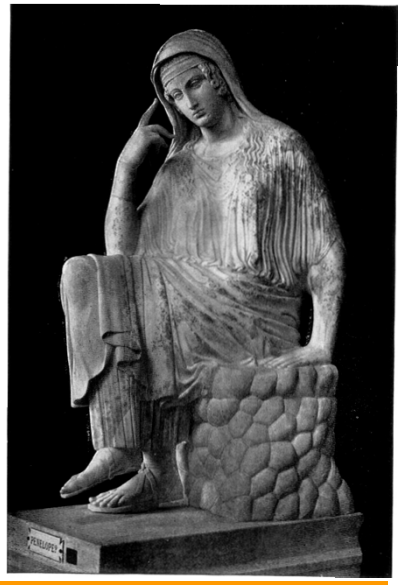
The PENELOPE/penEasy system

Structure, installation and operation

EUTEMPE-RX module 03

Monte Carlo simulation of x-ray imaging and dosimetry

Barcelona, June 2017



Statue of Penelope
in the Vatican
(source: Wikipedia)

What is PENELOPE?

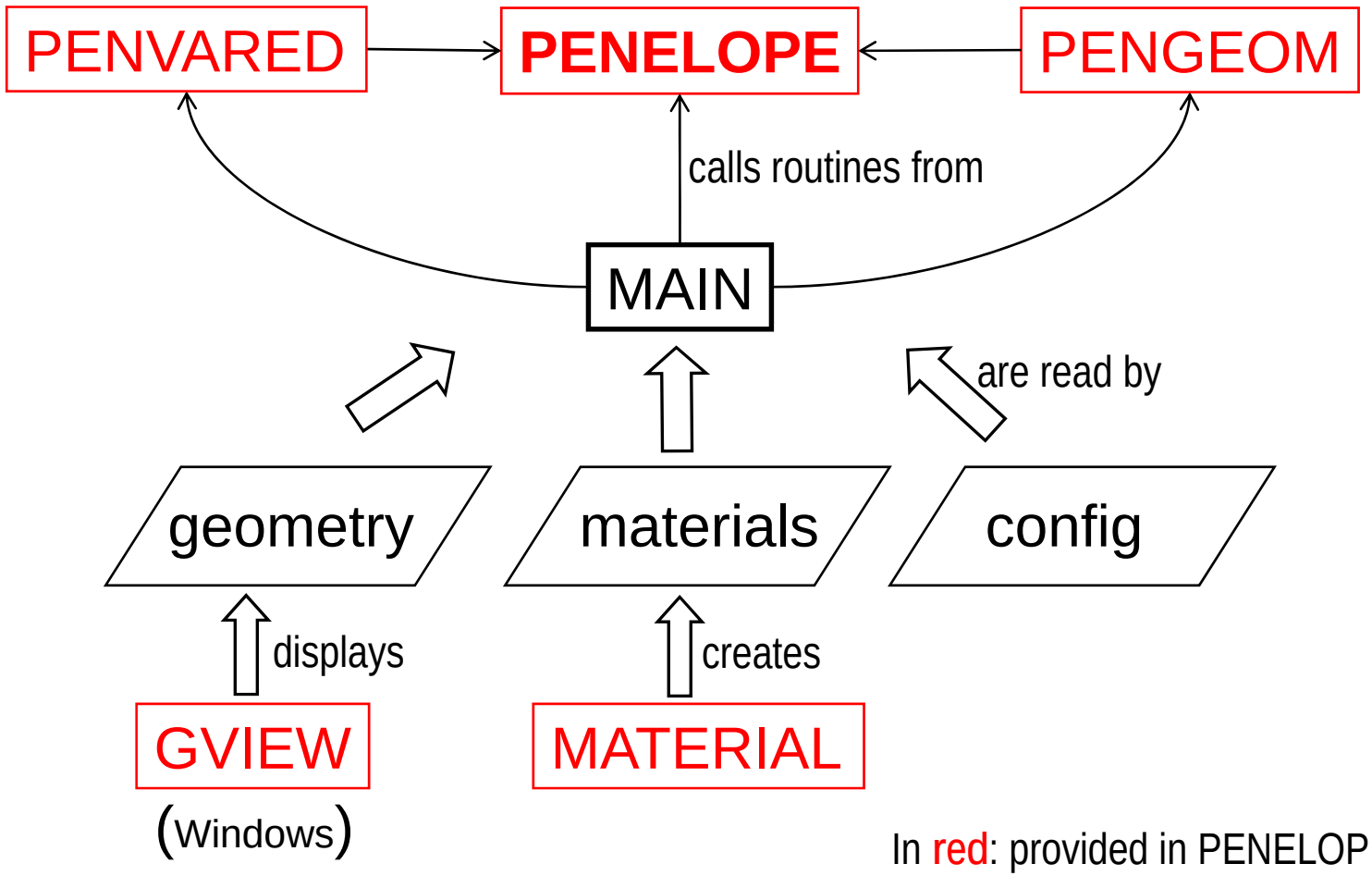
- Software package for the **Monte Carlo simulation of coupled γ-e$^{\pm}$ transport.**
- Capable of handling arbitrary material systems and **quadric geometries.**
- Works in the energy range $50\ \mathrm{eV} < E < 1\ \mathrm{GeV}$
- Includes auxiliary "tools" (geometry viewers, variance-reduction, EMFs).
- Subroutine package in Fortran.
- Developed by

  Francesc Salvat (Universitat de Barcelona)

  José M Fernández-Varea (Universitat de Barcelona)

  Josep Sempau (Universitat Politècnica de Catalunya)

Code structure



In red: provided in PENELOPE package
In black: provided by the user

What is penEasy?

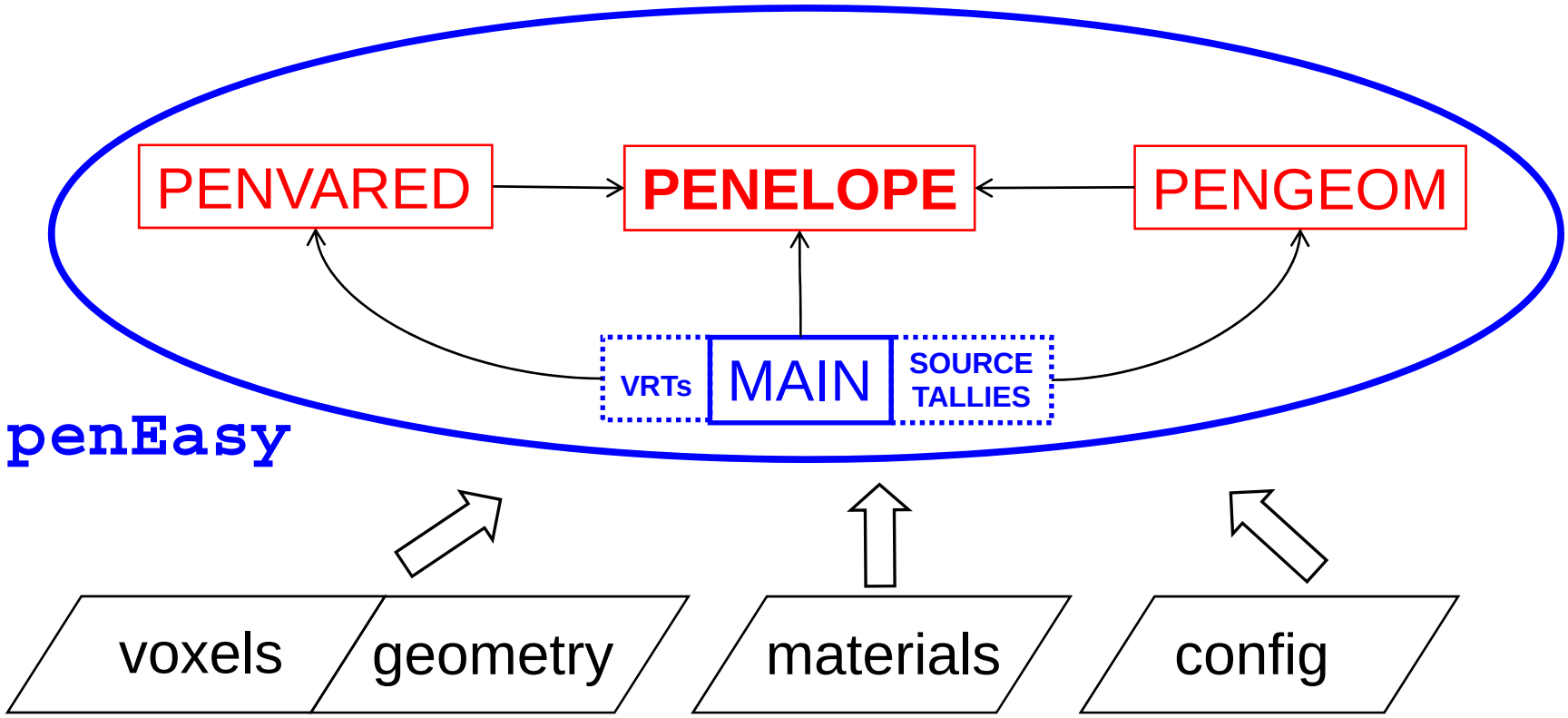
- A general-purpose **main program for PENELOPE.**
- It has two goals:

  1) To provide a set of ready-made **source models** and **tally schemes** applicable to a variety of practical situations. Users must provide a configuration data file, **no programming** is required.

  2) To supply a structured and modular code that, if needed, facilitates its adaptation by end users, reducing the programming effort to a minimum.

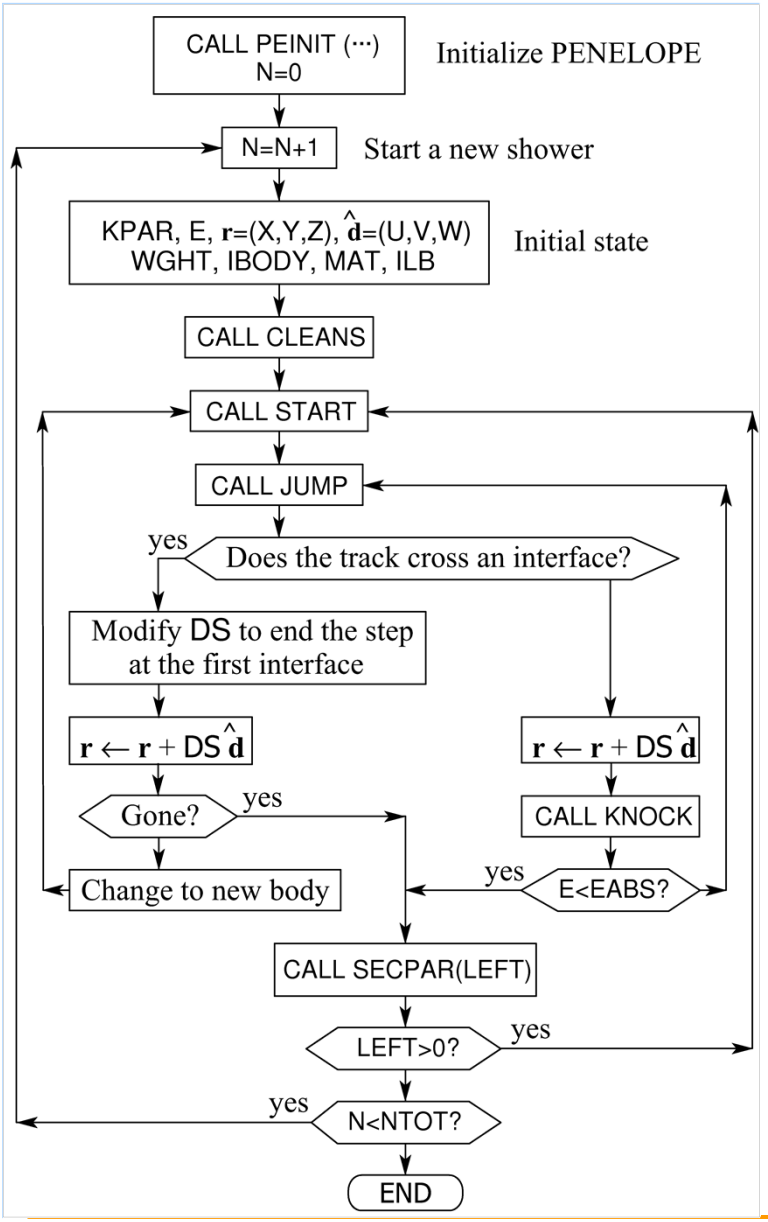
- Extends PENELOPE's **variance reduction** and introduces **voxelized geometries**
- penEasy, like PENELOPE, is written in Fortran.
- Developed by J Sempau (Universitat Politècnica de Catalunya).

Code structure



In blue: provided by penEasy

main program




```
program main
call init
n = 0
history: do
  n = n+1
  call CLEANS
  call source
  particle: do
    call SECPAR(left)
    if (left.eq.0) exit particle ! Empty
    call START
    interact: do
      call JUMP(dsmax(mat),ds)
      call STEP(ds,dsef,ncross)
      if (ncross.ne.0) then
        if (mat.eq.0) exit interact ! Gone
        call START
        cycle interact
      endif
      call KNOCK(de,icol)
      if (e.lt.eabs(kpar,mat)) exit interact
    enddo interact
  enddo particle
  if (n.ge.nhist) exit history ! Done
enddo history
end
```

MODULE TRACK_mod: E,X,Y,Z,U,V,W,WGHT,KPAR,IBODY,MAT,...

penEasy main

```
!*******************************************************
!*    MAIN
!*******************************************************
      program main
      implicit none
      integer*4 kpar,ibody,mat,ilb
      real*8 e,x,y,z,u,v,w,wght
      common/track/e,x,y,z,u,v,w,wght,kpar,ibody,mat,ilb(5)
      logical endsim,absorb,forcing,isforcing
      integer*4 ncross,icol,left
      real*8 n,ds,dsef,de,dsmax

      write(*,'(a)')
     & '>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>'
      write(*,'(a)')
     & '>>>> This is penEasy v.2008-06-15 >>>>'
      write(*,'(a)')
     & '>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>'
      call initime
      call init
      call treset
      n = 0.0d0
```

```
history: do
  n = n+1.0d0
  call noverflow(n)
  call cleans
  call tally(1,n)
  call source(n)

  particle: do
    call secpar(left)
    if (left.eq.0) exit particle
    call tally(-99,-e)
    if (absorb()) cycle particle
    call start

    interact: do
      if (absorb()) exit interact
      call jump(dsmax(),ds)
      call stepx(ds,dsef,ncross)
      if (ncross.eq.0) then
        call tally(3,ds)
      else
        call tally(4,dsef)
        if (mat.eq.0) exit interact
        call start
        cycle interact
      endif
      call knockx(de,icol)
      call tally(-icol,de)
    enddo interact
  enddo particle

  call tally(6,n)
  if (endsim(n)) exit history
enddo history
call report(n)
end
```

Example: tallyEnergyDeposition.F

```
subroutine EDPtally(mode,eloss)
use EDPmod
use TRACK_mod, only : mat,wght
use PENELOPE_mod, only : nmat
implicit none
integer mode
real*8 eloss
integer i

if (.not.active) return

if (mode.le.0.and.mat.gt.0) then        ! There's energy to be deposited
  edptmp(mat) = edptmp(mat)+eloss*wght ! Update temporary E counter
else if (mode.eq.6) then                ! End-of-history bookkeeping
  do i=1,nmat                           ! For all existing materials
    if (edptmp(i).eq.0.0) cycle         ! Skip void counters
    edep(i)   = edep(i) +edptmp(i)      ! Xfer counter to mean&variance
    edep2(i)  = edep2(i)+edptmp(i)**2
    edptmp(i) = 0.0                     ! Clear to start a fresh history
  enddo
endif
end
```

PENELOPE distribution

- PENELOPE is open and free software available through the OECD Nuclear Energy Agency, http://www.oecd-nea.org. (In North America http://www.ornl.gov).
- The NEA organises an annual course in Barcelona. There is a discussion forum at http://www.nea.fr/lists/penelope.html.
- References:

a) F. Salvat, *PENELOPE, A Code System for Monte Carlo Simulation of Electron and Photon Transport,* OECD Nuclear Energy Agency, Issy-les-Moulineaux, France, 2015.

