Acceleration methods for Monte Carlo simulations

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Outline

1.	VRT1 (dose)	Last Vertex Spliting (LVS) + Track Length Estimator (TLE)
2.	VRT2 (image)	Free-flight Angular Acceptance (FFAA)
3.	GAN (dose)	GAN Linac source
4.	GAN (image)	cGAN SPECT

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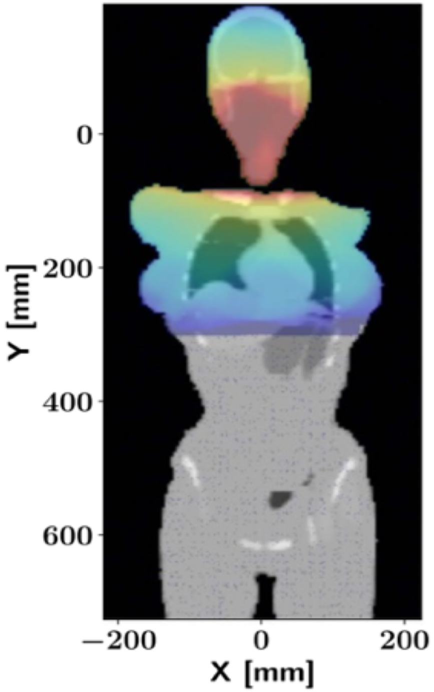
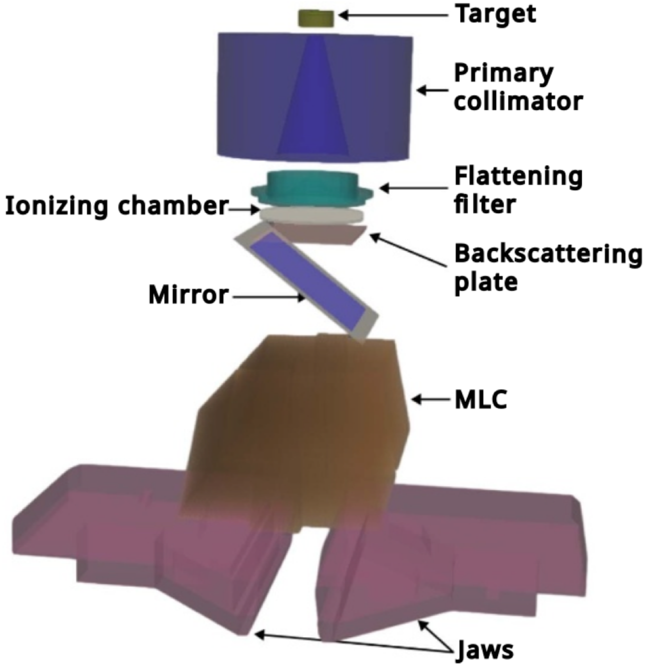
Goal: out-of-field dose estimation

Complete treatment plan: 5k hours (10% at 50cm)





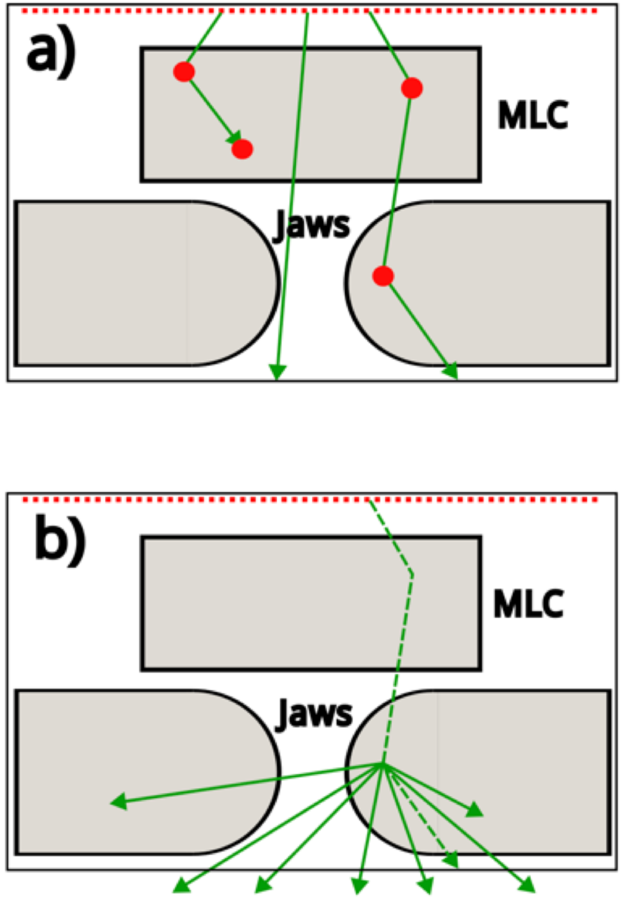
GUSTAVE ROUSSY CANCER CAMPUS GRAND PARIS

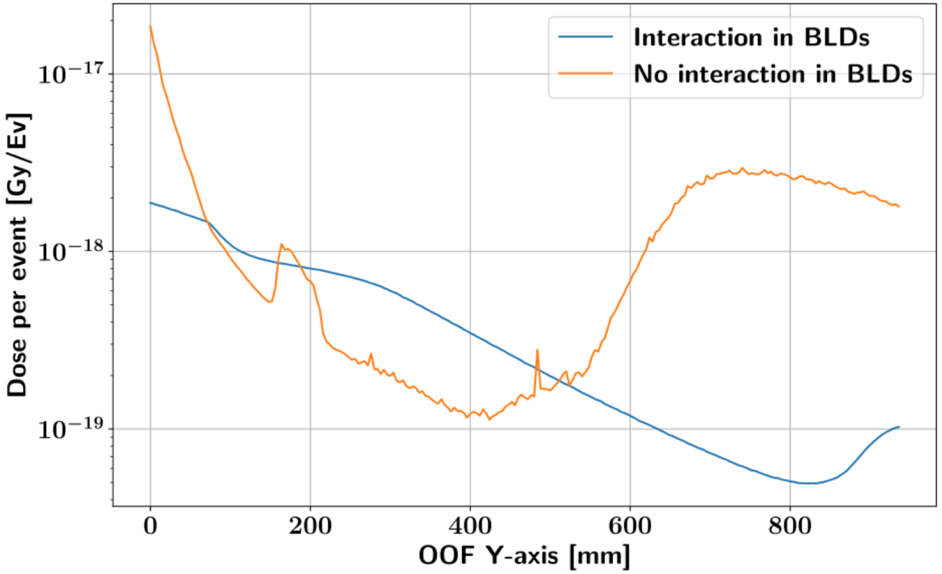
RHU

INVESTIR L'AVENIR

Monte Carlo simulation

Last Vertex Splitting (**LVS**) + Track Length Estimator (**TLE**)

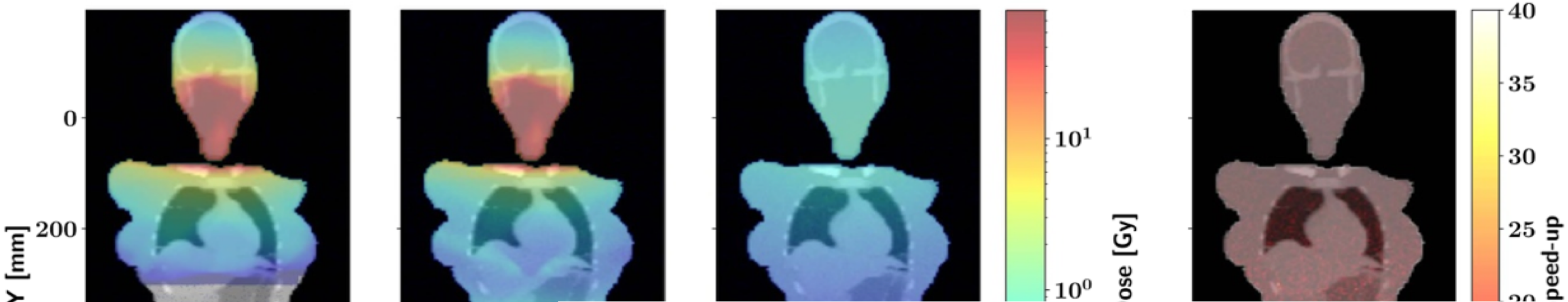




$$D_i^{\text{TLE}} = \frac{E \times \mu_{\text{en}}(E, m_i) \times L_i}{\rho_i \times V}$$

