HPC serving
High Energy and Medical Physics

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HPC Workshop, 23 May 2022
Sharjah, UAE

Outline

- Research Computing at Texas A&M University at Qatar
- HPC case studies: for HEP and MedPhys
- Remarks and summary

HPC?

High Performance Computing is the **aggregation of computing** elements to deliver **much higher performance** computing power

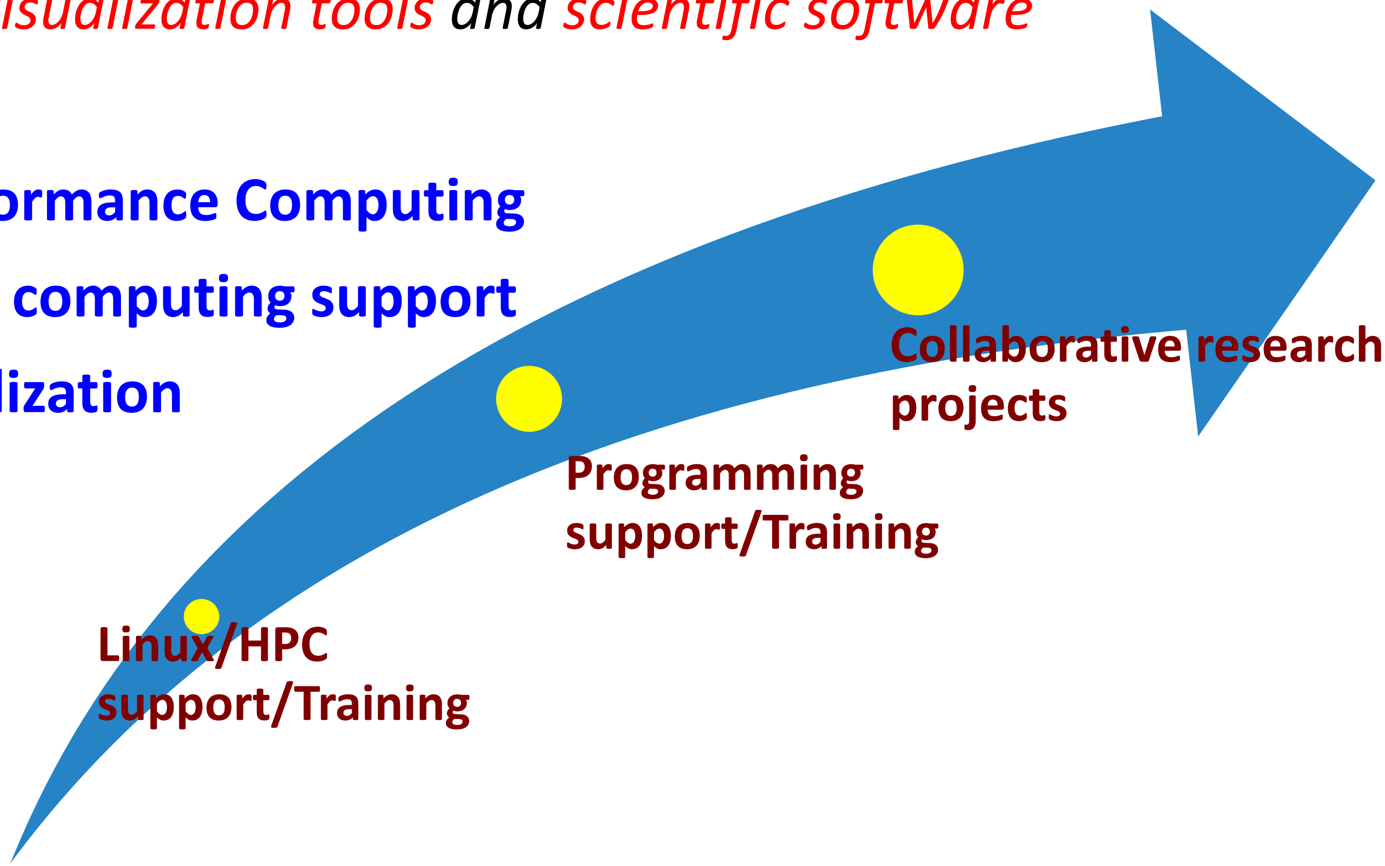
→ Solve problems that cannot be handled by commodity computers or desktops

RC at TAMUQ

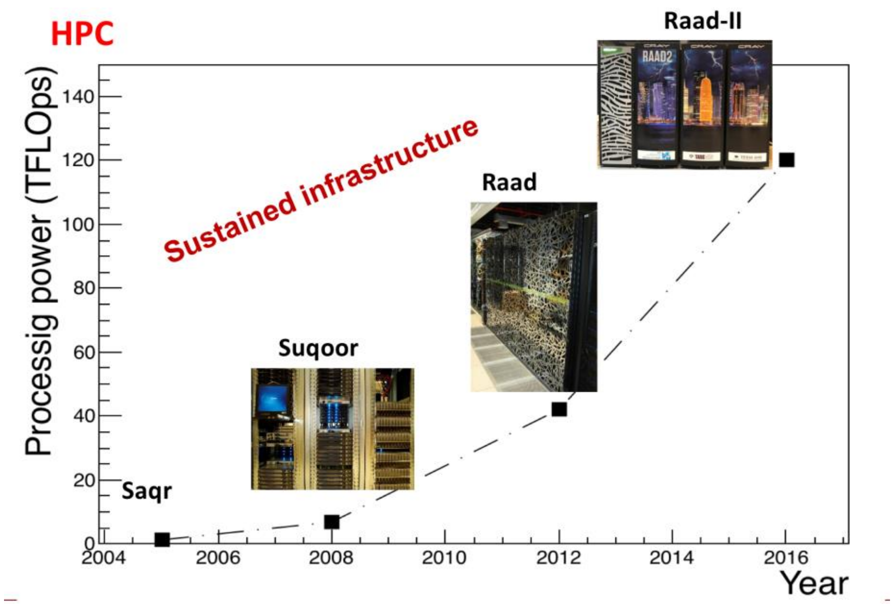
Research Computing group formed in 2008

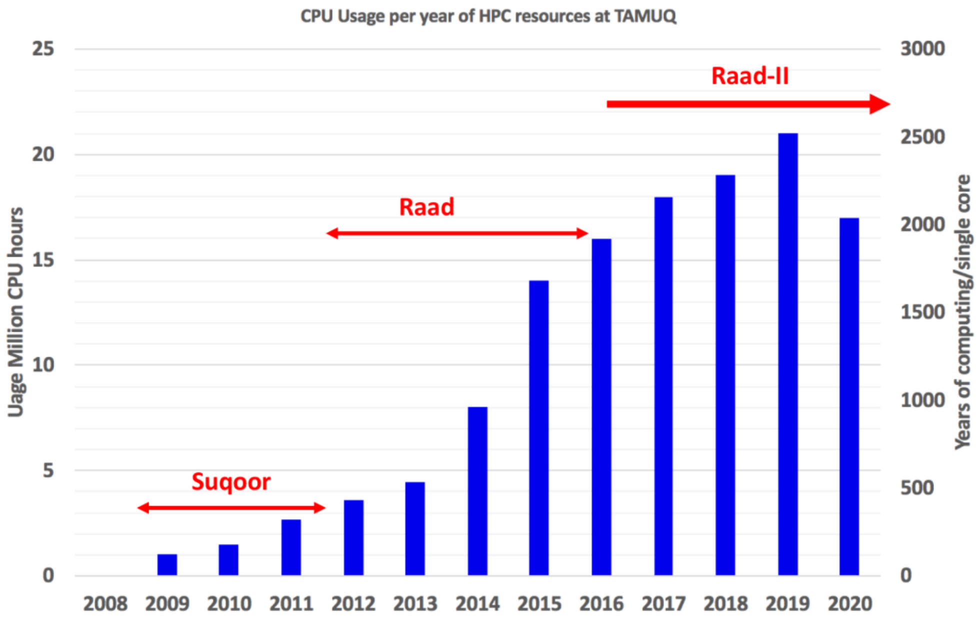
Mission: *Foster scientific research by providing researchers With advanced resources in terms of computational power, Storage capability, visualization tools and scientific software*

- **High Performance Computing**
- **Scientific computing support**
- **3D Visualization**



Sustained HPC Infrastructure





130 million CPU hours

الصندوق القطري لرعاية البحث العلمي
Qatar National Research Fund
Member of Qatar Foundation

HPC training programs

- Linux
- Scripting and programming (shell, python, C/C++…)
- Usage of HPC (batch software…)
- User interface for novice users
- Parallel programming
- Scientific programming
- GPU programming (e.g. CUDA)
- Python for AI
- Containers in HPC clusters

HPC capacity building

- Capstone project for undergraduates
- Helping Master and PhD students in their computational work
- Bringing new users to the HPC (user engagement)
- Attracting talents

HPC: service key areas locally and globally

- Environmental and climate science
- Oil&Gas applications
- Photovoltaics technologies
- Advanced Materials
- Life Science
- Computational Medicine
- Cybersecurity
- Information and Communication Technologies
- High Energy and Nuclear Physics
- Artificial Intelligence
- Others
- Training and Education

- 600+ Peer-reviewed journal
- 300+ International conference
- 300 Users trained: Linux/Supercomputing
- 120 Current Users

200+ publications/proc. used the HPC in 2020 and 2021 only

HPC: Not only a machine: it’s an ecosystem

Manpower	Hardware	Security	Software/application	Governance	Logistic
• Administration, • Daily support • Planning • executing • training • Docs	• replacing old equipment, • expanding existing one, • emerging technologies	• Data security and retention • Long and short term backup	• licensing • porting, compiling, optimizing • Common repositories • application requirement	• Policies • Roadmap update • Implement and enforce policies	• Networking • Data center issues

Updated roadmap for the future →

Consolidating the High Performance Computing Ecosystem to Prepare Qatar for Peta & Exa-scale Computing in the Data Intensive Era

Authors: Research Computing team at TAMUQ
August 2018, Doha.

TASC: Advanced Scientific Computing Center

HPC: Ecosystem

- We started the International Computational Science and Engineering Conference
- Three conferences alerady: ICSEC15, ICSEC17 and ICSEC19
- Selected papers published in the Journal of Computational Science
- **Fourth (ICSEC23) will be launched soon**

High Energy Physics

Particle/High Energy Physics:

❑ What' s?

