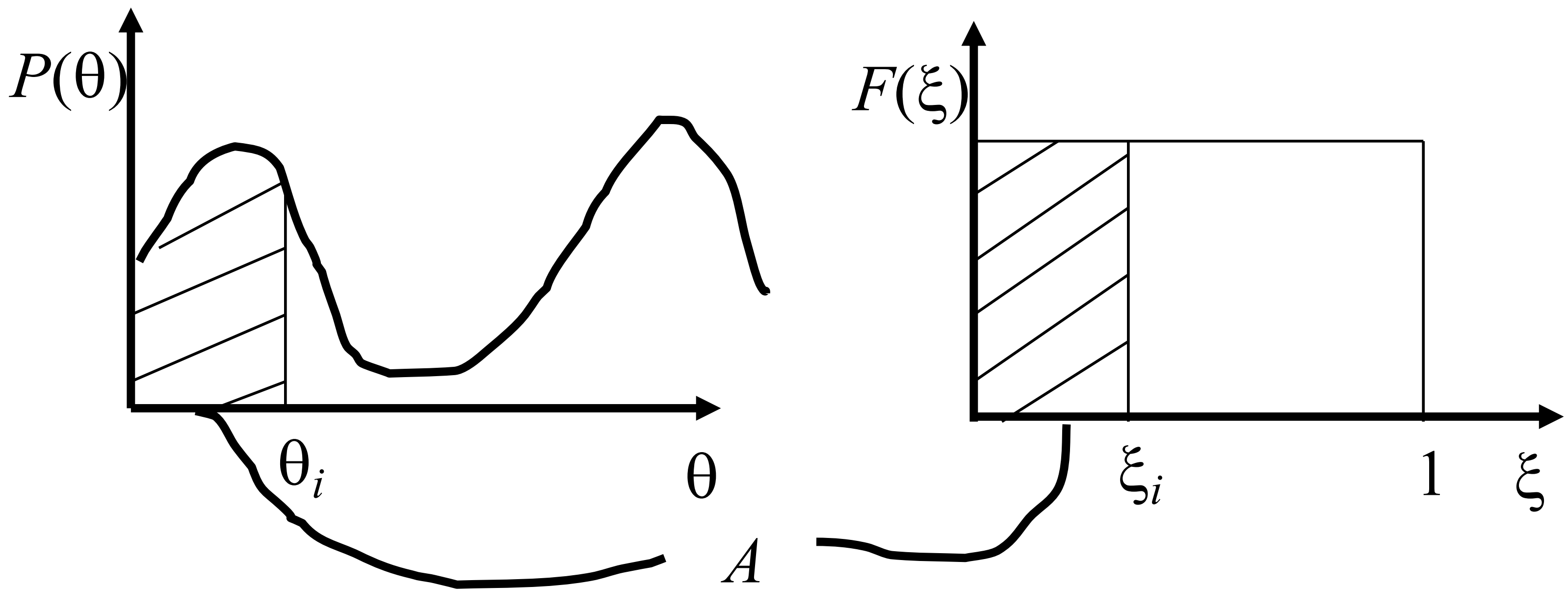
Monte Carlo Sampling

Sampling from PDFs: given $F(x)$ in analytic or tabulated form, generate a random number ξ in the range (0,1) and solve the equation to get the randomly sampled value X

