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Accelerating C++ applications in Medical Physics

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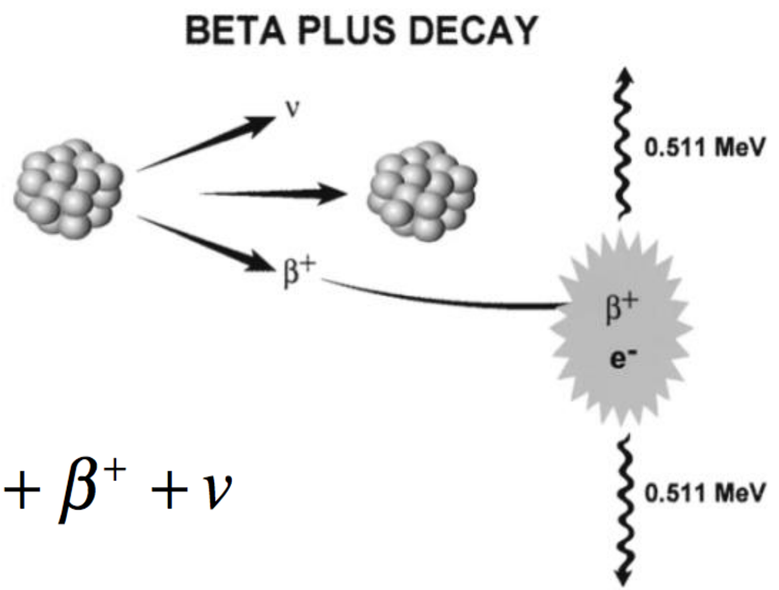
Outline

- **Positron Emission Tomography (PET)**
  - What is a **PET** scanner?
  - Detector simulation, data acquisition/analysis and image reconstruction in **PET (**GATE simulations and data analysis**)**
- **Acceleration tools:**
  - Intel® Threading Building Blocks
  - OpenMP API (**Open M**ulti-**P**rocessing **A**pplication **P**rograming **I**nterface)
  - NVIDIA CUDA®
- **Case Studies:**
  1. Parallelism in GATE
  2. Image Reconstruction: OpenMP vs TBB
  3. MLEM Acceleration
- **Conclusions**

Positron Emission Tomography (PET)

Positron Emission Tomography (PET)

- Radioactive nucleus decays in a β+ reaction.
- β+ annihilates -> two antiparallel 511 keV photons emitted.

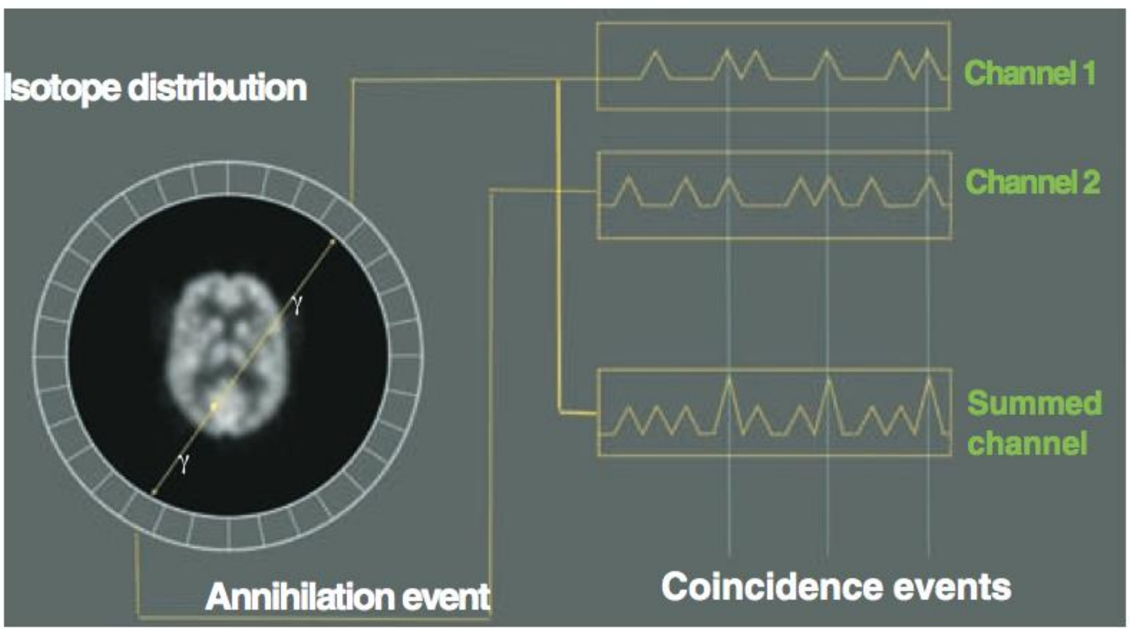


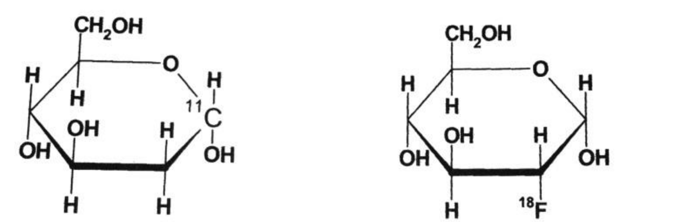
$$p \rightarrow n + \beta^{+} + \nu$$

In *Basics of PET Imaging Physics, Chemistry, and Regulations*, **Gopal B. Saha**

Positron Emission Tomography (PET)

- Detection of the two photons in the same time window is called a **coincidence** event, and the line is called **LOR** (line of response).
- A patient is injected with a radiotracer (usually FDG, a radioactive replacement of the deoxyglucose) that accumulates in a region of interest.
- The detection of coincident events allows the image reconstruction.

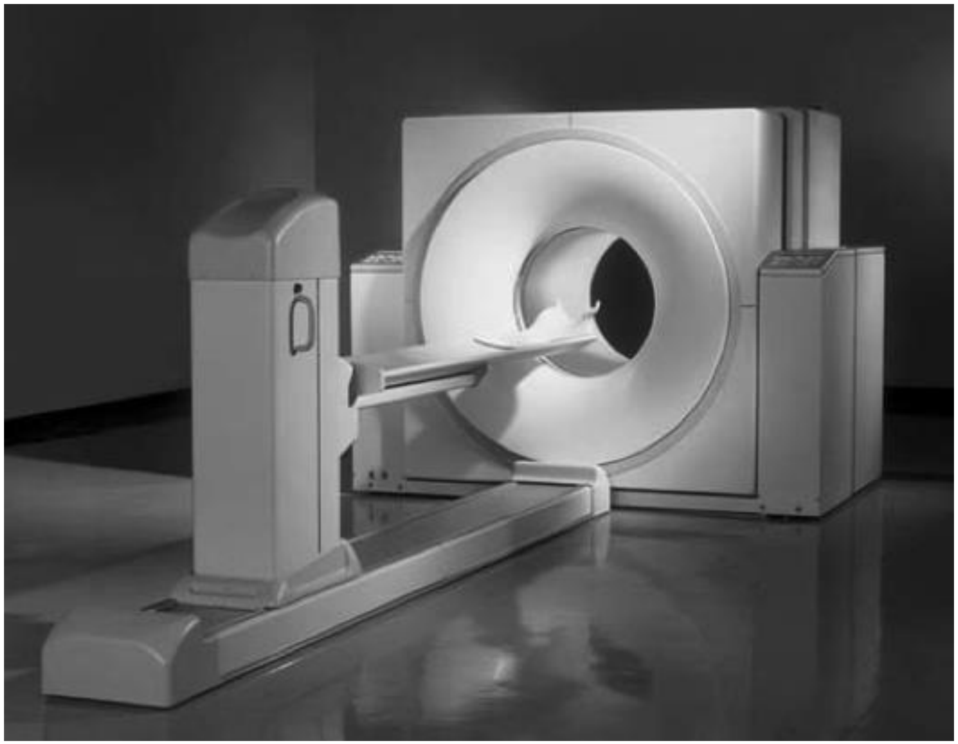


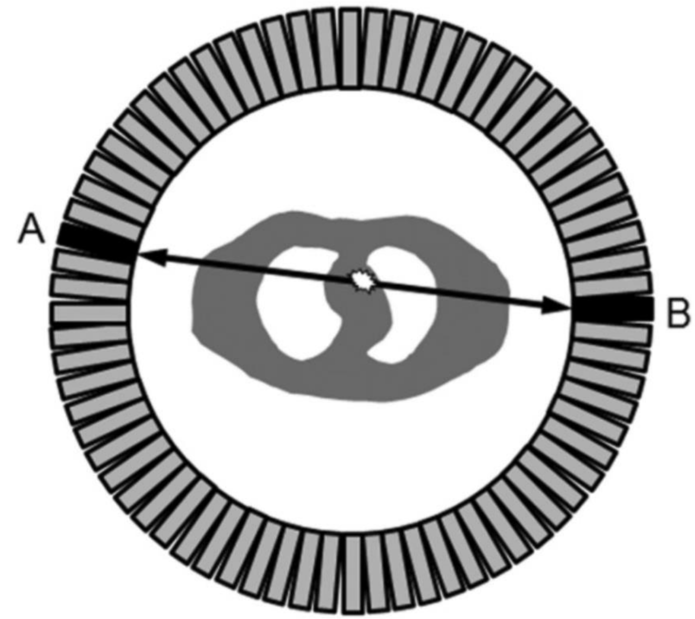


2-desoxi-D-[1-^{11}C]glicose

2-[^{18}F]fluoro-2-desoxi-D-glicose

PET Scanner





In *Nuclear Medicine Physics: A Handbook for Teachers and Studends*, **D. L Bailey, J. L Humm, A. Todd-Pokropek and , A. van Answegen, International Atomic Energy Agency**

