Python for Data Science 2

Lecture 15- Data/Models at the Large Hadron Collider

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ATLAS Computing

Full Simulation

KHz
Generation
mHz
Simulation
Hz
Digitization

Fast Simulation

KHz
Generation
Hz
Fast Simulation

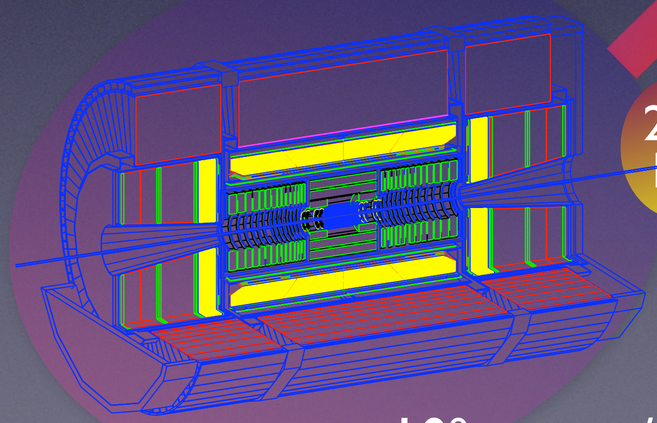
Data Store

New

cHz
Reconstruction

50% ATLAS CPU resources used for simulation

High-level Trigger



200 Hz

10^9 events/year

Data Base

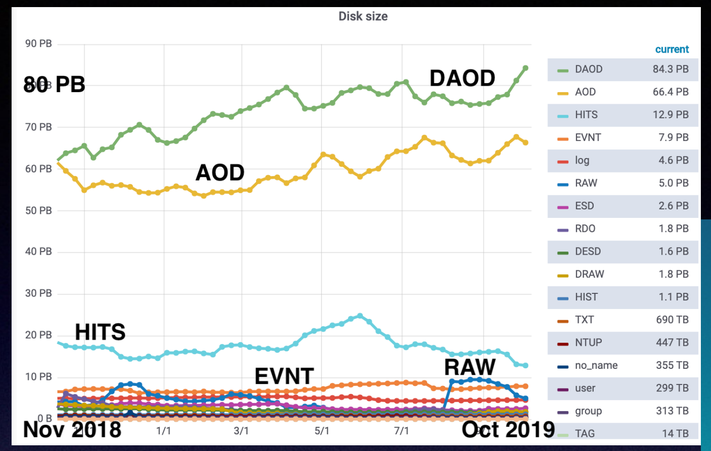
KHz
Hz
Algorithmic Analysis

MHz
Interactive Analysis

Statistical Analysis

Data Analysis & Calibration

The Event Data Model



Reconstruction Output.
Intended for calibration.
1000 KB/event.
Cells,Hits, Tracks,
Clusters,Electrons, Jets, ...

Raw Channels.
1.6 MB/event.

Event Summary Data

Raw Data Objects

Data refinement

Analysis Object Data

Intended for Analysis.
~500 KB/event.
"Light-weight" Tracks,
Clusters,Electrons, Jets,
Electron Cells, Muon
HitOnTrack,...

Derived Physics Data

Intended for "interactive" Analysis.
~10-50 KB/event.
What-ever is necessary for a specific analysis/ calibration/study.

The Computing Model

- Resources Spread Around the GRID

•Interactive Analysis
•Plots, Fits, Toy MC, Studies, ...

Tier 3

DPD

•Reprocessing of full data with improved calibrations 2 months after data taking.
•Managed Tape Access: RAW, ESD
•Disk Access: AOD, fraction of ESD

Tier 2

AOD

•Derive 1st pass calibrations within 24 hours.
•Reconstruct rest of the data keeping up with data taking.