Monte Carlo simulation

Speedup around x10



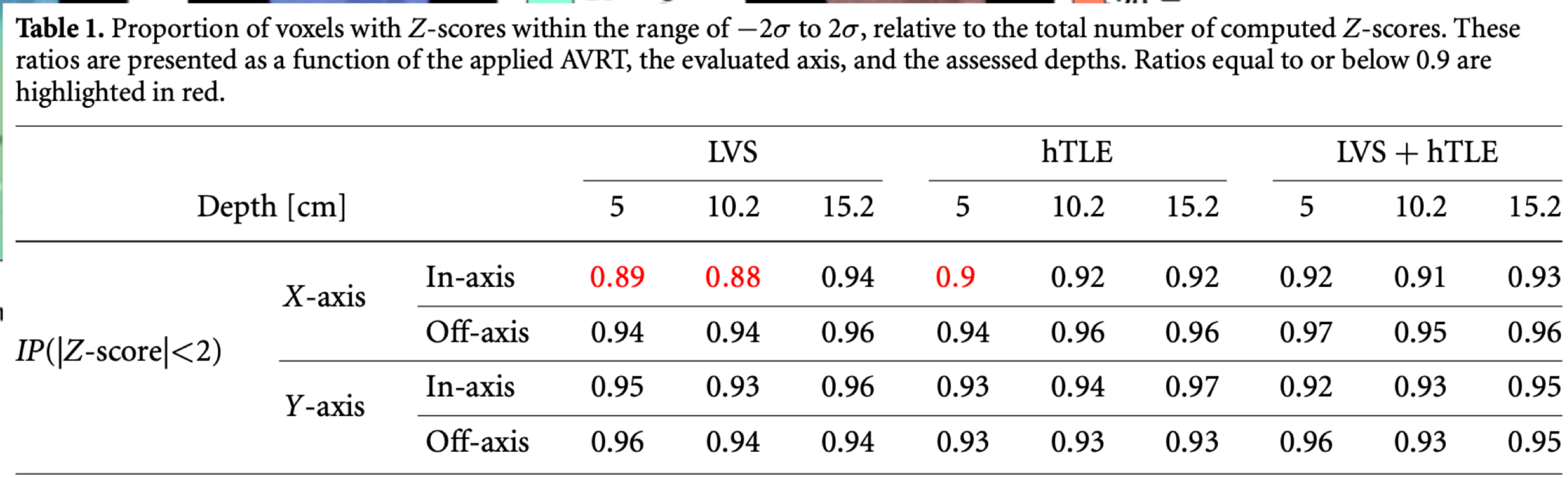


Table 1. Proportion of voxels with Z-scores within the range of -2σ to 2σ, relative to the total number of computed Z-scores. These ratios are presented as a function of the applied AVRT, the evaluated axis, and the assessed depths. Ratios equal to or below 0.9 are highlighted in red.

			LVS			hTLE			LVS + hTLE		
Depth [cm]			5	10.2	15.2	5	10.2	15.2	5	10.2	15.2
$IP(\|Z\text{-score}\|<2)$	X-axis	In-axis	0.89	0.88	0.94	0.9	0.92	0.92	0.92	0.91	0.93
		Off-axis	0.94	0.94	0.96	0.94	0.96	0.96	0.97	0.95	0.96
	Y-axis	In-axis	0.95	0.93	0.96	0.93	0.94	0.97	0.92	0.93	0.95
		Off-axis	0.96	0.94	0.94	0.93	0.93	0.93	0.96	0.93	0.95

Conclusion

- Variance Reduction Techniques (combined)
- Speedup x10 (from 5k hours to 300 hours)
- Available open-source in GATE

- Ready to generate a training database for AI

[Baldacci *et al*, ZMP 2014]
[Smekens *et al*, PMB 2014]
[Jacquet *et al*, PMB 2025]

Outline

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2.	**VRT2 (image)**	**Free-flight Angular Acceptance (FFAA)**
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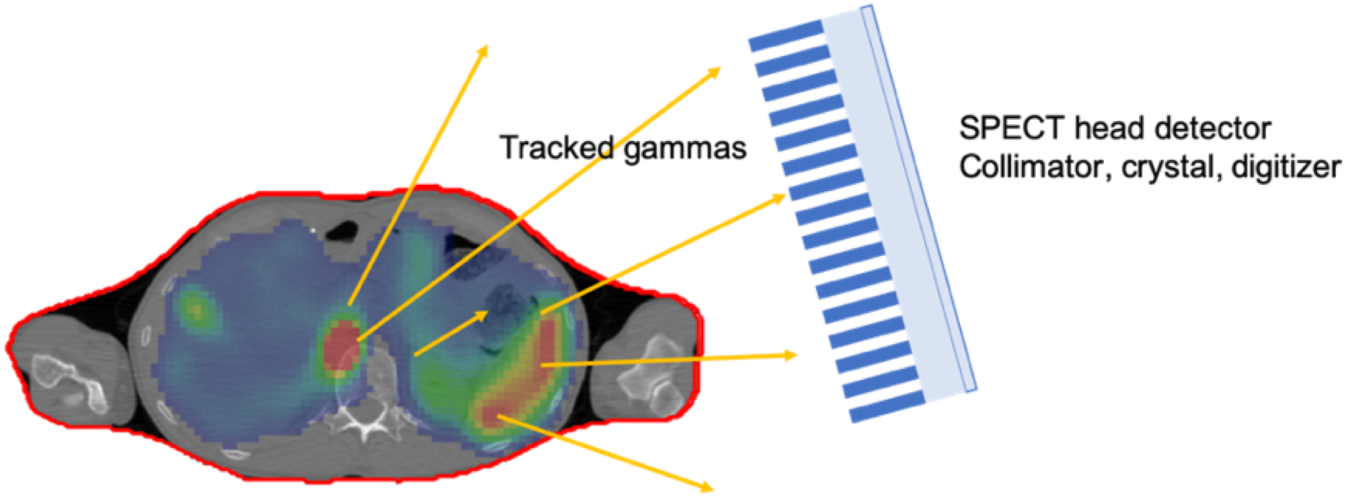
Goal: SPECT imaging

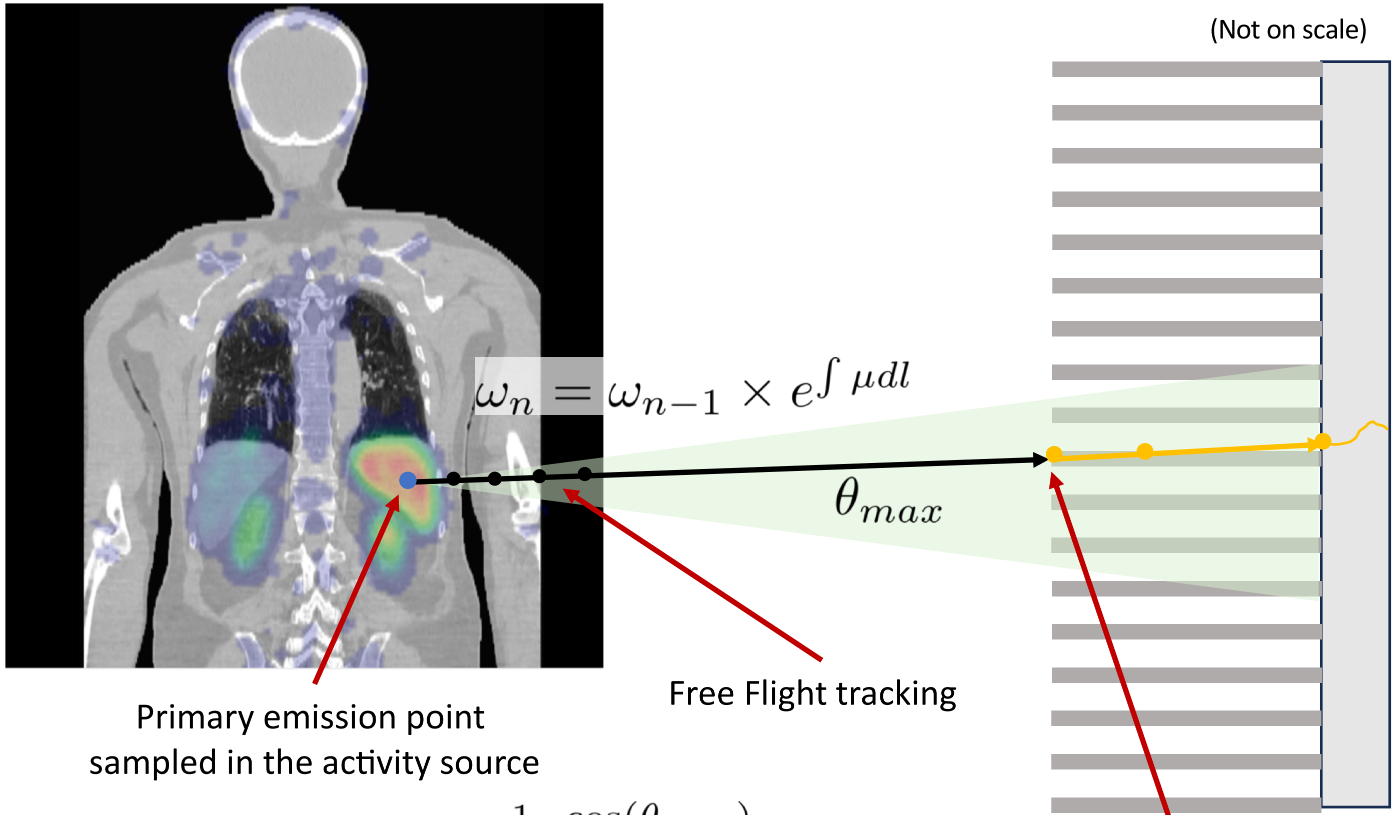
- Very slow MC simulations
- Track 1e5 particle for 1 count