Applications

Functional clinical studies

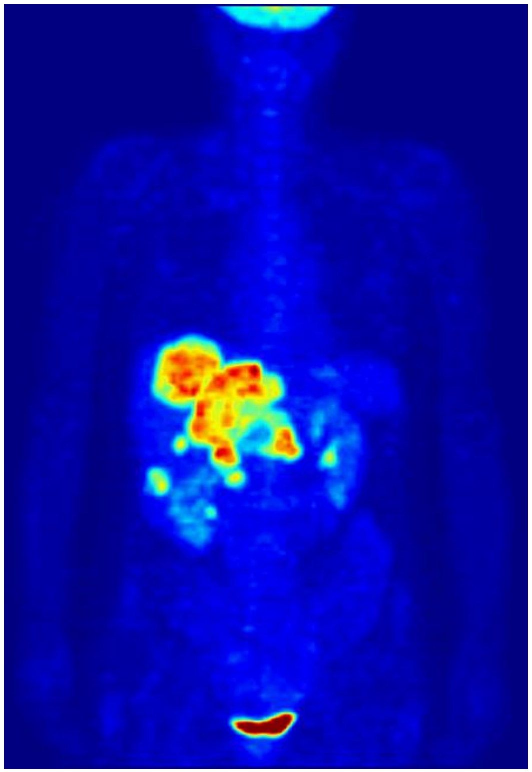
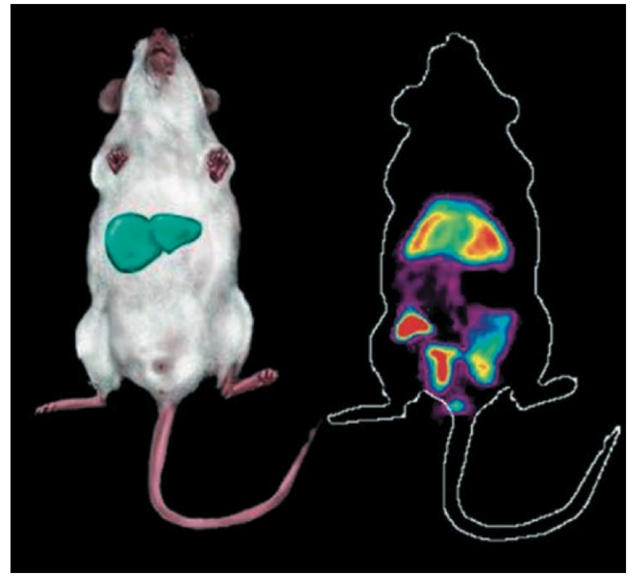


Image from Jens Maus (http://jens-maus.de/)

- Oncology
- Cardiology
- Neurology

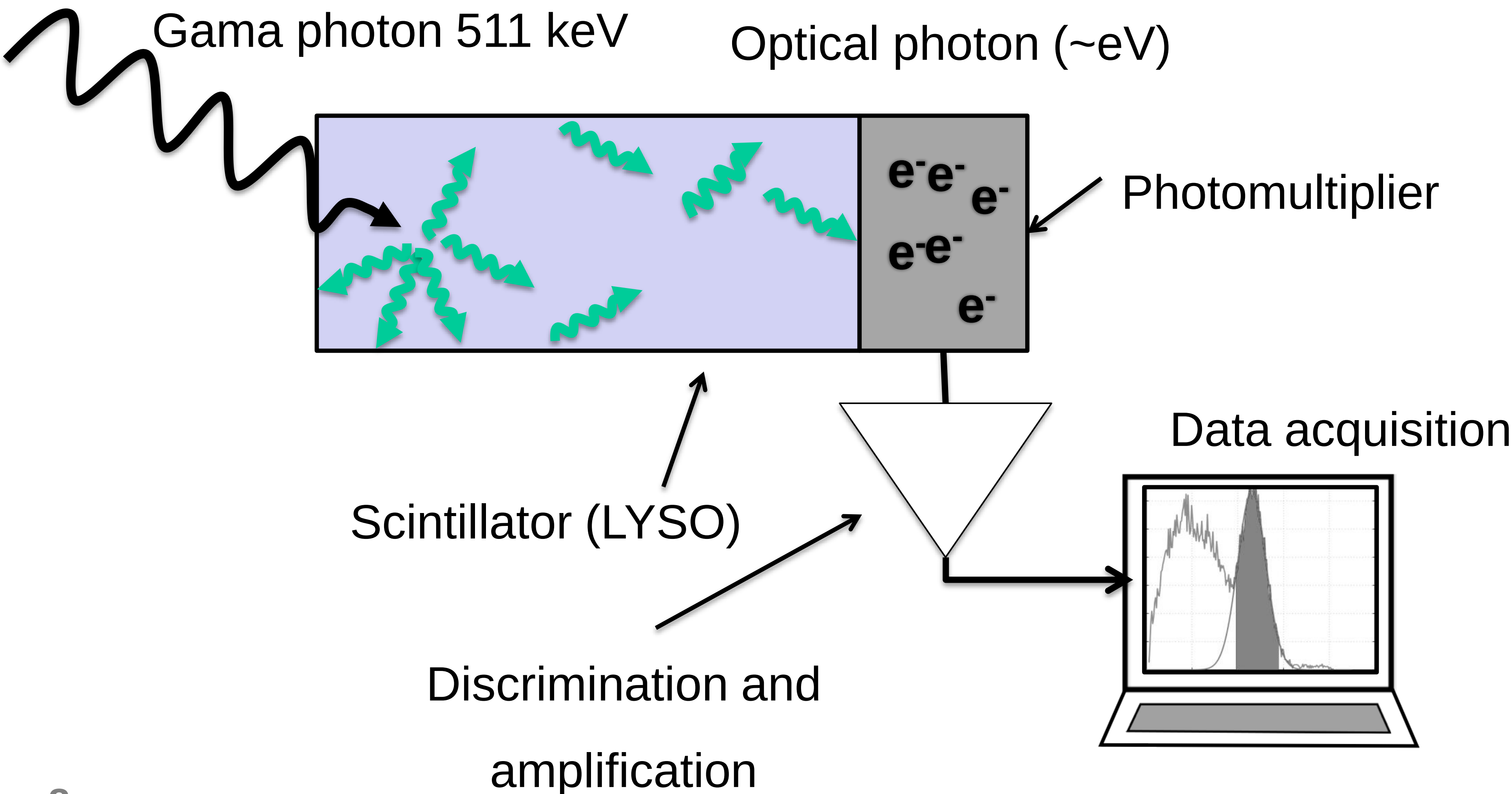
Pre-clinical research



- New drugs
- Diseases research

From *Emission Tomography: The fundamentals of PET and SPECT.*

Data Acquisition



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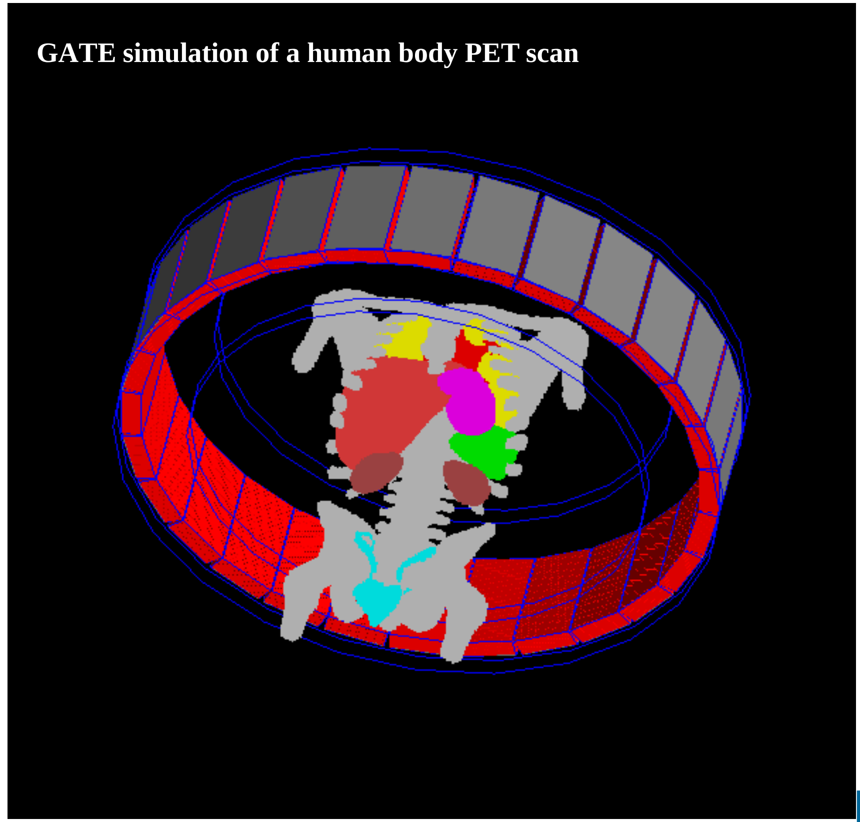
PET Simulations

