Monte Carlo Simulations: Efficiency Improvement Techniques and Statistical Considerations

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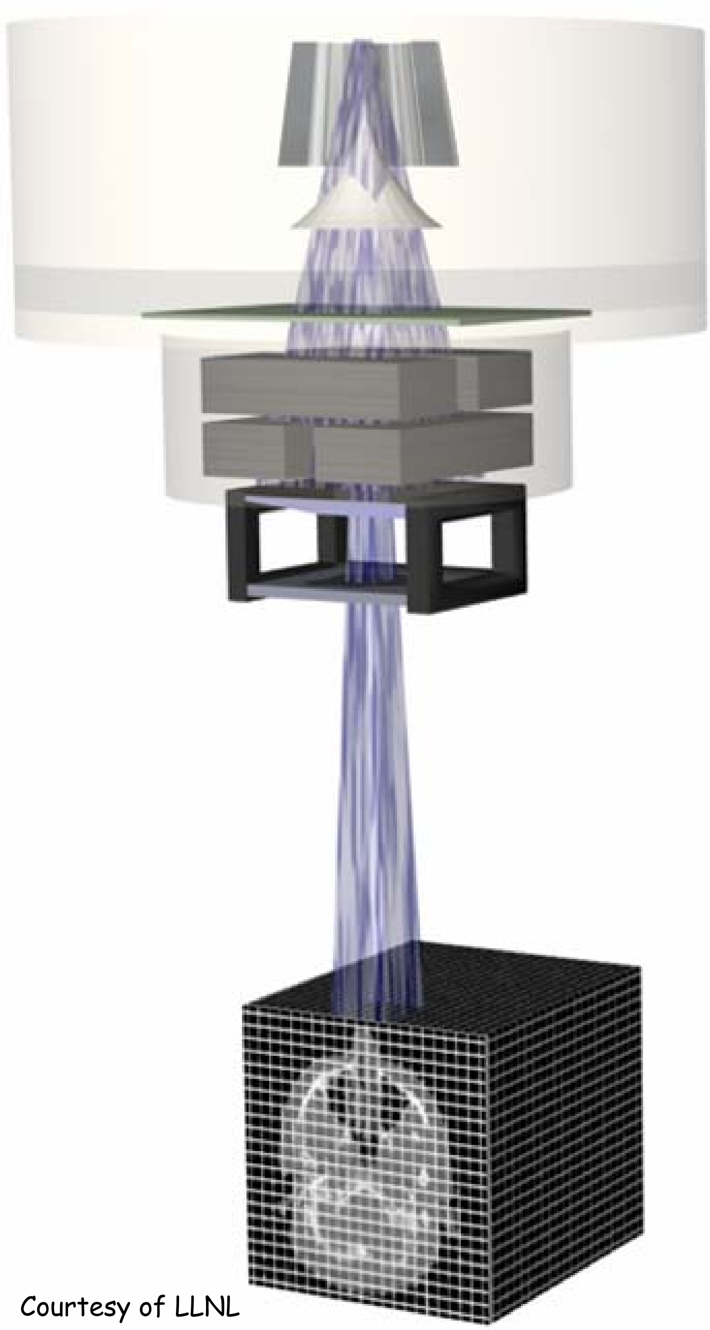

Courtesy of LLNL

If linac simulations take too long …

- Divide the beam into treatment-independent and treatment-dependent components
- Simulate treatment-independent components
  - characterize phase space distribution with a beam model
- Simulate treatment-dependent components and the patient CT together

Courtesy of LLNL

If linac simulations can be made fast enough …
Do all at once …

- Simulate treatment-independent linac components, treatment-dependent components and the patient CT together

Metrics of Efficiency

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

T: computing time to obtain a variance σ^2

σ^2: variance on the quantity of interest

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Q: How can one increase the efficiency?

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

A: By reducing the computing time that it takes to obtain a sufficiently small variance on the quantity of interest

...

easier said than done!

Variance of what?

- Variance of a quantity of interest averaged over a region
- Examples:
  - ICCR (2000) benchmark suggested by Rogers and Mohan (see http://www.irs.inms.nrc.ca/benchmark_need/benchmark_need.html):

$$\sigma^2 = \frac{1}{n}\sum_{i=1}^{n}\left(\frac{\Delta D_i}{D_i}\right)^2 ,$$

$D_i > 0.5\ D_{max}$

  - fluence in 1x1 cm^2 regions in beam
  - dose on central axis or profile, etc.

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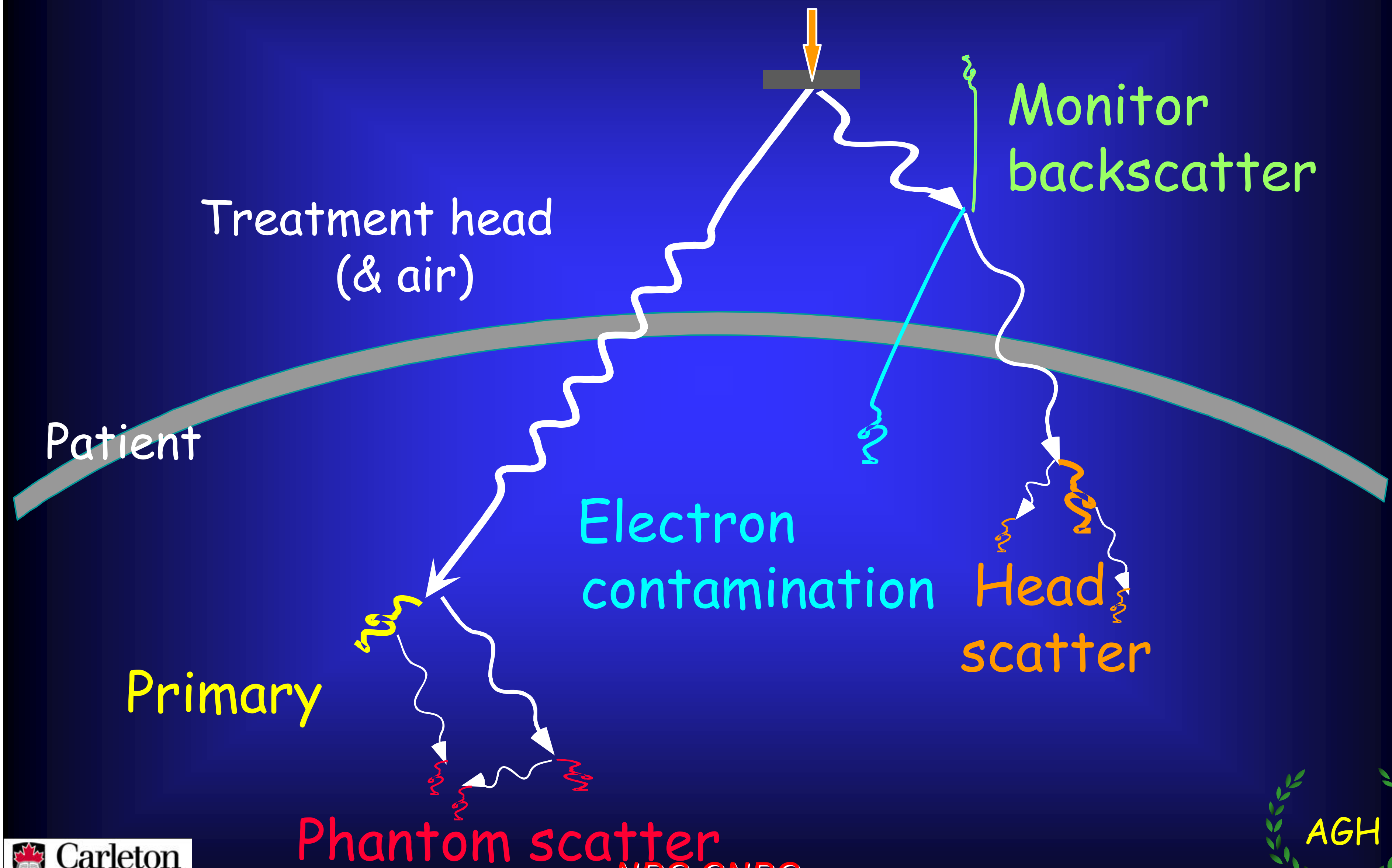
Statistical Uncertainties

- Without them MC calculated values would be … useless
- Prerequisite to efficiency estimation
- Central limit theorem
- The batch method
- The history-by-history method
- Pick independent particles … otherwise correlation
- Only those particles are **independent** that belong to different histories
- Note particle's origin when recycling phase-space files
- Latent Variance

Histories …



Monitor backscatter
Treatment head (& air)
Patient
Electron contamination
Head scatter
Primary
Phantom scatter
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Uncertainties: Computational Considerations

$$\sigma_{\overline{X}} = \sqrt{\frac{\sum_{i=1}^{N}(X_i - \overline{X})^2}{N(N-1)}}$$

$$\sigma_X^2 = \frac{\langle X^2 \rangle - \langle X \rangle^2}{N-1}$$

$$\langle X \rangle = \frac{1}{N}\sum_{i=1}^{N} x_i, \qquad \langle X^2 \rangle = \frac{1}{N}\sum_{i=1}^{N} x_i^2$$

Making the history-by-history technique computationally feasible

- Trick by Salvat

```
IF(HIST.NE.LASTHI(K)) THEN
  Q(K) = Q(K)+QTEMP(K)
  Q2(K)= Q2(K)+QTEMP(K)**2
  QTEMP(K) = DELTAQ
  LASTHI(K)= HIST
ELSE
  QTEMP(K) = QTEMP(K)+DELTAQ
ENDIF
```

```
IF(nhist=X_last) THEN
  X_tmp=X_tmp+delta
ELSE
  X=X+X_tmp
  X2=X2+(X_tmp)**2
  X_tmp=delta
  X_last=nhist
ENDIF
```

Sempau et al, Phys Med Biol 46:1163-1186

Latent Variance

- Divide the dose calculation into 2 phases; A, B

"A" -> the linac simulation resulting in a phase-space

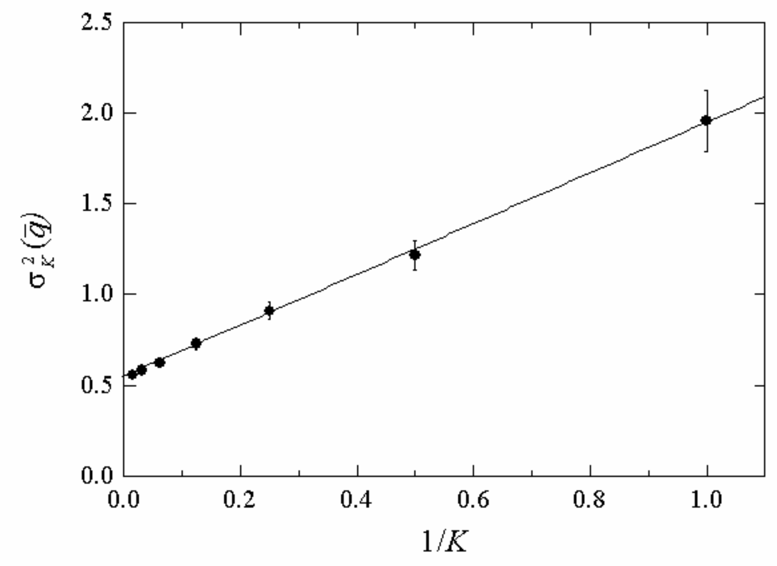
"B" -> the dose calculation using the phase-space

$$\sigma^2(\overline{q}) = \frac{1}{N}(A + B)$$

$$A = \sum_b \langle q_b\rangle^2 \langle n_b^2\rangle + \sum_{a\neq b} \langle q_a\rangle \langle q_b\rangle \langle n_a n_b\rangle - \langle q\rangle^2$$

$$B = \sum_b \sigma^2(q_b)\langle n_b^2\rangle$$

$$\sigma_K^2(\overline{q}) = \frac{1}{N}(A + BK^{-1}).$$



Sempau et al, Phys Med Biol 46:1163–1186

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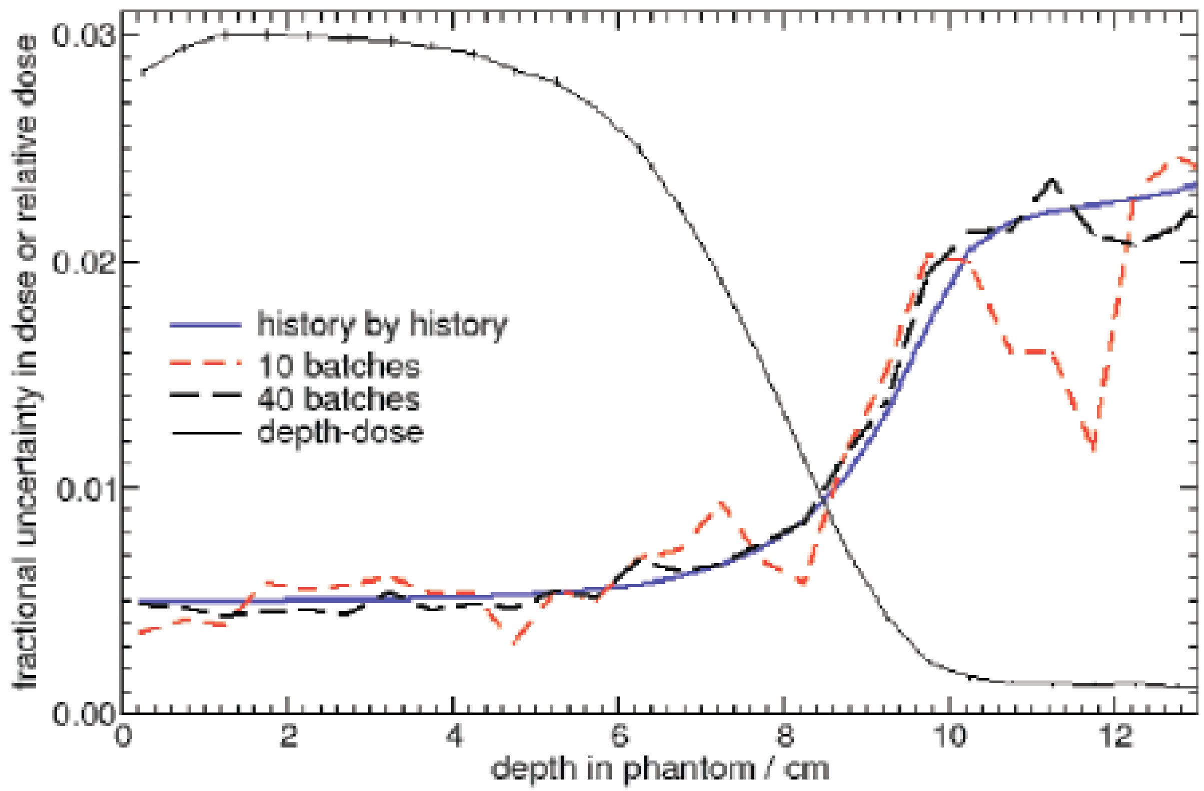
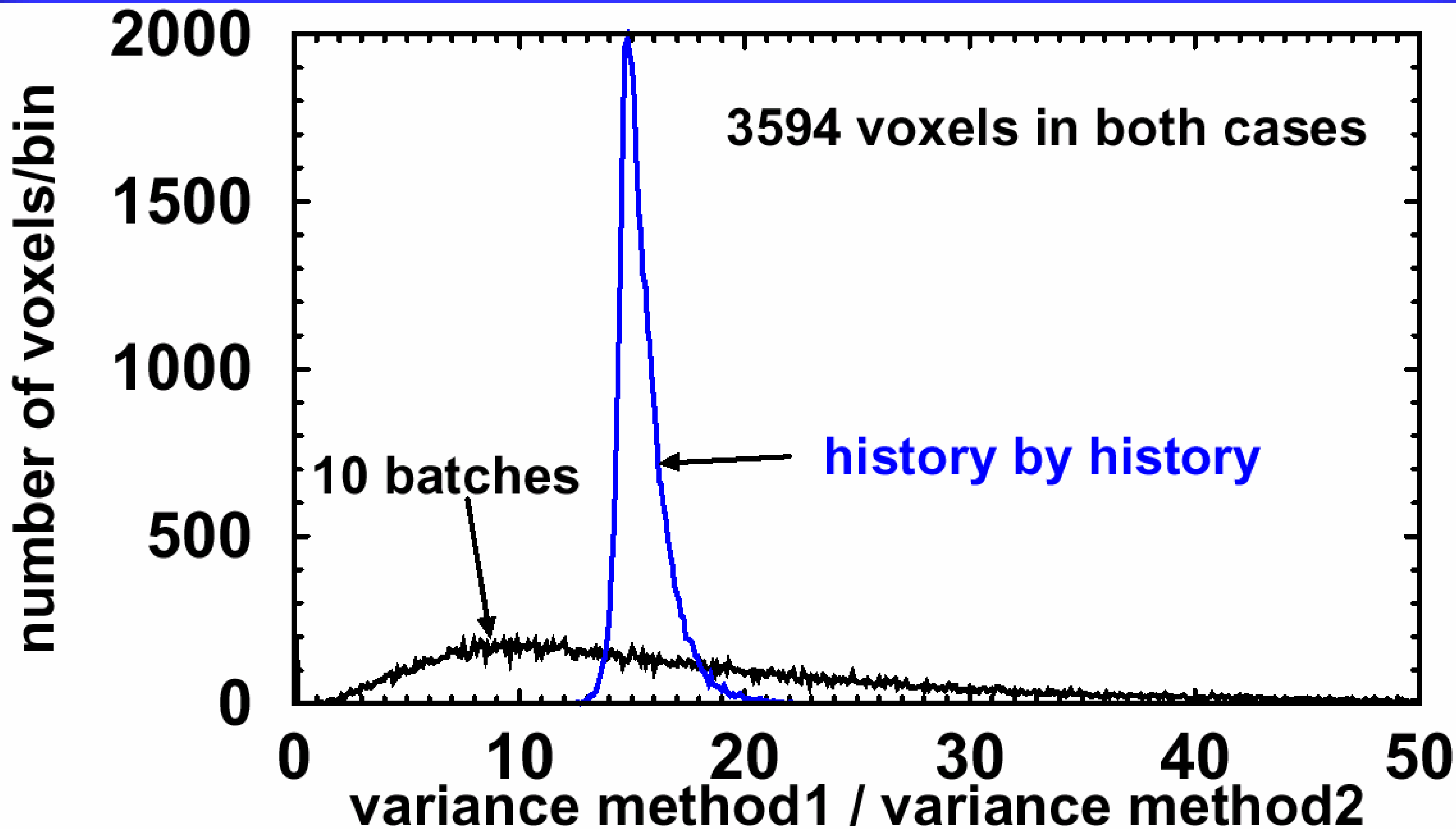
History-by-history and batch methods



Walters, Kawrakow and Rogers, Med Phys 29: 2745-2752

Advantage of history by history



Dose in a brachytherapy phantom: from Gultekin Yegin

Codes used in radiotherapy

- ITS
- MCNP
- PENELOPE
- GEANT4
- No VRTs -> EGS and ITS/ETRAN same efficiency
- Other systems slower
- BEAMnrc code significantly more efficient, still not fast enough for routine RTP

