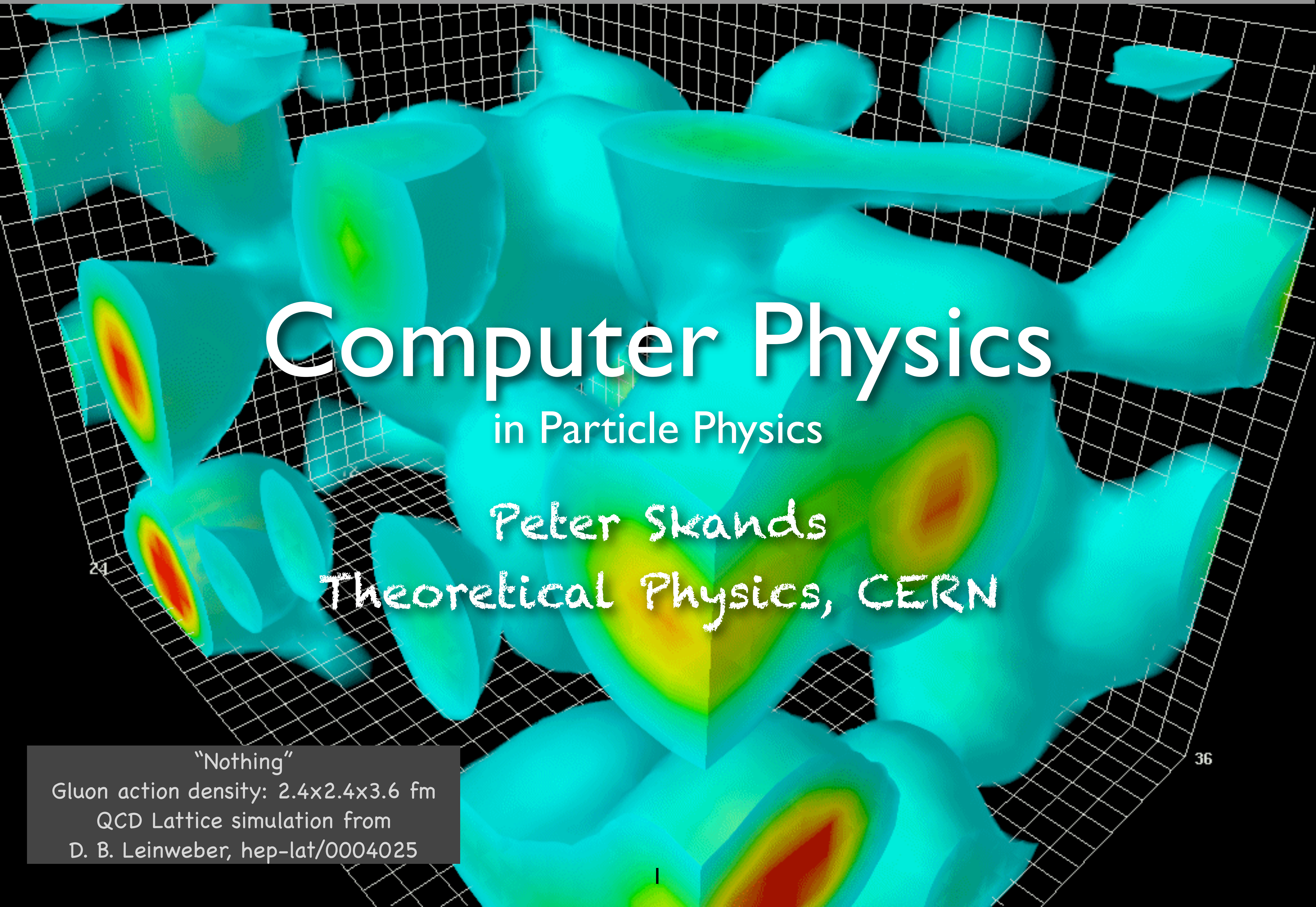


Computer Physics

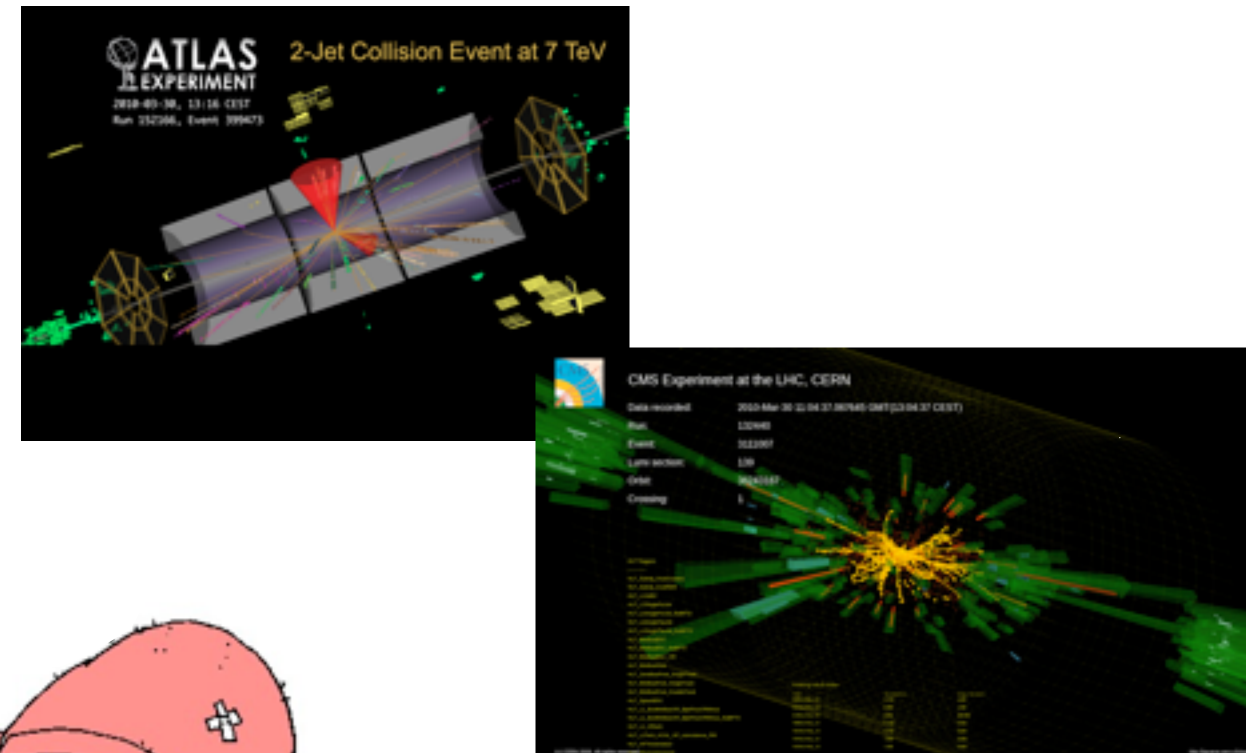
in Particle Physics

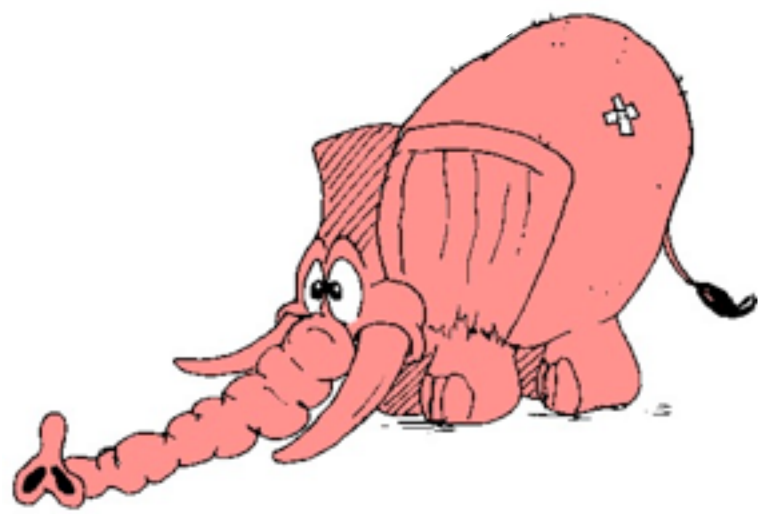
Peter Skands
Theoretical Physics, CERN

"Nothing"
Gluon action density: 2.4x2.4x3.6 fm
QCD Lattice simulation from
D. B. Leinweber, hep-lat/0004025

