Inclusive lepton fluxes and numerical methods

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HELMHOLTZ RESEARCH FOR GRAND CHALLENGES

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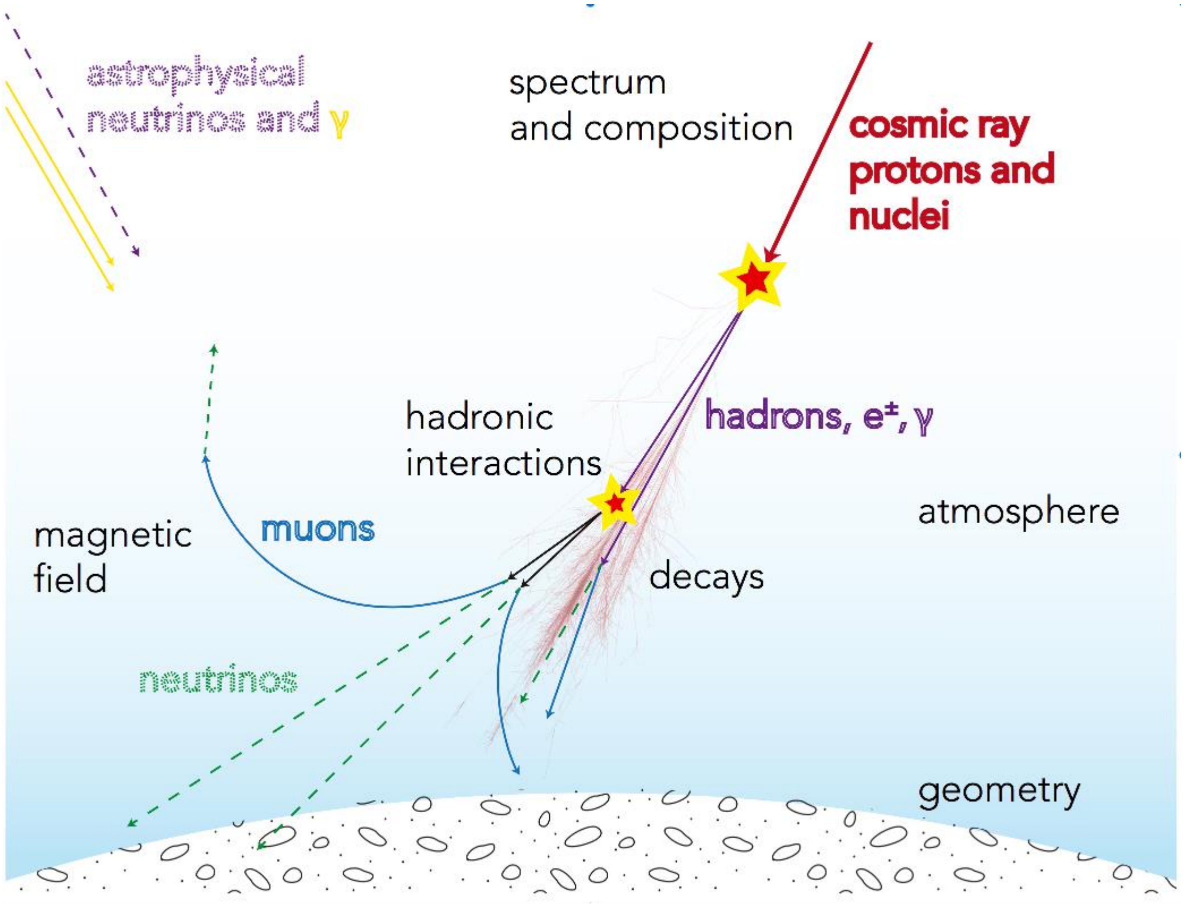
Atmospheric leptons: muons & neutrinos



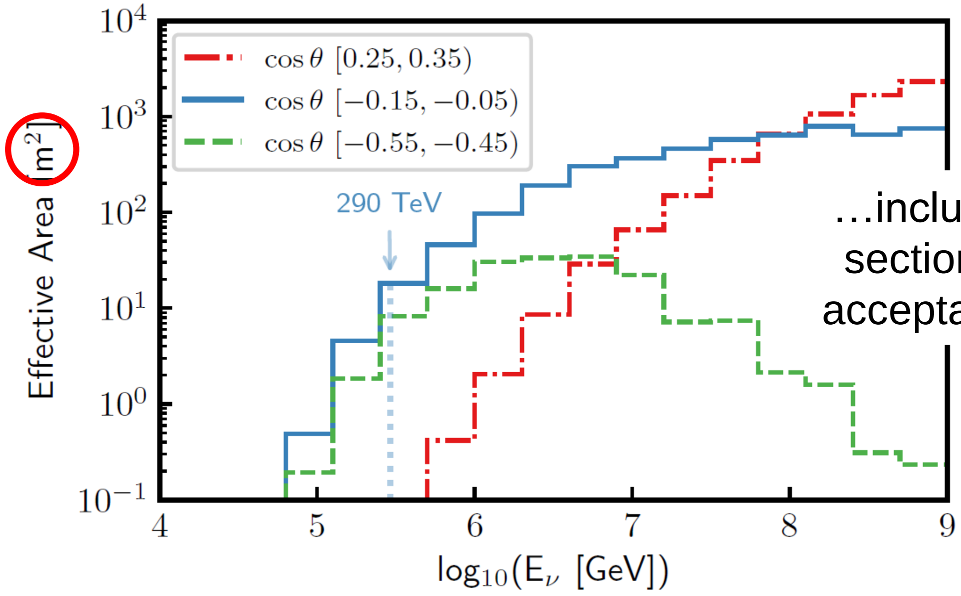
- For <u>high precision</u> calculations all phenomena need accurate modeling
- Uncertain "ingredients":
  - Cosmic ray spectrum and composition
  - Hadronic interactions
  - Atmosphere (dynamic, depends on use case)
  - (Rare) decays
  - Geometry, magnetic fields, solar modulation
- No clear prescription how to handle uncertainties.
- Energy range MeV – EeV!

Typical application

Inclusive, differential Flux of particles per unit area, angle and time

$$\Phi = \frac{\mathrm{d}\phi}{\mathrm{d}E} = \frac{\mathrm{d}N}{\mathrm{d}E\ \mathrm{d}A\ \mathrm{d}\Omega\ \mathrm{d}t}\,, \qquad [\Phi] = \frac{\text{particles}}{\text{GeV s sr cm}^2}$$

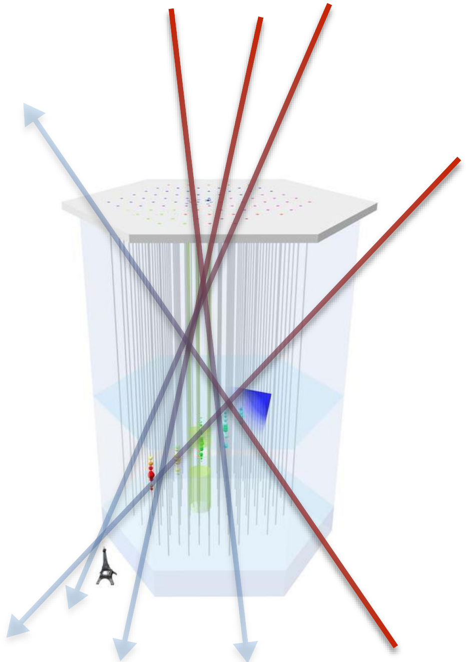
Effective area: converts physical units to event numbers



…includes interaction cross sections, trigger efficiency, acceptance, mis-tagging etc.

IceCube+, Science eeat1378 (2018)

Flat or volumetric detector (e.g. IceCube)



How many signal or background events do I expect?

$$N_{\text{events}} = 4\pi\ T \int_0^\infty \mathrm{d}E\ \Phi_{\nu_\mu}(E) A_{\nu_\mu,\text{eff}}(E)$$

Integrated over full sky (4π) for <u>isotropic</u> flux. T=10 years for example

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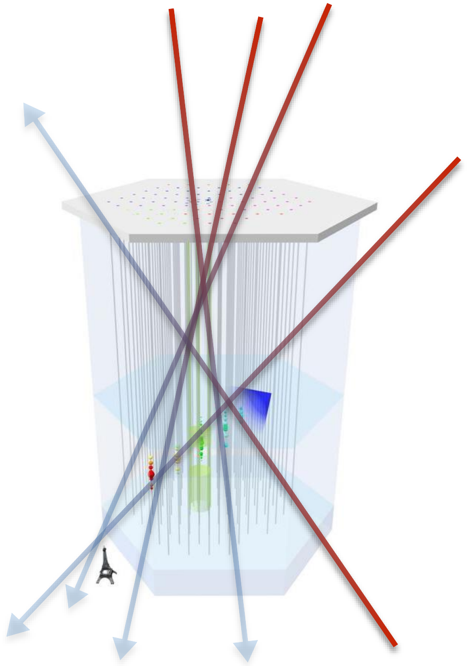

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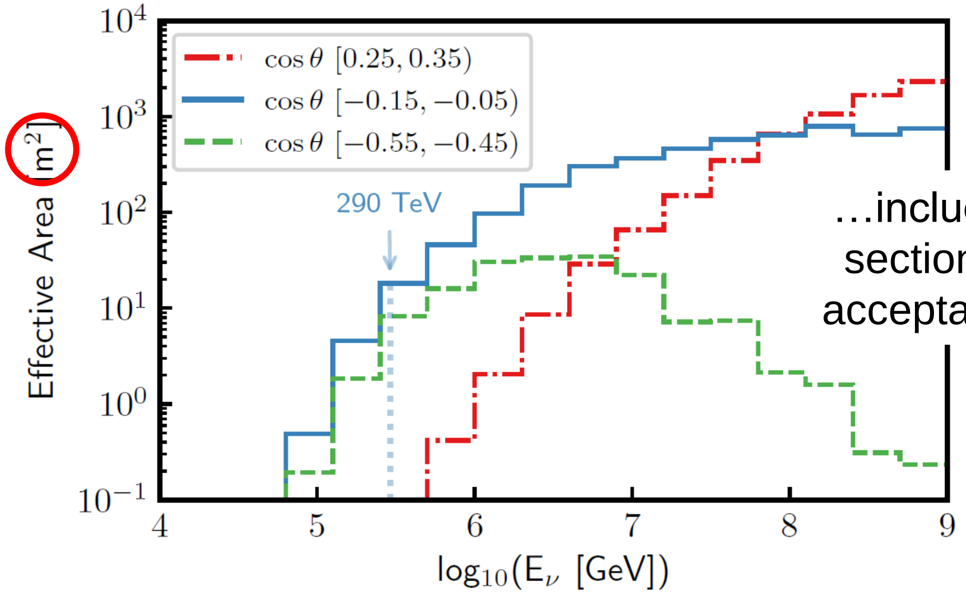

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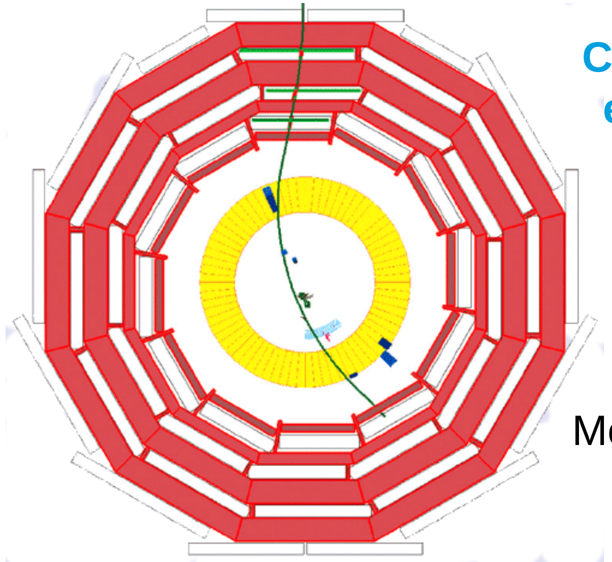
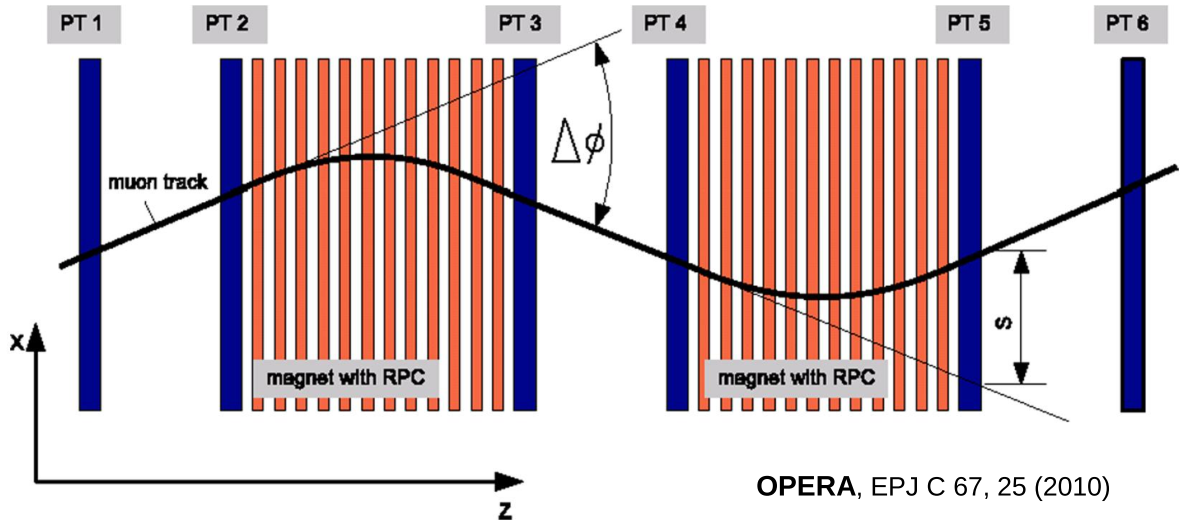
Atmospheric single muons vs. muon bundles

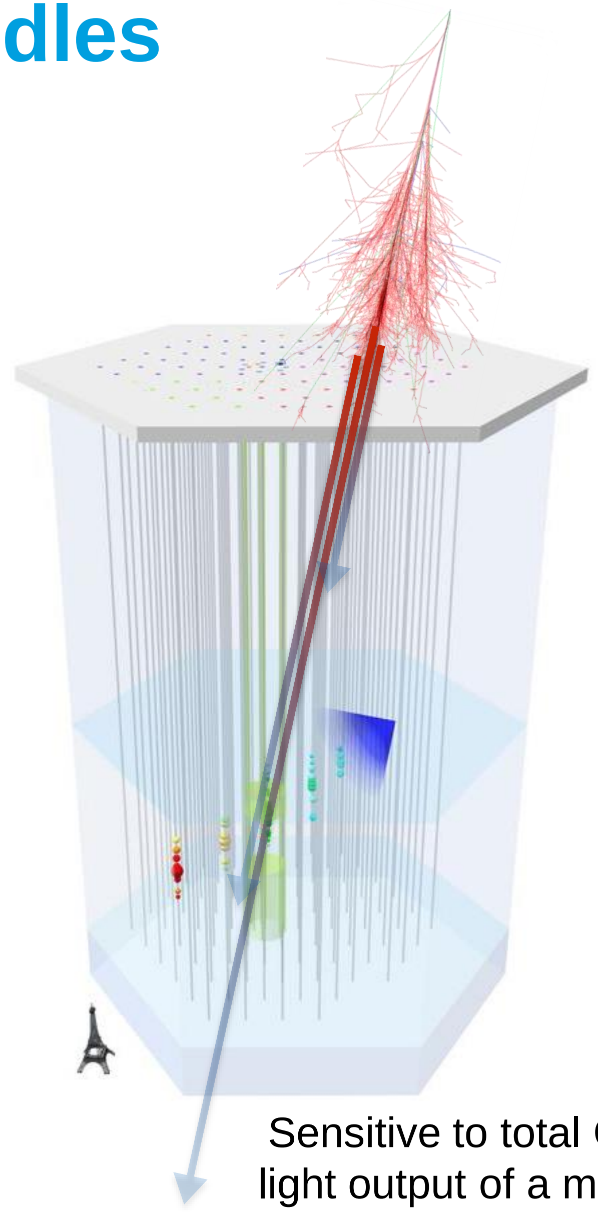


Cosmic (muon) event in CMS

Resolves individual muons
in a bundle of muons.
Measurement of individual momenta



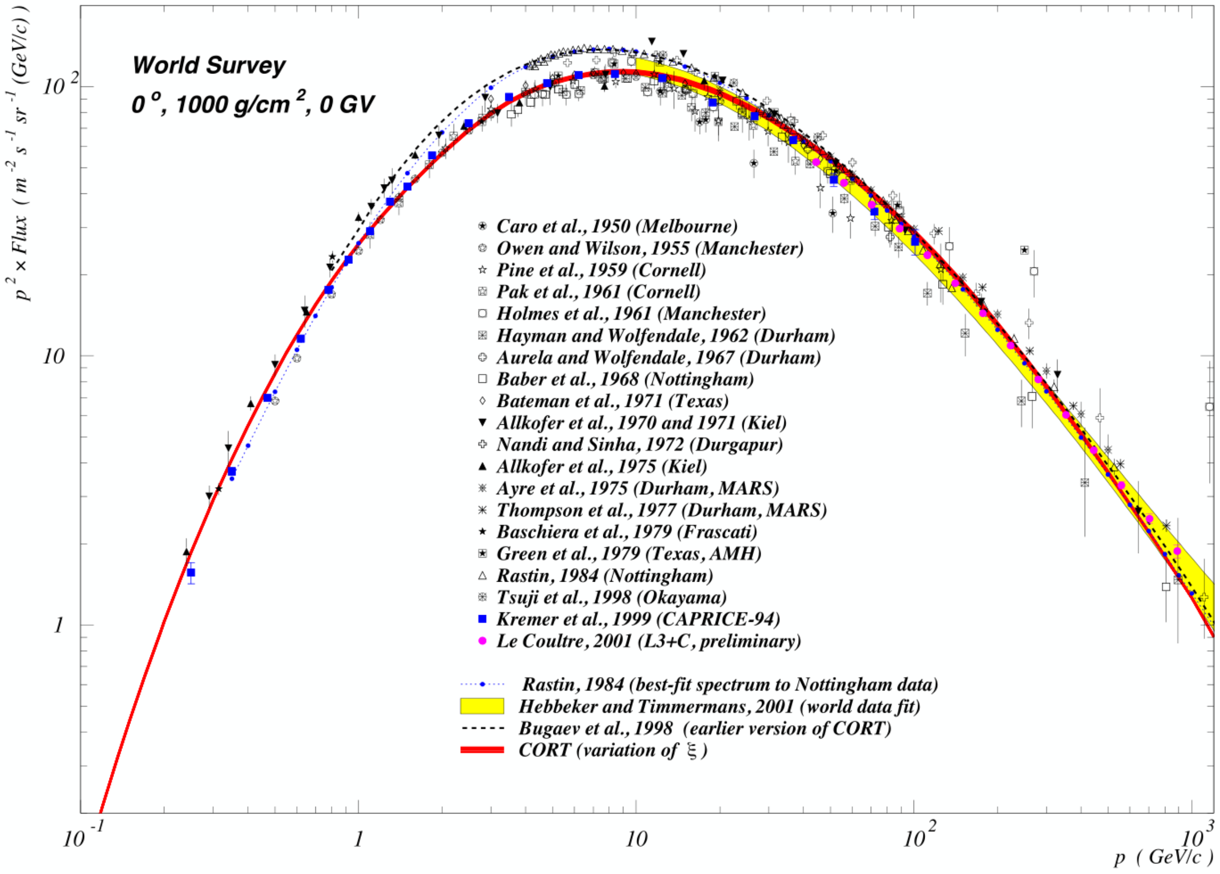
OPERA, EPJ C 67, 25 (2010)

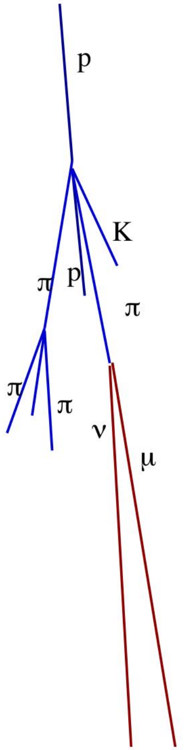


Sensitive to total Cherenkov
light output of a muon bundle
~ multiplicity x energy

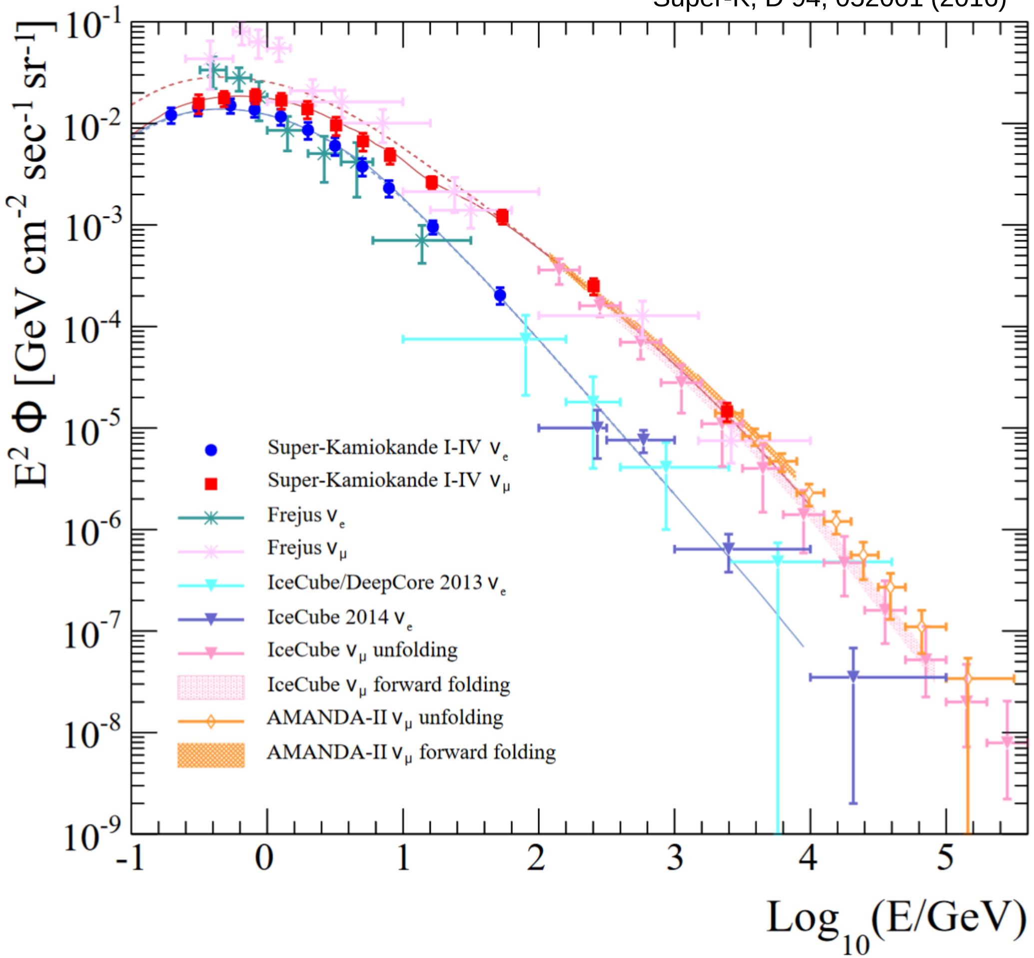
Inclusive spectra of (single) muons and neutrinos

PDG, 2015





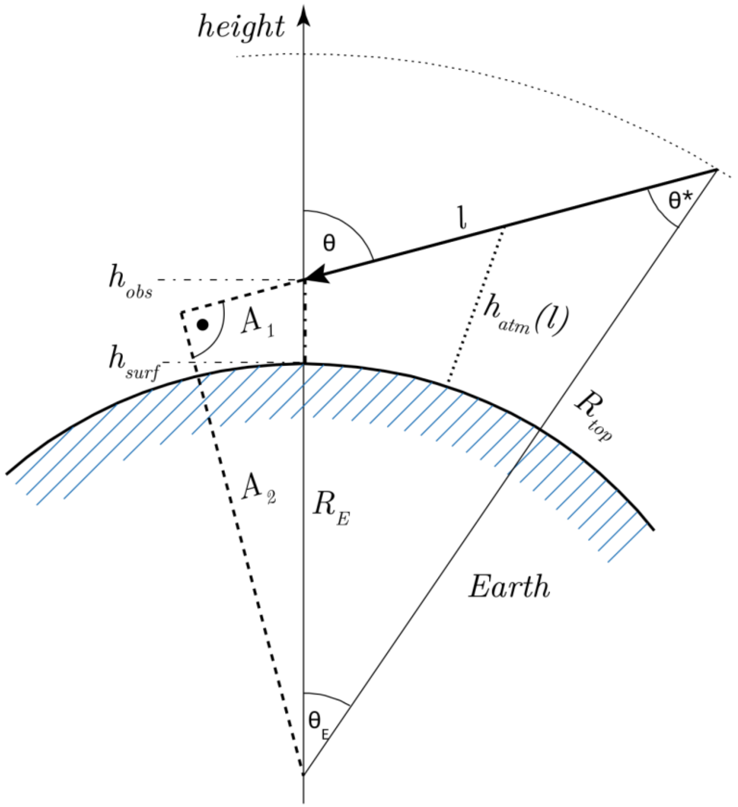
Super-K, D 94, 052001 (2016)

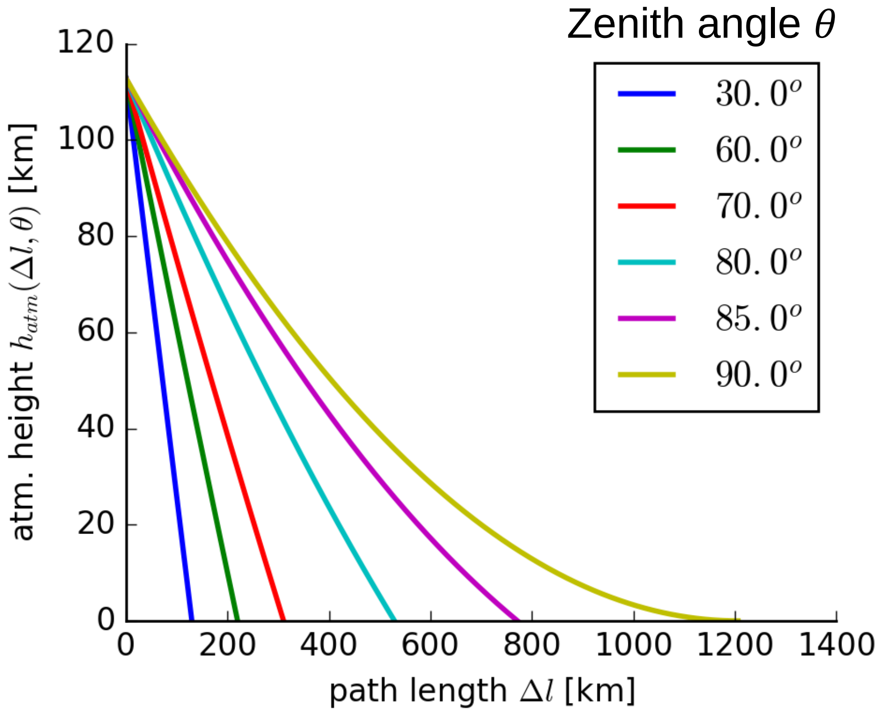


- Power-law-like spectra, similar for muons and neutrinos
- (muons : muon neutrinos : electron neutrinos) ~ (1 : 0.2 : 0.01) @ 100 GeV
- Low-energy muons suppressed due to decays

Atmospheric depth

From MCEq.geometry docs @
https://mceq.readthedocs.io/





can be > 30 km

(Slant) depth, independent of zenith angle

$$X(h_0) = \int_0^{h_0} \mathrm{d}k\ \rho_{\text{air}}(\ell)$$

1D transport equation for protons through matter

$$\frac{\mathrm{d}\Phi_\mathrm{p}(E,X)}{\mathrm{d}X} = -\frac{\Phi_\mathrm{p}(E,X)}{\lambda_{\mathrm{int,p}}(E)} + \int_E^\infty \mathrm{d}E' \, \frac{\Phi_\mathrm{p}(E',X)}{\lambda_{\mathrm{int,p}}(E')} \frac{\mathrm{d}N_{\mathrm{p}\to\mathrm{p}}(E')}{\mathrm{d}E'}$$

- **"Approximation A":**
  - $\lambda_{int} \neq f(E)$; constant interaction cross section
  - ${}^{dN}/_{dx} \neq f(E)$; Feynman scaling
  - power-law spectra
  - No continuous losses
  - see book by Gaisser, Engel, Resconi (2016)

Solve via separation of variables with substitution $x = E/E'$

$$\Phi_\mathrm{p}(E,X) = A(X)E^{-\gamma} \Rightarrow \frac{\mathrm{d}A(X)}{\mathrm{d}X} = -\frac{A(X)}{\lambda_{int,p}}\left[1 - \underbrace{\int_0^1 x^{\gamma-1}\frac{\mathrm{d}N_{p\to p}}{\mathrm{d}x}}\right]$$

$$\boxed{\Phi_\mathrm{p}(X) = A(0)e^{-X/\Lambda}E^{-\gamma}} \Leftarrow = -\frac{A(X)}{\lambda_{\mathrm{int,p}}}[1 - Z_\mathrm{pp}]$$

sink source

$$\frac{\mathrm{d}\Phi_\mathrm{p}(E,X)}{\mathrm{d}X} = \boxed{-\frac{\Phi_\mathrm{p}(E,X)}{\lambda_{\mathrm{int,p}}}} + \boxed{Z_\mathrm{pp}\frac{\Phi_\mathrm{p}(E,X)}{\lambda_{\mathrm{int,p}}}}$$

$$= \boxed{-\frac{\Phi_\mathrm{p}(E,X)}{\lambda_{\mathrm{int,p}}}} + \boxed{S(\mathrm{p}\to\mathrm{p})}$$

New transport equation under Appr. A

notation from P. Lipari (1993)

Cascade equation for pions

$$\frac{\mathrm{d}\Phi_\pi(E,X)}{\mathrm{d}X} = \underbrace{-\frac{\Phi_\pi(E,X)}{\lambda_{\mathrm{int},\pi}} - \frac{\Phi_\pi(E,X)}{\lambda_{\mathrm{dec},\pi}}}_{\text{sink}} + \underbrace{\sum_{\mathrm{hadrons}} S(\mathrm{h}\to\pi,E)}_{\text{source}}$$

Mother/source hadrons for pions (w/o rare processes)

$$\sum_{\mathrm{hadrons}} S(\mathrm{h}\to\pi,E) = S(\mathrm{p}\to\pi,E) + S(n\to\pi,E) + S(\pi\to\pi,E)$$

$$= Z_{\mathrm{p}\pi}\frac{\Phi_\mathrm{p}(E,X)}{\lambda_{\mathrm{int},p}} + Z_{\mathrm{n}\pi}\frac{\Phi_\mathrm{n}(E,X)}{\lambda_{\mathrm{int},n}} + Z_{\pi\pi}\frac{\Phi_\pi(E,X)}{\lambda_{\mathrm{int},n}}$$

Cascade equation for charged pions in a couple (p,n,pion) system

$$\frac{\mathrm{d}\Phi_\pi}{\mathrm{d}X} = \boxed{-\frac{\Phi_\pi}{\lambda_{\mathrm{int},\pi}} - \frac{\Phi_\pi}{\lambda_{\mathrm{dec},\pi}}} + \boxed{\boxed{Z_{\mathrm{p}\pi}\frac{\Phi_\mathrm{p}(E,X)}{\lambda_{\mathrm{int},p}} + Z_{\mathrm{n}\pi}\frac{\Phi_\mathrm{n}(E,X)}{\lambda_{\mathrm{int},n}}} + Z_{\pi\pi}\frac{\Phi_\pi(E,X)}{\lambda_{\mathrm{int},n}}}$$

Coupling to cascade equations of other particles

Lepton production channels

conventional

$$p, A + \mathrm{air} \rightarrow \pi^{\pm}, \pi^{0}, \mathrm{K}^{\pm}, \mathrm{K}^{0}_{\mathrm{S,L}}$$

muons and muon neutrinos

$$\pi^{\pm}, K^{\pm} \rightarrow \mu^{\pm}\nu_{\mu}(\bar{\nu}_{\mu})$$

electron neutrinos

$$K^{\pm}, K^{0}_{L} \rightarrow [\pi^{\pm}, \pi^{0}]e^{\pm}\nu_{e}(\bar{\nu}_{e})$$

prompt

$$p, A + \mathrm{air} \rightarrow \mathrm{D}, \Lambda_{\mathrm{C}} \rightarrow \nu_{\mu}, \nu_{\mathrm{e}}, \mu$$

Subset of dominant decay channels

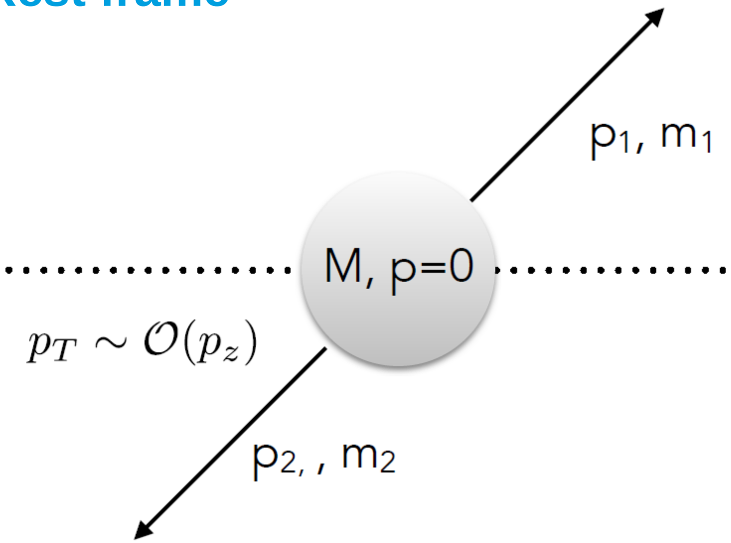
decay channel	branching ratio (BR)
$\mu^{-} \rightarrow e^{-}\bar{\nu}_{e}\nu_{\mu}$	100 %
$\pi^{+} \rightarrow \mu^{+}\nu_{\mu}$	99.9877 %
$K^{0}_{e3} : K^{0}_{L} \rightarrow \pi^{\pm}e^{\mp}\nu_{e}$	40.55 %
$K^{0}_{\mu 3} : K^{0}_{L} \rightarrow \pi^{\pm}\mu^{\mp}\nu_{\mu}$	27.04 %
$K^{+} \rightarrow \mu^{+}\nu_{\mu}$	63.55 %
$K^{+}_{e3} : K^{+} \rightarrow \pi^{0}e^{+}\nu_{e}$	5.07 %
$K^{+}_{\mu 3} : K^{+} \rightarrow \pi^{0}\mu^{+}\nu_{\mu}$	3.353 %
$D^{+} \rightarrow \overline{K}^{0}\mu^{+}\nu_{\mu}$	9.2 %
$D^{0} \rightarrow K^{-}\mu^{+}\nu_{\mu}$	3.3 %

+ *charge conjugates*

http://pdg.lbl.gov

Simplest case: 2-body decay

Rest frame

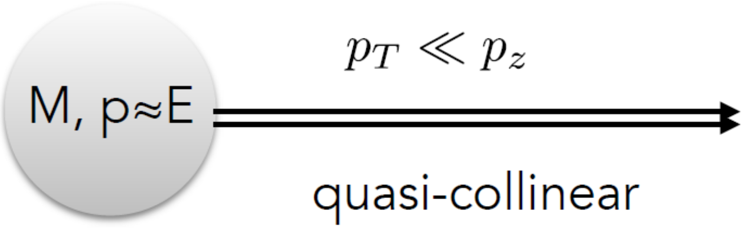


$$\boldsymbol{p}^*_M = \boldsymbol{0}$$

$$|\boldsymbol{p}_1| = -|\boldsymbol{p}_2|$$

In analogy to production spectrum weighted moment or Z-factor

Frame boosted in z direction



Example: $M \to \mu\nu$

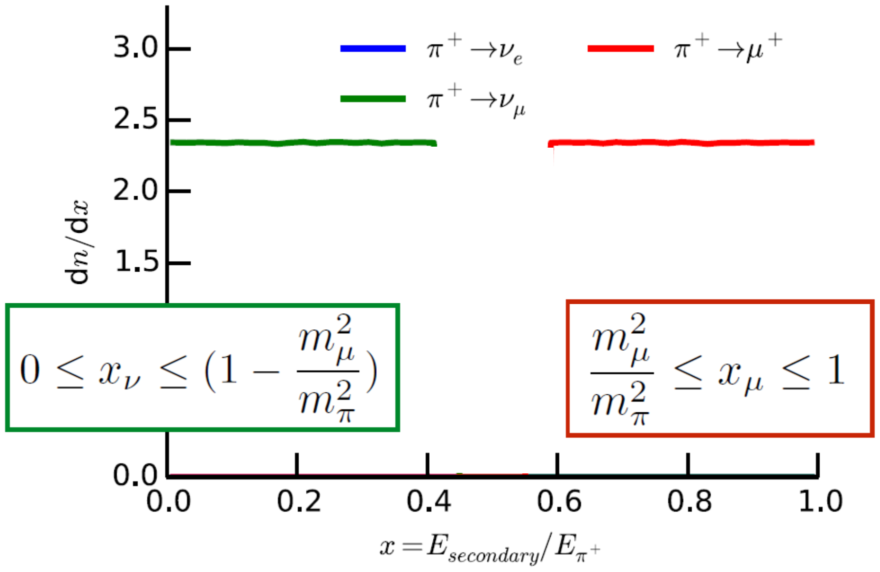
$$E_M \cdot \frac{m_\mu^2}{M^2} \leq E_\mu \leq E_M \,, \qquad x_i = \frac{E_i}{E_M}$$