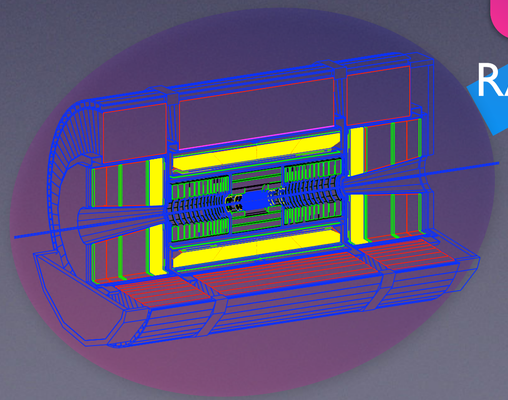
Tier 1

RAW/
AOD/
ESD

Tier 0

•Production of simulated events.
•User Analysis
•Disk Store

RAW



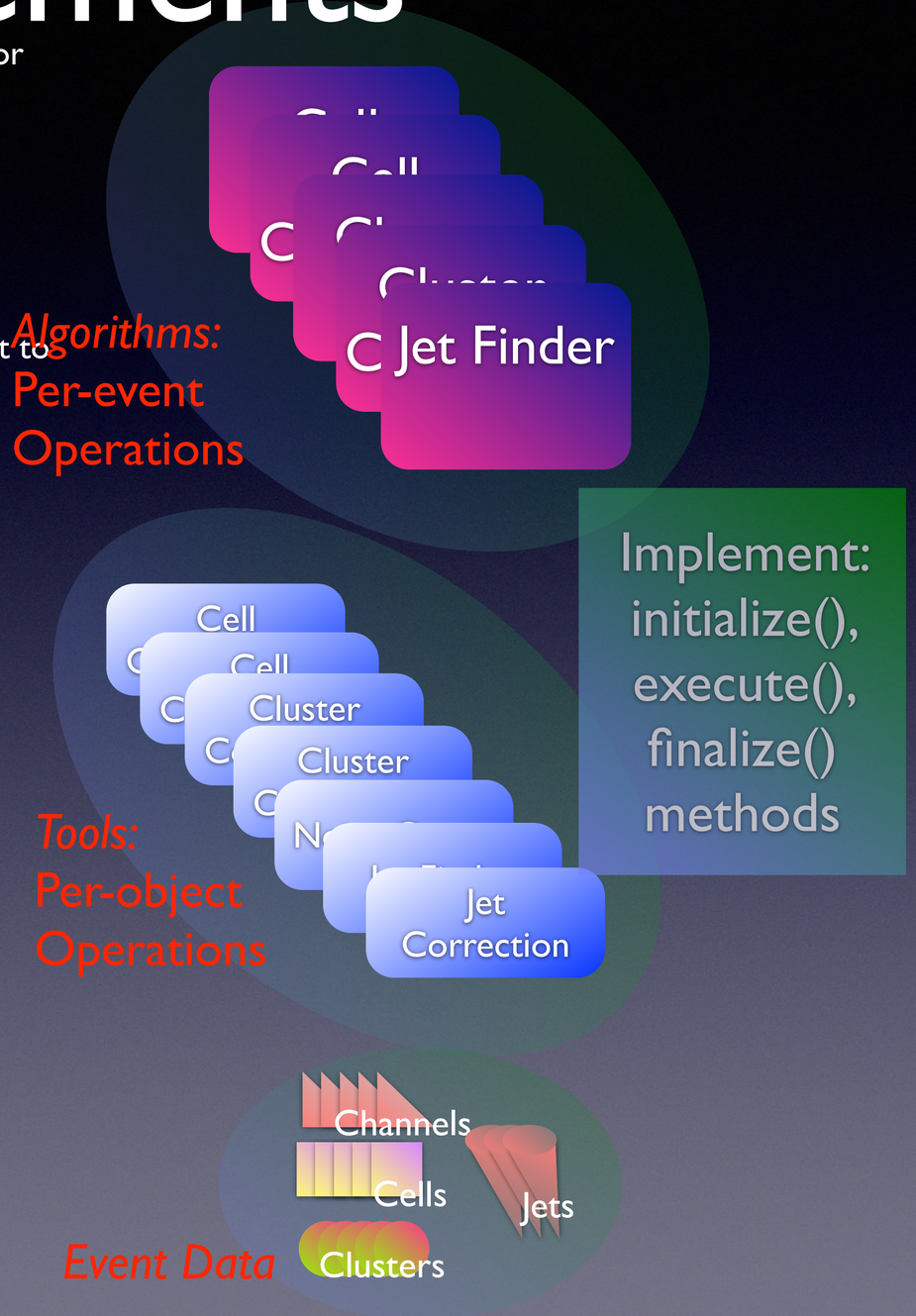
CERN Analysis Facility

•Primary purpose: calibrations
•Small subset of collaboration will have access to full ESD.
•Limited Access to RAW Data.

ATLAS Software Fundamentals

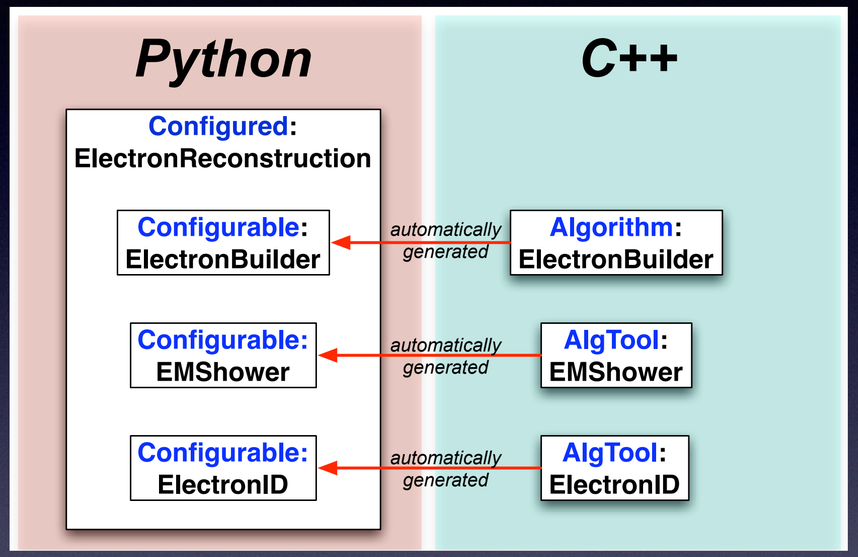
Framework Elements

- Athena is an extended version of LHCb's Gaudi framework used for high-level trigger, simulation/reconstruction, and analysis.
- Principles... separation of:
  - Data and algorithms
  - Transient (in memory) and Persistent (on disk) data (in contrast to CMS)
- Elements:
  - *Algorithms*- one execute per event, managed by framework.
  - *Tools*- multiple executes per event.
  - Event Data
  - Services
    - StoreGate- Transient Data Store- Mechanism for communication between Algorithms
    - Tool Service- Tool Factory
    - Interval of validity
    - Histogram Service
    - POOL- Persistency

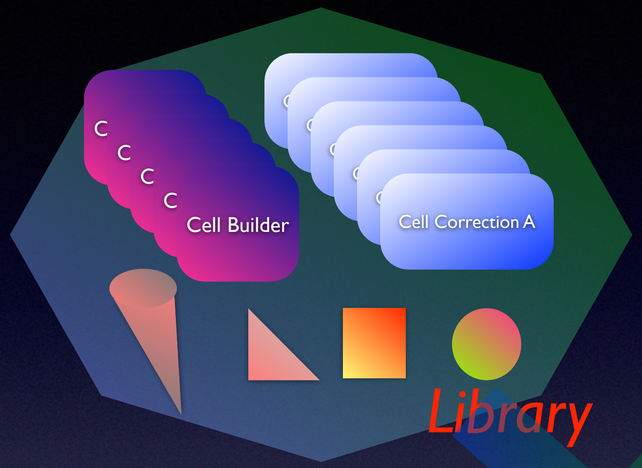


Configuration

- Framework elements (eg Algorithms, Tools, Services) declare properties which can be set at runtime
- Application defined in python:
  - Load libraries
  - Instantiate tools/algs, configure properties
  - Define input/output
- Configurables:
  - Auto-generated python reflection of C++ components
  - Build configuration purely in python, persistify the configuration, build application later.
  - Build higher level abstractions in python



- Any application (eg reconstruction) is a specific configuration of a library of framework elements.



The Framework

```
Input="TheData"
Algorithms+=CellBuilder(In="LArgChannels",Out="Cells1")
Algorithms+=CellCalibrator(In="Cells1",Out="Cells2")
CellCalibrator+=CellCorrectionA()
CellCalibrator+=CellCorrectionB()
Algorithms+=ClusterBuilder(In="Cells2",Out="Clusters1",MinEnergy=10*GeV)
....
```