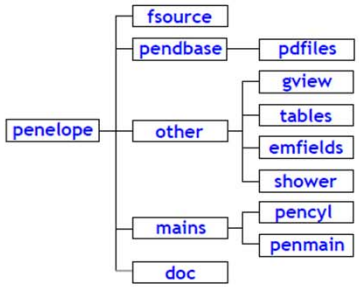
b) J. Sempau, E. Acosta, J. Baró, J. M. Fernández-Varea and F. Salvat, *An algorithm for Monte Carlo simulation of coupled electron-photon transport*, Nucl. Instrum. Meth. B 132 (1997) 377-390.

c) J. Baró, J. Sempau, J. M. Fernández-Varea and F. Salvat, *PENELOPE: An algorithm for Monte Carlo simulation of the penetration and energy loss of electrons and positrons in matter*, Nucl. Instr. and Meth. B 100 (1995) 31-46.

A short tutorial

Tutorial for PENELOPE (version 2014)

The distribution package has the following directory structure and contents:



\fsource Fortran source files of the PENELOPE code system:

penelope.f … Transport/physics simulation routines.

rita.f ... Routines for random sampling from single-variate distributions.

pengeom.f … Quadric geometry package.

penvared.f … Variance-reduction routines.

material.f … The main program for creating cross-section data files.

timer.f … Portable timing routines.

\pendbase Files necessary for creating material cross-section data files. The PENELOPE data-base of interaction cross-section data is contained in subdirectory **\pdfiles** (do not remove or alter any of the files in directory **\pdfiles**). The executable binaries **material.exe**, **tables.exe**, and **shower.exe** must be placed in directory **\pendbase**.

\other Additional software for quadric geometry visualisation (**\gview**), for displaying particle tracks on the screen of the computer (**\shower**), for generating and displaying tables of interaction cross sections and other transport properties (**\tables**), and a routine package for simulating radiation transport in static electromagnetic fields (**\emfields**).

\mains This directory contains two subdirectories with the steering main programs **pencyl** and **penmain**. Several **examples** are provided for each main program, with the corresponding sets of input, geometry, and material data files in separate subdirectories. Gnuplot scripts for visualisation of simulation results from the example main programs are also included in the subdirectories **\gscripts**.

\doc Documentation of the code system. It includes the following files:

tutorial.pdf … This file.

penelope-2014-NEA.pdf … Official release by the OECD Nuclear Energy Agency Data Bank of PENELOPE documentation, distributed together with version 2014. This is the reference to be used in any publication. Cite it as:

F. Salvat, "*PENELOPE–2014: A Code System for Monte Carlo Simulation of Electron and Photon Transport*" (OECD Nuclear Energy Agency, Issy-les-Moulineaux, France, 2015).

Have this document at hand in the initial stages when using PENELOPE.

The manual

Data Bank
NEA/NSC/DOC(2015)3
www.oecd-nea.org

PENELOPE-2014: A Code System for Monte Carlo Simulation of Electron and Photon Transport

Workshop
Barcelona, Spain
29 June-3 July 2015

Freely available at http://www.nea.fr

OECD
BETTER POLICIES FOR BETTER LIVES

NEA
NUCLEAR ENERGY AGENCY

penEasy distribution

- penEasy is open and free software available from
  http://www.upc.es/inte/downloads/penEasy.htm

- The Spanish Medical Physics Society (http://www.sefm.es) organises a biennial course in Barcelona (in Spanish).

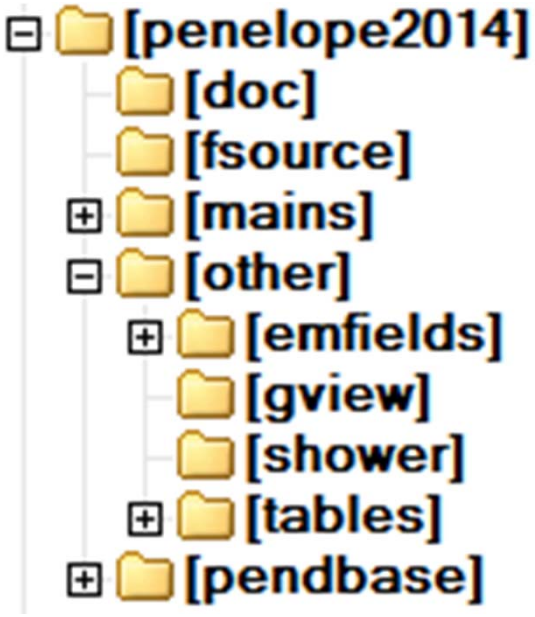
- Reference:

  J. Sempau, A. Badal and L. Brualla, A PENELOPE-based system for the automated Monte Carlo simulation of clinacs and voxelized geometries--application to far-from-axis fields, Med. Phys 38 (2011) 5887-5895.

- Documentation is available as text files in the distribution package.

PENELOPE installation

Step 1: unzip the package



Manual & Tutorial

Fortran code

Main programs: PENCYL & PENMAIN

Fortran routines for transport in EM fields

Geometry viewers and geometry examples

Program to display particle tracks in a slab

Program to display cross sections

Database to build material files

Step 2: compile

(A Unix/Linux system is assumed here)

- Compile **MATERIAL**

```
$ cd ~/penelope/fsource
$ gfortran material.f -o material.exe -O (=Optimize)
$ mv (move) material.exe ../pendbase/.
```

- Compile **TABLES**

```
$ cd ~/penelope/other/tables
$ cp (copy) ../../fsource/penelope.f .(in current dir)
$ gfortran tables.f -o tables.exe -O
$ rm (remove) penelope.f
```

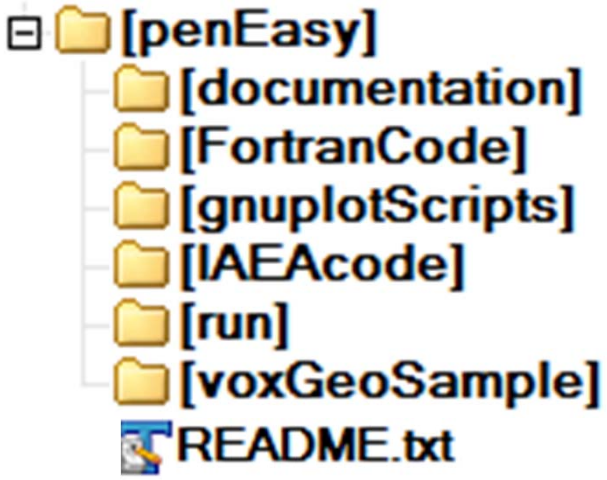
- Move **SHOWER**

```
$ cd ~/penelope/other/shower
$ mv (move) shower.exe ../../pendbase/.
```

(note that **shower.exe** runs under Windows only)

penEasy installation

The only step: unzip the package



Documentation for source models and tallies

Fortran code

Scripts to display simulation results

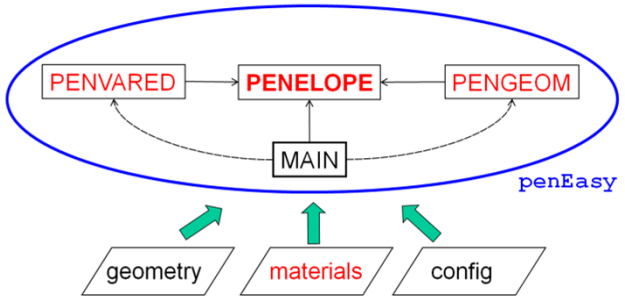
IAEA PSF format (see *https://www-nds.iaea.org/phsp)*

EXE for Windows systems & config file example

Example of voxelized geometry

Brief user's manual

How to run a job



The following files must be present in the working directory:

x.GEO : The (quadrics) geometry file

x.MAT : Material data files, one for each material

penEasy.IN : Configuration file (source, tallies, VRTs and transport parameters)

penEasy.EXE : The simulation program (Windows system assumed)

