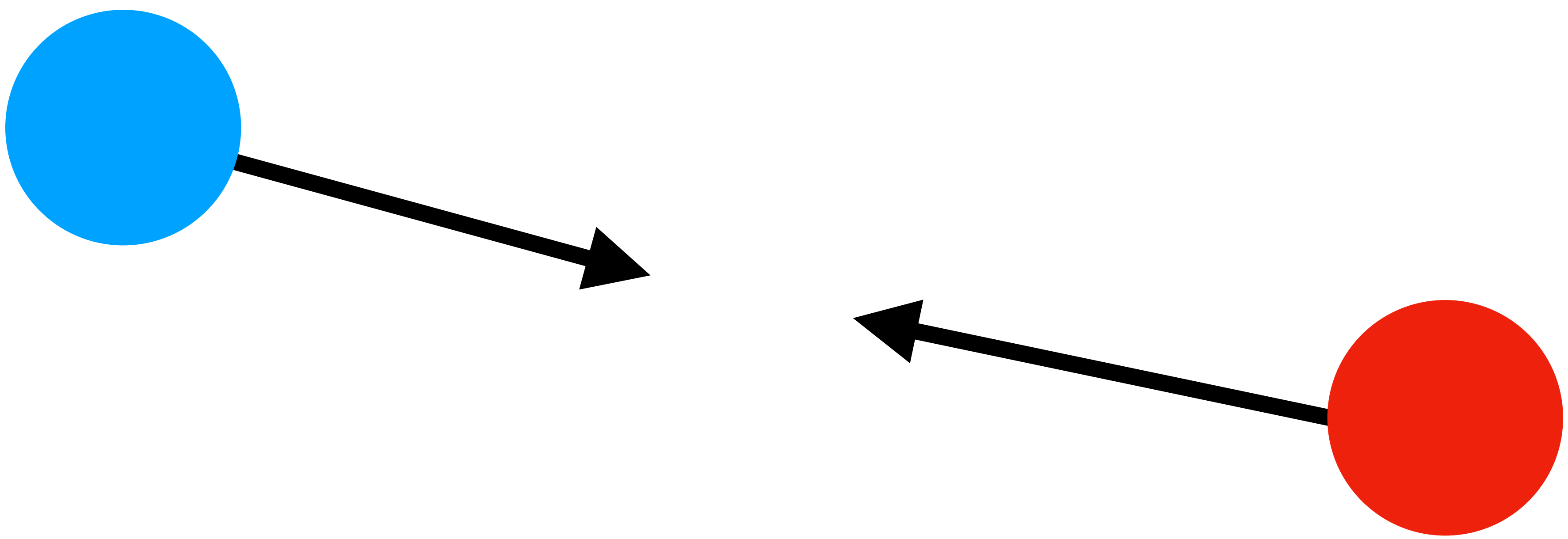
Lecture 18: Monte Carlo methods

What do we need for Simulation?

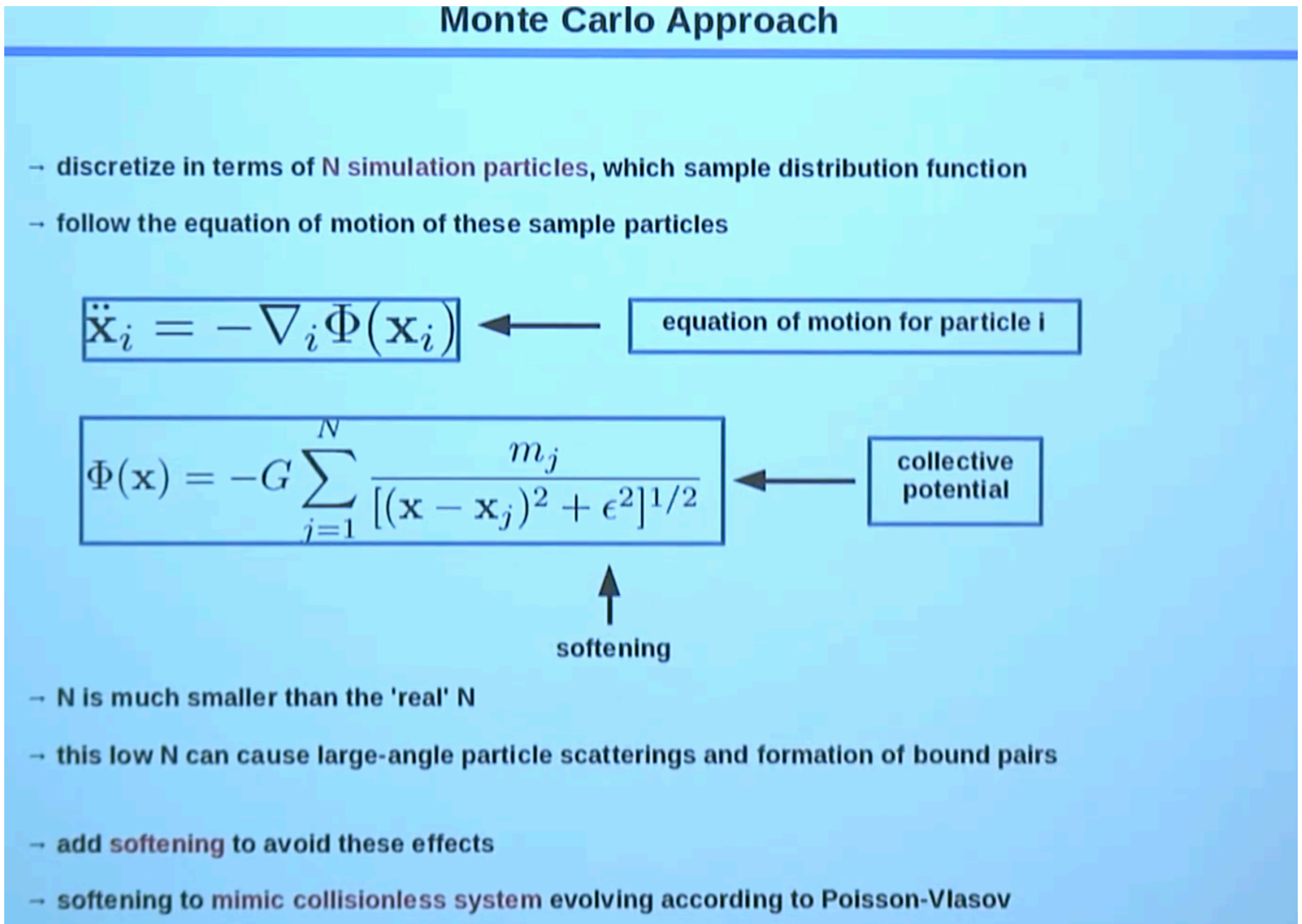


$$F = \frac{G m_1 m_2}{|\vec{r}_1 - \vec{r}_2 + \epsilon|^3} \left(\vec{r}_1 - \vec{r}_2\right)$$

- To simulate this on a computer we will add a “softening” term

This is how DM/galaxies are modeled

- Instead of treating matter as a fluid
  - Discretize matter into chunks and solve n-body problem



3 body Problem: History

- The original two body probelm was solved in 18th century
  - Work done by Netwon, Bernoulli Bros, Euler, Laplace,…
    - All started on the 3 body problem and built on the two body
- King Oscar II decided to make a competition:
  - For his 60th birthday he bestowed a prize on who could solve the n-body problem

3 body Problem: History

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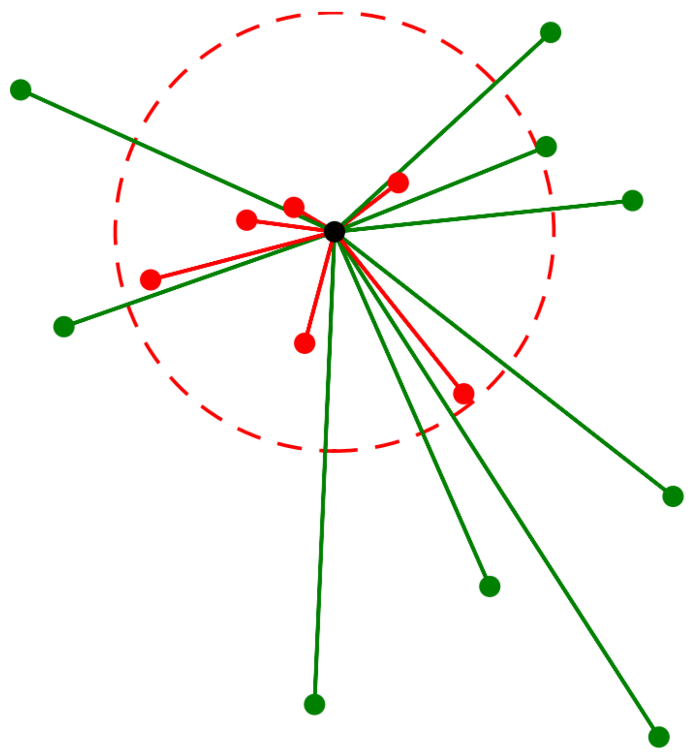
  - For his 60th birthday he bestowed a prize on who could solve the n-body problem

Henri Poincare →

He proved no solution existed!

Going to N-body

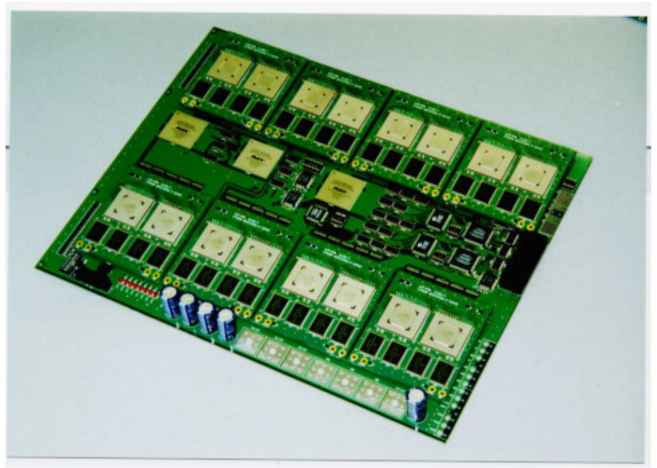
- The challenge of solving this numerically for n-body
  - This scales with the number of bodies N^2
  - Requires the computations of all pairwise distances

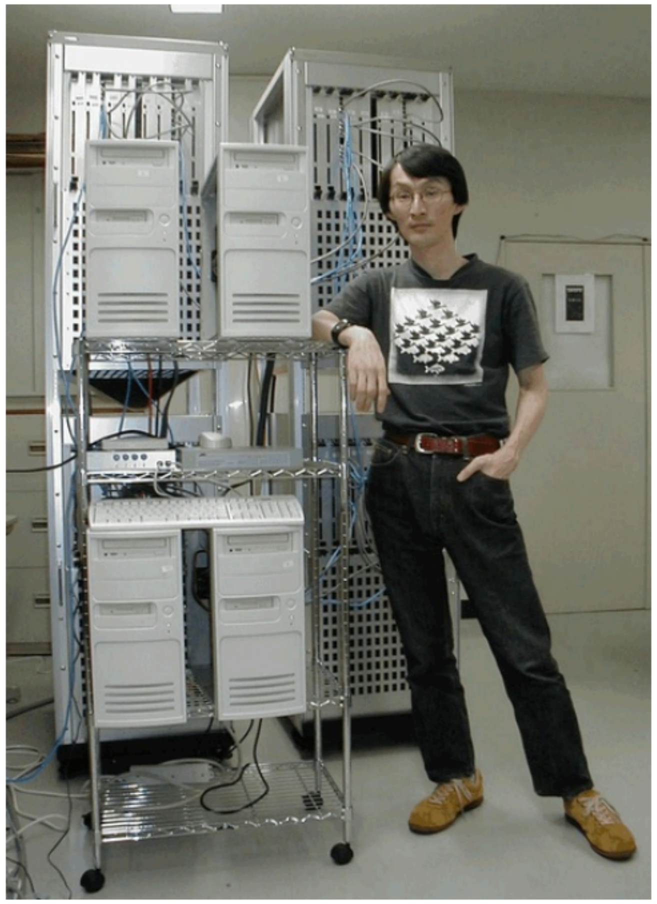


- For N=1000 (1 Million/step computations)
- For $N=10^6$ Something ridiculous

Historical Solutions

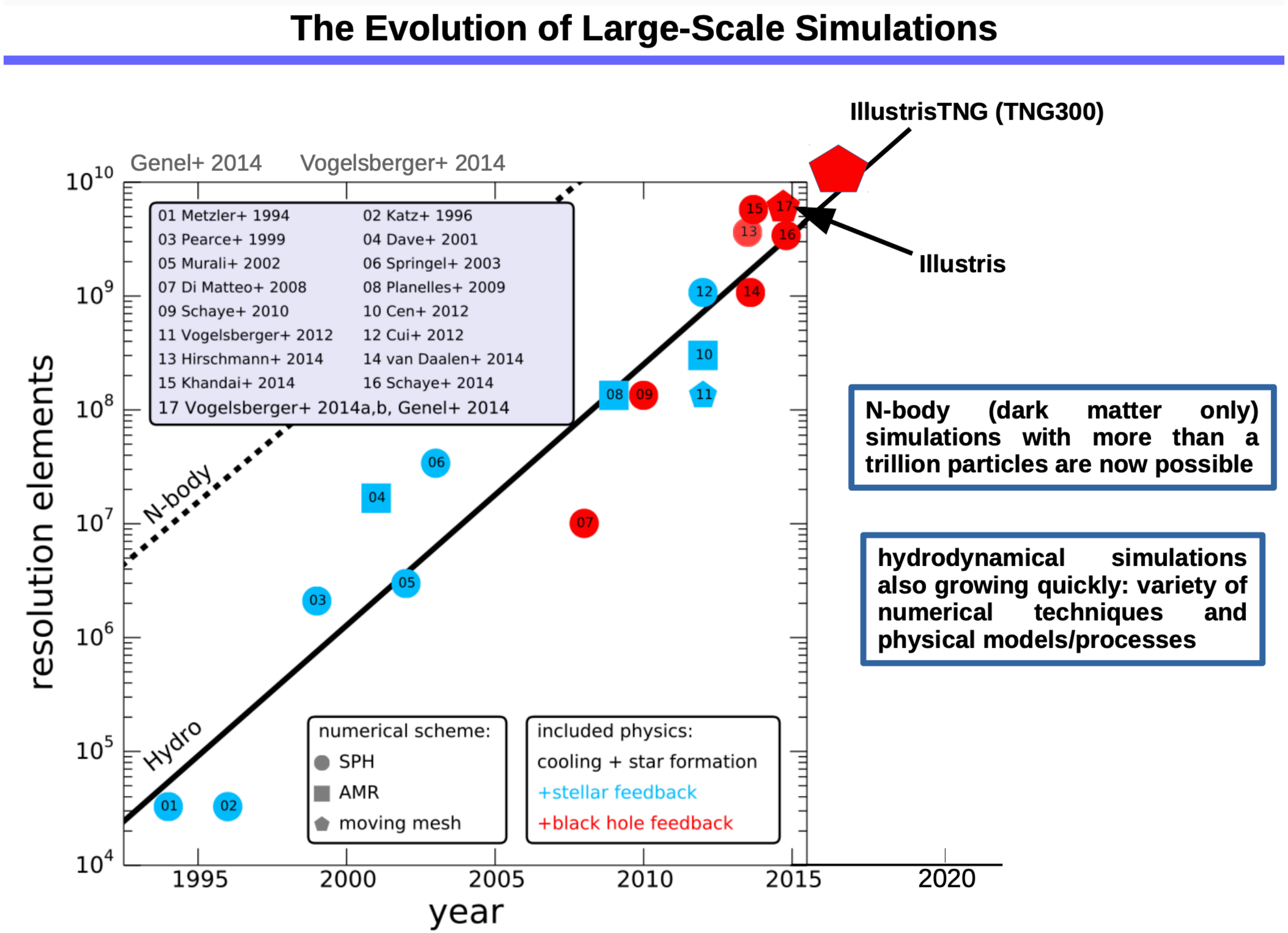
- One approach has been to build dedicated computing hardware
  - Dedicated hardware that can do large-scale parallel computation
  - Focused specifically on n-body simulation
  - GRAPE boards (GRAvity PipelinE)
- Now done with GPUs





