Whirlwind tour of Monte Carlo simulation for particle physics

Presented by Jackie Brosamer

(most slides by Zach Marshall)

Physics 290E

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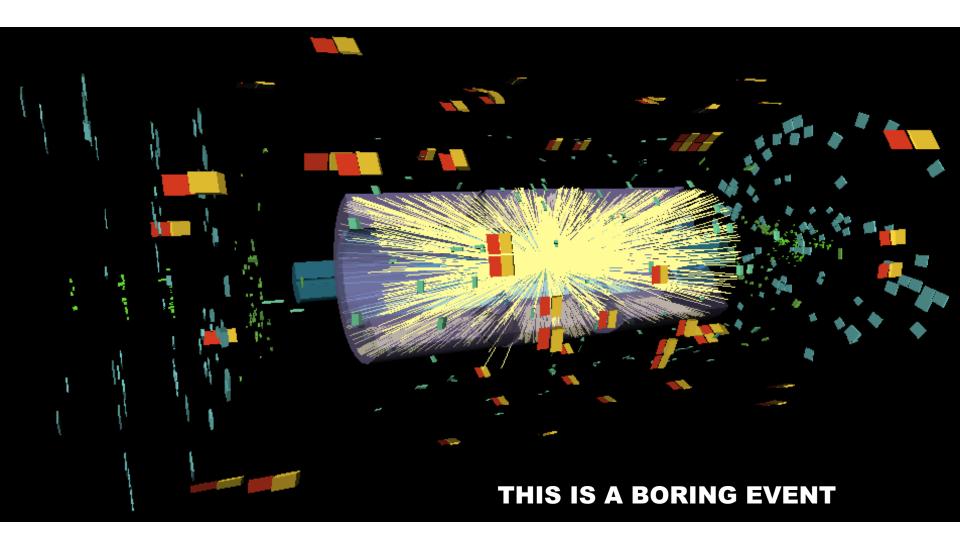
Outline and Disclaimers

- I'm going to try to tell you how to write a simulation from scratch
 - We'll spend few words about how to use the data you measure to improve your simulation ("tuning") at the end
- I'm about to blitz through about 15 different topics that usually each get their own workshops. STOP
 ME if you have questions, please.
- For obvious reasons, this talk is going to be *super* biased towards the LHC and ATLAS. But I can try to answer questions about other problems as well!

Why Simulate Anything

- We can (usually) only build one detector
 - What will we miss because of our detector design?
 - How would a slightly different detector affect things?
 - How will the detector stand up to radiation damage?
- Most detectors only measure voltages, currents, and times
 - It's an *interpretation* to say that such-and-such a particle caused such-and-such a signature in the detector
 - We can use simulation to correct our observables and understand our (in)efficiencies
- There is only one right answer in nature
 - What would new physics look like in our detector?
 - Could we find it under realistic conditions?
 - What are the biggest problems, and how do we ease them?
- A good simulation is the way to demonstrate to the world that you understand your detector and the physics you are studying

Write Me a Simulation for This:

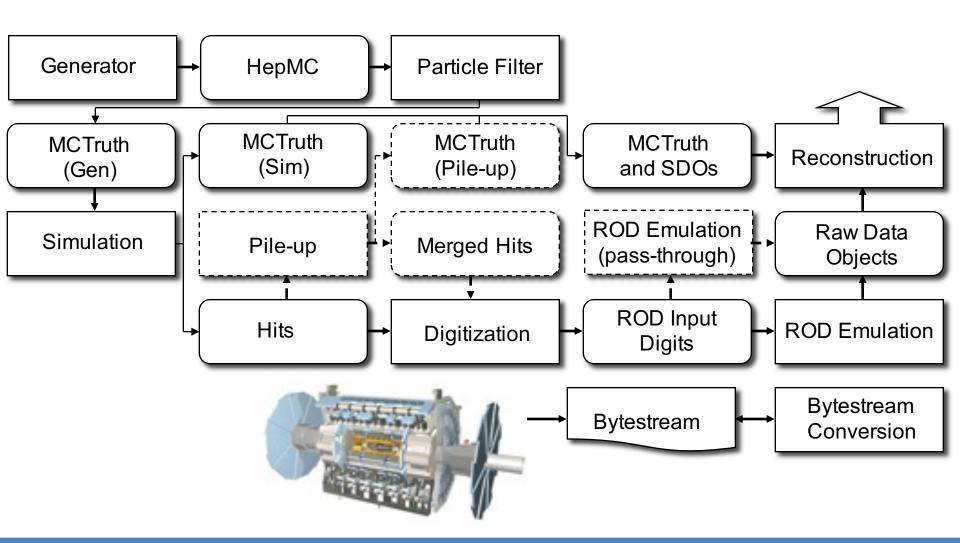


Simulation Basics

- 1. Break the problem up as much as possible
 - Do you understand *all the steps* of the system?
- 2. For each piece of the problem, write some code
 - Did you remember all the effects for each step?
- 3. Spend enough time on each piece that you get the accuracy that you need out of them
 - Not a moment longer!!
- 4. Cross your fingers and press the button

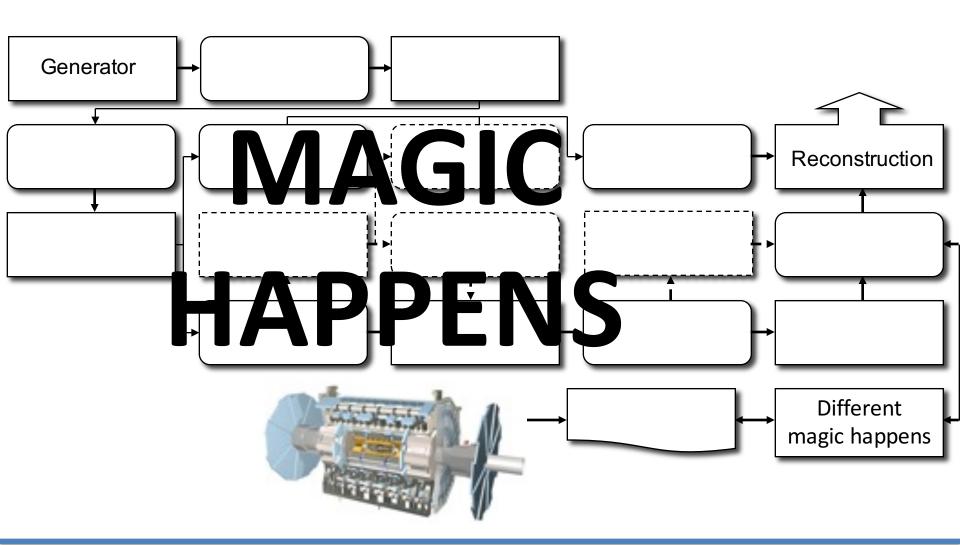
How does this look at the LHC?

Our LHC Simulation: The Dream



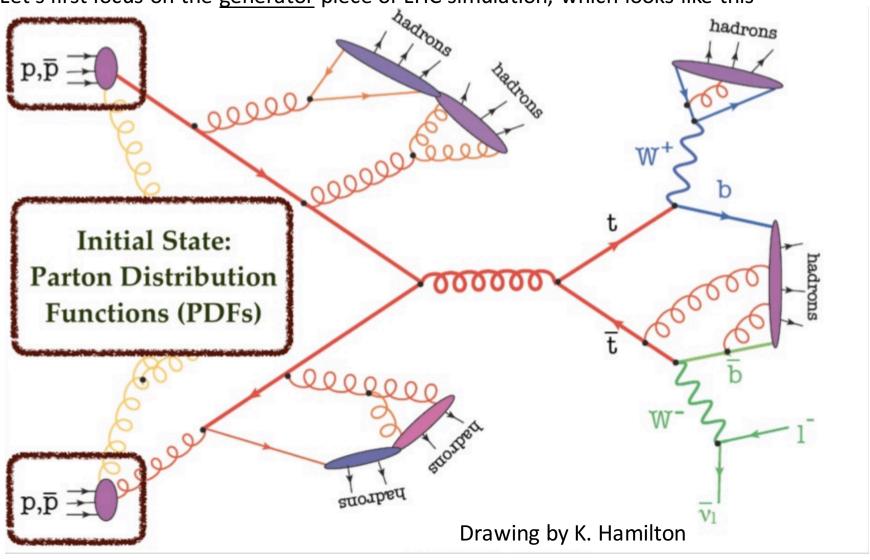
Our LHC Simulation: The Reality?