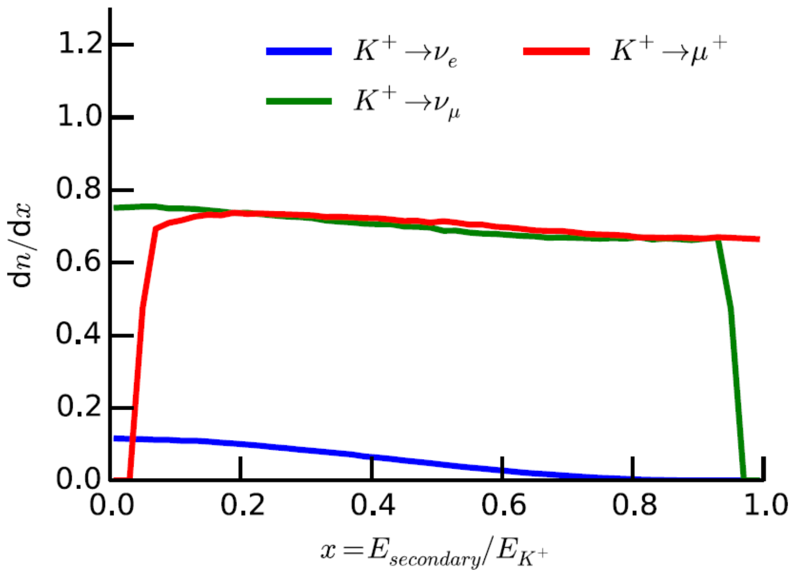
scaling = independent of the absolute value of E_M

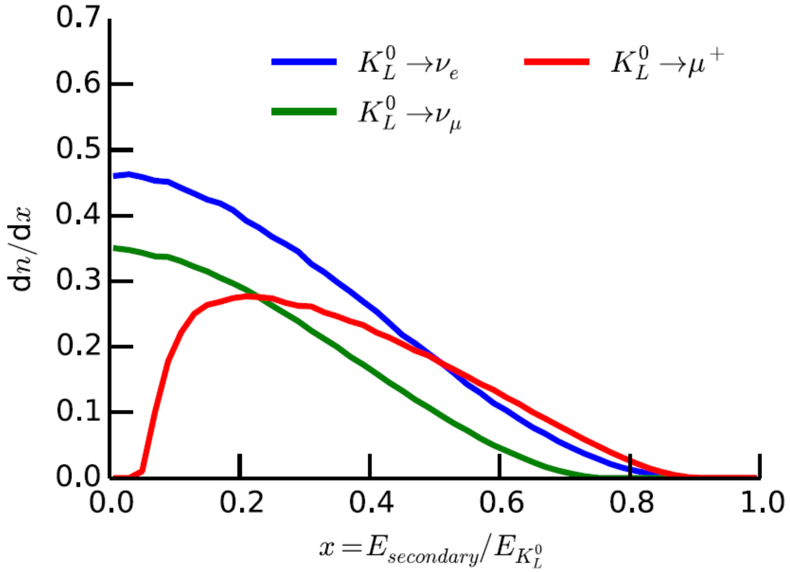
$$0 \leq x_\nu \leq (1 - \frac{m_\mu^2}{M^2}) \qquad \frac{m_\mu^2}{M^2} \leq x_\mu \leq 1$$

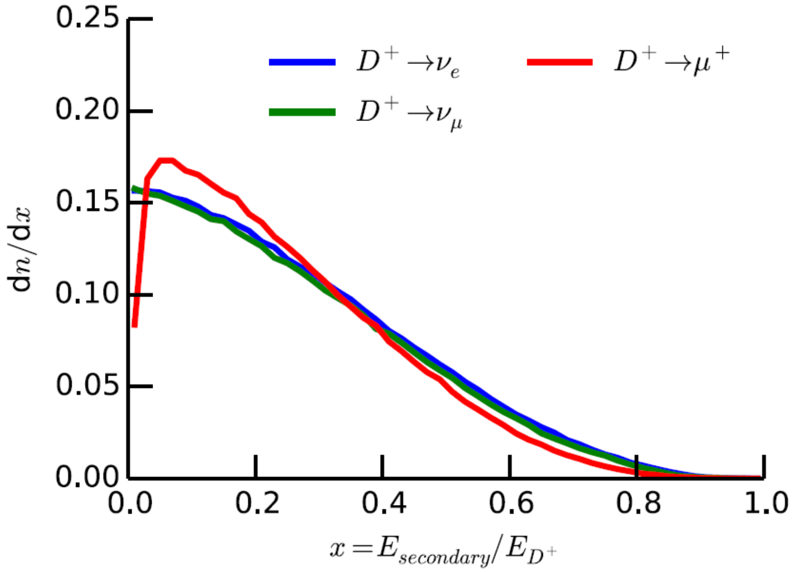
$$\boxed{Z^D_{M\to l} = BR(M \to l) \int_0^1 dx \; x^{\gamma-1} \frac{dN_{M\to l}}{dx}}$$

Energy distributions in decays (sampled from PYTHIA 8)









Cascade equations for inclusive muons and neutrinos

$$\frac{\mathrm{d}\Phi_\pi}{\mathrm{d}X} = \boxed{-\frac{\Phi_\pi}{\lambda_{\mathrm{int},\pi}} - \frac{\Phi_\pi}{\lambda_{\mathrm{dec},\pi}}} + \boxed{Z_{\mathrm{p}\pi}\frac{\Phi_\mathrm{p}(E,X)}{\lambda_{\mathrm{int},p}} + Z_{\mathrm{n}\pi}\frac{\Phi_\mathrm{n}(E,X)}{\lambda_{\mathrm{int},n}}} + Z_{\pi\pi}\frac{\Phi_\pi(E,X)}{\lambda_{\mathrm{int},n}}$$

Coupling to other hadrons

Cascade equation for muons, assuming only charged pions as sources and no continuous losses

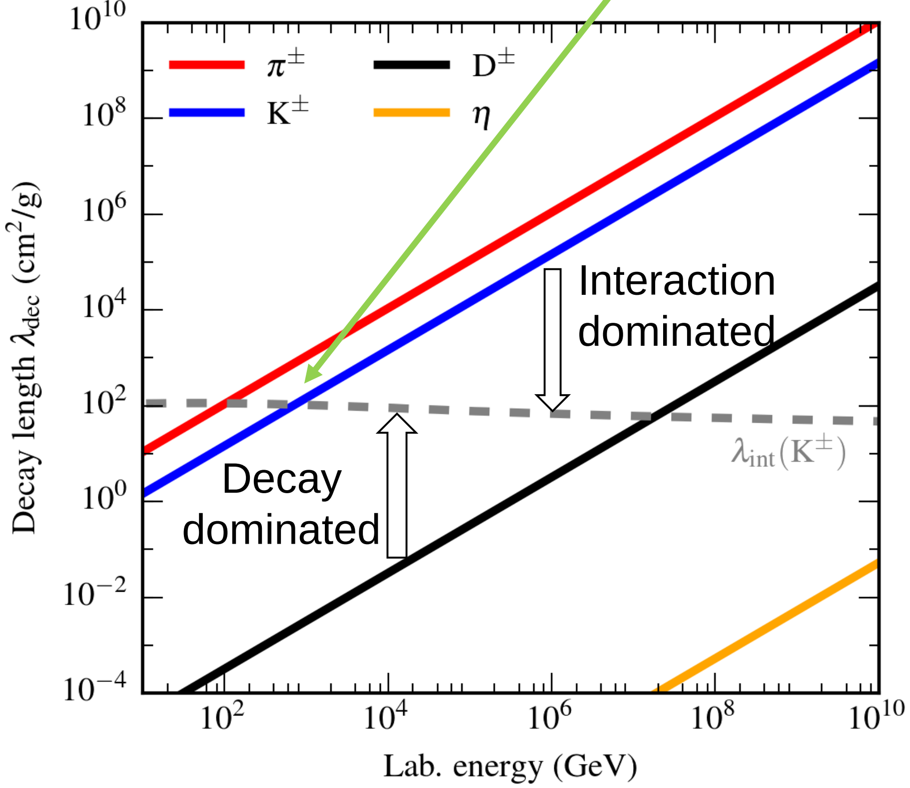
$$\frac{\mathrm{d}\Phi_\mu}{\mathrm{d}X} = -\frac{\Phi_\mu}{\lambda_{\mathrm{dec},\mu}} + S(\pi \to \mu) = \boxed{-\frac{\Phi_\mu}{\lambda_{\mathrm{dec},\mu}}} + \boxed{Z^{\mathrm{D}}_{\pi\to\mu}\frac{\Phi_\pi}{\lambda_{\mathrm{dec},\pi}}}$$

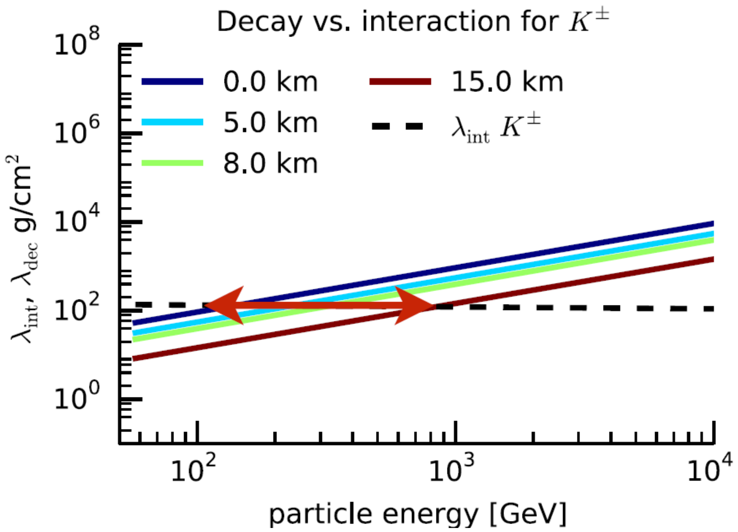
Same thing for neutrinos except that they don't decay

$$\frac{\mathrm{d}\Phi_{\nu_\mu}}{\mathrm{d}X} = S(\mu \to \nu_\mu) + S(\mu \to \nu_\mu) = \boxed{Z^{\mathrm{D}}_{\mu\to\nu_\mu}\frac{\Phi_\mu}{\lambda_{\mathrm{dec},\mu}} + Z^{\mathrm{D}}_{\pi\to\nu_\mu}\frac{\Phi_\pi}{\lambda_{\mathrm{dec},\pi}}}$$

Interactions vs. decays

$$\lambda_{\mathrm{dec},h}(E,X) = \frac{c\tau_h E \rho_{\mathrm{air}}(X)}{m_h c^2} = \frac{E X \cos\theta}{E_{\mathrm{crit},h}}$$





Critical energy depends on density

Int. length not density dependent. Why?

$$\lambda_{\mathrm{int},h}(E) = \frac{\langle m_{\mathrm{air}} \rangle}{\sigma^{\mathrm{prod}}_{h-\mathrm{air}}(E)}$$

particle	E_{crit} [GeV]
$\mu^\pm$	1.0
$\pi^\pm$	115
K_L^0	205
$K^\pm$	850
K_S^0	1.2E+05
$D^\pm$	4.3E+07

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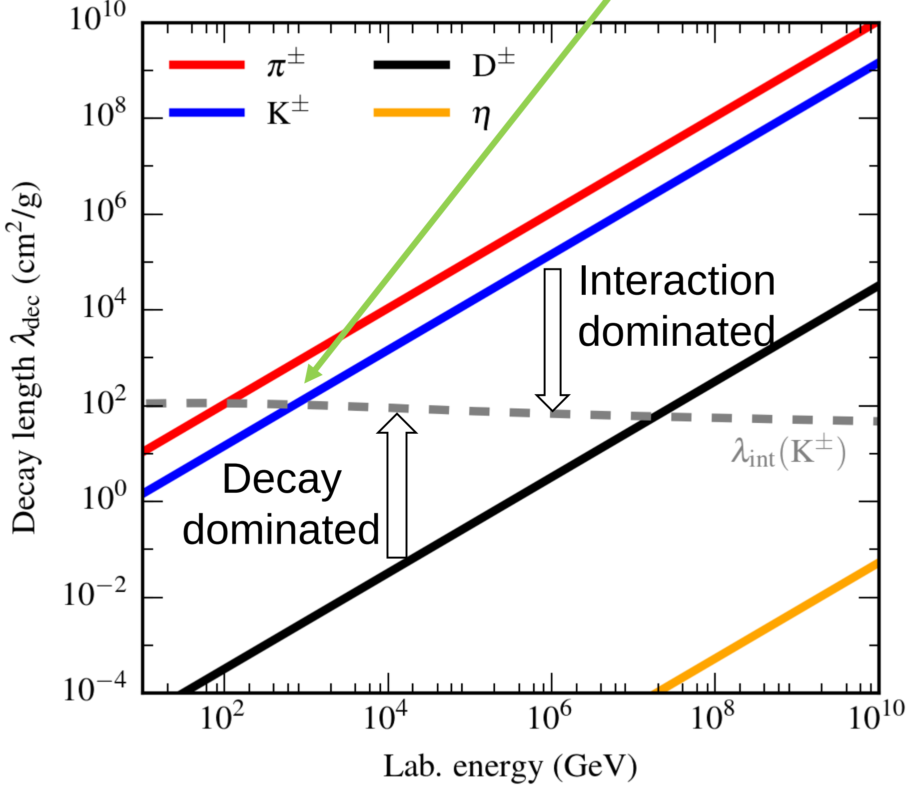

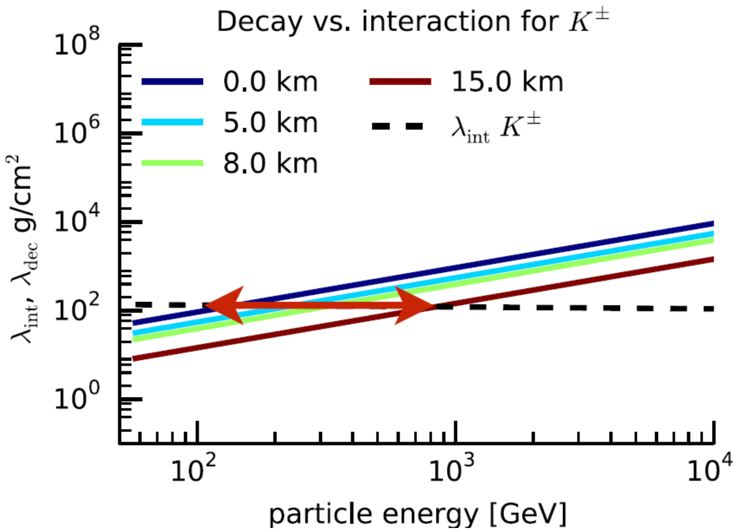

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$$\frac{\mathrm{d}X}{\mathrm{d}\ell} = \rho(\ell) \propto e^{\ell}$$

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Analytical solutions

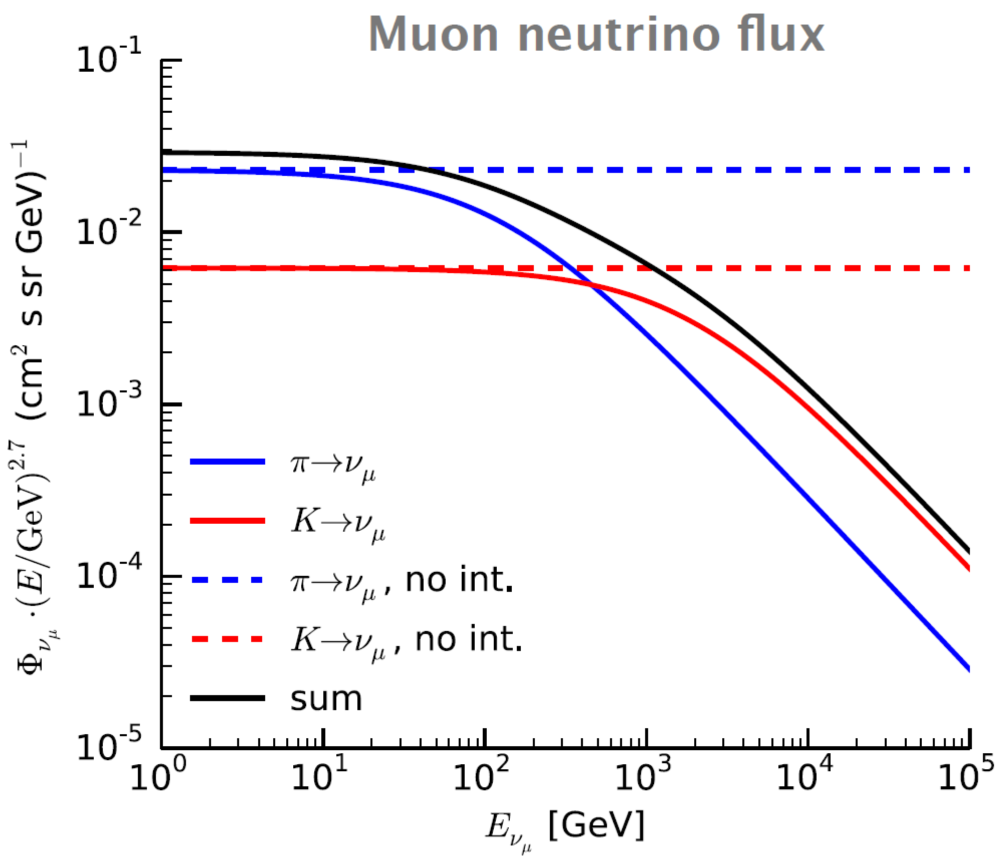
Asymptotic **low-energy solution** (pion interactions negligible)

$$\Phi_\nu(X) \propto E^{-\gamma}$$

Asymptotic **high-energy solution** (pion decays negligible)

$$\Phi_\nu(X) \propto E^{-\gamma-1}$$

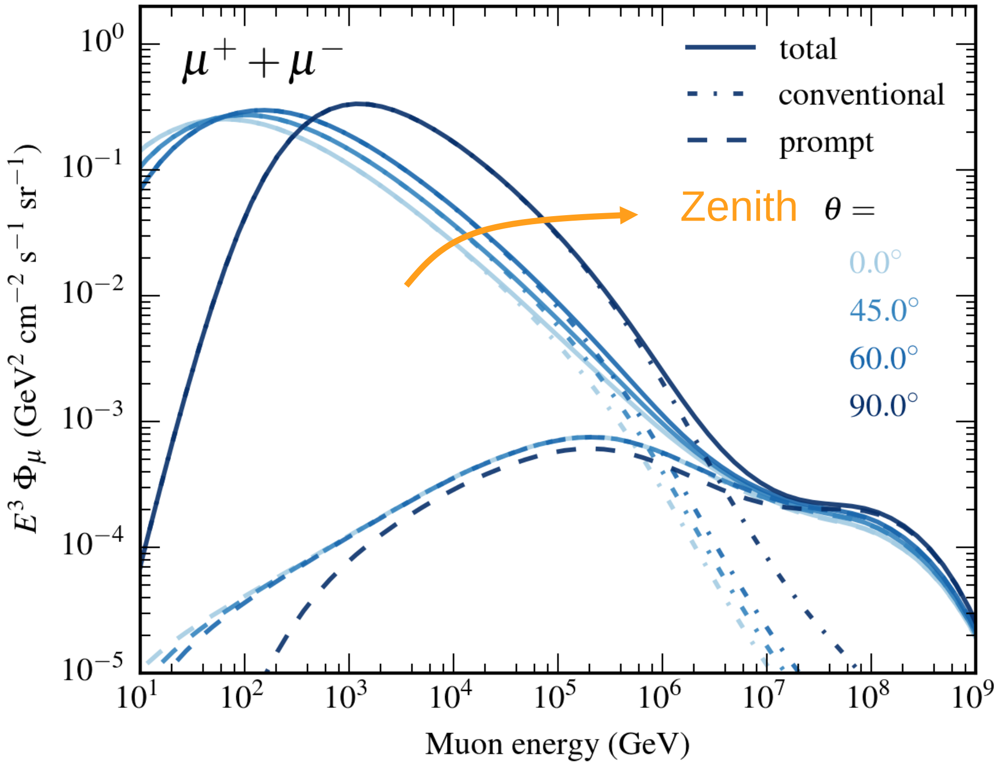
Interpolation $$\frac{\Phi_{\text{low}}\Phi_{\text{high}}}{\Phi_{\text{low}} + \Phi_{\text{high}}}$$

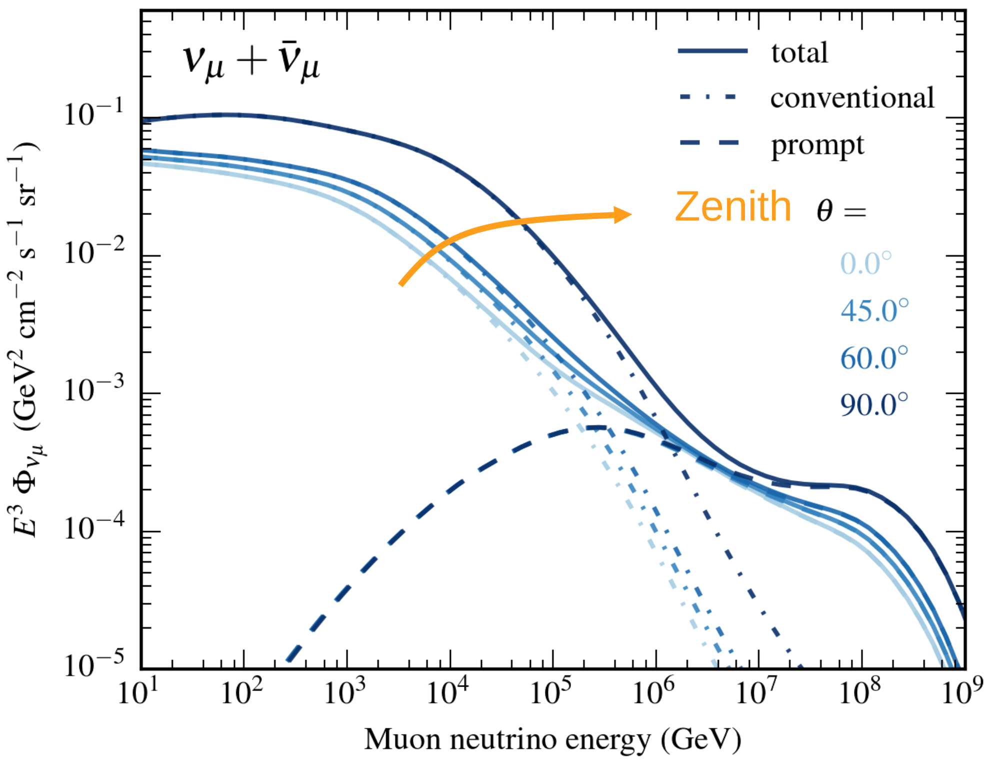


$$\boxed{\Phi_\nu(E) = \frac{\phi_N(E)}{1 - Z_{NN}} \left(\frac{\mathcal{A}_{\pi\nu}}{1 + \mathcal{B}_{\pi\nu} E \cos\theta/\varepsilon_\pi} + \frac{\mathcal{A}_{K\nu}}{1 + \mathcal{B}_{K\nu} E \cos\theta/\varepsilon_K} \right)}$$

see book by Gaisser, Engel, Resconi (2016) for full story

Zenith angle: Modified competition of decay and interactions

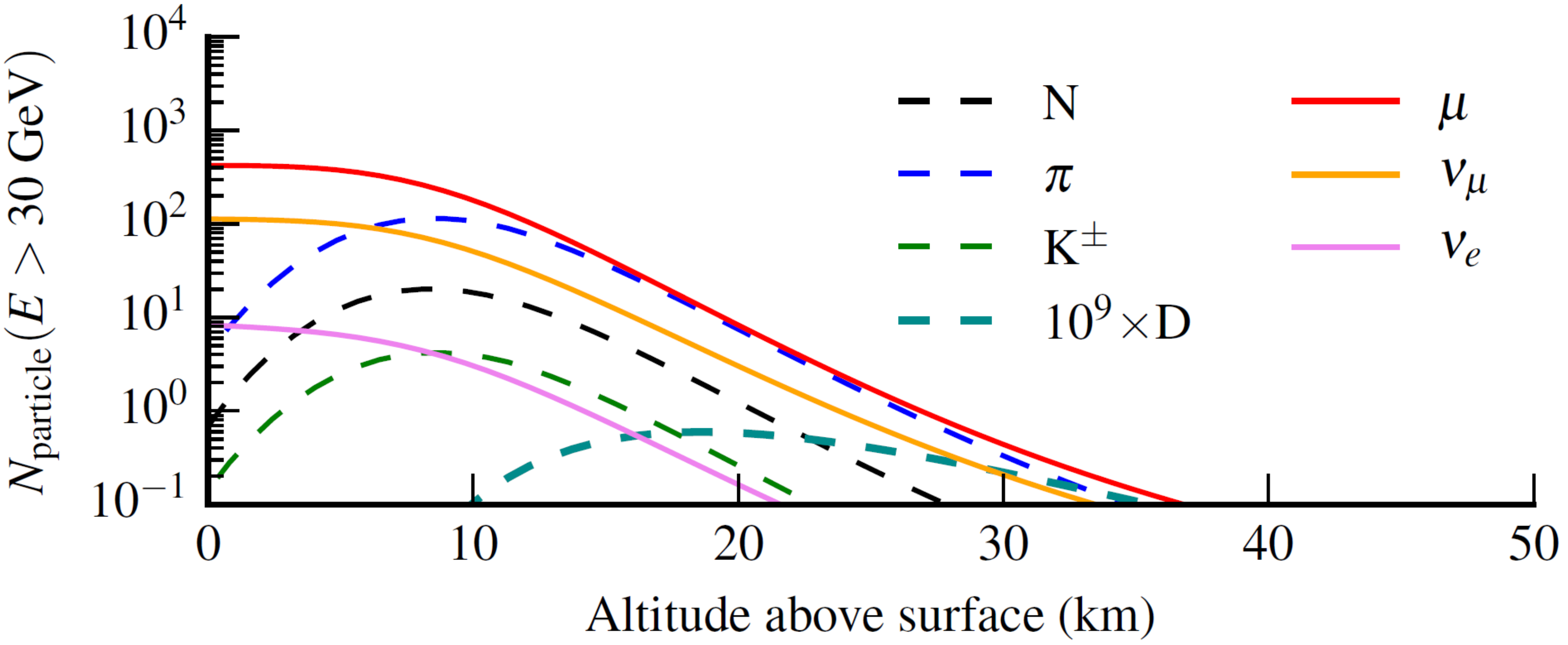




conventional: from decays of light and strange hadrons (longer lived)

prompt: from decays of short lived hadrons, mostly charm and bottom (no high-energy asymptotics)

Longitudinal evol. of 10 PeV proton interacting in atmosphere



Made with MCEq,
hands-on tomorrow

General form of 1D cascade equations in the atmosphere

System of PDE for each particle species *h* ($\leq 62 \times$ #E-bins in MCEq) *:*

$$
\begin{aligned}
\frac{\mathrm{d}\Phi_h(E,X)}{\mathrm{d}X} = &-\frac{\Phi_h(E,X)}{\lambda_{\mathrm{int},h}(E)} \\
&-\frac{\Phi_h(E,X)}{\lambda_{\mathrm{dec},h}(E,X)} \\
&-\frac{\partial}{\partial E}\left(\mu(E)\Phi_h(E,X)\right) \\
&+\sum_k \int_E^\infty \mathrm{d}E_k \; \frac{\mathrm{d}N_{k(E_k)\to h(E)}}{\mathrm{d}E}\frac{\Phi_k(E_k,X)}{\lambda_{\mathrm{int},k}(E_k)} \\
&+\sum_k \int_E^\infty \mathrm{d}E_k \; \frac{\mathrm{d}N^{\mathrm{dec}}_{k(E_k)\to h(E)}}{\mathrm{d}E}\frac{\Phi_k(E_k,X)}{\lambda_{\mathrm{dec},k}(E_k,X)}
\end{aligned}
$$

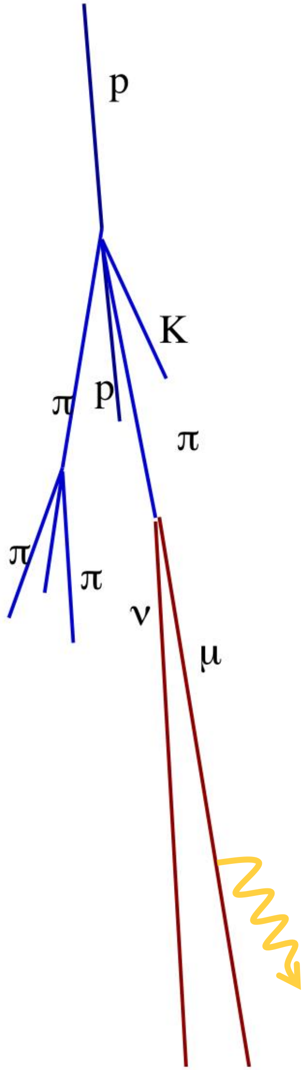
Interactions with air

Decays

Energy losses (radiative)

Re-injection from interactions

Re-injection from decays



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\end{aligned}
$$

cosmic ray physics

atmospheric physics

particle physics

Interactions with air

Decays

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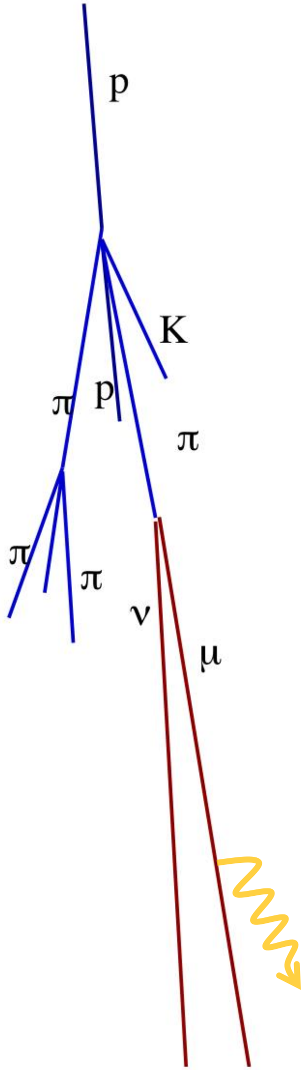
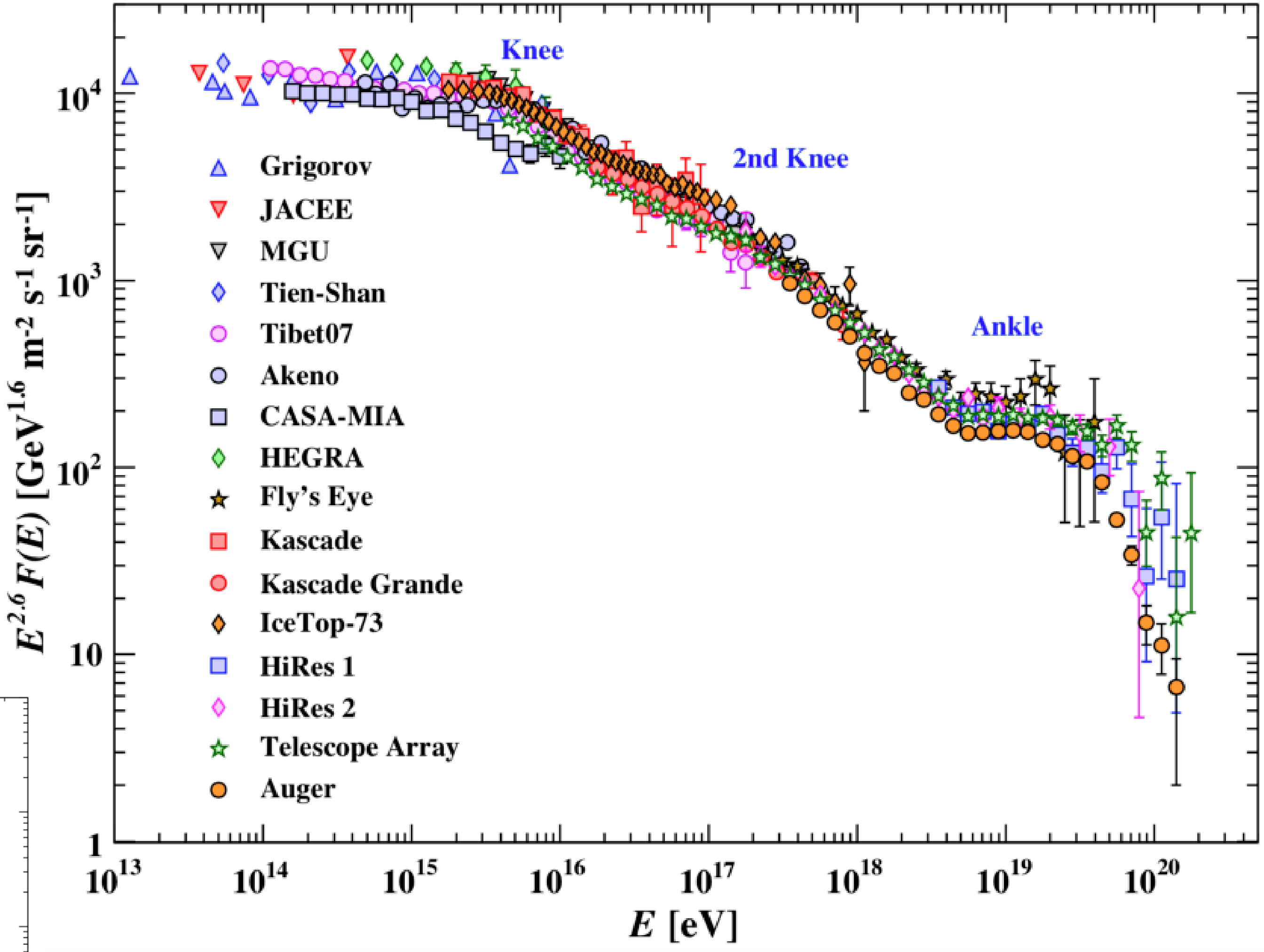
Re-injection from decays

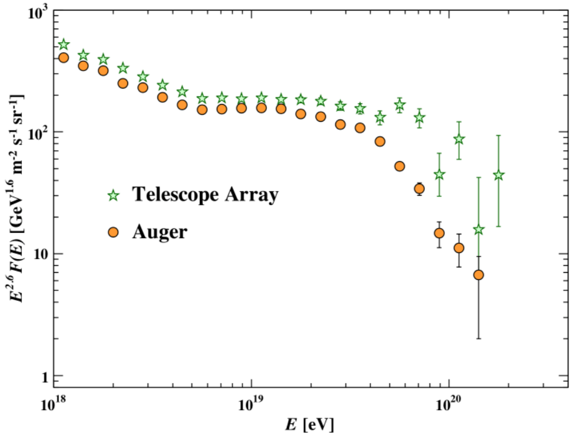


Reality: non-power-law Cosmic Ray spectra

PDG.lbl.gov

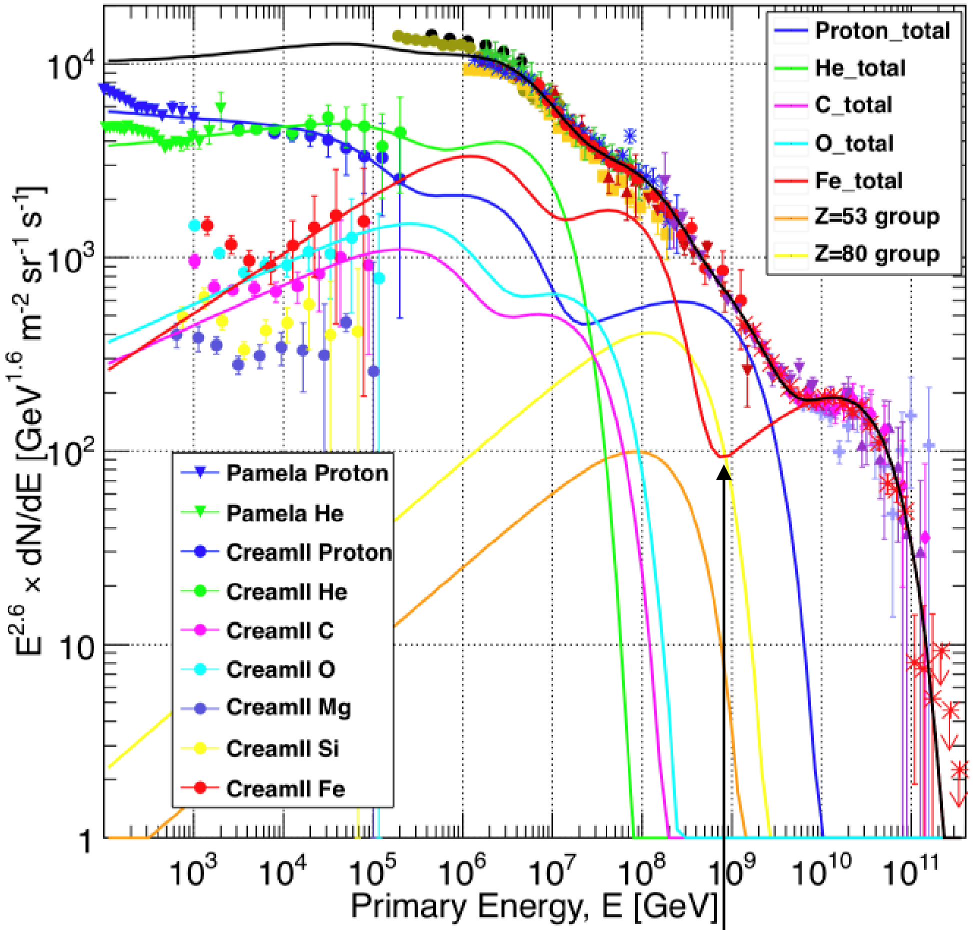
- Approx. series of broken power-laws
- **Fluxes of mass groups from indirectly from air-showers**
- Origin of features is disputed (lecture by P. Blasi). Might come from characteristics of
  - the accelerator itself
  - the transport through interstellar/-galactic medium
  - the superposition of different types of accelerators

