# Statistical Methods in Particle Physics

## 4. Monte Carlo Methods

Heidelberg University, WS 2020/21

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# Monte Carlo method

- Any method which solves a problem by generating suitable random numbers
- Useful for obtaining numerical solutions to problems which are too complicated to solve analytically
- The most common application of the Monte Carlo method is Monte Carlo integration
- Pioneers
  - Enrico Fermi
  - Stanislaw Ulam
  - John von Neumann
  - Nicholas Metropolis

https://en.wikipedia.org

Enrico Fermi

Stanislaw Ulam

J. von Neumann

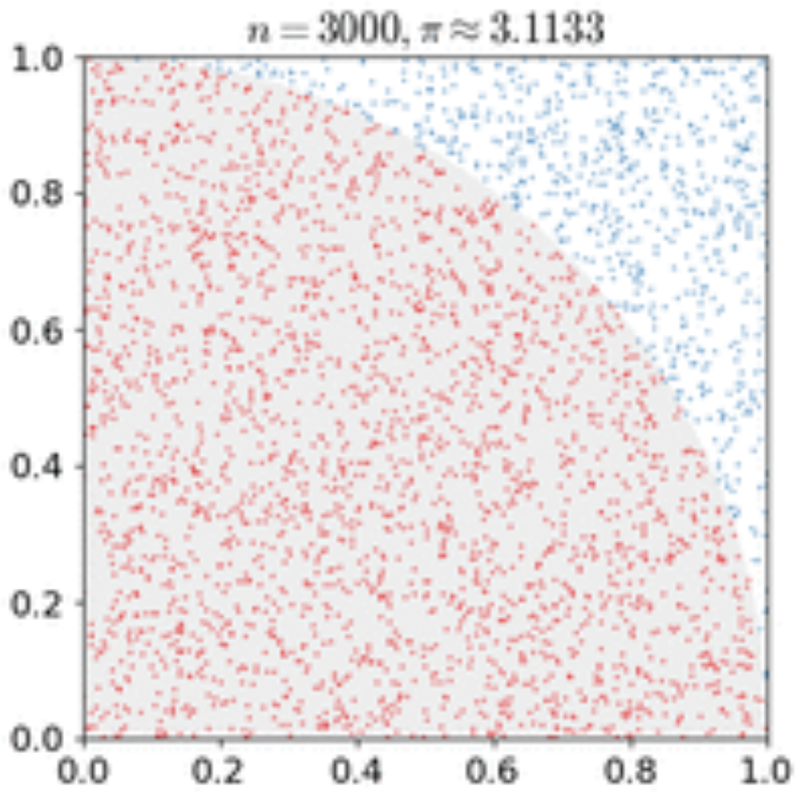
N. Metropolis

http://mathworld.wolfram.com/MonteCarloMethod.html

# Monte Carlo method: Examples

[from Bohm, Zech: Introduction to Statistics and Data Analysis for Physicists]

- Area of a circle
- Volume of the intersection of a cone and a torus
  - Hard to solve analytically
  - Easy to solve by scattering points homogeneously inside a cuboid containing the intersect
- Efficiency of particle detection with a scintillator
  - Produced photons are reflected at the surfaces and sometime absorbed
  - Almost impossible to calculate analytically for different parameters like incident angle, particle energy, …
  - Monte Carlo simulation is the only sensible approach



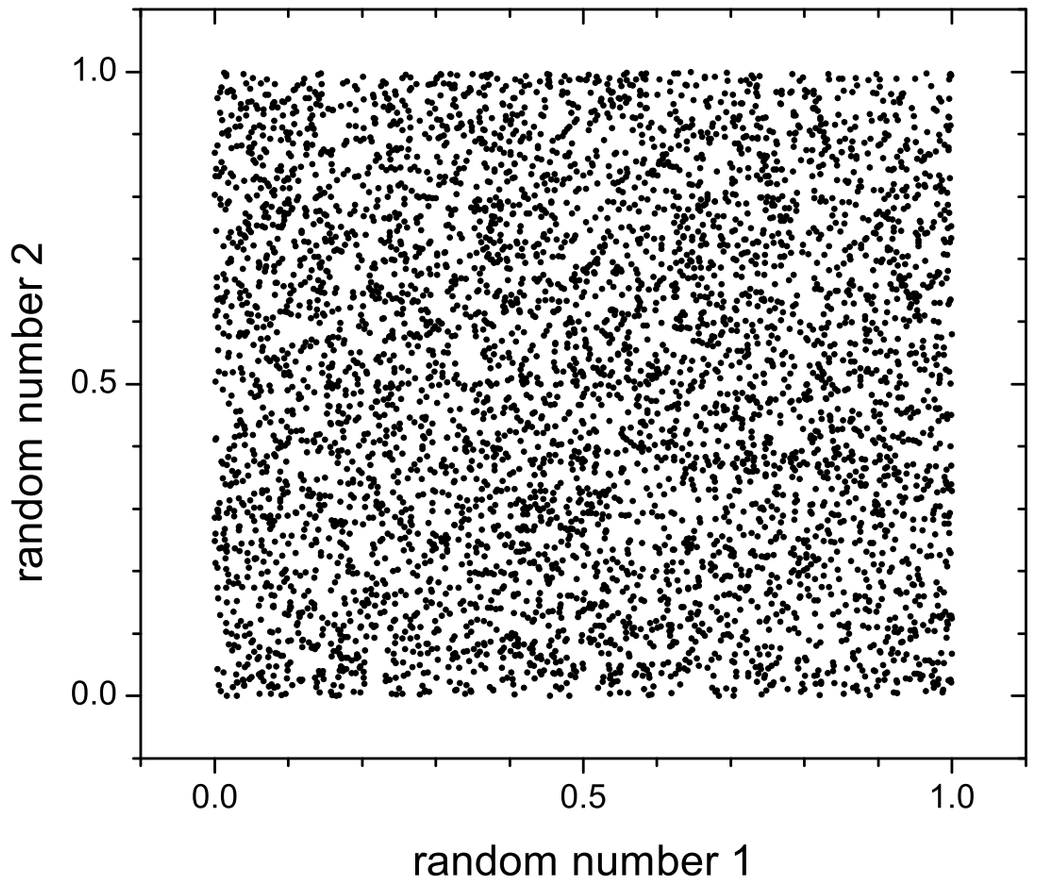
# Pseudo-random numbers

- Principle: Use insignificant digits of an operation to generate next number
  - choose large integers λ and $m$, $\lambda < m$
  - choose integer $n_0 < m$ (“seed”)
  - uniformly distributed random numbers $r_i$:

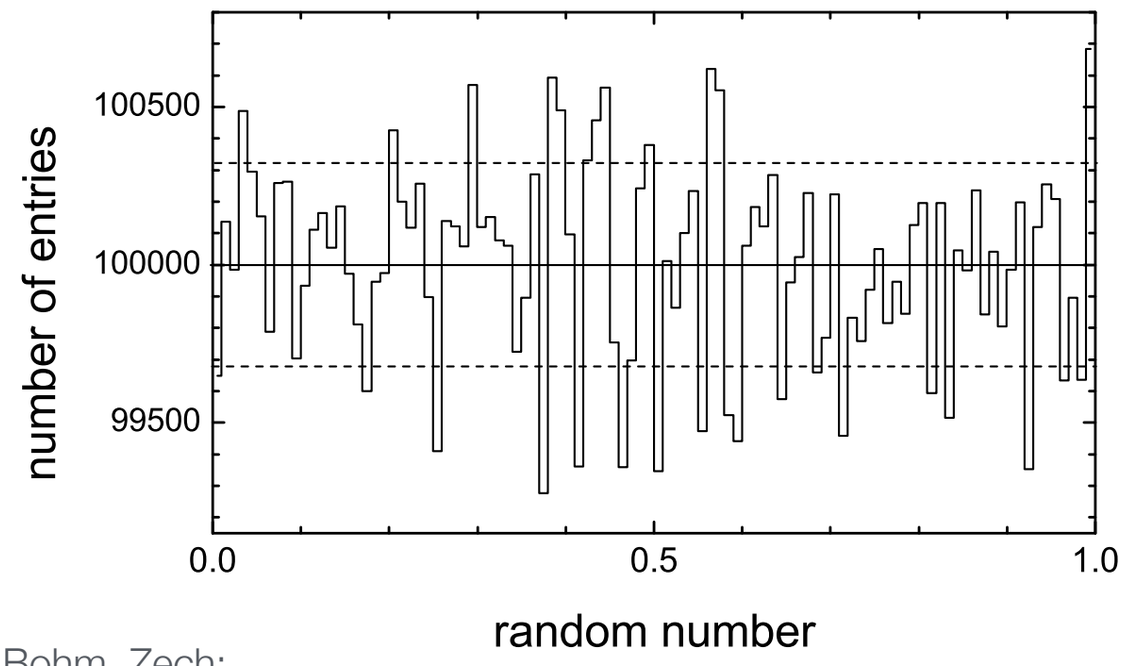
$$n_{i+1} = \lambda n_i \bmod m$$

$$r_i = n_i / m, \quad r_i \in [0, 1]$$

“Multiplicative linear congruential algorithm“
(period at maximum $m$ – 1)




- *Mersenne twister*
  - Invented 1997 by M. Matsomoto and T. Nishimura
  - Sequence repeats after $2^{19937}$ calls, i.e., never …
- Quality checks
  - Frequency of occurrence
  - Plot correlations between consecutive random numbers




Bohm, Zech:
http://www-library.desy.de/preparch/books/vstatmp_engl.pdf

# Box-Muller algorithm for creating Gaussian distributed random numbers

1. Generate two uniformly distributed random numbers $u_1$ and $u_2$ in the range [0,1]

2. Set

$$\phi = 2\pi u_1, \qquad r = \sqrt{-2 \ln u_2}$$

3. Then

$$z_1 = r \cos\phi \quad \text{and} \quad z_2 = r \sin\phi$$

are two independent rv's following a standard normal distribution

Why?

$$u_2(r) = e^{-\frac{r^2}{2}}$$

$$\frac{dp}{dr} = \frac{dp}{du_2} \cdot \left|\frac{du_2}{dr}\right| = e^{-\frac{r^2}{2}} r$$

$$dp = \underbrace{\frac{1}{2\pi} e^{-\frac{r^2}{2}} r \, dr \, d\phi}_{\text{2d standard normal distribution in polar coordinates}} = \underbrace{\frac{1}{2\pi} e^{-\frac{z_1^2+z_2^2}{2}} dz_1 \, dz_2}_{\text{2d standard normal distribution in cartesian coordinates}}$$

# Random Numbers from distributions: Inverse transform method

Consider a distribution $f$ from which we want to draw random numbers. Let $u(r)$ be the uniform distribution in [0, 1]:

$$\int_{-\infty}^{x} f(x')\,\mathrm{d}x' = \int_{0}^{r(x)} u(r')\,\mathrm{d}r' = r(x)$$

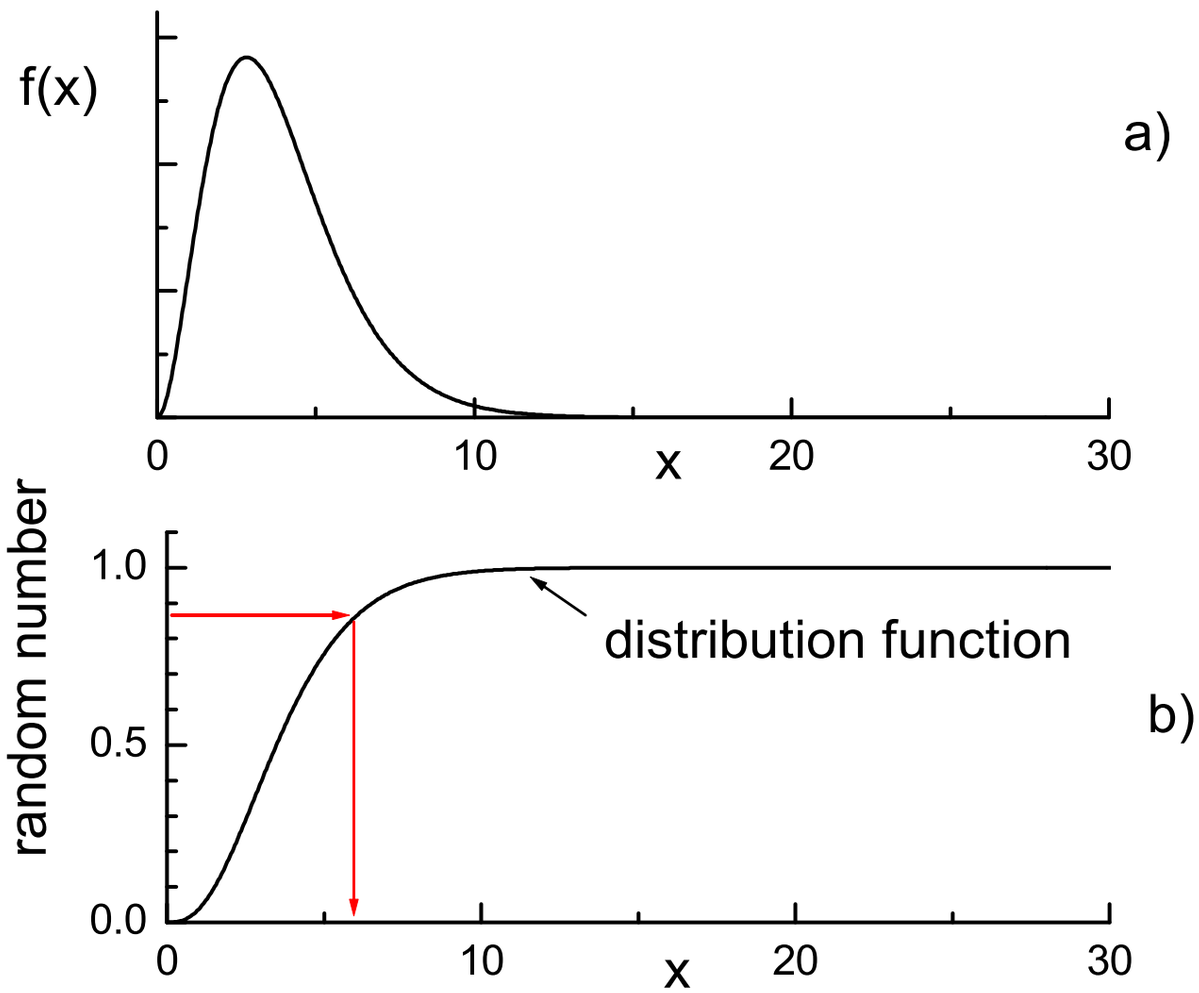
With $F(x)$ = cumulative distr.:

$$F(x) = r$$

We get the random number $x$ from the inverse of the cumulative distribution:

$$x(r) = F^{-1}(r)$$

Bohm, Zech:
http://www-library.desy.de/preparch/books/vstatmp_engl.pdf




Cross check:

$$\frac{\mathrm{d}p}{\mathrm{d}x} = \underbrace{\frac{\mathrm{d}p}{\mathrm{d}r}}_{=1}\frac{\mathrm{d}r}{\mathrm{d}x} = \frac{\mathrm{d}F(x)}{\mathrm{d}x} = f(x) \qquad \square$$