$$\xi = \int_{x_{\min}}^{X} F(x)\,\mathrm{d}x = C(X) \quad \Rightarrow \quad X$$

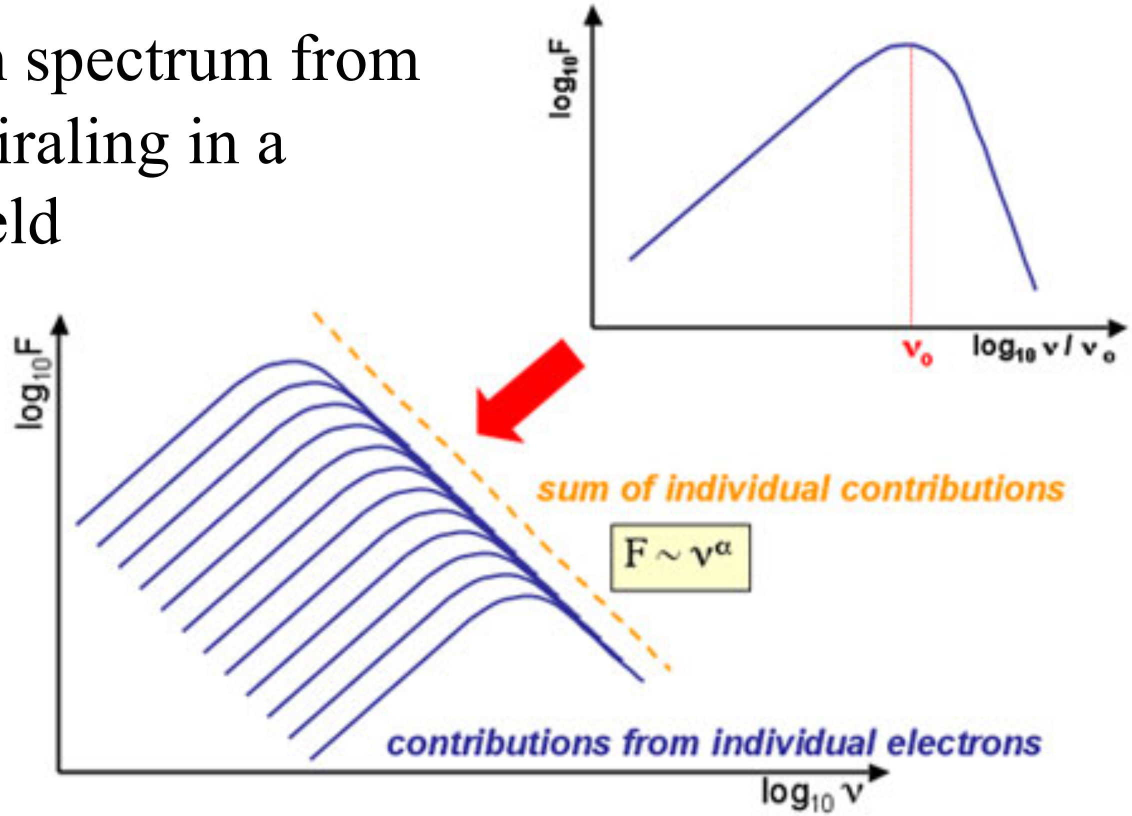
Solve this analytically, numerically, or by clever means…



Power Law Spectrum

- General power law spectrum: $y = a\,x^n + c$
- Choose random frequency ν_R from a power law spectrum: $F(\nu) \sim \nu^{-\alpha}$ with $\nu_1 < \nu < \nu_2$

Synchrotron spectrum from electrons spiraling in a magnetic field



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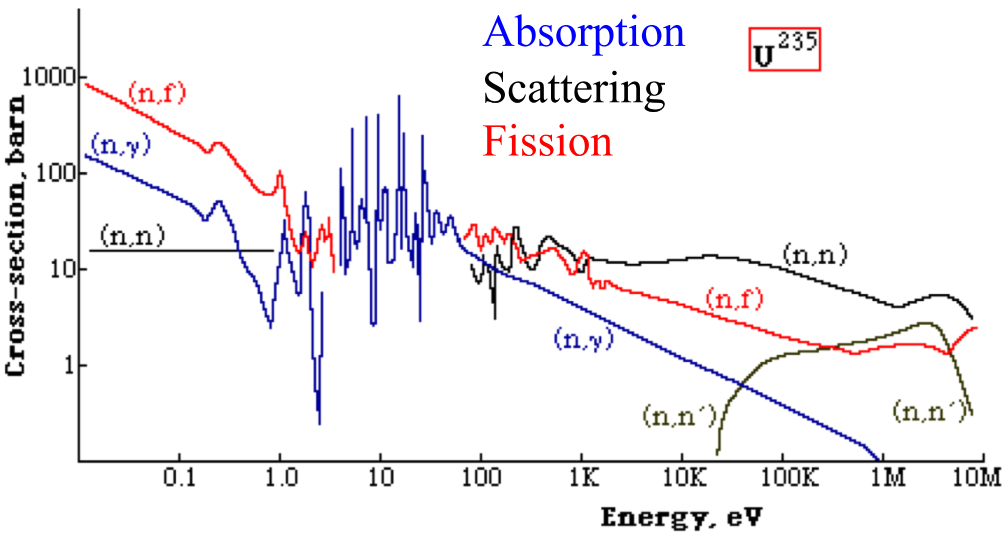
$$\boxed{\xi = \frac{\int_{\nu_1}^{\nu_R} \nu^{-\alpha}\,\mathrm{d}\nu}{\int_{\nu_1}^{\nu_2} \nu^{-\alpha}\,\mathrm{d}\nu} = \frac{\left[\nu^{1-\alpha}\right]_{\nu_1}^{\nu_R}}{\left[\nu^{1-\alpha}\right]_{\nu_1}^{\nu_2}} \quad \Rightarrow \quad \nu_R = \left(\nu_1^{1-\alpha} + \xi\left[\nu_2^{1-\alpha} - \nu_1^{1-\alpha}\right]\right)^{1/(1-\alpha)}}$$

Neutron Interactions

- Choose interaction event to be: absorption, scattering, or fission



$\sigma_T = \sigma_A + \sigma_S + \sigma_F$

ran = ξ

if (ran .lt. σ_A/σ_T) then

  neutron absorbed

elseif(ran .lt. $(\sigma_A+\sigma_S)/\sigma_T$) then

  neutron scattered

else

  fission event

endif

Tabulated Spectrum

- Solar spectrum: example of using numerical integration
- Given arrays of wavelengths, $\lambda(i)$, and corresponding flux values, $F(i)$, with $i = 1, 2, \ldots N$
- Numerical integration by trapezoidal rule:

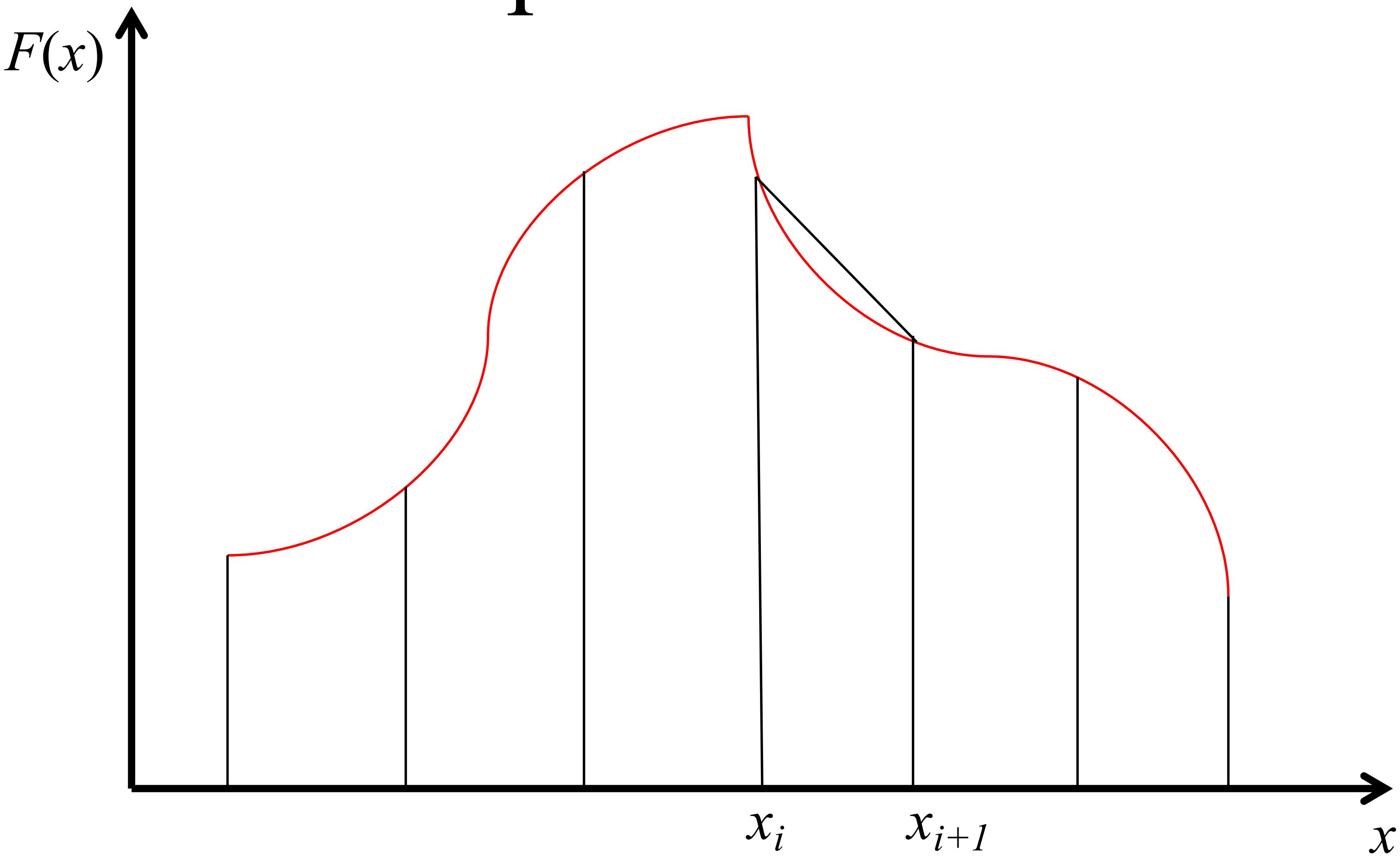
$$\int F(\lambda)\, d\lambda \approx \sum_{i=1}^{N-1} \frac{1}{2}\left(F_{i+1} + F_i\right)\left(\lambda_{i+1} - \lambda_i\right)$$

```
sum = 0
do i=1, N-1
  sum = sum + 0.5*[F(i+1)+F(i)]*[lam(i+1)-lam(i)]
end do
```

- Numerically compute and store the cumulative distribution function $C(i)$:

$$C(\lambda) = \int_{\lambda_{\min}}^{\lambda} F(\lambda')\, d\lambda' \Big/ \int_{\lambda_{\min}}^{\lambda_{\max}} F(\lambda')\, d\lambda'$$

Trapezoidal Rule



$$\text{Area} = [x_{i+1} - x_i]\,[F(x_i) + F(x_{i+1})]\,/\,2$$

Tabulated Spectrum

- Recall that $C(\lambda)$ increases monotonically from 0 to 1
- Also recall Monte Carlo sampling:

$$\xi = \int_{\lambda_{\min}}^{\lambda} F(\lambda')\,\mathrm{d}\lambda' = C(\lambda) \quad \Rightarrow \quad \lambda$$