Collider Physics

Comparisons to Collider observables

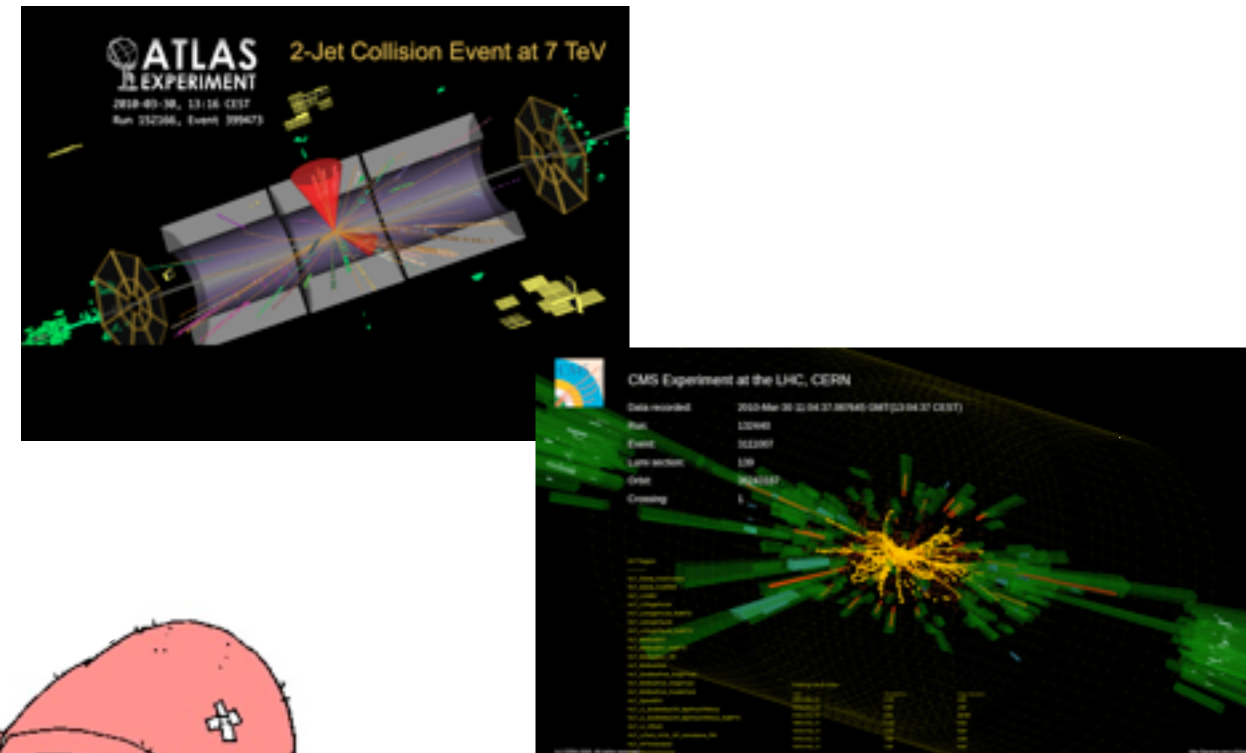


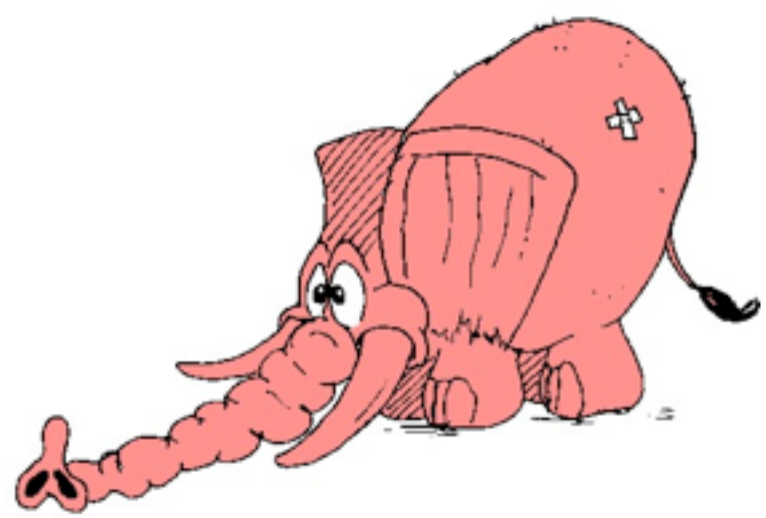


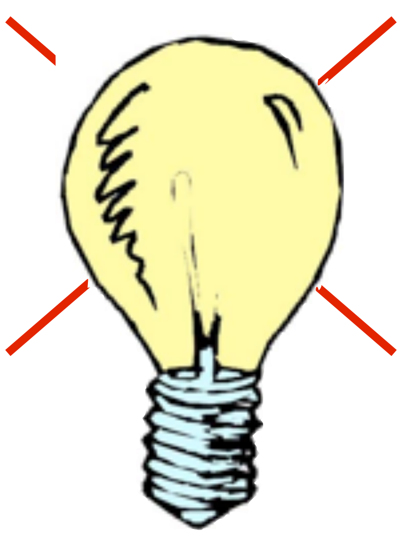
L=...

Collider Physics

Comparisons to Collider observables





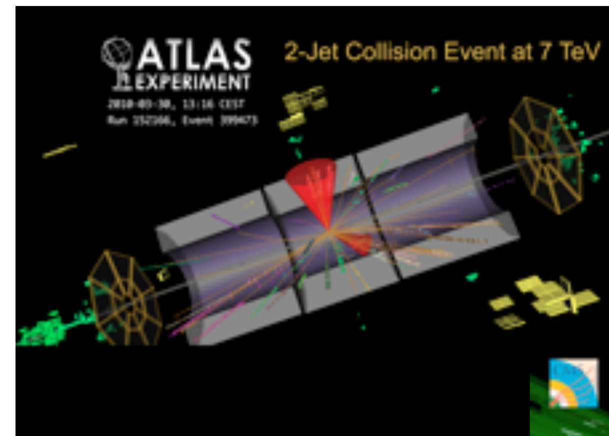


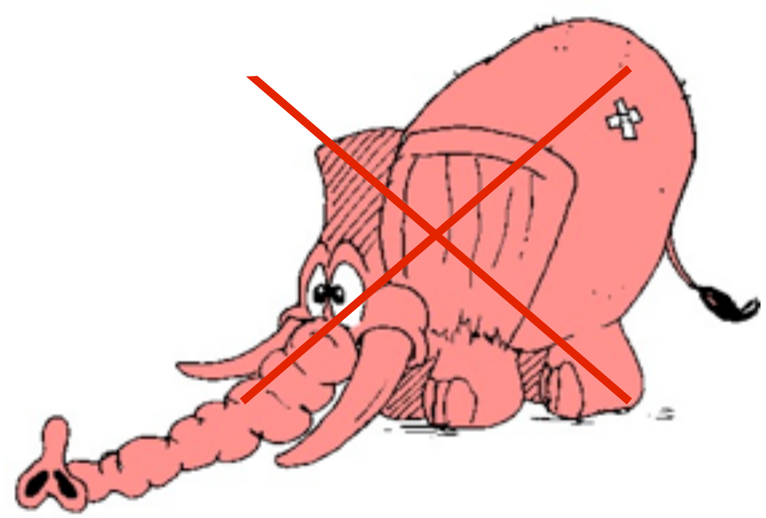
L=...

A) Theoretical Idea is wrong

Collider Physics

Comparisons to Collider observables





L=...

A) Theoretical Idea

B) SM Physics Model is wrong

Topics

Lecture 1:

Numerical Integration
Monte Carlo methods
Importance Sampling
The Veto Algortihm

+ on Friday

Practical Exercises:

PYTHIA 8 kickstart
(get the instructions)

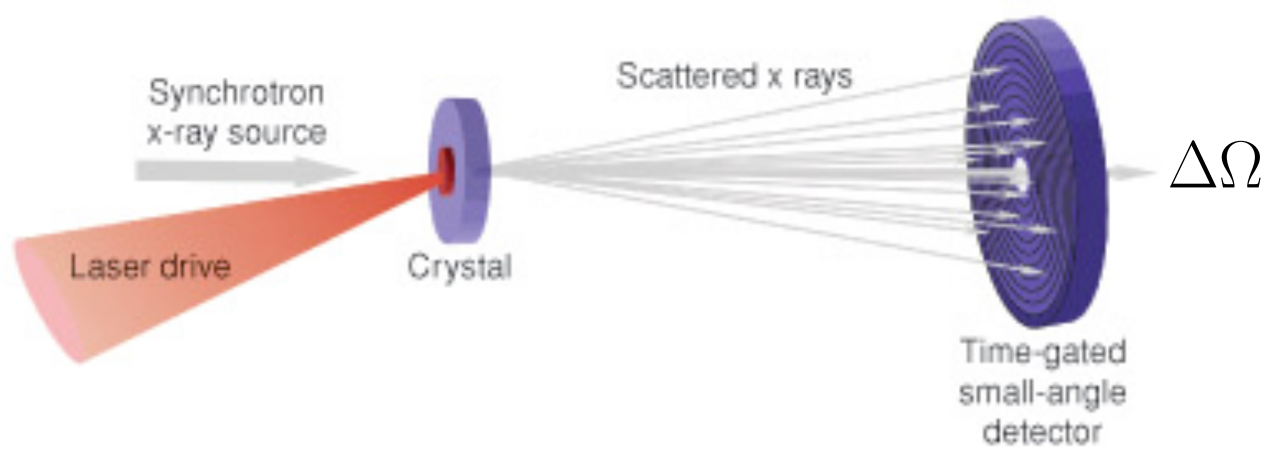
Lecture 2:

Application of these methods to simulations of collider physics: Monte Carlo Event Generators

Why Integrals?

Think: scattering experiments

→ Integrate differential cross sections over specific phase space regions



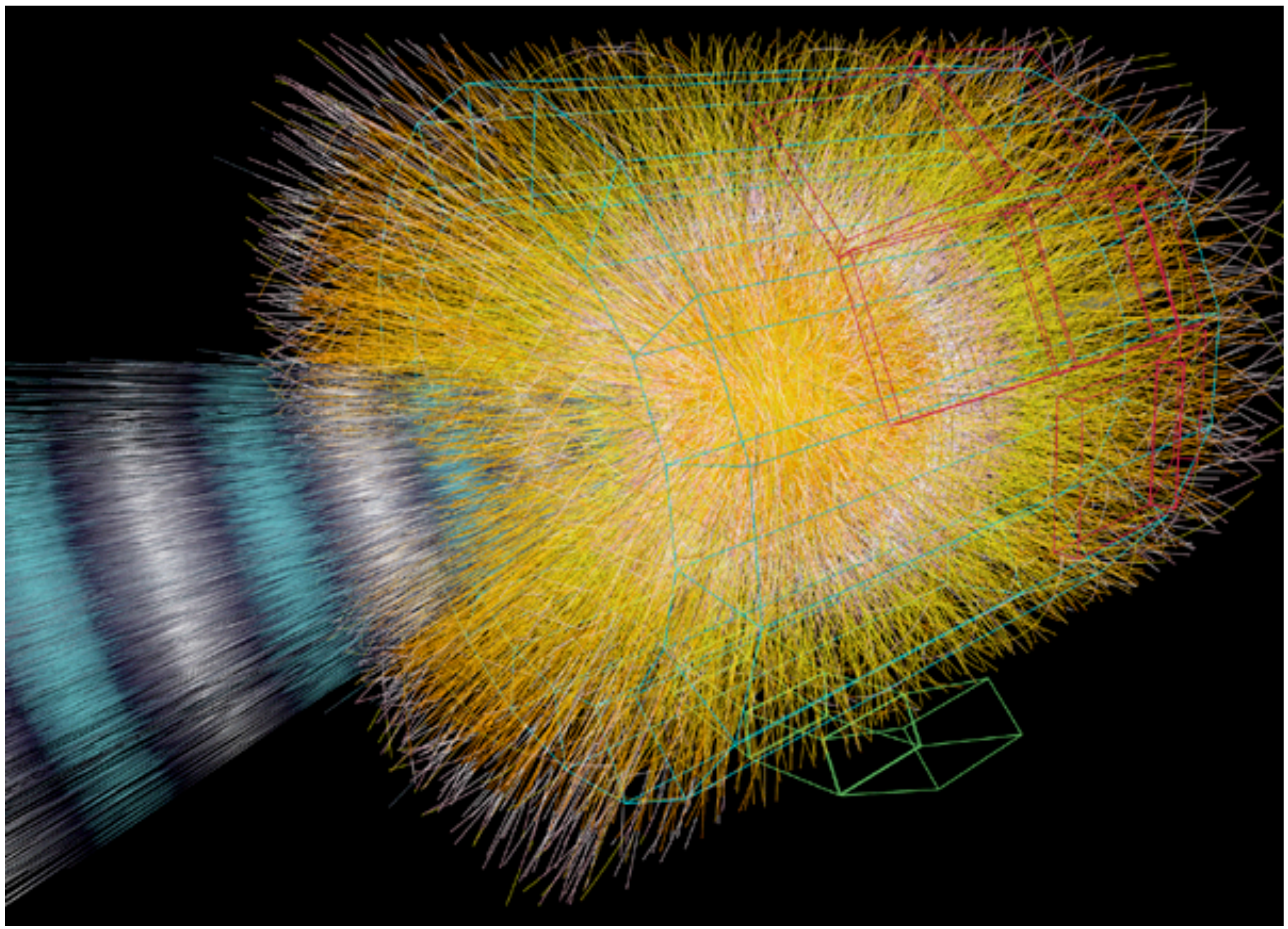
Predicted number of counts = integral over solid angle

$$N_{\mathrm{count}}(\Delta\Omega) \propto \int_{\Delta\Omega} \mathrm{d}\Omega \frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}$$

