Lecture 18:
Monte Carlo methods

Machine Learning Diffeq

- Recently within ML community :
  - The concept of Physics informed ML emerged

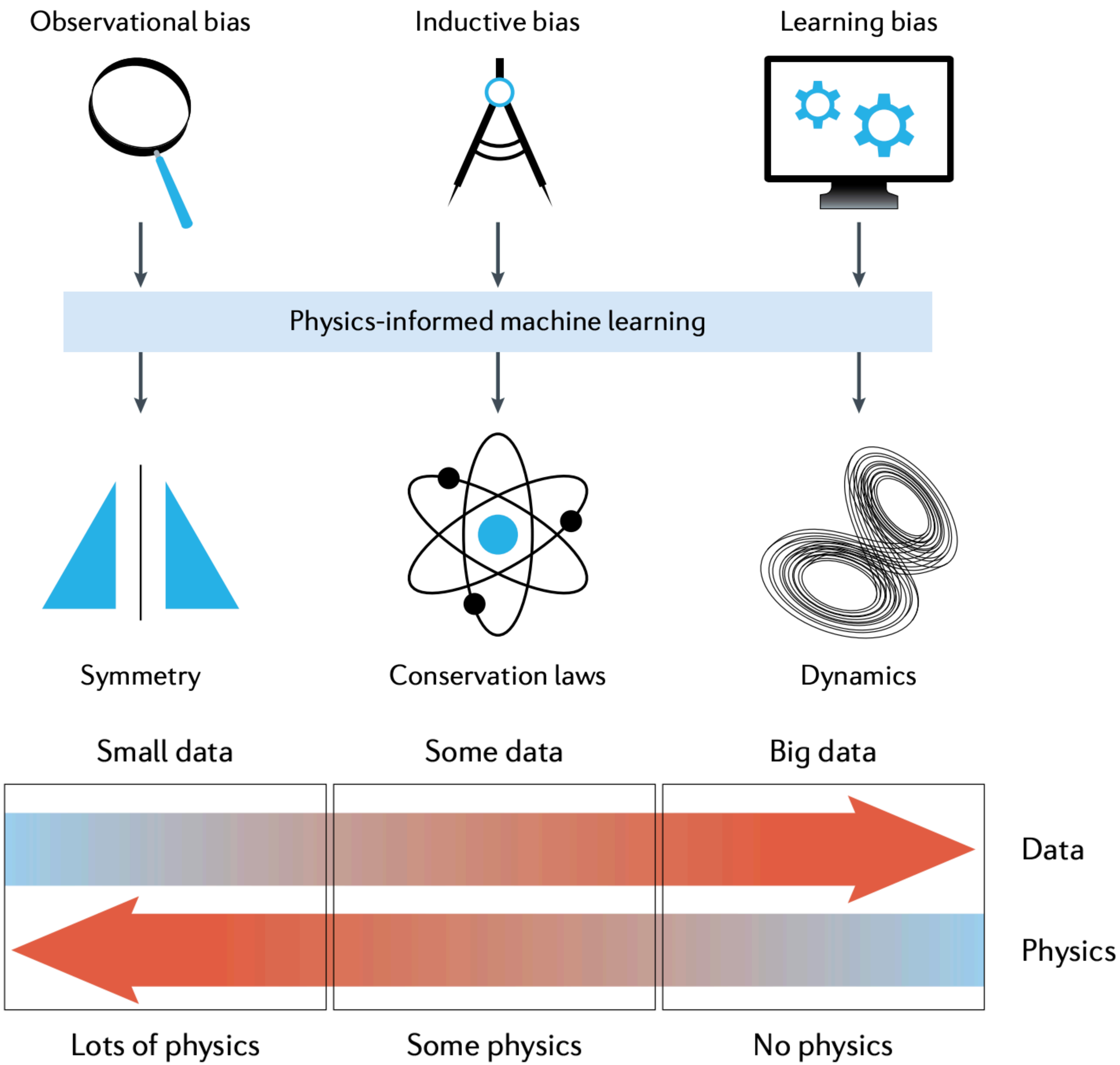
Strategy: $\mathscr{L}_{total} = \mathscr{L}_{NN} + \mathscr{L}_{\text{Diffeq}}$

$$\ddot{\theta} + \mu\dot{\theta} + k\theta = 0$$

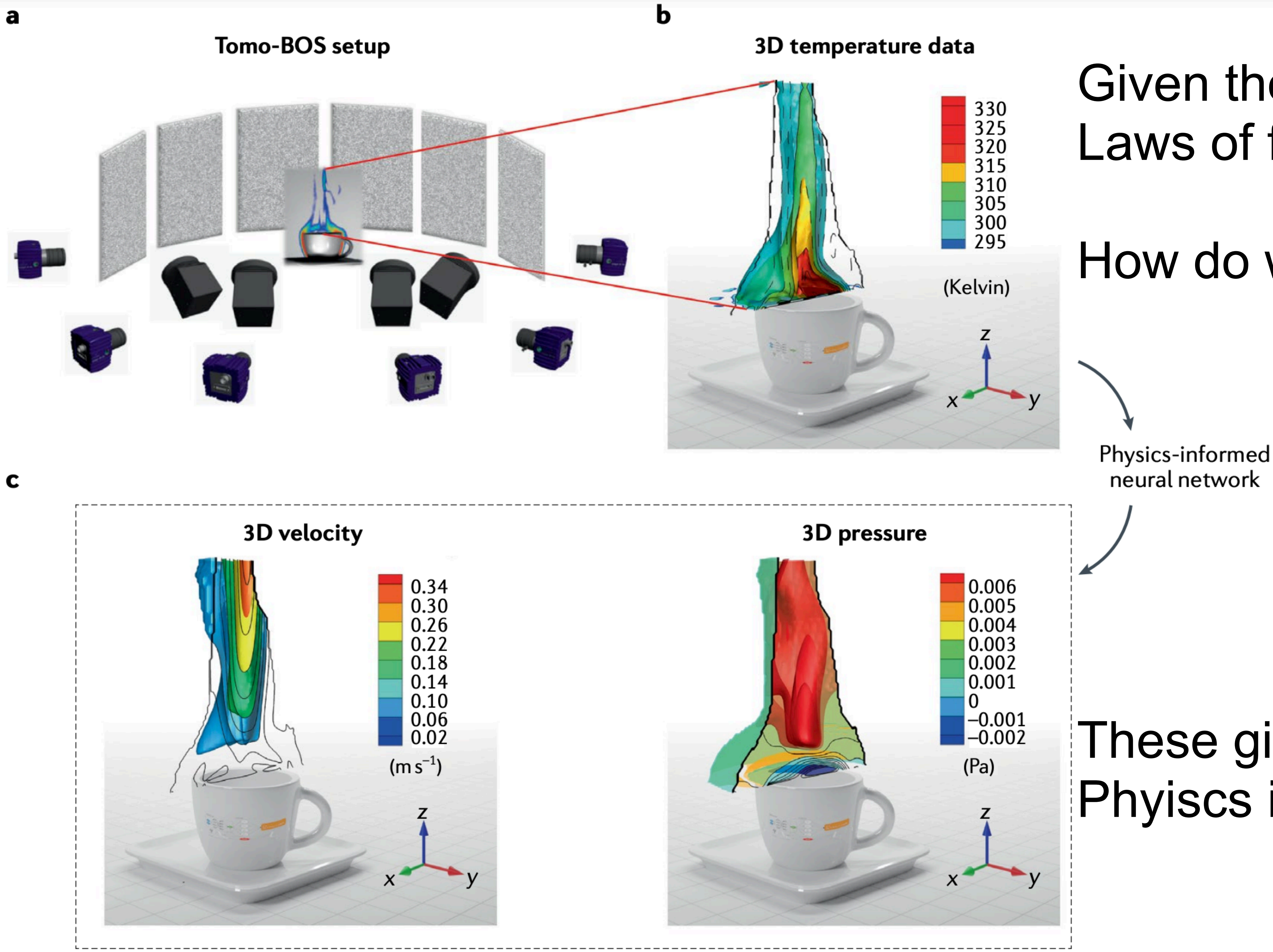
$$\boxed{\mathscr{L}_{\text{Diffeq}} = \left(\ddot{\theta} + \mu\dot{\theta} + k\theta\right)^2}$$