# Example I

Linear function:

$$f(x) = 2x, \qquad 0 \leq x \leq 1$$
$$F(x) = x^2 \quad \rightarrow \quad x = \sqrt{r}$$

Exponential:

$$f(x) = \gamma e^{-\gamma x}, \qquad x \geq 0$$
$$F(x) = 1 - e^{-\gamma x} \quad \rightarrow \quad x = -\frac{\ln(1-r)}{\gamma}$$

One can store *F*(x) as a histogram if there is no analytical solution, cf. root's `GetRandom()` function:

```
root [0] TF1 f("f", "x^3/(exp(x)-1)", 0., 15.);
root [1] cout << f.GetRandom() << endl;
13.9571
```

# Inverse transform method using histograms in Python

```
def get_random(f, xmin, xmax, n_samples):
    """Generate n_samples random numbers within range [xmin, xmax]
    from arbitrary continuous function f
    using inverse transform sampling
    """

    # number of points for which we evaluate F(x)
    nbins = 10000

    # indefinite integral F(x), normalize to unity at xmax
    x = np.linspace(xmin, xmax, nbins+1)
    F = integrate.cumtrapz(f(x), x, initial=0)
    F = F / F[-1]

    # interpolate F^{-1} and evaluate it for
    # uniformly distributed rv's in [0,1[
    inv_F = interpolate.interp1d(F, x, kind="quadratic")
    r = np.random.rand(n_samples)
    return inv_F(r)
```

[random_numbers_from_distribution.ipynb]

# Example II: Uniform points on a sphere

$$\frac{\mathrm{d}p}{\mathrm{d}\Omega} = \frac{\mathrm{d}p}{\sin\theta\,\mathrm{d}\theta\,\mathrm{d}\phi} = \mathrm{const} \equiv k \qquad \frac{\mathrm{d}p}{\mathrm{d}\theta\,\mathrm{d}\phi} = k\sin\theta \equiv f(\phi)g(\theta)$$

Distributions for θ and ϕ:

$$f(\phi) \equiv \frac{\mathrm{d}p}{\mathrm{d}\phi} = \mathrm{const} = \frac{1}{2\pi}, \qquad 0 \le \phi \le 2\pi$$

$$g(\theta) \equiv \frac{\mathrm{d}p}{\mathrm{d}\theta} = \frac{1}{2}\sin\theta, \qquad 0 \le \theta \le \pi$$

Calculating the inverse of the cumulative distribution we obtain:

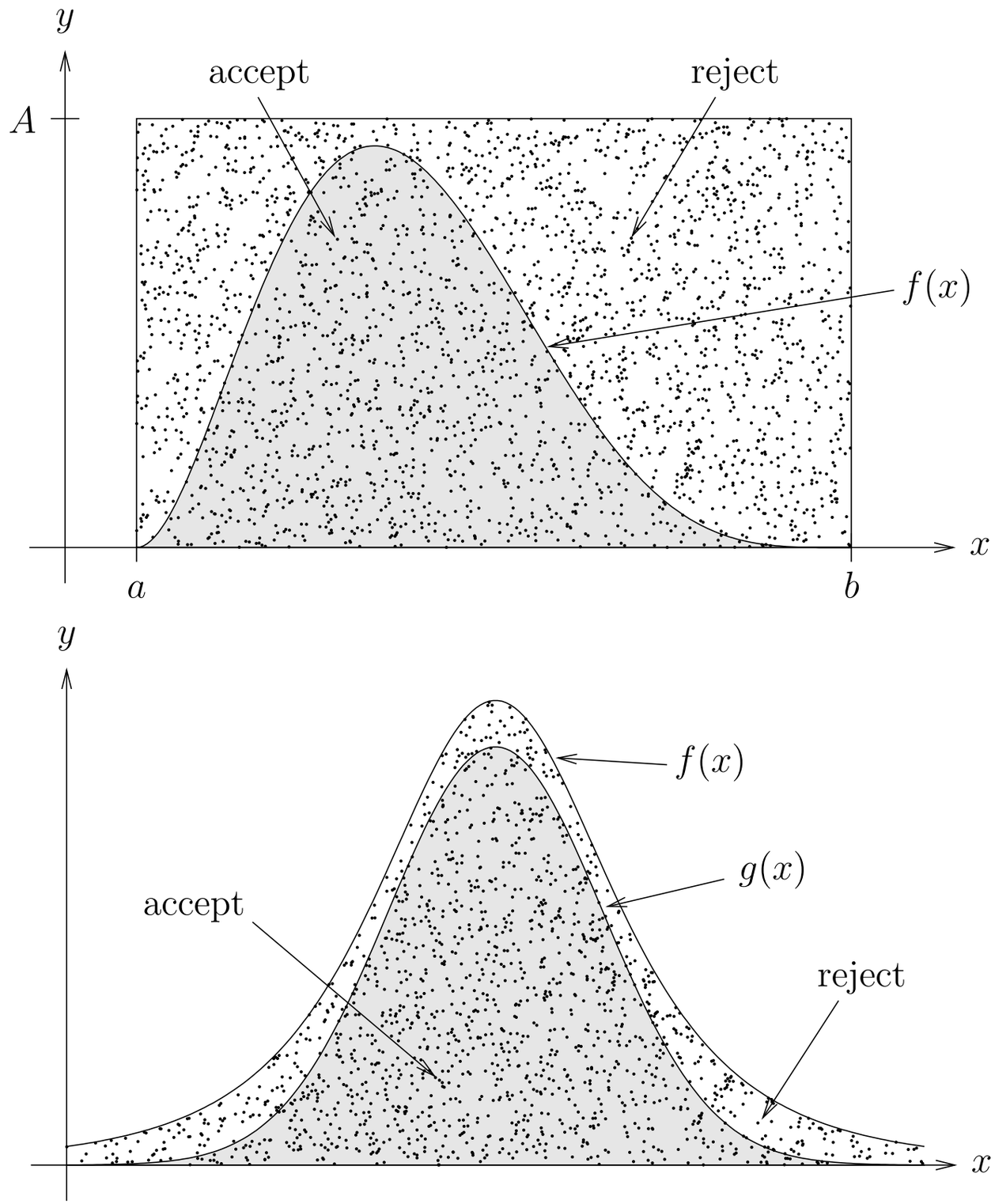
$$\phi = 2\pi r_1$$

$$\theta = \arccos(1 - 2r_2) \qquad [\text{as } G(\theta) = \frac{1}{2}(1 - \cos\theta)]$$