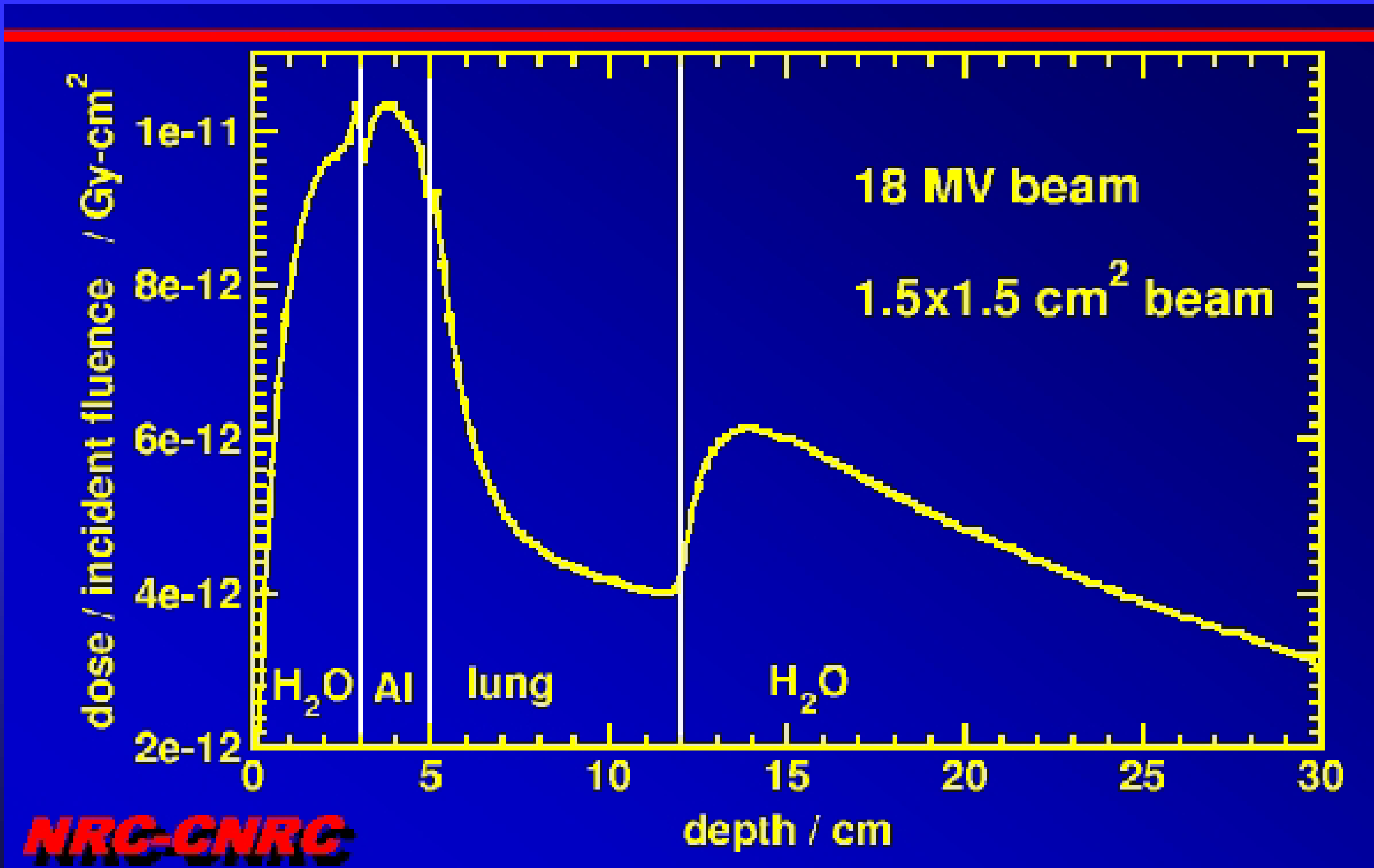
BEAMnrc

- a general purpose user-code for simulation of radiotherapy beams
- built on EGSnrc
- freely available for non-commercial use
- lots of built in variance reduction to enhance efficiency, especially for accelerator photon beams

Codes designed to be more efficient

- The Macro Monte Carlo (MMC) code
- The PEREGRINE code
- Voxel Monte Carlo (VMC/xVMC)
- VMC++
- MCDOSE
- The Monte Carlo Vista (MCV) code system
- The Dose Planning Method (DPM)
- and other codes (Keall and Hoban 1996; Wang, Chui, and Lovelock 1998).

Comparative accuracy of dose calculation



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How fast are current codes?

Monte Carlo code	Time estimate (minutes)	% max. diff. relative to ESG4/PRESTA/DOSXYZ
ESG4/PRESTA/DOSXYZ	42.9	0, benchmark calculation
VMC++	0.9	± 1
MCDOSE (modified ESG4/PRESTA)	1.6	± 1
MCV (modified ESG4/PRESTA)	21.8	± 1
RT_DPM (modified DPM)	7.3	± 1
MCNPX	60.0	max. diff. of 8% at Al/lung interface (on average ± 1% agreement)
Nomos (PEREGRINE)	43.3*	± 1*
GEANT 4 (4.6.1)	193.3**	± 1 for homogeneous water and water/air interfaces**

*Note that the timing for the PEREGRINE code also includes the sampling from a correlated-histogram source model and transport through the field-defining collimators.
** See Poon and Verhaegen (2005) for further details.

Chetty et al. (2006). "Issues associated with clinical implementation of Monte Carlo-based treatment planning: Report of the AAPM Task Group No. 105. *Med Phys*

AEIT vs VRT

• Distinguish between a technique that achieves the improved efficiency through the use of approximations

→ approximate efficiency improving technique (AEIT)

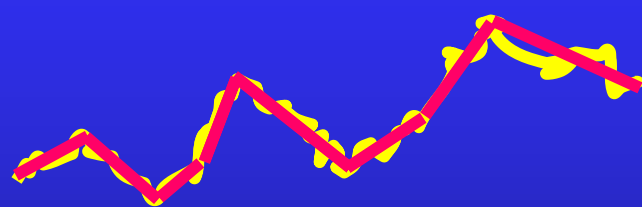
• And a technique that does not alter the physics in any way when it increases the efficiency

→ true variance reduction technique (VRT)

AEITs used in the treatment head simulation

- Condensed History Technique (CHT)
- Range Rejection
- Transport Cutoffs

Condensed History Technique (CHT)



In previous talk Iwan talked about this in detail …

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Condensed History Technique (CHT)

- 10^6 elastic and inelastic collisions until locally absorbed
- Berger (1963) introduced the condensed history technique
- "step-size" dependence
- Is an AEIT
- Two main components very strongly influence the simulation speed and accuracy :
  - the "electron-step algorithm"
    ("transport mechanics")
  - the boundary-crossing algorithm

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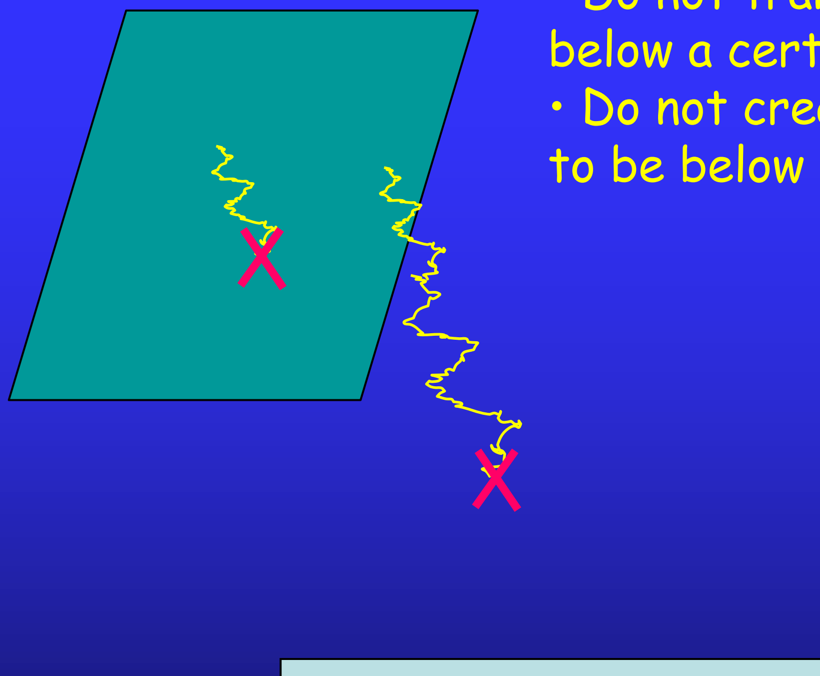
Range Rejection

- Discard an electron if its residual range is smaller than the distance to the nearest boundary
- Region Rejection:
  Discard more aggressively when "far" away from the region of interest

- Suggested 1.5 MeV cutoff for 6 MV and up
- By tagging bremsstrahlung photons generated outside target
- Speed up -> a factor of 3
- Negligible (< 0.2%) underestimation of the calculated photon fluence

Transport Cutoffs

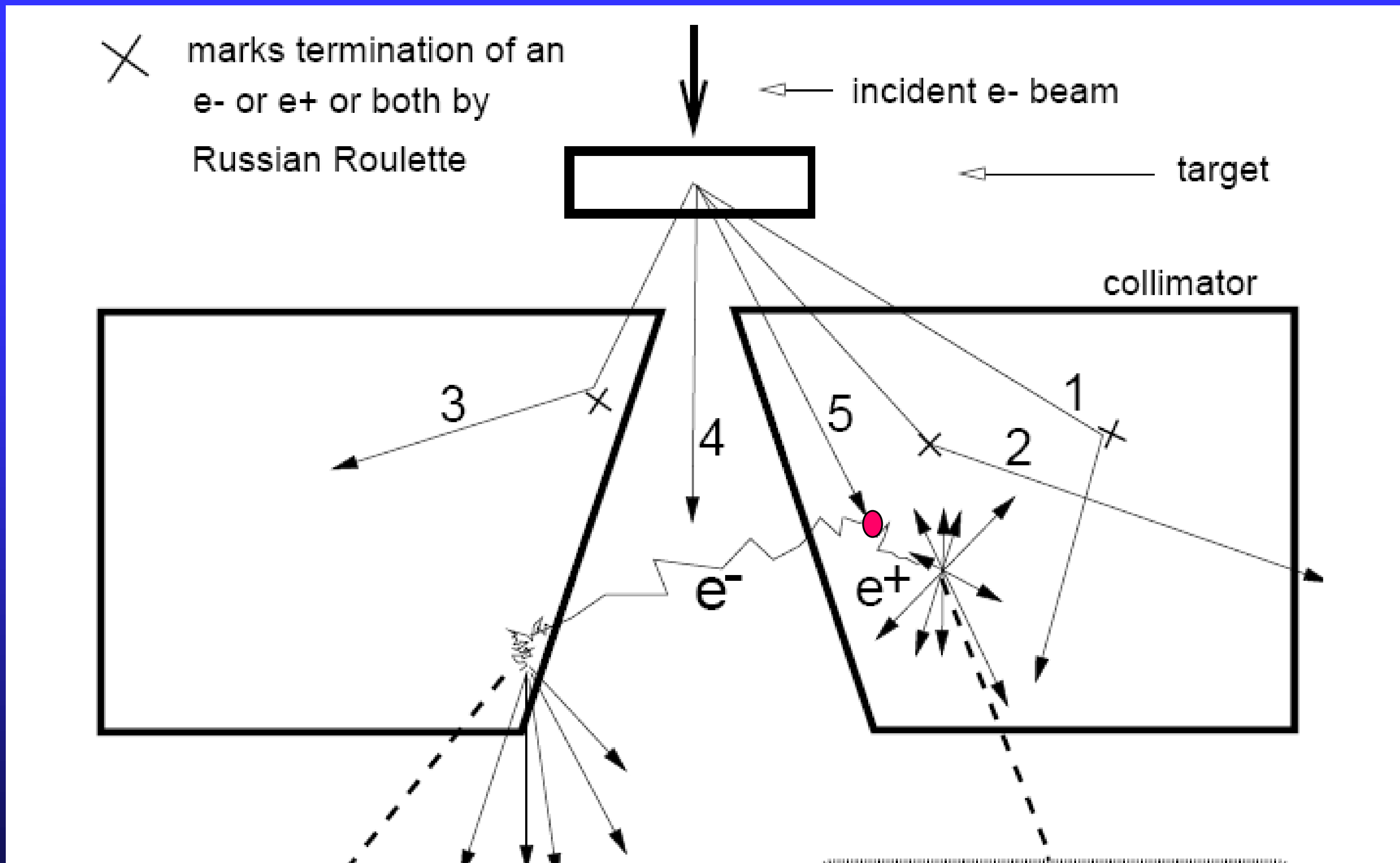


- Do not transport further, if the energy drops below a certain threshold (ECUT & PCUT)
- Do not create secondaries if their energy is going to be below a certain threshold (AE & AP)

Splitting and Russian Roulette

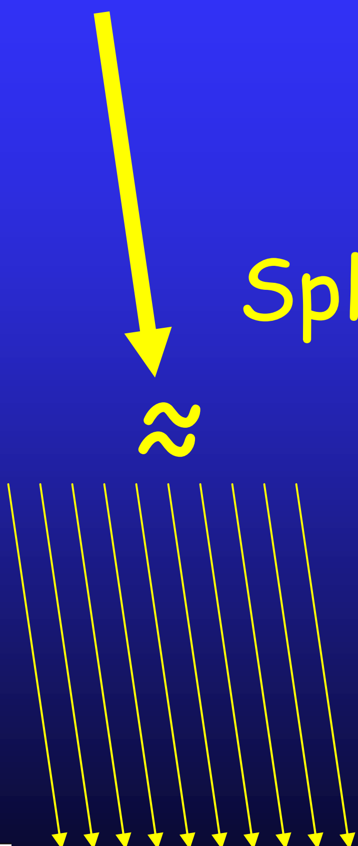
- Originally proposed by J. von Neumann and S. Ulam
- The most powerful VRTs used in Treatment Head Simulations

Splitting and Roulette; a schematic



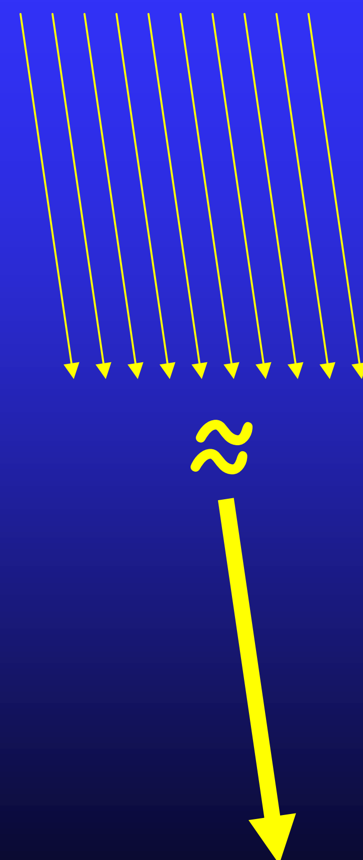
Splitting, Roulette & Particle Weight

$1\ w_i = 10\ w_f$



Split!

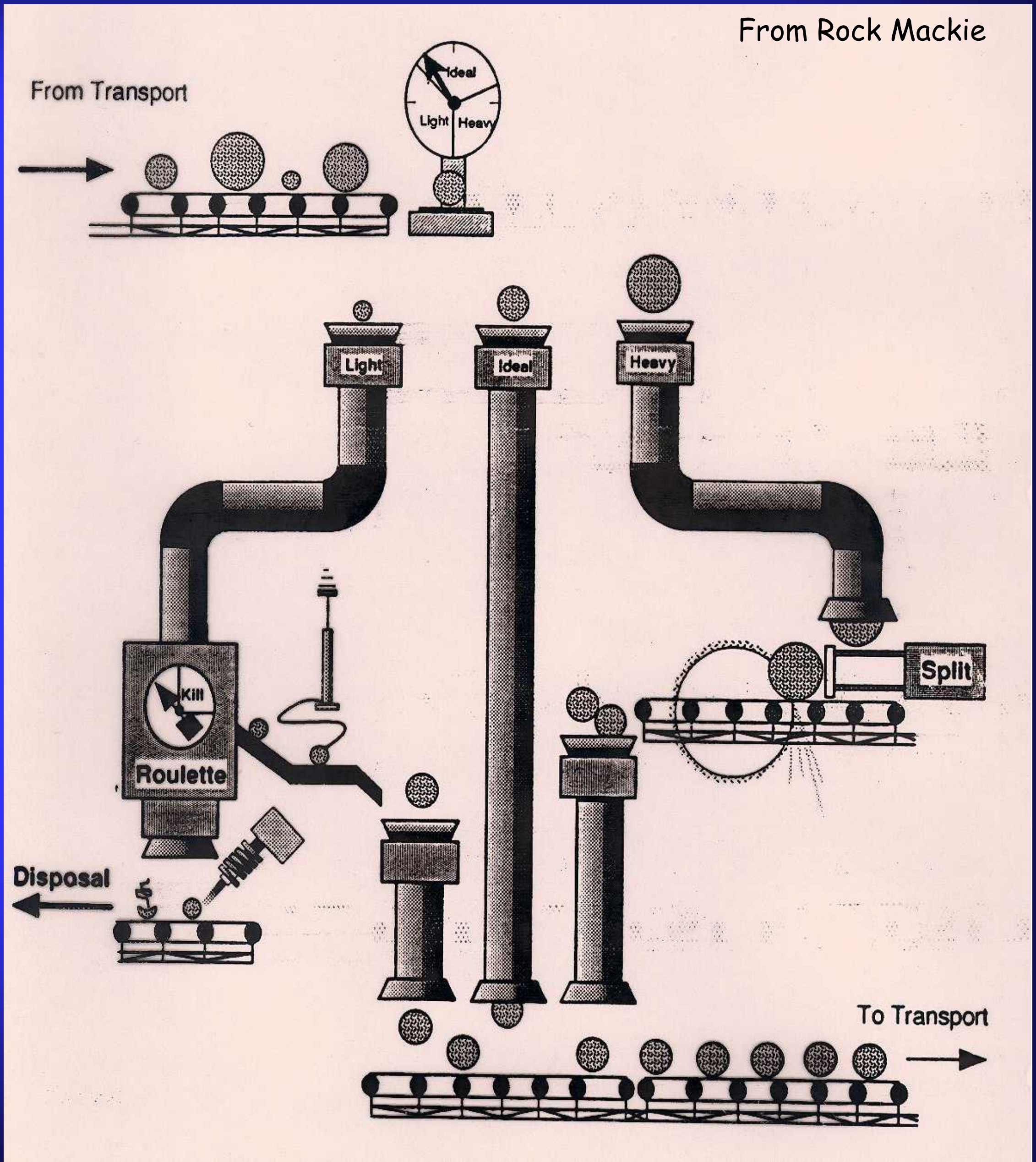
$10\ w_i = 1\ w_f$



Roulette!