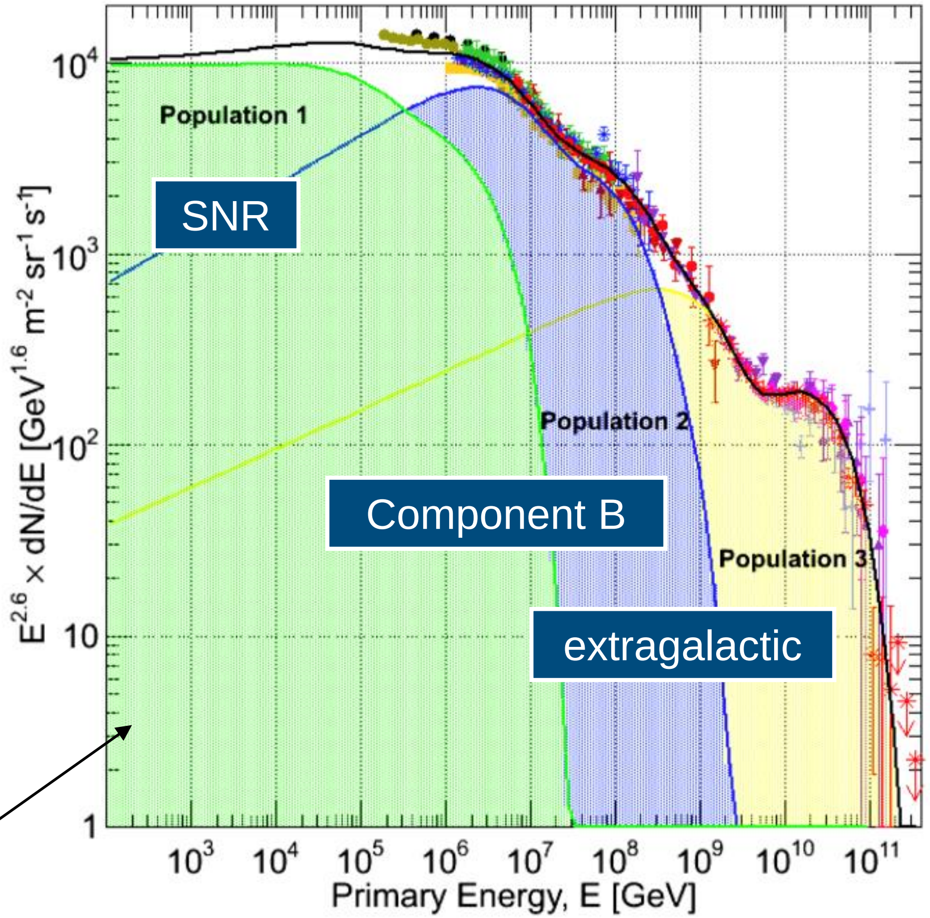




Typical Cosmic Ray Flux models

T. Gaisser, T. Stanev and S. Tilav, Front.Phys.(Beijing) 8 (2013) 748-758





$$\phi_i(E) \;=\; \Sigma_{j=1}^{3}\, a_{i,j}\, E^{-\gamma_{i,j}} \times \exp\left[-\frac{E}{Z_i R_{c,j}}\right]$$

Contemporary models

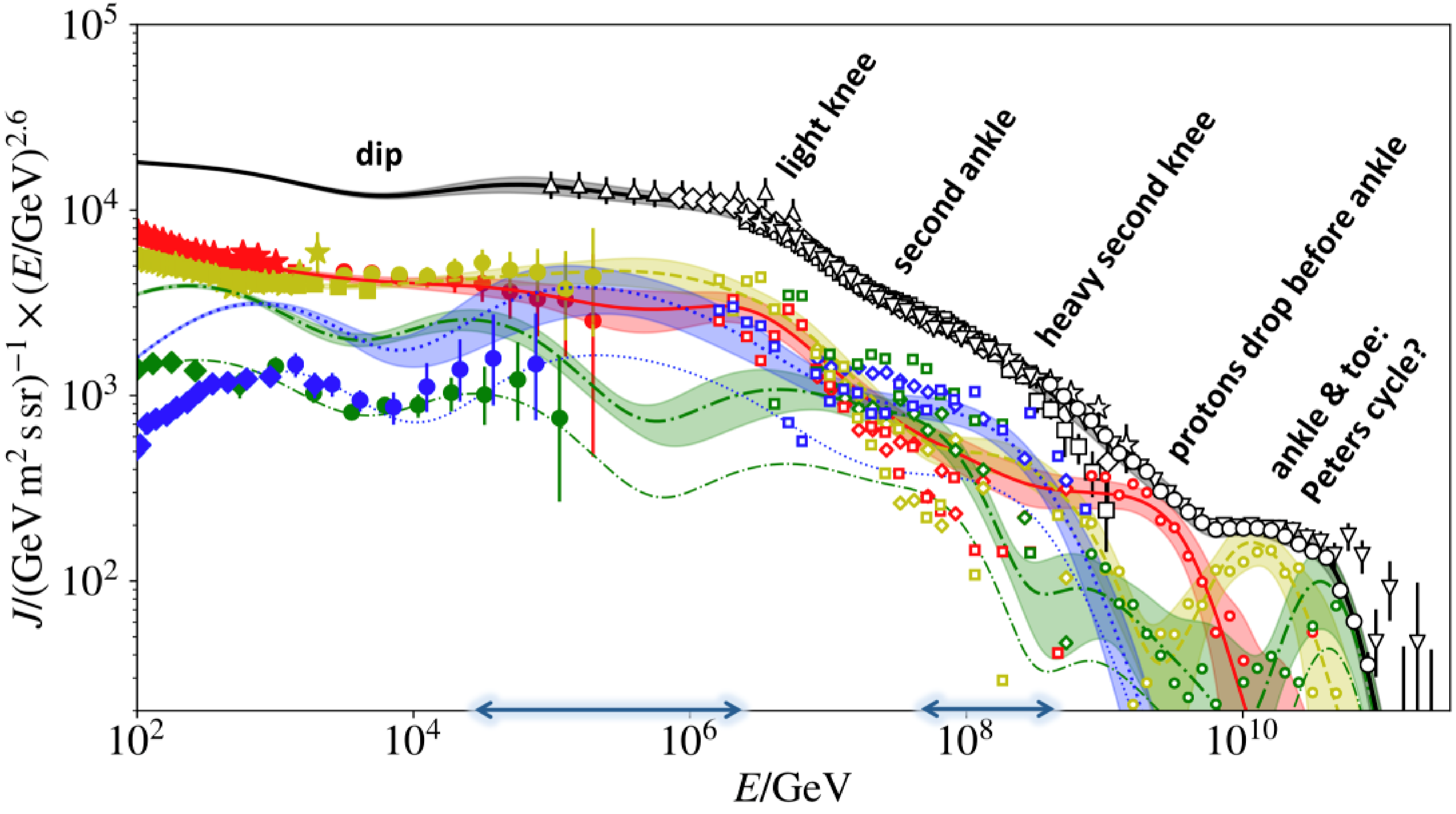
Short name	Reference	Description	Valid range [GeV]
H3a	[13]	three astrophysical populations, broken power laws, five mass groups, heavier composition at ultra-high energies (UHE)	$10^3 - 10^{11}$ GeV
H4a	[13]	same as H3a but with proton composition at UHE	$10^3 - 10^{11}$ GeV
GST-3	[44]	three population, broken power-law fit heavier composition between knee and ankle (second knee)	$10^3 - 10^{11}$ GeV
GST-4	[44]	like GST-3 but with an fourth extragalactic proton component at UHE	$10^3 - 10^{11}$ GeV
GH	[45]	power-law model with five mass groups, often used in atmospheric neutrino flux calculations below knee energies [12, 46, 11]	$<$ PeV
cHGp	[14, 45, 13]	combination of GH at low energy and H4a above	tens -10^{11} GeV
cHGm	[14, 45, 13]	like cHGp but with H3a instead of H4a	tens -10^{11} GeV
Polygonato	[47]	broken power-law fit, based on renormalization of various cosmic ray measurements up to knee energies	few TeV – PeV
ZS	[48, 49]	original model by Zatsepin and Sokolskaya, also including re-fitted parameters by the PAMELA collaboration	tens GeV – PeV
TIG	[28]	simple broken power law spectrum of nucleons (protons)	TeV – PeV
GSF	add..	Global Spline Fit to recent cosmic ray observations with errors	10 GeV -10^{12} GeV

Models in MCEq/CRFluxModels:
https://github.com/afedynitch/CRFluxModels

- Models are constructed from different sets of data
- Systematic uncertainties are rarely taken into account (Polygonato & **GSF**)

The Global Spline Fit (GSF)

H. Dembinski et al.
PoS(ICRC2017)533

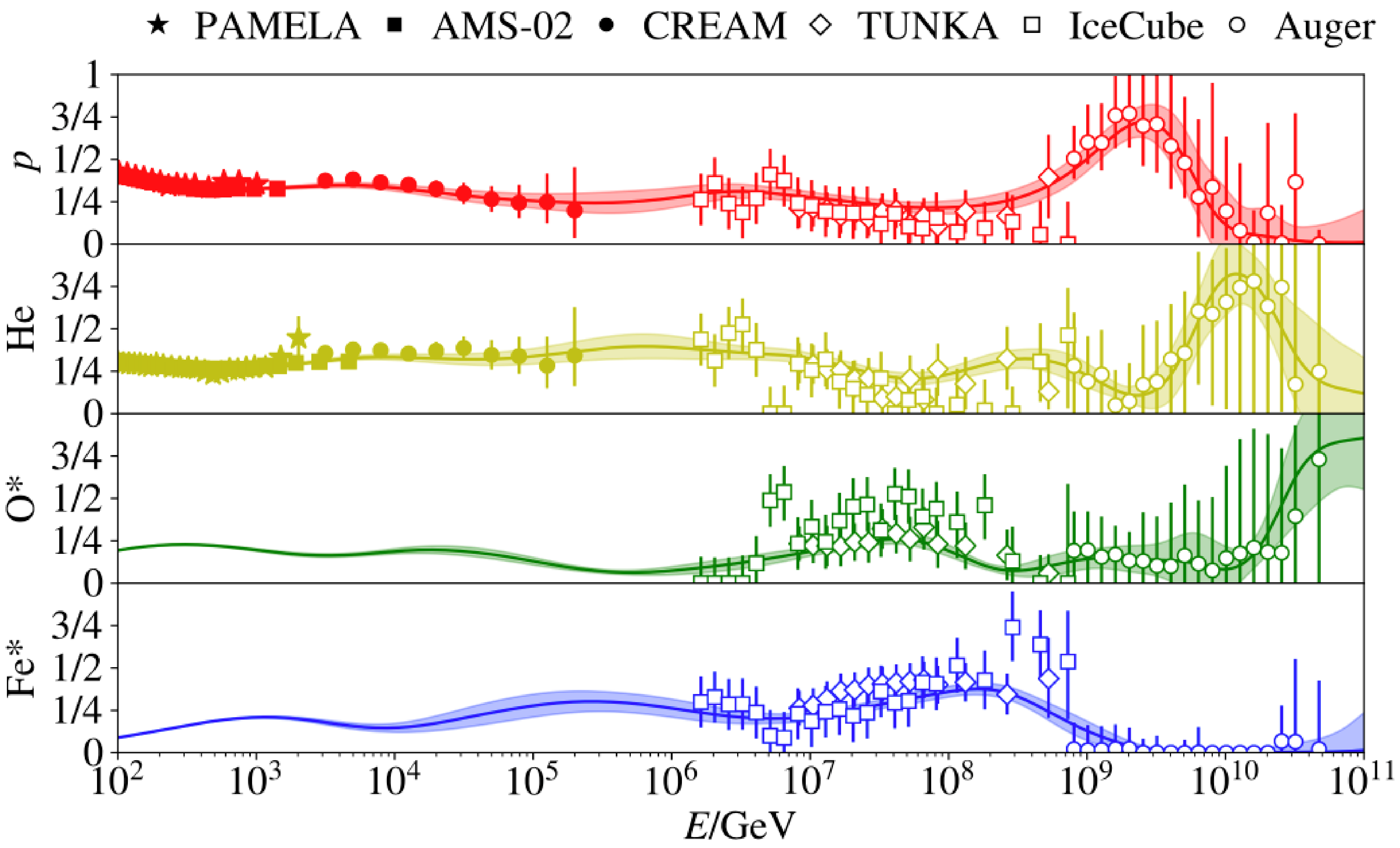


More composition data needed

Fitted composition data

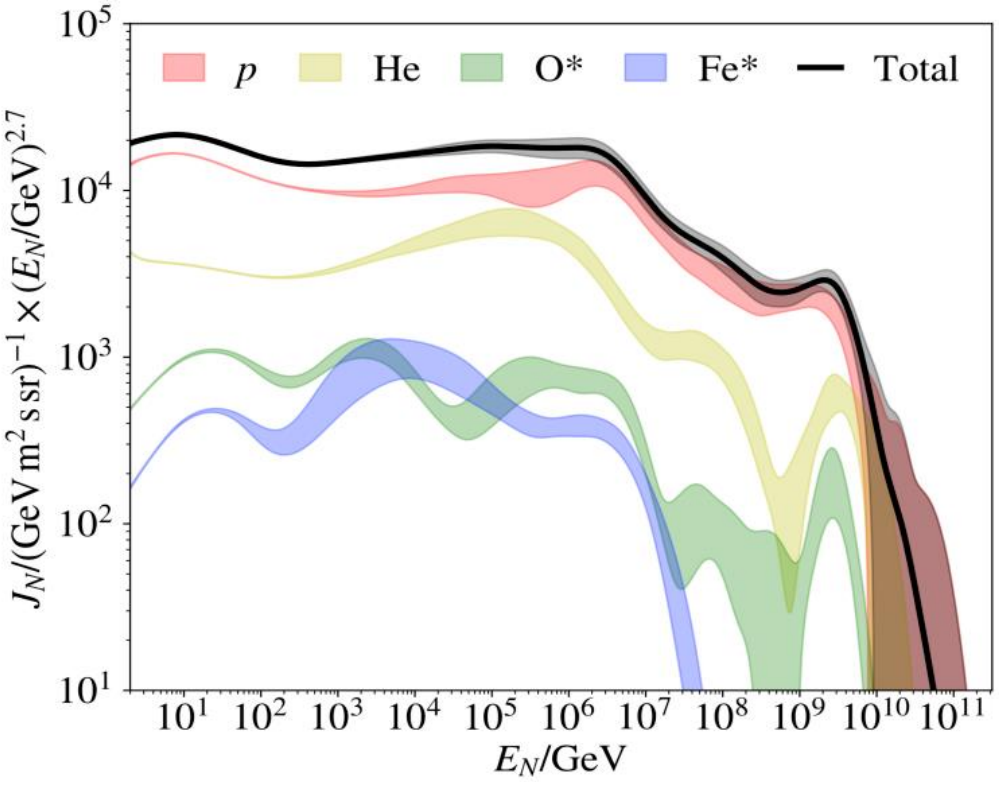
4-mass group experiments

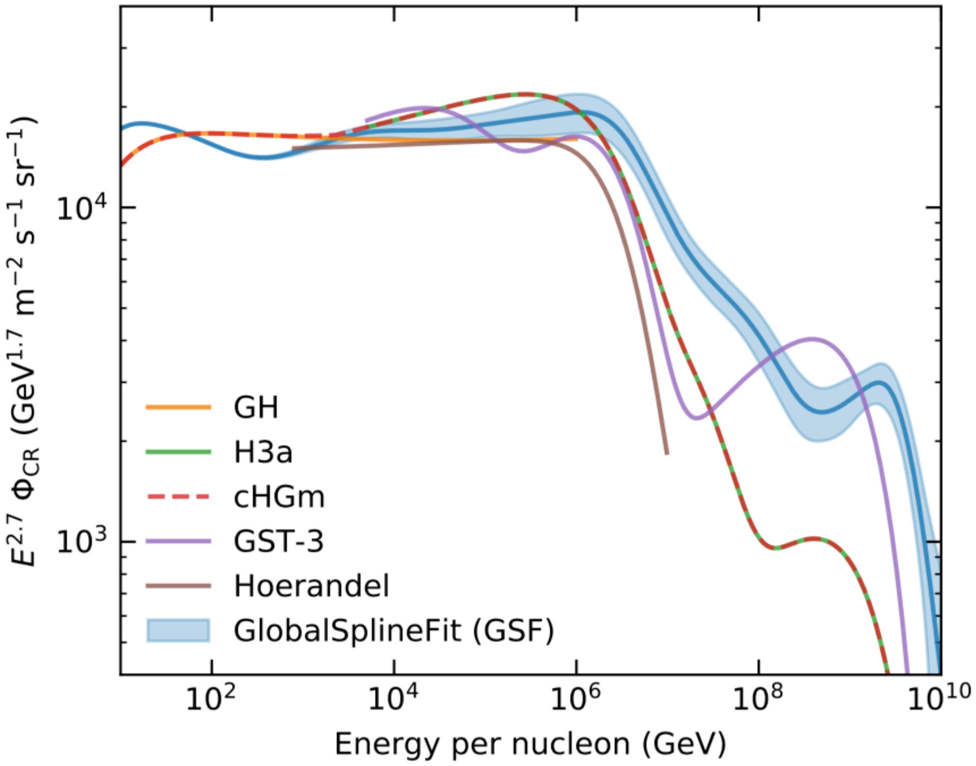
H. Dembinski et al.
PoS(ICRC2017)533



Required quantity: nucleon flux (not particle or nucleus flux)

AF et al, PoS(ICRC2017)1019





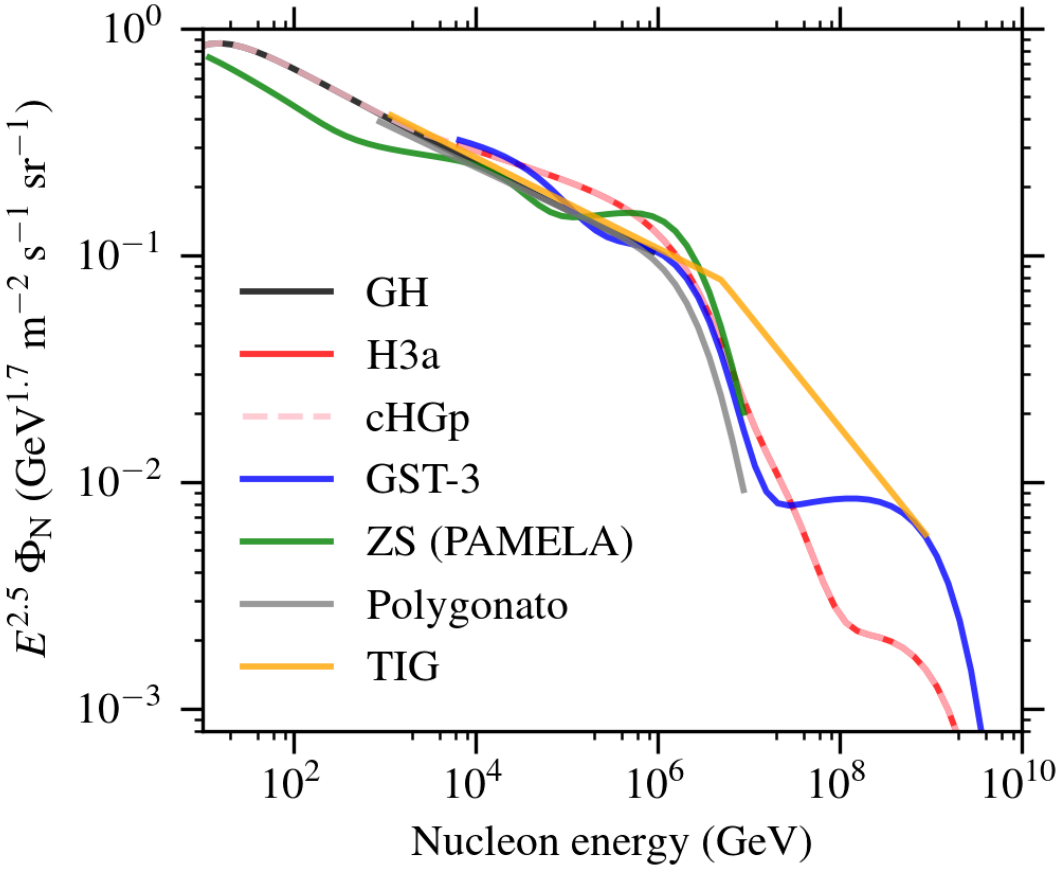
Dominated by proton flux.
Details of sub-leading elements not important.

Superposition model:
Nucleus of mass A = A nucleons with E/A

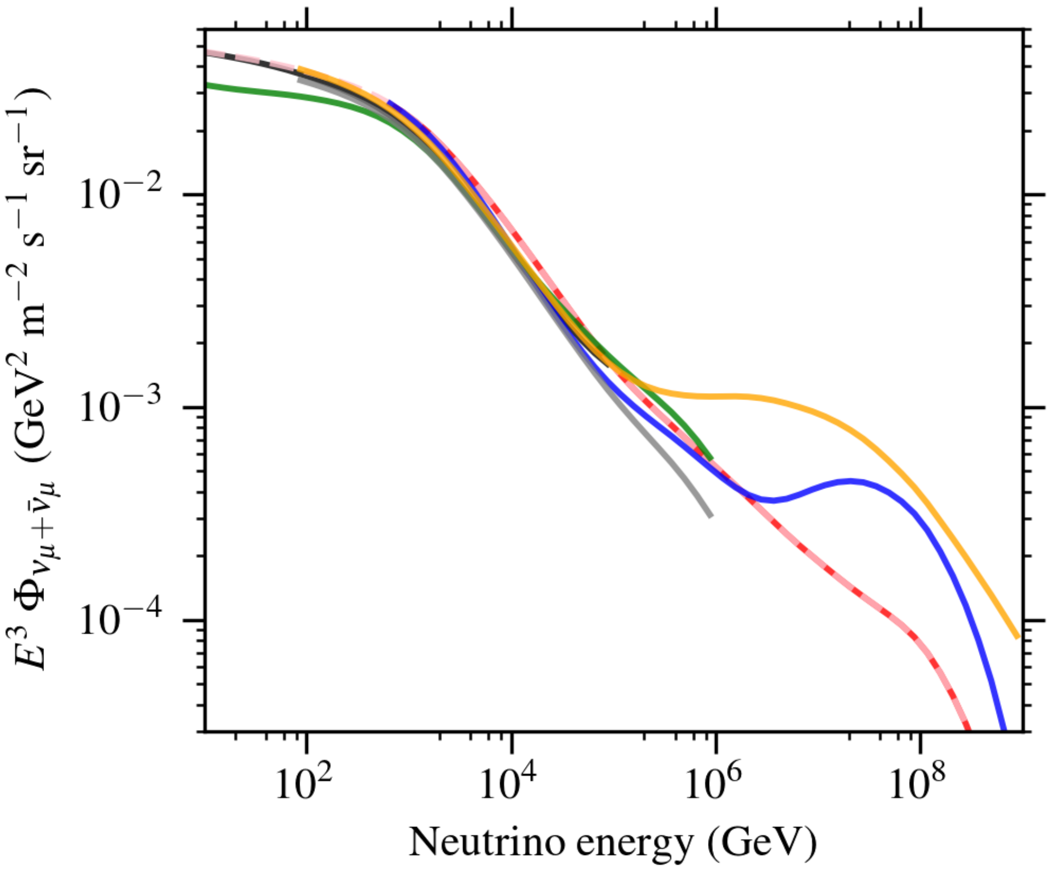
$$\phi_N(E_N) = \sum_{nuclei} A_i^2\ \phi_i(E \cdot A)$$

Impact on atmospheric neutrino flux

Cosmic ray nucleon flux

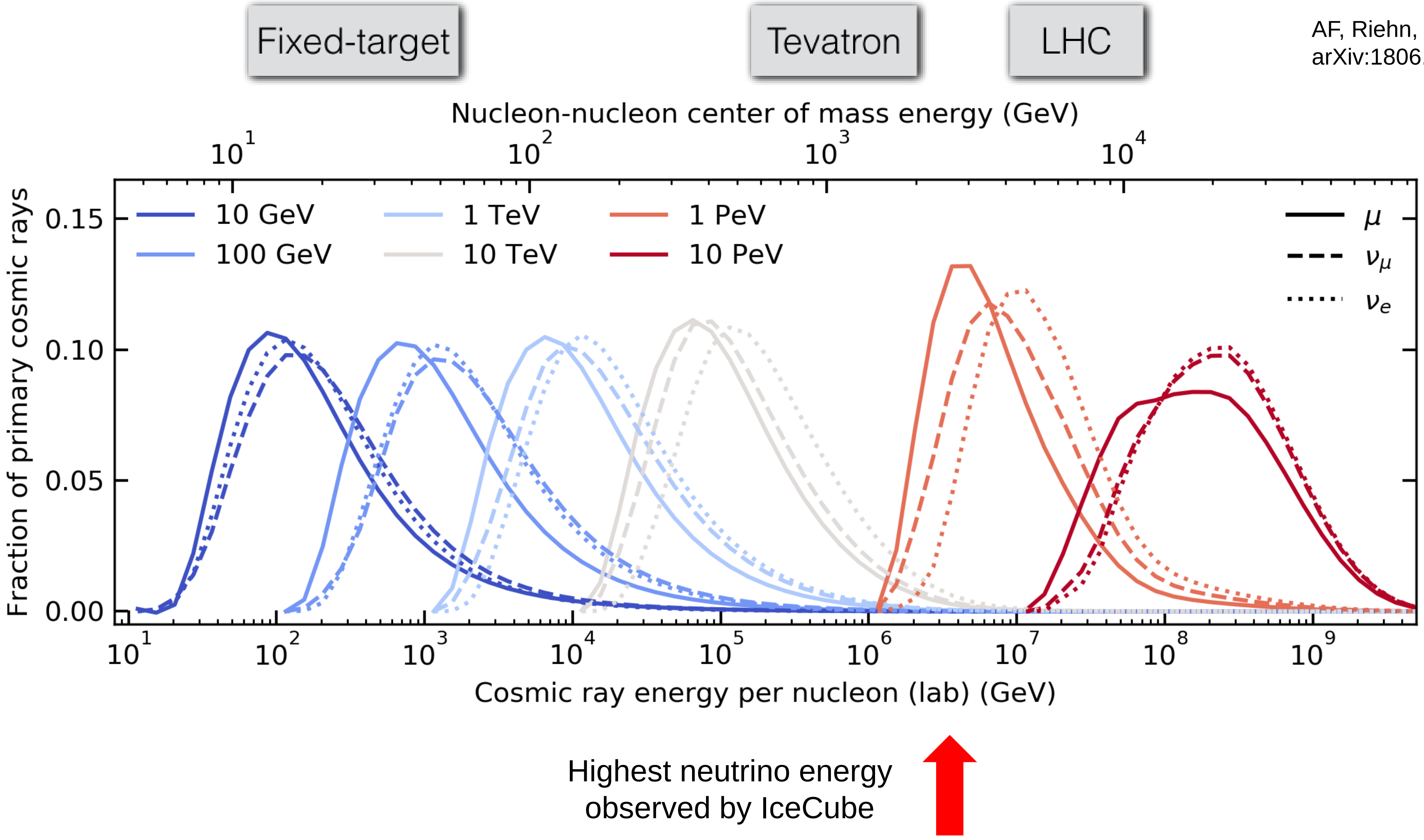


Atmospheric neutrino flux



Relation between lepton and cosmic ray energy

AF, Riehn, Engel, Gaisser, Stanev
arXiv:1806.04140



If energy is not a problem…

Kinematic variables

$$\theta = \arctan \frac{p_T}{p_z}$$

$$\eta = -\ln(\tan \frac{\theta}{2})$$

$$x_{\mathrm{lab}} = \frac{E_{\mathrm{secondary}}}{E_{\mathrm{primary}}} \approx \frac{p_{z,\mathrm{secondary}}}{E_{\mathrm{primary}}}$$

For atmospheric leptons

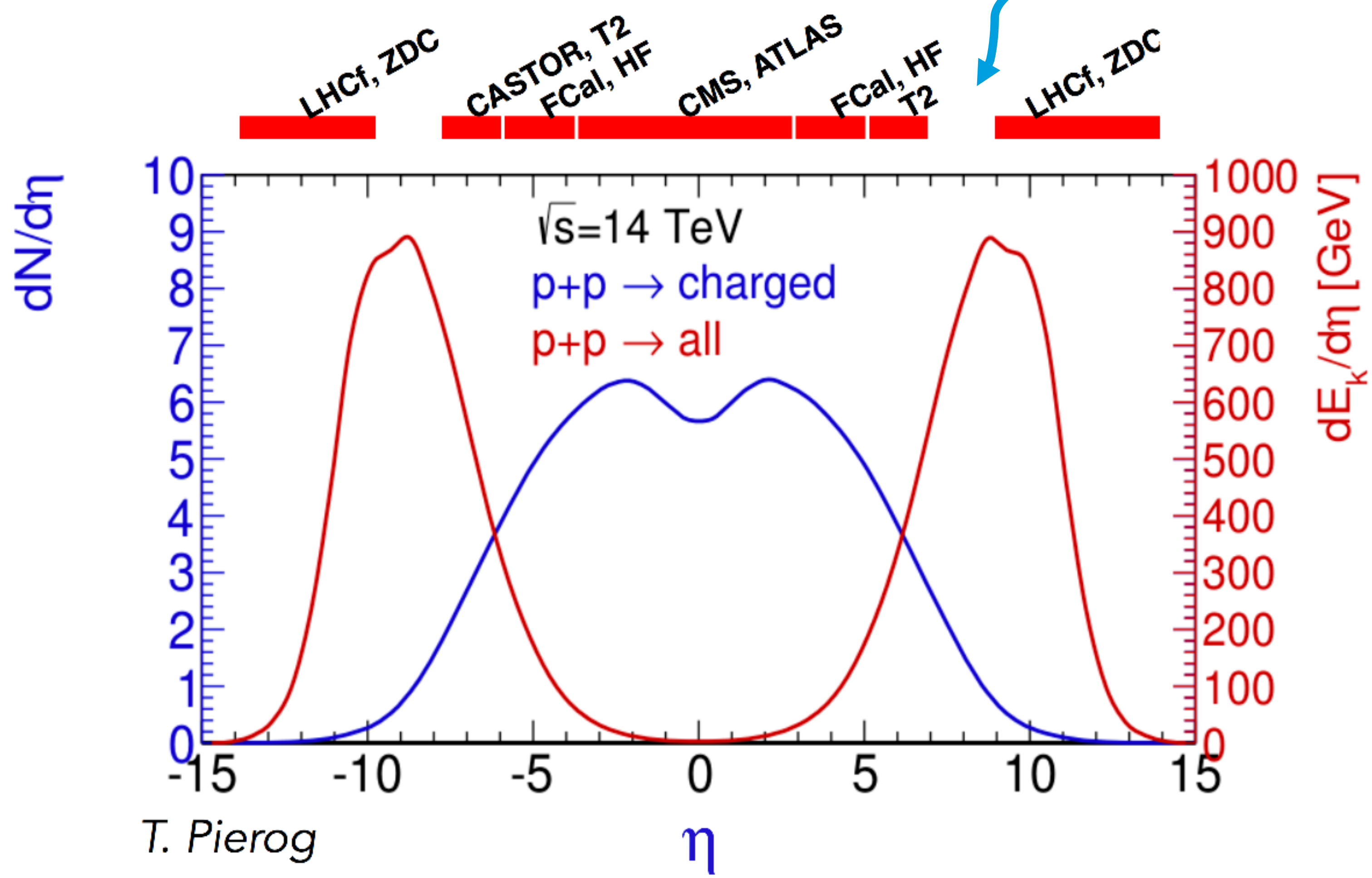
$$p_z \sim \mathrm{TeV} - \mathrm{PeV}$$

$$p_T \sim \text{few GeV}$$

$$\theta \sim \mu\mathrm{rad}$$

$$\boxed{x_{\mathrm{lab}} > 0.1, \quad \eta \to \infty}$$

Beam pipe!



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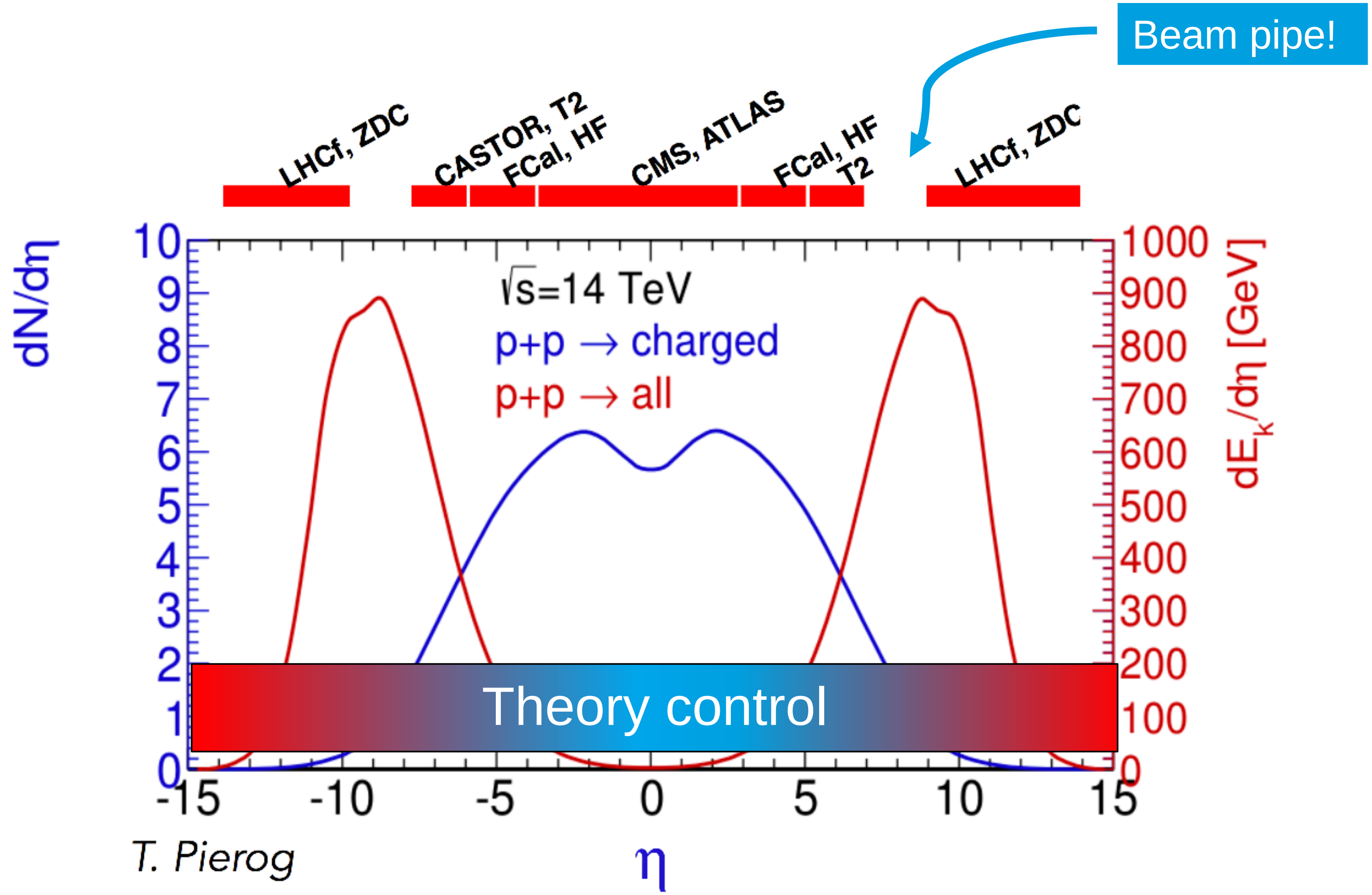
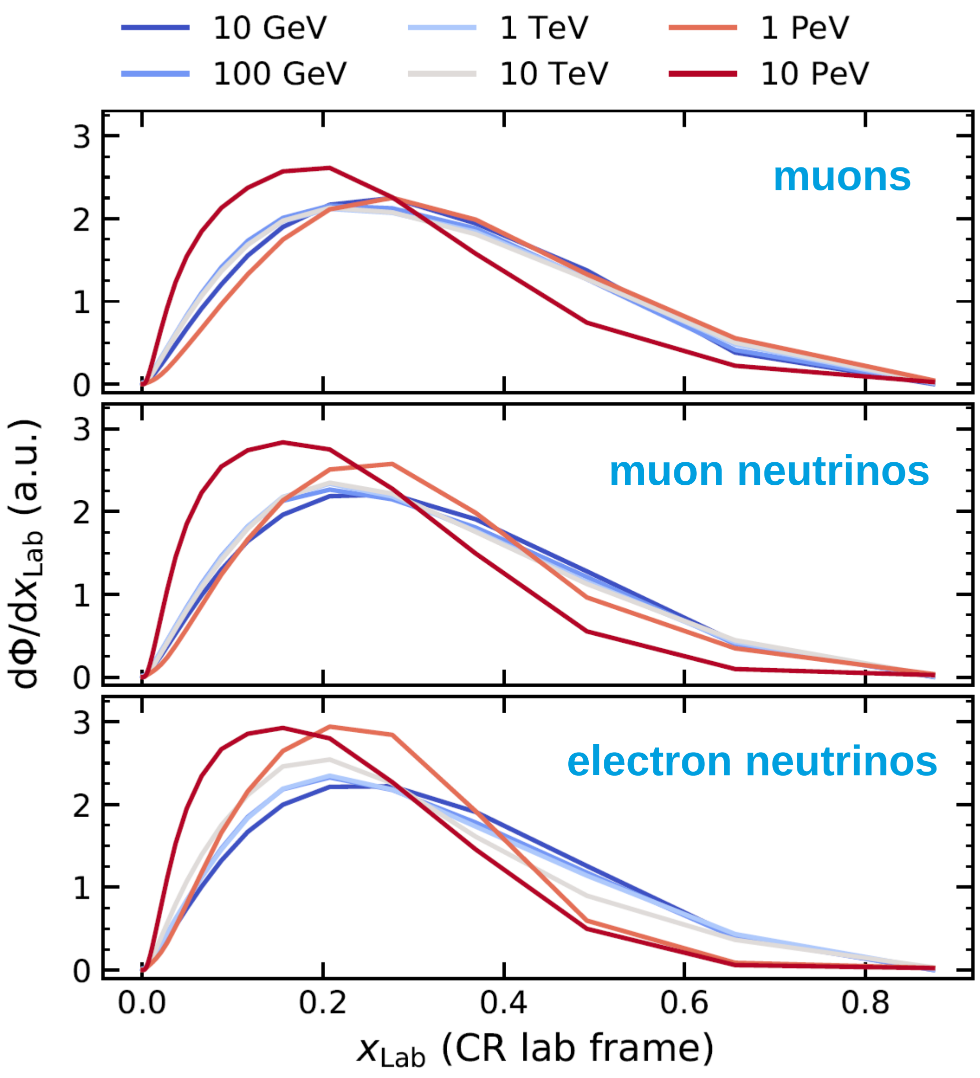


Relevant particle production phase space



AF, Riehn, Engel, Gaisser, Stanev
arXiv:1806.04140

- Atmospheric leptons are sensitive mostly to $x_{lab} > 0.1$
- Reason: steepness of primary CR spectrum

How much of this phase-space is seen by LHCb ("forward experiment")?

