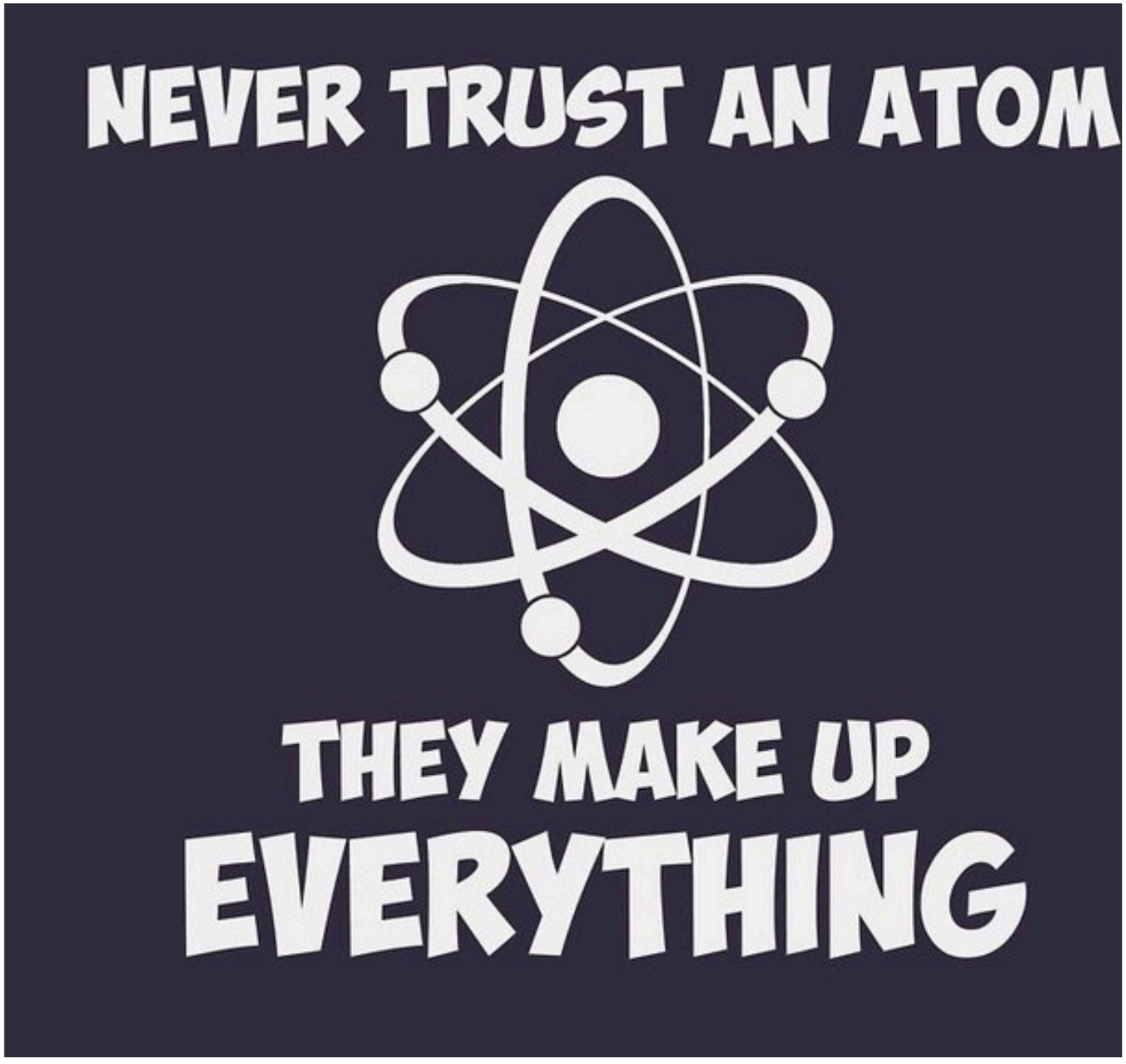
Unravelling proton structure with hyperoptimised machine learning