In particle physics:

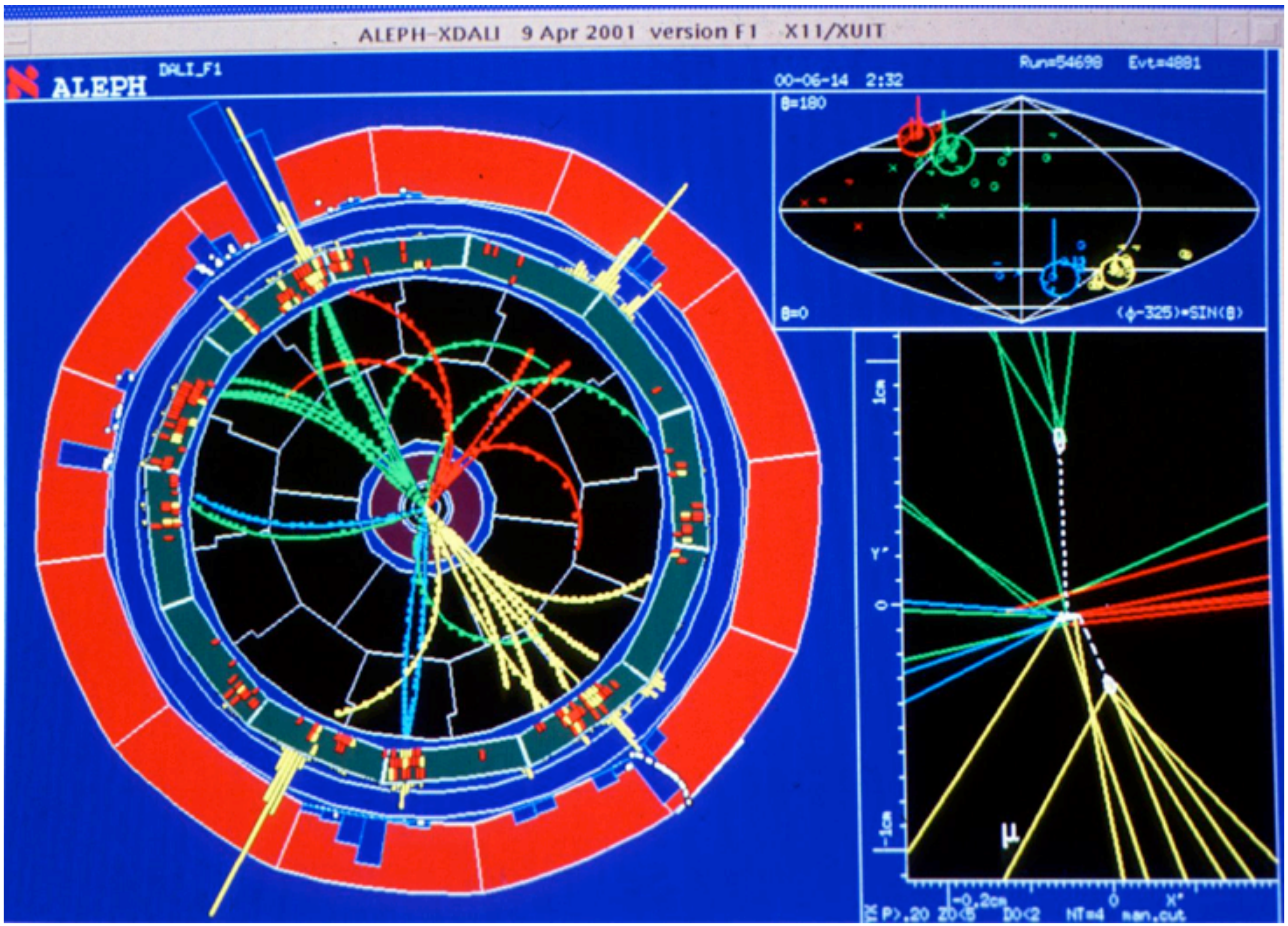
sum (= integrate) over all quantum histories

ALICE Collision



More complicated integrals ...

Why Numerical?



4-jet event in ALEPH at LEP (a Higgs candidate)

Now compute the backgrounds …

Why Numerical?

Part of Z → 4 jets ...

5.3 Four-parton tree-level antenna functions

The tree-level four-parton quark-antiquark antenna contains three final states: quark-gluon-gluon-antiquark at leading and subleading colour, A_4^0 and $\tilde{A}_4^0$ and quark-antiquark-quark-antiquark for non-identical quark flavours B_4^0 as well as the identical-flavour-only contribution C_4^0. The quark-antiquark-quark-antiquark final state with identical quark flavours is thus described by the sum of antennae for non-identical flavour and identical-flavour-only. The antennae for the $qgg\bar{q}$ final state are:

$$A_4^0(1_q,3_g,4_g,2_{\bar{q}}) = a_4^0(1,3,4,2) + a_4^0(2,4,3,1)\,, \qquad (5.27)$$

$$\tilde{A}_4^0(1_q,3_g,4_g,2_{\bar{q}}) = \tilde{a}_4^0(1,3,4,2) + \tilde{a}_4^0(2,4,3,1) + \tilde{a}_4^0(1,4,3,2) + \tilde{a}_4^0(2,3,4,1)\,, \qquad (5.28)$$

$$\begin{aligned}
a_4^0(1,3,4,2) = \frac{1}{s_{1234}}\Bigg\{ & \frac{1}{2s_{13}s_{24}s_{34}}\left[2s_{12}s_{14} + 2s_{12}s_{23} + 2s_{12}^2 + s_{14}^2 + s_{23}^2\right] \\
&+ \frac{1}{2s_{13}s_{24}s_{134}s_{234}}\left[3s_{12}s_{34}^2 - 4s_{12}^2s_{34} + 2s_{12}^3 - s_{34}^3\right] \\
&+ \frac{1}{s_{13}s_{24}s_{134}}\left[3s_{12}s_{23} - 3s_{12}s_{34} + 4s_{12}^2 - s_{23}s_{34} + s_{23}^2 + s_{34}^2\right] \\
&+ \frac{3}{2s_{13}s_{24}}\left[2s_{12} + s_{14} + s_{23}\right] + \frac{1}{s_{13}s_{34}}\left[4s_{12} + 3s_{23} + 2s_{24}\right] \\
&+ \frac{1}{s_{13}s_{134}^2}\left[s_{12}s_{34} + s_{23}s_{34} + s_{24}s_{34}\right] \\
&+ \frac{1}{s_{13}s_{134}s_{234}}\left[3s_{12}s_{24} + 6s_{12}s_{34} - 4s_{12}^2 - 3s_{24}s_{34} - s_{24}^2 - 3s_{34}^2\right] \\
&+ \frac{1}{s_{13}s_{134}}\left[-6s_{12} - 3s_{23} - s_{24} + 2s_{34}\right] \\
&+ \frac{1}{s_{24}s_{34}s_{134}}\left[2s_{12}s_{14} + 2s_{12}s_{23} + 2s_{12}^2 + 2s_{14}s_{23} + s_{14}^2 + s_{23}^2\right] \\
&+ \frac{1}{s_{24}s_{134}}\left[-4s_{12} - s_{14} - s_{23} + s_{34}\right] + \frac{1}{s_{34}^2}\left[s_{12} + 2s_{13} - 2s_{14} - s_{34}\right] \\
&+ \frac{1}{s_{34}^2s_{134}^2}\left[2s_{12}s_{14}^2 + 2s_{14}^2s_{23} + 2s_{14}^2s_{24}\right] - \frac{2s_{12}s_{14}s_{24}}{s_{34}^2s_{134}s_{234}} \\
&+ \frac{1}{s_{34}^2s_{134}}\left[-2s_{12}s_{14} - 4s_{14}s_{24} + 2s_{14}^2\right] \\
&+ \frac{1}{s_{34}s_{134}s_{234}}\left[-2s_{12}s_{14} - 4s_{12}^2 + 2s_{14}s_{24} - s_{14}^2 - s_{24}^2\right] \\
&+ \frac{1}{s_{34}s_{134}}\left[-8s_{12} - 2s_{23} - 2s_{24}\right] + \frac{1}{s_{134}^2}\left[s_{12} + s_{23} + s_{24}\right] \\
&+ \frac{3}{2s_{134}s_{234}}\left[2s_{12} + s_{14} - s_{24} - s_{34}\right] + \frac{1}{2s_{134}} + \mathcal{O}(\epsilon)\Bigg\}\,, \qquad (5.29)
\end{aligned}$$