Jun Makino with GRAPE-6

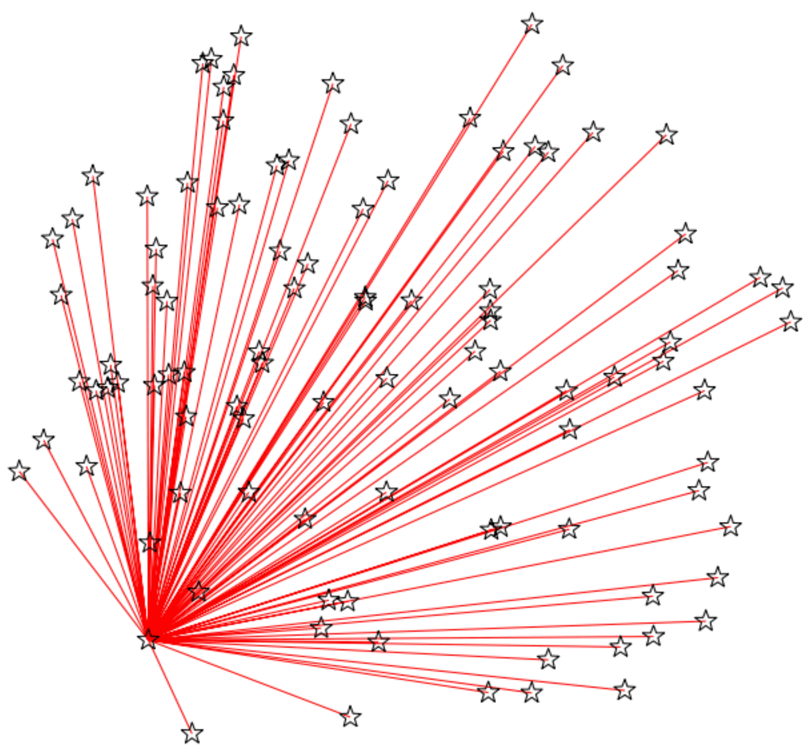
Scaling of n-body

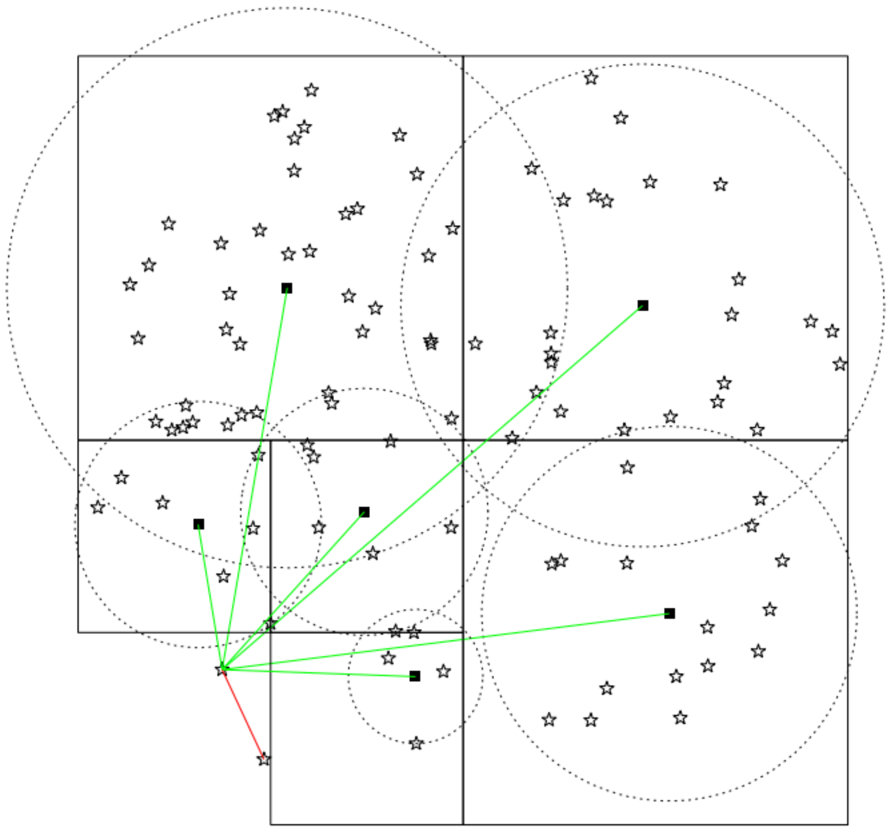


- M. Vogelsberger(https://indico.cern.ch/event/736594/contributions/3184103/attachments/1738225/2812076/talk_vogelsberger.pdf)

How do you deal with N-body?

- Barne’s-Hut Algorithm re-rank stars into a tree structure
  - Structure is a grid over the whole space

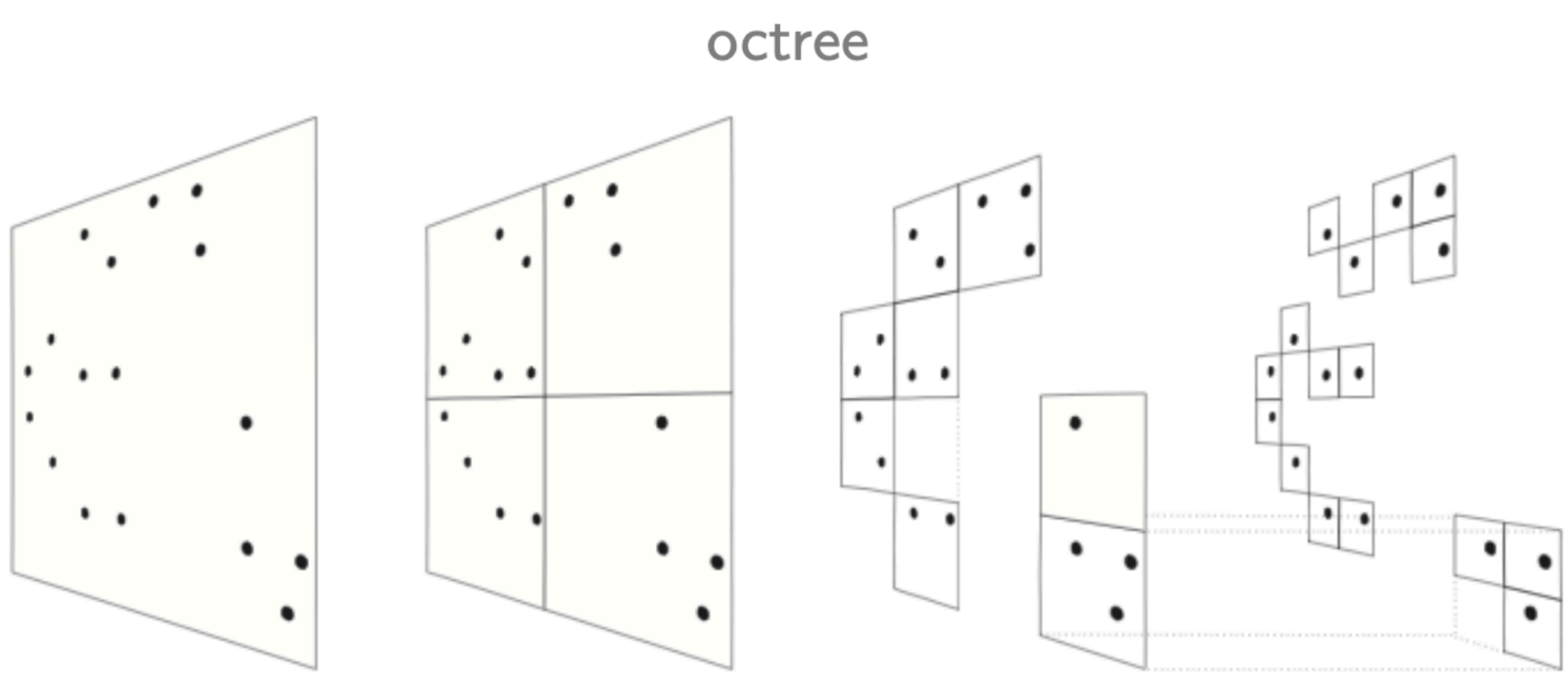


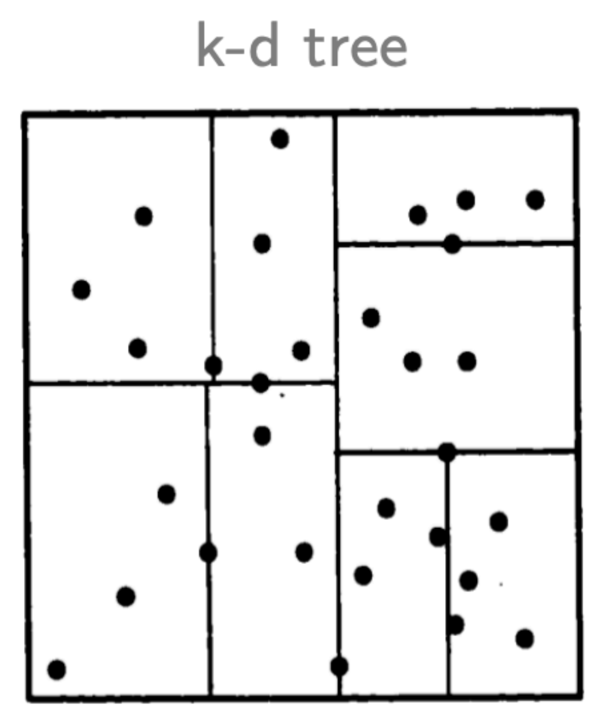


[from Dehnen & Read 2011]

Tree Construction

- QuadTree/OctTree
  - Split each square(cube) into 4(8) sub regions
- KD Tree
  - Use the data to draw equal numbered regions in space

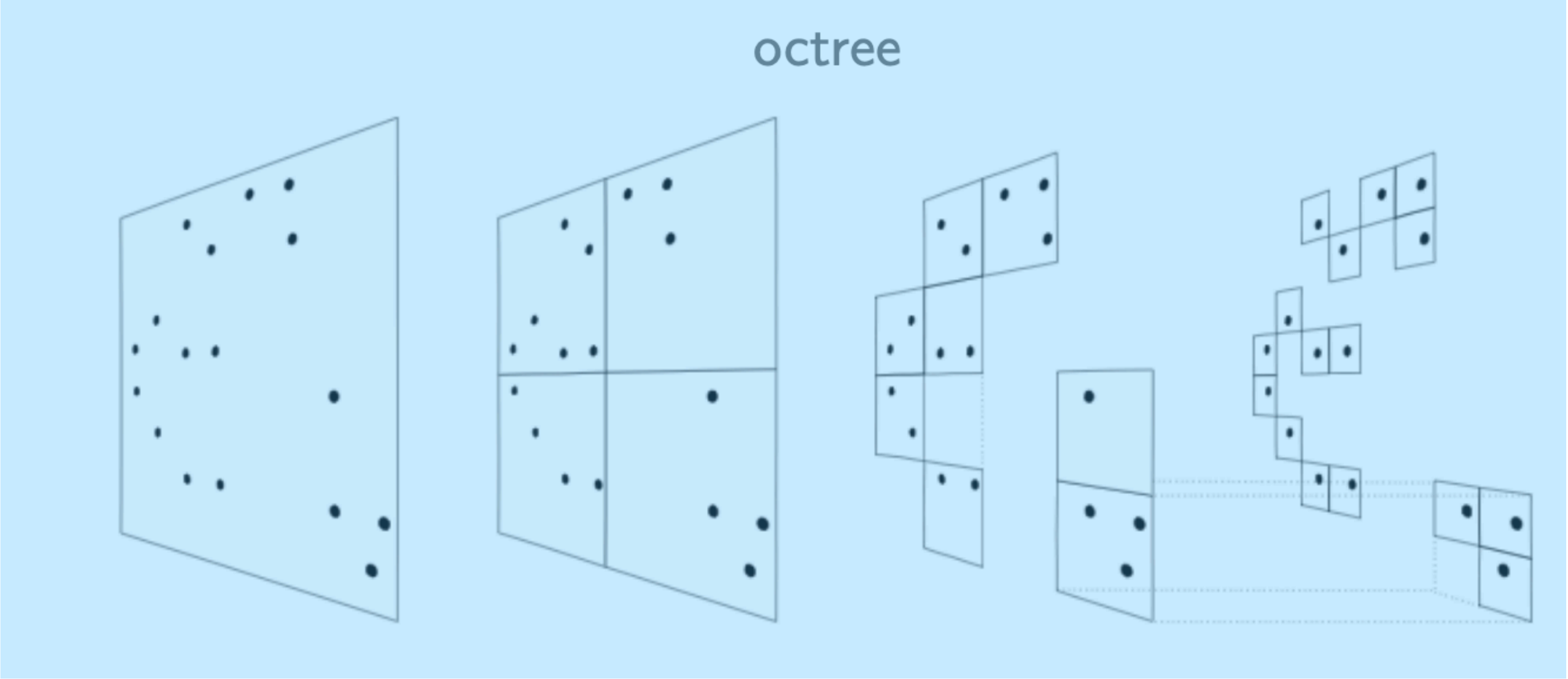


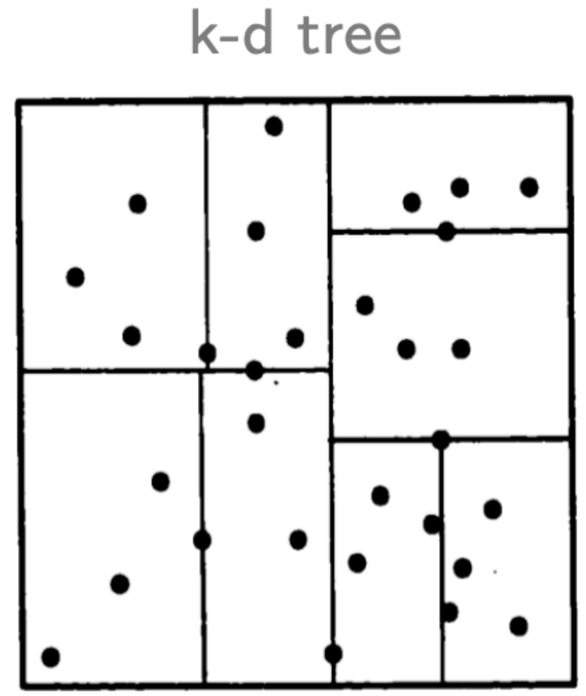


Tree Construction

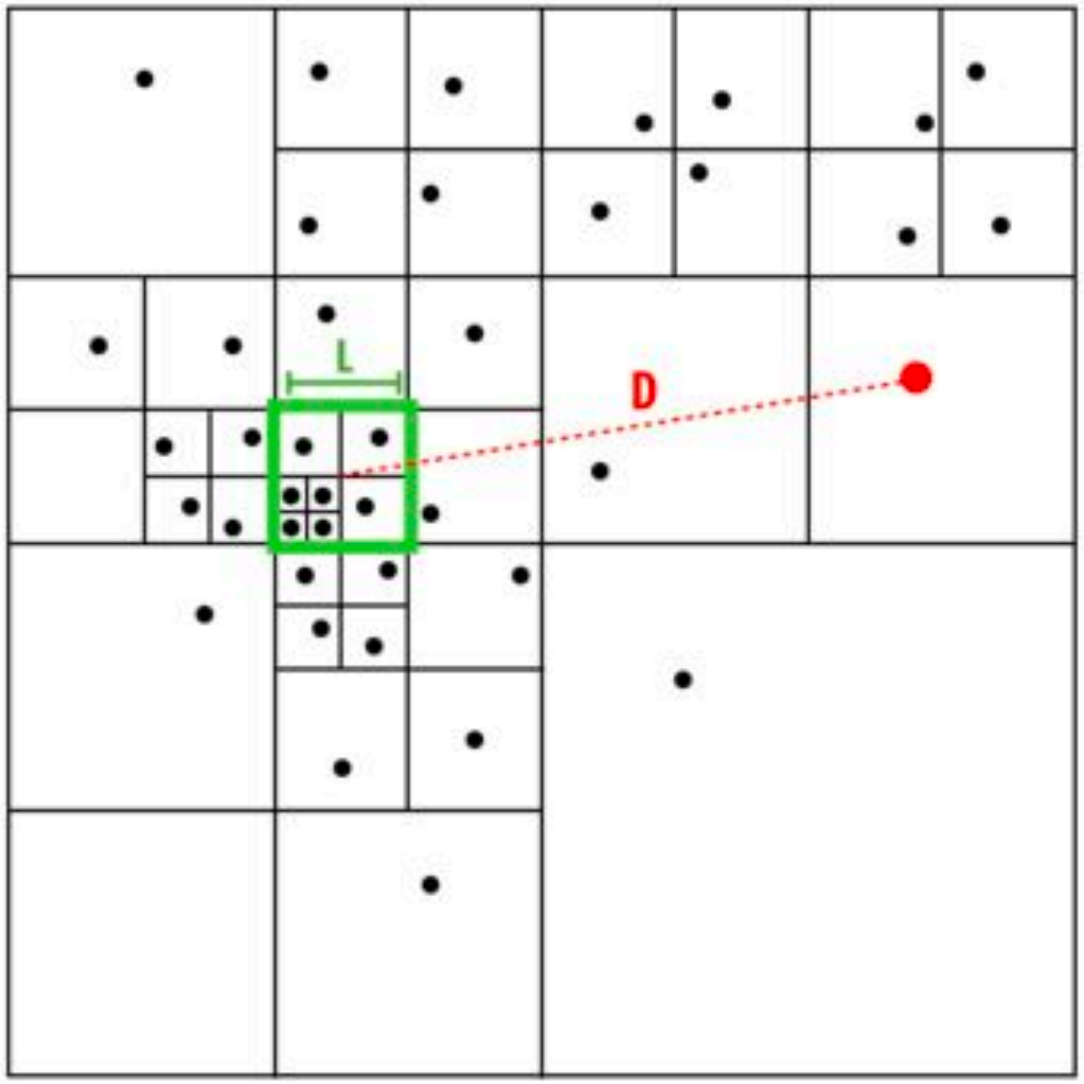
- QuadTree/OctTree
  - Split each square(cube) into 4(8) sub regions
- KD Tree
  - Use the data to draw equal numbered regions in space

