Joint ICTP-IAEA Workshop on Monte Carlo Radiation Transport and Associated Data Needs for Medical Applications
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Lecture 13

Variance reduction techniques

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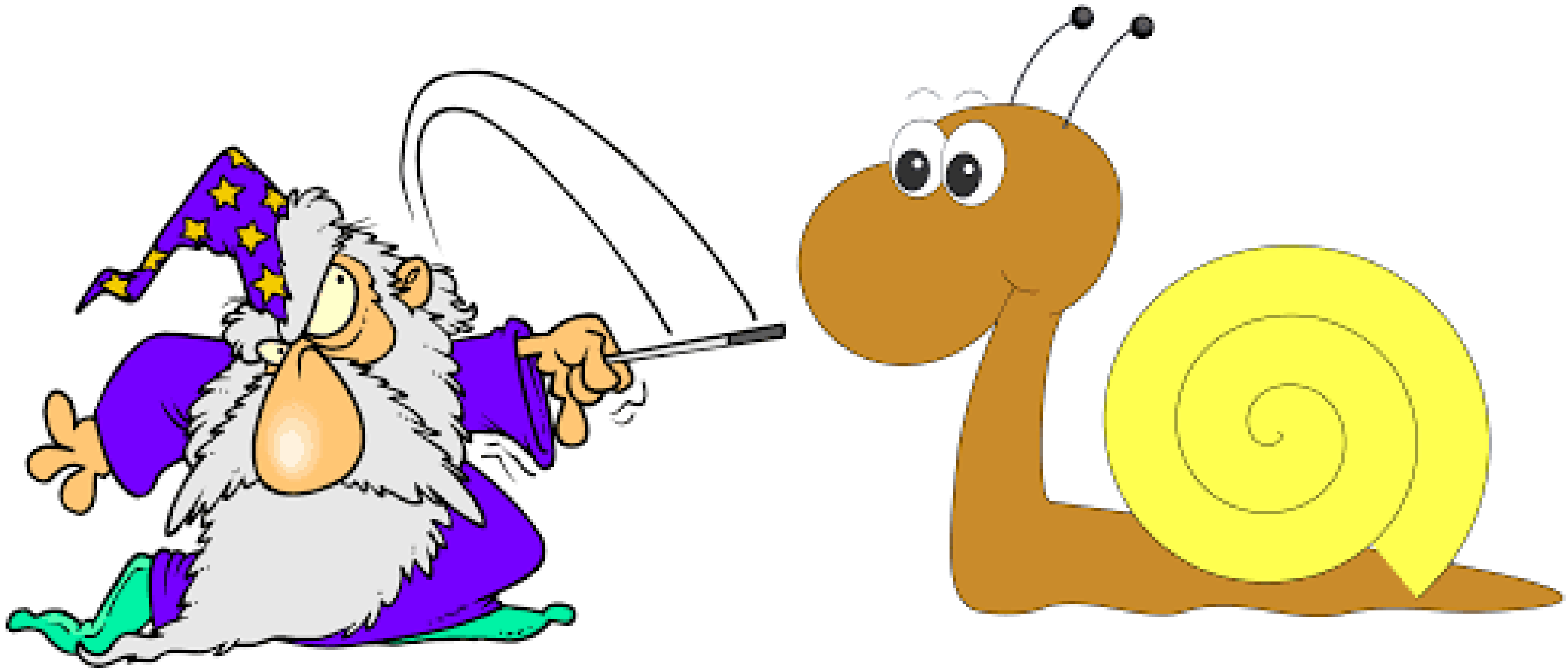
The black art of fast Monte Carlo simulations



The black art of fast Monte Carlo simulations

Hello (Monte Carlo) 12d world!

More dimensions = more efficient

$$r^2 = \sum_{i=1}^{d} x_i^2$$

Beyond 4 dimensions, Monte Carlo wins !

Monte Carlo

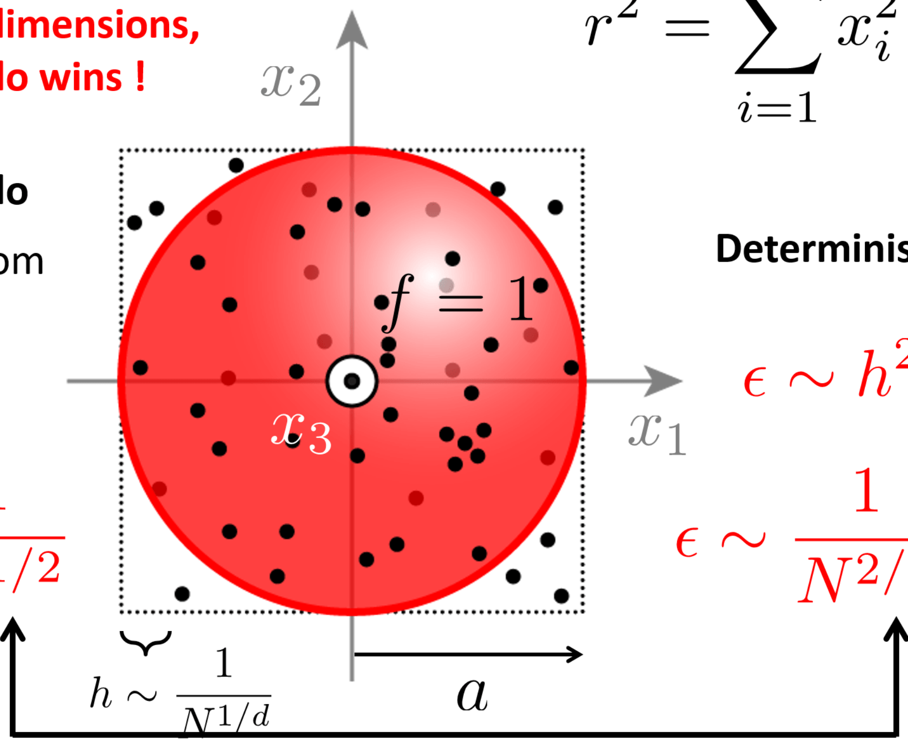
It is a random sampling process, so we have