Juan Rojo
VU Amsterdam & Theory group, Nikhef

Nikhef's Lunch Talk

26/01/2021

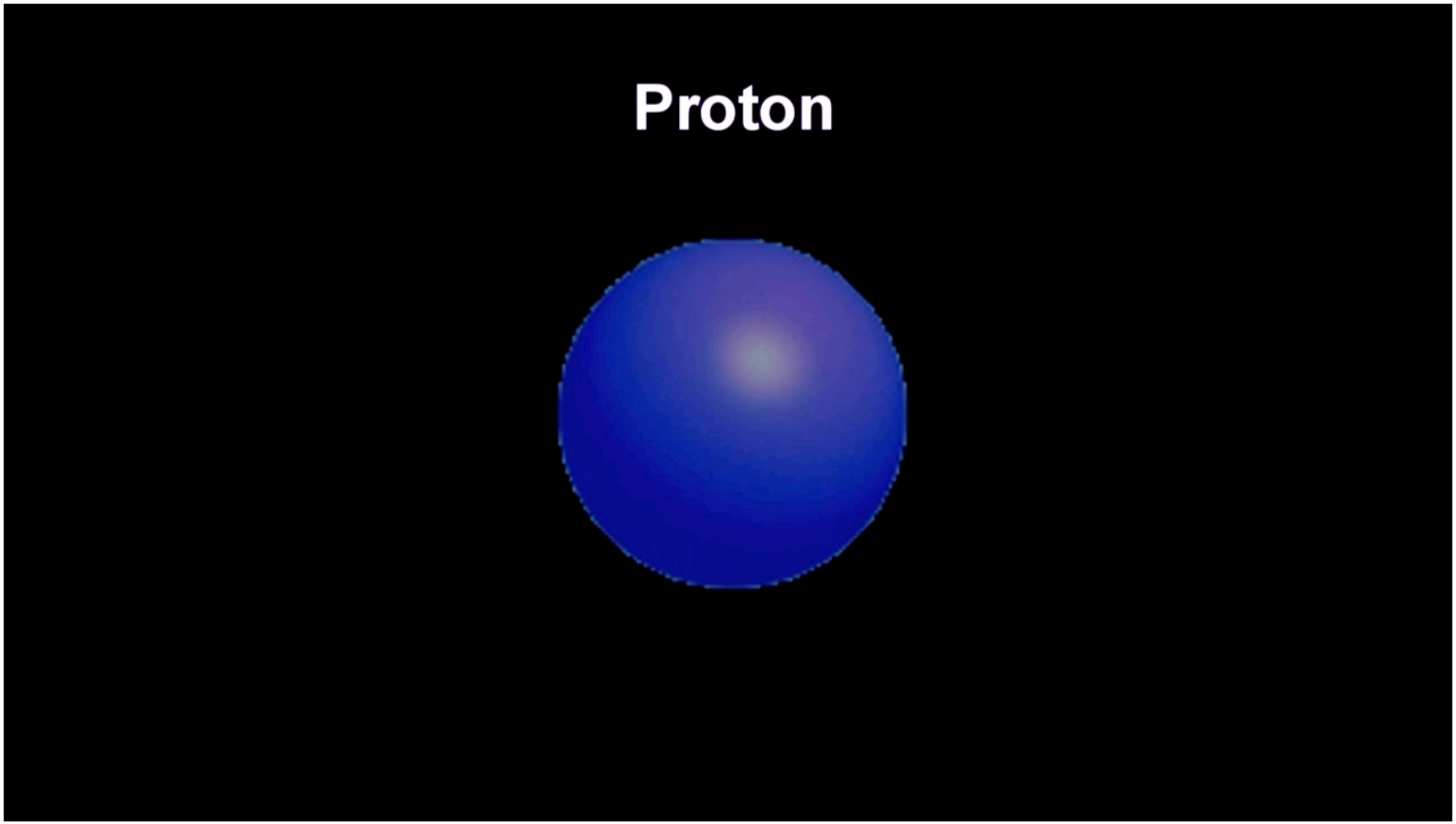
eScience's Accelerating Scientific Discoveries (ASDI2020)



protons compose > 99% of all visible mass in Universe, yet there remain **fundamental open questions** about them!

Why proton structure?

proton: QCD bound state of **quarks** and **gluons**

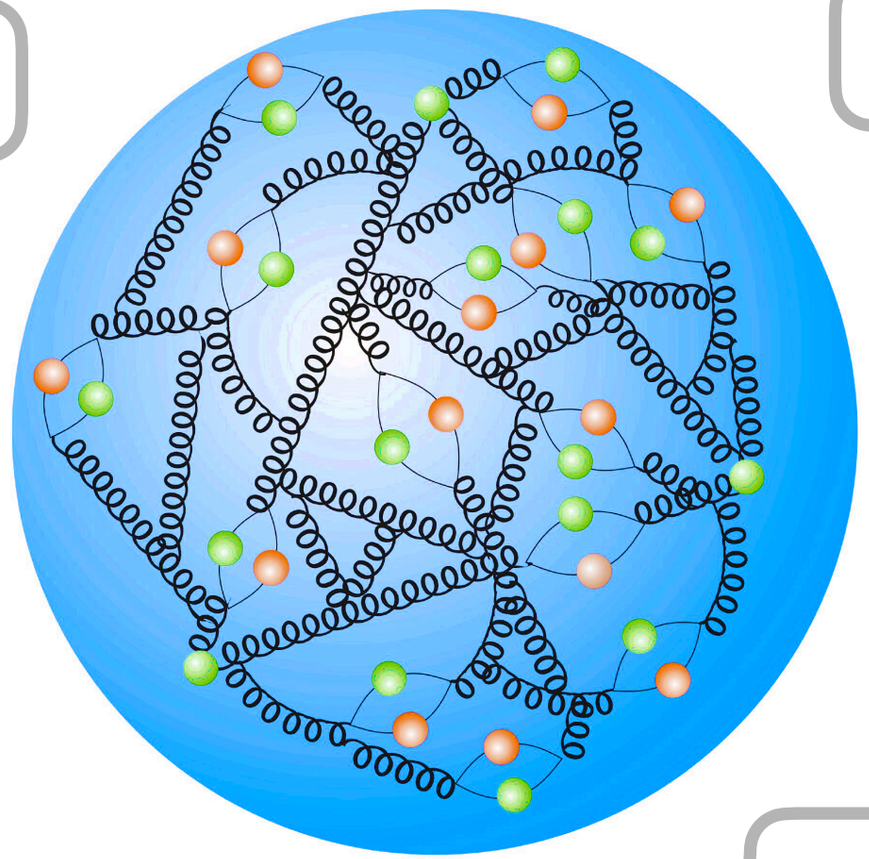


Why proton structure?

proton: QCD bound state of **quarks** and **gluons**

Origin of mass?

Origin of spin?



Gluon-dominated matter?

3D imaging?

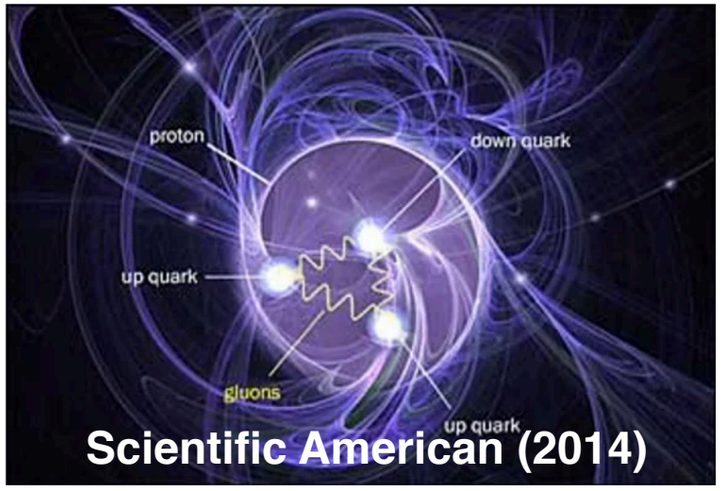
Heavy quark content?

