

Ferramentas Computacionais para Cálculos Dosimétricos

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<https://sites.google.com/site/tcff01/>



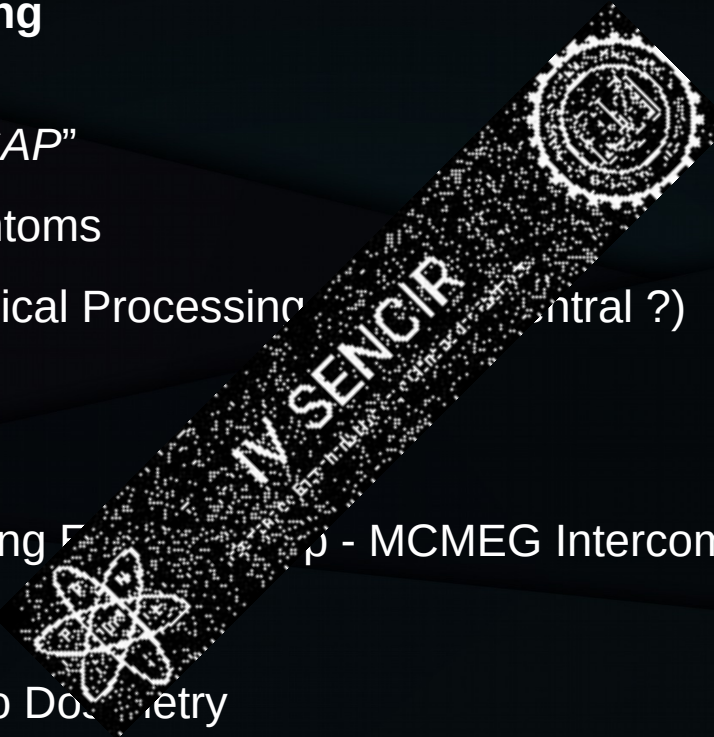
6, 7 e 8 de novembro de 2018

Escola de Engenharia da UFMG

IV SENCIR - Semana de Engenharia Nuclear e
Ciências das Radiações

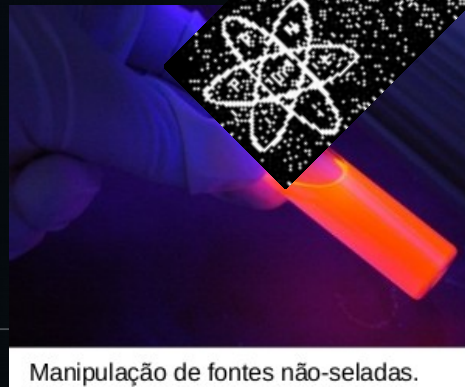
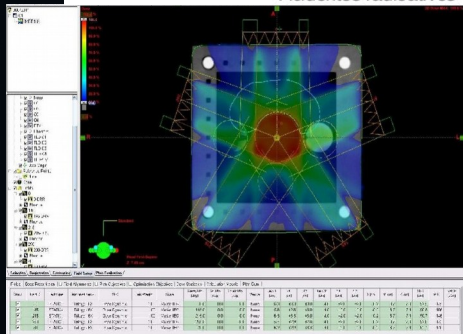
Overview

- **Computational Modelling**
 - Introduction MC “ASAP”
 - Computational Phantoms
 - CPU x GPU (Graphical Processing Central ?)
- **Applications:**
 - Monte Carlo Modelling F_{eff} - MCMEG Intercomparison
 - Internal Dosimetry
 - Radiotherapy - Nano Dosimetry
- **What else ? FYI**



Introduction

- Métodos para simulação computacional vêm sendo desenvolvidos e utilizados em todo o mundo desde meados do século XX.
- Tais métodos compreendem de modelos matemáticos a técnicas computacionais que permitem estudar, simular e analisar aplicações em diversas áreas do conhecimento.



STATISTICAL METHODS IN NEUTRON DIFFUSION

By R. D. RICHTMYER and J. VON NEUMANN

LAMS-551, 1947

There is reproduced here some correspondence on a method of solving problems in which data are chosen at random to represent a number of neutrons in a reacting system. The history of these neutrons and their progeny is followed by detailed calculations of the motions and collisions of these neutrons, and various variables being introduced at certain points in such a way as to represent the occurrence of various processes with the correct probabilities. If the history is followed through a long enough chain reaction thus represented may be regarded as a representative sample of the chain reaction in the system in question. The results may be analyzed statistically to obtain various average quantities of interest for comparison with experiments or for design problems.

This method is designed to deal with problems of a more complicated nature than conventional methods based, for example, on the Boltzmann equation. For example, it is not necessary to restrict neutron energies to a single value or even to a finite number of values and one can study the distribution of neutrons or of collisions of any specified type not only with respect to space variables but with respect to other variables, such as neutron velocity, direction of motion, time. Furthermore, the data can be used for the study of fluctuations and other statistical phenomena.

THE INSTITUTE FOR ADVANCED STUDY

PRINCETON, NEW JERSEY

School of Mathematics

March 11, 1947

Mr. R. Richtmyer
Post Office Box 1663
Santa Fe, New Mexico

Introduction

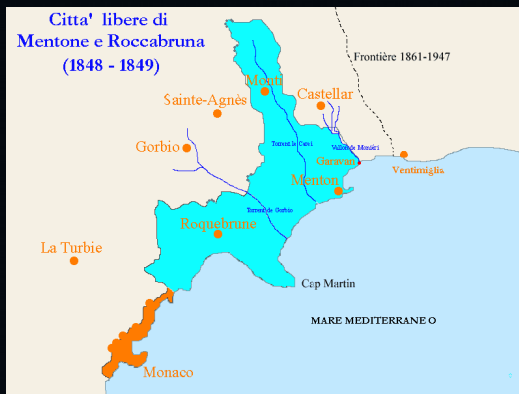


Define-se como Método de Monte Carlo (MMC) qualquer método de uma classe de métodos estatísticos que se baseiam em amostragens aleatórias para obter resultados numéricos, isto é, repetindo sucessivas simulações em um elevado número de vezes para calcular as probabilidades de que possíveis eventos ocorram.

A simulação conhecida como Método de Monte Carlo foi introduzida por Stanislaw Ulam, John von Neumann e Nicholas Metropolis no final da Segunda Guerra Mundial em um projeto do National Laboratory no New Mexico, USA, para estudar a difusão de nêutrons em material físsil.
[Metropolis, 1952]



Officially named "Casino de Monte-Carlo", the Monte Carlo is a gambling and entertainment complex located in Monaco.

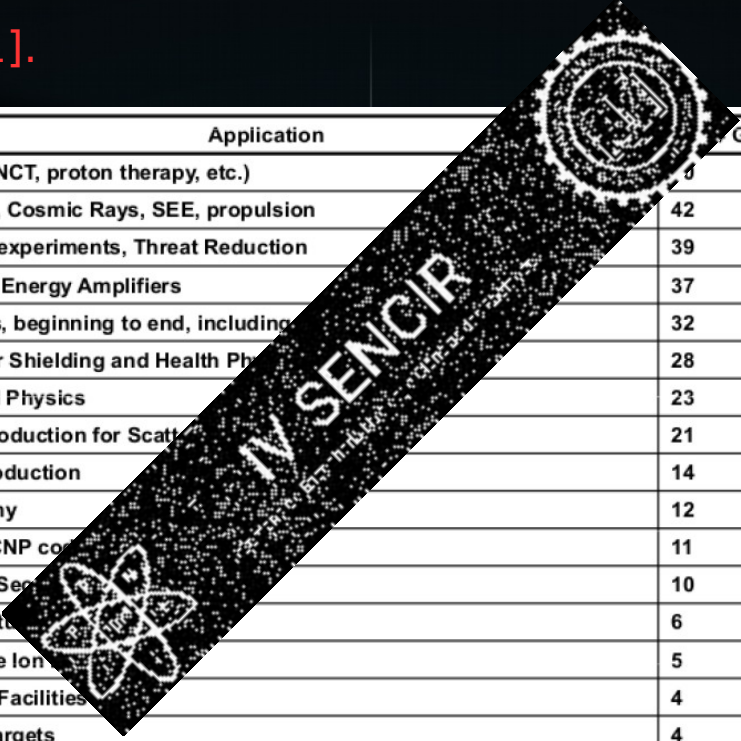


Cassino de Monte Carlo



Introduction

“Computation has become a third way of doing science and complements both theory and experiment” [1].



Application	Groups	Percent
Medical (BNCT, proton therapy, etc.)	15	15
Spacecraft, Cosmic Rays, SEE, propulsion	42	12
Detectors, experiments, Threat Reduction	39	11
ATW, ADS, Energy Amplifiers	37	11
Fuel cycles, beginning to end, including	32	9
Accelerator Shielding and Health Ph	28	8
Theoretical Physics	23	7
Neutron Production for Scatt	21	6
Isotope Production	14	4
Radiography	12	4
MCNPX/MCNP co	11	3
Homeland Sec	10	3
Materials st	6	2
Radioactive Ion	5	1
Irradiation Facilities	4	1
Neutrino Targets	4	1
Light Sources, electron machines	3	1

[1] H. Gould, J. Tobochnik, and W. Christian, *An Introduction to Computer Simulation Methods: Applications to Physical Systems*, 3rd ed., Addison-Wesley, 2007, ISBN: 978-0805377583, 720 pages.

[2] Book: Monte Carlo Techniques in Radiation Therapy by Joao Seco & Frank Verhaegen. January 1, 2013

Introduction

“Medicine” area leveling out, at greater than 2100 publications/year...[2]

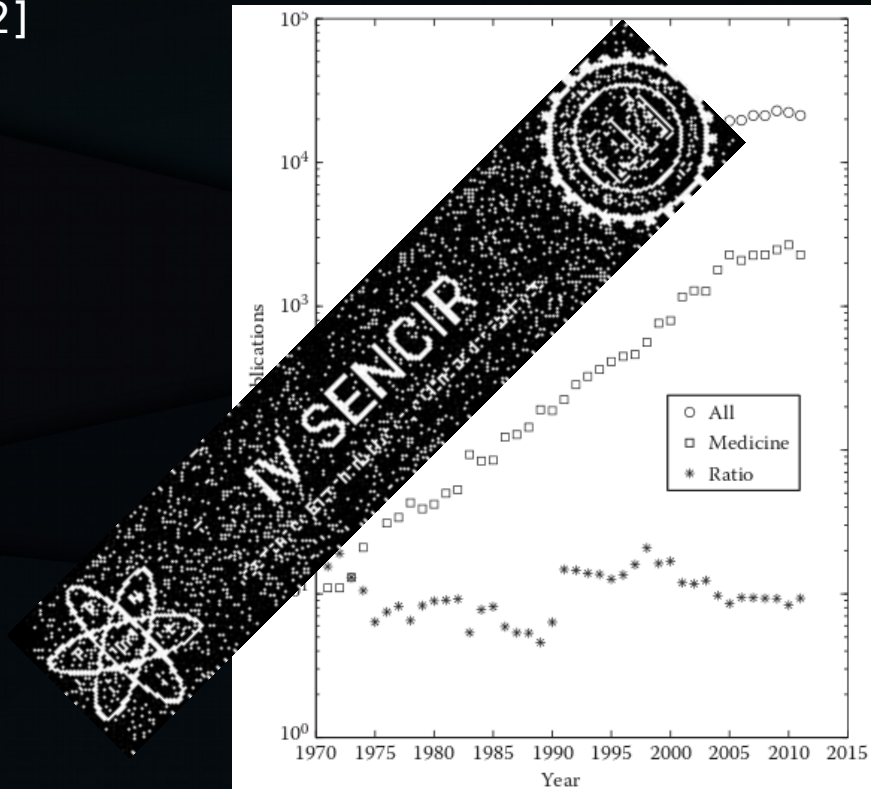


FIGURE 1.2 The number of papers published per year garnered from the Web of Knowledge (“All”) and MedLine (“Medicine”). Martin Berger, on a beach near Erice, 1987. (Photograph courtesy of Ralph Nelson.)

[2] Book: Monte Carlo Techniques in Radiation Therapy
by Joao Seco & Frank Verhaegen January 1, 2013

Introduction

M&S computacional ↔ experimento computacional

Laboratory experiment	Computation
sample	program
physical apparatus	program
calibration	calibration
measurement	analysis
data analysis	analysis

O ponto inicial da M&S computacional é o desenvolvimento de um:

- ... modelo ideal do sistema físico de interesse
- ... especificar um procedimento ou algoritmo para implementação do modelo em um computador e
- ... decidir o que se deseja medir ("tally score").

Os resultados de uma simulação computacional podem servir de ponte, conectando o experimentos laboratorial e a teoria utilizada para os cálculos do experimentos.

Introduction: MC

Porque Simular?

... desenvolver uma teoria ?

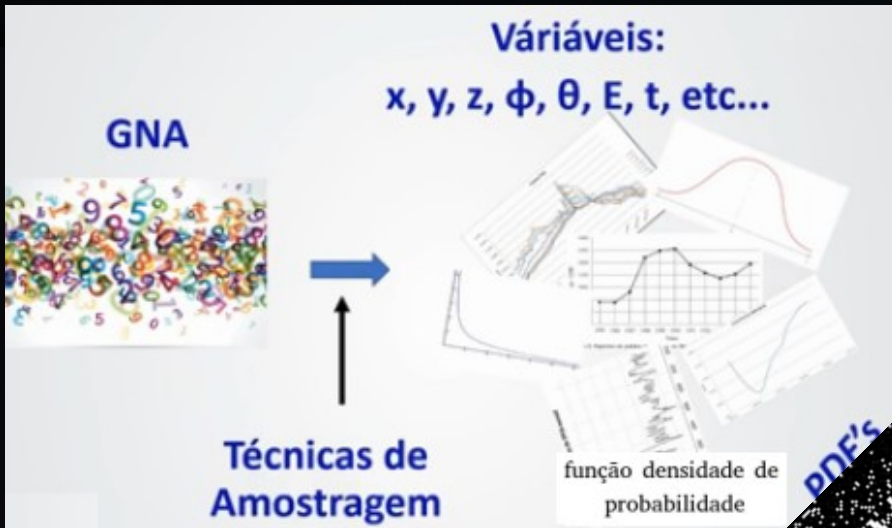
... fazer coisas que não são fisicamente ou numericamente possíveis dentro do sistema em estudo, etc....

... ajuda a entender um sistema real antes de ele ser construído?

Simulações são como experimentos em laboratórios, ou seja, **são ferramentas que podem ser utilizadas para entender fenômenos naturais.**

O objetivo de toda investigação de um fenômeno natural é buscar explicações concisas que possam estabelecer conclusões lógicas sobre este fenômeno.

Introduction: Como funciona ?



A **função densidade de probabilidade** $f(x)$:

- descreve a distribuição de uma **variável aleatória contínua** X .

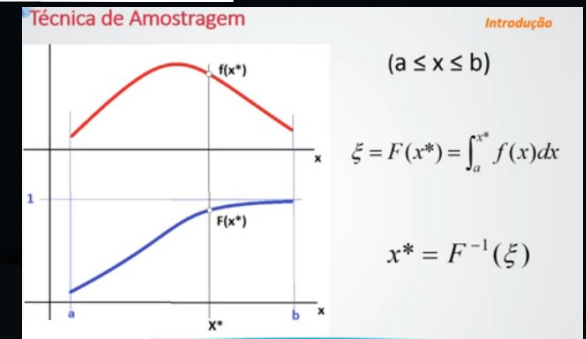
Se um intervalo tem grande probabilidade de conter X :

- $f(x)$ apresenta valores altos.

