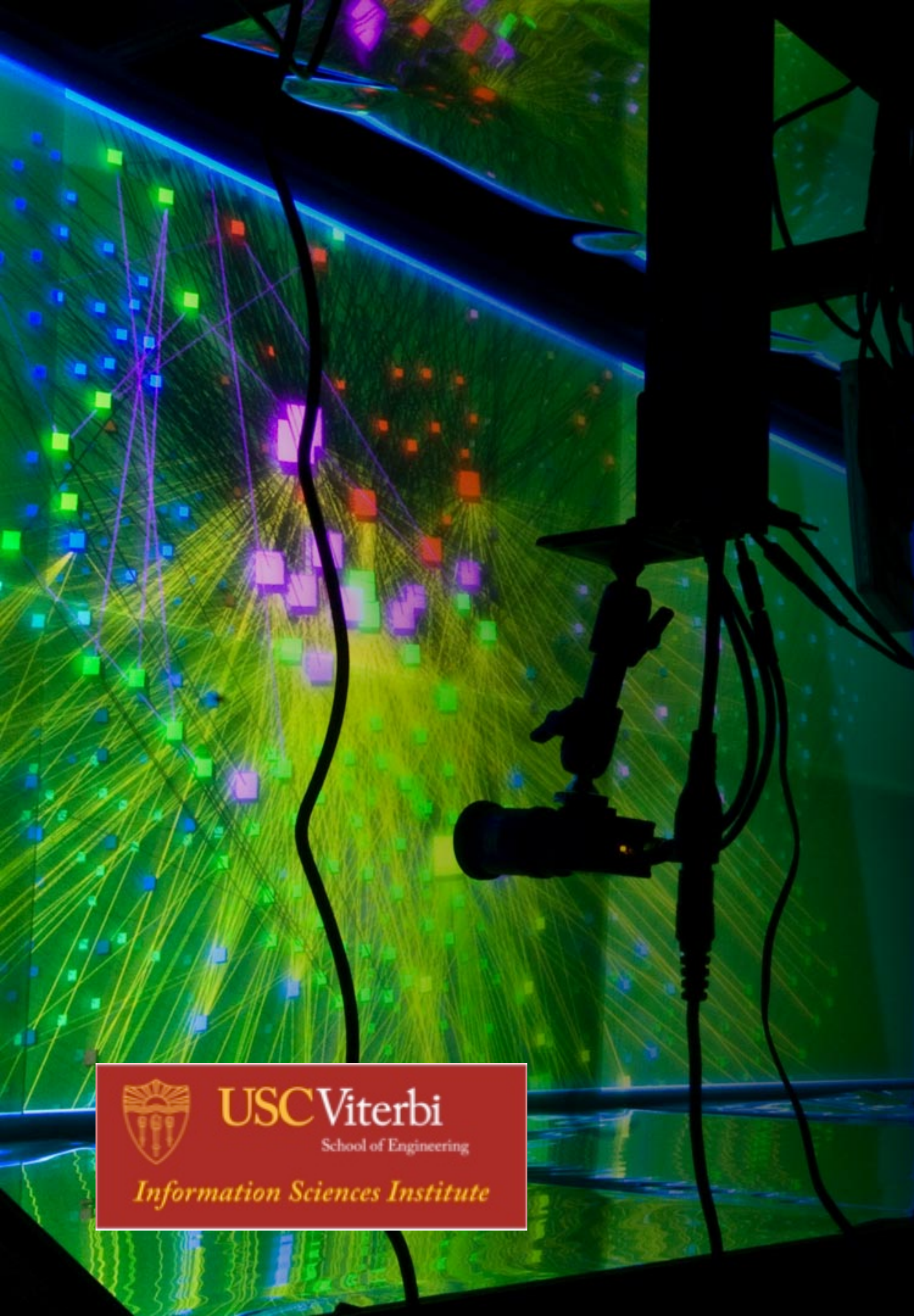

GEANT4 Hadronic Cross Section Optimizations

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RESEARCH ENGAGEMENT INNOVATION

Background CrossSection Calculation

*51 real events simulated in ~2 hours (provided by Soon)

- Hadronic CrossSections
  - ~10% of total wall clock time*
  - Deep call chain with no hot spots
    - Reduce call chain length
    - Reduce time spent in calculation