Nuclear modifications?

The proton in the spotlight

THE SCIENCES

Proton Spin Mystery Gains a New Clue



Non-zero gluon polarisation

NEWS PARTICLE PHYSICS

The inside of a proton endures more pressure than anything else we've seen

For the first time, scientists used experimental data to estimate the pressure inside a proton

BY EMILY CONOVER 1:18PM, MAY 16, 2018

Nucleon pressure

The proton keeps surprising us as an endless source of **fundamental discoveries**

QUANTUM PHYSICS

Decades-Long Quest Reveals Details of the Proton's Inner Antimatter

27 |

Twenty years ago, physicists set out to investigate a mysterious asymmetry in the proton's interior. Their results, published today, show how antimatter helps stabilize every atom's core.

Antimatter asymmetry @ SeaQuest

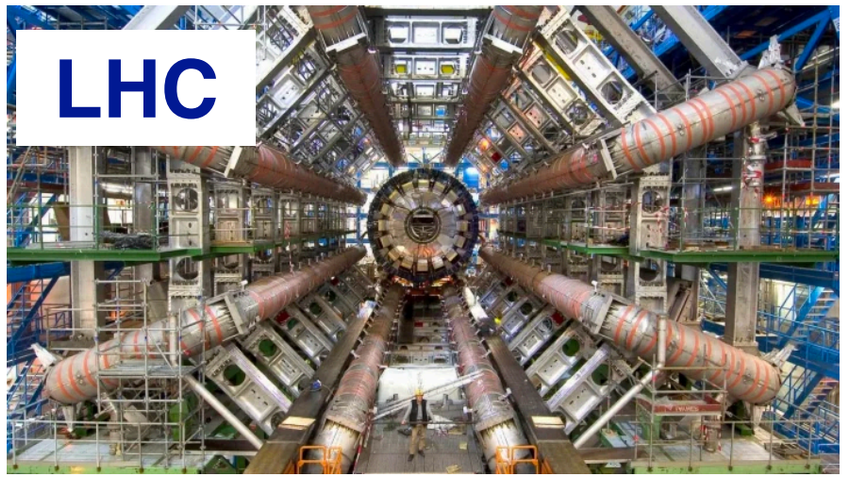
After 40 years of studying the strong nuclear force, a revelation

BFKL dynamics

This was the year that analysis of data finally backed up a prediction, made in the mid 1970s, of a surprising emergent behaviour in the strong nuclear force

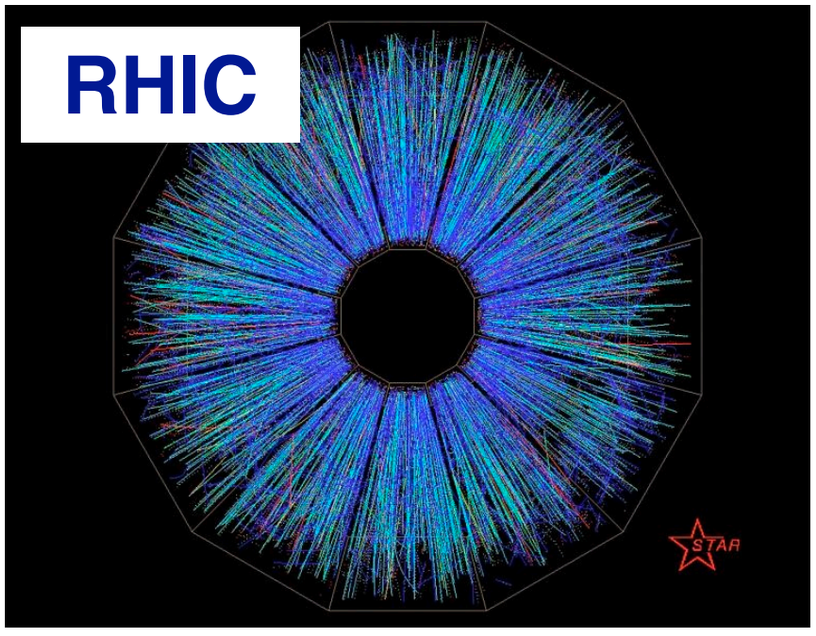
What about proton structure?

knowledge of **quark and gluon substructure of protons** also essential for:



New **elementary particles**
beyond the **Standard Model?**

Origins and properties of
cosmic neutrinos?

