ML/AI activities at Nikhef Theory

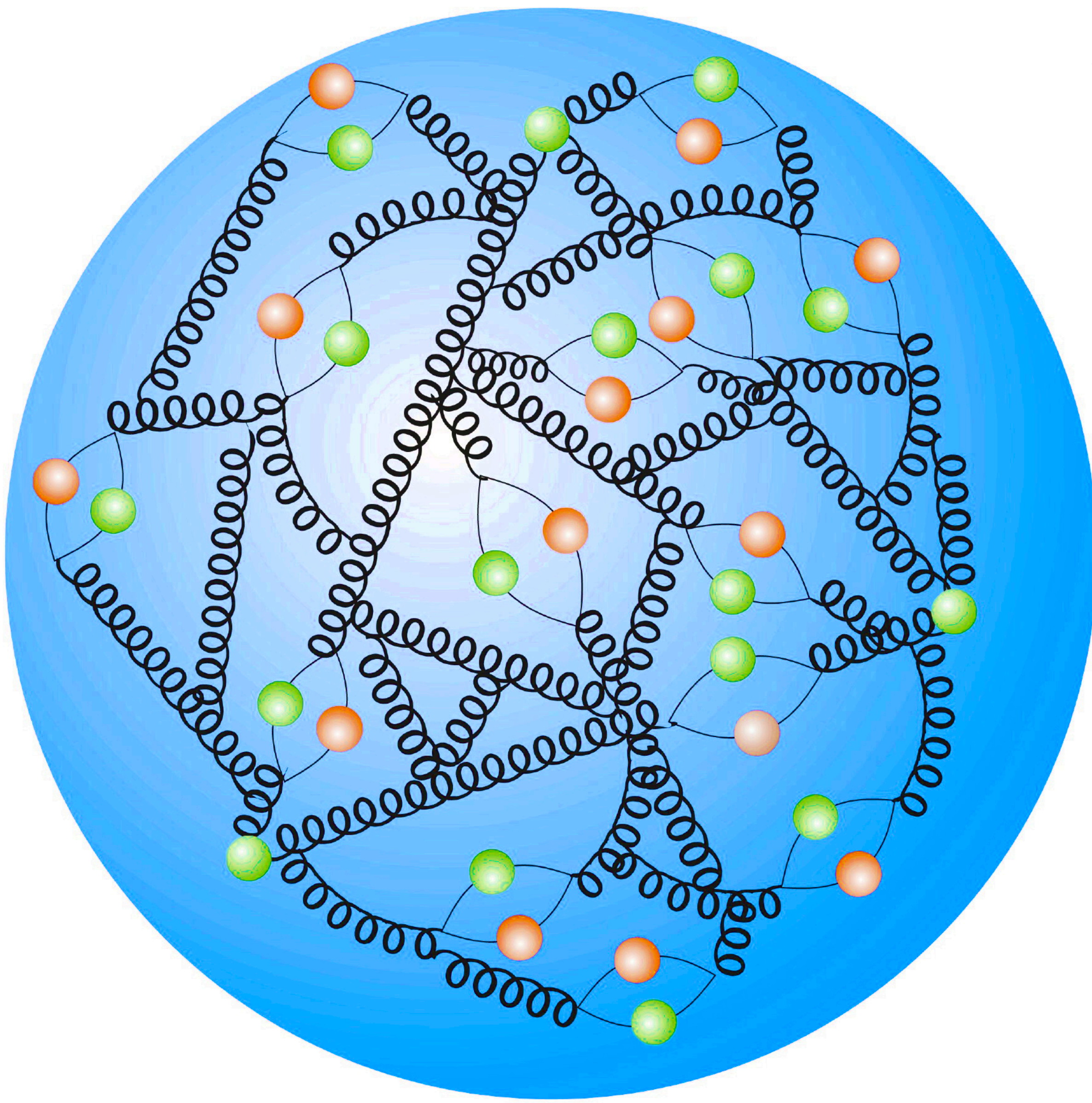
Juan Rojo, VU Amsterdam & Nikhef

Nikhef ML/AI Working Group - Kick-off Meeting

Nikhef, 6th September 2024

The many faces of the proton

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



- **Valence quarks (up and down)** give the proton its quantum numbers (e.g. electric charge)

$$|\Psi\rangle \approx |uud\rangle$$

$$Q_p = +1 \qquad \begin{array}{l} Q_u = +2/3 \\ Q_d = -1/3 \end{array}$$

- **Sea quarks (antiup, antidown, strange, …)** arise from quantum fluctuations

- Tightly held together by **gluons,** can only be broken in extremely energetic collisions

Parton Distributions

$$g(x, Q)$$

Probability of **finding a gluon inside a proton**, carrying a fraction ***x*** of the proton momentum, when probed with energy ***Q***

x: fraction of proton momentum carried by gluon

Energy of hard-scattering reaction**:** inverse of resolution length

Dependence on *x* fixed by **non-perturbative QCD dynamics**: extract from experimental data

$$g(x, Q_0, \{a_g\}) = f_g(x, a_g^{(1)}, a_g^{(2)}, \ldots)$$

constrain from data

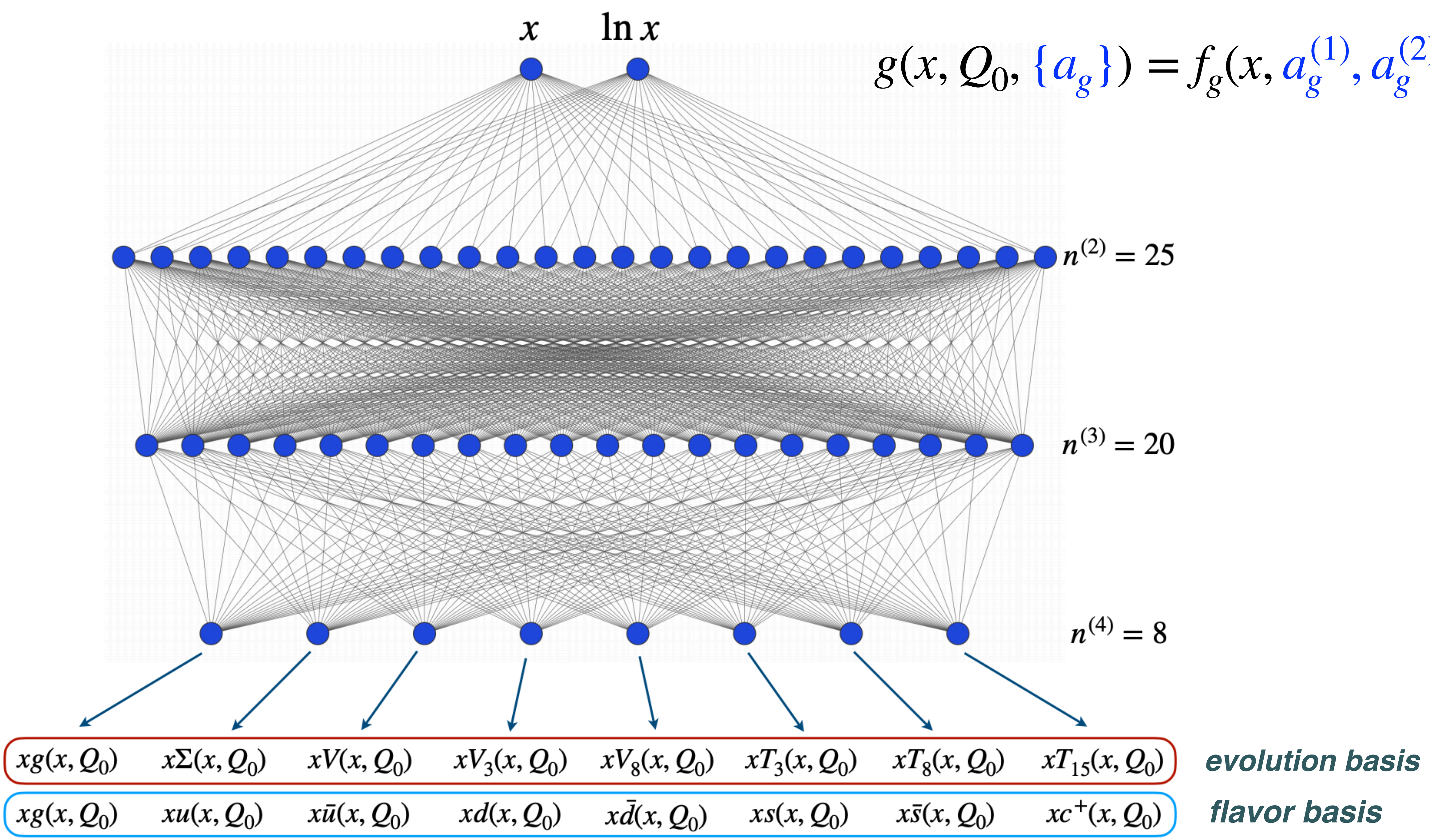
- Dependence with **resolution scale *Q***: DGLAP evolution, computable from first principles

