MY ACTIVITIES AS NGS USER SINCE APRIL 2004

MARY PW CHIN

Department of Physics, University of Surrey, Guildford

UNIVERSITY OF SURREY

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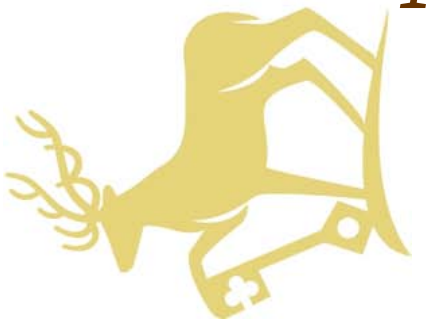
WHY WE NEED NGS

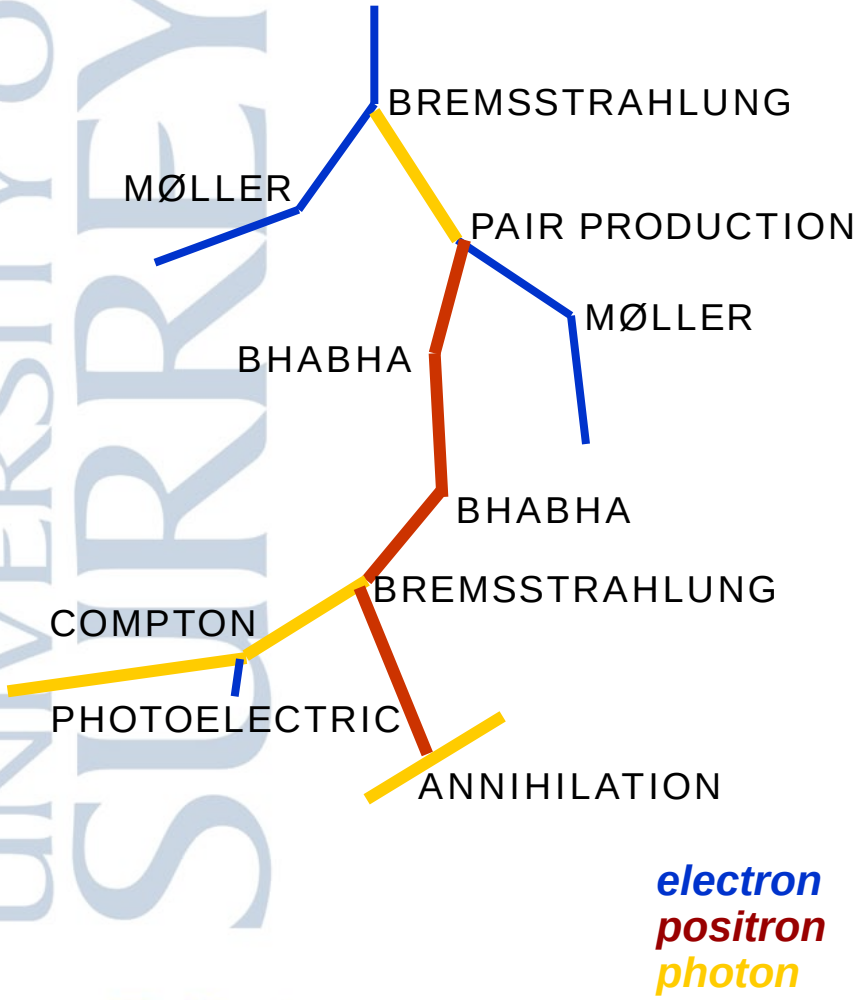
HOW WE USE NGS

APPLICATIONS

NotSoRandom THOUGHTS



PROBLEM STATEMENT

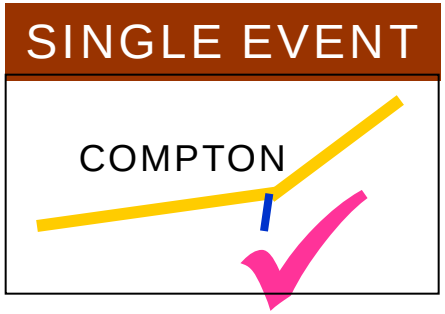


