

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

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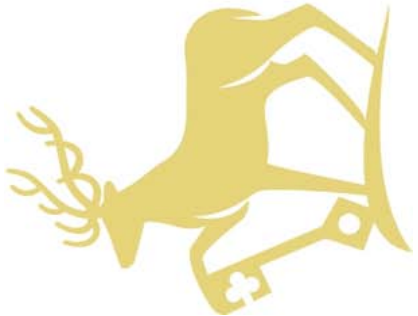
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OUR RECIPE

VALIDATION

GLITCHES & FIXES

APPLICATIONS



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EMBARASSING

**ASSUMES
RADIATION
HISTORIES DON'T
CROSS-TALK**
discussed in paper

NOT EMBARASSING

PVM / MPI

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FLEXIBLE

An Embarrassingly Parallel **Framework** for

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RESOURCE BROKER / GRID MIDDLEWARE

✓ Condor

✓ gLite

✓ Nimrod

FILE SYSTEM

✓ Shared

✓ Non-shared

MONTE CARLO CODE

✓ Pre-installed

✓ Not installed

OPERATING SYSTEM

✓ *nix, *nux, *rix

✓ Windows

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IDENTIFY LIGHT-WEIGHT FILESYSTEM FOR EACH
MONTE CARLO CODE.

IDENTIFY EXECUTION LINE FOR NON-
INTERACTIVE RUN. PREFERABLY FREE FROM
HARDCODED PATHS & ENVIRONMENT
VARIABLES.

DETAILED IN PAPER



EXECUTABLE +
ARGUMENTS

RESOURCE BROKING examples

FILES IN +
FILES OUT

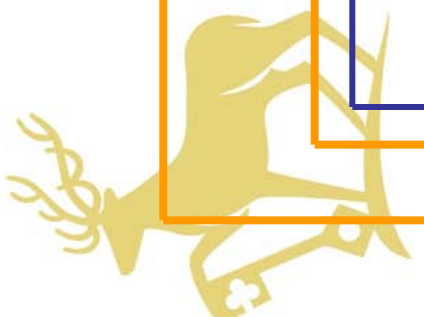
STDOUT +
STDERR

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

gLite

```
universe = vanilla  
Executable = imp.bat  
Arguments = cf$(Process)  
transfer_input_files = mcnp.exe, X11.dll, barpol.dat, bertin, el03, endf66a,  
gdr.dat, la150u, la150h, mcplib04, phtlib, rmccs, endl92, xmdir, cf$(Process)  
requirements = (OpSys == "WINNT51" && Memory >= 1000 && Disk >= 5000000)  
Rank = KFlops  
Output = $(Process).out  
Error = $(Process).err  
should_transfer_files = yes  
when_to_transfer_output = on_exit_or_evict  
queue 100
```

Condor



COMBINING OUTPUT FILES IS EASY

#!/usr/bin/perl

use POSIX qw(ceil floor);

@files = <\$ARGV[0]*m>;



AUTOMATED DIRECTORY SCAN

\$splits = 0;

foreach \$file(@files) {

\$splits++;

open(MCTAL,\$file) || die "OOPSY \$file not found.\n";

if (\$splits==1) {

\$line = <MCTAL>;

while (substr(\$line,0,4) ne 'ntal') {\$line = <MCTAL>;}

@temp = split /\s+/, \$line;

\$ntal = \$temp[1];



}

for (\$tally=0; \$tally<\$ntal; \$tally++) {

\$line = <MCTAL>;

if (\$splits==1) {

while (substr(\$line,0,5) ne 'tally') {\$line = <MCTAL>;}

@temp = split /\s+/, \$line;

\$tallylabel[\$tally] = \$temp[1];

while (\$#temp!=1 || \$temp[1]<=1) {

@temp = split /\s+/, <MCTAL>;

}

\$bins[\$tally] = \$temp[1];

\$j = 0;

while (\$j < \$bins[\$tally]) {

@temp = split /\s+/, <MCTAL>;

for (\$i=1; \$i<=#temp; \$i++) {

\$sticks1[\$j][\$tally] = \$temp[\$i];

\$j++;