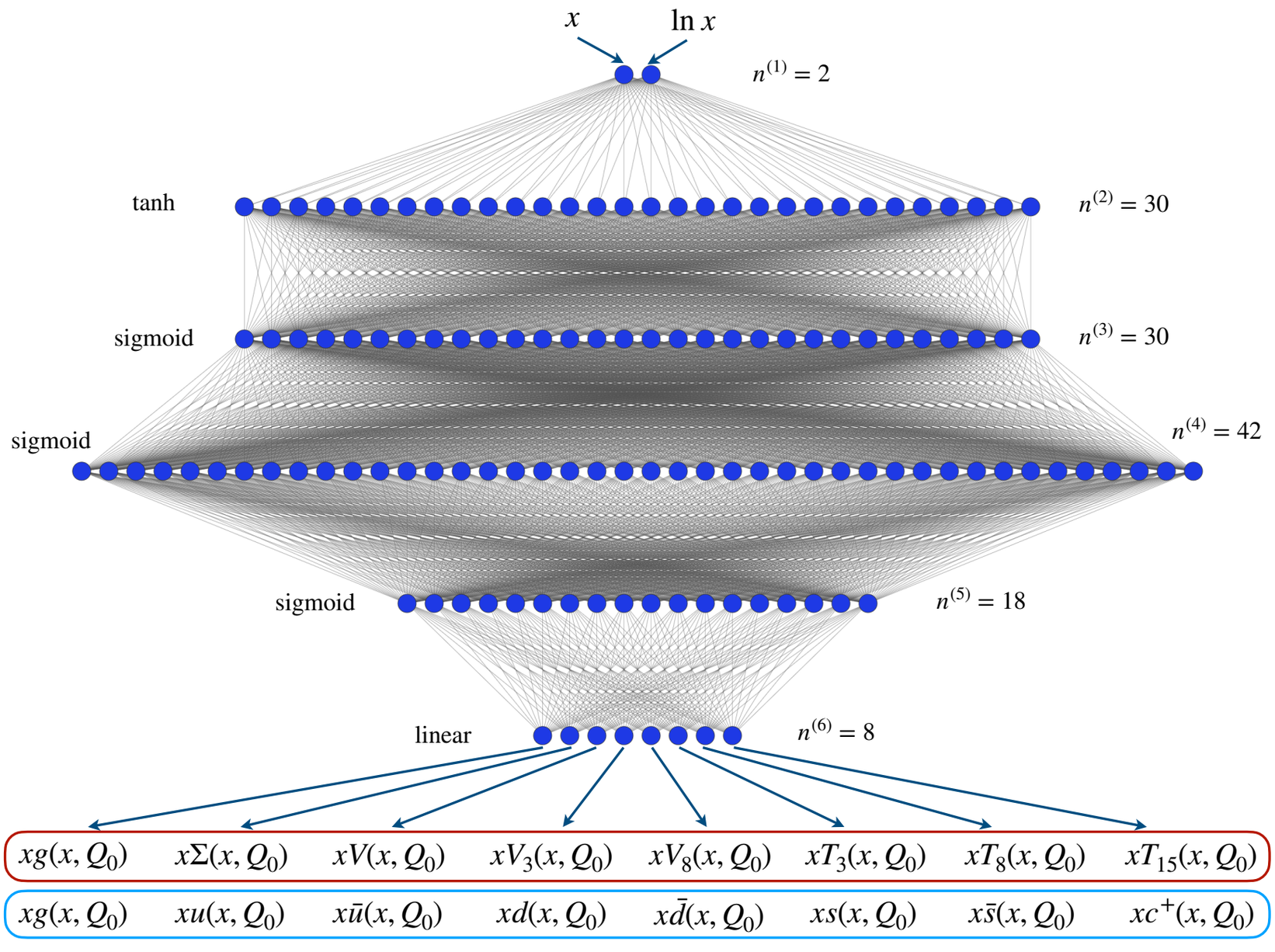


Nature of **Quark-Gluon Plasma**
in **heavy-ion collisions?**

From proton structure to machine learning

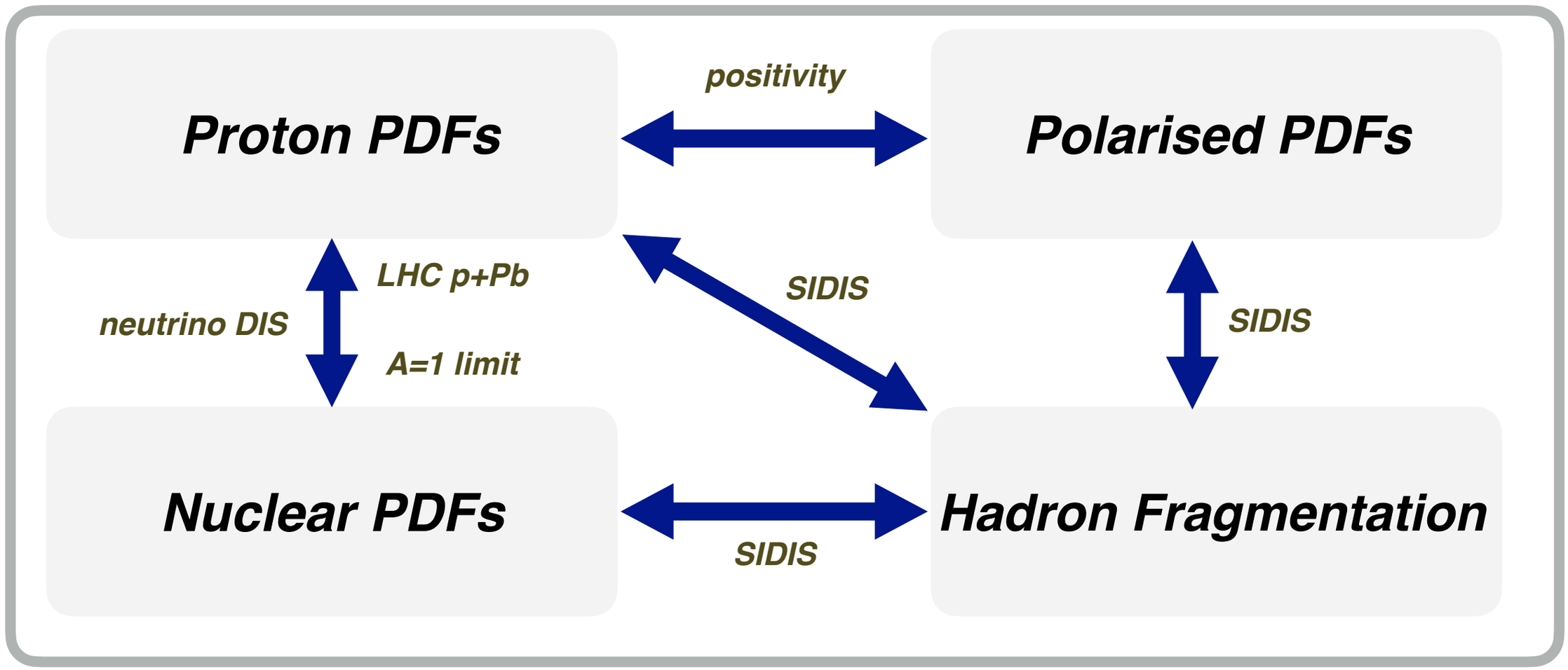
- The proton structure is described by quantities known as **parton distributions,** which need to be extracted from data