Just requires that we know the bounds of the space

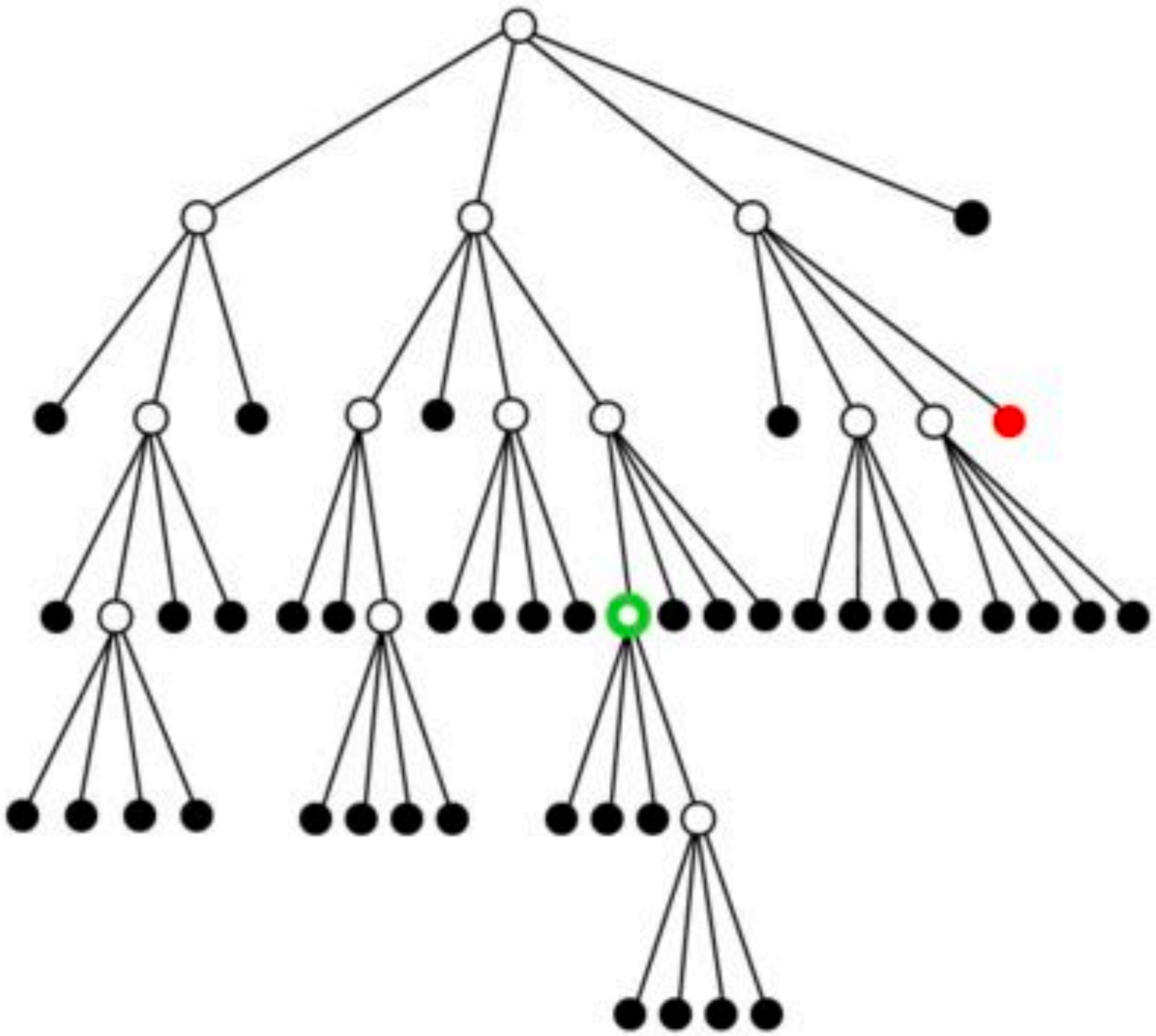




Visualizing Tree



Spatial Domain



Quad-Tree Representation

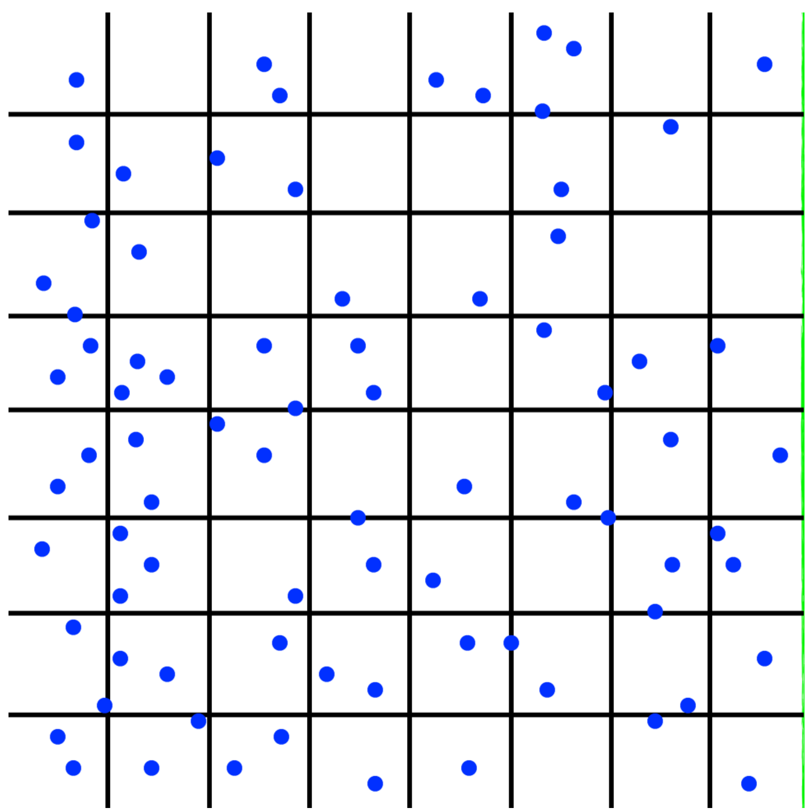
Note that for the big grids, this equates to Gauss' law style an apporach
Treat each square as a star w/total mass at mass weighted center

Barnes-Hut Algorithm

- We can follow a step by step construction of this :
  - 1. Construct tree structure with bounds
  - 2. Loop over stars and fill tree structure
  - 3. Loop over stars and compute distance
    - Full n-body computation for nearby trees only
  - 4. Step forward everything
- The above process is N log(N) in comptuational time

Larger Scale Concept

- For the really large scale n-body dynamics
  - To get global motion
  - Grid up the whole space and Fourier transform it
  - Evolve the system in Fourier space

FFT()

Solve for the Graviational Potential in Fourier space

Step Potential

Larger Scale Concept

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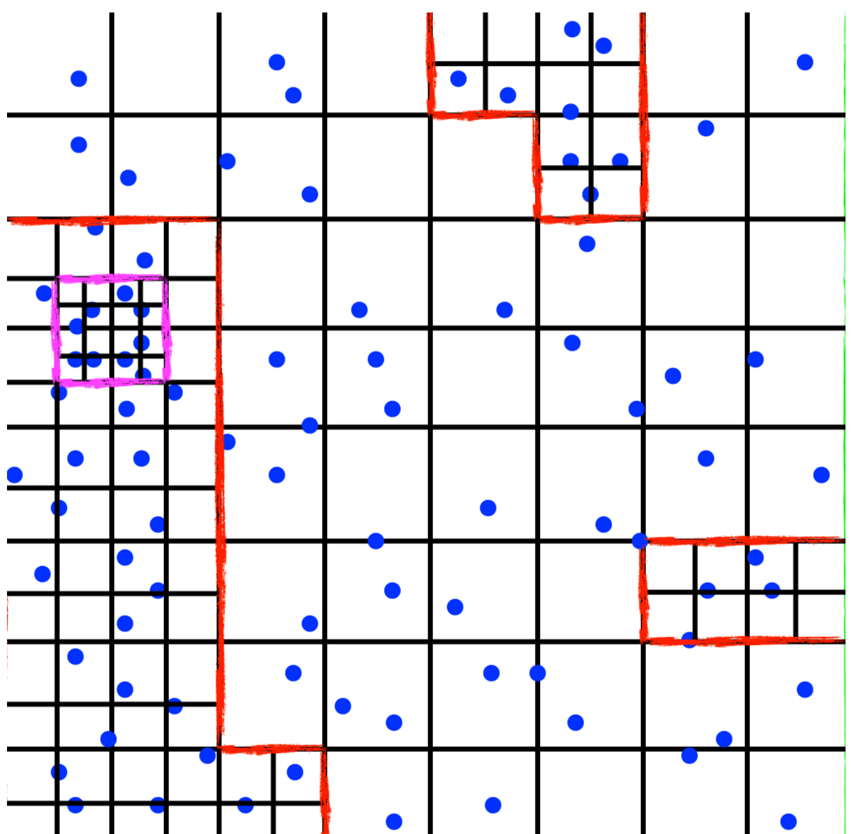
FFT(



)

Solve for the Graviational Potential in Fourier space

Step Potential

http://iac.edu.mx/data/events/2016/simschool/Li-L2.pdf

Lecture 18:
Monte Carlo methods

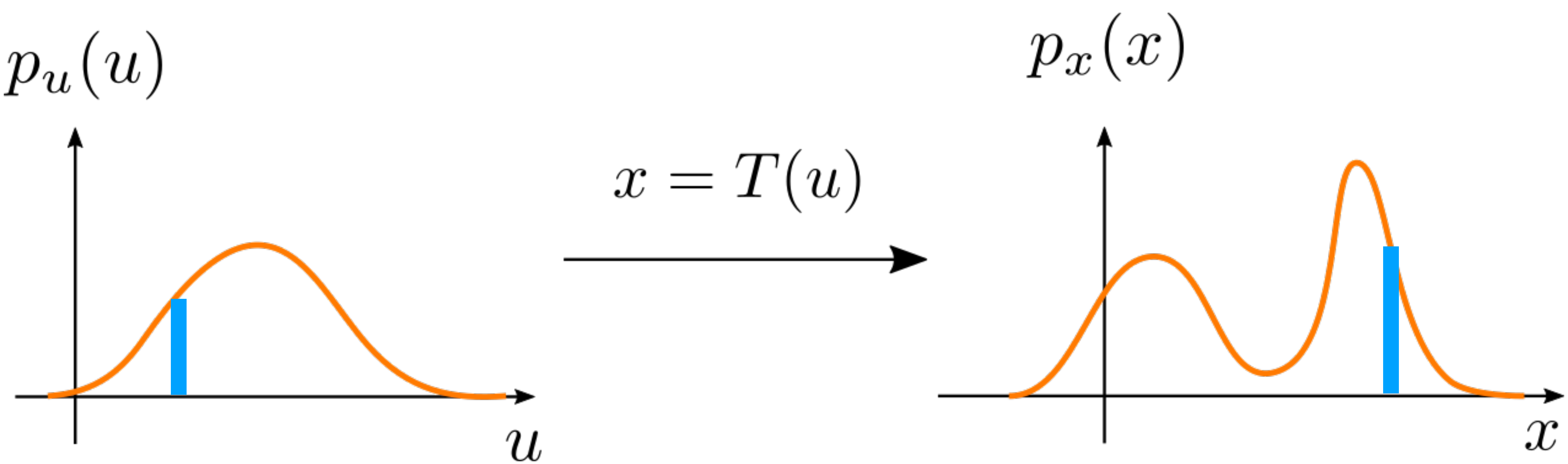
Monaco

Monte Carlo(MC)

- Have been seeing Monte Carlo methods throughout class
  - Any time we randomly sample thats an MC method
  - Effectively we are just rolling the die

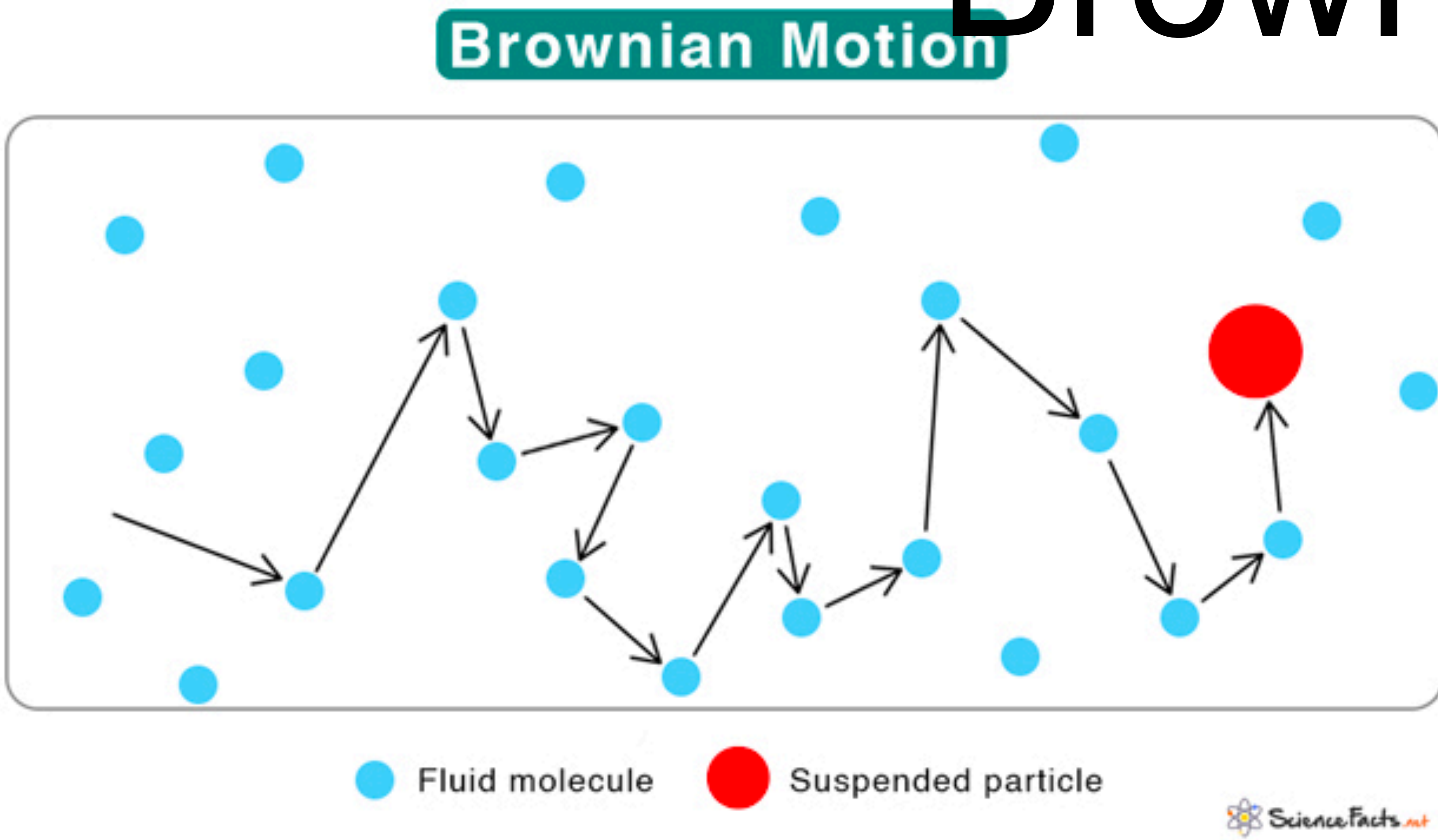
Monte Carlo vs Integration

- Monte Carlo is a form of integrator
  - However non-deterministic and varies over distribution



- Monte Carlo typically used when
  - we can't model things analytically any more
  - Replace a whole distribution with just an event (small region