Step1: primary photon

Step1:

- Non interacting (primary) photon
- FF + AA towards the detector
- Conventional MC in the collimator/detector



(Not on scale)

$$\omega_n = \omega_{n-1} \times e^{\int \mu dl}$$

Primary emission point sampled in the activity source

Free Flight tracking

Conventional tracking (in the detector)

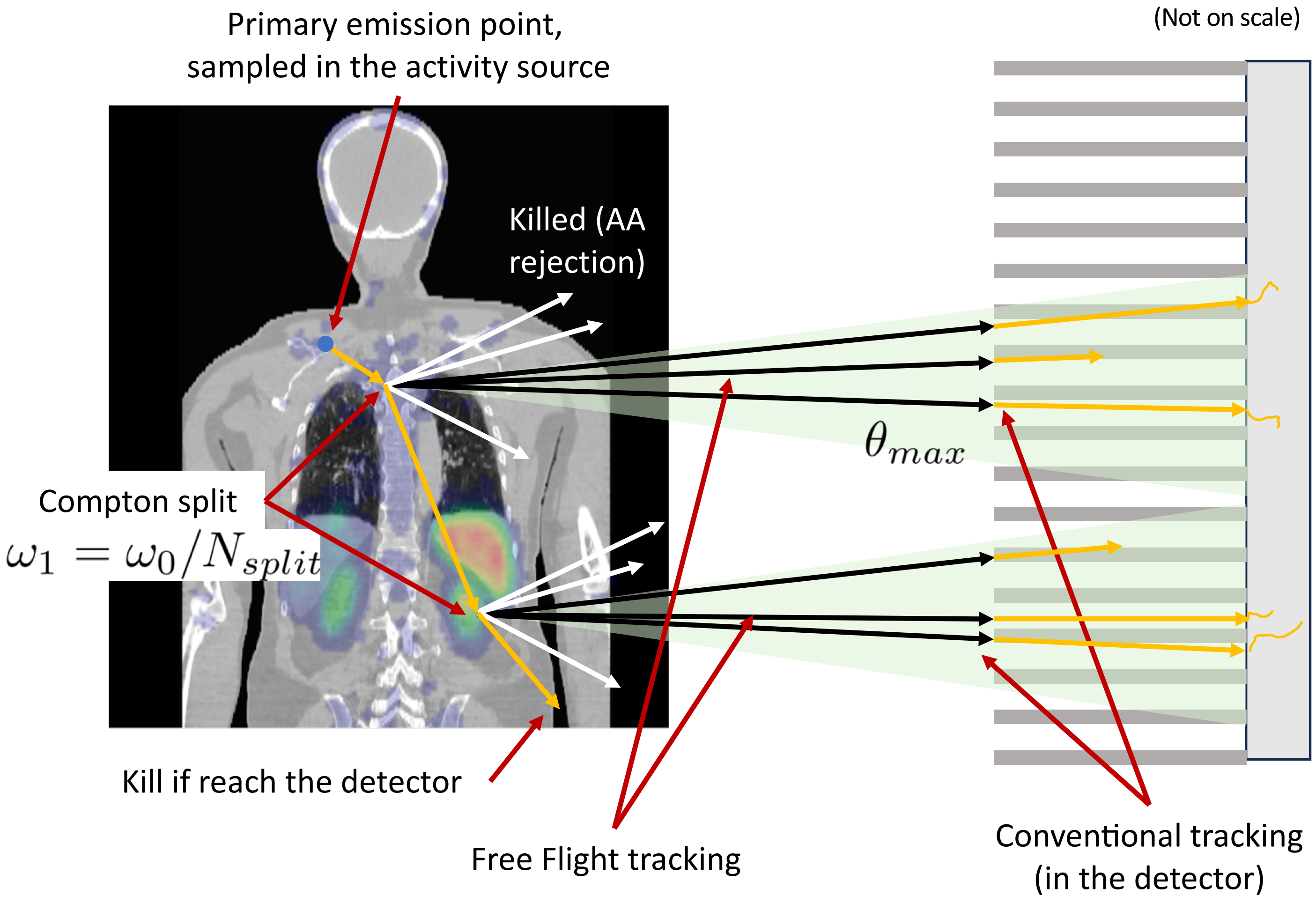
$$\omega_0 = 1 \qquad \omega_1 = \omega_0 \times \frac{1-\cos(\theta_{max})}{2}$$

Free Flight + Angular Acceptance FFAA

Step2: Scattered photons

Step2:

- Scattered photon, spliting factor
- FF + AA toward the detector

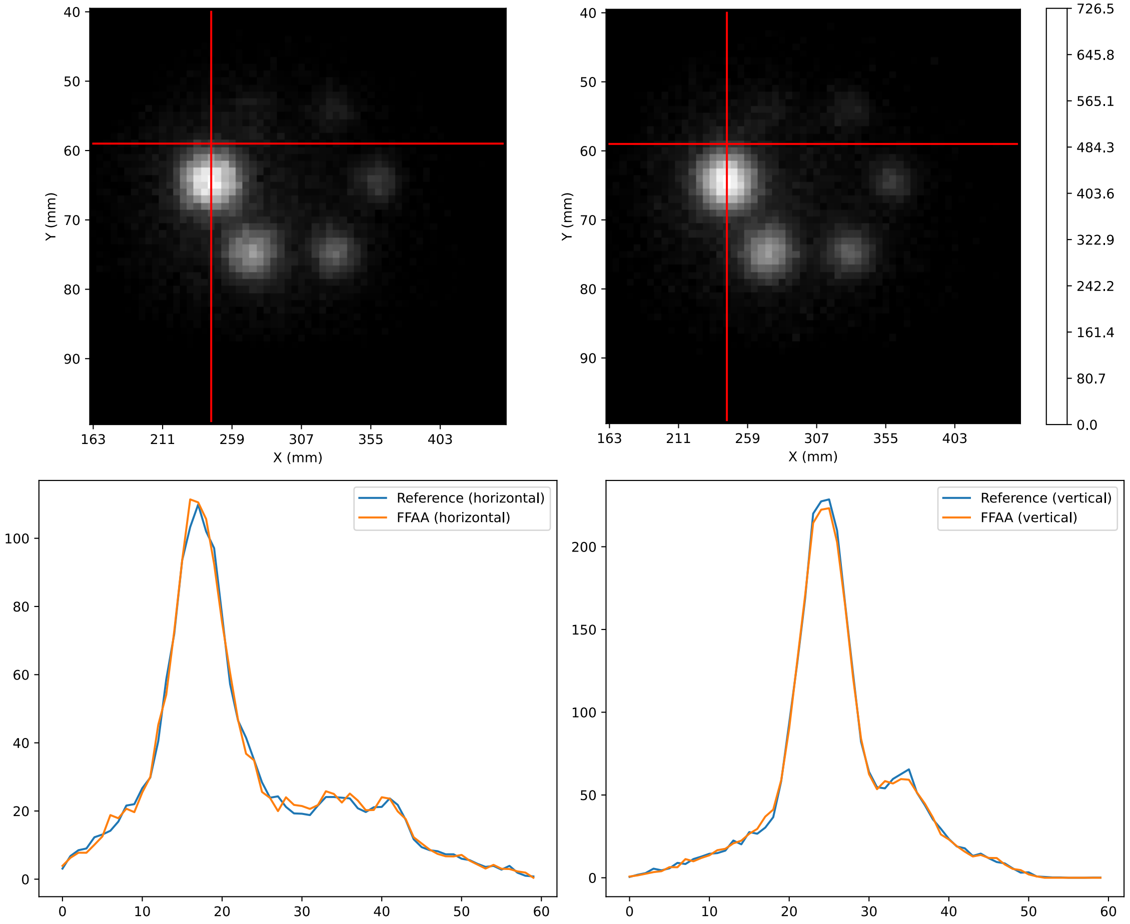


(Not on scale)
Primary emission point, sampled in the activity source
Killed (AA rejection)
θ_{max}
Compton split
$\omega_1 = \omega_0 / N_{split}$
Kill if reach the detector
Free Flight tracking
Conventional tracking (in the detector)