$$\epsilon \sim \frac{1}{N^{1/2}}$$

Deterministic

$$\epsilon \sim h^2$$

$$\epsilon \sim \frac{1}{N^{2/d}}$$

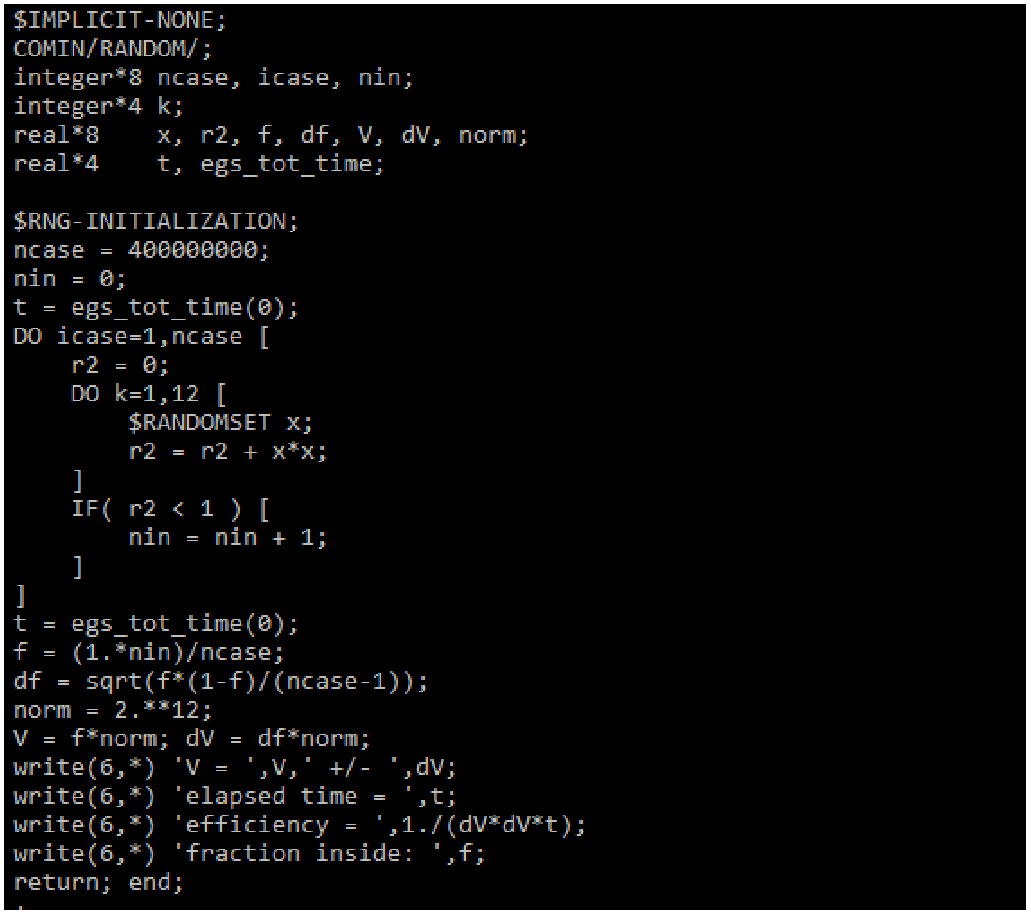


Definition of efficiency

$$\varepsilon = \frac{1}{T\sigma^2}$$

- σ is an estimate of the uncertainty of the quantity of interest, *e.g.*
  - The uncertanty of the 12d sphere volume
  - The uncertainty of the photon fluence in a region of interest
  - The uncertainty of the dose at $d_{\max}$
  - ...
- T is the total CPU time for the calculation.
- As $\sigma^2 \propto 1/N$ and $T \propto N$, the efficiency is independent of the number of samples N used to determine it
- Efficiency comparisons only make sense for the same situation on the same hardware

Version 0

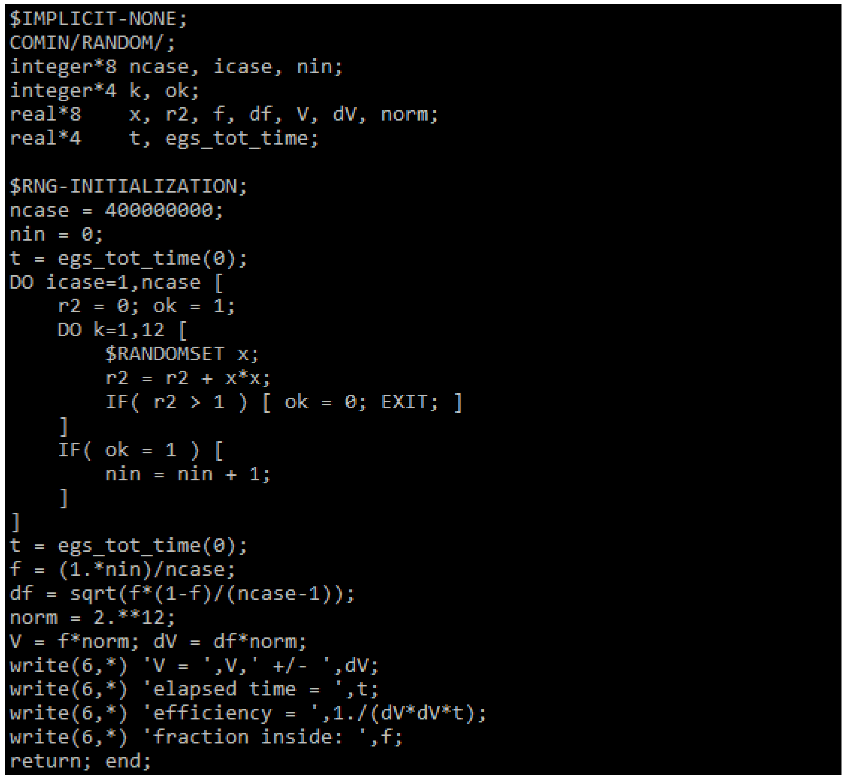


```
$IMPLICIT-NONE;
COMIN/RANDOM/;
integer*8 ncase, icase, nin;
integer*4 k;
real*8    x, r2, f, df, V, dV, norm;
real*4    t, egs_tot_time;

$RNG-INITIALIZATION;
ncase = 400000000;
nin = 0;
t = egs_tot_time(0);
DO icase=1,ncase [
    r2 = 0;
    DO k=1,12 [
        $RANDOMSET x;
        r2 = r2 + x*x;
    ]
    IF( r2 < 1 ) [
        nin = nin + 1;
    ]
]
t = egs_tot_time(0);
f = (1.*nin)/ncase;
df = sqrt(f*(1-f)/(ncase-1));
norm = 2.**12;
V = f*norm; dV = df*norm;
write(6,*) 'V = ',V,' +/- ',dV;
write(6,*) 'elapsed time = ',t;
write(6,*) 'efficiency = ',1./(dV*dV*t);
write(6,*) 'fraction inside: ',f;
return; end;
```

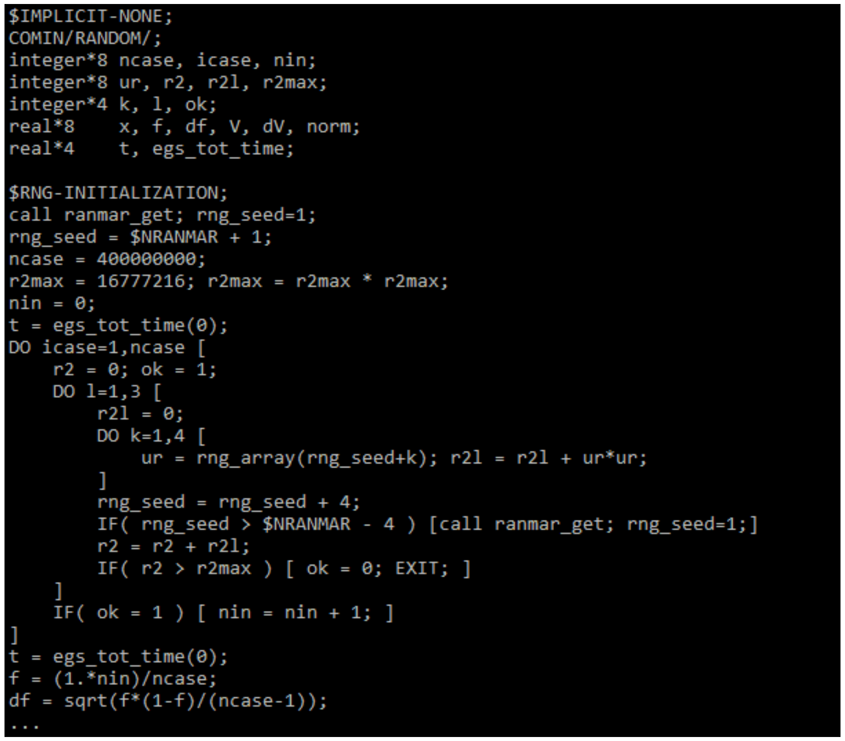
$$\varepsilon = 2.5 \times 10^3\,\mathsf{s}^{-1} \equiv \varepsilon_0$$

