

AGATA PSA basis with AGATAGeFEM

Joa Ljungvall

June 15, 2026

I have a question and asked AI...

"I'm making a presentation for how to calculate AGATA psa basis with AGATAGeFEM. Can you make a summary slide in emacs org mode that are to be exported into beamer PDF about the code AGATAGeFEM?"

Question posed to Mistral "le chat", cnrs account. And ChatGPT without connecting.

AGATAGeFEM: A Geant4-based Framework for AGATA (according to Mistral)

Purpose: Simulate gamma-ray tracking and PSA (Pulse Shape Analysis) basis calculation for AGATA detectors.

- Key Features:
 - Geant4 integration for detector geometry and physics.
 - Customizable PSA algorithms for AGATA's segmented HPGe detectors.
 - Outputs: Energy deposition, pulse shapes, and basis vectors for PSA.

AGATAGeFEM: A Geant4-based Framework for AGATA (according to Mistral)

Workflow (according to Mistral)

- 1 Define AGATA detector geometry and segmentation.
- 2 Simulate gamma-ray interactions using Geant4.
- 3 Extract pulse shapes and energy depositions.
- 4 Calculate PSA basis vectors for signal decomposition.

AGATAGeFEM: A Geant4-based Framework for AGATA (according to Mistral)

Why AGATAGeFEM? (according to Mistral)

- Optimized for AGATA's high-resolution gamma-ray spectroscopy.
- Flexible for testing new PSA algorithms.
- Open-source and community-driven (CNRS/IN2P3).

AGATAGeFEM: A Geant4-based Framework for AGATA (according to Mistral)

Key Code Components (according to Mistral)

- `AGATADetectorConstruction`: Detector geometry.
- `AGATAPSAManager`: PSA basis calculation.
- `AGATAEventAction`: Event processing and data output.

AGATAGeFEM: A Geant4-based Framework for AGATA (according to Mistral)

Next Steps (according to Mistral)

- Validate PSA basis with experimental data.
- Integrate machine learning for advanced PSA.
- Collaborate with AGATA collaboration for benchmarking.

AGATAGeFEM: Pulse-Shape Basis Generation for AGATA (according to ChatGPT)

Purpose

- Generate realistic pulse-shape databases (PSA bases) for AGATA HPGe detectors.
- Simulate detector response from first principles:
 - Electric field (E)
 - Weighting fields (Φ_W)
 - Charge-carrier transport
 - Induced segment signals

AGATAGeFEM: Pulse-Shape Basis Generation for AGATA (according to ChatGPT)

Main Features

- Detailed AGATA crystal geometry (A/B/C types, bore-hole variations).
- Finite Element Method (FEM) solution of:
 - Poisson equation (electric field)
 - Laplace equation (weighting fields)
- Adaptive meshing and parallel execution (MPI + multithreading).
- Charge drift using anisotropic electron/hole mobility models.
- Generation of PSA libraries and neutron-damage correction coefficients.

AGATAGeFEM: Pulse-Shape Basis Generation for AGATA (according to ChatGPT)

PSA Basis Workflow

- 1 Define crystal geometry and segmentation.
- 2 Compute electric and weighting fields.
- 3 Simulate charge-carrier trajectories.
- 4 Calculate pulse shapes on a 3D interaction grid.
- 5 Generate neutron-sensitivity corrections.
- 6 Export AGAPRO/Bart-format PSA basis.

AGATAGeFEM: Pulse-Shape Basis Generation for AGATA (according to ChatGPT)

Outputs

- `.pulsesraw` : simulated pulse shapes
- `.trajectories` : charge drift trajectories
- `.ns` : neutron correction coefficients
- `.dat` : final PSA basis used by AGATA analysis

AGATAGeFEM uses FEM directly on the detector mesh, avoiding interpolation errors and enabling accurate pulse-shape modelling for AGATA PSA.

AGATAGeFEM - how did the AI do?

Mistral

- Mistral is tangentially talking about the correct subject but got all mixed up. Not capable of differentiating between a feature (couple AGATAGeFEM with AGATA g4 simulations) and the code itself. Would have failed an exam. A small plus for the "Next steps" slide.