RADIATION INTERACTIONS WITH MATTER
eg BODY TISSUES

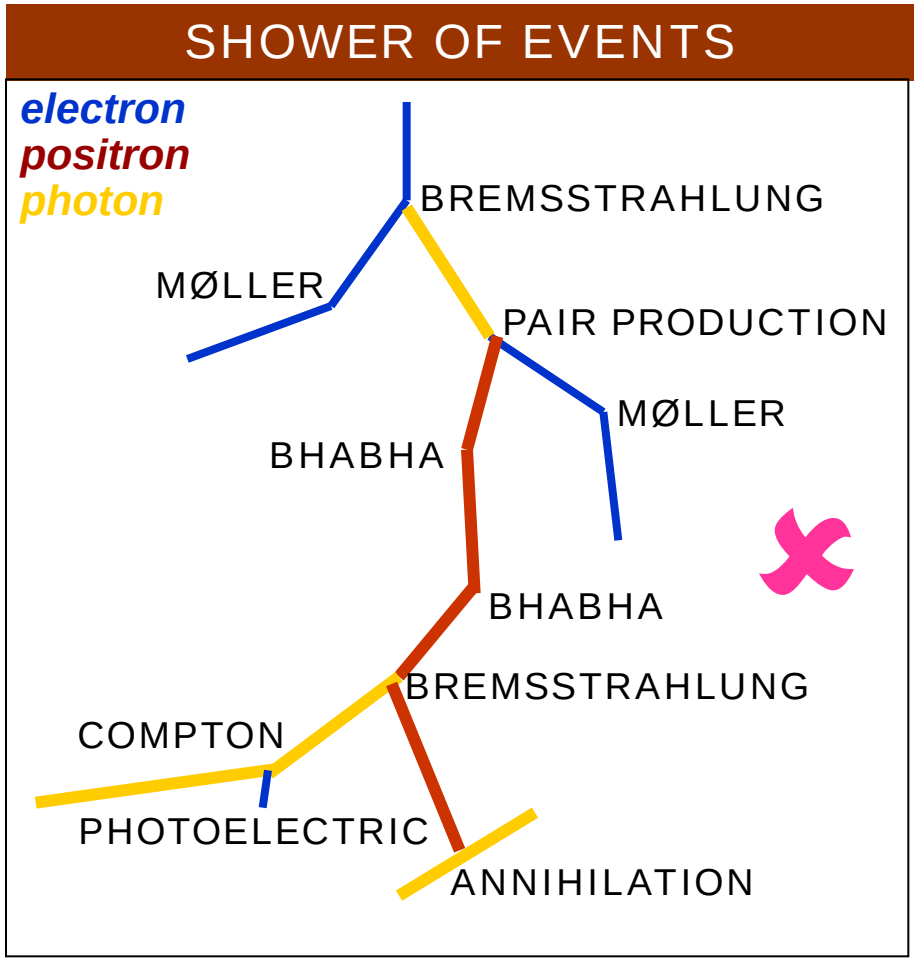
LOTS & LOTS OF EVENTS

EACH EVENT, EACH PARTICLE IS RANDOM: BIRTH, DEATH, ENERGY, DIRECTION

WHY MONTE CARLO

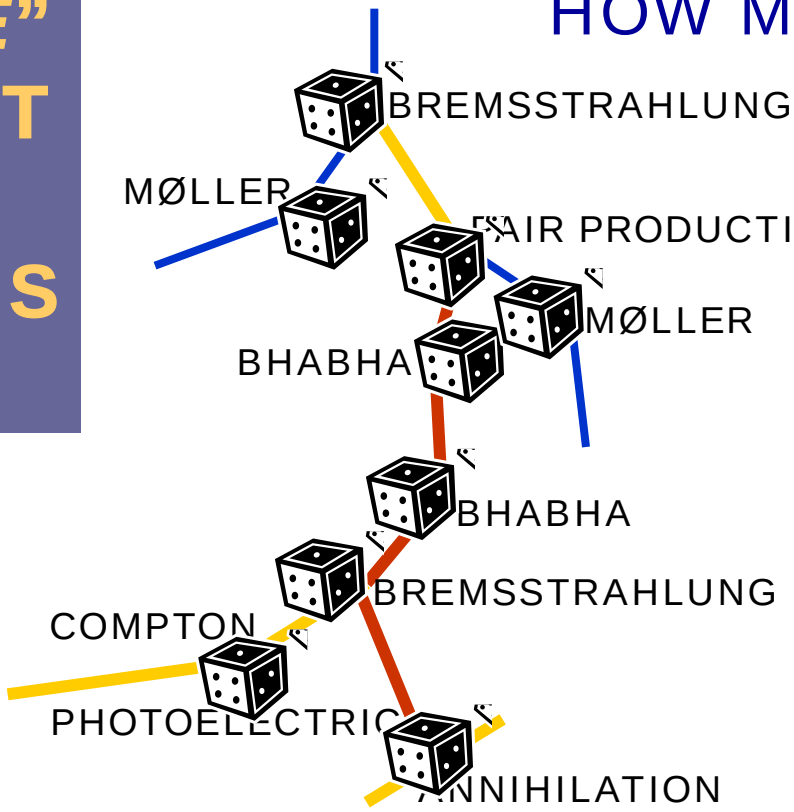


DETERMINISTIC EQUATIONS



HOW MONTE CARLO WORKS

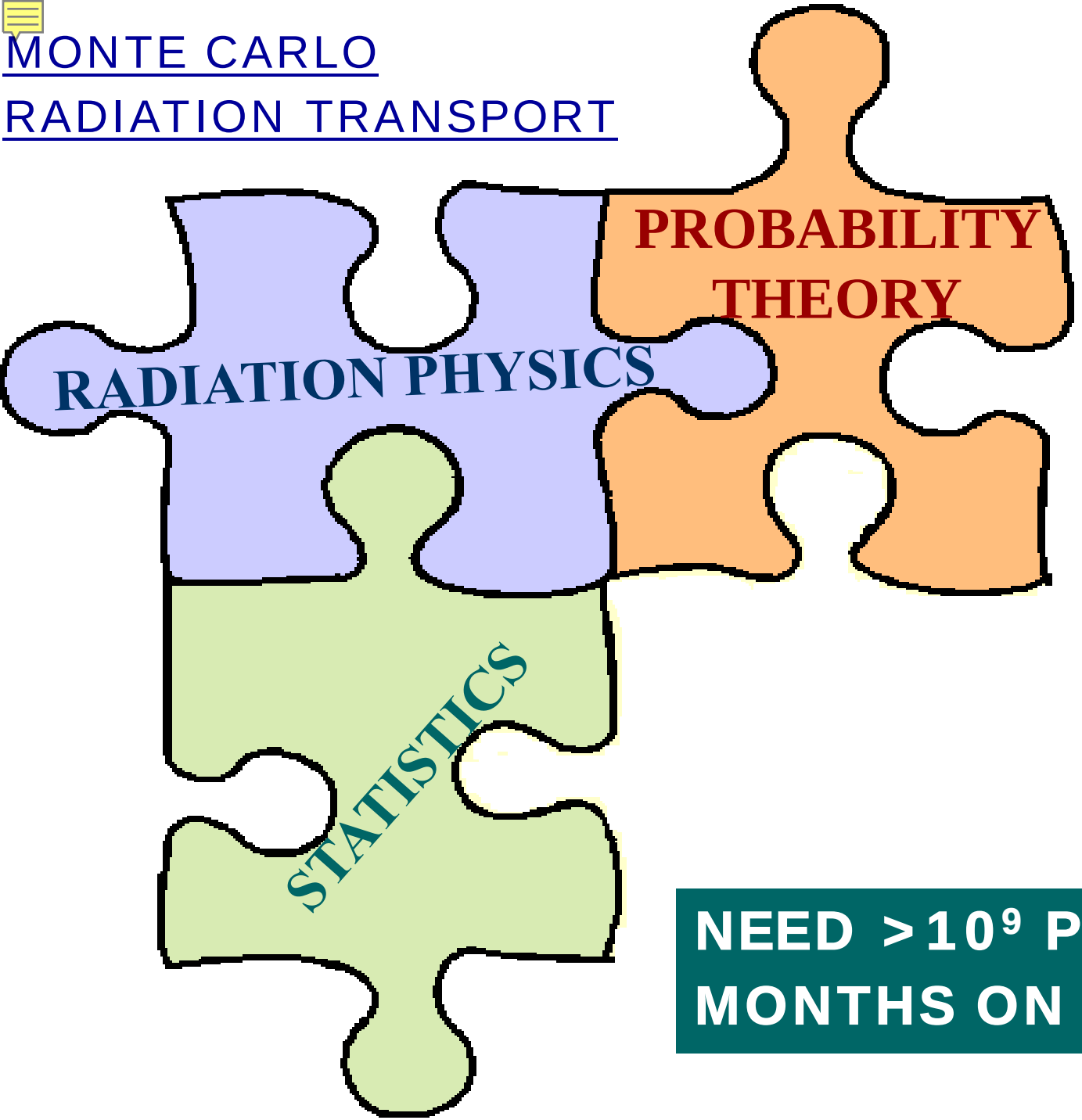
"THROW DICE" AT EACH POINT TO DECIDE WHAT HAPPENS NEXT