- **Energy conservation** and **quark number conservation** are fixed boundary conditions

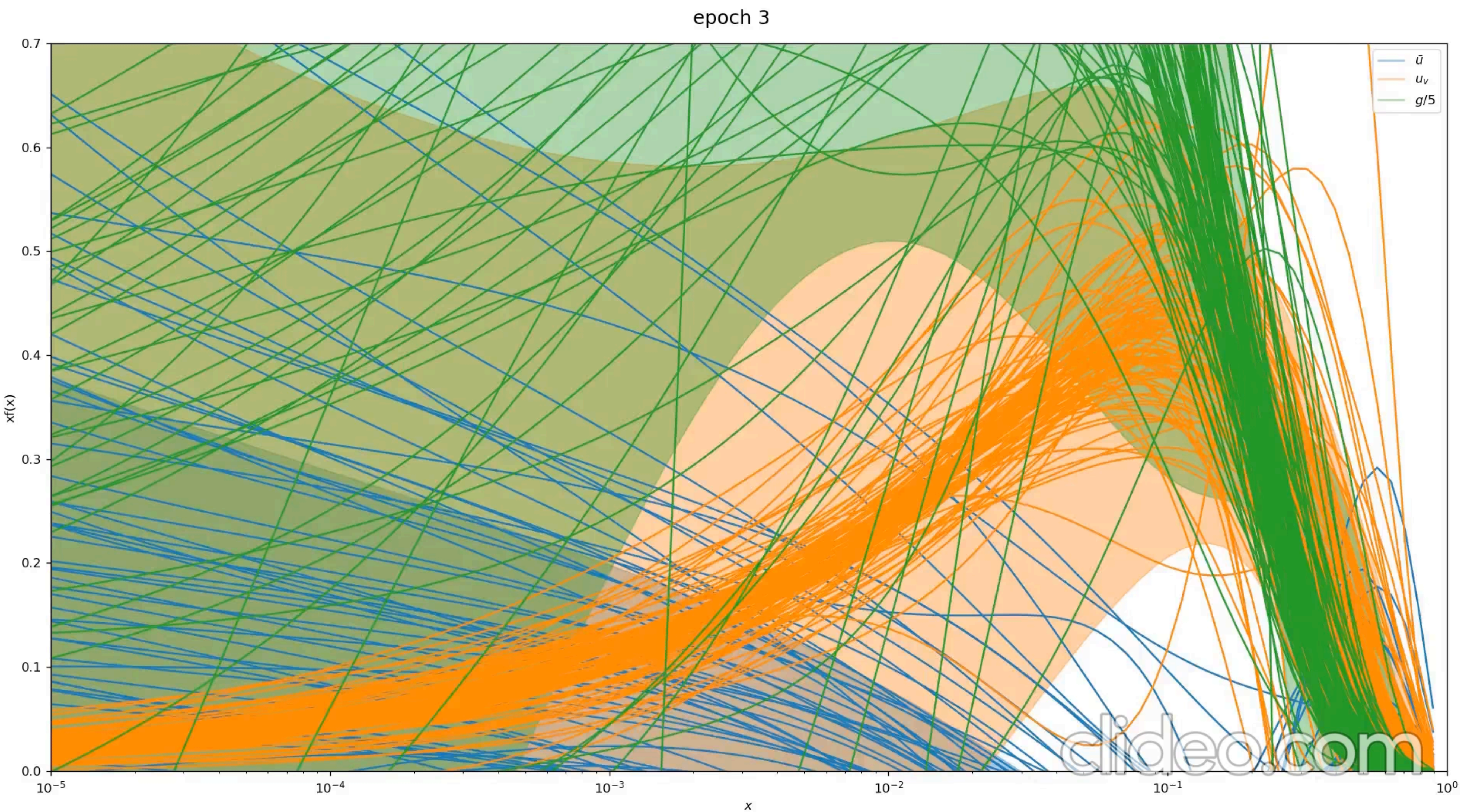
ML Proton Structure

- Model-independent PDF parametrisation with neural networks as **universal unbiased interpolants**
- **Stochastic Gradient Descent** via TensorFlow for neural network training
- Automated model **hyperparameter optimisation:** NN architecture, minimiser, learning rates …

$$g(x, Q_0, \{a_g\}) = f_g(x, a_g^{(1)}, a_g^{(2)}, \ldots)$$



Machine Learning PDFs



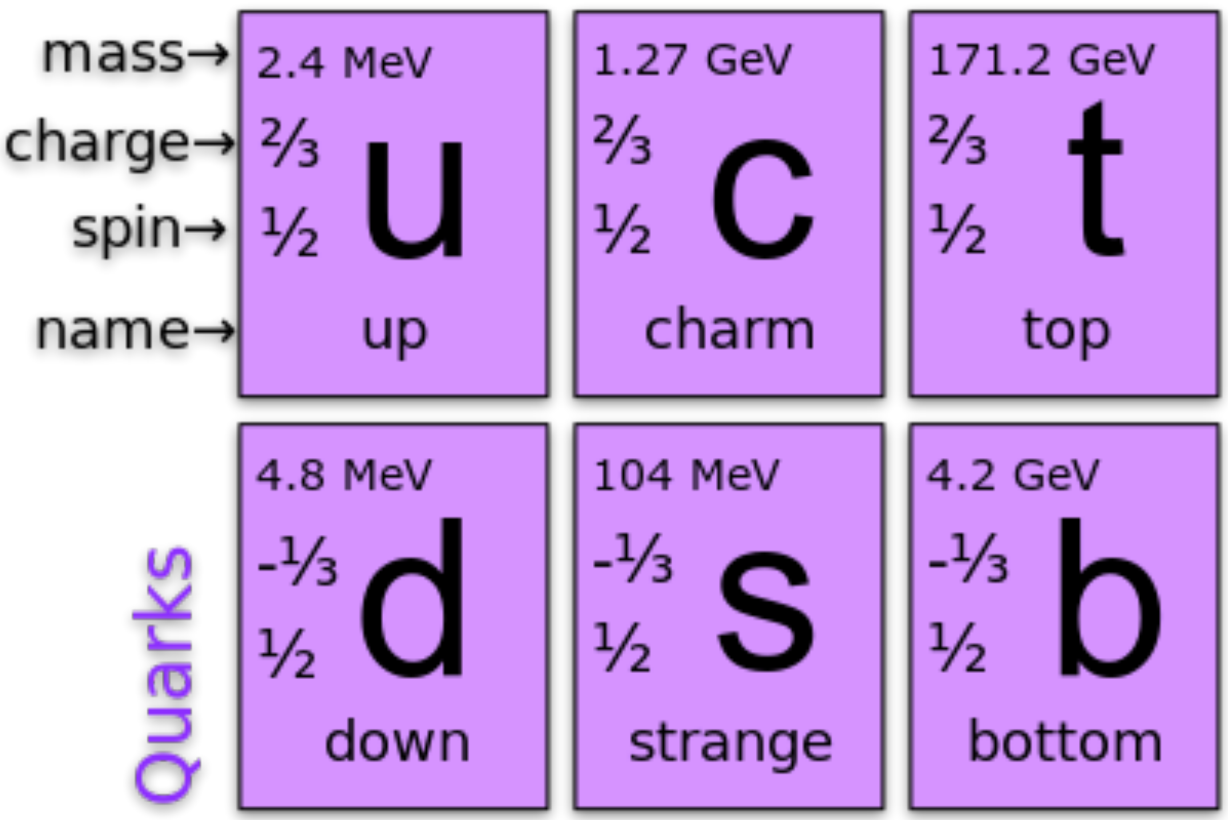
Error estimate based on **Monte Carlo replica method** (band: standard deviation over the MC replicas)