Constraint on Differential Equation
Aim to approximate learning

Physics Informed ML



Physics Informed ML

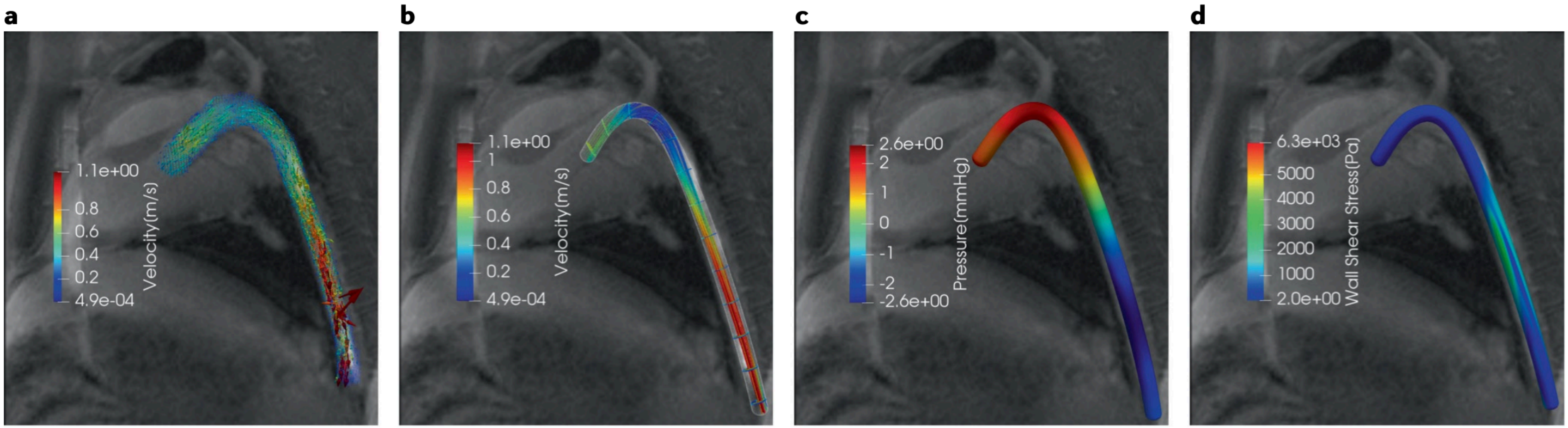


Given the
Laws of fluid flow

How do we model flow

These give us
Phyiscs informed ML

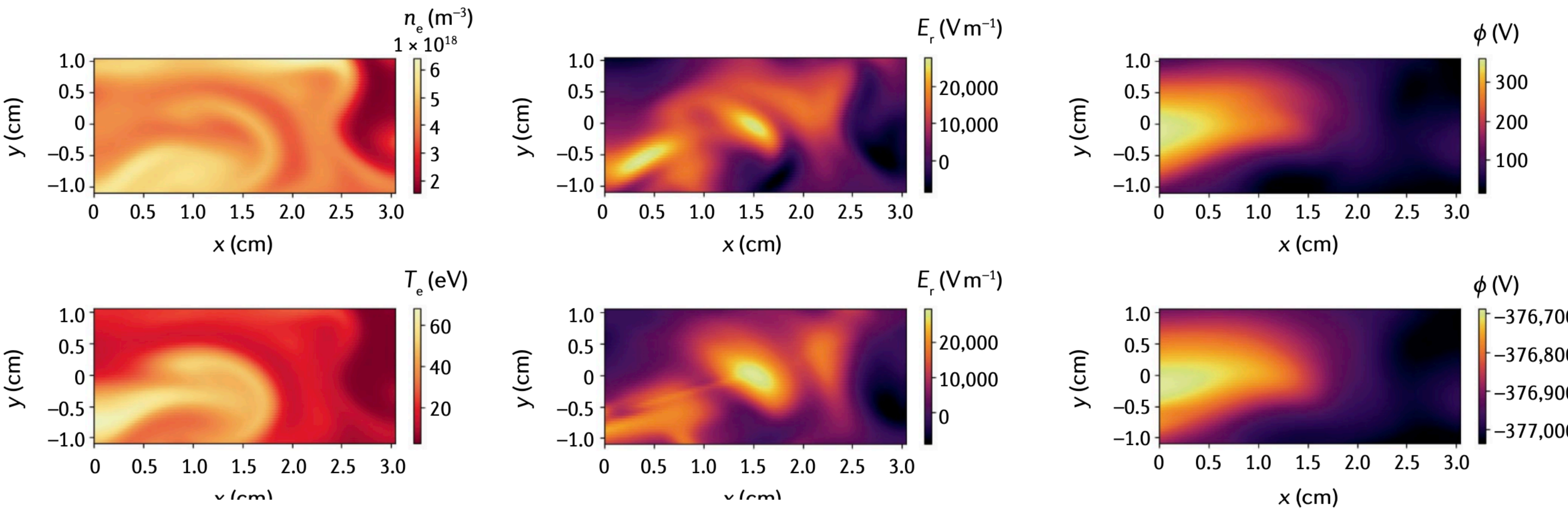
Physics Informed ML

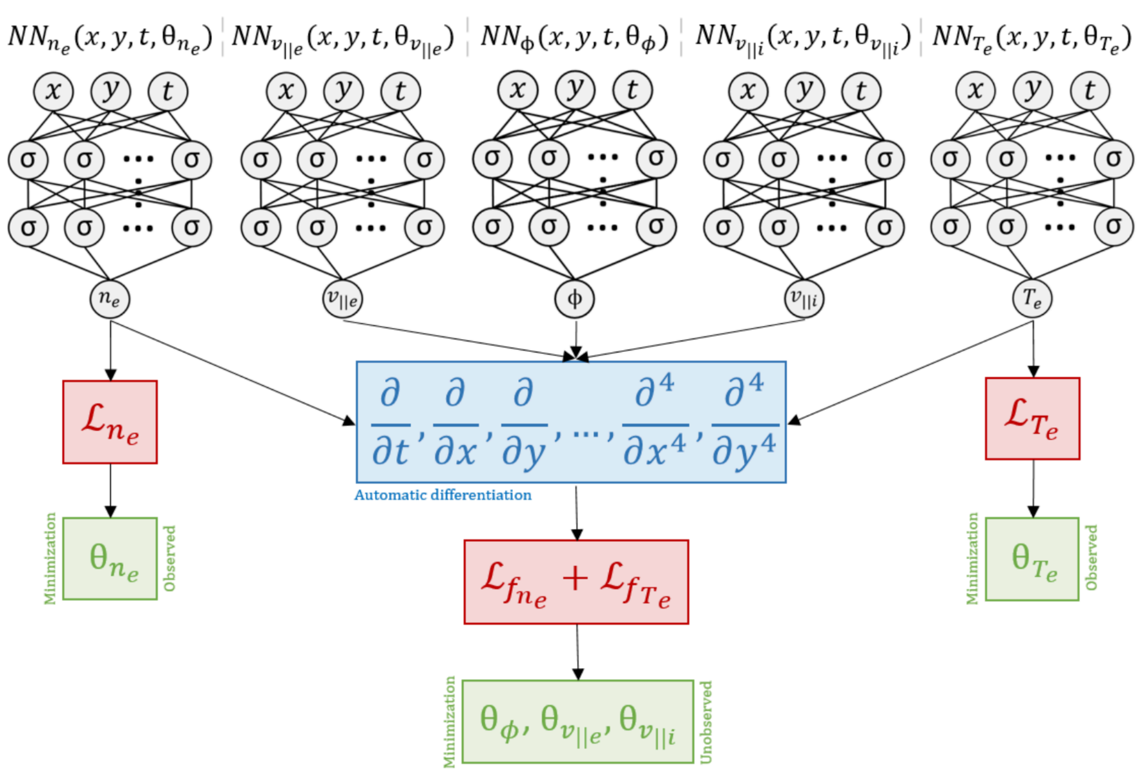


Navier Stokes equation to extrapolate blood flow in system

Navier Stokes equation to extrapolate blood flow in system

Physics Informed ML



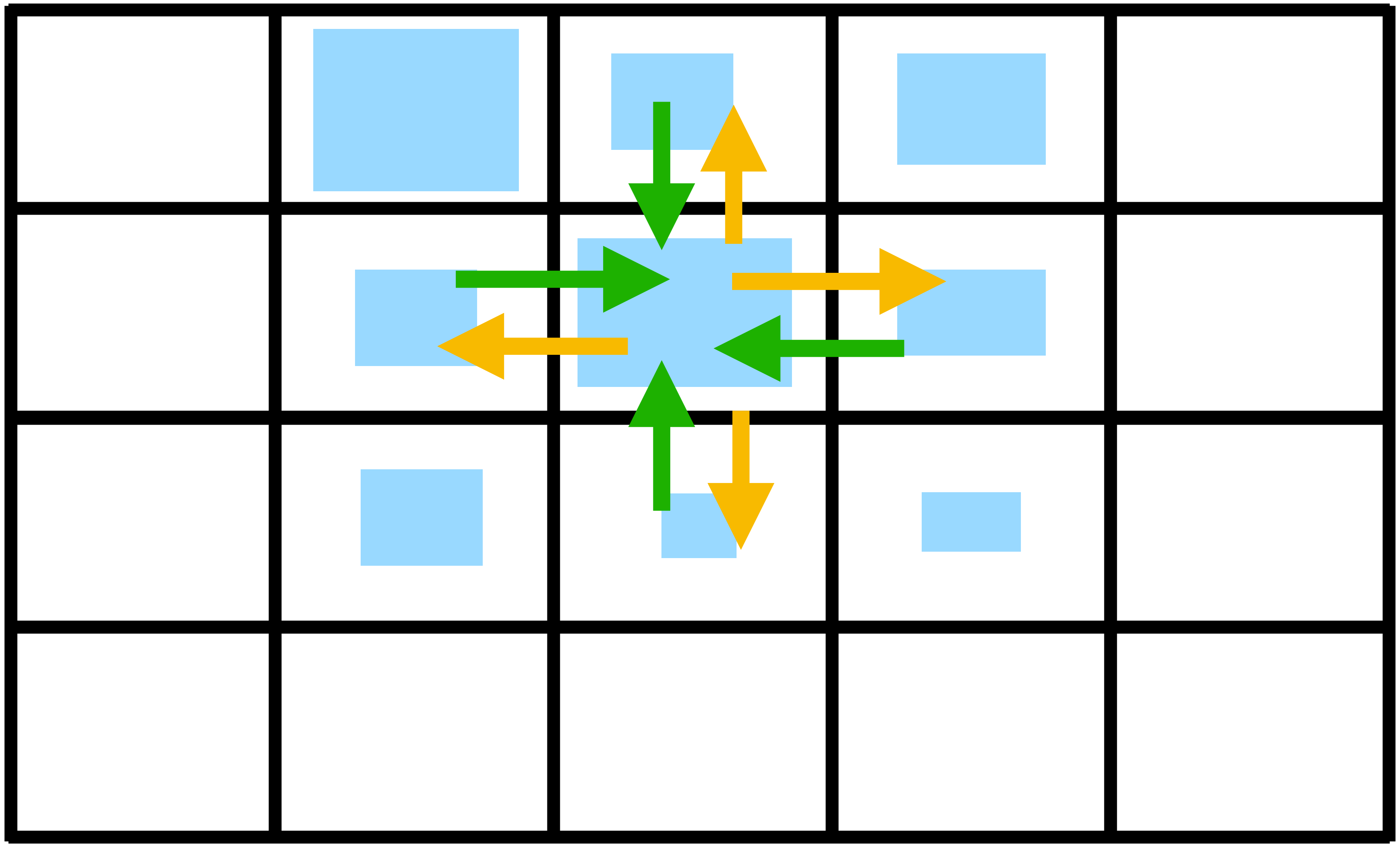


$$\mathcal{L}_{n_e} = \frac{1}{N_0} \sum_{i=1}^{N_0} |n_e^*(x_0^i, y_0^i, z_0^i, t_0^i) - n_{e,0}^i|^2,$$

$$\mathcal{L}_{T_e} = \frac{1}{N_0} \sum_{i=1}^{N_0} |T_e^*(x_0^i, y_0^i, z_0^i, t_0^i) - T_{e,0}^i|^2,$$

Hydrodynamics

- Hydrodynamics we want to consider motion along a grid
- Each grid has a density
  - We consider motion in and out of specific grid



For Galactic Matter

- Unlike Dark matter, standard model interacts with each other
- Need to consider particle interactions in addition to gravity
  - These are governed by fluid flow adding particle interactions
  - When simulating you do n-body dynamics
    - However you need to save density information of body
    - When bodies collide need to solve fluid flow dyanmics

Berger's Equation

- We will consider a few simple fluid equations:

- $\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = \nu\frac{\partial^2 u}{\partial x^2}$ (Burger's equation)

    - U is velocity and ν is the viscosity

Fluid Equations

- Inviscid Fluid flow is governed by the Euler Equations
  - Aka Navier-stokes with zero viscosity

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) = 0$$

CONTINUITY

$$\frac{\partial \rho u}{\partial t} + \nabla \cdot (\rho u \otimes u) + \nabla p = -\rho \nabla \phi$$

MOMENTUM

$$\frac{\partial \rho e}{\partial t} + \nabla \cdot \left[\rho u \left(e + p/\rho\right)\right] = -\rho u \cdot \nabla \phi$$