$$\begin{aligned}
\tilde{a}_4^0(1,3,4,2) = \frac{1}{s_{1234}}\Bigg\{ & \frac{1}{s_{13}s_{24}s_{134}s_{234}}\left[\frac{3}{2}s_{12}s_{34}^2 - 2s_{12}^2s_{34} + s_{12}^3 - \frac{1}{2}s_{34}^3\right] \\
&+ \frac{1}{s_{13}s_{24}s_{134}}\left[3s_{12}s_{23} - 3s_{12}s_{34} + 4s_{12}^2 - s_{23}s_{34} + s_{23}^2 + s_{34}^2\right] \\
&+ \frac{s_{12}^3}{s_{13}s_{24}(s_{13}+s_{23})(s_{14}+s_{24})} + \frac{1}{s_{13}s_{24}(s_{13}+s_{23})}\left[\frac{1}{2}s_{12}s_{14} + s_{12}^2\right] \\
&+ \frac{1}{s_{13}s_{24}(s_{14}+s_{24})}\left[\frac{1}{2}s_{12}s_{23} + s_{12}^2\right] + \frac{1}{s_{13}s_{24}}\left[3s_{12} + \frac{3}{2}s_{14} + \frac{3}{2}s_{23}\right] \\
&+ \frac{1}{s_{13}s_{134}^2}\left[s_{12}s_{34} + s_{23}s_{34} + s_{24}s_{34}\right] + \frac{2s_{12}^3}{s_{13}s_{134}s_{234}(s_{13}+s_{23})} \\
&+ \frac{1}{s_{13}s_{134}s_{234}}\left[3s_{12}s_{34} - s_{24}s_{34} - 2s_{34}^2\right] \\
&+ \frac{1}{s_{13}s_{134}(s_{13}+s_{23})}\left[s_{12}s_{24} + s_{12}s_{34} + 2s_{12}^2\right] \\
&+ \frac{1}{s_{13}s_{134}}\left[-s_{23} - s_{24} + 2s_{34}\right] + \frac{1}{s_{13}s_{234}(s_{13}+s_{23})}\left[s_{12}s_{14} + s_{12}s_{34} + 2s_{12}^2\right] \\
&+ \frac{1}{s_{13}s_{234}}\left[-2s_{12} - 2s_{14} + s_{24} + 2s_{34}\right] \\
&+ \frac{2s_{12}^3}{s_{13}(s_{13}+s_{23})(s_{14}+s_{24})(s_{13}+s_{14})} \\
&+ \frac{1}{s_{13}(s_{13}+s_{23})(s_{13}+s_{14})}\left[s_{12}s_{24} + 2s_{12}^2\right] \\
&+ \frac{1}{s_{13}(s_{14}+s_{24})(s_{13}+s_{14})}\left[s_{12}s_{23} + 2s_{12}^2\right] \\
&+ \frac{2s_{12}}{s_{13}(s_{13}+s_{14})} - \frac{2}{s_{13}} + \frac{1}{s_{134}^2}\left[s_{12} + s_{23} + s_{24}\right] \\
&+ \frac{1}{s_{134}s_{234}}\left[s_{12} - s_{34}\right] + \frac{1}{s_{134}} + \mathcal{O}(\epsilon)\Bigg\}\,. \qquad (5.30)
\end{aligned}$$

First computed by K. Ellis, D. Ross, A. Terrano, Nucl.Phys.B178 (1981) 421
This version from Gehrmann-de-Ridder, Gehrmann, Glover, JHEP 0509(2005)056

Why Numerical?

The non-identical quark antenna is:

$$B_4^0(1_q, 3_{q'}, 4_{\bar{q}'}, 2_{\bar{q}}) = b_4^0(1,3,4,2) + b_4^0(2,3,4,1) + b_4^0(1,4,3,2) + b_4^0(2,4,3,1)\ , \quad (5.37)$$

with a sub-antenna function given by

$$b_4^0(1,3,4,2) = \frac{1}{s_{1234}}\left\{ \frac{1}{s_{34}^2 s_{134}^2}\left[s_{12}s_{13}s_{14} + s_{13}s_{14}s_{23} - s_{13}^2 s_{24}\right] + \frac{1}{s_{34}^2 s_{134} s_{234}}\left[-s_{12}s_{13}s_{24} + s_{13}s_{14}s_{23} - s_{13}s_{24}^2\right] + \frac{1}{s_{34}s_{134}^2}\left[s_{12}s_{13} + s_{13}s_{23}\right] + \frac{1}{2s_{34}s_{134}s_{234}}\left[2s_{12}s_{13} + s_{12}^2\right] + \frac{s_{12}}{2s_{134}s_{234}} + \mathcal{O}(\epsilon)\right\} . \quad (5.38)$$

The identical-flavour-only quark-antiquark-quark-antiquark antenna is:

$$C_4^0(1_q, 3_q, 4_{\bar{q}}, 2_{\bar{q}}) = c_4^0(1,2,3,4) + c_4^0(1,4,3,2)\ , \quad (5.42)$$

$$c_4^0(1,2,3,4) = \frac{1}{s_{1234}}\left\{ -\frac{s_{12}s_{13}s_{14}}{2s_{23}s_{34}s_{123}s_{134}} + \frac{1}{2s_{23}s_{34}s_{134}s_{234}}\left[-s_{12}s_{13}s_{24} + s_{13}s_{14}s_{24}\right] - \frac{s_{13}s_{24}^2}{2s_{23}s_{34}s_{234}^2} - \frac{s_{12}s_{13}}{s_{23}s_{123}s_{134}} + \frac{1}{2s_{23}s_{123}s_{234}}\left[-s_{12}s_{14} - s_{12}s_{34} - s_{12}^2 + s_{13}s_{24}\right] + \frac{1}{2s_{23}s_{134}s_{234}}\left[s_{12}s_{14} + s_{12}s_{34} + s_{12}^2 + s_{13}s_{24}\right] - \frac{s_{13}}{2s_{123}s_{134}} + \frac{1}{s_{23}s_{234}^2}\left[s_{12}s_{24} + s_{14}s_{24}\right] + \frac{1}{2s_{123}s_{234}}\left[-s_{12} + s_{14}\right] + \mathcal{O}(\epsilon)\right\} . \quad (5.43)$$

Integrate over 4-particle phase space …

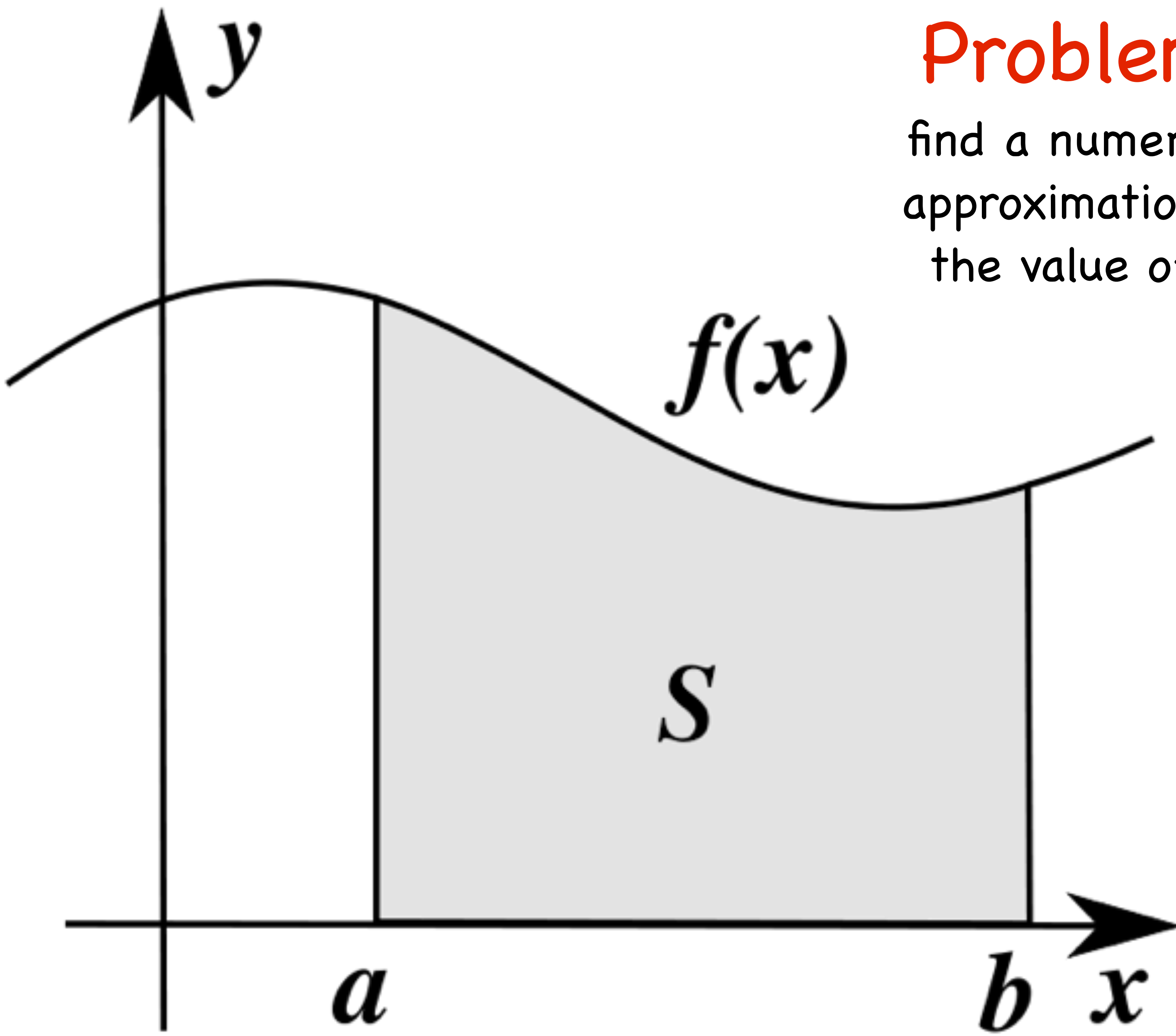
This is one of the simplest processes … computed at lowest order in the theory.

