Varying Geant4 Model Parameters with Bertini Cascade as the 1st Use Case - status report -

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Outline

- Motivation
- Software Toolkit
- Bertini as the 1st use case
- Recent efforts
  - Process-level Bertini variants and comparison vs multiple experimental datasets
  - ”Pilot” simulation of LArIAT test beam setup using Bertini variants
  - “Pilot” simulation of the SimplifiedCalorimeter
- Plans for near future
- Summary

Motivation

- Strong interest from the users community:
  - Study and understand how sensitive Geant4 predictions are to varying parameters of models involved in the simulation project
  - Study specific detector effects
  - Make steps towards calculating systematic uncertainties
  - ...
- Benefit to Geant4
  - Explore Geant4 predictions sensitivity in many areas
  - Benchmark variants vs multiple experimental datasets (if available)
  - Refine ranges of parameters validity
  - Potential input to optimize model parameters
  - …

Software Toolkit Features

- User-friendly API to vary one or multiple parameters of Geant4 physics models involved in the simulation studies
- Flexible run-time configurable workflow
- Full-scale Geant4 application with run-time geometry input in GDML format
  - Only one instance per job due to technicalities of physics lists
- Single interaction simulation (process level)
  - Multiple instances of the same model can run in the same job
- Comprehensive bookkeeping
  - When running a full-scale application, results from different variants can be appended to one output as long as the metadata are consistent
- Example analysis modules - easy-to-extend collection of tools
- Development towards collective comparison of multiple variants of the resulting physics observables vs experimental data (via programmatic access to DoSSiER)
- Documentation (always work in progress ^_^)

Bertini as 1st Use Case (I)

- Largely employed to model processes through the MeV range and/or in the several-GeV range
- Offers reasonably ready model configuration interface – documented in the technical note by Dennis W.:
  - https://cdcvs.fnal.gov/redmine/attachments/download/32147/Bertini_params.pdf
- (Initial) List of Bertini modifiable parameters:
  - Cross Section Scale
  - Nuclear Radius Scale
  - Fermi Momentum Scale
  - Shadowing Radius (trailing effect)
  - Gamma Quasi-Deuteron Scale
  - Use PreCompound switch (false/true)
  - Do Coalescence switch (false/true)
- It is known that modifying some parameters have significantly larger impact on the Bertini simulated results while modifying others will induce relatively small variations in the results

Bertini as 1st Use Case (II)

- The two “sensitive” parameters and some of their history:
  - Cross Section Scale = multiplicative factor is applied to the internal cross sections used in the Bertini model of the nucleus. Here “internal" means the cross section that an incident particle sees as it travels though the target nucleus; it is not necessarily the free-space cross section
    - Default setting: 1
    - (Current) Allowed range of variations: 0.05 – 2.
    - Dennis W. is the best expert to explain specific details of how internal cross sections are implemented in Bertini cascade
  - Radius Scale = scale factor for the nuclear radius
    - Default setting: radius_scale=2.82 (well, 2.8197 to be precise)
    - “Literature value”: 1
    - (Current) Reasonable range of variations is 2.82 to 1.
- NOTE: I bet other hadronic models may have their own little secrets up the sleeve

Recent Efforts

- Exploring Bertini model sensitivity to Radius Scale and Cross Section Scale settings:
  - Simultaneous benchmarking of Bertini prediction variants vs HARP and ITEP771 experimental data, including initial statistical analysis

    NOTE: data are taken directly from DoSSiER, via programmatic access
  - Efforts to refine Bertini parameters ranges
  - Initial indications towards possible improving Bertini tune
- Initial steps towards exploring sensitivity of full-scale detector simulation:
  - "Proof-of-principle" study to explore sensitivity of LArIAT test beam simulation to Bertini parameters variations (effect on the simulated energy deposition in small LAr TPC)
  - Exploring possibility to use SimplifiedCalorimeter application to study the effect of model parameter variations on hadronic showers

Modeling Single Interactions with Bertini Variants

- Modeling selected proton- or pion-nucleus interactions at intermediate energy with different settings:
  - 5 GeV/c proton + Pb -> pions (HARP), p, n (ITEP771)
  - 5GeV/c pi- + Pb -> pions (HARP), p,n (ITEP771)
- Radius Scale settings: 2.1 (75%), 1.4 (50%), 1. (35%)
- Cross Section Scale settings: 2., 0.5, 0.1, 0.05
- Combinations of the above variants
- Results are obtained in a form of chi2/ndf:
  - chi2 is calculated for each variant for MC vs data spectra as a sum