ENERGY

mass density

specific energy

fluid velocity

thermal pressure

acceleration

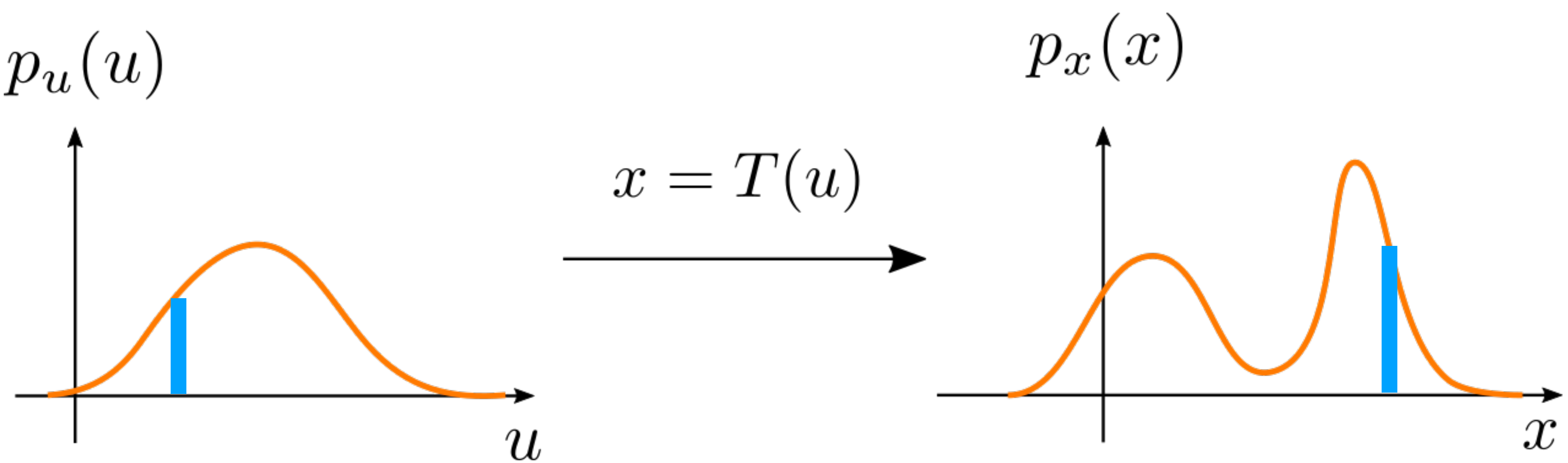
Monaco

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

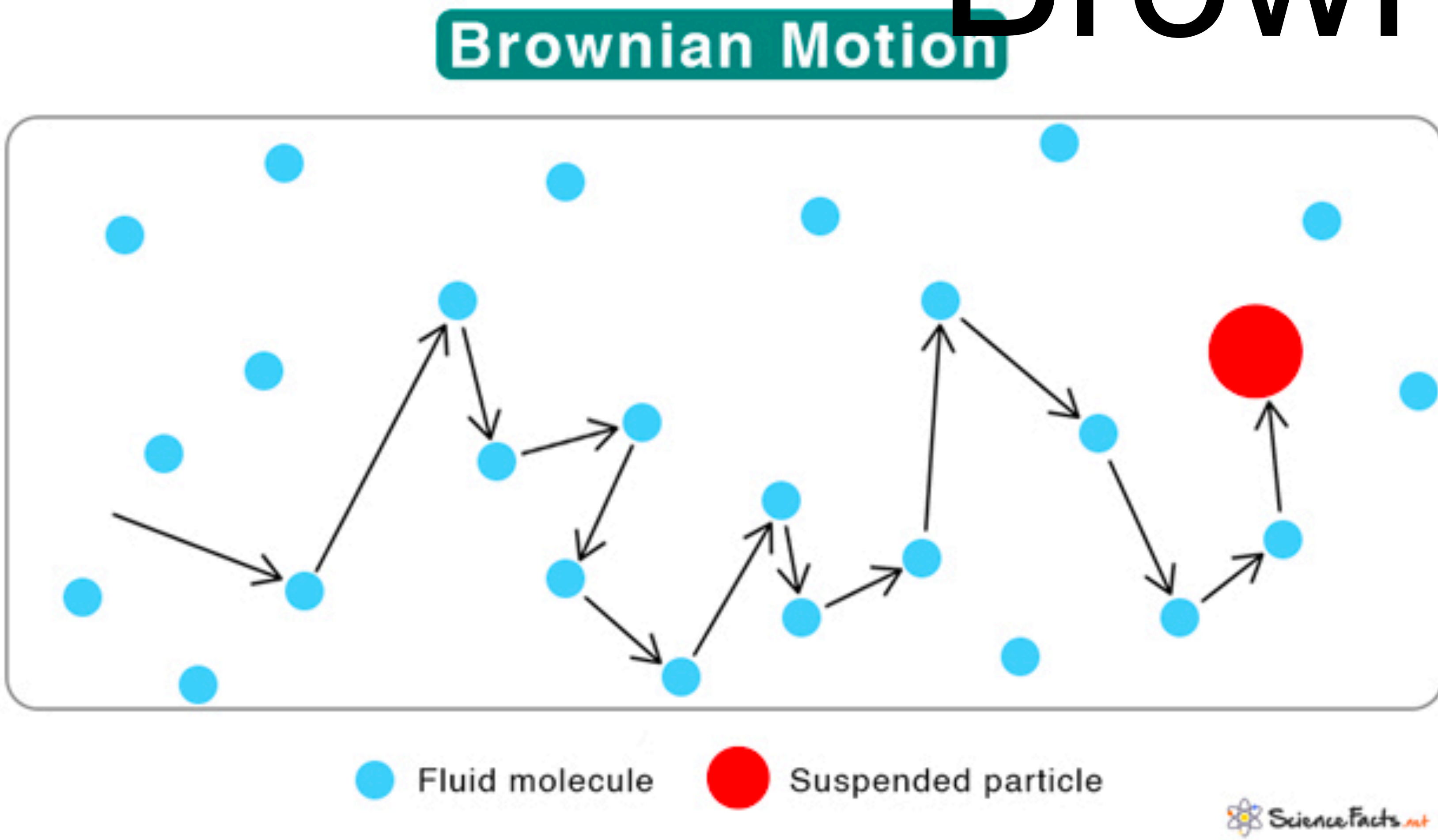
Monte Carlo vs Integration

- 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

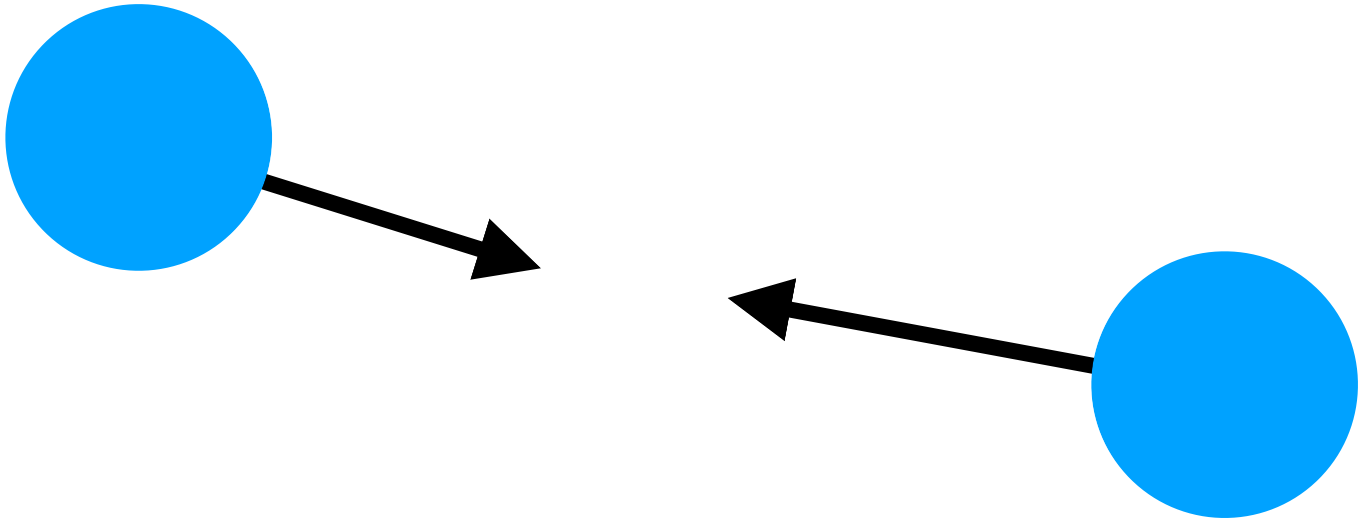


$$f(v_x, v_y, v_z) = \left[\frac{m}{2\pi kT}\right]^{3/2} e^{-m(v_x^2+v_y^2+v_z^2)/2kT}$$
$$= \left[\frac{m}{2\pi kT}\right]^{3/2} e^{-mv^2/2kT}$$

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

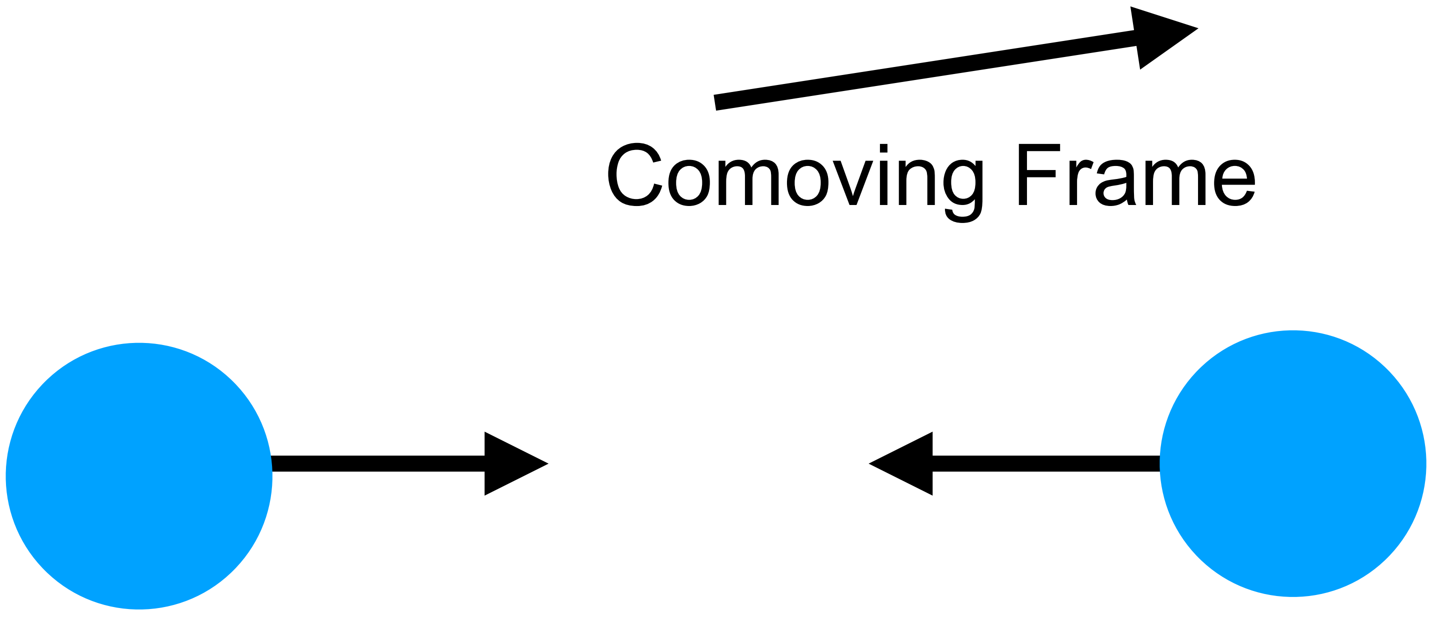
The motion at each step



Elastic Collision

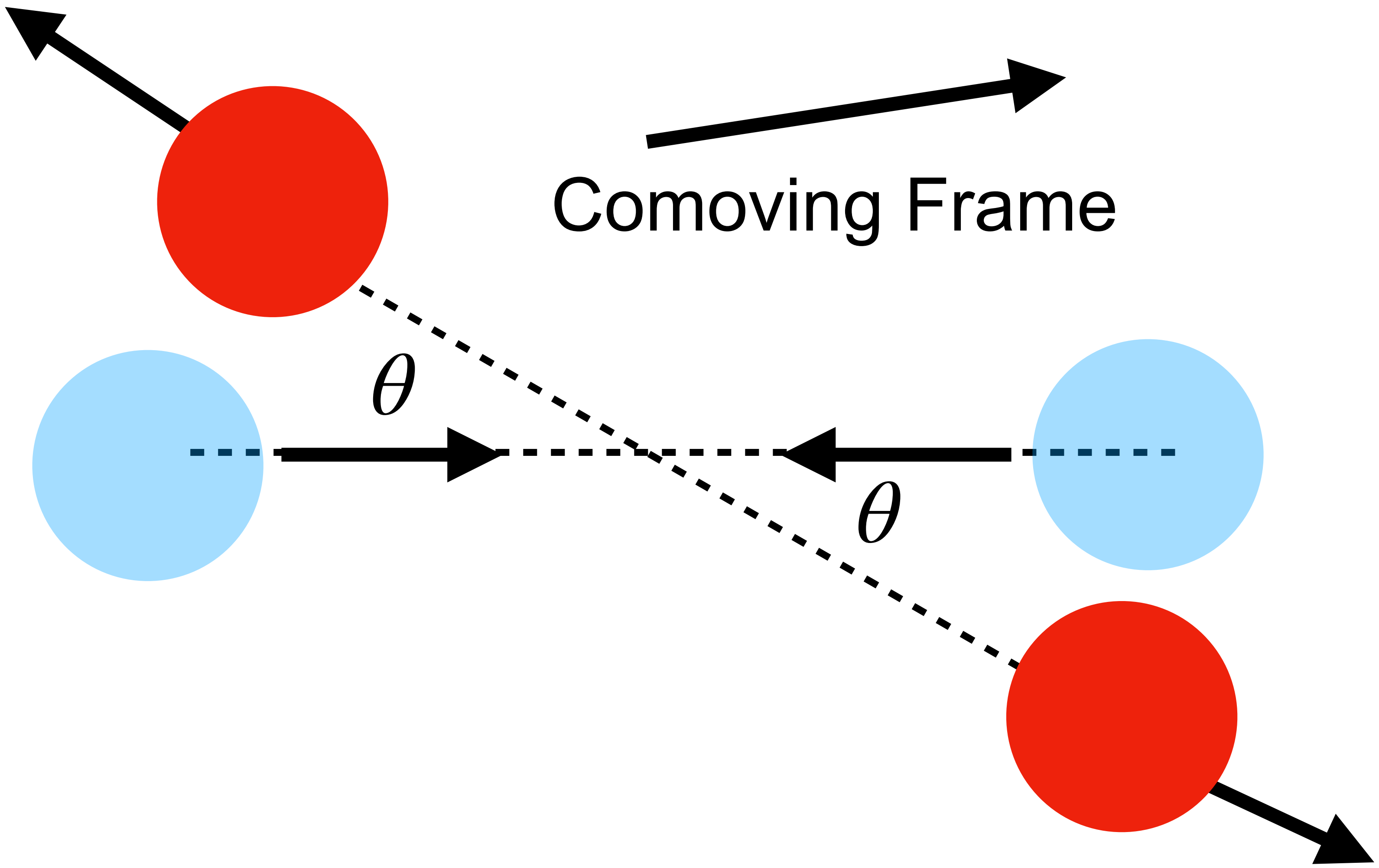
- Just sample particle collisions at each step