Versions 1 & 2



```
$IMPLICIT-NONE;
COMIN/RANDOM/;
integer*8 ncase, icase, nin;
integer*4 k, ok;
real*8    x, r2, f, df, V, dV, norm;
real*4    t, egs_tot_time;

$RNG-INITIALIZATION;
ncase = 400000000;
nin = 0;
t = egs_tot_time(0);
DO icase=1,ncase [
    r2 = 0; ok = 1;
    DO k=1,12 [
        $RANDOMSET x;
        r2 = r2 + x*x;
        IF( r2 > 1 ) [ ok = 0; EXIT; ]
    ]
    IF( ok = 1 ) [
        nin = nin + 1;
    ]
]
t = egs_tot_time(0);
f = (1.*nin)/ncase;
df = sqrt(f*(1-f)/(ncase-1));
norm = 2.**12;
V = f*norm; dV = df*norm;
write(6,*) 'V = ',V,' +/- ',dV;
write(6,*) 'elapsed time = ',t;
write(6,*) 'efficiency = ',1./(dV*dV*t);
write(6,*) 'fraction inside: ',f;
return; end;
```

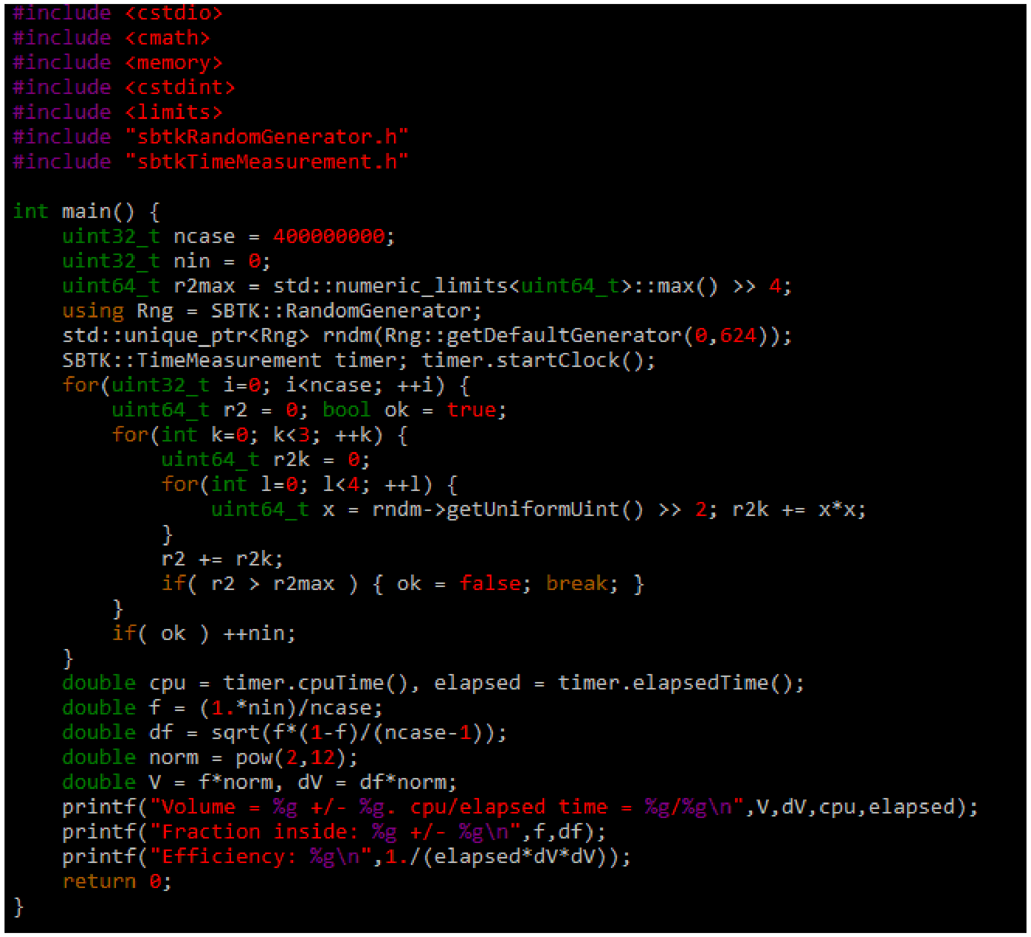


```
$IMPLICIT-NONE;
COMIN/RANDOM/;
integer*8 ncase, icase, nin;
integer*8 ur, r2, r2l, r2max;
integer*4 k, l, ok;
real*8    x, f, df, V, dV, norm;
real*4    t, egs_tot_time;

$RNG-INITIALIZATION;
call ranmar_get; rng_seed=1;
rng_seed = $NRANMAR + 1;
ncase = 400000000;
r2max = 16777216; r2max = r2max * r2max;
nin = 0;
t = egs_tot_time(0);
DO icase=1,ncase [
    r2 = 0; ok = 1;
    DO l=1,3 [
        r2l = 0;
        DO k=1,4 [
            ur = rng_array(rng_seed+k); r2l = r2l + ur*ur;
        ]
        rng_seed = rng_seed + 4;
        IF( rng_seed > $NRANMAR - 4 ) [call ranmar_get; rng_seed=1;]
        r2 = r2 + r2l;
        IF( r2 > r2max ) [ ok = 0; EXIT; ]
    ]
    IF( ok = 1 ) [ nin = nin + 1; ]
]
t = egs_tot_time(0);
f = (1.*nin)/ncase;
df = sqrt(f*(1-f)/(ncase-1));
...
```

$$\varepsilon = 3.8 \times 10^3\,\mathsf{s}^{-1} \approx 1.5 \times \varepsilon_0 \qquad \varepsilon = 8.2 \times 10^3\,\mathsf{s}^{-1} \approx 3.3 \times \varepsilon_0$$

Version 3 (C++, single-threaded)

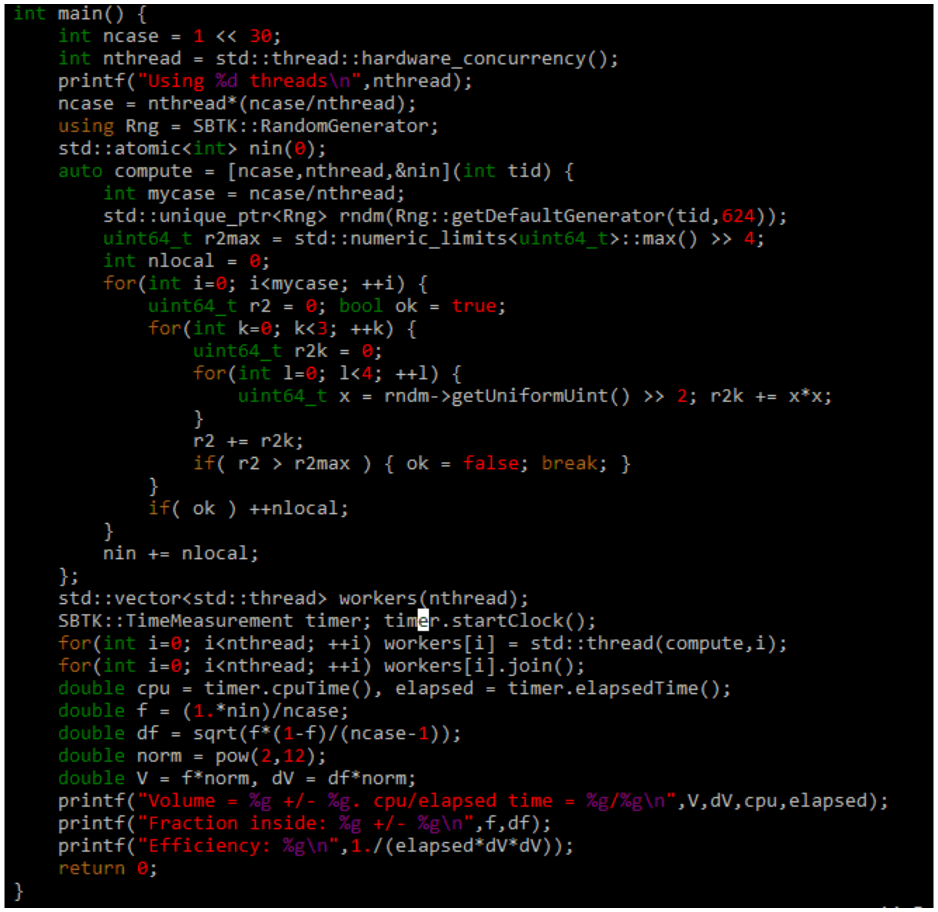


```
#include <cstdio>
#include <cmath>
#include <memory>
#include <cstdint>
#include <limits>
#include "sbtkRandomGenerator.h"
#include "sbtkTimeMeasurement.h"

int main() {
    uint32_t ncase = 400000000;
    uint32_t nin = 0;
    uint64_t r2max = std::numeric_limits<uint64_t>::max() >> 4;
    using Rng = SBTK::RandomGenerator;
    std::unique_ptr<Rng> rndm(Rng::getDefaultGenerator(0,624));
    SBTK::TimeMeasurement timer; timer.startClock();
    for(uint32_t i=0; i<ncase; ++i) {
        uint64_t r2 = 0; bool ok = true;
        for(int k=0; k<3; ++k) {
            uint64_t r2k = 0;
            for(int l=0; l<4; ++l) {
                uint64_t x = rndm->getUniformUint() >> 2; r2k += x*x;
            }
            r2 += r2k;
            if( r2 > r2max ) { ok = false; break; }
        }
        if( ok ) ++nin;
    }
    double cpu = timer.cpuTime(), elapsed = timer.elapsedTime();
    double f = (1.*nin)/ncase;
    double df = sqrt(f*(1-f)/(ncase-1));
    double norm = pow(2,12);
    double V = f*norm, dV = df*norm;
    printf("Volume = %g +/- %g. cpu/elapsed time = %g/%g\n",V,dV,cpu,elapsed);
    printf("Fraction inside: %g +/- %g\n",f,df);
    printf("Efficiency: %g\n",1./(elapsed*dV*dV));
    return 0;
}
```