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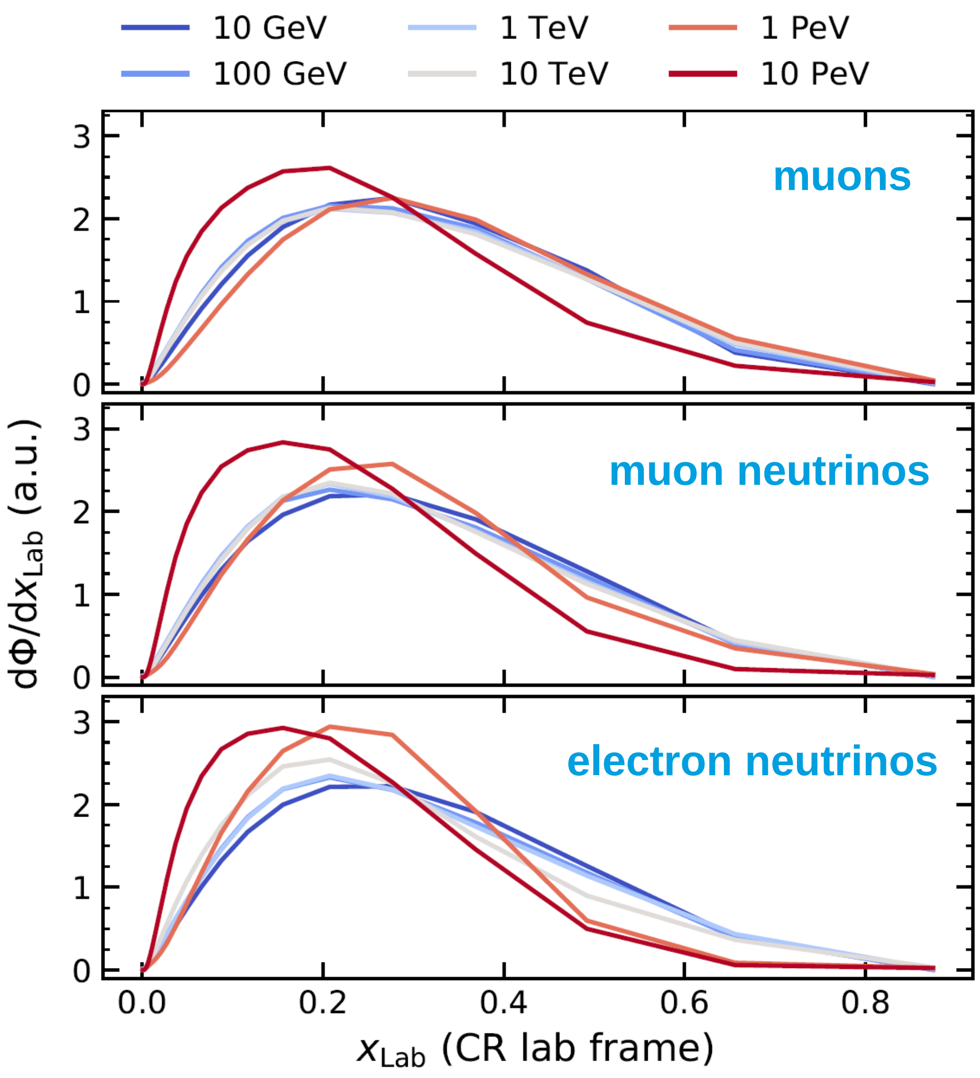

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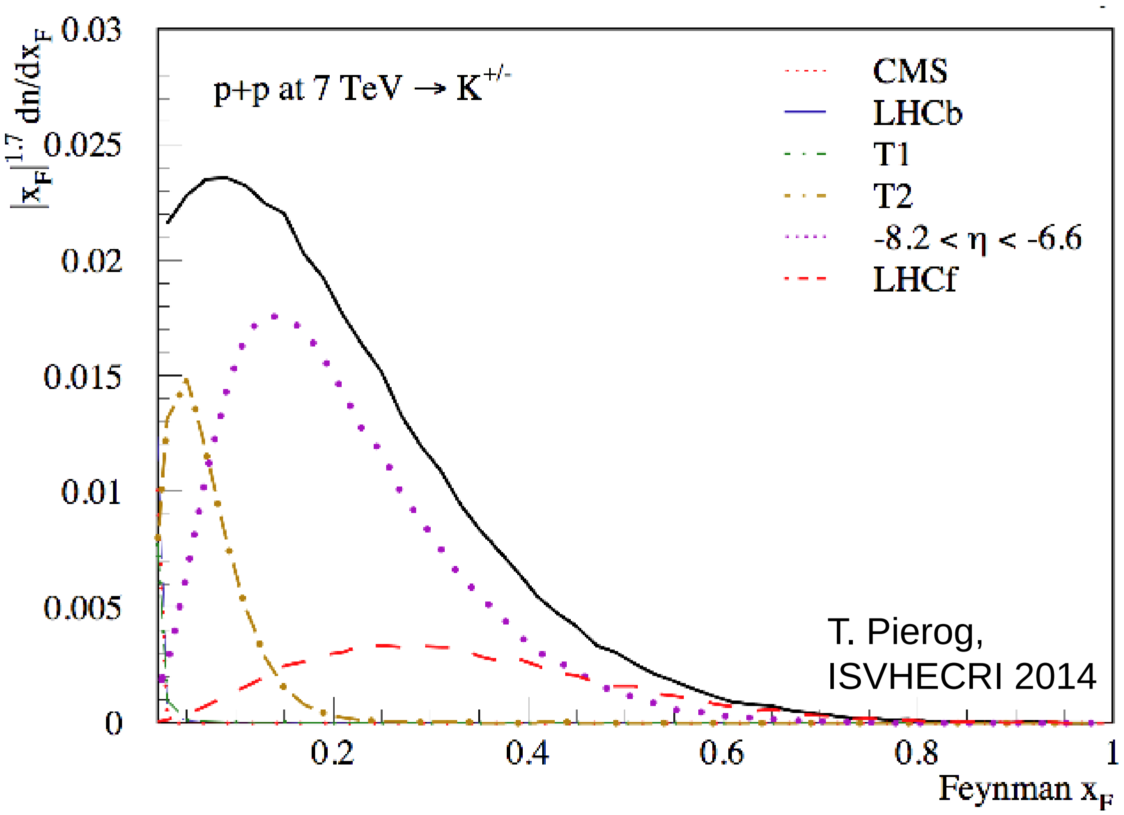
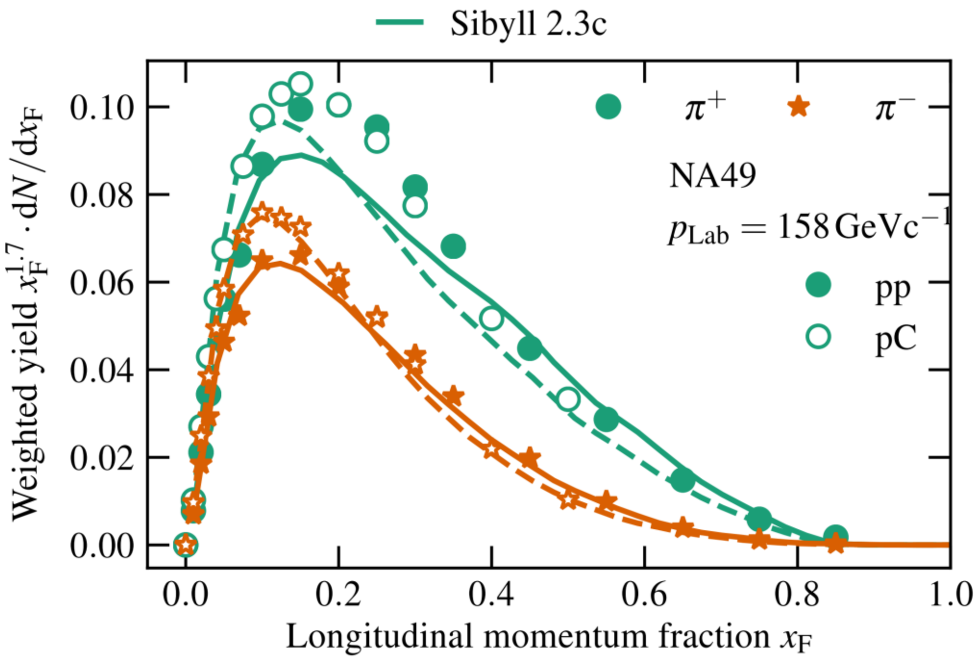
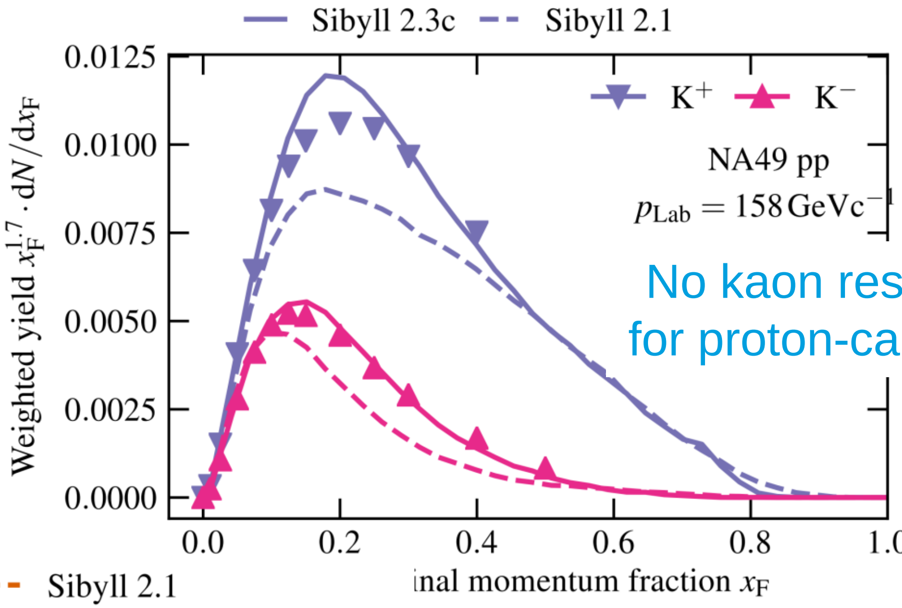


How much of this phase-space is seen by LHCb (“forward experiment”)?

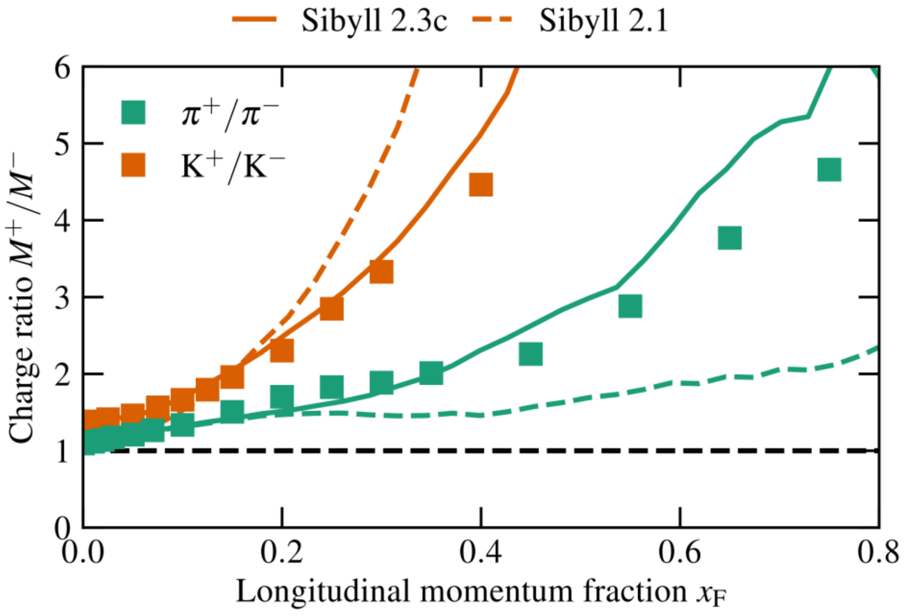
Fixed-target data with large phase space coverage crucial

… but only at low energy, extrapolation model dependent





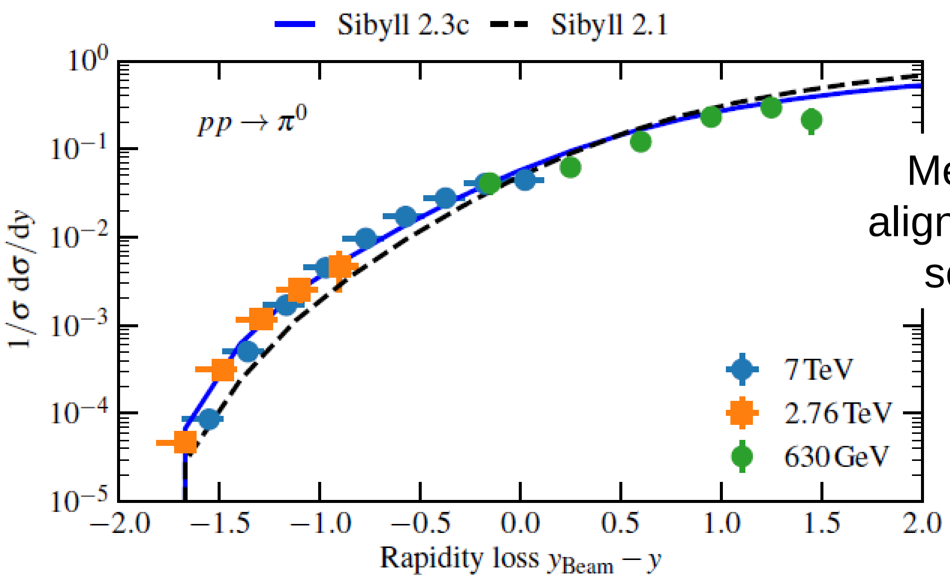
No kaon results for proton-carbon



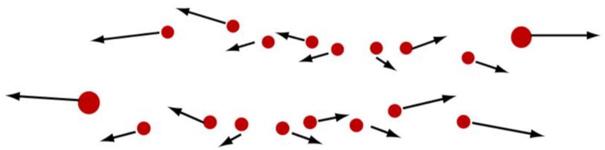
AF, Riehn, Engel, Gaisser, Stanev
arXiv:1806.04140

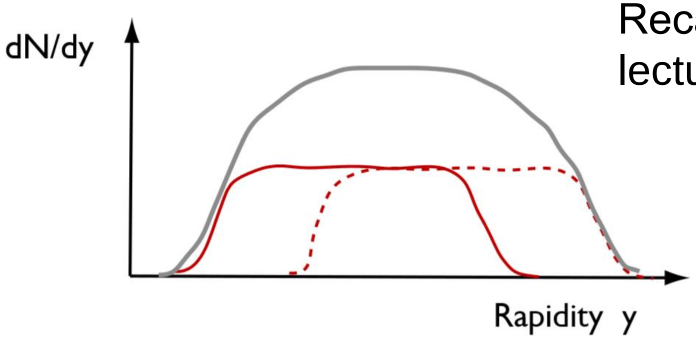
Feynman scaling

AF, F. Riehn, R. Engel, T. Gaisser, T. Stanev
arXiv:1806.04140

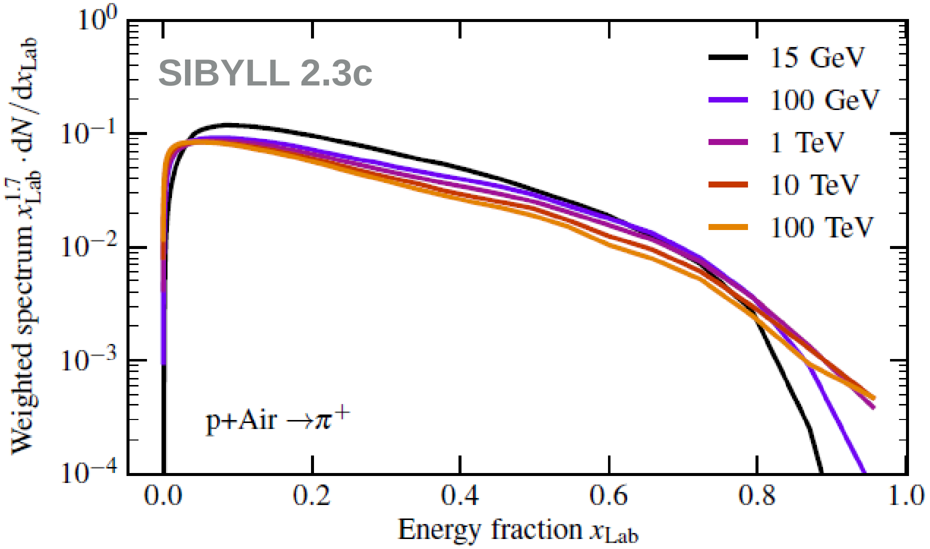


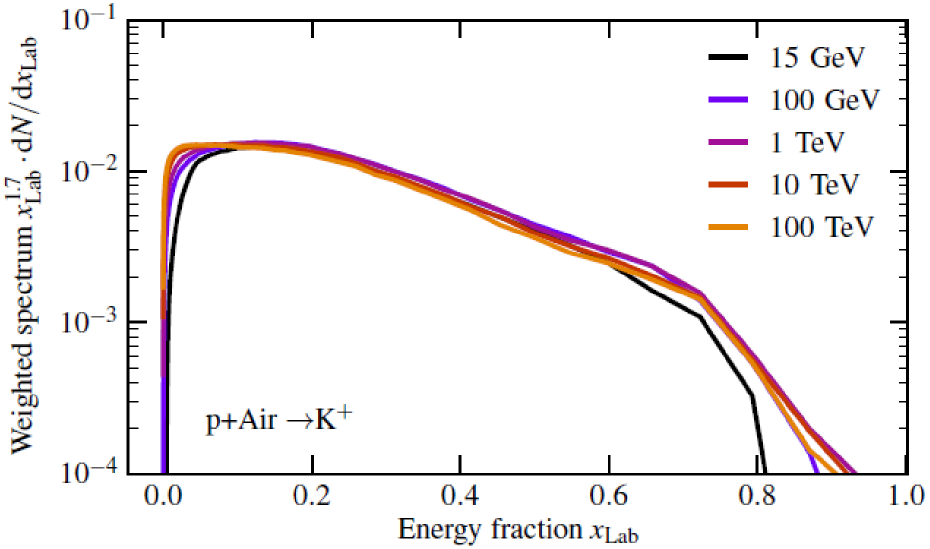
Measurements aligned if Feynman scaling holds





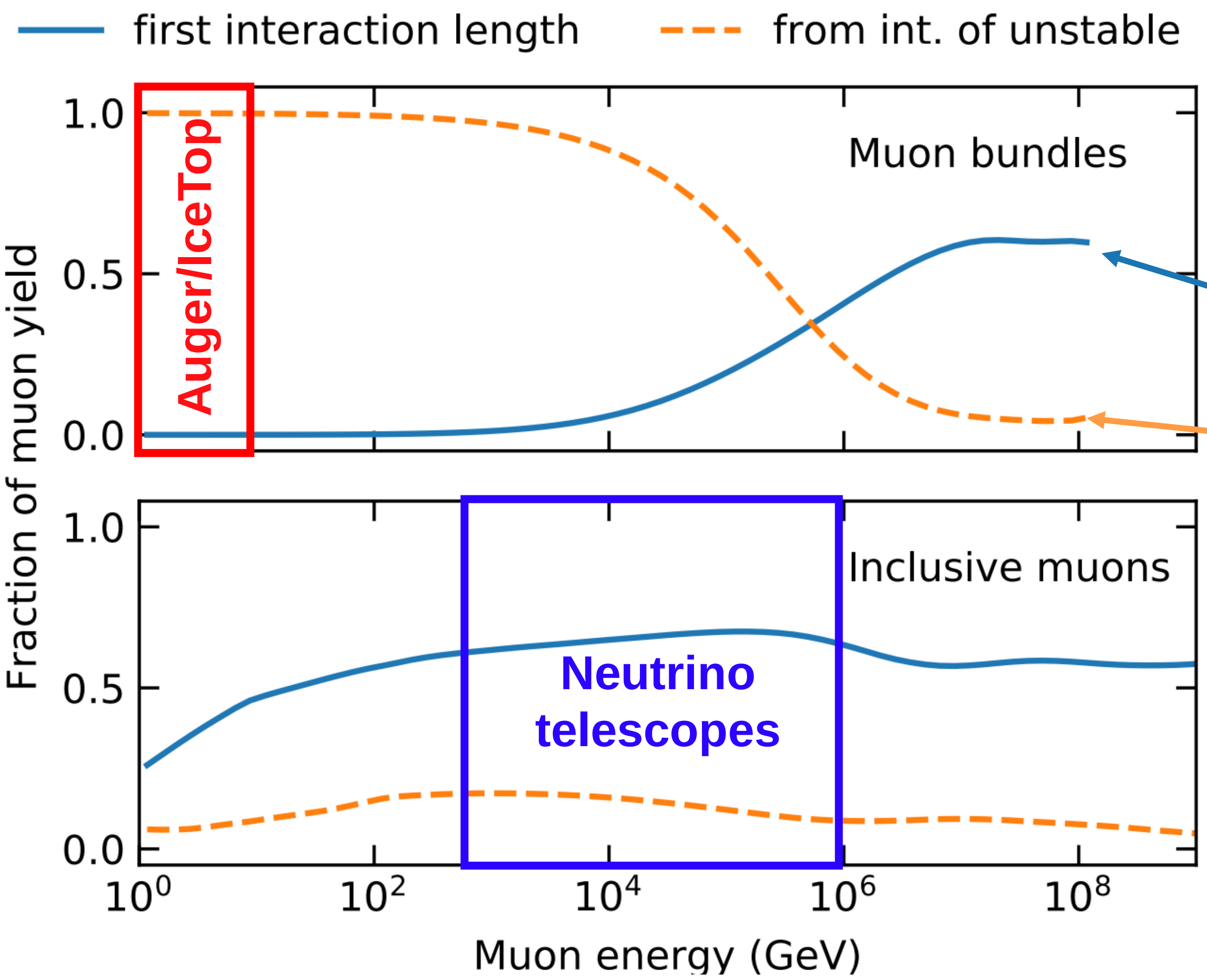
Recall R. Engel's lecture on Monday



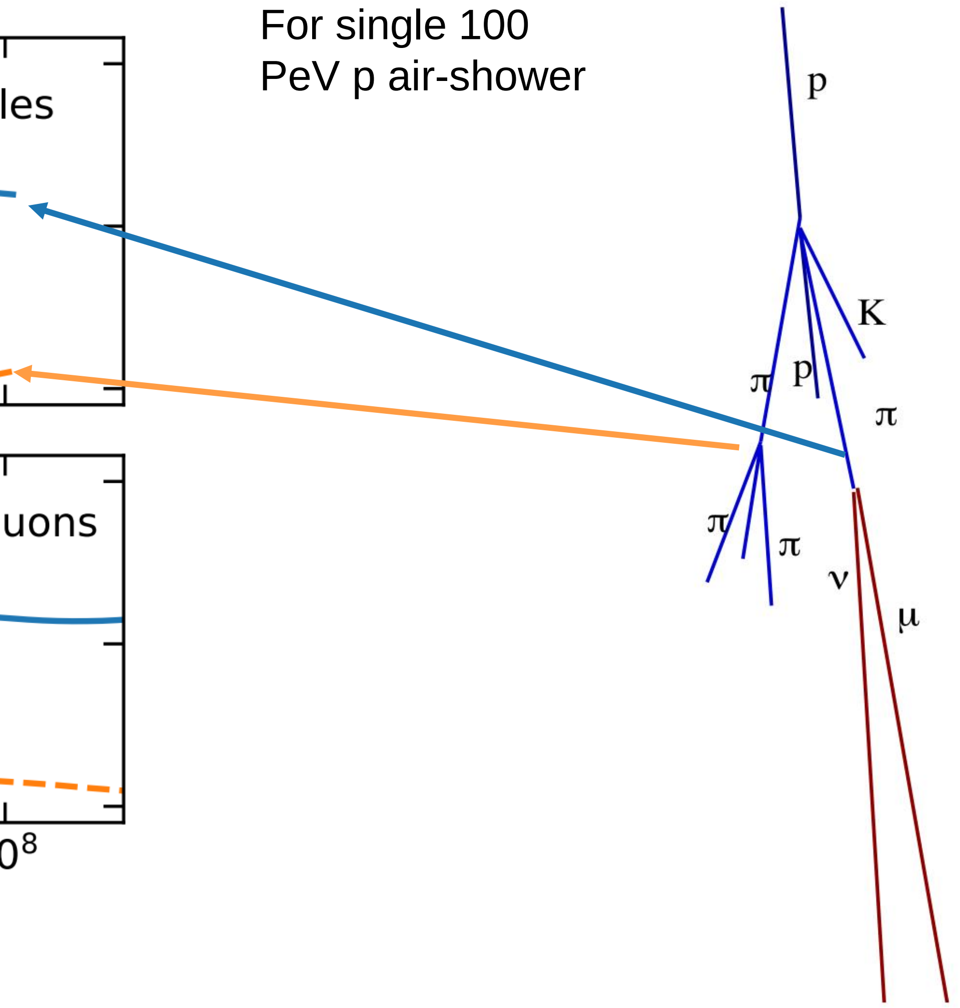


Air-showers & inclusive leptons sensitive to different physics

arXiv:1806.04140

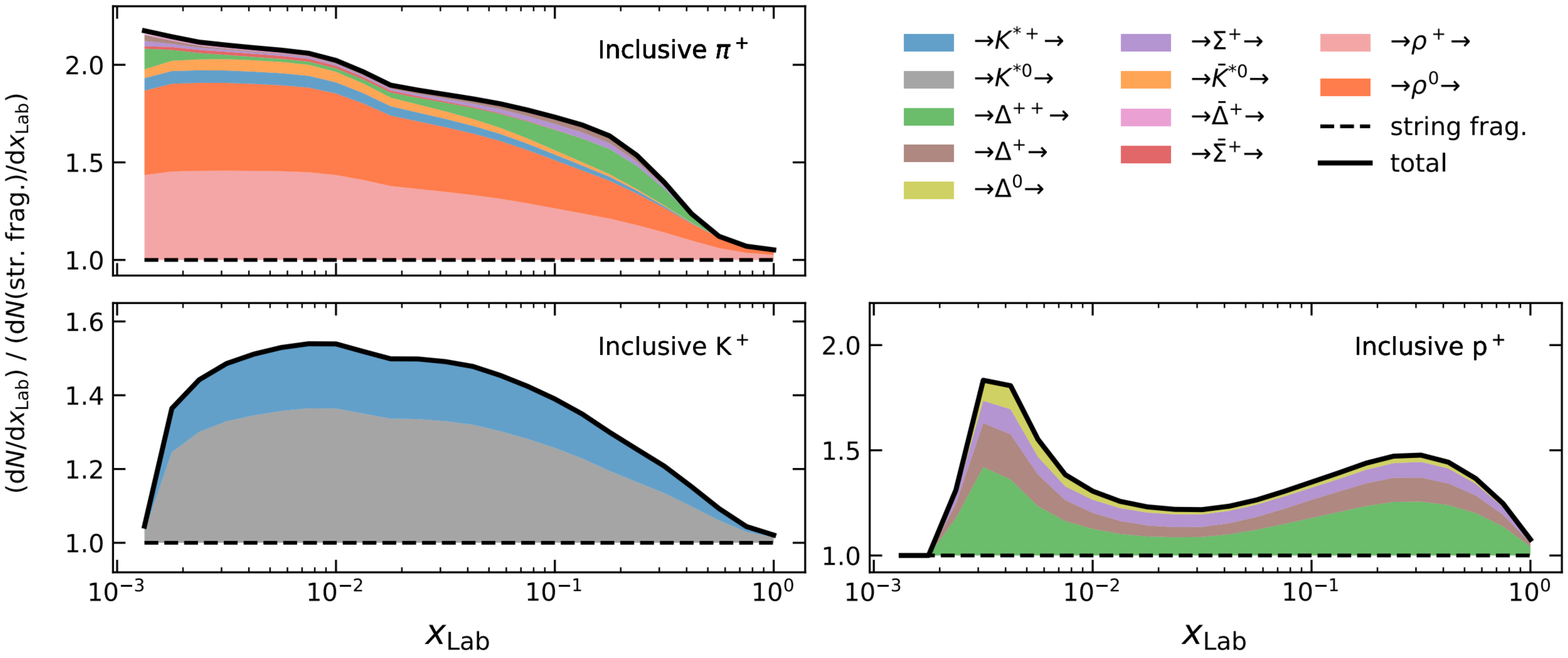


For single 100 PeV p air-shower



More than just pions and kaons

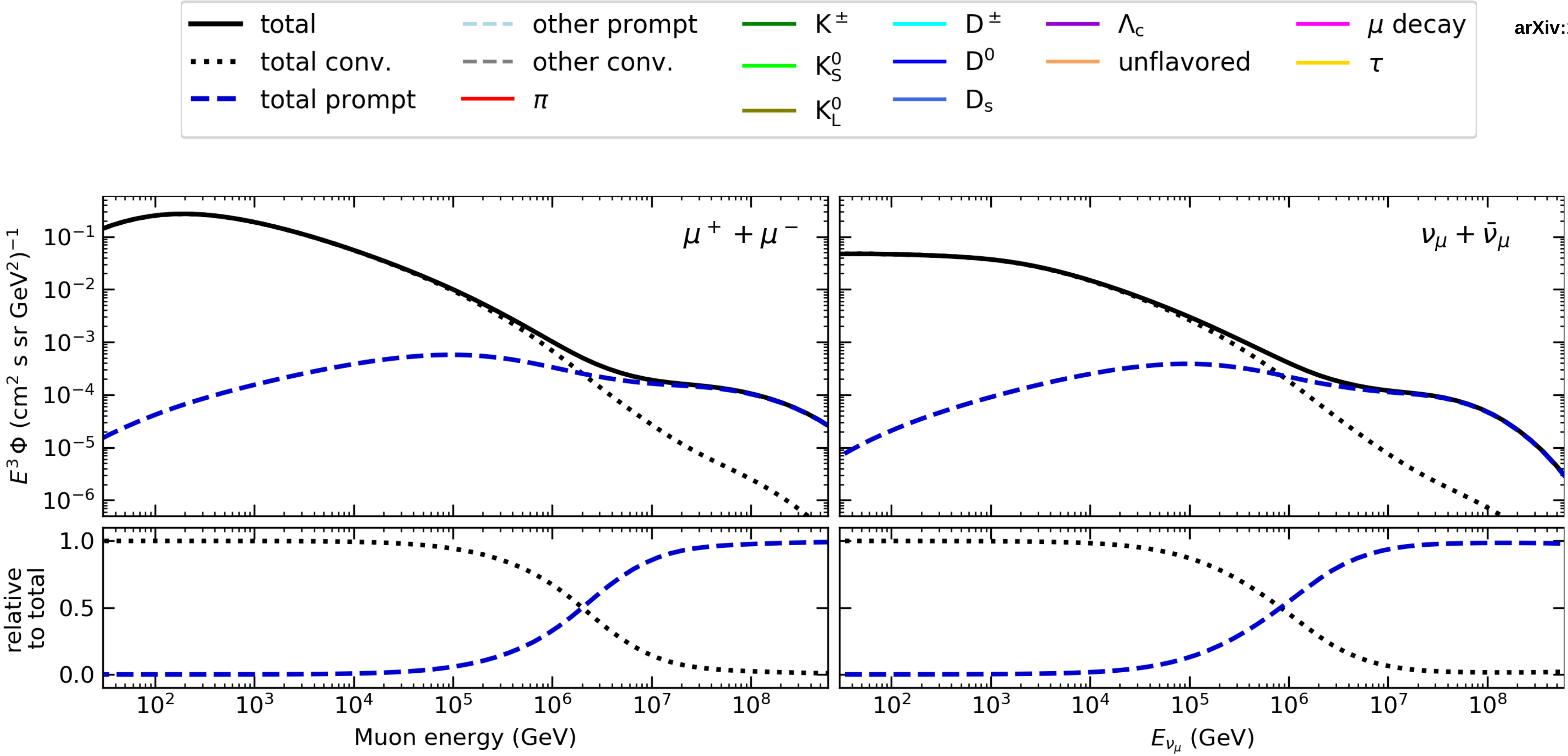
arXiv:1806.04140



No simple tuning/systematic parameters within one interaction model! Many features related to each other.