ChatGPT

- ChatGPT got it right. In the "PSA Basis Workflow" list there is a point to many (3 and 4 are the same thing). Would have passed the exam.

Input data

What is the same for each (type of) crystal?

- The geometry (true to <0.5 mm)
- Crystallographic axes
- Can, mounting in can etc (not even known to us)

What is different?

- Impurity concentrations
- Bias voltage

What have we sometimes varied to test PSA?

- The bore hole radius

Input data

Where do we find the info?



Parc des Tamaris, 1 Chemin de la Rivière,
67083 Le Galstern

MT	Site	Type	Model	Level	Page
	LGM	P	137	C	1

Établissement de Lingolshausen / Lingolshausen Facility

AGATA Canister B025 – Detector performance and operating manual

AGATA Canister B025

Detector performance and operating manual



23/11/2016

**MIRION TECHNOLOGIES (CANBERRA) SPECIALTY
DETECTORS**

Das Unternehmen und/oder seine Warenzeichen sind Marken. Diese reproduktion des Textes ist ein Verstoß gegen die CANBERRA-
Copyright-Richtlinien in Bezug auf die Marken. Alle Rechte vorbehalten. © MIRION TECHNOLOGIES (CANBERRA) 2016

Note, this presentation shows how to add a base for a new crystal, so only "different" is shown, i.e. impurity concentrations.

Input data

Where do we find the info?



MT	Entité LGH	Type P	Numéro 117	Version C	Page 14
----	---------------	-----------	---------------	--------------	------------

Parc des Tanneries, 1 Chemin de la Roseaie,
67380 Lingolsheim

Etablissement de Lingolsheim / Lingolsheim Facility

AGATA Canister B025 – Detector performance and operating manual

3. AGATA Canister B025 performance

3.1 Crystal characteristics

Canister reference number	B025
Crystal reference number	75271
Diameter ^(a) [mm]	79.8
Length ^(a) [mm]	89.9
Weight ^(a) [g]	2043
Net impurity (n-type) concentration ^(b) [10^{10} cm^{-3}]	Front: 1.31 Rear: 0.29
Mobility ^(b) [m^2/Vs]	Front: 3.24 Rear: 3.27
Depletion voltage ^(a) [V]	3250

^a Crystal characteristics after processing and encapsulation

^b Crystal characteristics before any process

^c Detector front (closed end) corresponds to the grown crystal tail

3.2 Depletion profile

Input data

Where do we find the info?



MT	Entité LGH	Type P	Numéro 117	Version C	Page 15
----	---------------	-----------	---------------	--------------	------------

Parc des Tanneries, 1 Chemin de la Roseraie,
67380 Lingolsheim

Etablissement de Lingolsheim / Lingolsheim Facility

AGATA Canister B025 – Detector performance and operating manual

3.3 Specification sheet

	MT	ENTITE DET	TYPE F	N° 157	VERSION D	Page 1/1
1. Chemin de la Roseraie 67380 Tanneries		Etablissement de Lingolsheim/ Lingolsheim facility				

SPECIFICATION SHEET FOR IRREGULAR AGATA DETECTOR	
Canister S/N:	B025
Crystal S/N:	75271

Full volume performances	Guaranteed specifications
Depletion voltage	+ 3250 V
Operating high voltage (positive)	+ 5000 V
FWHM at 1.33 MeV (⁶⁰ Co)	2.43 keV ≤ 2.35 keV
Efficiency	83 %
FWTM/FWHM at ⁶⁰ Co	2.08 ≤ 2.0
Peak / Compton ratio	69
FWHM at 122 keV (⁵⁷ Co)	1.01 keV ≤ 1.35