$$\varepsilon = 12.5 \times 10^3 \approx 5 \times \varepsilon_0$$

Version 4 (C++, multi-threaded)



```
int main() {
    int ncase = 1 << 30;
    int nthread = std::thread::hardware_concurrency();
    printf("Using %d threads\n",nthread);
    ncase = nthread*(ncase/nthread);
    using Rng = SBTK::RandomGenerator;
    std::atomic<int> nin(0);
    auto compute = [ncase,nthread,&nin](int tid) {
        int mycase = ncase/nthread;
        std::unique_ptr<Rng> rndm(Rng::getDefaultGenerator(tid,624));
        uint64_t r2max = std::numeric_limits<uint64_t>::max() >> 4;
        int nlocal = 0;
        for(int i=0; i<mycase; ++i) {
            uint64_t r2 = 0; bool ok = true;
            for(int k=0; k<3; ++k) {
                uint64_t r2k = 0;
                for(int l=0; l<4; ++l) {
                    uint64_t x = rndm->getUniformUint() >> 2; r2k += x*x;
                }
                r2 += r2k;
                if( r2 > r2max ) { ok = false; break; }
            }
            if( ok ) ++nlocal;
        }
        nin += nlocal;
    };
    std::vector<std::thread> workers(nthread);
    SBTK::TimeMeasurement timer; timer.startClock();
    for(int i=0; i<nthread; ++i) workers[i] = std::thread(compute,i);
    for(int i=0; i<nthread; ++i) workers[i].join();
    double cpu = timer.cpuTime(), elapsed = timer.elapsedTime();
    double f = (1.*nin)/ncase;
    double df = sqrt(f*(1-f)/(ncase-1));
    double norm = pow(2,12);
    double V = f*norm, dV = df*norm;
    printf("Volume = %g +/- %g. cpu/elapsed time = %g/%g\n",V,dV,cpu,elapsed);
    printf("Fraction inside: %g +/- %g\n",f,df);
    printf("Efficiency: %g\n",1./(elapsed*dV*dV));
    return 0;
}
```

$\varepsilon = 84.2 \times 10^3\,\text{s}^{-1} \approx 33.7 \times \varepsilon_0$ (8 threads on a 4-core laptop)

Can we do better?

$$V = \int\limits_{-1}^{1} \mathrm{d}x_1 \cdots \mathrm{d}x_{12} \Theta\left(1 - x_1^2 - \cdots - x_{12}^2\right) \tag{1.1}$$

$$= 2^{12} \int\limits_{0}^{1} \mathrm{d}x_1 \cdots \mathrm{d}x_{12} \Theta\left(1 - x_1^2 - \cdots - x_{12}^2\right) \tag{1.2}$$

$$= 2^{24} \int\limits_{0}^{1} \frac{\mathrm{d}x_1}{2\sqrt{x_1}} \cdots \frac{\mathrm{d}x_{12}}{2\sqrt{x_{12}}} \Theta\left(1 - x_1^2 - \cdots - x_{12}^2\right) \left(\prod_{i=1}^{12} x_i\right)^{1/2} \tag{1.3}$$

$$= 2^{24} \int\limits_{0}^{1} \mathrm{d}\eta_1 \cdots \mathrm{d}\eta_{12} \Theta\left(1 - \eta_1^4 - \cdots - \eta_{12}^2\right) \left(\prod_{i=1}^{12} \eta_i\right) \tag{1.4}$$

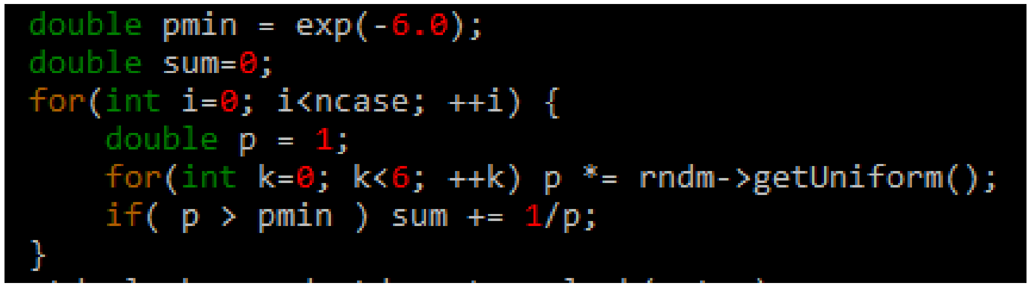
$$\varepsilon = 362.1 \times 10^3\,\mathsf{s}^{-1} \approx 145 \times \varepsilon_0$$

Can we do even better?

$$V = 2^{12}\int_0^1 \mathrm{d}x_1\cdots\mathrm{d}x_{12}\Theta\left(1-x_1^2-\cdots-x_{12}^2\right) \tag{1.5}$$

$$= 2^{12}\int_0^\infty\int_0^{2\pi} r_1\mathrm{d}r_1\mathrm{d}\phi_1 e^{-6r_1^2}\cdots r_6\mathrm{d}r_6\mathrm{d}\phi_6 e^{-6r_6^2}\Theta\left(1-\sum_{i=1}^6 r_i^2\right)\exp\left(6\sum_{i=1}^6 r_i^2\right) \tag{1.6}$$

$$= \left(\frac{\pi}{6}\right)^6\int_0^1 \mathrm{d}\eta_1\cdots\mathrm{d}\eta_6\Theta\left(\prod_{i=1}^6\eta_i-e^{-6}\right)\left(\prod_{i=1}^6\eta_i\right)^{-1} \tag{1.7}$$