- In my research I use **deep learning tools** to parametrise parton distributions (PDFs) and related quantities such as nuclear PDFs (nPDFs) and hadron fragmentation functions (FF)



Goal of ASDI project

Determine **simultaneously proton, deuteron,** and **heavy nuclear PDFs** together with **polarised PDFs** and **fragmentation functions**



Essential to boost our understanding of the **strong nuclear force** and to lay the groundwork for the science of the upcoming **Electron Ion Collider**

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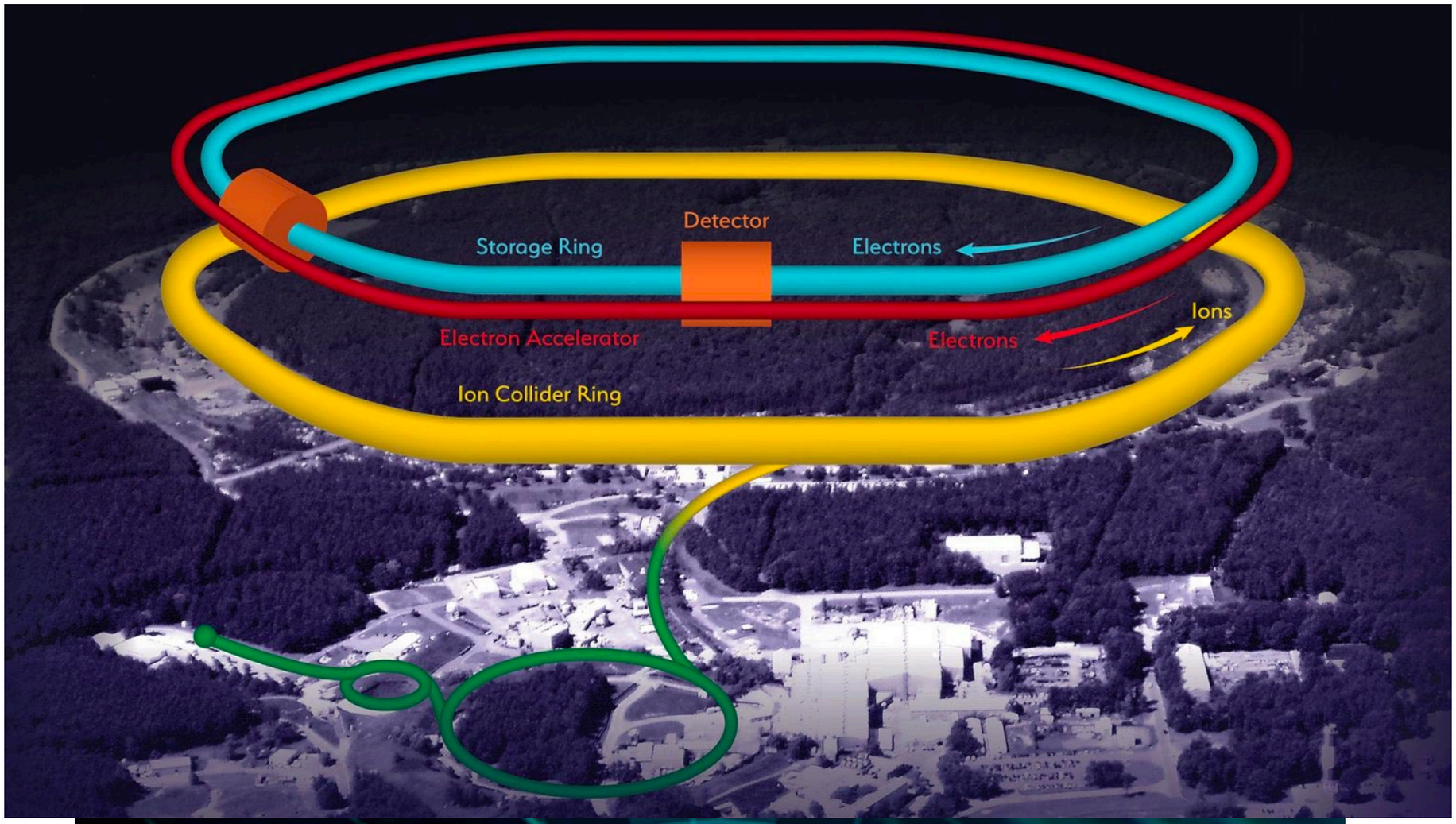
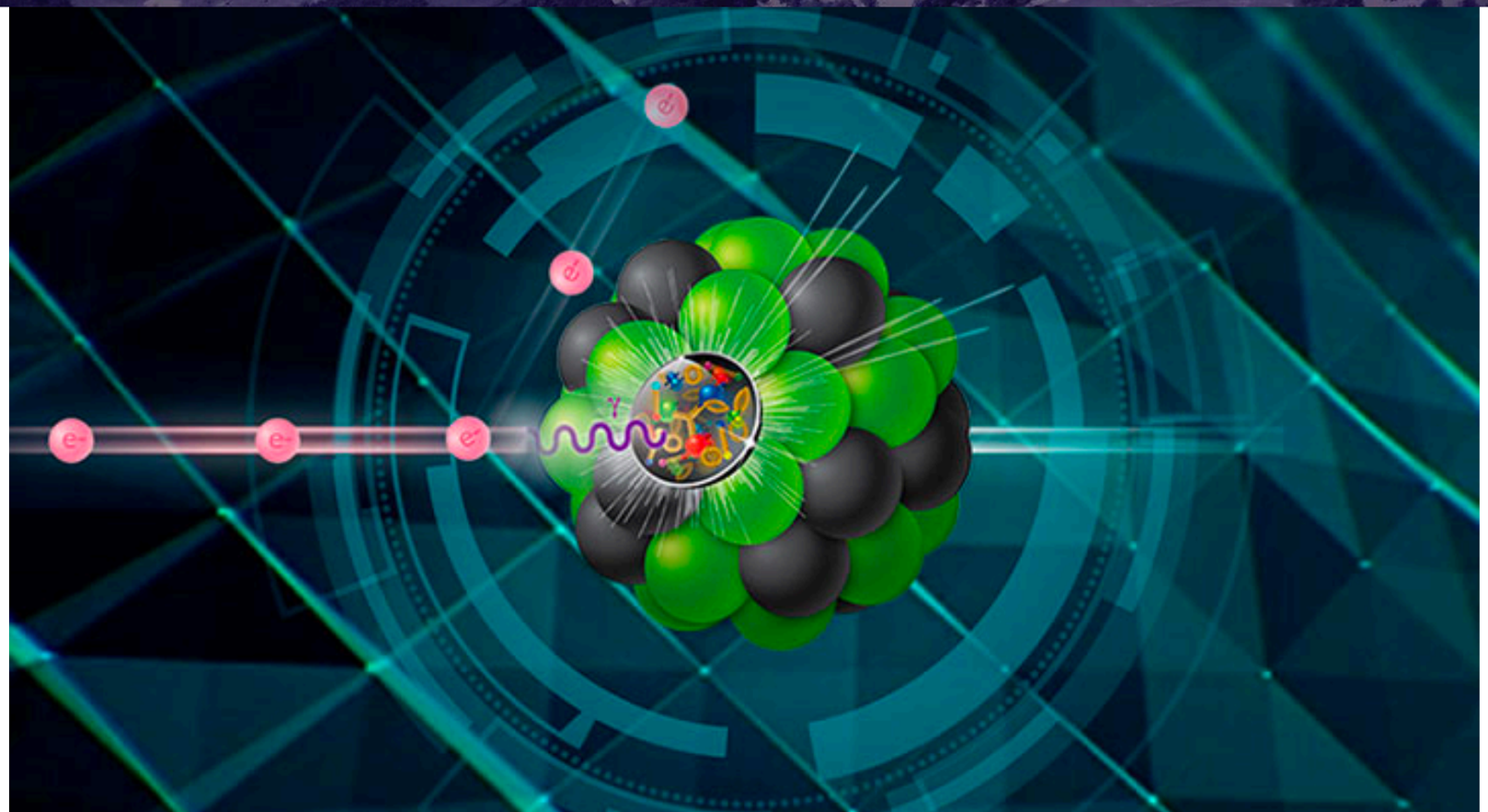
	standard approach	universal QCD analysis
fragmentation functions	$N(p+p\to\pi)\propto\sum_{i,j,k}\widetilde{\sigma}_{ij\to k}\otimes f_i^{(p)}\otimes f_j^{(p)}\otimes f_{k\to\pi}$	$N(p+p\to\pi)\propto\sum_{i,j,k}\widetilde{\sigma}_{ij\to k}\otimes f_i^{(p)}\otimes f_j^{(p)}\otimes f_{k\to\pi}$