Weight Management for:

Splitting and Russian Roulette

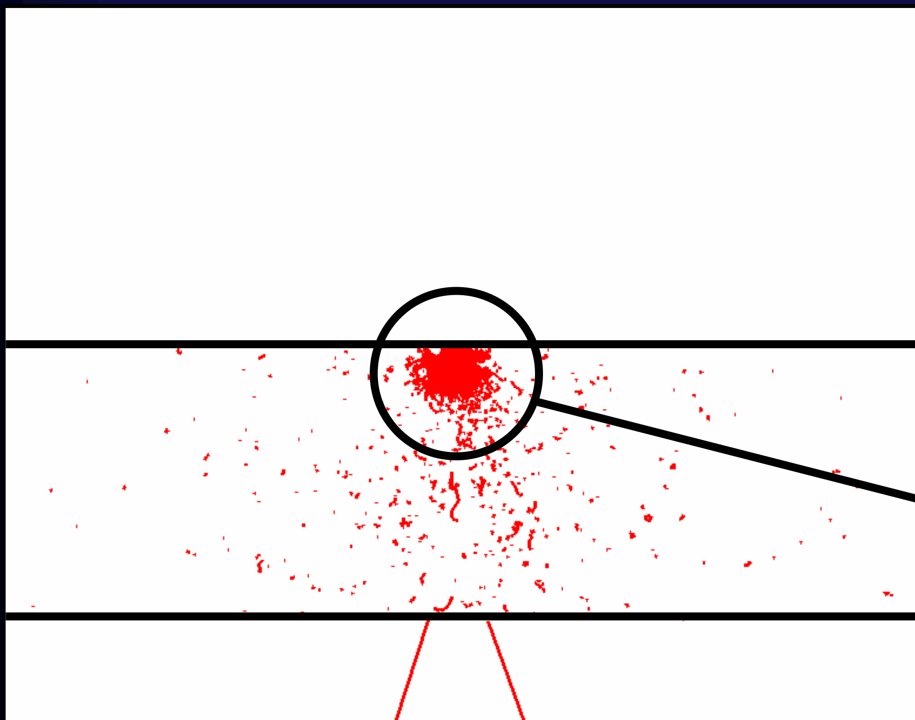


Courtesy of Jinsheng Li, Fox Chase CC

Splitting-based VRTs developed for BEAM/BEAMnrc

- Uniform Bremsstrahlung Splitting (UBS)
- Selective Bremsstrahlung Splitting (SBS)
- Directional Bremsstrahlung Splitting (DBS)

Electrons incident on and transported in the tungsten target …



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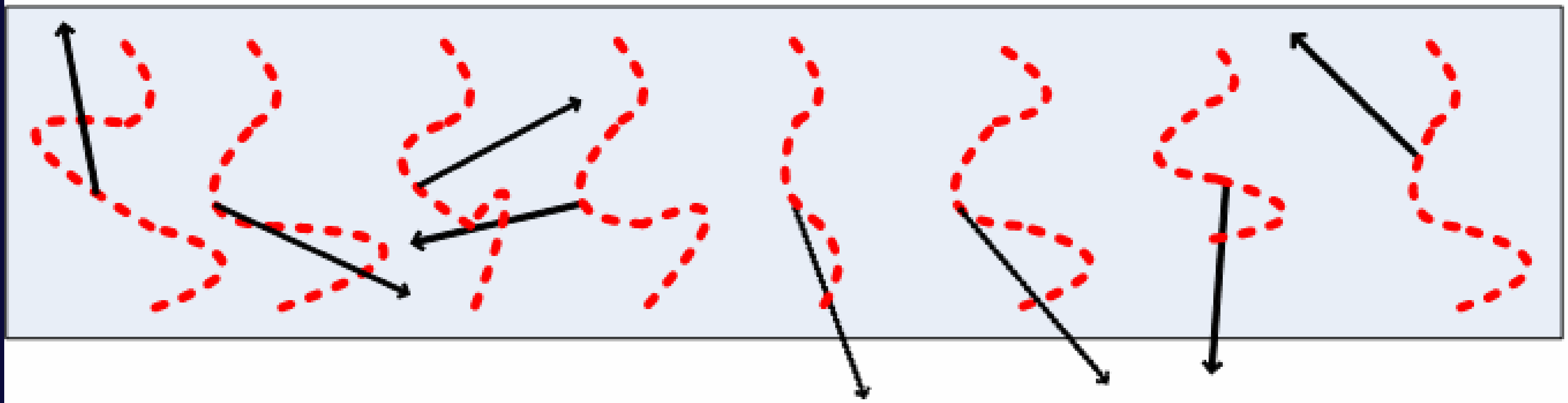
No Splitting



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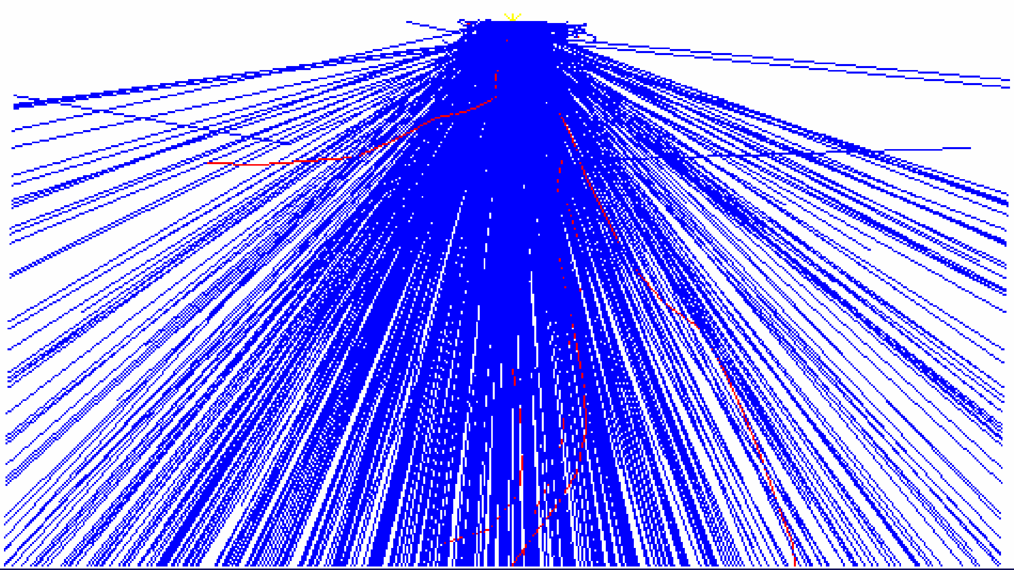
And the resulting brem photons …



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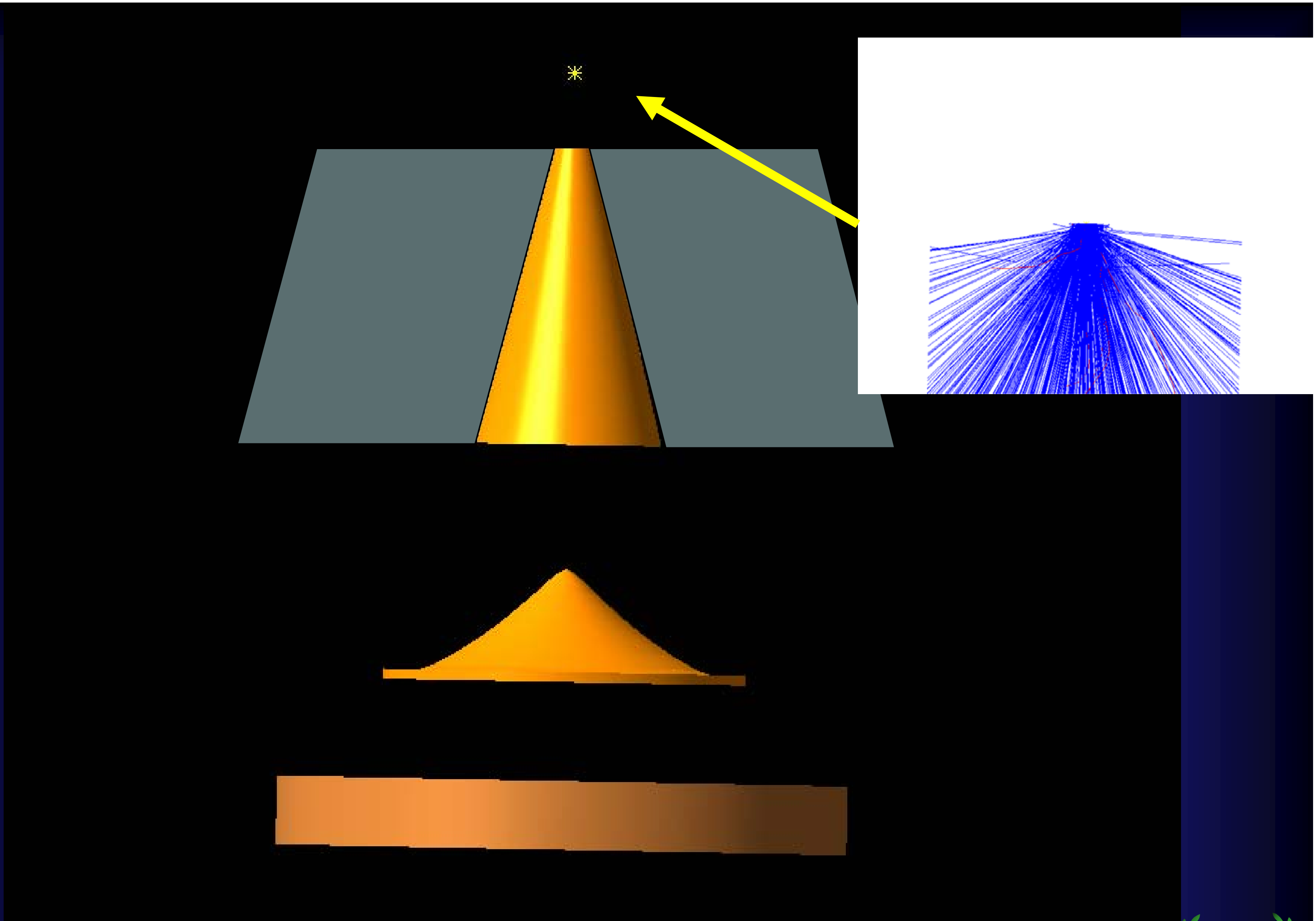
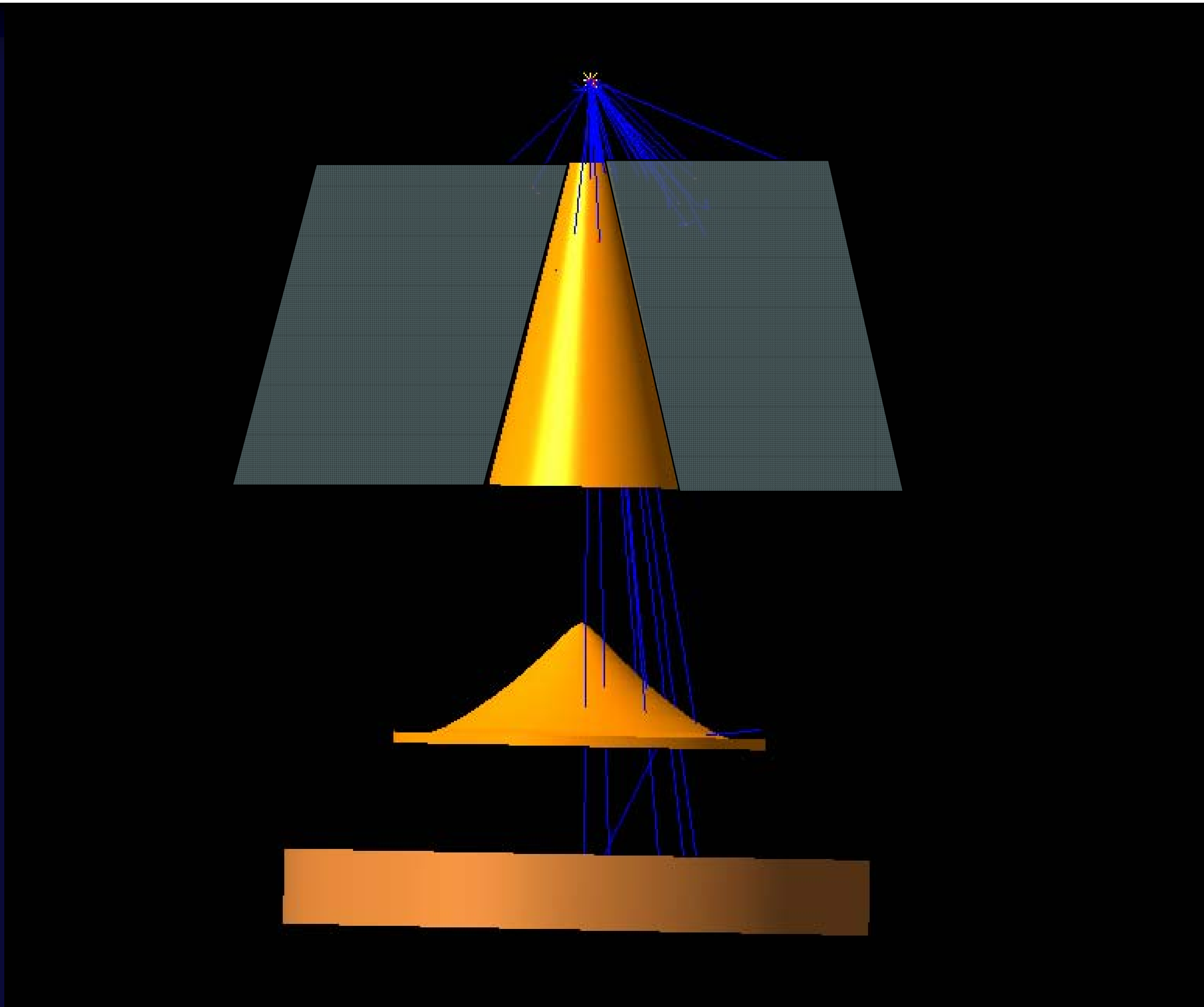
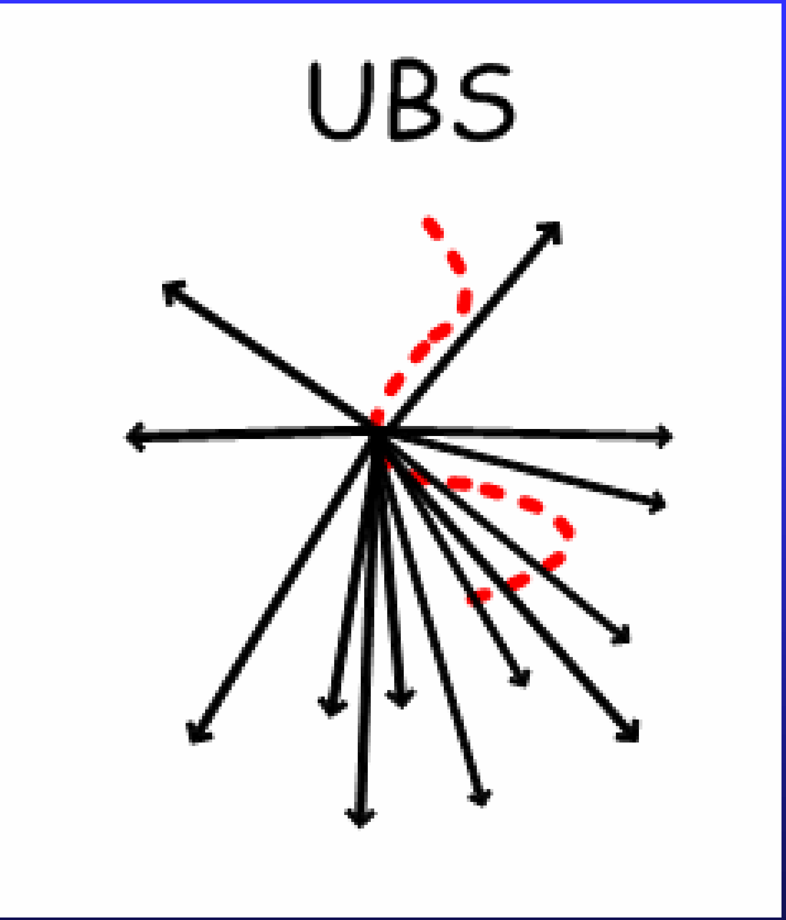




Uniform Brems Splitting



Particle weights:

1/N

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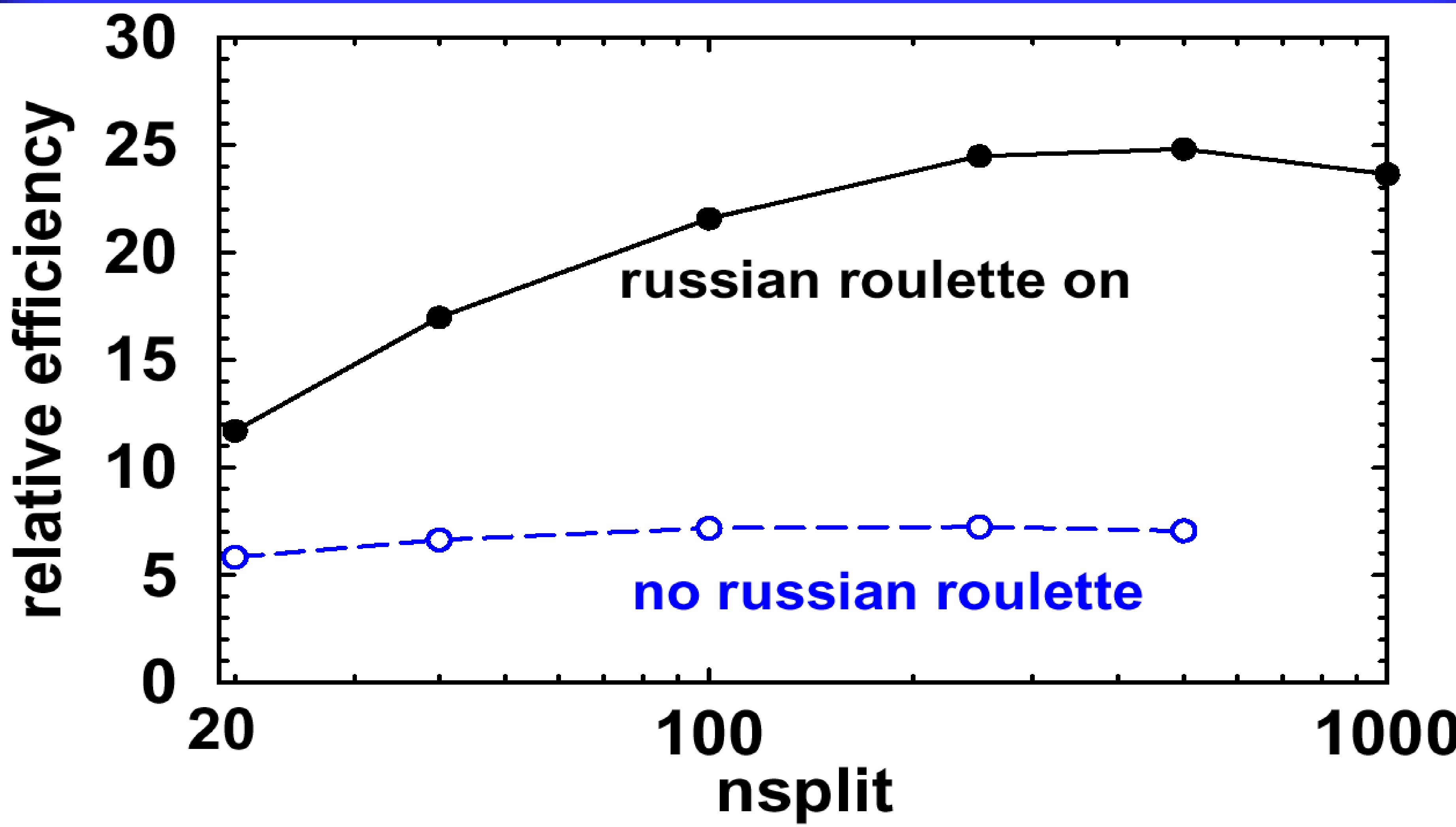
Uniform Brems Splitting



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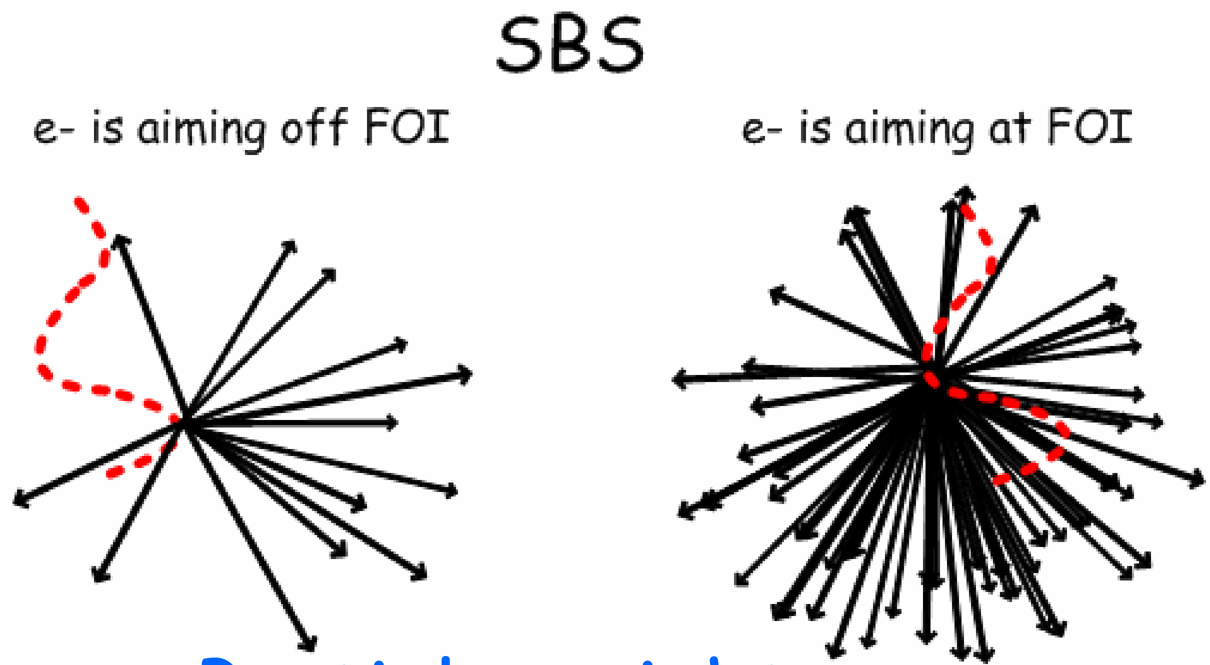
Selective Brems Splitting