- **Simulations plays an important role in Medical Research**
  - Develop and optimize new scanners and techniques
    - PET-CT, PET-MRI, PET-CT-MRI, SPECT-CT, Optical Imaging, etc
  - Discover of new drugs
    - Biomarkers
  - Study of diseases and new treatments.
    - Cancer, Alzheimer's
    - Radiotherapy and Hadrontherapy

GATE

- **GATE (G**eant4 **A**pplication for **T**omographic **E**mission**)**[1,2]
  - Monte Carlo application
  - Allows the use of simplified macros as primary input mechanism (no C++ knowledge is needed for most of the applications);



[1] Jan, S. et al., **"Gate: a simulation toolkit for PET and SPECT"**
[2] Santina, G. et al., "**Evolution of the GATE project: new results and developments** "

GATE Architecture

1.Defining the geometry

⇩

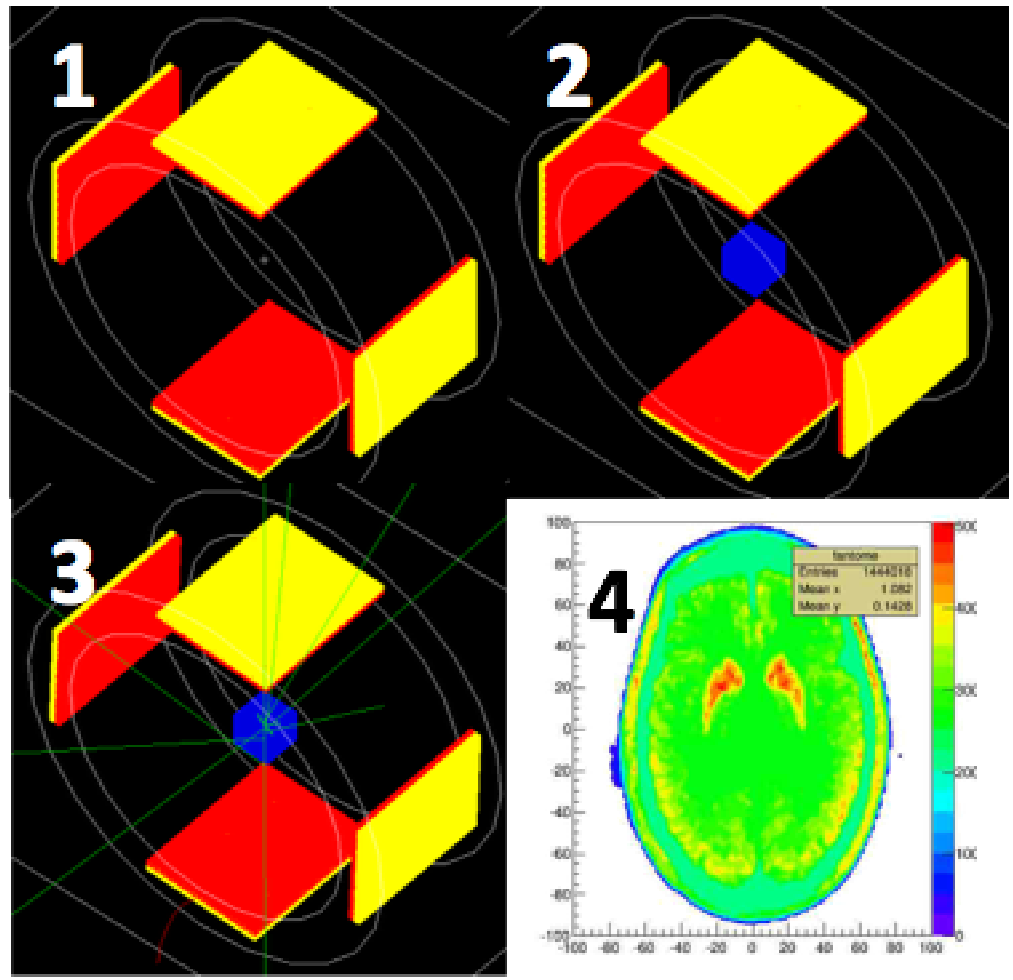
2.Defining the source/ phantom

⇩

3.Start acquisition/ simulation

⇩

4.Analysis and image reconstruction



GATE simulation

- **Geant4 engine is used for generate and tracking particles**
- **In a typical simulation:**
  - Source with 300 MBq ^{18}F-FDG generates ~ 10^{11} decays during a 30 min scan (plus secondary particles)
  - Each event (decay) is independent – Monte Carlo simulation
  - Very time consuming to track all this particles
- **Parallelization first approach:**
  - Spit job into smaller jobs (time slices) in a grid

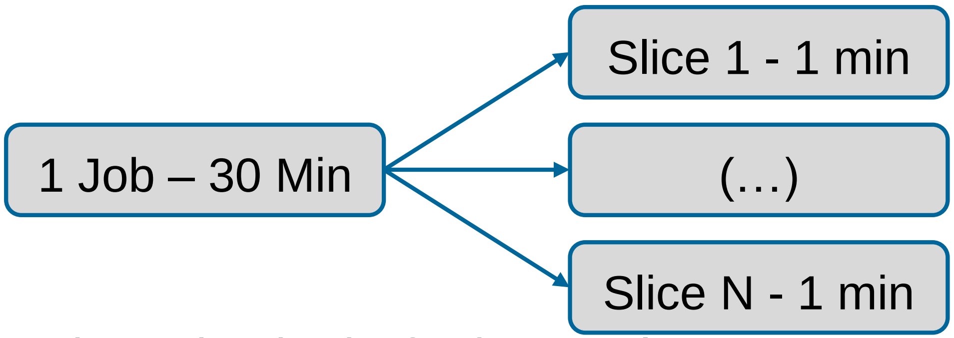


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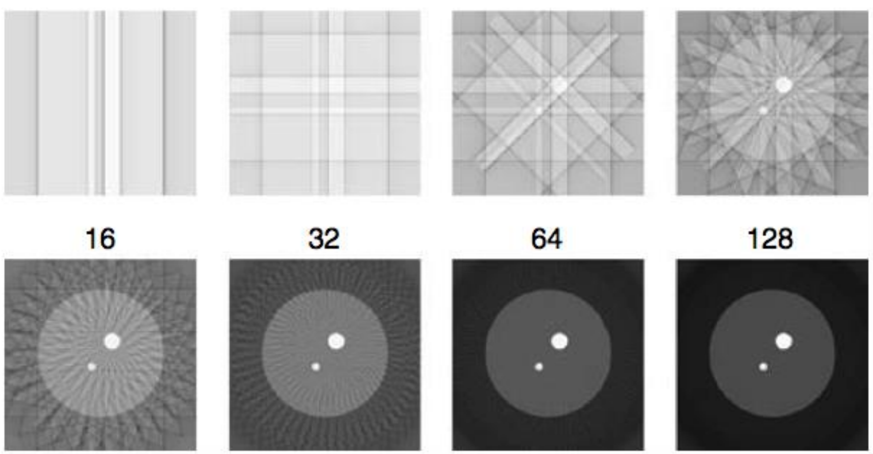
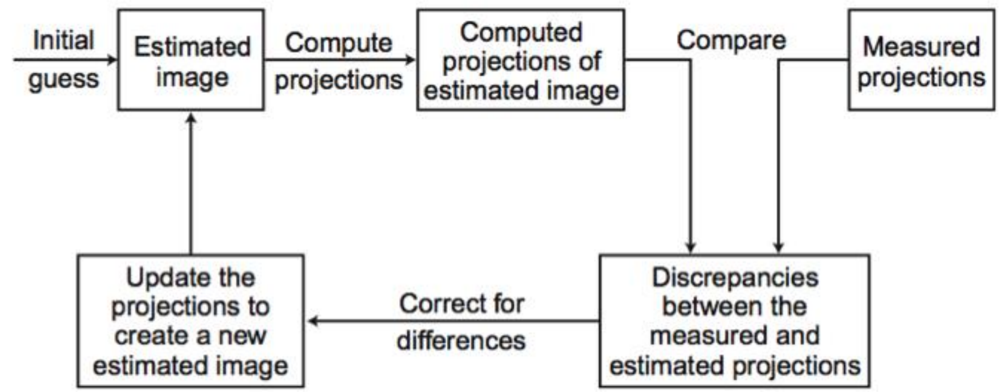
Image Reconstruction algorithms

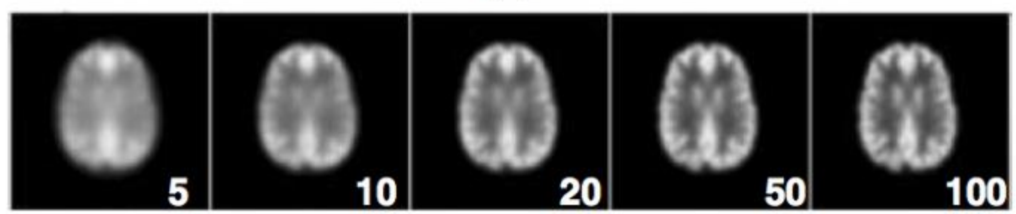
- Analytic methods (fast, simpler and easier to implement). E.g. Retroprojections.
- Iterative methods (slower, more complex but usually with better performance)