nuclear PDFs	$N(p+\mathrm{Pb}\to W)\propto\sum_{i,j}\widetilde{\sigma}_{ij\to W}\otimes f_i^{(p)}\otimes f_j^{(A)}$	$N(p+\mathrm{Pb}\to W)\propto\sum_{i,j}\widetilde{\sigma}_{ij\to W}\otimes f_i^{(p)}\otimes f_j^{(A)}$
proton PDFs	$N(\nu+\mathrm{Pb}\to\mu^+\mu^-)\propto\sum_{i}\widetilde{\sigma}_{i\to\mu^+\mu^-}\otimes f_i^{(p)}\times\left(\frac{f_i^{(A)}}{f_i^{(p)}}\right)$	$N(\nu+\mathrm{Pb}\to\mu^+\mu^-)\propto\sum_{i}\widetilde{\sigma}_{i\to\mu^+\mu^-}\otimes f_i^{(p)}\times\left(\frac{f_i^{(A)}}{f_i^{(p)}}\right)$

theory fitted fixed

theory fitted

Essential to boost our understanding of the **strong nuclear force** and to lay the groundwork for the science of the upcoming **Electron Ion Collider**


Detector
Storage Ring
Electrons
Ions
Electron Accelerator
Electrons
Ion Collider Ring