➢ Study the elementary constituents of matter

➢ the interaction between them

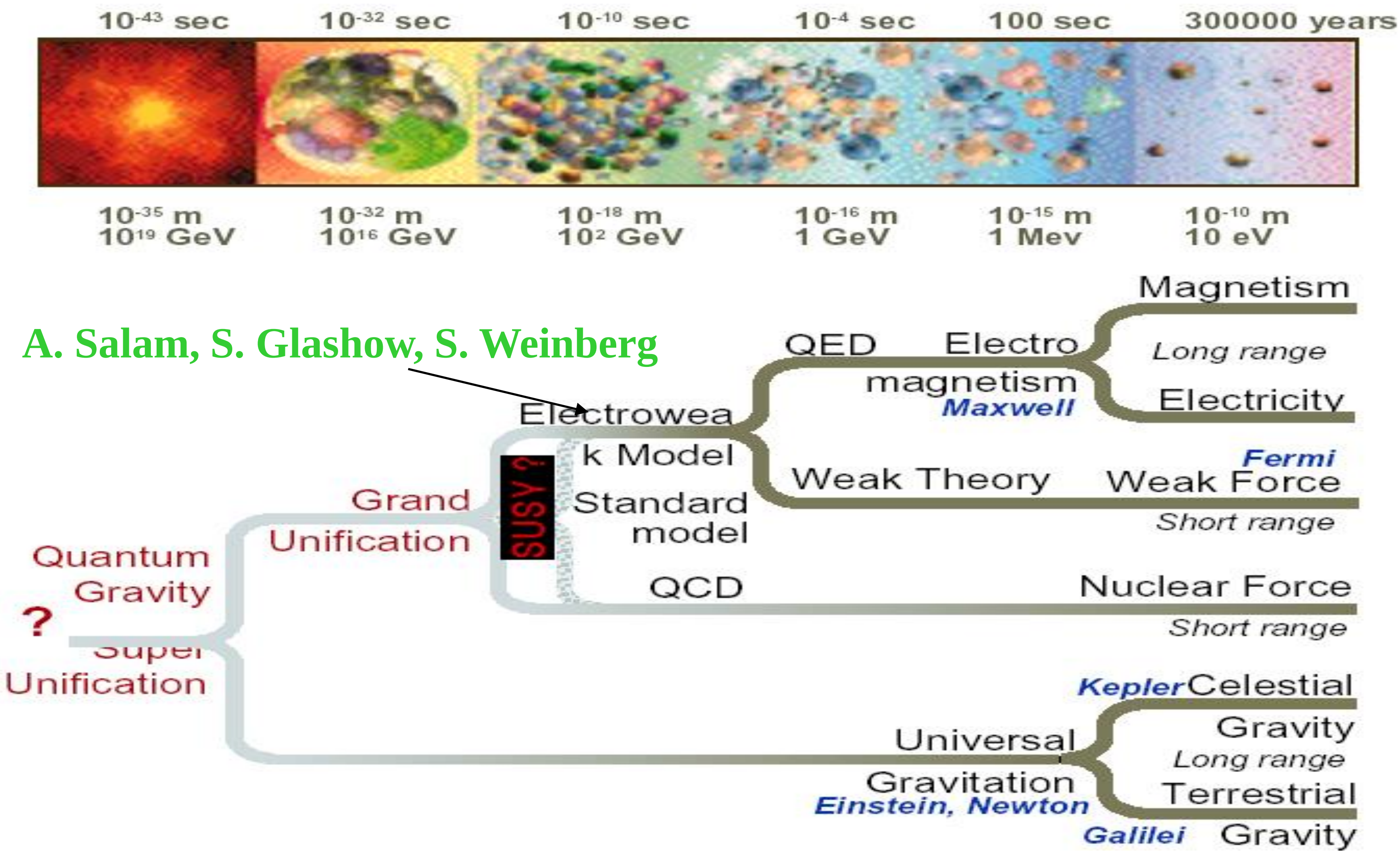
❑ How?

➢ accelerate particles

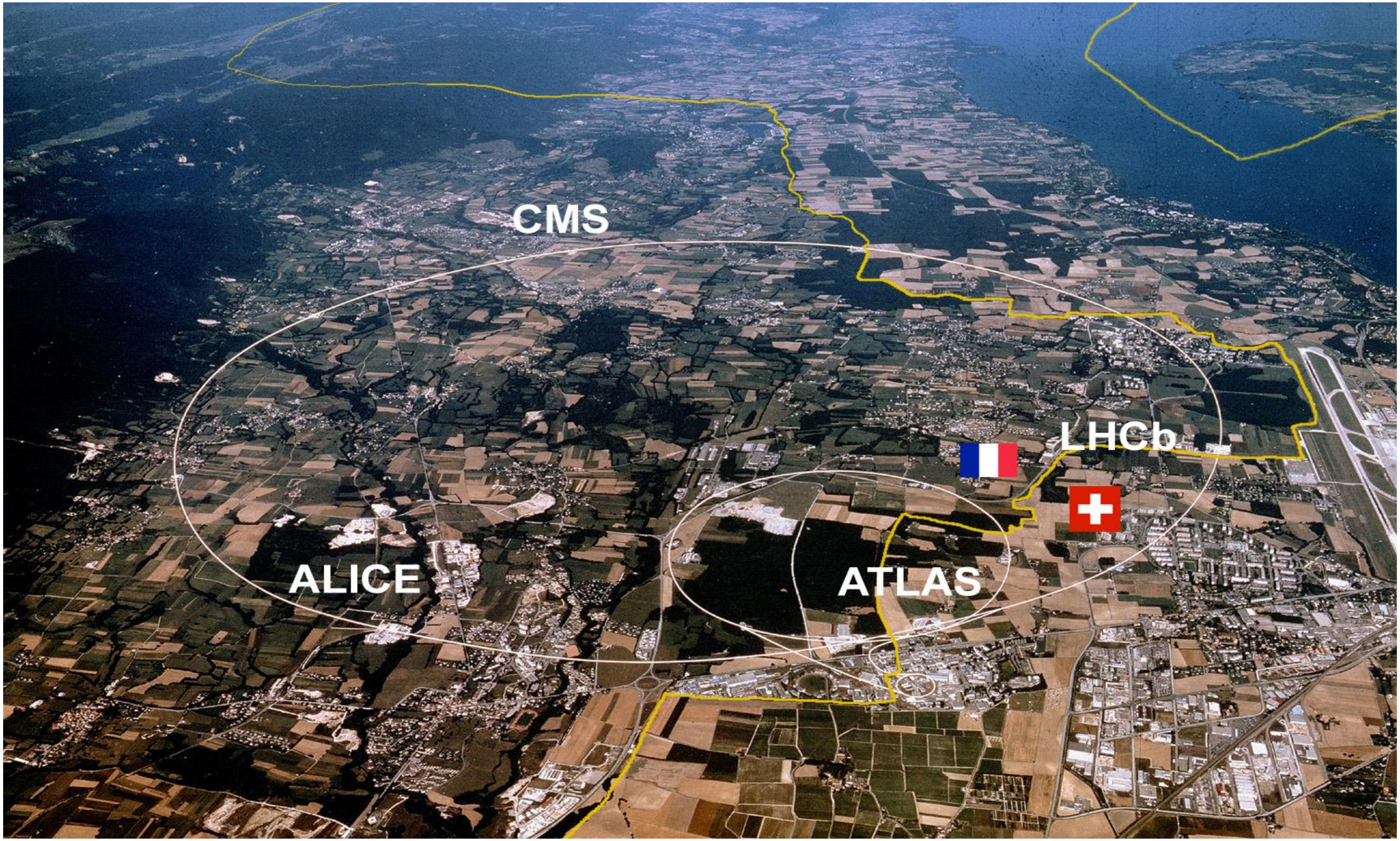
➢ make them collide with each other or with a fixed target

➢ detect and study the collision products

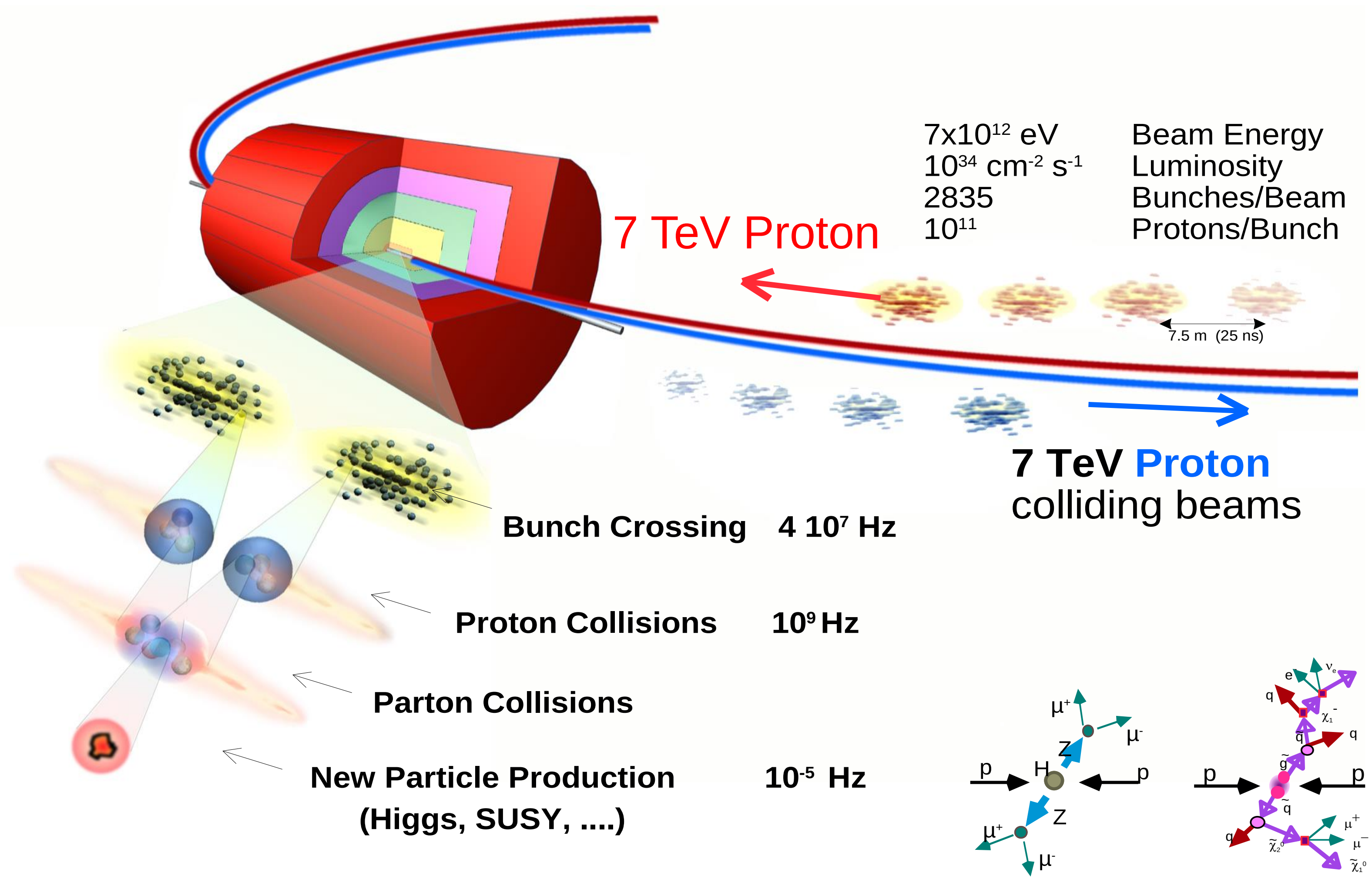
Evolution: Unification?