The motion at each step



Elastic Collision
In COM Frame

The motion at each step



Elastic Collision
In COM Frame

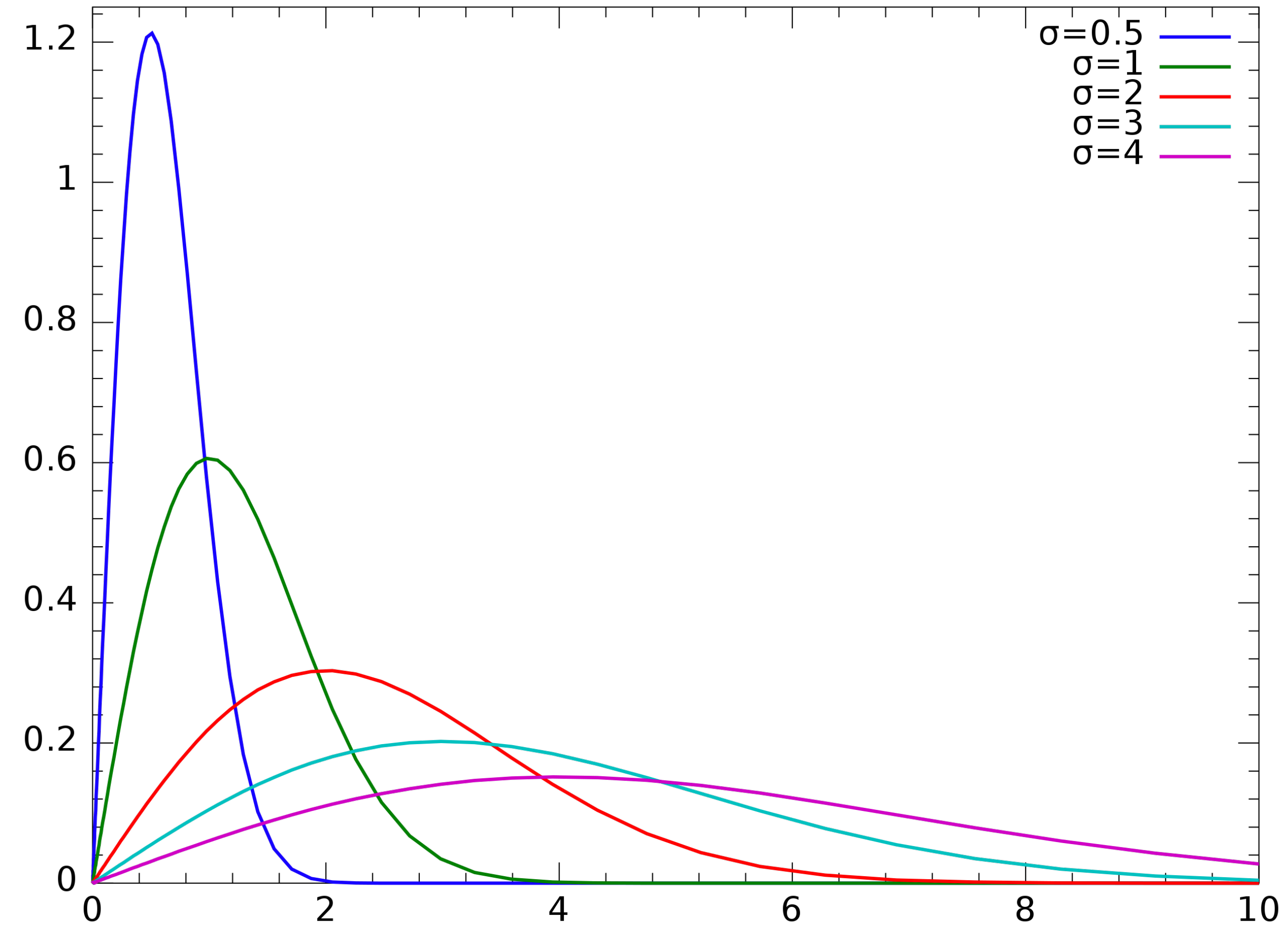
Rayleigh Distribution

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

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

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

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

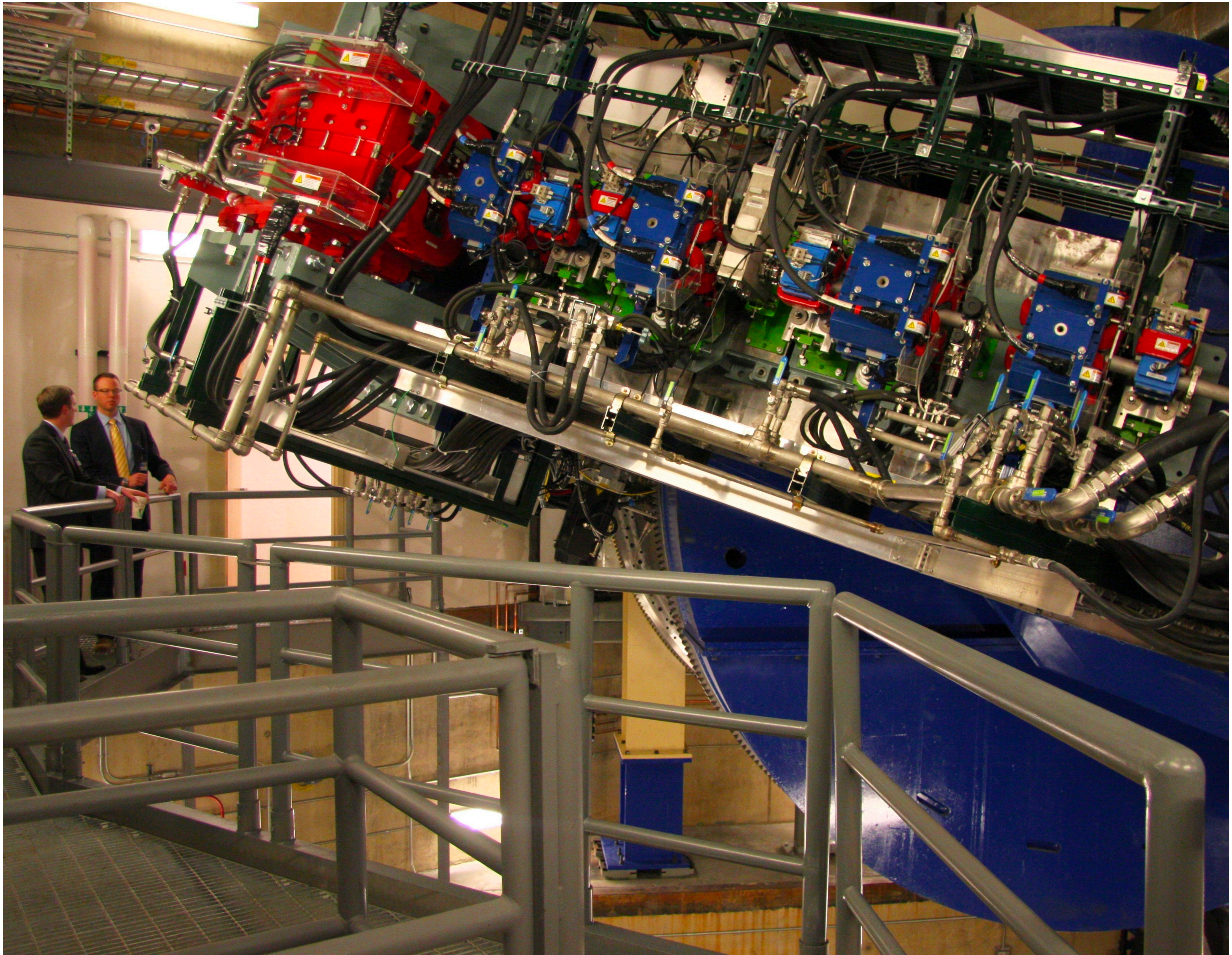


Proton Therapy

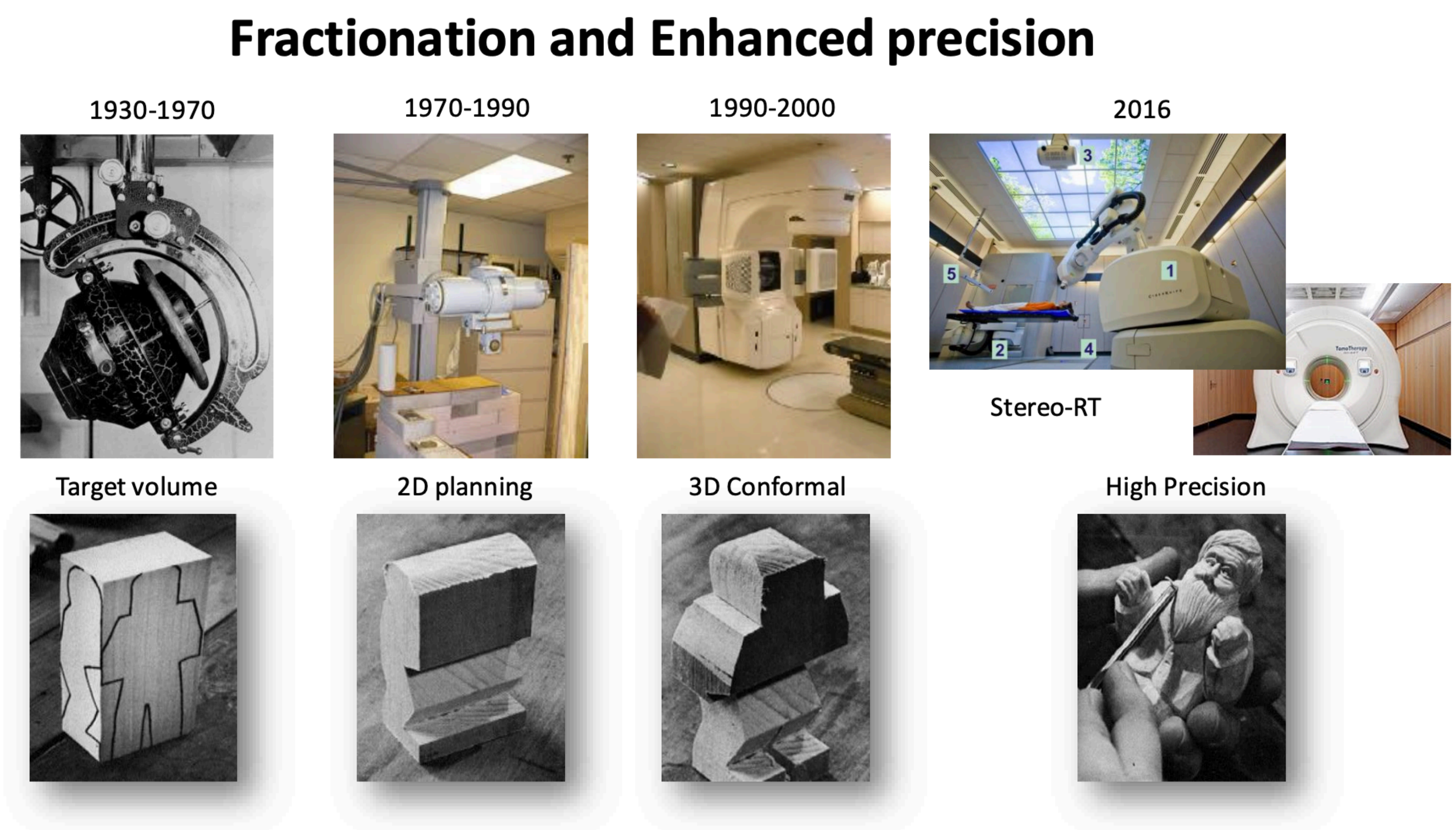
Proton Therapy Center at MGH

Typical Device

Mayo Clinic



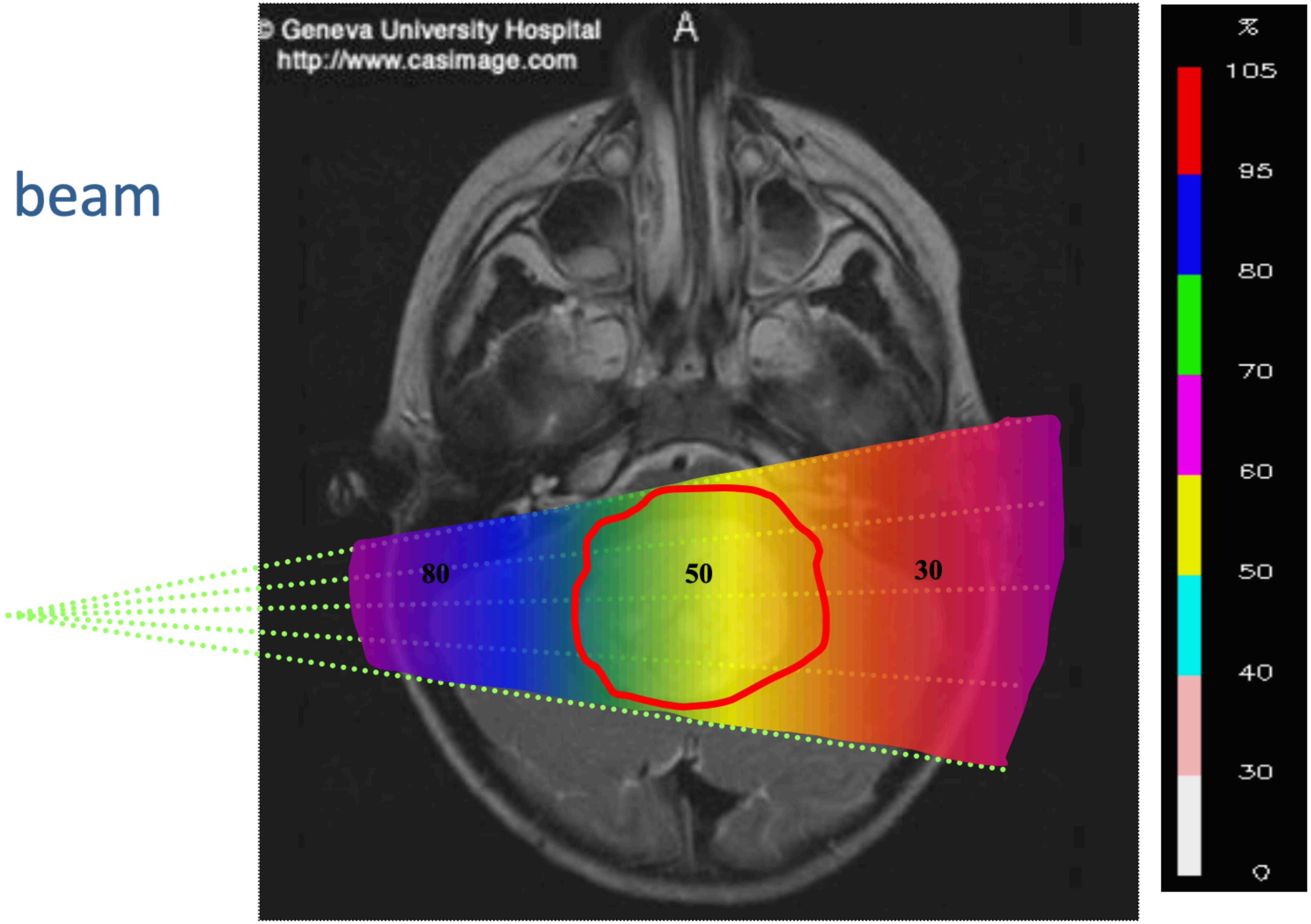
Radiation Therapy



- 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