Hadrons contributing to muonic leptons

arXiv:1806.04140



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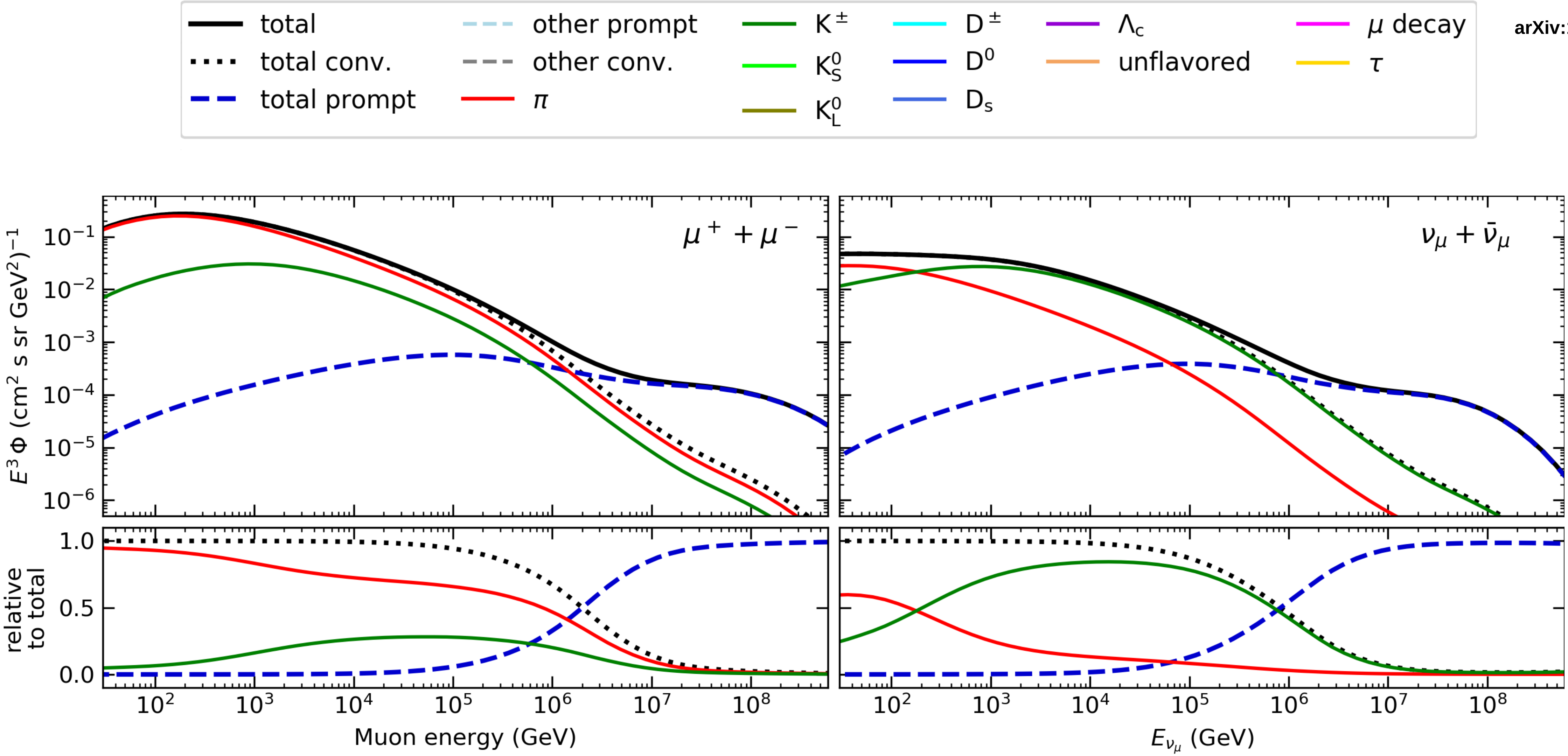

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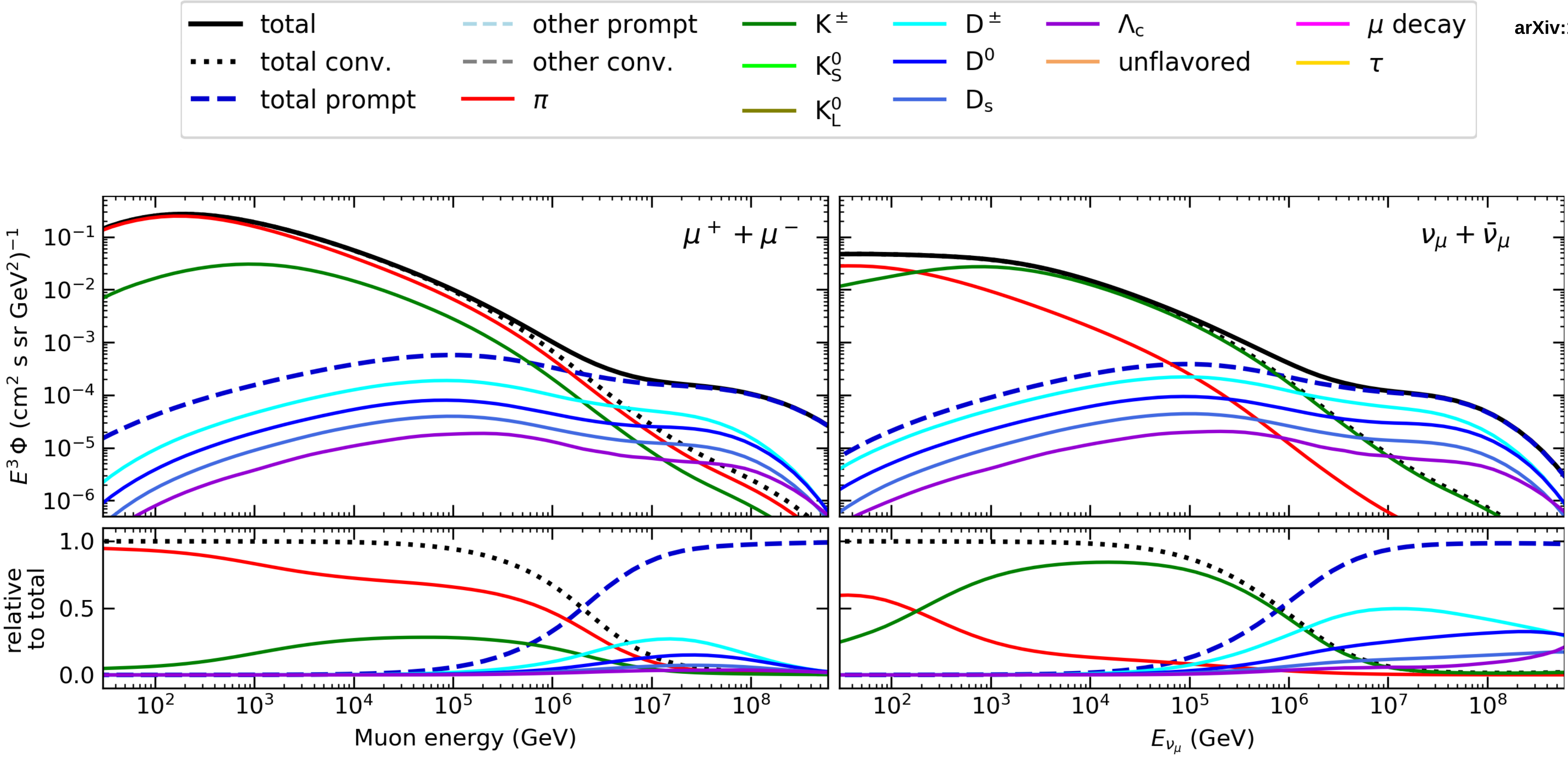

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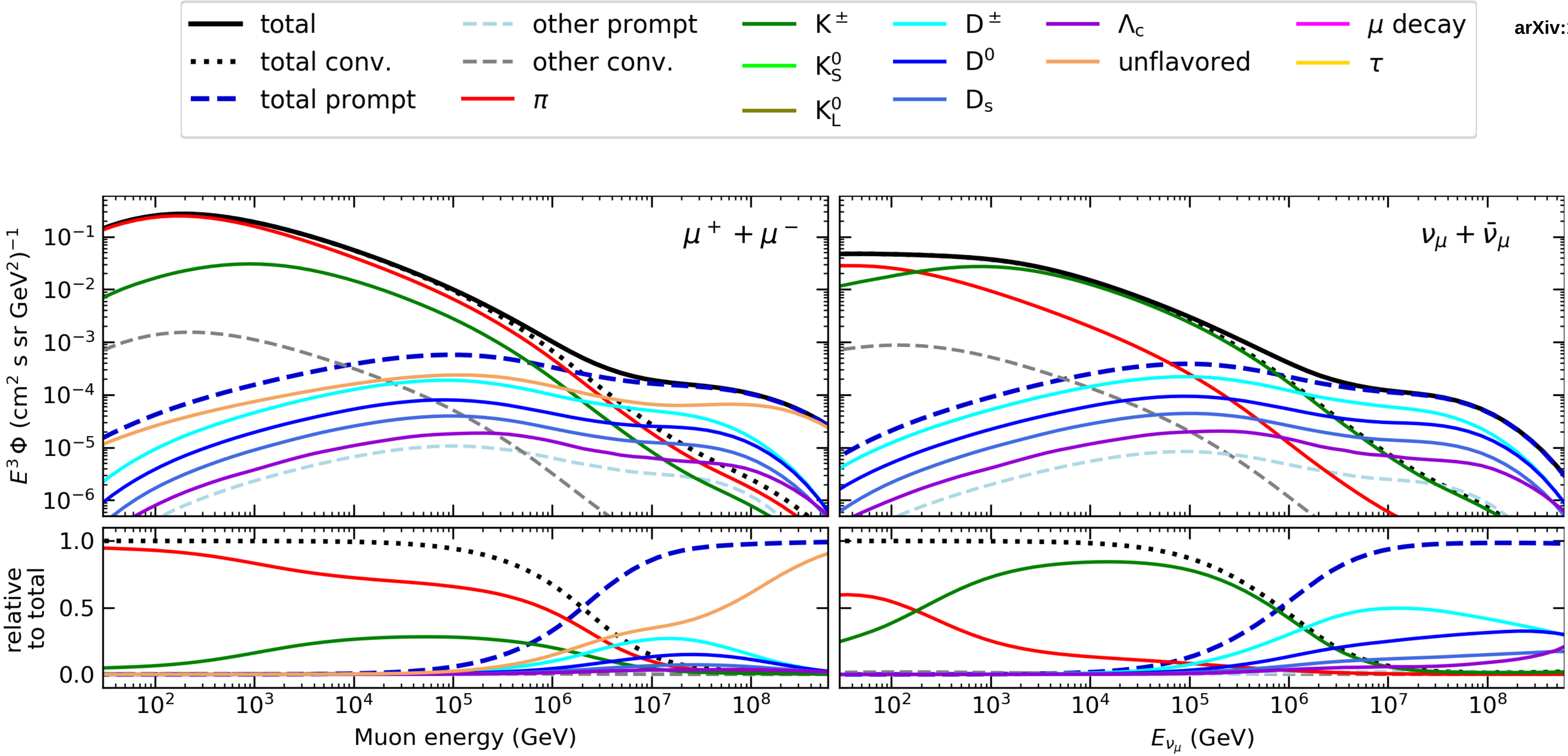
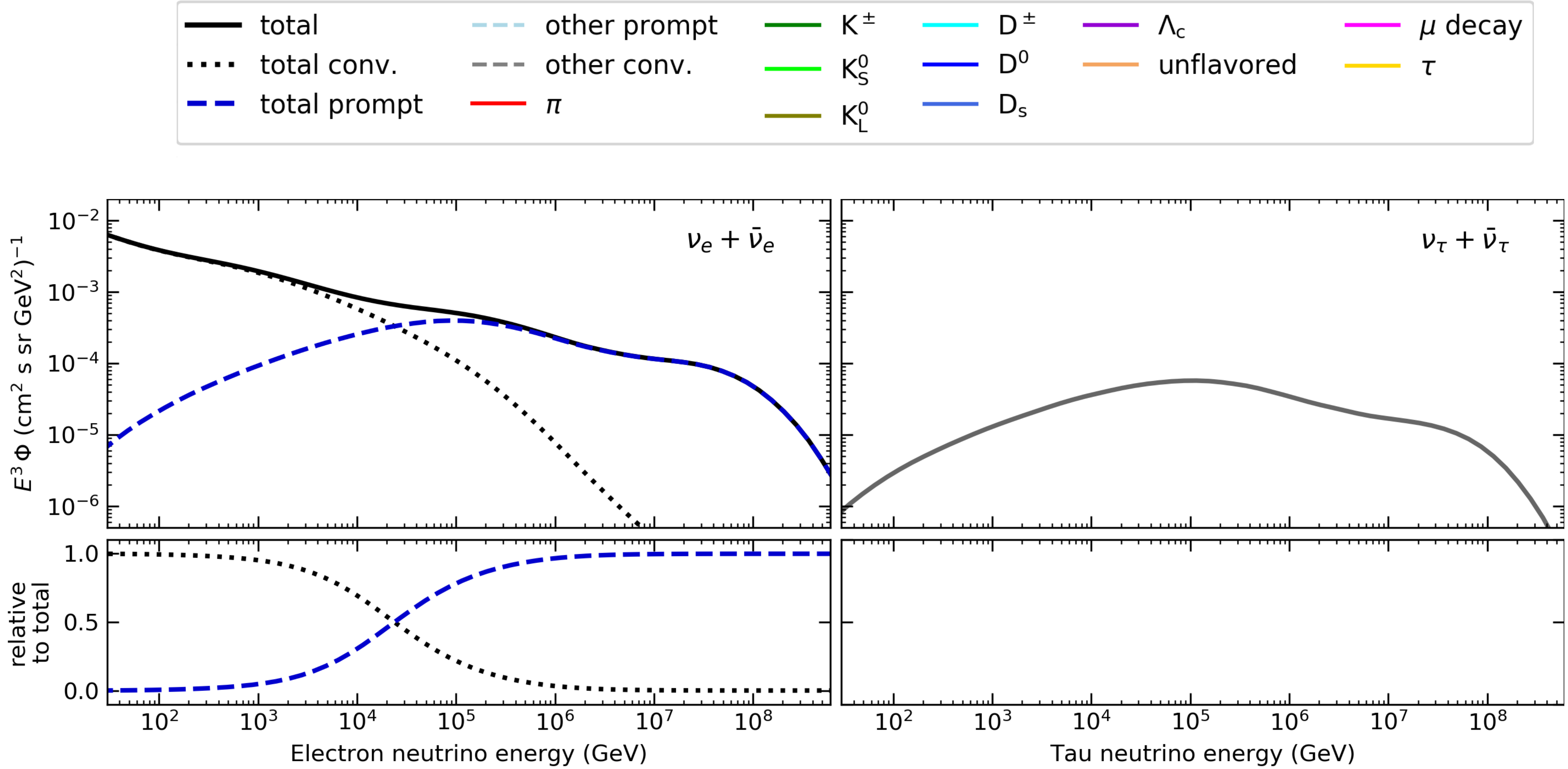


Hadrons contributing to electron and tau neutrinos

arXiv:1806.04140



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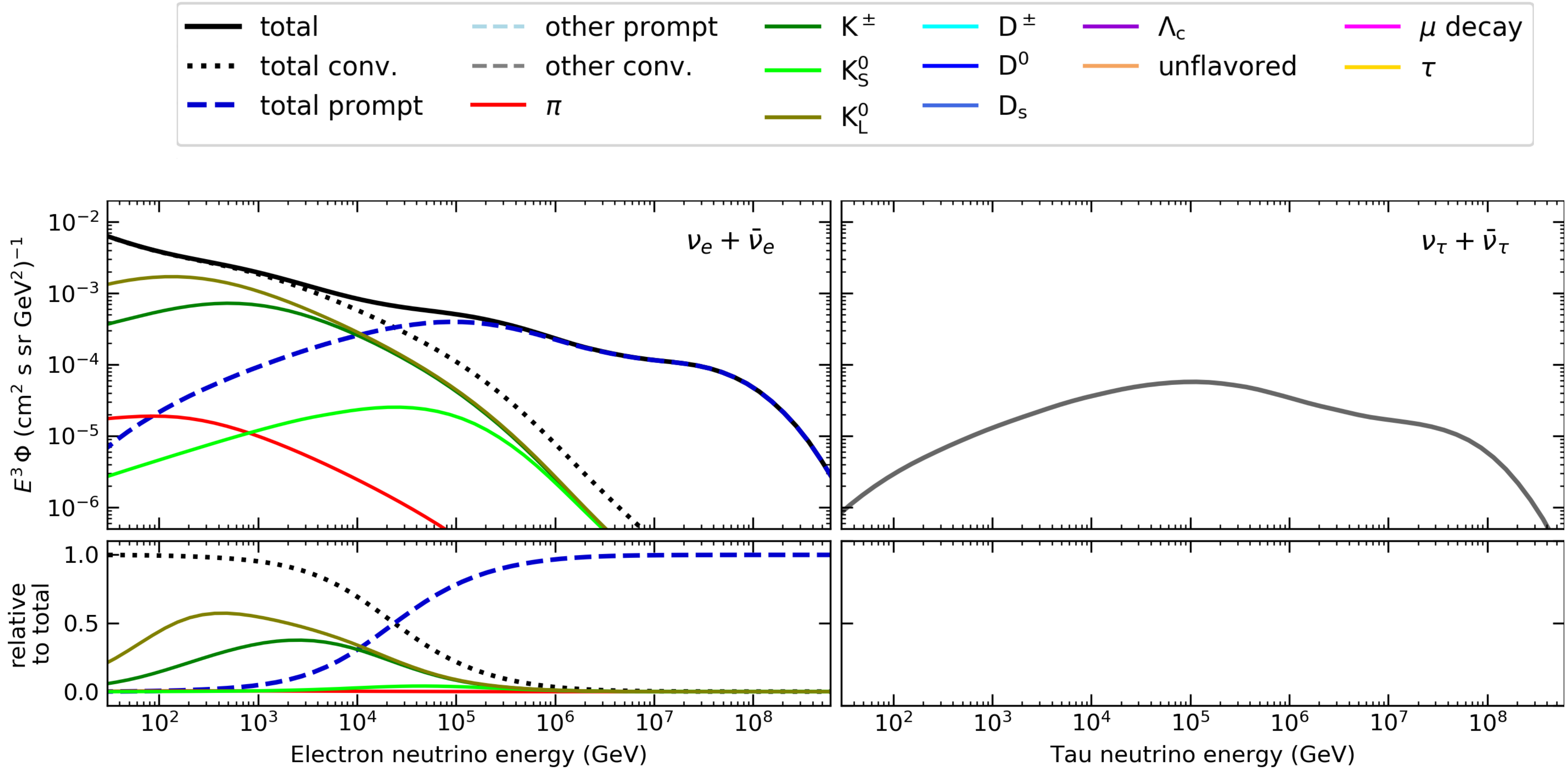

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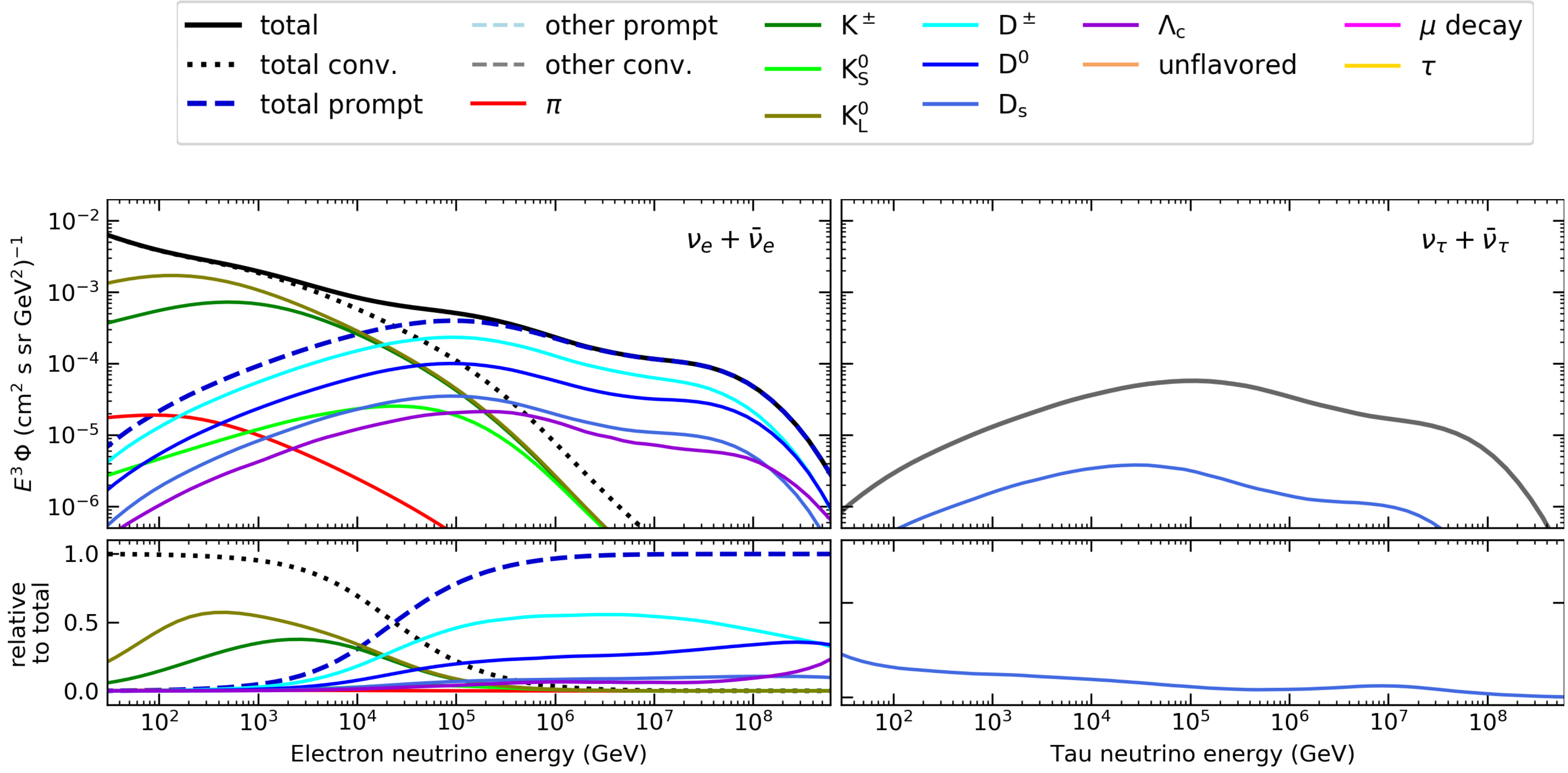

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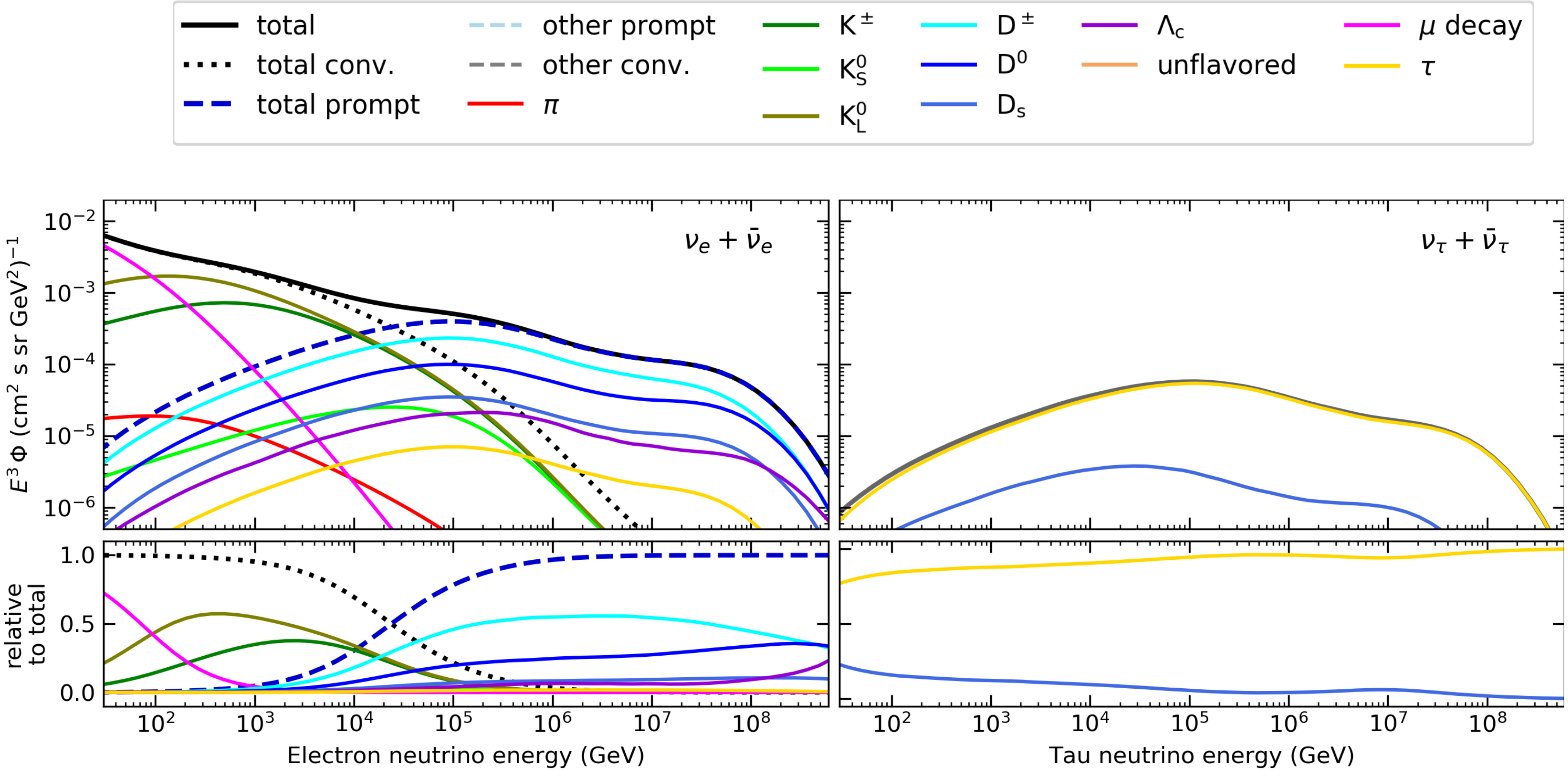

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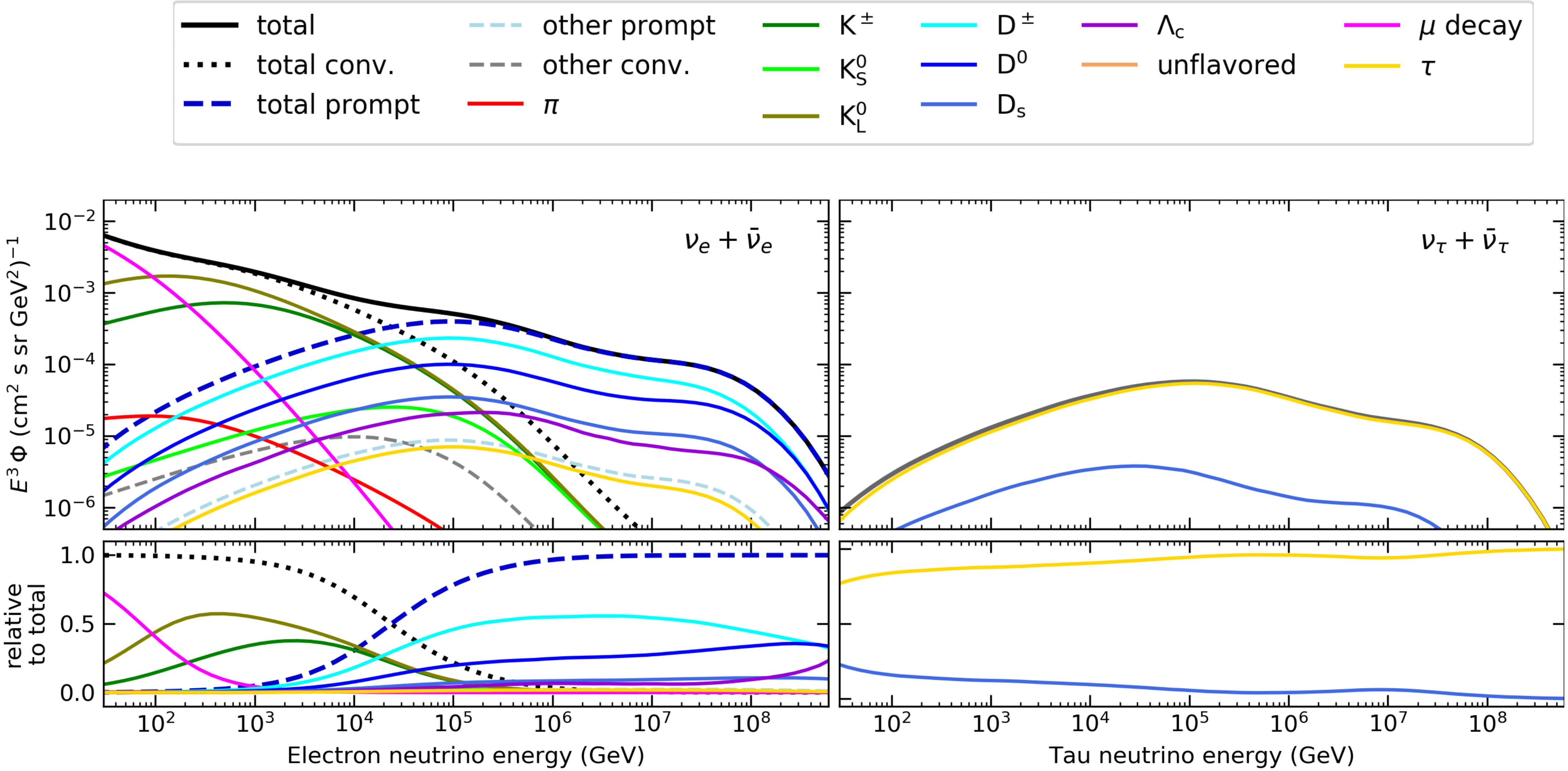
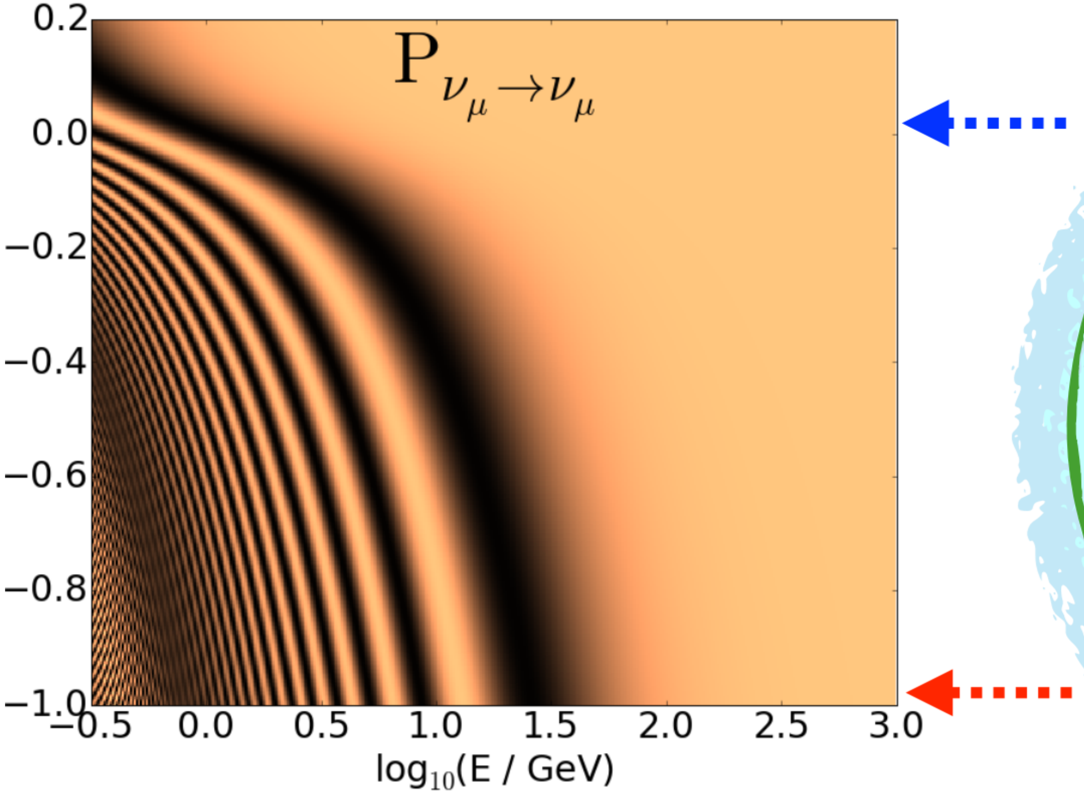
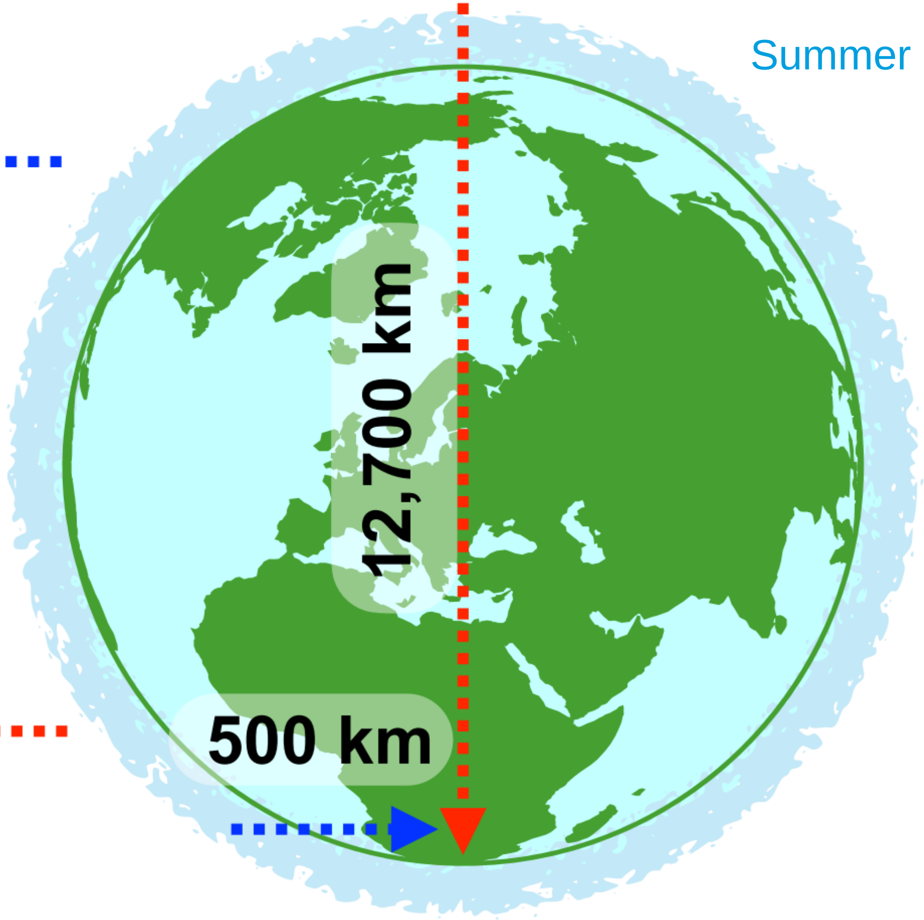


Neutrino properties manifest as pattern in E-θ plane





Summer Blot

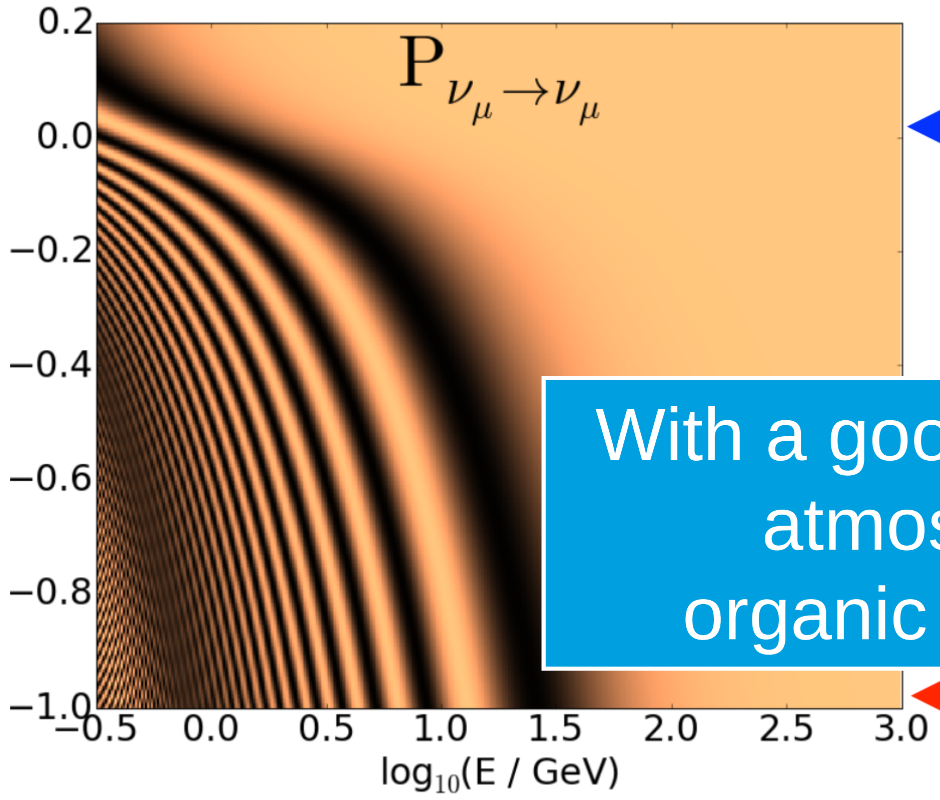
Normal mass ordering

$\theta_{23}=\pi/2$

$\Delta m^2_{32}= 2.51 \times 10^{-3}\ eV^2$

$$P(\nu_\mu \to \nu_\mu) \approx 1 - \sin^2(2\theta_{23}) \sin^2\left(\Delta m^2_{32} \frac{L}{4E_\nu}\right)$$

Neutrino properties manifest as pattern in E-θ plane



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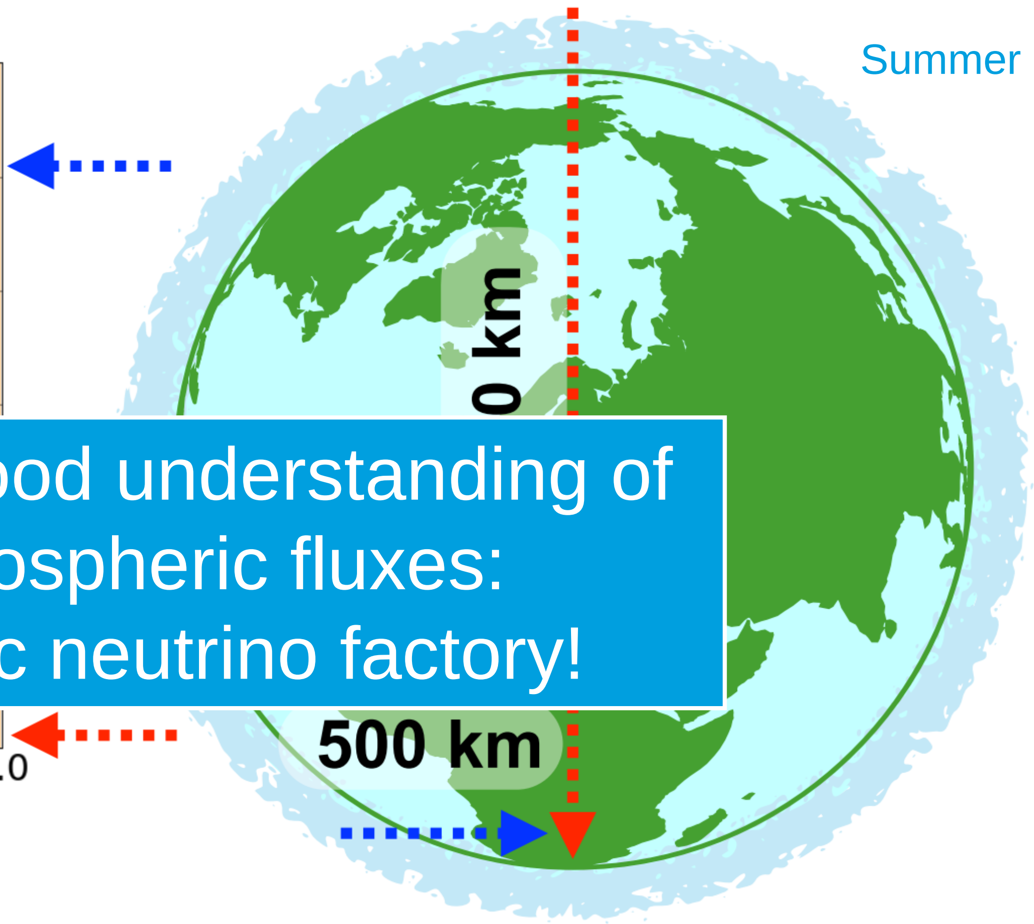

With a good understanding of atmospheric fluxes:
organic neutrino factory!