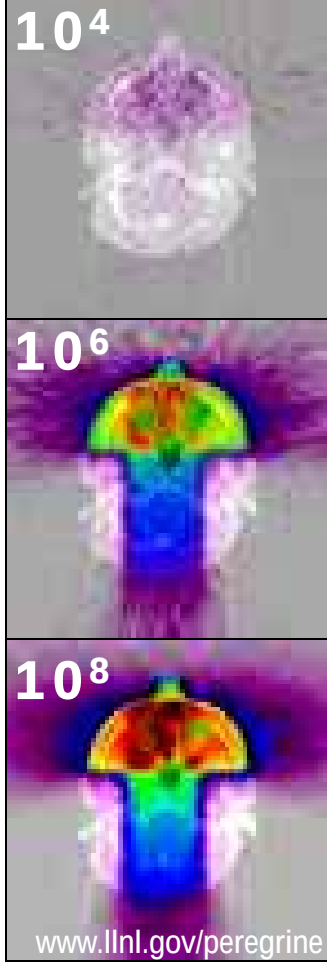


electron
positron
photon

REPEAT WITH TRILLIONS OF PARTICLES ENTERING THE BODY

MONTE CARLO RADIATION TRANSPORT





NEED >10^9 PARTICLES & MONTHS ON A DESKTOP!

Different MONTE CARLO codes or *housebrands*

An Embarassingly Parallel Framework for Running EGSnrc/BEAMnrc/DOSXYZnrc, FLUKA, MCNP/MCNPX, GEANT4 & PENELOPE on Grid & Cluster Computers

Chin MPW *et al* 2007 Proc. XVth Int Conf on the Use of Computers in Radiation Therapy, ed Bissonnette J, University of Toronto, Toronto pp 93-7

-------- supersedes ---------

Chin MPW *et al* 2004 Proc. XIVth ICCR "Implementation of BEAMnrc Monte Carlo simulations on the Grid" ed Yi BY, Ahn SD, Choi EK, Ha SW, Jeong Publishing, Seoul

Different MONTE CARLO codes

or *housebrands*

European Organization for Nuclear Research (CERN)

Istituto Nazionale di Fisica Nucleare (INFN)

An Embarassingly Parallel Framework for

National Research Council Canada (NRCC)

Stanford Linear Accelerator Centre (SLAC)

Running EGSnrc/BEAMnrc/DOSXYZnrc,

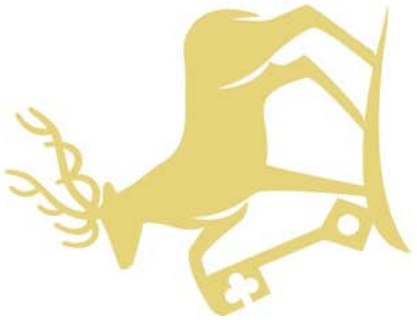
Los Alamos National Laboratory (LANL)

FLUKA, MCNP/MCNPX, GEANT4 &

European Organization for Nuclear Research (CERN)

PENELOPE on Grid & Cluster Computers

Universitat de Barcelona



Different MONTE CARLO codes or *housebrands*

An Embarassingly Parallel Framework for

electron, positron, photon

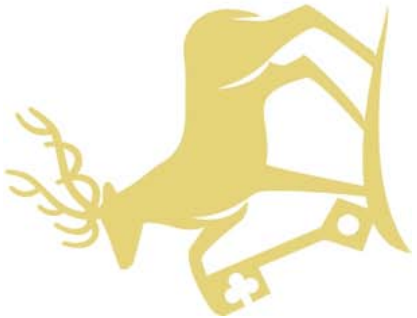
Running EGSnrc/BEAMnrc/DOSXYZnrc,

more particle types

FLUKA, MCNP/MCNPX, GEANT4 &

even more particle types

PENELOPE on Grid & Cluster Computers



FROM SINGLE DESKTOP TO *N* NODES

SKELETON OF INPUT FILE

....

....

....

....

NumberOfHistories xxx

RandomNumberSeed yyy

...

...

other parameters

...

...

...