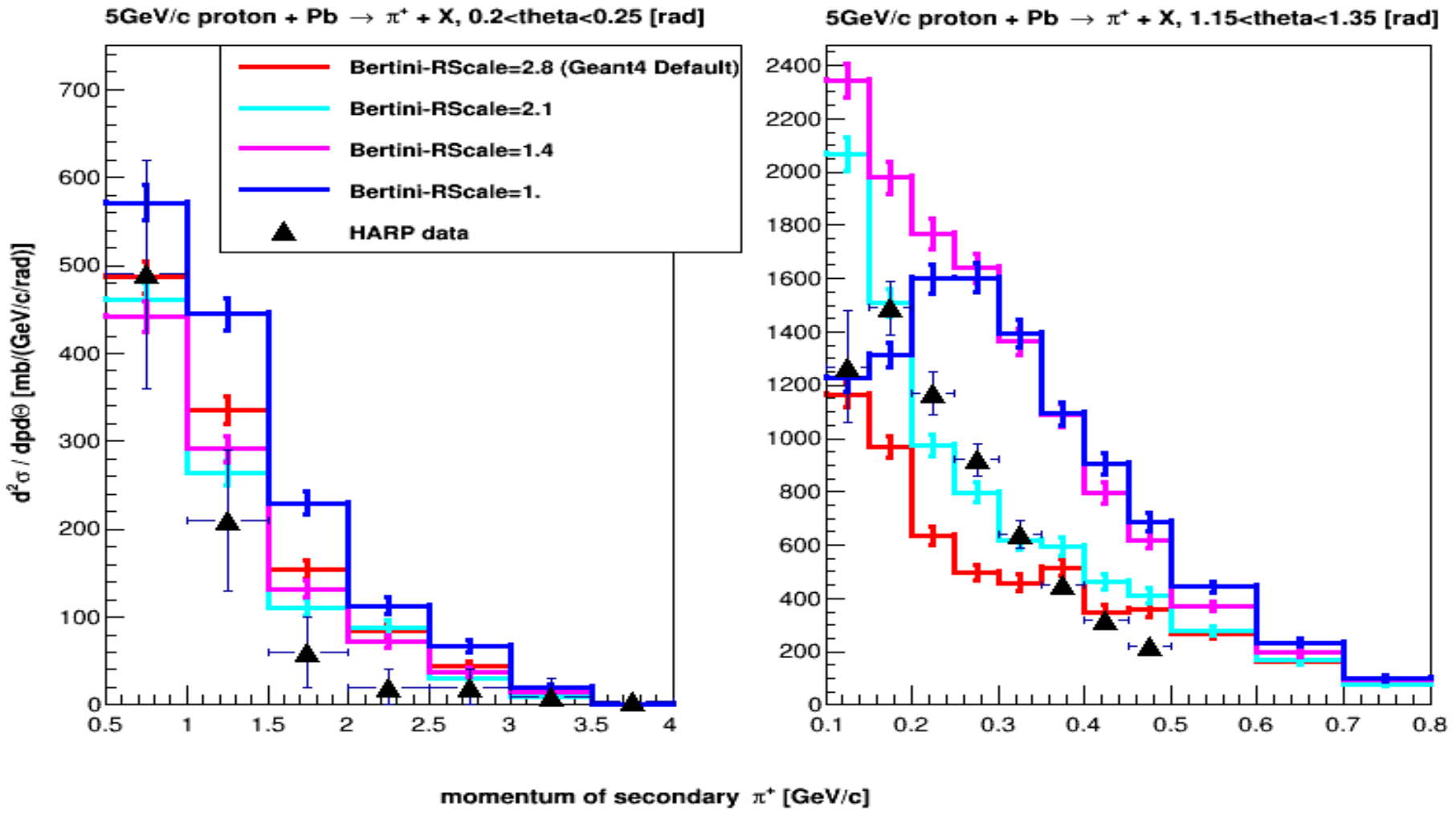
    Σ((Xi-Yi)/(σxi+σyi))**2

    where X=sim., Y=exp.data; i=1,N, N=number of exp.data points

  NOTE: when chi2 is large, it is difficult to make comparisons; however, it is the only metric we have at the moment
- Selected results are included in the following slides, for illustration
- Additional results can be found in the presented at the Geant4 Hadronic group meeting: http://indico.cern.ch/event/549952/contributions/2249243/attachments/1312951/1965416/G4HAD-July20-2016-ModelParams.pdf

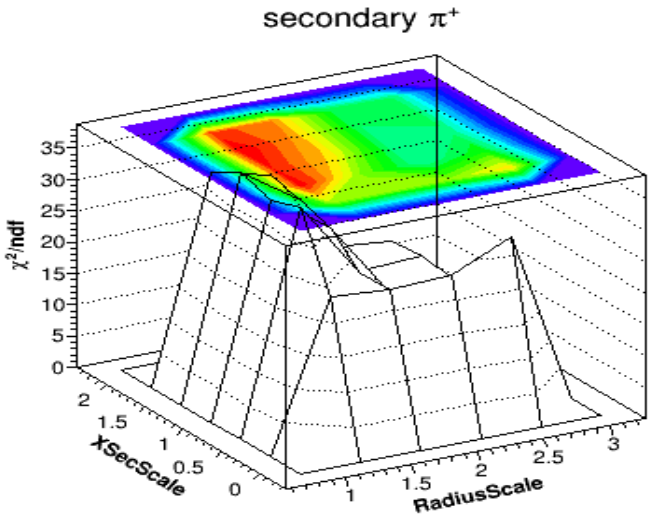
5GeV/c proton + Pb -> π^+ + X

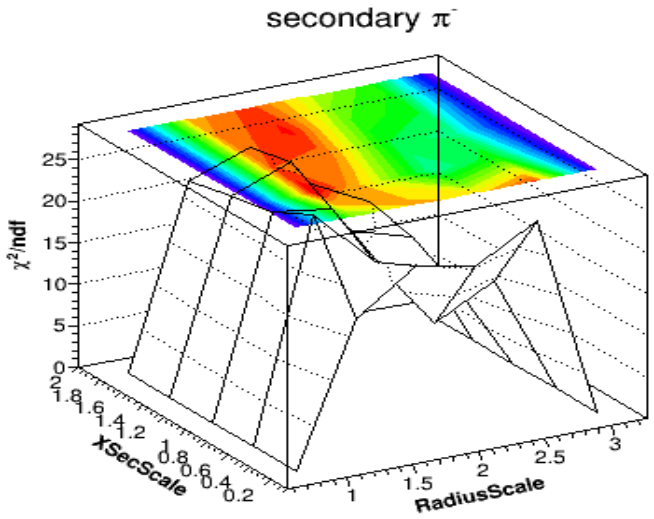
Selected simulated momentum spectra of secondary π^+ in different bins of the polar angle are compared with HARP data