A Configuration

EventSelector Service

Cell Builder

Channels

Cells

Cell Correction A

Cell Correction B

Cell Calibrator

Cells

Cluster Builder

Clusters

Cluster Correction A

Cluster Correction B

Cluster Calibrator

Clusters

Noise Cutter

Jet Finder

Jet Correction

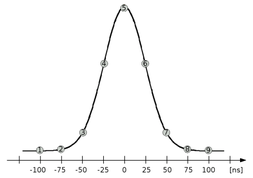
Jet Finder

Jets

Transient Data Store

HEP Data

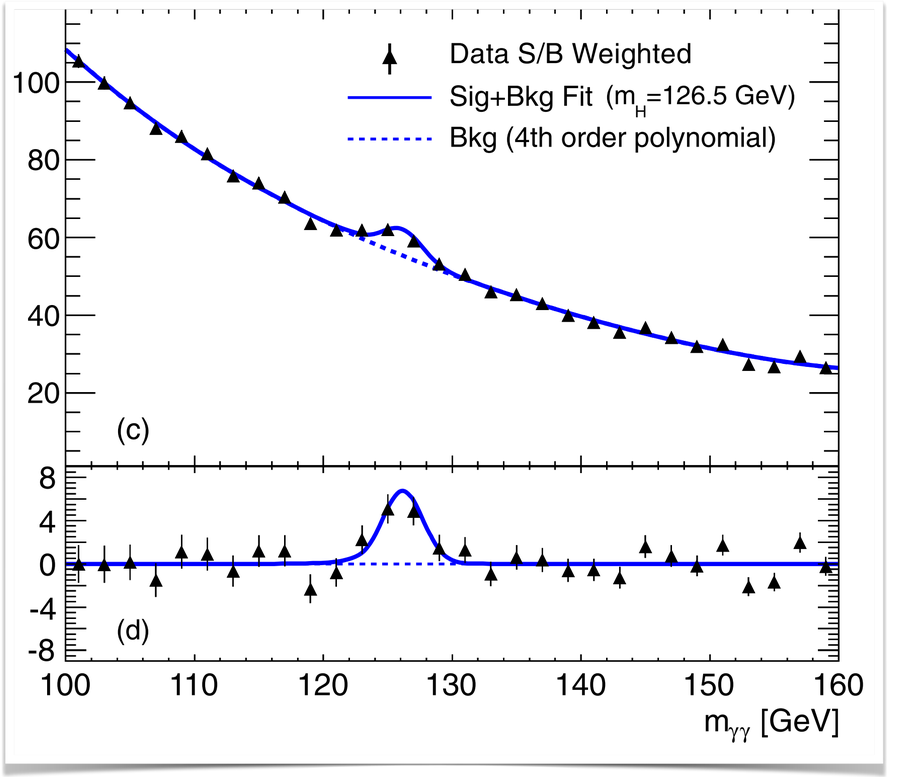
- The lowest-level (raw) data we generally have are the digitized outputs of detectors… e.g. voltages.
- Reconstruction is a series of sequential algorithms that construct features from outputs of the previous algorithm.
  - “raw” ⟶ “features”
- Highest level of Reconstruction output is usually particle candidates.
- Analysis, usually
  - choosing candidates ⟶ 4-vectors, separated by PID
  - 4-vectors ⟶ kinematic features (e.g. masses)
  - kinematic features ⟶ signal/background
  - statistical analysis ⟶ hypothesis test, limits, measurements
    - Background estimation
    - Lots of systematics



“Traditional” use of ML in HEP

HEP Data Analysis (Very Simplified)

- Lets say you are looking for the Higgs decaying to 2 photons.
  - Rare process. Large backgrounds
    - reducible: e.g. not really 2 photons, but look like it.
    - irreducible: e.g. really 2 photons, but not from Higgs.
- Data: 40M events/sec → 1000 events/sec stored by trigger → AOD format
- Simulation: Large samples of “signal” events +
- Derived Physics Data (DPD) (Reduce data size)
  - Select stored events with 2 energetic photons
  - Store only relevant information
- Compute features (invariant mass, angles, …)
- Select subset of events very likely to be Higgs (appropriate features) and not background.
  - Compute efficiency of selection.
- Use Statistical Fitting techniques to determine number of Higgs events in sample.
- Divide by efficiency → # of Higgs → 2 photon decays produced in LHC.



Physics Models

What is a “Model”?

- The context of science, data science, machine learning, etc, the word model is often used…
  - e.g disease transmission model, plate model, Standard Model of particle physics, neutral network model, …
- In science, models often try to capture some phenomena in a mathematical or heuristic way.
  - There are likely assumptions in a model, which often are simplifications
- Why? to understand, define, quantify, visualize, simulate, predict, …
- Often the general knowledge of a discipline (e.g. particle physics), is captured in a model.
  - It therefore represents what is known.
- Scientific research then becomes the iterative process of
  - comparing the model predictions with experimental results
  - improve the model
- Key is to understand what experiments to best reveal the weaknesses of these models.

- To understand the most fundamental phenomena in nature, the Physicists application of the scientific method:

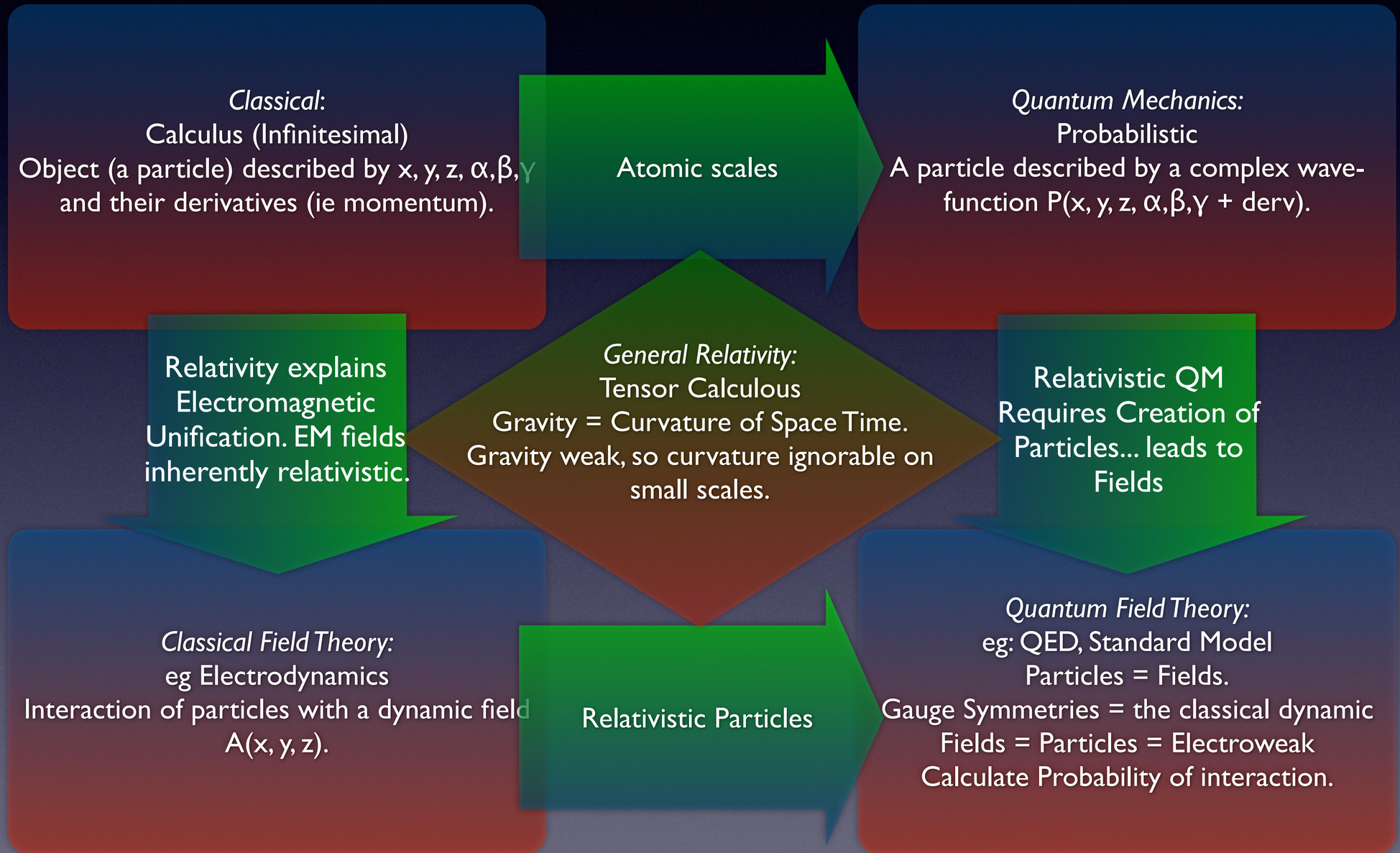
  1. Build Models

  - The **Standard Model of HEP** describes the building blocks of matter and their interactions.
    - SM requires the existence of a set of fundamental particles with very specific properties.
      - Tested and validated through experiments, including some of the most precise measurements ever.
    - Yet, has **failures**, e.g. no Dark Matter. Not compatible with Gravity.
    - And, has **inconsistencies**: e.g. both SM predicts the Higgs mass to be big and requires it to be small.
  - Models are **expressed mathematically**
    - Ideally build on a minimal set of rules (principles/laws)
    - SM Mathematical Framework: Quantum Field Theory- Way beyond this class.
      - Renormalization: encapsulating unknown (effects at high energy) in measurable parameters.
      - SM is a Model with **19 parameters**. Masses of particles. Strengths of forces. etc…
        - None are fundamental like speed of light or Planck's constant.

  2. **Build new model that tackle inconsistencies**.

  3. **Create experiments (target weaknesses in the model)**

Physics Models



Building the SM

Field Theory + Quantum Mechanics + Relativity = Quantum Field Theory

Ingredients

1. Leptons + Quarks

FERMIONS matter constituents spin = 1/2, 3/2, 5/2, ...

Leptons spin = 1/2

Flavor	Mass GeV/c^2	Electric charge
ν_e electron neutrino	$<1\times10^{-8}$	0
e electron	0.000511	−1
ν_μ muon neutrino	<0.0002	0
μ muon	0.106	−1
ν_τ tau neutrino	<0.02	0
τ tau	1.7771	−1

Quarks spin = 1/2

Flavor	Approx. Mass GeV/c^2	Electric charge
u up	0.003	2/3
d down	0.006	−1/3
c charm	1.3	2/3
s strange	0.1	−1/3
t top	175	2/3
b bottom	4.3	−1/3

2. Three Local Gauge Symmetries

- Each Symmetry implies existence of a new set of boson (spin 1) fields
- These bosons "carry" the Forces

Unified Electroweak spin = 1

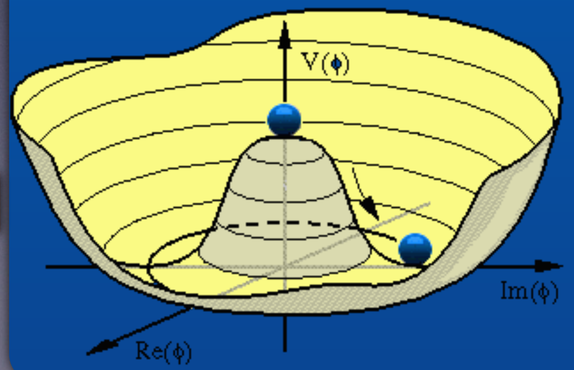
Name	Mass GeV/c^2	Electric charge
γ photon	0	0
W^-	80.4	−1
W^+	80.4	+1
Z^0	91.187	0

Strong (color) spin = 1

Name	Mass GeV/c^2	Electric charge
g gluon	0	0

3. Higgs Mechanism

- Every particle interacts with a scalar (spin 0) field
- This field has non-zero Vacuum Expectation Value
  - Breaks symmetry between E&M and Weak Forces
  - Gives masses to all particles w/o breaking Gauge Symmetries

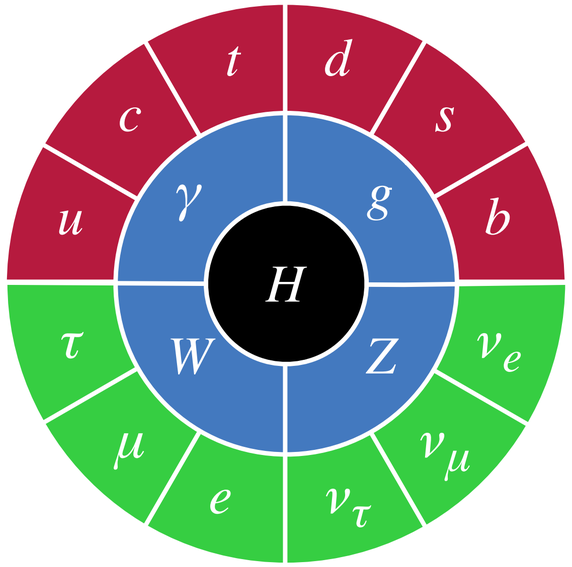


Standard Model

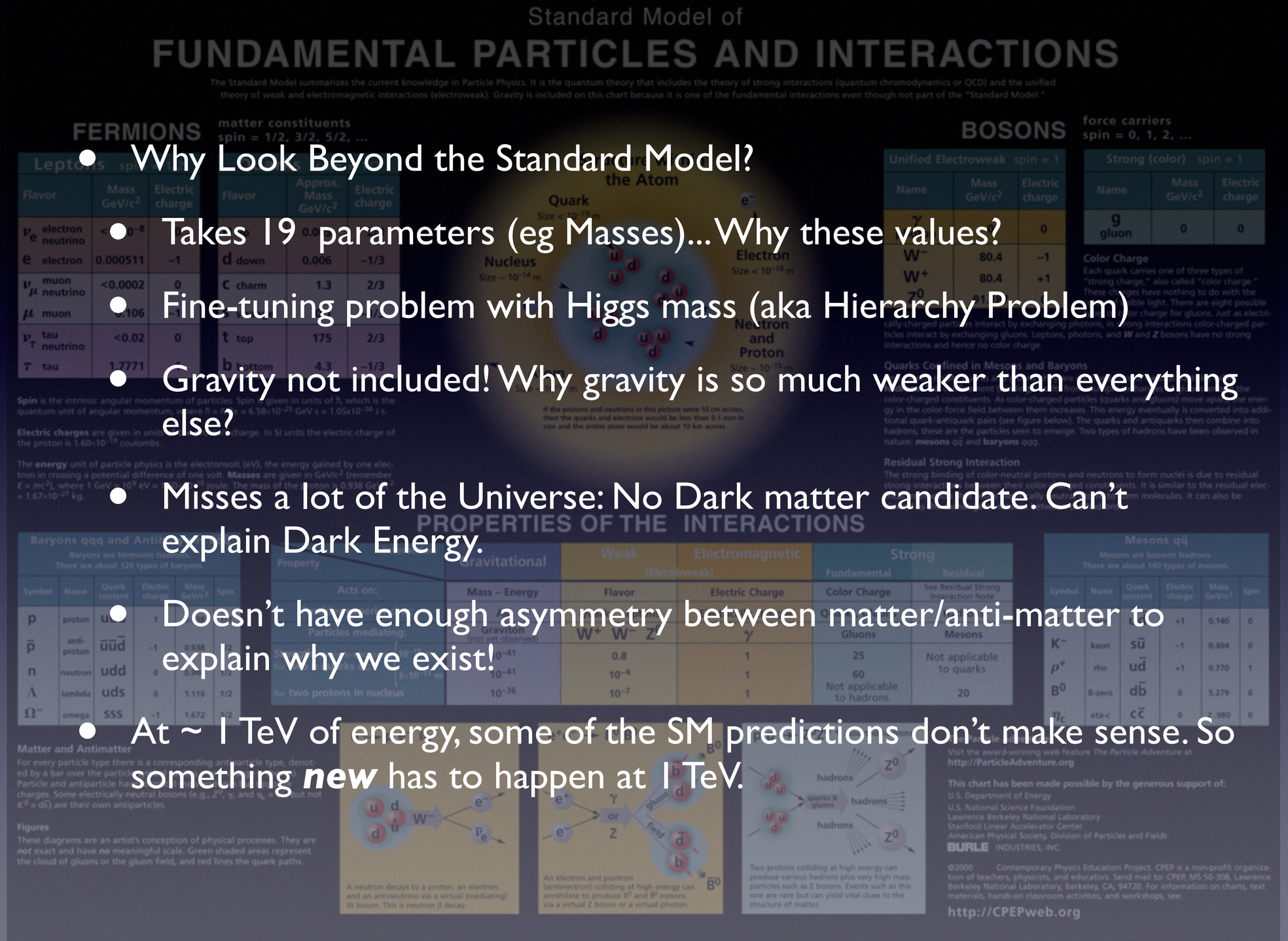
Agreement with all experimental results so far