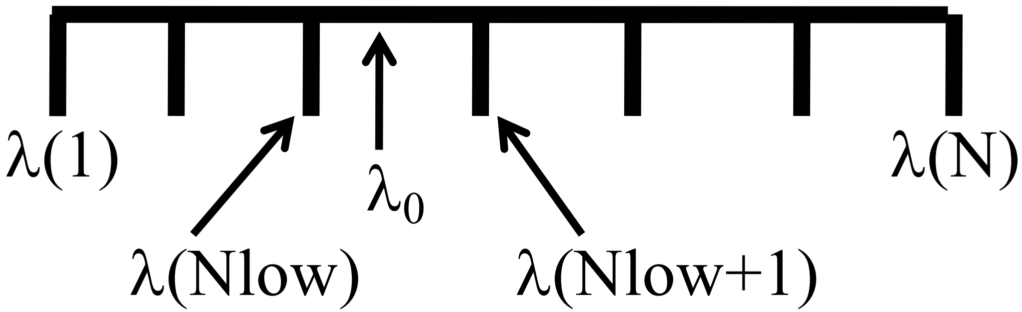
- So, given a random number ξ, search $C(i)$ to find C values that bracket ξ, and the corresponding indices i, i+1
- Interpolate to get wavelength and flux corresponding to ξ, e.g., linear interpolation:

$$\lambda = \lambda(i) + \left[\lambda(i+1) - \lambda(i)\right] \frac{\xi - C(i)}{C(i+1) - C(i)}$$

$$F = F(i) + \left[F(i+1) - F(i)\right] \frac{\lambda - \lambda(i)}{\lambda(i+1) - \lambda(i)}$$

Search an array by bisection

Given a wavelength, λ_0, search an array of wavelengths $\lambda(i)$, where i = 1, 2, … N, to find the λs and i-values that bracket λ_0



When exit the do-loop, λ_0 will be bracketed by the indices i = Nlow and i = Nlow + 1,
$\lambda(\mathrm{Nlow}) < \lambda_0 < \lambda(\mathrm{Nlow} + 1)$

```
Nup = N
Nlow=1
mid=(Nup+Nlow)/2
do while(Nup – Nlow .gt. 1)
  mid=(Nup+Nlow)/2)
  if (lam0 .gt. lam(mid)) then
     Nup=Nup
     Nlow=mid
  else
     Nup=mid
     Nlow=Nlow
  endif
end do
```

Setting the opacity

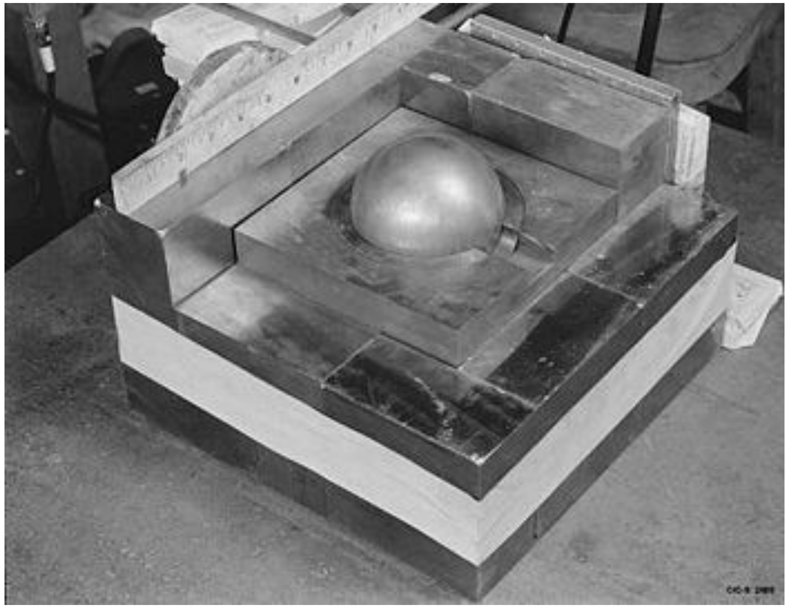
- If Monte Carlo simulation has source emitting a spectrum, then need to set optical properties (cross sections, opacities, etc) for the ensuing random walk for the wavelength randomly sampled from the spectrum
- Wavelength λ randomly sampled from source spectrum, find bracketing location as above in array of wavelengths for cross sections, interpolate to get optical properties:

$$\sigma(\lambda) = \sigma(i) + \left[\sigma(i+1) - \sigma(i)\right] \frac{\lambda - \lambda(i)}{\lambda(i+1) - \lambda(i)}$$

Volume emission from uniform sphere

- Choose x, y, z randomly in the range (-1, 1)
- Reject if $x^2 + y^2 + z^2 > 1$
- Choose new random set of x, y, z until $x^2 + y^2 + z^2 < 1$