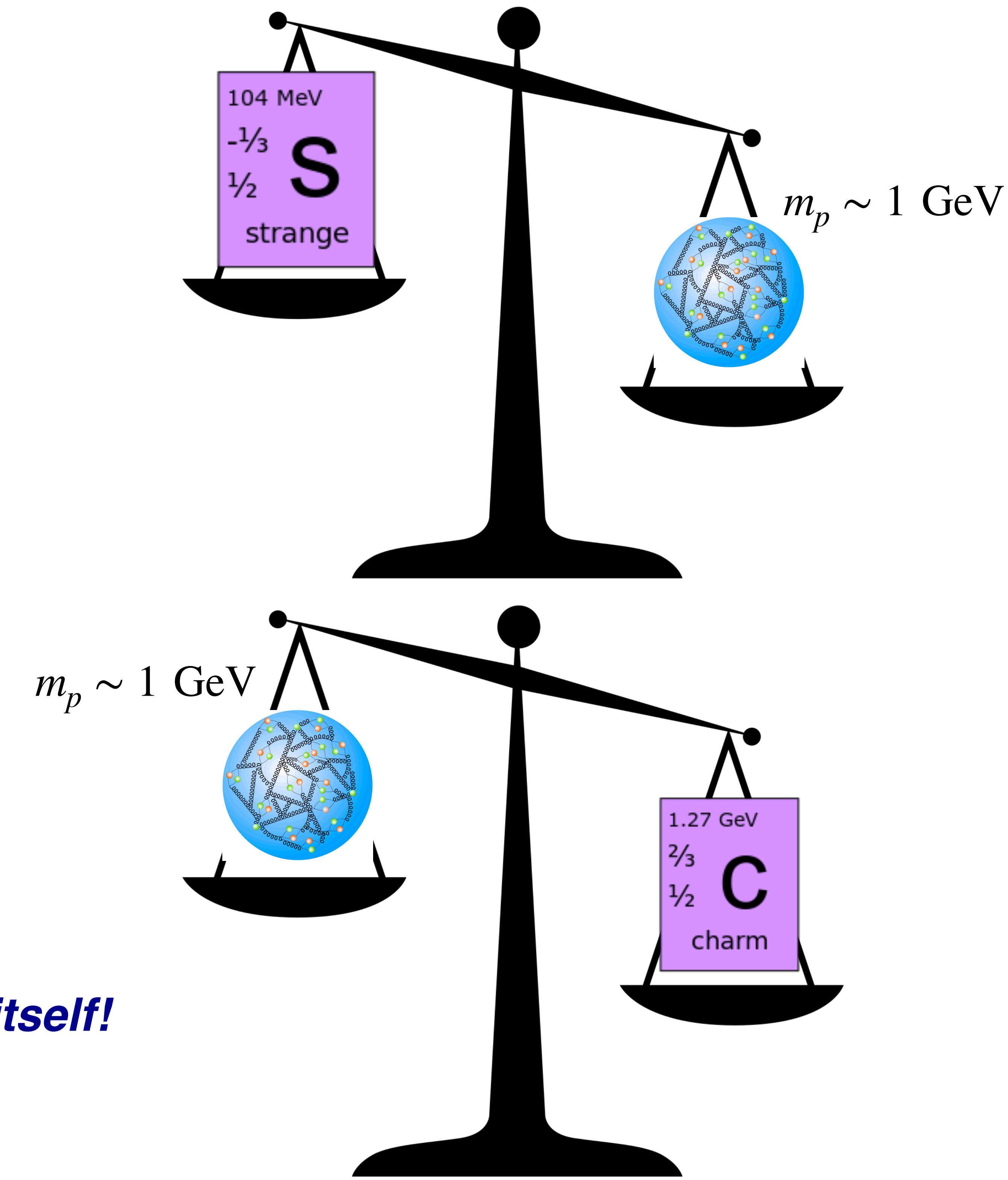
each curve is a separately trained neural network

The charm content of the proton

common assumption: the proton wave function does not contain charm quarks

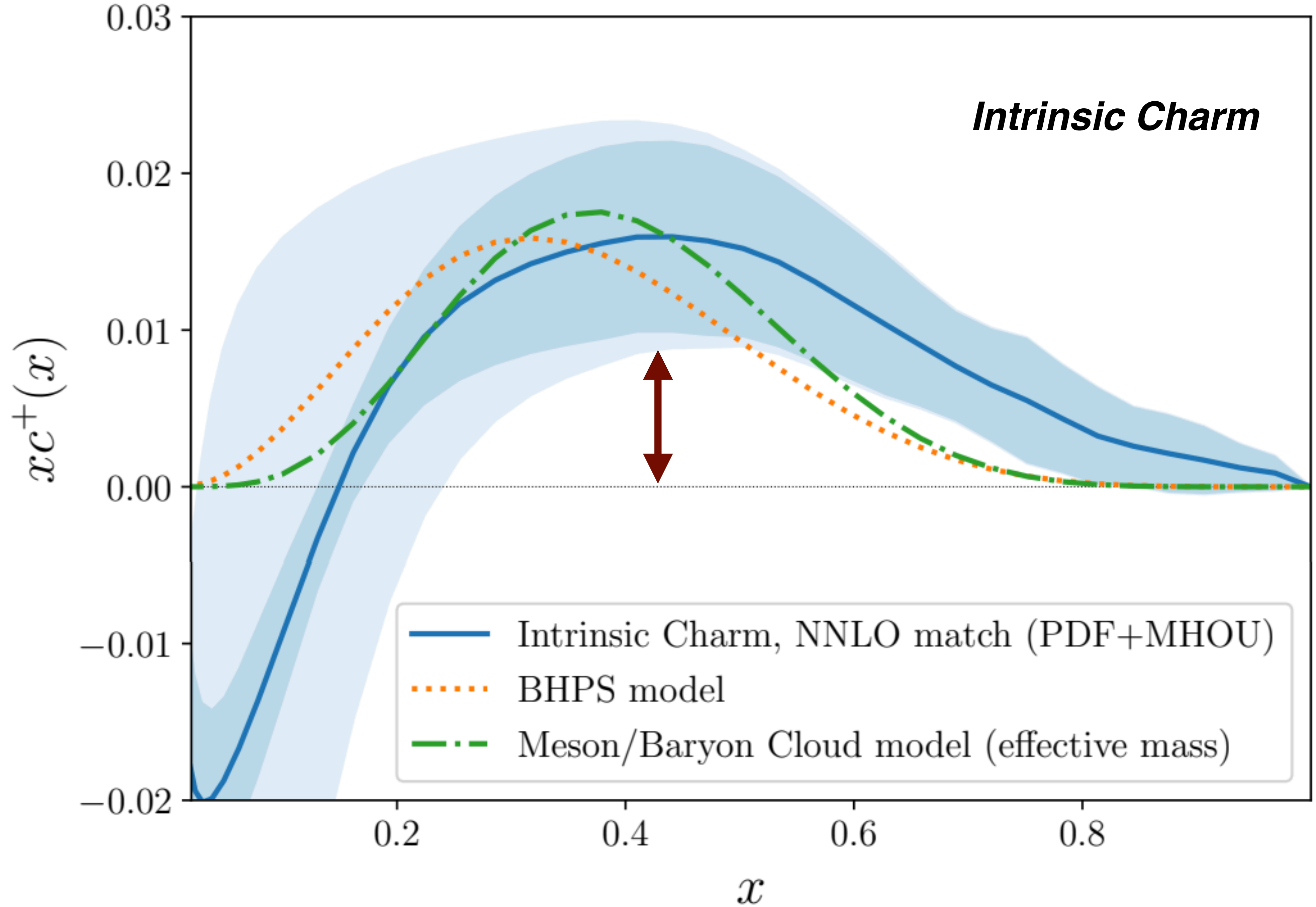
the proton contains **intrinsic up, down, strange (anti-)quarks** but **no intrinsic charm quarks**