Brownian Motion



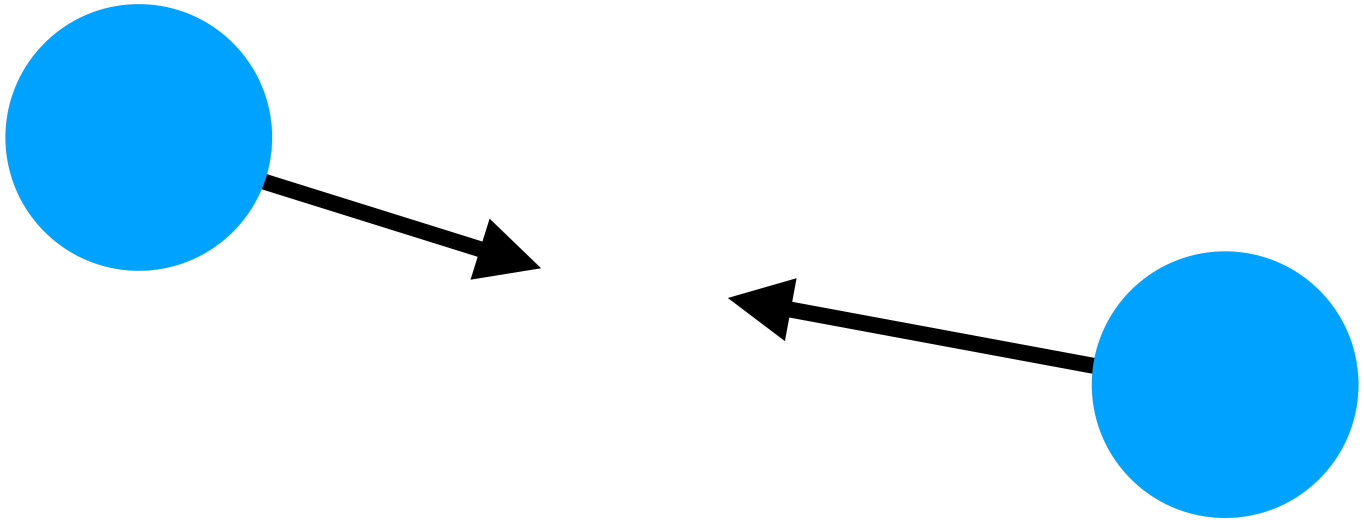
$$f(v_x, v_y, v_z) = \left[\frac{m}{2\pi kT}\right]^{3/2} e^{-m(v_x^2+v_y^2+v_z^2)/2kT}$$

$$= \left[\frac{m}{2\pi kT}\right]^{3/2} e^{-mv^2/2kT}$$

using $v^2 = v_x^2 + v_y^2 + v_z^2$

- At each step
  - We just randomly sample the velocity from a Gaussian
  - We can do this many times to look at overall motion

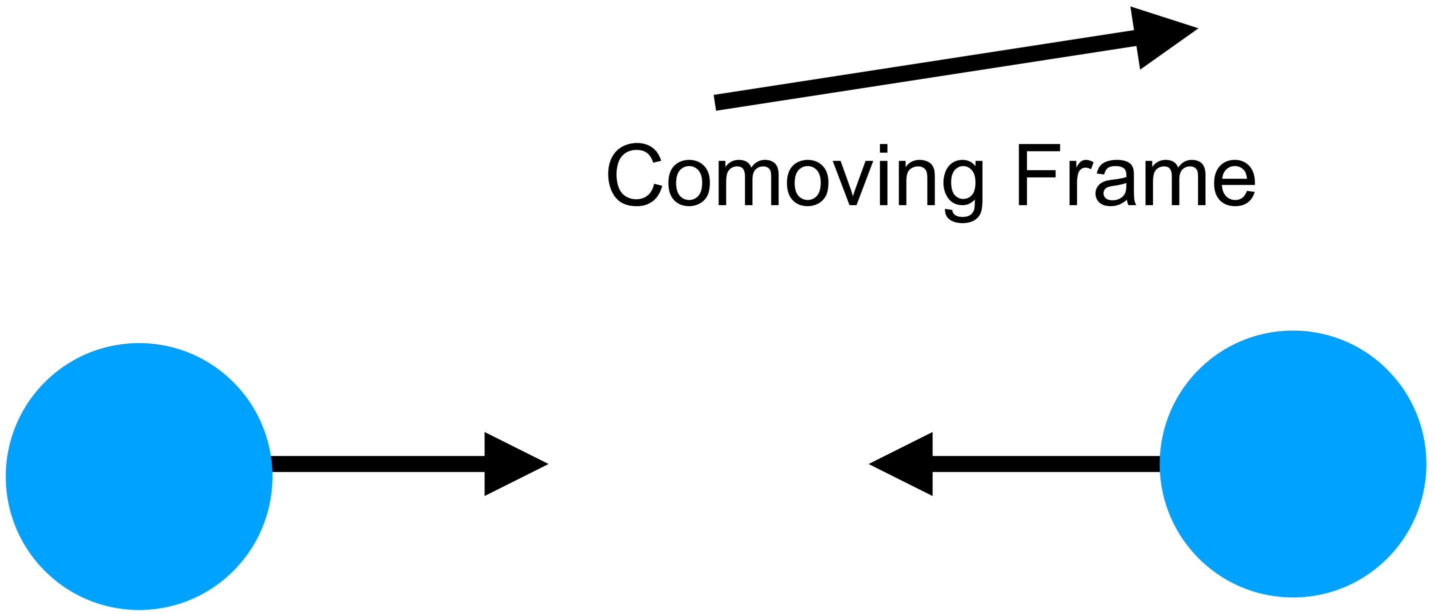
The motion at each step



Elastic Collision

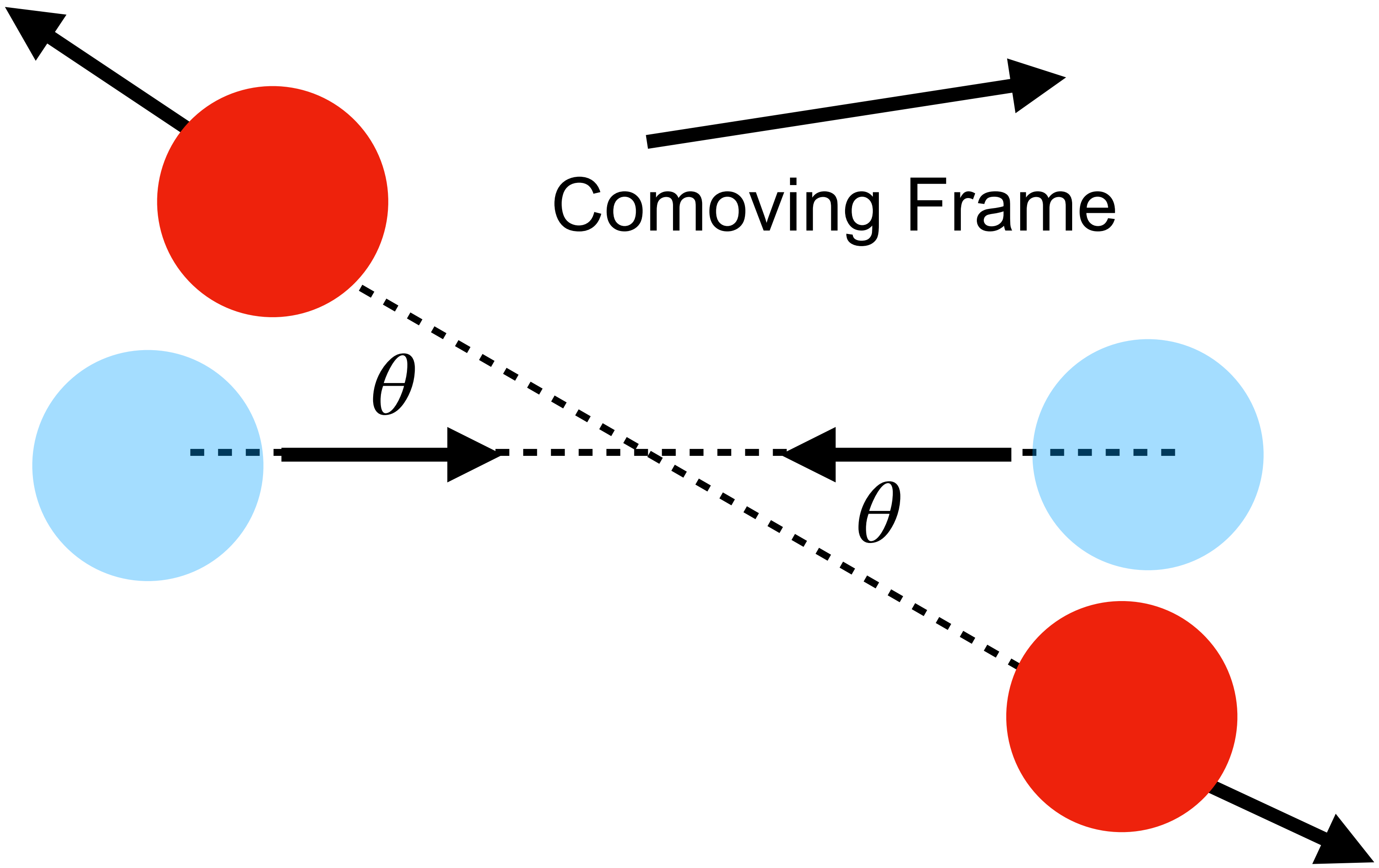
- Just sample particle collisions at each step

The motion at each step



Elastic Collision
In COM Frame

The motion at each step



Elastic Collision
In COM Frame

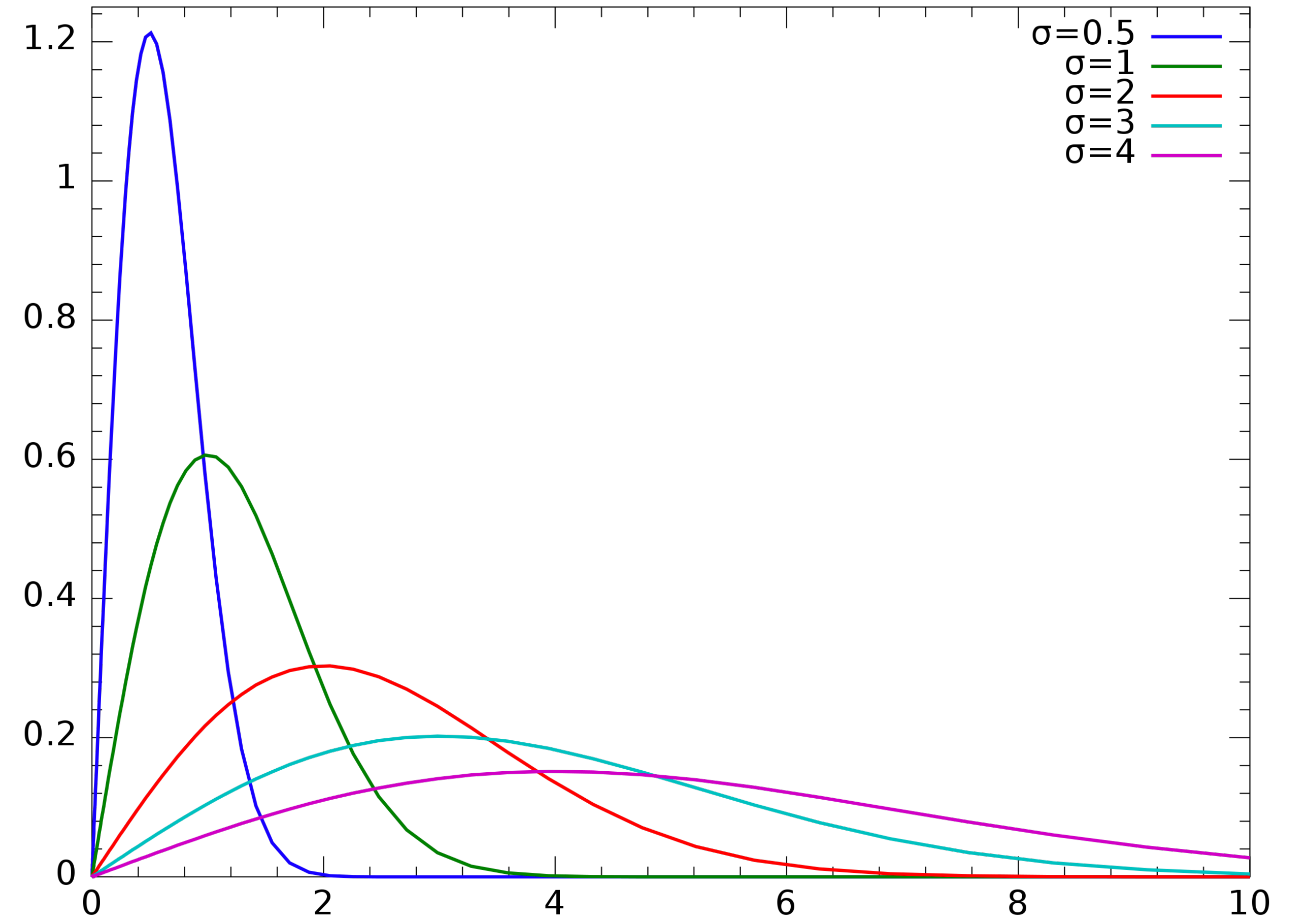
Rayleigh Distribution

Rayleigh is a distribution of the radius in a 2D Gaussian

$$f_U(x;\sigma) = f_V(x;\sigma) = \frac{e^{-x^2/(2\sigma^2)}}{\sqrt{2\pi\sigma^2}}.$$

$$f(x;\sigma) = \frac{x}{\sigma^2} e^{-x^2/(2\sigma^2)}, \quad x \geq 0,$$

$$F_X(x;\sigma) = \frac{1}{2\pi\sigma^2} \int_0^{2\pi} \int_0^x r e^{-r^2/(2\sigma^2)} \, dr \, d\theta = \frac{1}{\sigma^2} \int_0^x r e^{-r^2/(2\sigma^2)} \, dr.$$



