

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

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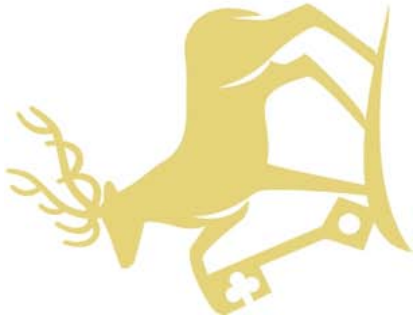
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OUR RECIPE

VALIDATION

GLITCHES & FIXES

APPLICATIONS



An **Embarassingly Parallel** Framework for
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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

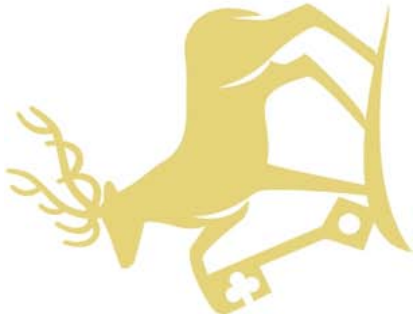
✓ Not installed

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

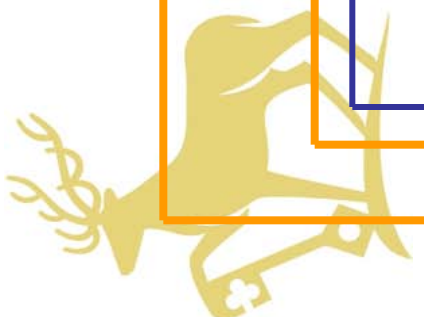
STDOUT +
STDERR

```
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++;
```

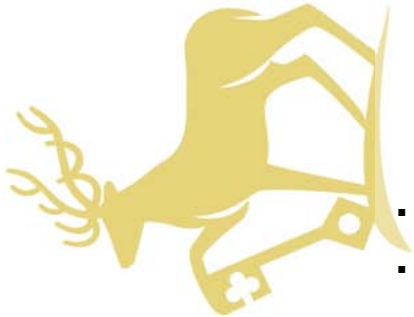
```
                }
```

```
            }
```

TRAP WANTED VARIABLES 

SKIP UNWANTED LINES

THIS IS A COMPLICATED EXAMPLE OF
MULTIPLE MULTI-DIMENSIONAL TALLY



VALIDATION / SECURITY

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LESS CONTROL

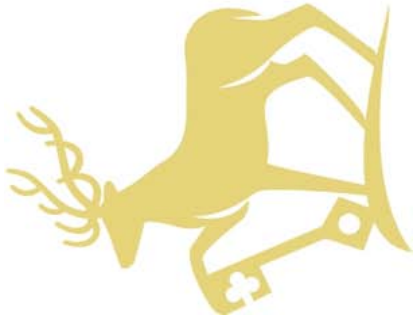
MORE UNKNOWN

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
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```
Jo
```