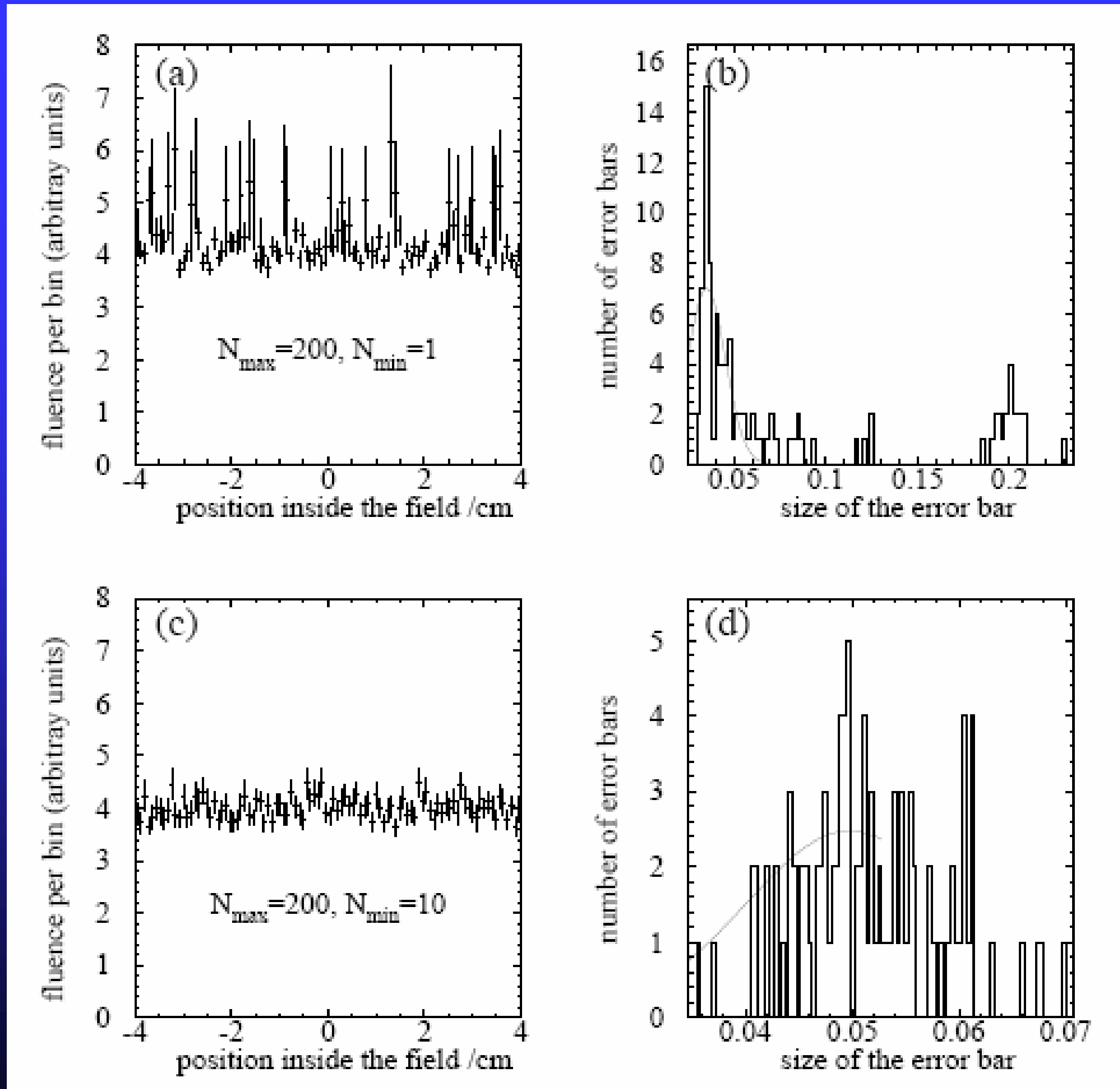
Particle weights:

Vary between $1/N_{min}$ and $1/N_{max}$

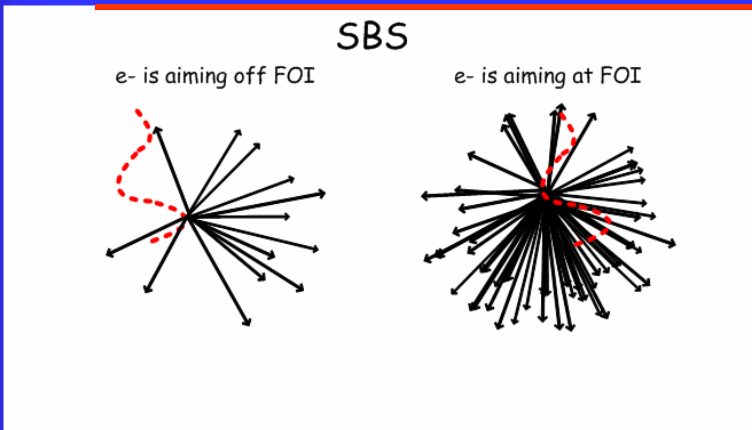
Fat Particles

Distribution that has fat particles

No fat particles

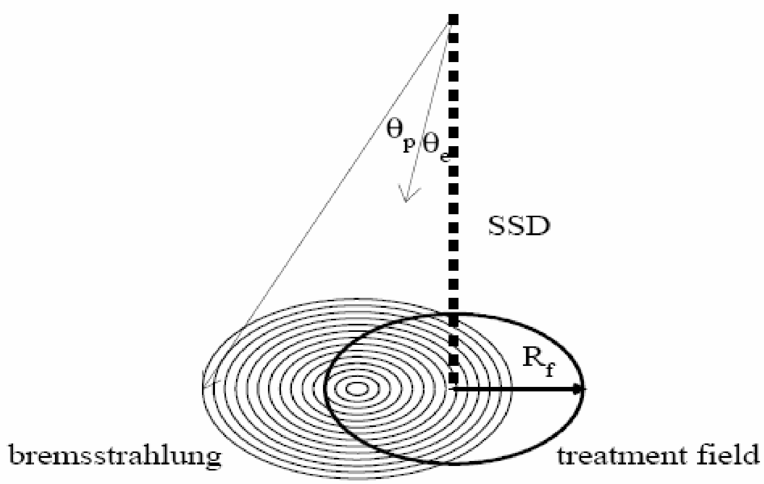


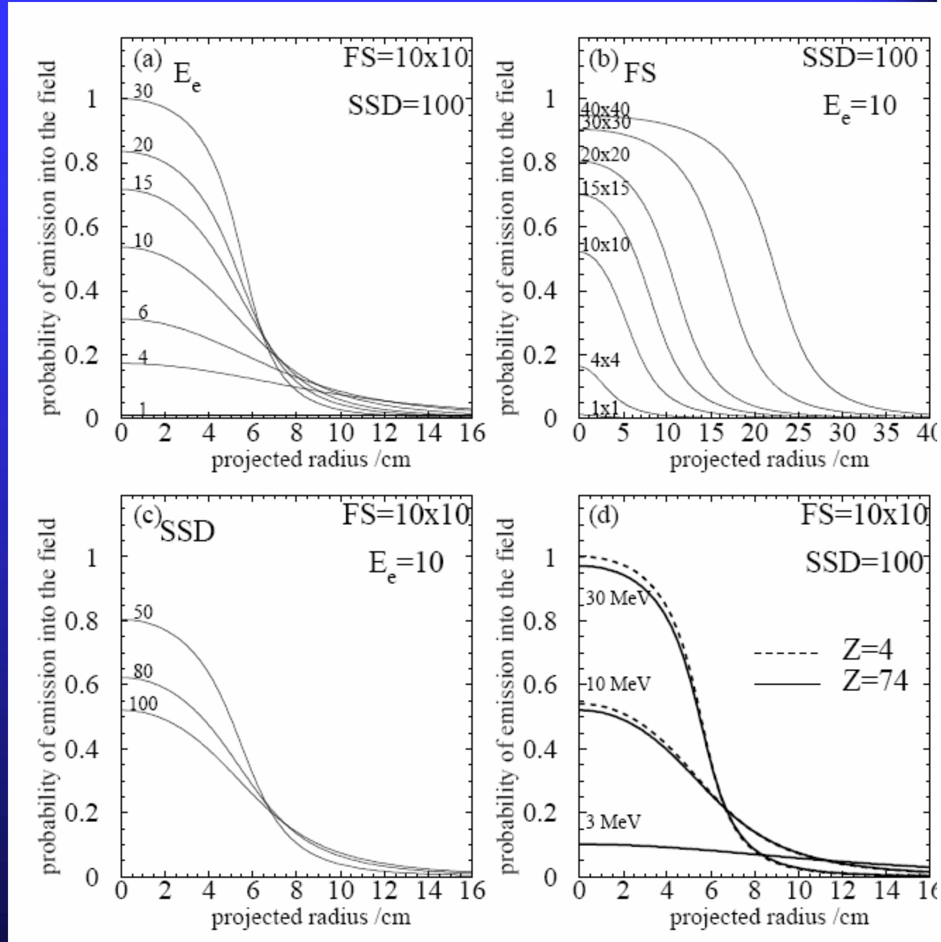
Selective Brems Splitting



Probability of photon emission towards treatment field

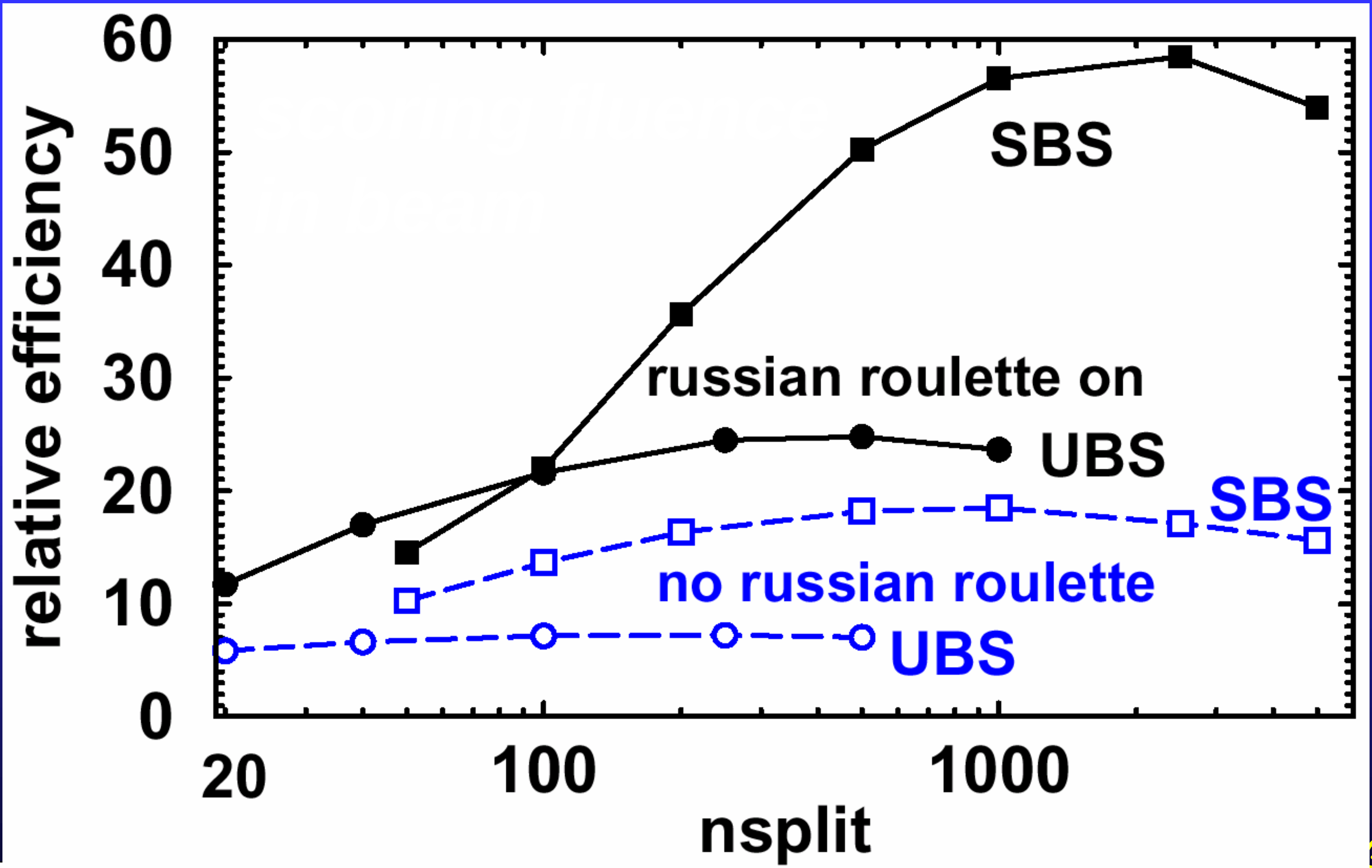
$$P(R_e , E_e , R_f , SSD) = \frac{\int_{\theta_{min}}^{\theta_{max}} d\sigma/d\theta_p \; f(\theta_p) \; d\theta_p}{\int_0^{\pi} d\sigma/d\theta_p \; d\theta_p}$$





Sheikh-Bagheri (1999)

Selective Brem Splitting (SBS)



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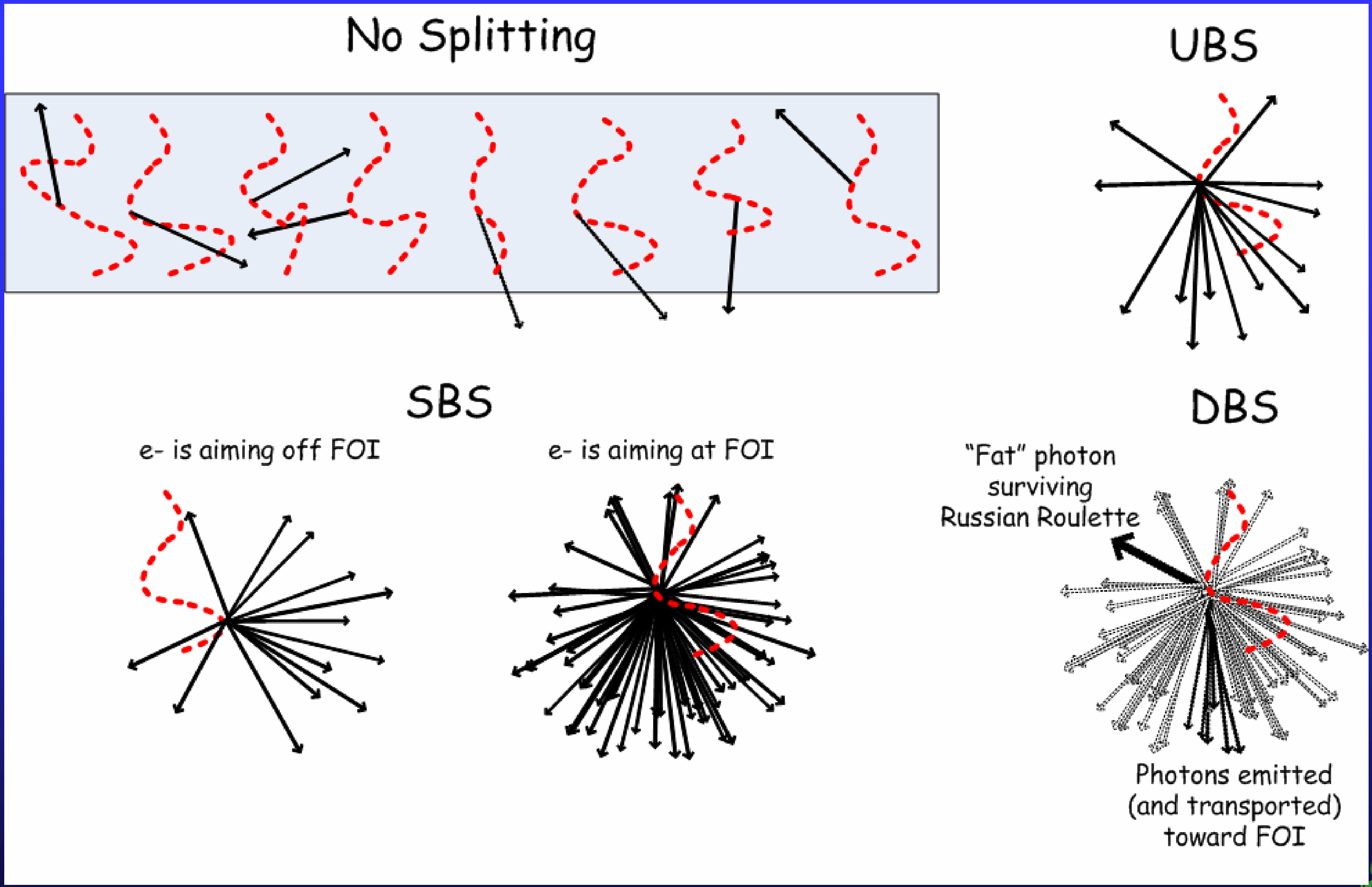
The evolution of splitting routines



Directional Brem Splitting (DBS)

-goal: all particles in field when reach phase space have same weight

Procedure

i) brem from all fat electrons split nsplit times

ii) if photon aimed at field of interest, keep it, otherwise Russian roulette it:

if it survives, weight is 1 (i.e. fat)

iii) if using only leading term of Koch-Motz angular dist'n for brem: **do_smart_brems** and similar tricks for other interactions