From *Emission Tomography: The fundamentals of PET and SPECT.*



(a)



(b)

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Image Reconstruction Methods

- **The “inverse” problem of the acquisition. Why?**
- **Analytical :**
  - Involves the reconstruction of an image from its X-Ray transform
  - Deterministic problem, usually “ignoring” real data.
  - Efficient and non-iterative algorithms

  →
  - Backprojection
  - Filtered Backprojection
- **Iterative :**
  - Start with a guessing image
  - Finite iterations over images
  - Requires heavier calculations
  - Suitable for more complex problems

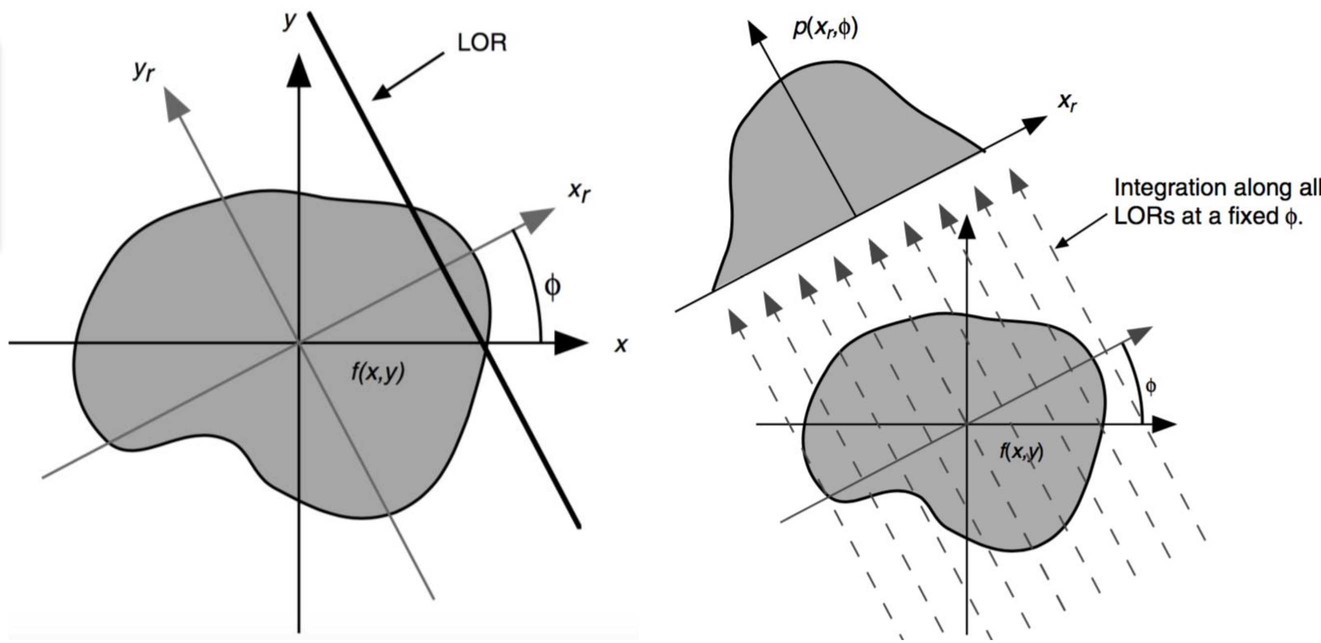
  →
  - MLEM
  - OSEM

Analytical reconstruction

- **Uses X-Ray transforms :**
  1. Returns all the possible line integrals of an image f(x,y). 2D example:
     - The X-Ray transform is the operation $f(x,y) \to p(x_r,\phi)$
     - $p(x_r,\phi)$ is the 1D projection of f(x,y) for a given angle ϕ

$$p(x_r,\phi) = \int_{-\infty}^{\infty} f(x,y)\,dy_r$$

$$\begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} \cos\phi & -\sin\phi \\ \sin\phi & \cos\phi \end{bmatrix} \begin{bmatrix} x_r \\ y_r \end{bmatrix}$$



From *Emission Tomography: The fundamentals of PET and SPECT*

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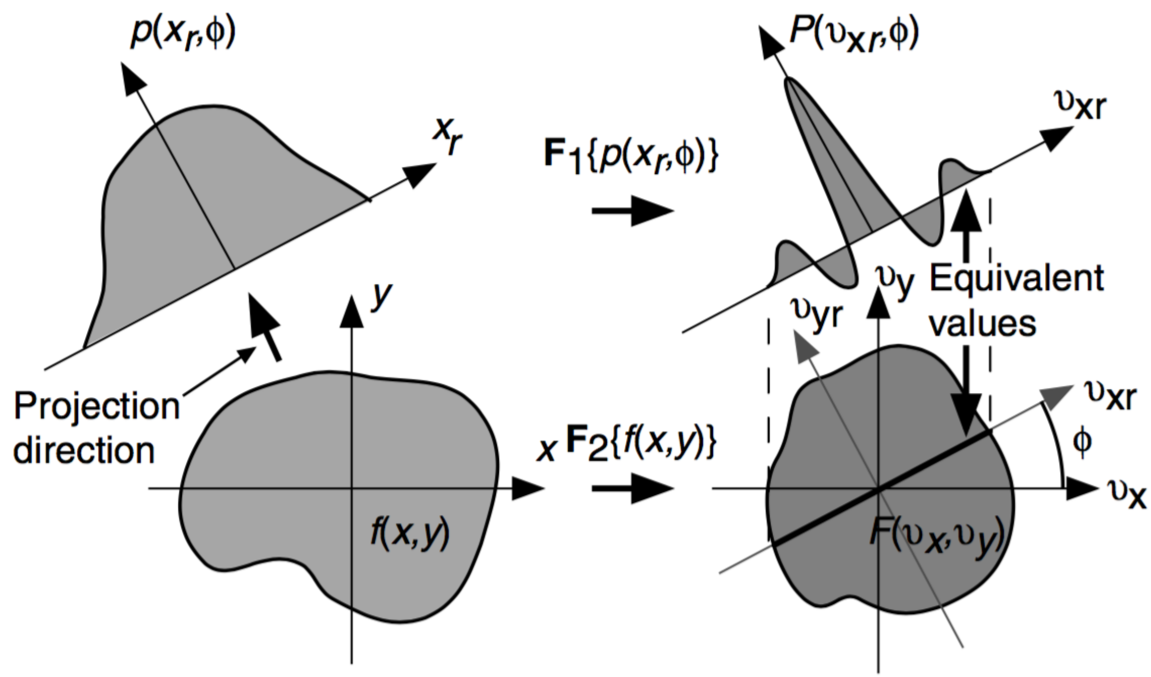
Analytical reconstruction

- **Uses X-Ray transforms :**
  2. Central slice theorem
     - Gives relation between 2-D Fourier transform of image and 1-D Fourier transform of its projections along the detector axis

$$P(\upsilon_{xr},\phi) = F(\upsilon_x,\upsilon_y)\Big|_{\upsilon_{yr}=0}$$

1-D FT for projections along axis at angle ϕ

2-D FT of the image + central slice



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Analytical reconstruction

- **Uses X-Ray transforms :**
  3. 2-D FBP algorithm
     - Compute 1-D FT of the projections along the detector axes
     - Apply:
       - ‘Ramp-filter’ in the frequency space (1-D Convolution)
       - 1-D iFT to obtain filtered projections
       - Back-projection operator to obtain the image

$$f(x,y)=\int_{0}^{\pi}\int_{-\infty}^{\infty}|\upsilon_{xr}|P(\upsilon_{xr},\phi)e^{i2\pi x_r \upsilon_{xr}}\,d\upsilon_{xr}\,d\phi$$

     - Parallelization can be obtained, for example:
       - Projections for different ϕ may be calculated in different processors

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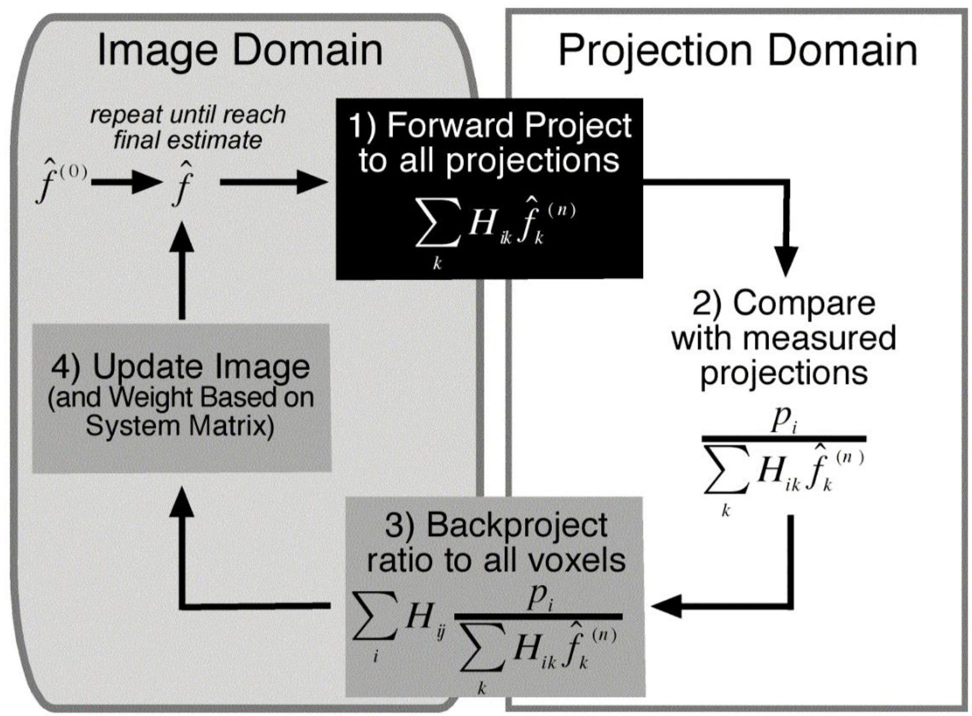
Iterative Reconstruction