Upshot: ϕ and cos θ need to be distributed uniformly

# Random numbers from distributions: Acceptance-rejection method

- Algorithm
  - Generate random number *x* uniformly between *a* and *b*
  - Generate second random *y* number uniformly between 0 and *A*
  - Accept *x* if *y* < f(*x*)
  - Repeat many times
- The efficiency of this algorithm can be quite small
- Improvement possible by choosing a majorant, i.e., a function which encloses *g*(x) and whose integral is known ("importance sampling")



# Random numbers from multivariate Gaussian (1)

Random number from multivariate normal distribution $f(\vec{x}; \vec{\mu}, V)$:

1. Calculate the Cholesky decomposition $V = AA^{\mathrm{T}}$
2. Draw $z_1, z_2, \ldots, z_n$ from the standard normal distribution $N(0,1)$ and let $\vec{z} = (z_1, z_2, \ldots, z_n)$
3. Output $\vec{x} = \vec{\mu} + A\vec{z}$

Cholesky decomposition:

A symmetric positive-definite matrix $V$ can be written as

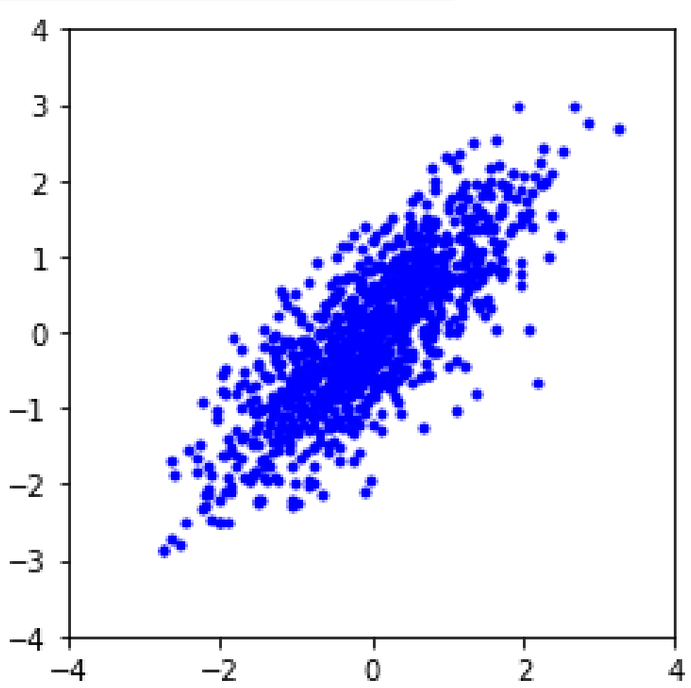
$$V = AA^{\mathrm{T}}$$

where $A$ is a real lower triangular matrix with positive diagonal entries.

# Random numbers from multivariate Gaussian (2)

[random_numbers_mv_normal_distr.ipynb]

```
# example: 2d normal distribution
mu = np.array([0., 0.]) # mean
cov = np.array([[1, 0.8], [0.8 , 1]]) # cov. matrix

# Cholesky decomposition, A = lower triangular matrix
A = np.linalg.cholesky(cov)

# number of random vectors
n = 1000

# random numbers following standard normal distr.
# Ndim rows, N columns (here Ndim = 2)
z = np.random.normal(size=(2, n))

# matrix with Ndim rows (here Ndim = 2):
# [[mu1, mu1, ...], [mu2, mu2, ...]]
mean = np.repeat(mu, n).reshape(2,n)

# matrix of random vectors
# vector i: (rand[1][i], rand[2][i])
rand = mean + np.dot(A, z)
```

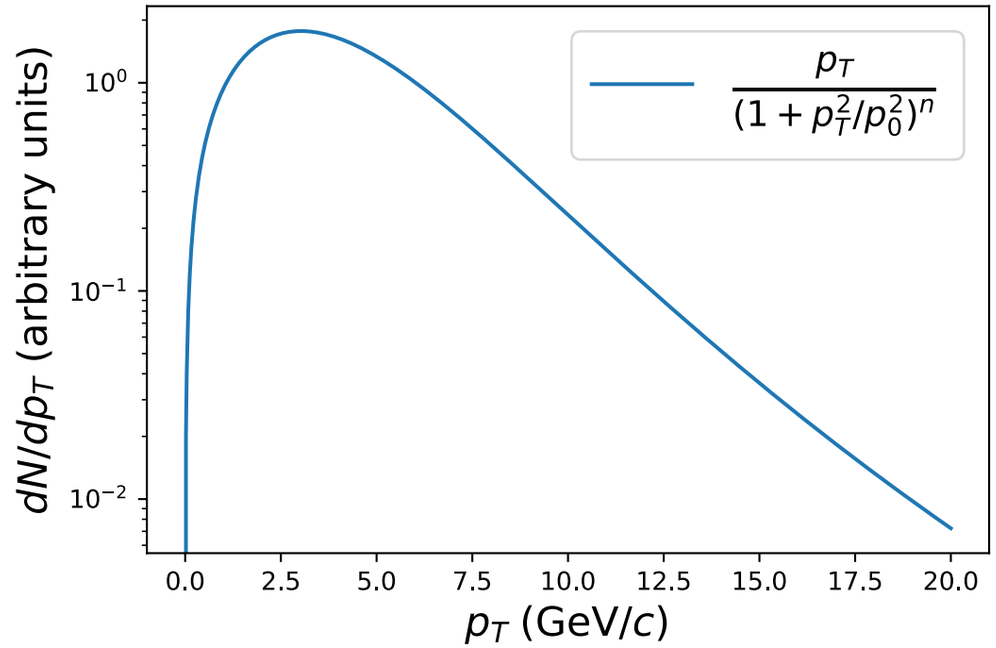


# Weighting method

Sometimes it is not practical to generate random numbers from a distribution $f(x)$

- for instance, because in the range of interest it varies by several orders of magnitude
- take $p_T$ spectra as an example: would take long to get sufficient statistics at high $p_T$

Typical $p_T$ spectrum, e.g., of a J/ψ meson




In this case the weighting method may be useful:

1. Generate uniformly distributed random numbers $x_i$ in interval of interest $[x_{\min}, x_{\max}]$
2. Assign a weight $w_i = f(x_i)$ to event $i$
3. Fill histogram, e.g. for those events that pass certain cuts, with weight $w_i$, i.e., histogram counter is incremented by $w_i$, not by 1

More general: define a distribution $h(x)$ which is easy to sample but not necessarily uniform, draw $x_i$ from $h$, and set $w_i = f(x_i)/h(x_i)$.