This is most people's view of the situation



MC event generation

Let's first focus on the generator piece of LHC simulation, which looks like this



Before we talk about simulating QCD

PROLOGUE: QCD REVIEW

QCD=SU(3) [nonabelian] gauge theory

$$\mathcal{L} = \underbrace{\bar{q}_{\alpha}^{a,j}}_{\alpha\beta} [i\,\gamma_{\alpha\beta}^{\mu}\,(\delta_{ab}\,\partial_{\mu} + i\,\underline{g}_{\mathrm{s}} t_{ab}^{r}\underline{g}_{\mu}^{r}) - m_{j}\,\delta_{ab}\,\delta_{\alpha\beta}] \underbrace{q_{\beta}^{b,j}}_{\beta} - \frac{1}{4}F_{\mu\nu}^{r}\,F^{r,\mu\nu}$$
 spin ½ quarks spin 1 gluons

$$\alpha, \beta, \ldots = 1, 2, 3, 4$$
 Dirac index $\mu, \nu, \ldots = 1, 2, 3, 4$ space time index $a, b, \ldots = 1, \ldots, N_{\rm C} = 3$ quark color index $r, s, \ldots = 1, \ldots, N_{\rm C}^2 - 1 = 8$ gluon color index $j, k, \ldots = 1, \ldots, N_{\rm F}$ flavor index .

coupling constant (only free parameter)

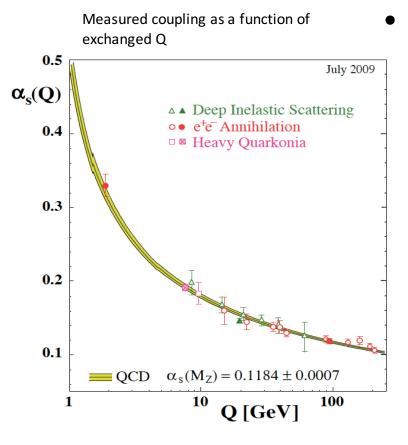
From T. Hebbeker
$$F^r_{\mu\nu}=\partial_\mu g^r_
u -\partial_
u g^r_\mu -g_{
m s}f^{rst}_
u g^s_\mu g^t_
u$$
 SU(3)

QCD Feynman diagrams

From T. Hebbeker

$$F^r_{\mu
u} = \partial_\mu g^r_
u - \partial_
u g^r_\mu - g_{
m s} f^{rst} g^s_\mu g^t_
u$$

Running of QCD coupling constant



$$\alpha_S(Q) = \frac{12\pi}{(33 - 2N_f) \ln\left(\frac{Q^2}{\Lambda^2}\right)}$$

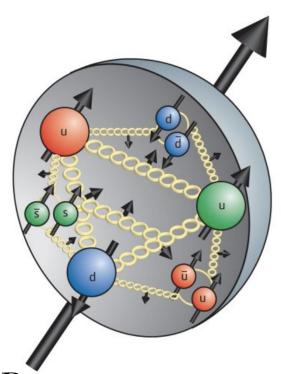
The QCD coupling (αs) depends on the energy and distance of interaction: it "runs"

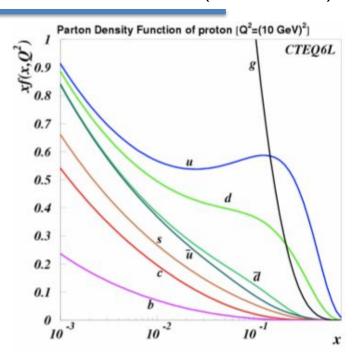
Partons (quarks and gluons) have "asymptotic freedom"

- At small R (<<1fm, αs<1),
 partons can be described as individual free particles using perturbative QCD
- At small R (>~1fm, αs~1),
 partons exist only in bound,
 colorless states called hadrons

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Parton density functions (PDFs)



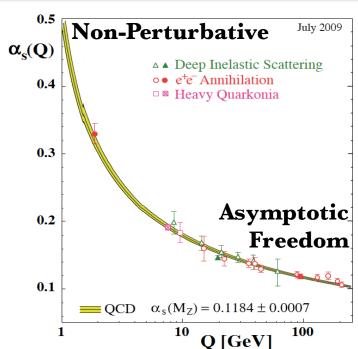


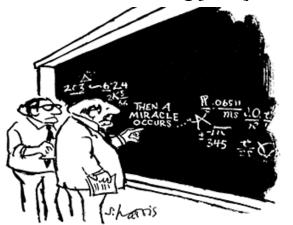
- Protons are composite particles composed of a collection of quarks and gluons
- PDFs are experimentally measurements of what fraction of the proton's momentum the different partons have

So you want to write a simulation? Start with a...

MONTE CARLO GENERATOR

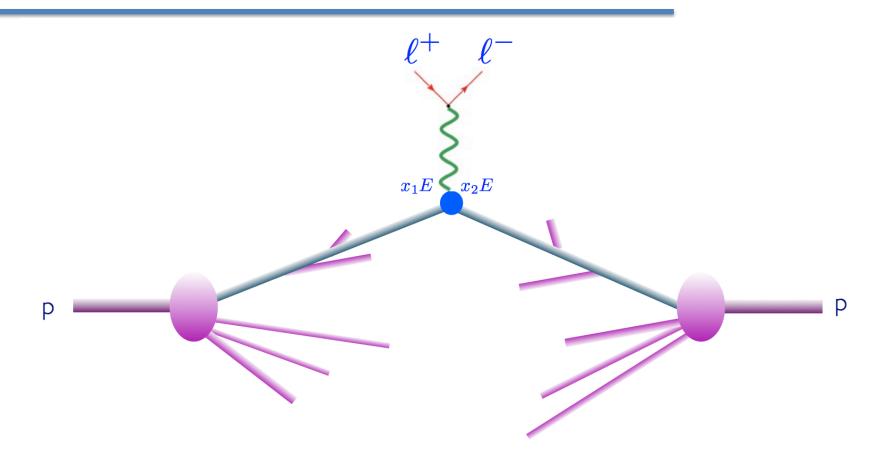
Start from the Strong Force



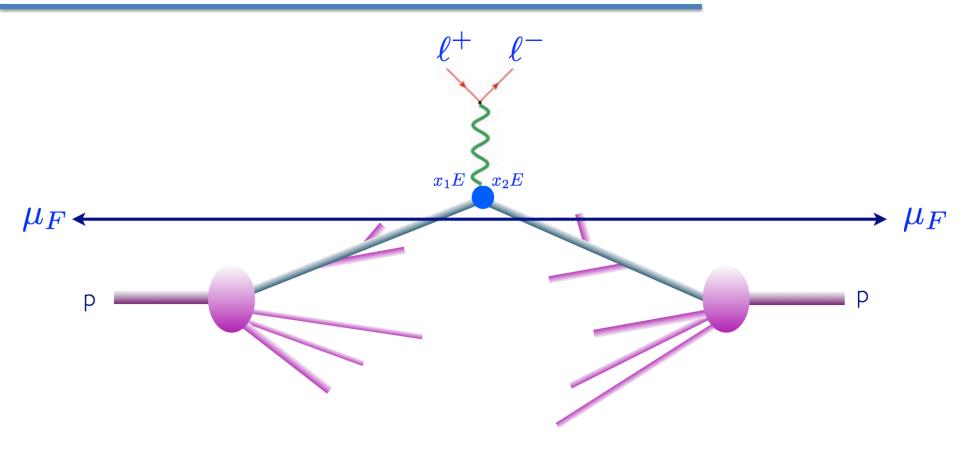


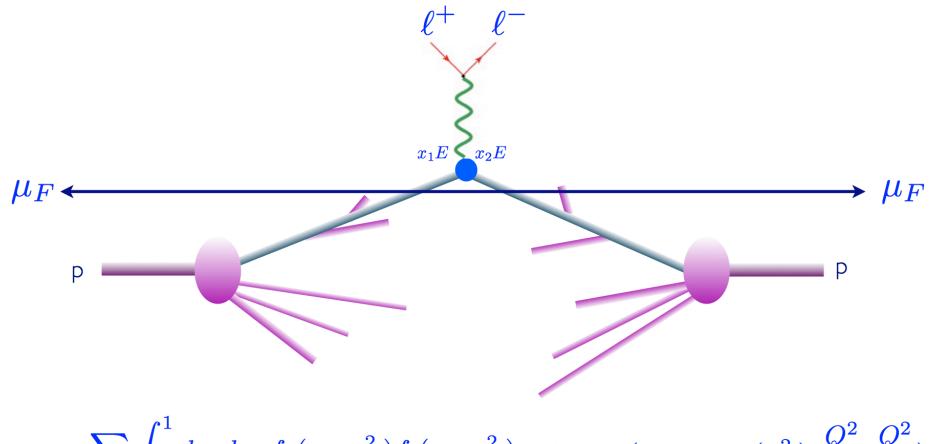
"I think you should be more explicit here in step two."