Scope	WALLCLOCK (us).[0,0] (E)	WALLCLOCK (us).[0,0] (I)
Experiment Aggregate Metrics	1.29e+09 100 %	1.29e+09 100 %
main		1.29e+09 100 %
131: G4UImanager::ApplyCommand(char const*)		1.28e+09 99.3%
422: G4UIcommand::DoIt(G4String)		1.28e+09 99.3%
210: G4UIcontrolMessenger::SetNewValue(G4UIcommand*, G4String)		1.28e+09 99.3%
277: G4UImanager::ExecuteMacroFile(char const*)		1.28e+09 99.3%
234: G4UIbatch::SessionStart()		1.28e+09 99.3%
215: G4UIbatch::ExecCommand(G4String const&)		1.28e+09 99.3%
170: G4UImanager::ApplyCommand(char const*)		1.28e+09 99.3%
422: G4UIcommand::DoIt(G4String)		1.28e+09 99.3%
210: G4RunMessenger::SetNewValue(G4UIcommand*, G4String)		1.28e+09 99.3%
287: G4RunManager::BeamOn(int, char const*, int)		1.28e+09 99.3%
155: G4RunManager::DoEventLoop(int, char const*, int)		1.26e+09 97.1%
237: G4RunManager::ProcessOneEvent(int)		1.26e+09 97.1%
264: G4EventManager::DoProcessing(G4Event*)	9.34e+05 0.1%	1.26e+09 97.1%
185: G4TrackingManager::ProcessOneTrack(G4Track*)	2.98e+06 0.2%	1.25e+09 96.6%
125: G4SteppingManager::Stepping()	5.61e+06 0.4%	1.17e+09 90.8%
180: G4VProcess::AlongStepGPIL(G4Track const&, double, double, double&, G4GPILSelection*)	2.27e+05 0.0%	5.64e+08 43.6%
458: G4Transportation::AlongStepGetPhysicalInteractionLength(G4Track const&, double, double, double&, G4GPILSelection*)	9.47e+06 0.7%	5.20e+08 40.2%
321: G4PropagatorInField::ComputeStep(G4FieldTrack&, double, double&, G4VPhysicalVolume*)	1.00e+07 0.8%	3.45e+08 26.7%
286: G4ChordFinder::AdvanceChordLimited(G4FieldTrack&, double, double, CLHEP::Hep3Vector, double)	2.51e+06 0.2%	2.29e+08 17.7%
202: G4MagInt_Driver::AccurateAdvance(G4FieldTrack&, double, double, double)	2.40e+06 0.2%	1.17e+08 9.1%
185: G4ChordFinder::FindNextChord(G4FieldTrack const&, double, G4FieldTrack&, double&, double, double*, CLHEP::He	4.28e+06 0.3%	9.35e+07 7.2%
323: G4MultiLevelLocator::EstimateIntersectionPoint(G4FieldTrack const&, G4FieldTrack const&, CLHEP::Hep3Vector const	2.29e+06 0.2%	1.02e+08 7.9%
210: G4ChordFinder::ApproxCurvePointV(G4FieldTrack const&, G4FieldTrack const&, CLHEP::Hep3Vector const&, double	1.02e+06 0.1%	6.01e+07 4.6%
298: G4VIntersectionLocator::IntersectChord(CLHEP::Hep3Vector const&, CLHEP::Hep3Vector const&, double&, double	8.82e+05 0.1%	1.52e+07 1.2%

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Cross Section Usage

- Cross section calculation is used to:
  - Determine (probabilistically) whether an interaction occurs in traversing a particular geometric volume.
  - Then determine reaction and outcomes.
- CrossSectionDataStore instances created for 65 different processes.
  - Each of these uses different models for different energy domains, particles, materials.
  - Data is (usually) represented in sub-classes of G4PhysicsVector.
- We have been working on increasing the performance of the CrossSection calculations.