PARTICLE PHYSICS: 19 PARAMETERS

$$\begin{aligned}\mathcal{L}_{SM} = & \underbrace{\frac{1}{4}\mathbf{W}_{\mu\nu}\cdot\mathbf{W}^{\mu\nu} - \frac{1}{4}B_{\mu\nu}B^{\mu\nu} - \frac{1}{4}G^{a}_{\mu\nu}G^{\mu\nu}_{a}}_{\text{kinetic energies and self-interactions of the gauge bosons}} \\ & + \underbrace{\bar{L}\gamma^{\mu}(i\partial_{\mu} - \frac{1}{2}g\tau\cdot\mathbf{W}_{\mu} - \frac{1}{2}g'YB_{\mu})L + \bar{R}\gamma^{\mu}(i\partial_{\mu} - \frac{1}{2}g'YB_{\mu})R}_{\text{kinetic energies and electroweak interactions of fermions}} \\ & + \underbrace{\frac{1}{2}\left|(i\partial_{\mu} - \frac{1}{2}g\tau\cdot\mathbf{W}_{\mu} - \frac{1}{2}g'YB_{\mu})\,\phi\right|^{2} - V(\phi)}_{W^{\pm},Z,\gamma,\text{and Higgs masses and couplings}} \\ & + \underbrace{g''(\bar{q}\gamma^{\mu}T_{a}q)\,G^{a}_{\mu}}_{\text{interactions between quarks and gluons}} + \underbrace{(G_{1}\bar{L}\phi R + G_{2}\bar{L}\phi_{c}R + h.c.)}_{\text{fermion masses and couplings to Higgs}}\end{aligned}$$



Symbol	Description	Value
m_e	Electron mass	511 keV
m_μ	Muon mass	105.7 MeV
m_τ	Tau mass	1.78 GeV
m_u	Up quark mass	1.9 MeV
m_d	Down quark mass	4.4 MeV
m_s	Strange quark mass	87 MeV
m_c	Charm quark mass	1.32 GeV
m_b	Bottom quark mass	4.24 GeV
m_t	Top quark mass	172.7 GeV
θ_{12}	CKM 12-mixing angle	13.1°
θ_{23}	CKM 23-mixing angle	2.4°
θ_{13}	CKM 13-mixing angle	0.2°
δ	CKM CP-violating Phase	0.995
g_1	U(1) gauge coupling	0.357
g_2	SU(2) gauge coupling	0.652
g_3	SU(3) gauge coupling	1.221
θ_{QCD}	QCD vacuum angle	~0
v	Higgs vacuum expectation value	246 GeV
m_H	Higgs mass	125 GeV



- Why Look Beyond the Standard Model?
- Takes 19 parameters (eg Masses)... Why these values?
- Fine-tuning problem with Higgs mass (aka Hierarchy Problem)
- Gravity not included! Why gravity is so much weaker than everything else?
- Misses a lot of the Universe: No Dark matter candidate. Can't explain Dark Energy.
- Doesn't have enough asymmetry between matter/anti-matter to explain why we exist!
- At ~ 1 TeV of energy, some of the SM predictions don't make sense. So something ***new*** has to happen at 1 TeV.