A probabilidade de ocorrer entre a e b é determinada pela integral da função densidade de probabilidade $f(x)$ sobre esse intervalo.



1. GNA - Gerador de números aleatórios
Ou processos estocásticos
2. PDFs
3. Técnicas de amostragem
4. Estimador de erros
5. Técnicas de redução de variância
6. Vetorização e Computação Paralela



Introduction: Example

Linear Congruential Generator (LCG)

é um algoritmo que produz uma sequência de números pseudo-aleatórios.

- Mais utilizado
- Período máximo de 2^n para números de n-bits

- $X_{n+1} = (aX_n + c) \bmod m$

- a, c, m são constantes
- X_0 é a semente

```
#include <stdio.h>
#include <termios.h>
#include <stdlib.h> // necessário para rand()
#include <time.h> // necessário para time()

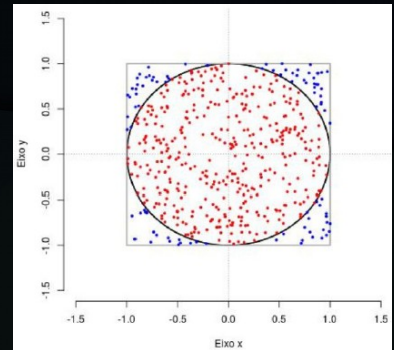
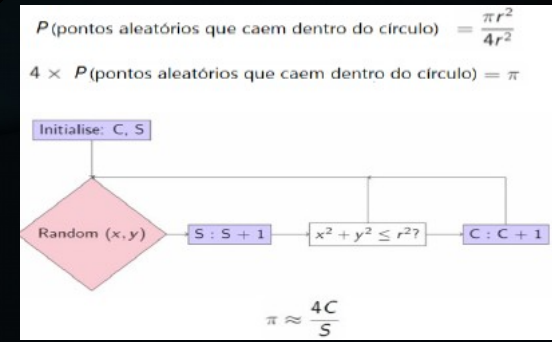
int main(void)
{
    int i;
    printf("Gerando 10 números aleatórios\n");

    /* srand(time(NULL)) inicializa o gerador de números aleatórios com o
    valor da função time(). Cada vez que é chamado, é calculado como sendo o
    total de segundos desde o início de janeiro de 1970 até a data
    atual. Devido a isso, o valor da "semente" será diferente. */

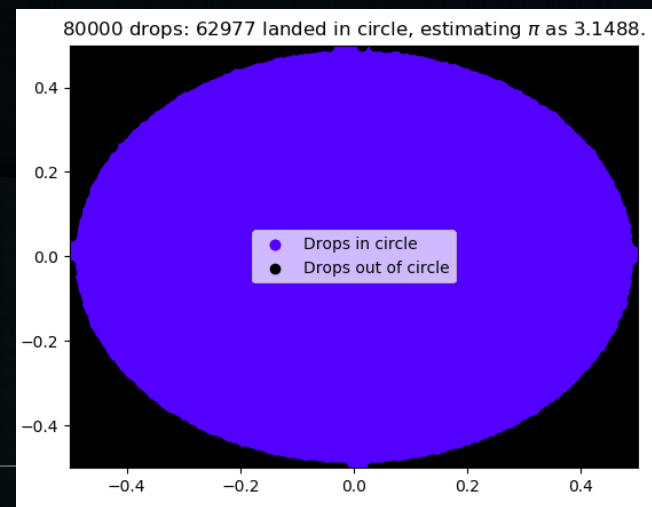
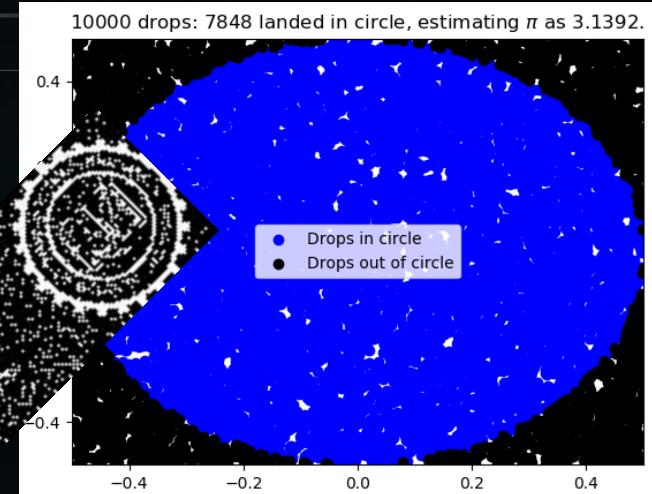
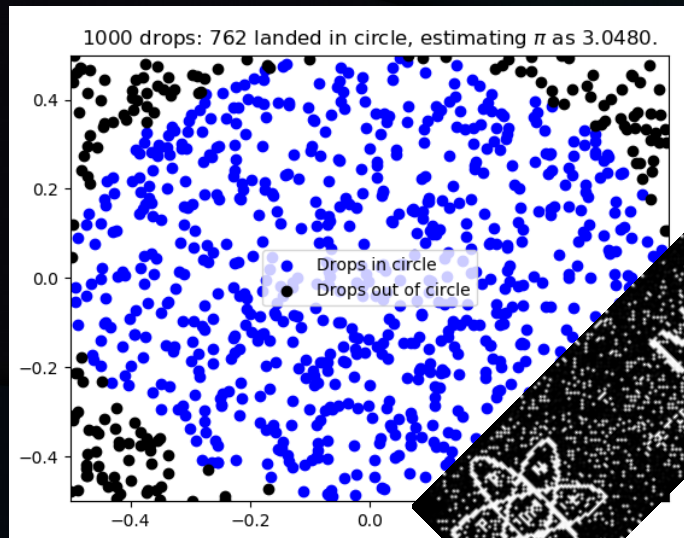
    srand(time(NULL));

    for (i = 0; i < 10; i++)
    {
        /* Gerando números aleatórios entre zero e 100 */
        printf("%d\n", rand() % 100);
    }

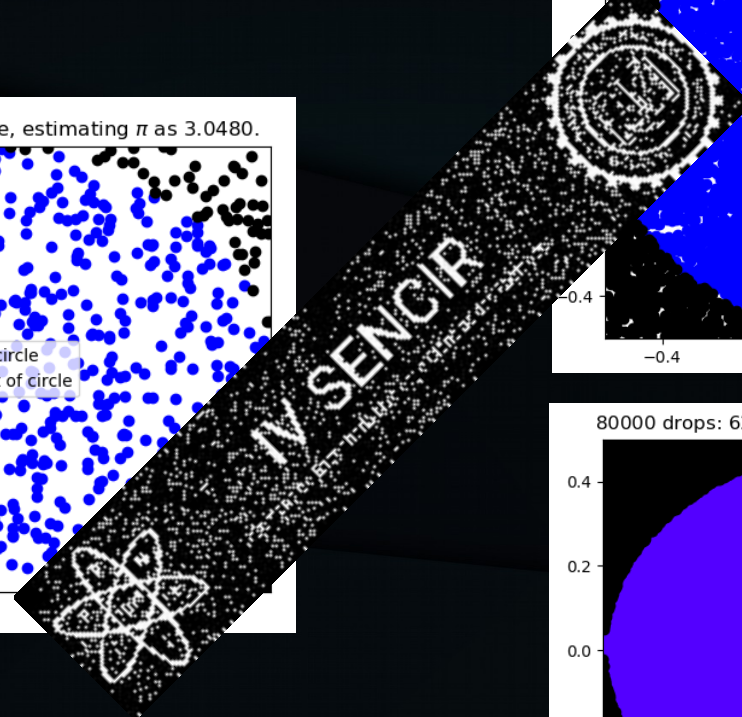
    getchar();
    return 0;
}
```



Introduction: Example

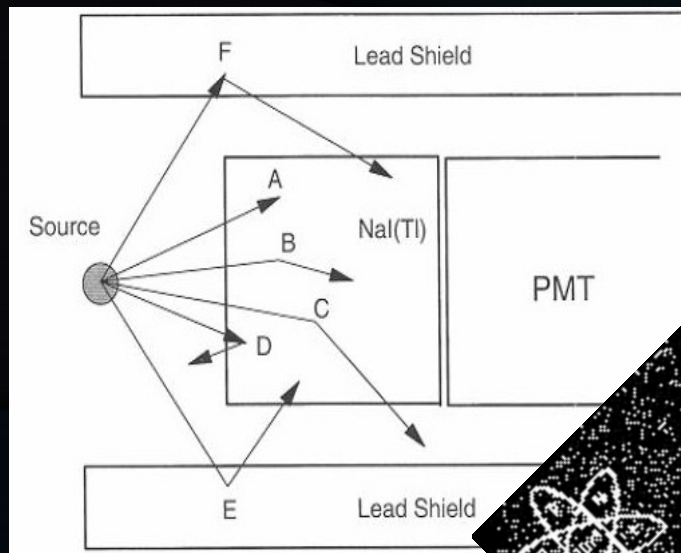


$$\pi = 3.1415926$$

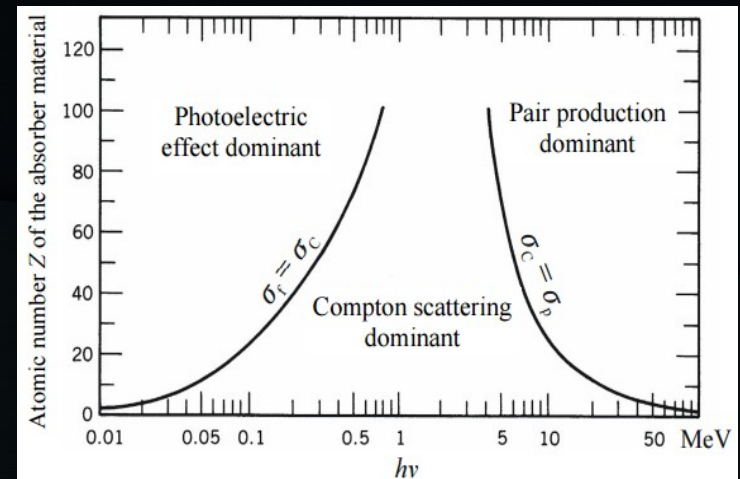


Introduction: MC example

Typical case of Nuclear Instrumentation



Importance of the three major types of γ interactions processes for different absorber Z and photon energies.

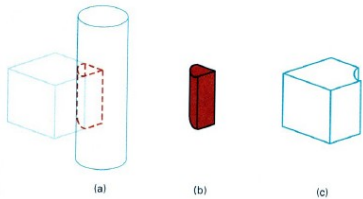


Introduction: MC geometry

Constructive Solid Geometry (CSG):

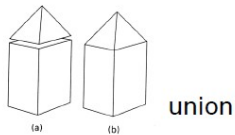
...the common approach of radiation transport codes
 ...set of primitives (blocks, cones, cylinders, ...)

new solid is defined by applying mathematical operations;



intersection

difference



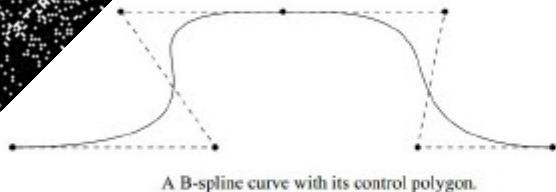
union

Mnemonic	Type	Description	Equation	Card Entries
F	Plane	General	$Ax + By + Cz - D = 0$	A B C D
FX		Normal to x-axis	$x - D = 0$	D
FY		Normal to y-axis	$y - D = 0$	D
FZ		Normal to z-axis	$z - D = 0$	D
SO	Sphere	Centered at Origin	$x^2 + y^2 + z^2 - R^2 = 0$	
S		General	$(x - \bar{x})^2 + (y - \bar{y})^2 + (z - \bar{z})^2 - R^2 = 0$	
SX		Centered on x-axis	$(x - \bar{x})^2 + y^2 + z^2 - R^2 = 0$	
SY		Centered on y-axis	$x^2 + (y - \bar{y})^2 + z^2 - R^2 = 0$	
SZ		Centered on z-axis	$x^2 + y^2 + (z - \bar{z})^2 - R^2 = 0$	
C/X	Cylinder	Parallel to x-axis	$(y - \bar{y})^2 + (z - \bar{z})^2 - R^2 = 0$	
C/Y		Parallel to y-axis	$(x - \bar{x})^2 + (z - \bar{z})^2 - R^2 = 0$	
C/Z		Parallel to z-axis	$(x - \bar{x})^2 + (y - \bar{y})^2 - R^2 = 0$	
CO		On x-axis	$y^2 + z^2 - R^2 = 0$	
CY		On y-axis	$x^2 + z^2 - R^2 = 0$	
CO		On z-axis	$x^2 + y^2 - R^2 = 0$	
K/X	Cone	Parallel to x-axis	$\sqrt{(y - \bar{y})^2 + (z - \bar{z})^2} = R - H x - \bar{x} $	
K/Y		Parallel to y-axis	$\sqrt{(x - \bar{x})^2 + (z - \bar{z})^2} = R - H y - \bar{y} $	
K/Z		Parallel to z-axis	$\sqrt{(x - \bar{x})^2 + (y - \bar{y})^2} = R - H z - \bar{z} $	
KO		On x-axis	$\sqrt{y^2 + z^2} = R - H x $	
KY	On y-axis	$\sqrt{x^2 + z^2} = R - H y $		
KZ	On z-axis	$\sqrt{x^2 + y^2} = R - H z $		

Boundary Representation (BREP)

New... Systems: Computer graphic and animated films industry.

... (rational B-Spline)
 ... (Micro, QuickDraw 3D, etc..)



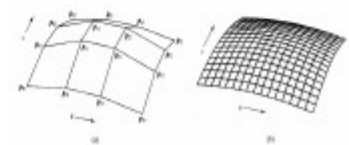
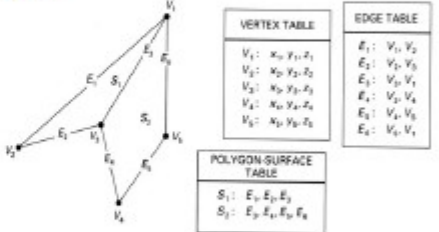
A B-spline curve with its control polygon.

$$C(u) = \frac{\sum_{i=0}^n N_{i,p}(u)w_i P_i}{\sum_{i=0}^n N_{i,p}(u)w_i} \quad a \leq u \leq b$$

where P_i are the control points, w_i are the weights and $N_{i,p}$ are the B-spline basis functions defined on the non-periodic and non-uniform knot vector,

Polygon mesh surfaces:

...is representing by connecting faces, edges and vertices.