To run the code execute the following command:

```
penEasy.exe < penEasy.in > penEasy.out 2> zz.err
```

Read input from config file

Write output to file

Write system errors to file

Geometry file .GEO (quadrics)

Edited by user

```
c >>>> Anode >>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>
c
0000000000000000000000000000000000000000000000000000000000000000000000000
SURFACE (   1)
INDICES=( 0, 0, 0, 1, 0)
0000000000000000000000000000000000000000000000000000000000000000000000000
SURFACE (   2)
INDICES=( 0, 0, 0, 1, 0)
Z-SHIFT=(-0.20                    ,   0)
0000000000000000000000000000000000000000000000000000000000000000000000000
SURFACE (   3)
INDICES=( 1, 1, 0, 0,-1)
X-SCALE=(+10.0                    ,   0)
Y-SCALE=(+10.0                    ,   0)
0000000000000000000000000000000000000000000000000000000000000000000000000
BODY    (   1)  Anode base cylinder
MATERIAL(   1)
SURFACE (   2), SIDE POINTER=(+1)
SURFACE (   1), SIDE POINTER=(-1)
SURFACE (   3), SIDE POINTER=(-1)
```

Geometry file .VOX (voxels)

Edited by user or computer-generated

```
[SECTION VOXELS HEADER v.2008-04-13]
 500   320   260          No. OF VOXELS IN X,Y,Z
 0.1   0.1   0.1          VOXEL SIZE (cm) ALONG X,Y,Z
 1                        COLUMN NUMBER WHERE MATERIAL ID IS LOCATED
 2                        COLUMN NUMBER WHERE THE MASS DENSITY IS LOCATED
 1                        BLANK LINES AT END OF X,Y-CYCLES (1=YES,0=NO)
[END OF VXH SECTION]
#
# Slice k=1
# y index=1
1 1.205E-03
1 1.205E-03
1 1.205E-03
1 1.205E-03
1 1.205E-03
1 1.205E-03
1 1.205E-03
1 1.205E-03
1 1.205E-03
1 1.205E-03
1 1.205E-03
```

Material data file .MAT

Generated by program MATERIAL

```
PENELOPE (v. 2014)  Material data file ..............
Material: TUNGSTEN  (74)
Mass density = 1.93000000E+01 g/cm**3
Number of elements in the molecule =  1
  atomic number = 74,  atoms/molecule = 1.00000000E+00
Mean excitation energy = 7.27000000E+02 eV
Number of oscillators = 19 (E/P inelastic model)
  1  6.00000000E+00  0.00000000E+00  2.28694232E+01   0  30
  2  1.40000000E+01  3.68571429E+01  7.63536287E+01  74  30
  3  4.00000000E+00  4.10000000E+01  8.32699456E+01  74  30
  4  2.00000000E+00  5.10000000E+01  1.02397800E+02  74  30
  5  2.00000000E+00  8.00000000E+01  1.60094699E+02  74  30
  6  6.00000000E+00  2.48000000E+02  4.95518981E+02  74  14
  7  4.00000000E+00  2.61000000E+02  5.21346345E+02  74  13
  8  4.00000000E+00  4.28000000E+02  8.54698448E+02  74  12
  9  2.00000000E+00  4.95000000E+02  9.88396214E+02  74  11
 10  2.00000000E+00  5.99000000E+02  1.19603670E+03  74  10
 11  6.00000000E+00  1.81100000E+03  3.61596551E+03  74   9
 12  4.00000000E+00  1.87400000E+03  3.74173676E+03  74   8
 13  4.00000000E+00  2.28300000E+03  4.55835747E+03  74   7
```

Do NOT edit this file!

Configuration file .IN

Edited by user

```
# >>>> CONFIG FILE FOR penEasy >>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>
#
# CASE DESCRIPTION:
#   X-ray tube simulation.
#
# LAST UPDATE:
#   2015-02-17 by JS

[SECTION CONFIG v.2006-08-01]

[SECTION SOURCE BOX ISOTROPIC GAUSS SPECTRUM v.2006-08-01]

[SECTION SOURCE PHASE SPACE FILE v.2008-06-01]

[SECTION PENGEOM+PENVOX v.2008-06-01]

[SECTION PENELOPE v.2008-02-20]

[SECTION TALLY SPATIAL DOSE DISTRIB v.2006-08-01]
...

[SECTION INTERACTION FORCING v.2008-05-15]
...
```

Developments based on PENELOPE/penEasy

clonEasy + seedsMLCG

A Badal & J Sempau, Comput. Phys. Commun. 175 (2006)

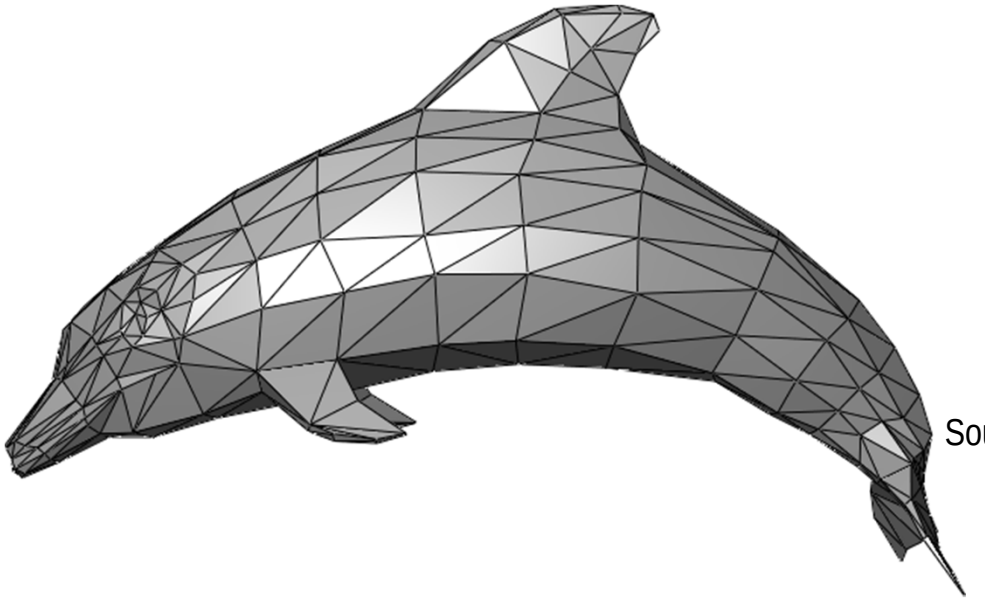
- clonEasy: Linux scripts package for **parallelization** of MC simulations
  Requirements to become a clone: IP + ssh + Fortran

- seedsMLCG: generates **non-overlapping sequences of random numbers** using an MLCG, for parallel execution

- Open source and free:
  http://www.upc.es/inte/downloads/clonEasy.htm
  http://www.upc.es/inte/downloads/seedsMLCG.htm

penMesh

Simulates **triangle mesh geometries** (*e.g.*, from CAD programs) with penEasy.