1 input file

↓

N input files

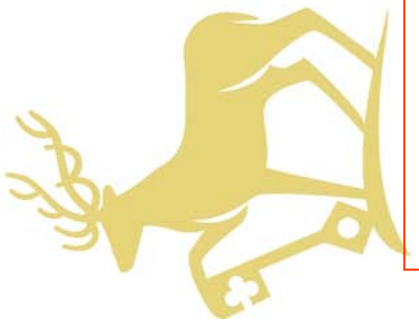
xxx histories

↓

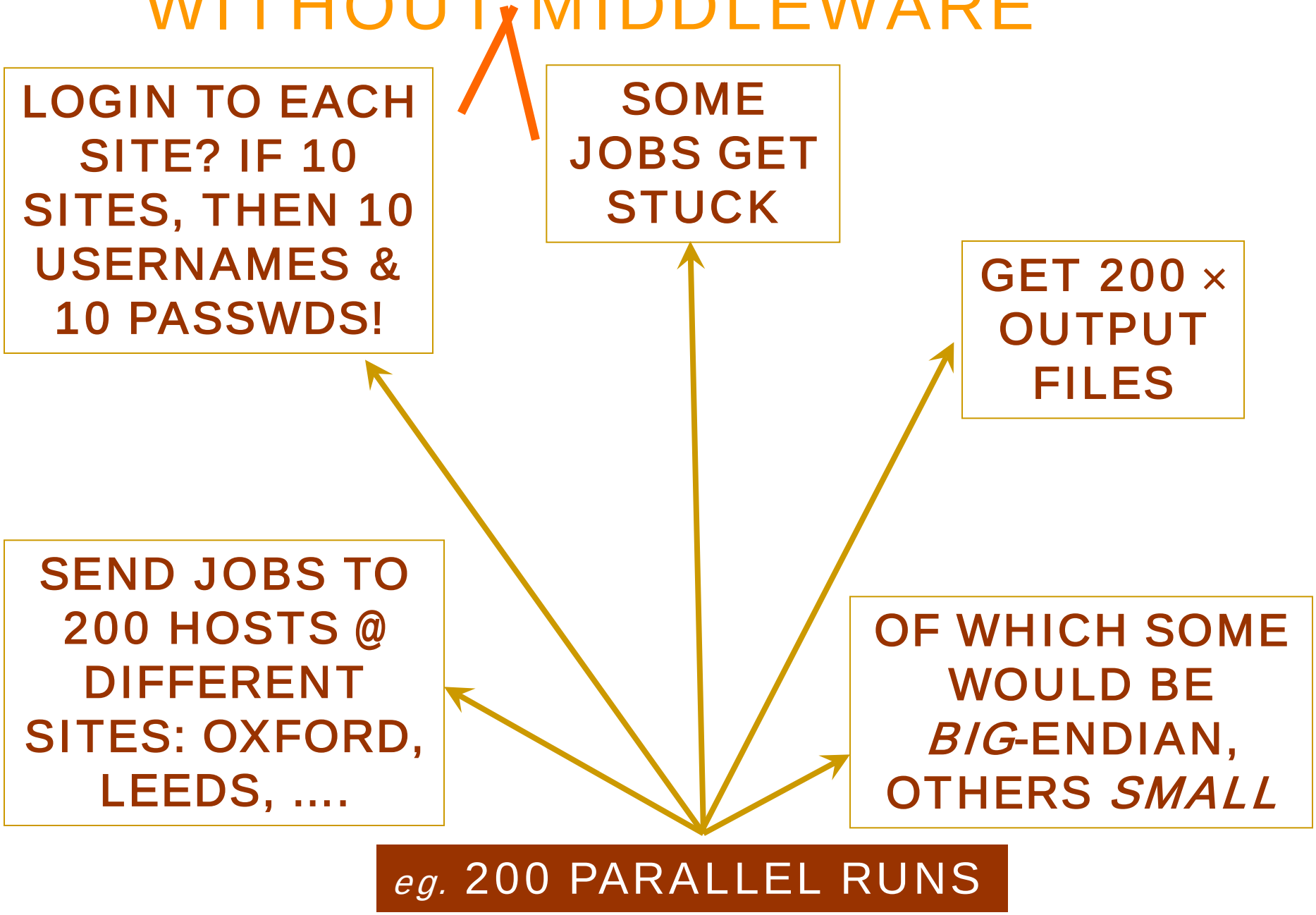
xxx/*N* histories

EACH INPUT FILE MUST HAVE DIFFERENT SEED.

NEEDS PARAMETER SWEEPING. NIMROD DOES THIS WELL.



GOOD WITHOUT MIDDLEWARE



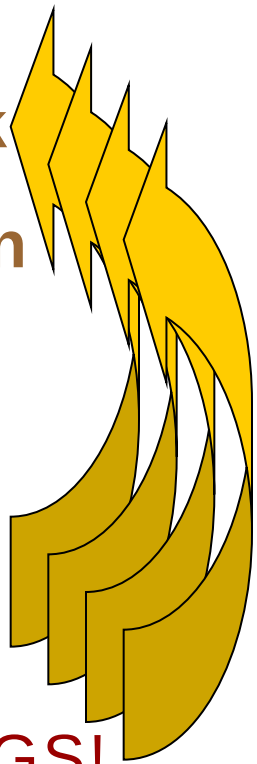

GOOD
WITHOUT MIDDLEWARE
LOGIN TO EACH SITE? IF 10 SITE
USE
10
SOME JOBS GET
COMPLETE MESS
SEN
20
DIFFERENT SITES: OXFORD, LEEDS, ...
OME
WOULD BE *BIG*-ENDIAN, OTHERS *SMALL*
eg. 200 PARALLEL RUNS

GOOD WITHOUT MIDDLEWARE

SOME JOBS GET STUCK

AM I SUPPOSED TO

- **identify which, among the 200, got stuck**
- **identify which nodes are they running on**
- **logon to each node to kill the process**
- **find which nodes are not busy**
- **restart each job on each free node**



I TOOK 3 YEARS... THANKS TO THE NGS!

GOOD

WITHOUT MIDDLEWARE

SOME JOBS GET

PEOPLE WOULD NEED 20 YEARS TO DO THEIR PhD

find which nodes are not busy

- restart each job on each free node

I TOOK 3 YEARS... THANKS TO THE NGS!

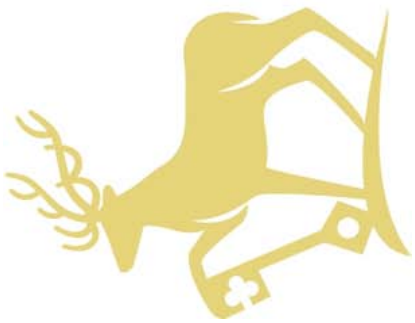
RESOURCE BROKERS

WHAT WE LOOK FOR

CAN BE MESSY OTHERWISE

- **jobs never return, occupy resource forever**
- **completed jobs get reported as queueing, shadows still occupy resource**

- **(SELF-HEALING) QUEUEING**
- **PARAMETER SWEEPING**
- **STAGING FILES OUT**
- **EXECUTION LINE (COMMAND + ARGUMENTS)**
- **STAGING FILES IN**



RESOURCE BROKERS
WHAT WE LOOK FOR

Used CONDOR & NIMROD, tried gLite & gridSAM. CONDOR most reliable.

So that we can run jobs on nodes NOT PRE-INSTALLED WITH THE CODE

- **(SELF-HEALING) QUEUEING**
- **PARAMETER SWEEPING**
- **STAGING FILES OUT**
- **EXECUTION LINE (COMMAND + ARGUMENTS)**
- **STAGING FILES IN**

RESOURCE BROKING examples

EXECUTABLE + ARGUMENTS

FILES IN + FILES OUT

STDOUT + STDERR

gLite

```
Type = "Job";
JobType = "Normal";
Executable = "imp.sh";
StdOutput = "myjob.out";
StdError = "myjob.err";
InputSandbox = {"imp.sh","imp.tar.gz“,”mcnpx.exe”,”X11.dll”,”barpol.dat ”,
      “bertin”,”el03”,”endf66a”,”gdr.dat”,”la150u”,”la150h”,”mcplib04”,”
      phtlib”,”rmccs”,”endl92”,”xsdir”};
OutputSandbox = {"myjob.err","myjob.out"};
Arguments = "ong3 7 100";
RetryCount = 7;
ShallowRetryCount = -1
```

Condor

```
universe = vanilla
Executable = imp.bat
Arguments = cf$(Process)
transfer_input_files = mcnpx.exe, X11.dll, barpol.dat, bertin, el03, endf66a,
gdr.dat, la150u, la150h, mcplib04, phtlib, rmccs, endl92, xsdir, cf$(Process)
requirements = (OpSys == "WINNT51" && Memory >= 1000 && Disk >= 50000000)
Rank = KFlops
Output = $(Process).out
Error = $(Process).err
should_transfer_files = yes
when_to_transfer_output = on_exit_or_evict
queue 100
```

The Monte Carlo Method: Versatility Unbounded in a Dynamic Computing World
Chattanooga, Tennessee, April 17-21, 2005, on CD-ROM, American Nuclear Society, LaGrange Park, IL (2005)

UNIVERSITY OF SURREY

WE DO REPORT OUR USE OF THE NGS

A MONTE CARLO SOLUTION FOR EXTERNAL BEAM PHOTON RADIOTHERAPY VERIFICATION

P W Chin and D G Lewis
Department of Medical Physics, Velindre Cancer Centre
Cardiff, Wales, United Kingdom.
mary.chin@physics.org; dg.lewis@physics.org

J P Giddy
Welsh e-Science Centre, Cardiff University
Cardiff, Wales, United Kingdom.
j.p.giddy@wesc.ac.uk

ABSTRACT

In this work, Monte Carlo (MC) simulations provide an answer to the surging clinical need for verifying complex radiation treatments. As will be demonstrated, this solution attained accuracy (2% in dose prediction) and versatility (over a wide range of clinical setups) known to be unachievable by other techniques. The solution is not impeded by long runtimes since it has been successfully implemented on the Grid. It can therefore be clinically productive. Implementation on the UK National Grid Service will be reported. This work also draws from MC simulation information beyond physical measurements, such as details about radiation interactions in a radiotherapy imager. Aided by this knowledge, we designed a simplified, substitute imager which reduces MC runtimes. It can also be useful for other dosimetric computation techniques where detailed modelling is unavailable. Additionally, we report a MC study on how a general assumption in non-MC techniques leads to inaccurate dose prediction.