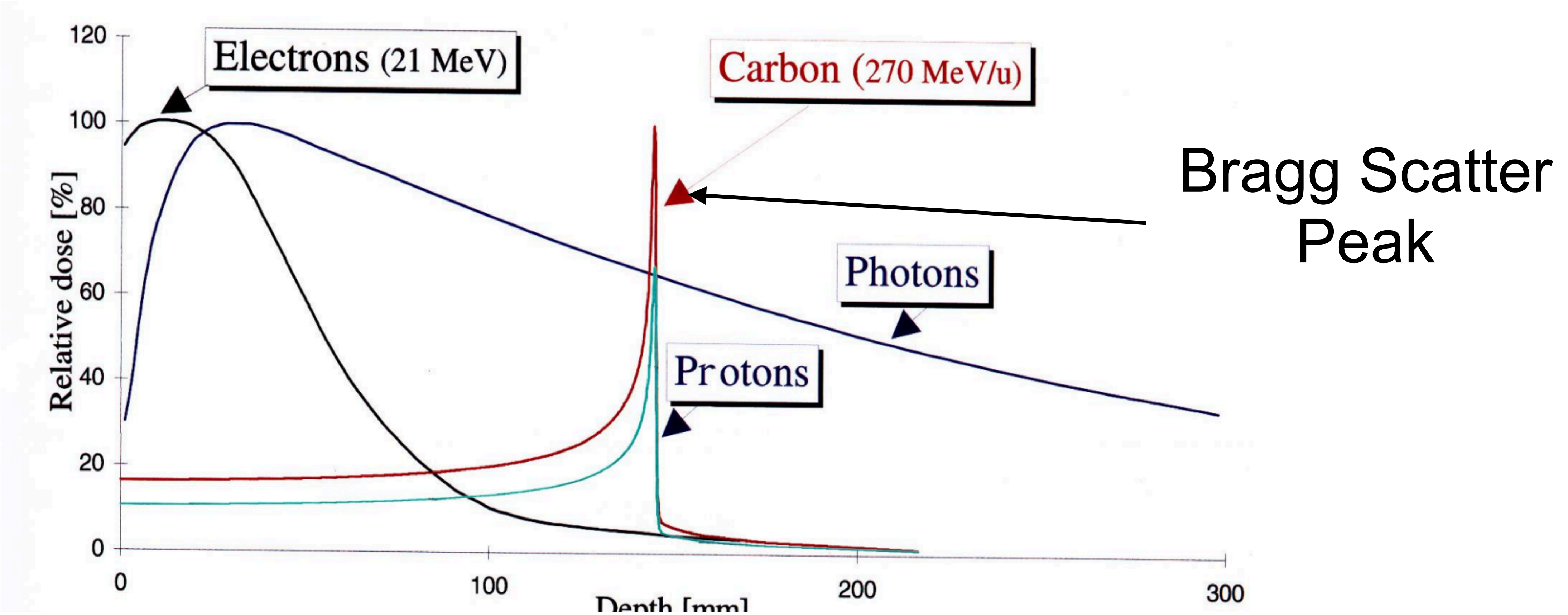
Classical Radiotherapy with X-rays

single beam

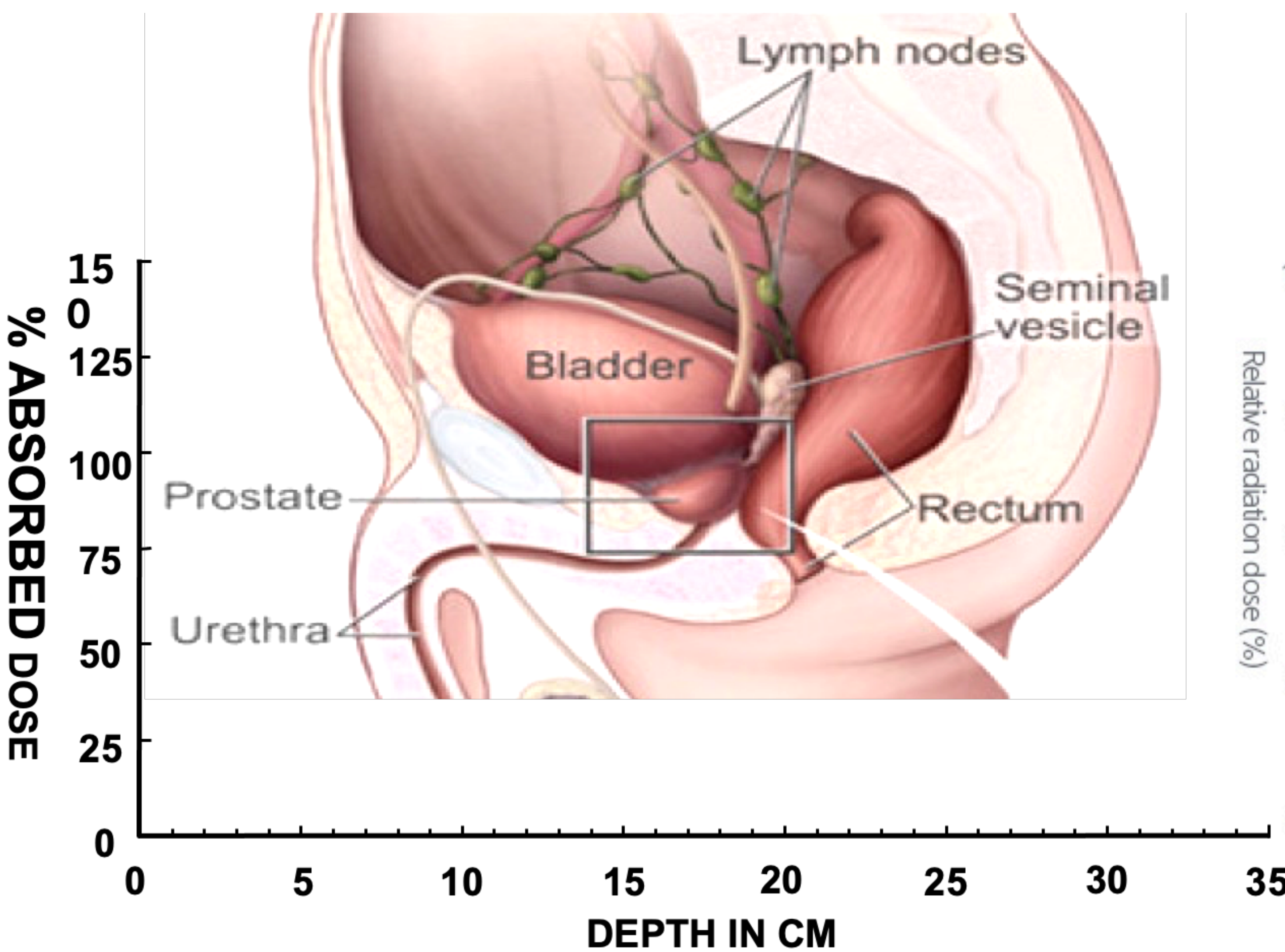


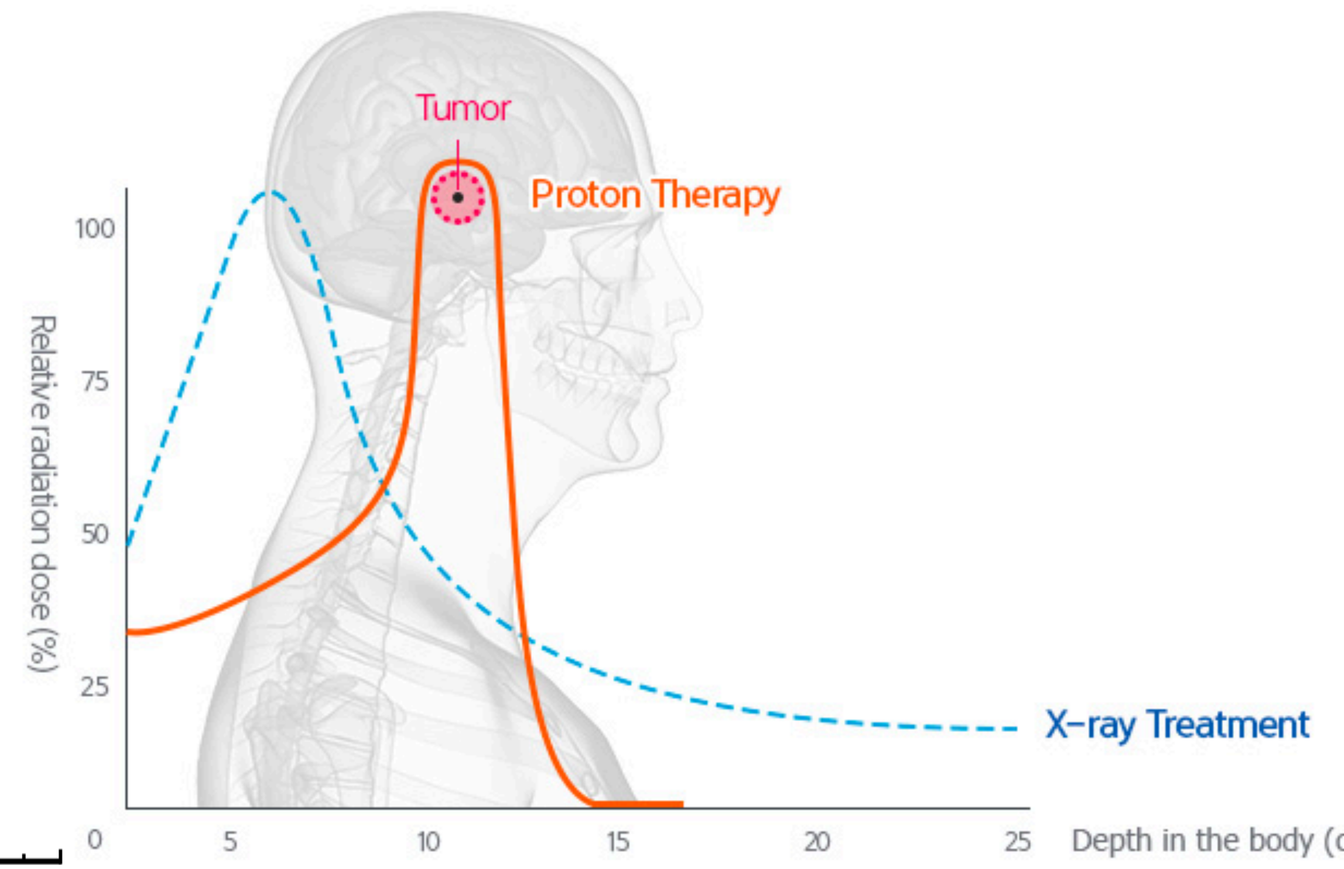
Hadron Therapy

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



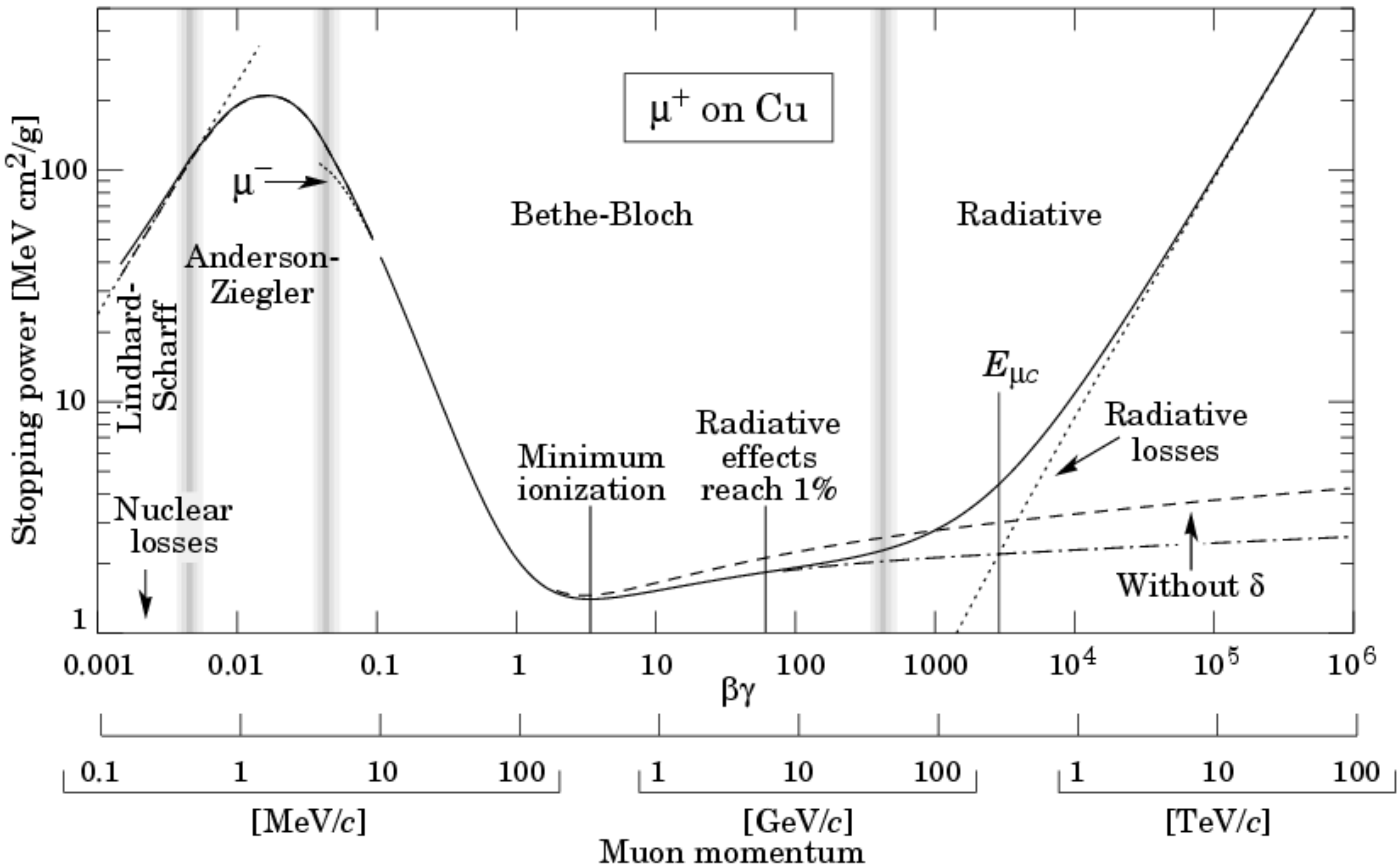
Proton Therapy





Bethe-Bloch Equation

- Charged Particles in matter are goverened by this equation



Protons Governed

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

density

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

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

[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]