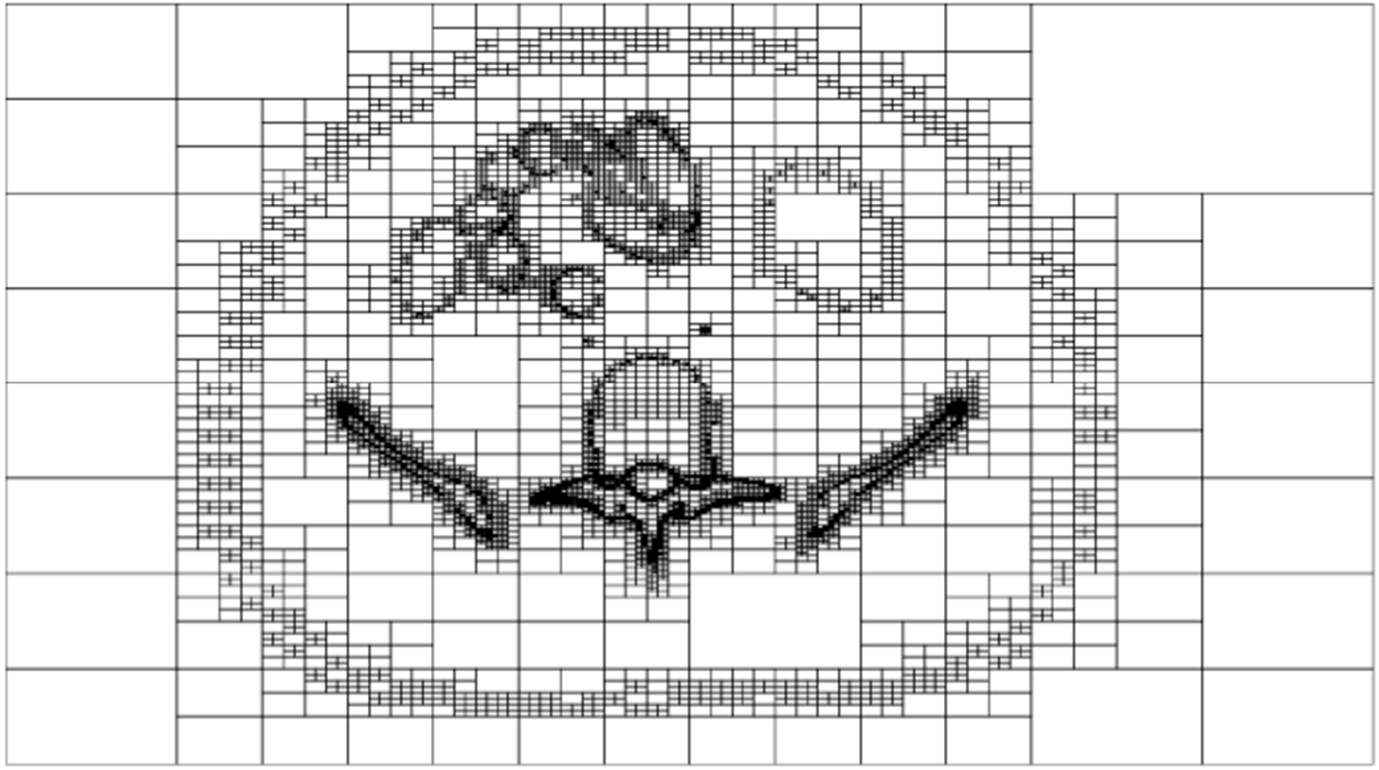
Source: Wikipedia

Developed by Andreu Badal and Iacovos Kyprianou (U.S. Food & Drug Admin.)

A Badal *et al.*, *penMesh -- Monte Carlo Radiation Transport Simulation in a Triangle Mesh Geometry,* IEEE Trans. Med. Imag. 28 (2009) 1894-1901

Open source and free: **https://code.google.com/p/penmesh**

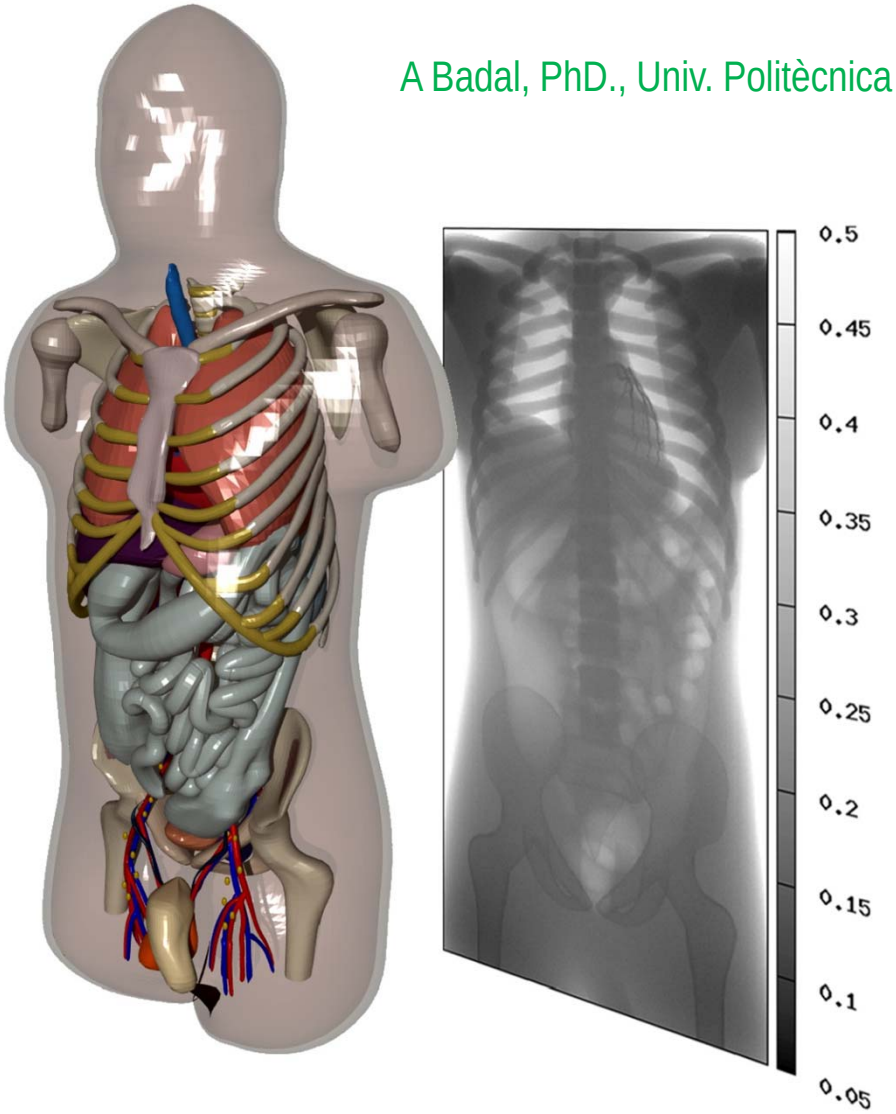
Deals with **highly complex objects** by having recourse to an **octree structure**



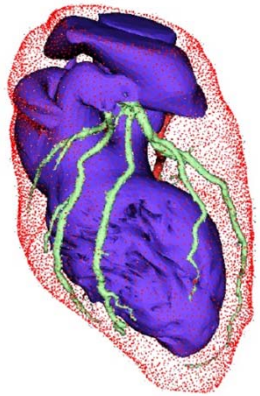
A Badal *et al*., Radiotherapy and Oncology 86

Coded in C++ to be linked with PENELOPE/penEasy's Fortran

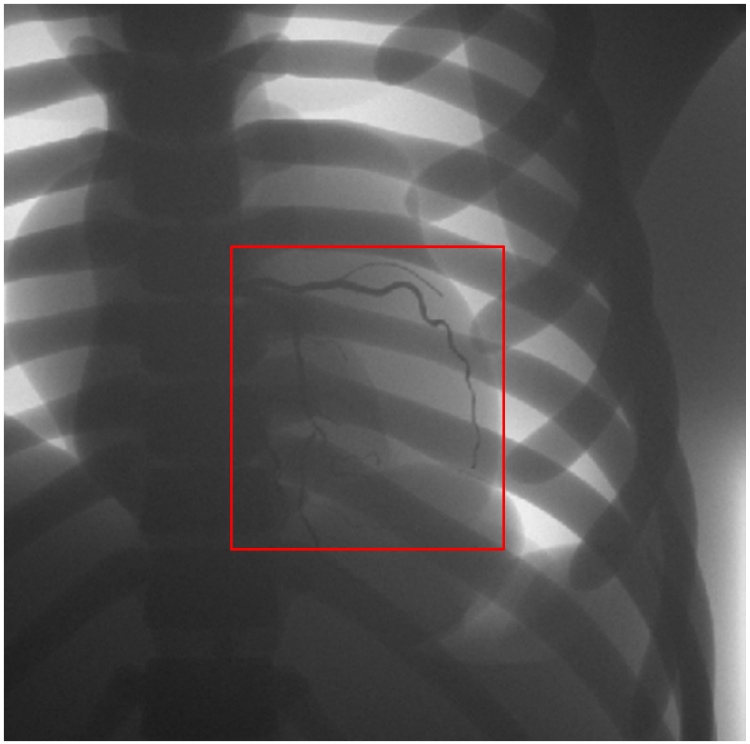
A Badal, PhD., Univ. Politècnica Catalunya 2008



High-resolution tessellated version of the NCAT phantom (W. P. Segars, Ph.D., Univ. North Carolina 2001). 330 closed triangle meshes, with over 5 million triangles were defined.