HEP Data Model

Data Model

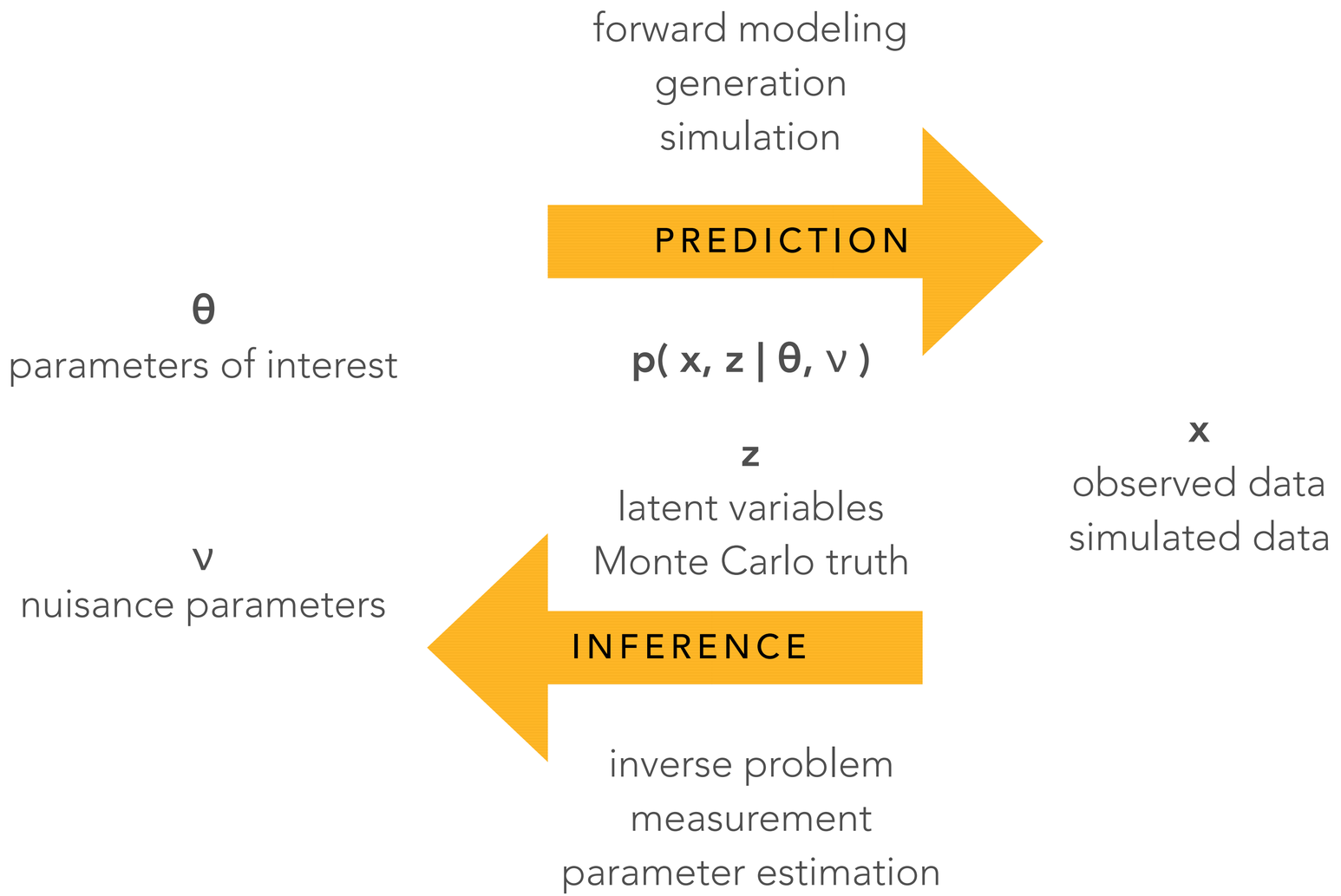
- Lets formalize what we mean by a ***dataset*** with a Probabilistic Model:
  - Assumption: Observed **Data is a mixture of *M* different processes** (M=2: signal/background)
  - Data set of *N* **data points**, $\{\{x_d\}_i\}$ (For SUSY N = 5M)
    - each $\{x_d\}_i$ consisting of (i goes from 0 → 5M, d = 18 observables, if we exclude “signal”)
      - *d* **observations** $\{x_d\}$
      - probability f_j of uniquely coming from one of *M* **classes** (if $N_s = 10$, $N_b = 100$ → $f_s = 10/110$, $f_b = 1\text{-}f_s$)
        - each class has label c_j is indexed by j (c_j = s or b)
        - dependent on parameters $\{\alpha_k\}_j$ (some **parameters of of interest**, some **nuisance parameters**)
    - Dependent on other parameters $\{\beta_l\}$

- $\Longrightarrow P(\{x\}|\theta) = P(\{x\}|\{f_j, c_j, \{\{\alpha_k\}_j\}, \{\beta_l\}) = \sum_j f_j P(\{x\}|c_j, \{\alpha_k\}_j, \{\beta_l\})$

- $P(\{x\}|\theta) = P(\{x\}|\{f_j, c_j\}) = \sum_j f_j P(\{x\}|c_j) = f_s P(\{x\}|s) + (1\text{-}f_s) P(\{x\}|b)$

What is it good for?

- If we know $P(X|\theta)$, what is it good for? (Statistical Inference)
  - ***Prediction***: Assume $\theta \Longrightarrow$ distribution of $\{x_d\}$.
  - ***Classification***: Observation $\{x_d\} \Longrightarrow$ most likely class c
  - ***Regression***: Dataset $\{\{x_d\}_i\} \Longrightarrow$ parameters of interest $\{\alpha_j{}^k\}$ or $\{\beta_l\}$
  - ***Hypothesis test***: Dataset $\{\{x_d\}_i\} \Longrightarrow$ is H_1 true (or H_0 null hypothesis)


forward modeling
generation
simulation
PREDICTION
θ
parameters of interest
p(x, z | θ, ν)
z
latent variables
Monte Carlo truth
x
observed data
simulated data
ν
nuisance parameters
INFERENCE
inverse problem
measurement
parameter estimation

Data Analysis

- Objectives:
  - ***Searches*** (hypothesis testing): Likelihood Ratio Test (Neyman-Pearson lemma)
  - ***Limits*** (confidence intervals): Also based on Likelihood
  - ***Measurements***: Maximum Likelihood Estimate

$$\frac{P(x|H_1)}{P(x|H_0)} > k_\alpha$$

- ***Likelihood***

$$p(\{x\}|\theta) = \mathrm{Pois}(n|\nu(\theta)) \prod_{e=1}^{n} p(x_e|\theta)$$

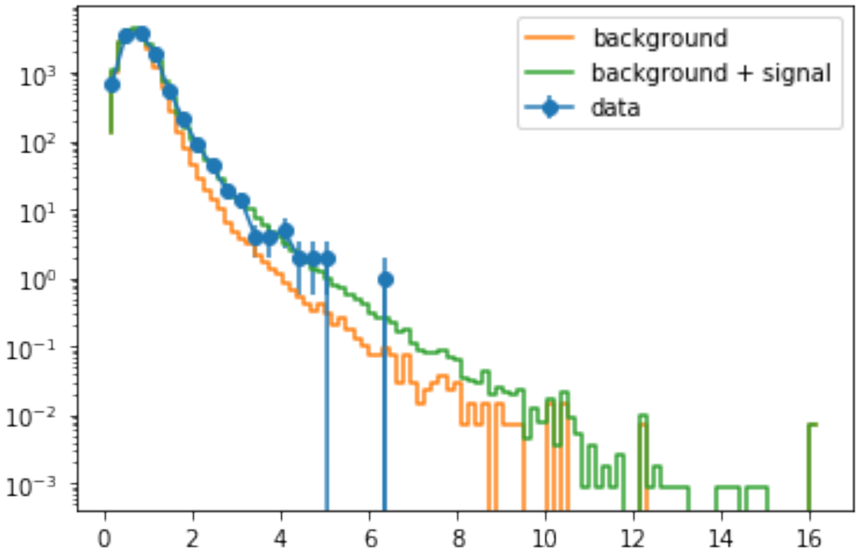
  - *n* Independent Events (*e*) with Identically Distributed Observables ({*x*})
  - Significant part of Data Analysis is ***approximating the likelihood*** as best as we can.