# Monte Carlo Integration

## Naïve Monte Carlo integration:

$$\underbrace{\int_a^b f(x)\,\mathrm{d}x}_{=:\,I} = (b-a)\int_a^b f(x)\,\underbrace{u(x)}_{\text{uniform distribution in } [a,b]}\,\mathrm{d}x = (b-a)\langle f(x)\rangle \approx \underbrace{(b-a)\cdot\frac{1}{n}\sum_{i=1}^{n} f(x_i)}_{=:\,\hat{I}}$$

$x_i$: uniformly distributed random numbers

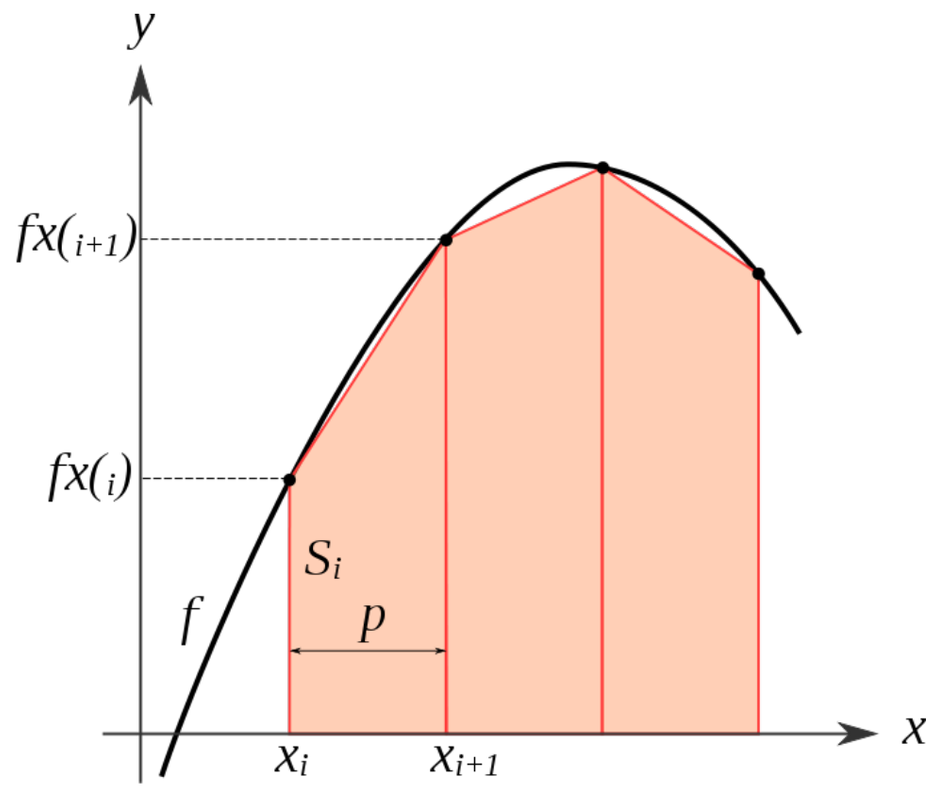
## Typical deviation from the true value of the integral (standard deviation)

$$V[\hat{I}] = \frac{(b-a)^2}{n^2} V[\sum_{i=1}^{n} f(x_i)] = \frac{(b-a)^2}{n^2}\cdot n\cdot\sigma^2[f] \quad \rightarrow \quad \sigma[\hat{I}] = \frac{b-a}{\sqrt{n}}\sigma[f]$$

# Monte Carlo Integration: Multidimensional integrals

## Trapezoidal rule in one dimension

- accuracy improves as $1/n^2$ with the number of points
- Much better than $1/\sqrt{n}$ scaling of the MC methods




https://en.wikipedia.org/wiki/Trapezoidal_rule

## Monte Carlo integration in *d* dimensions:

$$I = \int_\Omega f(\vec{x})\,\mathrm{d}\vec{x}, \quad \Omega \subset \mathbb{R}^d, \qquad V = \int_\Omega \mathrm{d}\vec{x}$$

$$I \approx \hat{I} = V\frac{1}{n}\sum_{i=1}^{n} f(\vec{x}_i), \qquad \sigma[\hat{I}] \approx V\frac{\sigma[f]}{\sqrt{n}}$$ ← same as in 1d case

## Trapezoidal rule in *d* dimension:

- accuracy improves as $1/n^{2/d}$ with the number of points
- for $d > 4$ the dependence on $n$ is better for MC integration

For multidimensional integrals MC integration outperforms other numerical integration methods

# Metropolis-Hastings algorithm (1)

Bayesian inference often involves marginalization of a high-dimensional posterior distribution:

$$P(\theta_0|\text{data}) = \int P(\theta_0, \theta_1, ..., \theta_n|\text{data})\, d\theta_1 ... d\theta_n$$

Typically, the integral cannot be solved in closed form. Moreover, repeated one-dimensional integration becomes inefficient ("curse of dimensionality").

Idea: sample distribution many times and consider only parameter of interest.

Method: Markov Chain Monte Carlo (MCMC)

MCMC has revolutionized Bayesian analysis.

A sequence of random numbers is a Markov chain if the probability of the next number only depends on the previous one:

$$f(x_{n+1}|x_n, x_{n-1}, ..., x_0) = f(x_{n+1}|x_n)$$

# Metropolis-Hastings algorithm (2)

Goal: sample from a distribution $f(\vec{x})$ known up to a normalization constant.

Take initial $\vec{x}_0$ with $f(\vec{x}_0) > 0$ and repeat the following steps many times:

1. Generate candidate $\vec{y}$ according to proposal distribution $q(\vec{y} \mid \vec{x}_k)$
2. Generate uniformly distributed random number $r$ in [0, 1] and set

$$\vec{x}_{k+1} = \begin{cases} \vec{y}, & \text{if } r \leq \alpha(\vec{x}_k, \vec{y}) \\ \vec{x}_k, & \text{otherwise} \end{cases}$$

where

$$\alpha(\vec{x}, \vec{y}) = \min\left\{1, \frac{f(\vec{y})\, q(\vec{x} \mid \vec{y})}{f(\vec{x})\, q(\vec{y} \mid \vec{x})}\right\}$$

$\alpha(\vec{x}, \vec{y})$ is called the acceptance probability.

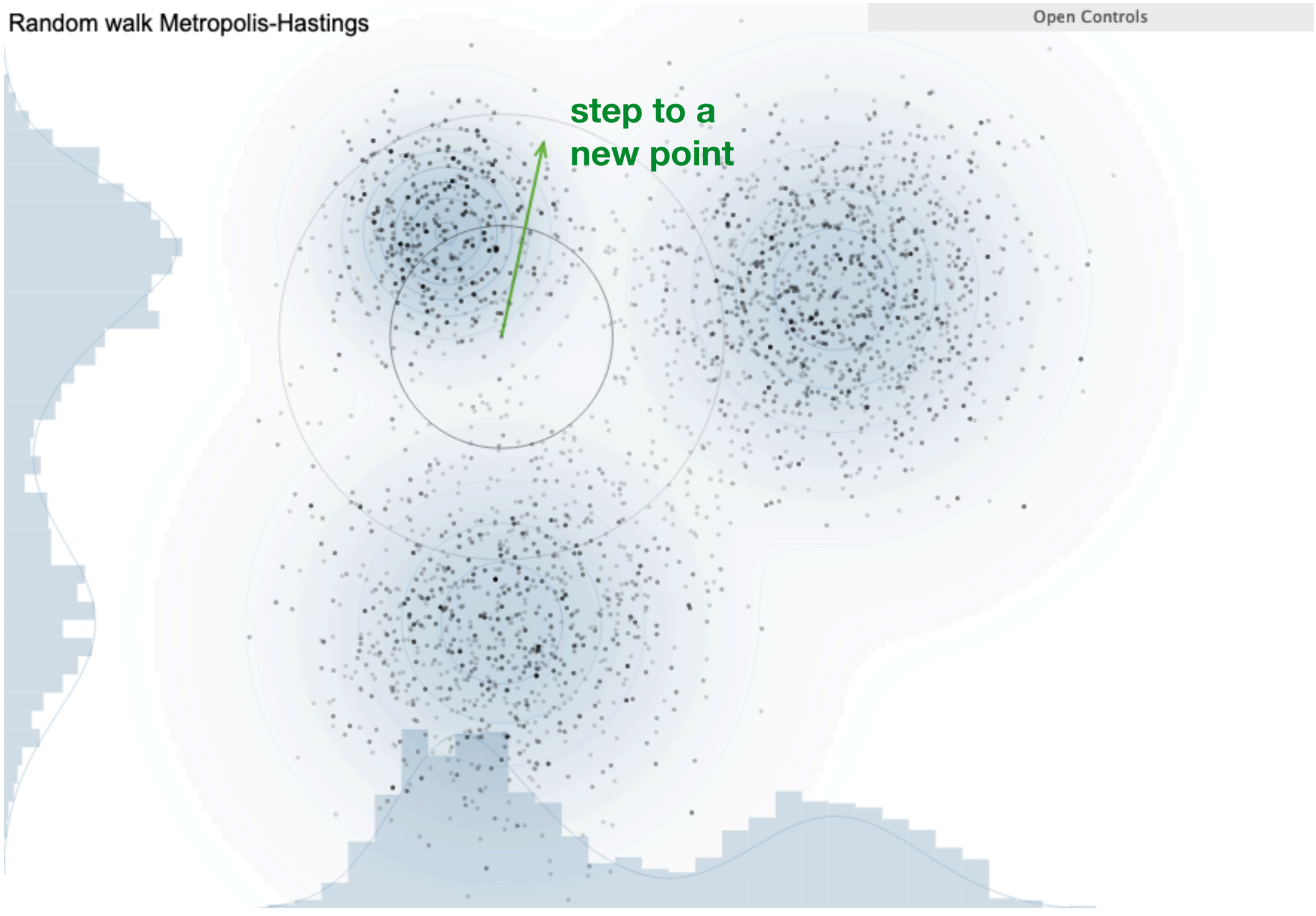
# Metropolis-Hastings algorithm (3)