}

}

TRAP WANTED VARIABLES

THIS IS A COMPLICATED EXAMPLE OF
MULTIPLE MULTI-DIMENSIONAL TALLY

VALIDATION / SECURITY

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LESS CONTROL

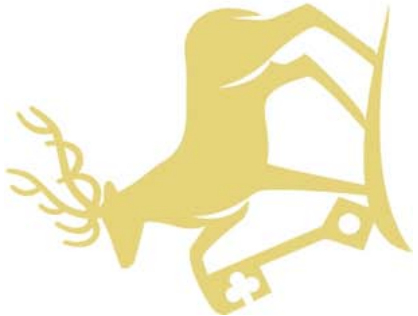
MORE UNKNOWN

PRE-RUN OPTION

WRAP JOB WITH TEST(S) SIMILAR TO
MCNP/MCNPX TEST SUITE.

POST-RUN EXERCISE

CHECK STATISTICAL DISTRIBUTION OF
RESULTS FROM EACH EXECUTION NODE



WHEN THINGS GO WRONG

```
Connecting to host ngsrb01.ngs.rl.ac.uk, port 7772
```

```
Logging to host ngsrb01.ngs.rl.ac.uk, port 9002
```

```
**
```

```
"J
```

```
re
```

```
Jo
```

```
-
```

```
-
```

```
-
```

```
- Jobs completed and returned but still queueing
```

THERE'S A
SOLUTION TO
EVERY
PROBLEM

change resource broker!



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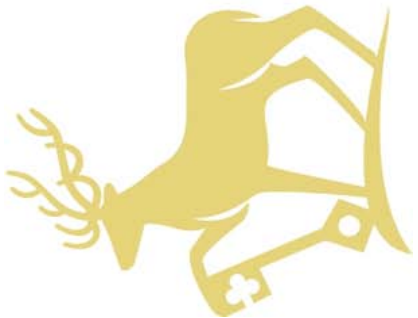
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SO MANY CODES?

SO MANY COMPUTERS?

I'VE GOT TO EXPLAIN
WHAT WE DO



2006/07 MONTE CARLO 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

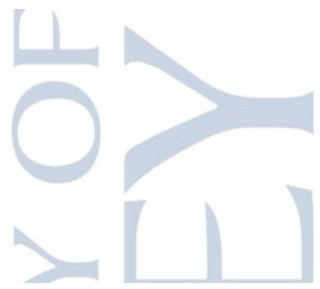
Chin & Spyrou *to present at* 12th Int Conf Modern Trends in Activation Analysis 16-21 Sep 2007 Tokyo

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 180° apart, not polyenergetic positrons with radiation histories of their own. Without prior assumptions, we investigated electron-positron annihilation, we tallied the positron energy and position. Results from 106 radiation histories, a positron source as 1.58 MeV, producing photons with energies 0.30 to 2.20 MeV, 79° to 180° apart. From 106 radiation histories, photon annihilation at energies as high as 0.56 MeV, producing 0.33 to 1.27 MeV photons. Results occurred in-flight in the chest and the text mention any deviation from 180°, or state that 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.