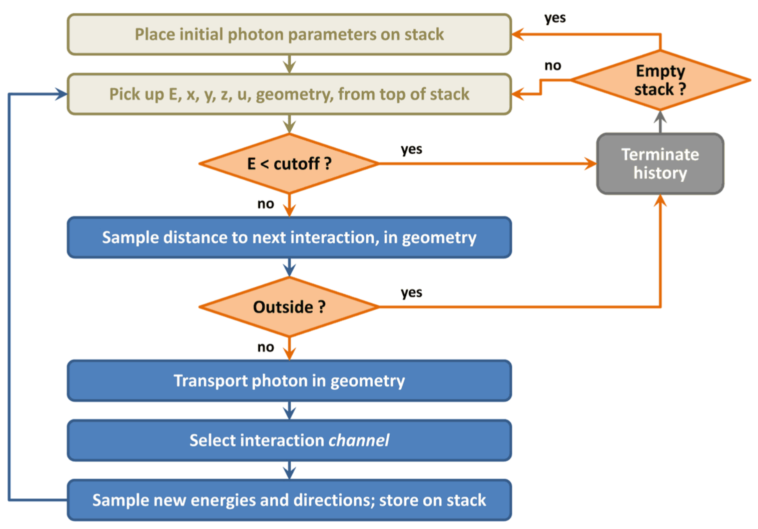

```
double pmin = exp(-6.0);
double sum=0;
for(int i=0; i<ncase; ++i) {
    double p = 1;
    for(int k=0; k<6; ++k) p *= rndm->getUniform();
    if( p > pmin ) sum += 1/p;
}
```

$$\varepsilon = 6.8 \times 10^7\,\mathsf{s}^{-1} \approx 27000 \times \varepsilon_0$$

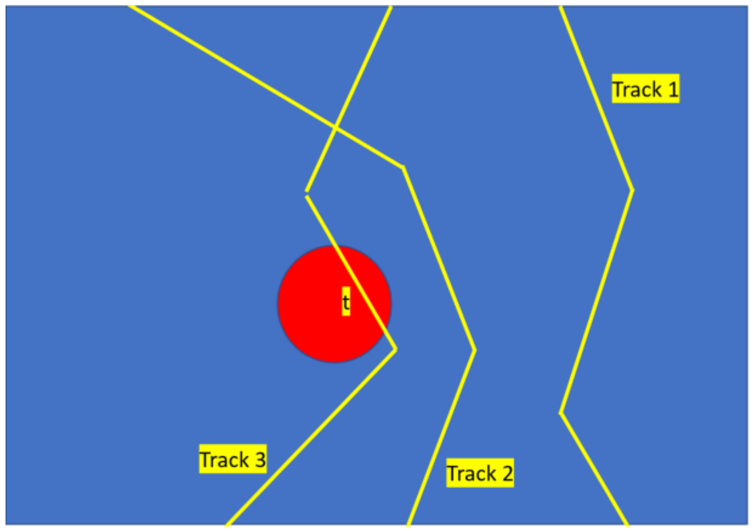
Hello (Monte Carlo) 12d world - Summary

- Speed-up compared to naive implementation: 27,000!
- Better coding: factor of ~ 5
- Parallel implementation: factor of ~ 6 (on 4-core laptop)
- Clever algorithm: factor of ~ 900

What do points in a sphere have in common with radiation transport?


Place initial photon parameters on stack
Pick up E, x, y, z, u, geometry, from top of stack
E < cutoff ?
yes
no
Sample distance to next interaction, in geometry
Outside ?
yes
no
Transport photon in geometry
Select interaction *channel*
Sample new energies and directions; store on stack
Empty stack ?
yes
no
Terminate history

Consider tracks with 2 interactions



Track 1: $(\lambda_1, \theta_1, \phi_1, \lambda_2, \theta_2, \phi_2) \rightarrow 0$
Track 2: $(\lambda_1, \theta_1, \phi_1, \lambda_2, \theta_2, \phi_2) \rightarrow 0$
Track 3: $(\lambda_1, \theta_1, \phi_1, \lambda_2, \theta_2, \phi_2) \rightarrow t$

$\Rightarrow$ Points in 6d space

There are many known VRTs

- Proper selection of available/development of new VRTs is the bread and butter of MC simulations
- Many papers since the veray early days of MC radiation transport
- Some commonly used tecniques are
  - Particle splitting
  - Russian Roulette
  - Interaction forcing
  - Exponential transforms
  - Correlated sampling
  - Importance and/or stratified sampling
  - Cross section enhancement
  - ...

VRT in the EGSnrc package

- Forcing photon interactions (BEAMnrc, CAVRZnrc)
- Bremsstrahlung splitting (BEAMnrc)
- Russian Roulette (BEAMnrc, cavity, egs_chamber)
- Bremsstrahlung cross section enhancement (BEAMnrc)
- Photon splitting (DOSXYZnrc, CAVRZnrc, cavity)
- Photon cross section enhancement (egs_chamber)
- Correlated sampling (egs_chamber)

Explorer

Explorer

Particle splitting

- In a MC simulation, one can split a particle into N identical particles at any time
- Each of the daughter particles gets $1/N$ of the statistical weight of the original particle
- Each daughter particle can then be transported separately thus improving the information gain
- Typical application: particles arriving in a region that is only rarely visited during a simulation or in combination with Russian Roulette
- Particle splitting is a true VRT, it does not modify the physics in any way

Russian Roulette (RR)

- RR is the reverse of particle splitting: at any time one can terminate a particle trajectory with a given probability p (*i.e.* play a RR game with the particle where the survival probability is p)
- If the particle survives, its statistical weight is increased by $1/p$.
- A particle surviving a RR game represents all other particles killed in the game
- Typical application: avoid transporting particles that contribute nothing or very little to the quantity of interest
- RR is a true VRT, it does not modify the physics in any way

Bremsstrahlung splitting

figures/brem_split-eps-converted-to.pdf

Approach A: $E_{after} = E_{in} - E_{\gamma 1}$ (or $E_{\gamma 2}$ or $E_{\gamma 3}$)

Approach B: $E_{after} = E_{in} - \overline{E}_{\gamma}$

Which is correct?

Bremsstrahlung splitting is simply Particle splitting + RR

Step 1 Split electron into N electrons, each having a weight of $1/N$

Step 2 Sample 1 bremsstrahulung photon for each of the N electrons $\Rightarrow N\ \gamma$'s

Step 3 Play RR with the electrons with $p = 1/N \Rightarrow$ 1 electron with weight 1 survives on average

$\Rightarrow$ Approach A is correct

Note: Energy conservation is only fulfilled *on average* and not on event-by-event basis

$\Rightarrow$ Not suitable if event-by-event energy conservation is important

Example: bremsstrahlung splitting in kV beams

figures/eff_rel_ubs_vs_dbs-eps-converted-to.pdf

From [Mainegra-Hing and Kawrakow, Med. Phys. 33, (2006) 2683]

Photon forcing

- Consider a photons passing through a geometry (or region) with a thickness of X mfp
- Fraction of photons interacting in the geometry will be $1 - e^{-X}$
- Fraction of photons leaving without interaction will be e^{-X}

$\Rightarrow$ Split photon into an interacting portion (weight $1 - e^{-X}$) and a non-interacting portion (weight e^{-X})

$\Rightarrow$ Transport the non-interacting portion to end of geometry (or region)

$\Rightarrow$ Force mfp to interaction to be between 0 and X for interacting portion

$$\gamma\text{-mfp} = -\ln(1 - \text{RN}(1 - e^{-X}))$$

Used *e.g.* in CAVRZnrc for simulations related to the primary air kerma standard.

