Exploring the nature of matter

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Christopher Newport U. & Jefferson Lab

Colloquium at
Old Dominion University
29 October 2024

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Outline

- **Intro: what are we made of?** (And how do we know?)
  - Quarks & gluons
  - Quantum Chromodynamics (QCD)
  - Color confinement

- **Dynamical mass generation**
  - How are massive particles created out of nearly massless quarks?

- **Parton Distributions Functions (PDFs) in the proton**
  - Quark and gluons at the "edge of confinement"
  - Global QCD analysis

    ⟶ Theory + Experiment + Data/Computer Science

- **Perspectives**

Acknowledgments

- **My CTEQ-JLab (CJ) collaboration colleagues:**
  - **Matteo Cerutti** (CNU)**, Xiaoxian Jing** (Meta), **Ishara Fernando** (UVa), W.Melnitchouk (JLab), J.F.Owens (Florida State U.)
  - C.E. Keppel & Sanghwa Park (JLab), **Shujie Li** (LBL), P. Monaghan (CNU)

- **My other collaborators:**
  - **C. Costa, A. Simonelli** (JLab), A. Bacchetta (Pavia U., Italy), **A. Krause** (ODU), A. Signori (Torino U., Italy)
  - **[nCTEQ]** F. Olness (Southern Methodist U.), R. Ruiz (Cracow, Poland), I.Schienbein (Grenoble)

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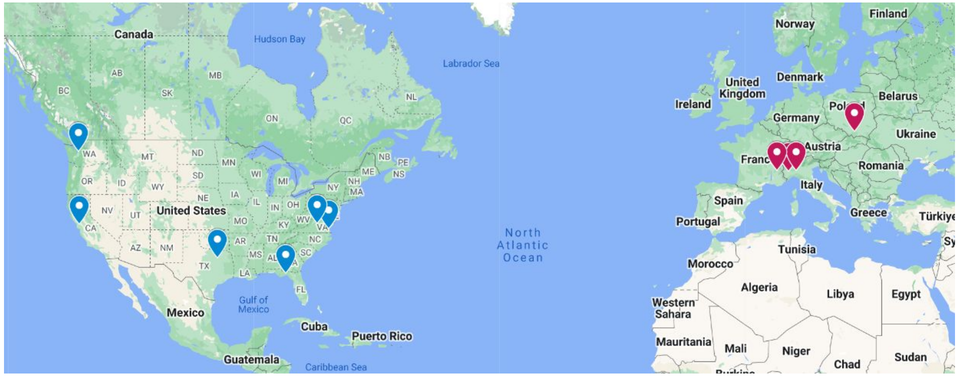
  - DE-AC05-06OR23177 (JLab theory)
  - APS-Simons travel grant

- **Artwork:** Bernhard Musch (2009)
  Scattering discussion: R. Ruiz (2024)



General References

QCD global analysis from protons to nuclei:

- **Accardi,** *PoS DIS2015 (2015) 001*
- **Jimenez-Delgado, Melnitchouk, Owens,** *J.Phys.G40 (2013) 093102*
- **Ethier, Nocera,** *Ann.Rev.Nucl.Part.Sci. (2020) 70, 1-34*

QCD global analysis and statistical methods:

- **Kovarik, Nadolsky, Soper,** *Rev.Mod.Phys. 92 (2020) 4, 045003*
- **Buckley, White and White,** "Practical Collider Physics", IOP publishing 2021

References - technical

Inclusive Jet functions & dynamical mass generation

- **Accardi, Costa, Signori,** *Phys.Rev.D 108 (2023) 114011*
- **Accardi, Signori,** *Phys.Lett.B 798 (2019) 134993* & *Eur.Phys.J.C 80 (2020) 825*
- **Accardi, Bacchetta,** *Phys.Lett.B 773 (2017) 632*