Normal mass ordering

$\theta_{23} = \pi/2$

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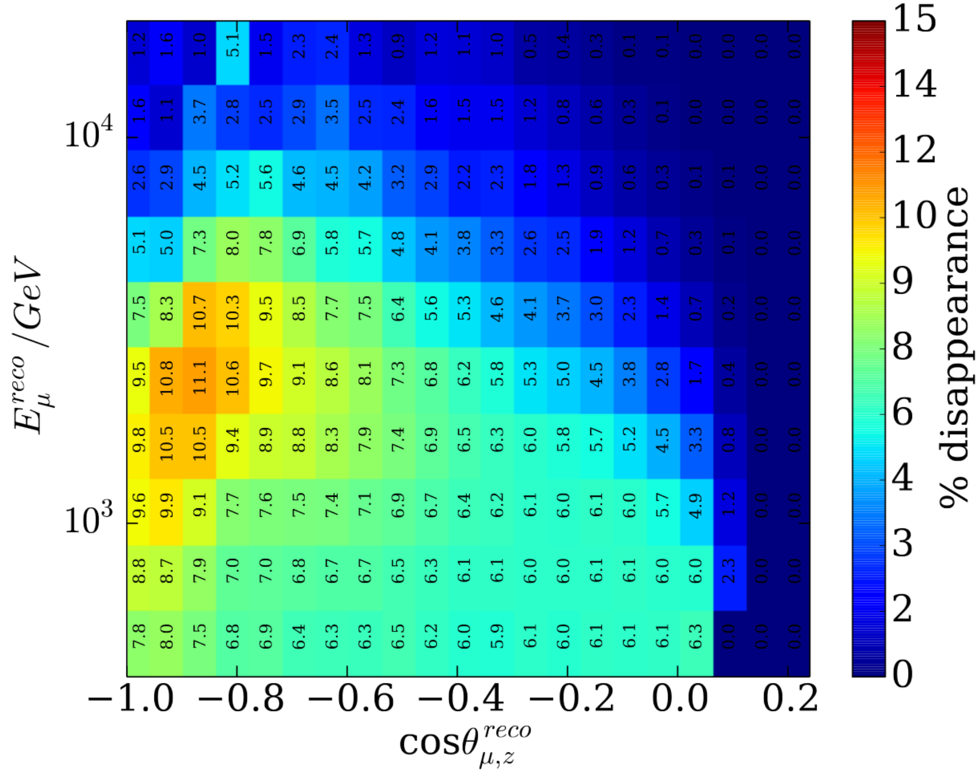
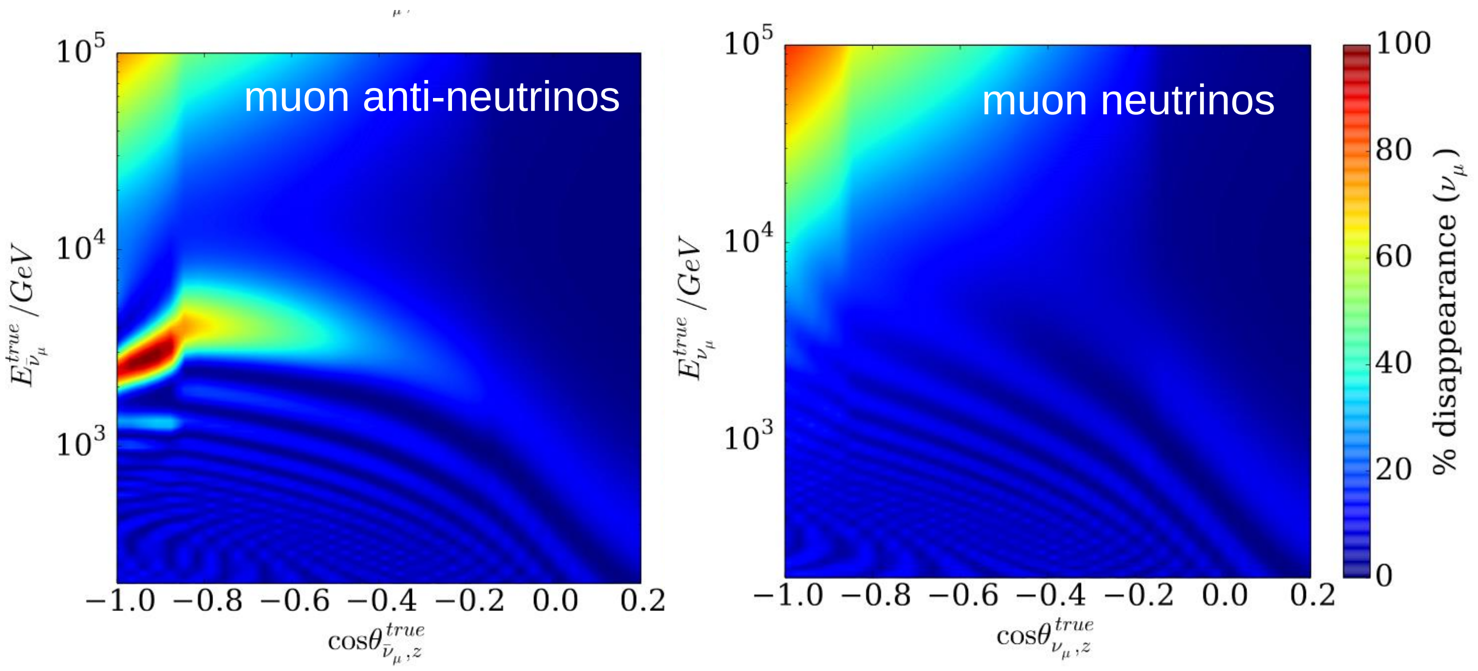
$$P(\nu_\mu \rightarrow \nu_\mu) \approx 1 - \sin^2(2\theta_{23}) \sin^2\left(\Delta m^2_{32} \frac{L}{4E_\nu}\right)$$

Non-standard oscillations with high energy neutrinos

Relative rate change due to sterile neutrinos in IceCube > 100 GeV



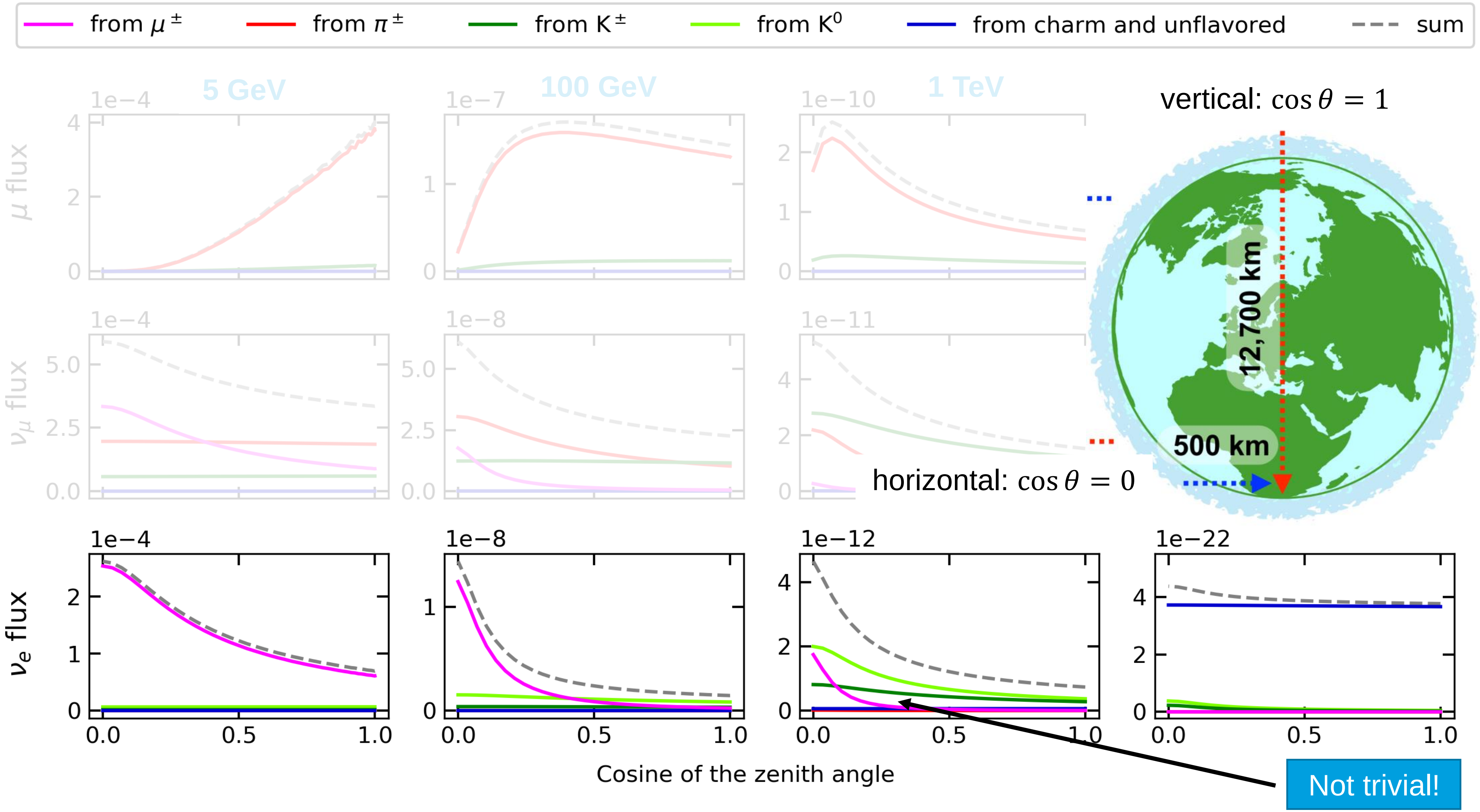
IceCube, Phys. Rev. Lett. 117, 071801 (2016)



Atmospheric flux		
ν flux template	discrete (7)	
ν / $\bar{\nu}$ ratio	continuous	0.025
π / K ratio	continuous	0.1
Normalization	continuous	none[1]
Cosmic ray spectral index	continuous	0.05
Atmospheric temperature	continuous	model tuned

Uncertainties physically correlated and related to hadronic, cosmic ray or atmospheric model

Different hadronic components shape the zenith distribution



AF, F. Riehn, R. Engel, T.K. Gaisser, T. Stanev, in prep. (2018)

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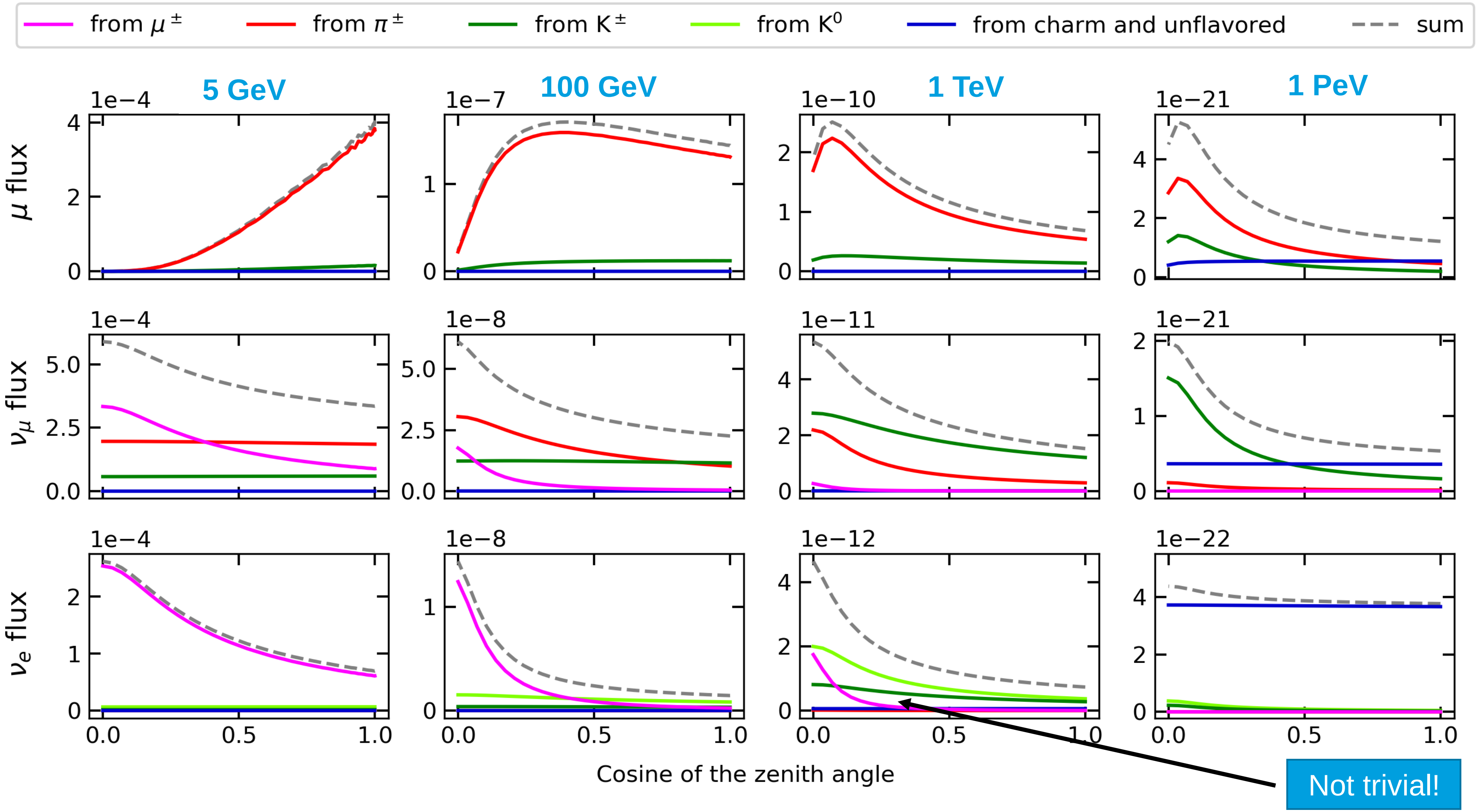

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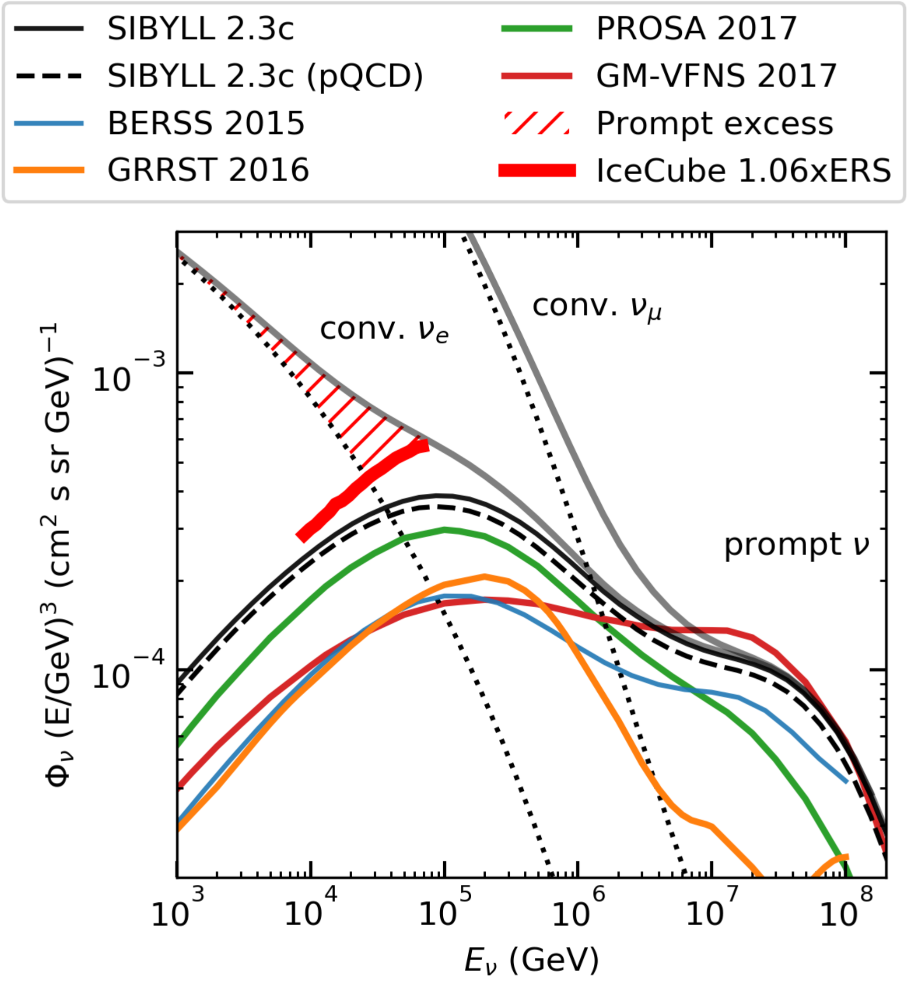
Signatures of the prompt neutrino flux



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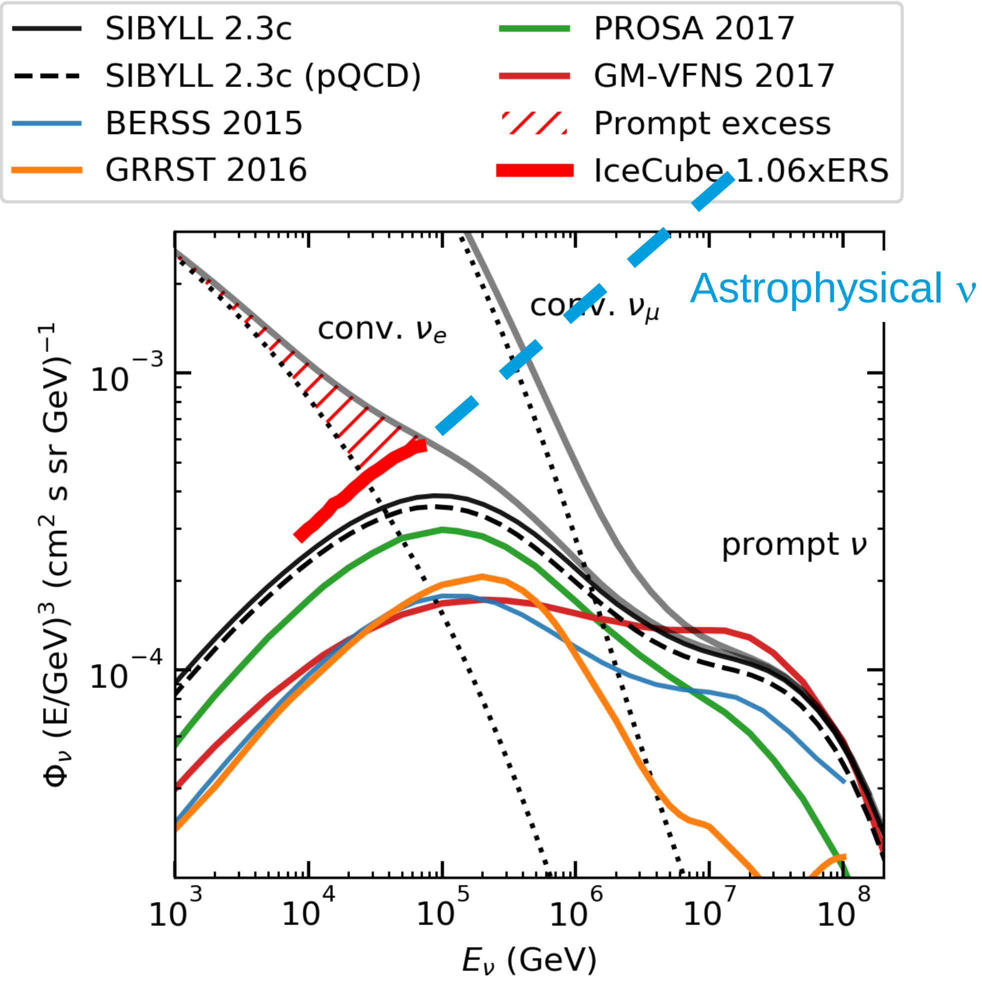

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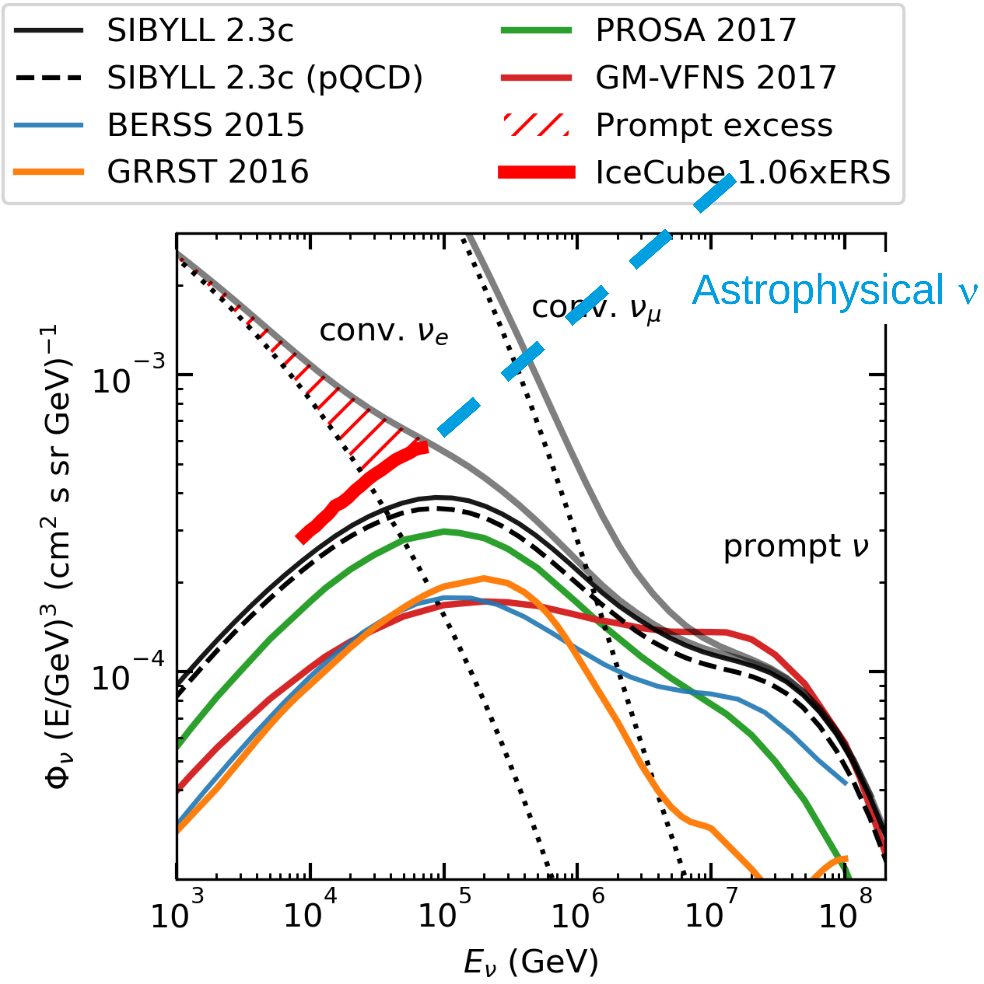

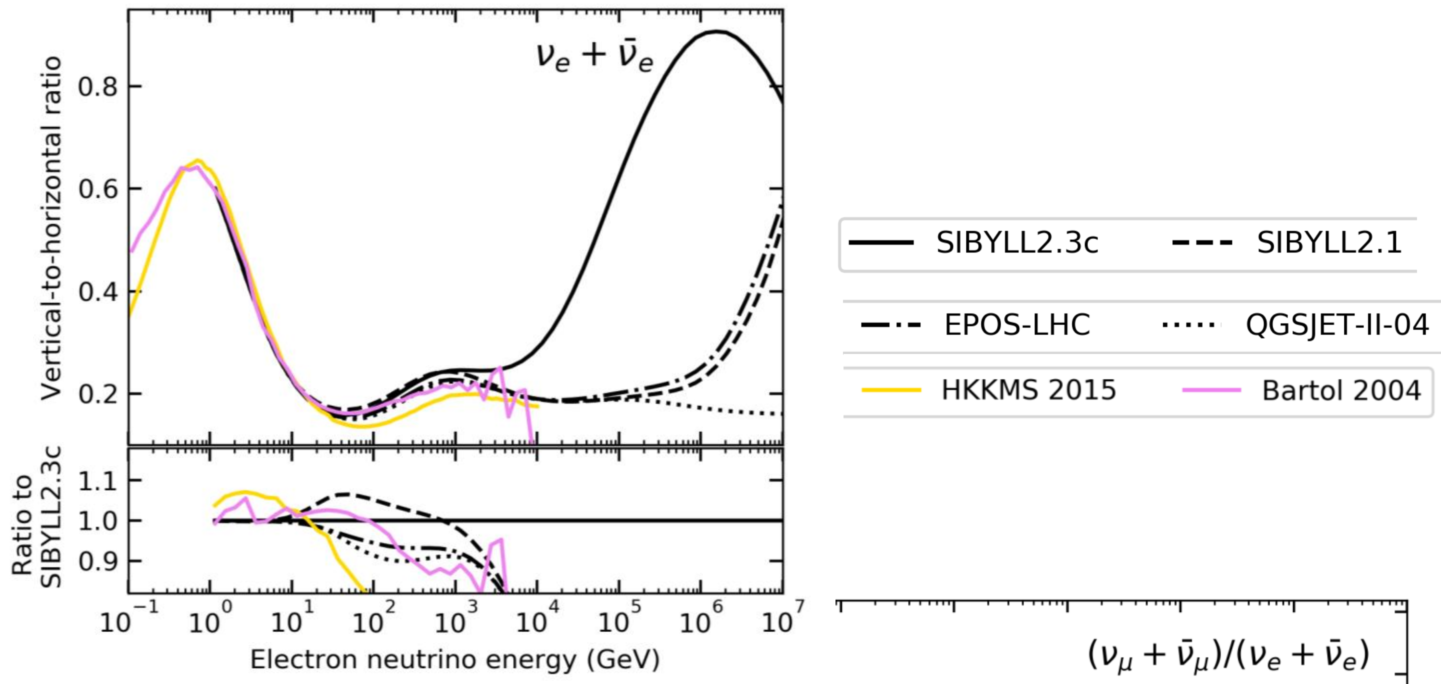

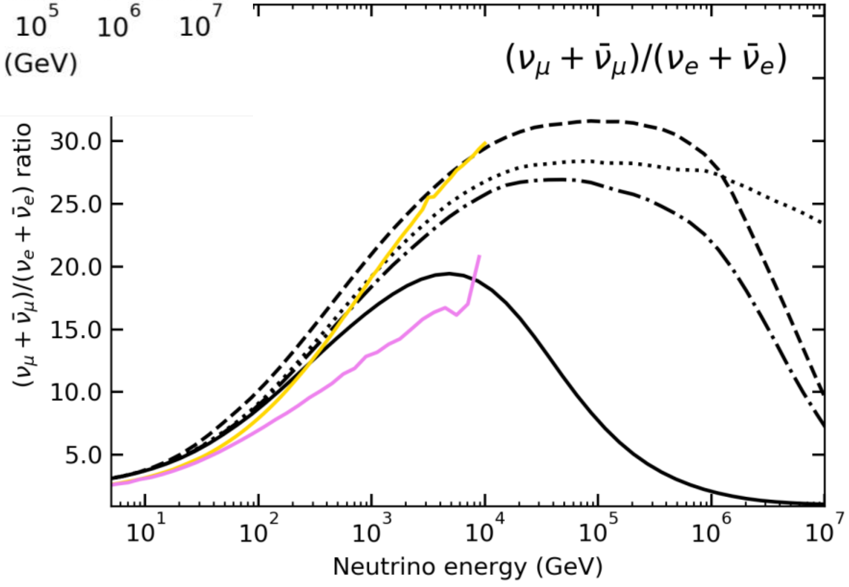

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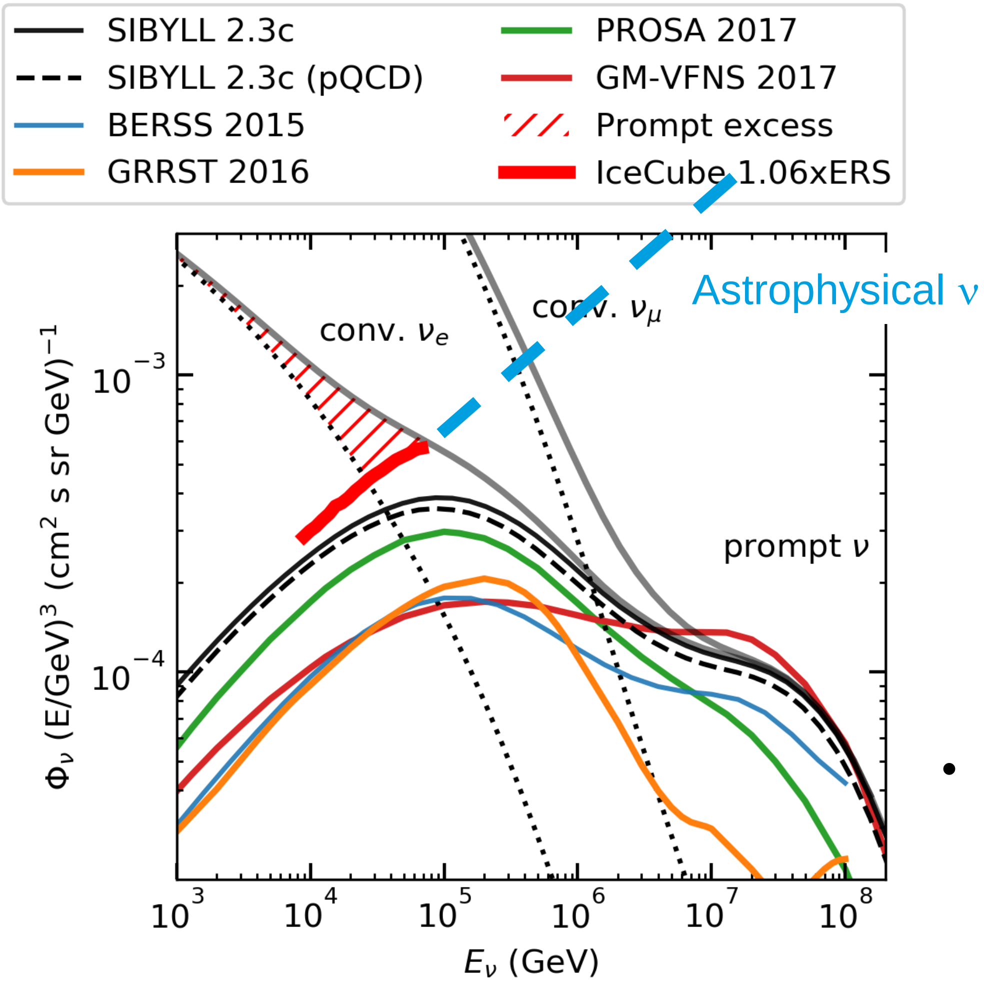

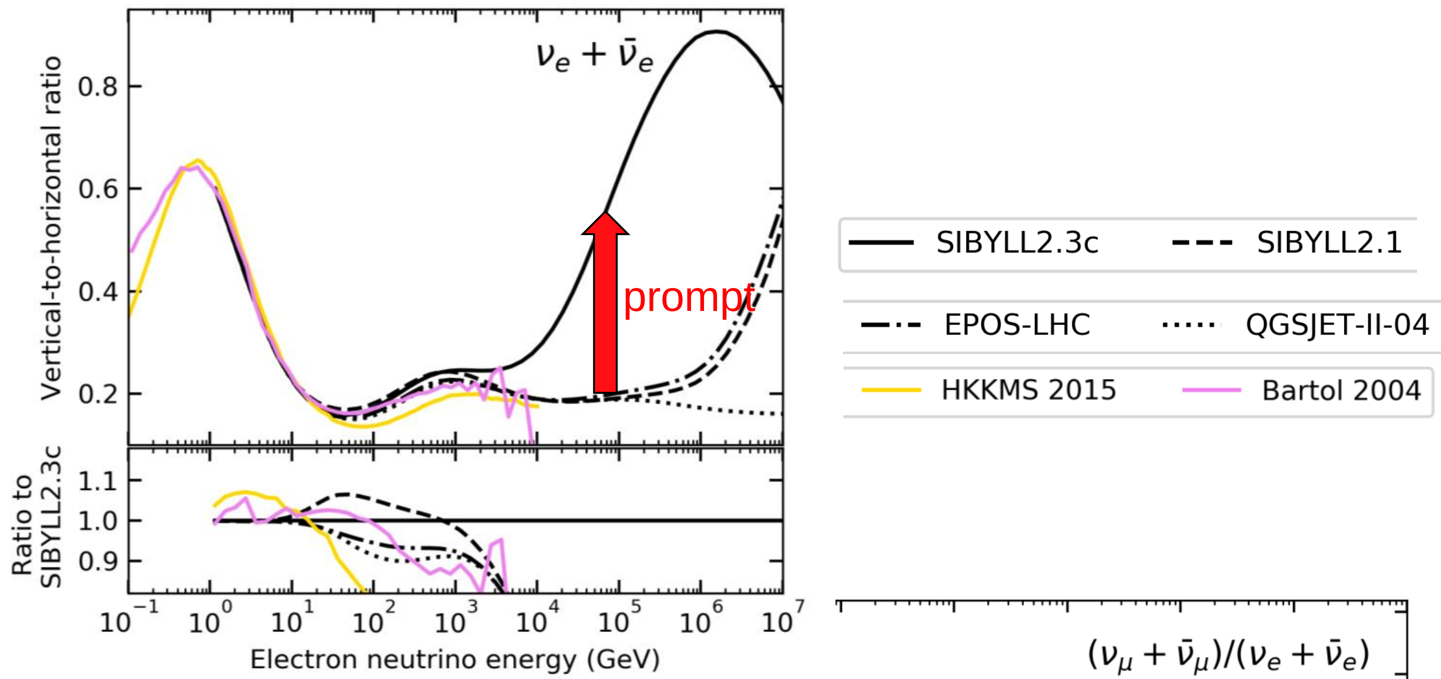

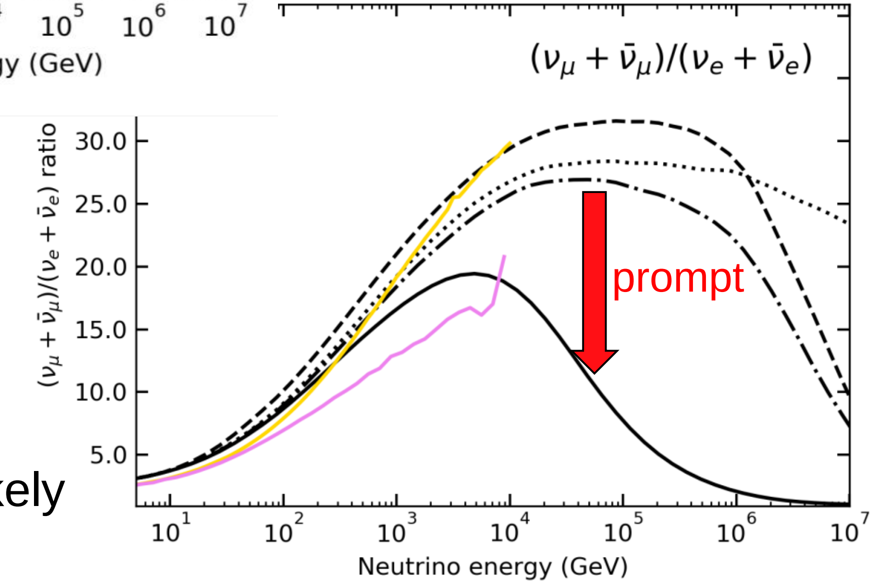

- Sensitive variables
  - Up-horizontal ratio
  - Track/cascade ratio
- Detection of flux excess unlikely

Why investing time in learning numerical methods

- Sure that your (computational) research won’t change, if your code would run instead of 2h/2 min/40 seconds just **2 seconds** or **tens of milli-seconds**?

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- Sure that your (computational) research won't change, if your code would run instead of 2h/2 min/40 seconds just **2 seconds** or **tens of milli-seconds**?
- Imagine you want to allow (many ~ 5-20) uncertain and degenerate physical parameters to float in a fit to data or vary all to derive systematic uncertainties
  - Not well suited are MC (requires statistics), or some hybrid simulations (require precomputed tables)
  - Often many "local minima" (few seconds or minutes/evaluation too much for direct minimizers or MCMC)
  - Common solution: "effective" methods or approximations instead of fitting or scanning parameters on fine grids
  - Effective methods require additional time to check if approximations are valid, etc.
- Trivially parallel programs (cluster jobs) do not solve this problem: assume, 1000 jobs for hypercube of 3 parameters needed. Adding a 4th parameter requires ~20000 jobs, a 5th one is impossible already
- Numerical methods, **if applicable to a physical problem**, can accelerate solutions by orders of magnitude

Moores' law or what?