- Different iterative methods are available. Ex: **ML-EM, OSEM, …**
- **Maximum Likelihood - Expectation Maximization (ML-EM)**
  - First introduced for image reconstruction in 1982 by Shepp and Vardi, remains the **basis** algorithm for iterative statistical image reconstruction
  - It leads to the iterative equation and chart[1]

$$\hat{f}_j^{(n+1)} = \frac{\hat{f}_j^{(n)}}{\sum_{i'} H_{i'j}} \sum_i H_{ij} \frac{p_i}{\sum_k H_{ik} \hat{f}_k^{(n)}}$$

Image at iteration n+1



[1] *PET Image Reconstruction,* A. Alessio, and P. Kinahan, Available at http://faculty.washington.edu/aalessio/papers/alessioPETRecon.pdf

Acceleration tools

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Acceleration tools

- Many tools and approaches have been developed in the last years to extract as much performance as the recent computers can give.
- Some examples:
  - **Multi-thread (sharing memory)**: e.g. OpenMP, TBB, CUDA
  - **Multi-CPU (splitting memory):** e.g. MPI
  - **Intrinsic parallelism:** split the work in smaller parts
- Monte Carlo simulations are well suitable for intrinsic parallelism[1].

[1] A. Dubois, S. Stute and S. Jan **"Accelerating GATE simulations"** GATE Training, INSTN-Saclay, October 2015

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Data parallelism vs Task Parallelism

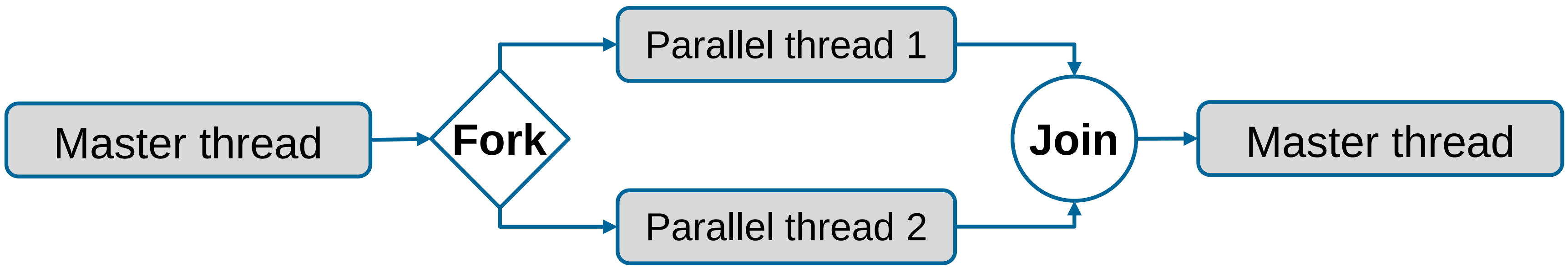
- We can think about parallelism in two ways:
  - **Task parallelism:** Simultaneous execution of different tasks on the same or different data
  - **Data parallelism:** Simultaneous execution of the same task/function (single instruction, multiple data – SIMD) for various elements on a ensemble
- The use of one or the other approach depends on the user application, usually the use both is the best option

OpenMP

- **First released in 1997**
  - Designed to ensure an ordered access of different threads to shared data and to be a standard notation **among different SMP** (Symmetric multiprocessing) architectures.
  - Supports **Fortran, C and C++.**
  - It's implemented in many **commercial** and **Open Source** compilers.
  - It's a set of compiler directives, library routines and environment variables as **an extension** of C, C++ and Fortran standard compilers.
  - For simple applications, **only few code** lines may be needed.

OpenMP

- Uses the Fork-join[1] model of parallel execution



- **For-loop example C++:**

```
//Typical C++
for (int i = 0; i < 8; ++i) {
 do_some_task(i);
}
```

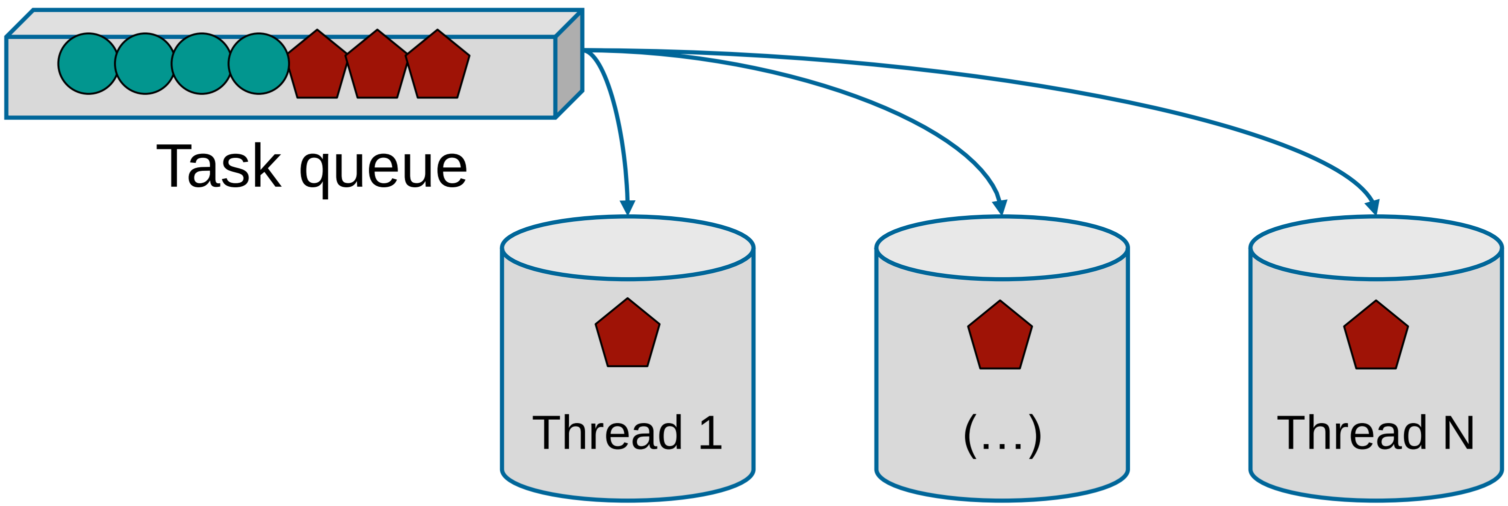
```
//C++ with OpenMP
#include <omp.h>

omp_set_num_threads(8);
#pragma omp parallel for
for (int i = 0; i < 8; ++i) {
 do_some_task(i);
}
```

[1]M. E. Conway. *A multiprocessor system design*. In Proceedings, November 12-14 1963

Intel® Threading Building Blocks

- ***"Is a popular software C++ template library that simplifies the development of software applications running in parallel***" from https://www.threadingbuildingblocks.org/faq
- Unlike OpenMP, TBB makes use of the typical programming style of C++
- It is focused for **tasks** instead of **threads**



Intel® Threading Building Blocks

- **For-loop example C++:**

```
#include "tbb/tbb.h"
using namespace tbb;

void Application(size_t size) {
  parallel_for(size_t(0), size, size_t(1) , [=](size_t i) {
     do_some_task(i);
  });
}

int main(){
  const size_t size = 8;
  Application(size);
  return 0;
}
```

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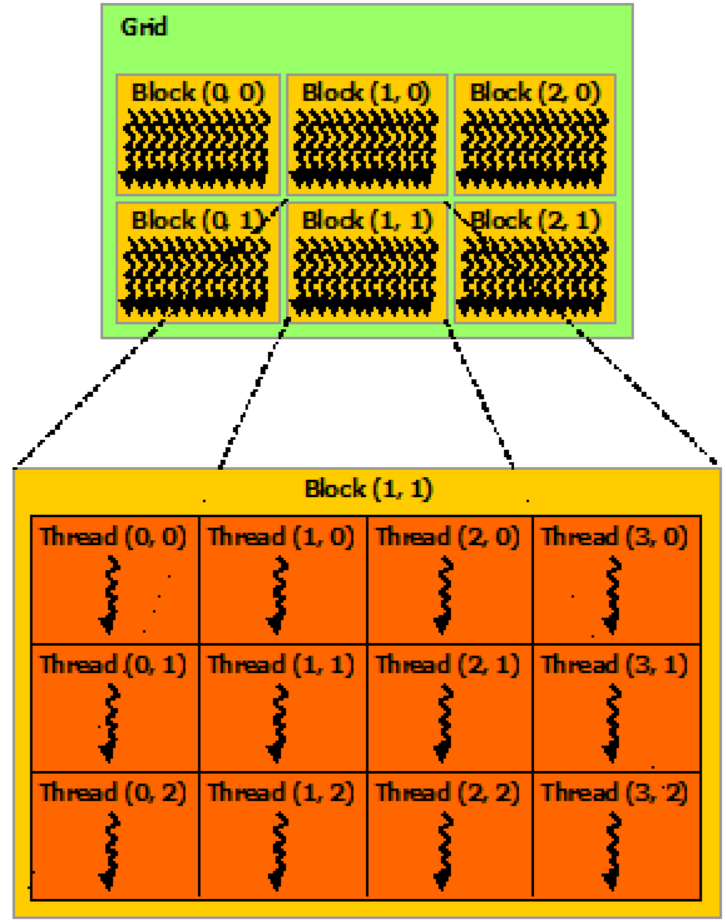
CUDA®