- The LHC collides protons that means we're dealing with QCD
- That means that one size does not fit all
- There are parts of the process where QCD will be a perturbative theory
 - This will be the easy part, and the popular part to work on
- There are part of the process where QCD will be non-perturbative
 - Here be dragons
 - Lots of lore, little knowledge



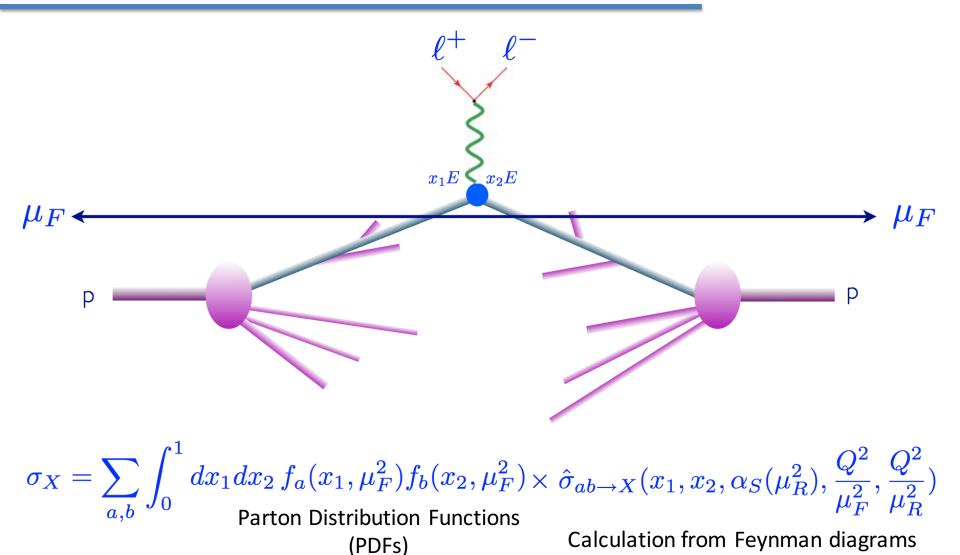
*from Fabio Maltoni





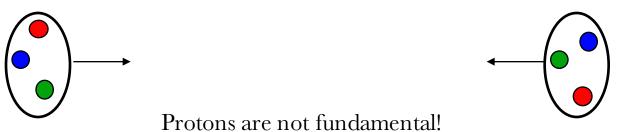
$$\sigma_X = \sum_{a,b} \int_0^1 dx_1 dx_2 f_a(x_1, \mu_F^2) f_b(x_2, \mu_F^2) \times \hat{\sigma}_{ab \to X}(x_1, x_2, \alpha_S(\mu_R^2), \frac{Q^2}{\mu_F^2}, \frac{Q^2}{\mu_R^2})$$

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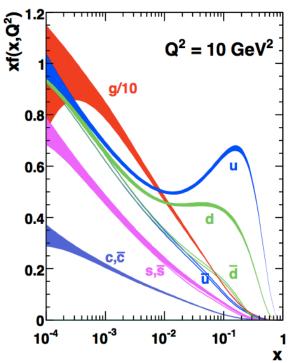
Parton Distribution Functions

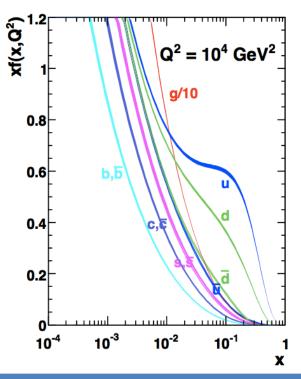


We need to know what exactly we are colliding...

MSTW 2008 NNLO PDFs (68% C.L.)

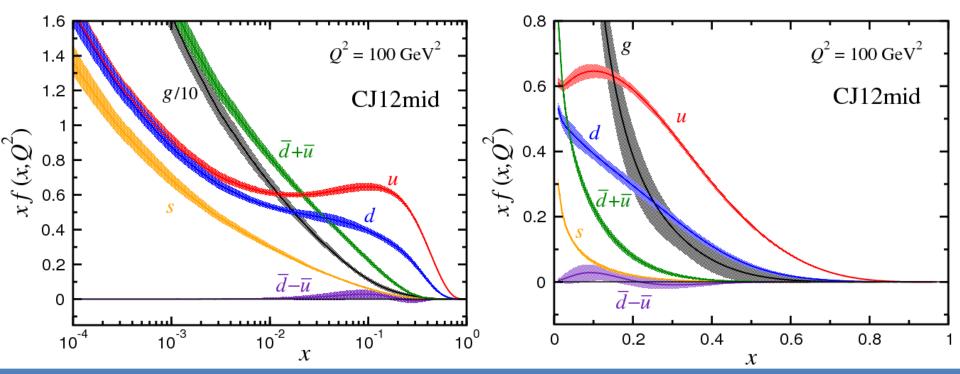
- Distributions of the partons within them have been well studied
- Described by the fraction of proton momentum carried by the parton (x) and the momentum transfer of the interaction (Q²)





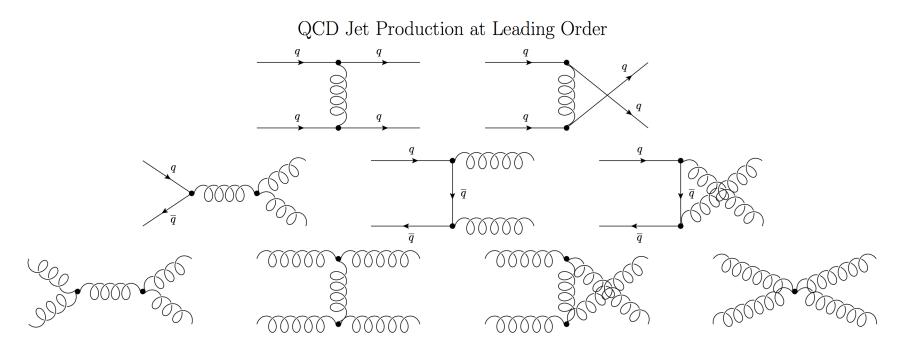
Other Options

- Proton structure is very much *not* an understood thing
 - There are aspects that we have a pretty good handle on
- CTEQ and MSTW/MRST are the two biggest players, and they have fundamental disagreements about some issues
 - This is only going to get more complicated... where is the top?



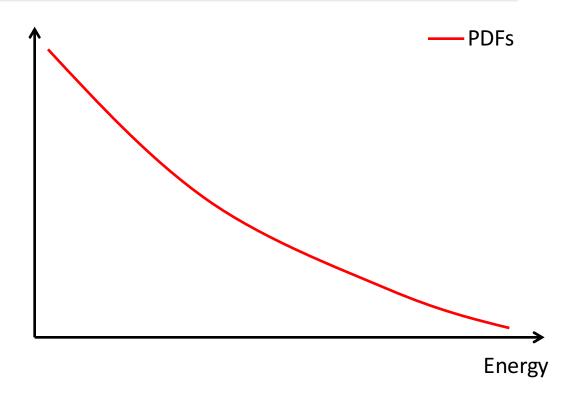
Cross Section History

• IN THE BEGINNING... there was $2 \rightarrow 2$

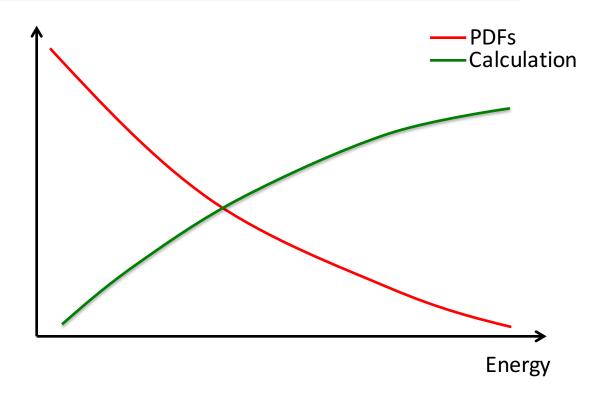


- But of course, we don't observe any of these things!
 - Let's start here, and we'll come back to more accurate models in a few minutes

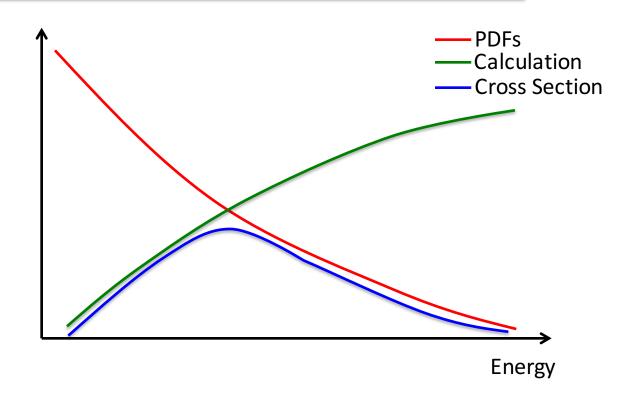
Making an Event



Making an Event



Making an Event

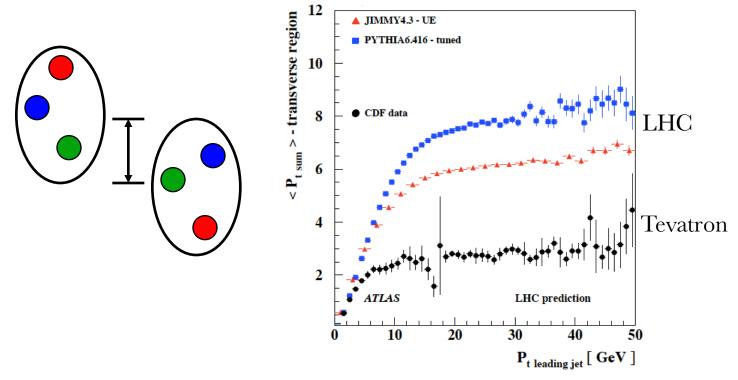


Now all we do is sample from that distribution, and we have an event!