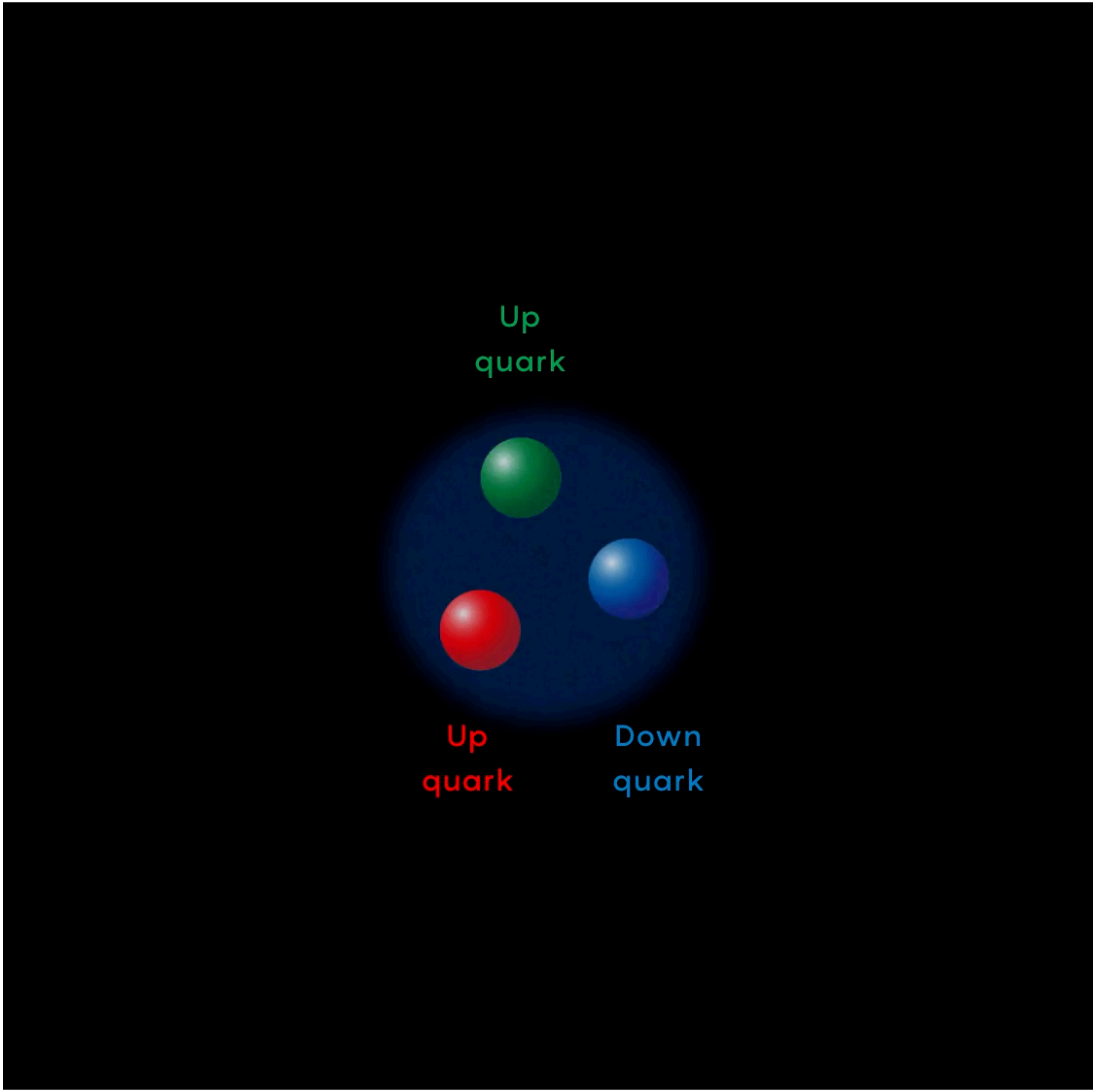
charm quarks heavier than the proton itself!

Intrinsic Charm in the Proton



The 3FNS charm PDF displays **non-zero component** peaked at large-*x* which can be identified with **intrinsic charm**

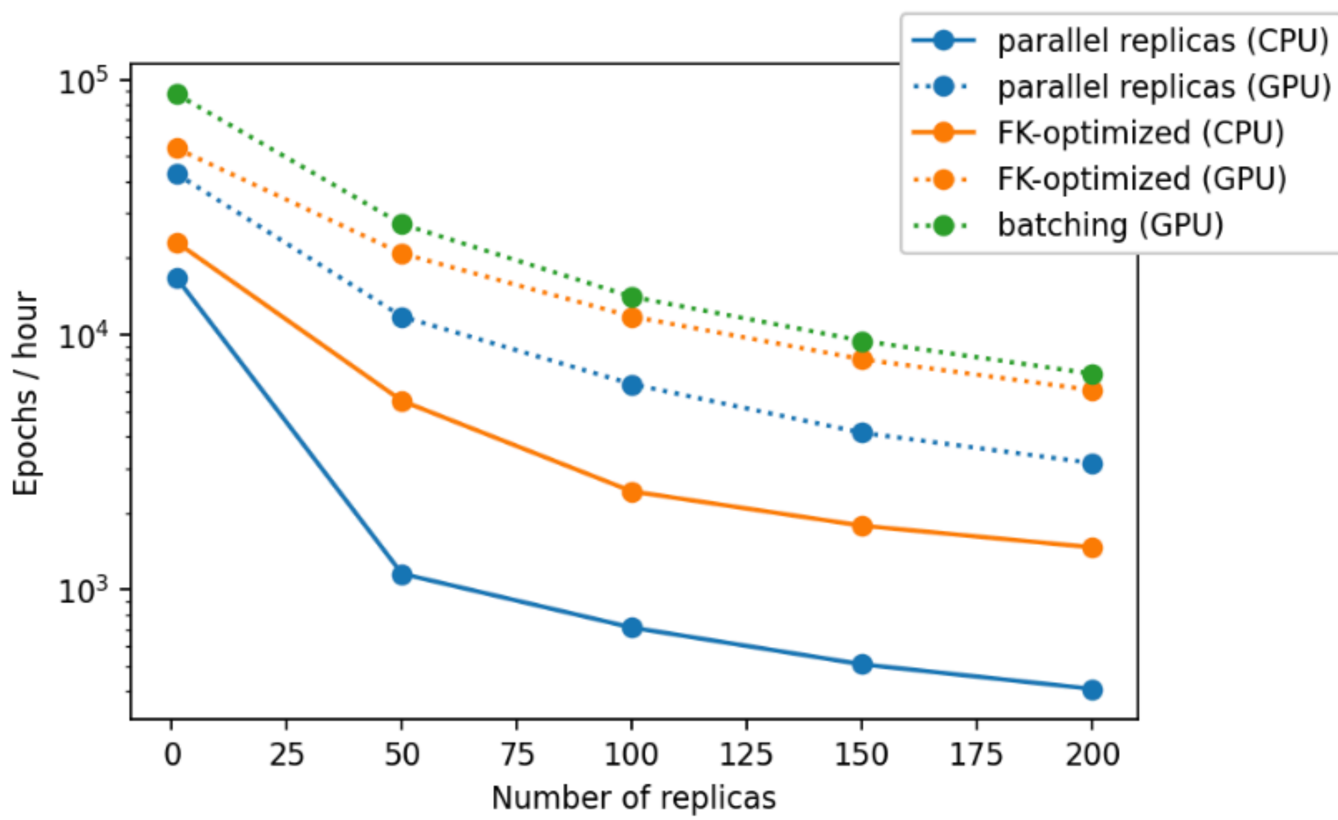
JR et al, Evidence for intrinsic charm quarks in the proton, ***Nature* (2022)**