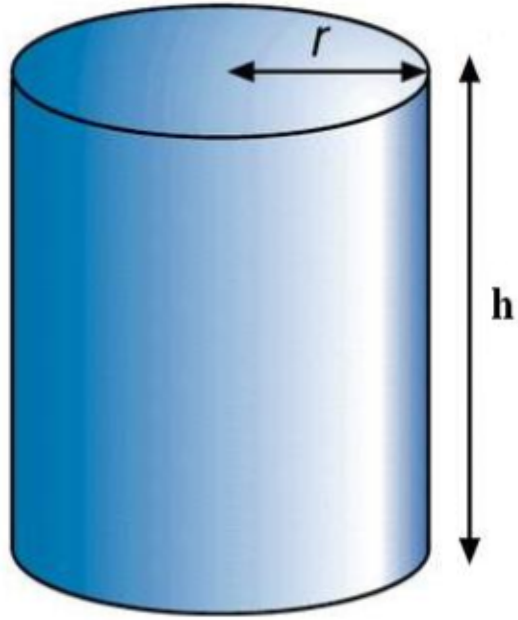
- OR sample from volume element $\mathrm{d}V = r^2 \sin\theta \,\mathrm{d}r \,\mathrm{d}\theta \,\mathrm{d}\phi$
- Choose r, θ, ϕ from appropriate pdfs – group tutorial exercise



Can use this algorithm
to select source locations for
neutrons when computing
critical mass of a Uranium sphere

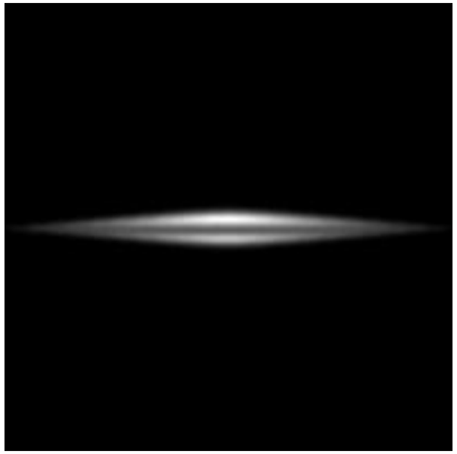
Cylinders or rods

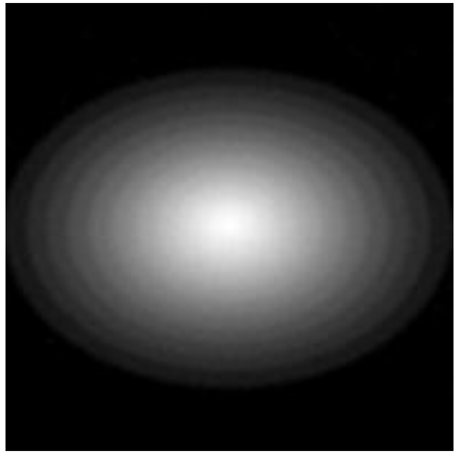
- Choose z using: $z = \xi h$
- Choose x, y randomly in the range $(-r, r)$
- Reject if $x^2 + y^2 > r^2$
- Choose new random set of x, y until $x^2 + y^2 < r^2$



- OR choose z as above, but sample r, θ from appropriate pdfs for uniformly sampling points within a circle – group tutorial exercise

Emission from a galaxy with stellar emission approximated as a smooth emissivity: $j(r, z) \sim \exp(- |z| / Z) \exp(- r / R)$. Defined over $0 < r < R_{\max}$, $0 < z < Z_{\max}$





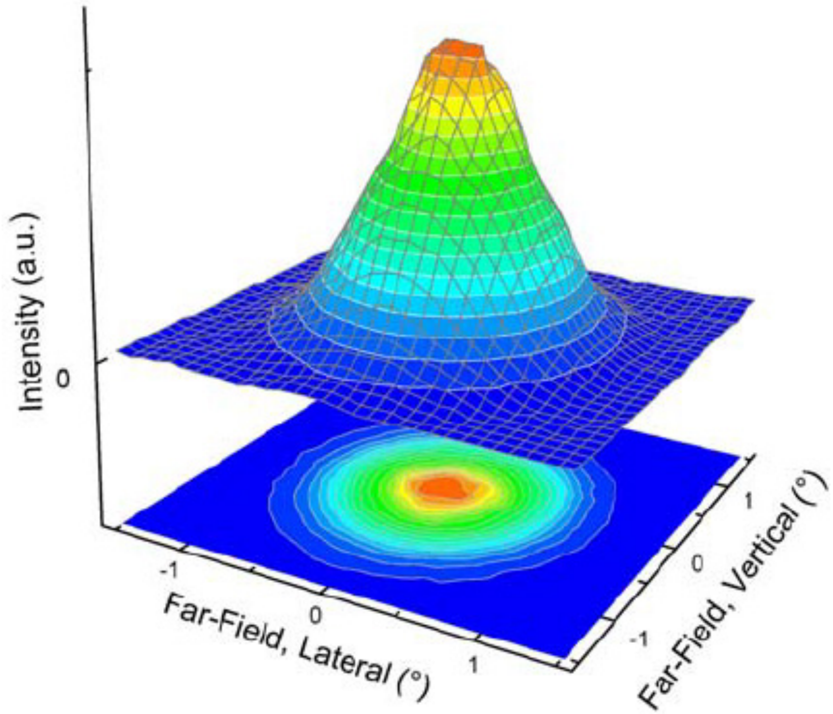
Split into separate probabilities for r and z