- The algorithm generates a *correlated* sequence of points (not suited for many applications, but okay for marginalization)
- If a finite initial sequence of points is discarded, the remaining points can be shown to follow $f(\vec{x})$
- Not easy to figure out when the sequence has started to converge to $f(\vec{x})$
- The proposal function $q(\vec{y} \mid \vec{x})$ can be almost anything. Often, a multi-dimensional Gaussian is used.
- Often the proposal function is symmetric, i.e., $q(\vec{y} \mid \vec{x}) = q(\vec{x} \mid \vec{y})$. Then the acceptance probability reduces to

$$\alpha(\vec{x}, \vec{y}) = \min\left\{1, \frac{f(\vec{y})}{f(\vec{x})}\right\}$$

  and a step to a higher $f(\vec{y})$ is always taken.
- Original Metropolis algorithm suggested symmetric proposal functions, Hastings modified original rules by using non-symmetric functions.

# Metropolis-Hastings algorithm: Visualization

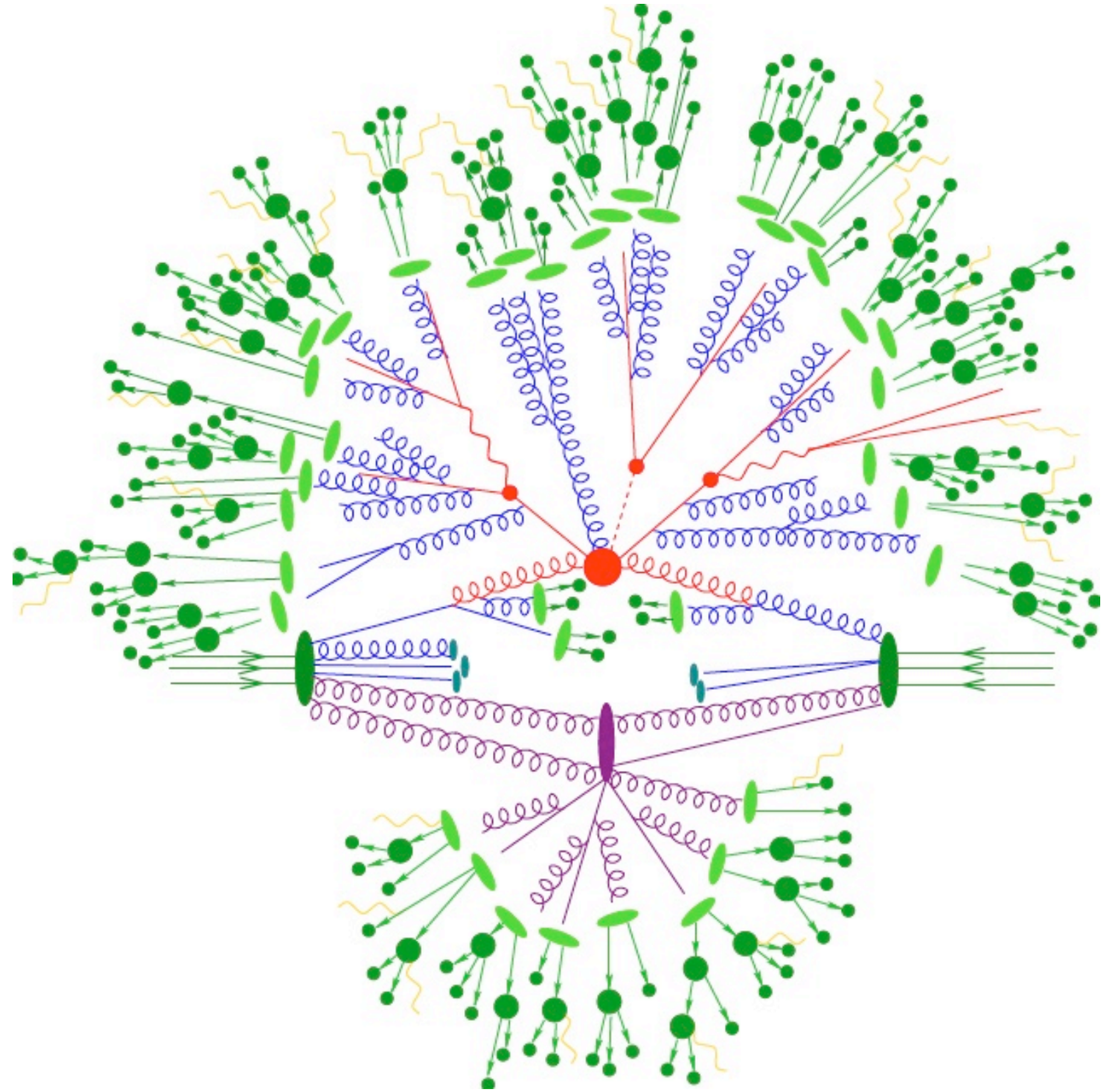



https://chi-feng.github.io/mcmc-demo

# Monte Carlo simulation I: Event generators (Pythia, Sherpa, …)

## Examples: Pythia

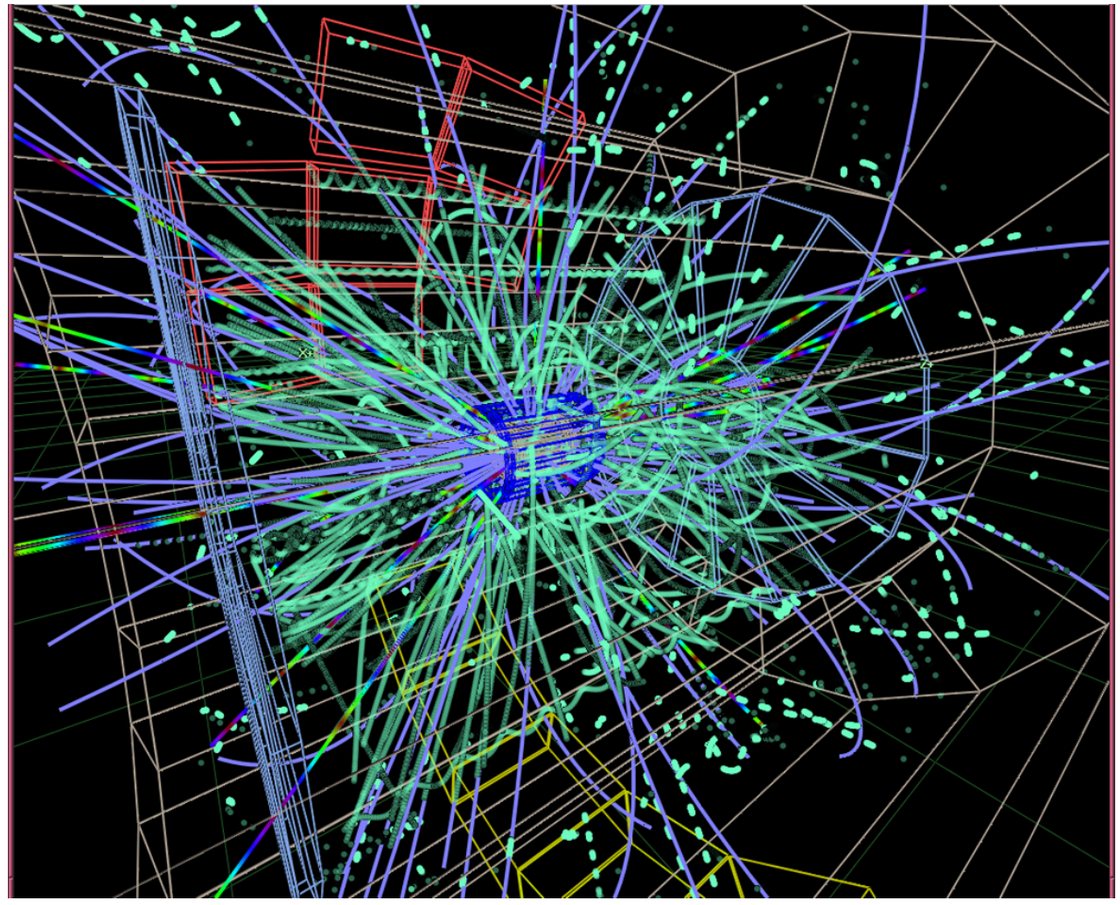
- Simulation of pp and $e^+e^-$ collision on quark and gluon level
- Hard and soft interactions, parton showers, fragmentation and particle decay