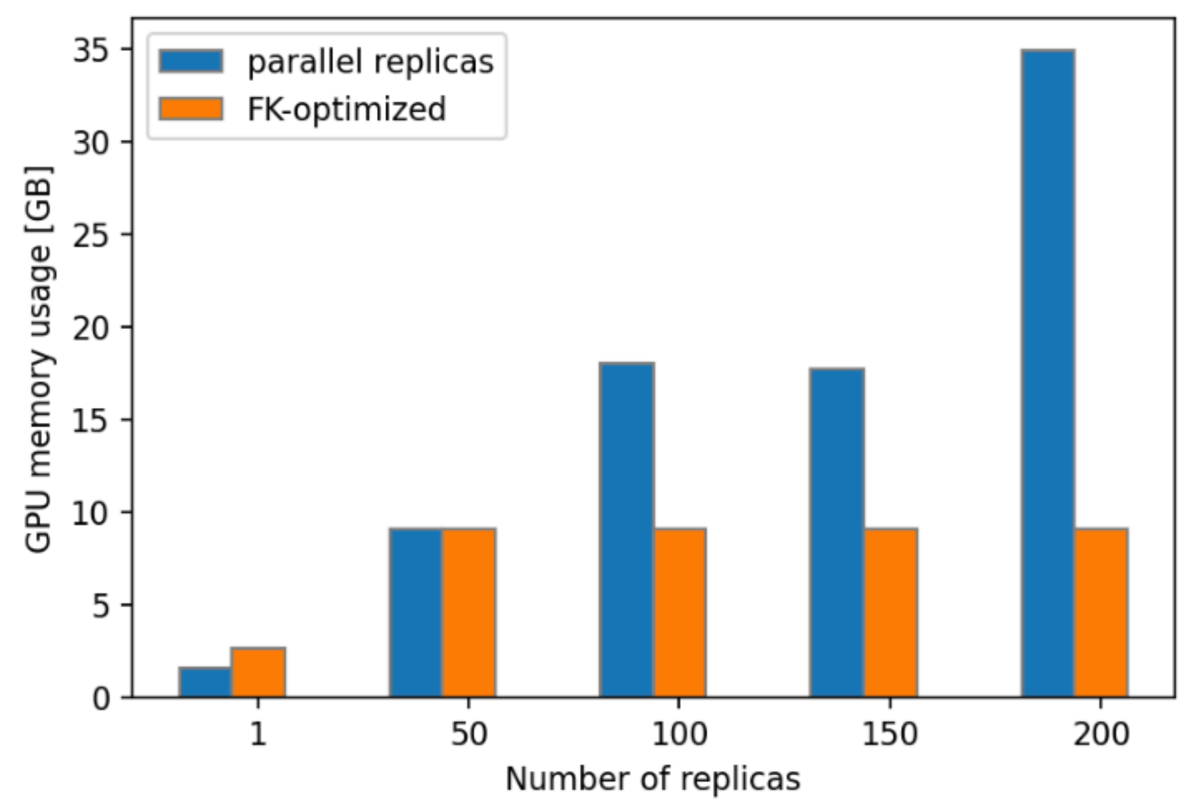


credits: https://www.quantamagazine.org/inside-the-proton-the-most-complicated-thing-imaginable-20221019/

GPU & Hyperparameter Optimisation

- Deploy NNPDF machinery on GPUs & optimise performance: **factor speed 200 improvement!**
- Also ensure CPU memory consumption keep reasonable
- Develop new strategies for **hyperparameter optimisation** based on the full posterior probability distribution, not only on first moment as most approaches





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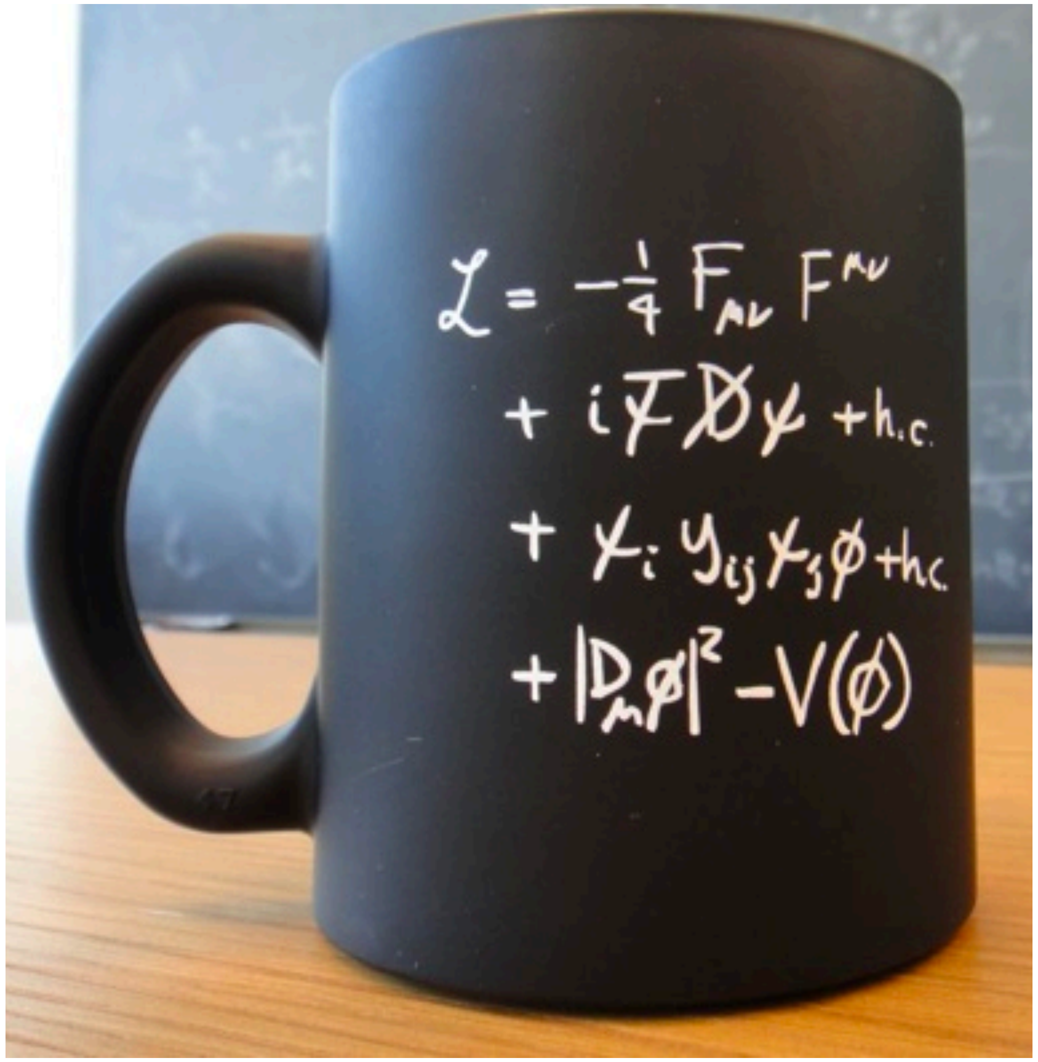
The Standard Model as an Effective Theory

The Standard Model EFT is defined by:

- **Particle (matter) content**: quarks and leptons
- **Gauge** (local) symmetries and their eventual breaking mechanisms
- **Lorentz** invariance and other global symmetries
- Linearly realised $SU(2)_L$ EW symmetry breaking
- **Validity only up to certain energy scale *Λ***



$$\mathcal{L}_{\text{SMEFT}}(\{c_i\}, \Lambda) = \mathcal{L}_{\text{SM}} + \sum_{d=5}^{\infty} \sum_{i=1}^{N_d} c_i^{(d)} \frac{\mathcal{O}_i^{(d)}}{\Lambda^{d-4}}$$

EFT coupling constants, to be determined from **data**

All possible operators of **mass-dimension *d*** consistent with above requirements

Statistically optimal observables from ML

Optimal observables depend on **all kinematic variables** and **all EFT coefficients**

$$r_\sigma(\boldsymbol{x}, \boldsymbol{c}) \equiv \frac{f_\sigma(\boldsymbol{x}, \boldsymbol{c})}{f_\sigma(\boldsymbol{x}, \boldsymbol{0})} = 1 + \sum_{j=1}^{n_{\rm eft}} r_\sigma^{(j)}(\boldsymbol{x}) c_j + \sum_{j=1}^{n_{\rm eft}} \sum_{k \geq j}^{n_{\rm eft}} r_\sigma^{(j,k)}(\boldsymbol{x}) c_j c_k$$

parametrised with **neural networks** trained to Monte Carlo simulations & benchmarked with exact calculations

$$\hat{r}_\sigma(\boldsymbol{x}, \boldsymbol{c}) = 1 + \sum_{j=1}^{n_{\rm eft}} \mathrm{NN}^{(j)}(\boldsymbol{x}) c_j + \sum_{j=1}^{n_{\rm eft}} \sum_{k \geq j}^{n_{\rm eft}} \mathrm{NN}^{(j,k)}(\boldsymbol{x}) c_j c_k$$

extendable to **arbitrary number** of kinematic variables and EFT coefficients: training can be parallelised

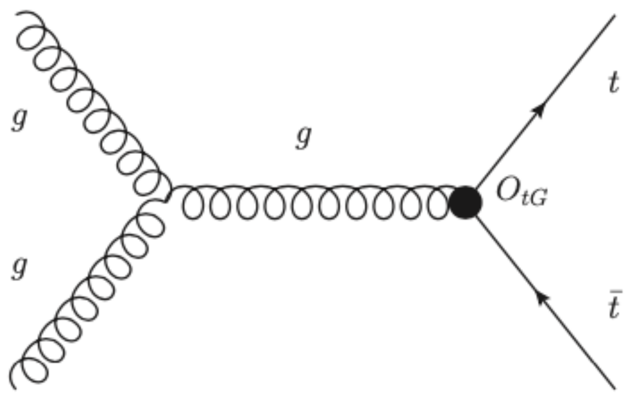
methodological uncertainties (e.g. finite training samples) assess with the **replica method**