Introduction

Dentre os vários programas computacionais existentes, baseados no método de MC para transporte de partículas, destacam-se:

MCNPx - Monte Carlo N-Particle Transport Code System – (RSIC, Los Alamos, USA)

EGSnrc - Electron-Gamma Shower - National Research Council (Canada)

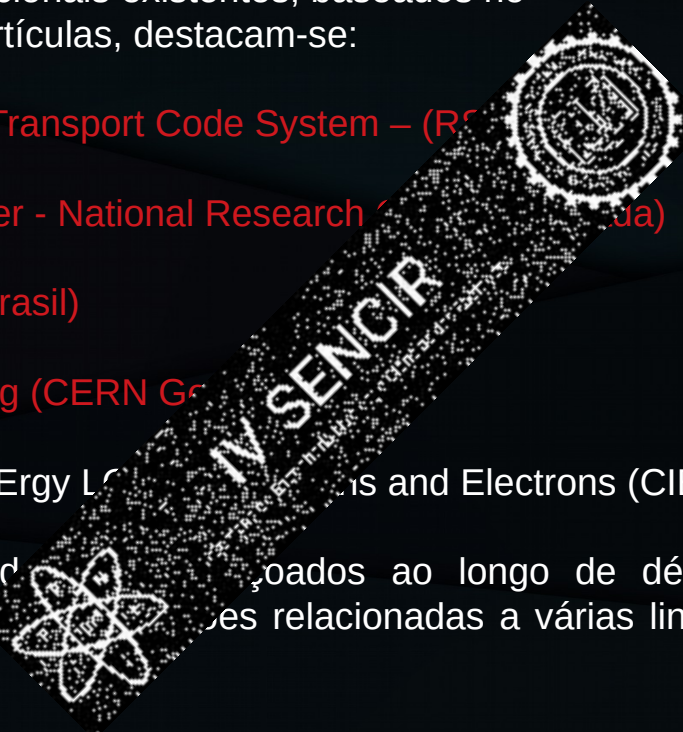
VMC - Visual Monte Carlo (IRD, Brasil)

GEANT4 - GEometry ANd Tracking (CERN Geneva)

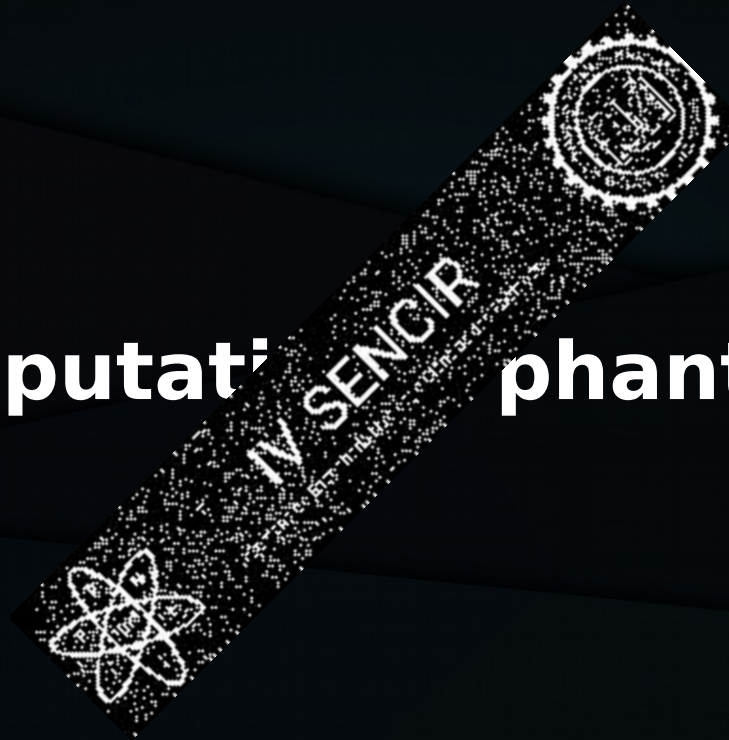
PENELOPE - Penetration and ENergy Losses of Electrons and Electrons (CIEMAT, Espanha), etc.

Estes programas foram desenvolvidos e aperfeiçoados ao longo de décadas de pesquisas e hoje são amplamente usados para simulações de problemas relacionados a várias linhas de pesquisas, em especial na área da **física médica**.

Normalmente, este tipo de simulação exige um **tempo computacional** e **quantidade de memória** demasiadamente elevados e uma forma de melhorar o desempenho dessas aplicações é utilizar a *Multicore central processing unit* (CPU) Cluster ou *Graphics processing unit* (GPU).

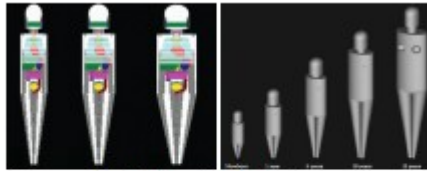


Computational phantoms

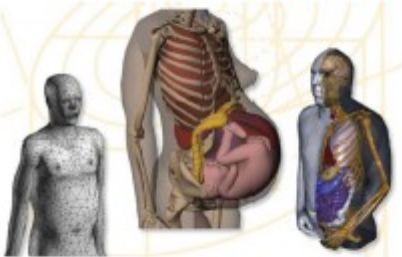


Computational phantoms

- 1 - Constructive Solid Geometry (CSG)
Voxel Geometry (VOXEL) (Medical images)
Mathematical/Stylized
- 2 - Boundary Representation (BREP)
NURBS Surface
Surface Mesh Approximation (MESH)



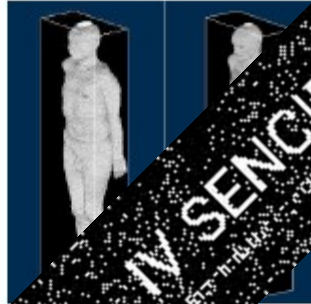
1- Mathematical phantoms



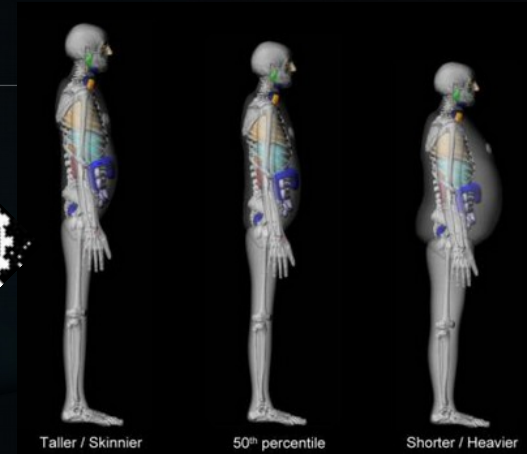
2- BREP phantoms (Xie George Xu, 2009)



2- FASH Surface (Kramer et al. 2009)



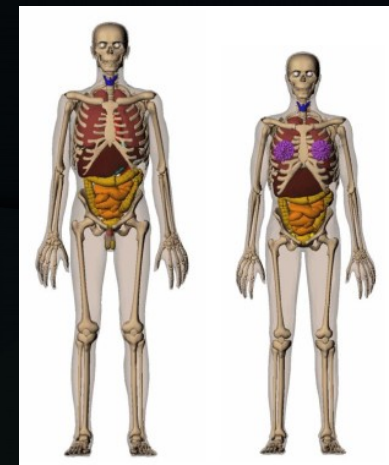
89



Taller / Skinnier

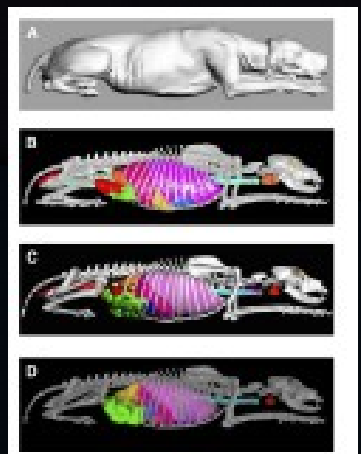
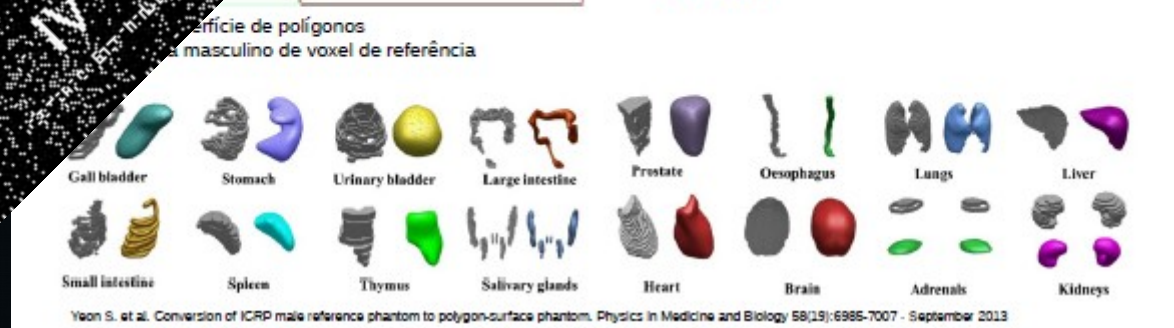
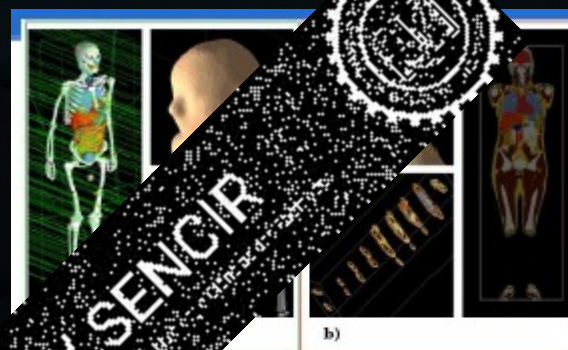
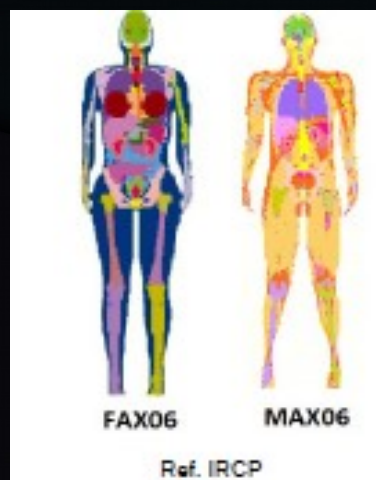
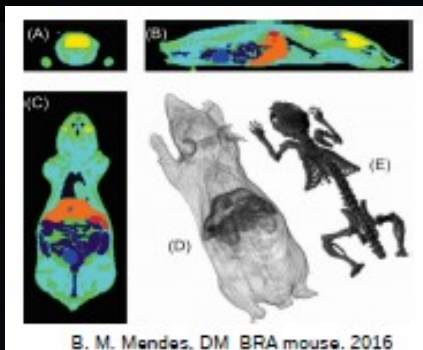
50th percentile

Shorter / Heavier



University of Florida Hybrid Adult Male and Female
UFHADM and UFHADDF phantoms

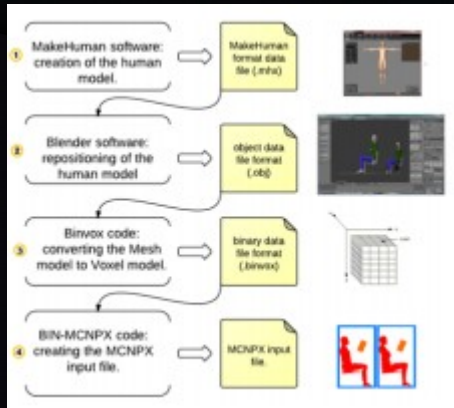
Computational phantoms



<http://jnm.snmjournals.org/content/49/3/446.full.pdf>

- A nova geração de fantasmas permite a criação do Avatar ou humanoíde (objeto mesh) mas ...como modelar os possíveis volumes e diferentes formas dos órgão internos para cada indivíduo?!

Computational phantoms



MakeHuman



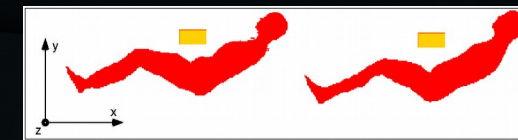
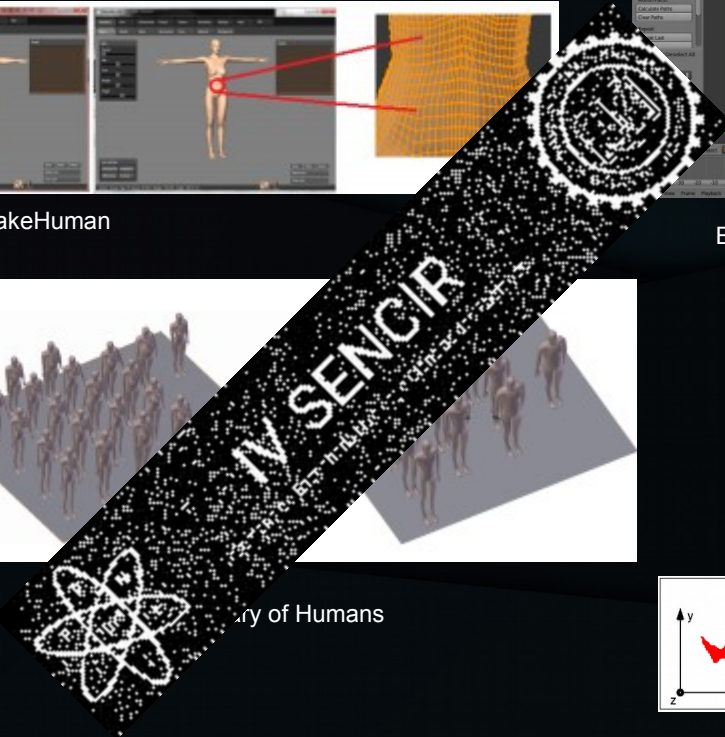
Blender



Binvox



Library of Humans

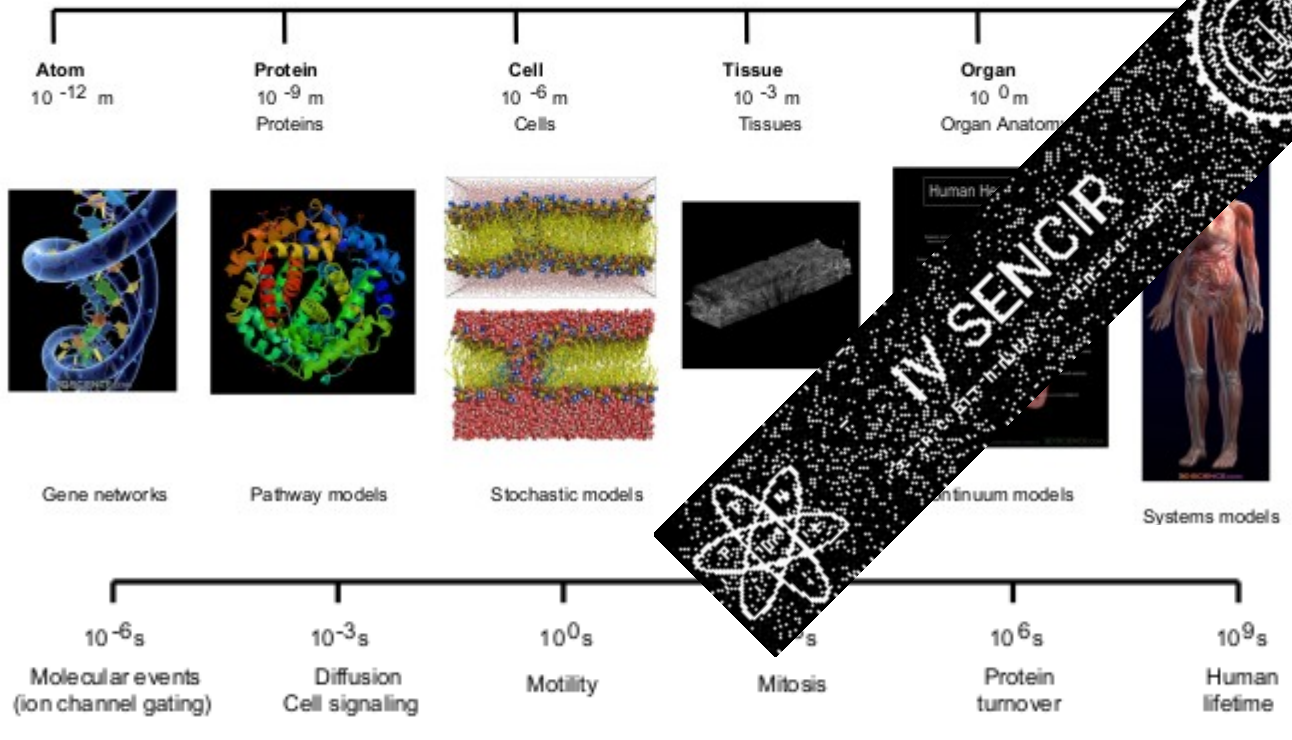


Fonseca T, Bogaerts R., Lebacqz A., Mihailescu C., Ribeiro M. R. and Vanhavere F. "MaMP and FeMP - computational mesh phantoms applied for studying the variation of WBC efficiency using a NaI(Tl) detector". Journal of Radiological Protection. 2014.