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

$m_e = 511\ \text{keV}$
[Electron mass]

$\beta = v/c$
[Velocity]

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

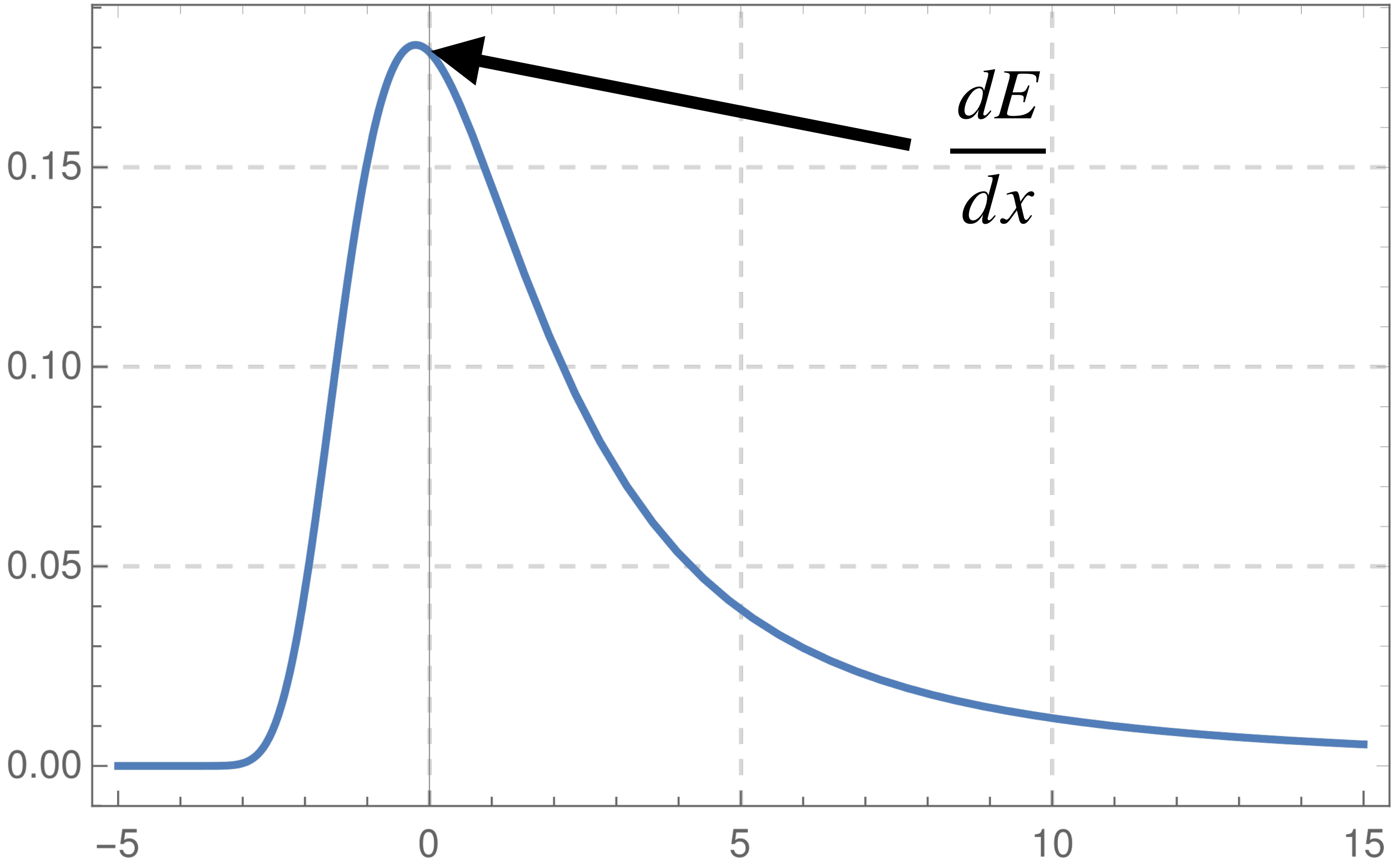
Validity:

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

Actual Energy Loss

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

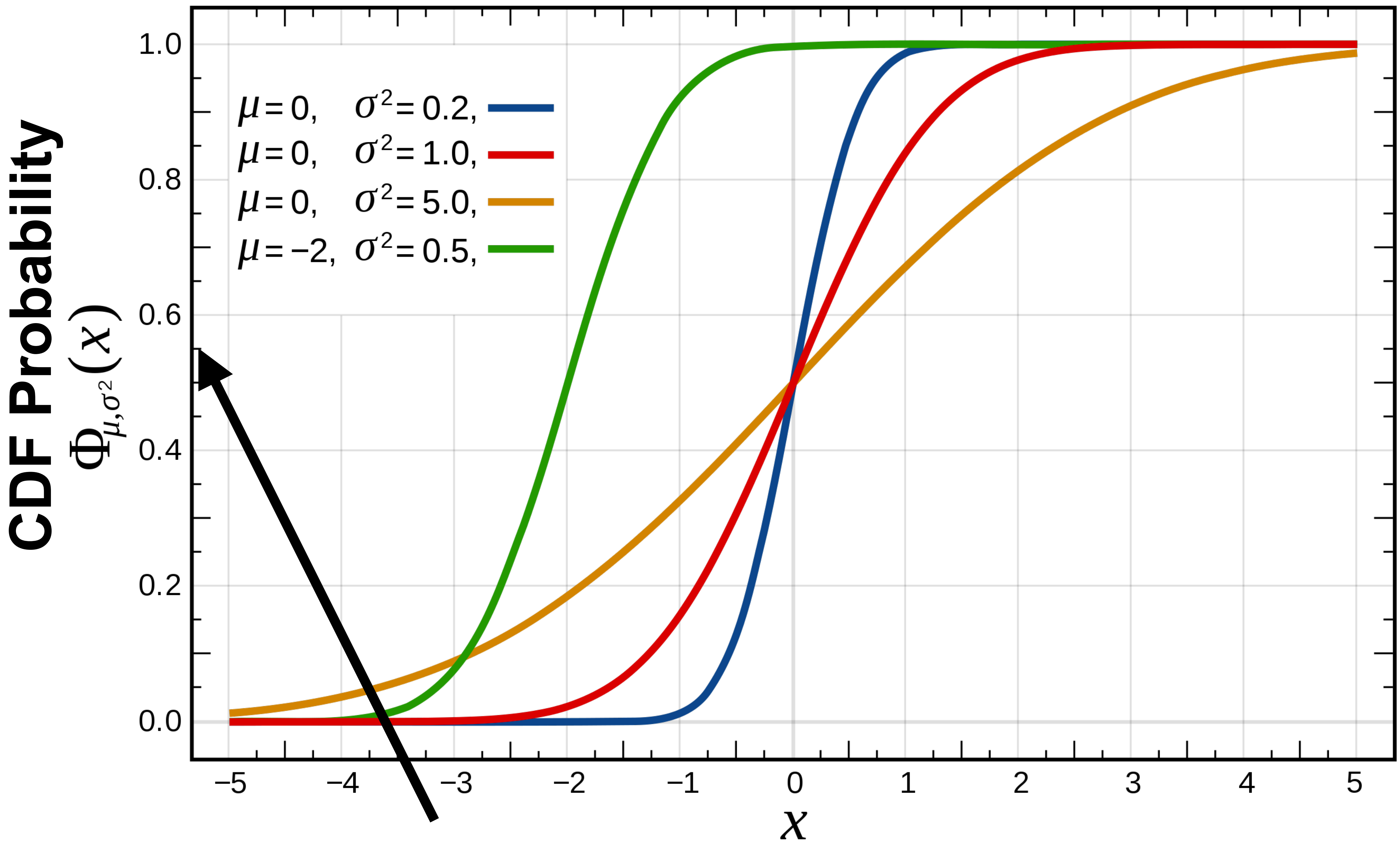
$$p(x) = \frac{1}{2\pi i} \int_{a-i\infty}^{a+i\infty} e^{s\log(s)+xs}\, ds,$$



Average of this distribution gives Bethe-Bloch

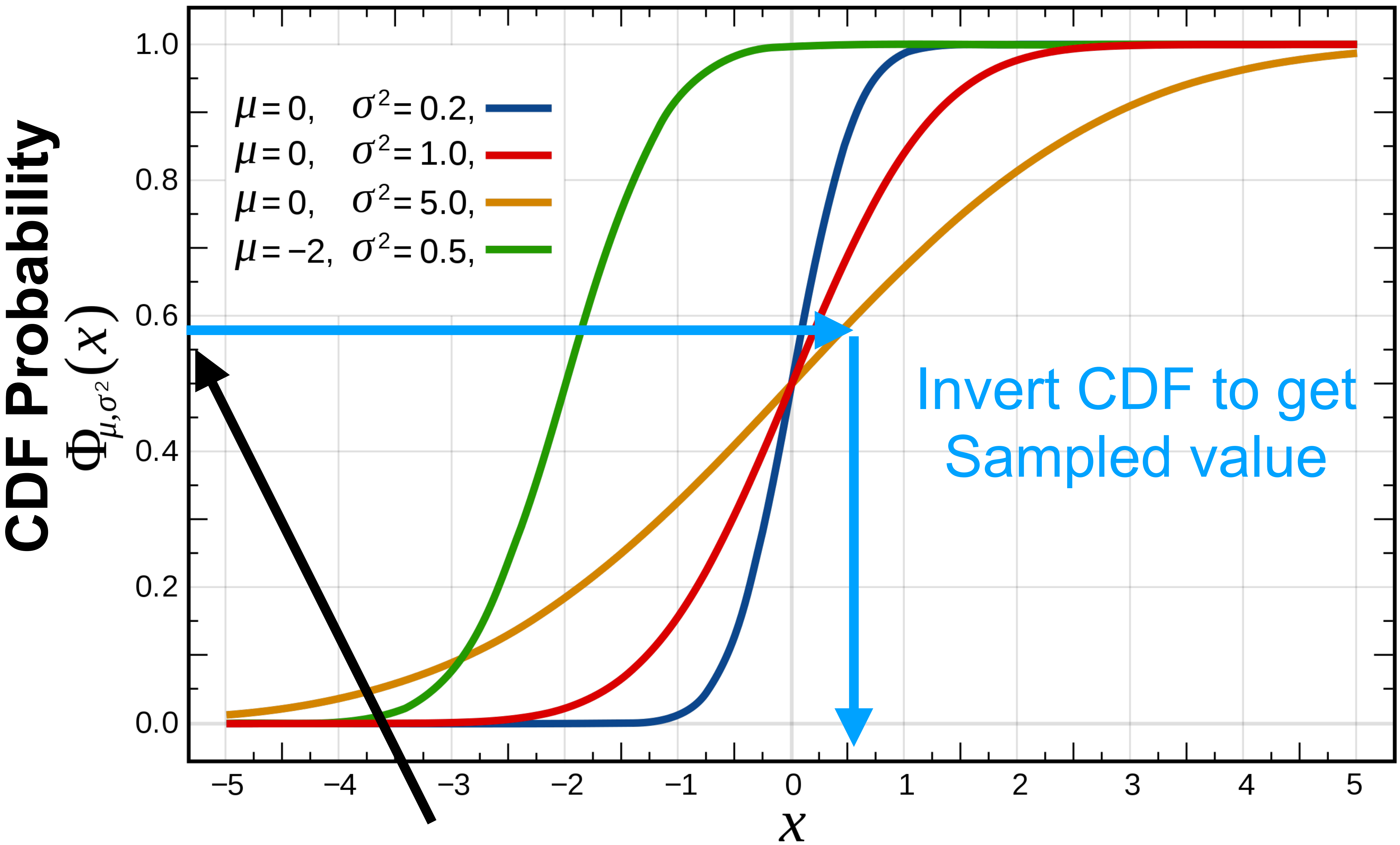
We can sample this
At each step

Sampling a Distribution



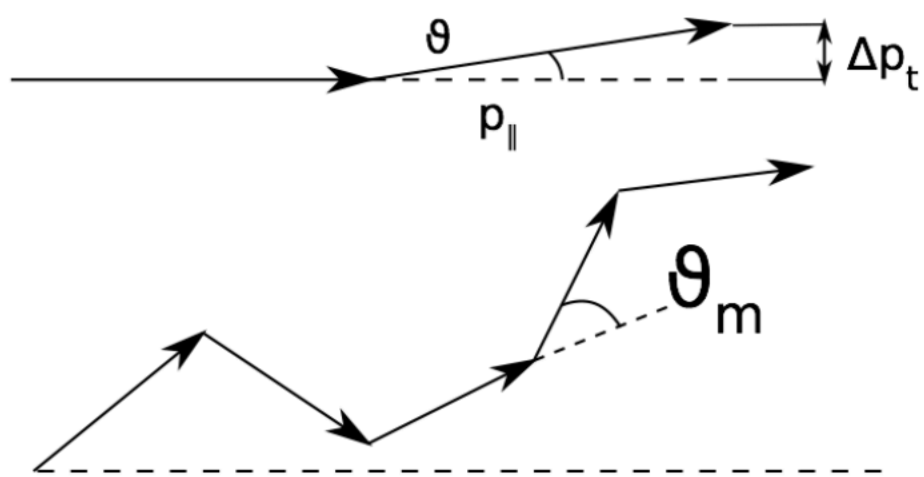
Sample from a p-value from 0 to 1 (flat 0 to 1)