$$\xi = \frac{\int_0^r \exp(-r/R)\,\mathrm{d}r}{\int_0^{R_{\max}} \exp(-r/R)\,\mathrm{d}r} = \frac{[1-\exp(-r/R)]}{[1-\exp(-R_{\max}/R)]}$$

$$\Rightarrow \quad r = -R\log\left(1-\xi\,[1-\exp(-R_{\max}/R)]\right)$$

Laser beams

- Techniques for sampling from collimated laser beams, e.g., Gaussian beam profile…



Launching from a collimated beam

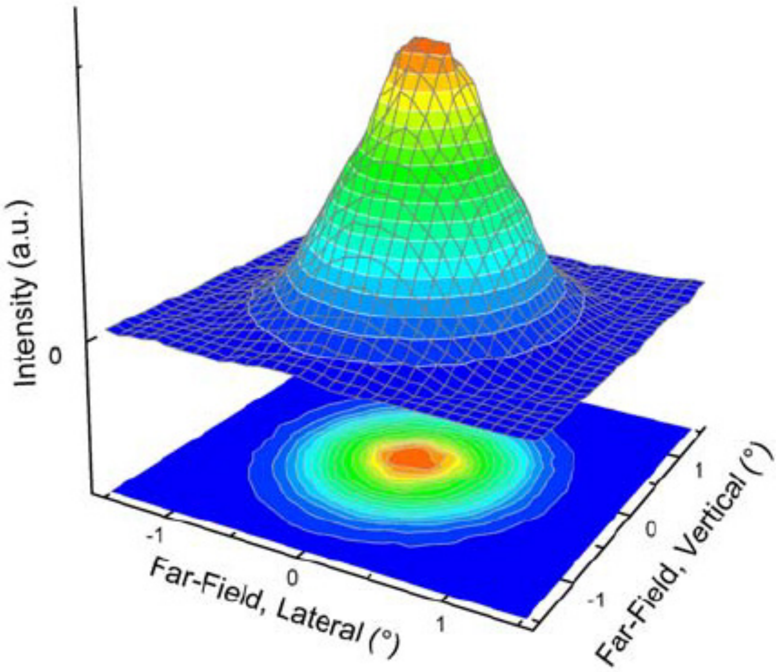
- For a circular beam of uniform intensity can use rejection method to sample (*x, y*) launch positions of photons
- Choose x, y randomly in the range ($-R$, R)
- Reject if $x^2 + y^2 > R^2$
- Choose new random set of x, y until $x^2 + y^2 < R^2$

- Gaussian beam profile: $\exp[-(r/b)^2]$
- Choose (r, ϕ) by:

$$r = b\sqrt{-\ln(\xi)}$$

$$\phi = 2\pi\xi$$

- See Jacques (2009) review eq 5.27
- Use trigonometry to get (*x, y*)



Clever techniques…

- Not as crucial now, but something still to consider when trying to speed up codes – be efficient!
- Cost of evaluating functions: addition < division < exponentials < trig functions, etc
- Cashwell & Carter (1977) – Third Monte Carlo Sampler, contains algorithms for sampling lots of functions

Isotropic emission or scattering

- Choosing isotropic direction cosines
- Simple method:

$$\mu = \cos\theta = 2\xi - 1$$

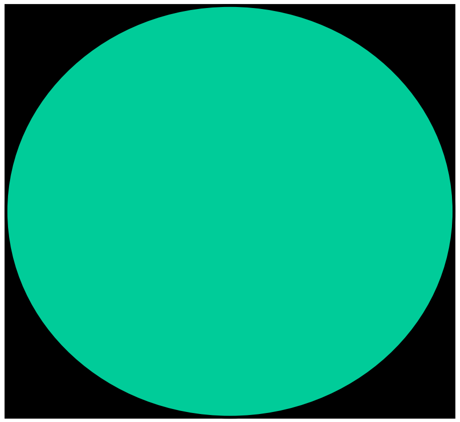
$$\phi = 2\pi\,\xi$$

$$n_x = \sqrt{1-\mu^2}\,\sin\phi$$

$$n_y = \sqrt{1-\mu^2}\,\cos\phi$$

$$n_z = \mu$$

- From John von Neumann, to avoid evaluating sin ϕ, cos ϕ:



Choose $x = 2\xi - 1$, $y = 2\xi - 1$ (different ξs!!)
Reject if $x^2 + y^2 > 1$
$\cos\phi = x/\mathrm{sqrt}(x^2 + y^2)$, $\sin\phi = y/\mathrm{sqrt}(x^2 + y^2)$
Double angle formula avoids taking square root:
$\cos\phi = (x^2 - y^2)/(x^2 + y^2)$, $\sin\phi = 2xy/(x^2 + y^2)$

- Efficiency = π / 4

Energy of fission neutrons

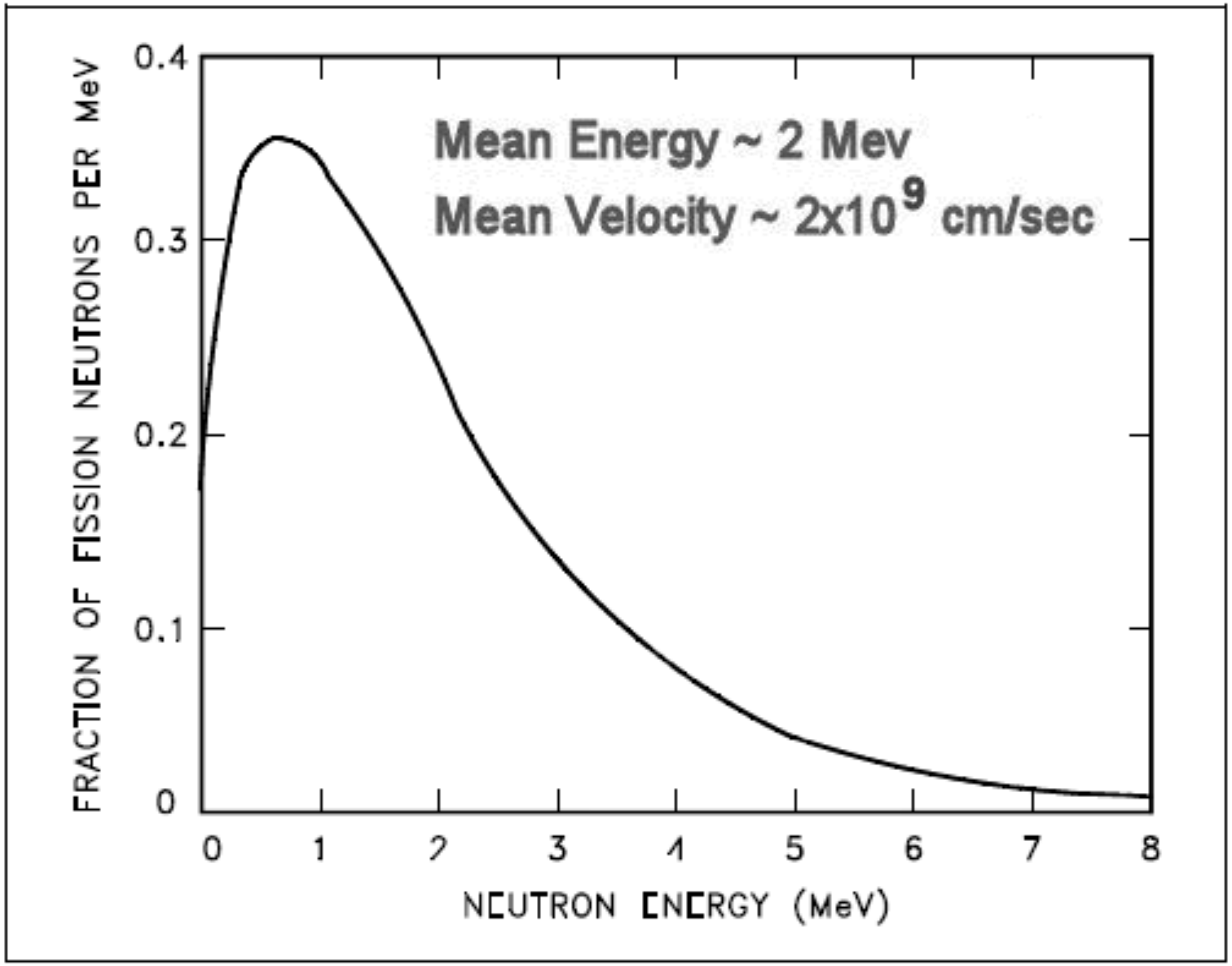
Fission produced by an incident neutron of energy E_0. Sample energy E from the normalised fission spectrum, which can be approximated by the Maxwell spectrum:

$$X(E) = \frac{2}{\pi^{1/2}} T(E_0)^{-3/2} E^{1/2} \mathrm{e}^{-E/T(E_0)}$$

where $T(\mathrm{E}_0)$ is the nuclear temperature (in energy units) which is tabulated as a function of energy in nuclear data tables. Use three random numbers to get:

$$E = T(E_0)\left[-\ln\xi_1 - \left(\ln\xi_2\right)\cos^2\left(\frac{\pi}{2}\xi_3\right)\right]$$

U235 Fission Spectrum



Prompt Fission Neutron Energy Spectrum for
Thermal Fission of Uranium-235

Blackbody Radiation

Sample frequency ν from Planck function. Use the normalised Planck function with $x = h\nu/kT$