High Energy Physics

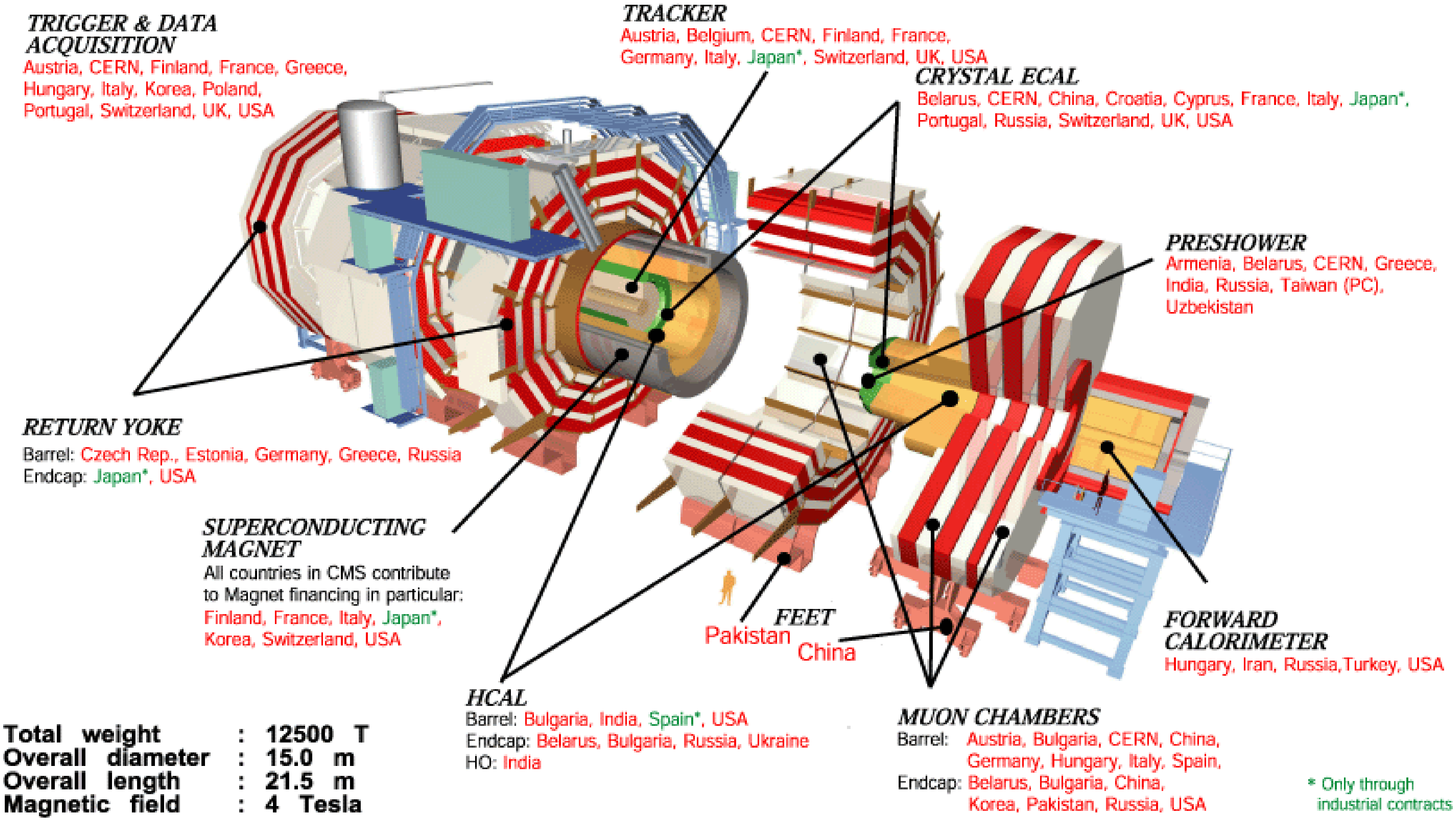


LHC: some parameters



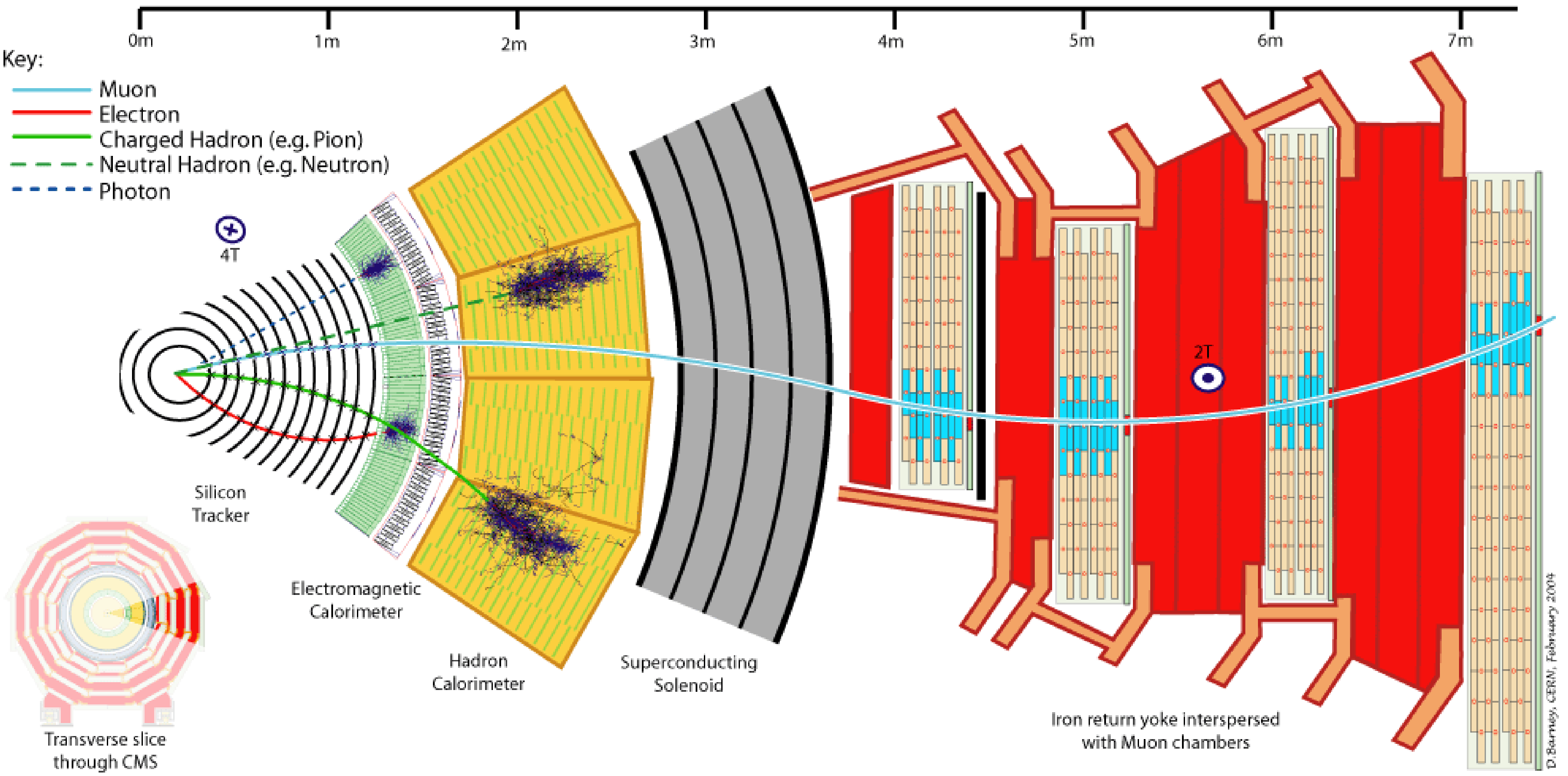
Selection of 1 event in 10,000,000,000,000

CMS components and collaborators

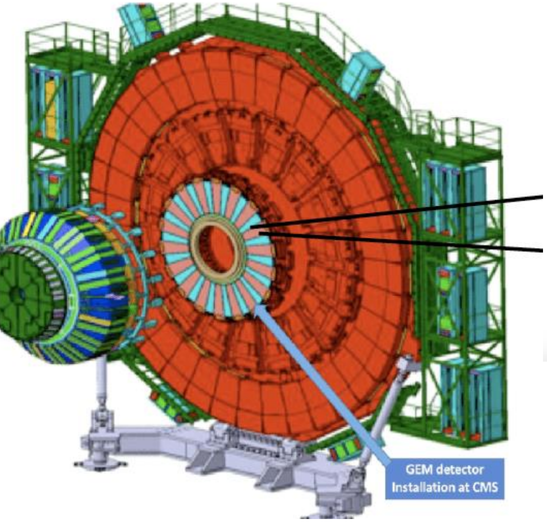


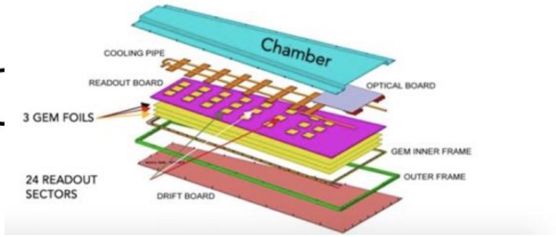
Total weight	**:**	**12500**	**T**
Overall diameter	**:**	**15.0**	**m**
Overall length	**:**	**21.5**	**m**
Magnetic field	**:**	**4**	**Tesla**