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

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

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

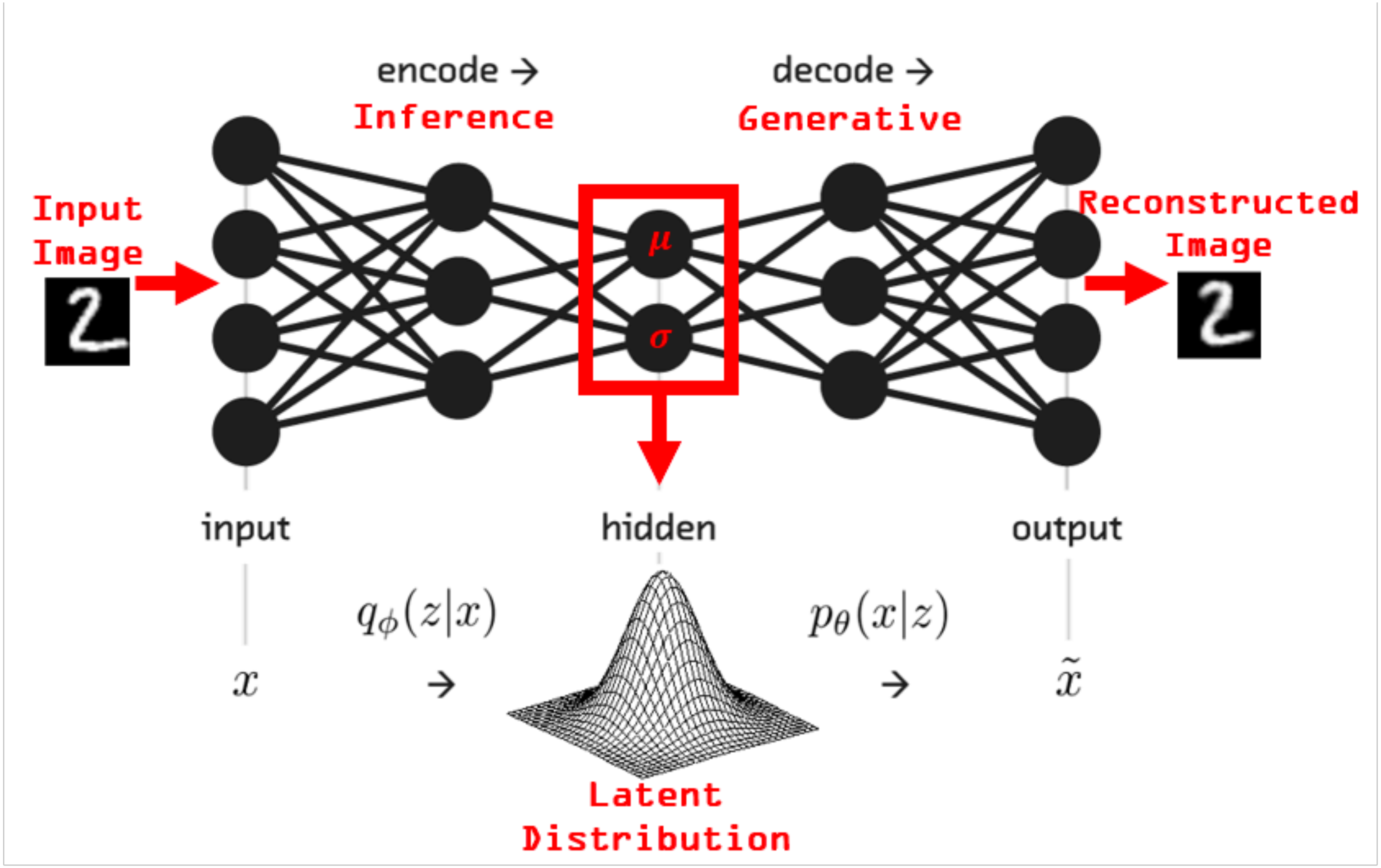
$$\sqrt{\langle \theta^2(x) \rangle} = \theta_{\text{rms}}^{\text{plane}} = \frac{13.6 \text{ MeV}}{\beta p c} z \sqrt{\frac{x}{X_0}} \left(1 + 0.038 \ln \frac{x}{X_0}\right)$$

- 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



VAE

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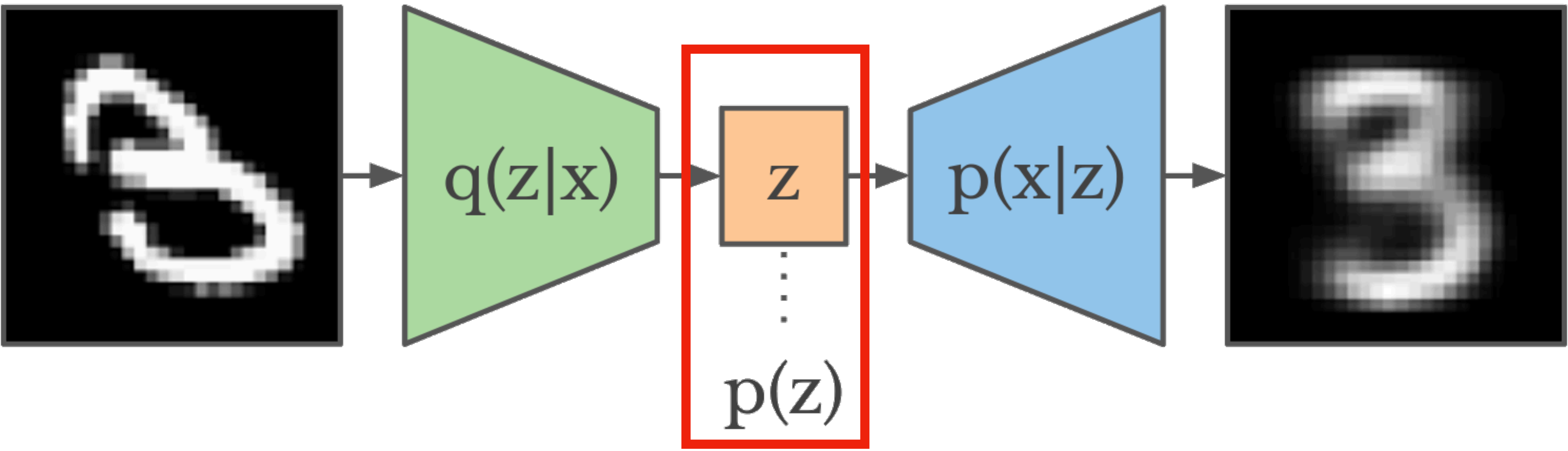
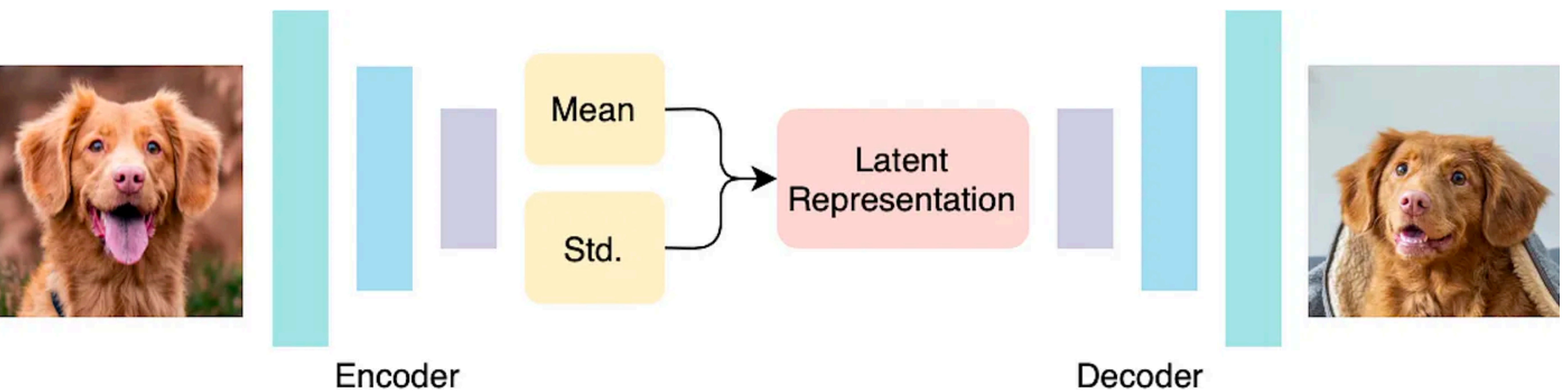
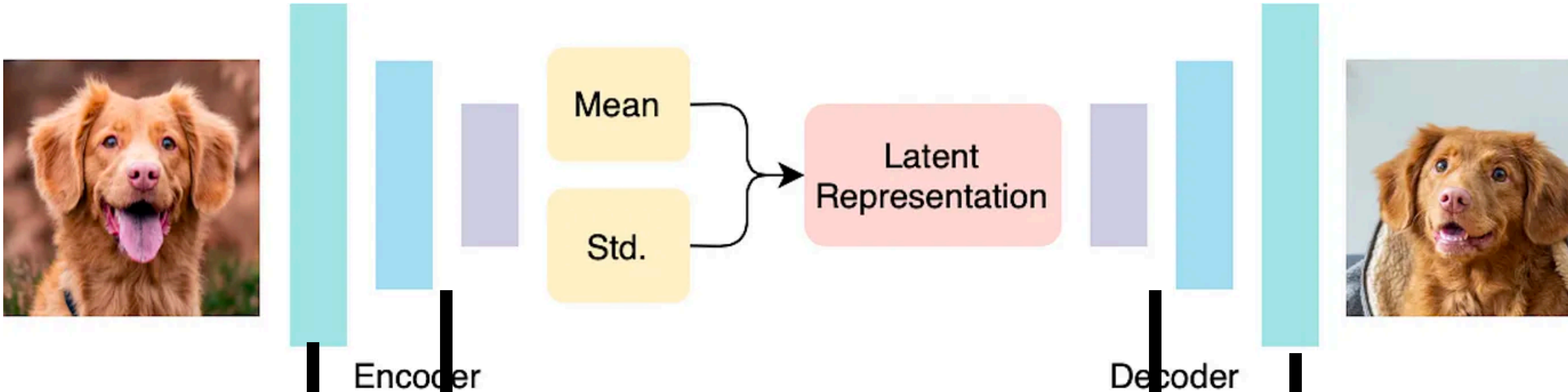