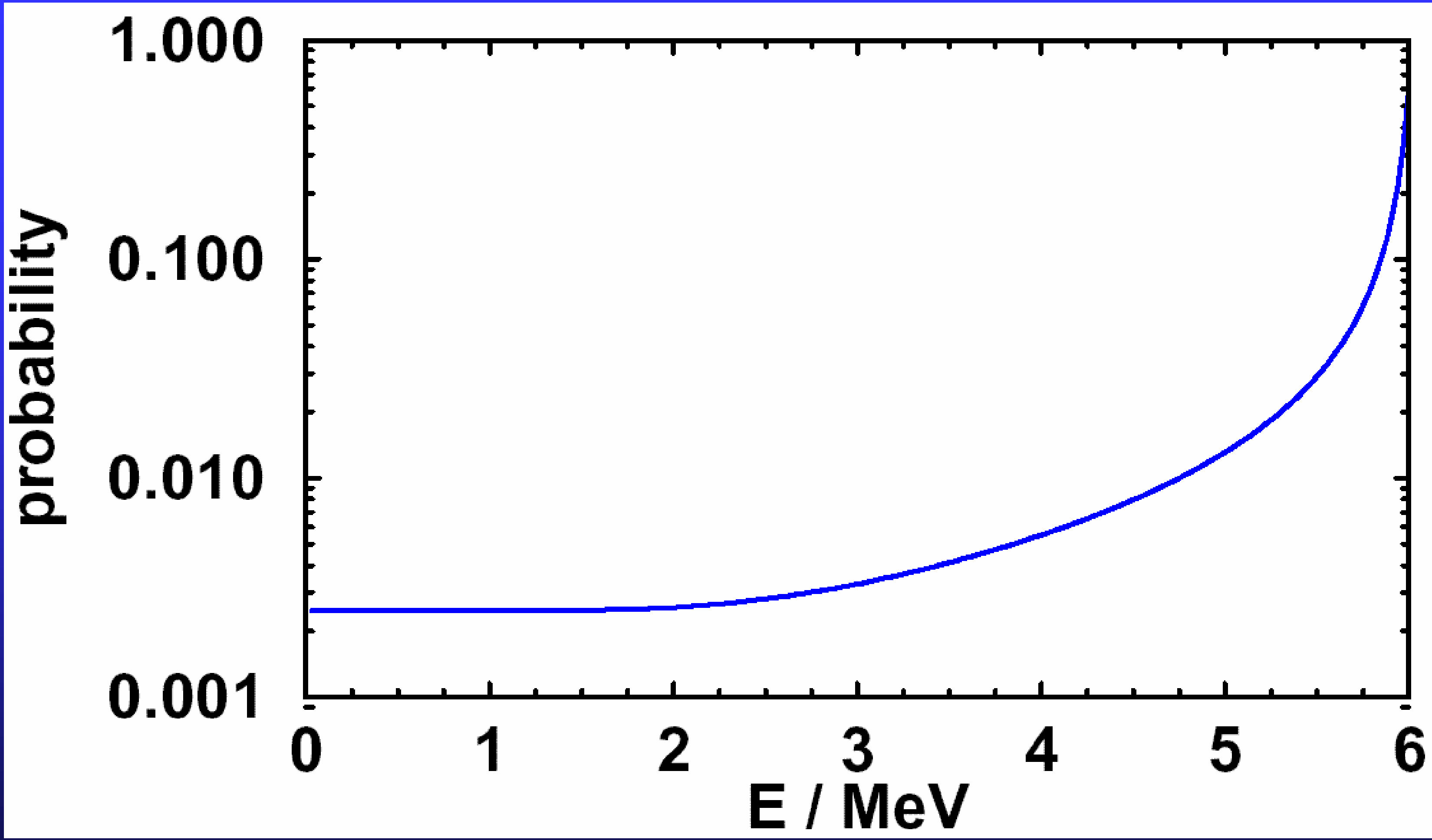
do_smart_brems

do_smart_brems calculates how many of the nsplit brem photons will head to the field and only generates those photons;

+

samples 1 photon from the entire distribution (if not heading into the field, kept with weight 1)

Probability of photon heading at field



DBS (cont)

Play similar tricks for other quantities

- e+ annihilation: (**uniform_photons**)
- Compton scattering:
  (**do_smart_compton** if Klein Nishina)
- Pair production/photo-effect: (Russian roulette **before** sampling)
- Fluorescence: (**uniform_photons**)

DBS (cont)

Photons

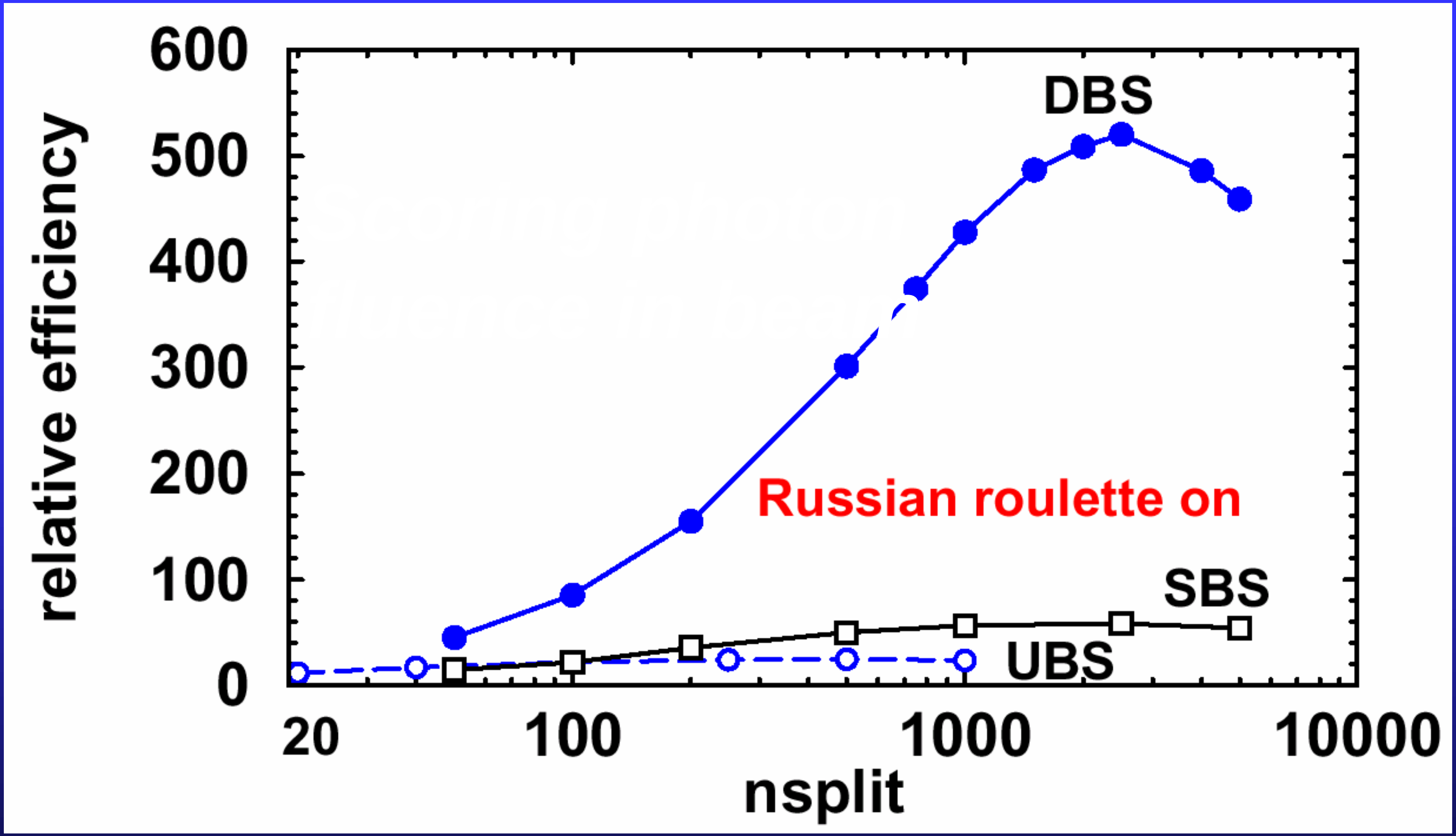
- reaching field have weight 1/nsplit
- outside field are fat