- Some manufacturers present amazing numbers of floating point performance for their hardware products
- Can I use this somehow in my calculations?
- **Often you can not,** if you write:

PERFORMANCE SPECIFICATION FOR NVIDIA TESLA P100 ACCELERATORS

	P100 for PCIe-Based Servers
Double-Precision Performance	4.7 TeraFLOPS
Single-Precision Performance	9.3 TeraFLOPS
Half-Precision Performance	18.7 TeraFLOPS

```
for (int i=0; i < get_upper_idx(); ++i){
    ...
    x[i] = x[i]*x[i] + y[i,i];
    ...
}
```

```
int IMAX = 100000;

for (int i=0; i < IMAX; ++i){
    ...
    x[i] = calculate_something();
    if (x[i] < 5)
        break;
    else ...
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Compiler doesn't know N-iterations during compile-time

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Termination condition depends on intermediate result

Usually, a simple branch in the loop is enough to break optimization

Parallelization where you might don't expect it

Transport/cascade equations require <u>many</u> convolutions at each step

$$\frac{\mathrm{d}\Phi_h(E,X)}{\mathrm{d}X} = \quad \dots$$
$$+\sum_k \int_E^\infty \mathrm{d}E_k \, \frac{\mathrm{d}N_{k(E_k)\to h(E)}}{\mathrm{d}E} \frac{\Phi_k(E_k,X)}{\lambda_{\mathrm{int},k}(E_k)}$$
$$+\sum_k \int_E^\infty \mathrm{d}E_k \, \frac{\mathrm{d}N^{\mathrm{dec}}_{k(E_k)\to h(E)}}{\mathrm{d}E} \frac{\Phi_k(E_k,X)}{\lambda_{\mathrm{dec},k}(E_k,X)}$$

Matrix expression for convolution using midpoint rule

$$c(E_i) = \int_{E_i}^\infty \mathrm{d}E' b(E_i,E')a(E')$$
$$\approx \sum_{j=E_i}^{E_N} \Delta E'_j \; b(E_i,E'_j)a(E'_j) = \sum_j B_{ij}a_j$$

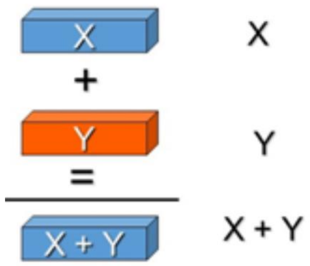
Then, for any dim. of c $\boxed{\vec{c} = \mathbf{B} \times \vec{a}}$

Well,
matrices … sure …
I write loops
…obviously

Ordinary loops and calls to a Linear Algebra library are not the same

Vectorization

```
double *x, *y, *z;
for (i=0;  i<n;  i++)      z[i] = x[i] + y[i];
```



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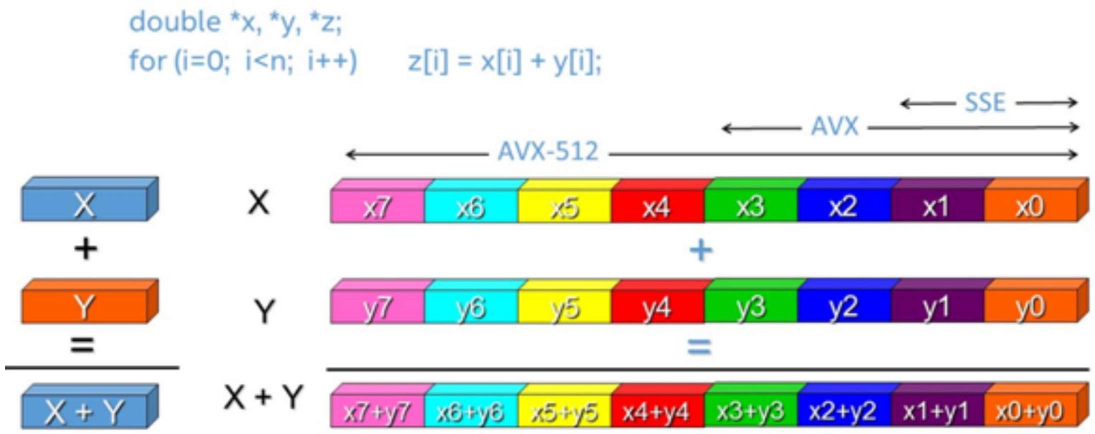

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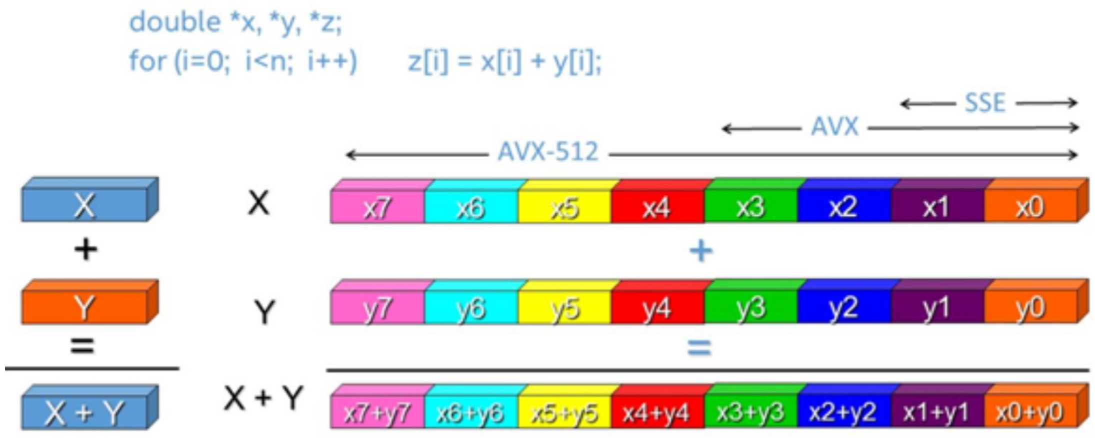

> Features you might get:

- 2-8 Float operations per clock instead of 1
- Addition + multiplication in 1 clock instead of 2
- Coalesced memory access (higher RAM/Cache FPU bandwidth)
- SMP (Multicore), easy GPU, packed math, …

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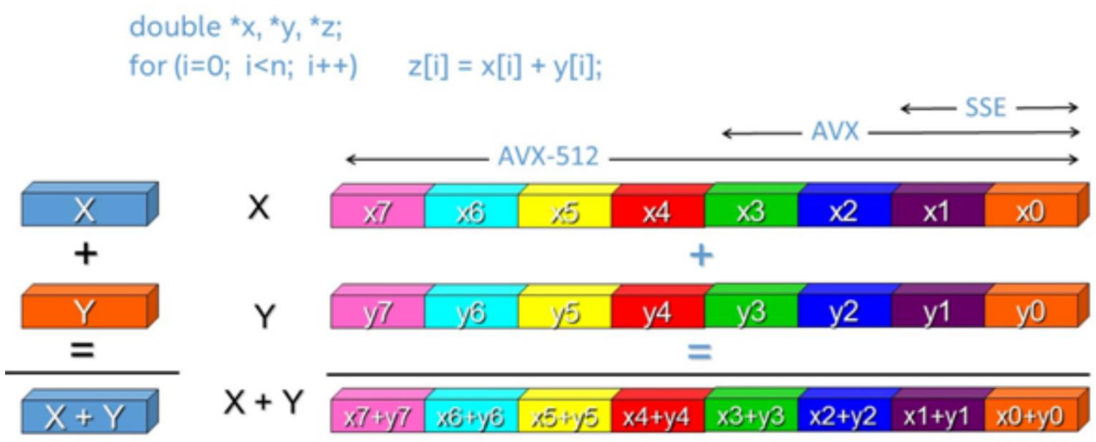

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> We are not computer scientist and we **don't** want to

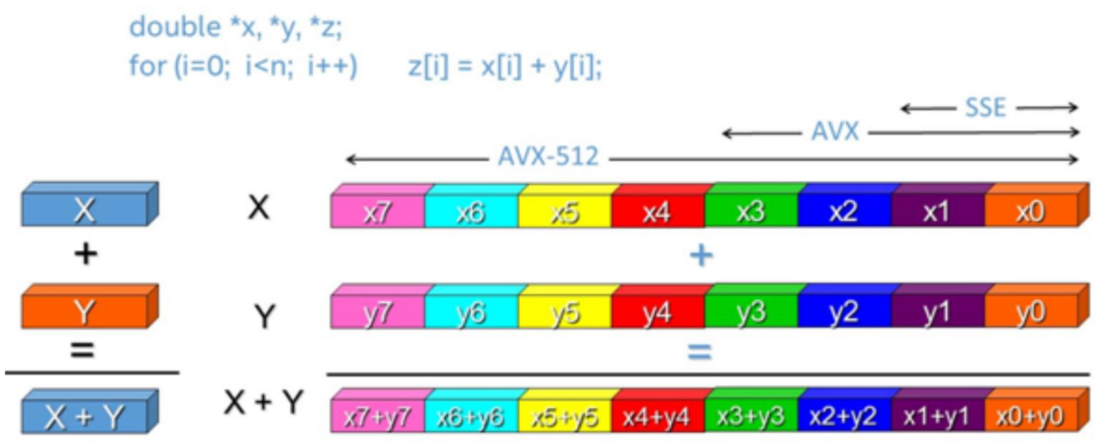
- spend a significant fraction of life-time to study all these new technologies/APIs
- Look at profiler/optimization reports each time we wrote a line of code

> However, it is much easier to accelerate just matrix expressions (other techniques often not worth the additional dev time)

> Many packages available: MKL, Magma, CUBLAS/cuSparse

Ordinary loops and calls to a Linear Algebra library are not the same

Vectorization



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> However, it is much easier to accelerate just matrix expressions (other techniques often not worth the additional dev time)

> Many packages available: MKL, Magma, CUBLAS/cuSparse

It's all just marketing!

Some case…

Should be pretty fast, right?

```
SUBROUTINE MATMULOPT(M, N, DATA, VEC, RES)
  INTEGER M, N, I, J
  DOUBLE PRECISION DATA(10000,10000)
  DOUBLE PRECISION VEC(10000), RES(10000)
intent(out) :: RES

  DO J=1,N
      DO I=1,M
          RES(J) = DATA(I,J)*VEC(I) + RES(J)
      END DO
  END DO

END
```

Some case…

Should be pretty fast, right?

```fortran
SUBROUTINE MATMULOPT(M, N, DATA, VEC, RES)
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      END DO
  END DO

END
```

- This example is brute force
- Run on a tablet, workstation typically higher gain
- Linear algebra has many interesting features (sparse matrices, efficient solvers, etc.)

```
In [3]: m,n, data, vec = 10000,10000, np.random.random((10000,10000)), np.random.random(10000)

In [4]: dataf = np.asfortranarray(data)

In [5]: vecf = np.asfortranarray(vec)

In [6]: %timeit fortrantest.matmulopt(m,n,dataf,vecf)
10 loops, best of 3: 130 ms per loop

In [7]: %timeit np.dot(data.T, vec)
10 loops, best of 3: 35.4 ms per loop
```

gfortran-7 -O3 vs. numpy linked to Intel MKL

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      END DO
  END DO

END
```

- This example is brute force
- Run on a tablet, workstation typically higher gain
- Linear algebra has many interesting features (sparse matrices, efficient solvers, etc.)

Well,
… great …
but my “matrices” are neither random, nor dense!

```
In [3]: m,n, data, vec = 10000,10000, np.ra                    n(10000)

In [4]: dataf = np.asfortranarray(data)

In [5]: vecf = np.asfortranarray(vec)

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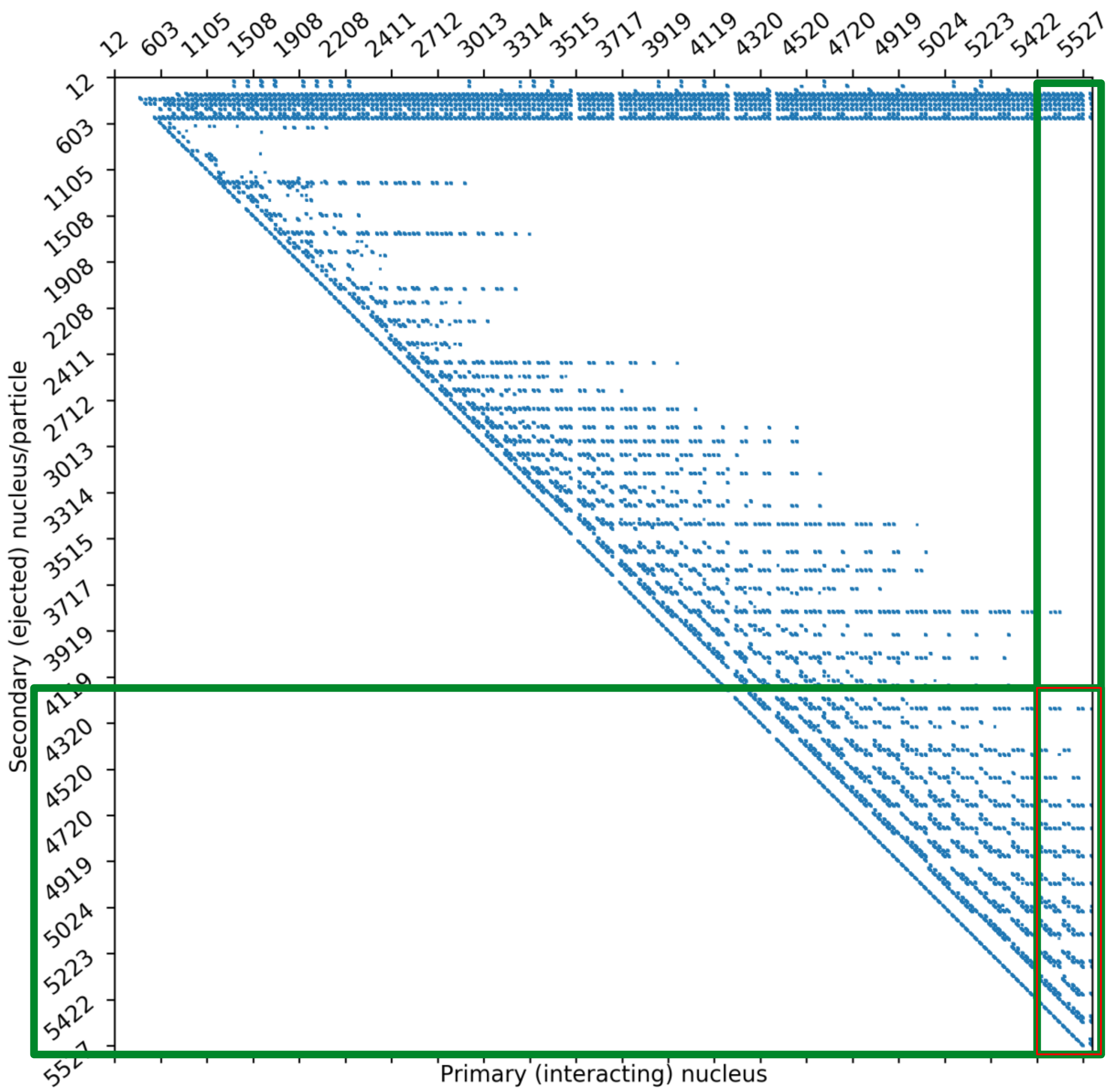
gfortran-7 -O3 vs. numpy linked to Intel MKL

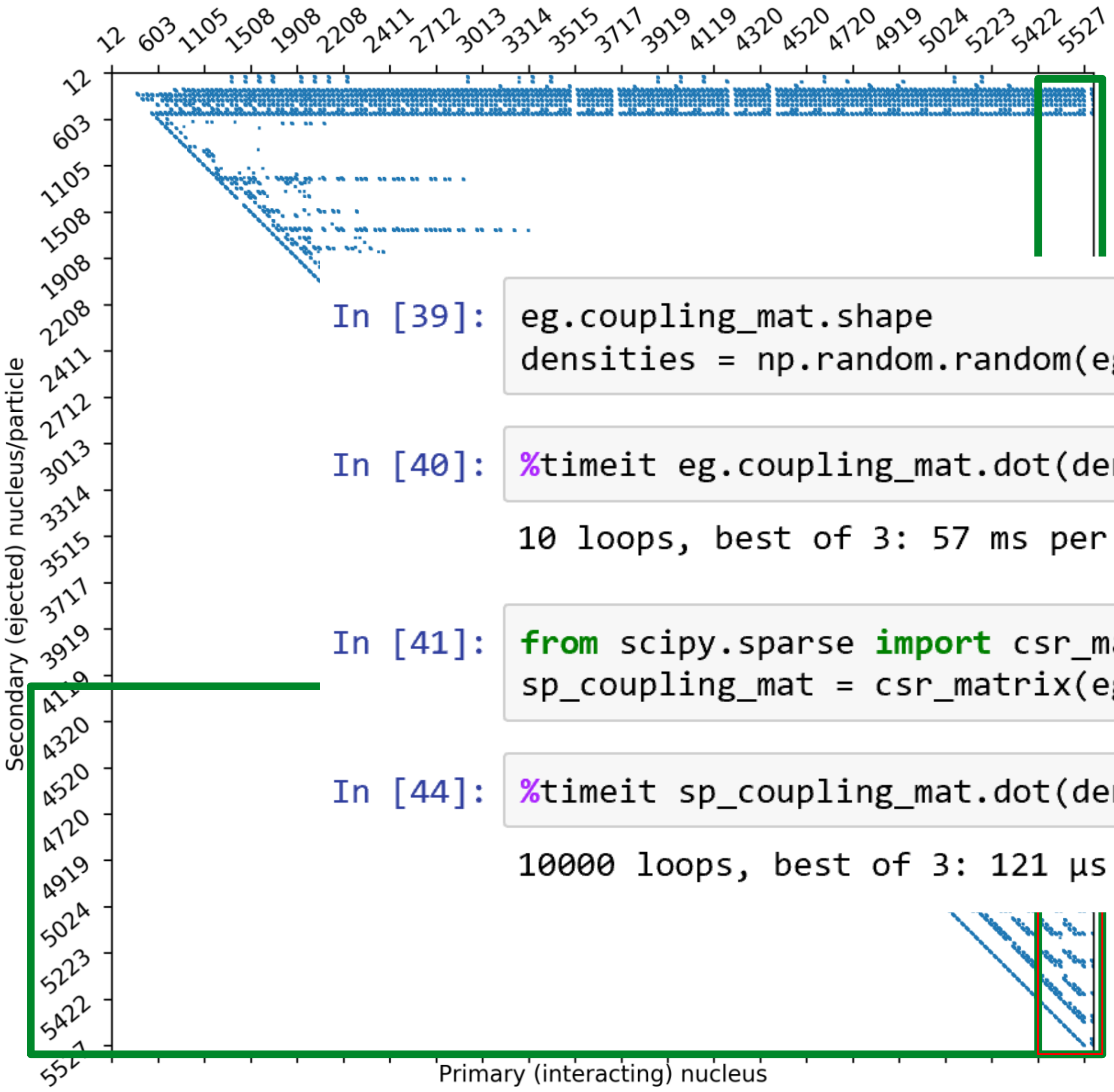
More realistic case: propagation coupling matrix



- IDs: A*100 + Z
- Each element represents an injection rate
- Interacting elements are rows
- Ejected elements are columns

All possible disintegration channels of iron(ish) isotopes (1n, 2n, 1n1p emissions etc.)

More realistic case: propagation coupling matrix




```
In [39]: eg.coupling_mat.shape
         densities = np.random.random(eg.coupling_mat.shape[0])

In [40]: %timeit eg.coupling_mat.dot(densities)
10 loops, best of 3: 57 ms per loop

In [41]: from scipy.sparse import csr_matrix
         sp_coupling_mat = csr_matrix(eg.coupling_mat)