Key Words: Radiotherapy, Verification, EPID, EGSnrc, BEAMnrc, Grid computing, Radiation detectors, Phantom design

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2.5 Simulations on the UK National Grid Service

Serial computation of millions of histories requires long runtimes, which is clinically impractical. However, the lack of dependencies between individual particle histories makes it simple to distribute history ranges to different processors to shorten the overall runtime. We have previously Grid-enabled EGSnrc, BEAMnrc and DOSXYZnrc simulations [13]. Recently, we gained access to the UK National Grid Service (NGS), the core production-level grid created under the UK e-Science program. It uses grid middleware (the Globus Toolkit) to provide secure remote access to a collection of hardware, software and support resources available to the UK

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The NGS provides access to 168 dedicated dual 3.06 GHz Intel Xeon nodes (336 processors in total) spread over four UK sites. Using the NGS, and in competition with other users' computations, the DOSXYZnrc simulation took less than 3 hours to complete. This is a 50-fold increase in the speed of computation, and brings the runtime much closer to an acceptable time frame for clinical operation.

The use of the NGS allowed us to achieve this speed-up without purchasing additional resources, and the time and costs of installing and maintaining a computational cluster ourselves. In a clinical setting, the capital and labour costs of obtaining this computational power and the expertise to run it are usually unavailable.

4/12

Additionally, we report a MC study on how a general assumption in non-MC techniques leads to inaccurate dose prediction.

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2006/07 ACTIVITIES

PATIENT DOSE CALCULATIONS

EGS / BEAM / DOSXYZ nrc

Vanderstraeten, Chin, Fix et al 2007 Conversion of CT numbers into tissue parameters for Monte Carlo dose calculations: a multi-centre study *Phys. Med. Biol. 52(3)*

POSITRON PHYSICS

EGSnrc & PENELOPE

Chin & Spyrou 2007 Monte Carlo investigation of positron annihilation in medical positron emission tomography
Nucl. Instr. Meth. A doi:10.1016/j.nima.2007.05.200

ION BEAMS

FLUKA & GEANT4

Chin & Spyrou *to present at* Int Conf Biomedical Applications of High Energy Ion Beams 30 July – 2 August 2007 Guildford

BORON NEUTRON CAPTURE THERAPY

MCNPX

Alfuraih, Chin & Spyrou *to present at* 12th Int Conf Modern Trends in Activation Analysis 16-21 Sep 2007 Tokyo

NUCLEAR ACTIVATION

FLUKA & MCNPX

Chin & Spyrou *to present at* 12th Int Conf Modern Trends in Activation Analysis 16-21 Sep 2007 Tokyo

NEUTRON SHIELDING

MCNPX

Chin & Spyrou *to present at* American Nuclear Society Winter Meeting 11-15 Nov 2007 Washington

PET TEXTBOOKS DIDN'T TELL US

Abstract

A number of Monte Carlo codes are available for simulating positron emission tomography (PET), however, physics approximations differ. A number of radiation processes are deemed negligible, some without rigorous investigation. Some PET literature quantify approximations to be valid, without citing the data source. The radiation source is the first step in Monte Carlo simulations, for some codes this is 511 keV photons 180º apart, not polyenergetic positrons with radiation histories of their own. Without prior assumptions, we investigated electron-positron annihilation under clinical PET conditions. Just before annihilation, we tallied the positron energy and position. Right after annihilation, we tallied the energy and separation angle of photon pairs. When comparing PET textbooks with theory, PENELOPE and EGSnrc, only the latter three agreed. From 106 radiation histories, a positron source of 15O in a chest phantom annihilated at as high as 1.58 MeV, producing photons with energies 0.30 to 2.20 MeV, 79º to 180º apart. From 106 radiation histories, a 18F positron source in a head phantom annihilated at energies as high as 0.56 MeV, producing 0.33 to 1.18 MeV photons 109º to 180º apart. 2.5% and 0.8% annihilation events occurred in-flight in the chest and the head phantoms respectively. PET textbooks typically either do not mention any deviation from 180°, or state a deviation of 0.25º or 0.5º. Our findings are founded on the well-established Heitler cross sections and relativistic kinematics, both adopted unanimously by PENELOPE, EGSnrc and GEANT4. Our results highlight the effects of annihilation in-flight, a process sometimes forgotten within the PET community.