Fonseca T. R Bogaerts, John Hunt, F Vanhavere. "A methodology to develop computational phantoms with adjustable posture for WBC calibration". Physics in Medicine and Biology 11/2014; 59(22)

Computational phantoms

Computational models for medical devices integrate different processes over a wide range of spatial scales... [and...](#)



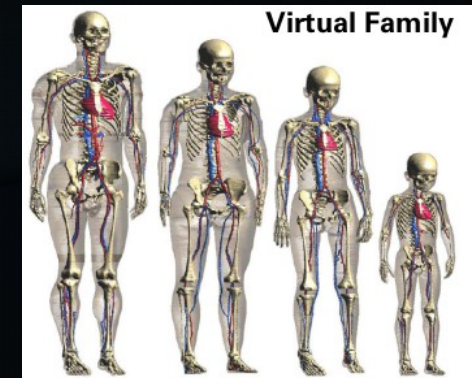
... temporal scales

Computational phantoms: Future!

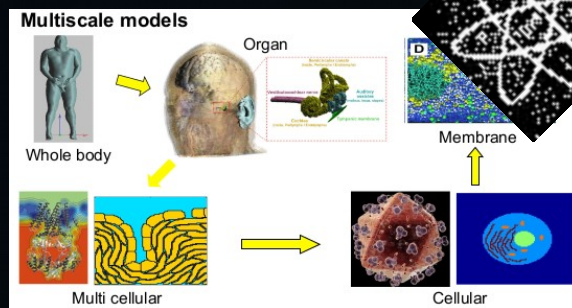
Requirements for computational phantom & modelling for the next generation of medical devices

- need to combine all fields of human macro-, micro- and nano- dosimetry
- need to combine all fields of human macro-, micro- and nano- physics, anatomy
- need to include biomechanical tissue engineering, e.g. vibration assessment
- electric, magnetic and electromagnetic tissue response and assessment
- chemical tissue response and chemical tissue damage assessment
- thermal dosimetry and non-linear tissue damage model
- needs anatomical models to cover the entire patient
 - the virtual family, the virtual classroom

**A multitude of disciplines must be coped with:
Medical devices combine problems of physics,
electrodynamics, thermodynamics,
anatomy, biology and chemistry**

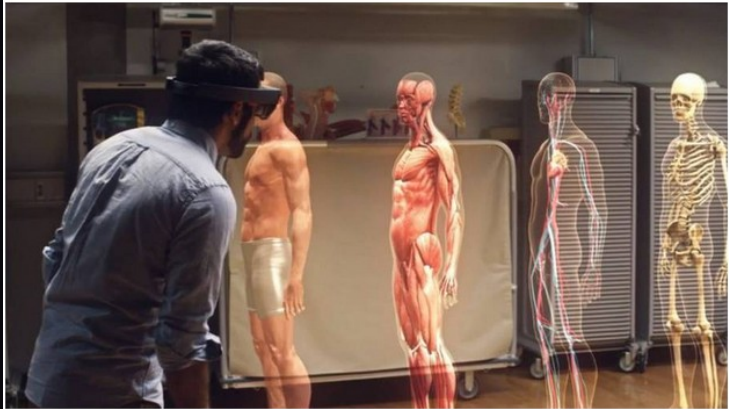


Virtual Patient



Computational phantoms: Future!

By: Kirsty Wynn



Accurate Holograms are helping surgeons plan complex surgeries. Photo / Microsoft

Experts gather in Rotorua to discuss latest technological breakthroughs.
Holograms of accurate human skeletons, layered with muscle and organs, veins and vessels are among technological breakthroughs tipped to revolutionise health care.

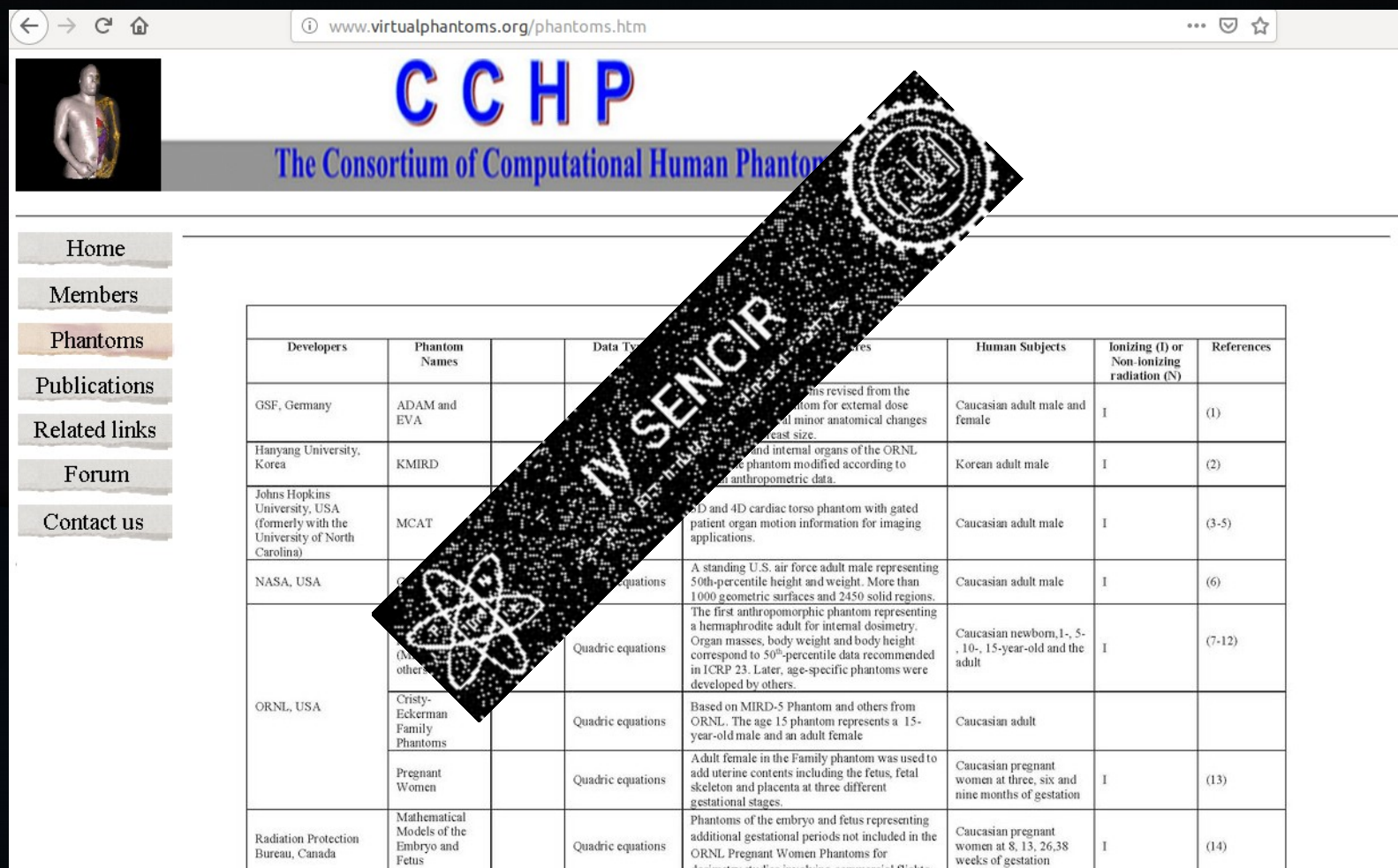
November, 5 2018- Health and technology experts → the latest trends – including the holograms which are already being used overseas instead of cadavers to train medical students, and by surgeons to plan operations.



LucinaAR childbirth simulator

<https://healthcentral.nz/holograms-and-virtual-doctors-in-our-medical-future/>
<https://caehealthcare.com/hololens/> video

Computational phantoms: Future!



The screenshot shows the website for the Consortium of Computational Human Phantoms (CCHP). The page features a navigation menu on the left with links to Home, Members, Phantoms, Publications, Related links, Forum, and Contact us. The main content area displays a table listing various computational phantoms, their developers, data types, human subjects, and references. A large, stylized watermark reading 'IV SENCIR' is overlaid diagonally across the table.

Developers	Phantom Names	Data Type	Human Subjects	Ionizing (I) or Non-ionizing radiation (N)	References
GSF, Germany	ADAM and EVA	...	Caucasian adult male and female	I	(1)
Hanyang University, Korea	KMIRD	...	Korean adult male	I	(2)
Johns Hopkins University, USA (formerly with the University of North Carolina)	MCAT	...	Caucasian adult male	I	(3-5)
NASA, USA	...	Quadratic equations	Caucasian adult male	I	(6)
ORNL, USA	(MIRD) and other	Quadratic equations	Caucasian newborn, 1-, 5-, 10-, 15-year-old and the adult	I	(7-12)
	Cristy-Eckerman Family Phantoms	Quadratic equations	Caucasian adult		
	Pregnant Women	Quadratic equations	Caucasian pregnant women at three, six and nine months of gestation	I	(13)
Radiation Protection Bureau, Canada	Mathematical Models of the Embryo and Fetus	Quadratic equations	Caucasian pregnant women at 8, 13, 26, 38 weeks of gestation	I	(14)

Computational phantoms: Drawback

Problemas!!

1- Geração de número **pseudoaleatórios!!**

2- **Cluster:** vários computadores, espaço físico e localização, manutenção específica, etc.

3- **Alto custo** operacional: compra de vários computadores, processadores, refrigeração das máquinas, no-breaks, software de gerenciamento de filas, etc.

4- **Tempo computacional: Cenário**

Contaminação interna com Fluor-18 (utilizado em diagnóstico médico) → Simulação de cálculo de dose em todos os órgãos do fantoma Golem e Laura feminino (com milhões de voxels)

→ ~5 dias num cluster com 222 núcleos

Cluster Orion com 37 máquinas AMD Phenom II X6 1100T com clock de 3,3 GHz de 16 GB de memória, num total de 222 núcleos. (LN / IRD/CNEN)

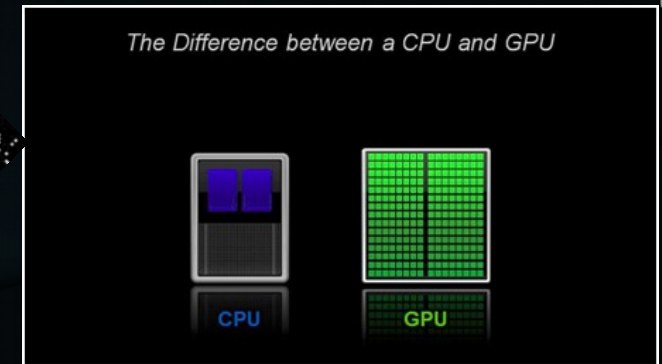
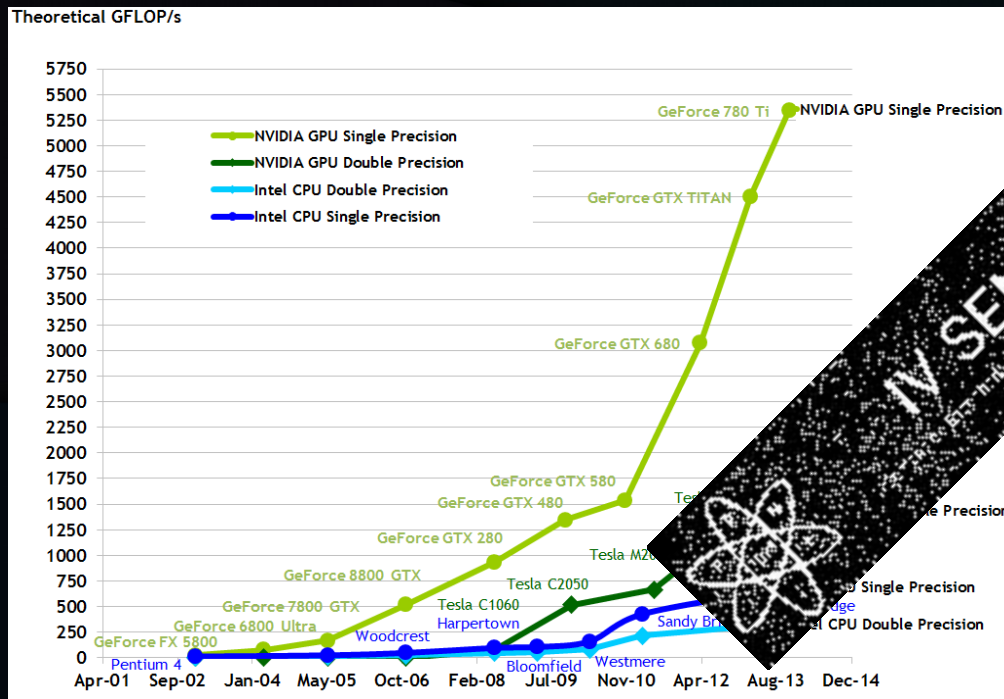
Golem → Masculino, 1.76 m 73 kg 1.9 Milhões de voxels (36.5 mm³)

Laura → Feminino, 1.63 m 60 kg 3.9 Milhões de voxels (15.2 mm³)



Computational phantoms: CPU x GPU

Capacidade de processamento de uma GPU tem se mostrado muito superior em relação à uma CPU nos últimos anos.



Common programming languages **CUDA**

(**NVIDIA-CUDA 2008**) and

standard libraries (**OpenCL**: www.khronos.org/opencv)

→ these are developing, and enabling processing in data-intensive problems many orders of magnitude faster than using conventional CPUs.

The recent of the OpenCL library for porting to popular statistical analysis packages reflects a future for algorithmic advances that are immediately available to the larger research community.

Convincente Link

Computational phantoms: CPU x GPU



Capacidade de processamento de uma GPU tem se mostrado superior em relação à uma CPU nos últimos anos.

Projeto em aberto para mestrado!!!