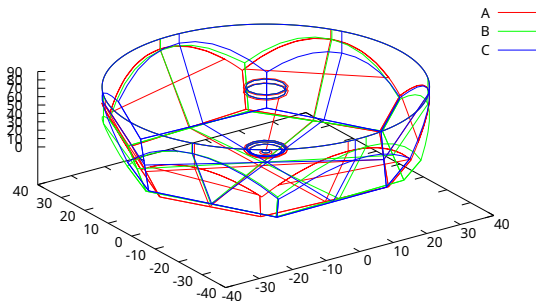
Outer contacts performances	At 60 keV (²⁴¹ Am)		At 1.33 MeV (⁶⁰ Co)					
	Max value ≤ 1.30 keV		Max value : ≤ 2.30 keV					
	Mean value ≤ 1.20 keV		A	B	C	D	E	F
50 keV	1.05	0.95	0.99	0.95	0.94	0.94	0.94	0.94
122 keV	2.07	2.07	2.08	2.02	2.13	2.13	2.12	2.12

Input files

Geometry

Geometry goes into two files, e.g. for a B type crystal (files are found in AGATAGeFEM/AGATAGeometries)

- AGATAGreen.list
- AGATAGreen.list.extra



Input files

Impurity concentration and bias voltage

The we found in the manual go into the [ABC]0[0-6][0-9]_Gaps file, in this case the B025_Gaps (all already calculated crystals are found in AGATAGeFEM/inputfiles)

```

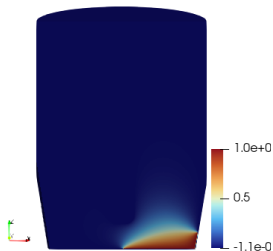
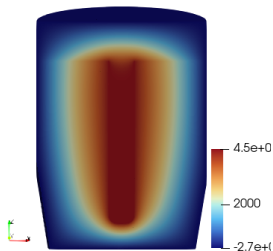
! <-Indicates that we use planes for seg. input.
#Unit: [deg] #Elastic[deg] #start[mm] #stop[mm] #Electrod[V] #Qlowinnerr [#]/mm3 #Qlowouterr [#]/mm3 #Qhighinn
err [#]/mm3 #Qhighouterr [#]/mm3 #epsilon #cycles #global refinmets
#Udcis 0 0 0 90 0 1e7 1.5e7 4.3e6 4.3e6 16 4 1
UCore_2 0 0 0 90 0 1e7 1.5e7 4.3e6 4.3e6 16 4 1
UCore_1 0 0 0 90 0 1e7 1.5e7 4.3e6 4.3e6 16 4 1
UCore 5000 0 0 0 90 0 1e7 1.5e7 4.3e6 4.3e6 16 4 1
WCORE 1 0 0 90 0 0 0 0 0 0 1 1 1
WA0 0 1 5 0 0 1 -7.75 -1.79769e+308 1.79769e+308 0 0 -1 0 -1 -1.79769e+308 1.79769e+308 -0.456798 -0.889414 0.0167063 0.511077 -1.797
69e+308 1.79769e+308 -0.494778 0.868571 -0.027925 -0.480922 -1.79769e+308 1.79769e+308 -0.997664 -0.068311 0 -0.578989 -1.79769e+3
08 1.79769e+308 0 0 0 0 1 1 1
WA1 0 1 5 0 0 1 -20.75 -1.79769e+308 1.79769e+308 0 0 -1 8.25 -1.79769e+308 1.79769e+308 -0.456798 -0.889414 0.0167063 0.461077 -1
.79769e+308 1.79769e+308 -0.494778 0.868571 -0.027925 -0.530922 -1.79769e+308 1.79769e+308 -0.997664 -0.068311 0 -0.578989 -1.7976
9e+308 1.79769e+308 0 0 0 0 1 1 1
WA2 0 1 5 0 0 1 -35.75 -1.79769e+308 1.79769e+308 0 0 -1 21.25 -1.79769e+308 1.79769e+308 -0.456798 -0.889414 0.0167063 0.461077 -1
.79769e+308 1.79769e+308 -0.494778 0.868571 -0.027925 -0.530922 -1.79769e+308 1.79769e+308 -0.997664 -0.068311 0 -0.578989 -1.797
69e+308 1.79769e+308 0 0 0 0 1 1 1
WA3 0 1 5 0 0 1 -55.75 -1.79769e+308 1.79769e+308 0 0 -1 36.25 -1.79769e+308 1.79769e+308 -0.456798 -0.889414 0.0167063 0.461077 -1
.79769e+308 1.79769e+308 -0.494778 0.868571 -0.027925 -0.530922 -1.79769e+308 1.79769e+308 -0.997664 -0.068311 0 -0.578989 -1.797
69e+308 1.79769e+308 0 0 0 0 1 1 1