Large-x fits with nuclear corrections & applications

- **CJ15:** Accardi et al., *PRD 93 (2016) 114017*
    - Accardi, DNP 2020 / Fernando, GHP 2021 / Accardi, APS 2022
- **$F_2(n)$:** Li, Accardi et al., *Phys.Rev.D 109 (2024) 074036*

Light quark asymmetry fits

- **CJ15a:** Accardi, Owens, Melnitchouk, *Phys.Lett.B 801 (2020) 135143*
- **CJ22:** Accardi, Jing, Owens, Park, *Phys.Rev.D 107 (2023) 113005*

PDF uncertainties

- **Hunt-Smith, Accardi, Melnitchouk, Sato, Thomas, White,** *Phys.Rev.D 106 (2022) 036003*

References - recent and in prep.

Inclusive Jet functions & dynamical mass generation

- Simonelli, Accardi, Cerutti, Costa, Signori
  "Unveiling the Collins-Soper kernel in inclusive DIS at threshold"
  - Rigorous QCD factorization with jet functions

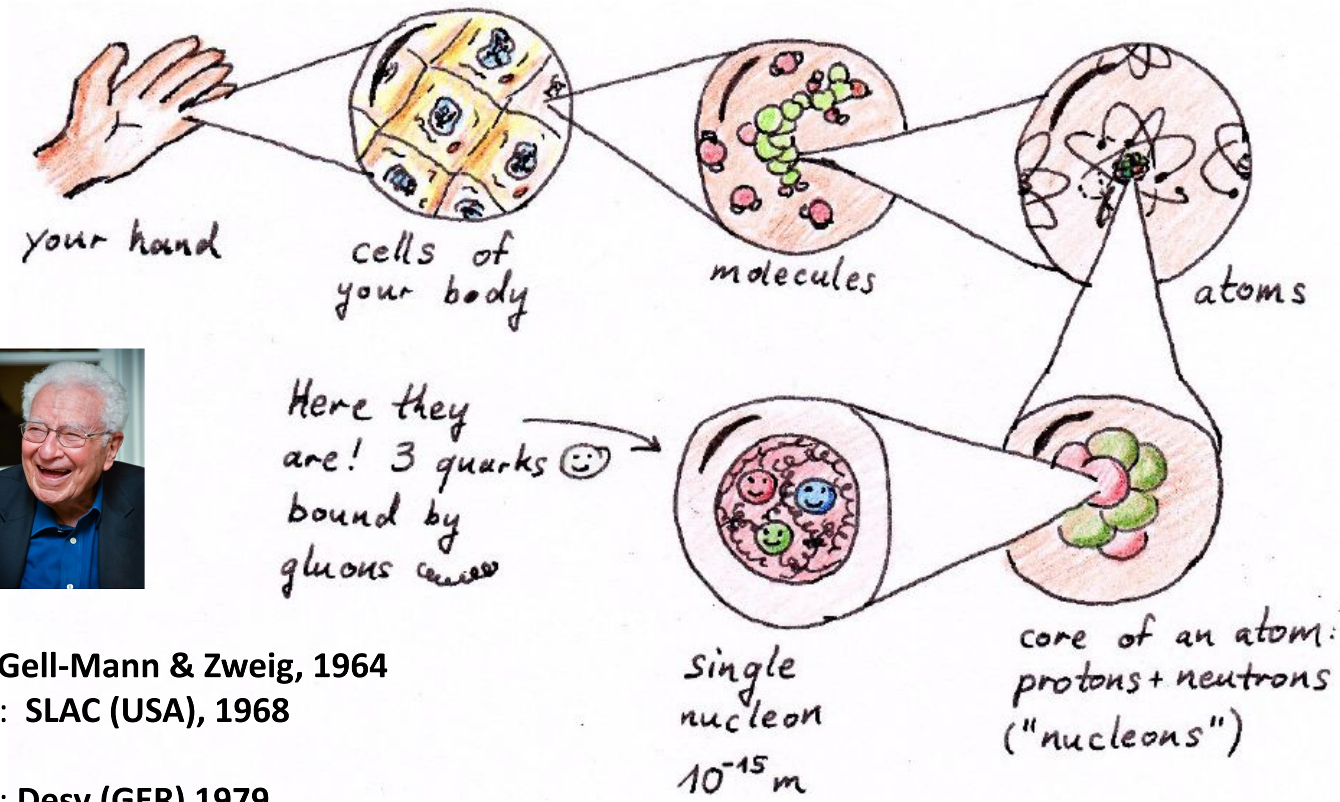
Large-x fits with power and nuclear corrections & applications