Two strategies

- Improved caching of CrossSection results
  - 1 cache entry per ***triple*** (process/particle/material)
  - Completed (In the pipeline toward production code)
- Surrogate model for CrossSection calculations
  - Prototype completed
  - Initial results are promising

Caching CrossSection Results

- Currently, there is a 1-entry cache per process for XC calculations.
- Observation
  - There is an interleaving of recent calls to GetCrossSection with the same sets of particle, material, process, and energy.
  - Results in same cross section value
  - True even though energy is a double! (The physics is causing this.)
- Optimization
  - Expanded cache recent the most recent cross section for particle, material, process triple.
- Measurements
  - 17% of calls would benefit from this cache
  - 29% of GetCrossSection cycles are from these calls.
  - ~18k triples total
  - ~3k triples would benefit

Caching CrossSection Results

- Implementation
  - Hashtable per process (i.e. per CrossSectionDataStore)
    - std::unordered_map
  - One cache entry for each particle/material pair
    - Key
      - material
      - particle definition
    - Value
      - particle energy
      - cross section (including xsecelm)

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Modified CrossSection Calculation

```
G4double G4CrossSectionDataStore::GetCrossSection(part,mat){
  ...
    entry = process_cache_map[(part,mat)];
    if(entry->energy == part->GetKineticEnergy()){
       xsecelm = entry->xsecelm;
       crossSection = entry->crossSection;
    } else
       //Calculate CrossSection the regular way (including xsecelm)
       ...
       entry->xsecelm = xsecelm;
       entry->crossSection = crossSection;
    }
    return crossSection;
}
```

Caching CrossSection Results

- Performance increase
  - 1.8% reduction in wall clock time (51 real events simulated over 2+ hours)
- Presented at Hadronic working group
  - What is the state of this being put in the production code?

Surrogate Model: XS Usage

In the Hadronic section of the code:

- Particle/Material/Process Triples
  - 50% of cycles in ~10 triples
  - 90% of cycles in ~85 triples
  - Total ~18k triples
- Implementing for tens of triples can utilize fast path for nearly all of the calls.

Surrogate Model

- The cross section of an interaction between a particle and a complex material is (re-computed) on each call.
  - Look up each isotope. Use element and isotope abundance tables to weight the result.
- Typical materials
  - Air, Stainless steel, $PbZO_4$, Cu, Teflon, Circuit boards, …
- Stainless ={ ^{12}C, ^{13}C, (^{14}C), ^{54}Fe, (^{55}Fe), ^{57}Fe,^{58}Fe, ^{60}Fe, (^{50}Cr), ^{52}Cr, ^{53}Cr, ^{54}Cr, ^{55}Mn, ^{58}Ni, ^{60}Ni, ^{61}Ni, ^{62}Ni, ^{64}Ni, ^{28}Si, ^{29}Si, ^{30}Si}
- Previous versions of G4 used "pseudoelements" based on natural abundances. This was judged in adequate for the "what happened" calculations.

Building the Surrogate Model

- Create fast path for CrossSection calculations (offline or in initialization).
  - Identify common (particle, material, process) triples.
    - The number chosen depends on how much extra storage can be used.
  - Create Surrogate Model
    - Over sample using existing physics model.
    - Down sample to a simpler model with bounded error.
      - Evenly spaced sample points in E, ln(E), or log(E)
      - Or piecewise linear with adaptively placed nodes (Douglas-Peucker method).
    - Solve a linear system to adjust Y values to remove bias from the sign of the errors in each interval.
    - Represent the reduced model using existing G4PhysicsVector sub-classes.
- For triples where the fast path exists, use it for the mean free path (interaction length) calculations.
  - Single query of a G4PhysicsVector
- When an interaction occurs (rare)
  - Perform original physics calculations