Electrons in the field

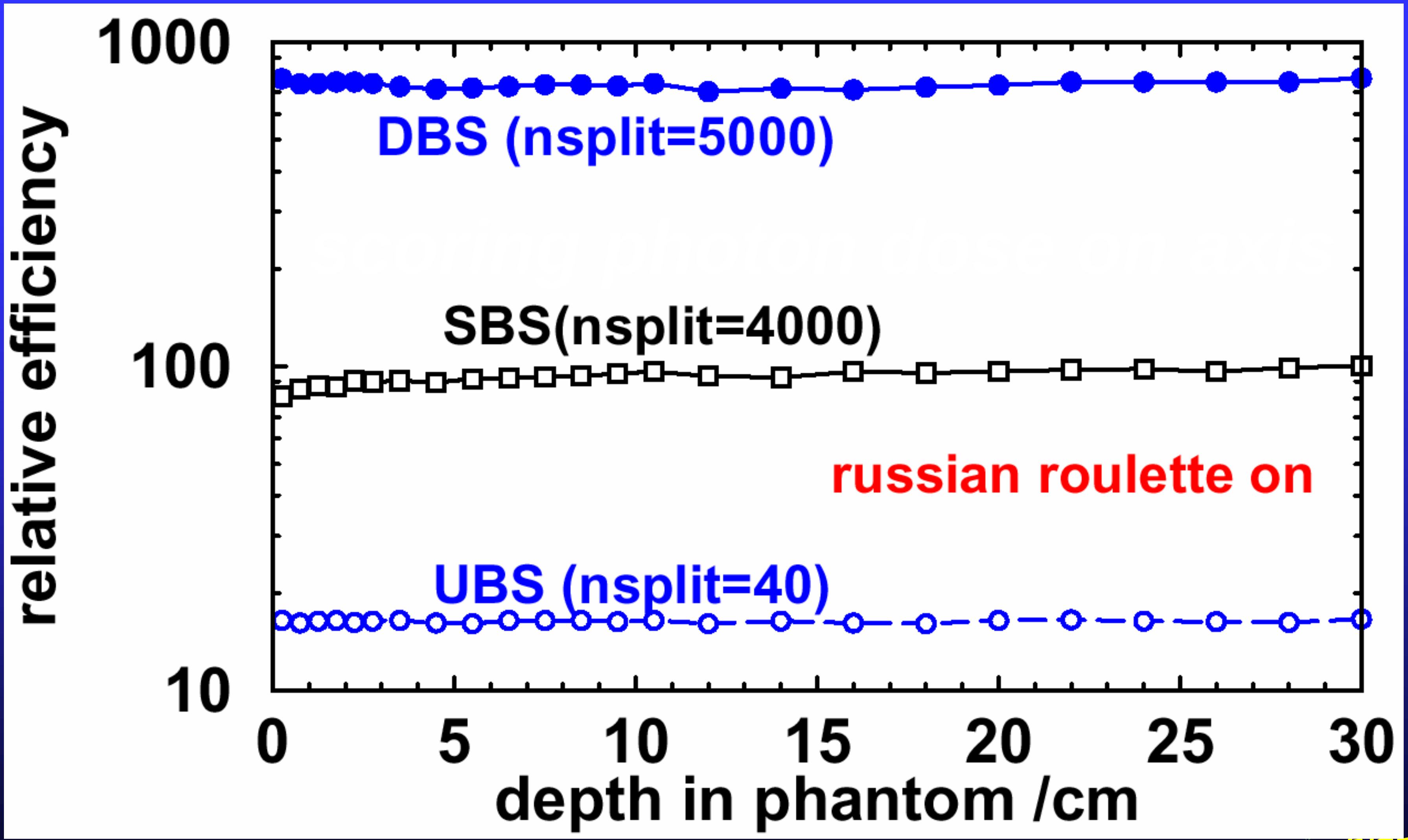
-usually fat

-a few have weight 1/nsplit from interactions in the air

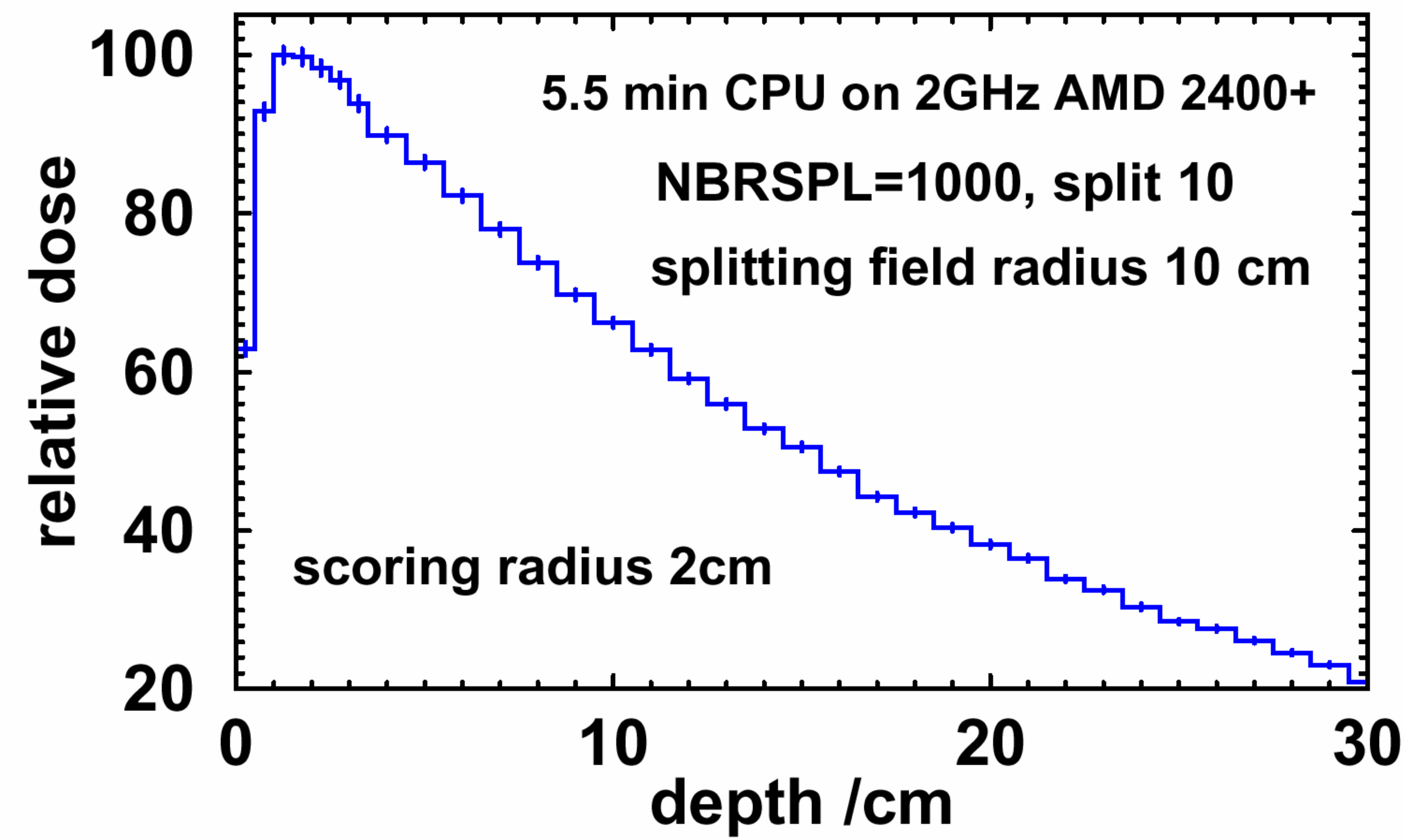
Efficiency of fluence calcs



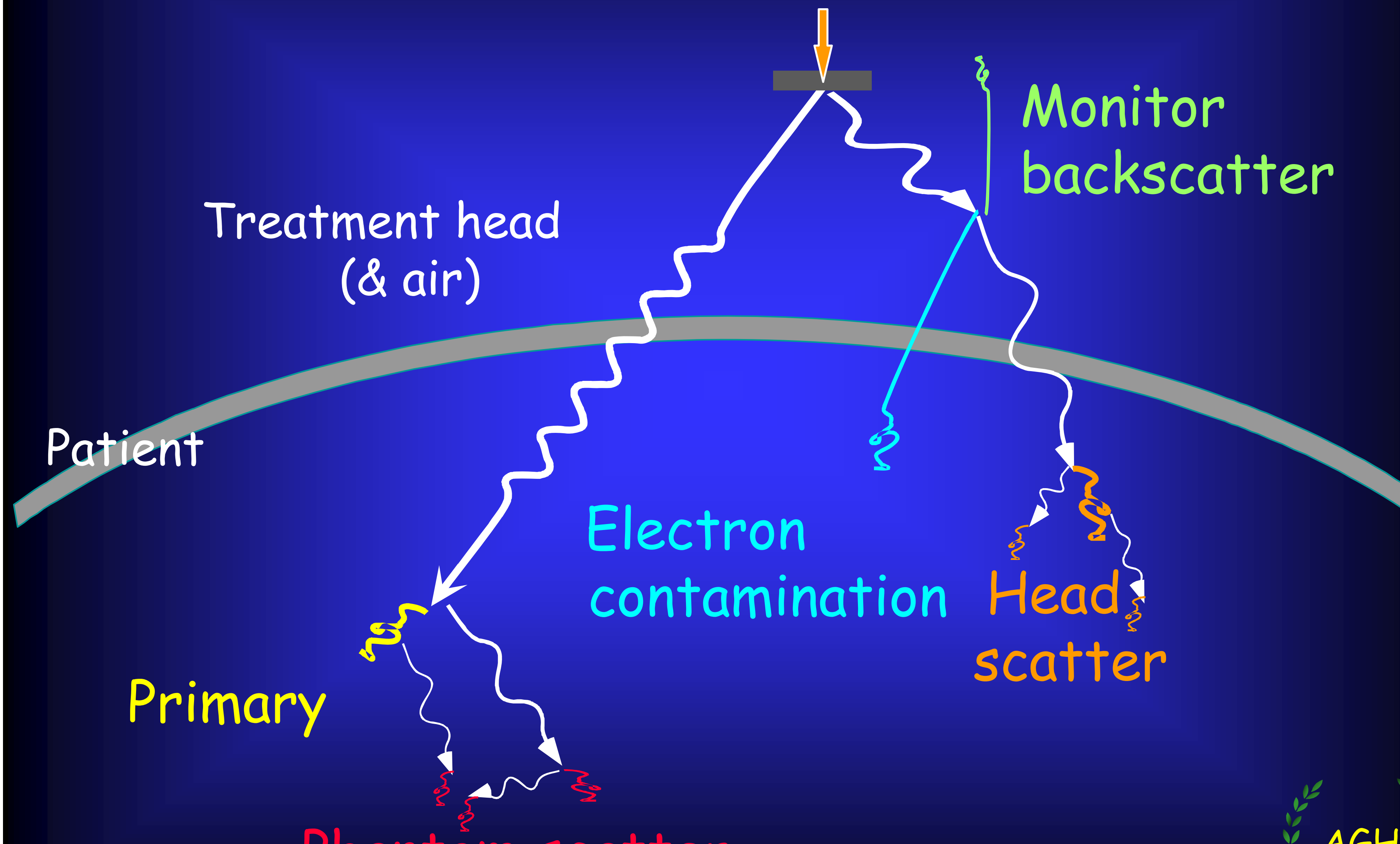
Efficiency of phantom dose calcs



6 MV, 10x10 cm^2



Electron contamination …



Electron problem

Unlike UBS and SBS,

DBS efficiency gain for electrons is only 2

Basis of the solution

-electrons are, almost entirely, from flattening filter and below

-major gains are from "taking care" of electrons in primary collimator

Electron solution

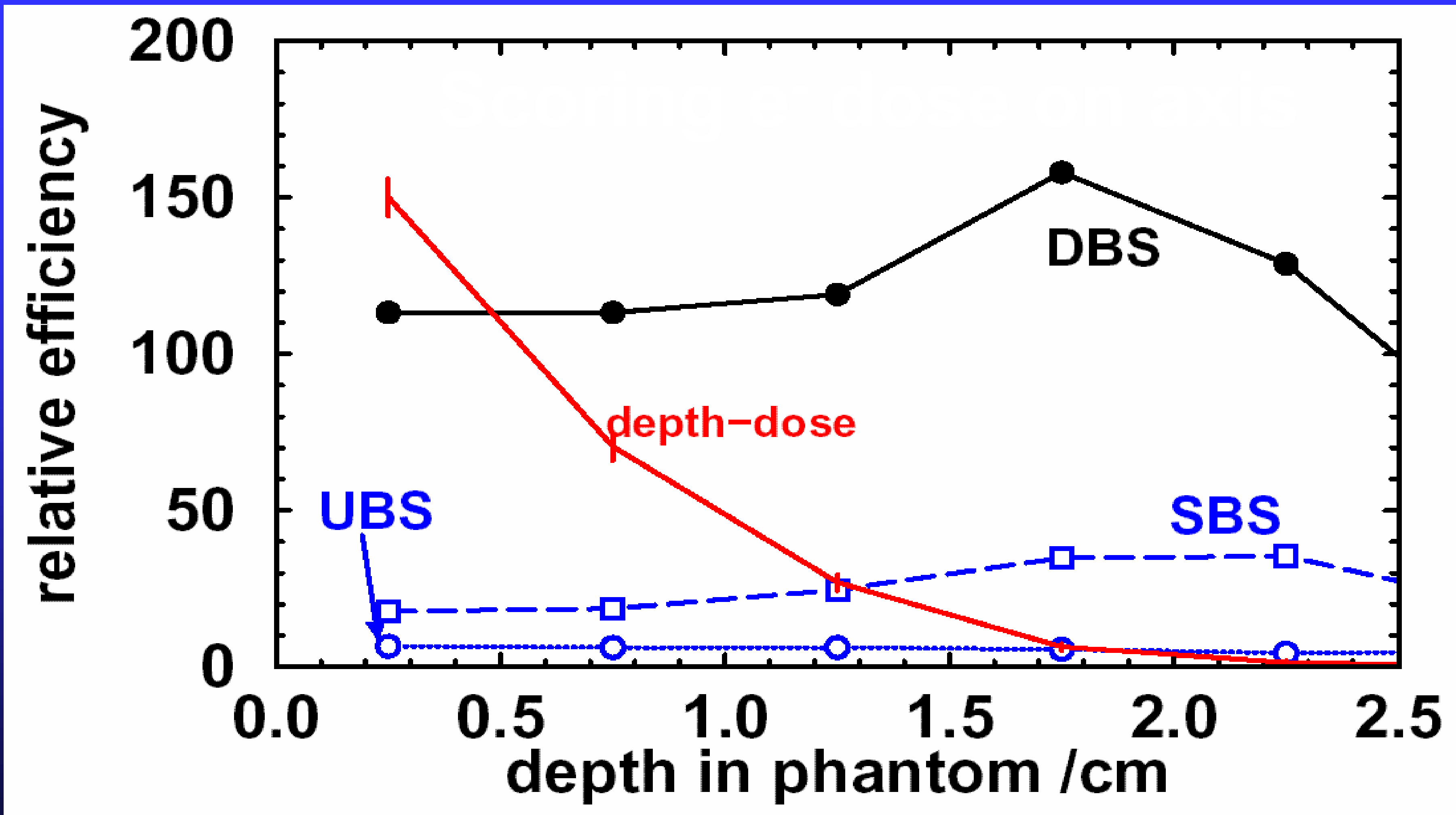
Introduce 2 planes

Splitting plane: split weight 1 charged particles nsplit times

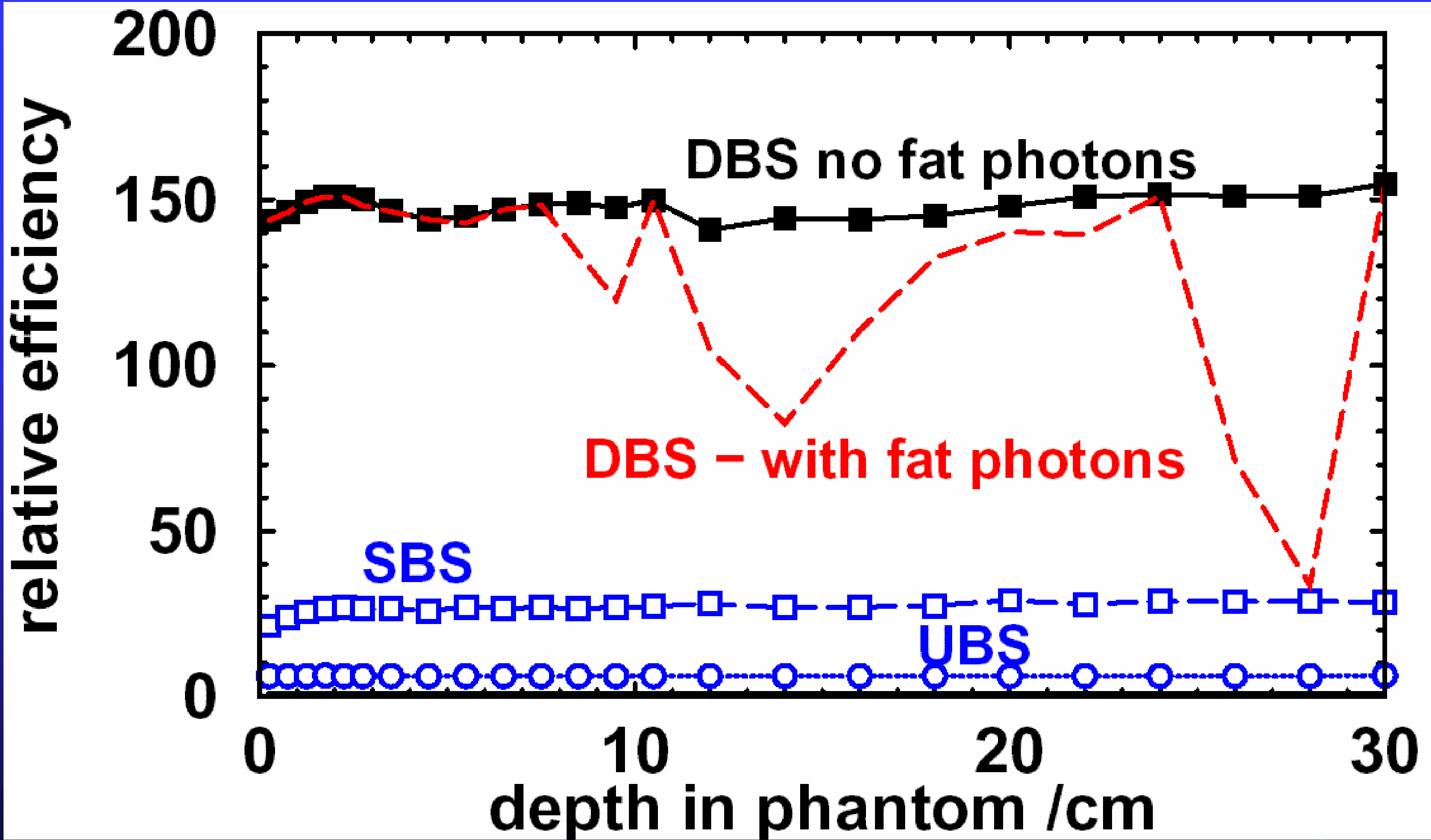
(may distribute symmetrically)

Russian roulette turned off below a certain plane and all fat photon interactions split nsplit times

Efficiency increase for e^-



Efficiency: total dose



DBS summary

DBS improves BEAMnrc's efficiency by a factor of 800 (10 vs SBS) for photon beams (ignore small dose from photons outside field).

For total dose calculations the efficiency improves by a factor of 150 (5 vs SBS)

SBS is optimized for greater nsplit than previously realized (5000)

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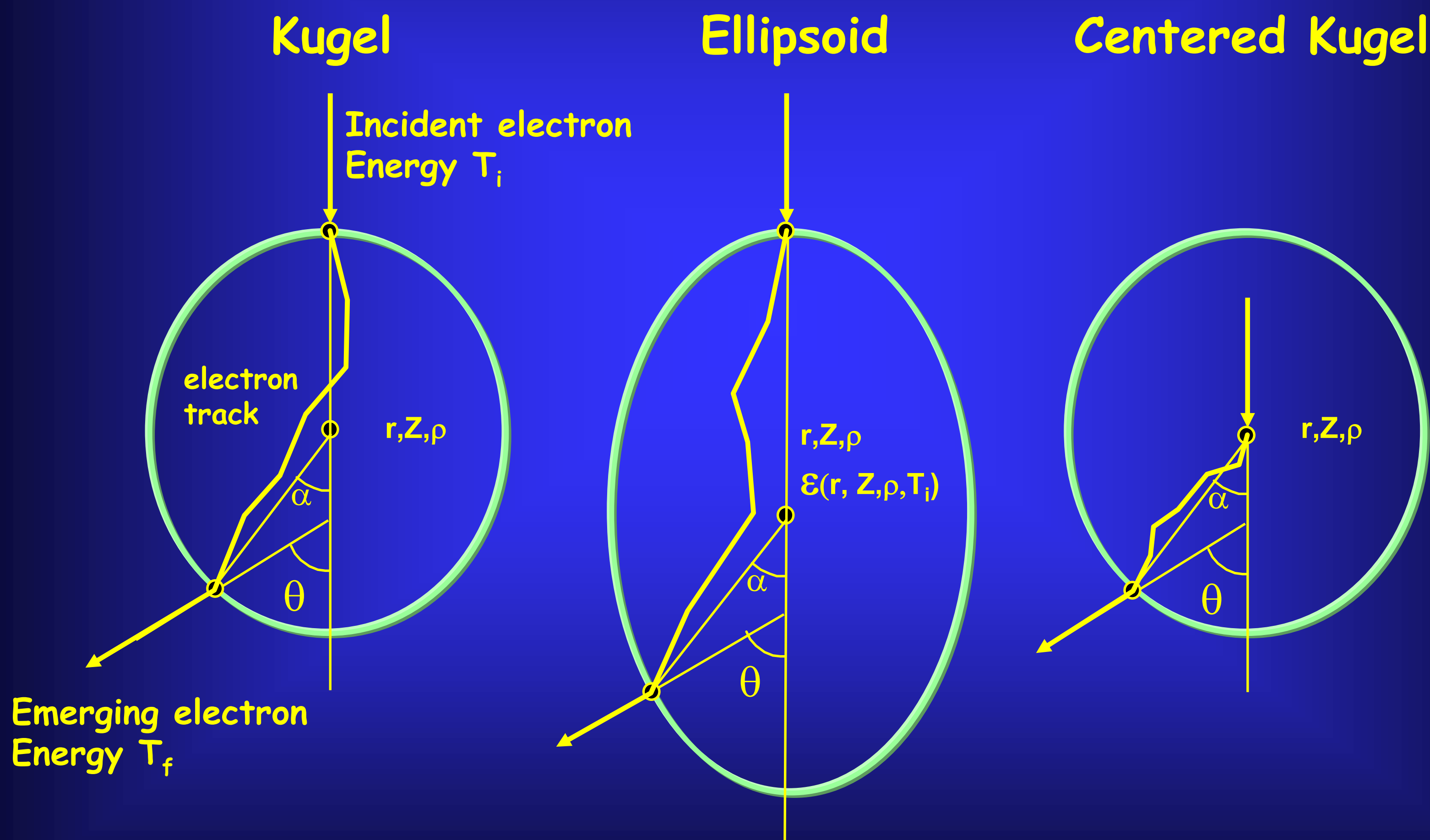
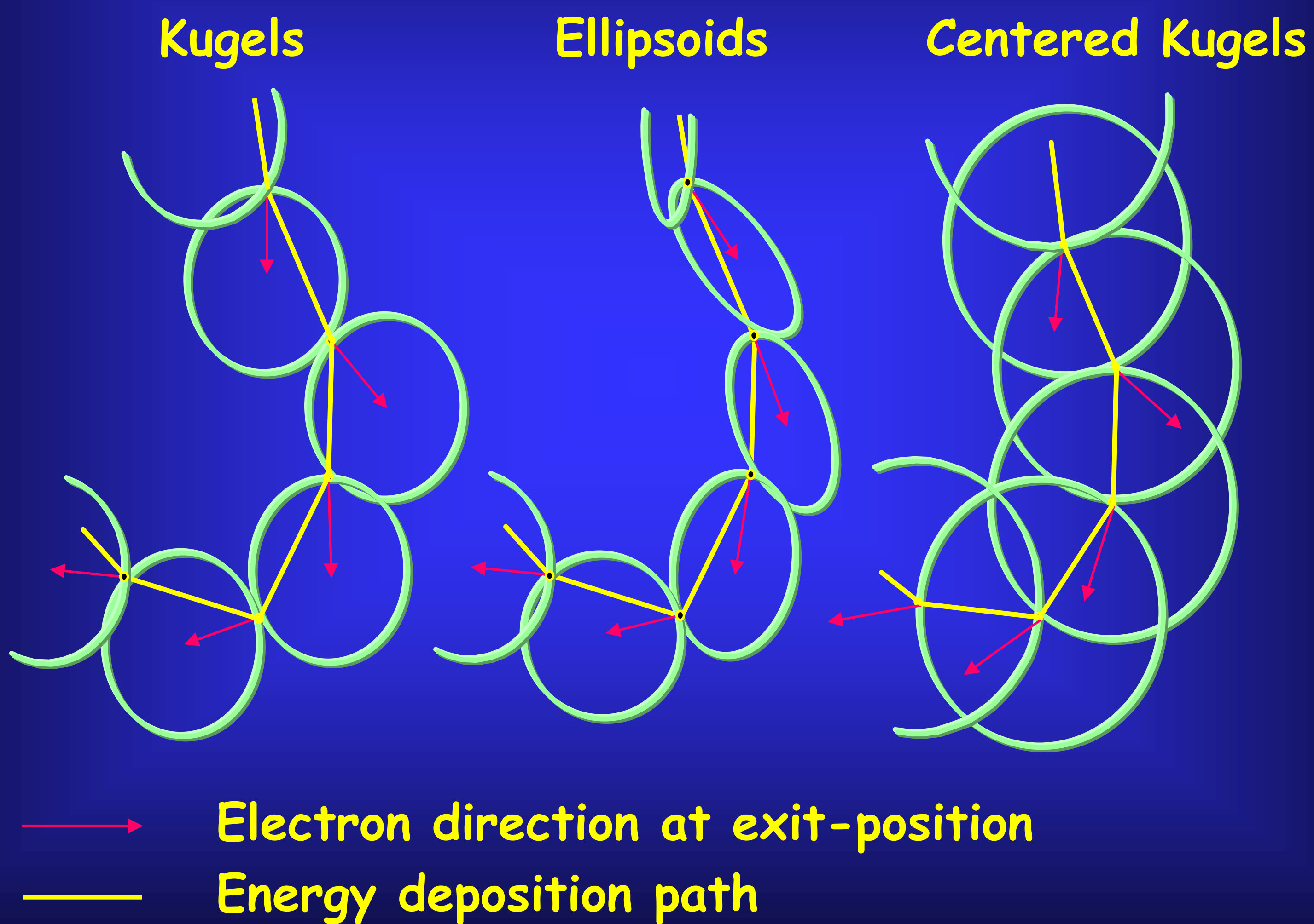
Efficiency Improvement Techniques Used in Patient Simulations

- Macro Monte Carlo
- History Repetition
- Boundary-Crossing Algorithms
- Precalculated Interaction Densities
- Woodcock Tracing
- Photon Splitting Combined with Russian Roulette
- Simultaneous Transport of Particle Sets (STOPS)
- Quasi-Random Sequences
- Correlated Sampling

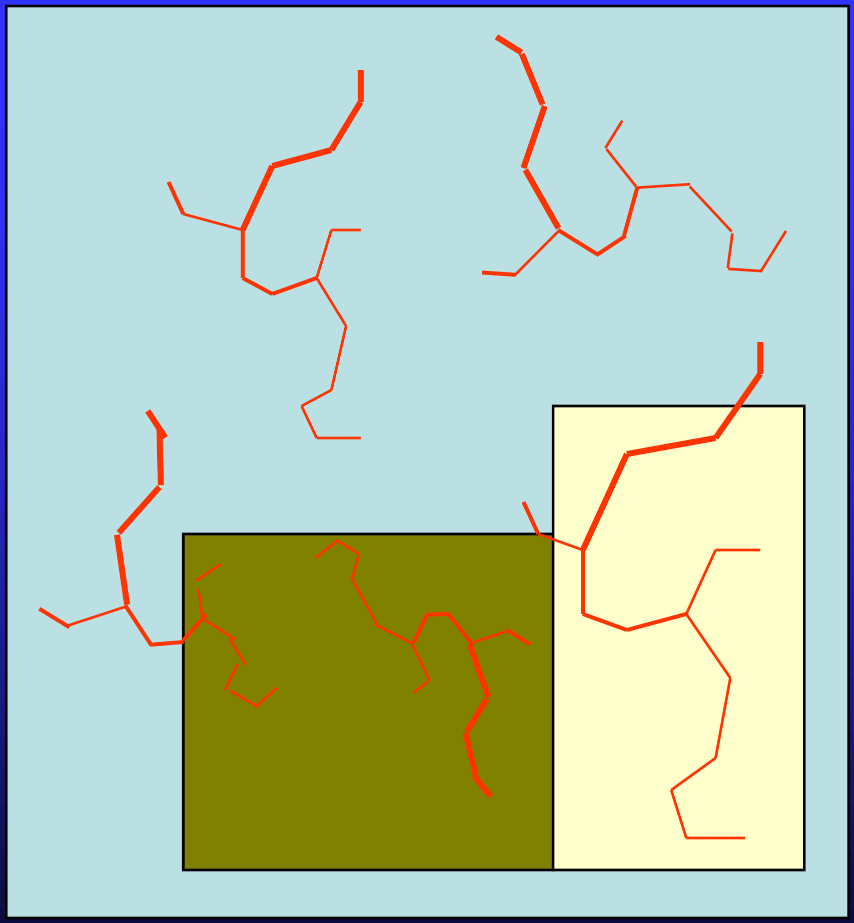
Macro Monte Carlo (MMC)

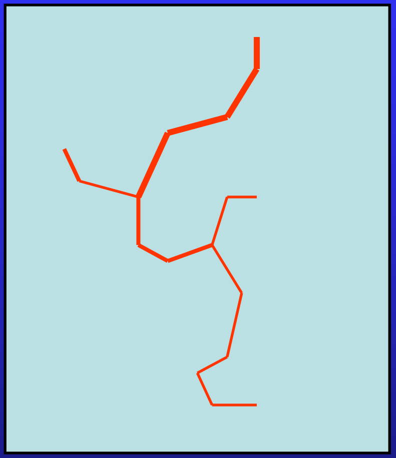


Macro Monte Carlo



Electron Track Repeating





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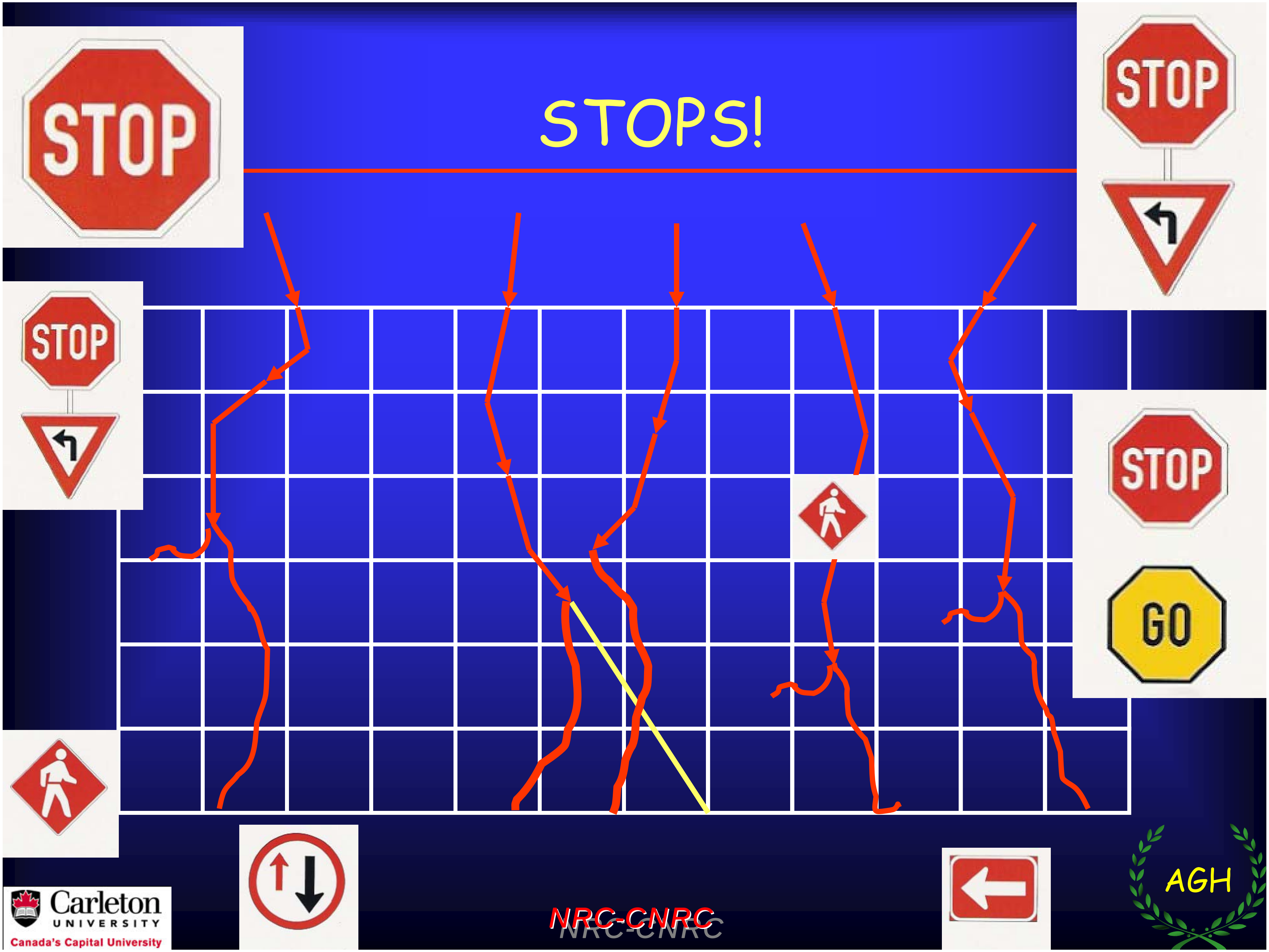
STOPS