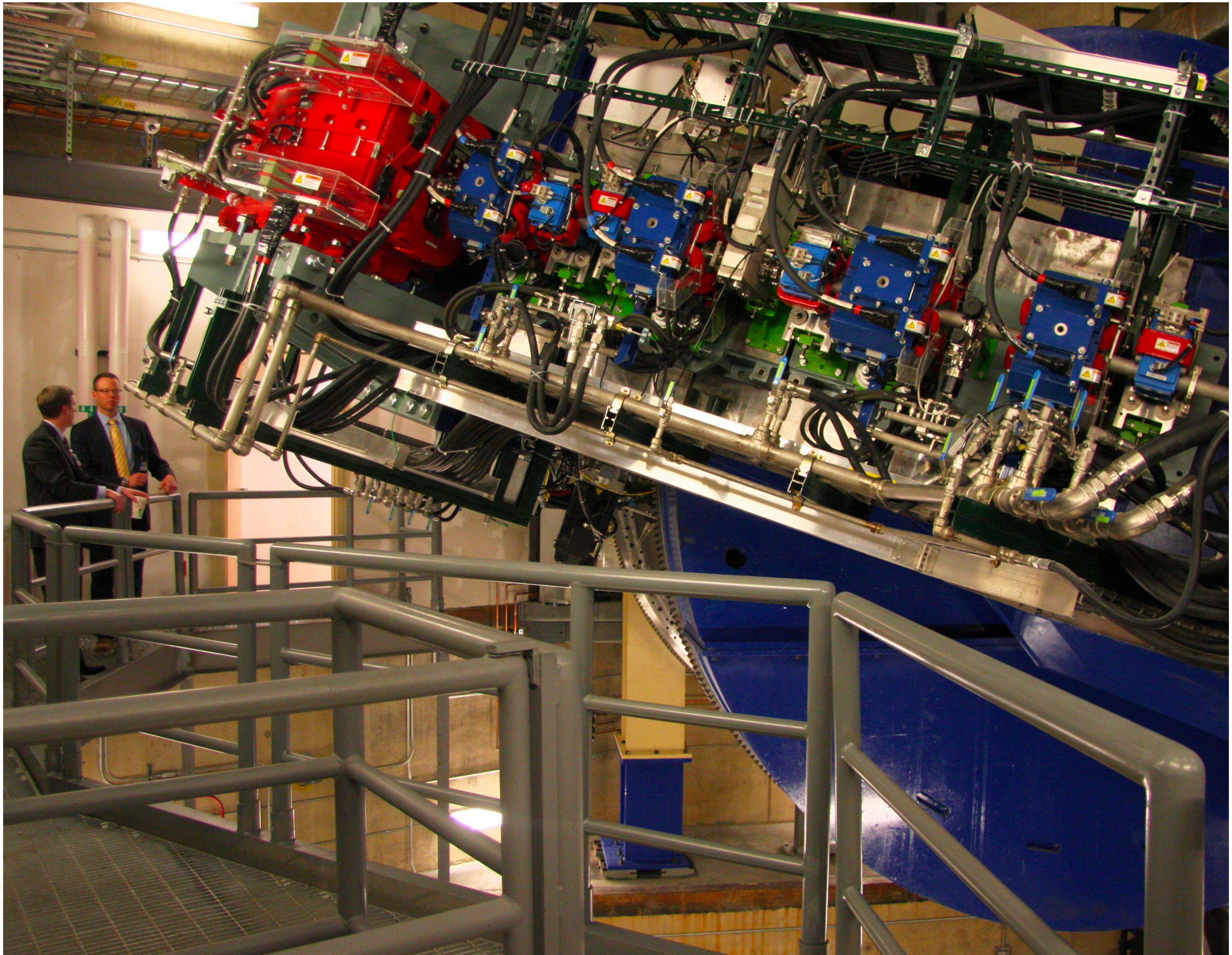
Proton Therapy

Proton Therapy Center at MGH

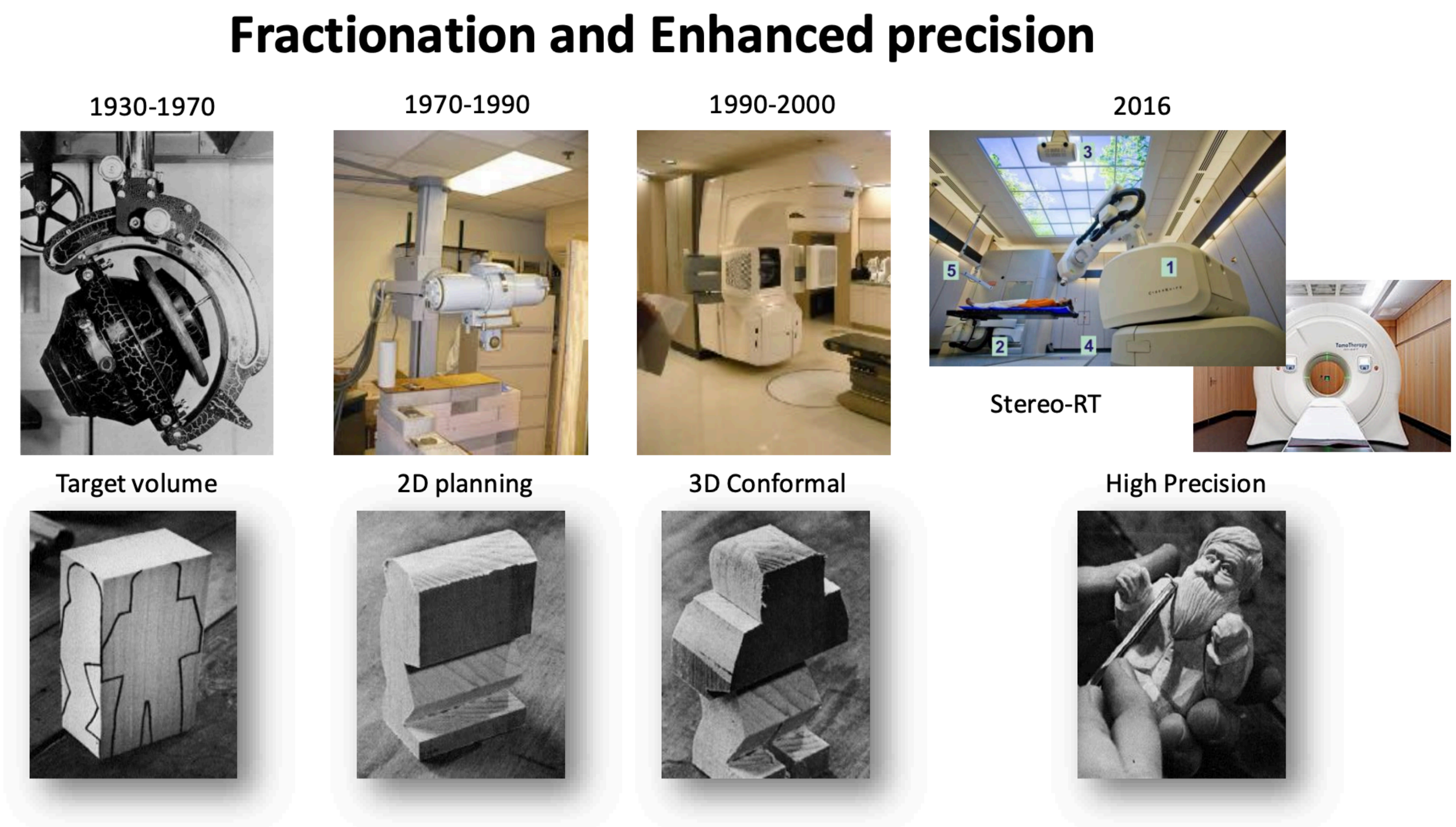
Typical Device

Particle Therapy Centre

Mayo Clinic



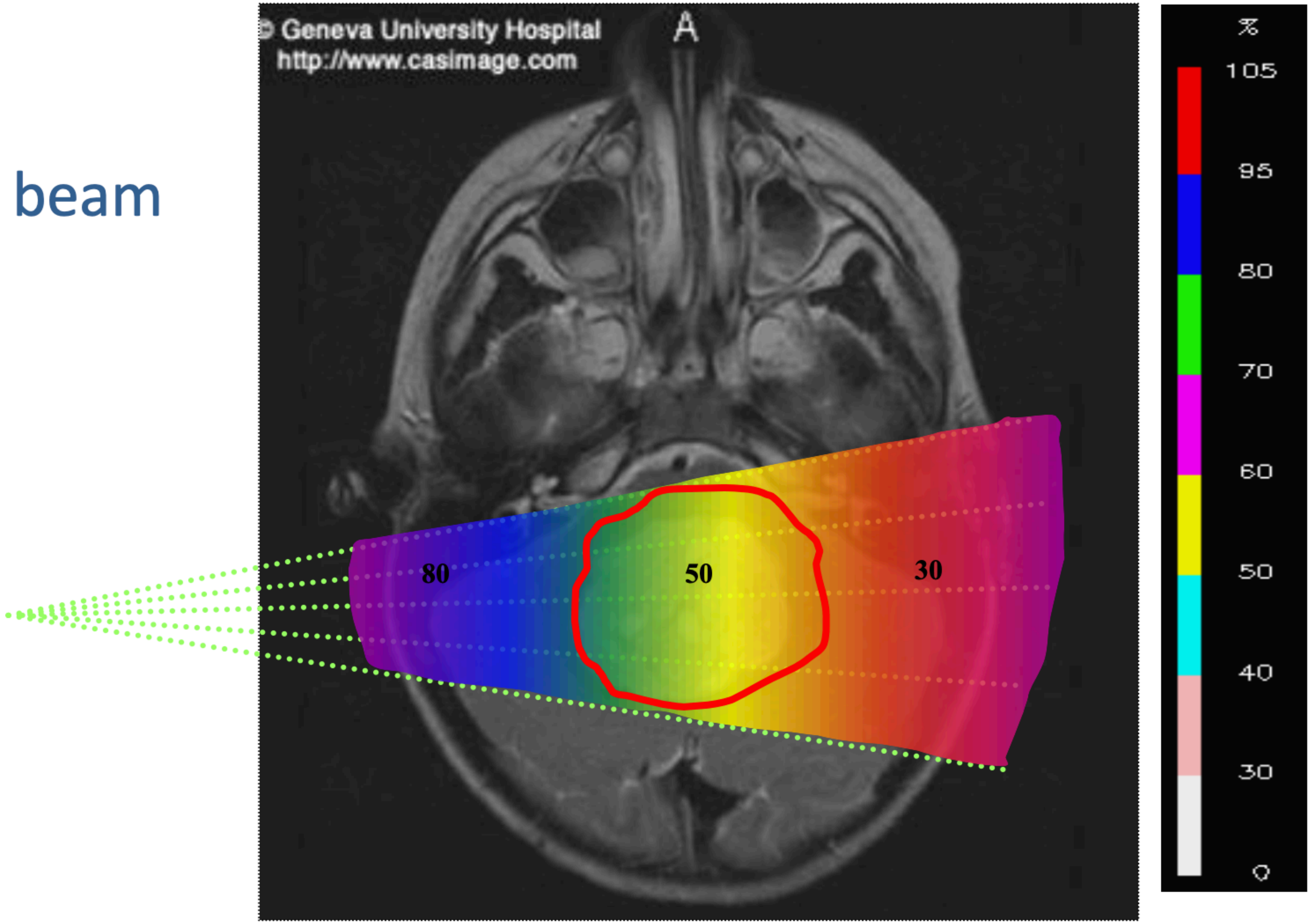
Radiation Therapy



- To fight Cancer
  - Radiation therapy has had a long history of usage
  - Radiation is sent to a tumor to kill it
  - Critical when you can’t cut the tumor out