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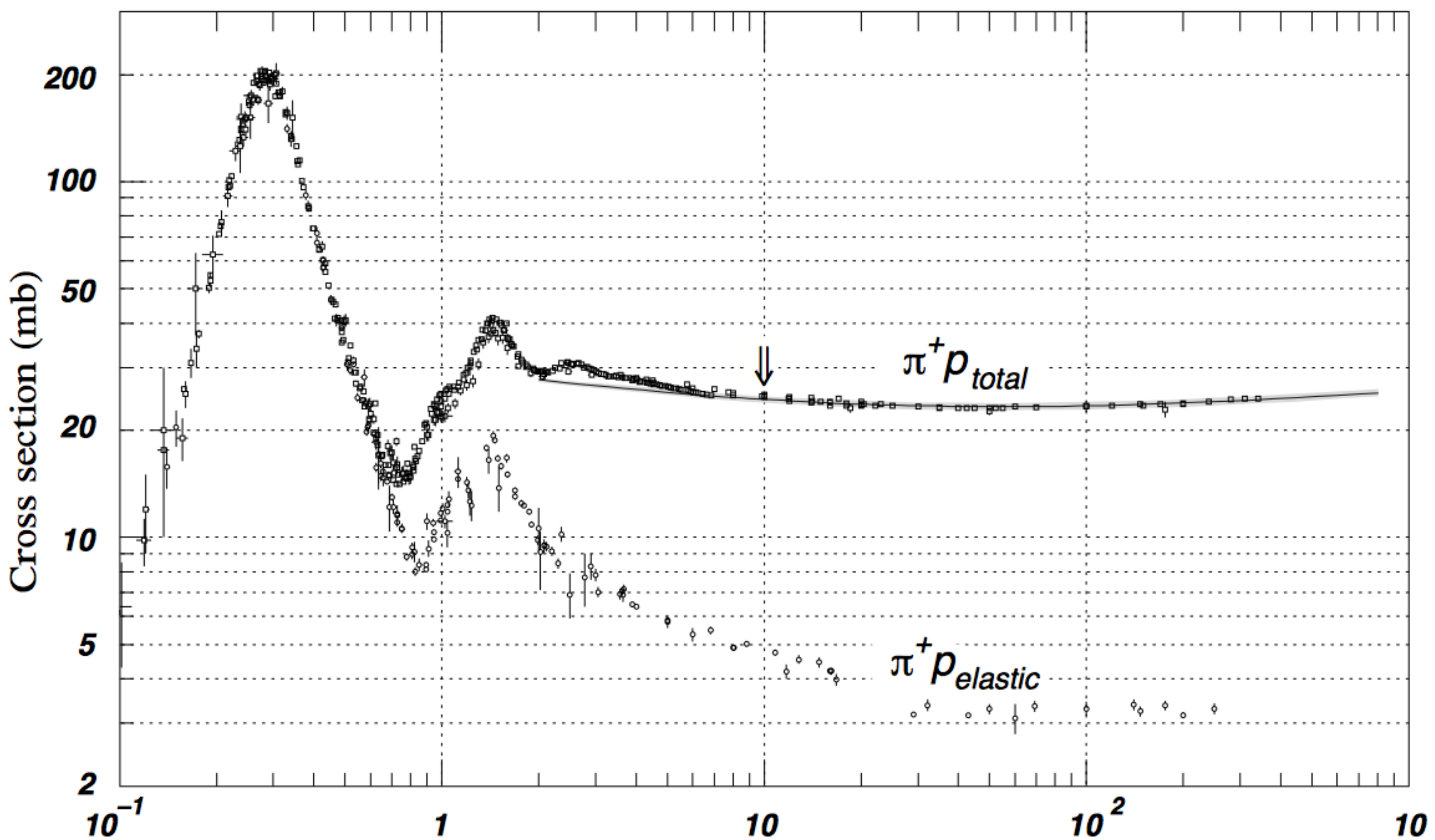
Building the Surrogate Model

Over sample the existing code.