```
-
```

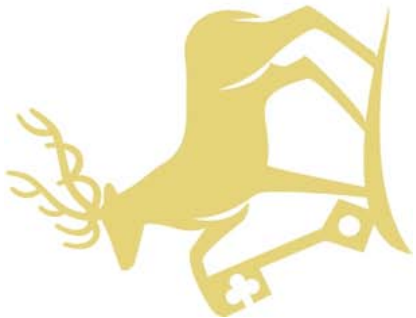
```
-
```

```
-
```

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

THERE'S A
SOLUTION TO
EVERY
PROBLEM

change resource broker!



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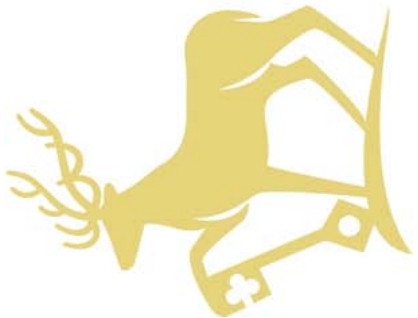
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SO MANY CODES?

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

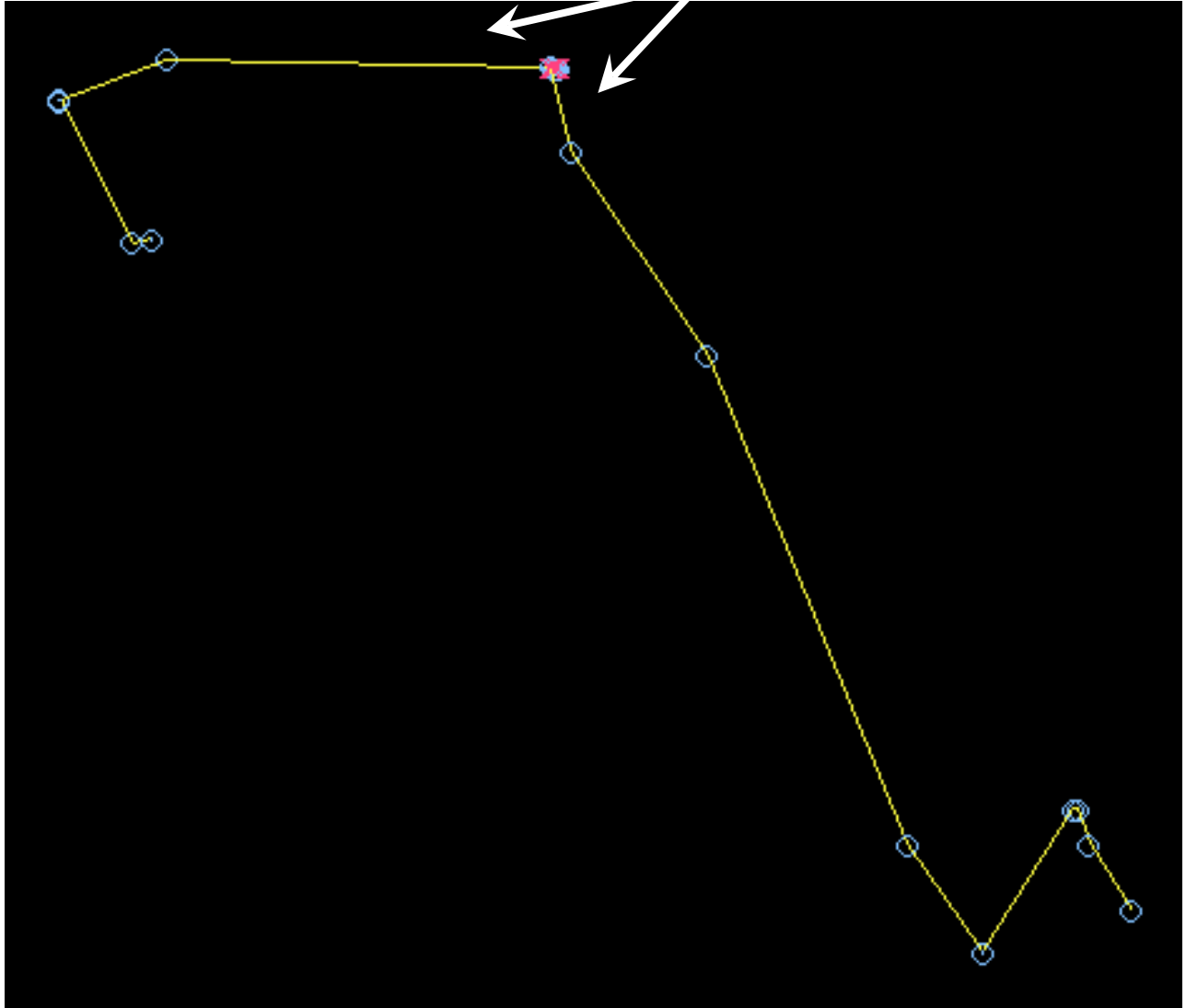
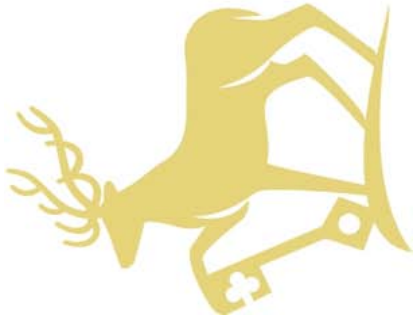
Chin & Spyrou *to present at* American Nuclear Society Winter Meeting 11-15 Nov 2007 Washington



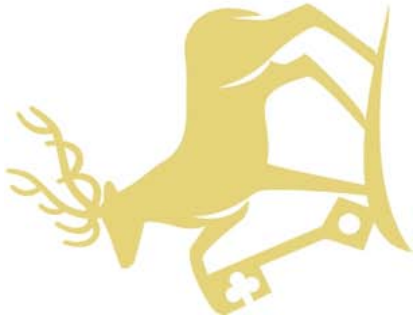
Positron about to decay in flight	1	0.606	1	2	0.155,0.023,500.314	-0.122,-0.592, 0.797
Resulting photons	1	0.979	0	2	0.155,0.023 500.314	-0.311, 0.020, 0.950
NOT THERMALISED?		0.649	0	2	0.155,0.023 500.314	0.282,-0.935,-0.213

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

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m o r e ...

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