Triangle-mesh based heart model



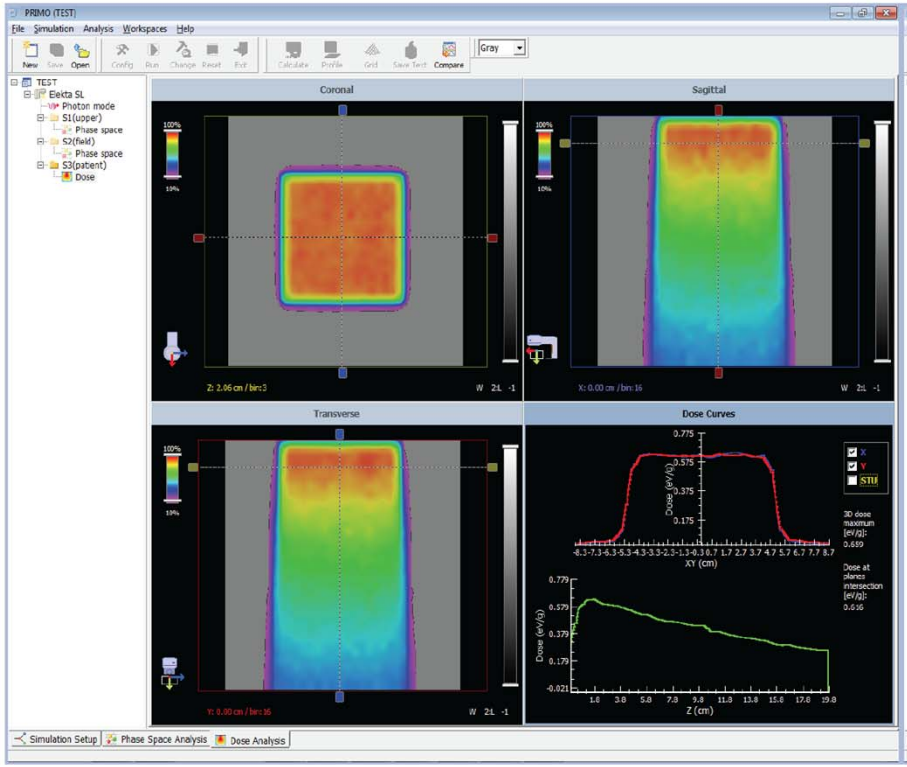
Simulated coronary angiography image at 60 kVp with iodine contrast

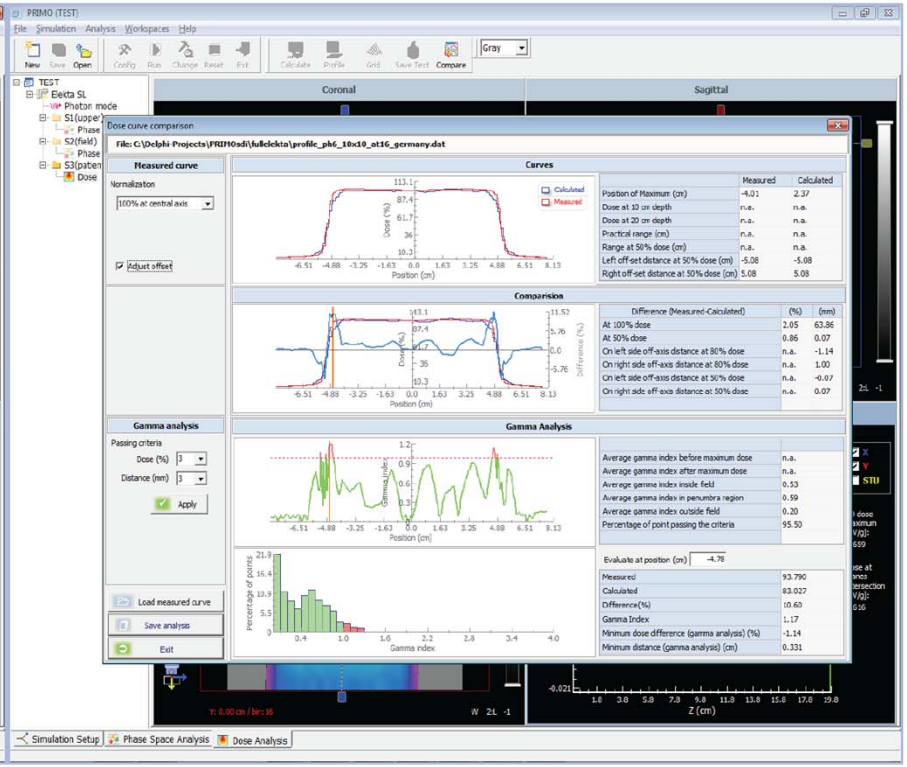
PRIMO

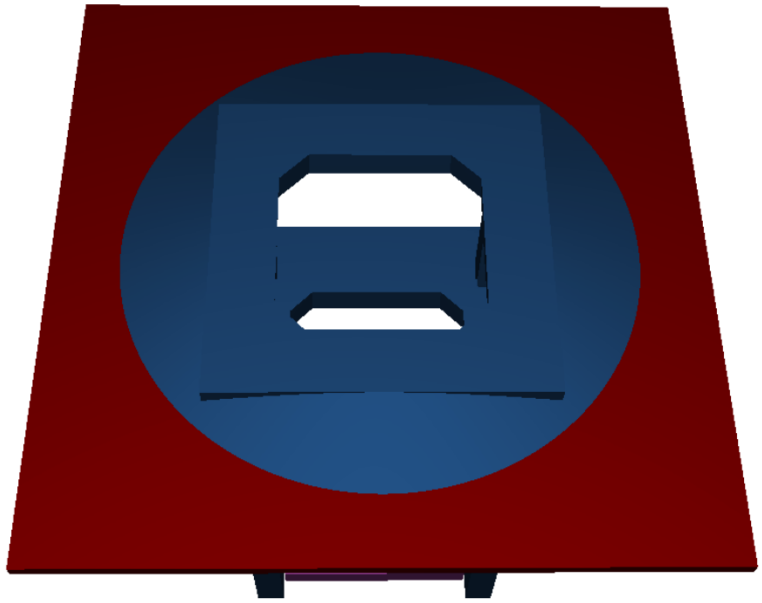
Simulation of Varian and Elekta linacs and patient/phantom dose distributions.