Now compute the quantum corrections: Z → 5, 6, …

And higher orders of quantum fluctuations (quantum loops) …

And hadronization, hadron decays, detector response, …

Numerical Integration

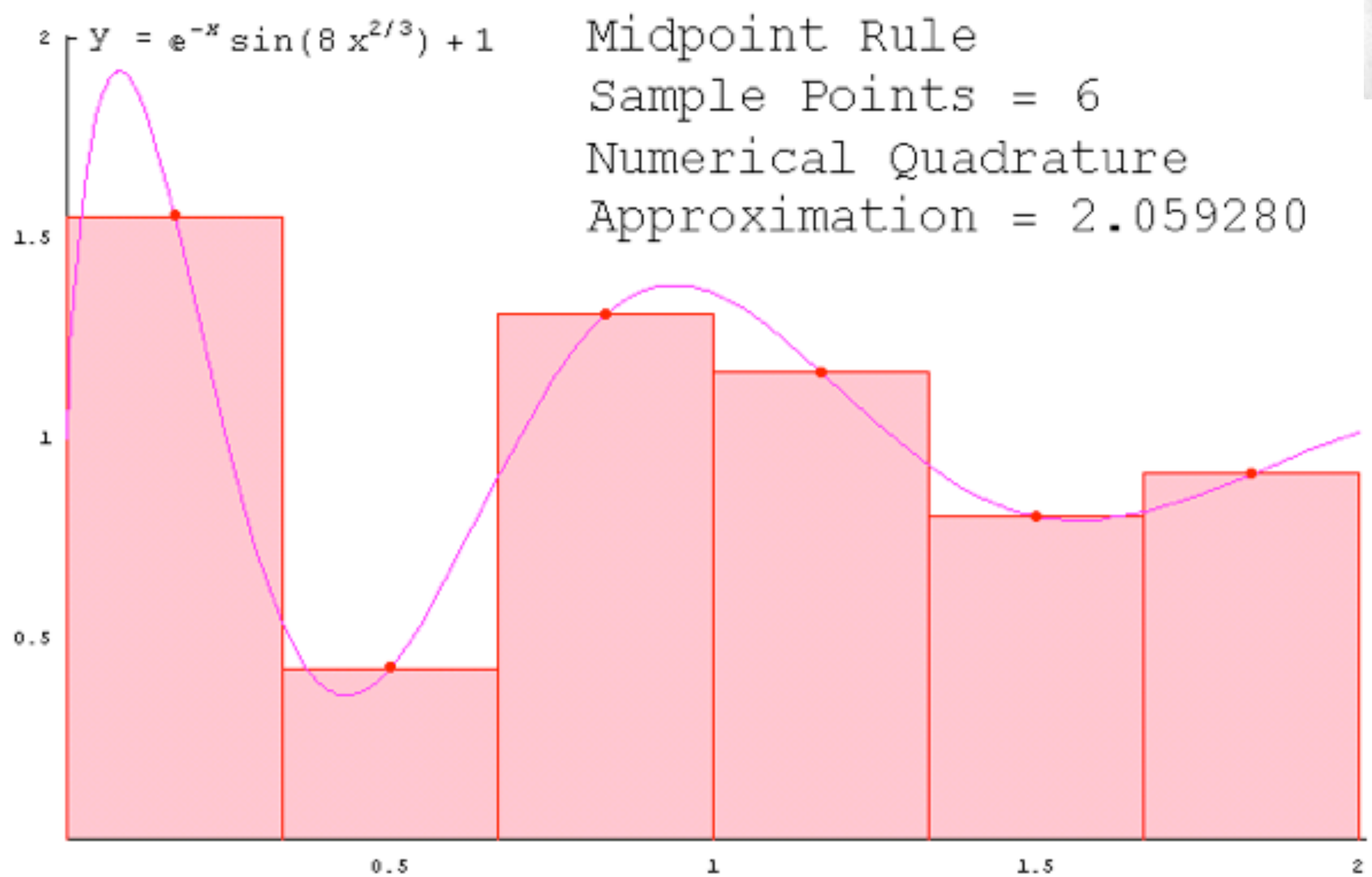


Problem:

find a numerical approximation to the value of S

Riemann Sums

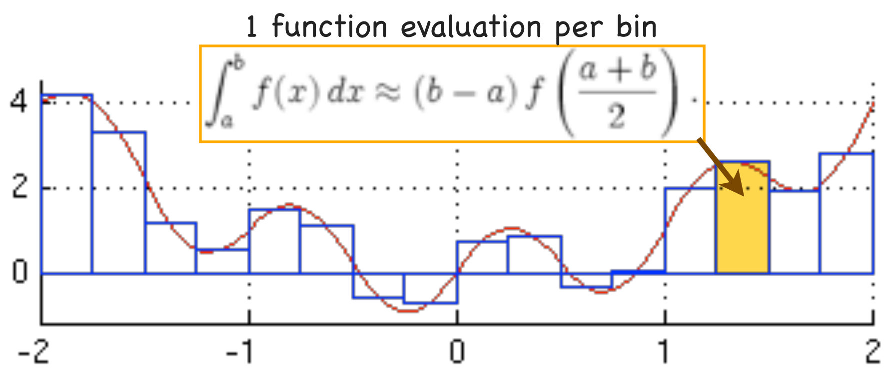
$$\int_a^b f(x)\mathrm{d}x = \lim_{n\to\infty}\sum_{i=1}^{n} f(t_i)(x_{i+1} - x_i)$$



B. Riemann, (1826-1866)

Numerical Integration in 1D

Fixed-Grid n-point Quadrature Rules:

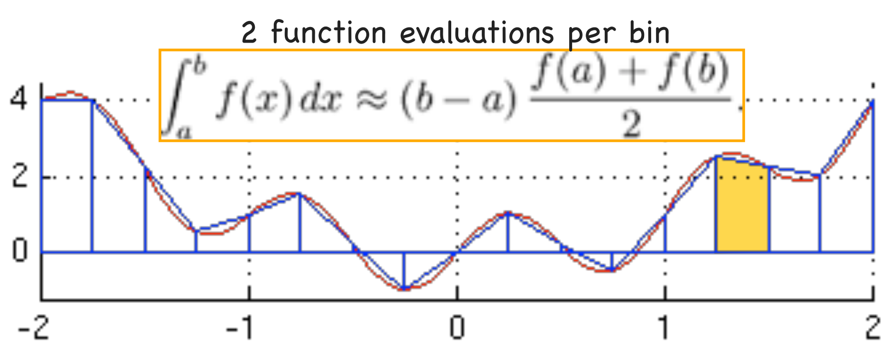


Midpoint (rectangular) Rule:

Divide into N "bins" of size Δ

Approximate f(x) ≈ constant in each bin

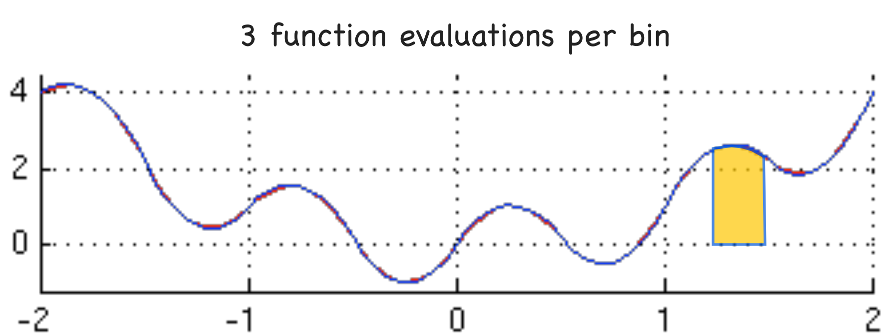
Sum over all rectangles inside your region



Trapezoidal Rule:

Approximate f(x) ≈ linear in each bin

Sum over all trapeziums inside your region



Simpson's Rule:

Approximate f(x) ≈ quadratic in each bin

Sum over all simpsons inside your region

etc ...

Convergence Rate

The most important question:

How long do I have to wait?

(How many points do I need for a given precision)?

Uncertainty as a function of number of points	n_{eval} / bin	Approx Conv. Rate (in 1D)
Trapezoidal Rule (2-point)	2	$1/n^2$
Simpson's Rule (3-point)	3	$1/n^4$
... m-point (Gauss quadrature)	m	$1/n^{2m-1}$

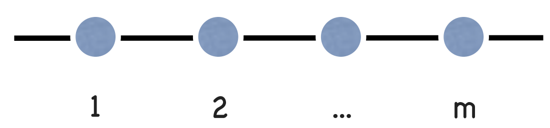
See, e.g., Numerical Recipes

See, e.g., F. James, "Monte Carlo Theory and Practice"

Higher Dimensions

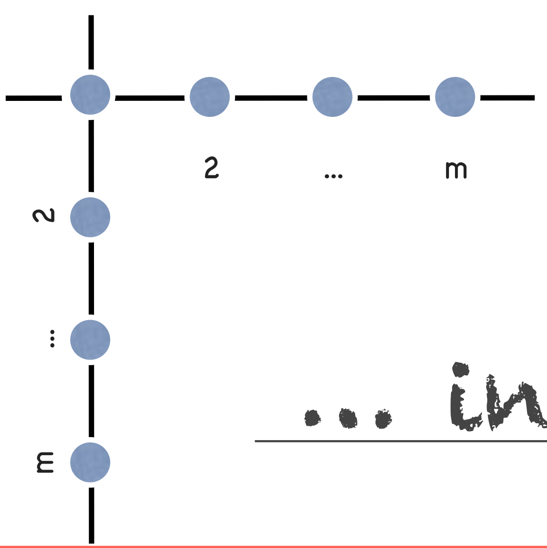
Fixed-Grid (Product) Rules scale exponentially with D

N-point rule in 1 dimension



→ m function evaluations per bin

... in 2 dimensions



→ m^2 evaluations per bin

... in D dimensions → N^D per bin

E.g., to evaluate a 12-point rule in 10 dimensions, need 1000 billion evaluations per bin

Convergence Rate

+ Convergence is slower in higher Dimensions!

→ More points for less precision 

Uncertainty as a function of number of points	n_{eval} / bin	Approx Conv. Rate (in D dim)
Trapezoidal Rule (2-point)	2^D	$1/n^{2/D}$
Simpson's Rule (3-point)	3^D	$1/n^{4/D}$
... m-point (Gauss rule)	m^D	$1/n^{(2m-1)/D}$

See, e.g., Numerical Recipes

See, e.g., F. James, Monte Carlo Theory and Practice

Monte Carlo

A Monte Carlo technique: is any technique making use of random numbers to solve a problem

Convergence:

Calculus: {A} converges to B
if an n exists for which
$|A_{i>n} - B| < \varepsilon$, for any $\varepsilon > 0$

Monte Carlo: {A} converges to B
if n exists for which
the probability for
$|A_{i>n} - B| < \varepsilon$, for any $\varepsilon > 0$,
is > P, for any P[0<P<1]

"This risk, that convergence is only given with a certain probability, is inherent in Monte Carlo calculations and is the reason why this technique was named after the world's most famous gambling casino. Indeed, the name is doubly appropriate because the style of gambling in the Monte Carlo casino, not to be confused with the noisy and tasteless gambling houses of Las Vegas and Reno, is serious and sophisticated."