(Simultaneous Transport Of Particle Sets)

- Several particles that have the same energy (but not position, direction, weight) form a "Particle Set" and are transported simultaneously
- This allows material independent quantities such as interpolation indices, azimuthal angles, maximum acceptable step-lengths, etc., to be calculated just once for the set
- Material dependent quantities such as MS angles and discrete interaction probabilities are sampled separately
- In particular, if one or more particles in the set undergo a different interaction, set is split into separate sets and each new set transported individually


STOPS!
STOP
STOP
STOP
STOP
GO
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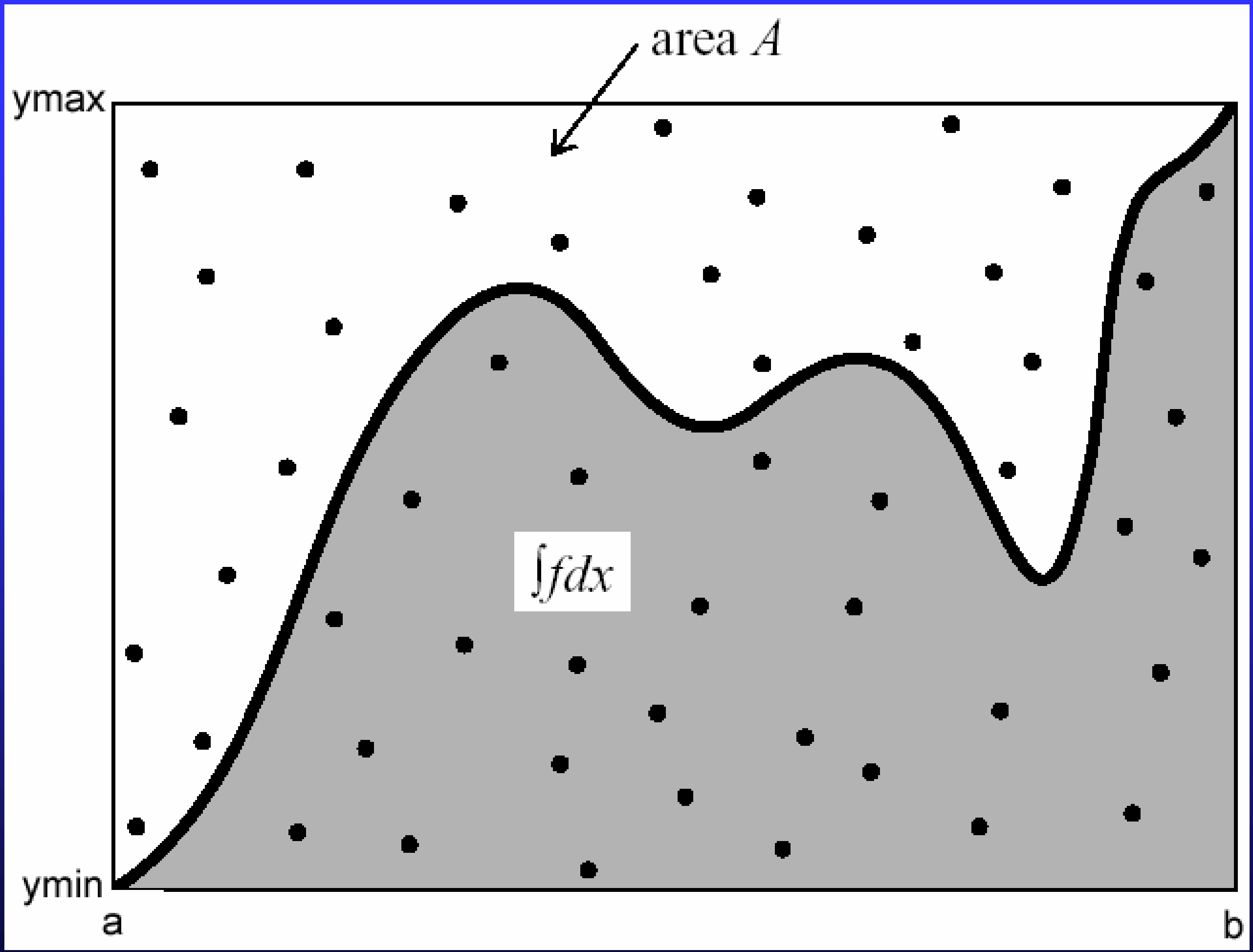
Faster Convergence Using Quasi RNs



$$I = \int_a^b f(x)\,dx$$

$$I_m = (b-a)\frac{1}{N}\sum_{i=1}^{N} f(x_i)$$

$$\lim_{N\to\infty} I_m = I$$

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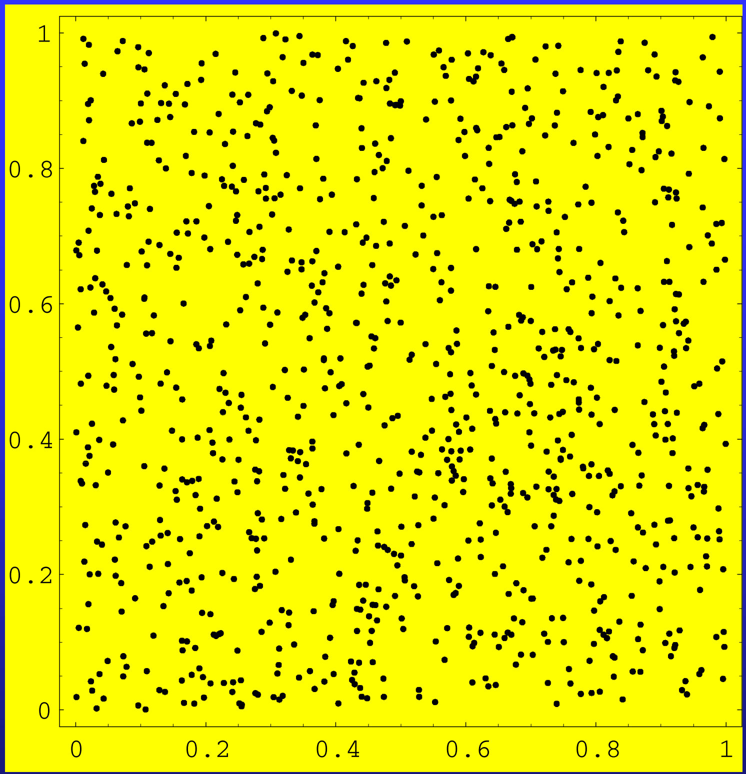
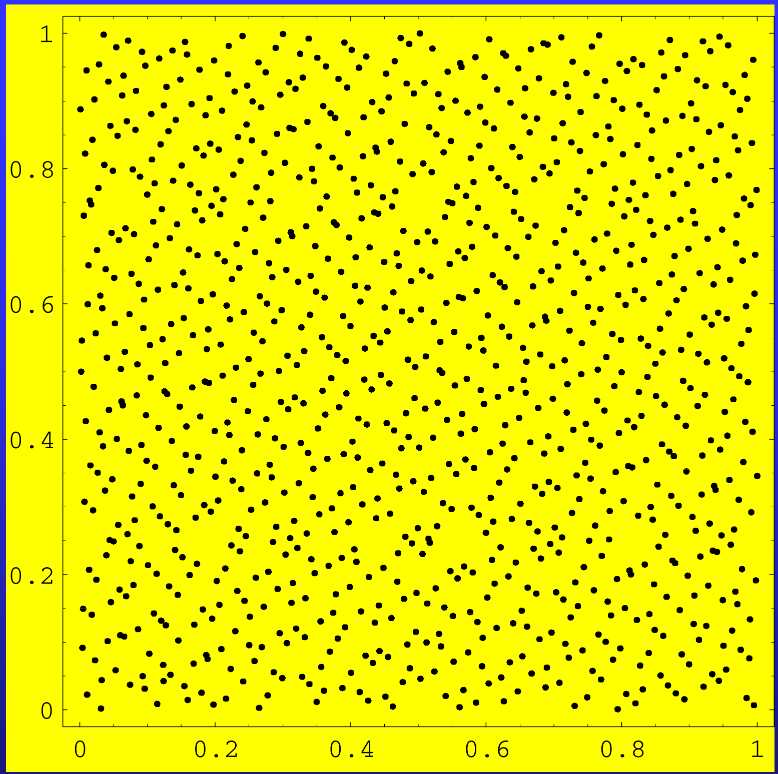
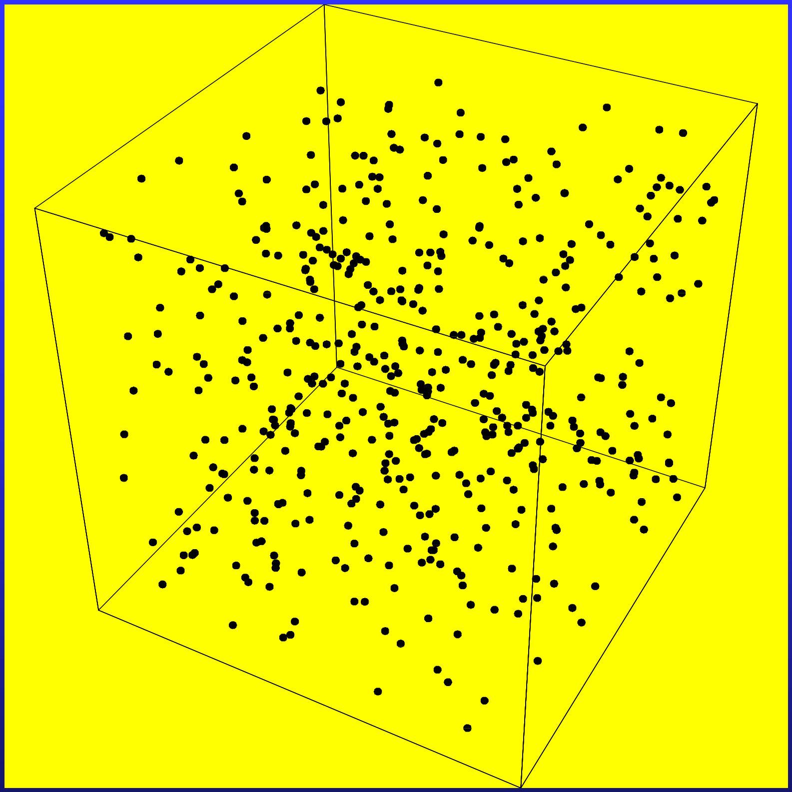
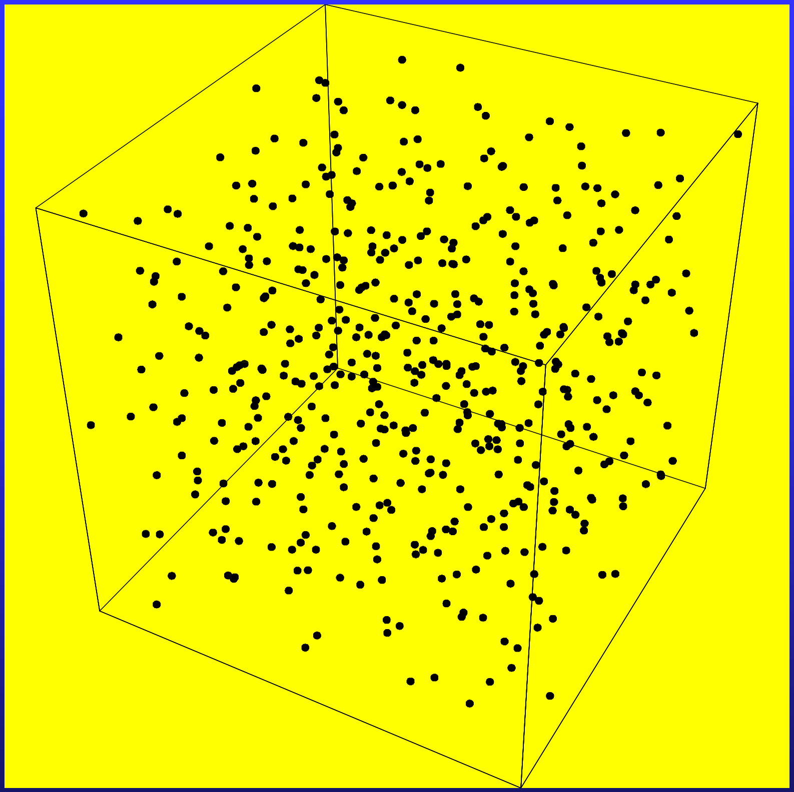
Pseudo-Random vs. Quasi-Random





Pseudo-Random vs. Quasi-Random in 3D





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NRC-CNRC

AGH

Less Frequently Used VRTs

- Forcing
- CNVR
- Correlated Sampling
- Exponential Transform

NRC-CNRC

Photon interaction forcing

- **Force to interact in a phantom**

$$N_\lambda = -\ln\{1-R[1-e^{-M_\lambda}]\}$$

M_λ is the thickness of the phantom in number of mean free paths

The new photon weight: $W' = W\{1-e^{-M_\lambda}\}$

- **Force to interact in a region of a phantom**

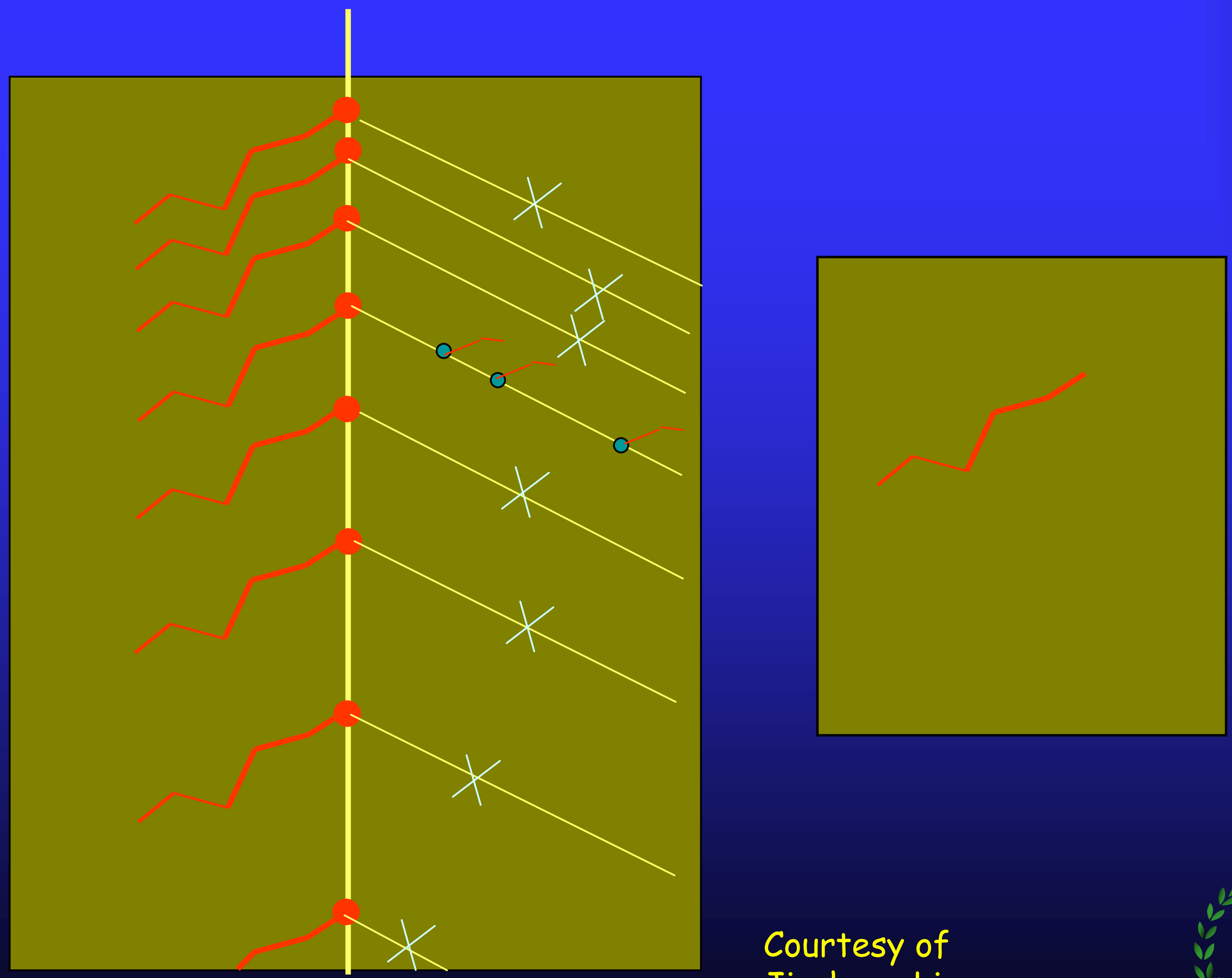
$$N_\lambda = M_{\lambda 1} - \ln\{1-R[1-e^{(M_{\lambda 1} - M_{\lambda 2})}]\}$$

$M_{\lambda 1}$ is the number of mean free paths to the near boundary of the region and $M_{\lambda 2}$ to the far boundary of the region.