Have to include (weighted appropriately) all the desired initial states and all the desired final states

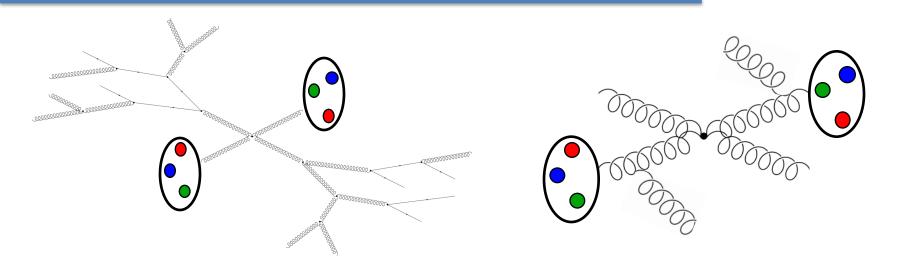
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The "Underlying Event"



- Additional parton-parton interactions are added
 - Probability rises with the 'overlap' between the protons
- These are particularly important at the LHC
 - Parton-parton cross section rises faster with center-of-mass energy than proton-proton cross section

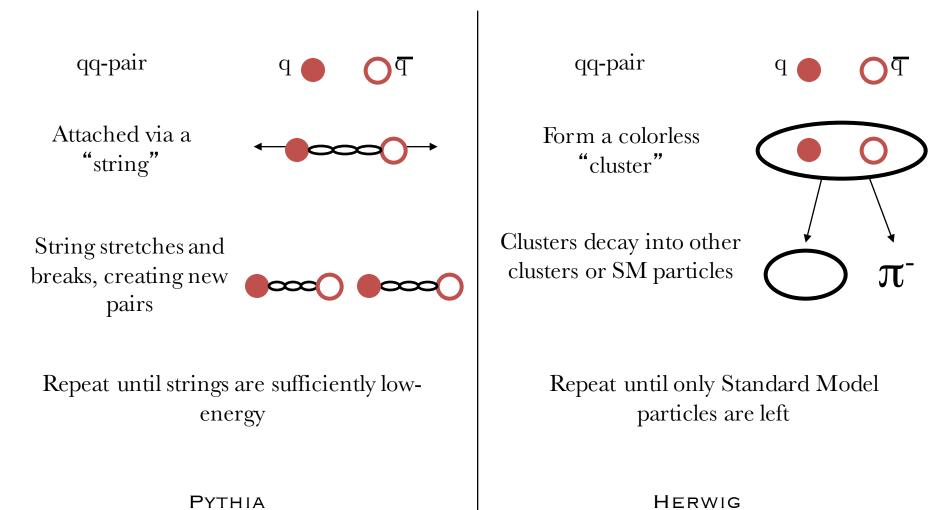
Parton Showers



- Partons are "evolved" down to ~1 GeV (the nonperturbative regime) using the DGLAP equations
 - Describe probability for one particle to branch into two
 - Accurate to leading logarithm
- Avoid double counting in two ways:
 - Showers must be strictly ordered in some variable
 - Common choices are Q^2 , p_T , or opening angle
 - Ensure that a shower does not move an event from one matrix element's phase-space into another
 - Create gg \rightarrow gqq in the matrix element *or* in the parton shower

Hadronization

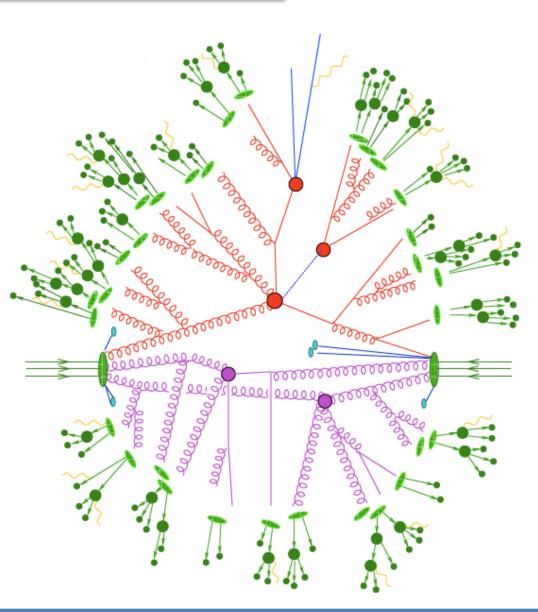
• Two approaches: string and cluster fragmentation



The Full Picture

- A generator is *meant* to go from a Lagrangian to that mess on the right
- The reality is WAY nastier than this
- Also, this picture is a bit misleading what QM process looks like that??

Really good generator paper: http://arxiv.org/abs/0911.5286



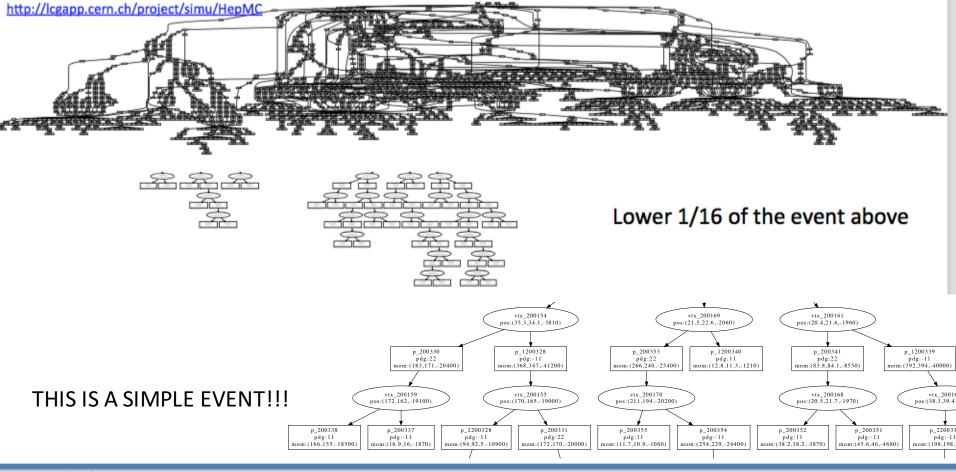
Four Types of Generators

- Some generators are used for cross-sections ONLY
 - These make matrix elements at most (most don't even do that)
 - MCFM is a very common one
- Most generators are used for matrix elements
 - These just give you parton (usually) four-vectors from the hard scatter
 - They (usually) give output in "public" HepMC format (almost human-readable, but it is a text file you can get this from a theorist)
 - Alpgen, MadGraph, MC@NLO, PowHeg are all pretty common
- Some can generate the rest of the event (or the whole event)
 - These give final state *particles*!! And we write EVNT (ATLAS) format.
 - Pythia/Herwig (fortran) and Pythia8/Herwig++/Sherpa (not fortran)
 - They include the parton shower, addition of multiple parton-parton interactions, initial state radiation, hadronization, and some decays
- Afterburners that improve the modeling of some observable
 - Tauola and Photos are super popular. Also EVTGEN and some HI stuff.
 - Jimmy should really be here it is an MPI afterburner for fHerwig

https://twiki.cern.ch/twiki/bin/viewauth/AtlasProtected/McGeneratorsForAtlas

Generator Myths and Evil

- The generator event record is NOT a connected tree of branchings
 - There may be loops, breaks, particles disappear or appearing...
 - Some generators in particular (Sherpa) omit some particles (Zs and Ws)
 - This is why you ALWAYS want to look at observables if they are available!!



Generator Myths and Evil

- The "hard process" in a generator is NOT just pQCD
 - Pythia in particular has many "tricks" to make the output agree with the data
 - Sherpa has tricks to make it "better than LO" (so we use an NLO PDF)
- Generally, matrix element generators run in two(+1) steps:
 - "Phase space integration" figure out what to generate
 - Matrix element generation, sometimes with weights according to where in phase space the event landed
 - [Optional: event unweighting, to try to remove the weights. Alpgen does this.]
 - Weights are >0, except in MC@NLO (virtual diagrams get negative weights)
 - This is why we like PowHeg
- Phase space integration is slow for high-multiplicity (days)
- Event generation (can be) relatively quick as long as you don't put some strange filter on the back end
 - ATLAS's lowest acceptable generation speed is ~5-10 events per DAY

Tuning

- All your generators are heavily *tuned* to reproduce data
 - Most of the hadronization data come from LEP
 - Most of the UE data come from the Tevatron and LHC
- There are NOT enough knobs to reproduce all data perfectly
 - fHerwig/Jimmy in particular has no knobs left
 - Big fight in the generator community: do we include more knobs or try to include models that fundamentally should reproduce the data and say they fail if they don't? We had to introduce *energy scaling* by hand in Herwig already!
 - The data are re-weighted to blow up low-p_T error bars and shrink high-p_T error bars and to emphasize different measurements in the tuning
 - The first step of tuning is actually selecting which knobs you will tune!
- ATLAS has quite a bit of tuning machinery in place
 - If you do a Standard Model measurement that is more than a cross-section, please write a Rivet routine to help the MC match your result!
- ATLAS has also dropped the ball on tuning quite a few times
 - MC11b was a TUNING problem, not a fundamental Pythia8 problem
 - Our constant struggle with Z samples started with a Z-p_T tuning problem, not from any fundamental difficulty modeling Z-bosons

Generators to Watch

MadGraph

- I really like the developers, and they are quite good
- They have big support for UFOs, which is probably the best theorist-experimentalist interface I've seen

• Sherpa

- ATLAS have basically never produced a bug-free Sherpa sample that
 I'm aware of but at least the developers are responsive! (We seem to
 be close-ish now...)
- They have big support for BlackHat, which is Lance Dixon's 4-vector generator that supports a *lot* of processes at NLO / NNLO

PowHeg

- Up side: some nice NLO modeling of various processes
- Down side: implemented process-by-process, so there is no good version control!