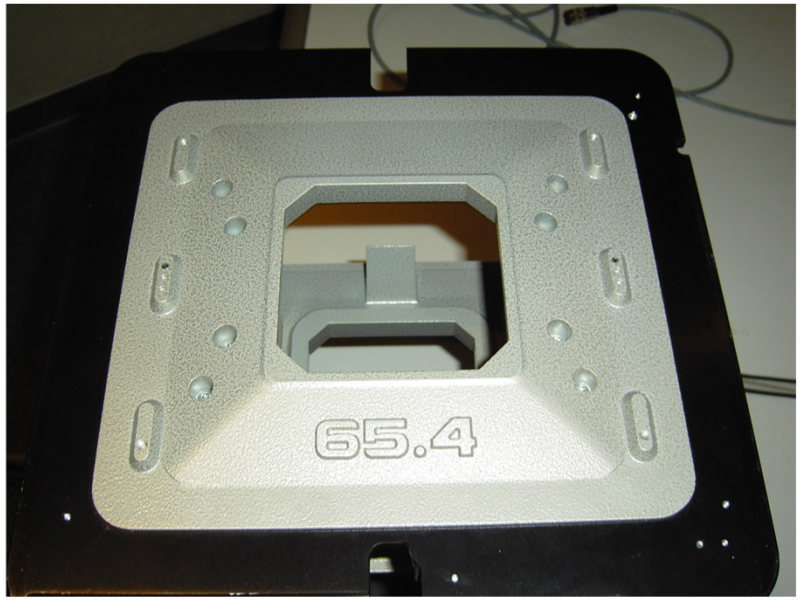
PRIMO

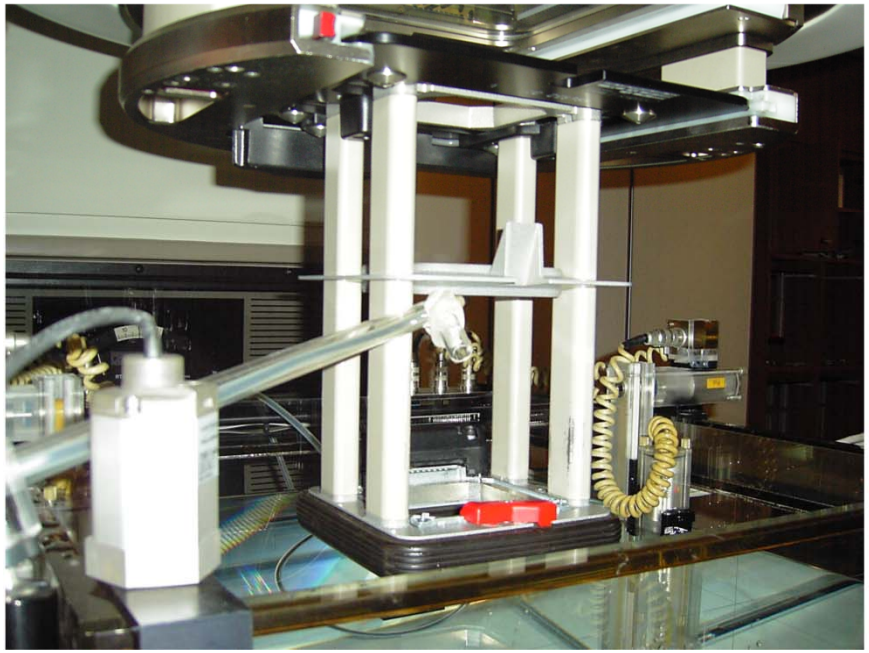
Linac-GLASS		Graphical user interface
penEasyLinac		Input files preparation for linacs
penEasy		MAIN: sources+tallies+VRTs
PENGEOM	penVox	Geometry
PENELOPE		Physics