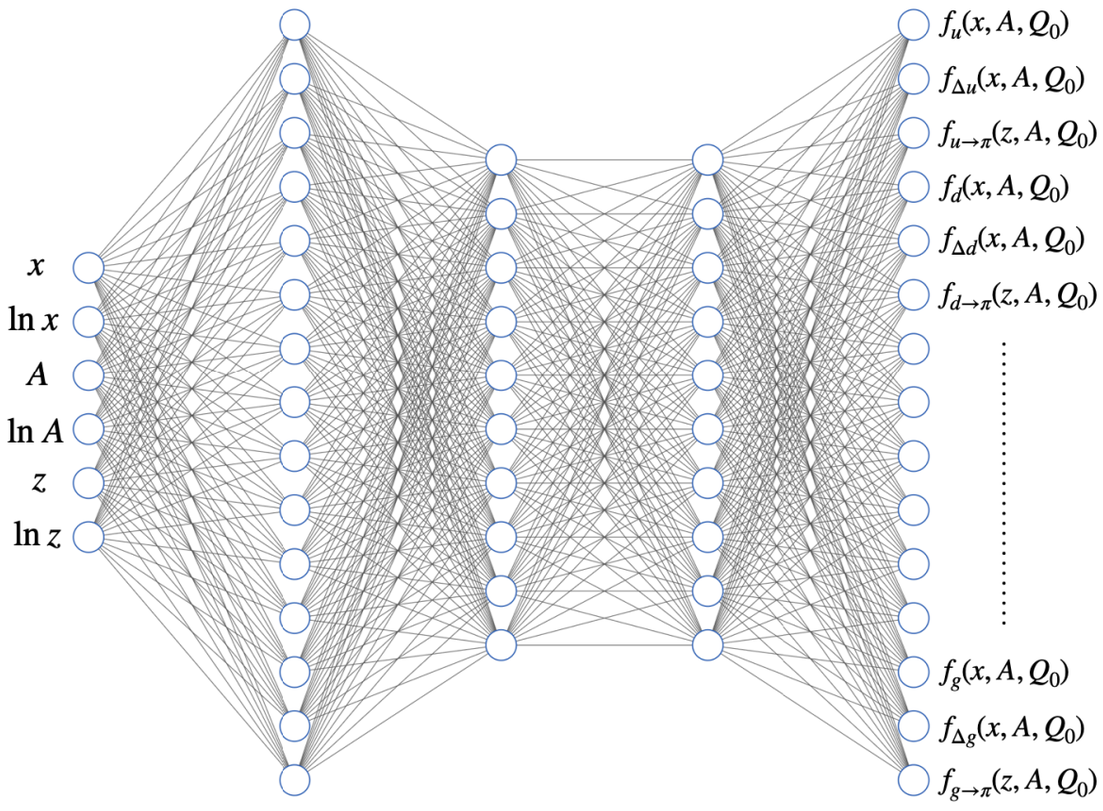
Challenges and eScience contribution

☑ ***Computing overhead from model training:*** extend NNPDF framework to run on **GPUs**, in particular the grid representation of QCD convolutions (current bottleneck)

☑ ***Algorithmic hyperoptimisation in ML:*** explore novel **ML hyperoptimisation strategies** leading to superior performance (tens of hyperparams considered)

☑ ***Efficient database management:*** organize, access, and exploit the hundreds (or thousands) of individual measurements of the universal fit while reducing their memory footprint,

☑ ***Dimensional reduction and data visualization***



brute-force calculation

$$N(p+\mathrm{Pb}\to\pi+X)\propto\sum_{i,j,k=u,d,g,\ldots}^{n_f}\int dx_1\int dx_2\int dz\,\widetilde{\sigma}_{ij\to k+X}(x_1,x_2,z,Q)\left(f_i(x_1,Q,1)\,f_j(x_2,Q,A_{\mathrm{Pb}})\,f_{k\to\pi}(z,Q,A_{\mathrm{Pb}})\right)$$

$$f_i(x,A,Q)=\sum_{j=u,d,g,\ldots}^{n_f}\int dQ'\int dz\,\Gamma_{ij}(x/x',Q'/Q_0)\,f_j(x',A,Q_0)$$