F. James, "Monte Carlo theory and practice", Rept. Prog. Phys. 43 (1980) 1145

Random Numbers and Monte Carlo

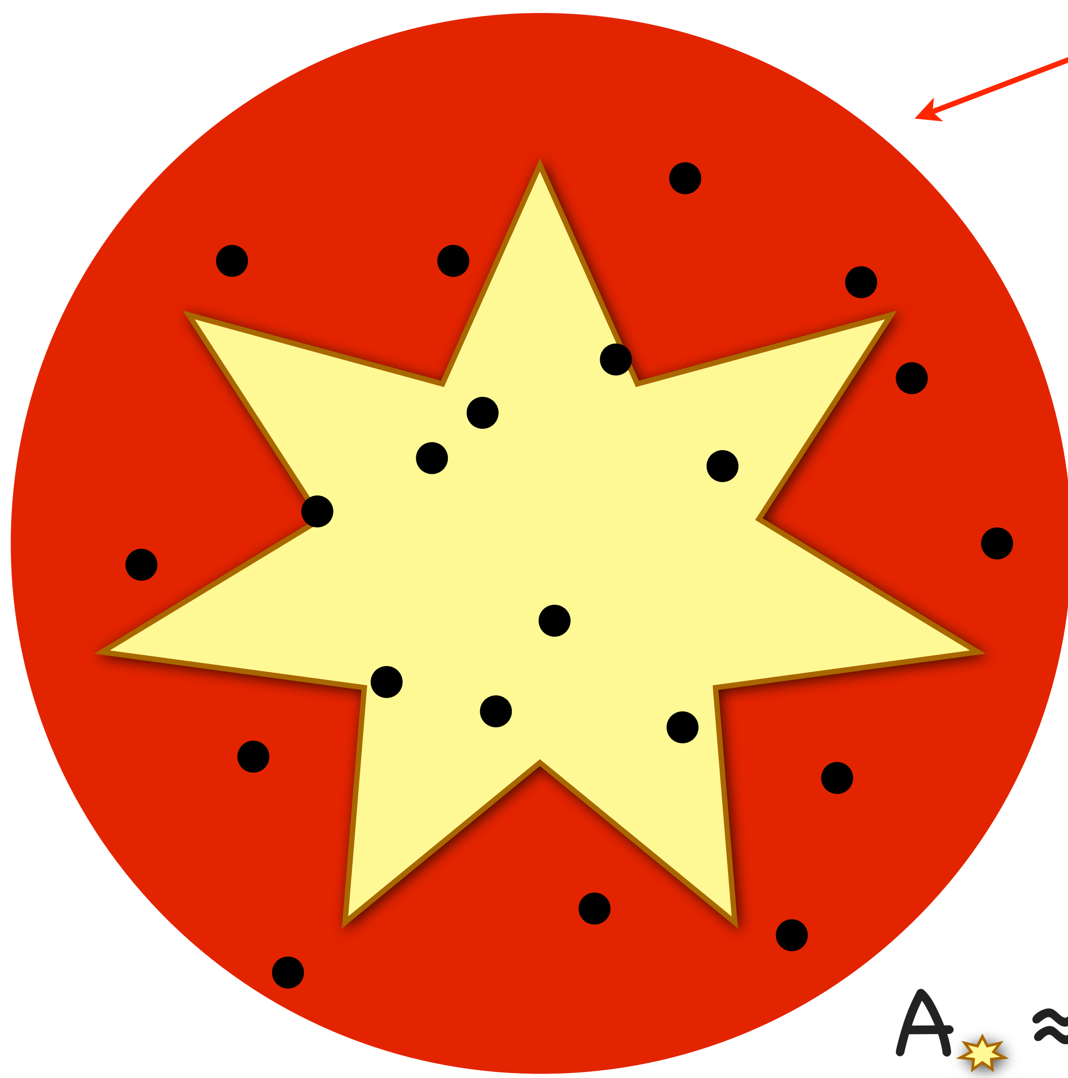
Example 1: simple function (=constant); complicated boundary

Example: you want to know the area of this shape:

Now get a few friends, some balls, and throw random shots inside the circle

(PS: be careful to make your shots truly random)

Count how many shots hit the shape inside and how many miss



Assume you know the area of this shape: πR^2 (an overestimate)

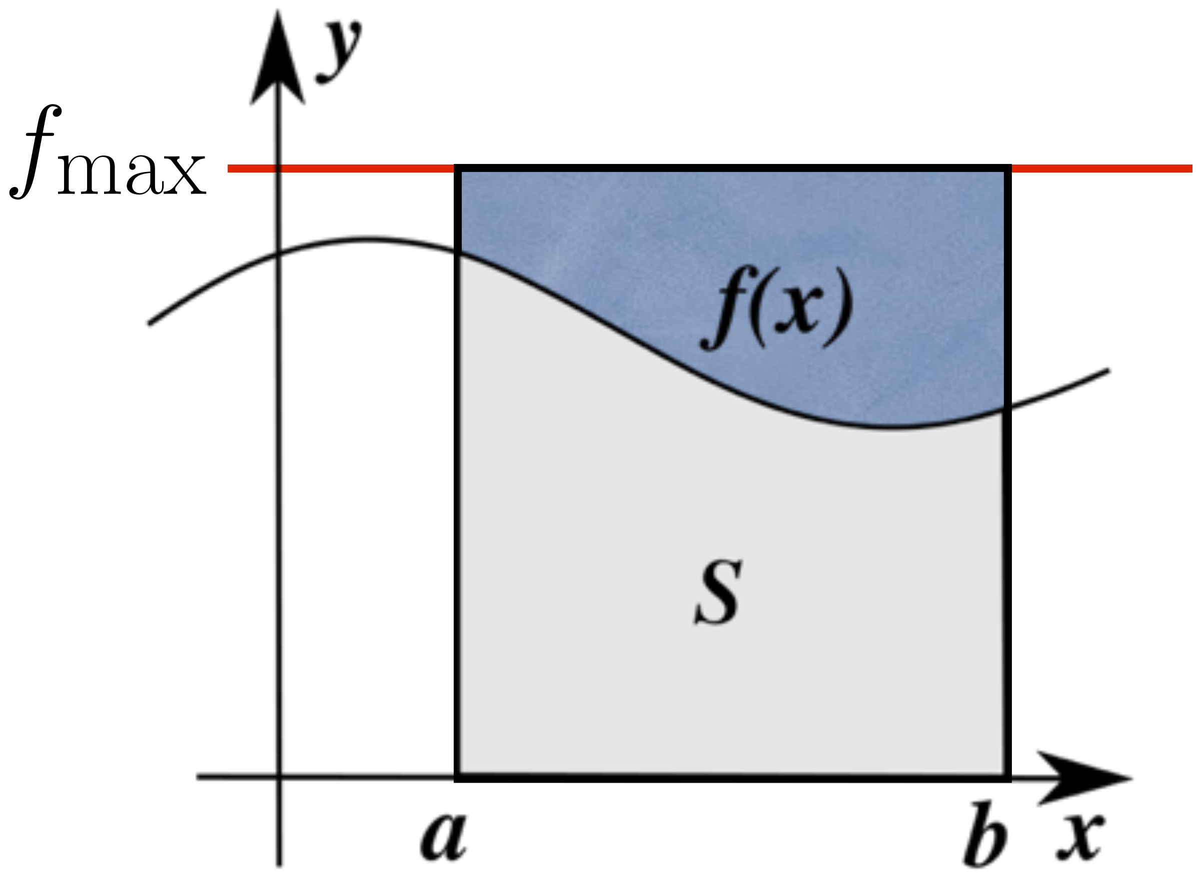
Earliest Example of MC calculation: Buffon's Needle (1777) to calculate π

G. Leclerc, Comte de Buffon (1707-1788)

$$A_{\star} \approx N_{hit}/N_{miss} \times \pi R2$$

Random Numbers and Monte Carlo

Example 2: complicated function; simple boundary



Start from overestimate,

$$f_{\max}$$

Generate uniformly distributed random points between a and b $\frac{f(x_i)}{f_{\max}} = P_{\text{hit}}$

The integral is then ≈ $(b-a)f_{\max}\,\frac{1}{n}\sum_{i=1}^{n}\frac{f(x_i)}{f_{\max}}$

area of rectangle — fraction that 'hit'

Justification

1. Law of large numbers

For a function, f, of random variables, x_i,

$$\lim_{n\to\infty} \frac{1}{n}\sum_{i=1}^{n} f(x_i) = \frac{1}{b-a}\int_a^b f(x)\mathrm{d}x$$

Monte Carlo Estimate — The Integral

For infinite n:
Monte Carlo is a consistent estimator

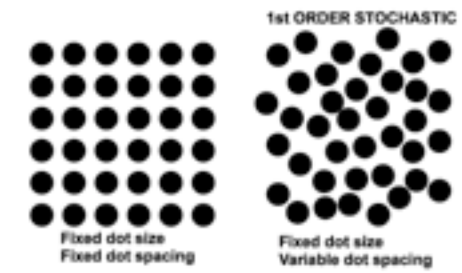
2. Central limit theorem

The sum of n independent random variables (of finite expectations and variances) is asymptotically Gaussian
(no matter how the individual random variables are distributed)

For finite n:
The Monte Carlo estimate is Gauss distributed around the true value