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NOT BACK-TO-BACK

NOT 511 keV

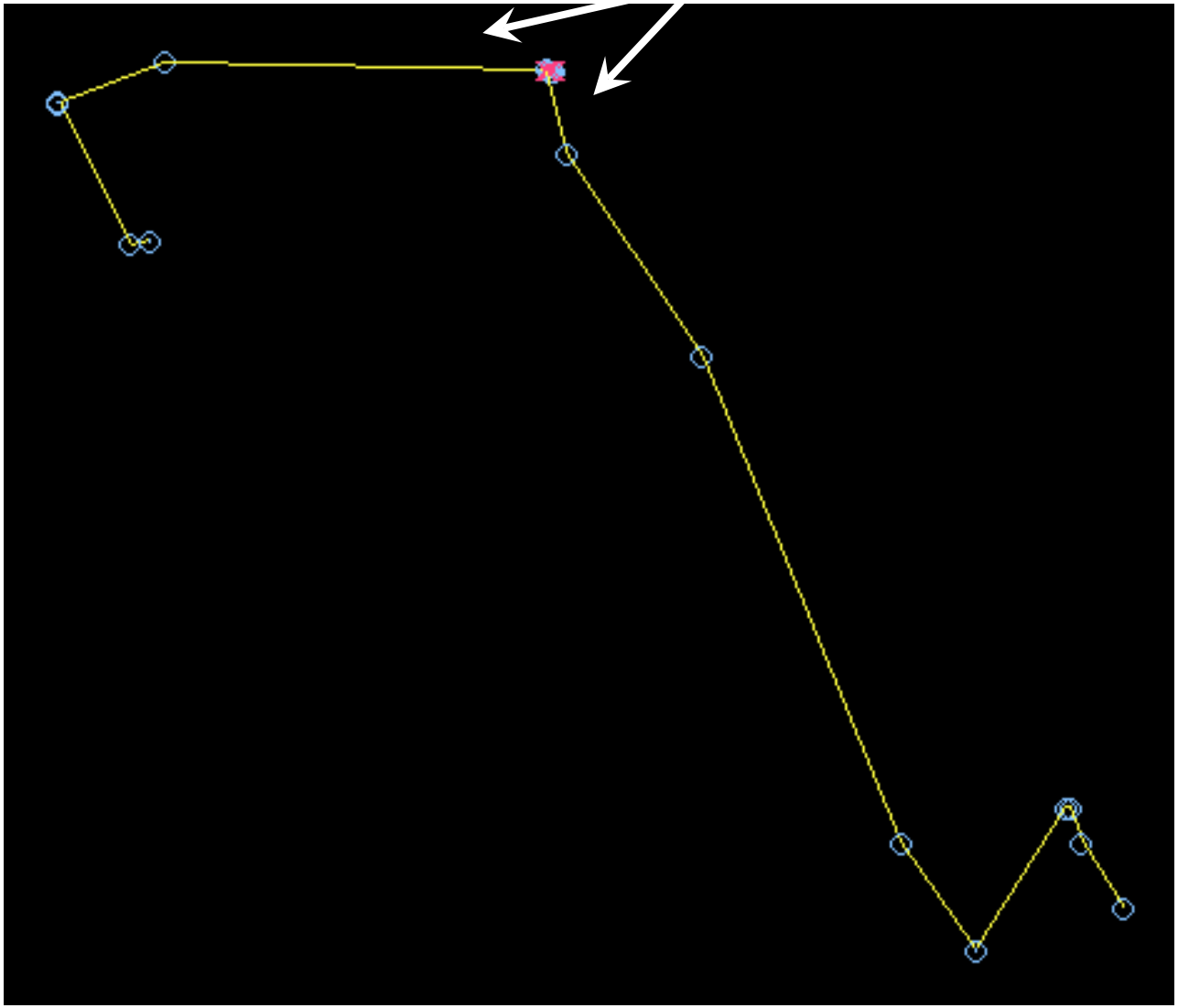
NOT THERMAL

Chin & Spyrou 2007 Monte Carlo investigation of positron annihilation in medical positron emission tomography
Nucl. Instr. Meth. A doi:10.1016/j.nima.2007.05.200

Positron about to decay in flight	1	0.606	1	2	0.155,0.023,500.314	-0.122,-0.592, 0.797
Resulting photons	1	0.979	0	2	0.155,0.023 500.314	-0.311, 0.020, 0.950
	2	0.649	0	2	0.155,0.023 500.314	0.282,-0.935,-0.213

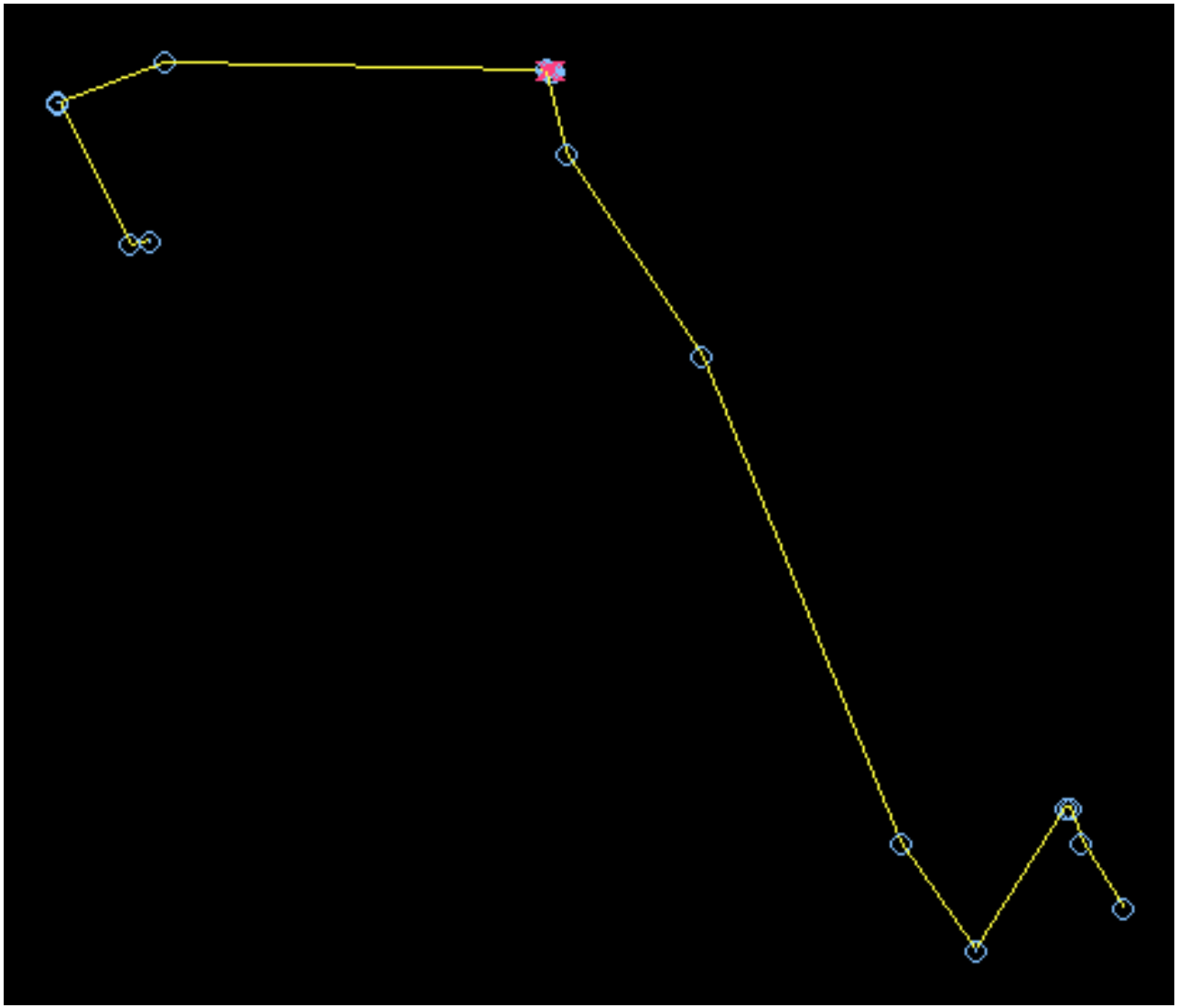
NOT THERMALISED?

NOT BACK-TO-BACK!