CUDA - GPU

2 x Graphics Card NVIDIA GeForce® GTX 1070
Core Clock 1620 MHz/ Base: 1620 MHz in OC Mode
Boost Clock 1594 MHz in Gaming Mode

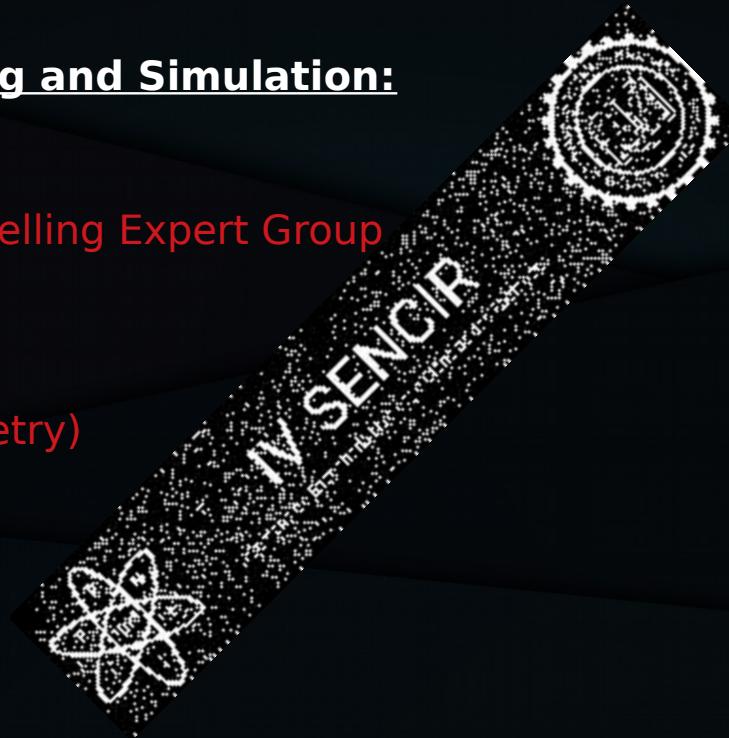
Architecture Turing
Process Technology 16 nm
Boost Clock 8008 MHz
Memory Size 8 GB
Memory Type GDDR5
Memory Bus 256 bit
Card Bus PCI-E 3.0 x 16

Implementar um GNA em C ou C++ & CUDA
Comparar tempo de processamento.

Criar um modelo de simulação simples utilizando um MC robusto e CUDA
Comparar resultados!

Applications

- Computational Modelling and Simulation:
- MCMEG – Monte Carlo Modelling Expert Group
- Internal dosimetry
- Radiotherapy (NanoDosimetry)
- Brachytherapy
- Neutron Dosimetry
- Mammography
- Radiologia Intervencionista



Application 1:

MCMEG - Monte Carlo Modelling Expert Group



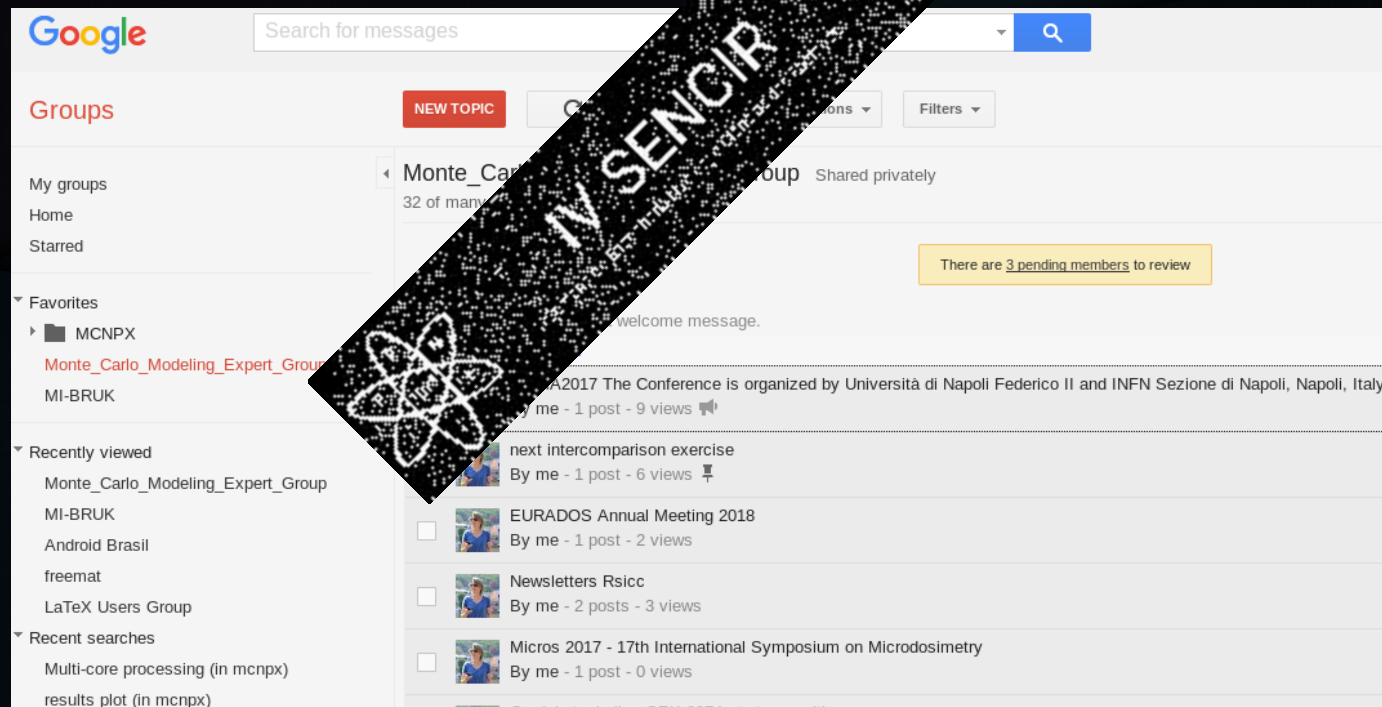
Application 1: MCMEG – Monte Carlo Modelling Expert Group

-> launched several computational inter-comparisons among different MC codes (MCNPX, GEANT4, PENELOPE, EGSnrc, VMC, etc...)

+52 Members, from different institutes around the world (Belgium, France, Germany, Italy, Mexico & Peru)

<https://groups.google.com/forum/#!forum/mcmeg>

Join Us!!



The screenshot displays the Google Groups interface for the 'Monte Carlo Modelling Expert Group'. The page includes a search bar at the top, a 'NEW TOPIC' button, and a list of group members and posts. A large, semi-transparent watermark for 'INSENCIR' is overlaid diagonally across the center of the screenshot.

Groups

Search for messages

NEW TOPIC

Monte Carlo Modelling Expert Group Shared privately

32 of many...

There are 3 pending members to review

welcome message.

2017 The Conference is organized by Università di Napoli Federico II and INFN Sezione di Napoli, Napoli, Italy.

By me - 1 post - 9 views

next intercomparison exercise

By me - 1 post - 6 views

EURADOS Annual Meeting 2018

By me - 1 post - 2 views

Newsletters Rsicc

By me - 2 posts - 3 views

Micros 2017 - 17th International Symposium on Microdosimetry

By me - 1 post - 0 views

Graduated controller GPC 2014 state monitoring

My groups

Home

Starred

Favorites

MCNPX

Monte Carlo Modeling Expert Group

MI-BRUK

Recently viewed

Monte Carlo Modeling Expert Group

MI-BRUK

Android Brasil

freemat

LaTeX Users Group

Recent searches

Multi-core processing (in mcnpX)

results plot (in mcnpX)

Application 1: MCMEG – Monte Carlo Modelling Expert Group

Responsáveis:

Profa. Dra. Telma C. Ferreira Fonseca (DEN/UFMG)

Dr. Bruno Mendes Melo (CDTN/CNEN)

Prof. Dr. Lucas Paixão Reis – Departamento De Anatomia e Fisiologia da Faculdade de Medicina da UFMG



The screenshot displays the MCMEG application interface. The top navigation bar includes the CNPq logo, the name of the institution (Universidade Federal de Minas Gerais), and the user name 'Telma / Lider'. The main content area is titled 'Dados do grupo' and contains a form for group identification. The form fields are as follows:

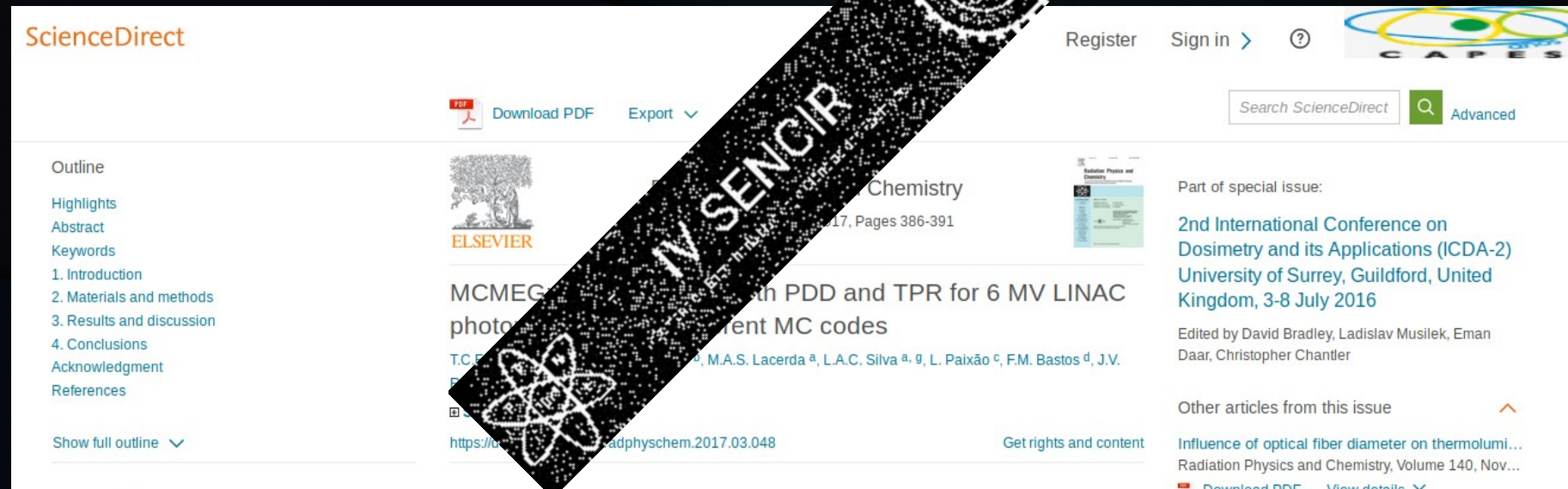
- Nome do grupo:** Monte Carlo Modeling Expert Group (MCMEG)
- Ano de criação:** 2016
- Instituição do grupo:** Universidade Federal de Minas Gerais
- Unidade:** Departamento de Engenharia Nuclear
- Grande área predominante:** Ciências Exatas e da Terra

A large, semi-transparent watermark with the text 'IV SENCIR' and a logo is overlaid diagonally across the center of the screenshot.

Application 1: MCMEG – Monte Carlo Modelling

Expert Group

First Intercomparison exercise launched in 2016 [4]



The screenshot shows a ScienceDirect article page. The article title is "MCMEG: Simulations of both PDD and TPR for 6 MV LINAC photon beam using different MC codes". The authors listed are T.C. Fonseca, B.M. Mendes, M.A.S. Lacerda, L.A.C. Silva, L. Paixão, F.M. Bastos, and J.V. Mendes. The article is from the journal "Radiation Physics and Chemistry", Volume 140, November 2017, Pages 386-391. The page includes a table of contents on the left, a search bar at the top right, and a section for "Part of special issue: 2nd International Conference on Dosimetry and its Applications (ICDA-2) University of Surrey, Guildford, United Kingdom, 3-8 July 2016".

[4] Fonseca TC, Mendes BM, Lacerda MA, Silva LA, Paixão L, Bastos FM, et al. MCMEG: Simulations of both PDD and TPR for 6MV LINAC photon beam using different MC codes. Radiat. Phys Chem 2017;140:386-391

Application 1: MCMEG – Monte Carlo Modelling Expert Group

Second Intercomparison exercise launched in 2017

MCMEG: Simulations of both PDD and TPR for 6 MV LINAC photon beam using different Monte Carlo codes.

Now, the second inter-comparison task the MCMEG is launching an exercise to assess the accuracy of Monte Carlo codes for organs at risk in physical and computational phantoms simulating a prostate cancer under a prostate cancer treatment plan for intensity modulated radiation therapy (IMRT).

Scope
This study will describe a comparative analysis of dose distribution for a prostate cancer phantom and its segmented CT images with prostate cancer treated with ionizing radiation. The intercomparison exercise will be done using IMRT. The IMRT plan will be used as protocol and the experimental process will be done at the Radiotherapy Department of the Hospital General de Garmy in BH/MG and the Monte Carlo codes used will be MCNP, EGSnrc, Geant4, and FLUKA.

The organs at risk will be assessed are the urinary bladder, rectum, sigmoid, and testis, as well as the volume of normal tissue. The following features will be compared to the simulation results: the mean dose in the target volume, the mean dose in the organs at risk, and organ volumes for each particular dose.

Best regards,
MCMEG team.

MCMEG: Intercomparison Exercise for Monte Carlo Codes in Radiotherapy Dose Assessment:

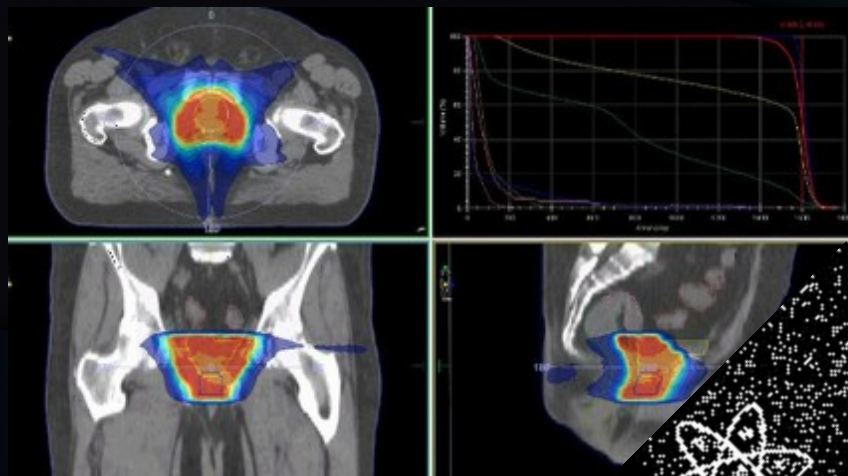
Presented at the ISRP-14 Participatory Workshop on Monte Carlo Simulation for Radiation Physics and Chemistry in Argentina in 2018.

Submission by December 15th of 2018 to the Journal of Radiation Physics and Chemistry

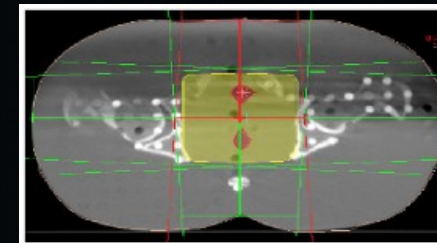
Application 1: MCMEG – Monte Carlo Modelling

Expert Group

Mestrado: Maria Angelina Mendes



Art Rando Phantom. Presents male pelvic phantom. Slice the prostate and organs at risk with details of position of cavities to insert the detectors. Positioning of three TLDs per hole.