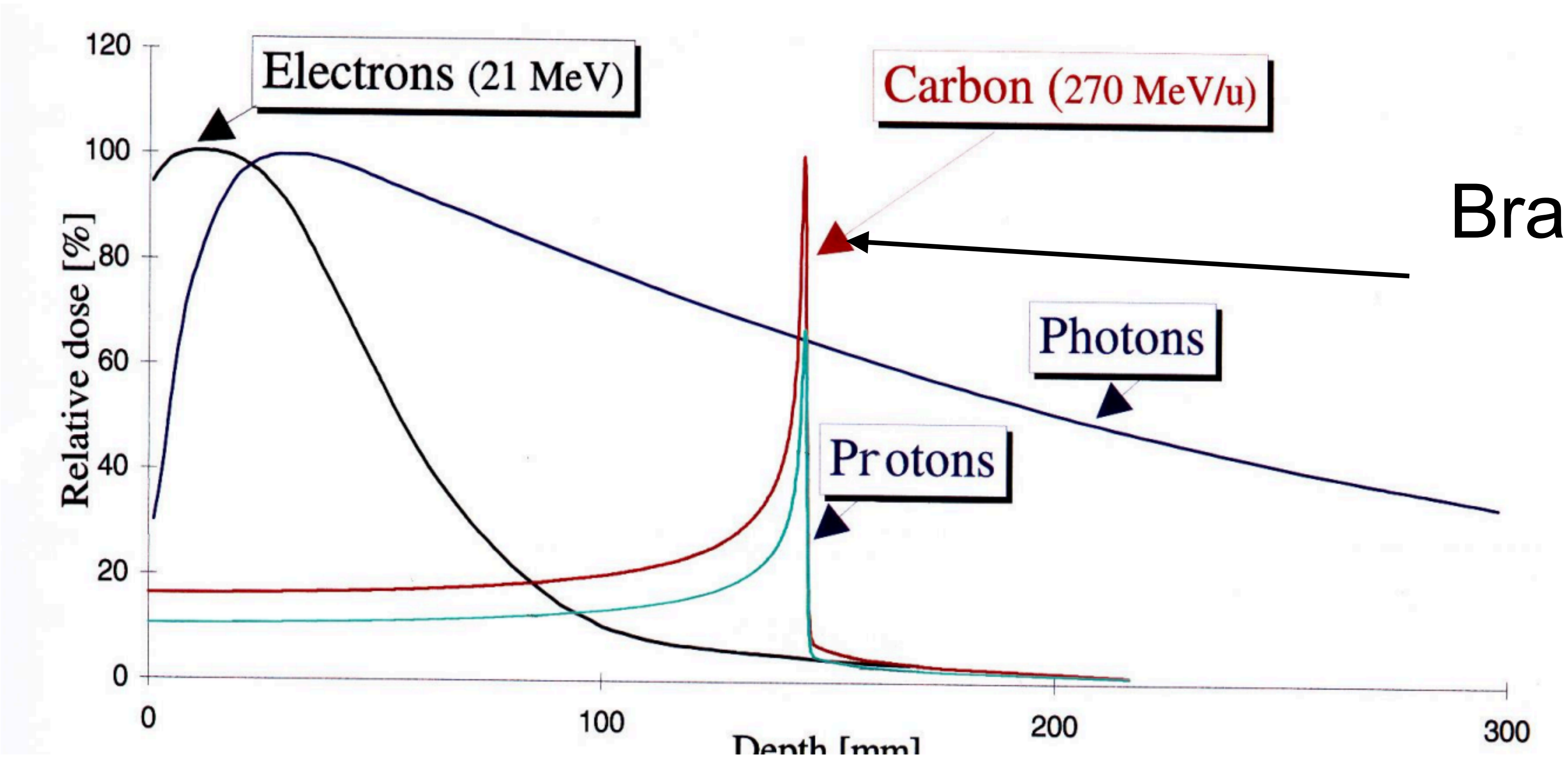
Classical Radiotherapy with X-rays

single beam



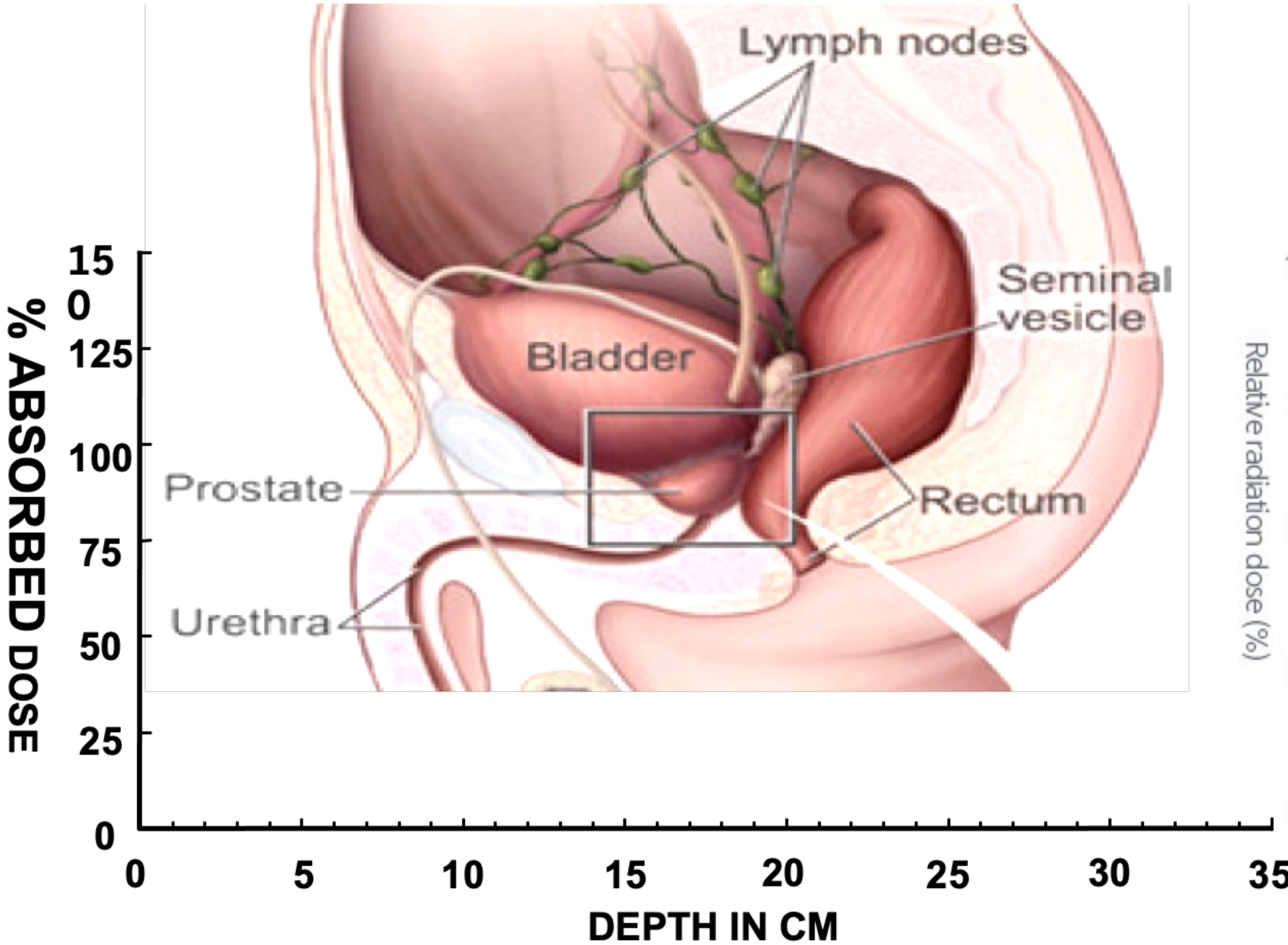
Hadron Therapy

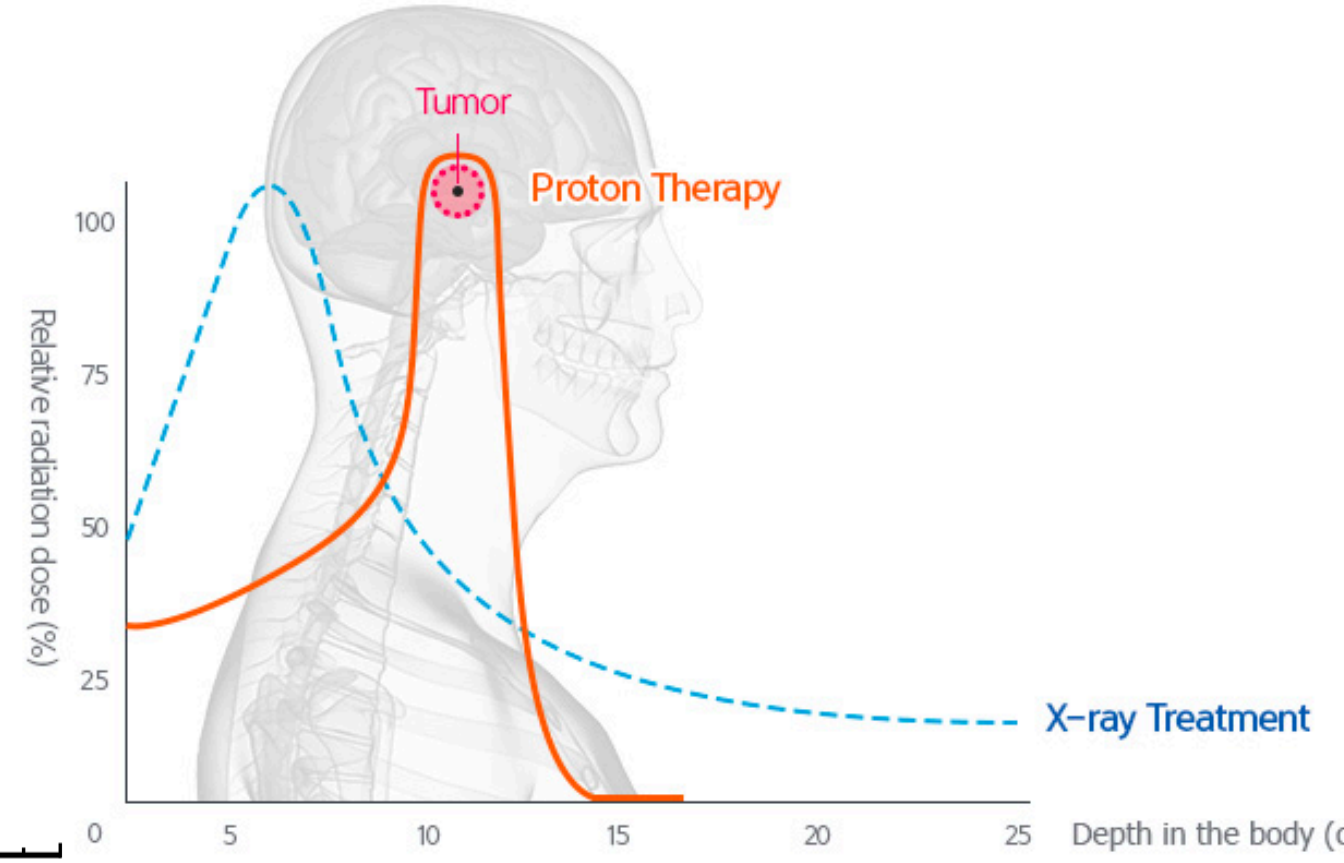
- Therapy
    - Hadrons allow you to control deposit
    - Can vary the depth of the hadrons through Bragg scatter



Bragg Scatter Peak

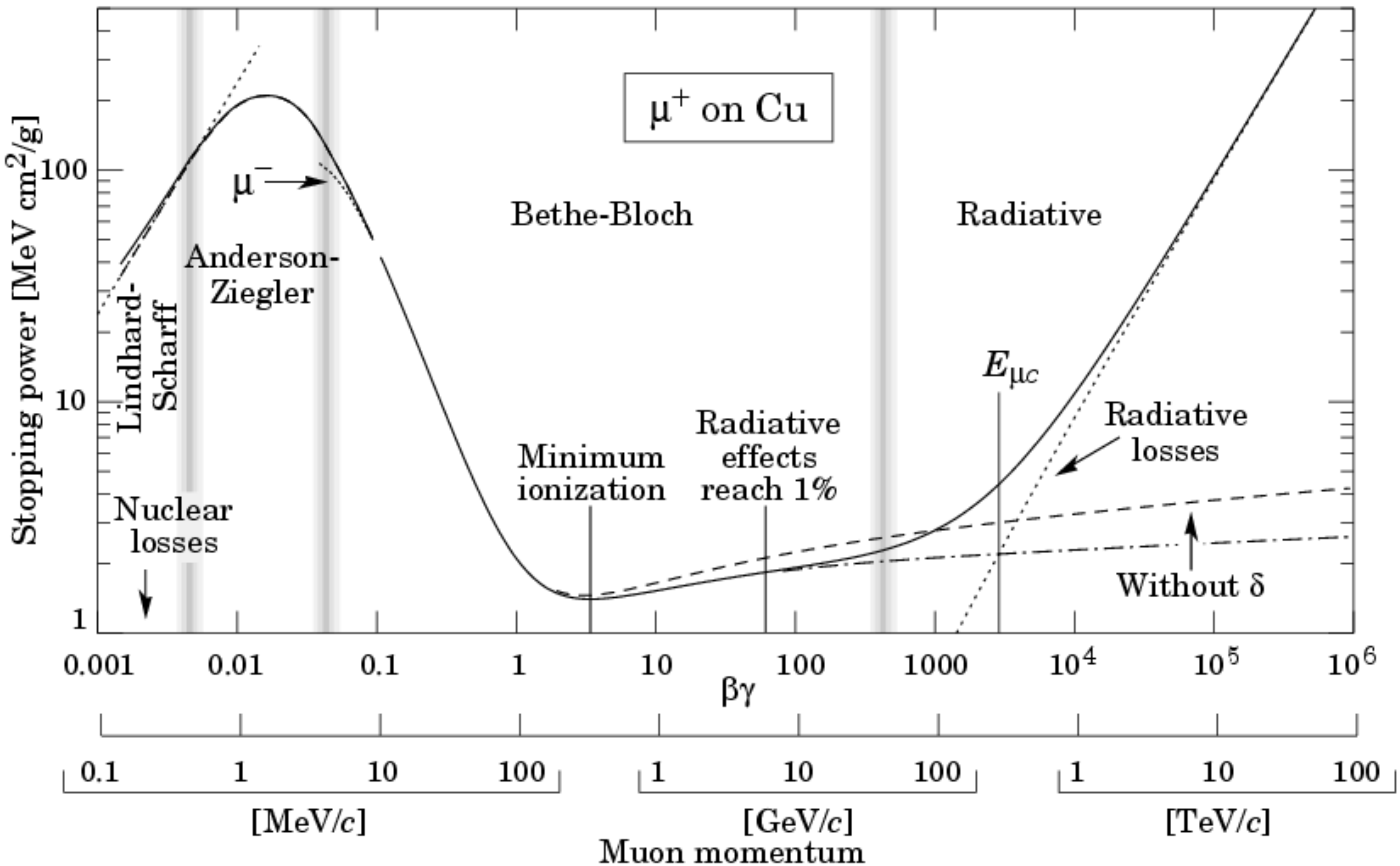
Proton Therapy





Bethe-Bloch Equation

- Charged Particles in matter are goverened by this equation



Protons Governed

$$-\left\langle \frac{dE}{dx} \right\rangle = Kz^2 \frac{Z}{A} \frac{1}{\beta^2} \left[\frac{1}{2} \ln \frac{2 m_e c^2 \beta^2 \gamma^2 T_{\max}}{I^2} - \beta^2 - \frac{\delta(\beta\gamma)}{2} \right] \quad [\cdot \rho]$$

density

$K = 4\pi N_A r_e^2 m_e c^2 = 0.307\ \mathrm{MeV\ g^{-1}\ cm^2}$

$T_{max} = 2 m_e c^2 \beta^2 \gamma^2 / (1 + 2\gamma\, m_e/M + (m_e/M)^2)$

[Max. energy transfer in single collision]

z : Charge of incident particle
M : Mass of incident particle

Z : Charge number of medium
A : Atomic mass of medium

I : Mean excitation energy of medium
δ : Density correction [transv. extension of electric field]

$N_A = 6.022 \cdot 10^{23}$
[Avogardo's number]

$r_e = e^2/4\pi\varepsilon_0 m_e c^2 = 2.8$ fm
[Classical electron radius]

$m_e = 511$ keV
[Electron mass]

$\beta = v/c$
[Velocity]

$\gamma = (1-\beta^2)^{-2}$
[Lorentz factor]

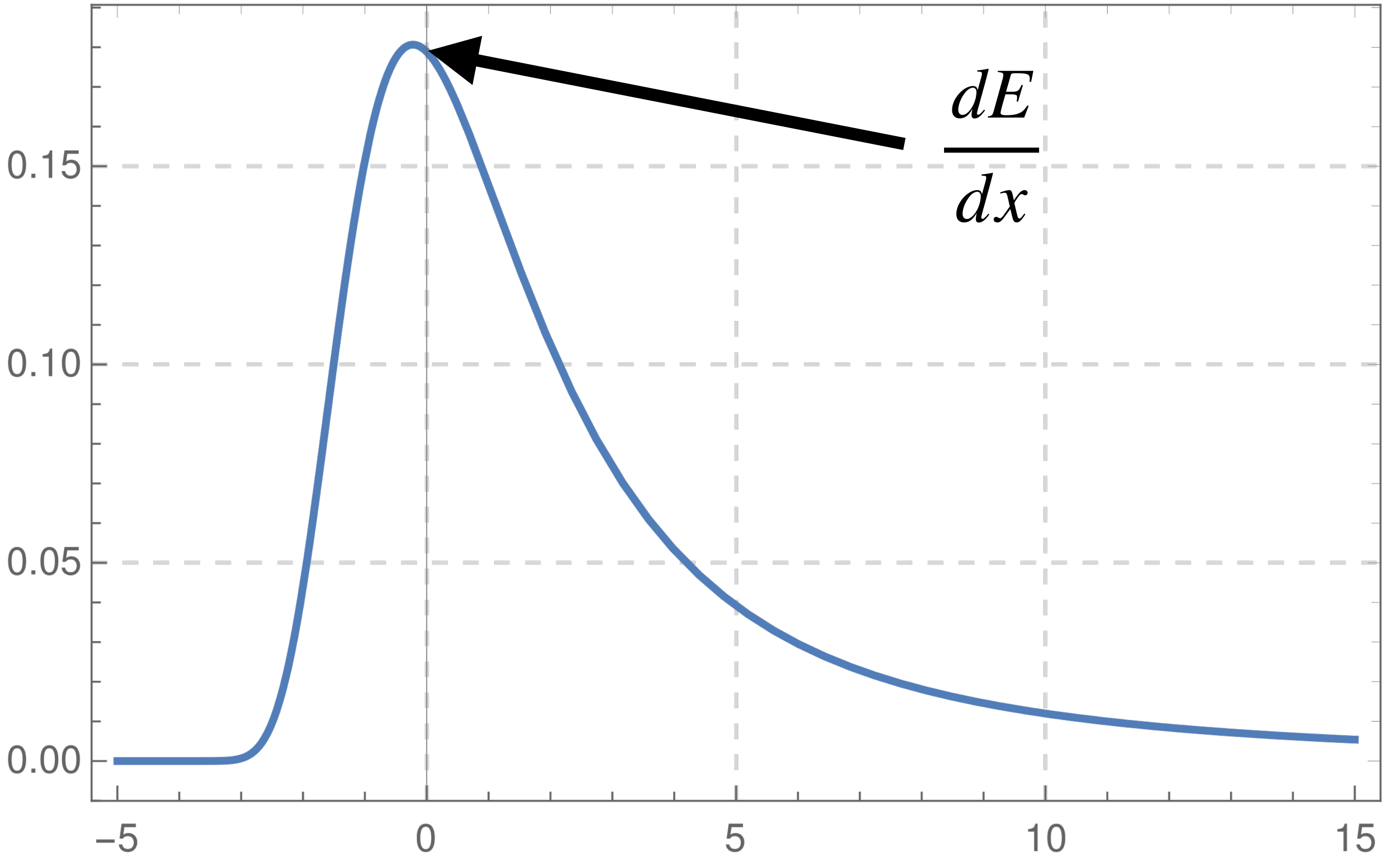
Validity:

$.05 < \beta\gamma < 500$
$M > m_\mu$

Actual Energy Loss

- As we step along we lose energy by the Landau distribution

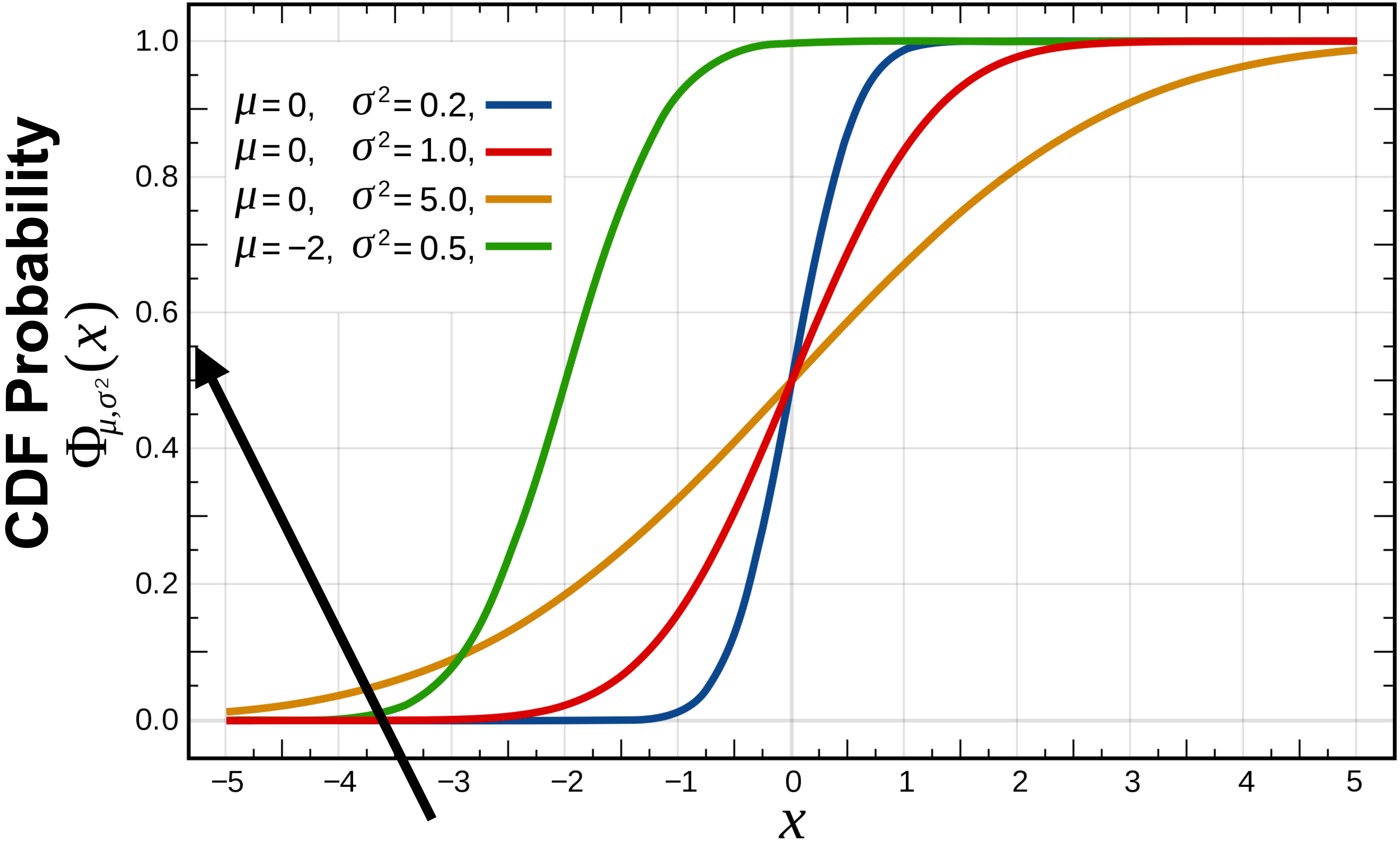
$$p(x) = \frac{1}{2\pi i} \int_{a-i\infty}^{a+i\infty} e^{s\log(s)+xs}\, ds,$$