- **Compute Unified Device Architecture,** introduced in November 2006 by NVIDIA
- ***"Is a parallel computing platform and programming model invented by NVIDIA",*** from http://docs.nvidia.com/cuda/cuda-c-programming-guide/index.html#introduction
- It allows the use of GPUs to solve complex parallelization problems that general CPUs have more difficulty/need more time to handle.
- To make use of it, the installation of a software environment is needed. Its possible to develop applications using different programming languages (C, C++, Fortran, Java, etc).
- Its being widely used in scientific applications nowadays.

CUDA®

- **Three major steps:**
  - Copy the data for processing from CPU memory to GPU memory
  - Execute the desired processing
  - Copy results back to the CPU memory

- The main concept
  - The used defines a function, called **kernel**, and each kernel, when called, is executed in **N threads** in parallel
  - Each thread has **an unique ID**
  - **Threads** can be grouped in **blocks**, and blocks in **grids** – the dimensions of each depends on the type of data for processing



[Ref]CUDA C Programming Guide: http://docs.nvidia.com/cuda/cuda-c-programming-guide/index.html#abstract

Case Study 1

Parallelism in GATE

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Parallelism in GATE

- Two possibilities for simulations acceleration:
  - **Time split**:
    - Events are dependent between them.
    - Jobs are separated in the time domain into smaller jobs and distributed among a queuing system.
    - Better for imaging applications, due to time dependant effects
  - **Events split:**
    - Events are independent
    - Each job will only simulate a fraction of the total number of events
    - More suitable for Dose Applications (Radiotherapy, Hadrontherapy) because no dependence between particles is demanding

Parallelism in GATE

- **Using multithreading capabilities with CUDA:**
  - Only **highly-demanding** parts of the simulation goes to CUDA kernels - hybrid simulation **CPU+GPU**
- **Phantom part uses CUDA**
  - One particle per thread
  - Specific kernels for physics effects
- **Detector part uses the CPU**
  - Time dependence is vital to simulate electronic chain, data acquisition and reconstruct images with accuracy
- Example: **Hybrid-GATE** project, funded for 36 months by the French National Research Agency, to accelerate GATE simulations using CPU/GPU capabilities

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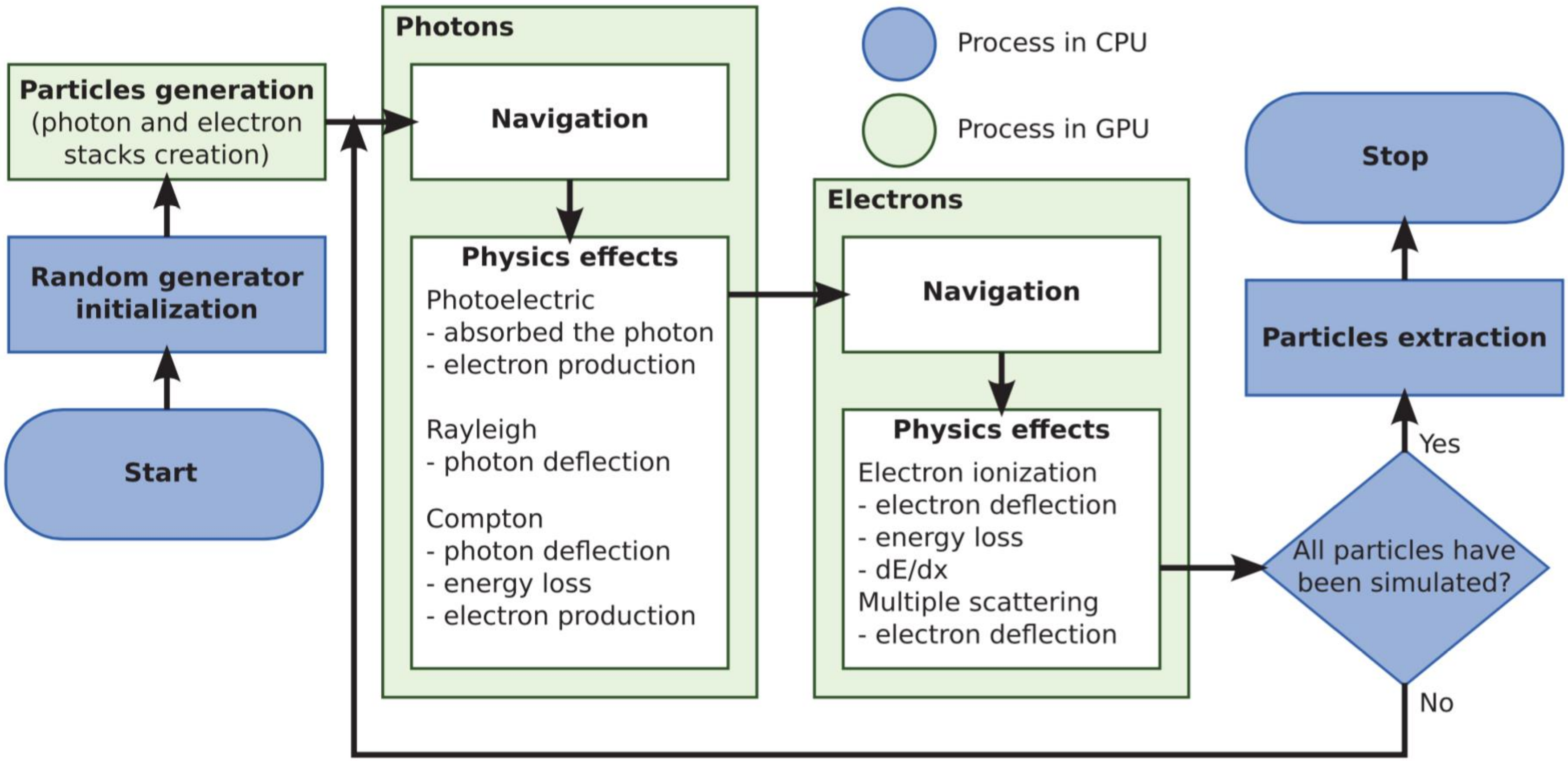
Parallelism in GATE

- Geant4 code has been moved to GPU (random number generator, photon physics effects, etc)[1]



[1] J. Bert, et al., “Geant4-based Monte Carlo simulations on GPU for medical applications”, Phys. Med. Biol. **58** (2013) 5593–5611

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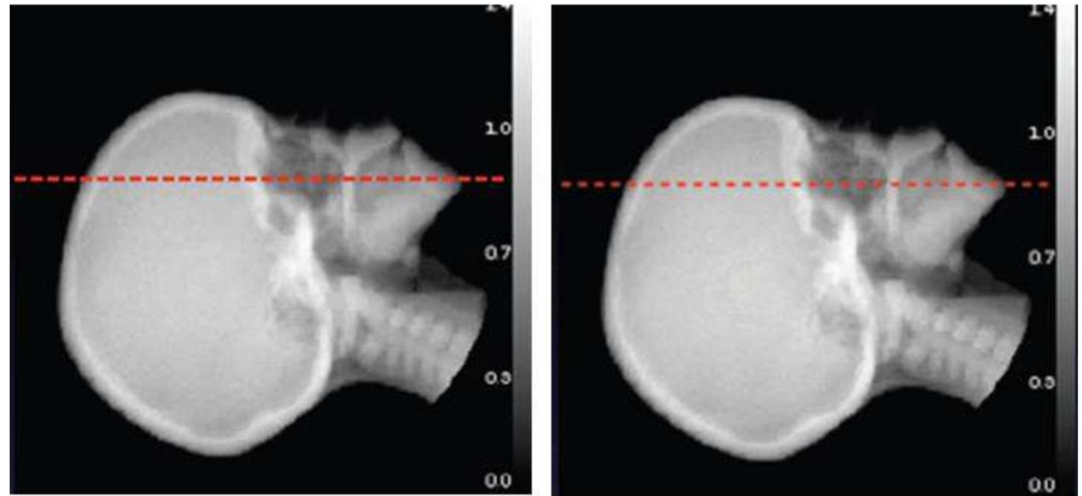
GATE CPU+GPU