Stat Shot: ATLAS Generators

- ~30 MC Generators (how many can you name?)
 - Actually, it's been over 50 in run 1, from my count!
 - >>50 Combinations (Powheg+Pythia vs Powheg+Jimmy)
 - Remember: pick the model that is as accurate as you need to describe the physics that is important to you!
- 34 000 samples in the last MC campaign
- MC for 2011: \sim 5B events
- MC for 2012: ~6.6B events
 - Fastest is a few minutes / 5k events. Slowest is 5 events per **DAY**
 - We record data at ~ 400 Hz, for reference \odot
- We are still getting better at event generation
 - That is one place where we really need help and better interactions with theorists and with each other

One down...

NOW WE HAVE A MODEL FOR PRODUCING HADRONS

On to the Simulation!

- The simulation is agnostic about what happened in the matrix element
- It *only* cares about "final state particles" (stable particles)
- What is "final state" depends on the experiment!!
 - ATLAS uses $c\tau < 10$ mm.
- Remember that your generator does not know *anything* about your detector geometry or magnetic field. So you don't want it to handle anything that would move through a detector element or bend significantly in a field

Simulation: Where do we begin?

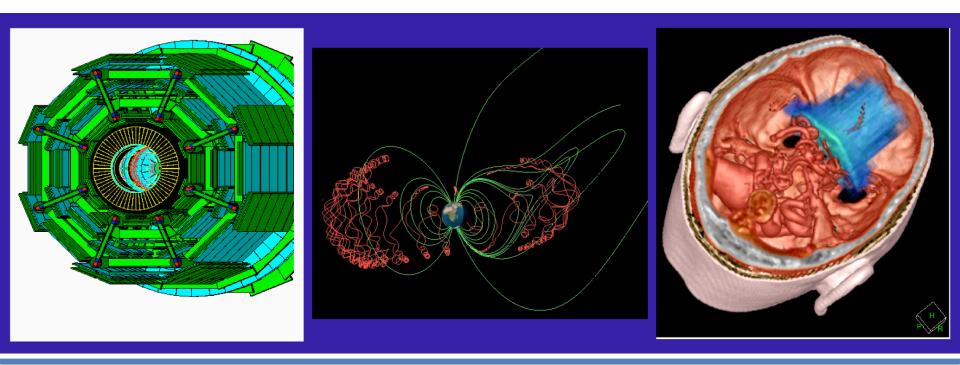
- There are two options for a detector simulation
- We can go straight for the final state
 - "A pion will look like such-and-such"
 - Smear things directly
 - These are *always* home-brewed
- We can simulate every little detail along the way
 - Usually we use either Geant4 (GEometry ANd Tracking) or FLUKA (public software)
- In ATLAS we try to do both
 - Actually we have half a dozen "kinds" of simulation that are combinations of these two approaches...

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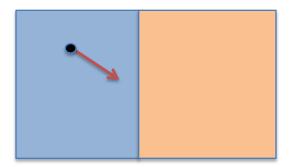
Geometry and Tracking

- People do all kinds of crazy stuff with Geant4
 - Space physics, medical physics, collider physics, nuclear physics, protein folding, radiation surveys...



Simulation Primer

• To Geant4, every problem looks like this:



- It has the concepts of:
 - Particle (if it isn't standard model, G4 has no idea about it!)
 - Material (you define everything except the elements)
 - Magnetic field (you define it at every point)
 - Physics process (you get to pick from their list!)
- It is *only a toolbox* it's up to you to put the pieces together
 - Don't expect it to be any smarter than you are.

Simulation Step 1



Question 1: What am I looking at, and what can it do?

Grab a particle from the 'stack' and see what type of particle it is

If necessary, figure out where it is

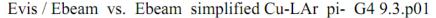
Nature is continous

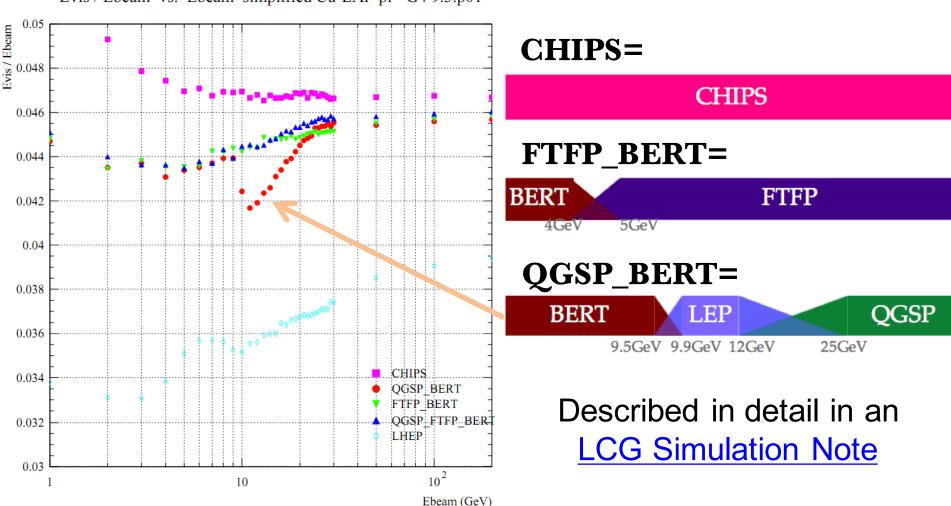
- But numerical models are not!
 - All processes become discrete, including "transportation"
- Use phenomenological models tuned to experimental data
 - Never solve a Lagrangian!!
- Some interactions are easy
 - Photon conversion
- Some are hard to model
 - The nucleus gets its own simulation!
- Some have a variety of models
 - ATLAS covers keV to TeV physics:
 - >9 orders of magnitude!!
 - Good in an energy range
 - Transitions can be problematic!!



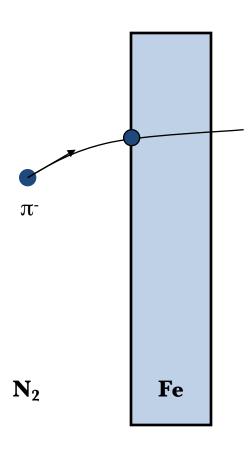
Different Models

Hadronic physics is really nasty stuff





Simulation Step 2

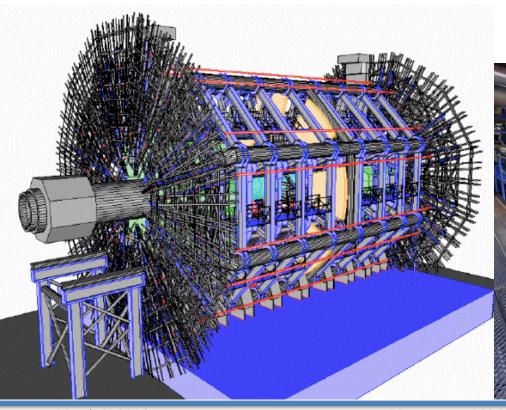


Question 2: How far may I go?

Never move farther than a volume boundary - the physics could change!!

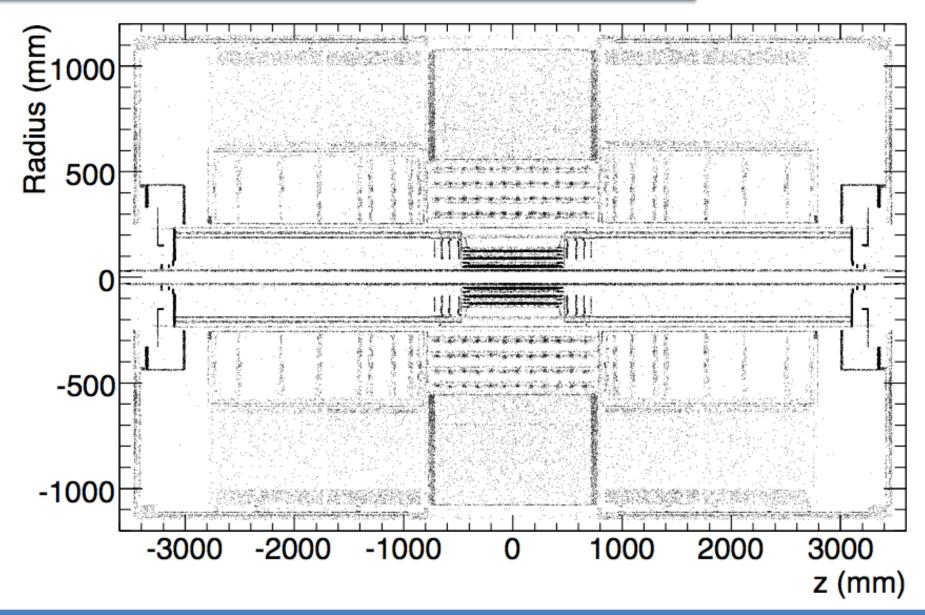
Detector Descriptions

- Need a consistent detector description
 - We are still making things more 'realistic'
 - But some things aren't worth worrying about
 - Once you are done: just weigh the detector!
 - Of course, with collisions, we can get fancier...