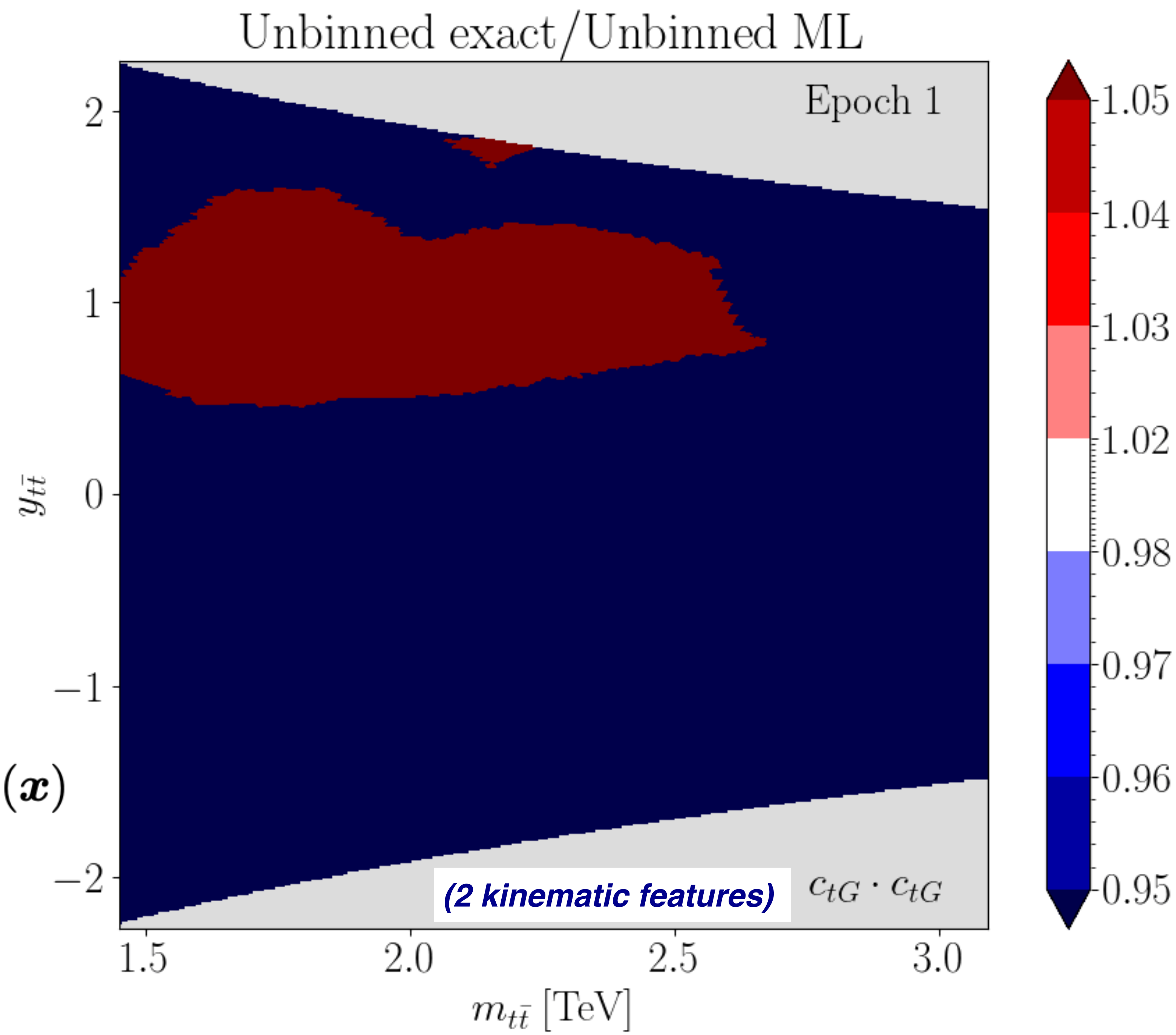
$$\hat{r}_\sigma^{(i)}(\boldsymbol{x}, \boldsymbol{c}) \equiv 1 + \sum_{j=1}^{n_{\rm eft}} \mathrm{NN}_i^{(j)}(\boldsymbol{x}) c_j + \sum_{j=1}^{n_{\rm eft}} \sum_{k \geq j}^{n_{\rm eft}} \mathrm{NN}_i^{(j,k)}(\boldsymbol{x}) c_j c_k \,, \qquad i = 1, \ldots, N_{\rm rep}$$

each replica trained to an independent set of MC events

representation of the probability distribution in the space of ML models

Neural network training





$$r_\sigma(\boldsymbol{x}, c_j^{(\mathrm{tr})}, c_k^{(\mathrm{tr})}) = 1 + c_j^{(\mathrm{tr})} c_k^{(\mathrm{tr})} \mathrm{NN}^{(j,k)}(\boldsymbol{x})$$

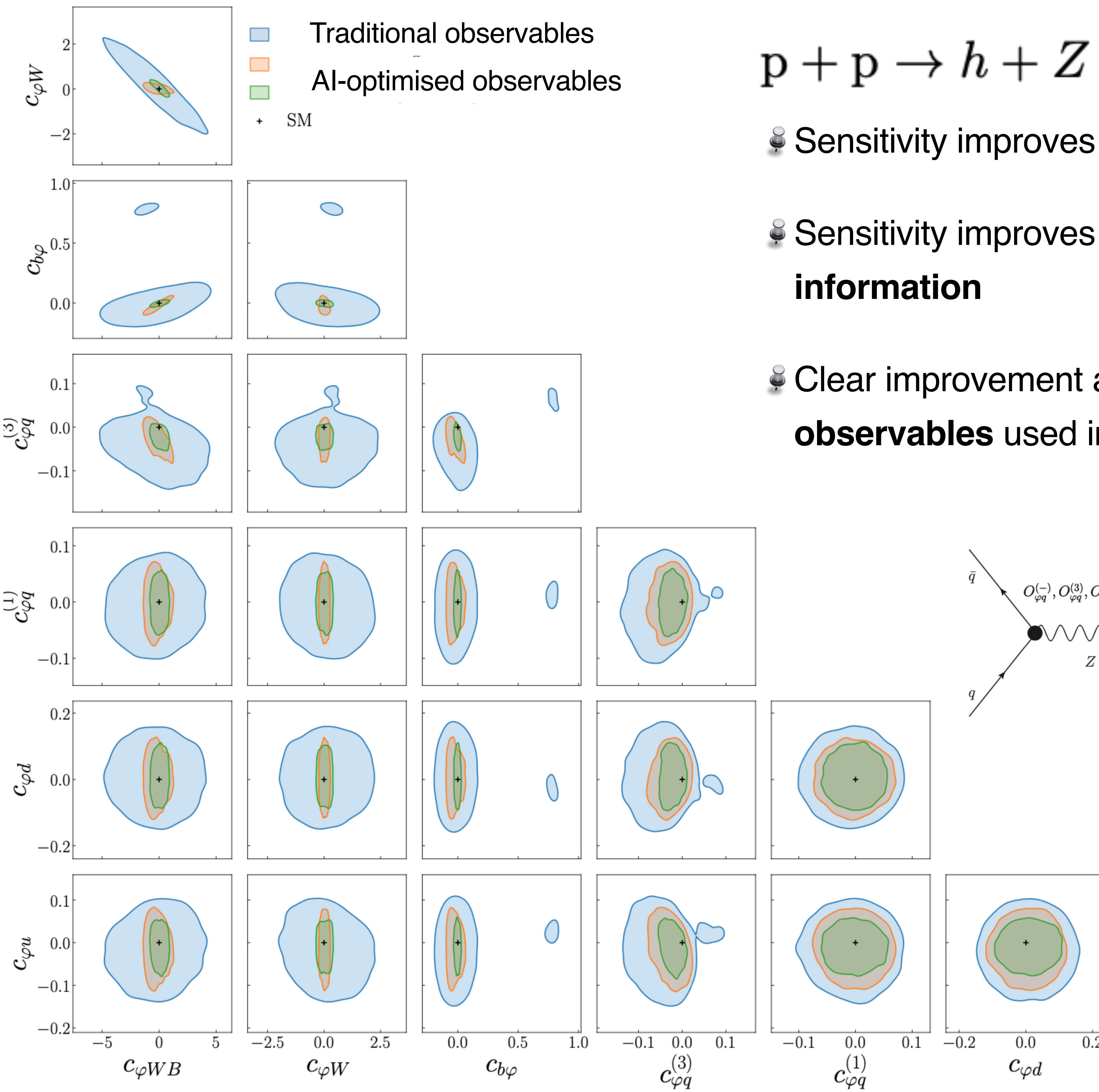
$$\boldsymbol{x} = (m_{t\bar{t}}, y_{t\bar{t}})$$