Photon splitting

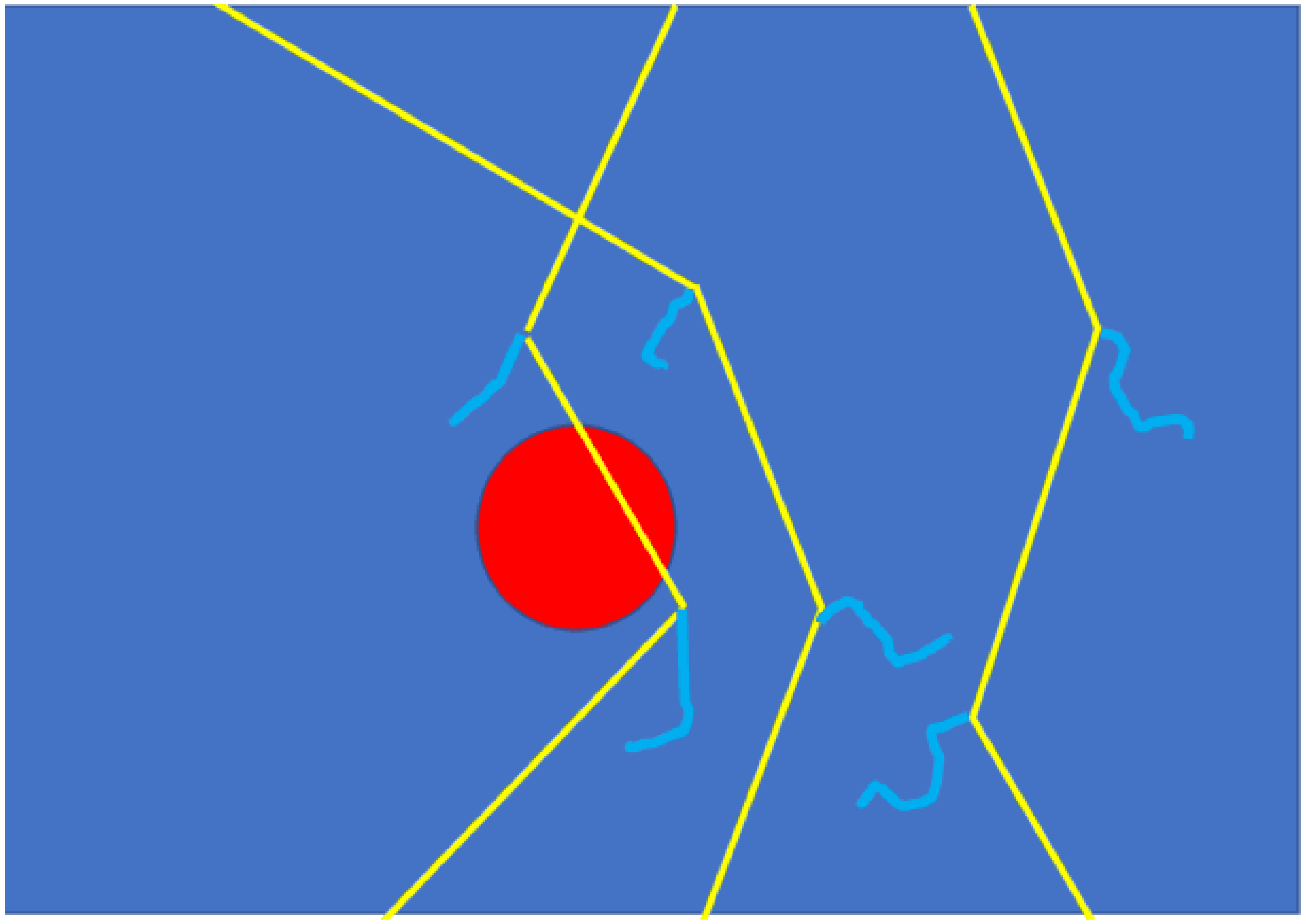
- λ is γ-mfp to an interaction. Normally $\lambda = -\ln(1-\eta)$
- With splitting on (splitting number N_s)

$$\lambda_i = -\ln\left(1 - \frac{\eta + i}{N_\mathrm{s}}\right) \ , \quad i = 0 \ldots N_\mathrm{s}$$

  i.e. we have interactions uniformly spread through the phantom and a single photon sets several electrons in motion

- Electrons have weight w/N_s (w = initial photon's weight)
- RR with scattered photons $\Rightarrow$ weight w if they survive
- Surviving scattered photons are split again
- Introduced for xVMC in Phys.Med.Biol **45** (2000) 2163
- Used in DOSXYZnrc, CAVRZnrc, cavity

Ion chamber simulations



Photon cross section enhancement (XCSE)

- Increase photon cross section in a (set of) region(s) by a factor of C
- When a photon interacts, split it into an interacting portion (weight $1/C$) and a non-interacting portion (weight $1 - 1/C$)
- Keep electrons set in motion (they have weight of w_0/C)
- Play RR with scattered photon(s) and non-interacting portion of initial photon, *i.e.*, if $\eta < 1/C$ keep scattered photon(s), else keep initial photon. Surviving photons have again weight w_0
- Used in egs_chamber
- Introduced in Med.Phys. 35 (2008) 1328

Photon cross section enhancement (XCSE)

figures/from_iwan_egs_chamber/tracks-eps-converted-to.pdf

Correlated sampling

figures/correlated-eps-converted-to.pdf

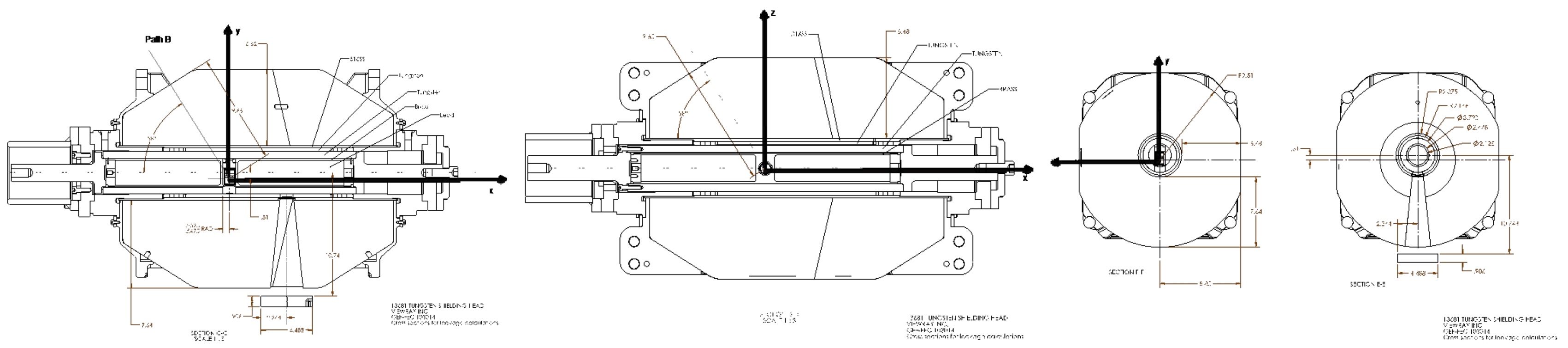
Efficiency gains due to

- Tracks not entering regions of interest only simulated in one geometry
- Correlation between tracks $\Rightarrow$ uncertainty on dose ratio can be significantly lower than individual dose uncertainties
- Available in egs_chamber

Approximate techniques

- Range rejection
- Use of high transport cutoff energies (ECUT, PCUT)
- Use of high secondary particle profuction thresholds (AE, AP)
- Use of simplified geometries
- The condensed history technique
- Use of approximate cross sections (*e.g.*, Klein-Nishina instead of bound Compton scattering, turn off spin effects in elastic scattering, etc.)
- Need to understand impact on accuracy very well!