Obtaining the Likelihood

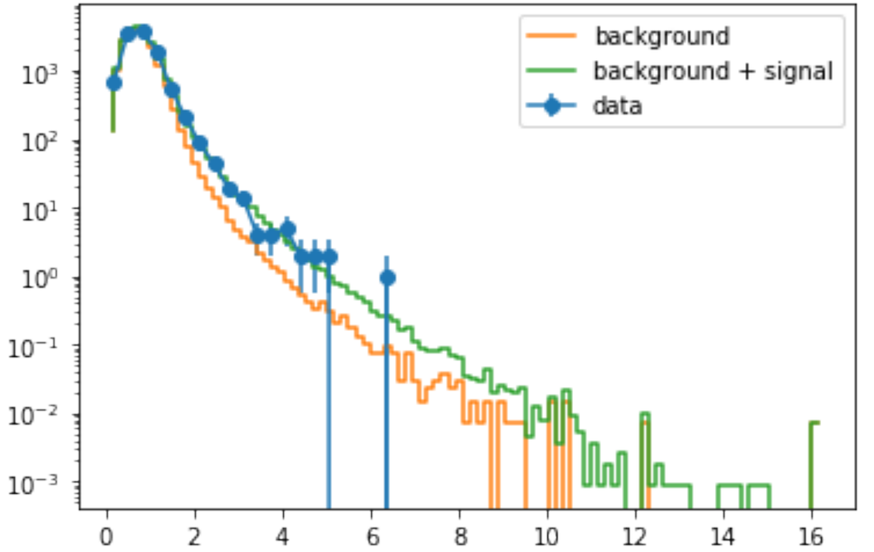
- How do we obtain $P(X|\theta)$?
  - In HEP, we have precise ***algorithmic simulations*** that generate $\{x_d\}$ given θ.
    - We estimate P by comparing observed x_d with simulated $\{x_d\}$.
  - We can build ***analytical first principle models***. *Matrix Element Method* is such a technique.
    - But it's technically difficult, computationally expensive, and only tractable with physics and detector simplifications.
  - We can build a statistical model P based on previous data.
    - We can using ML to learn P from simulation or data.

Data vs Simulation

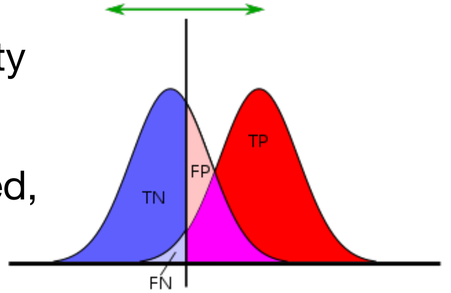
- The data you are playing with in the labs are simulated as opposed to data recorded in collisions.
- We will use it for 2 purposes:
  - Characterize $P(\{x\}|\theta)$ → establish strategy for searching for signal in real data
  - Create mock datasets ~ real data → test our statistical procedure
- The simulation does not have the ratio of signal to background you expect from nature.
  - Nearly same number of signal and background events.
  - Allows you to have similar statistical power in characterizing signal and background events.



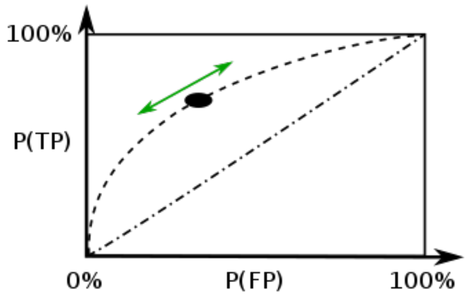
Hypothesis Test



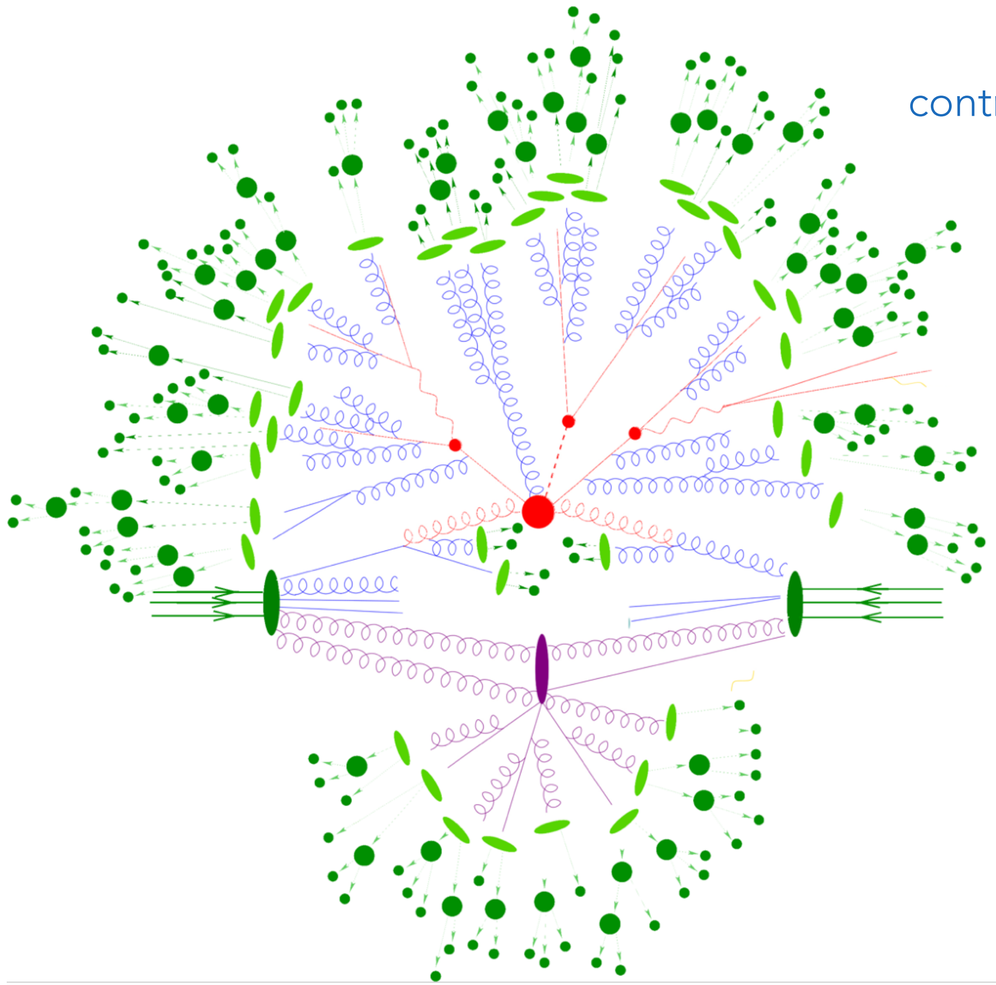
- H_0 = Null Hypothesis = Background Only
- H_1 = Test Hypothesis = Background + signal
- $P(x|f_s) = f_s\, P(x|s) + (1-f_s)\, P(x|b)$
  - $f_s = 0 \implies H_0, f_s > 0 \implies H_1$
- Remember this is a counting experiment → Expect Poisson Statistics. The uncertainty (standard deviation) on a count (e.g. n) is sqrt(n).
- Let's say you expect ~1000 events with f_s = .05 → ~ 950 background events expected, 50 signal events expected.
- Likelihood Ratio Test (Neyman-Pearson lemma) $\dfrac{P(x|H_1)}{P(x|H_0)} > k_\alpha$