NN training by minimising cross-entropy loss function

$$L[g(\boldsymbol{x}, \boldsymbol{c})] = -\sigma_{\mathrm{fid}}(\boldsymbol{c}) \sum_{i=1}^{N_{\mathrm{ev}}} \log(1 - g(\boldsymbol{x}_i, \boldsymbol{c})) - \sigma_{\mathrm{fid}}(\boldsymbol{0}) \sum_{j=1}^{N_{\mathrm{ev}}} \log g(\boldsymbol{x}_j, \boldsymbol{c}) \qquad g = (1 + r_\sigma)^{-1}$$

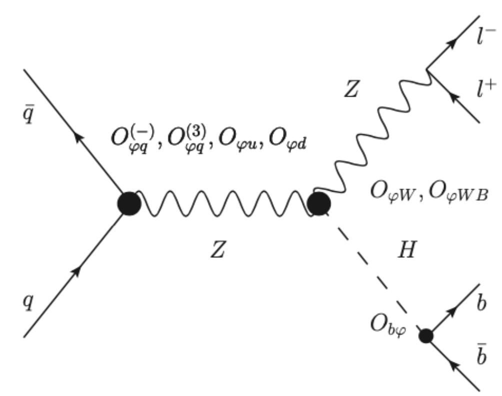
Results: Higgs+Z production

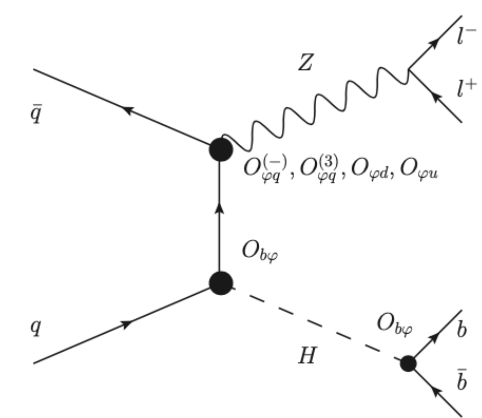
Marginalised 95 % C.L. intervals, $\mathcal{O}\left(\Lambda^{-4}\right)$ at $\mathcal{L} = 300\ \text{fb}^{-1}$



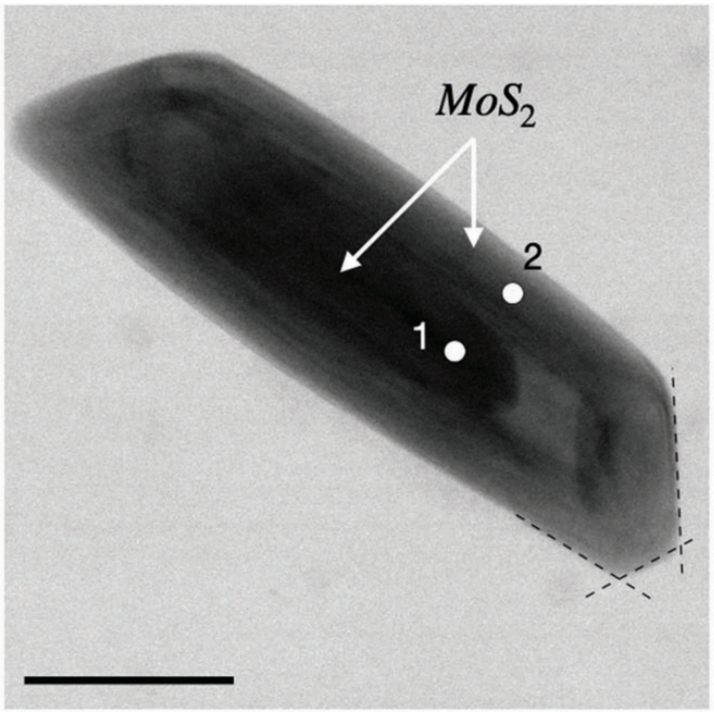
$$\mathrm{p} + \mathrm{p} \to h + Z \to b + \bar{b} + \ell^{+} + \ell^{-}$$

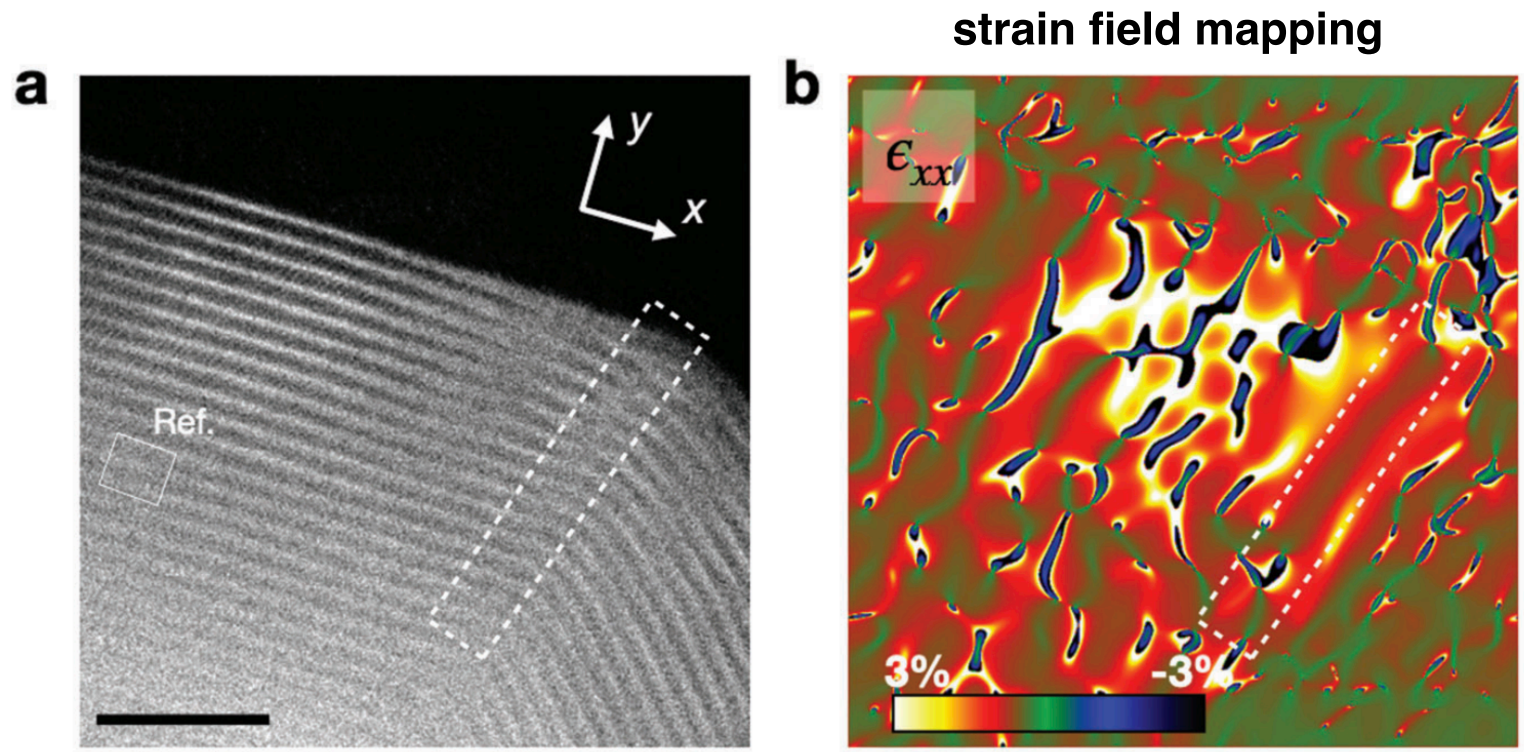
- Sensitivity improves in **unbinned analysis**
- Sensitivity improves when **using all kinematic information**
- Clear improvement as compared to **traditional observables** used in EFT fits