Example: shielding calculations

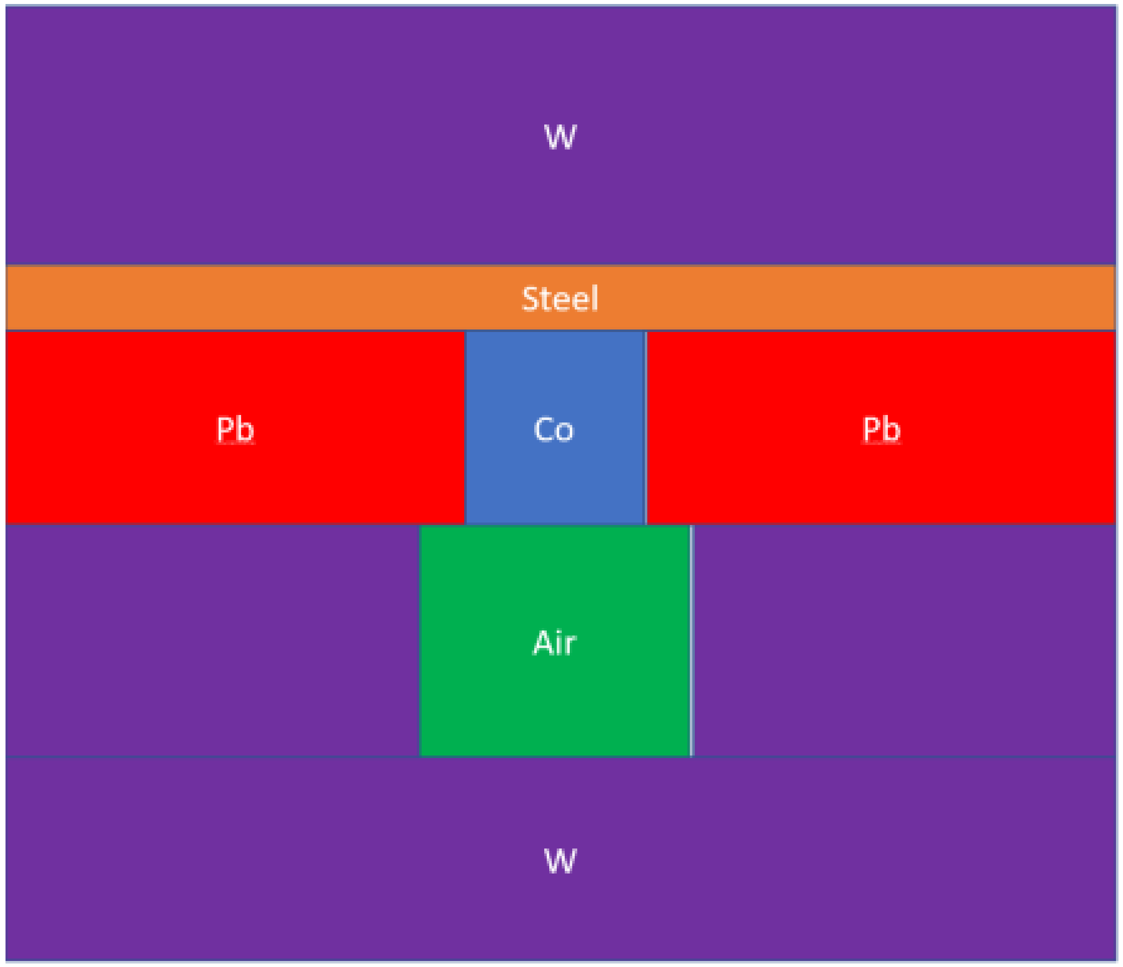


- 15,000 Ci source
- Original design: depleated uranium (DU)
- Design goal: replace DU with tungsten
- Goal: ≤ 1 mRad/h at 1 m from source to satisfy ICRP and IEC standards
- Constraint: new head must fit in existing gantry

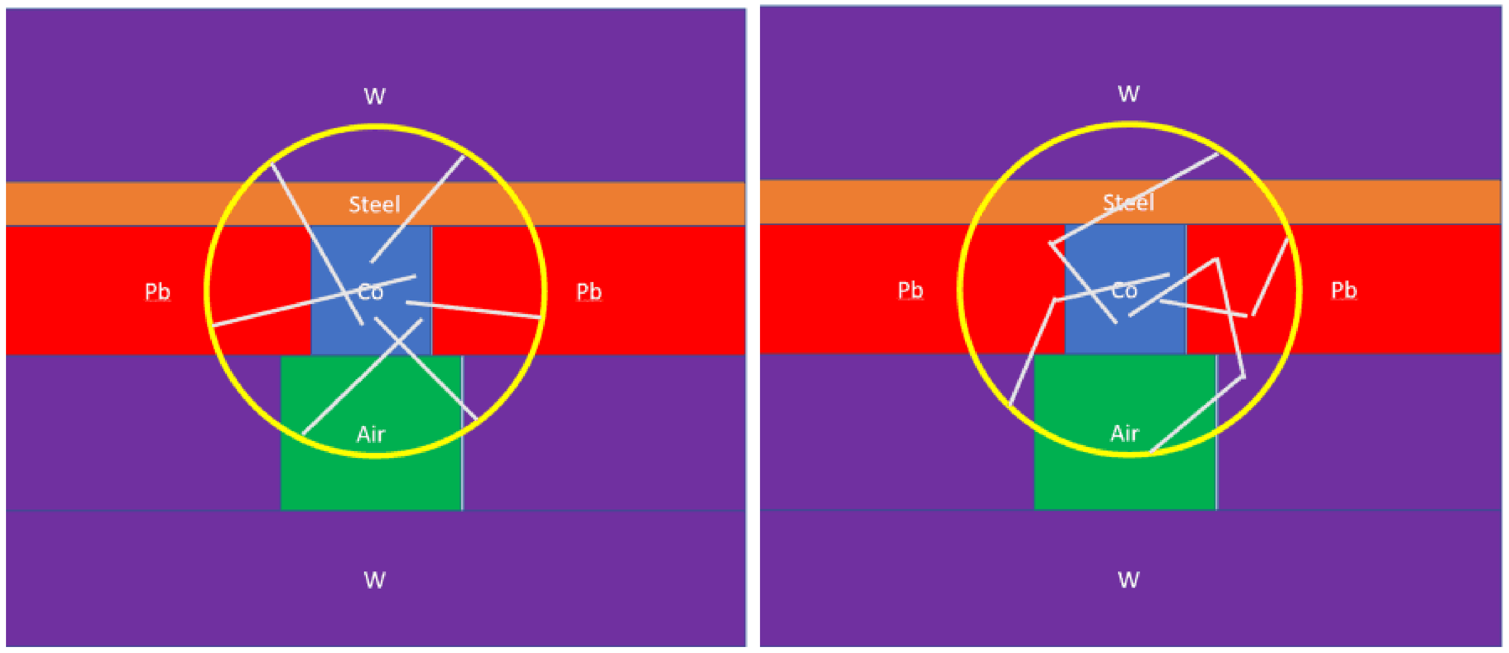
Seems Hopeless!

- ~ 1 out of 10^9 photons escape
- Need to simulate $\sim 10^{15}$ decays to get ~ 5% statistics in 25 cm^2 scoring regions at 1 m without using VRT
- All is scatter
- Highly heterogeneous geometry $\Rightarrow$ standard VRT's did not really work (at most a 10-fold acceleration)
- $\sim$ 2 year of computation on available computers
- Buy $500k+ cluster?

Divide et impera (Divide and Conquer)!



Divide et impera (Divide and Conquer)!



- Select N photons from source
- For each, place photon with weight $w_0 e^{-\lambda_i}$ at intersection with sphere
- Transport each photon. From each interaction, place scattered photon with weigth $w_0 e^{-\lambda_i}$ at intersection with sphere
- Discard transported photons when they reach sphere

Divide et impera (Divide and Conquer)!