In [44]: %timeit sp_coupling_mat.dot(densities)
10000 loops, best of 3: 121 µs per loop
```

- IDs: A*100 + Z
- represents an injection
- considered as dense rows
- nts are columns
- converted to sparse
- All possible disintegration channels of iron(ish) isotopes (1n, 2n, 1n1p emissions etc.)

General remarks

- Radiation and particle transport are often **sparse problems**
- Calls to special functions (like pow(x,y)) are very expensive, interpolation is expensive,….
- Formulating the kernel of you problem in algebraic expressions gives you a lot of performance for free, vectorization doesn't simply become marketing or impossible to afford due to dev time
- You can use GPUs, multi-core, etc., and if you need performance, you probably should, since CPU's won't accelerate much in the next decade
- If using vectorization, think deeply about required precision. Single or half precision may double or quadruple FLOPs on modern hardware

MCEq: Matrix Cascade Equations

A. Fedynitch, R. Engel, T. K. Gaisser, F. Riehn and S. Todor
PoS ICRC 2015, 1129 (2015), EPJ Web Conf. 99, 08001 (2015)
and EPJ Web Conf. 116, 11010 (2016)

$$\frac{\mathrm{d}\Phi_h(E,X)}{\mathrm{d}X} = -\frac{\Phi_h(E,X)}{\lambda_{\mathrm{int},h}(E)} - \frac{\Phi_h(E,X)}{\lambda_{\mathrm{dec},h}(E,X)} - \frac{\partial}{\partial E}(\mu(E)\Phi_h(E,X)) + \sum_\ell \int_E^\infty \mathrm{d}E_\ell \frac{\mathrm{d}N_{\ell(E_\ell)\to h(E)}}{\mathrm{d}E} \frac{\Phi_\ell(E_\ell,X)}{\lambda_{\mathrm{int},l}(E_\ell)} + \sum_\ell \int_E^\infty \mathrm{d}E_\ell \frac{\mathrm{d}N^{\mathrm{dec}}_{\ell(E_\ell)\to h(E)}}{\mathrm{d}E} \frac{\Phi_\ell(E_\ell,X)}{\lambda_{\mathrm{dec},l}(E_\ell,X)}$$

$$\frac{\mathrm{d}\Phi^h_{E_i}}{\mathrm{d}X} = -\frac{\Phi^h_{E_i}}{\lambda^h_{\mathrm{int},E_i}} - \frac{\Phi^h_{E_i}}{\lambda^h_{\mathrm{dec},E_i}(X)} - \vec{\nabla}_i(\mu^h_{E_i}\Phi^h_{E_i}) + \sum_{E_k \geq E_i}^{E_N} \sum_\ell \frac{c_{\ell(E_k)\to h(E_i)}}{\lambda^\ell_{\mathrm{int},E_k}} \Phi^\ell_{E_k} + \sum_{E_k \geq E_i}^{E_N} \sum_\ell \frac{\mathrm{d}_{\ell(E_k)\to h(E_i)}}{\lambda^\ell_{\mathrm{dec},E_k}(X)} \Phi^\ell_{E_k}$$

State (or flux) vector

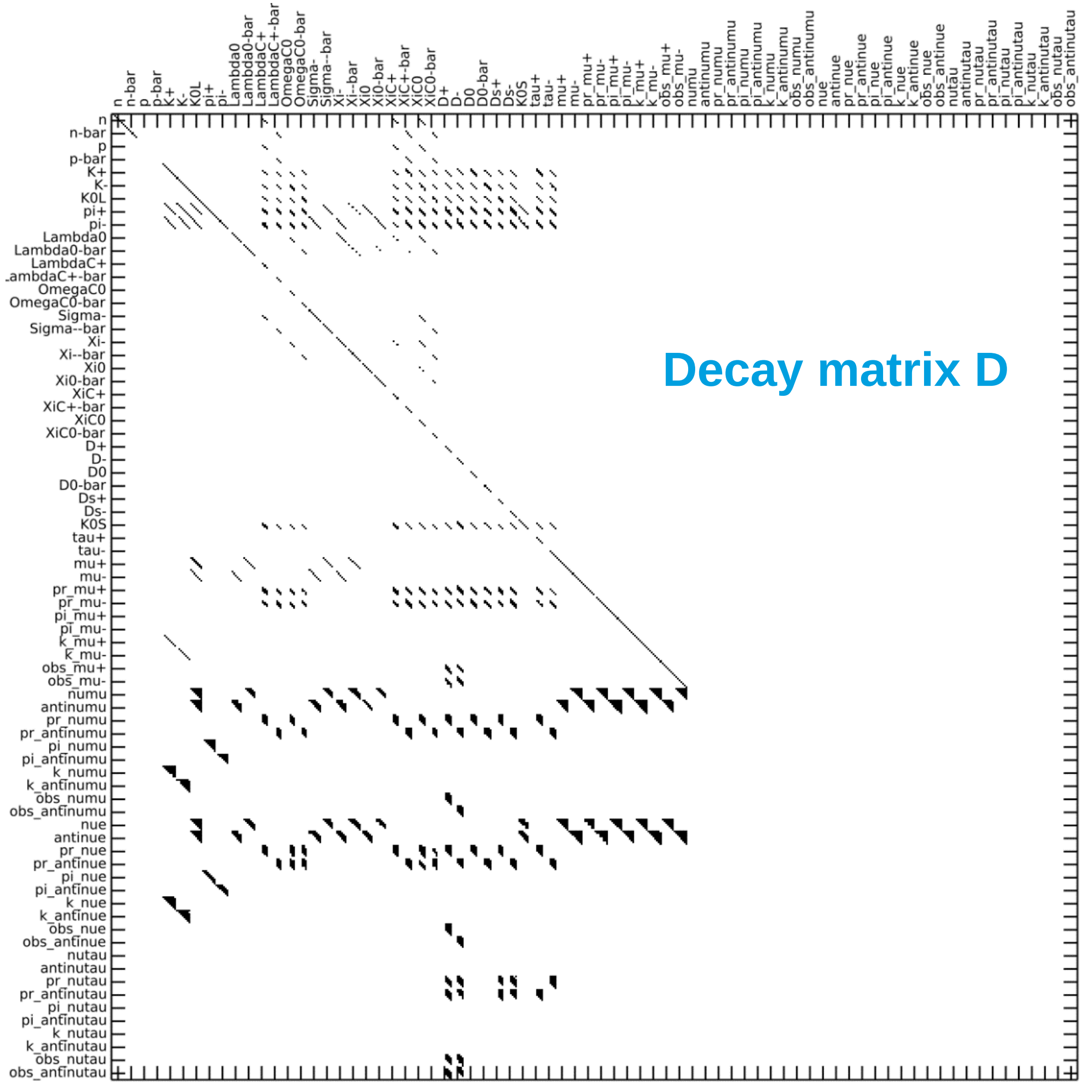
$$\vec{\Phi} = \left(\vec{\Phi}^{\mathrm{p}} \quad \vec{\Phi}^{\mathrm{n}} \quad \vec{\Phi}^{\pi^+} \quad \ldots \quad \vec{\Phi}^{\bar{\nu}_\mu} \quad \ldots\right)^T$$

$$\vec{\Phi}^{\mathrm{p}} = \left(\Phi^{\mathrm{p}}_{E_0} \quad \Phi^{\mathrm{p}}_{E_1} \quad \cdots \quad \Phi^{\mathrm{p}}_{E_N}\right)^T$$

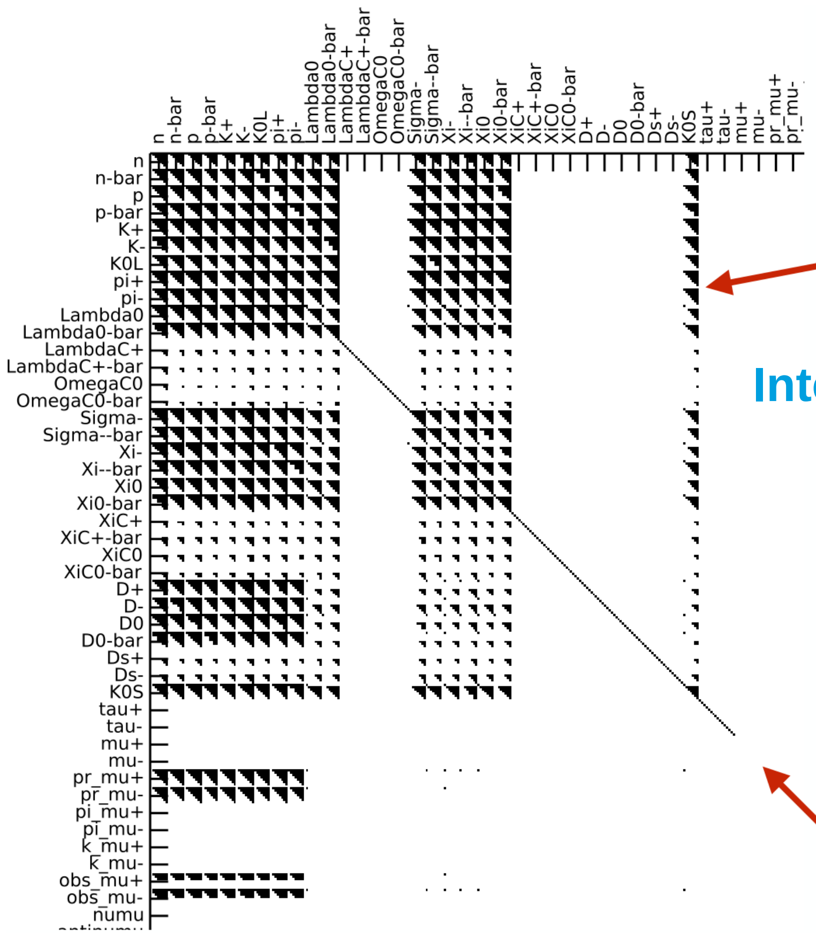
“Matrix form”

$$\frac{\mathrm{d}}{\mathrm{d}X}\vec{\Phi} = -\vec{\nabla}_E(\mathrm{diag}(\vec{\mu})\vec{\Phi}) + (-\mathbf{1} + \mathbf{C})\mathbf{\Lambda}_{\mathrm{int}}\vec{\Phi} + \frac{1}{\rho(X)}(-\mathbf{1} + \mathbf{D})\mathbf{\Lambda}_{\mathrm{dec}}\vec{\Phi}$$

Sparse matrix structure



Decay matrix D



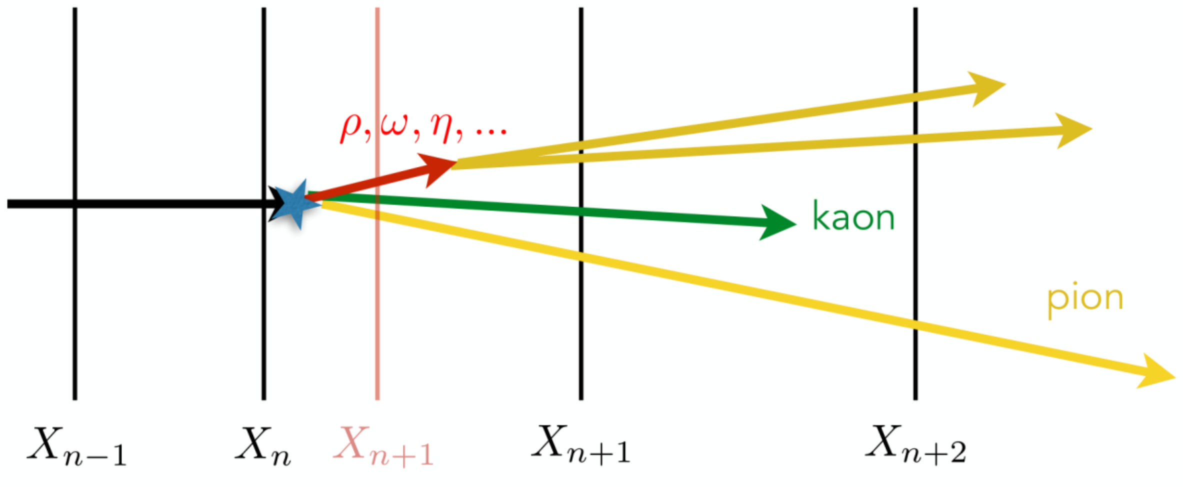
$$\frac{c_{k\to h}(E_i, E_k)}{\lambda_{int}^{(k)}(E_k)}$$

Interaction matrix C

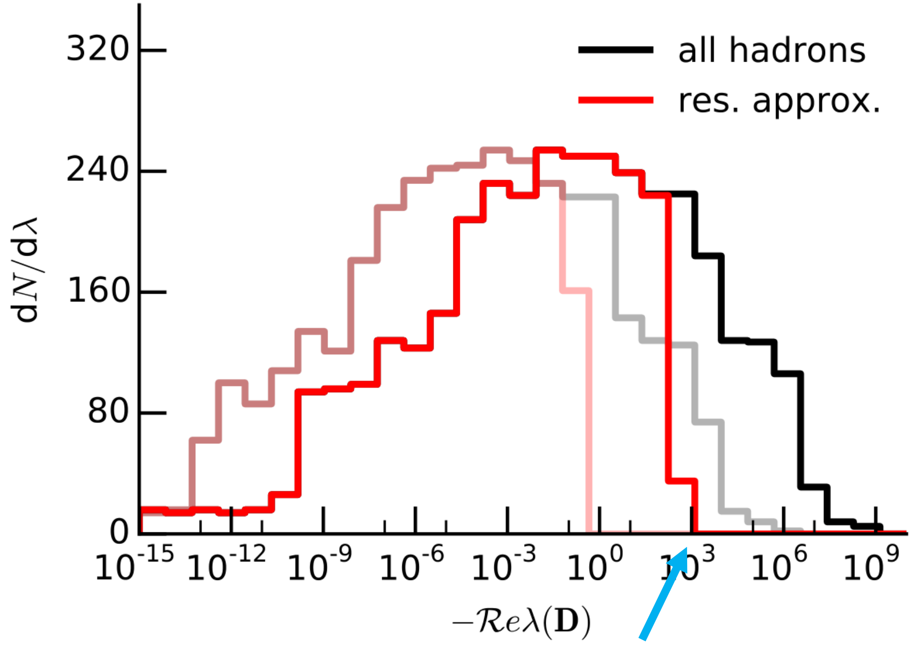
$$-\frac{\phi_h(E_i)}{\lambda_{int}^{(h)}(E_i)}$$

matrices are sparse → high performance

Short resonances and stiffness



Eigenvalues of matrix equation



Resonance approximation: integrate out fast decays

$$\vec{\Phi}^{\omega} = \Big(\underbrace{\Phi^{\omega}_{E_0} \quad \cdots \quad \Phi^{\omega}_{E_i}}_{\equiv 0} \;\Big|\; \Phi^{\omega}_{E_{i+1}} \cdots \quad \Phi^{\omega}_{E_N} \Big)^T$$

$\lambda_{dec} < t_{mix}\lambda_{int}$: treat as resonance

$\lambda_{dec} \geq t_{mix}\lambda_{int}$: transport as particle

Fastest eigenvalue controls integration step

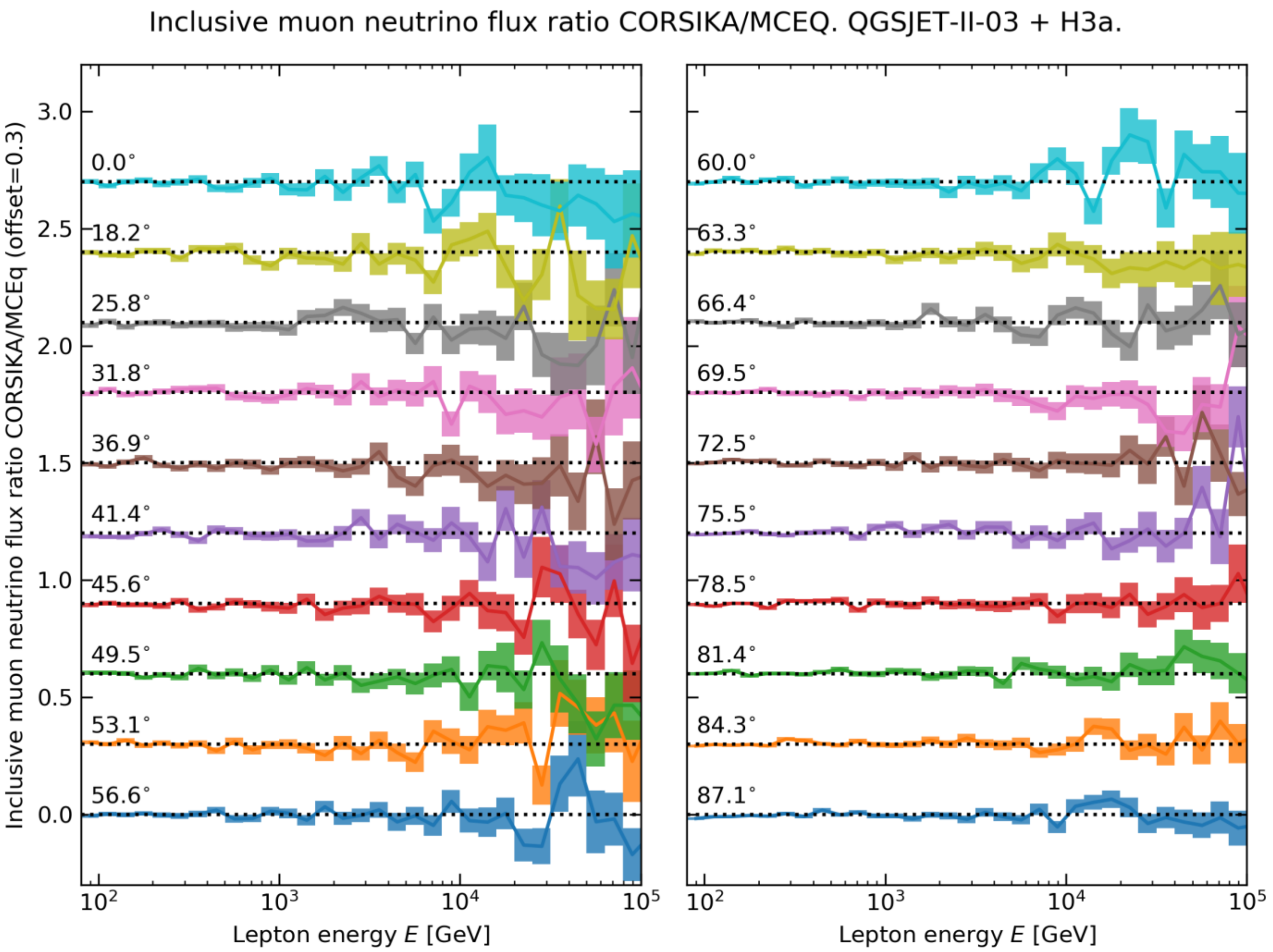
General solutions for linear ODE systems

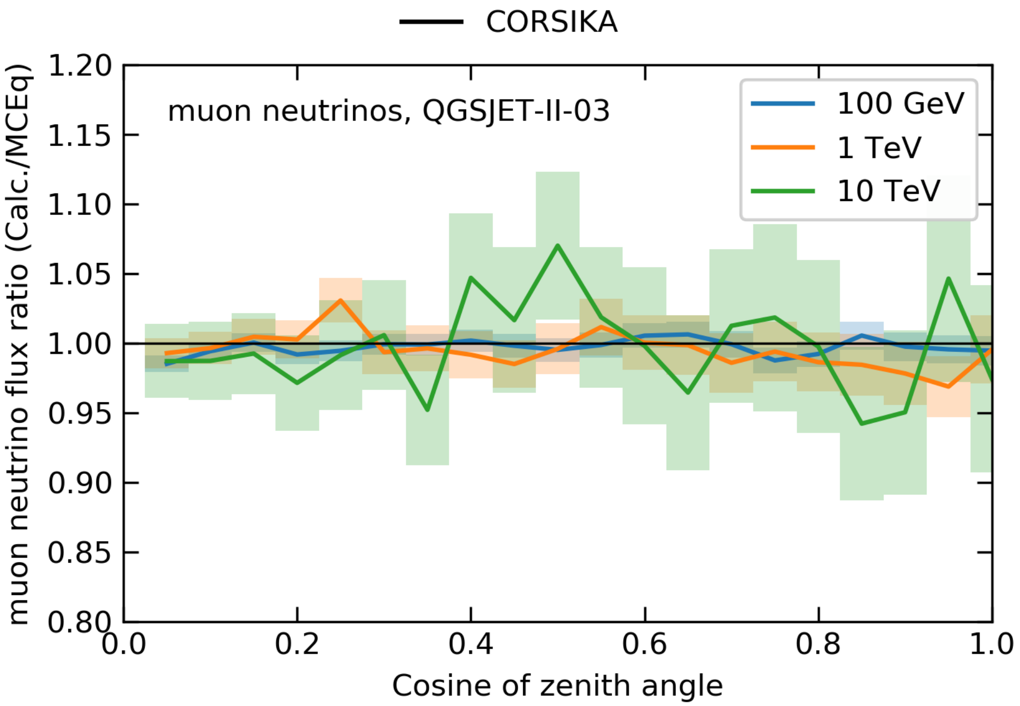
$$\vec{\Phi} = \sum_{i=1}^{n} c_i e^{\lambda_i^* X} \vec{\Psi}_i$$

Stability criterion for explicit integrators

$$\Delta X < \frac{2}{\lambda^*_{\max}}$$

MCEq vs (thinned) CORSIKA calculation in 1D



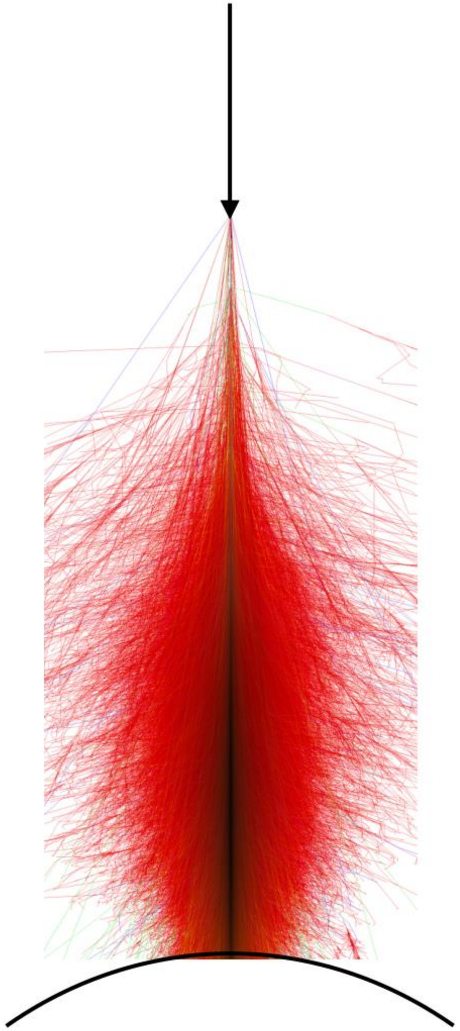


How do you actually compute inclusive fluxes with CORSIKA?

- MIT licensed @ https://github.com/afedynitch/MCEq

CORSIKA: A. Fedynitch, J. Becker Tjus and P. Desiati, PRD 2012
MCEq: Code paper, AF, R. Engel, in prep. for submission

Inclusive fluxes with CORSIKA



For various "inputs"

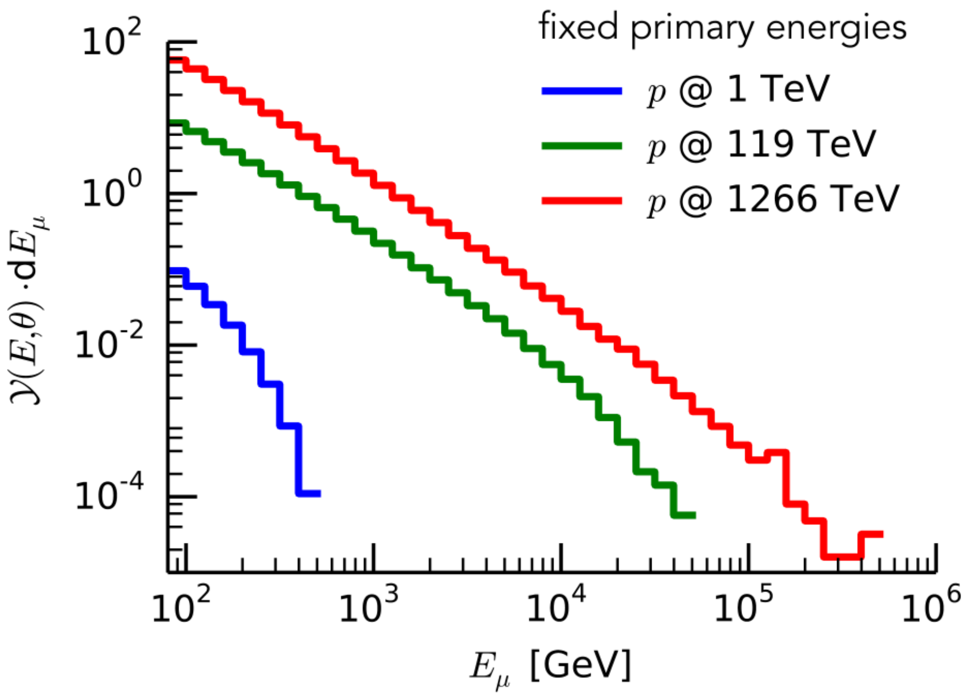
primary spectrum,
zenith angle,
composition

simulate "average" air-shower

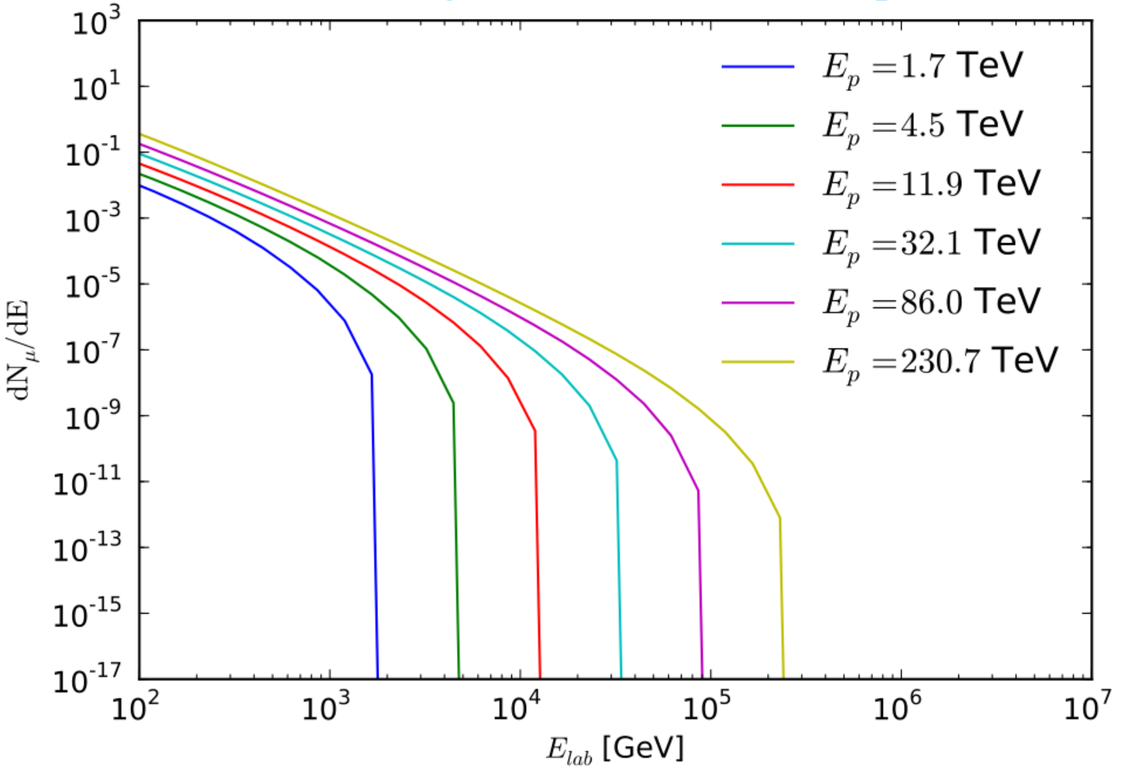
score energy spectrum of particles in virtual detector

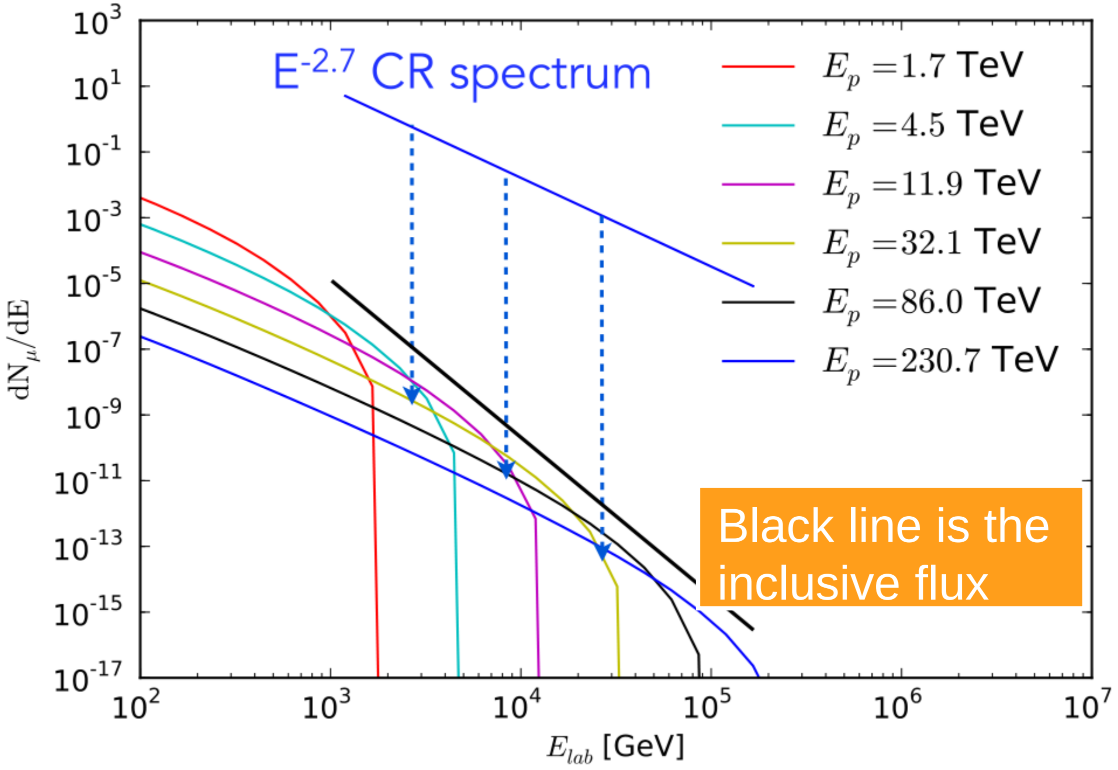
Obtain 1D Yield/Response function

$$\mathcal{Y}(E_0, Z_0, \theta, M, \dots)$$



Convolve yields with primary spectrum





$$\Phi_\mu(E_\mu, \theta) = \sum_p \sum_{E_i} w_p(E_i) \times \mathcal{Y}_{p\to\mu}(E_\mu, E_i, \theta)$$

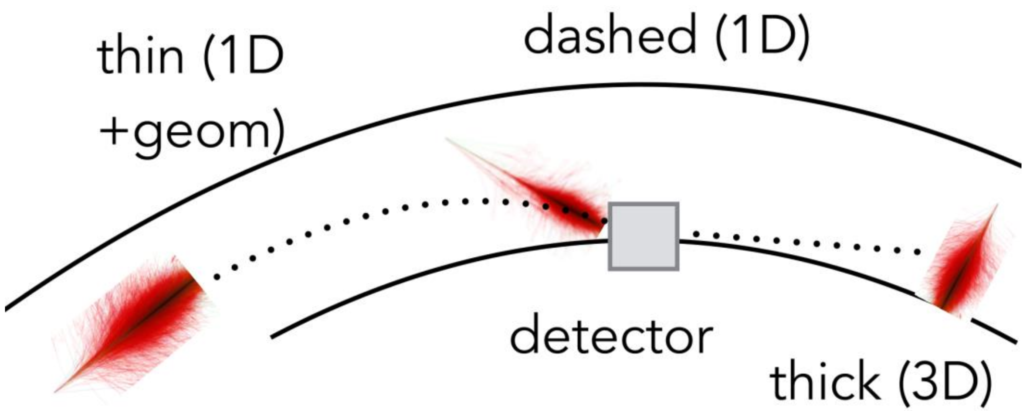
nuclei/
composition

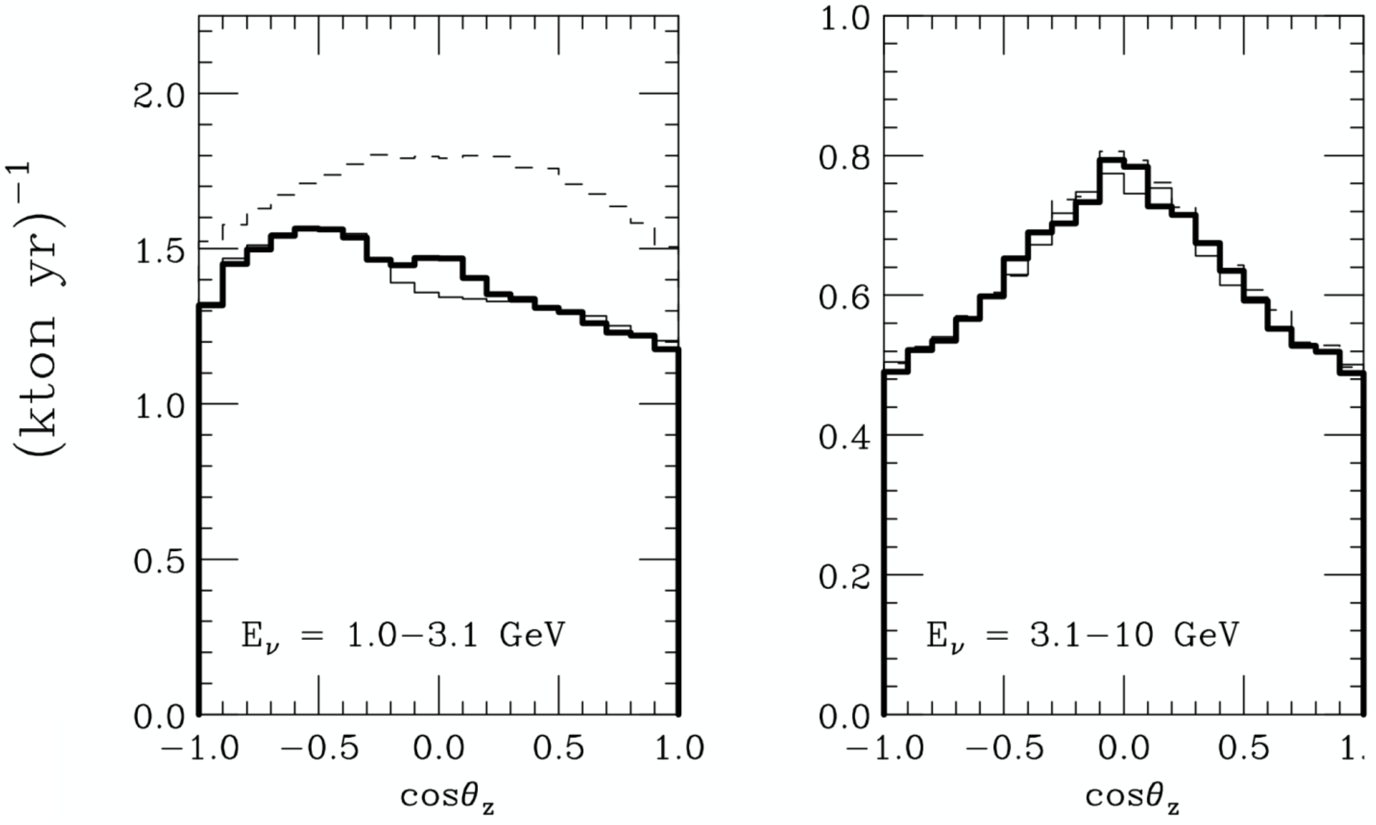
primary spectrum

from CORSIKA

$$w_p(E_i) = \frac{1}{N_p(E_i)} \int_{E_i}^{E_{i+1}} \Phi_p(E')dE', \qquad N_p(E_i) = \mathrm{NSHOW}$$

Low energies: limitation of 1D approach





A subset of 3D calculations

[1] G. Barr, P. Lipari, S. Robbins, and T. Stanev, International Cosmic Ray Conference 3, 1411 (2003).

[2] M. Honda, T. Kajita, K. Kasahara, and S. Midorikawa, Phys. Rev. D 83, (2011).

[3] M. Honda, T. Kajita, K. Kasahara, S. Midorikawa, and T. Sanuki, Phys. Rev. D 75, (2007).

*[4] [1] G. Battistoni, A. Ferrari, P. Lipari, T. Montaruli, P. R. Sala, and T. Rancati, Astroparticle Physics **12**, 315 (1999).*

[5] J. Wentz, I. M. Brancus, A. Bercuci, D. Heck, J. Oehlschläger, H. Rebel, and B. Vulpescu, Phys. Rev. D 67, 073020 (2003).

3D needed < ~ 5 - 10 GeV

AF, Riehn, Engel, Gaisser, Stanev
arXiv:1806.04140

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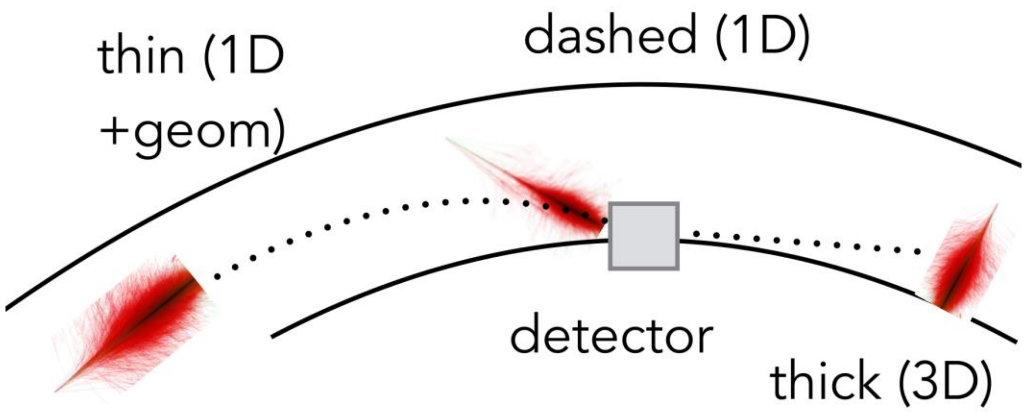

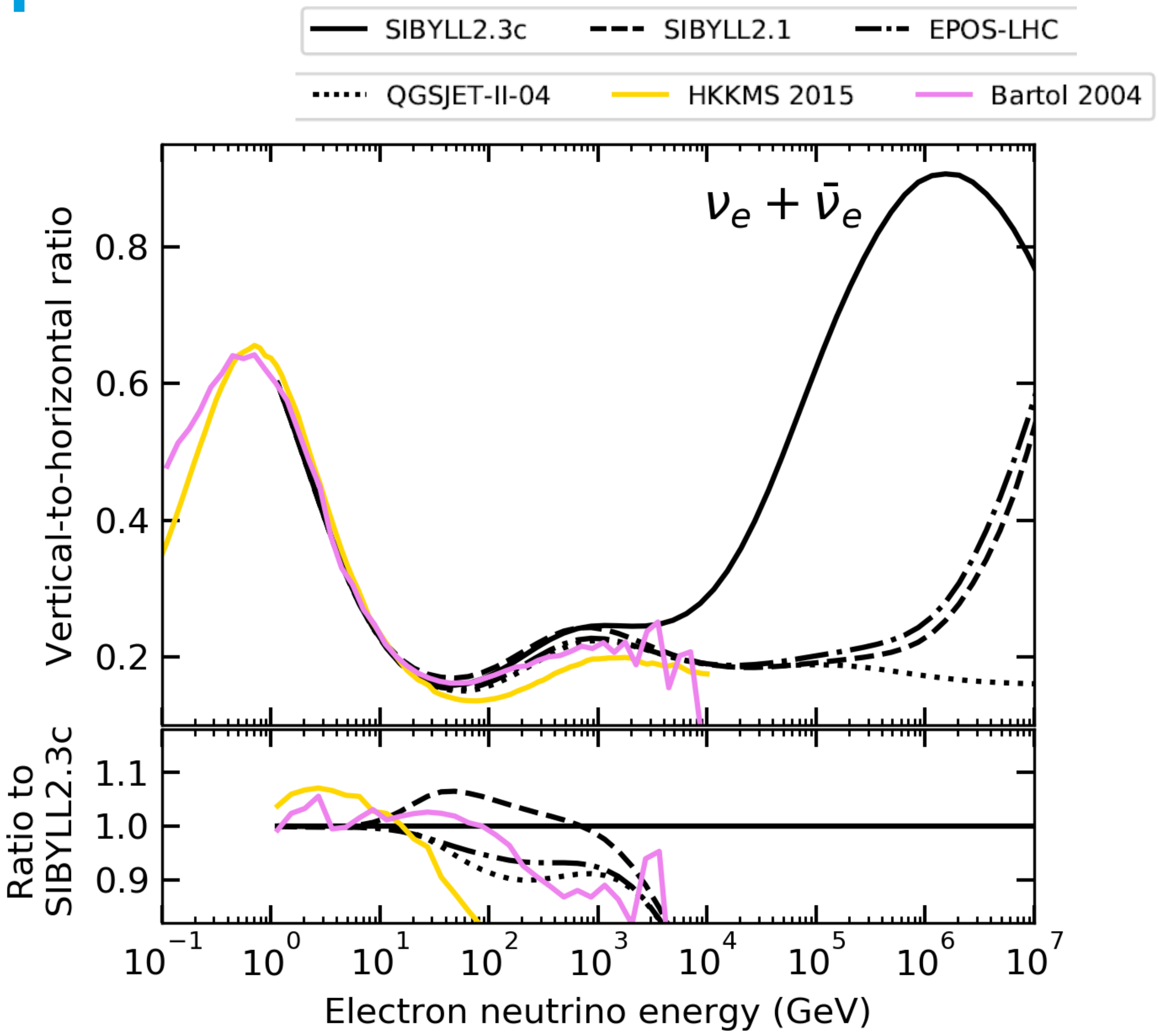

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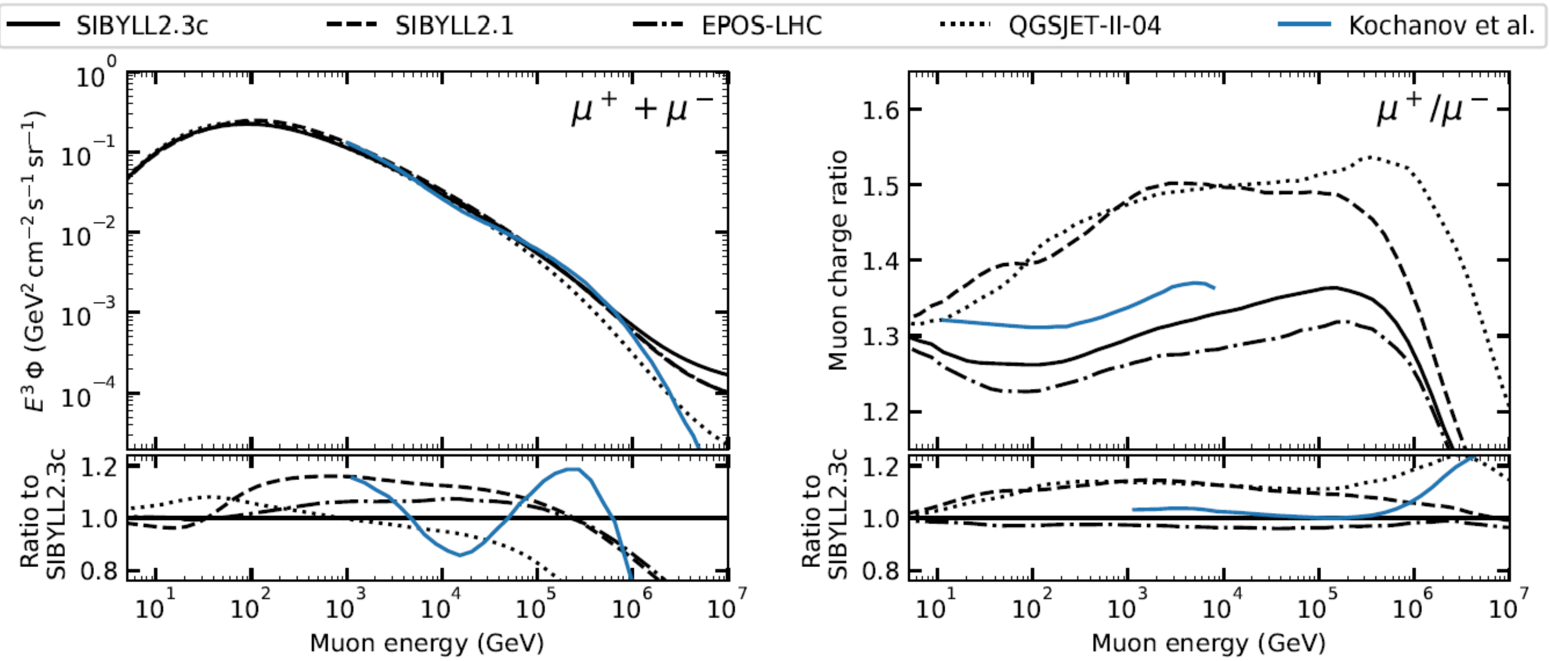
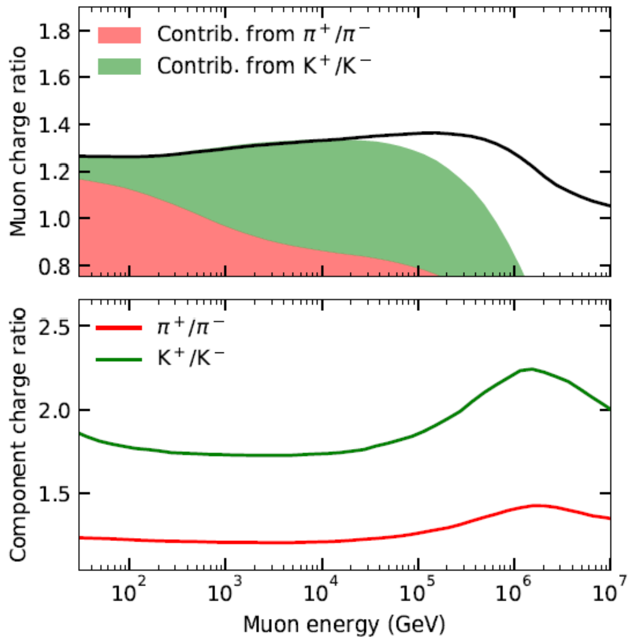
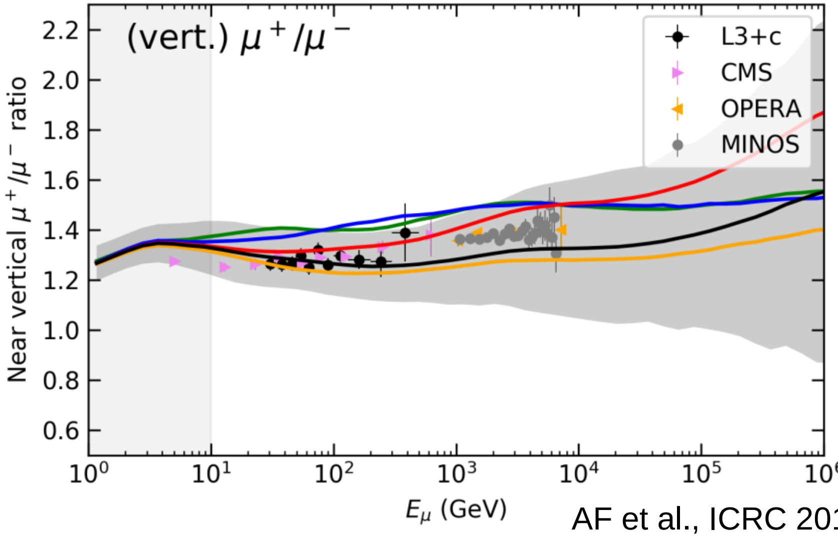
Impact of hadronic interaction model I

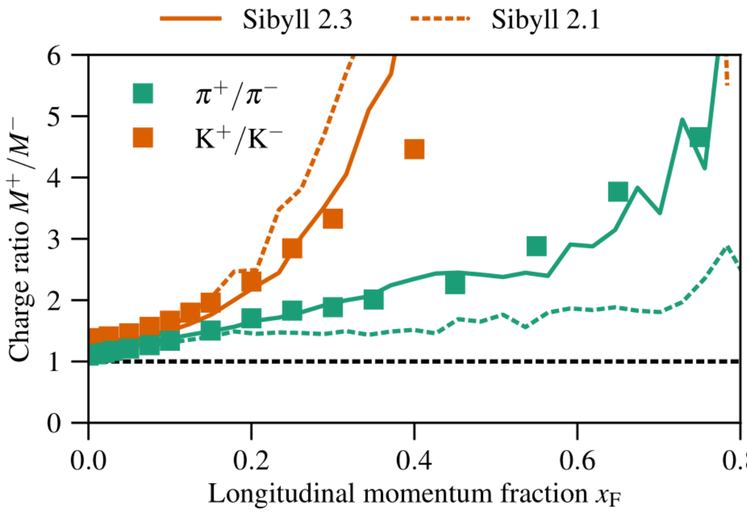




- Inclusive muons “still” uncertain
- Hard to get muon charge ratio right
- Hadronic uncertainties larger than measurement errors

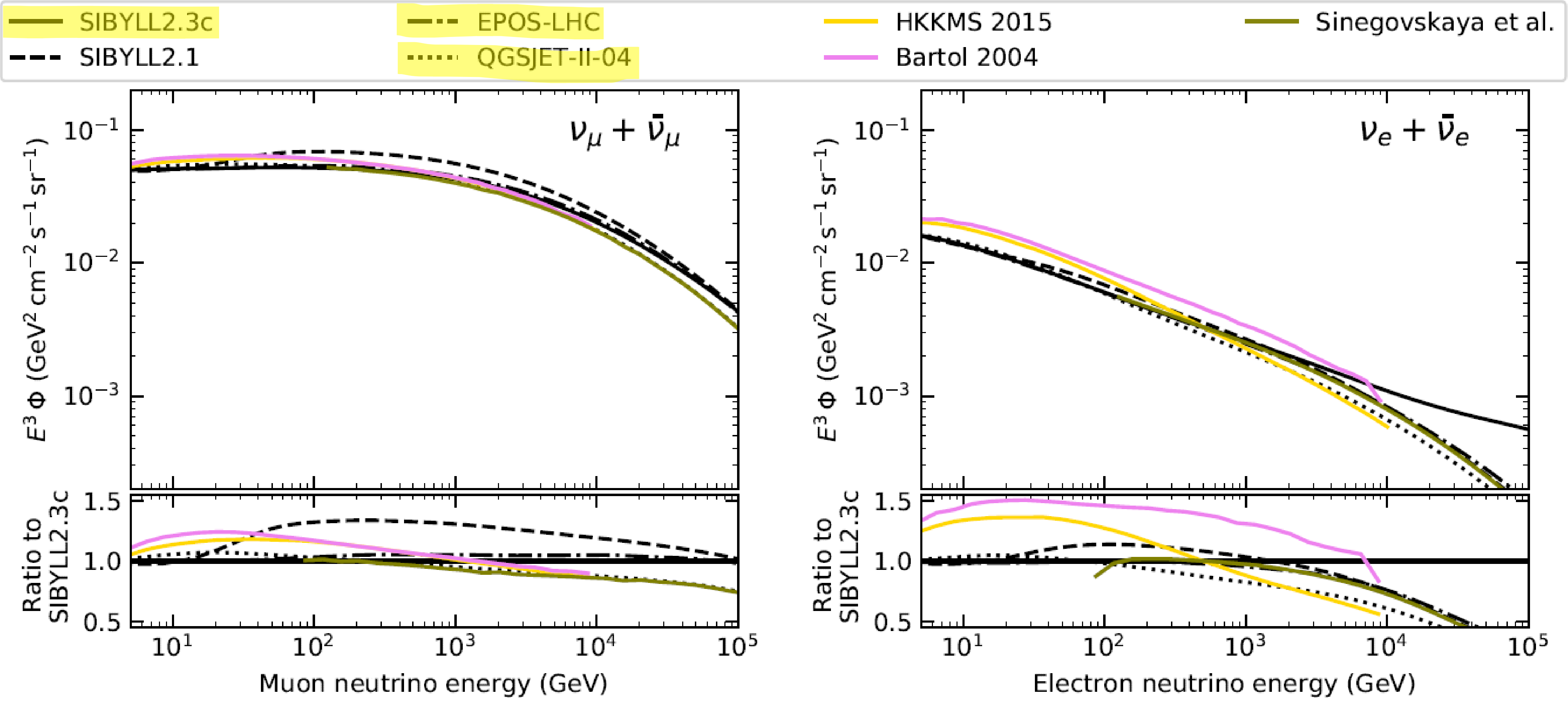


AF et al., ICRC 2017



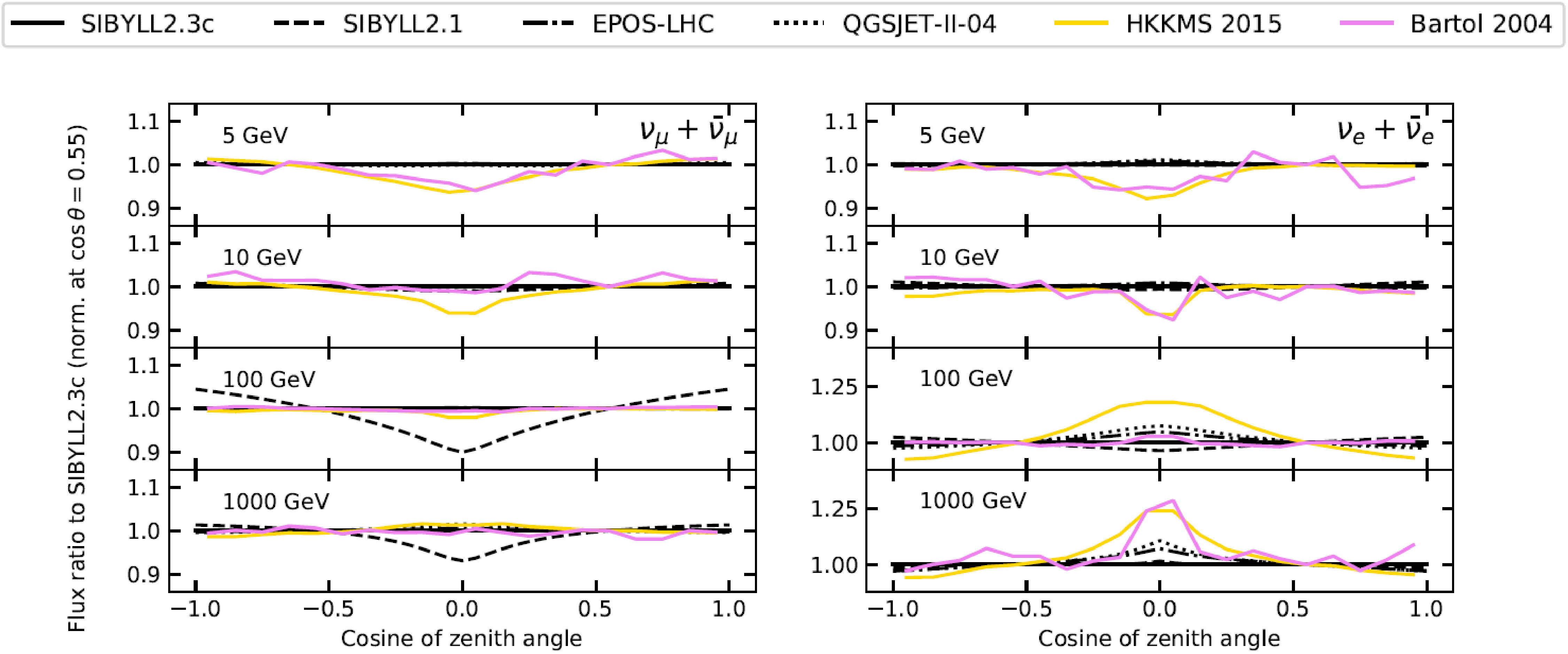
Post-LHC models indeed improve the situation

arXiv:1806.04140

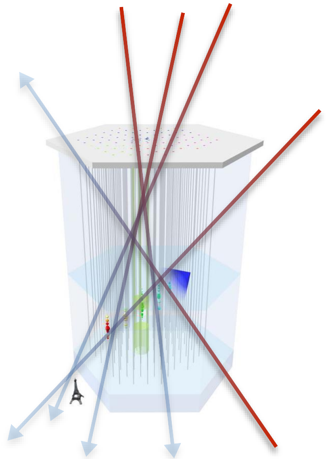


Calculation method more important for angular distributions

arXiv:1806.04140



Wrap-up



$$\frac{d\Phi_h(E,X)}{dX} = -\frac{\Phi_h(E,X)}{\lambda_{int,h}(E)} - \frac{\Phi_h(E,X)}{\lambda_{dec,h}(E,X)} - \frac{\partial}{\partial E}(\mu(E)\Phi_h(E,X)) + \sum_k \int_E^\infty dE_k \frac{dN_{k(E_k)\to h(E)}}{dE}\frac{\Phi_k(E_k,X)}{\lambda_{int,k}(E_k)} + \sum_k \int_E^\infty dE_k \frac{dN^{dec}_{k(E_k)\to h(E)}}{dE}\frac{\Phi_k(E_k,X)}{\lambda_{dec,k}(E_k,X)}$$