Average of this distribution gives Bethe-Bloch

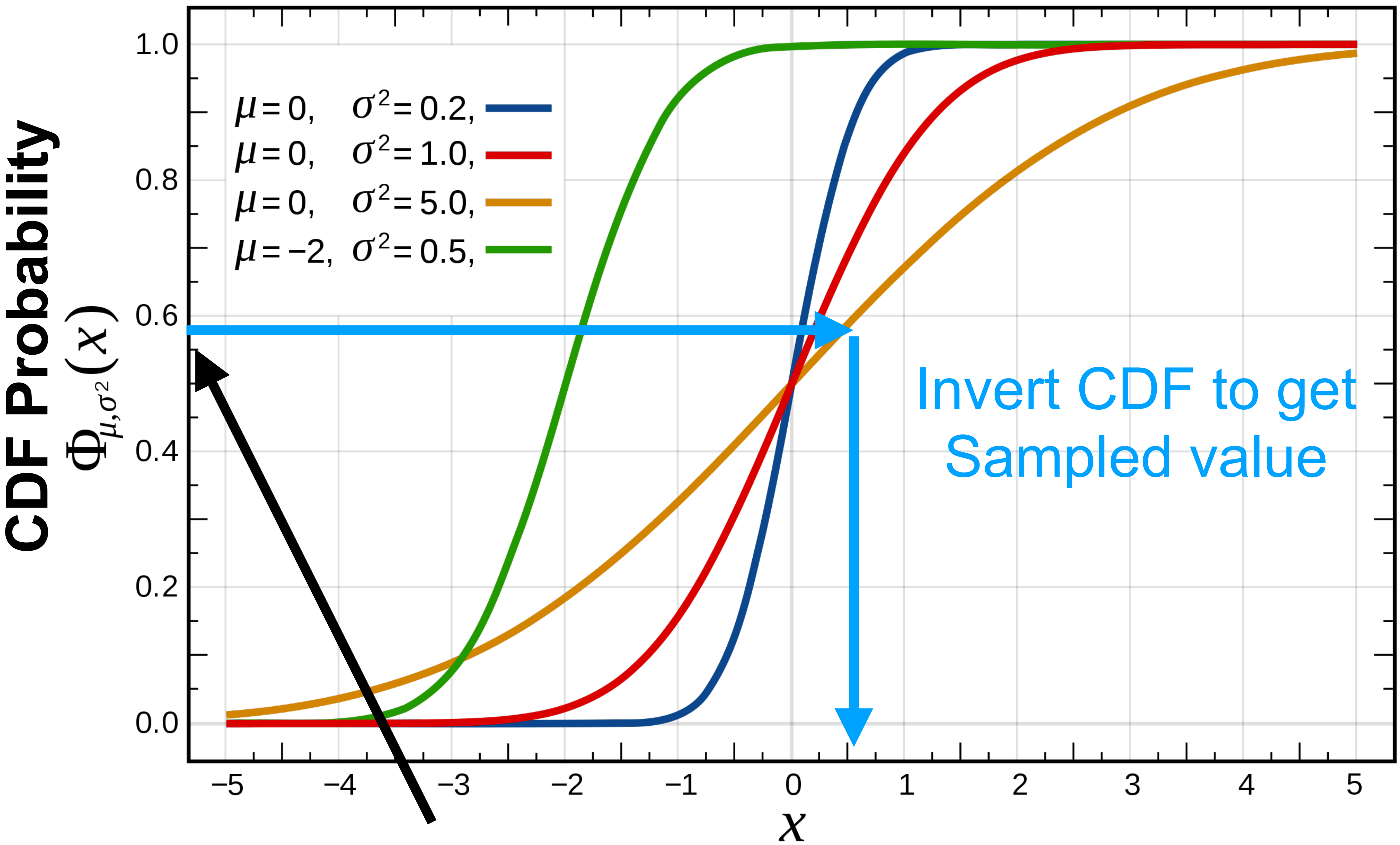
We can sample this At each step

Sampling a Distribution



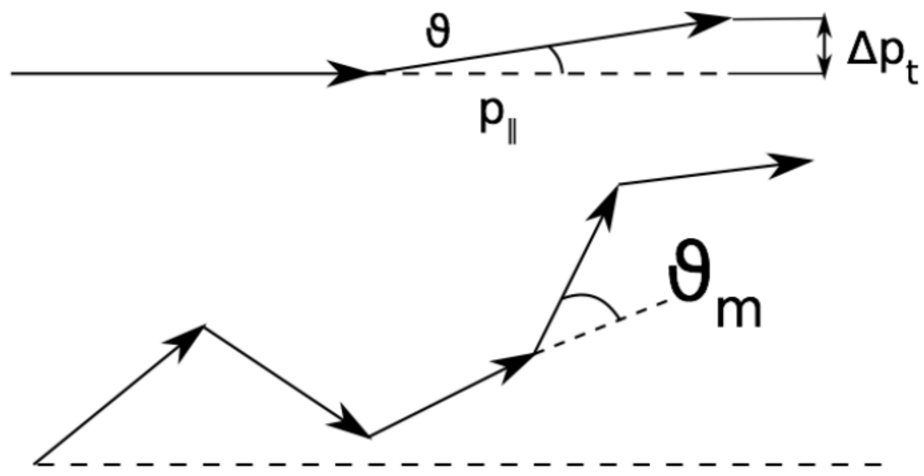
Sample from a p-value from 0 to 1 (flat 0 to 1)

Sampling a Distribution



Sample from a p-value from 0 to 1 (flat 0 to 1)

Multiple Scatter Particles



$$\theta \simeq \frac{\Delta p_\perp}{p_{||}} \simeq \frac{\Delta p_\perp}{p} = \frac{2Zze^2}{b}\frac{1}{pv}$$

after k collisions

$$\langle \theta_k^2 \rangle = \sum_{m=1}^{k} \theta_m^2 = k\langle \theta^2 \rangle$$

- Single collision (thin absorber): Rutherford scattering $d\sigma/d\Omega \propto \sin^{-4}\theta/2$
- Few collisions: difficult problem
- Many (>20) collisions: statistical treatment “Molière theory”

Multiple Scatter Particles

$$\theta \simeq \frac{\Delta p_\perp}{} \simeq \frac{\Delta p_\perp}{}$$

Obtain the mean deflection angle in a plane by averaging over many collisions and integrating over b:

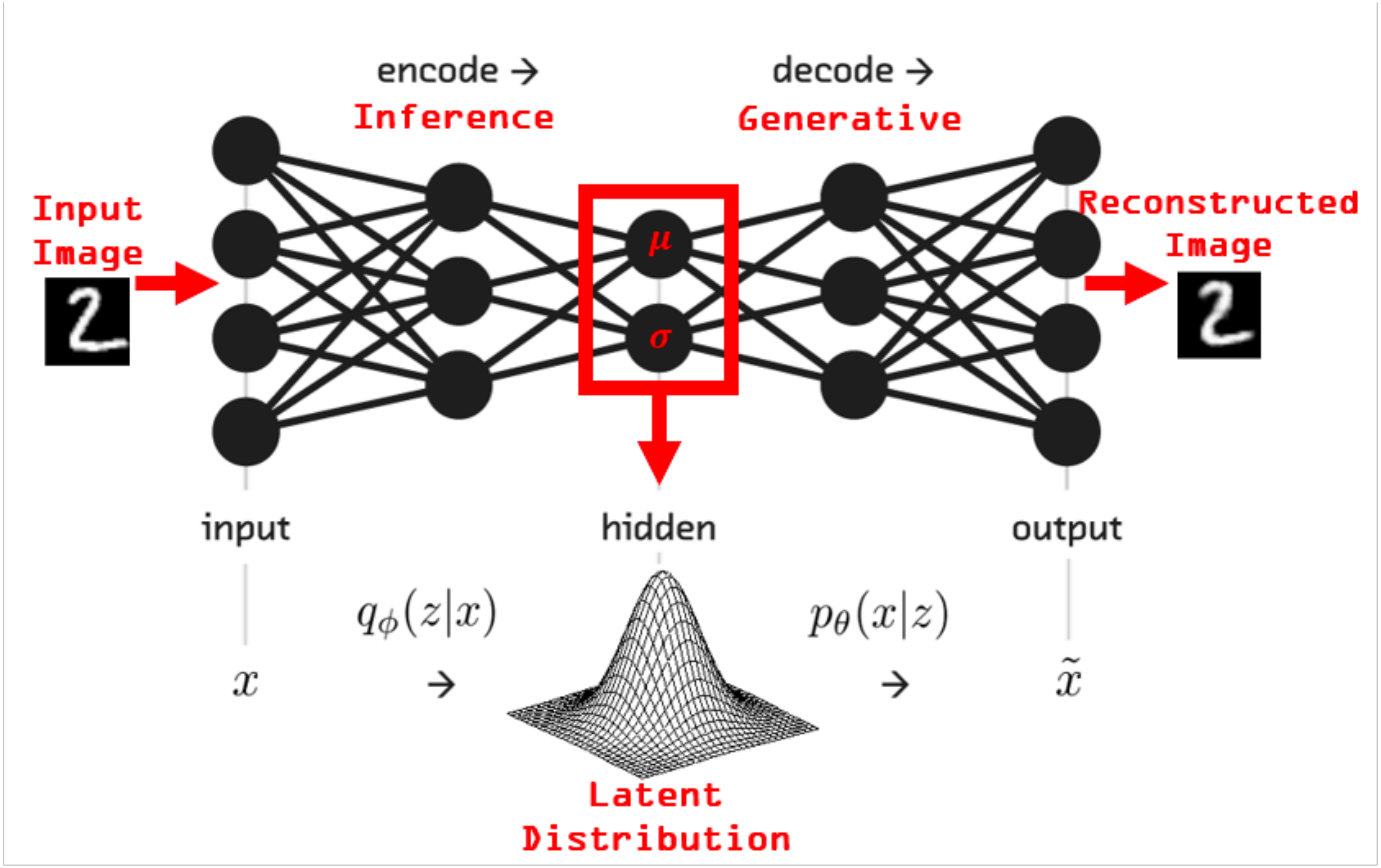
$$\sqrt{\langle \theta^2(x) \rangle} = \theta_{\text{rms}}^{\text{plane}} = \frac{13.6 \text{ MeV}}{\beta p c} z \sqrt{\frac{x}{X_0}} \left(1 + 0.038 \ln \frac{x}{X_0}\right)$$

- Material constant X_0: radiation length
- $\propto \sqrt{x} \rightarrow$ use thin detectors
- $\propto 1/\sqrt{X_0} \rightarrow$ use light detectors
- $\propto 1/\beta p \rightarrow$ serious problem at low momenta

In 3 dimensions: $\theta_{\text{rms}}^{\text{space}} = \sqrt{2}\, \theta_{\text{rms}}^{\text{plane}}$ $\quad 13.6 \rightarrow 19.2$

VAE

- Variational Autoencoder is a great way to model objects



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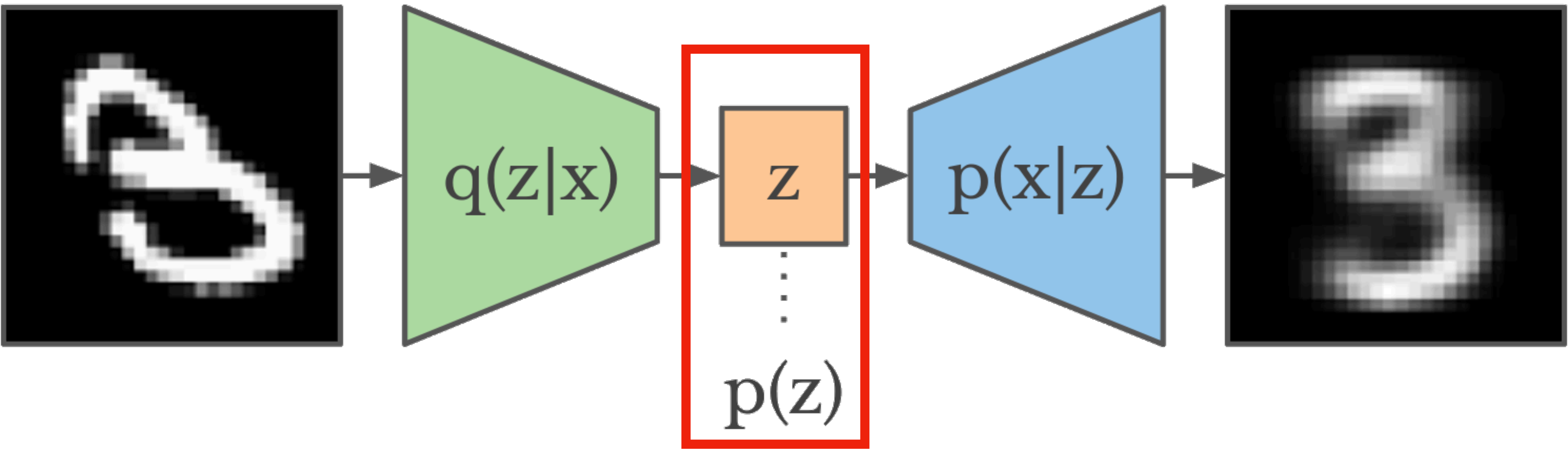
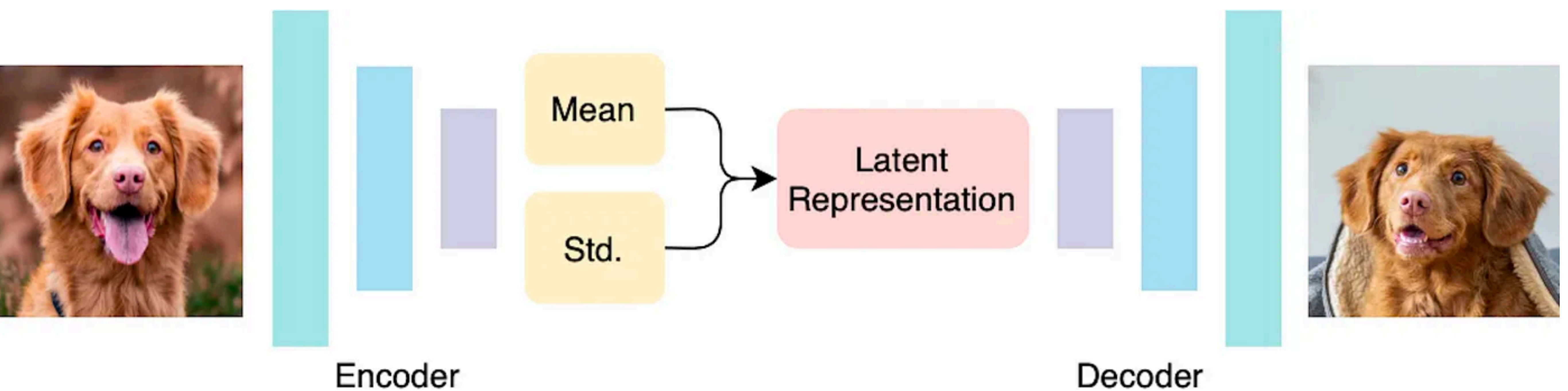
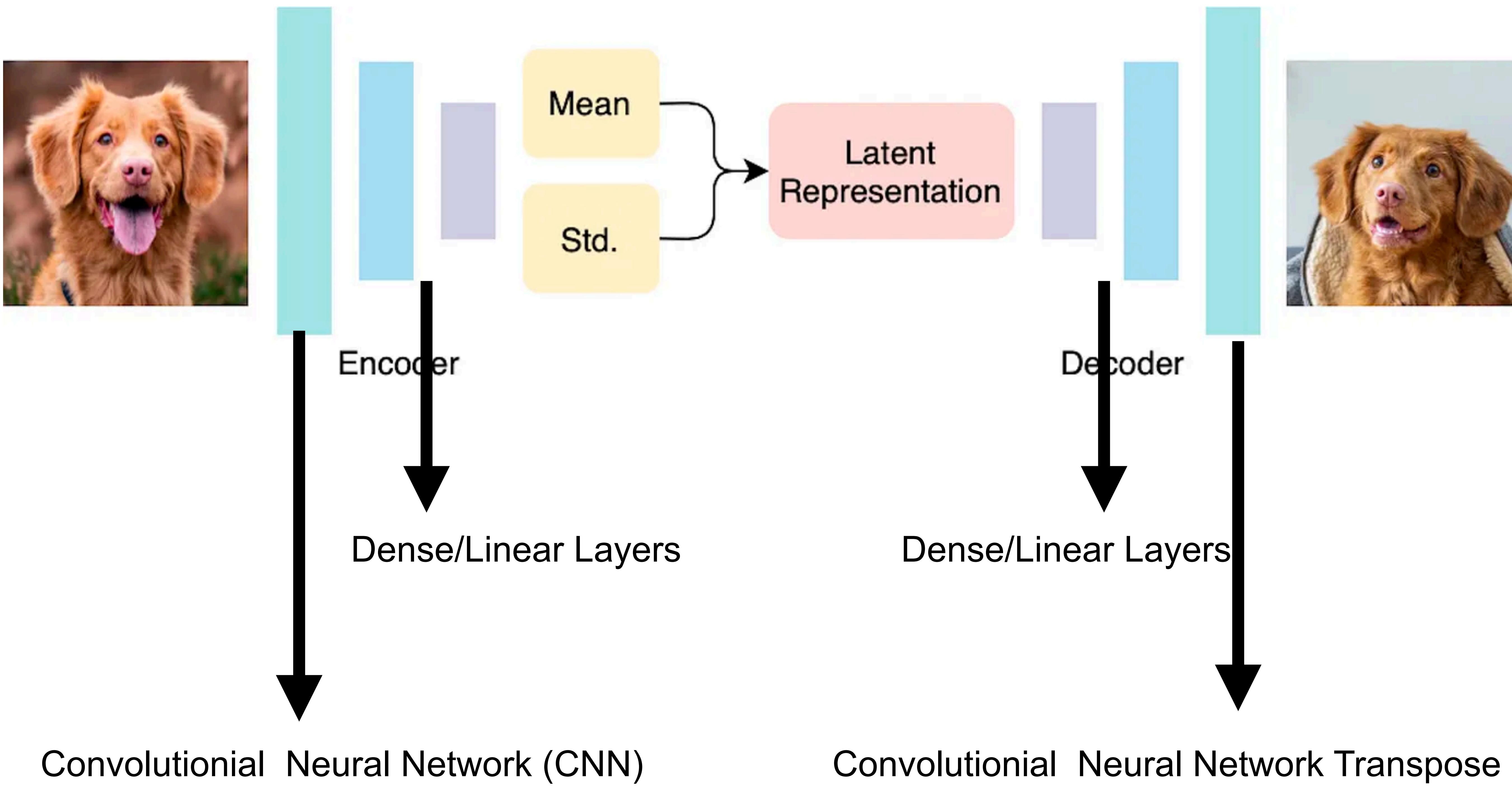


