u>

> state etectors

but usually parameters of the models have to be fitted to each individual detector





#### **Charge Drift Models**



#### **Charge Drift Models**

#### Charge drift model

# julia > cdm = ADLChargeDriftModel( ) julia > sim.detector = SolidStateDetector(sim.detector, cdm)

#### **Custom Charge Drift Model**

The user can implement and use his own drift model.

The first step is to define a struct for the model which is a subtype of SolidStateDetectors.AbstractChargeDriftModel:

using SolidStateDetectors using SolidStateDetectors: SSDFloat, AbstractChargeDriftModel using StaticArrays

struct CustomChargeDriftModel{T <: SSDFloat} <: AbstractChargeDriftModel{T}
 # optional fields to parameterize the model
end</pre>

The second step is to define two methods (getVe for electrons and getVh for holes), which perform the transformation of an electric field vector,  $fv::SVector{3,T}$ , into a velocity vector. Note, that the vectors are in cartesian coordinates, independent of the coordinate system (cartesian or cylindrical) of the simulation.

<pre>function SolidStateDetectors.getVe(fv::SVector{3, T}, cdm::CustomChargeDriftModel)::SVector{3, # arbitrary transformation of fv</pre>	1
return -fv	
end	
<pre>function SolidStateDetectors.getVh(fv::SVector{3, T}, cdm::CustomChargeDriftModel)::SVector{3,</pre>	1
# arbitrary transformation of fv	

#### Documentation on GitHub

https://juliaphysics.github.io/SolidStateDetectors.jl/stable/





return fv

end



#### **Charge Drift Simulation**

Drift velocity for electrons and holes:  $\mathbf{v}_{e,h}(\mathbf{r}) = \mu_{e,h} \, \mathbf{E}(\mathbf{r})$ 



Drift paths

#### **Charge Drift Simulation**

julia > locations = [CartesianPoint(0.035,0,0.02), CartesianPoint(-0.015,0,0.015)] julia > energies = [1000u"keV", 300u"keV"] julia > evt = Event(locations, energies) julia > drift\_charges!(evt, sim)



Drift paths

### **Pulse Shape Simulation Chain**



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### Weighting Potential Calculation

 $\Phi^w_i(\mathbf{r})$  is the so-called weighting potential for electrode i.

It describes how much charge is induced on the electrode depending on the position **r** of the charge carrier in the crystal.

$$\nabla \cdot (\epsilon_r(\mathbf{r}) \cdot \nabla \Phi_i^w(\mathbf{r})) = 0$$

Same algorithm as for the electric potential but:

- Charge density is set to 0
- The potential values at all contacts are set to 0, but only the potential value of contact i is set to 1.





#### Weighting Potential Calculation

julia > calculate\_weighting\_potential!(sim, 1)





#### **Signal Generation**

Shockley-Ramo Theorem  $Q_i^{ind}(\mathbf{r}_e(t),\mathbf{r}_h(t)) = q \cdot [\Phi_i^w(\mathbf{r}_e(t)) - \Phi_i^w(\mathbf{r}_h(t))]$ 



### **Pulse Shape Simulation Chain**





## **Pulse Shape Simulation Chain**

julia > using SolidStateDetectors, Unitful

```
julia > locations = [CartesianPoint(0.035,0,0.02)]
julia > energies = [1000u"keV"]
julia > evt = Event(locations, energies)
julia > simulate!(evt, sim)
```





### **Configuration File**

name: Point-contact detector units: length: mm angle: deg potential: V temperature: K grid: coordinates: cylindrical axes: r: to: 60 boundaries: inf phi: from: 0 to: 0 boundaries: left: periodic right: periodic z: from: -20 to: 60 boundaries: left: inf right: inf medium: vacuum



Constructive Solid Geometry **Documentation** on GitHub



Solid State





#### **Documentation on GitHub**



#### SolidStateDetectors.jl

Search docs

Electric Potential

Electric Field

Charge Drift

Weighting Potentials

Capacitances

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Plotting

Tutorials

Simulation Chain: Inverted Coax Detector

- Partially depleted detectors
- Electric field calculation
- Simulation of charge drifts
- Weighting potential calculation
- Detector Capacitance Matrix
- Detector waveform generation

Advanced Example: Custom Impurity Profile

API



#### Simulation Chain: Inverted Coax Detector

using Plots using SolidStateDetectors using Unitful

T = Float32

sim = Simulation{T}(SSD\_examples[:InvertedCoax])

plot(sim.detector, size = (700, 700))



Find the latest version of the documentation on GitHub: <u>https://juliaphysics.github.io/</u><u>SolidStateDetectors.jl/stable/</u>



## **Pulse Shape Simulation Chain**

julia > using SolidStateDetectors, Unitful

```
julia > locations = [CartesianPoint(0.035,0,0.02)]
julia > energies = [1000u"keV"]
julia > evt = Event(locations, energies)
julia > simulate!(evt, sim)
```





### **Undepleted Detectors**

julia > using SolidStateDetectors, Unitful

julia > calculate\_mutual\_capacitance(sim, (1, 2))





#### **GPU** Support

julia > using SolidStateDetectors, Unitful julia > using CUDAKernels, CUDA

```
julia > sim = Simulation{Float64}("BEGe.yaml")
```

```
julia > calculate_electric_potential!(sim, device_array_type = CuArray)
```

```
julia > calculate_electric_field!(sim)
```

```
julia > for i in 1:2
```

calculate\_weighting\_potential!(sim, i, device\_array\_type = CuArray) end

```
julia > locations = [CartesianPoint(0.035,0,0.02)]
julia > energies = [1000u"keV"]
julia > evt = Event(locations, energies)
julia > simulate!(evt, sim)
```





## **Simulating Group Effects**

julia > using SolidStateDetectors, Unitful

```
julia > locations = [CartesianPoint(0.035,0,0.02)]
julia > energies = [1000u"keV"]
julia > evt = Event(NBodyChargeCloud(locations, energies, 100))
julia > simulate!(evt, sim, diffusion = true, self_repulsion = true)
```