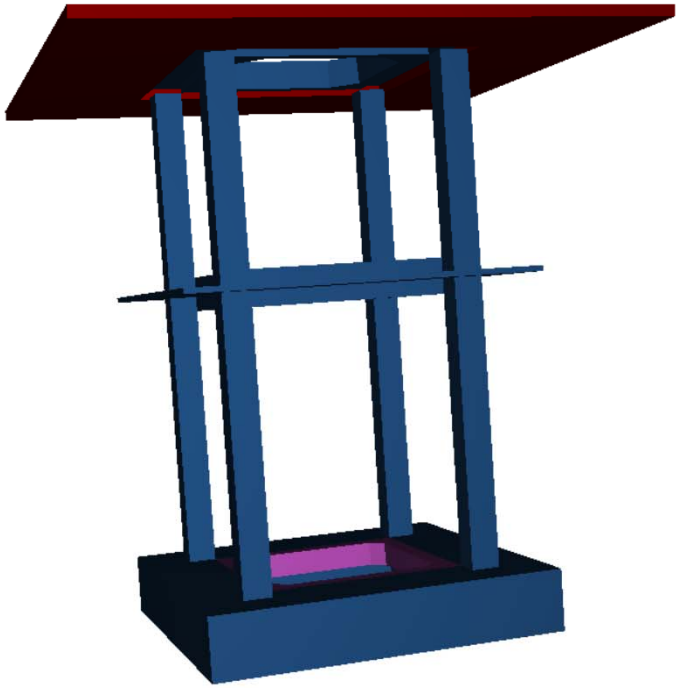


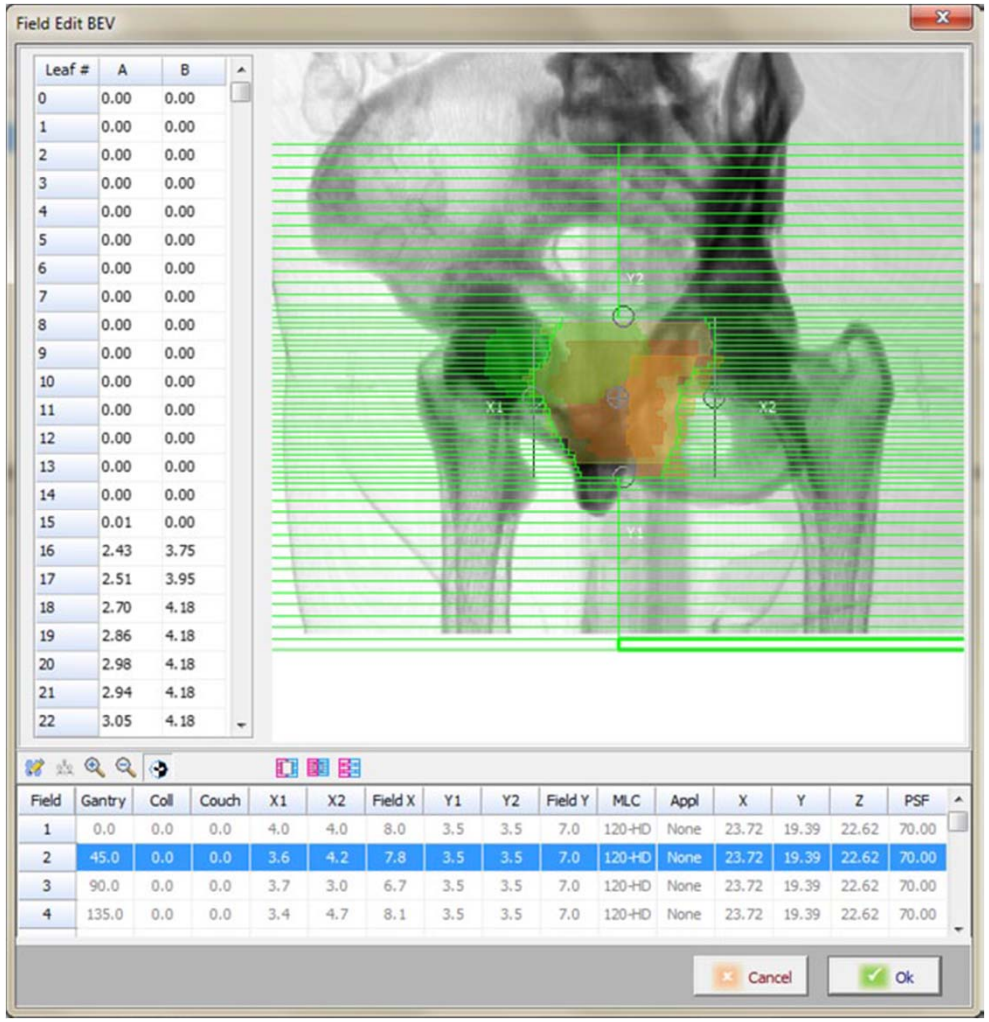


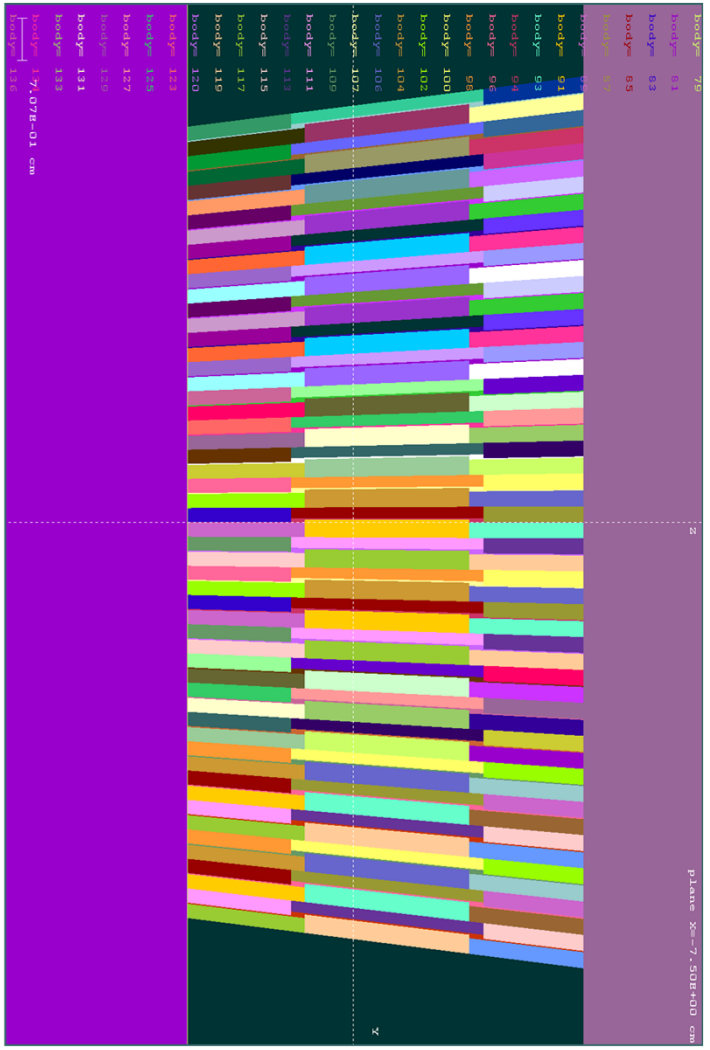



65.4









Includes multi-leaf collimators:

Varian 52 leaves, Millenium and 120 high-definition

Elekta

Supported linac models

PRIMO	commercial
Elekta SL	SL series
Elekta MLCi	SLi Plus, Axesse, Affinity, Synergy, Precise
Varian Clinac 600C	Clinac 600 C
Varian Clinac 600CD	Clinac 600 C/D
Varian Unique	Unique
Varian Clinac 2100	Clinac C series, TrueBeam (sect. 5.3)
Varian Clinac 2300	Clinac 2300 C/D
FakeBeam	TrueBeam 6- and 10-FFF beams

Imports DICOM-RT STRUCTs

Imports/exports external phase-space files in IAEA format

(see https://www-nds.iaea.org/phsp)

Runs in parallel on a single multi-core **64-bits windows system**

(parallel version for Linux clusters under development)

Typical timings:

- patient-dependent part only
- desktop computer, 8 processing cores
- $2 \times 2 \times 2$ mm^3 voxels
- average standard statistical uncertainty of 2%
- Computing time: **2 - 3 hours**

M. Rodriguez (UPC), J. Sempau (UPC) and L. Brualla (Universitätsklinikum Essen),

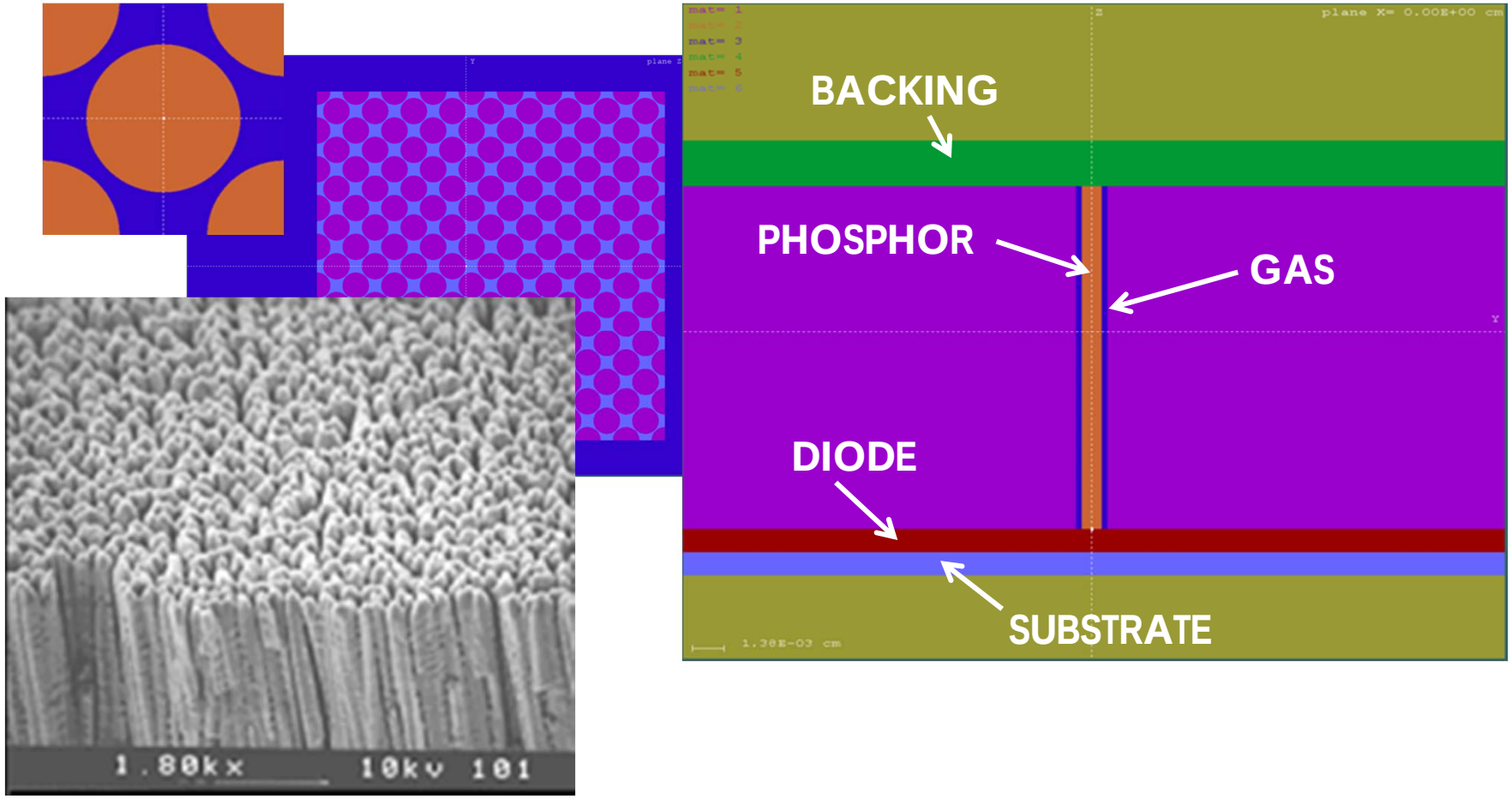
PRIMO -- A graphical environment for the Monte Carlo simulation of Varian and Elekta linacs,
Strahlenther. Onkol. 189 (2013) 881-886

Freely downloadable from

https://www.primoproject.net

MANTIS

Couples ionizing radiation with visible light to simulate **indirect detector structures.**



Developed by

A Badano & J Sempau, *MANTIS: combined x-ray, electron and optical Monte Carlo simulations of indirect radiation imaging systems,* Phys. Med. Biol. 51 (2006) 1545–1561

Open source and free: **https://code.google.com/p/mantismc**

An extension, **hybrid**MANTIS, that combines CPU(x-rays)+GPU(optical) computations has been developed by

Diksha Sharma, Andreu Badal and Aldo Badano, *hybridMANTIS: a CPU-GPU Monte Carlo method for modeling indirect x-ray detectors with columnar scintillators,* Phys. Med. Biol. 57 (2012) 2357-2372.

and is available at **http://code.google.com/p/hybridmantis**

Auxiliary tools for this course (freeware)

- Total Commander, a powerful file manager (shareware).
  http://www.ghisler.com

- Programmer's File Editor, or PFE. A simple, lightweight text editor.
  http://www.lancs.ac.uk/people/cpaap/pfe

- gfortran, the Fortran compiler from GNU.
  http://gcc.gnu.org/fortran
  http://users.humboldt.edu/finneyb/gfortran-windows-20140629.exe
  (as of 2015-03-16)

- Gnuplot, represents data graphically; intensively used by penEasy.
  http://www.gnuplot.info

Thank you.