Convergence

<u>MC convergence is Stochastic!</u>

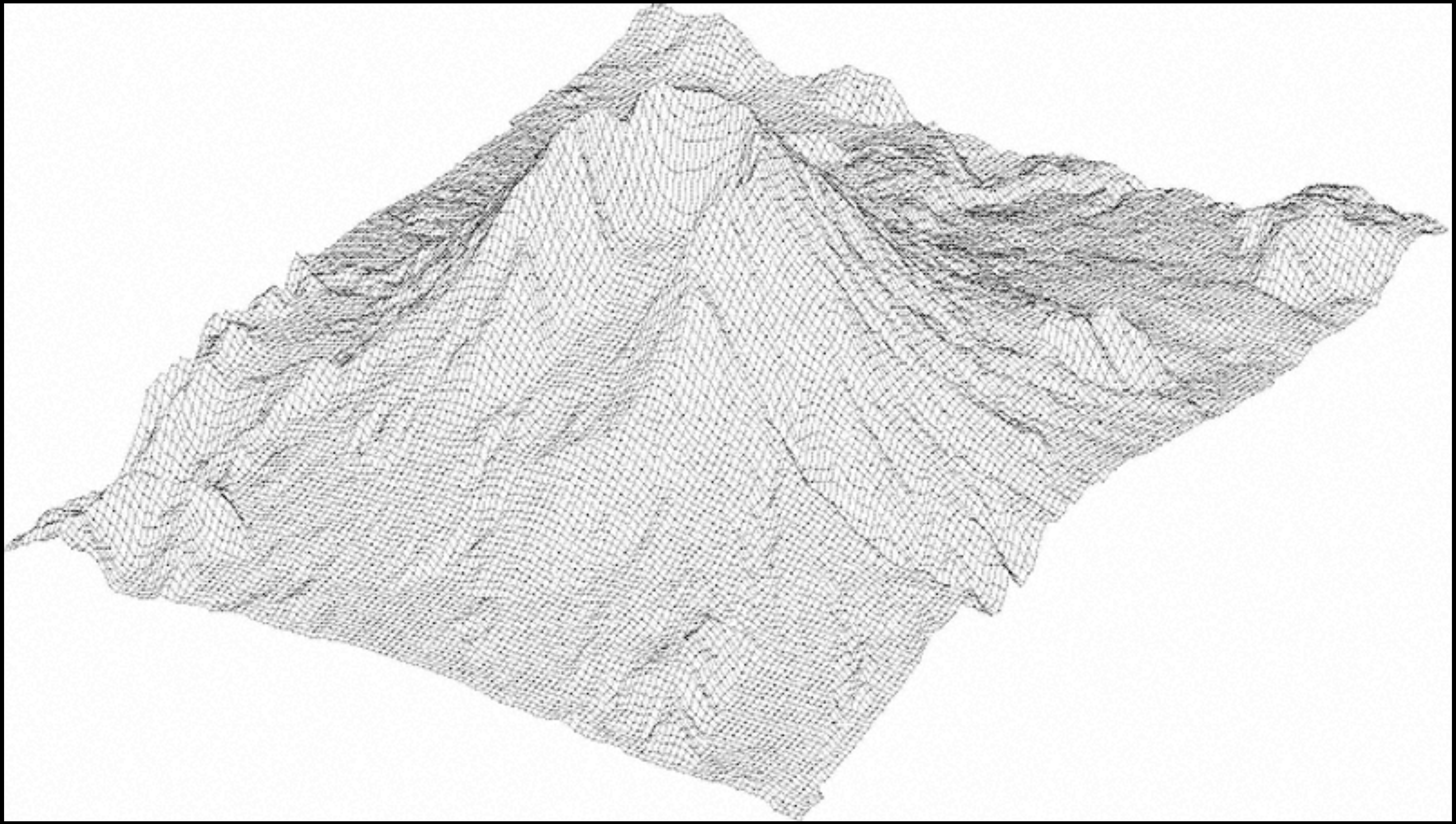


$\frac{1}{\sqrt{n}}$ in <u>any</u> dimension

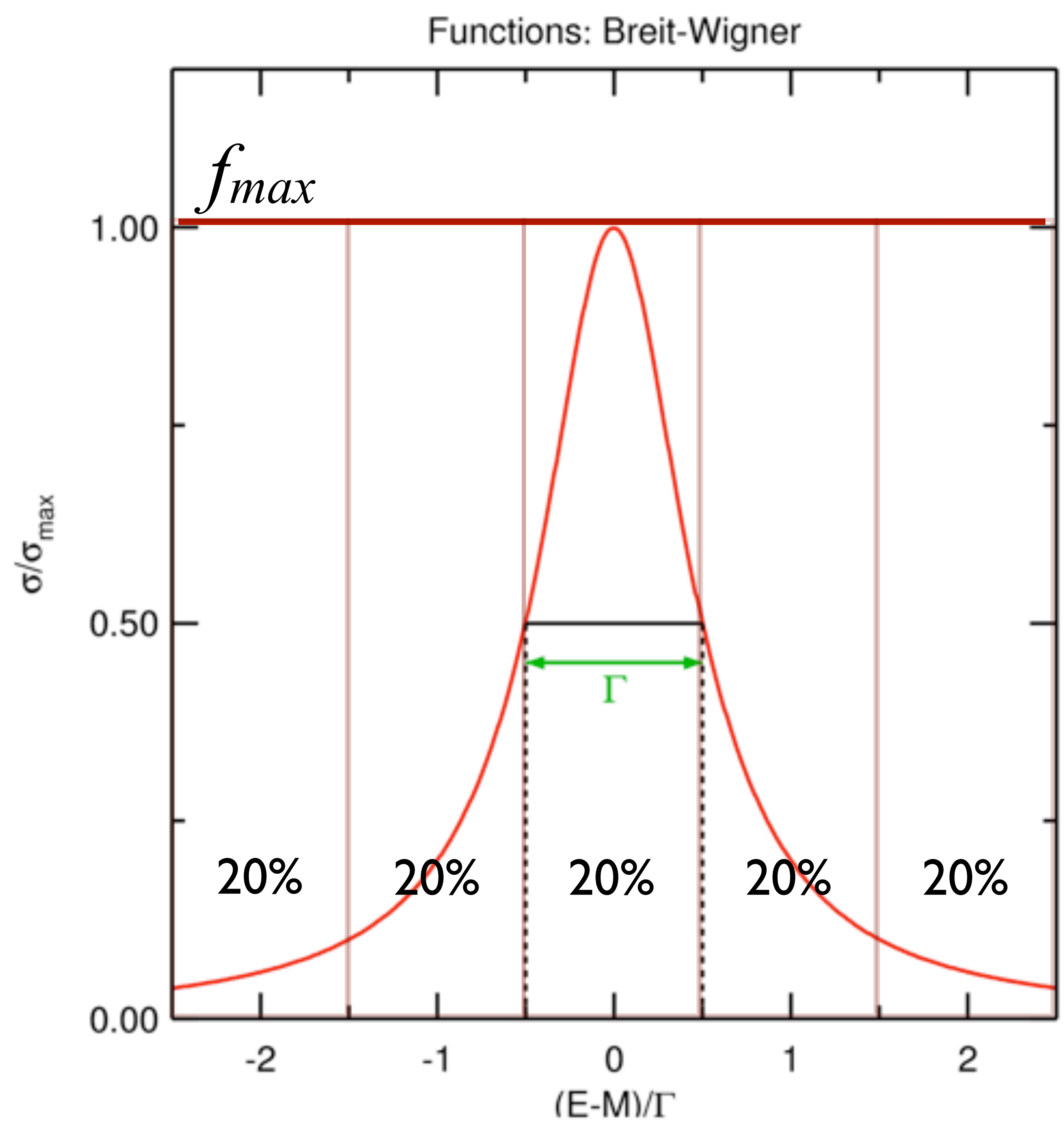
+ can re-use previously generated points (≈ nesting)

Uncertainty as a function of number of points	n_{eval} / bin	Approx Conv. Rate (in 1D)	Approx Conv. Rate (in D dim)
Trapezoidal Rule (2-point)	2^D	$1/n^2$	$1/n^{2/D}$
Simpson's Rule (3-point)	3^D	$1/n^4$	$1/n^{4/D}$
... m-point (Gauss rule)	m^D	$1/n^{2m-1}$	$1/n^{(2m-1)/D}$
Monte Carlo	1	$1/n^{1/2}$	$1/n^{1/2}$

Importance Sampling



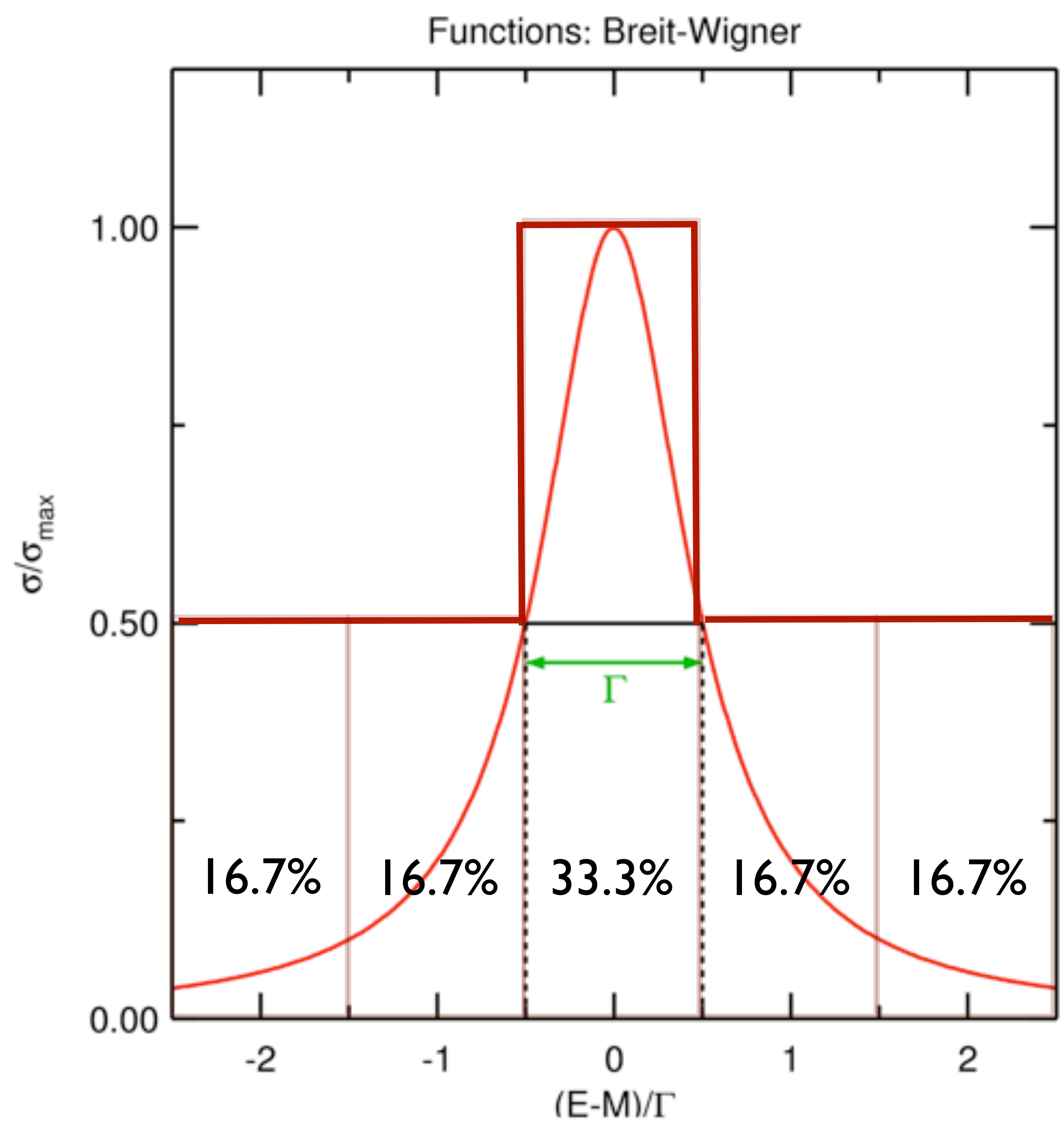
Peaked Functions



Precision on integral dominated by the points with f ≈ f_{max} (i.e., peak regions)