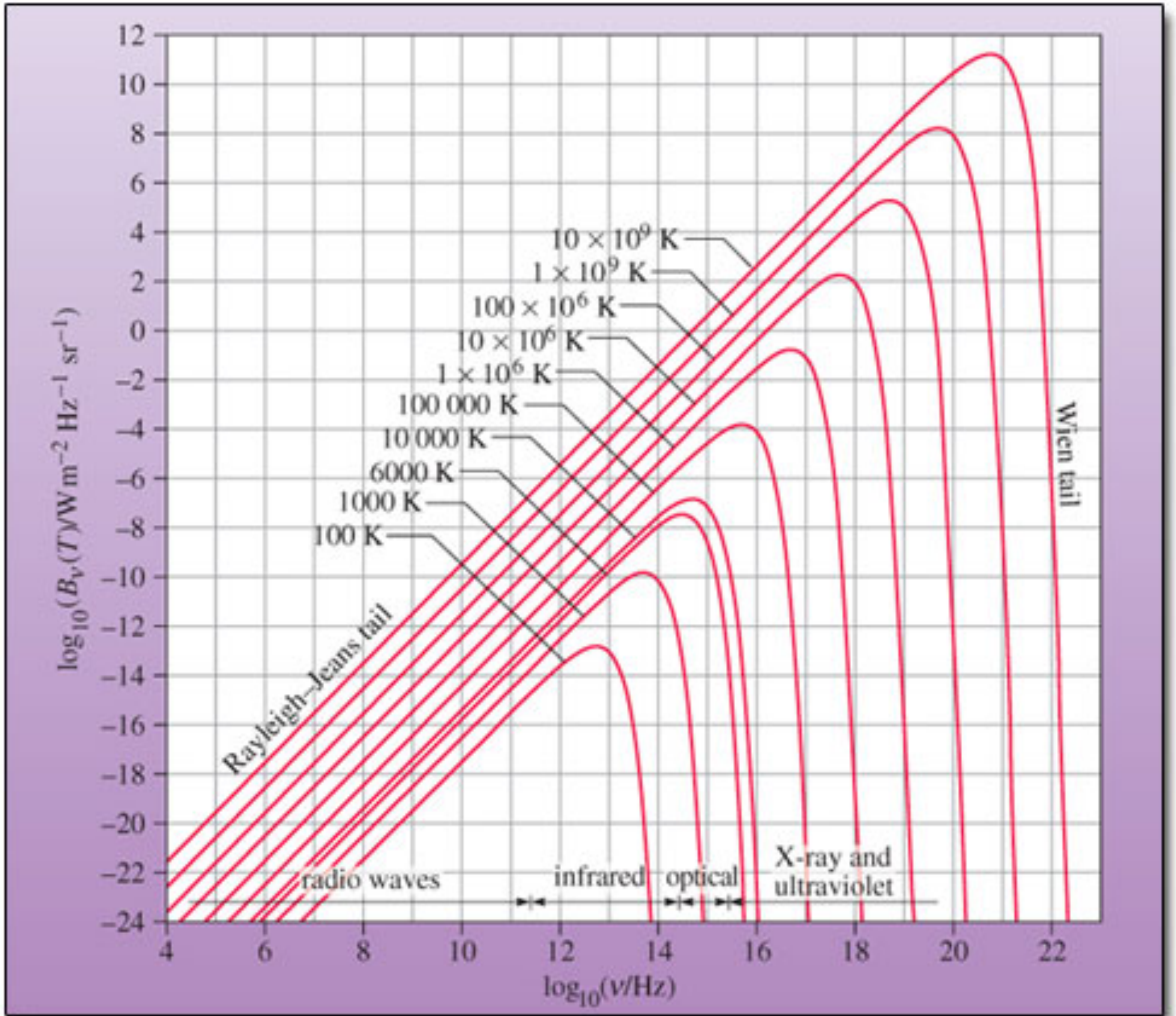
$$B_\nu(T) = \frac{2h\nu^3}{c^2}\frac{1}{e^{h\nu/kT}-1} \quad ; \quad b_x = \frac{15x^3}{\pi^4\left(\mathrm{e}^x - 1\right)}$$

Set: $$L = \min\left\{ l\,;\sum_{j=1}^{l} j^{-4} \geq \xi_0 \frac{\pi^4}{90} \right\}$$

The notation $\{x; F(x)\}$ means the set of all x satisfying $F(x)$

Then: $$x = -L^{-1}\ln\left(\xi_1\,\xi_2\,\xi_3\,\xi_4\right)$$

Blackbody Radiation



Scattering

- Isotropic scattering: neutrons, photons
- See later lectures for non-isotropic scattering, polarization, and rotating angles from scattering to lab frame
- Non-isotropic: electrons, dust, molecules, biological tissue
- Rayleigh, Thompson/Compton, Klein-Nishina, Mie theory, Heyney-Greenstein functions