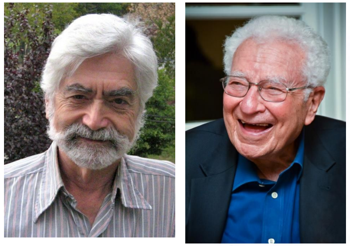
- Accardi, Cerutti, Fernando, Li, Owens, Park
  "Interplay of off-shell and higher-twist corrections in DIS at large x"
  - Non negligible QCD analysis systematic effects
  - Short version @ DIS 2024: *arXiv:2407.03589*
- Accardi, Krause
  "Testing large-x QCD analysis in a spectator model"

Introduction:
What are we made of?

What are we made of?

- **Quarks and gluons!**



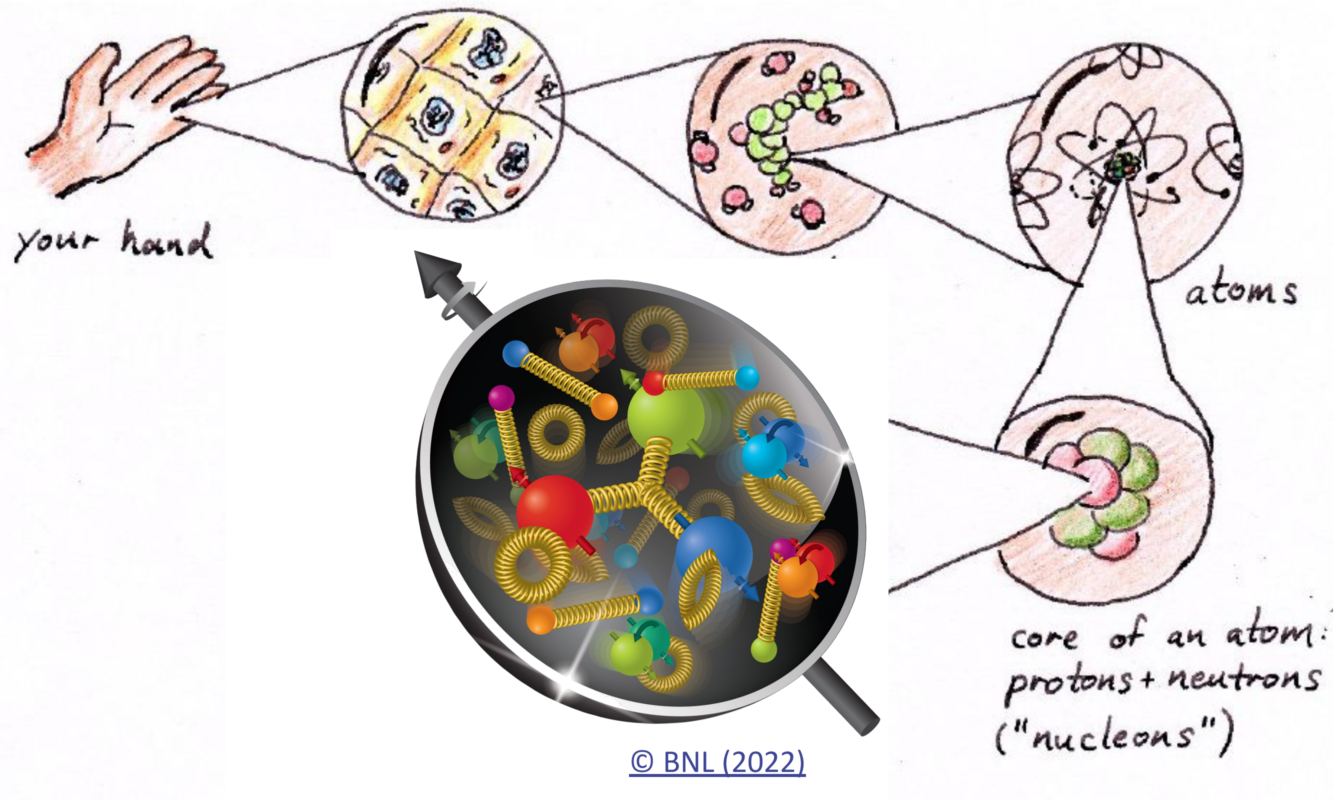


Quarks:
proposed: **Gell-Mann & Zweig, 1964**
discovered: **SLAC (USA), 1968**
Gluons:
discovered: **Desy (GER) 1979**

E. Rutherford, 1897, 1917

What are we made of?

- **Quarks and gluons!**



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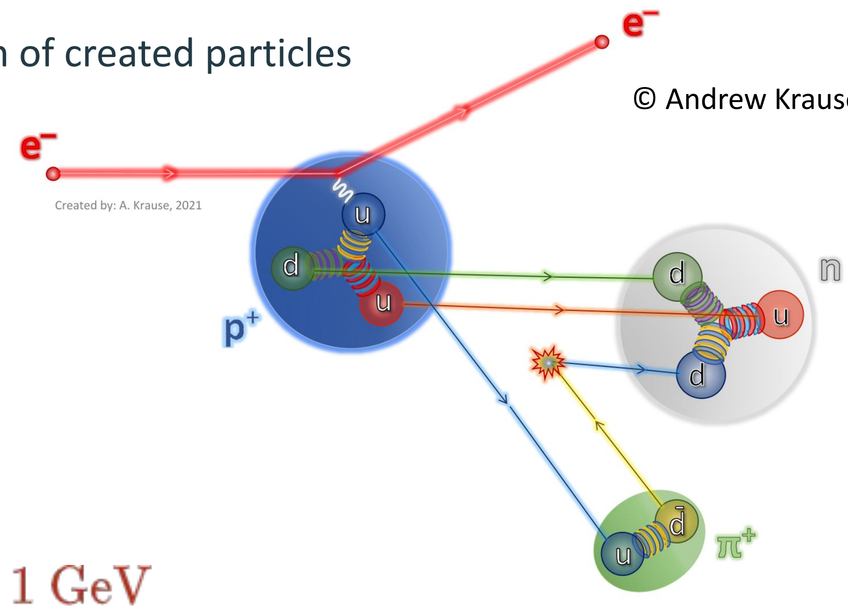
How do we know?

- **By using high-energy scattering as a microscope!** (actually, a femtoscope)
  - And also looking at the spectrum of created particles