Free Flight + Angular Acceptance FFAA

Results

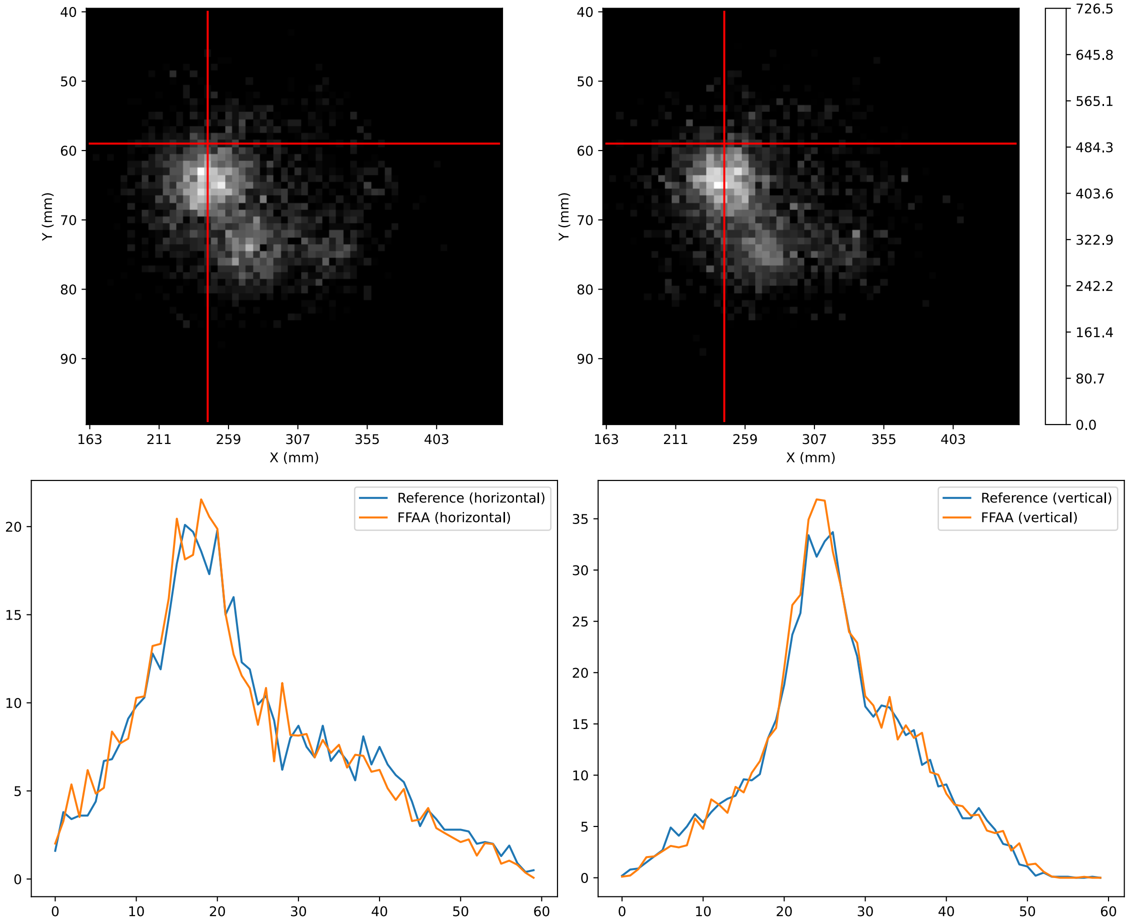
^{177}Lu 113 keV peak windows



Analog

FF-AA

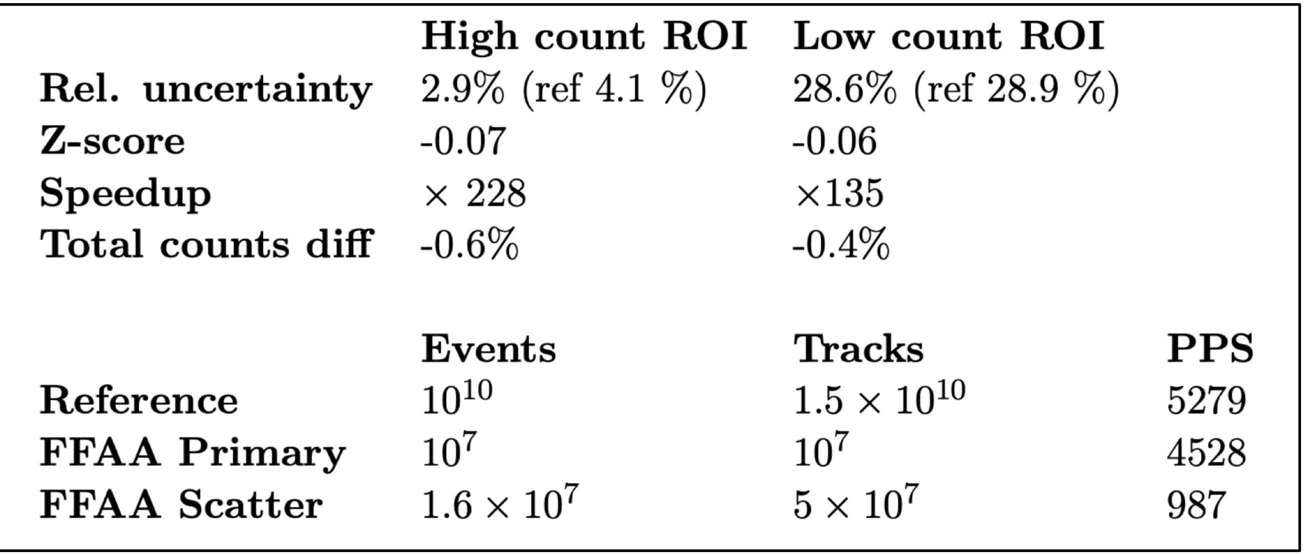
^{177}Lu upper scatter windows



Analog

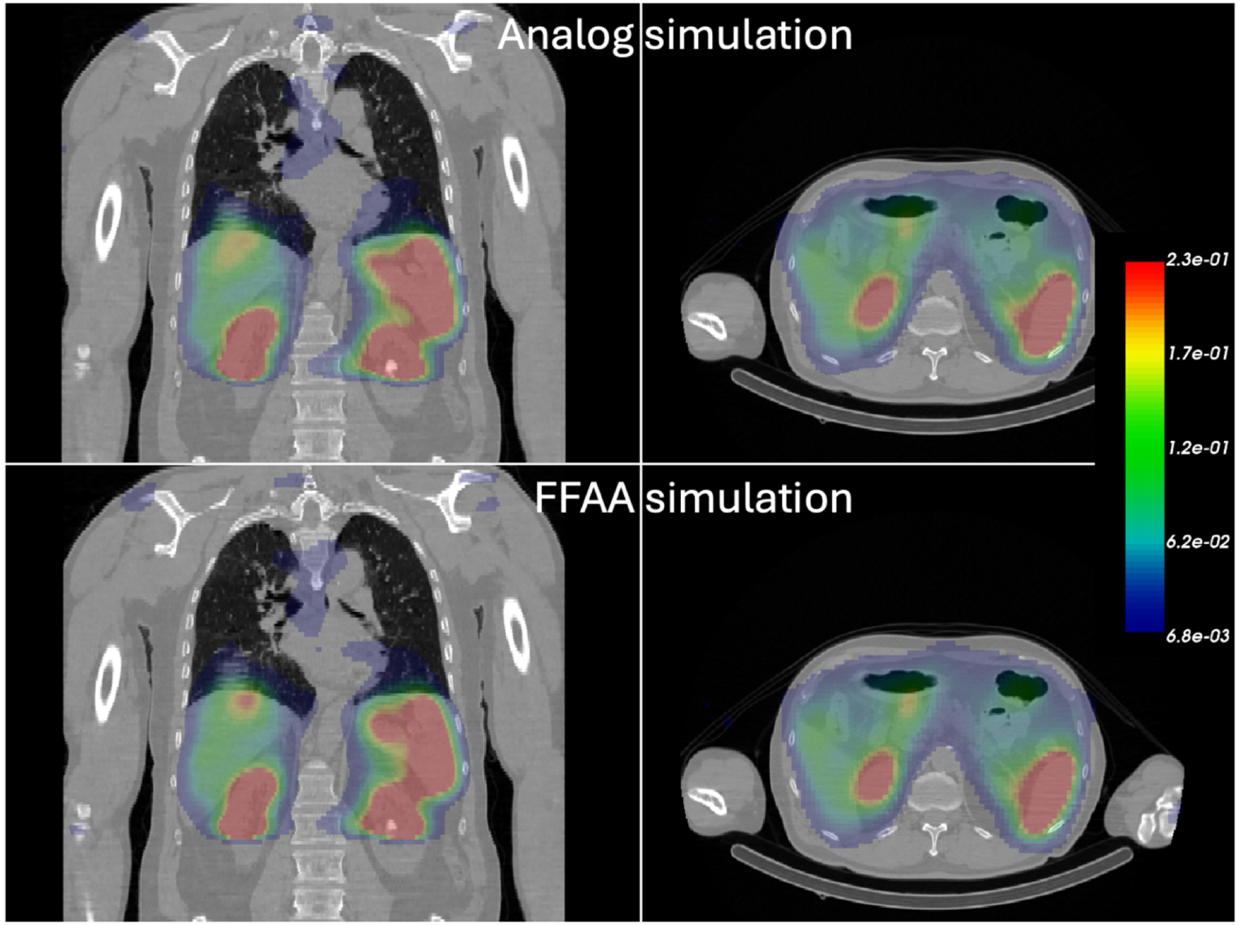
FF-AA

Results (reconstruction)



	High count ROI	Low count ROI
Rel. uncertainty	2.9% (ref 4.1 %)	28.6% (ref 28.9 %)
Z-score	-0.07	-0.06
Speedup	× 228	×135
Total counts diff	-0.6%	-0.4%

	Events	Tracks	PPS
Reference	10^{10}	1.5×10^{10}	5279