CMS cross section



Major upgrade





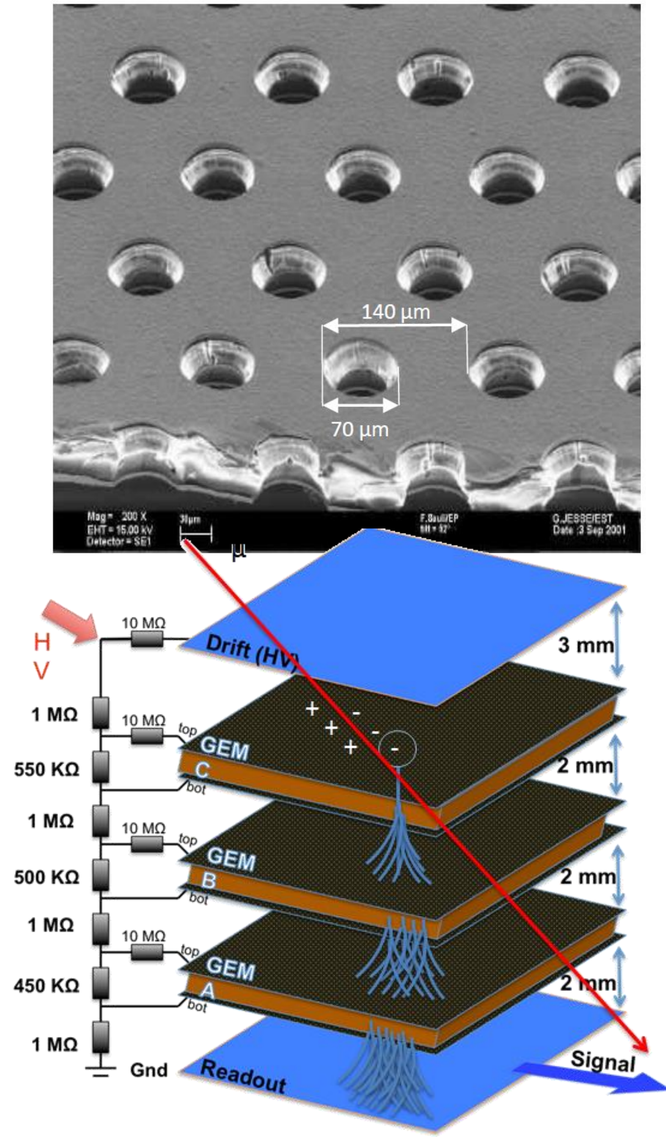
	GE1/1	GE2/1	ME0
Number of GEM chambers	144 chambers (72 superchambers)	72	36
Chamber dimensions (cm)	Long modules: 22.5 base, 128.5 length Short modules: 22.5 base, 113.5 length	53.3 base, 183.3 length	23.6 base, 78.8 length
Total readout channels	442,368	442,368	663,552
Pseudorapidity (η) coverage	$1.55 < \eta < 2.20$	$1.62 < \eta < 2.43$	$2.03 < \eta < 2.80$
Opening angle (degrees)	10	20	20
Status	Installation completed in Fall 2020	Design almost complete	Design and optimization in progress

1.5 M Electronic channels added to this area

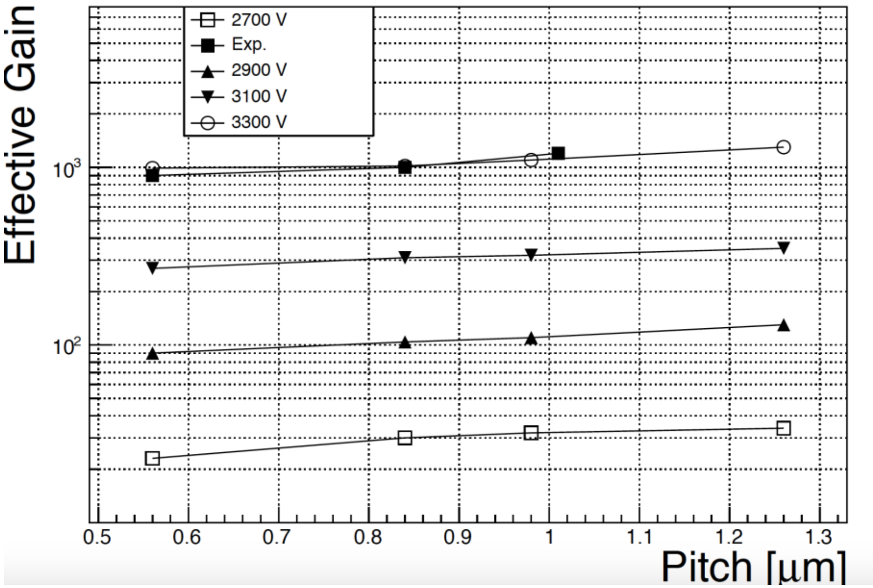
The Gas Electron Multiplier (GEM)

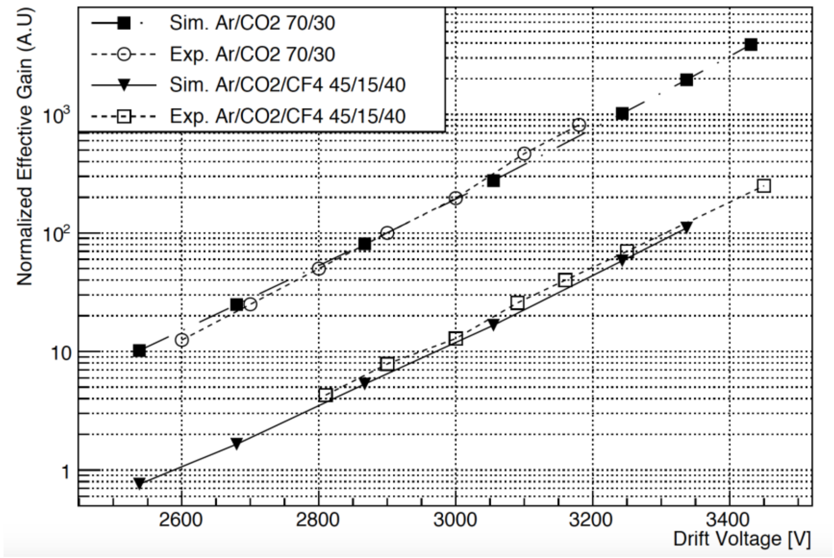
Spatial resolution	300 µm
Time resolution	10 ns
Detection Efficiency	97%
Long-term operation	> 10 years LHC-HL
Uniform response	<15-20% gain variation across the full area

Extensive R&D through simulation

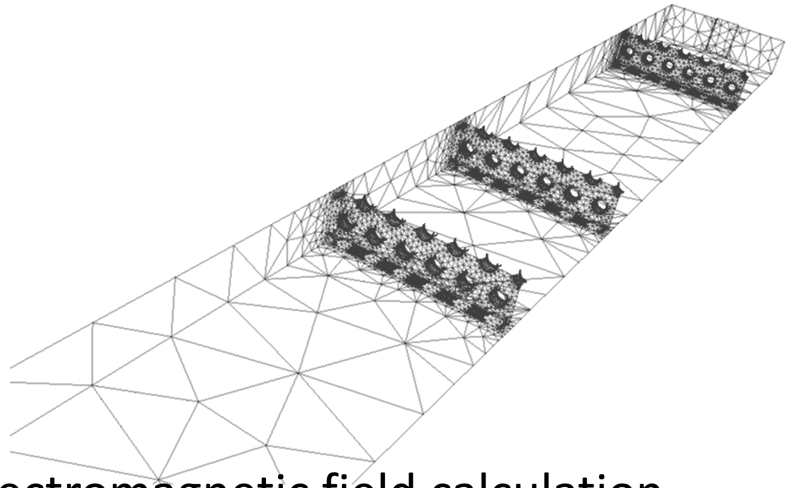


The Gas Electron Multiplier (GEM)





Involving students from mechanical engineering



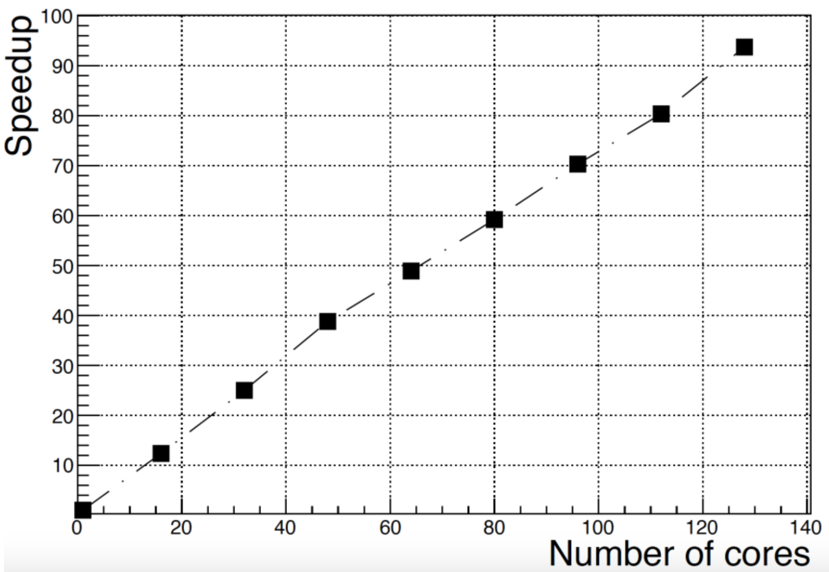
O. Bouhali et al., NIMA 832 (2016)

Electromagnetic field calculation

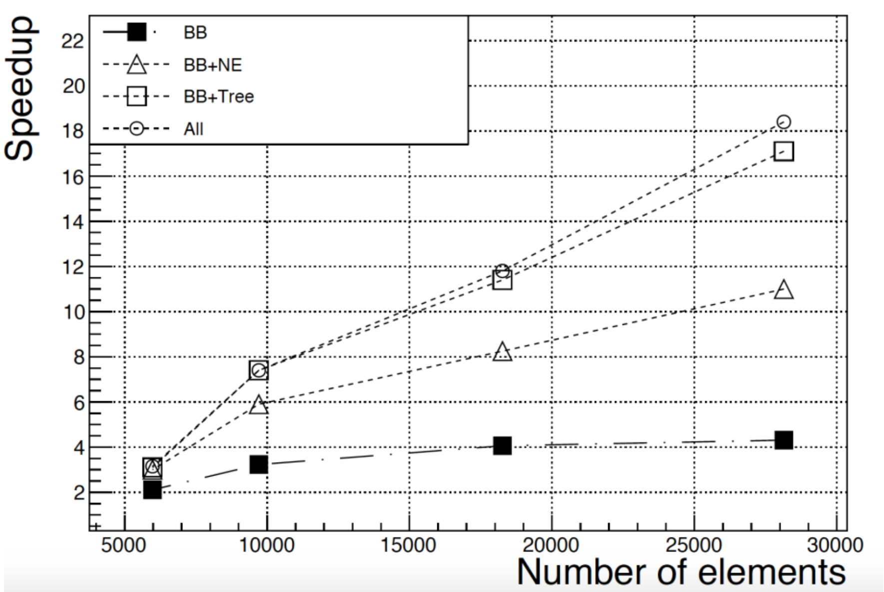
Software optimization

e.g.: Garfield software used for Detector simulation

Parallelization



Optimization



Involving students from electrical engineering

O. Bouhali Nucl. Instr. Meth 901 (2018)

Introduction: Medical Physics

Medical physics is a branch of Applied Physics

→ prevention, diagnosis and treatment of disease using physics principles and methods

Subfields of Medical Physics include:

- Radiation Oncology
- Medical Imaging
- Nuclear Medicine
- Radiation Protection (Health Physics)
- …

Medical Imaging techniques

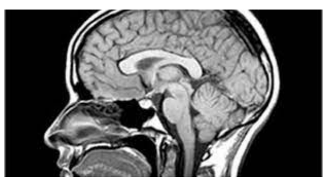
Examples are:

- X-ray

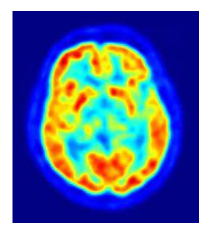
- Fluoroscopy, Ultrasound

- Computed Tomography (CT)

- MRI

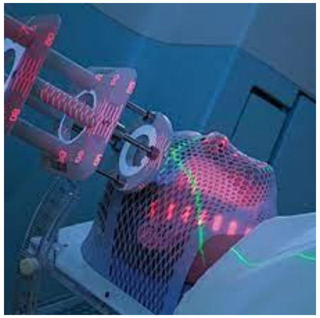


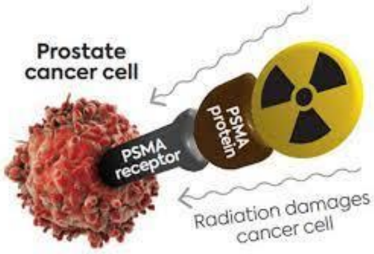
- PET (Positron Emission Tomography)



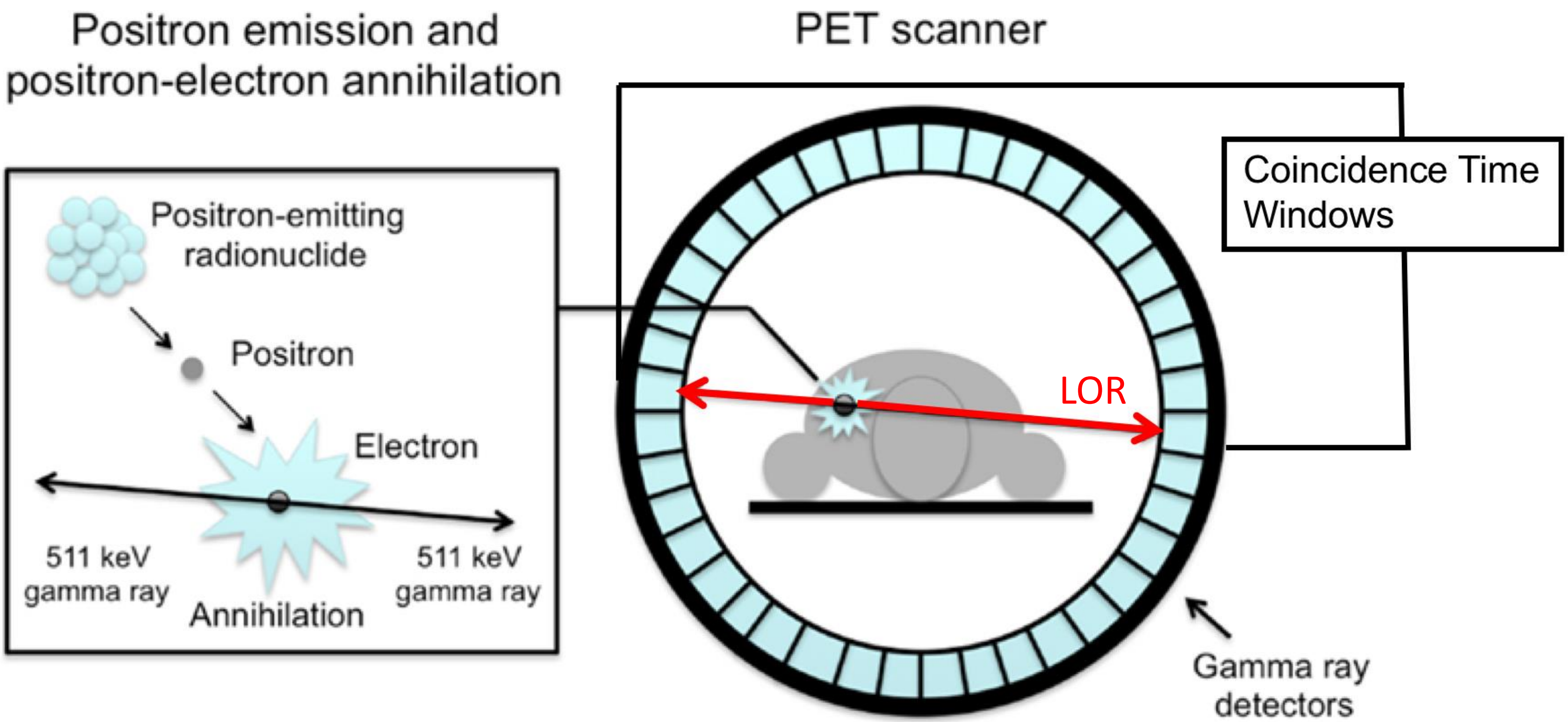
Medical physics: treatment techniques

- Radiation therapy
  - ➢ Conventional photon therapy
  - ➢ Proton Therapy
  - ➢ Ion Beam Therapy
- Radionuclide Therapy
- Theranostics





Principle of Positron Emission Tomography



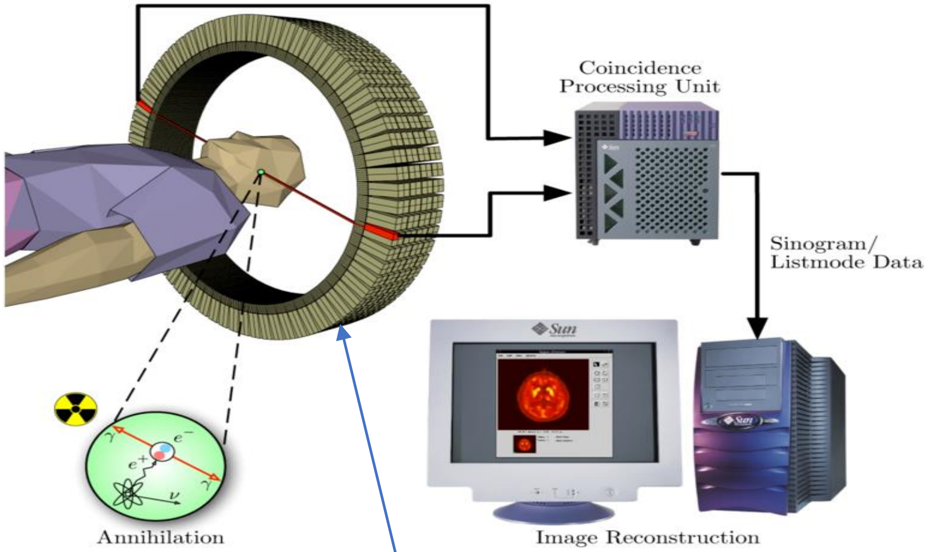
LOR: line connecting two detecting blocks

Total number of coincidences in each LOR is proportional to the radiotracer distribution

Modeling: PET imaging

Electron-Positron annihilation

$$e^{-} + e^{+} \rightarrow \gamma + \gamma$$



Block of scintillation crystals

Applications:

- Cardiac imaging
- Neuroimaging
- Oncology

Some elements of a PET scanner

Texas A&M at Qatar Advanced Scientific Computing Center

- Gamma ray detection system
  - Scintillation Crystal (efficiency, low noise, fast response)
  - Photo Multiplier (electric signal generation)
- Data Acquisition (fast acquisition, low latency)
- Image reconstruction (efficient and fast algorithm)
- Mechanical and electronic design

→ This requires extensive modeling and AI based optimization

Full simulation chain

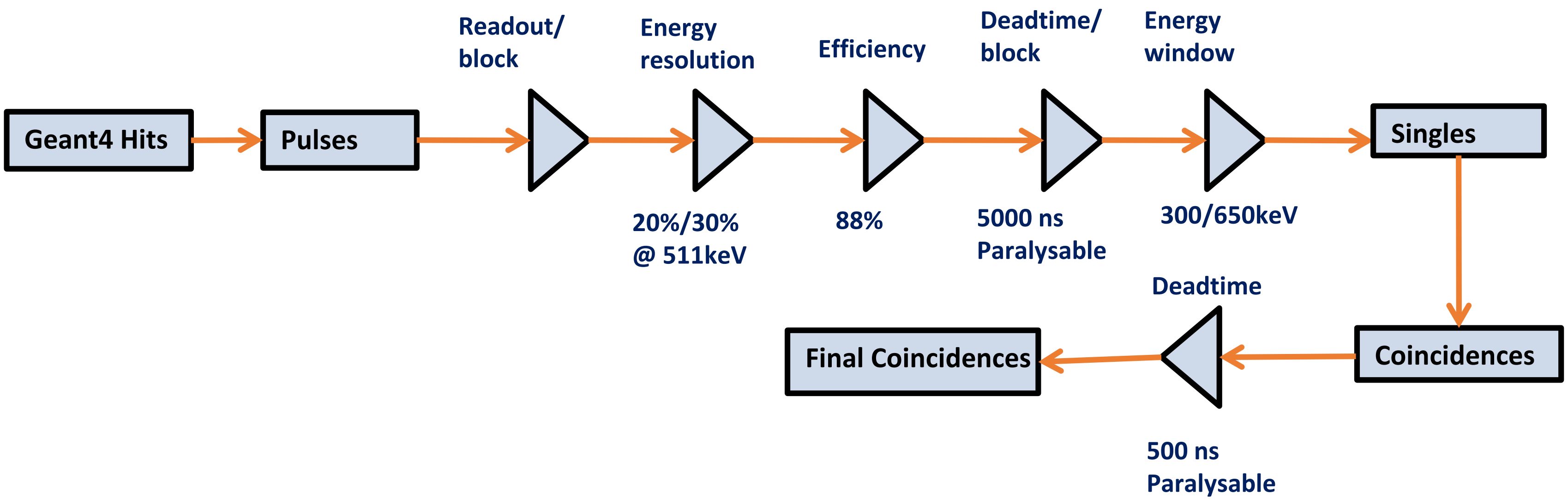
Modeling the PET system Geometry

- ✓ Nature and number of crystals
- ✓ Shapes and dimensions
- ✓ Geometry of the Phantom
- ✓ Geometry of the Radioactive Source

Setting the simulation Parameters

- ✓ Lowenergy models for Compton and Rayleigh
- ✓ Energy cuts: delta-ray 10 keV, X-rays 10 keV,
- ✓ Electron range cut 2 mm