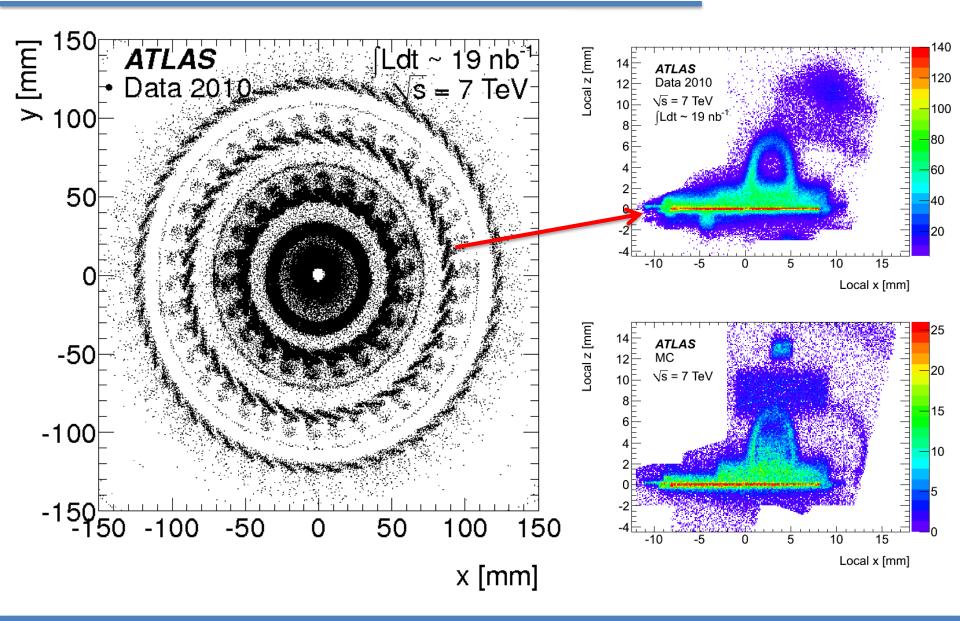




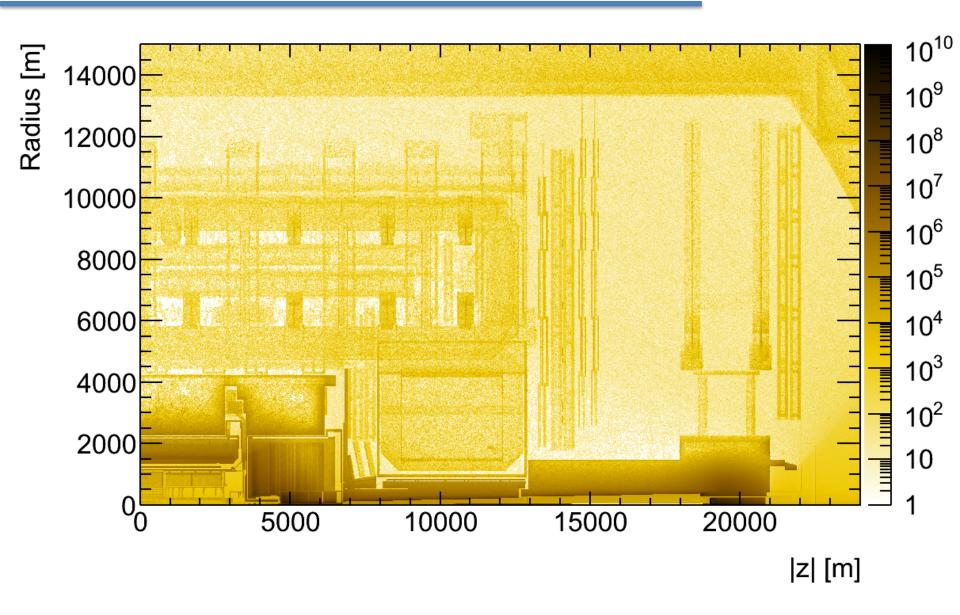
Photon Conversions



Hadronic Interactions

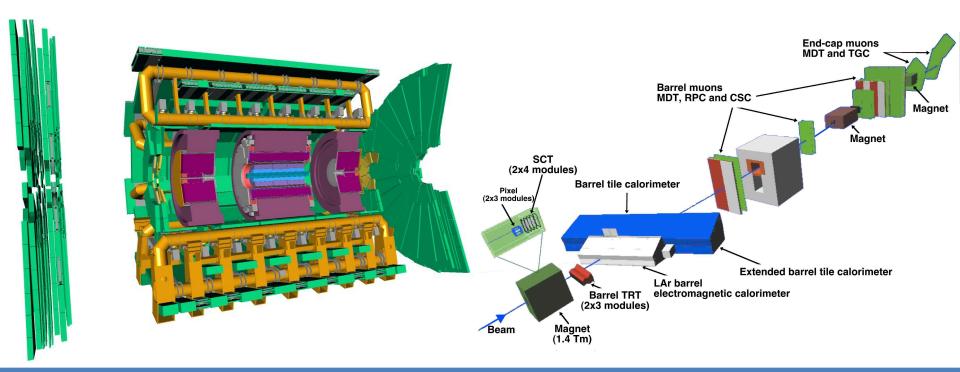


The Full Detector

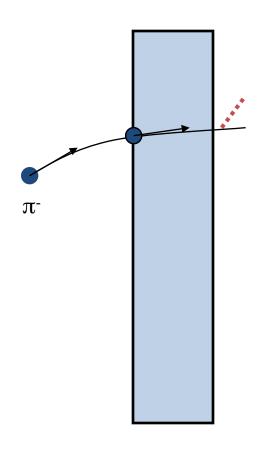


Strange Geometries

- We have commissioning layouts for cosmic ray data taking
 - See the calorimeter and muon wheel positions on the left there?
- We have layouts for test beams, IBL, NSW, Lucid, ZDC, ALFA
- If you want to simulate it, you had better write a geometry!



Simulation Step 3



Question 3: What will happen next?

Check on all physics models. For a pion, this means multiple scattering, bremsstrahlung, nuclear interactions, decay, ionization...

Add any new particles to the stack

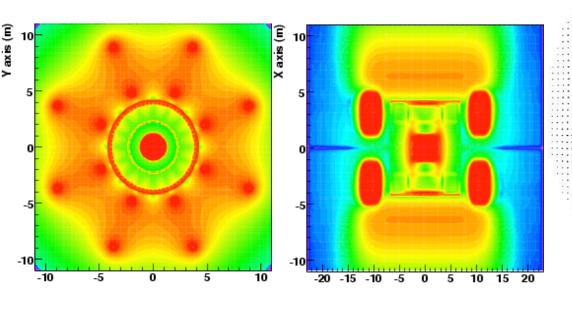
Adjust energy and momentum accordingly

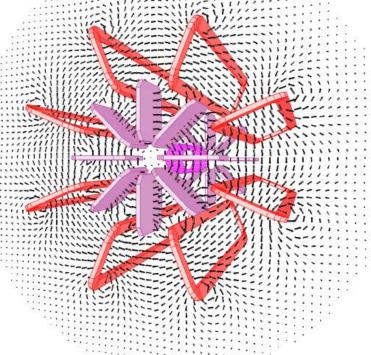
The Magnetic Field

- No hope for simulating on the fly must have a *map*
 - Do they match *reality*?
 - Do they match the *geometry*? (I always love finding a magnetic field map that has the wrong solenoid position...

 ATLAS keeps a handful of hall cubes on the detector to measure the field

- Parameterizes elsewhere



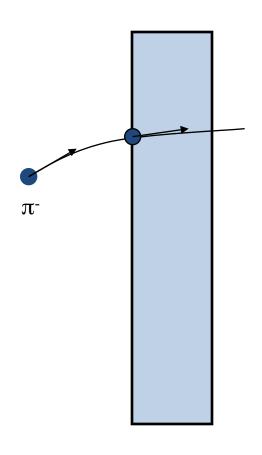


Where Do Those Steps Go?