FFAA Primary	10^{7}	10^{7}	4528
FFAA Scatter	1.6×10^{7}	5×10^{7}	987



Conclusion

- Revisited VRT for SPECT
- Free Flight concept from Geant4
- Angular Acceptance
- Speedup x100

- Available open-source in GATE
- Ready to generate database of SPECT for supervised deep reconstruction

[Sarrut *et al*,
submited PMB 2026]

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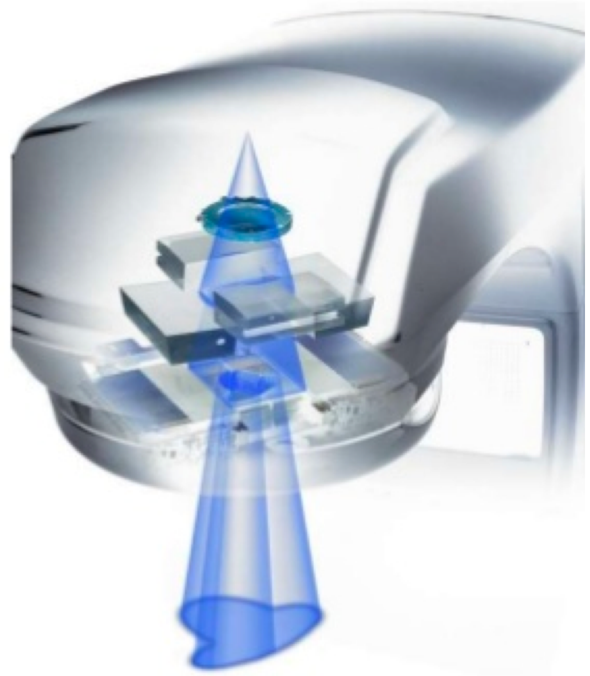
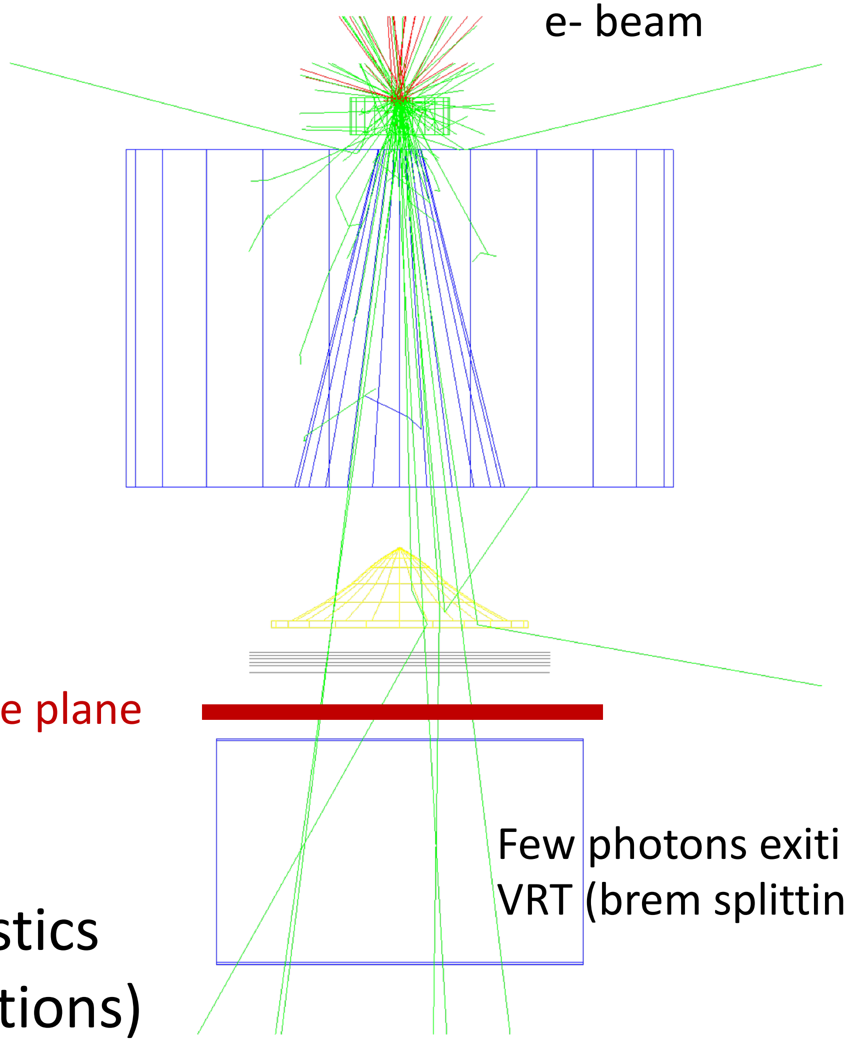
4. GAN (image) cGAN SPECT