Positron about to decay in flight	**1**	**0.606**	**1**	**2**	**0.155,0.023,500.314**	**-0.122,-0.592, 0.797**
Resulting photons	**1**	**0.979**	**0**	**2**	**0.155,0.023 500.314**	**-0.311, 0.020, 0.950**
	2	**0.649**	**0**	**2**	**0.155,0.023 500.314**	**0.282,-0.935,-0.213**

NOT 0.511



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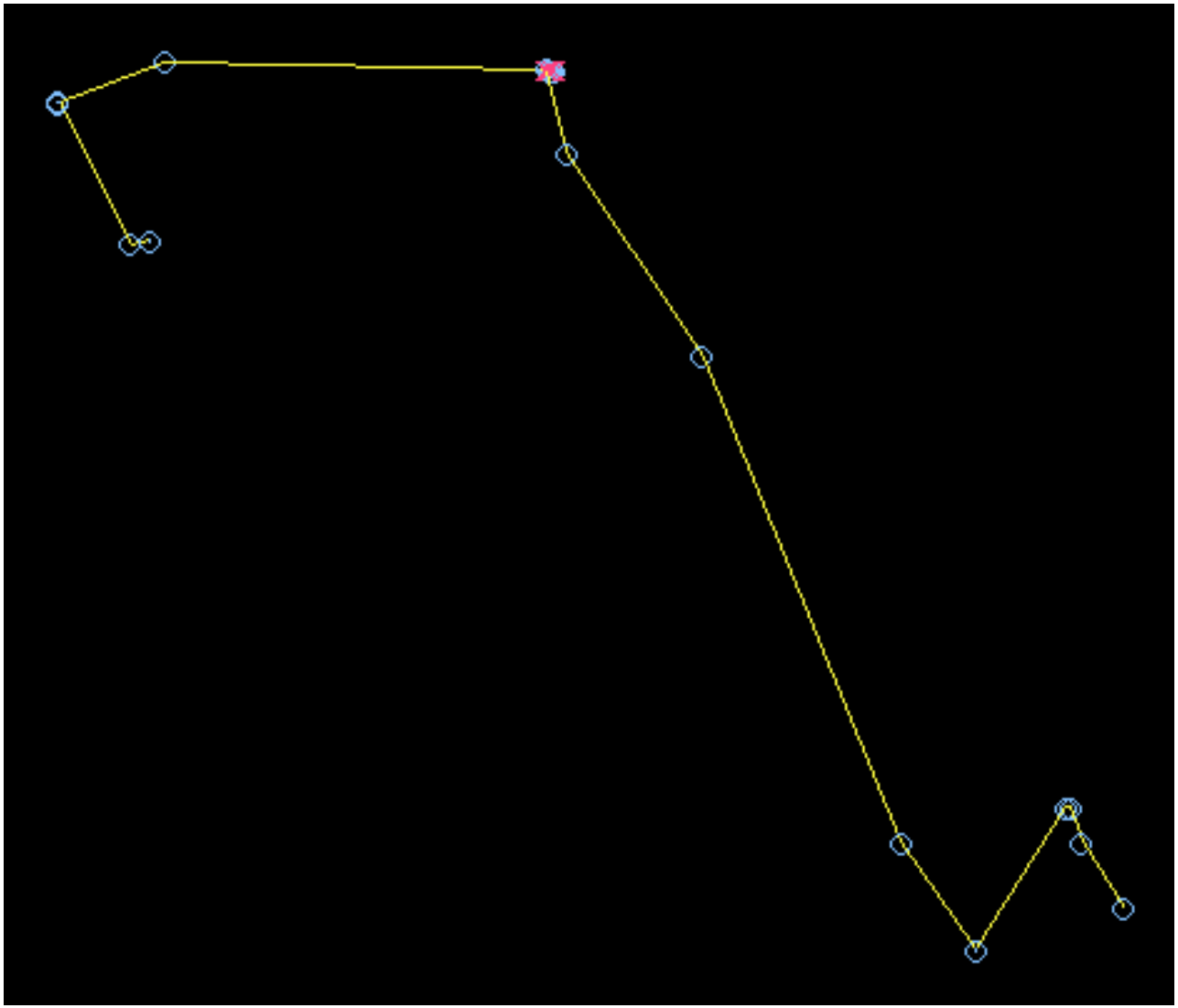
	2	**0.649**	**0**	**2**	**0.155,0.023 500.314**	**0.282,-0.935,-0.213**