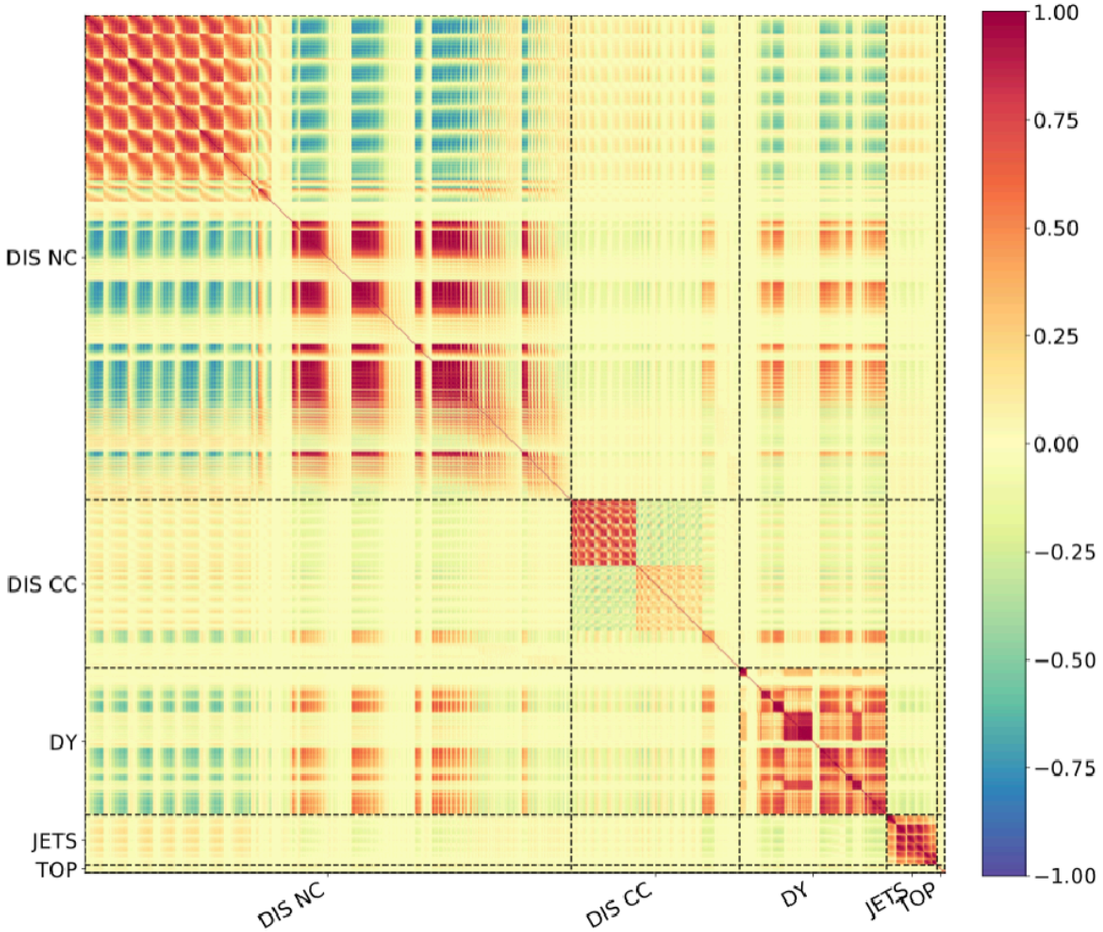
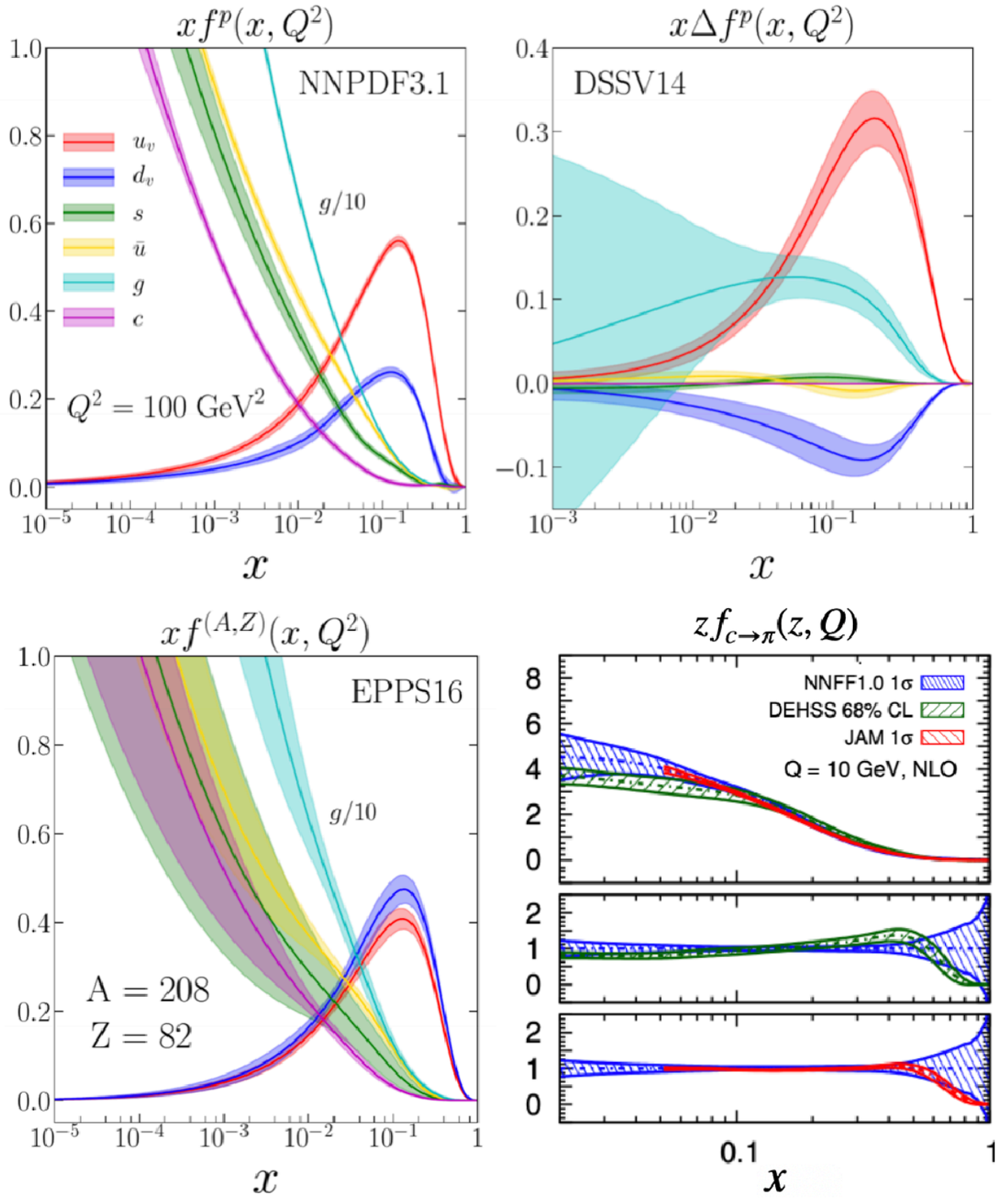
NN outputs

via grid interpolation (NNPDF method)

$$N(p+\mathrm{Pb}\to\pi+X)\propto\sum_{m,n,p=1}^{n_x}\sum_{i,j,k}^{n_f}\left(\mathbf{FK}_{m,n,p,i,j,k}\right)\times\left(f_i(x_m,Q_0,1)\,f_j(x_n,Q_0,A_{\mathrm{Pb}})\,f_{k\to\pi}(z_p,Q_0,A_{\mathrm{Pb}})\right)$$

sum over x,z grids — *sum over flavour*

Questions?



NNPDF3.1_th proton analysis