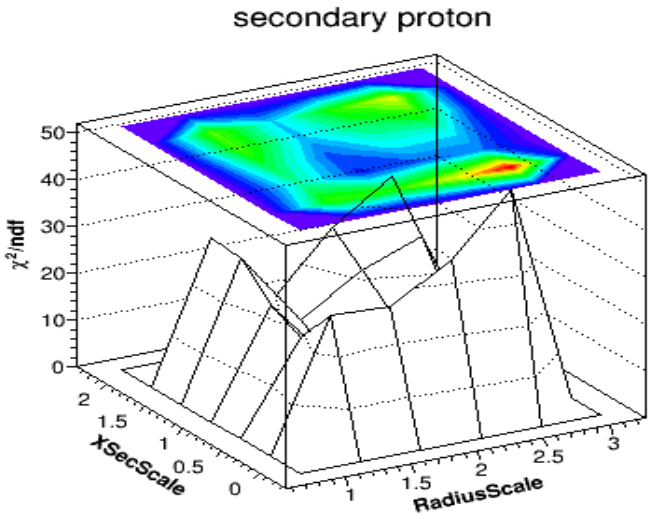


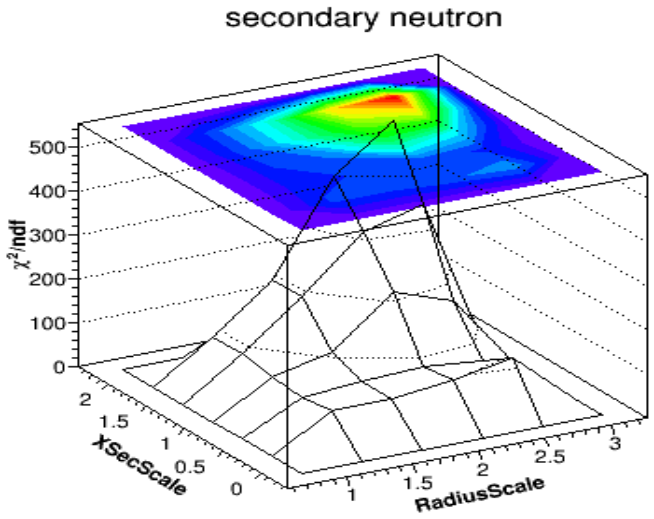
5GeV/c proton + Pb -> π^+/π^-/p/n + X (I)

For pions, integral chi2/ndf for each variant of Bertini is calculated vs HARP data
For baryons, integral chi2/ndf for each variant of Bertini is calculated vs ITEP771 data









5GeV/c proton + Pb -> π^+ / π^-

Tables contain integral chi2/ndf for each variant of Bertini as calculated vs HARP data

Radius Scale

XSec Scale

	D=2.82	75% (~2.1)	50% (~1.4)	35% (~1.)
D=1.	15.96	14.63	35.83	30.49
2.	14.88	17.39	39.73	16.94
0.5	20.65	13.39	23.48	42.63
0.1	34.31	28.66	12.77	13.68
0.05	35.50	33.04	22.64	10.35

π^+

	D=2.82	75% (~2.1)	50% (~1.4)	35% (~1.)
D=1.	10.17	12.95	29.23	17.02
2.	13.80	20.19	26.41	14.42
0.5	15.27	9.36	23.61	26.79
0.1	32.65	26.26	11.09	13.75
0.05	34.76	31.90	21.75	9.73

π^-

5GeV/c proton + Pb -> p/n

Tables contain integral chi2/ndf for each variant of Bertini as calculated vs ITEP771 data

Radius Scale

XSec Scale

	D=2.82	75% (~2.1)	50% (~1.4)	35% (~1.)
D=1.	14.06	15.04	2.90	47.15
2.	41.64	28.40	3.97	63.16
0.5	7.97	6.39	2.71	29.61
0.1	69.94	48.66	26.53	25.84
0.05	99.30	78.77	55.44	43.00

p

	D=2.82	75% (~2.1)	50% (~1.4)	35% (~1.)
D=1.	132.03	208.34	26.07	135.67
2.	596.85	438.57	22.02	170.81
0.5	19.13	42.13	28.16	91.76
0.1	162.75	123.35	71.18	67.32
0.05	201.08	176.07	135.28	113.26