0.606 + 0.511 + 0.511

= 0.979 + 0.649



Prediction of dose in radiotherapy patients

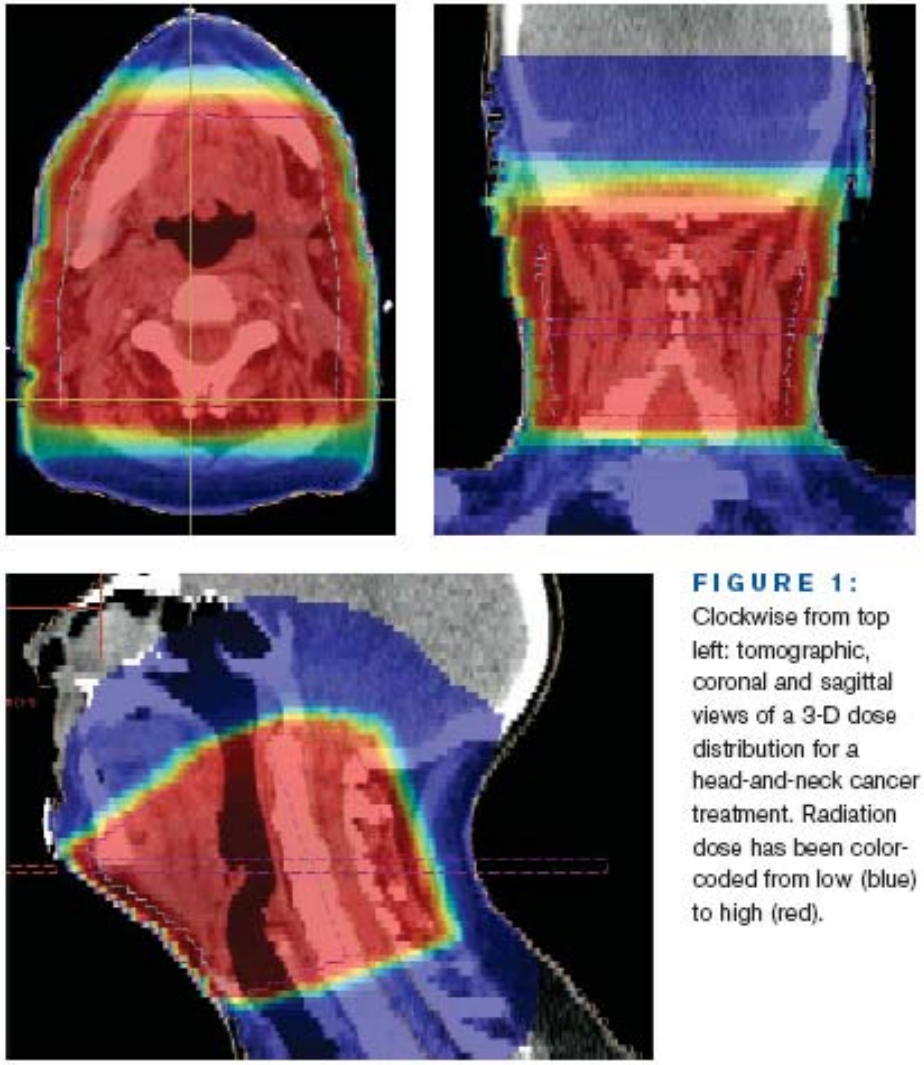


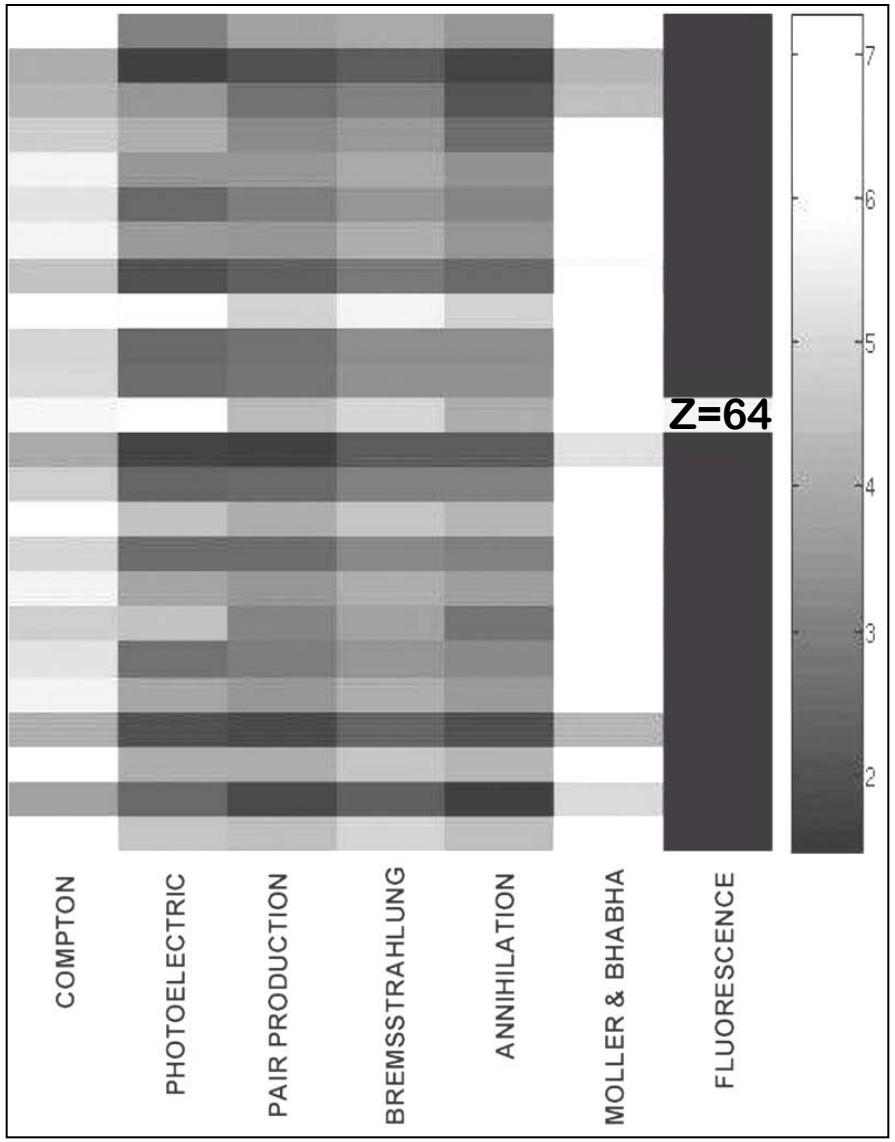
FIGURE 1: Clockwise from top left: tomographic, coronal and sagittal views of a 3-D dose distribution for a head-and-neck cancer treatment. Radiation dose has been color-coded from low (blue) to high (red).

Chin PW et al 2006 *Grid and cluster computing for radiotherapy* Scientific Computing

How do we know whether dose is delivered correctly?

Chin PW et al 2005 *A Monte Carlo solution for external beam photon radiotherapy verification* American Nuclear Society Topical Meeting in Monte Carlo. Chattanooga: American Nuclear Society

Radiation detection in amorphous silicon imager



Chin PW 2005 *Monte Carlo portal dosimetry* Medical Physics 32:3228

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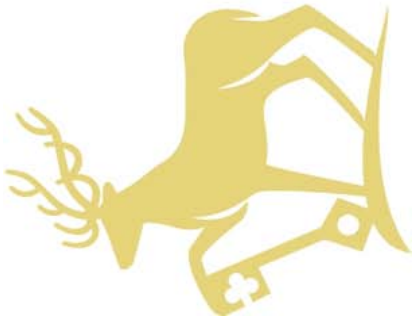

extra notes

1. as NGS user

2. as admin for local clusters

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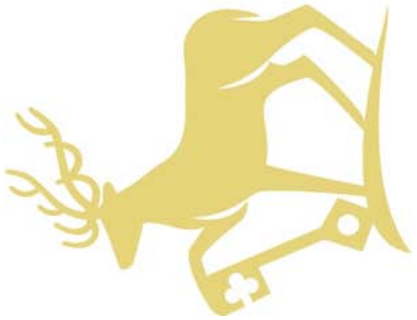
extra notes…

If I'm the only one using the resources, nice to monopolise!

If there are fellow users, great to share!



DESKTOP IS MINE, CLUSTER / GRID ISN'T

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extra notes...

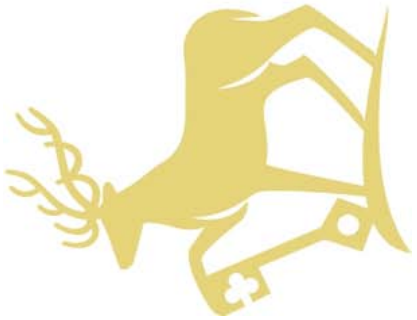
People take resources for granted, submit crap jobs carelessly

Never mind... if results isn't what we want, we can always repeat the simulations...

extra notes…

Setting up long jobs before disappearing for holidays never works…

- jobs crash
- the mind ends up *helping* the computers *run* the jobs



m o r e ...

http://www.marychin.org

me@marychin.org