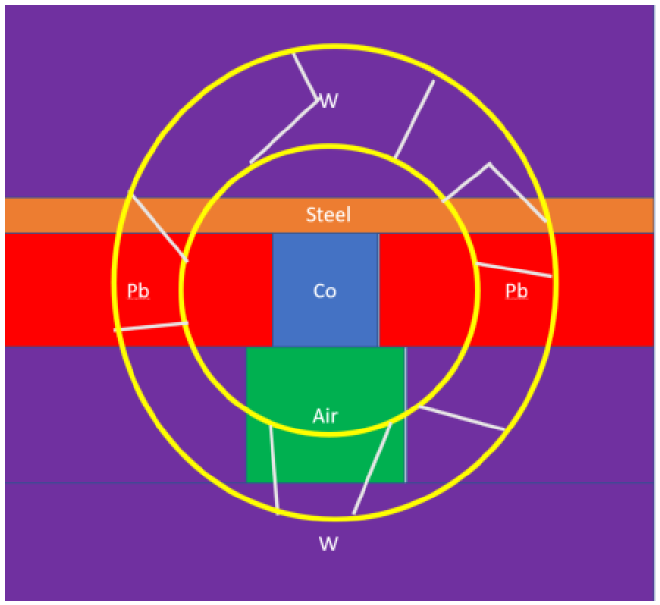
- Now have N_1 photons at first surface with weights w_i
- Compute average weight $\bar{w} = \sum w_i / N_1$
- Play RR with photons having $w_i < \bar{w}$ with survival probability $p = w_i / \bar{w}$
- Split photons with $w_i > \bar{w}$ into $w_i / \bar{w}$ photons

$\Rightarrow$ All photons now have weight $\bar{w}$

$\Rightarrow$ Photons “magically" concentrate along paths with less attenuation

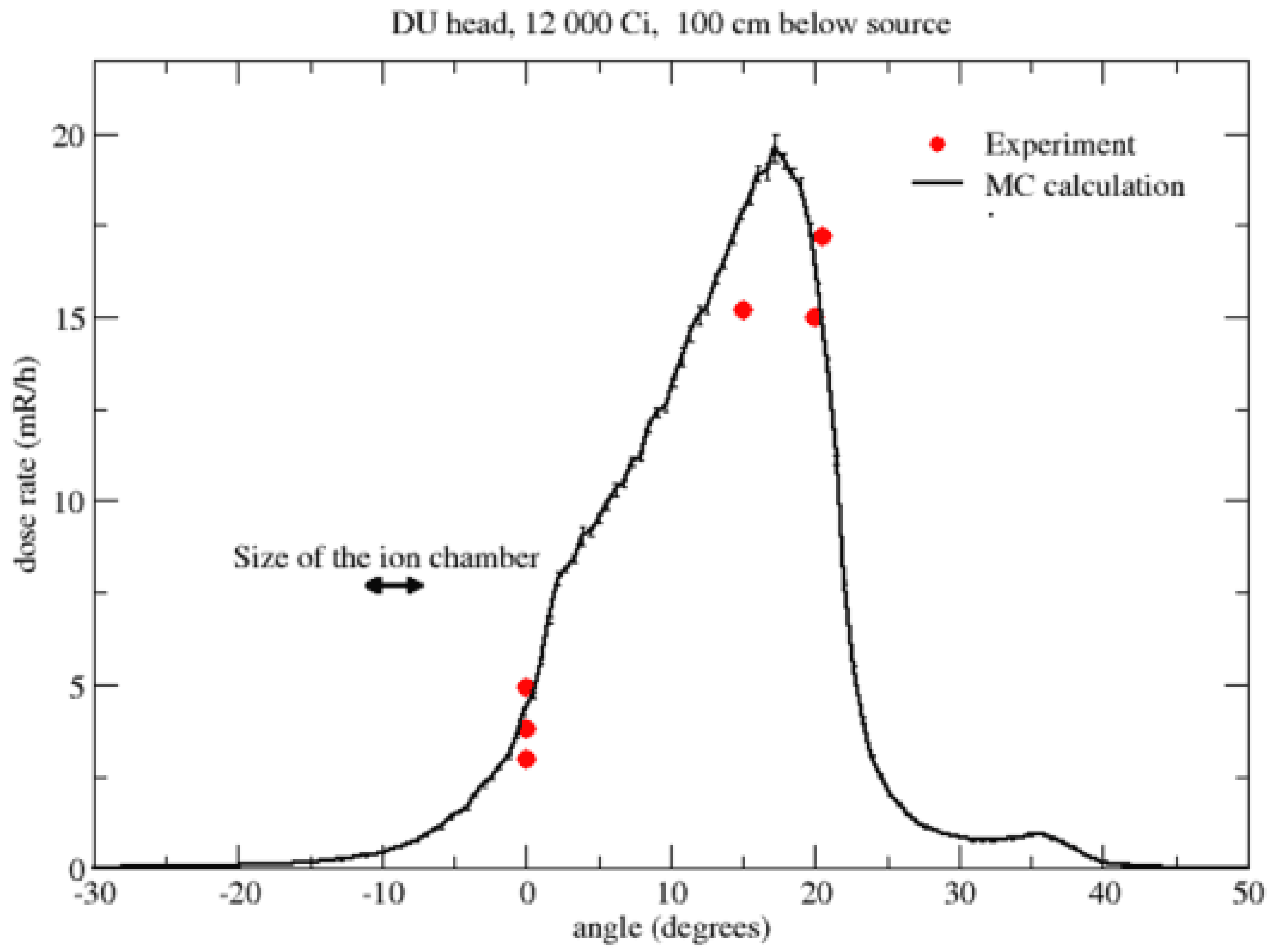
- Now add next surface
- Transport from first to second surface in the same way
- Repeat until exiting treatment head

Divide et impera (Divide and Conquer)!

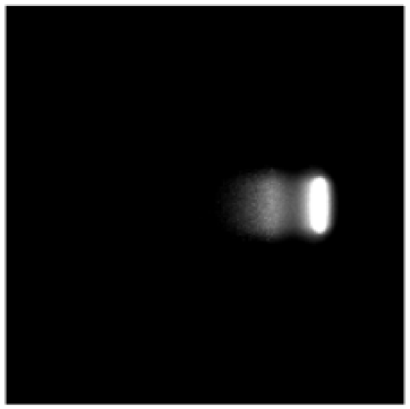


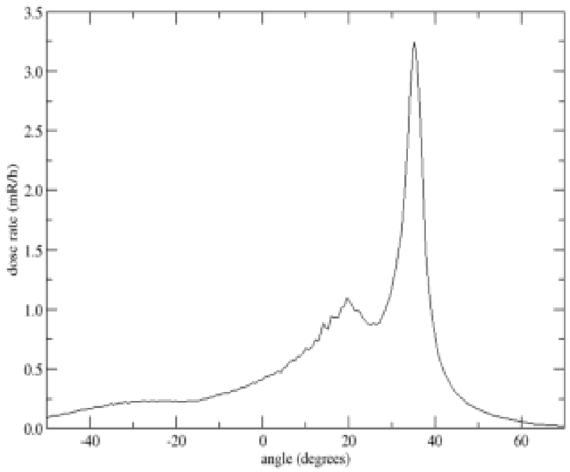
- 100 “bunches” of 10^6 photons are enough to get ~ 1% statistics!
- Note: each “bunch” is **one** statistically independent event
- 10-20 surfaces
- $\sim 10^6$ acceleration

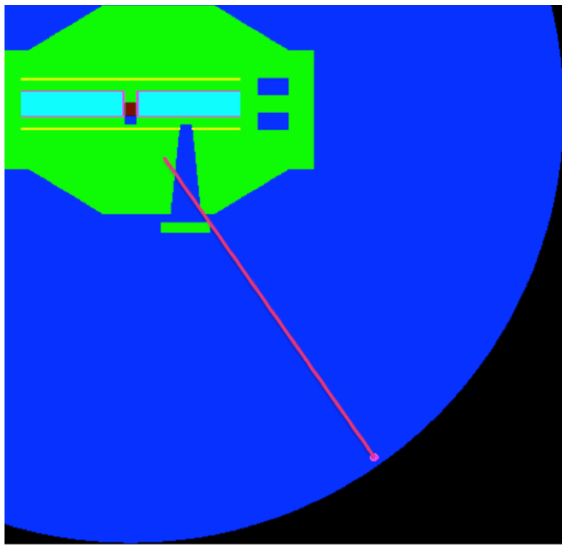
Comparison with measurements



Need to modify auxilary radiation shield







Summary

- VRT’s can increase the efficiency of MC simulations by orders of magnitude
- It is important to learn how to use the VRT’s available in the various EGSnrc user codes!