WA4 0 1 7 0 0 1 -71.75 -1.79769e+308 1.79769e+308 0 0 -1 54.25 -1.79769e+308 1.79769e+308 -0.456798 -0.889414 0.0167063 0.461077 -1
.79769e+308 58.8893 -0.494778 0.868571 -0.027925 -0.530922 -1.79769e+308 78.5237 -0.430081 -0.90279 -0.025 58.8893 1.79769e+308
-0.558222 0.829691 0.025 78.5237 1.79769e+308 -0.997664 -0.068311 0 -0.578989 -1.79769e+308 0 0 0 0 1 1 1
WA5 0 1 7 0 0 1 -90 -1.79769e+308 1.79769e+308 0 0 -1 72.25 -1.79769e+308 1.79769e+308 -0.456798 -0.889414 0.0167063 0.461077 -1.7
9769e+308 58.8893 -0.494778 0.868571 -0.027925 -0.530922 -1.79769e+308 78.5237 -0.430081 -0.90279 -0.025 58.8893 1.79769e+308 -0.
558222 0.829691 0.025 78.5237 1.79769e+308 -0.997664 -0.068311 0 -0.578989 -1.79769e+308 1.79769e+308 0 0 0 0 1 1 1
WB0 0 1 5 0 0 1 -7.75 -1.79769e+308 1.79769e+308 0 0 -1 0 -1 -1.79769e+308 1.79769e+308 0.494778 -0.868571 0.027925 1.03092 -1.79769e+3
08 1.79769e+308 -0.997306 -0.0682865 0.0268054 -0.328782 -1.79769e+308 1.79769e+308 -0.456861 -0.889538 0 0.211107 -1.79769e+308
1.79769e+308 0 0 0 0 1 1 1
WB1 0 1 5 0 0 1 -20.75 -1.79769e+308 1.79769e+308 0 0 -1 8.25 -1.79769e+308 1.79769e+308 0.494778 -0.868571 0.027925 1.03092 -1.79
769e+308 1.79769e+308 -0.997306 -0.0682865 0.0268054 -0.328782 -1.79769e+308 1.79769e+308 -0.456861 -0.889538 0 0.211107 -1.79769e
+308 1.79769e+308 0 0 0 0 1 1 1
WB2 0 1 5 0 0 1 -35.75 -1.79769e+308 1.79769e+308 0 0 -1 21.25 -1.79769e+308 1.79769e+308 0.494778 -0.868571 0.027925 1.03092 -1.7
9769e+308 1.79769e+308 -0.997306 -0.0682865 0.0268054 -0.328782 -1.79769e+308 1.79769e+308 -0.456861 -0.889538 0 0.211107 -1.79769
e+308 1.79769e+308 0 0 0 0 1 1 1
WB3 0 1 5 0 0 1 -55.75 -1.79769e+308 1.79769e+308 0 0 -1 36.25 -1.79769e+308 1.79769e+308 0.494778 -0.868571 0.027925 1.03092 -1.7
9769e+308 1.79769e+308 -0.997306 -0.0682865 0.0268054 -0.328782 -1.79769e+308 1.79769e+308 -0.456861 -0.889538 0 0.211107 -1.79769
e+308 1.79769e+308 0 0 0 0 1 1 1
WB4 0 1 5 0 0 1 -71.75 -1.79769e+308 1.79769e+308 0 0 -1 54.25 -1.79769e+308 1.79769e+308 0.494778 -0.868571 0.027925 1.03092 -1.797
69e+308 1.79769e+308 -0.997306 -0.0682865 0.0268054 -0.328782 -1.79769e+308 1.79769e+308 -0.456861 -0.889538 0 0.211107 -1.79769
e+308 1.79769e+308 0 0 0 0 1 1 1
WB5 0 1 5 0 0 1 -90 -1.79769e+308 1.79769e+308 0 0 -1 72.25 -1.79769e+308 1.79769e+308 0.494778 -0.868571 0.027925 1.03092 -1.7976
9e+308 1.79769e+308 -0.997306 -0.0682865 0.0268054 -0.328782 -1.79769e+308 78.6113 0.558222 -0.829691 0.025 78.5237 1.79769e+308 -0.99