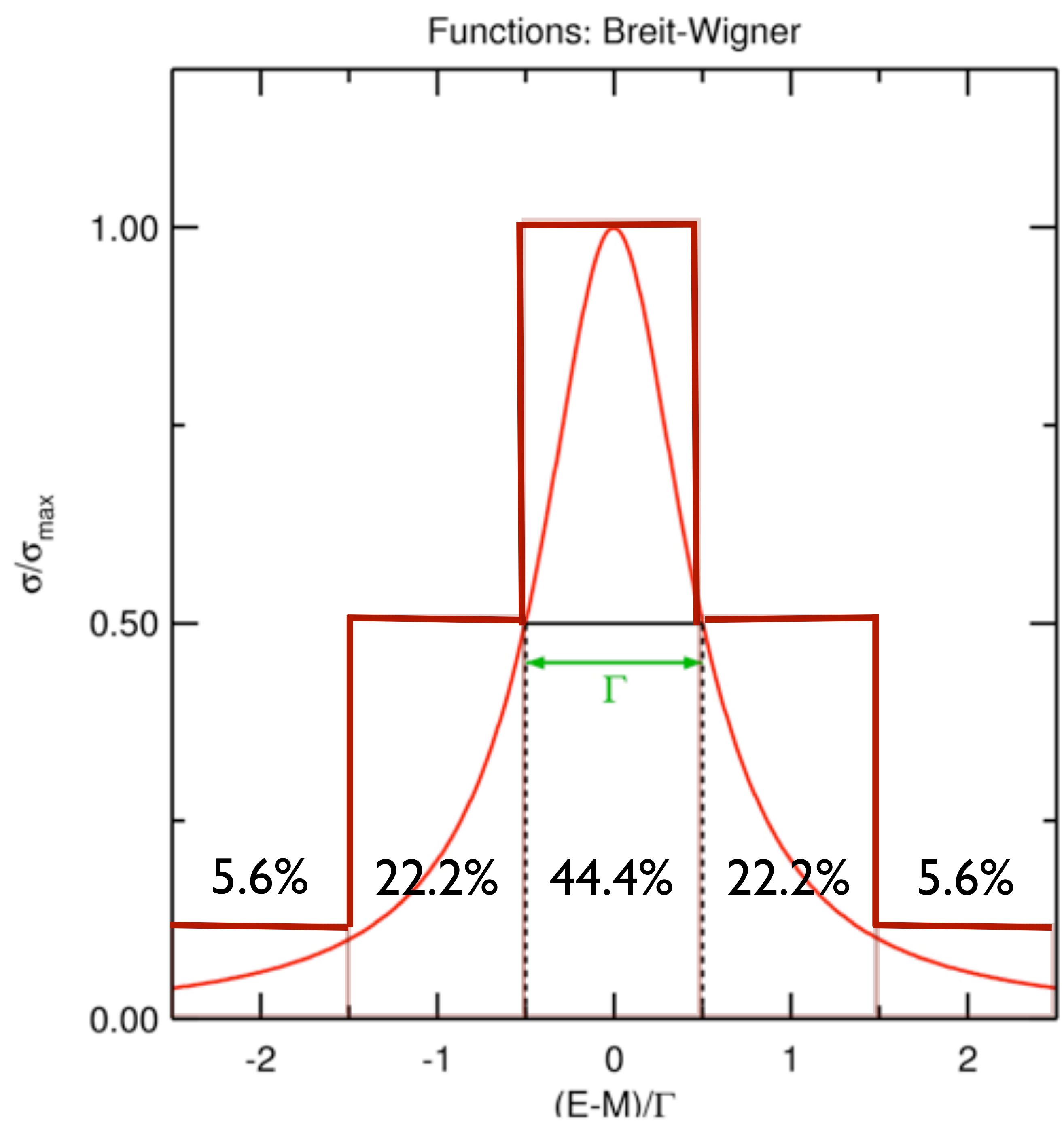
→ slow convergence if high, narrow peaks

Stratified Sampling



→ make it twice as likely to throw points in the peak
→ faster convergence for same number of function evaluations

Adaptive Sampling

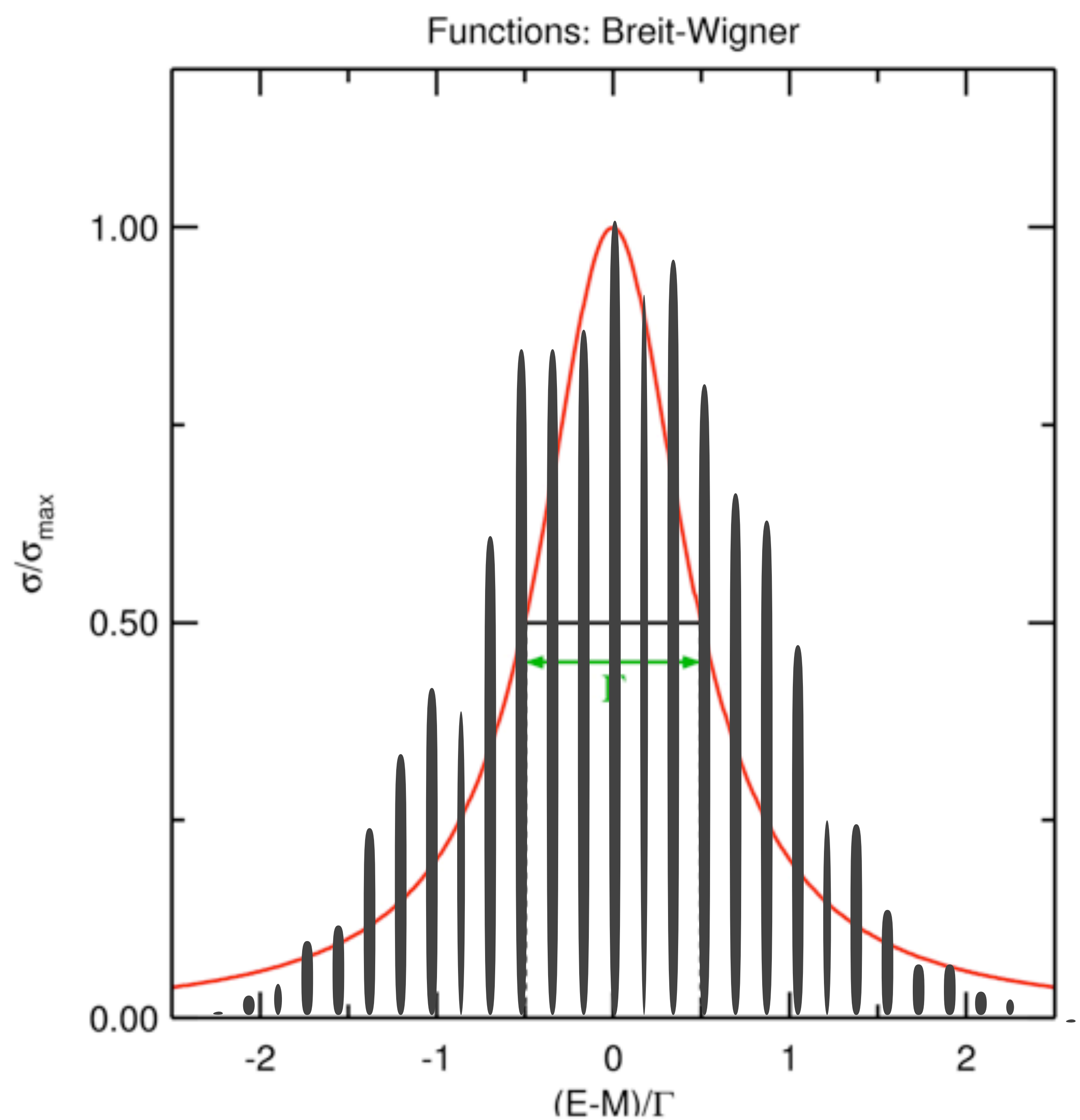


→ can even design algorithms that do this automatically as they run

→ Adaptive sampling

Importance Sampling

E.g., VEGAS algorithm, by G. Lepage



→ or throw points according to some smooth peaked function for which you have, or can construct, a random number generator
(here: Gauss)

Why does this work?

1) You are inputting knowledge: obviously need to know where the peaks are to begin with … (say you know, e.g., the location and width of a resonance)

2) Stratified sampling increases efficiency by combining n-point quadrature with the MC method, with further gains from adaptation

3) Importance sampling:

$$\int_a^b f(x)\mathrm{d}x = \int_a^b \frac{f(x)}{g(x)}\mathrm{d}G(x)$$

Effectively does flat MC with changed integration variables

Fast convergence if $f(x)/g(x) \approx 1$

The Veto Algorithm

Hit

Miss

How we do Monte Carlo

- **Take your system**
  - Set of radioactive nuclei
  - Set of hard scattering processes
  - Set of resonances that are going to decay
  - Set of particles coming into your detector
  - Set of cosmic photons traveling across the galaxy
  - …

How we do Monte Carlo

- **Take your system**
- **Generate a "trial"** event/decay/interaction/…
  - Not easy to generate random numbers distributed according to exactly the right distribution?
    - May have complicated dynamics, interactions …
    - → use a simpler "trial" distribution
      - Flat with some stratification
      - Or importance sample with simple overestimating function (for which you can generate random #s)

How we do Monte Carlo

- **Take your system**
- **Generate a "trial"** event/decay/interaction/…
  - Accept trial with probability f(x)/g(x)
    - f(x) contains all the complicated dynamics
    - g(x) is the simple trial function

no dependence on g in final result
- only affects convergence rate

  - **If accept:** replace with new system state
  - **If reject:** keep previous system state

And keep going: generate next trial …

Summary

Quantum Scattering Problems are common to many areas of physics:
To compute expectation value of observable: integrate over phase space

Complicated functions → Numerical Integration

High Dimensions → Monte Carlo (stochastic) convergence is fastest
Additional power by stratification and/or importance sampling

Additional Bonus → Veto algorithm → direct simulation of arbitrarily complicated reaction chains → next lecture

Recommended Reading

F. James

Monte Carlo Theory and Practice

Rept.Prog.Phys.43 (1980) p.1145

S. Weinzierl

Topical lectures given at the Research School Subatomic physics, Amsterdam, June 2000

Introduction to Monte Carlo Methods

e-Print: hep-ph/0006269

S. Teukolsky, B. Flannery, W. Press, T. Vetterling

Numerical Recipes *(in FORTRAN, C, …)*

http://www.nr.com/