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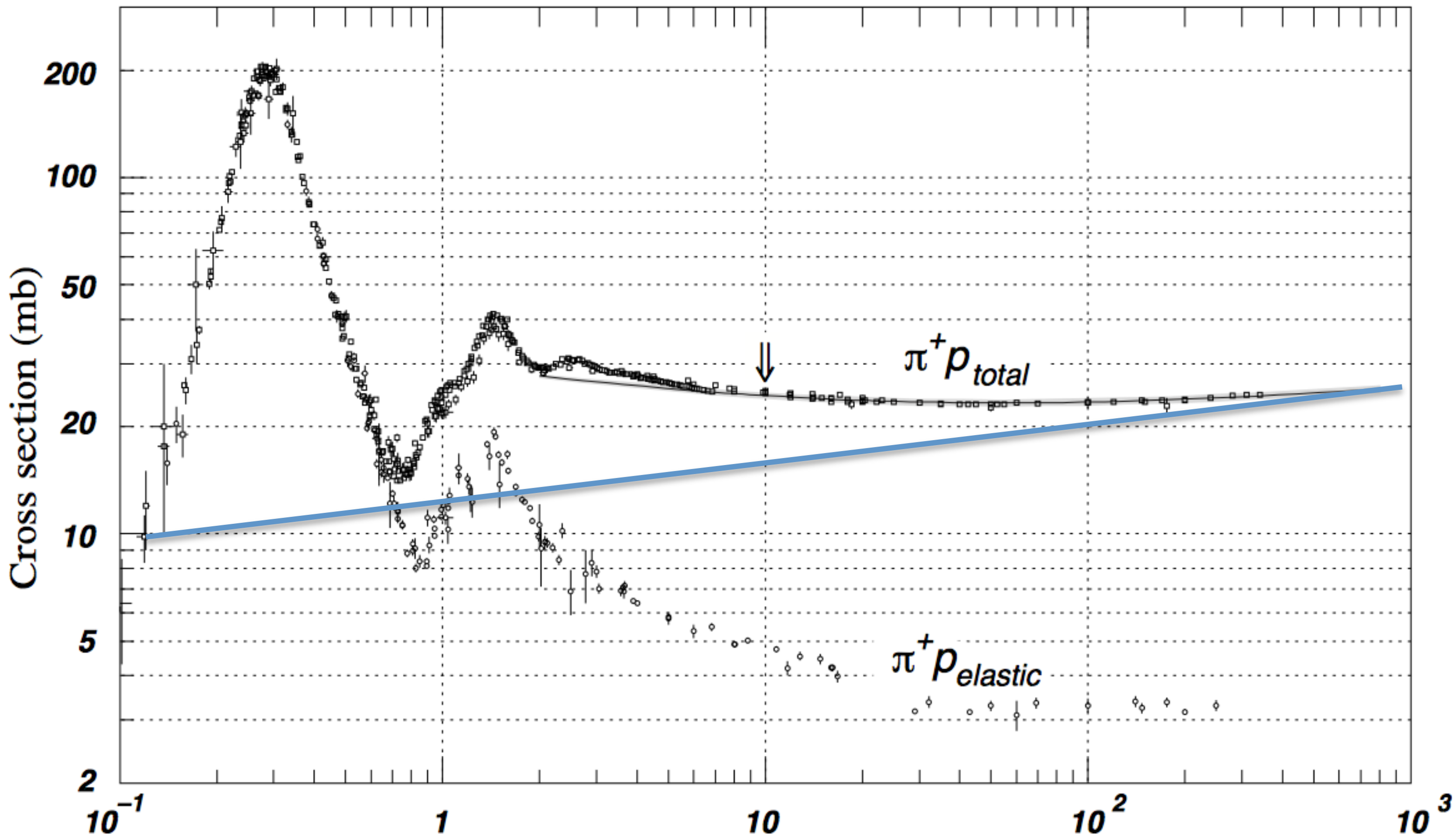
Douglas-Peucker Approximation.

Start with a piecewise-linear approximation.
In each segment, Add the point at the largest error.
Until total error is within the required bound.