Goal





e- beam

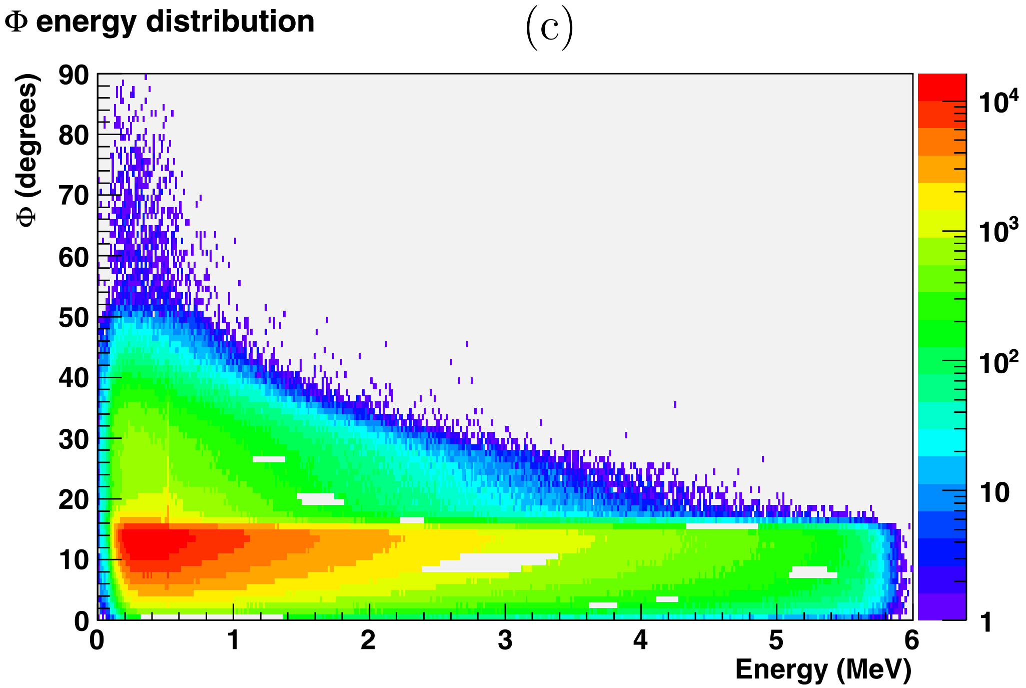
Phase space plane

Few photons exiting VRT (brem splitting)

Goal: determine beam characteristics (energy, position, direction distributions)

Phase Space (PHSP)

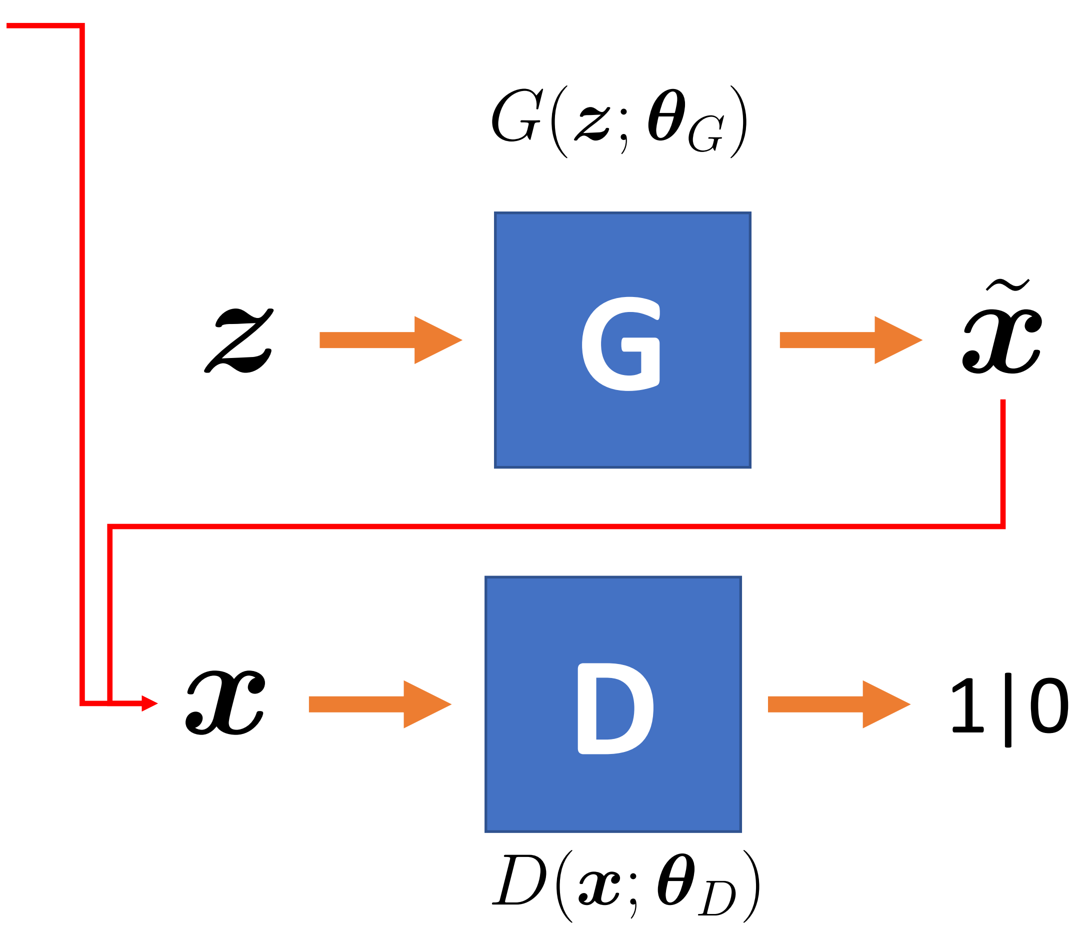
- Store beam properties as **Phase Space**
  - A PHSP is a list of particles (around 10^8, 10^9)
  - Properties: E, x, y, z, dx, dy, dz, w, (time)
- Advantages:
  - Computed only once
  - Fast to use
  - Can be shared
- Drawback
  - Several GB
  - When a cluster is used, should be shared among workers
  - Limited number of particles
- Need for an analytical model



Example of dependence of direction ϕ and energy

GAN: Generative Adversarial Network

- Training dataset $\boldsymbol{x} \in \mathbb{R}^d$
  - Dimension d=7 (E, X, Y, Z, dX, dY, dZ)
  - Samples of unknown p_{real}
- Generator + Discriminator
- Wasserstein GAN [Arjovsky 2017]



$G(\boldsymbol{z};\boldsymbol{\theta}_G)$
$\boldsymbol{z}$
G
$\tilde{\boldsymbol{x}}$
$\boldsymbol{x}$
D
1|0
$D(\boldsymbol{x};\boldsymbol{\theta}_D)$

$$J_D(\boldsymbol{\theta}_D, \boldsymbol{\theta}_G) = \mathbb{E}_{\boldsymbol{z}}[D(G(\boldsymbol{z}))] - \mathbb{E}_{\boldsymbol{x}}[D(\boldsymbol{x})]$$

$$J_G(\boldsymbol{\theta}_D, \boldsymbol{\theta}_G) = -\mathbb{E}_{\boldsymbol{z}}[D(G(\boldsymbol{z}))]$$