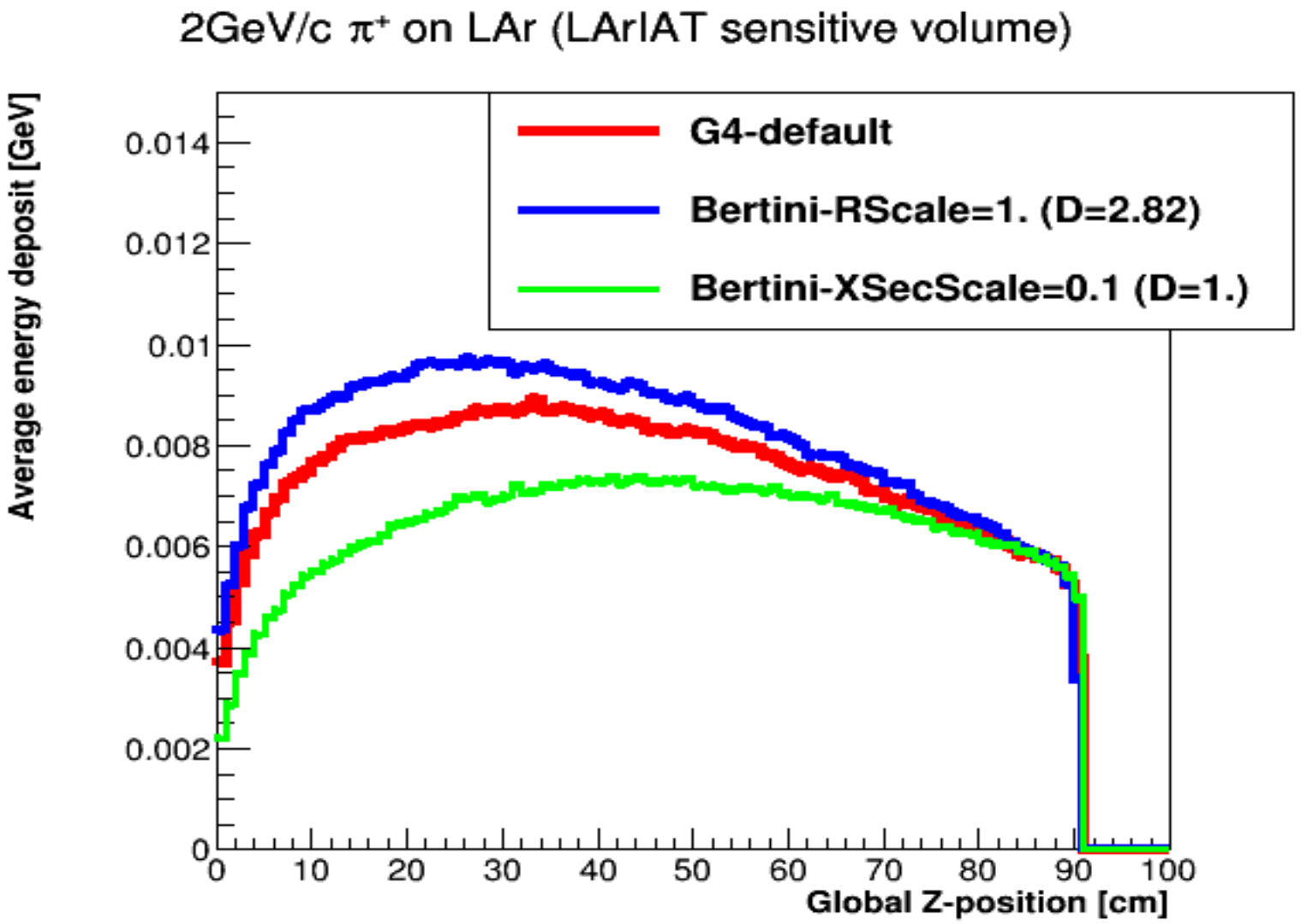
n

"Proof-of-Principle" Tests of Bertini's Variants on LArIAT Setup

- LArIAT geometry dumped in GDML form
  - Operational out-of-the box with the Geant4 application module
  - NOTE: sensitive volume is small LAr TPC – "leaky" containment
- Physics List: QGSP_FTFP_BERT (this is what LArIAT uses)
  - Largely Bertini-based
- Beam: π^+ of 2GeV/c (100K beam events)
- Bertini Variants:
  - Radius Scale = 1. (D=2.82; range of variations 1.-2.82)
    - Scale factor to define nuclear radius
  - Cross Section Scale = 0.1 (D=1.; range of variations 0.05-2.)
- NOTE: exaggerated settings to make effects of changes easy to see

LArIAT "Proof-of-principle" Study – Selected Results

Simulated Energy Deposit by a Hadronic Shower in LAr vs Shower Depth (Z)



SimplifiedCalorimeter and Bertini Parameters (I)

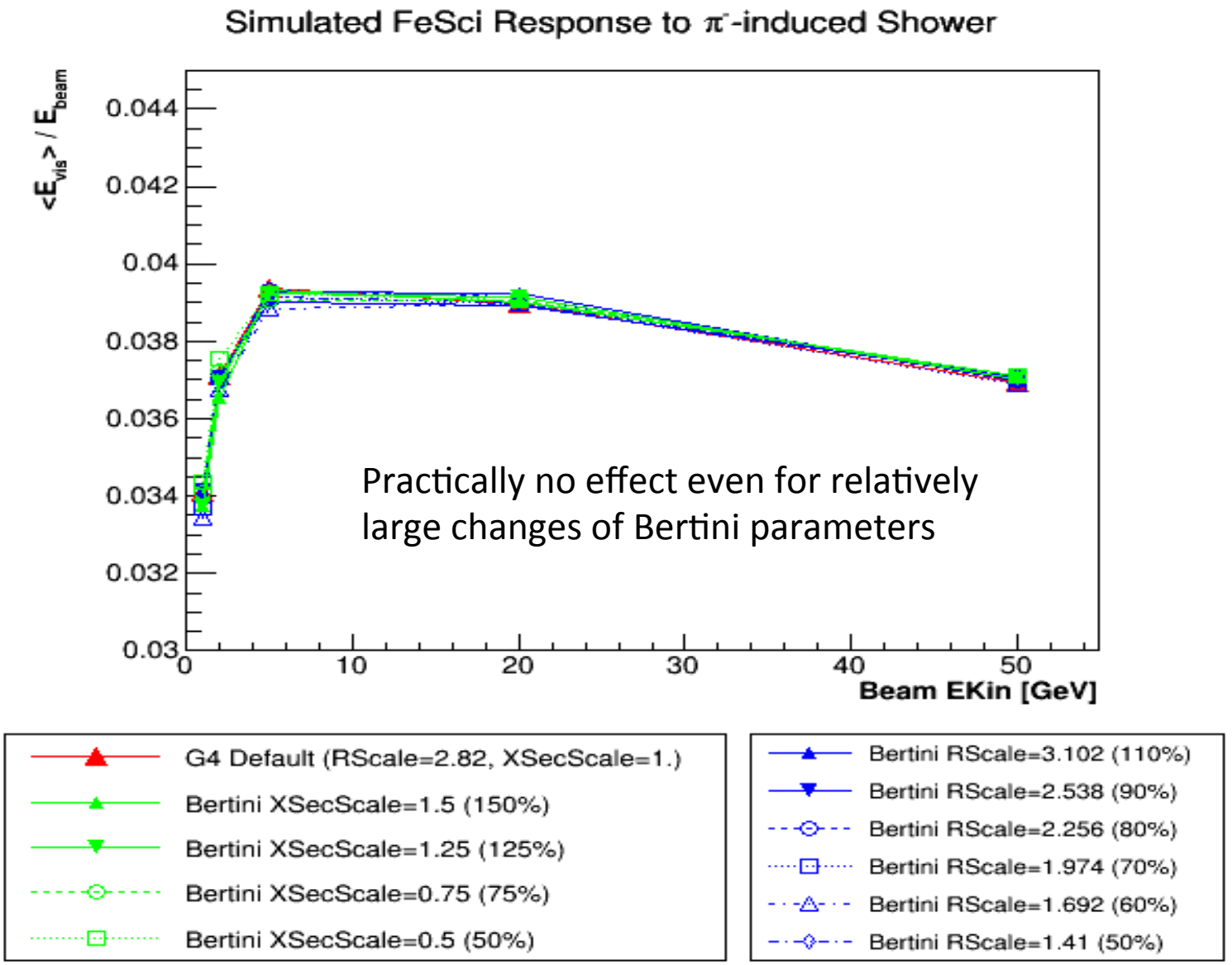
- Per initial email discussion with the SLAC team and Alberto R., we have decided to try SimplifiedCalorimeter application to see if hadronic showers are sensitive to variations of Bertini parameters
  - Many thanks to all for your support and encouragement !
- The application code is in SVN and is easy to obtain
- Fairly straightforward to get started
- Analysis involves some sophisticated details
  - Described in the note by Andrea D.:

    https://ep-dep-sft.web.cern.ch/sites/ep-dep-sft.web.cern.ch/files/documents/ShowerMoments.pdf
  - Assumes certain code infrastructure
- In principle, SimplifiedCalorimeter native app can be used (almost) directly but a few relatively small modifications will be needed to configure Bertini

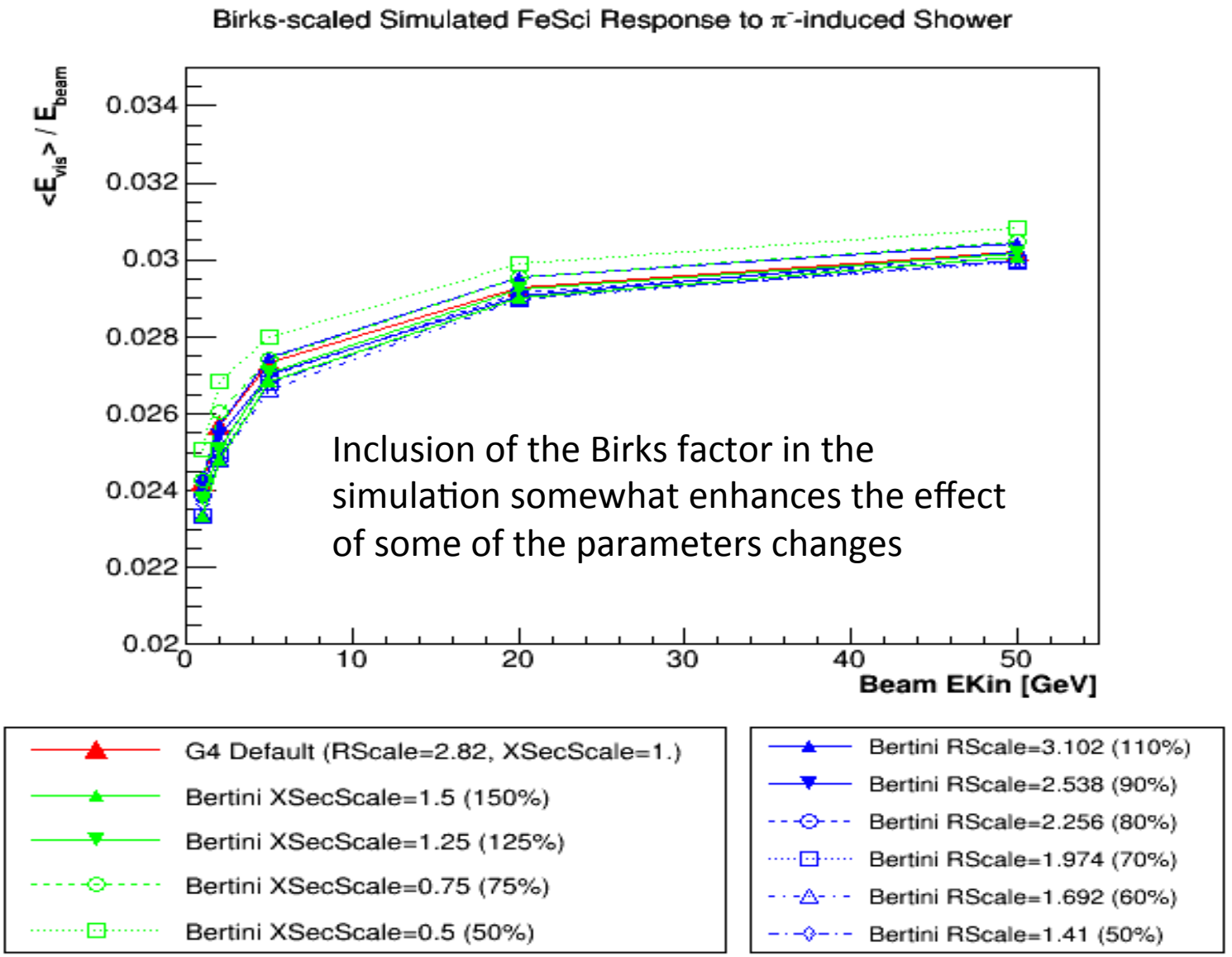
SimplifiedCalorimeter and Bertini Parameters (II)