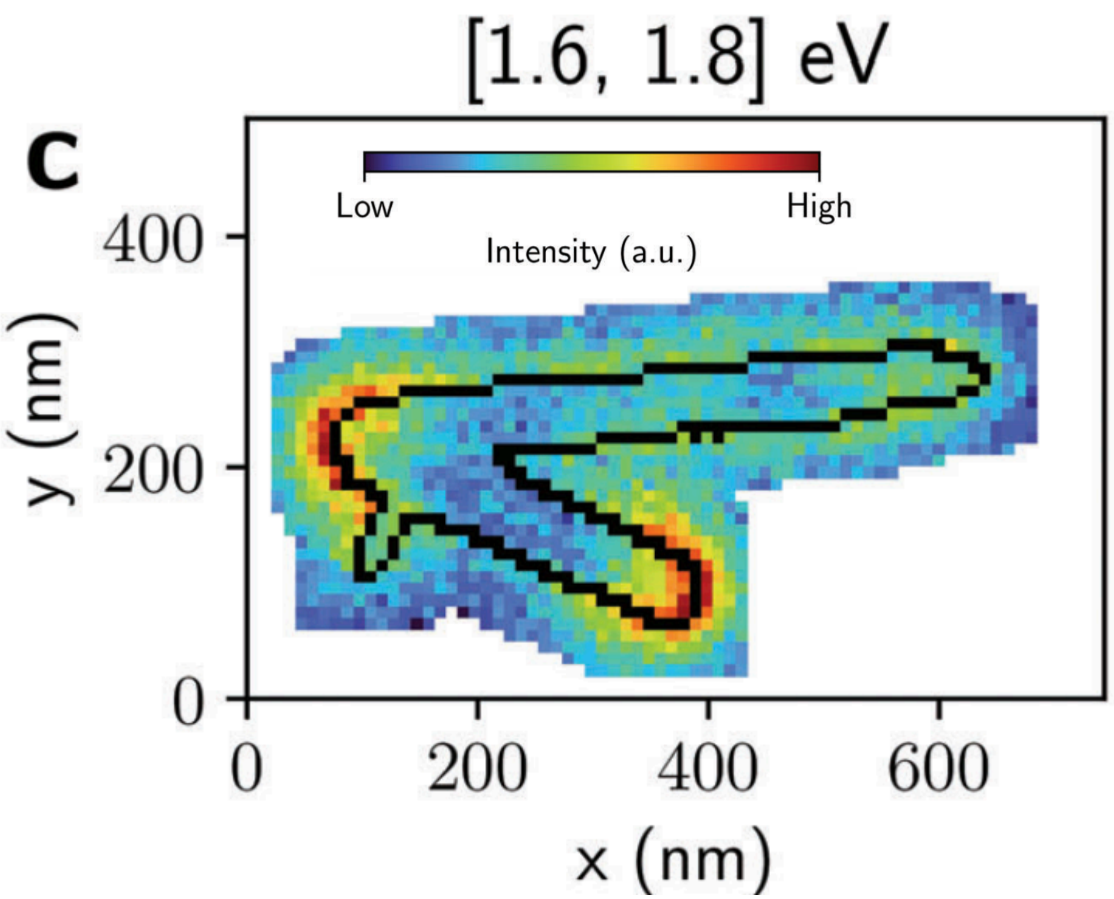




Applications to Material Science







- ☑ Background subtraction & anomaly detection problems from HEP arise also in material spectroscopy
- ☑ Direct correlation of **strain fields, band gap modulation, and exciton localisation** in 1D-MoS_2 nanostructures with different morphologies
- ☑ Developed EELSfitter ML framework together with TU Delft researchers

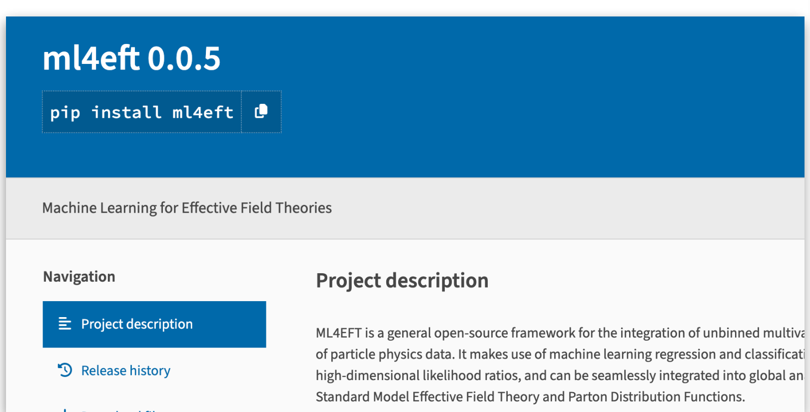
Summary and outlook

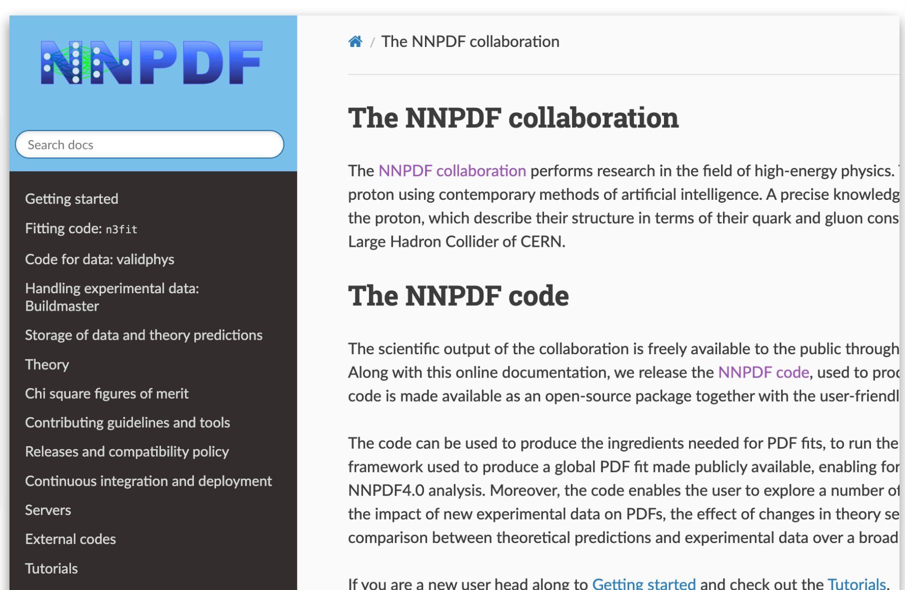
- Machine learning makes possible **identifying patterns in the data** whereby one can efficiently solve problems which are difficult of intractable with traditional approaches

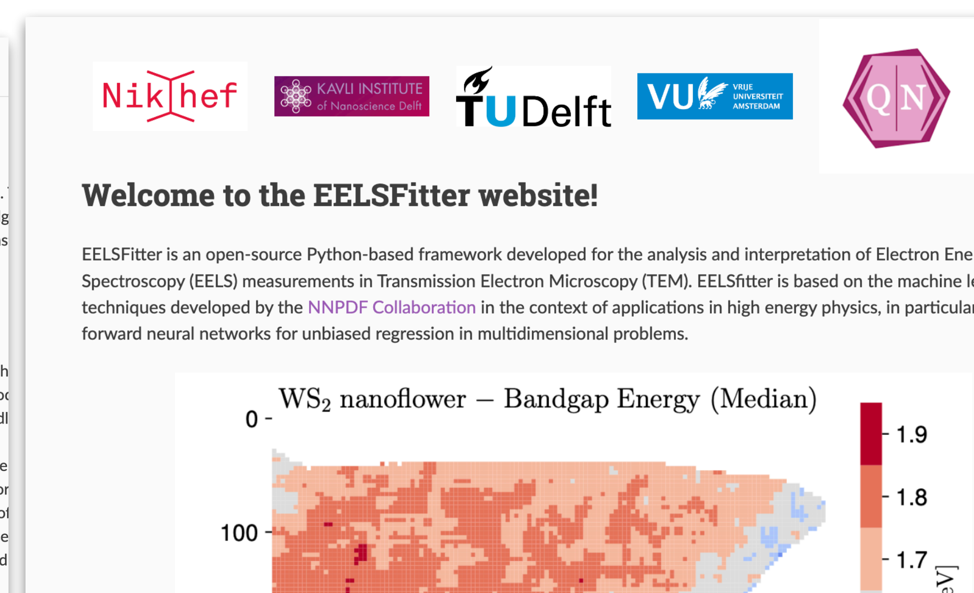
- **Enable discoveries** such as intrinsic charm quarks in the proton & make possible to **optimise the sensitivity of searches** for interesting phenomena hidden in the data

- Our technology is portable to many other problems, as demonstrated for their applicability to data analysis in **electron microscopy of quantum materials**

- Codes are **open source** and extensively documented, and have benefitted from contributions as well from BSc and MSc students in our groups







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Peter

Jaco

Giacomo

Tanjona

Tommaso