```

Steps that should be done at least one time

Calculate all weighting fields and auxiliary electric fields

This is already done for [ABC]001, including its electric field.



According to my present plans these will be accessible for download (automatic with Docker)

Steps that should be done for each basis

- Make a directory

In this directory

- The fields from above has to be linked, something like

```
for J in `ls ../../B001/B001_W*.field`
do
    ffn=$(basename $J)
    nfn=`echo $ffn | sed -e s:B001:B025:g`
    ln -sf $J $nfn
done
for J in `ls ../../B001/B001_UCore_[fb].field`
do
    ffn=$(basename $J)
    nfn=`echo $ffn | sed -e s:B001:B025:g`
    ln -sf $J $nfn
done
```

- The input file has to be copied, e.g. B025_Gaps
- The input file has to be modified according to

```
sed -i s:'W':'\&W':g B025_Gaps
sed -i s:'UCore_f':'\&UCore_f':g B025_Gaps
sed -i s:'UCore_b':'\&UCore_b':g B025_Gaps
```

to only calculate the UCore field

Steps that should be done for each basis

- The geometry files has to be copied, e.g. AGATAGreen.list*
- Run the AGATAGeFEM code

```
RunAGATampifields.py -f B025_Gaps -s AGATAGreen.list -r 0.9 -c 0.05 -o A001\
-N 1000000
```

- Copy input files for basis

```
cp ~/AGATAGeFEM/basesinputfiles/databaseinput .
cp ~/AGATAGeFEM/anisotropyfiles/anisotropy_completeRotZ045deg .
```

- Run the AGATAGeFEM code

```
AGATAGeFEM_CalculatingBase=true\
AGATAGeFEM_NumberOfThreads=16\
AGATAGeFEM_Writelibfield=YES\
AGATAGeFEM_tstop=1e-6\
AGATAGeFEM --calculateP B025\
anisotropy_completeRotZ045deg\
AGATAGreen.list\
databaseinput B025\
2> /dev/null
```

Steps that should be done for each basis

- Run calculating the neutron damage corrections

```
AGATAGeFEM_NumberOfThreads=16\  
AGATAGeFEM --NeutronSensitivity B025\  
anisotropy_completeRotZ045deg\  
AGATAGreen.list B025\  
2> /dev/null
```

- Convert into a correctly formatted basis file

```
AGATAGeFEM --convert -FJoa -PB025.pulsesraw -CB025.ns -ObaseB025.dat
```

DONE!

Improving on the above

- This procedure could be cut down to one line, i.e. produce a finished basis directly. But this does not really save time. Once fields are done a basis takes ~10 min all in all on a laptop.
- Instead, script the steps and automate with Docker.
- Separating the calculations is good for other uses of AGATAGeFEM.

Should we change basis format?

```
typedef struct {
float T0;           // time of interaction (in us)
float Eint;        // energy fractions == 1
float Pos[3];      // x y z (mm)
int  Trig;         // Core trigger time (sample index)
float Es[ 1+36     ]; // energy in segments (0=core)
float Tr[(1+36)*120]; // CC+nSeg traces given in steps of 5 ns. The first 10 samples are
} bbhit_t;
```

- 600 ns of trace with 5 ns steps
- Six of pretrigger points used for storing neutron correction data, out of which 2 are used
- Signals down sampled to 10 ns steps when read by the PSA algorithms.
- Trig is always as 50ns, Eint always 1
- Es is always [1 0 0 1 .. 0] with 1 at index hitseg.
- We could, without loss of information, cut the basis size on disk quite a lot