- "Pilot" study:
  - Used the software toolkit we develop
    - Convenient bookkeeping machinery that allows to combine multiple simulated variants in one source (file) which simplifies the analysis
    - Also to test the toolkit yet another time
  - FeSci geometry dumped in GDML form (addition of a couple of line of code)
  - Energy deposit recording via sensitive detector is fairly straightforward
  - Birks factor applied as in the original app, but non-scaled values were also recorded
  - **Approach to analysis is very simplistic at this stage** – it needs to be iterated with the experts how to perform full-scale analysis
  - FTFP_BERT physics list (maily FTF-based but shower goes through a few-GeV range)
  - pi- beam, Ekin=1,2,5,20,50GeV (5K events/variant)
  - Bertini variants were more "conservative" that in earlier studies:
    - RScale=110%,90,80,70,60,50
    - XSecScale=1.5,1.25,0.75,0.5

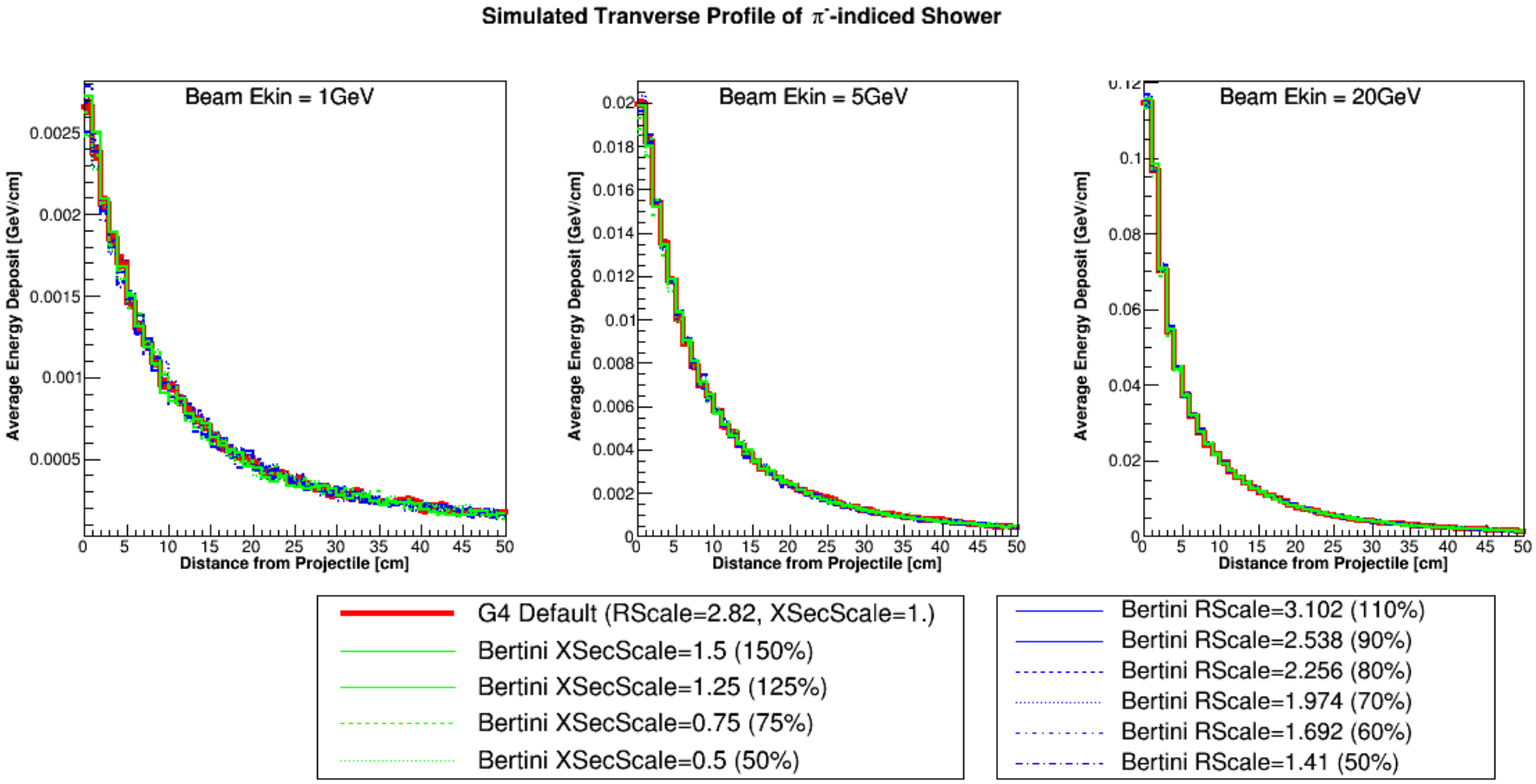
SimplifiedCalorimeter – Selected Results (I)