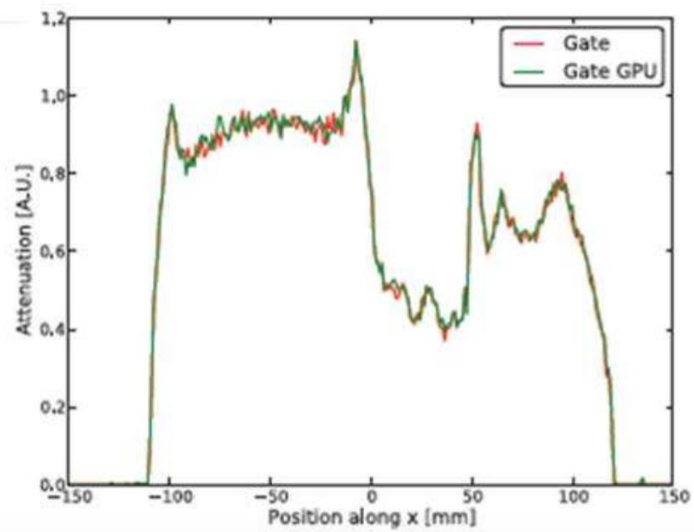
Voxelized phantom

GATE (CPU)
10^6 particles
~90 s

GATE (CPU+GPU)
10^6 particles
<2 s

GATE GATE-GPU





[1] J. Bert, et al., “Geant4-based Monte Carlo simulations on GPU for medical applications”, Phys. Med. Biol. **58** (2013) 5593–5611

Case Study 2

Image Reconstruction: OpenMP vs TBB

Image Reconstruction

OpenMP vs TBB

- **Image reconstruction is also usually a time consuming task.**
- **LM OSEM,** an iterative algorithm for 3D image reconstruction**:**
  - PET events (**LORs**) are split into s equally spaced subsets
  - For each subset $l \in 0, \ldots s-1$, is calculated f_{l+1}:

$$f_{l+1} = f_l c_l; \quad c_l = \frac{1}{A_N^t \mathbf{1}} \sum_{i \in S_l} (A_i)^t \frac{1}{A_i f_l}.$$

  - Where $f \in \mathbb{R}^n$ is a 3D image in vector form with dimensions $n = (X \times Y \times Z)$.
  - $\mathrm{A} \in \mathbb{R}^{mxn}$ and the element a_{ik} of the row A_i is the length of the LOR correspondent to the event i and the voxel k, calculated with Siddon's algorithm[1,2].

[1] P. Kegel , et al., "Using OpenMP vs. Threading Building Blocks for Medical Imaging on Multi-cores ", 15th International Euro-Par Conference, Delft, The Netherlands, August 25-28, 2009. Proceedings
[2]Siddon, R.L.: Fast calculation of the exact radiological path for a three-dimensional CT array. Medical Physics 12(2), 252–255 (1985)

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Image Reconstruction
OpenMP vs TBB

- **LM OSEM algorithm has 3 nested loops:**
  - 1 outer loop over all subsets
  - 2 inner loops, one for the summation, another for the iterations

Using OpenMP

```
for (int l = 0; l < subsets; l++) {
  /* read subset */

  /* compute c_l */
  #pragma omp parallel
  {
    #pragma omp for schedule(static)
    for (int i = 0; i < subset_size; i++) {
      ...
    }
  } /* end of parallel region */

  /* compute f_l+1 */
  #pragma omp parallel for schedule(static)
  for (int k = 0 ; k < image_size; k++) {
    if (sens[k] > 0.0 && c_l[k] > 0.0)
      f[k] = f[k] * c_l[k] / sens[k];  }  }
```

Race condition might happen here

Image Reconstruction
OpenMP vs TBB

- **LM OSEM algorithm has 3 nested loops:**
  - 1 outer loop over all subsets
  - 2 inner loops, one for the summation, another for the iterations

- For TBB, code modifications are needed

Using TBB

```
class ImageUpdate {
  double *const f, *const c_l;
  double *const sens,

public:
  ImageUpdate(double *f, double *sens, double *c_l) :
    f(f), sens(sens), c_l(c_l) {}

  void operator() (const blocked_range<int>& r) const {
    for (int k = r.begin(); k != r.end(); k++) {
      if (sens[k] > 0.0 && c_l[k] > 0.0)
        f[k] *= c_l[k] / sens[k];   }  }
};
```

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Image Reconstruction

OpenMP vs TBB

- **LM OSEM algorithm has 3 nested loops:**
  - 1 outer loop over all subsets
  - 2 inner loops, one for the summation, another for the iterations
- For TBB, code modifications are needed

Using TBB

```
for (int l = 0; l < subsets; l++) {
  /* read subset */

  /* compute c_l */
  parallel_for(
    blocked_range<int>(0, subset_size, GRAIN_SIZE),
    SubsetComputation(f, c_l, event_buffer, precision));

  /* compute f_l+1 */
  parallel_for(
    blocked_range<int>(0, image_size, GRAIN_SIZE),
    ImageUpdate(f, sens, c_l));   }
```

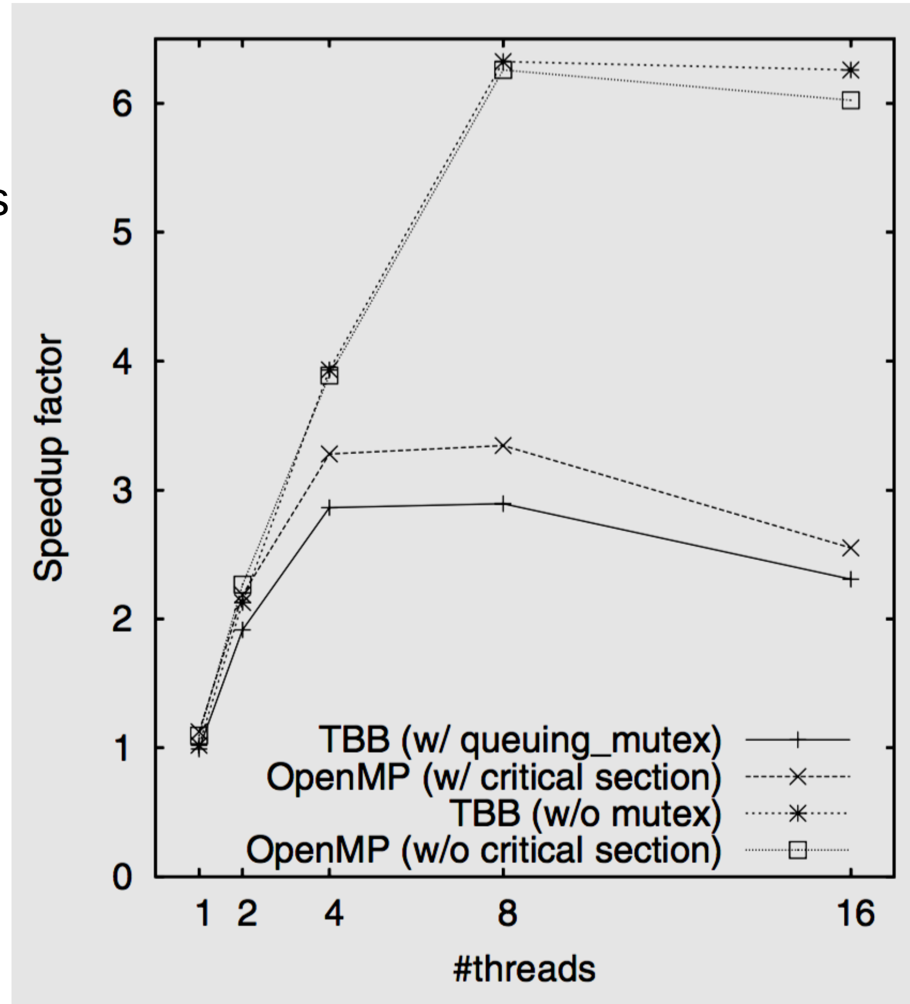
Image Reconstruction
OpenMP vs TBB

- **Implementation results:**

1. Preventing race conditions (using mutexes or critical sections), **OpenMP** has shown **better** performance over **TBB**.

2. Using **OpenMP** requires very little program redesign, contrary to **TBB**

3. **TBB** is more suitable for the design of new applications from the scratch, while **OpenMP** is preferable to redesign already developed code.