- Each iteration is called a "step"
- The number of steps dictates the speed of the simulation
 - The best code changes get us \sim 3-10% speed ups; the best physics changes get us 20-50% speed ups
- Most time just moving stuff around in the calorimeter
 - Here is the table for 50 ttbar events
- 50% of your simulation time is spent moving e^{\pm} and γ below 10 MeV

Process	Inner Detector	calorimeter	Muon System
Transportation	1.76×10^{6}	1.46×10^{7}	2.31×10^{5}
MSC	2.31×10^{5}	1.48×10^{7}	5,200
Photoelectric Effect	6,760	1.37×10^{6}	2.32×10^{5}
Compton Scattering	14,800	1.66×10^{6}	5.03×10^{5}
Ionization	1.03×10^{5}	4.81×10^{6}	9.71×10^{5}
bremsstrahlung	6,060	1.22×10^{6}	1.92×10^{5}
Conversion	416	86,800	18,100
Annihilation	271	87,000	18,500
Decay	212	1,670	402
Other Hadronic Interaction	2,190	6.66×10^{5}	1.23×10^{5}
Other Process	426	25,400	5,720
Total	2.13×10^{6}	3.93×10^{7}	2.69×10^{6}

Simulation Step 4



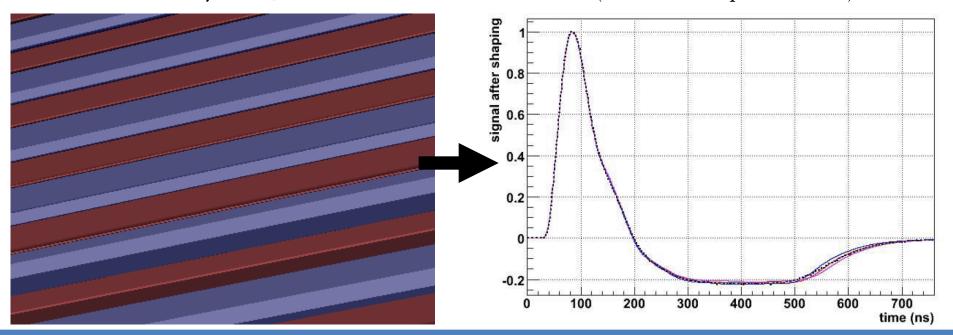
Question 4: Anything else to do?

The user is allowed a hook at the end of this "step" to perform any necessary action, for example to **make a record of energy deposition**

All particles are tracked to zero energy or their exit of your world (this is different from the old days of simulation...)

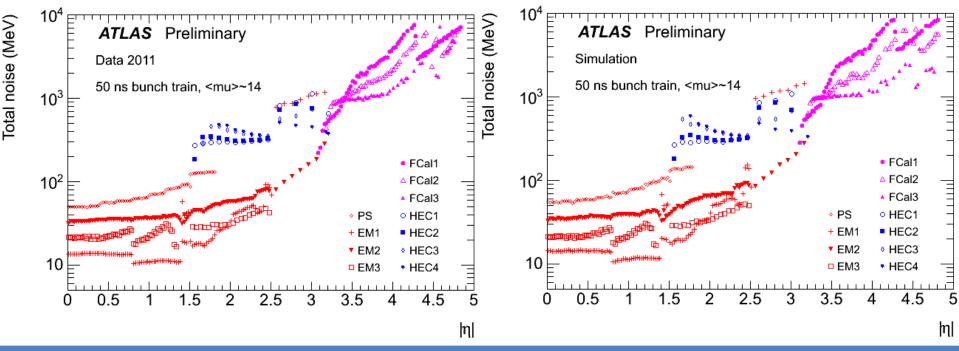
Detector Modeling: Digitization

- Geant4 has no idea how our detector *reacts* to particles
 - It only deposits *energy* with a position and time
- First we have to do some *energy collection*, then we have to do a *conversion* into something we can read out
 - How that's done depends completely on the detector
 - Have to take into account detector timing, pulse shapes, charge collection effects (sometimes conditions dependent)
- This is very hard, and all custom ATLAS code (with lots of parameters)



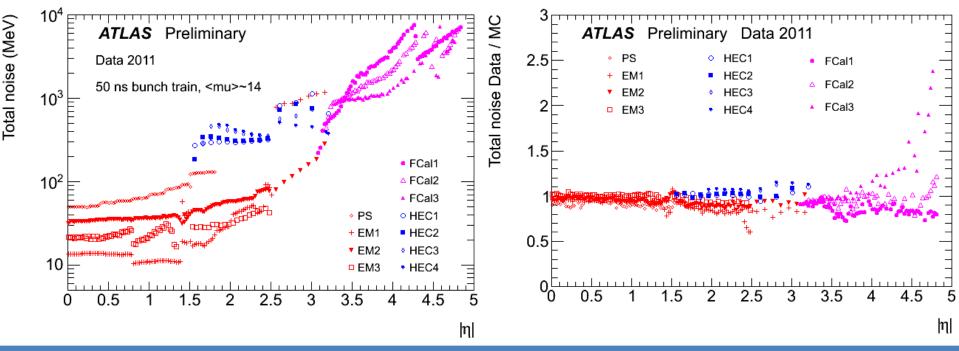
Modeling Noise

- One critical thing to get right is electronics noise
- You can imagine these models can get very complicated
 - Especially if you have to try to model channel cross-talk
- We are generally pretty good at this stuff, but there are still effects that we don't get right



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Things Change

- ATLAS has to deal with many types of "conditions"
 - Beam spot, misalignments, which parts are masked or disabled...
- To save time and energy, conditions are always applied as late as possible
 - Channels can be masked long after simulation finishes!
 - But moving the interaction region is a whole other story...
- Some misalignments have to be applied in the simulation
 - We have to be VERY careful that things don't overlap! Geant4 could get lost... and then the result is the bad kind of random



Exaggerated (10x) sagging in the EM barrel calorimeter

So you have finished your Monte Carlo!

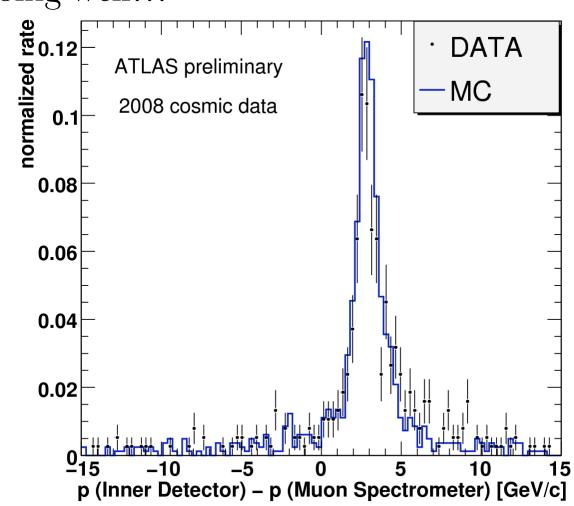
NOW PRESS THE BUTTON...

How Do You Know It Worked?

• When the simulation can recreate something it *was not designed for*, you're doing well...

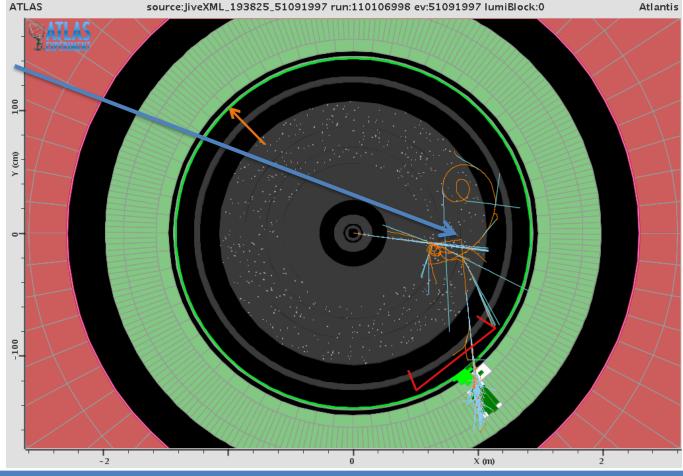
Cosmic rays are one interesting test. Use the simulation to propagate muons from the Earth's surface to the detector!

Here: energy loss in the calorimeter by a muon



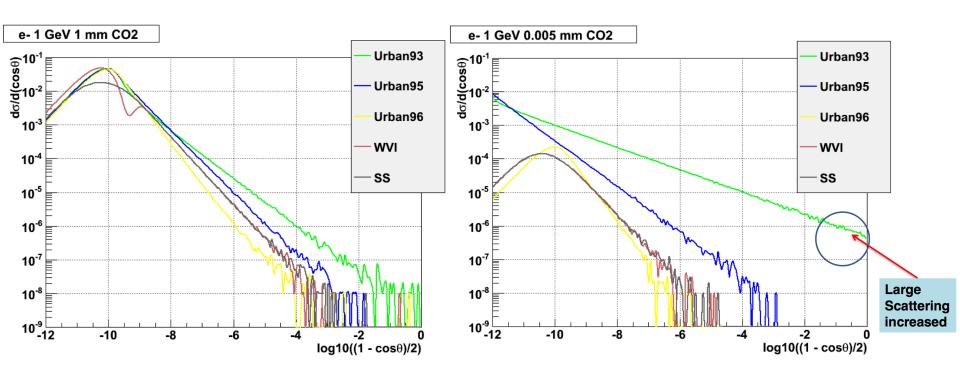
What Happens When It Didn't?

• A visualization of an ATLAS simulation bug



Extrapolating

- Turned out to be a "feature" in extrapolation of the multiple scattering parameterization
- Always know your model's region of validity!