Setting the Signal processor chain



Setting the Source Activity and the Acquisition Time

Simulation & Validation of clinical and micro-PET

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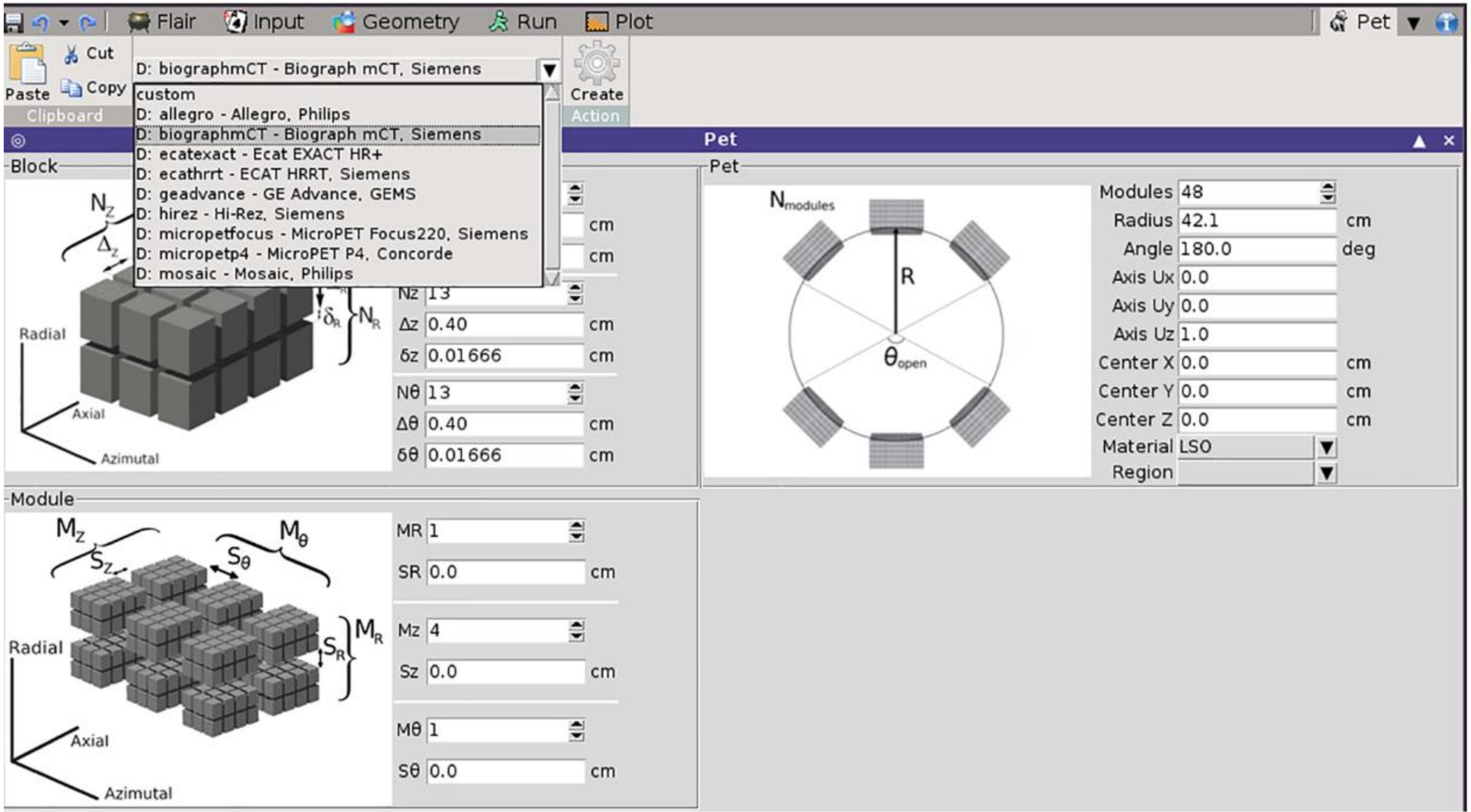
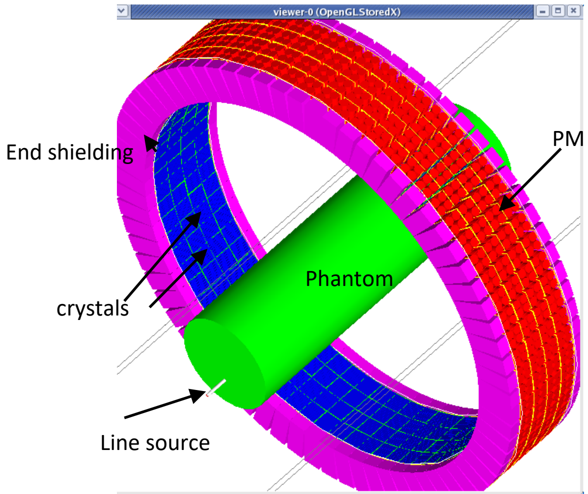
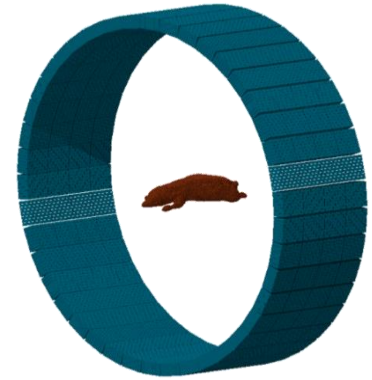


R.S. Augusto et al., Physica Medica, 54(2018)189-199

Simulation & Validation of clinical and micro-PET

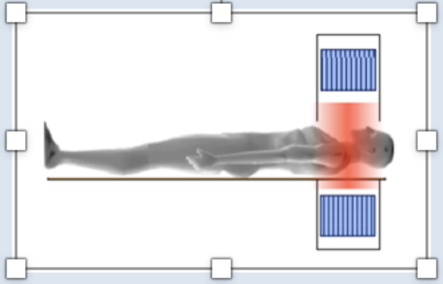




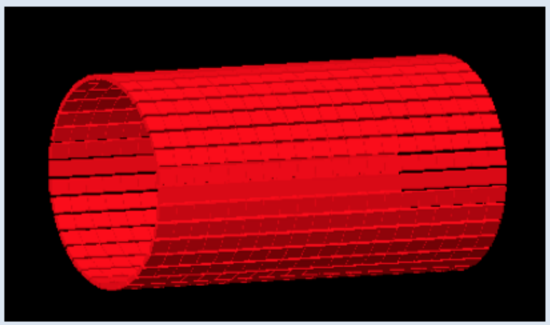
PET Scanner		Allegro		HR+		mCT		TF	
Performance Parameter		Exp.	Sim.	Exp.	Sim.	Exp.	Sim.	Exp.	Sim.
Spatial Resolution	Trans @1 cm	5.43	4.79	4,39	3.87	4.4	4.21	4.84	4.73
	Axial @1 cm	5.56	4.6	5.1	4.41	4.4	4.3	4.73	4.69
	Tang @10 cm	5.48	4.57	4,64	4.01	4.7	4.57	5.2	5.12
	Radial @10 cm,	5.70	4.86	5,65	4.7	5.2	4.95	5.2	5.08
Scatter Fraction (%)		42	42.2	48	44.3	33.2	30.5	30	31.5
Sensitivity (cps/MBq)	R=0 cm	4360	4790	6650	6877	4360	4790	7390	7640
	R=10 cm	4650	4850	7180	7235	4650	4850	7280	7564

R.S. Augusto et al., Physica Medica, 54(2018)189-199

Total Body PET (TBPET)



Only about 1-2% of emitted signal is detected in a conventional PET



104 cm (20 rings of 5cm each)

Solution: Scanner with an extended axial Field of View (FOV) that covers a larger part of the body.

Total Body PET (TBPET)

M. Abi Akl et al., ENAM 2017

M. Abi Akl, Middle East Medical Physics Conference (2nd best presentation)

M. Abi Akl et al., IEEE MIC 2019

O. Bouhali et al., FTMI, 2022

New device for Nuclear Medicine

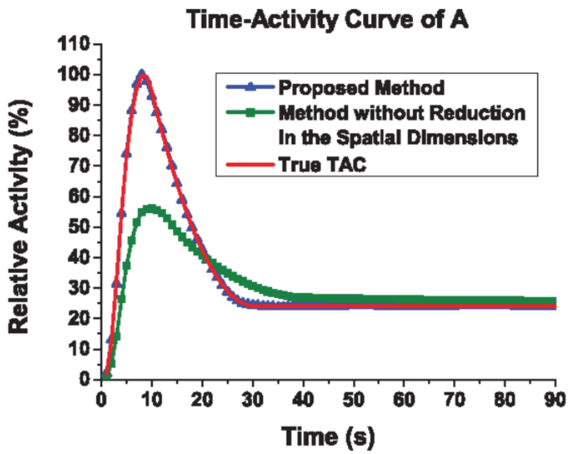
In nuclear medicine:

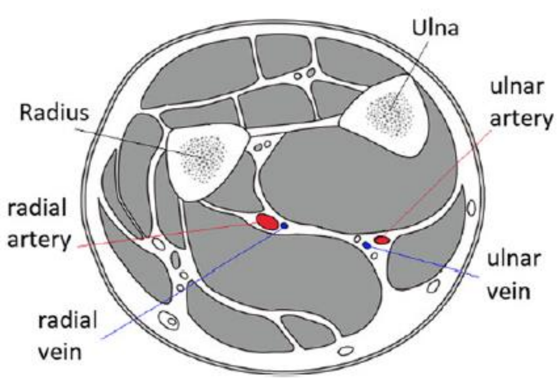
- Measuring the Blood Time Activity (BTAC) curve
  - ➢ Arterial blood sampling involves blood extractio
  - ➢ Uncomfortable for patients

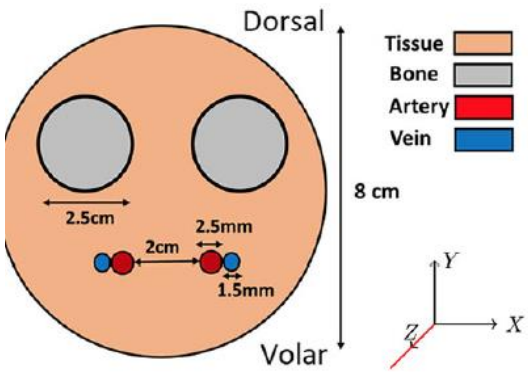
→ **Non-invasive arterial blood radioactivity device**