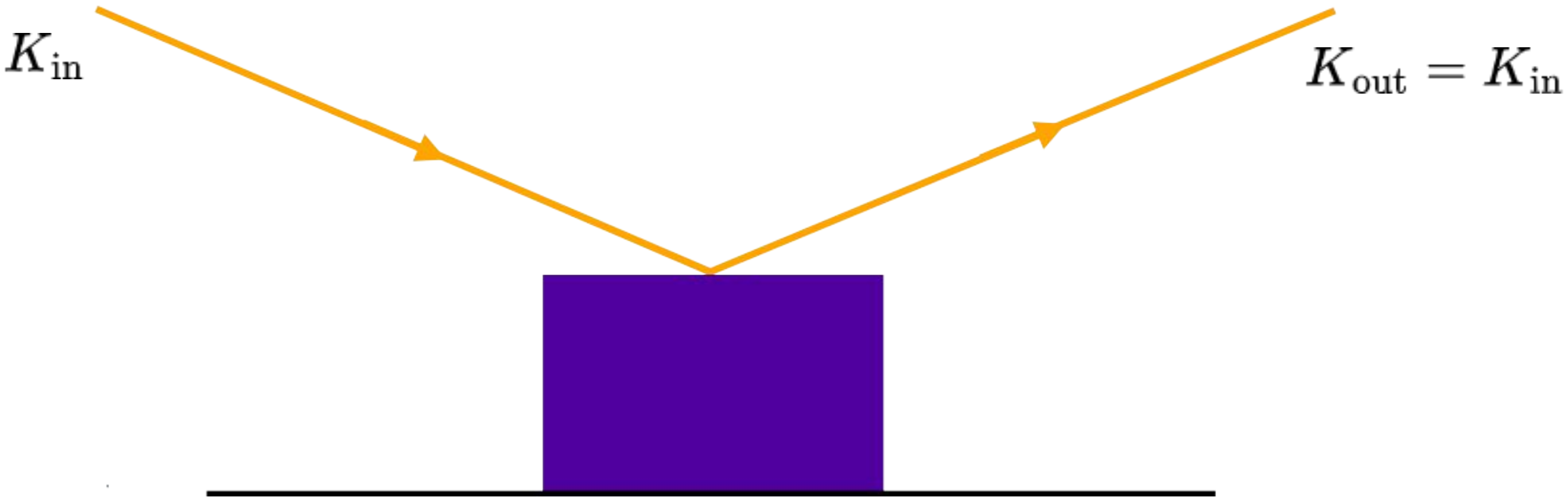
- Need a wavelength smaller than the proton's size:

$$\lambda \approx \frac{hc}{E} < 10^{-15}\ \mathrm{m}$$

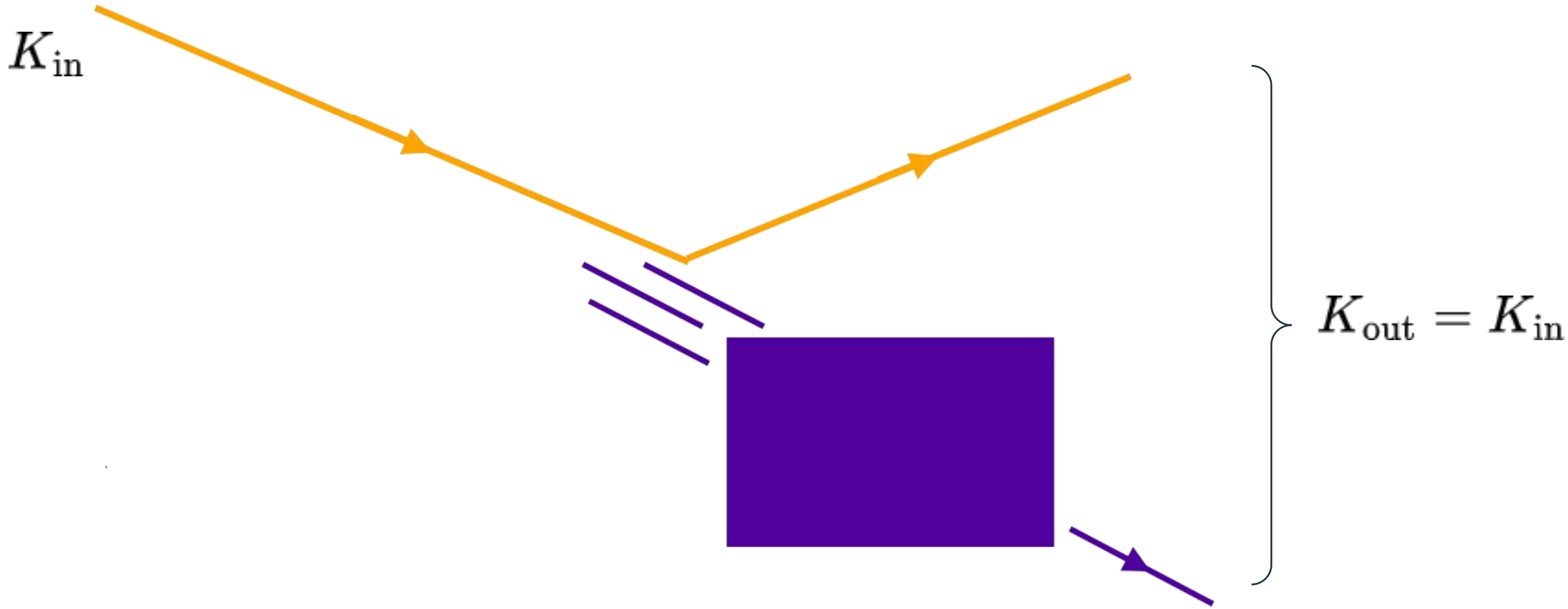
$$\Longrightarrow E > 1\ \mathrm{GeV}$$

1 eV =10^{-19} J : energy needed to move an electric of charge e = 10^{-19} C through a potential difference of 1 V