The positioning of four fields on the CT slice of RANDO phantom using Xio Treatment Planning System and the dose distribution is shown in yellow

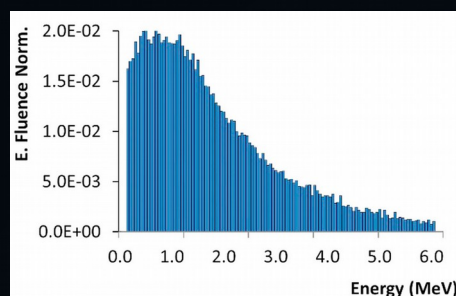
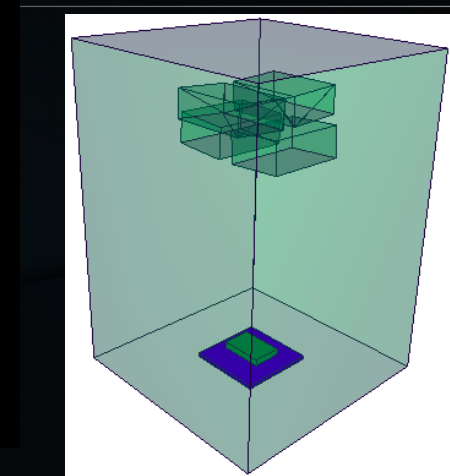
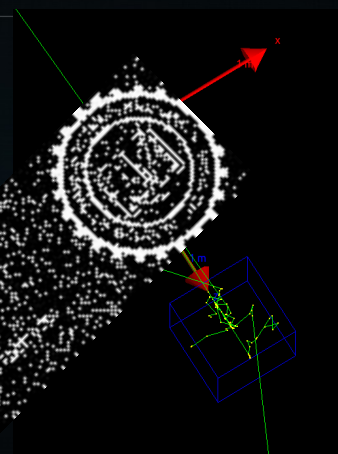
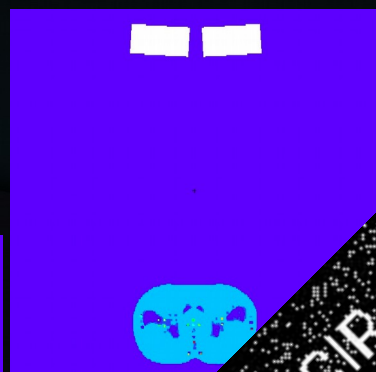
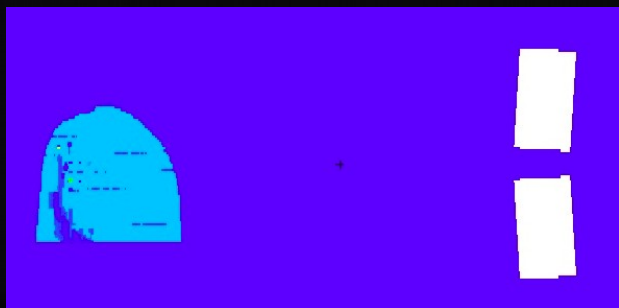
- A Comparison between Monte-Carlo Computations and Experimental Results Obtained With TLD Dosimetry for Art Rando Pelvic Phantom A Case Of Prostate Cancer And 3d- Conformal Radiation Therapy → CBFM 2018

- Processo de Preparo de um Sistema de Dosimetria para Análise da Dose Absorvida na Pelve De Um Simulador Antropomórfico Masculino → SENCIR4 2018

Application 1: MCMEG – Monte Carlo Modelling

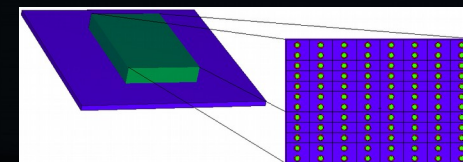
Expert Group

View plot on MCNPx
Alderson phantom + Jaws



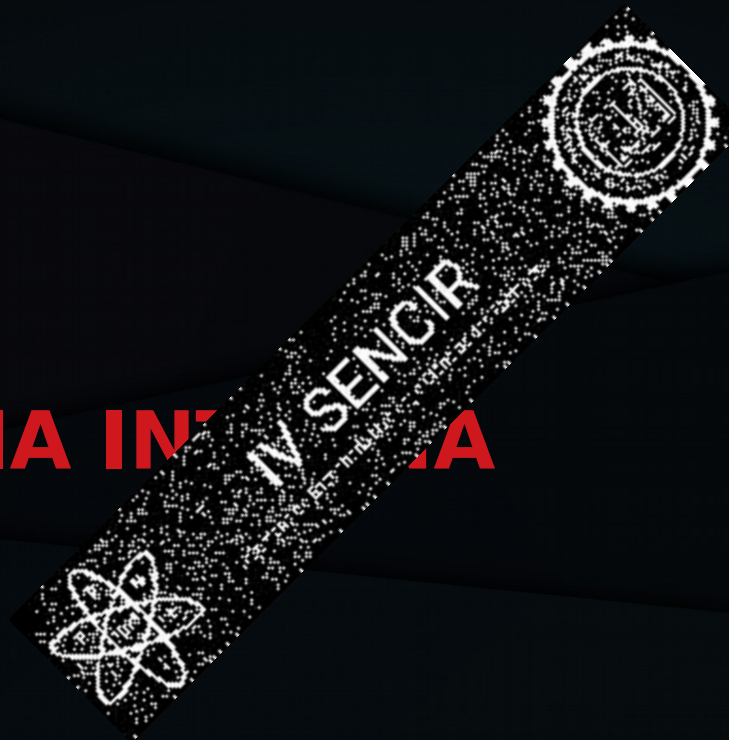
6MV Energy Spectrum

Calibration setup
View plot on TLDs + Jaws



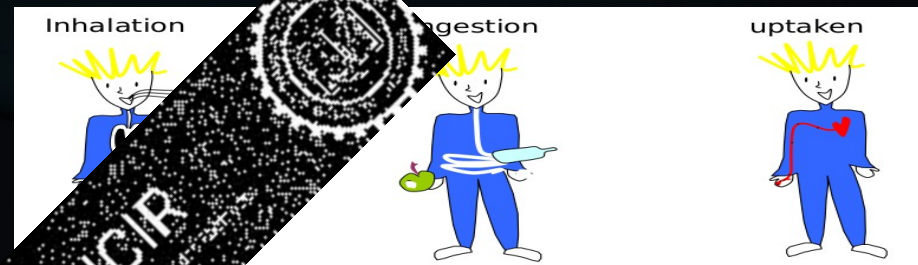
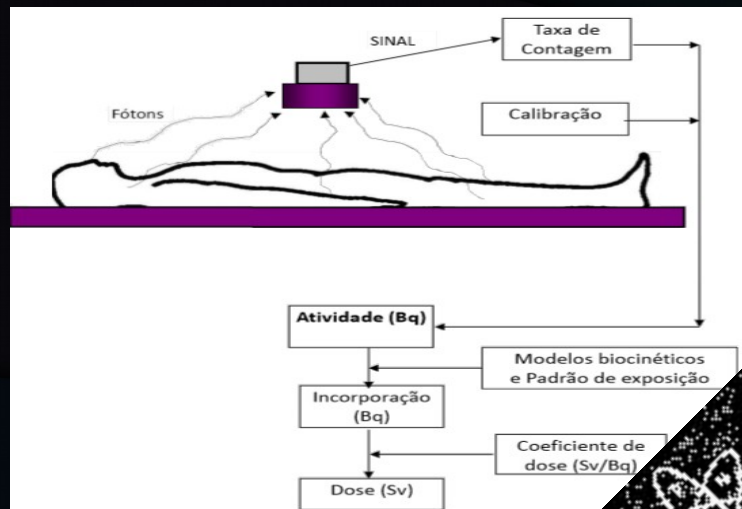
Application 2:

DOSIMETRIA INFANTIL



Application 2: Dosimetria Interna

Monitoração *In vivo* = monitoramento de trabalhadores que estão expostos a riscos de contaminação internos (IOEs).



dose interna → métodos de bioanálise *in vivo* e *in*

álise → modelos biocinéticos e dosimétricos = suposições

sobre o padrão de exposição:

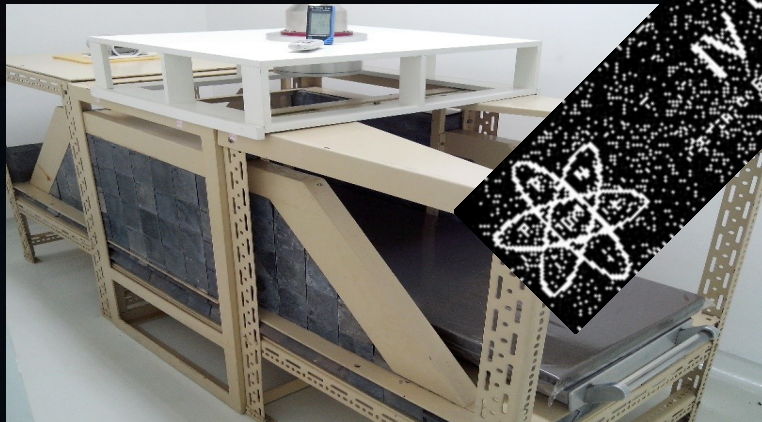
- incorporação única ou crônica
- via de incorporação (inalação, ingestão, injeção e absorção através da pele),
- forma química e o estado físico do material
- além das características aerodinâmicas, no caso de inalação de particulados e gases.

Application 2: **Dosimetria Interna**

Laboratório de Dosimetria Interna do CDTN

O sistema de medição direta de contaminação interna, faz parte de um sistema de espectrometria no qual os radionuclídeos no corpo humano pode ser detectados e sua atividade quantificada.

- Contador de Corpo Inteiro (CCI)
- Geometria para medição de crânio, tireoide, pulmão, etc.



CCI/LDI

Fonte: Acervo próprio

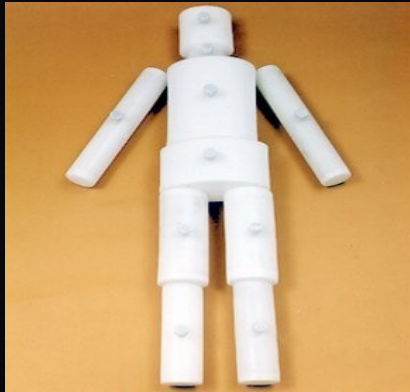


Geometria de Cabeça para ^{18}F -FDG

Monitoração de crânio

Application 2: **Dosimetria Interna**

Calibração: Simuladores físicos



Bottle Manikin Absorber (BOMAB) Phantom (Kramer, 1991).



Livermore Phantom et al., 1978).



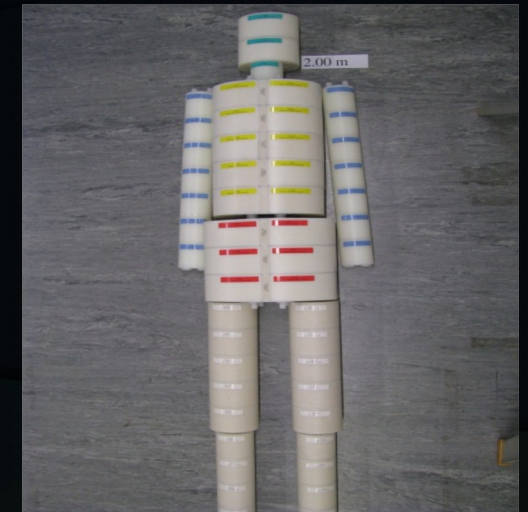
Japan Atomic Energy Research Institute - JAERI phantom.



Brain phantom for Fluorine-18 calibration -LDI/CDTN



Thyroid simulator
In vivo IRD/CNEN & LDI/CDTN



EMMA phantom
SCK-CEN, Mol Belgium (Lebacqz, 2011).

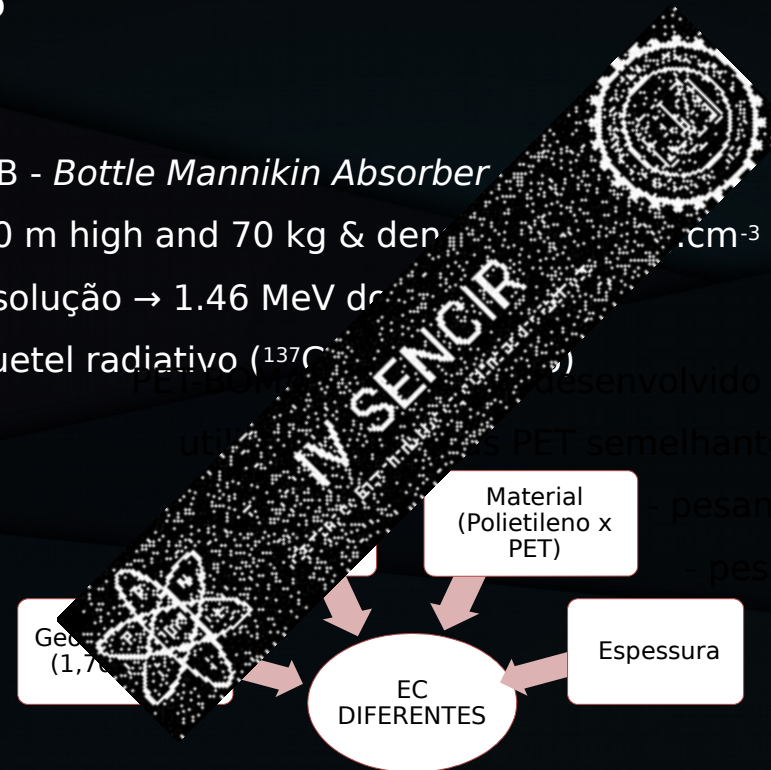
Application 2: Dosimetria Interna

Calibração CCI: 2015



BOMAB - *Bottle Mannikin Absorber*

- 1.70 m high and 70 kg & dens 1.03 g cm^{-3}
- KCl solução $\rightarrow 1.46 \text{ MeV dr}$
- coquetel radiativo (^{137}Cs)



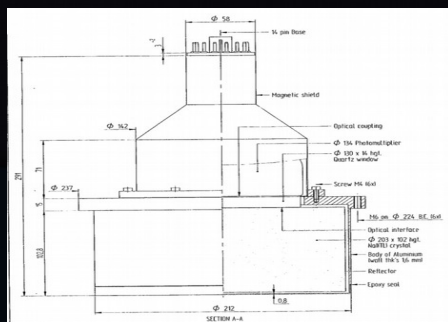
Paiva FG, Oliveira AH, Mendes BM, Pinto JR, Filho ND, Dantas BM, Dantas AL, Silva TA, Lacerda MA, Fonseca TC. Improvement of the WBC calibration of the Internal Dosimetry Laboratory of the CDTN/CNEN using the physical phantom BOMAB and MCNPX code. Appl Radiat Isot. 2016 Nov; 117:123-127. doi: 10.1016/j.apradiso.2015.12.059

Paiva, F. G., Fonseca, T. C. B., Mendes, B. M., Dantas, B., Dantas, A. L., Silva, T. A., Calibration of Whole Body Counter (WBC) of the LD/CNEN using two physical phantoms. Submitted to Physics and Chemistry, Agosto 2016.