→ **Device can be placed around the wrist**

→ **Complete simulation**

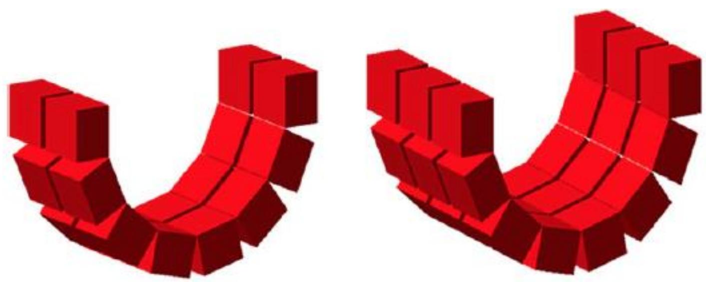




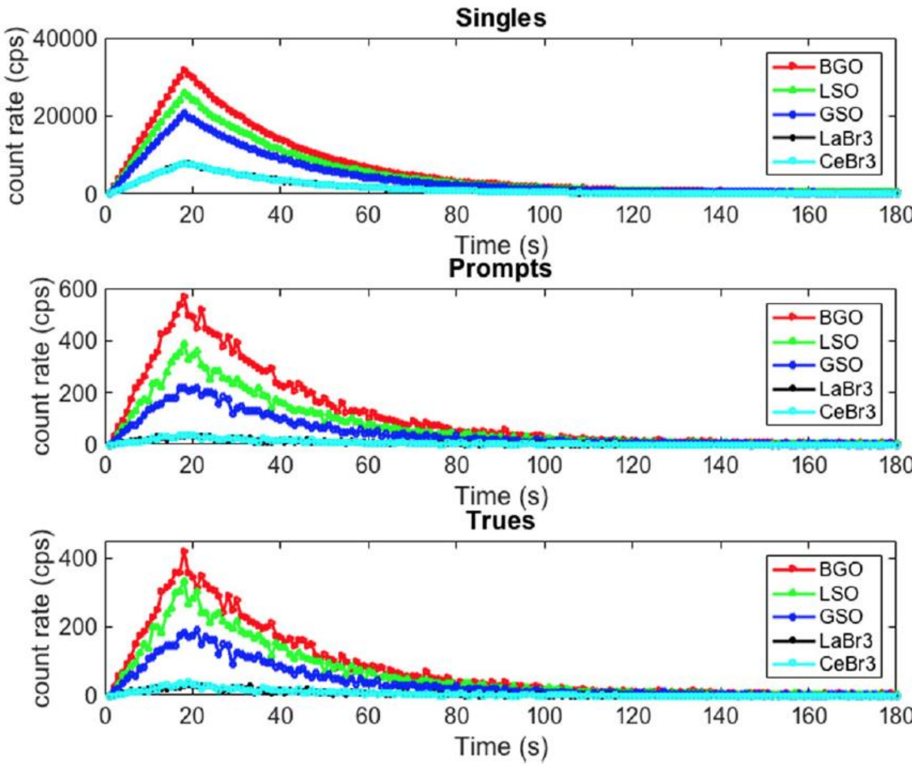


New device for Nuclear Medicine

Non-invasive arterial blood radioactivity device



2 detection planes   3 detection planes

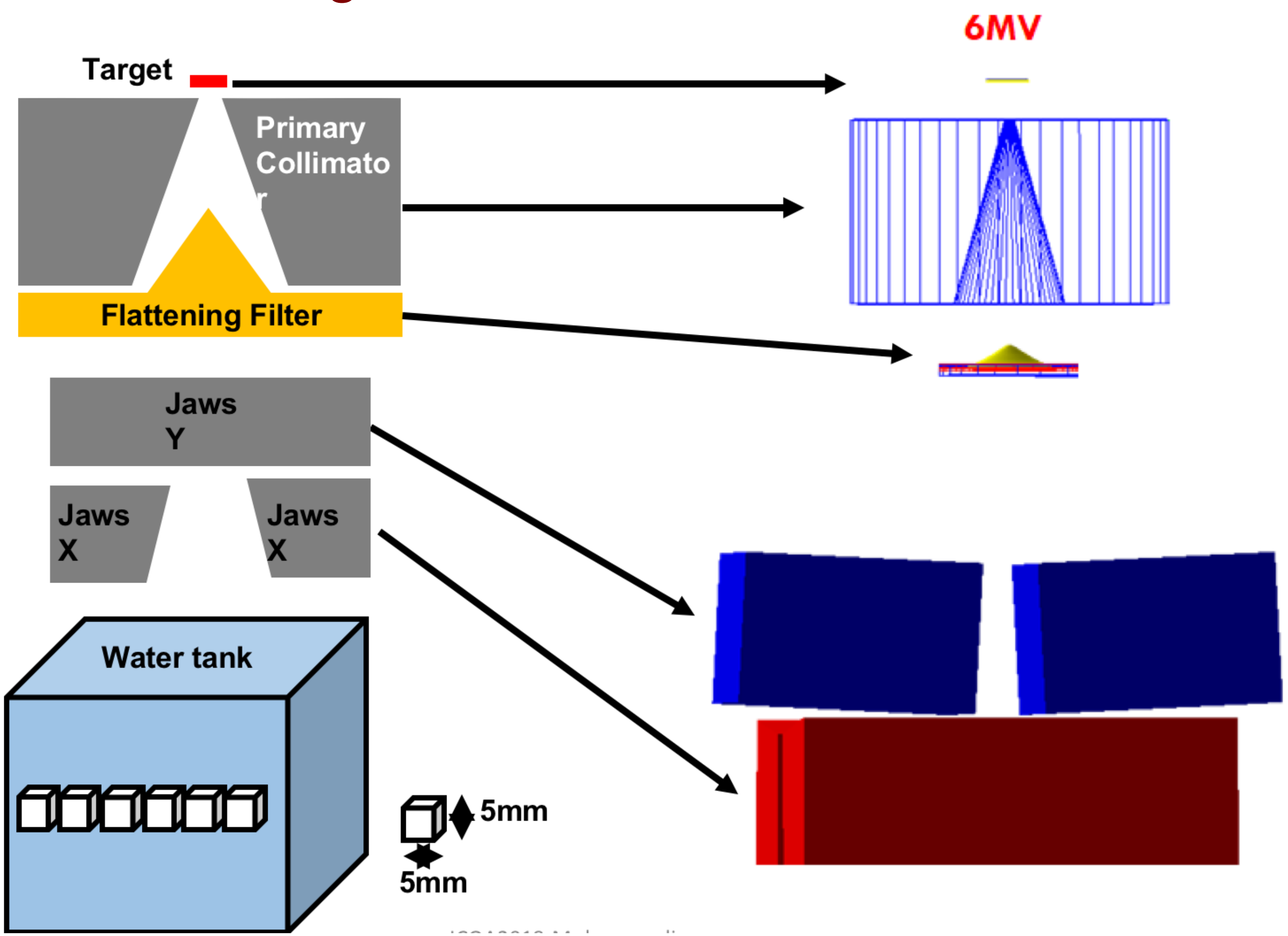


Y. Toufique, O. Bouhali, J. O'Doherty, Eur. J. Nucl. Moel. Med. (2020) 7:25

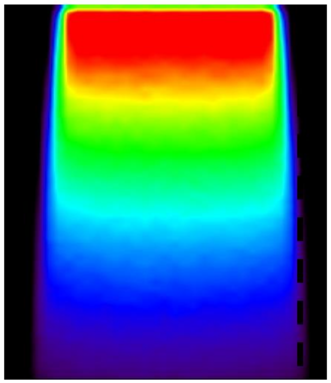
US Patent: **PCT/QA2020/050007**

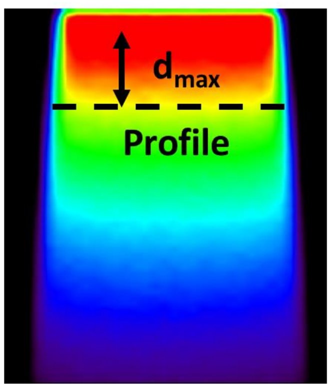
Radiation Therapy

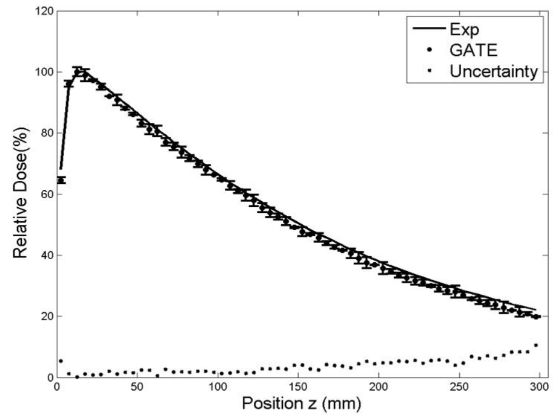
Modeling of a 6MV Varian Clinac



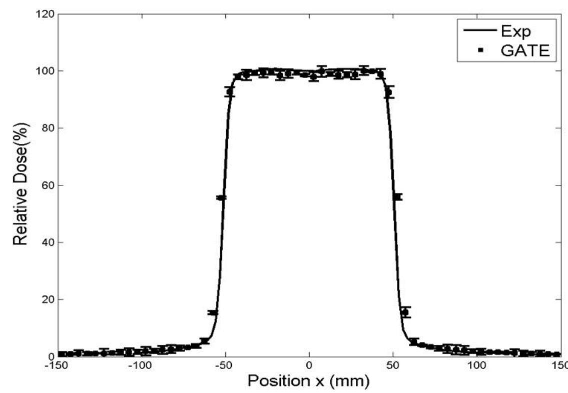
Results from dose profiles







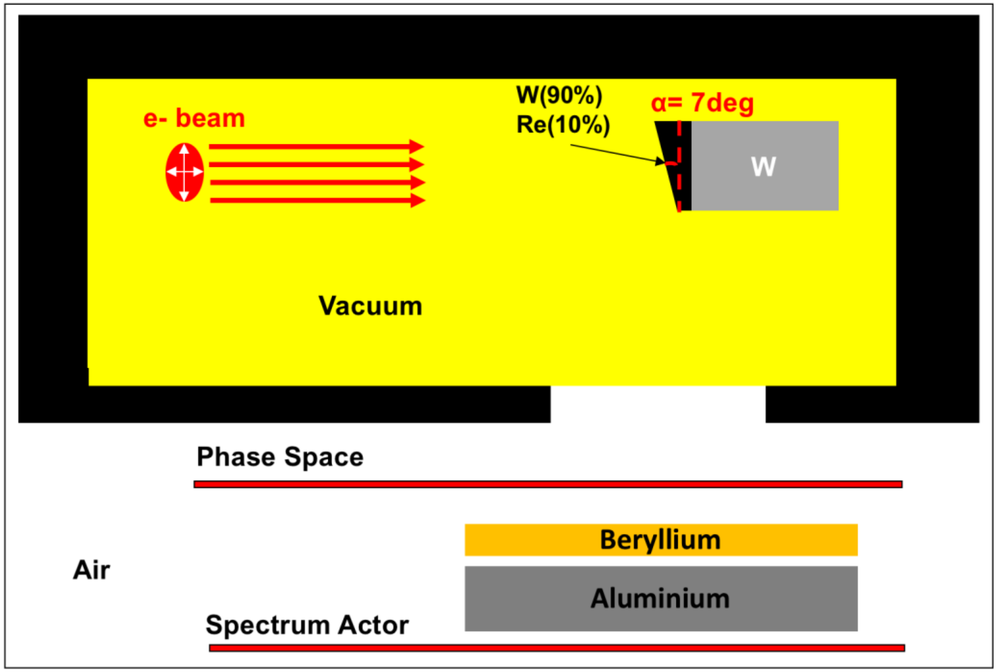
Percentage Depth Dose

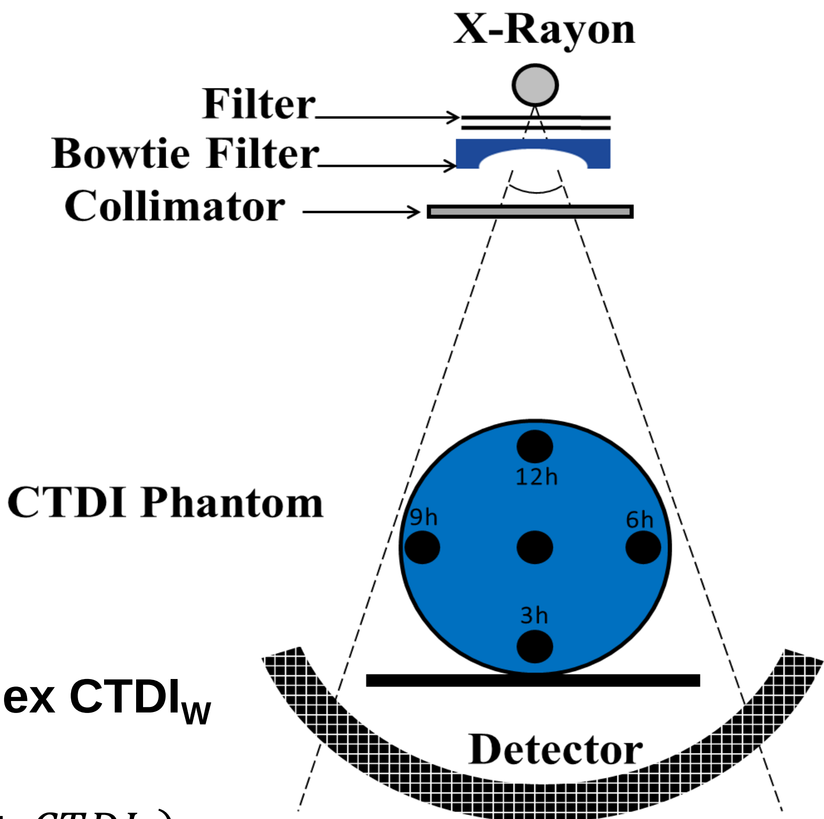


Dose profile

O. Bouhali et al., Computing in Biology and Medicine Conference, , London, 2019