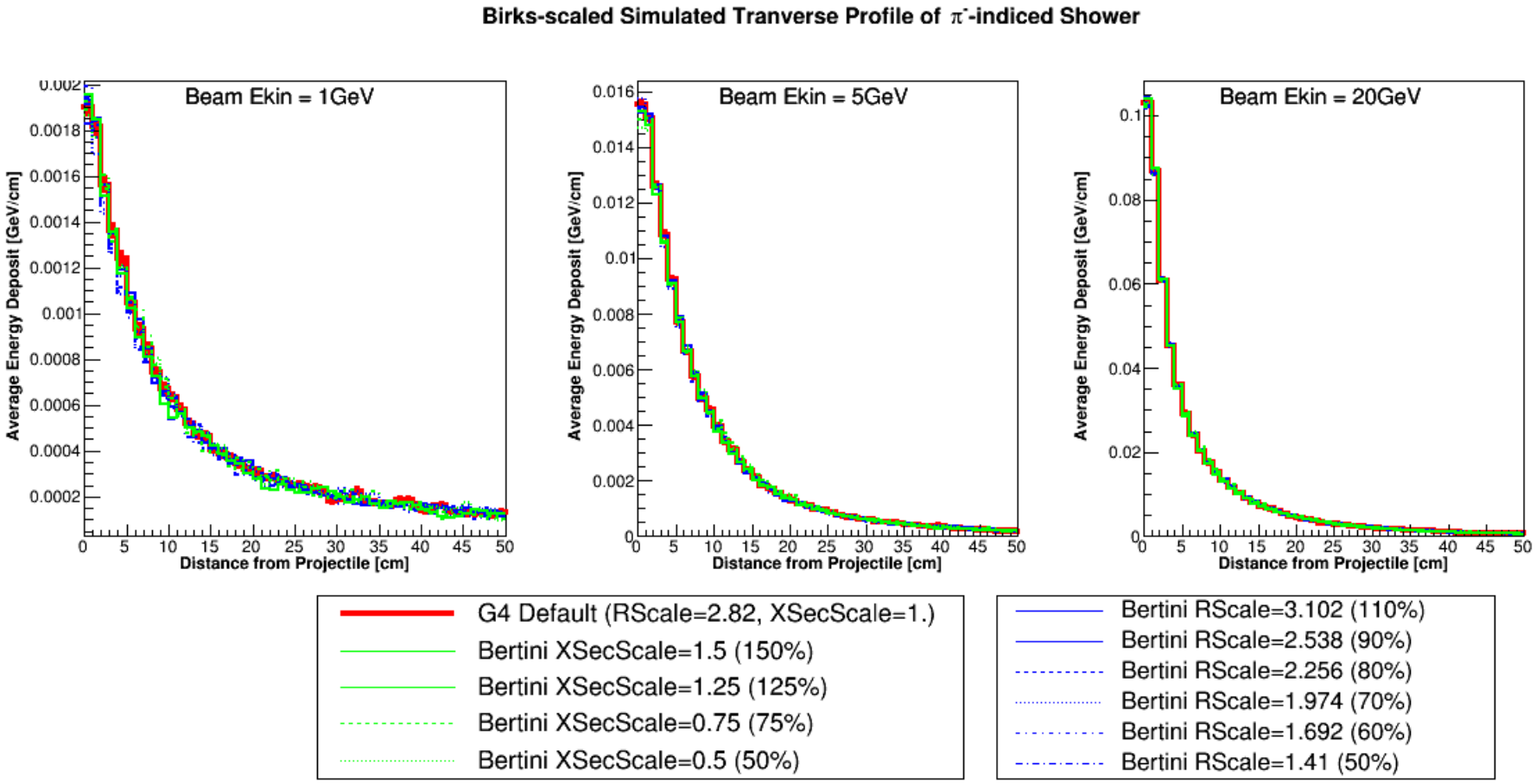
SimplifiedCalorimeter – Selected Results (II)



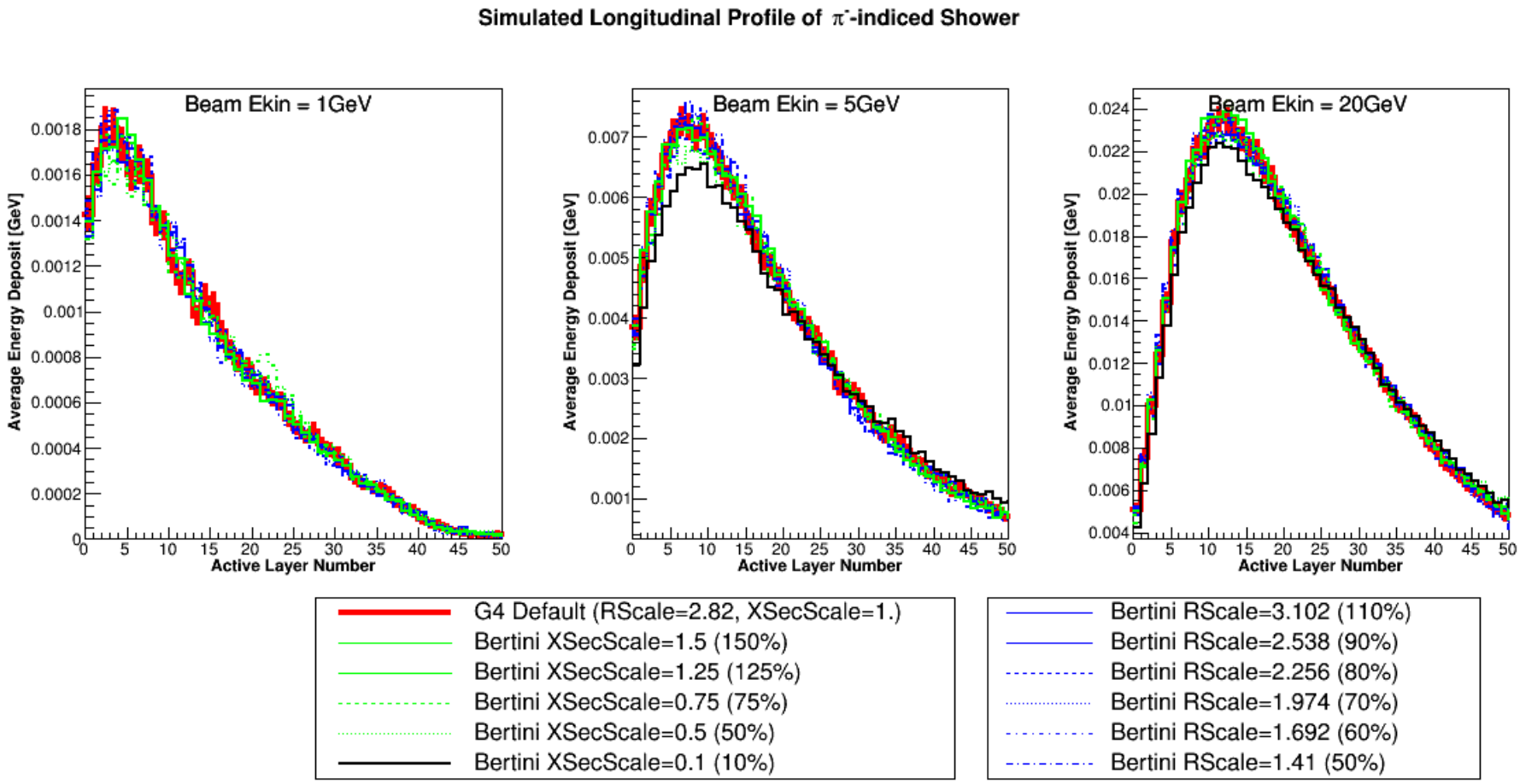
SimplifiedCalorimeter – Selected Results (III)