What Could Possibly Go Wrong??

- What is the production threshold for very low energy stuff?
- How long may a particle fly before you need to treat it with the detector simulation?
- Did the approximations you made apply?
- Have you checked for CRAZY things?
- Are the models all accurate enough for you?

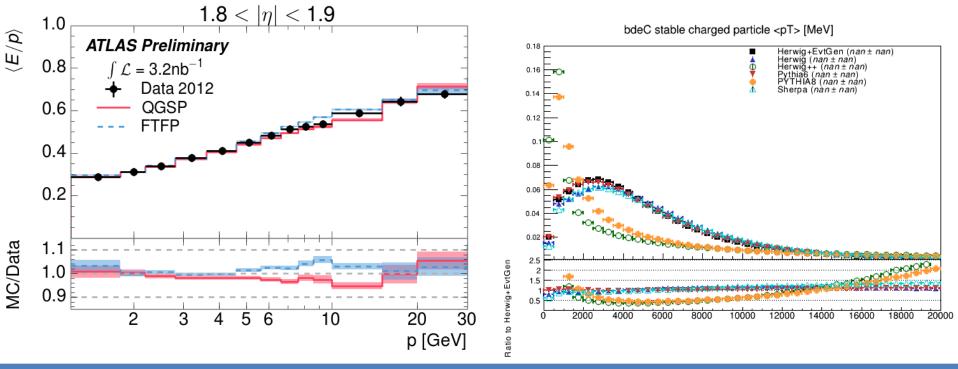
What Could Possibly Go Wrong??

- What is the production threshold for very low energy stuff?
 - Cost: ~6 months of simulation
- How long may a particle fly before you need to treat it with the detector simulation?
 - Cost: ~1 month of simulation
- Did the approximations you made apply?
 - Cost: ~1/2 month of simulation
- Have you checked for CRAZY things?
- Are the models all accurate enough for you?
 - Costs: Lots of sleepless nights and quite a few painful emails

Yup, been there, done that, got the T-shirt...

Feeding Back

- If your model isn't good enough, then find a measurement that can tell you something about *the specific reason* it isn't
- It's a rare treat when this works, and it takes some very creative thinking to come up with something that does the job



The Real Fun

- The best part of working on an MC is getting to learn everything
- Problems with the detector...
 - Did we install muon chambers upside down?
 - Do we know how big the gaps and shielding blocks are in our detector?
 - Did they accidentally build the ends of the detector differently?
 - Is there a leak, so that we might have to change detector gas?
- Problems with computing...
 - Random numbers ©
 - From float v double to trampolining in virtual classes
- Problems with the physics...
 - − What happens when a highly charged particle passes through the detector? ~100e kind of charged, like a monopole? Did we model those effects?
 - What is a quirk?
 - What's the rate of beam halo from the two sides of the detector?

Let's Stop Here...

- I've tried to run through all of the main issues with writing your own simulation
- There are a LOT of things that we could talk more about
 - The devil is in the details
 - ESPECIALLY in the details of how to make the data and the MC simulation that you've written line up

What are you most curious about?



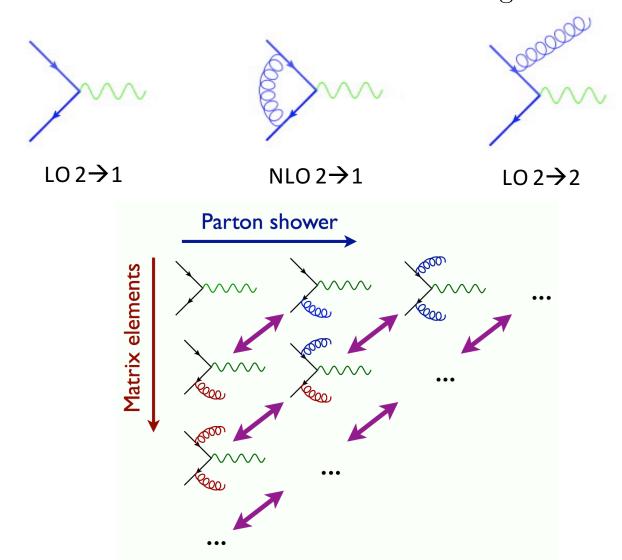
Is always tilted slightly to the left for some reason



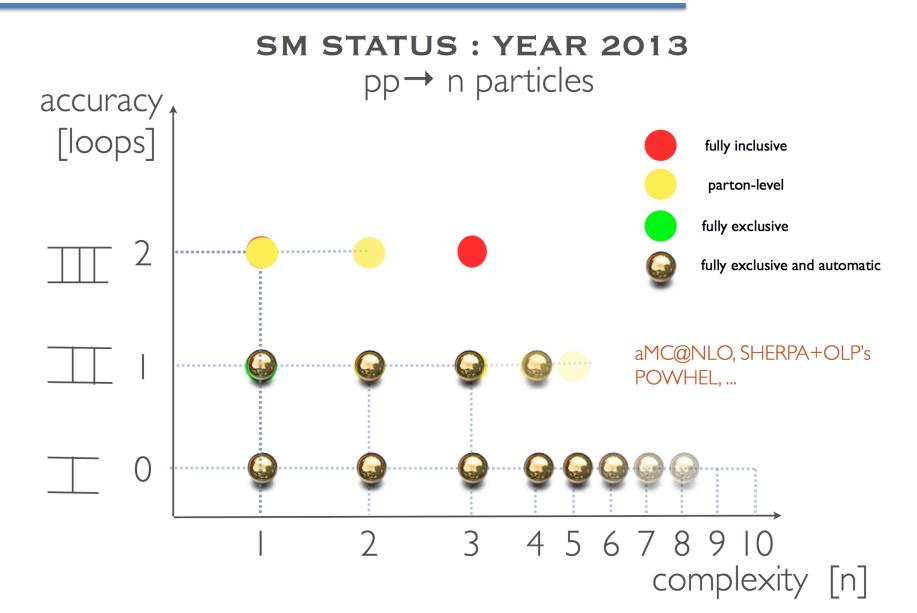


The Cross Section

• Here we want to use the most accurate thing we can



Generator Status



- At the core of MC method is ability to generate (pseudo)random numbers
 - □ Issue is generating truly random numbers
 - © Computers are (so far) deterministic
 - If each computer had an ADC, could use Josephson's noise
 - But in practice resort to pseudo-random sequences $x_{i+1} = f(x_i, x_{i-1}, ..., x_2, x_1)$
 - Requirements
 - Longest period possible

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We had serious discussions about this at the LHC (using thermal noise to generate random numbers) Why wouldn't you want to do it?

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Reproducibility! We want things to be random but reproducible!! 33

Random Numbers

- Ex: linear congruent generators
 - $^{\circ}$ Generate integers in range [0..*m*-1]

$$\mathfrak{F}_{n_{j+1}} = (a \ n_j + c) \ \% \ m$$

- Sequence is periodic, depends on increment c and modulus m
- © Ex: m = 2147483399, $a=40692 \rightarrow T=m-1 \approx 2 \times 10^9$
- Generate floats

$$r = n_{j+1}/m \in [0..1]$$

$$x = a + r(b-a) \in [a..b]$$

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Aside: Random Numbers

• These are multiplicative congruent generators

$$u_{i+1} = [u_i \times m] \mod 2^b$$

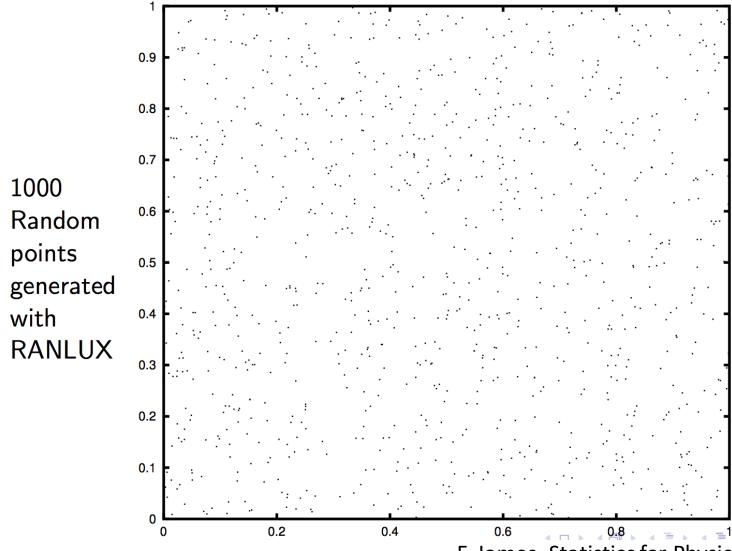
During the software development for the LEP experiments, two different physicists were surprised to see a simulated event exactly the same as one they had seen before. With a period of 10^9 , the probability of this happening is $10^{-4.5}$ per event.

• So they invented an upgrade with a period 2^{18} longer:

$$u_{i+1} = [(u_i + u_{i-1}) \mod 2^b \times m] \mod 2^b$$

What is Random? (I)

Looking at Random Point Sets



What is Random? (II)

Looking at Quasirandom Point Sets