Running machine: dual quad-core (AMD Opteron 2352, 2.1GHz with

Case Study 3

MLEM Acceleration

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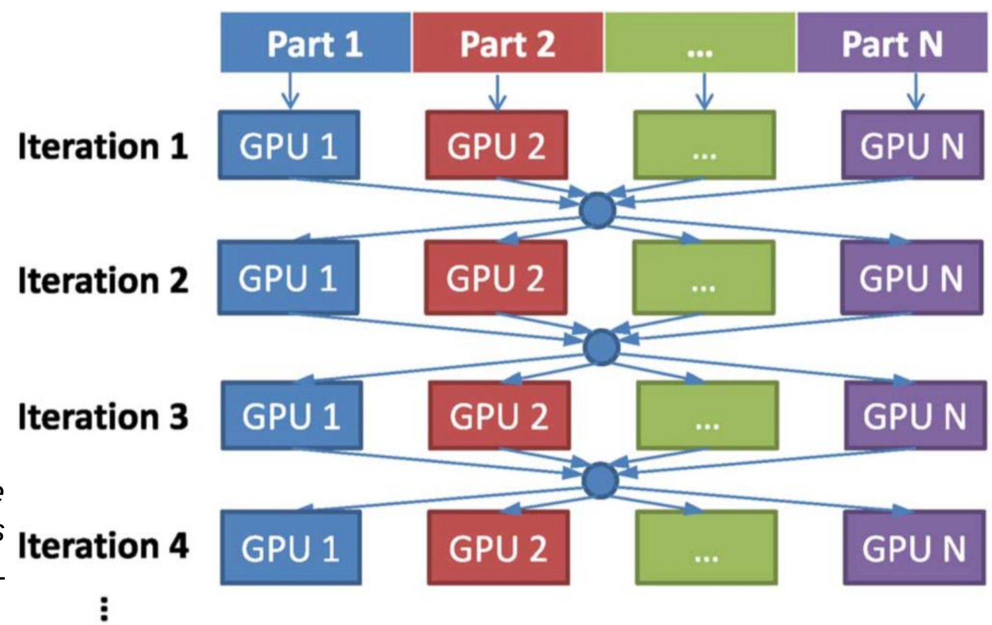
MLEM Acceleration

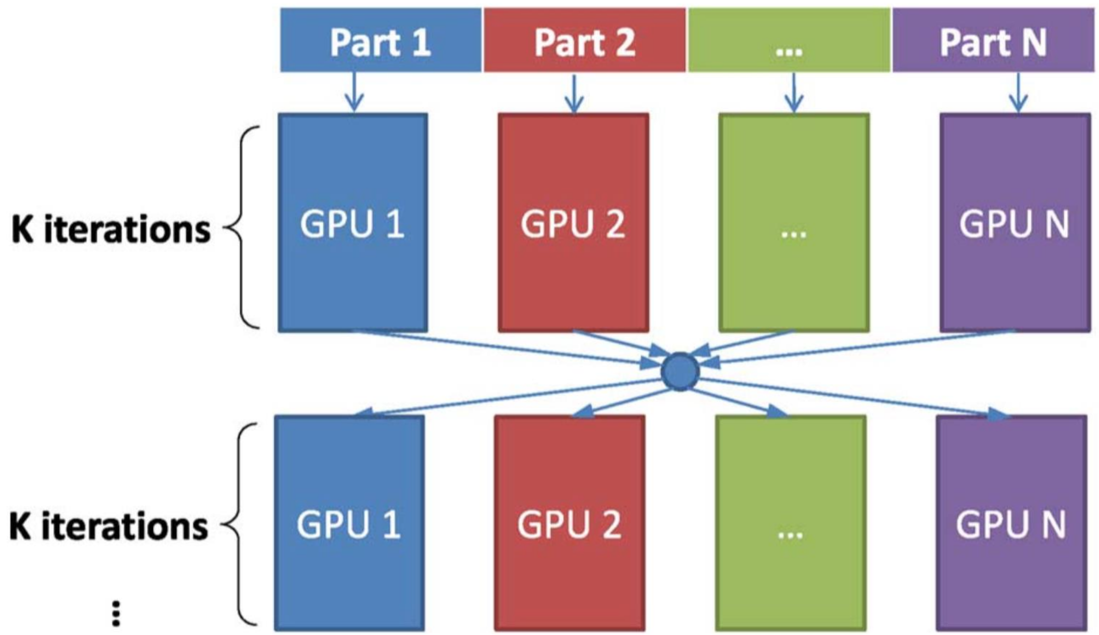
- The most of the time spent in projection and backprojection operations between the detected LORs and the image voxels.
- Acceleration of the method has been achieved in recent years, using single GPUs.
- Image reconstructions for real-time applications in hospitals demands even higher speed-up of calculations.
- Multi-GPUs systems are being used[1] but the communication between GPUs is a **bottleneck**.
- GeForce GTX 480 and GTX 285 were tested



[1] *Distributed MLEM: An Iterative Tomographic Image Reconstruction Algorithm for Distributed Memory Architectures* Craig S. Levin et al, IEEE TRANSACTIONS ON MEDICAL IMAGING, VOL. 32, NO. 5, MAY 2013

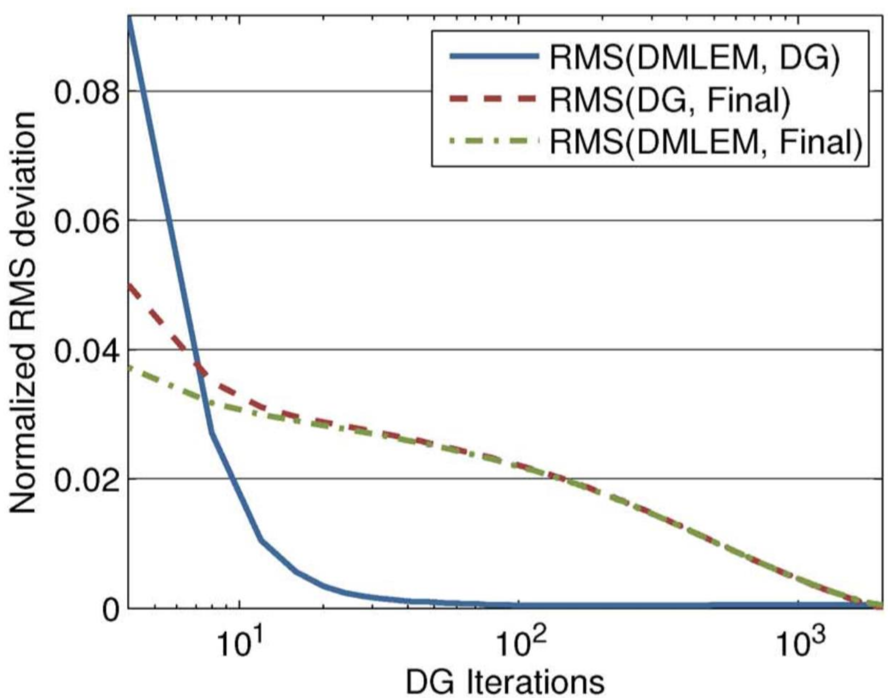
MLEM Acceleration

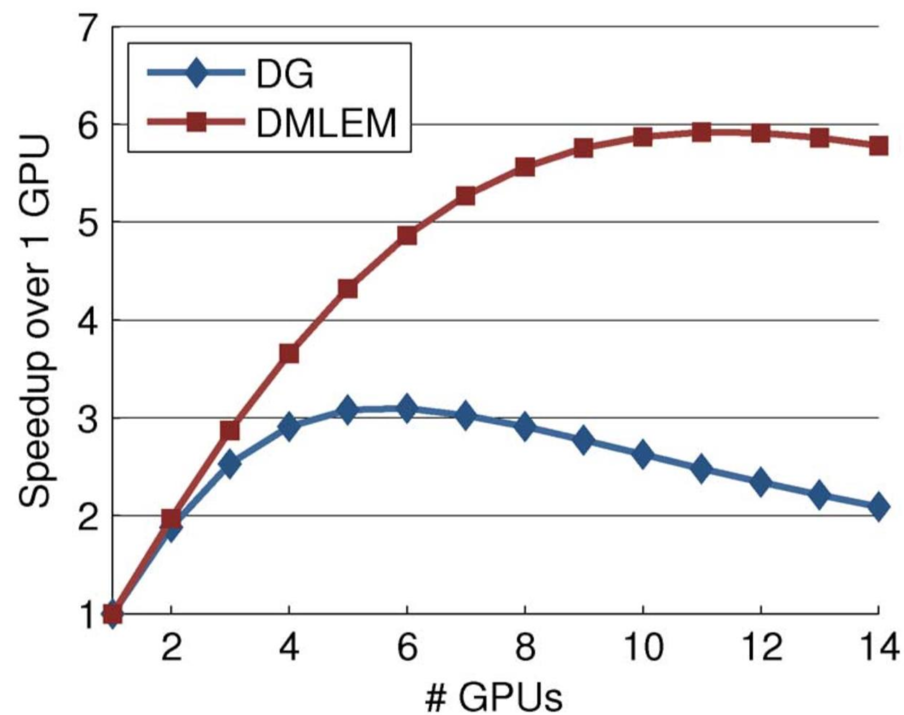
- In this work, the common MLEM (DG) algorithm is described as a special case of a general optimization problem
- A new MLEM (DMLEM) is derived by maximizing the same likelihood function as the common MLEM, but adapted to a multiGPU system
- The new algorithms performs several iterations in sub-problems of the original problem, but minimizing the same objective function



MLEM Acceleration

- Overall difference between images obtained with the two methods is negligible after the initial iterations
- Linear speedup with increase of GPUs is obtained in both methods for small number of GPUs, but saturation of DMLEM occurs later because of the reduced communication between independent nodes.





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Conclusions

- **In Medical Physics, several applications has taken advantage of the rapidly increase of the computation resources that are available, specially for:**
  - Simulation of the operation of existent and new **scanners.**
  - **Image reconstructions** both for scientific or preclinical research and in real time clinical practice.
- **New software tools has been used to accelerate these tasks:**
  - **OpenMP** and **TBB**, using the multi-CPU capabilities.
  - Nvidia **CUDA**, taking advantage of the power of graphic cards commonly available.
- **The use of one tool instead of the other will depend manly on:**
  - The desired **application** (new or renewed).
  - The available **resources** (time, funds, hardware).
  - The **will** of the person in charge.