NOT
BACK-TO-BACK

NOT
511 keV

NOT
THERMAL

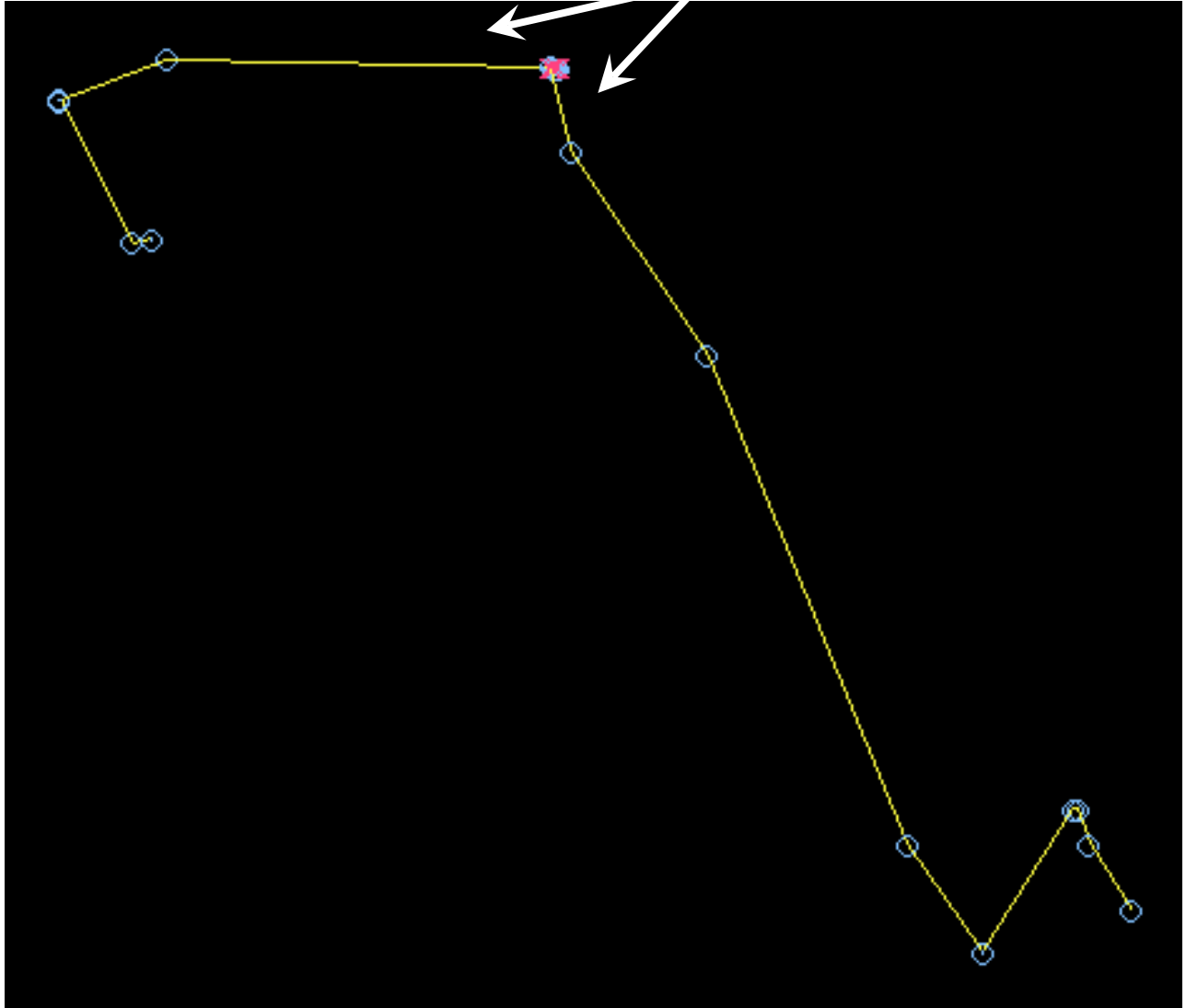
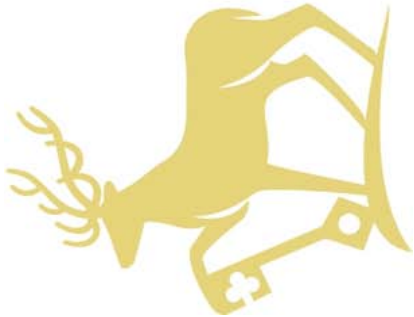
Chin & Spyrou 2007 Monte Carlo investigation of positron annihilation in medical positron emission tomography
Nucl. Instr. Meth. A doi:10.1016/j.nima.2007.05.200



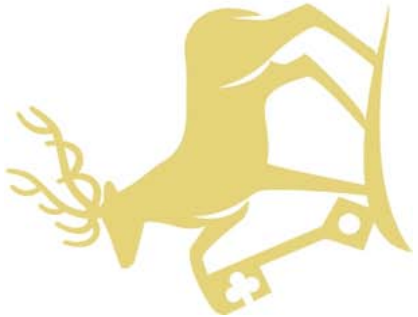
Positron about to decay in flight	1	0.606	1	2	0.155,0.023,500.314	-0.122,-0.592, 0.797
Resulting photons	1	0.979	0	2	0.155,0.023 500.314	-0.311, 0.020, 0.950
NOT THERMALISED?		0.649	0	2	0.155,0.023 500.314	0.282,-0.935,-0.213

$0.606 + 0.511 = 1.117$ NOT
 $= 0.979 + 0.649$ NOT BACK-TO-BACK!

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