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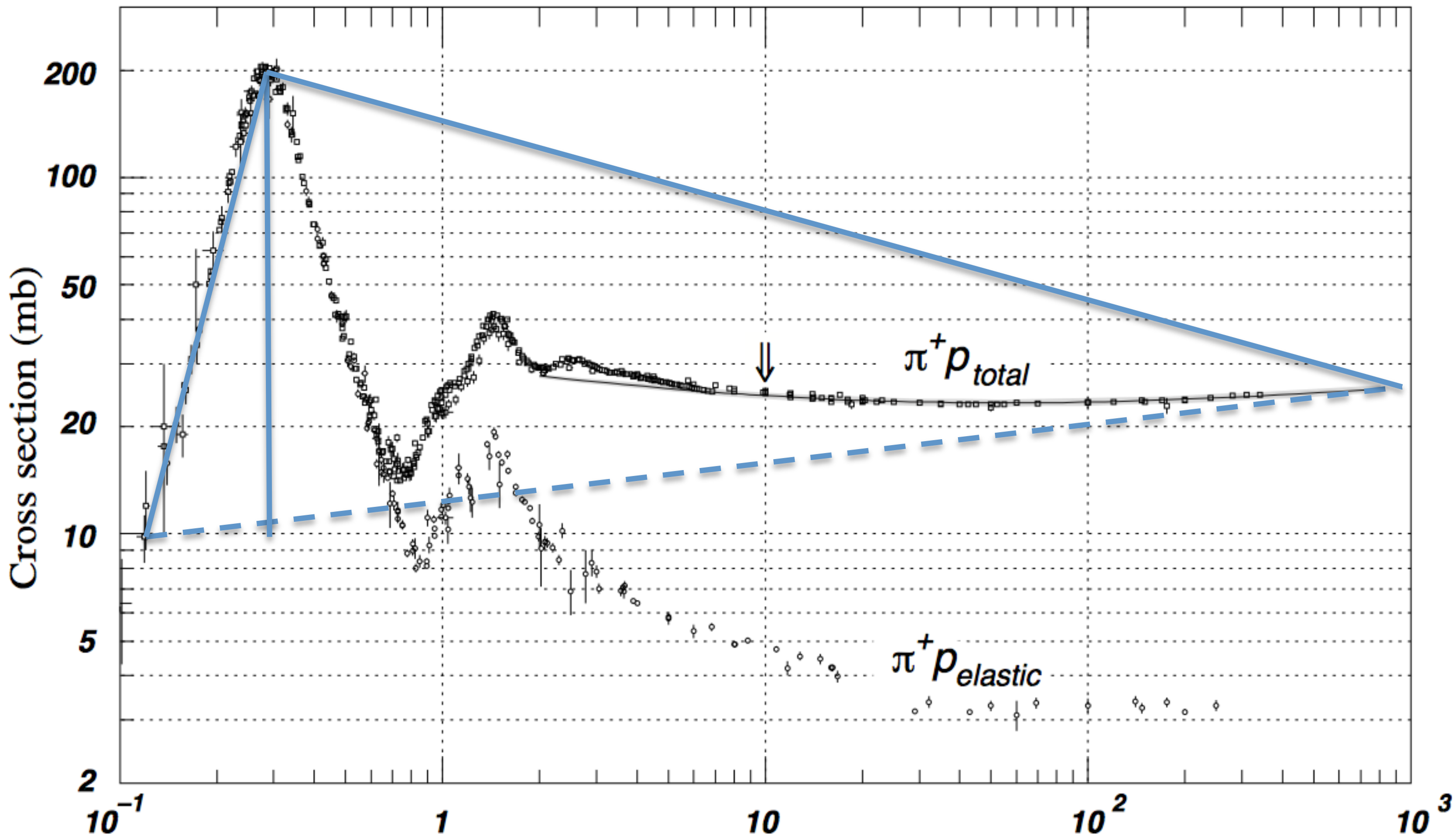