- Many applications
  - Test underlying physics, e.g., perturbative QCD
  - Calculate QCD background processes, e.g., in Higgs searches
  - Calculation of detector efficiencies



# Pythia

Output:

Four-vectors of of produced particles



Event listing (summary)

| I | particle/jet | KS | KF | orig | p_x | p_y | p_z | E | m |
|---|---|---|---|---|---|---|---|---|---|
| 1 | (u) | A | 12 | 2 | 0 | 0.000 | 0.000 | 10.000 | 10.000 | 0.006 |
| 2 | (ubar) | V | 11 | -2 | 0 | 0.000 | 0.000 | -10.000 | 10.000 | 0.006 |
| 3 | (string) | | 11 | 92 | 1 | 0.000 | 0.000 | 0.000 | 20.000 | 20.000 |
| 4 | (rho+) | | 11 | 213 | 3 | 0.098 | -0.154 | 2.710 | 2.856 | 0.885 |
| 5 | (rho-) | | 11 | -213 | 3 | -0.227 | 0.145 | 6.538 | 6.590 | 0.781 |
| 6 | pi+ | | 1 | 211 | 3 | 0.125 | -0.266 | 0.097 | 0.339 | 0.140 |
| 7 | (Sigma0) | | 11 | 3212 | 3 | -0.254 | 0.034 | -1.397 | 1.855 | 1.193 |
| 8 | (K*+) | | 11 | 323 | 3 | -0.124 | 0.709 | -2.753 | 2.968 | 0.846 |
| 9 | p~- | | 1 | -2212 | 3 | 0.395 | -0.614 | -3.806 | 3.988 | 0.938 |
| 10 | pi- | | 1 | -211 | 3 | -0.013 | 0.146 | -1.389 | 1.403 | 0.140 |
| 11 | pi+ | | 1 | 211 | 4 | 0.109 | -0.456 | 2.164 | 2.218 | 0.140 |

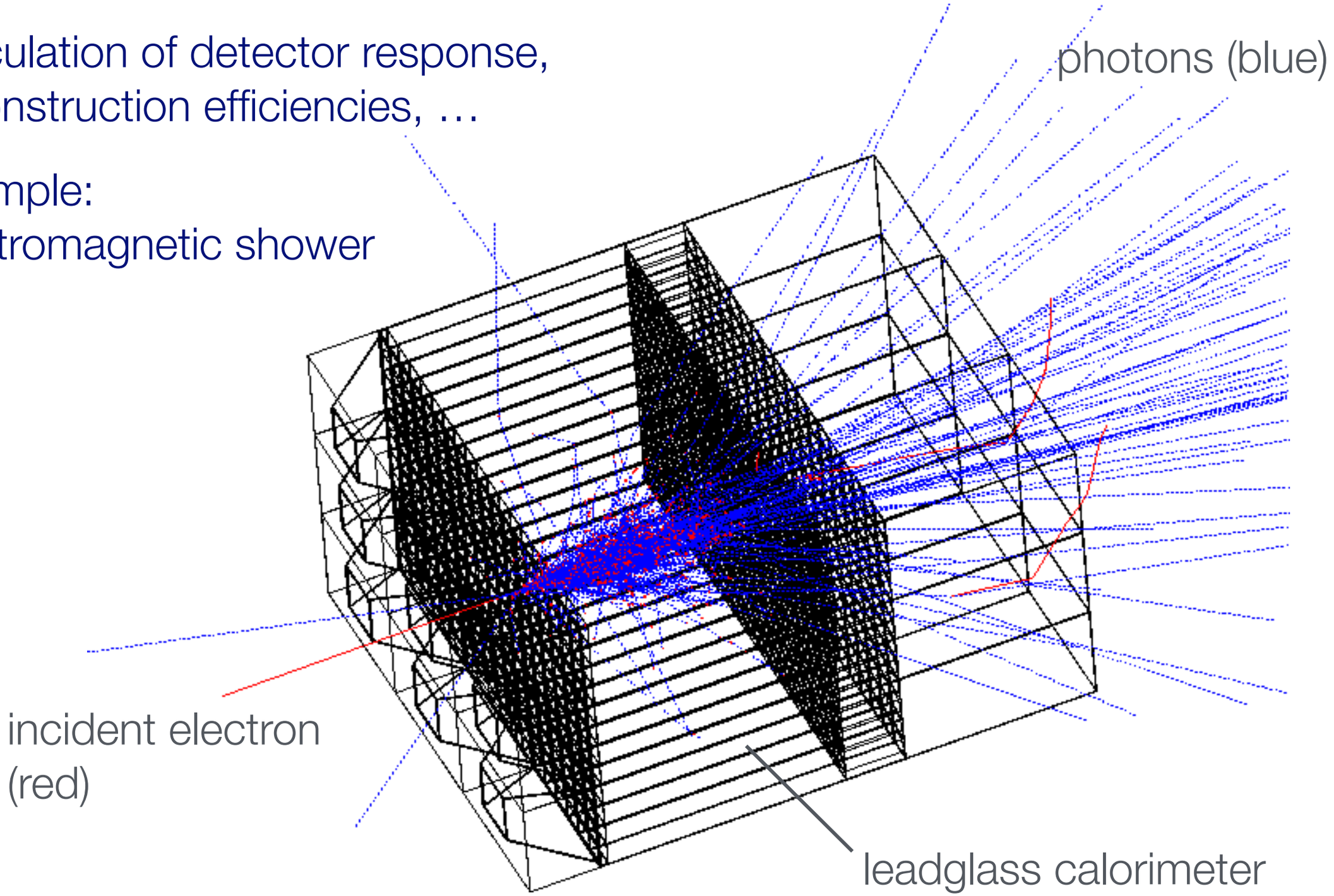
# Monte Carlo simulation II: Detector simulation with GEANT