Randomly sample a normal distribution in this space

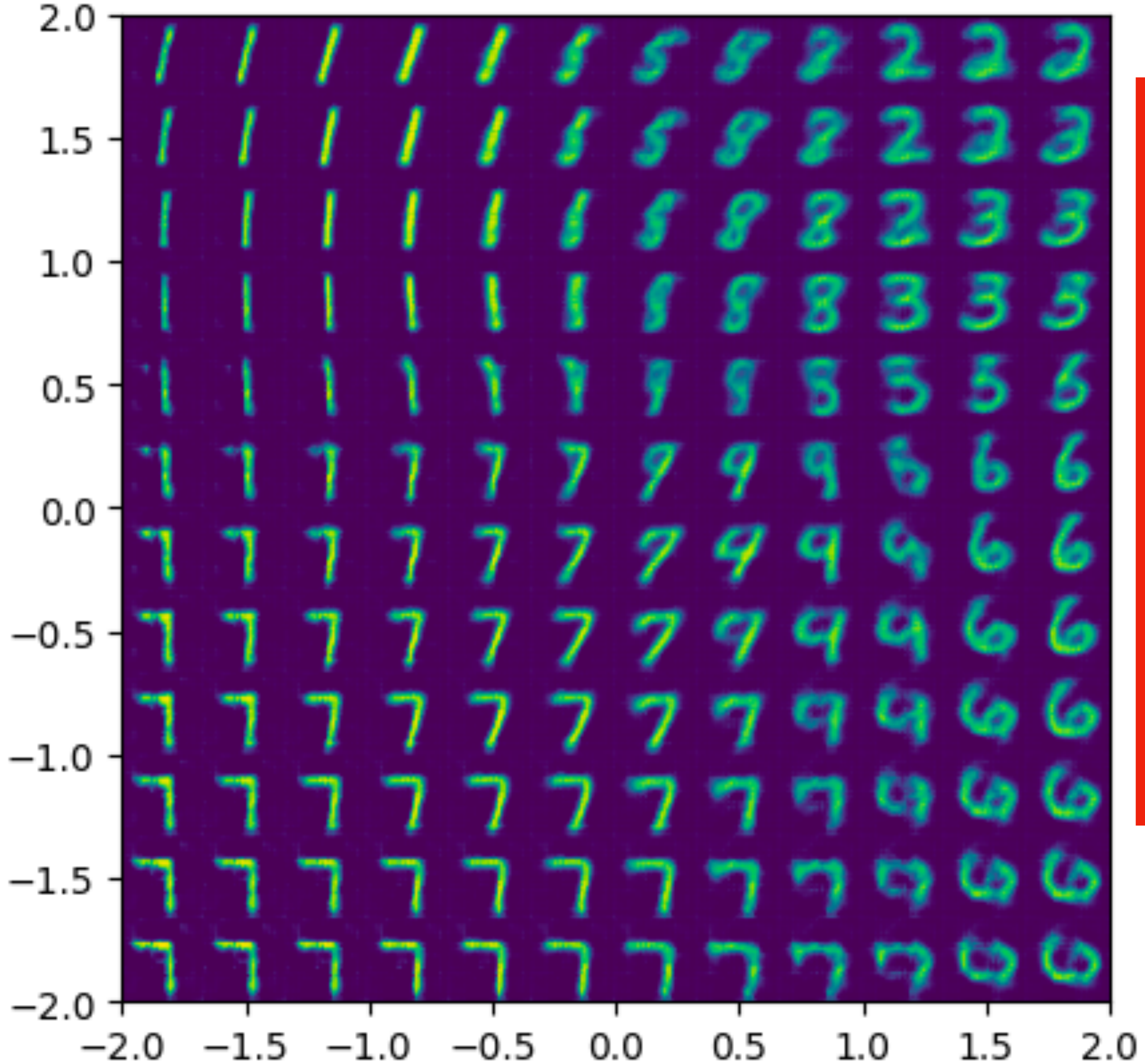


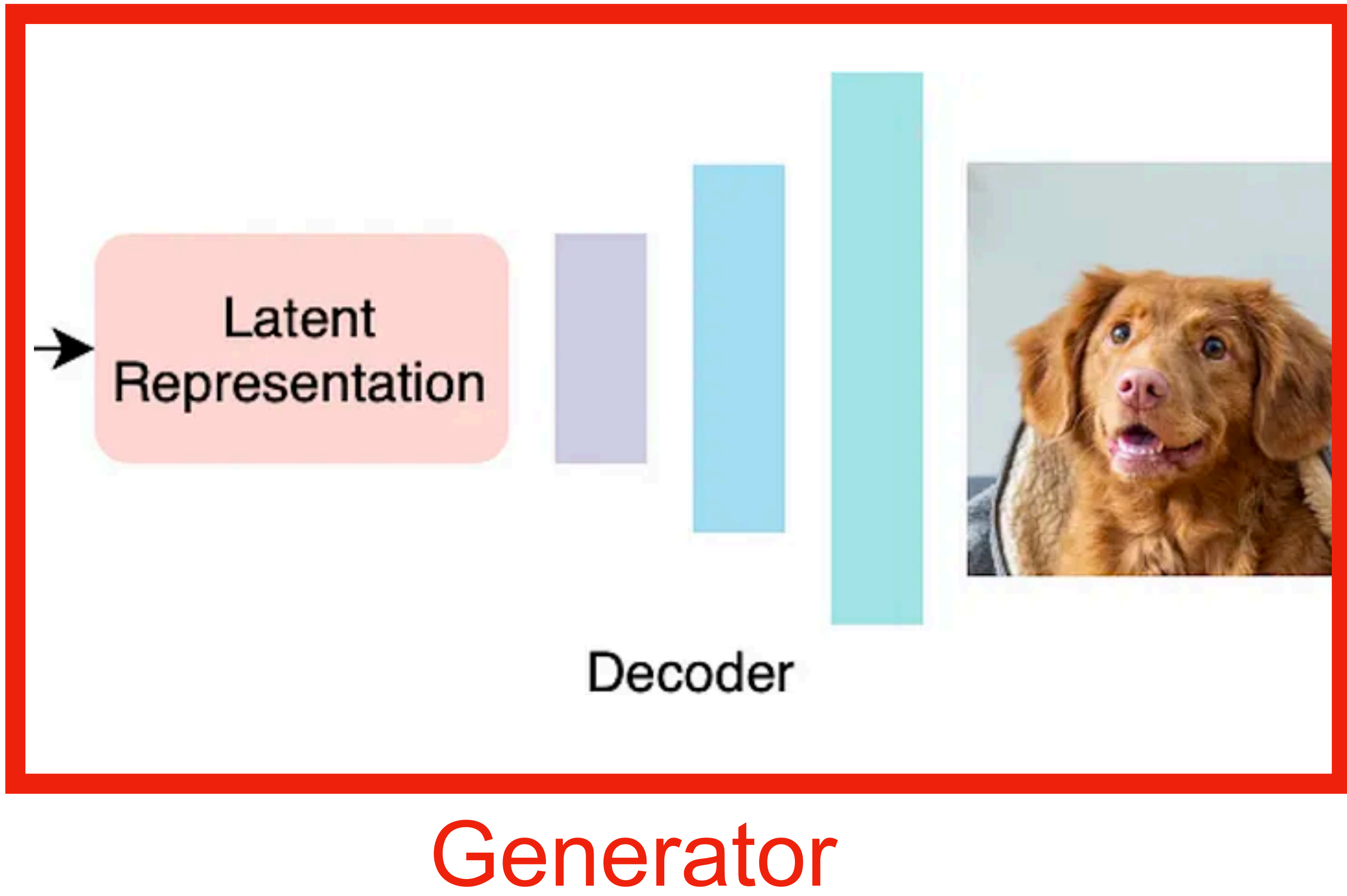
MNIST VAE encoder

- We will use a CNN to encode the data and process it



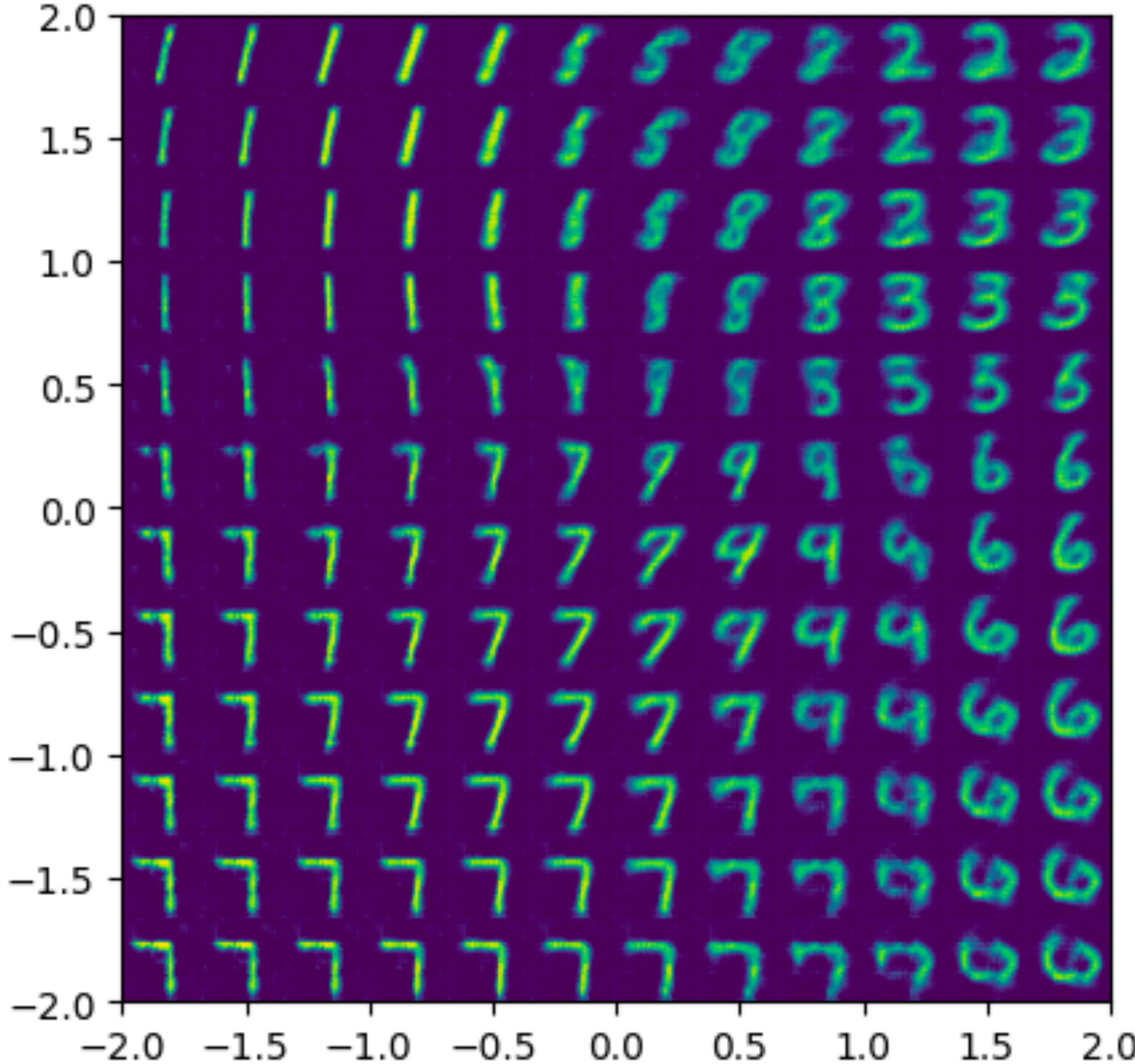
Exploring the latent space?

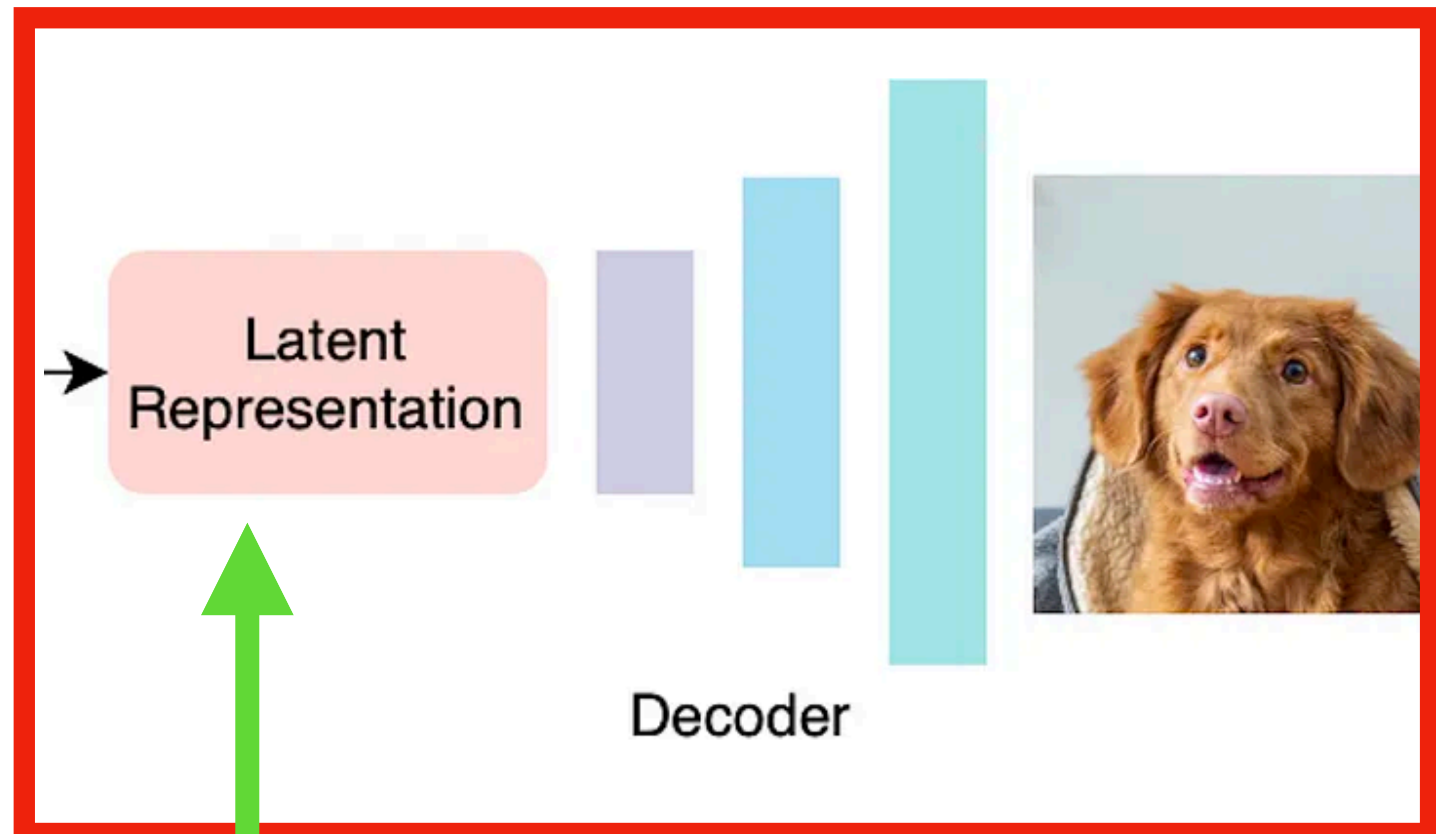




- We can sample the latent space as a generator

Conditional VAE





Generator

Variables that we would like to condition on

- Force known inputs into the VAE
  - That way our latent space has explicit knowledge of what is going on