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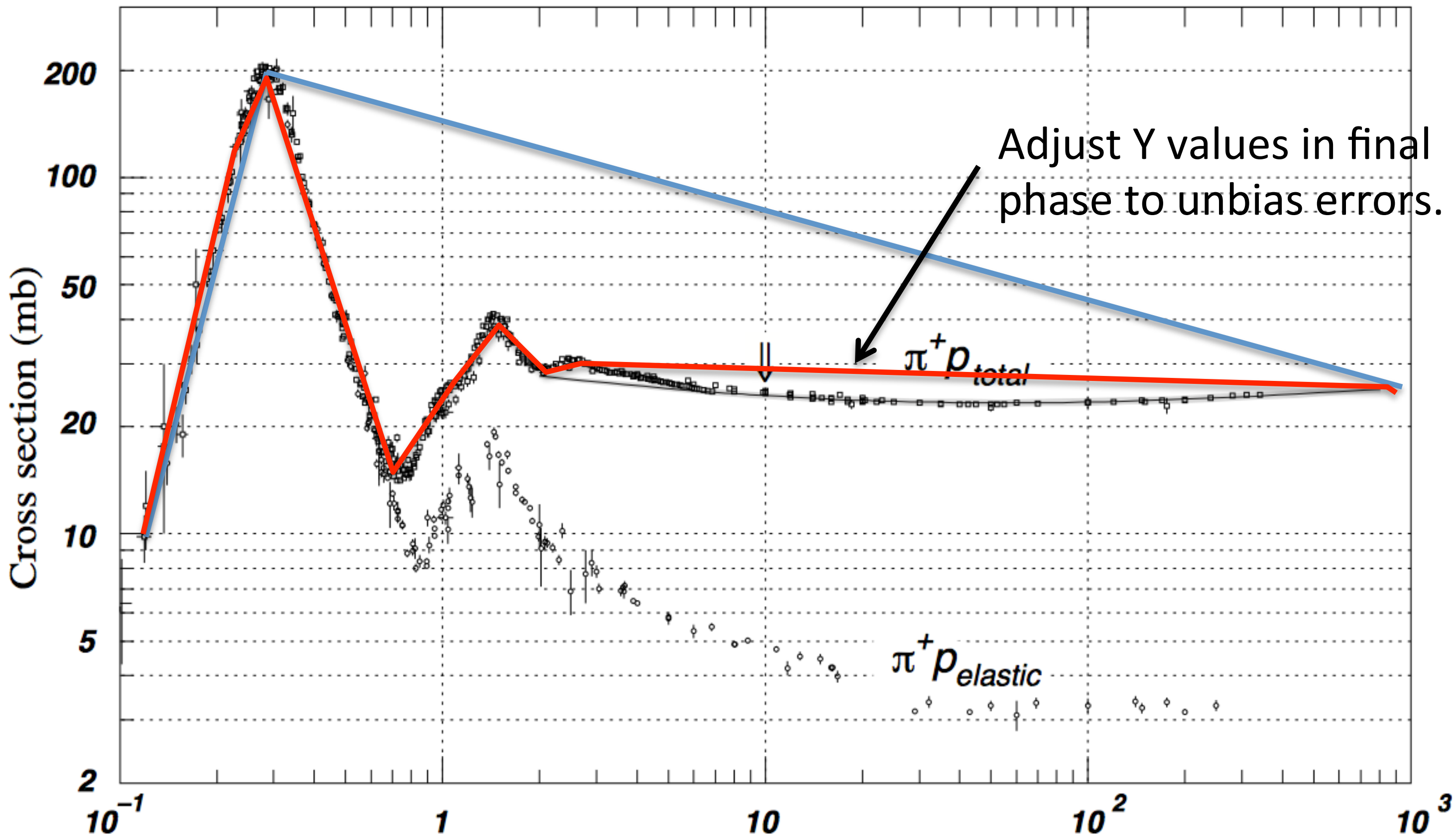

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Existing CrossSection Calculation

```
G4double G4CrossSectionDataStore::GetCrossSection(part,mat){
  ...
    if(mat == currentMaterial && part->GetDefinition() == matParticle
     && part->GetKineticEnergy() == matKinEnergy)
    { return matCrossSection; }

   //Calculate CrossSection the regular way (including xsecelm)
  ...
}

G4double G4CrossSectionDataStore::SampleZandA(part,mat){
  ...
    G4double cross = GetCrossSection(part, mat);
  ...
}
```

Modified CrossSection Calculation

```
G4double G4CrossSectionDataStore::GetCrossSection(part,mat,requireSlowPath){
  ...
    if(!requireSlowPath){
      fast_entry = (*fastPathMap)[searchkey];
    }
    if (!requireSlowPath && fast_entry != NULL){
      matCrossSection=GetCrossSectonFastPath(fast_entry,part);
    } else {
         //Calculate CrossSection the regular way (including xsecelm)
    }
  ...
}

G4double G4CrossSectionDataStore::SampleZandA(part,mat){
  ...
    G4double cross = GetCrossSection(part, mat, true);
  ...
}
```

Fast Path Usage: Runtime

Triples	Samples	Tolerance	Time	Percent Diff
90%	250K	1E-05	82:36	8.0%
90%	10K	1E-06	85:26	6.1%
90%	500K	1E-05	87:07	5.1%
90%	200K	1E-06	89:03	3.8%
Slow Path Only	N/A	N/A	94:57	0.0%
90%	2M	1E-06	99:18	-2.8%

Fast Path Usage: Cycles

Samples	Tol	Cyc/Op (fast)	Cyc/Op (slow)	Cyc/Op (avg)	Init Cycles	Cyc/Op (avg) w/ init	Total Calls
2M	1E-6	274	3982	839	2.77E+12	2731	1,468,837,903
1M	1E-6	252	3936	811	1.24E+12	1651	1,475,681,237
500K	1E-5	240	3873	786	2.58E+11	962	1,467,516,422
250K	1E-5	230	3981	801	1.23E+11	884	1,486,080,112
10K	1E-6	242	3882	820	6.17E+9	824	1,520,218,543

Questions?