http://geant4.cern.ch/

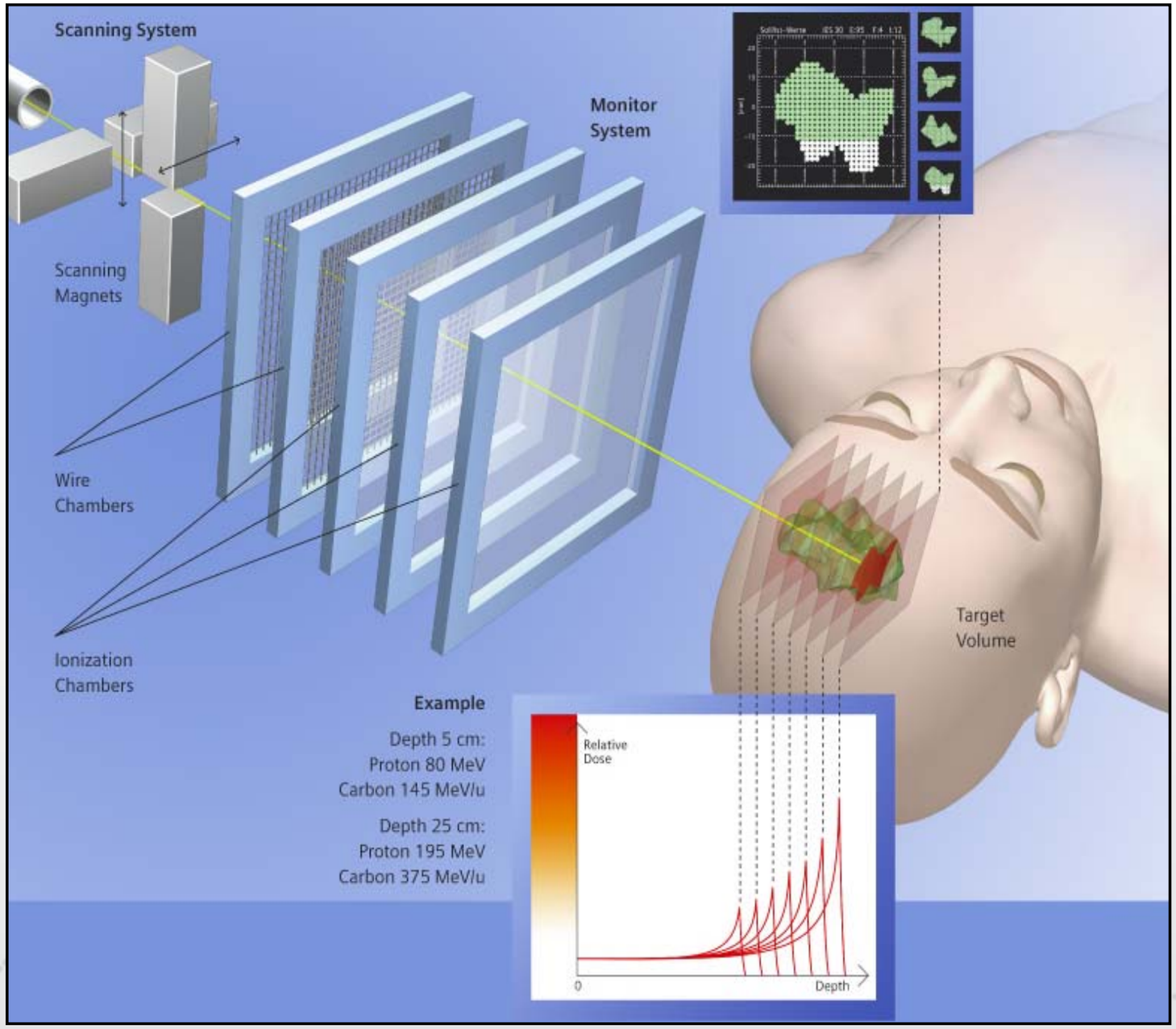
http://www.uni-muenster.de/Physik.KP/santo/thesis/diplom/kees

Calculation of detector response, reconstruction efficiencies, …

Example: electromagnetic shower

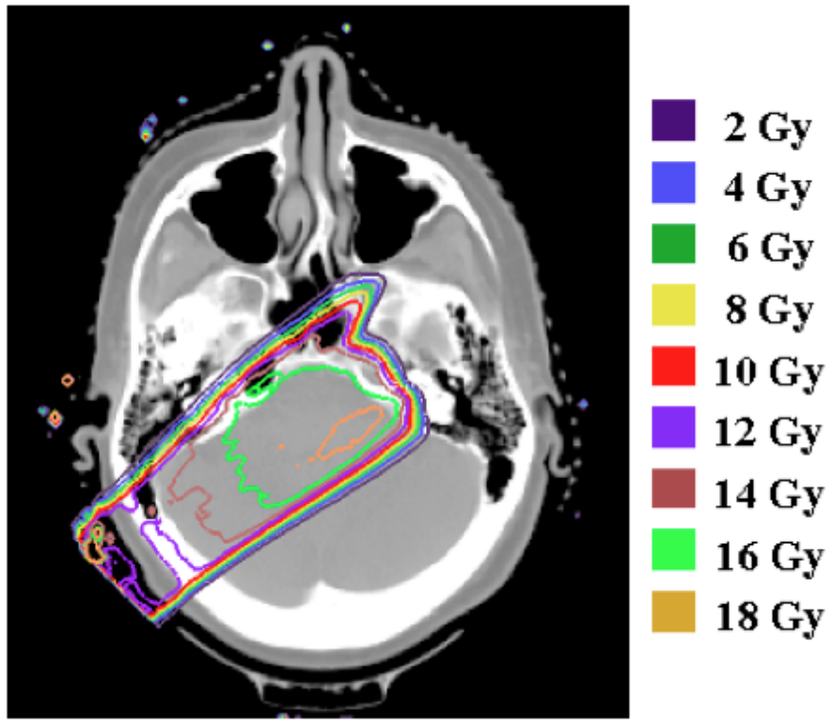


# Monte Carlo simulation III:
# Treatment planning in radiation therapy




Intensity-Controlled Rasterscan Technique, Haberer et al., GSI, NIM A,1993

Source: GSI




## Codes

- GEANT 4
- FLUKA
- …