The new photon weight: $W' = W\{e^{-M_{\lambda 1}} - e^{-M_{\lambda 2}}\}$

Courtesy of Jinsheng Li, Fox Chase CC

Combine Electron Track Repeating with Photon Interaction Forcing and Splitting



Courtesy of
Jinsheng Li,
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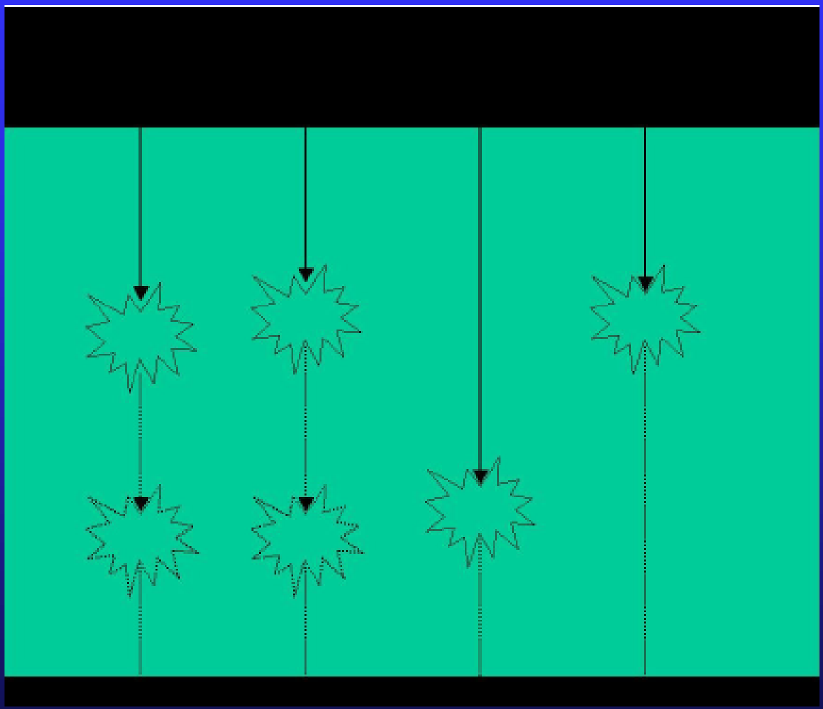
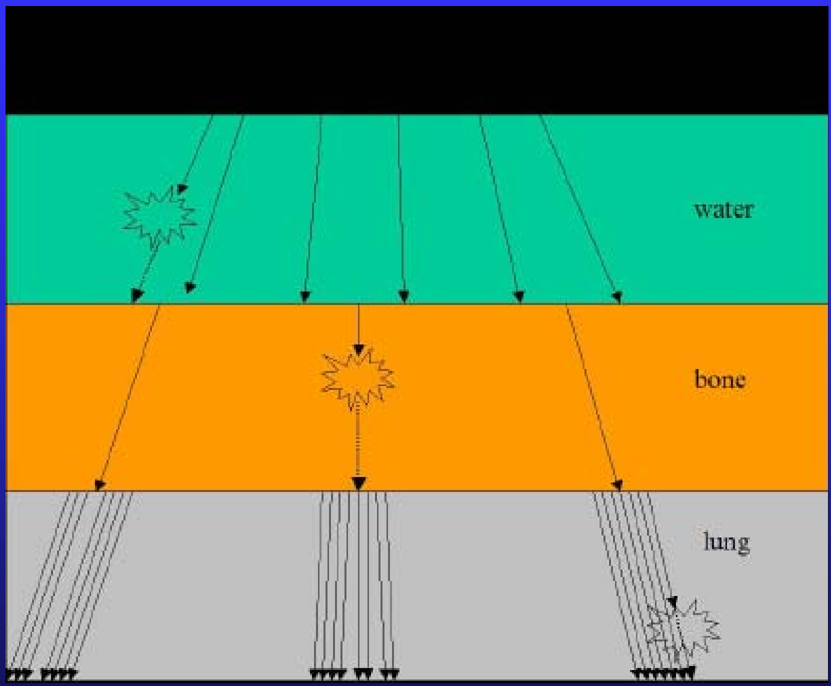
CNVR Technique

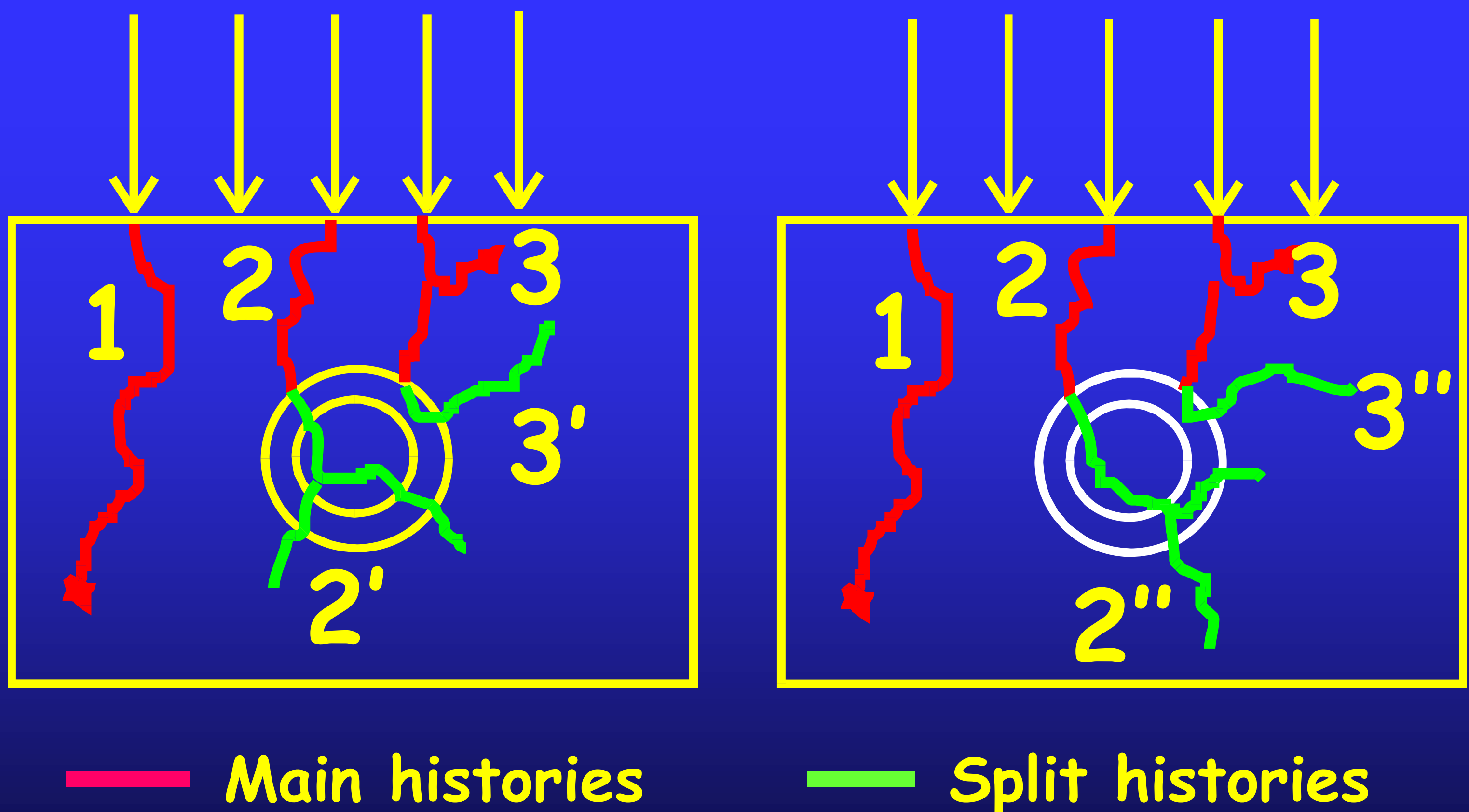
- Forces the primary photon fluence to be invariant with depth





Feng Ma, Paul Nizin – Baylor College of Medicine

Correlated Sampling



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Exponential Transform

- **Bias the sampling procedure to interact in the regions of interest**

$$N_\lambda = -\beta \ln R$$

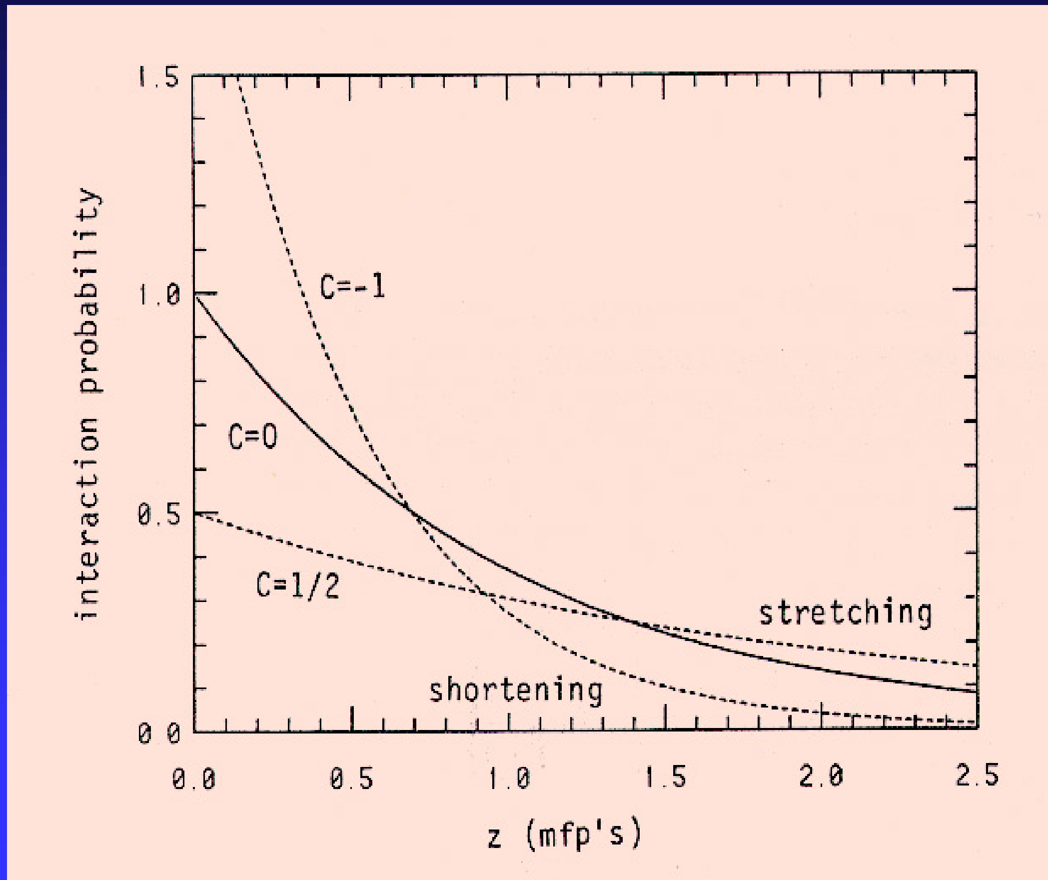
$$\beta = 1 / (1- C \cos\theta)$$

C is defined by the user, θ is the angle the photon makes with the direction of interest

The new weighting factor: $W' = W\, C\, e^{-N_\lambda \alpha \cos\theta}$

$C < 0$: smaller N_λ for surface problem, shortening

$0 < C < 1$: larger N_λ for shielding problem, stretching



Stretched (C = 1/2) and shortened (C = -1) distribution compared to an unbiased one (C = 0).
(From A.F. Bielajew and D.W.O. Rogers)

Courtesy of Jinsheng Li, Fox Chase CC

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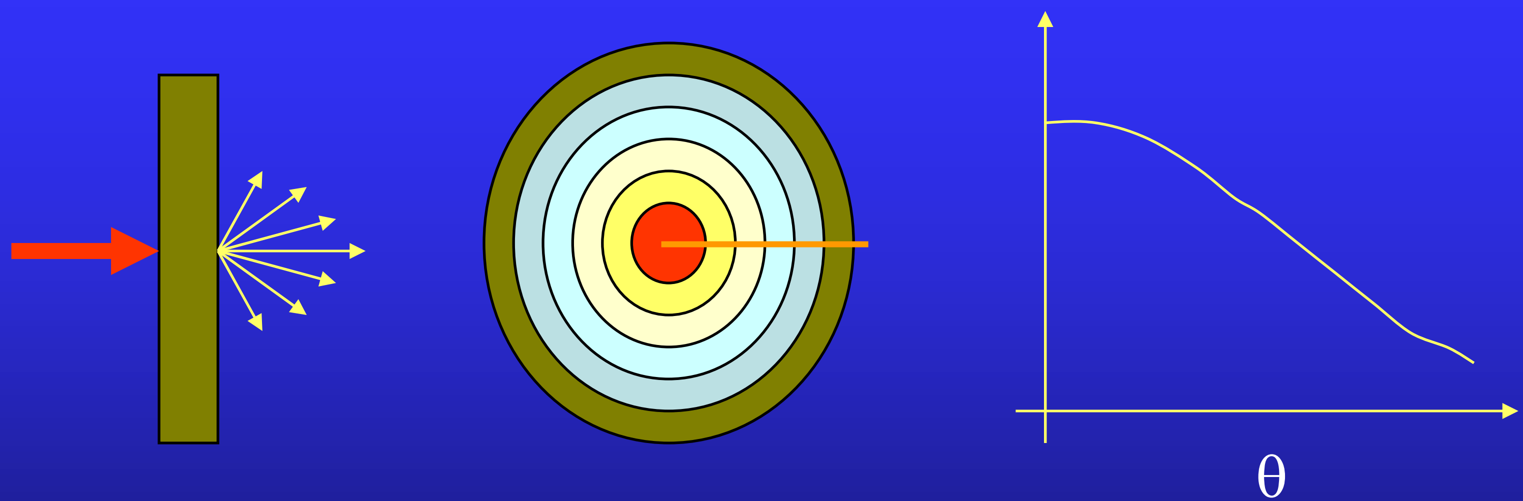
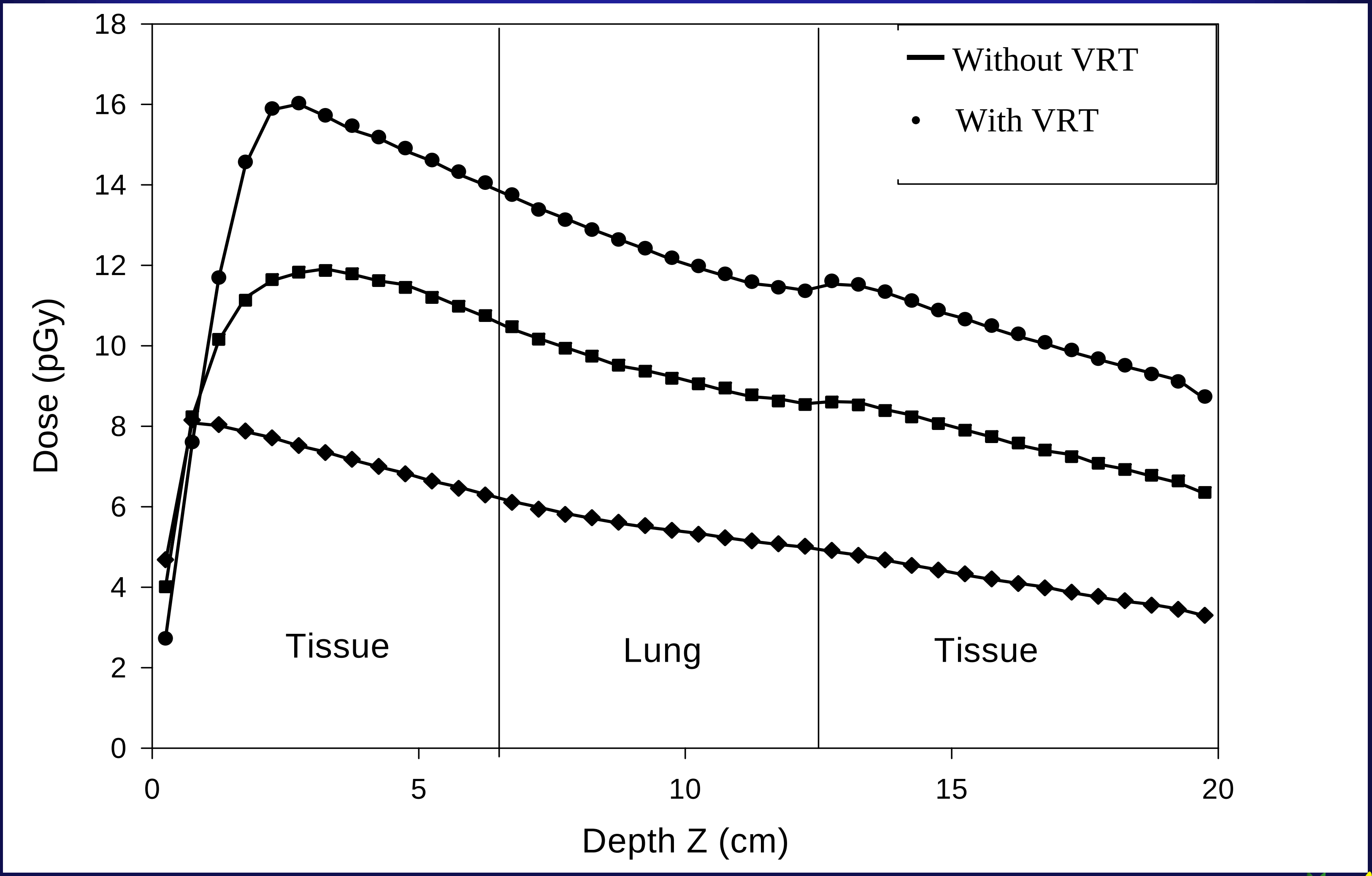
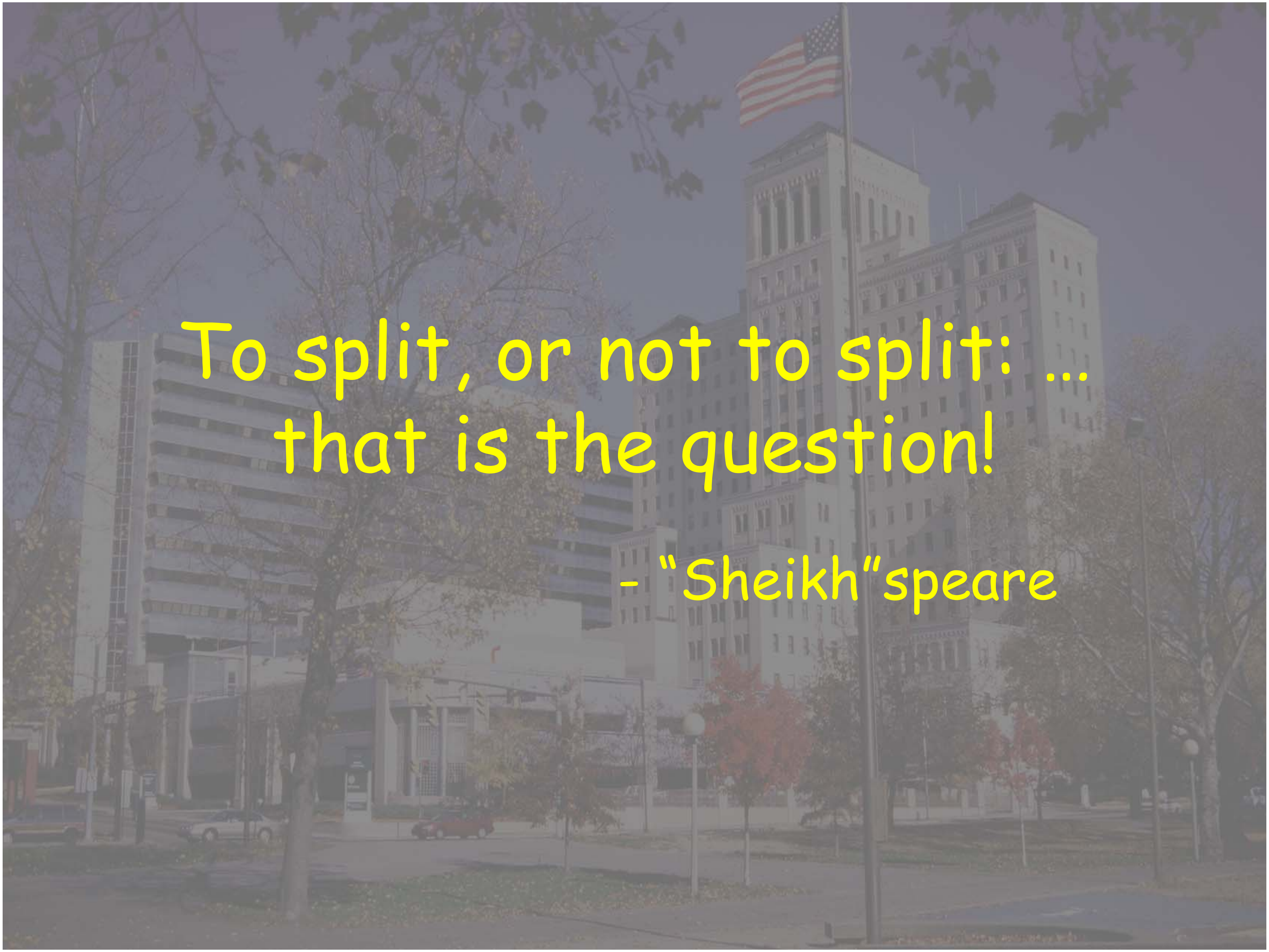
Use of Symmetry



Courtesy of Jinsheng Li, Fox Chase CC

PDD for Photon Beams





To split, or not to split: …
that is the question!

- "Sheikh"speare