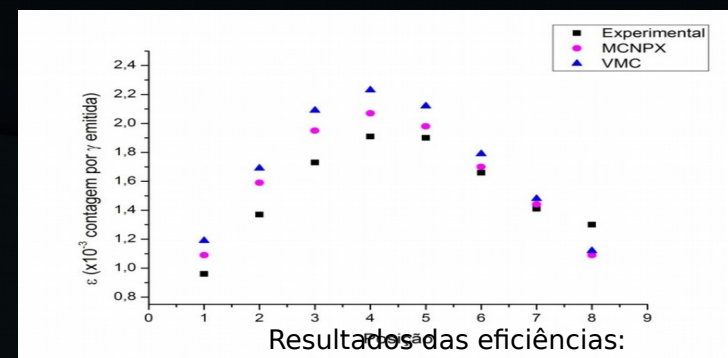
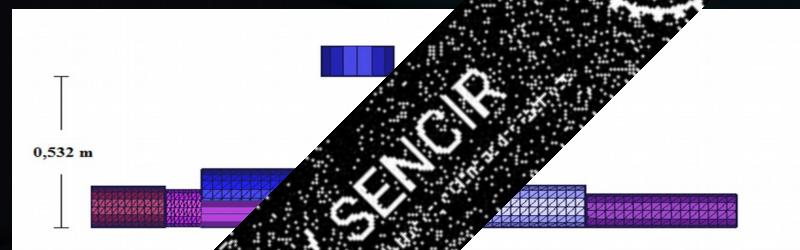
Application 2: Dosimetria Interna

Calibração CCI: WBC Virtual set-up

The physical WBC set-up was modeled and simulated using MCNP [Fonseca *et al*, 2015].



NaI(Tl) 8''x4'' Detector



Fonseca T. C. F.; Mendes M. B.; Paixão. L.; Bastos F. M.; J. A. Benavente, F. G. Paiva. Estudo comparativo entre simulações de um sistema de monitoração ocupacional interna utilizando diferentes códigos de Monte Carlo DOI: 10.15392/bjrs.v3i1.89 – Brazilian Journal of Radiation Sciences. 2015

Application 2: **Dosimetria Interna**

Calibração CCI: WBC Virtual set-up

Calibração do CCI com a biblioteca de fantomas: variação em altura e peso para população masculina e feminino.



[Conseca et al, 2014a,b]

Projeto em aberto para mestrado!!!

Application 2: Dosimetria Interna

Calibração Sistema: Monitoração de Crânio

Desenvolvimento de um fantoma físico de cérebro para dosimetria de trabalhadores sujeitos a incorporação de ^{18}F na produção do ^{18}F -FDG.

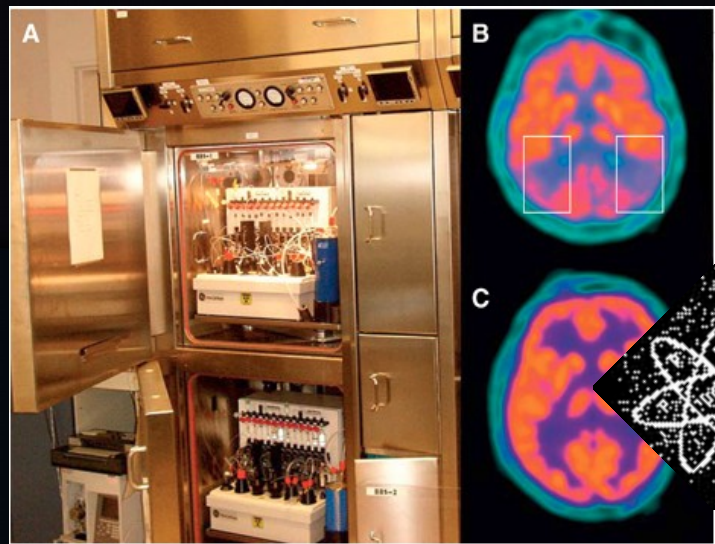
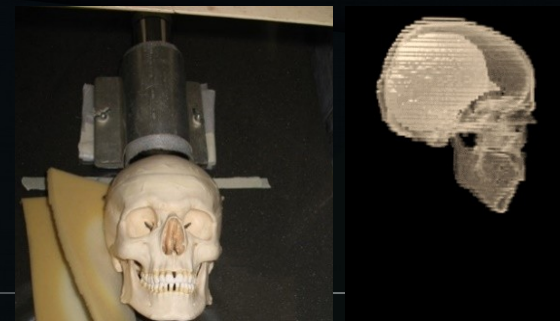


Imagem Molecular

Set-up monitoração



Biodistribuição do ^{18}F - FDG

Tabela 1: Dados Biocinéticos da ^{18}F -FDG

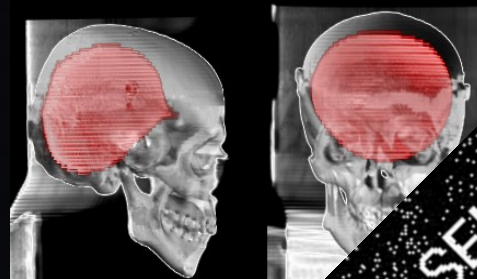
Residência	(h)	(s)	Normalizado	%
Bexiga	0.26	936	0.10446	10,4
Cérebro	0.21	756	0.08437	8,4
Coração	0.11	396	0.04419	4,4
Fígado	0.13	468	0.05223	5,2
Pulmão	0.079	284.4	0.03174	3,1
Outros	1.7	6120	0.68301	68,3
Total		8960.4	1.00000	

Application 2: Dosimetria Interna

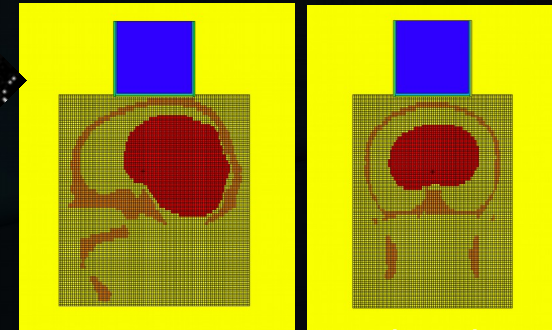
Calibração Sistema: Monitoração de Crânio



FC Ref. Masc



Imagens de



FC Computacional

Modelo	FC (Bq.CPS ⁻¹)
SiCab (experimental)	$\sim 2\%$ $34,0 \pm 0,7$
MV-SiCab (computacional)	$34,7 \pm 0,2$
RCP-AM (computacional)	$52,6 \pm 0,3$

MENDES, B. M.; FONSECA, T. C. F.; VITAL, K. D.; SILVA, T. A.; CAMPOS, T. P. R. MCNPx Computational Estimation of the Calibration Factor of an In Vivo Counter for 18F-FDG Activity Incorporated in the Brain. Applied Radiation and Isotopes, Jan. 2017

MENDES, B. M.; FONSECA, T. C. F.; Trindade B. M.; CAMPOS, T. P. R. Desenvolvimento e Validação de protocolos de Dosimetria Interna (PDI) baseados nos fantasmas voxelizados de referência do ICRP110. Brazilian Journal of Radiation Sciences, Vol5, N1 2017. 10.15392/bjrs.v5i1.243

Application 2: Dosimetria Interna



O processo de preenchimento do crânio com o material de ágar-ágar e ^{22}Na & ^{18}F



Fantoma computacional do ICRP
E a impressão 3D do modelo ICRP



BRAZILIAN JOURNAL
OF
RADIATION SCIENCES
05-01 (2017) 01-14



Desenvolvimento de protocolos de dosimetria interna empregando o código MCNPx e fantasmas voxelizados de referência da ICRP 110

B. M. Mendes^{1b}; T. C. F. Fonseca²; B. M. Trindade³; T. P. R. Campos³

¹ Seção de Dosimetria das Radiações – SECDOS, Centro de Desenvolvimento da Tecnologia Nuclear – CDTN/CNEN, 30.161-970, Belo Horizonte – MG, Brazil.

² Departamento de Engenharia Nuclear – DEN, Universidade Federal de Minas Gerais – UFMG,

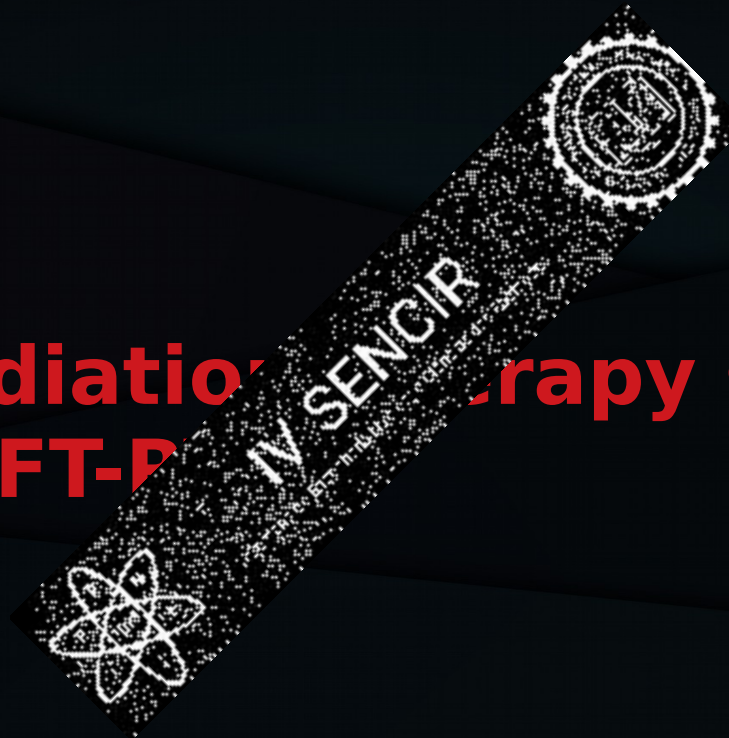
31270-901 Belo Horizonte - MG, Brazil

bmm@cdtn.br

KD Vital, BM Mendes, MA de Sousa Lacerda, TA da Silva, TCF Fonseca. Development of a physical head phantom using of a solid brain equivalent tissue for the calibration of the ^{18}F -FDG internal monitoring system. Radiation Physics and Chemistry 2018

Application 3:

Radiation Therapy software
SOFT-P

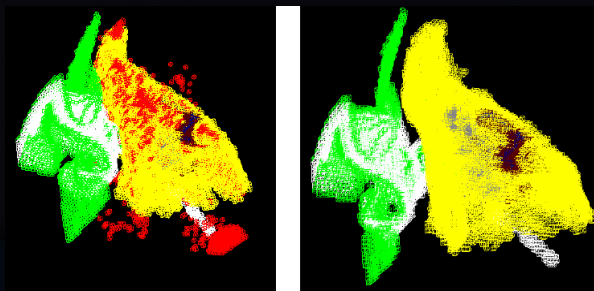


Application 3: SOFT-RT

SOFT-RT -> Sistema de simulação do protocolo IMRT

- C++ & OpenGL (*Open Graphics Library*) -> biblioteca (*Free Open Source*) de rotinas gráficas e de modelagem, para visualizações bi e tridimensionais

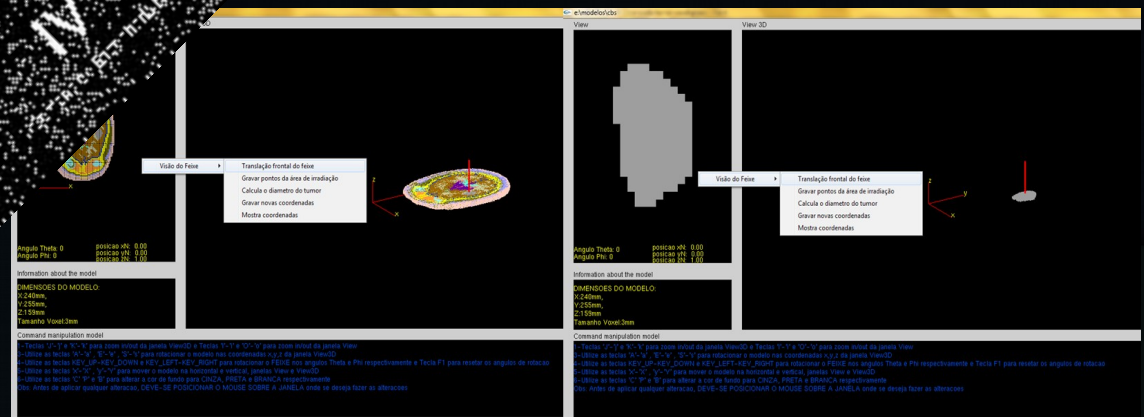
- Multiplataforma -> Windows & Linux OS



Modelo "Sistema-Auditivo"

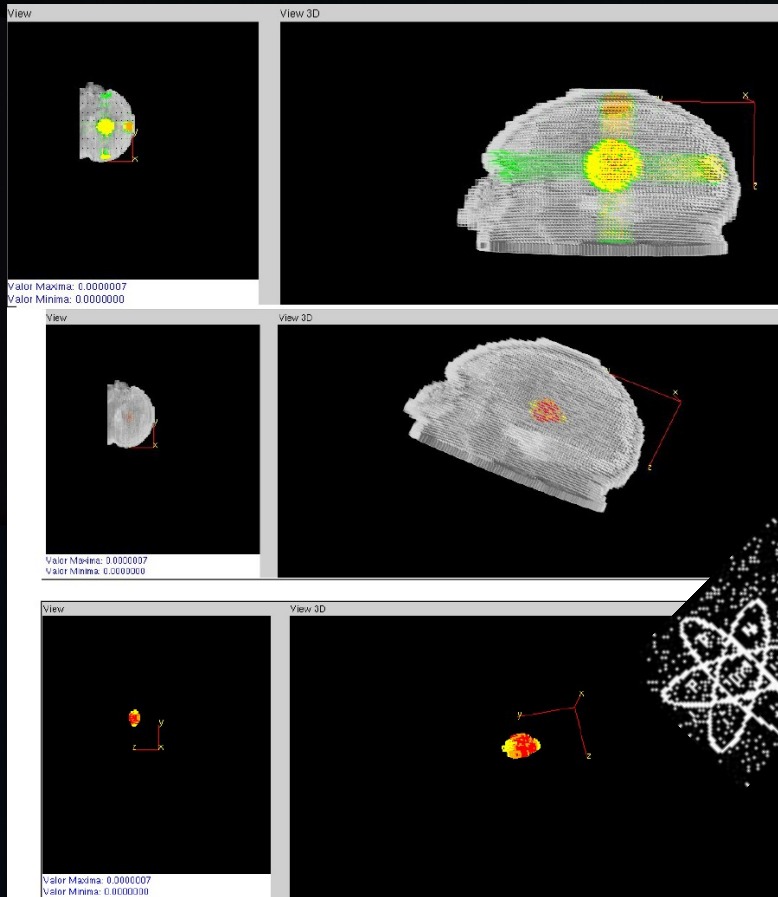


Modelo "Cabeça"



Tela principal – SOFT-RT

Application 3: SOFT-RT



Vermelhas - doses no intervalo de 80% a 100% da dose máxima

Amarelas - doses entre 50% a 80% da dose máxima

Verdes - doses entre 25% a 50%

Amarelo claro - doses entre 10% a 25%

Verde claro - doses entre 5% a 10%

Cinza - dose -> zero

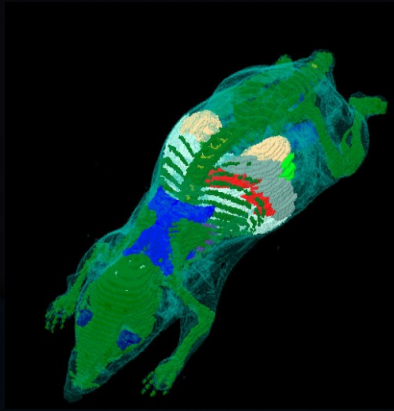
As cores de cinza foram definidas para os tecidos onde não foi solicitado o cálculo de dose.