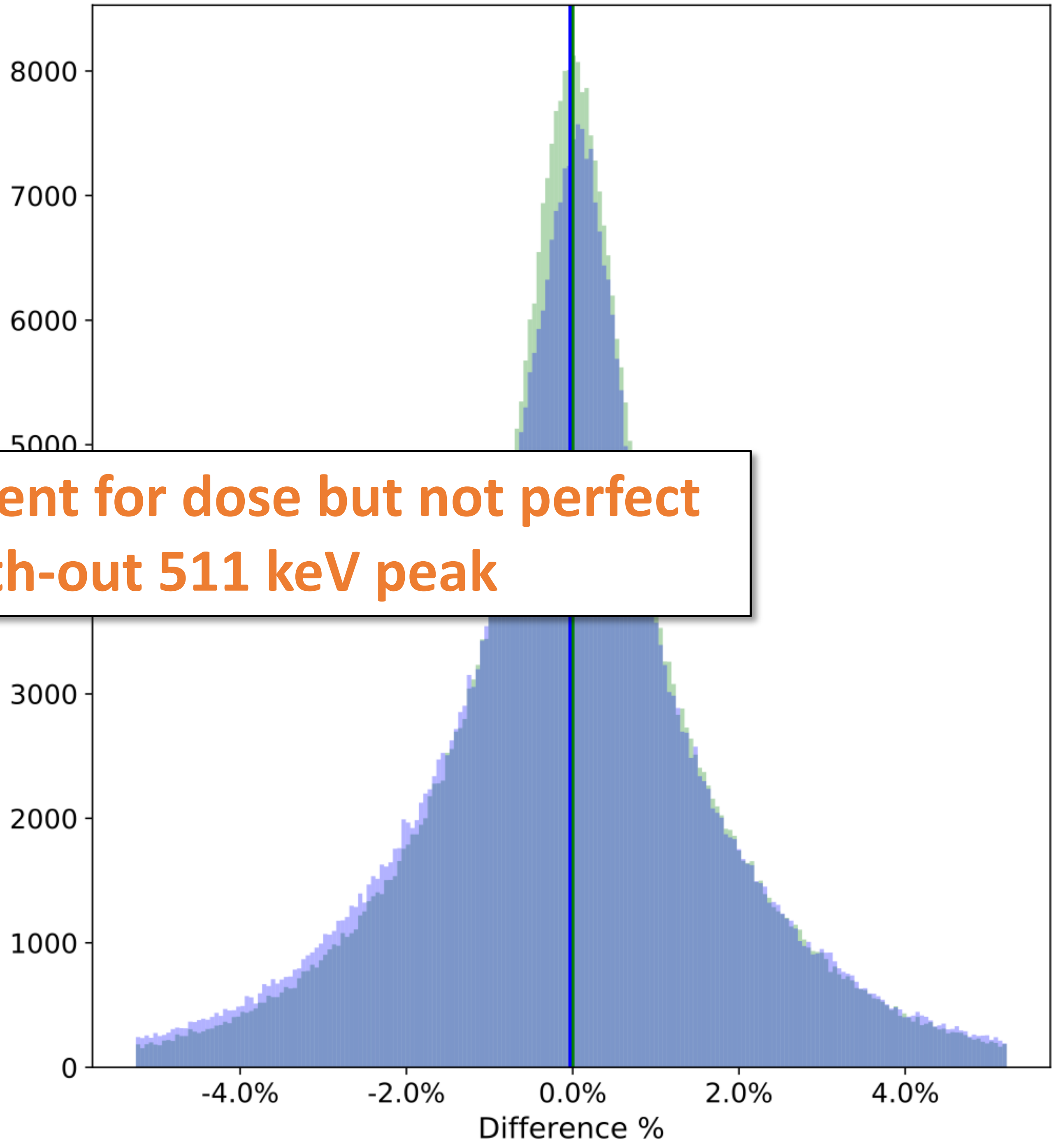
Results

Distributions of relative differences between

- PHSP1 and PHSP2
- PHSP1 and GAN

Vertical lines indicate the mean differences

Difference relative to the prescribed dose



- **Sufficient for dose but not perfect**
- **Smooth-out 511 keV peak**

Conclusion

- GAN as a particles generator (PHSP)
- From 5-10 GB to few MB
- Trained from Monte Carlo
- Available open-source in GATE

- Still difficult to train and control

[Sarrut *et al*, PMB 2019]

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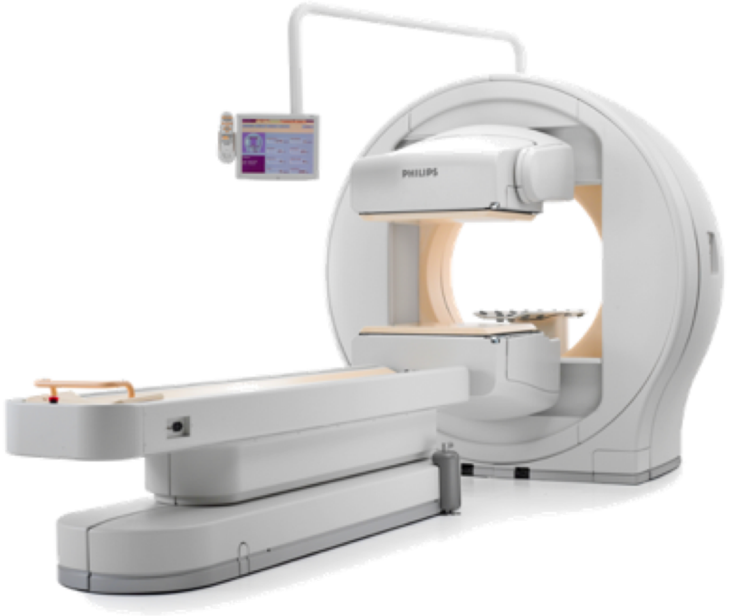
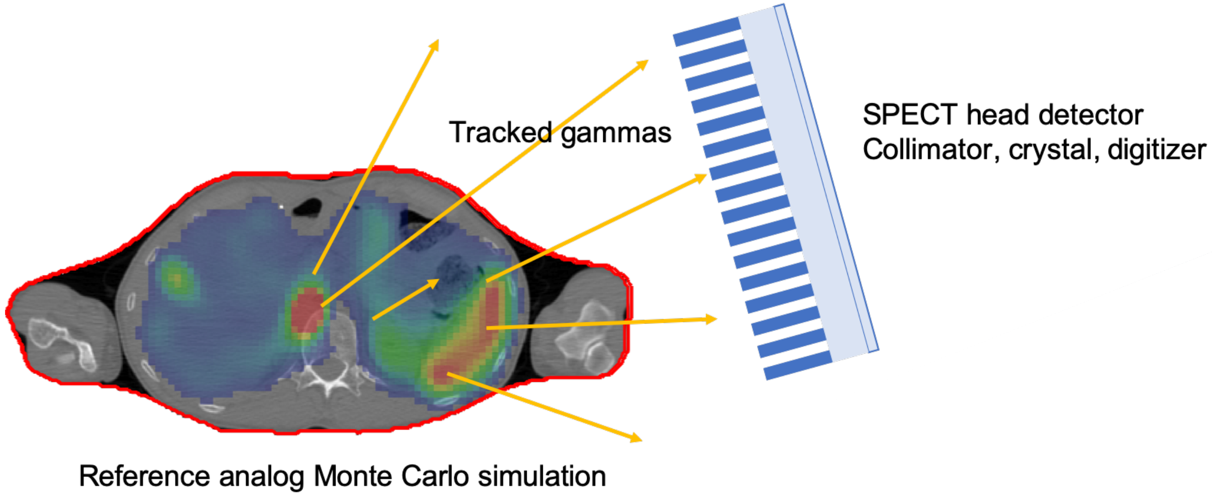
SPECT simulation

- Part1: from emission to patient exiting gamma
- Part2: track gamma inside the detector



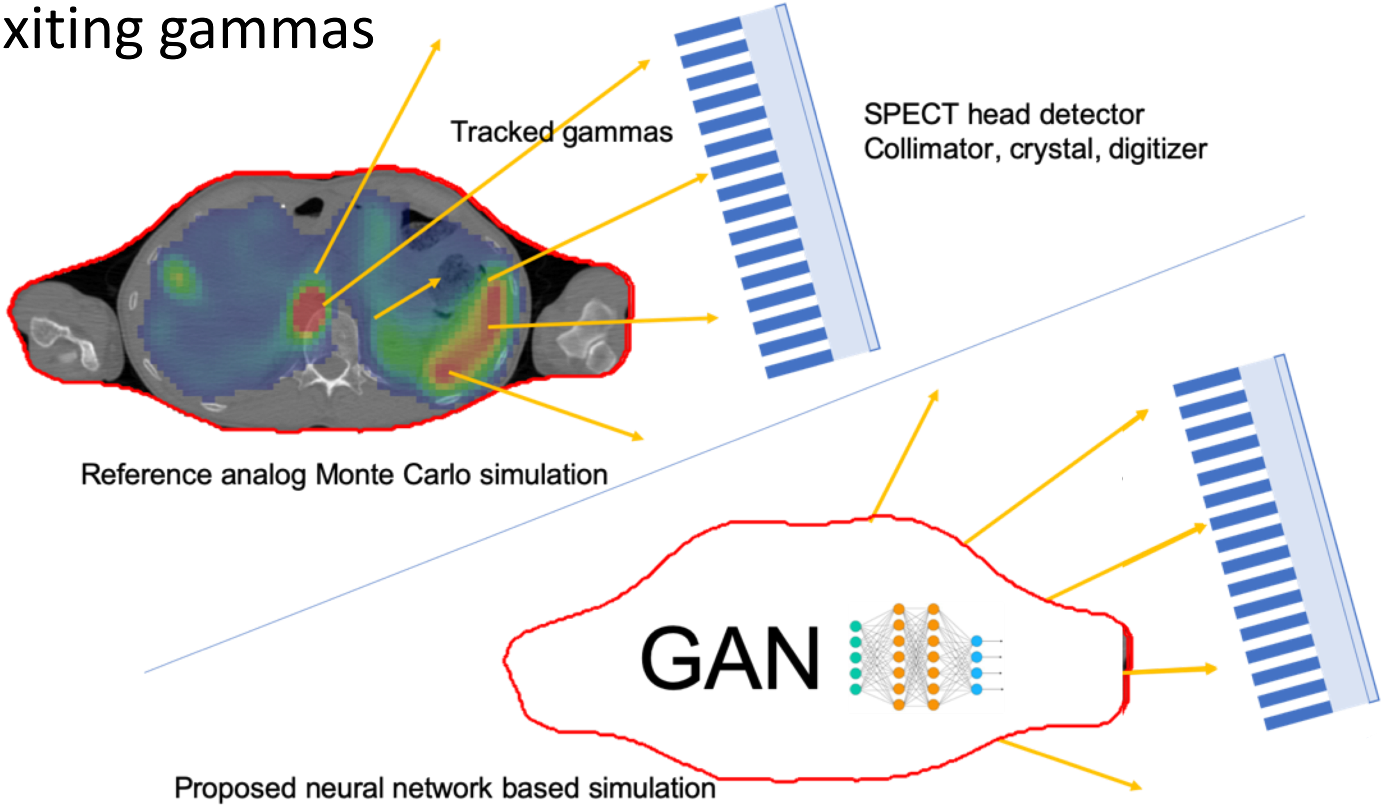


Tracked gammas
SPECT head detector
Collimator, crystal, digitizer
Reference analog Monte Carlo simulation