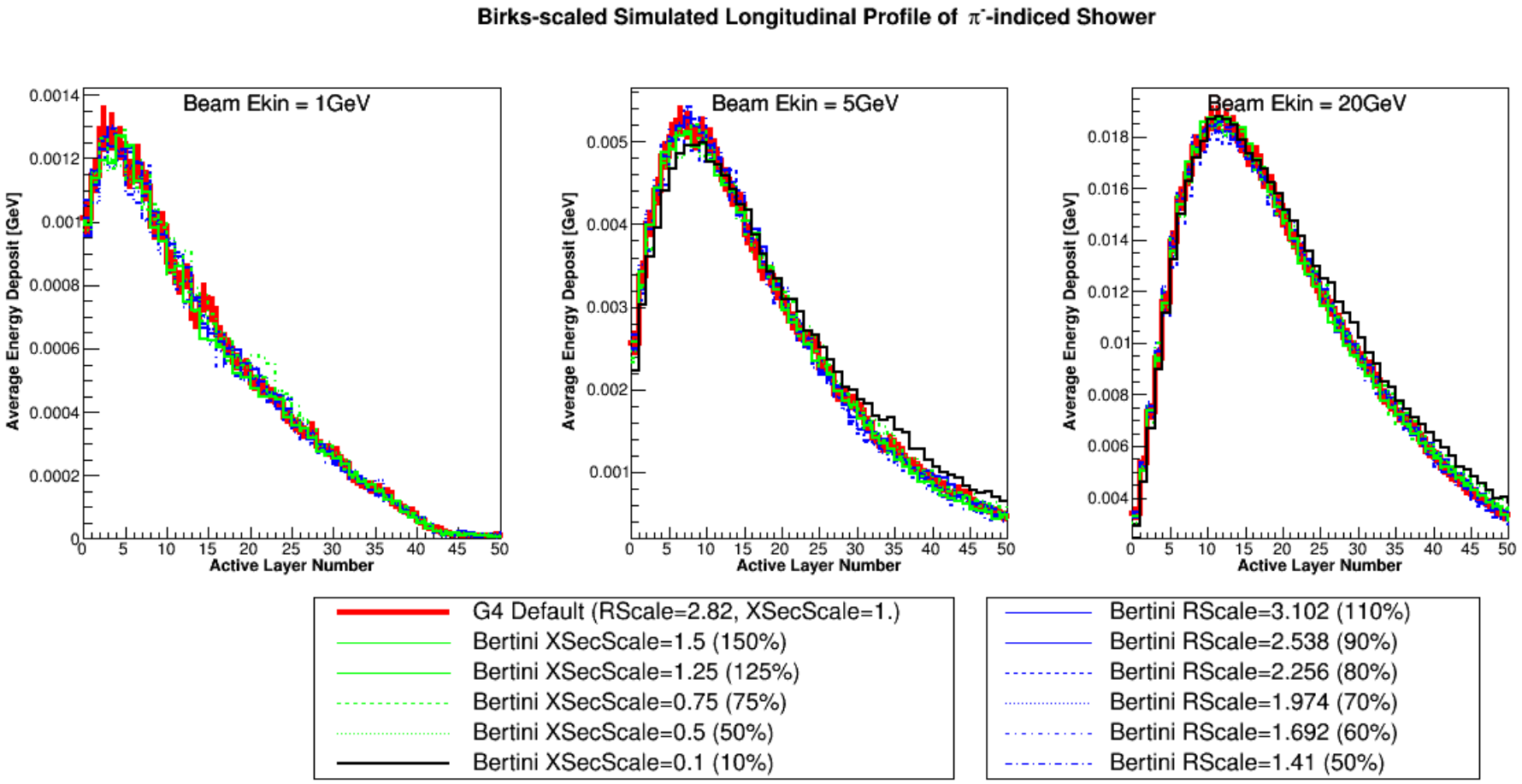
SimplifiedCalorimeter – Selected Results (IV)



SimplifiedCalorimeter – Selected Results (V)



SimplifiedCalorimeter – Selected Results (VI)



Near-term Plans

- Expand the “test bench” – more tests, more data
- Improve statistical analysis of multiple variants of Geant4 models
- Refine details of the simulation and analysis tools, as needed
- Other aspects may come up as we move forward

Summary

- Allowing modifications of the Geant4 hadronic models parameters is an important aspect and a serious challenge
  - Lots of analysis is needed to estimate the uncertainties in the simulation
- Work is underway, with Bertini Cascade model as the 1st use case
  - Exploring sensitivity of Bertini results to parameter variation when modeling single interaction
  - Exploring the impact of Bertini parameters variations on "bulk" effects modeled by full-scale applications (realistic geometry, use of physics list)
  - Working to better define validity range of Bertini parameters
  - There may be a chance to improve Bertini settings
- More work is in the plans
- Looking forward to involve other models shortly