Randomly sample a normal distribution in this space



MNIST VAE encoder

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



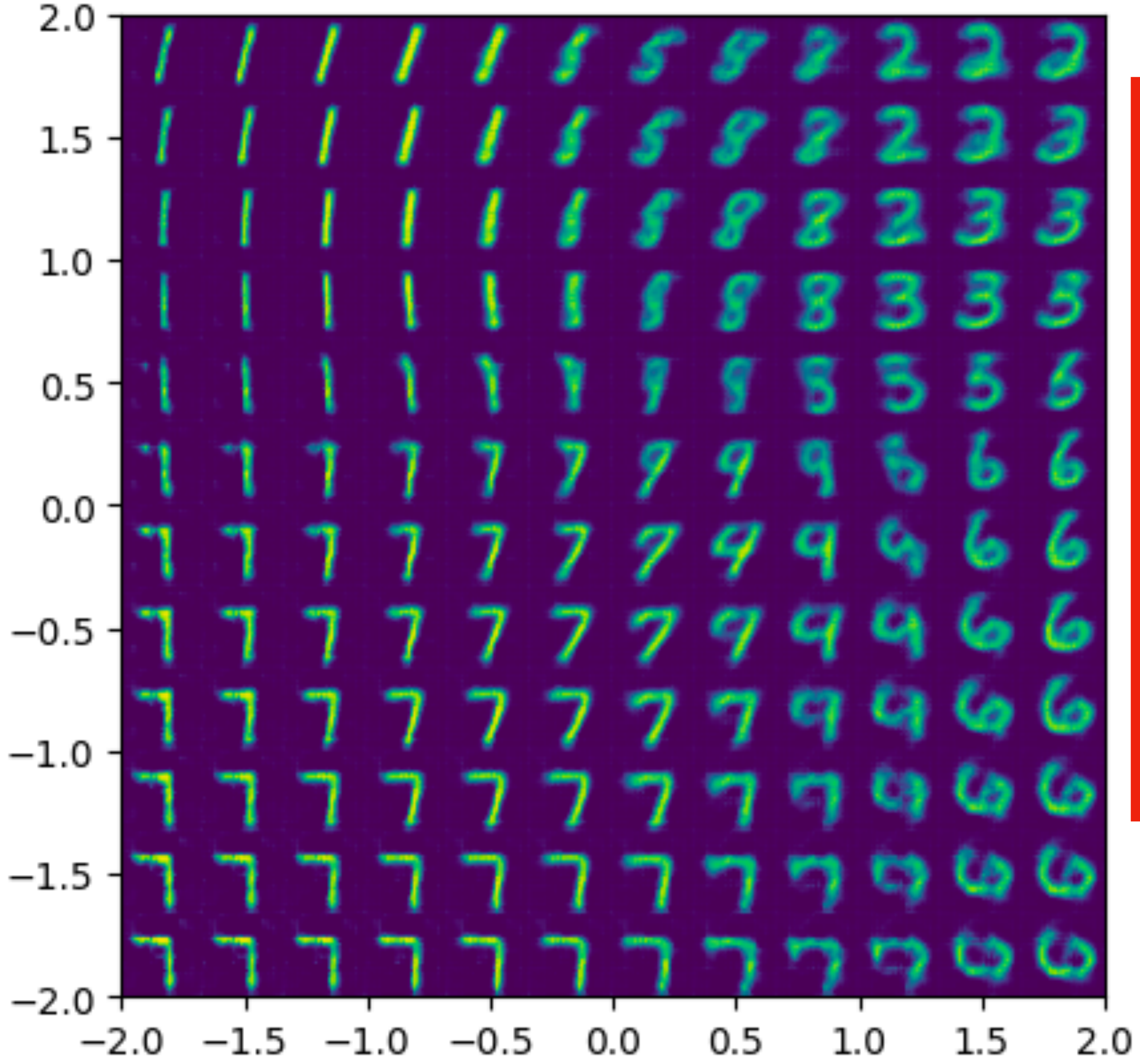
Dense/Linear Layers

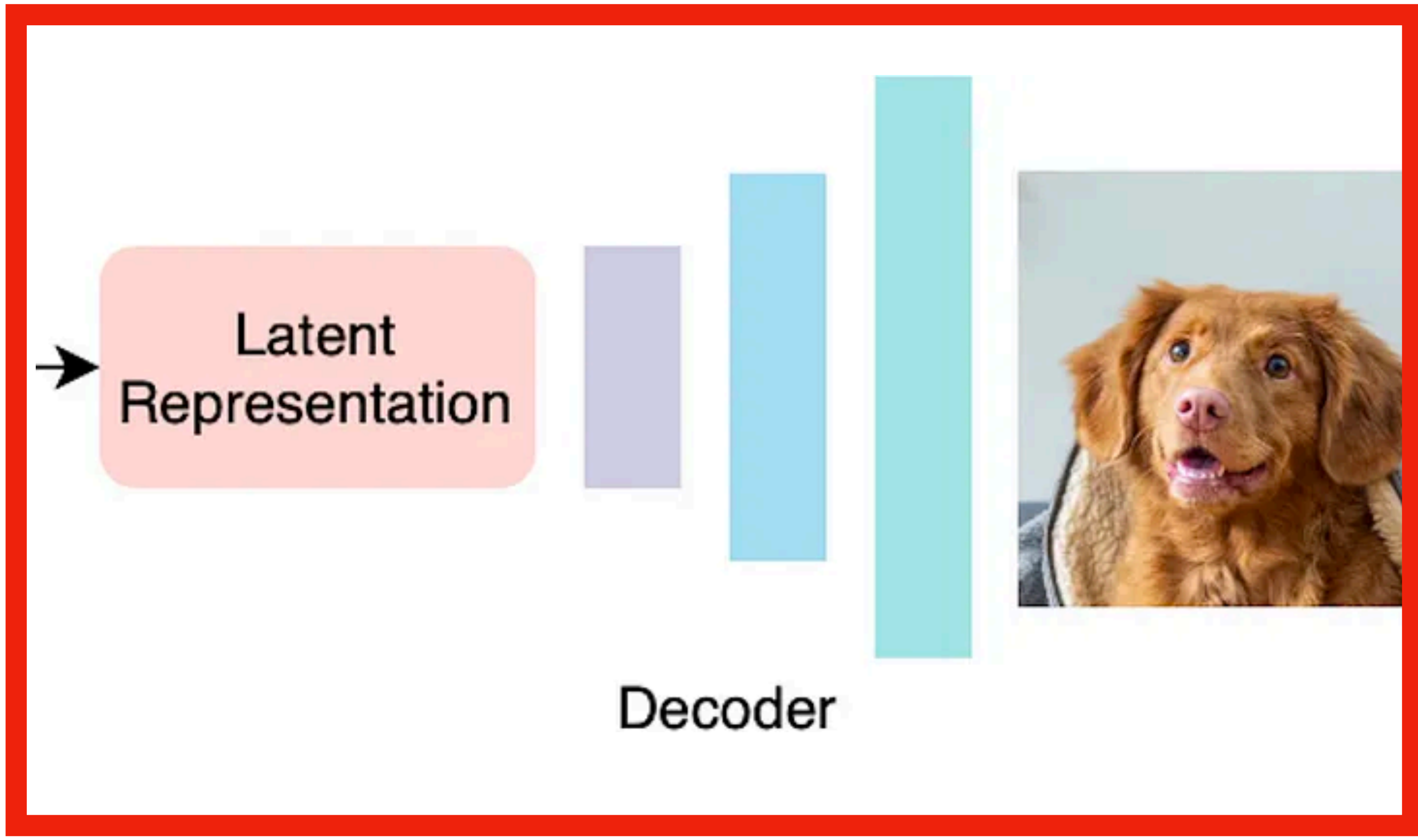
Dense/Linear Layers

Convolutionial Neural Network (CNN)

Convolutionial Neural Network Transpose

Exploring the latent space?

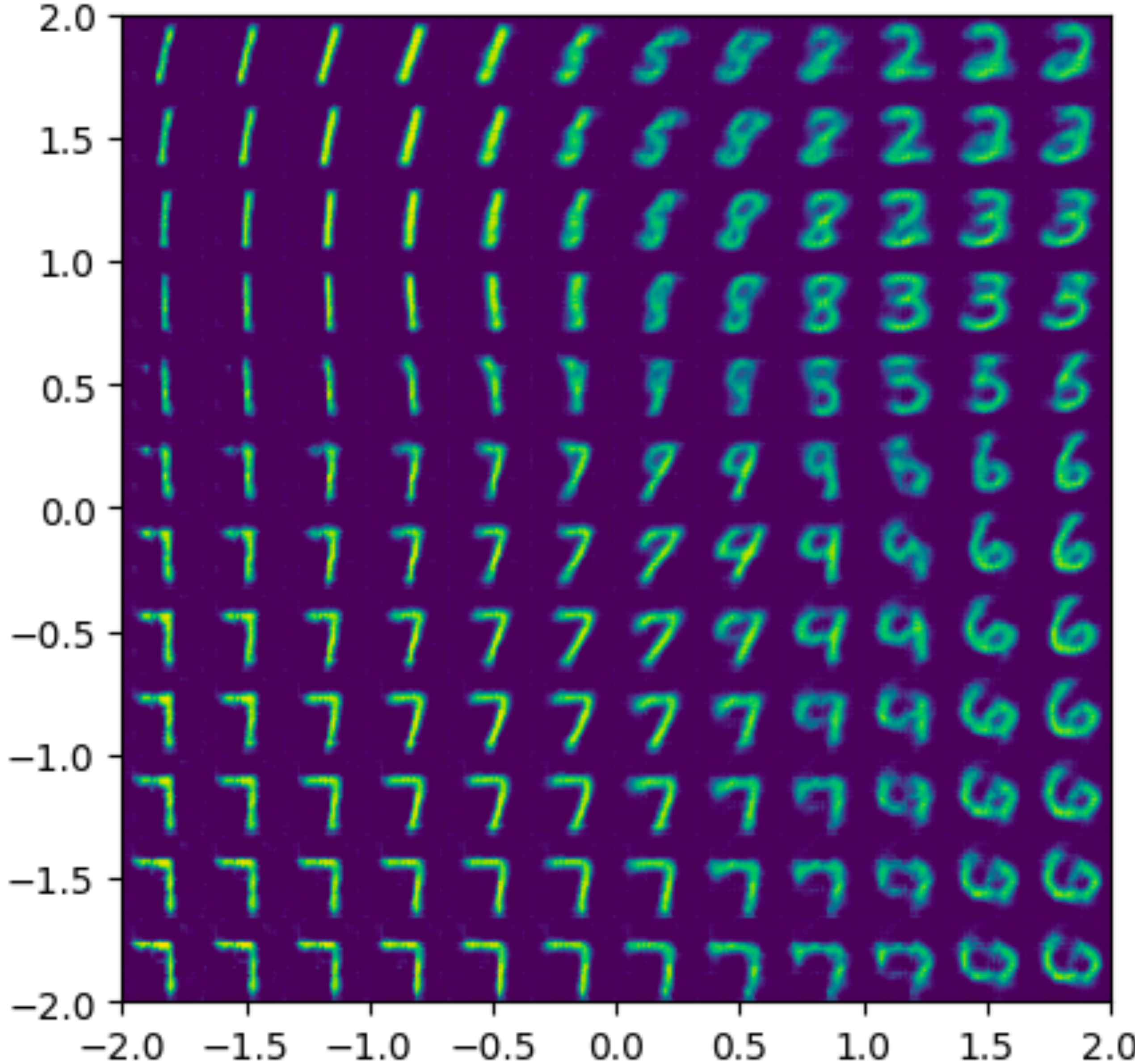


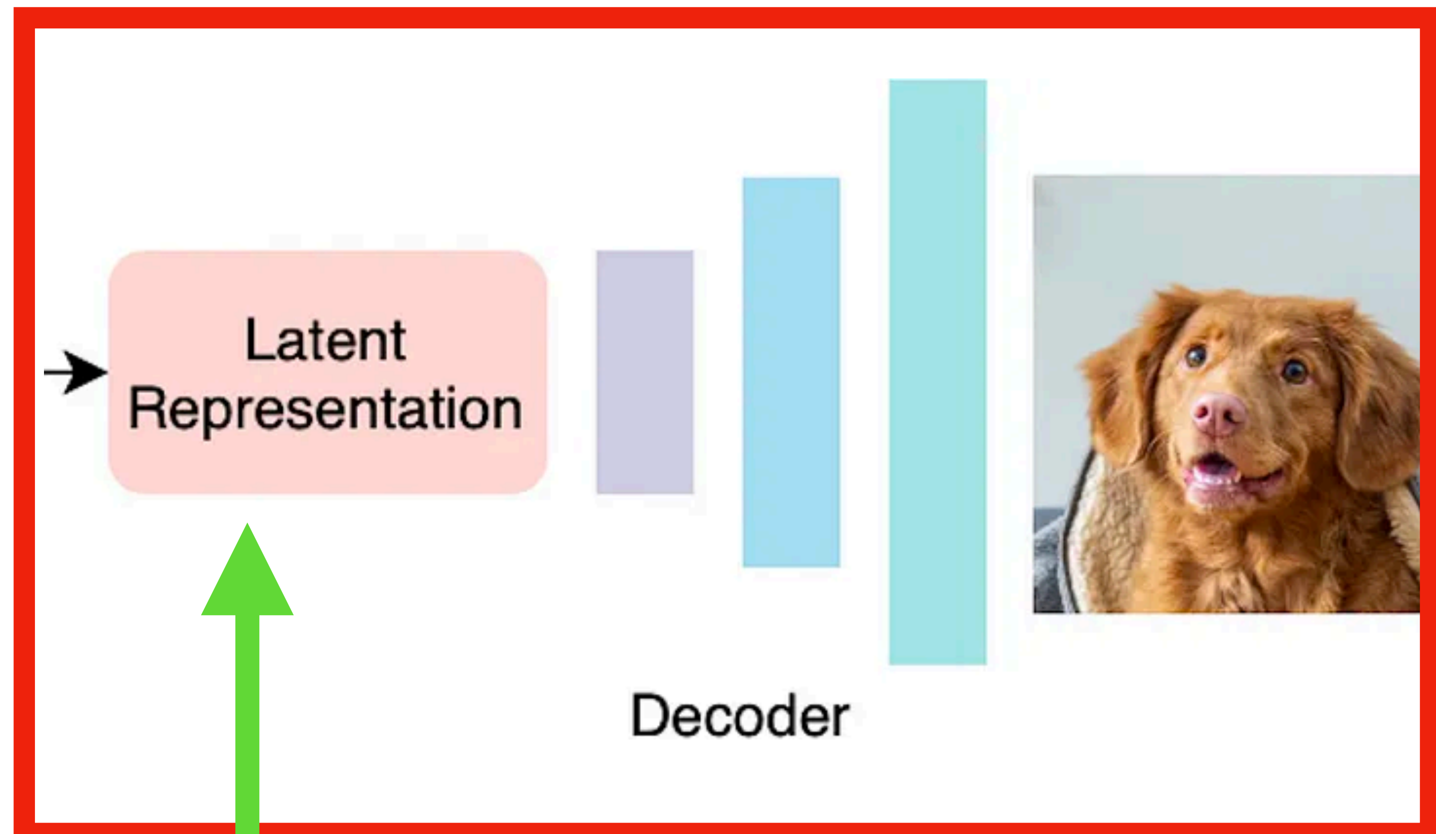


Generator

- 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