TP	FP
FN	TN



Simulation



pencil & paper calculable from first principles

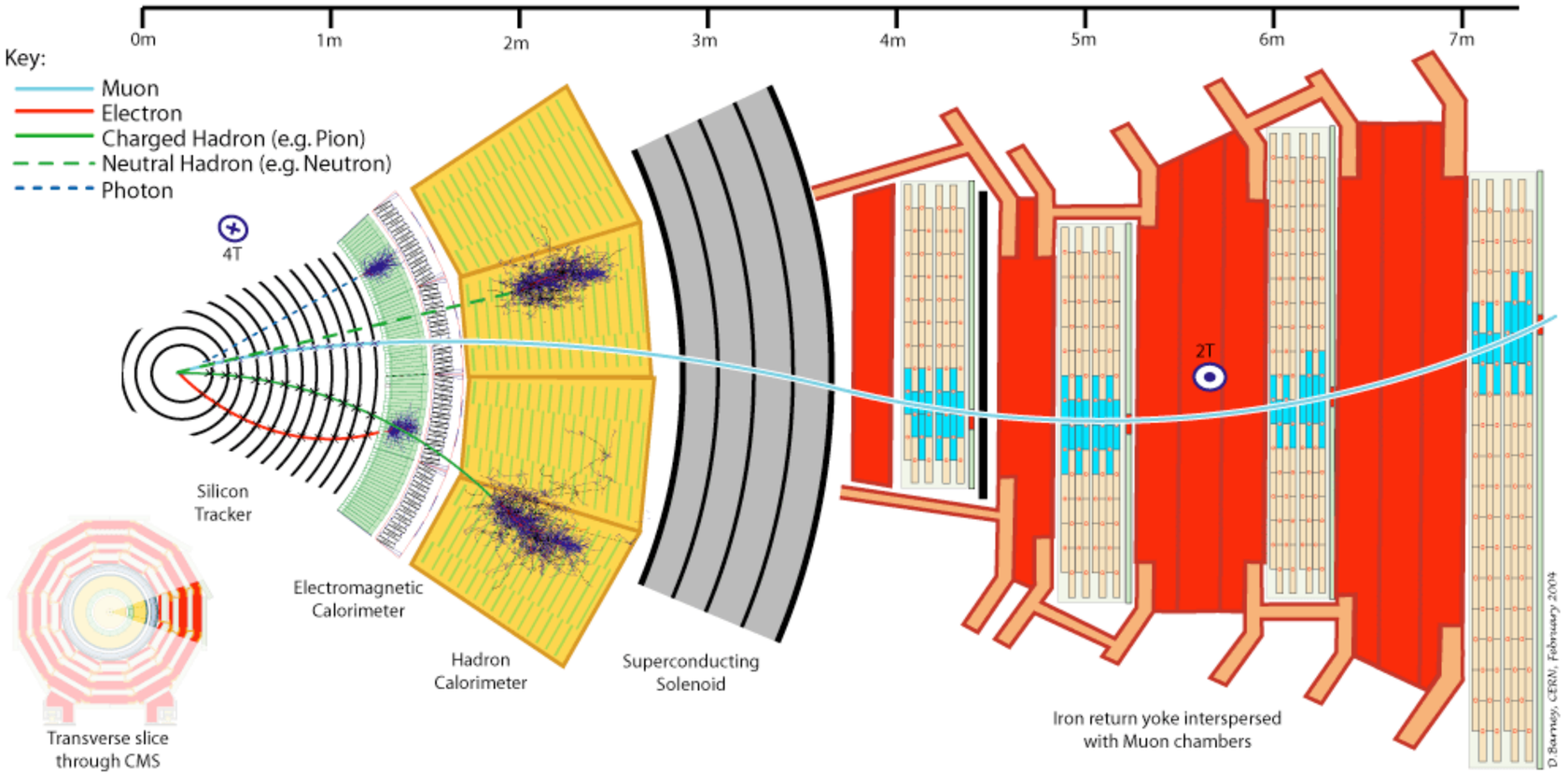
$p(z_1 \mid \theta)$

controlled approximation of first principles

$p(z_2 \mid z_1, \nu_1)$

phenomenological model

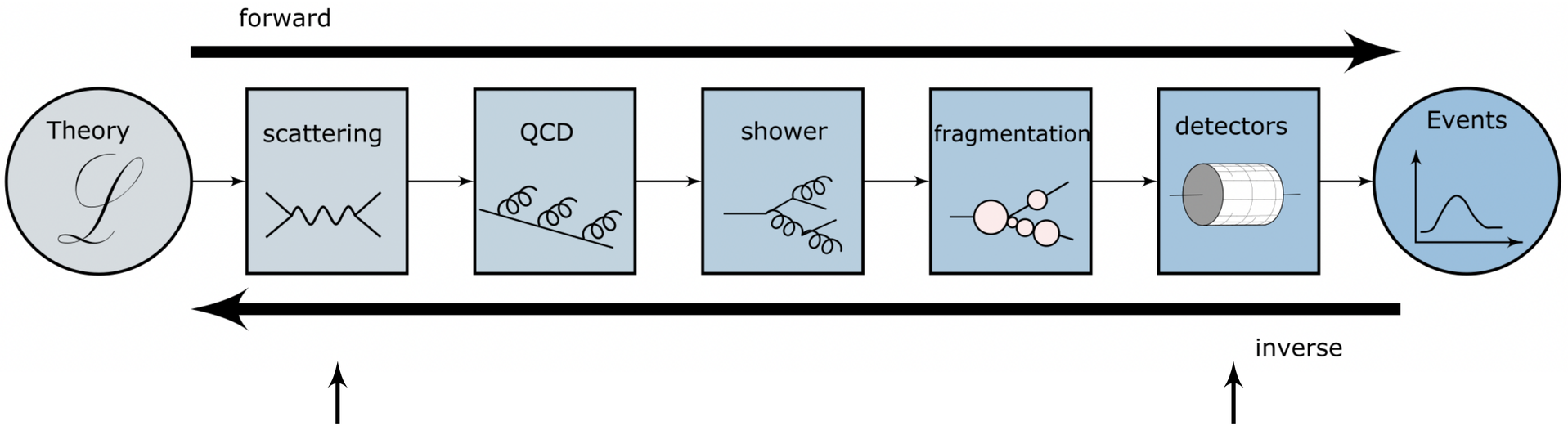
$p(z_3 \mid z_2, \nu_2)$



Detector Simulation **p(x | z3, ν_3):**

- detailed engineering (eg. CAD)
- in situ measurements of temperature, magnetic field, alignment, calibration constants
- first-principles description of interaction of particles with matter
- measured interaction of particles with matter

Simulation for LHC



Likelihood Approximations

- Need $P(\{x_d\}|\theta)$ of an observed event (i). The better we do, the more sensitive our measurements.
- Steps 2 (Hadronization) and 3 (Simulation) can only be done in the ***forward mode***…

  ➡ ***cannot evaluate the likelihood.***
- So we simulate a lot of events and generally use histograms (a crude *Probability Density Estimator (PDE) technique)*
  - $\{x_d\}$ = {100M Detector Channels} or even { particle 4-vectors } are too high dimensional.
    - Curse of dimensionality… more on this later
  - Instead we derive $\{x_d\}$ = { small set of physics motivated observables } → ***Lose information.***
    - ***Isolate signal*** dominating regions of $\{x_d\}$ → ***Lose efficiency.***
    - Sometimes use ***ML-based classifiers*** to further reduce dimensionality and improve significance
    - ***Profile the likelihood*** in 1 or 2 (ideally uncorrelated) observables.