M. Bendahman et al., under review, Oncology and radiology J.

Complete model of CT scan (SIDRA)



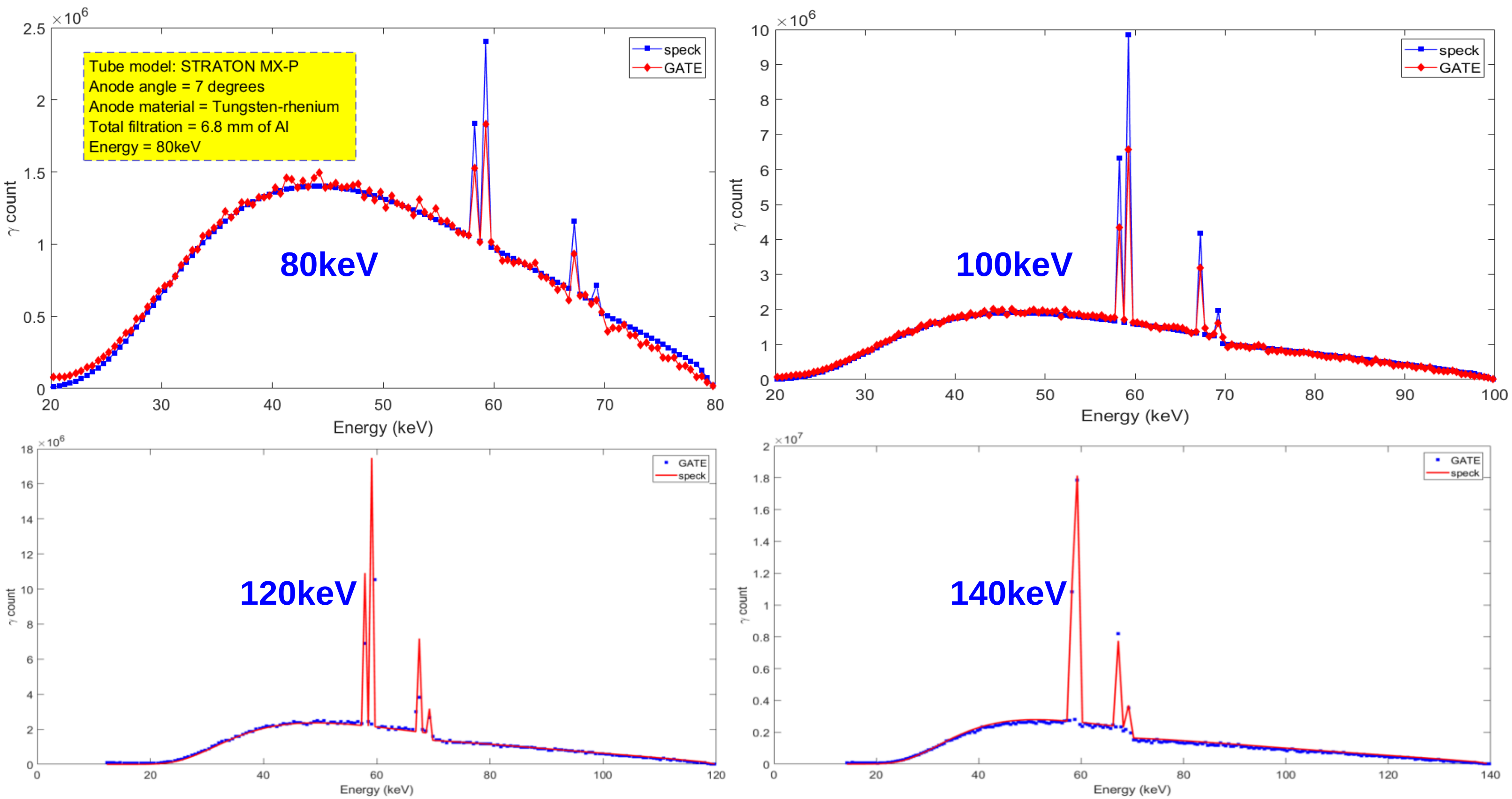


The weighted computed tomography dose index $CTDI_W$

$$CTDI_w = \frac{1}{3}CTDI_c + \frac{2}{3}(CTDI_{12} + CTDI_3 + CTDI_6 + CTDI_9)$$

Results: SOMATRON X-ray Tube

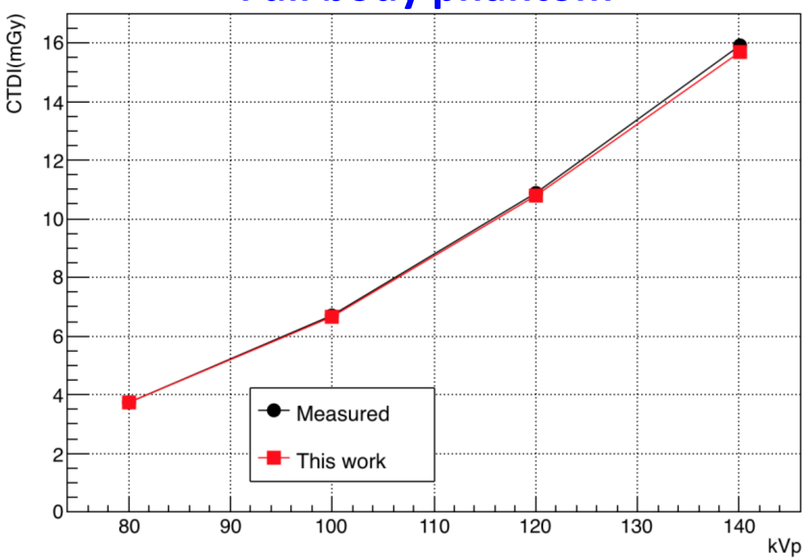
Comparison between simulated and measured data(SpeckCal)



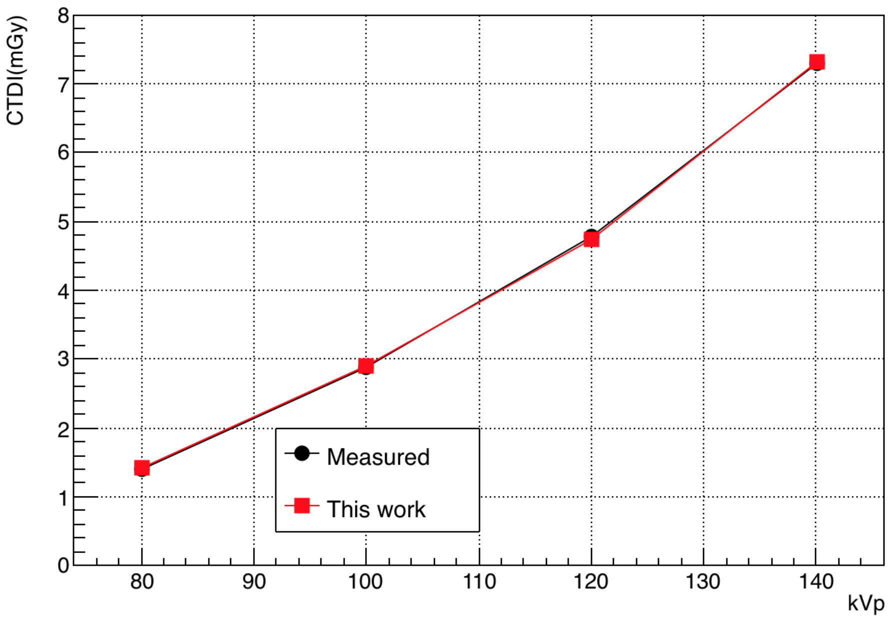
CT model: simulation versus experimental

Measurement done at SIDRA

Full body phantom



Head & Neck phantom



O. Bouhali et al., European Congress of Radiology, Vienna, March 2019

O. Bouhali et al., ECR, 2020

High Performance Computing:

→Is an ecosystem: **people**, **Infrastructure**, **Policies**, **Software**

→Critical for **research excellence** and efficient **capacity building**

Better HPC systems → better business value