Training dataset

Train a GAN to produce exiting gamma from a given source of activity

- Step1: run low stats MC, consider exiting gammas
- Step2: train a GAN
- Step3: use GAN a source


Tracked gammas
SPECT head detector
Collimator, crystal, digitizer
Reference analog Monte Carlo simulation
GAN
Proposed neural network based simulation

Conditional GAN

Train with one given **phantom** (CT, patient) …

… but with **homogeneous** activity

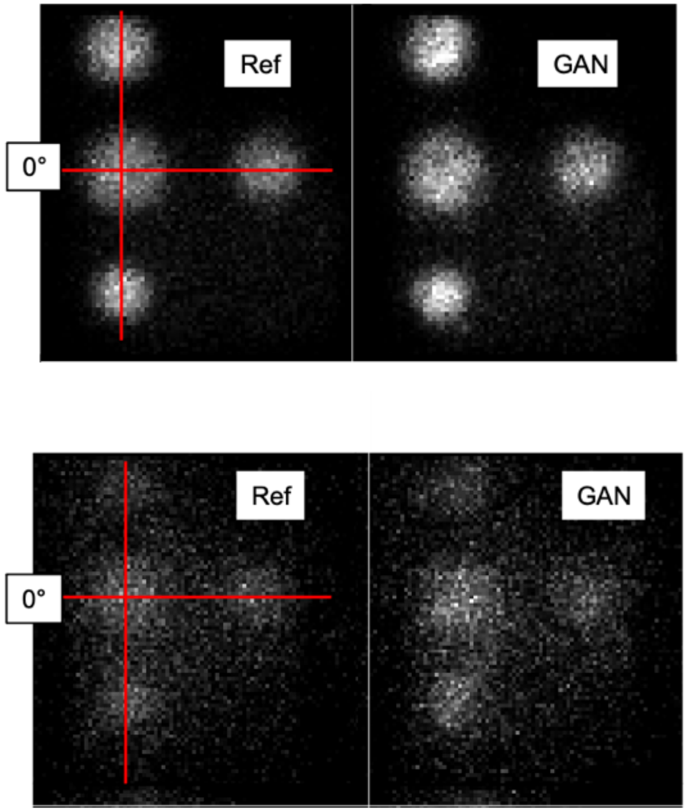
Conditional input activity map.

$$\mathcal{L}_{\mathcal{C}} = \mathbb{E}[C(G(\mathbf{z}|\mathbf{y}))] - \mathbb{E}[C(\mathbf{x}|\mathbf{y})] + \underbrace{\lambda\mathbb{E}[(\left\|\nabla_{\hat{\mathbf{x}}|\mathbf{y}}C(\hat{\mathbf{x}}|\mathbf{y})\right\|_2 - 1)^2]}_{GP \quad regularization}$$

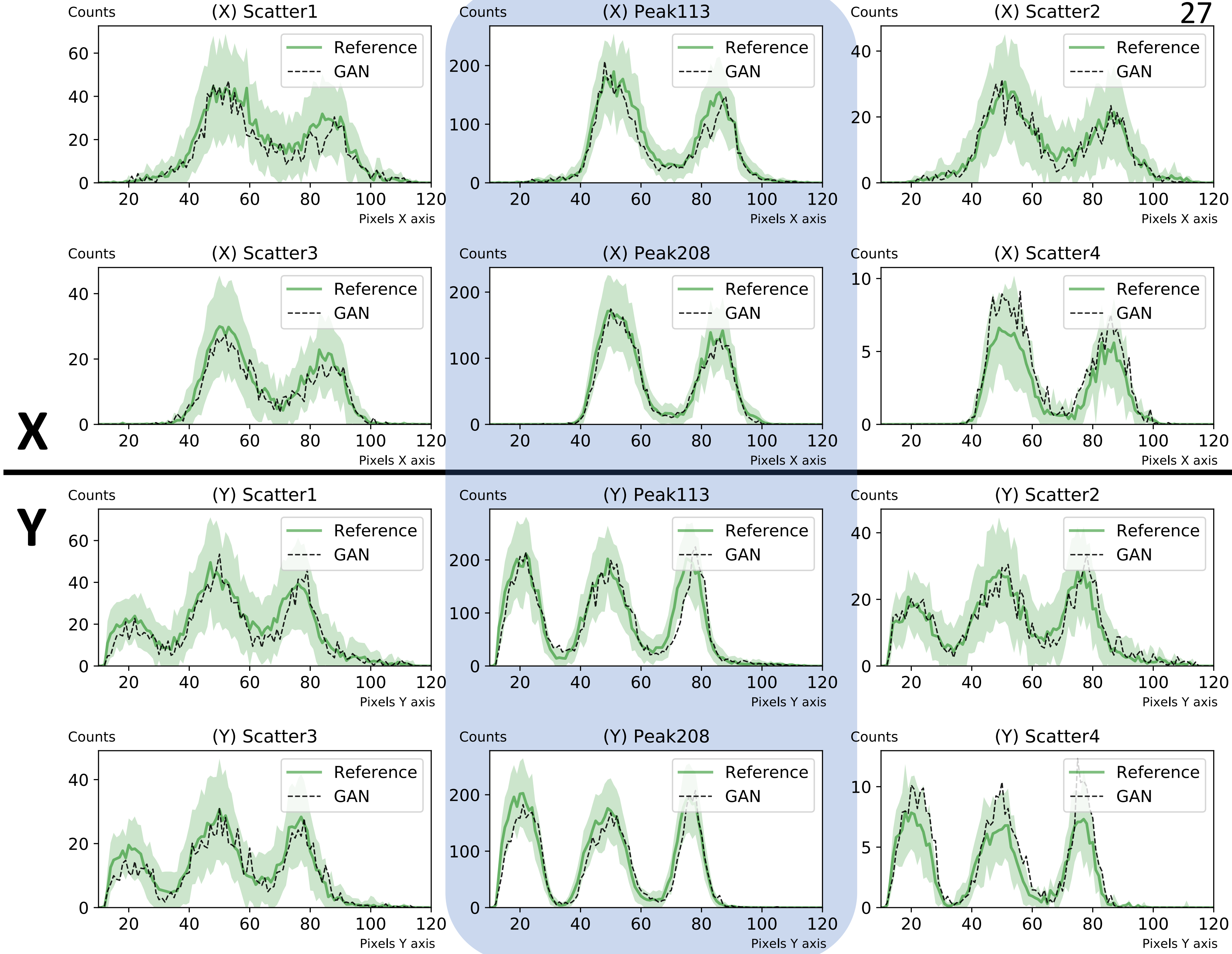
$$\mathcal{L}_G = -\mathbb{E}[C(G(\mathbf{z}|\mathbf{y}))]$$

[Saporta et al, PMB 2022]

Results



2D projections
Lu177 (1 peak & scatter)



Conclusion

- GAN as a particles generator …
- … conditioned with activity distribution
- Speedup x100

- Still need training with low-stat MC
- Still need re-training when CT change
- Still difficult to train and control
- Can be combined with NN ARF

- But potential for “differentiable MC” ?

[Sarrut *et al*, PMB 2021]
[Saporta *et al*, PMB 2022]
[Sarrut *et al*, PMB 2023]

Conclusion

- Monte Carlo still alive
- Still need acceleration methods
  - “Classical ones”: **VRT**
  - ”AI-based” : GAN, **Generative** ?
- To be included in reconstruction algorithms

- GATE is ready and open for research and industry