Validação do SOFT-RT
Projeto em aberto para mestrado!!!

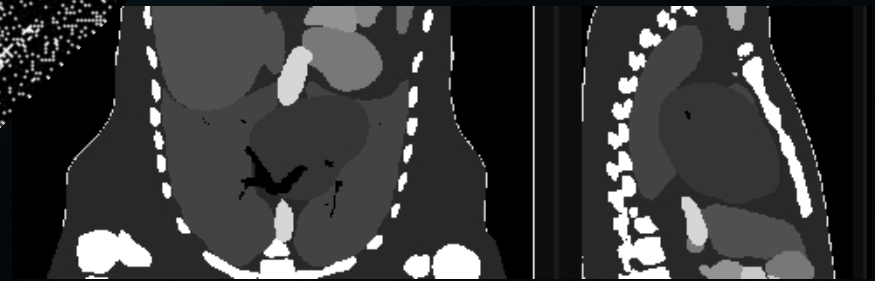
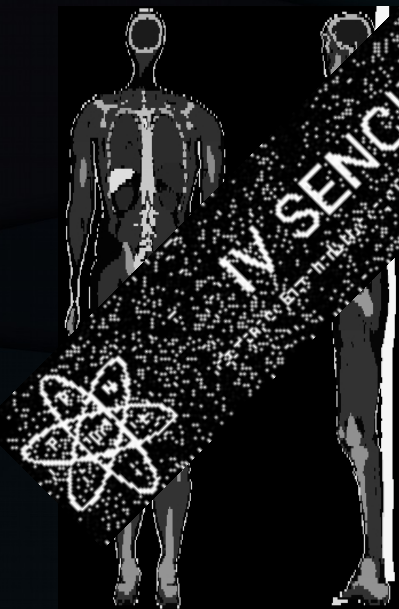
Application 4: EGSnrc

EGSnrc C++ class library (egspp) - Plugin IMAGEJ

A “in house” tool was developed to read the phantom binary file and write the voxel phantom structure according to egspp. Internal and external photon sources were considered and 4 voxel phantoms with different levels of complexity were taking into account: DM_BRA mouse phantom, Golem morphic phantom, and Case 5 XCAT model phantom from AAPM



3D view of DM_BRA mouse phantom (not all organs/tissues represented)



Coronal and sagittal views of Golem phantom

Prof. Dr. Lucas Paixão Reis – Departamento De Anatomia e Imagem – Faculdade de Medicina da UFMG

Accepted to be published as “Validation study of voxel phantom monte carlo simulations with EGSnrc C++ class library” to Braz. J. Rad. Sciences. In 2018

Application 5: Nano Dosimetria

Doutorado: Baljeet Seniwal

Modelagem e simulação computacional → Estruturas celulares em nível nanométricos

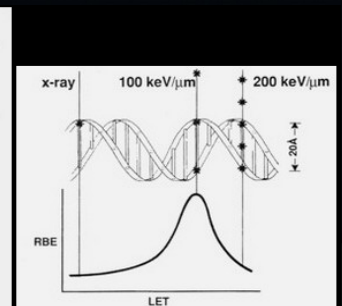
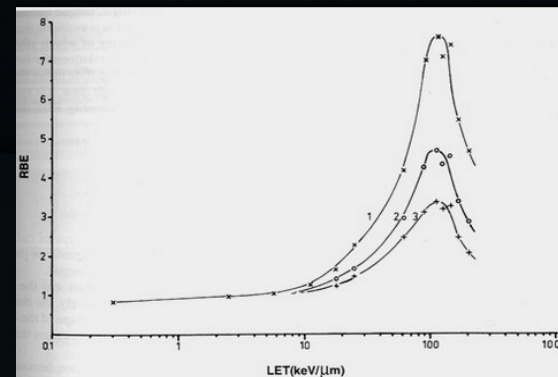
Estudo de caso:

Simulação celular para analisar como a densidade de ionização é alterada pela criação de fótons e elétrons secundários em AuNP (2-100nm), após interação com feixes de raios X, fótons de interesse clínico de 200 kV, Ir-192, Cs-137, 6 MV e Co-60.

Ouro metálico no citoplasma celular durante a radioterapia: interação de choque de absorção fotoelétrica no tecido alvo, o que contribui para o dano biológico letal. Emissão de elétrons Auger dentro do citoplasma.

Para a física médica, dentre os danos celulares causados pela radiação os mais importantes estão os relacionados à quebra da dupla hélice do DNA.

Principal objetivo: depositar uma quantidade de energia tal que haja a quebra dupla da fita de DNA para que não aconteça o reparo natural das células alvo (tumor).



**Maximum RBE
at 100KeV/uM**

RBE - Efetividade Biológica Relativa
LET - Transferência Linear de Energia

Application 5: Nano Dosimetria

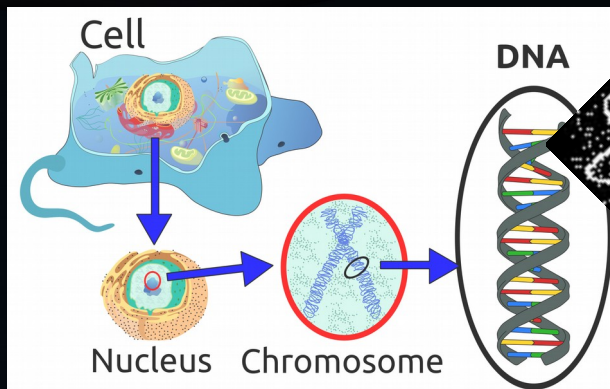
Implementar um código computacional para modelagem e simulação de estruturas celulares e/ou moleculares em nível nanométricos utilizando o código MC GEANT4 DNA Project.

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Soybeans as a Phytochemical Reservoir for the Production and Stabilization of Biocompatible Gold Nanoparticles

Ravi Shukla, Satish K. Nune, Nripen Chanda, Kavita Katti, Swapna Mekapothula, Rajesh R. Kulkarni, Wade V. Welshons, Raghuraman Kannan,* and Kattesh V. Katti*

DOSIMETRIA!!!



Laminin receptor specific therapeutic gold nanoparticles ($^{198}\text{AuNP-EGCg}$) show efficacy in treating prostate cancer

Ravi Shukla^a, Nripen Chanda^a, Ajit Zambre^a, Anandhi Upendran^{b,c}, Kavita Kattiⁱ, Rajesh R. Kulkarni^{a,d}, Satish Kumar Nune^a, Stan W. Casteel^e, Charles Jeffrey Smith^{a,f,g}, Jatin Vimal^h, Evan Boote^a, J. David Robertson^{d,g,i}, Para Kanⁱ, Hendrik Engelbrecht^g, Lisa D. Watkinson^{a,f}, Terry L. Carmack^{a,f}, John R. Lever^{a,f,j}, Cathy S. Cutler^{d,g,i,k}, Charles Caldwell^{k,l}, Raghuraman Kannan^{a,c,i}, and Kattesh V. Katti^{a,b,c,g,i}

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Feature Article

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nanoparticles in cancer therapy: therapeutic efficacy of AuNP nanoconstruct in prostate tumor-bearing mice

Ravi Shukla, PhD^a, Para Kan, MS^b, Lisa D. Watkinson, MS^c, Ravi Shukla, PhD^a, Terry L. Carmack, MS^e, Hendrik Engelbrecht, PhD^d, John R. Lever, PhD^c, Katti, BS^a, Genevieve M. Fent, DVM^c, Stan W. Casteel, DVM, PhD^c, Smith, PhD^{a,c,d}, William H. Miller, PhD^d, Silvia Jurisson, PhD^{b,c,e,f}, Evan Boote, PhD^a, J. David Robertson, PhD^{b,d,e,f}, Cathy Cutler, PhD^{b,d,e,f}, Marina Dobrovolskaia, PhD^g, Raghuraman Kannan, PhD^{a,h,*}, Kattesh V. Katti, PhD, DSc, FRSC^{a,d,h,*}

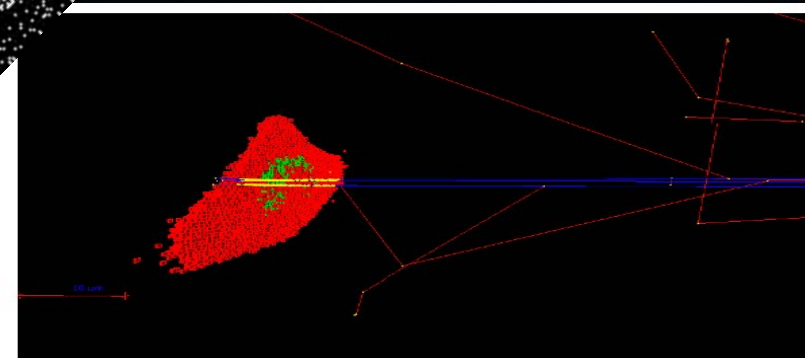
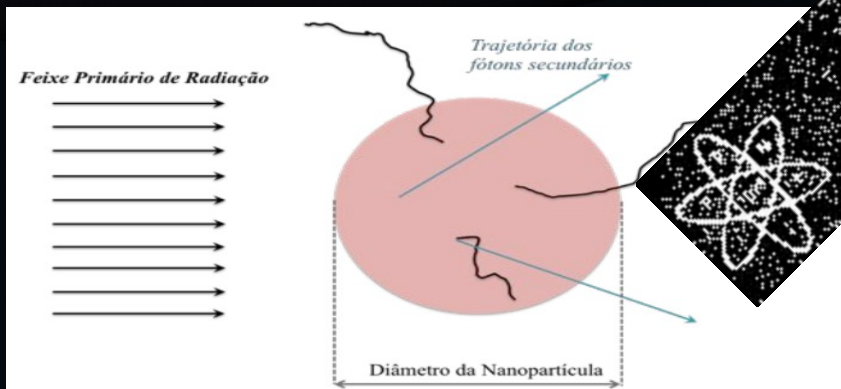
Prof. K. V. Katti, Prof. Dr. R. Kannan
Room 201, Alton Building Laboratories, 301, Business Loop 70W
University of Missouri-Columbia
Columbia, MO 65212 (USA)

Application 5: Nano Dosimetria

Geant4-DNA project:

The Geant4 general purpose particle-matter Monte Carlo simulations toolkit!

...modeling of early biological damage induced by radiation at the DNA scale.
Such developments are on-going in the framework of the Geant4-DNA project, originally initiated by the European Space Agency/ESTEC.
<http://geant4-dna.org>.



On-going developments include

- **Physics** processes in liquid water and other biological materials
- **Physico-chemistry** and **chemistry** processes for water radiolysis
- Molecular **geometries**
- Quantification of **damage** (such as single-strand, double-strand breaks, base oxidation...)

Application 5: Nano Dosimetria

O Geant4 « wholeNuclearDNA » extended/medical/dna

Extensão de modelos de física do Geant4 para a simulação de radiação em escala

Exemplo:

mostra como modelar um núcleo celular contendo um modelo de uma molécula de DNA.

Inputs:

Física eletromagnética (EM) na escala de baixa energia (eV^{\wedge})

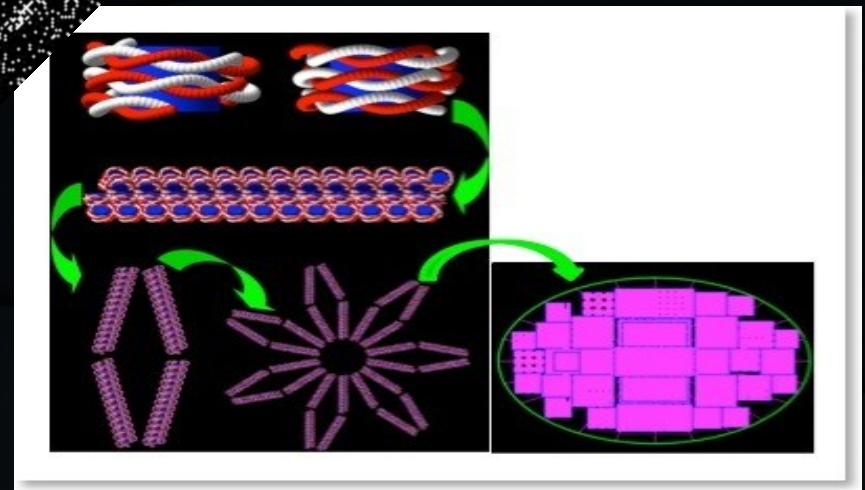
Processos Químicos (por exemplo Movimento Browniano)

- ✓ Criação de radicais livres que ajudam na quebra do DNA.

Outputs:

Deposição de energia local

Quantificação de danos do DNA



The Geant4-DNA Project

Application 5: Nano Dosimetria

Evolução em espaço e tempo do caminho percorrido por 1keV (elétron) em água líquida. Simulação: processo **Radiólise** é a dissociação das moléculas por radiação nuclear.

Primeiro: é gerado feixe de 1keV seguindo até os primeiros 100ns do estágio químico.

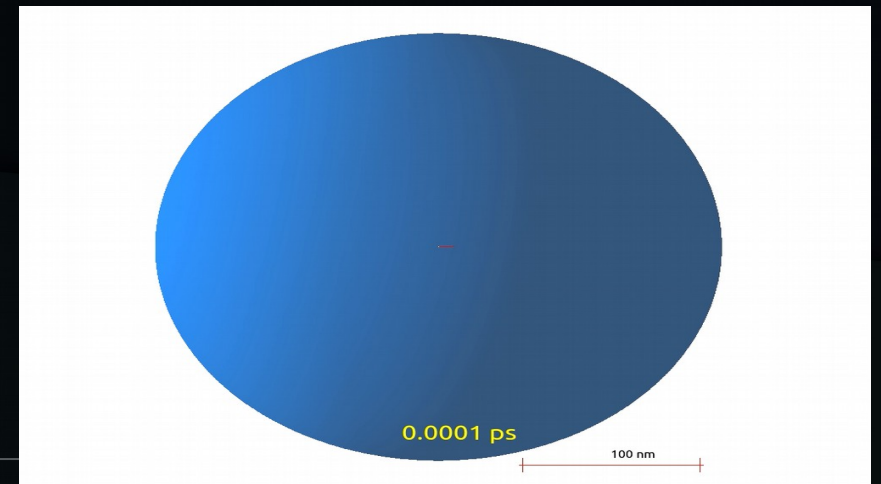
É possível perceber o estágio físico da ação da radiação modelado no pacote de física-DNA Geant4. A trilha percorrida de elétrons é totalmente freada e termalizada em uma esfera de 150 nm de água líquida. Os pontos amarelos correspondem a eventos de interação em

Em seguida, a simulação do estágio do efeito químico ocorrido para os primeiros 100ns é visualizado.

Reações entre diferentes espécies de radicais são mostradas em diferentes espaços e são mostrados em diferentes cores. Os pontos representam em diferentes espécies químicas.



[link](#)



The Geant4-DNA collaboration
Irradiation of a pBR322 plasmid, including radiolysis - courtesy of V. Stepan
(NPI-ASCR/CENBG/CNRS/IN2P3/ESA)

Geant4-DNA visualization: Evolution of 1 keV electron track in liquid water in space and time

Applications:

What else? FYI