Scattering 101: elastic

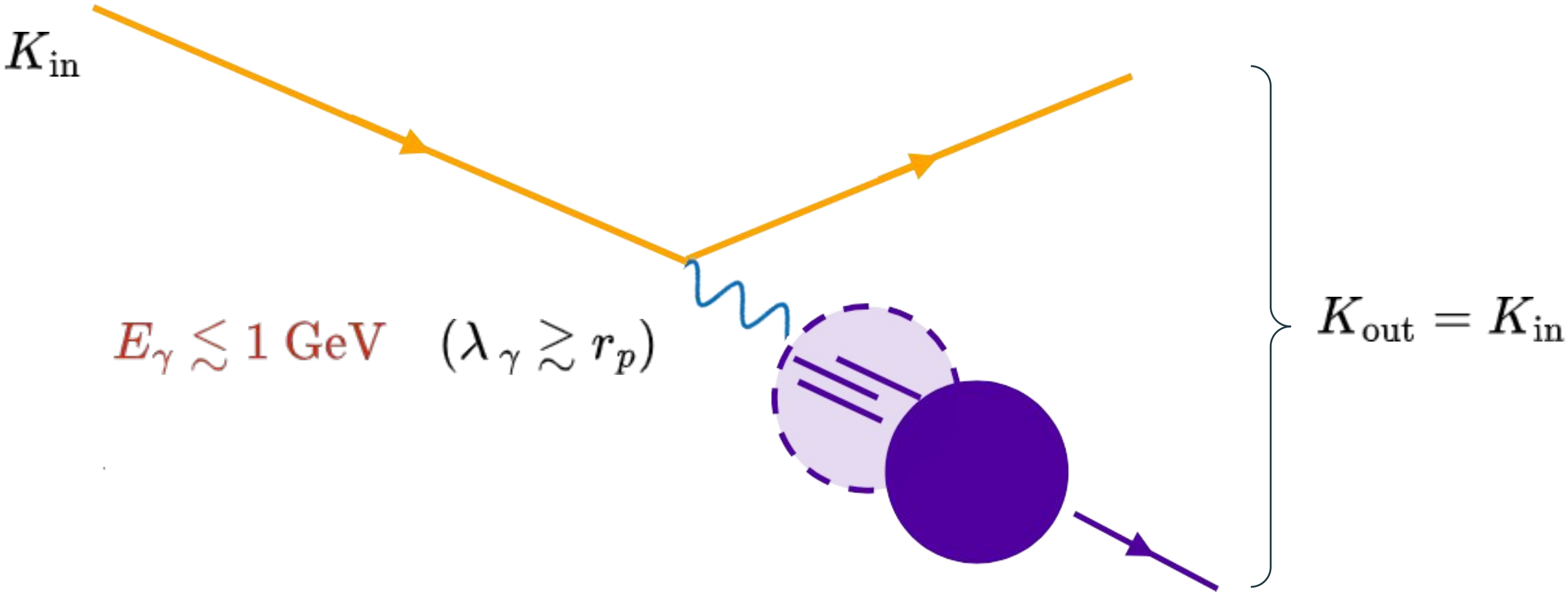


Scattering 101: elastic



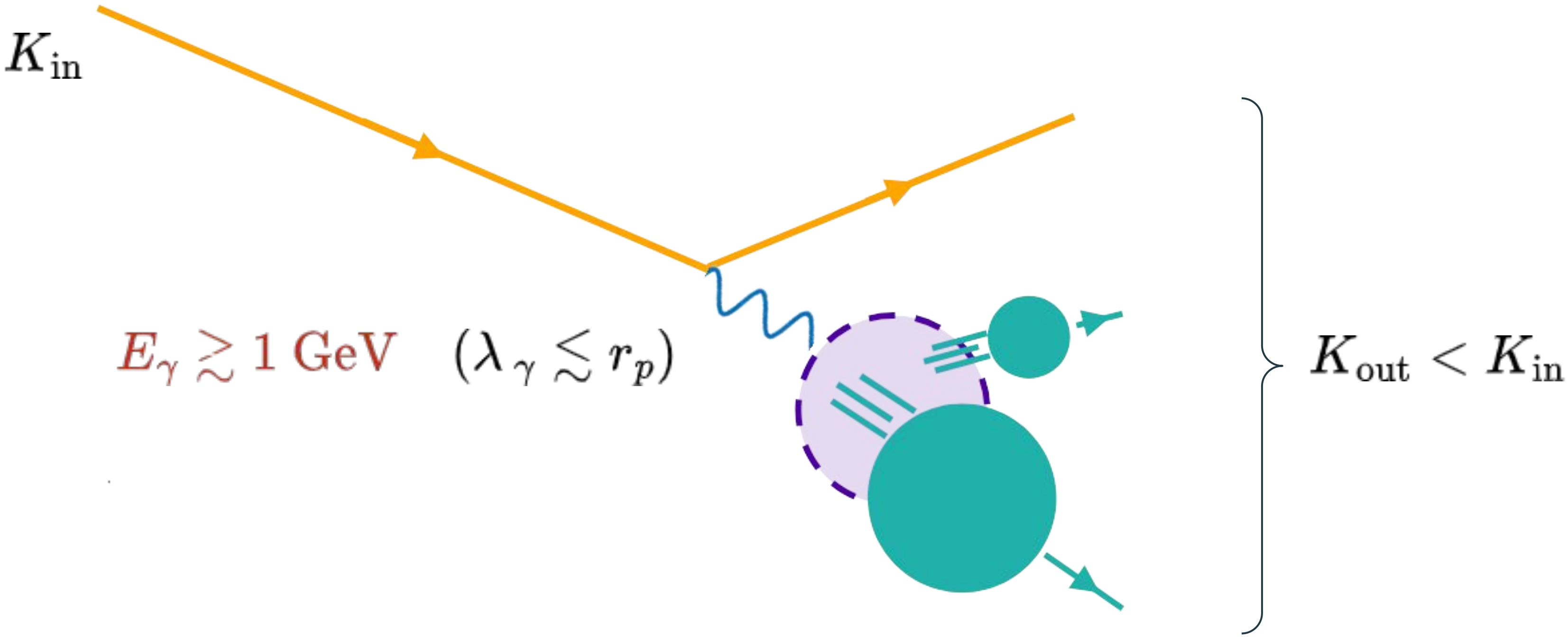
Electron-proton: elastic

- Exchanged photon wavelength: $\lambda_\gamma = h/p_\gamma \approx hc/E_\gamma$



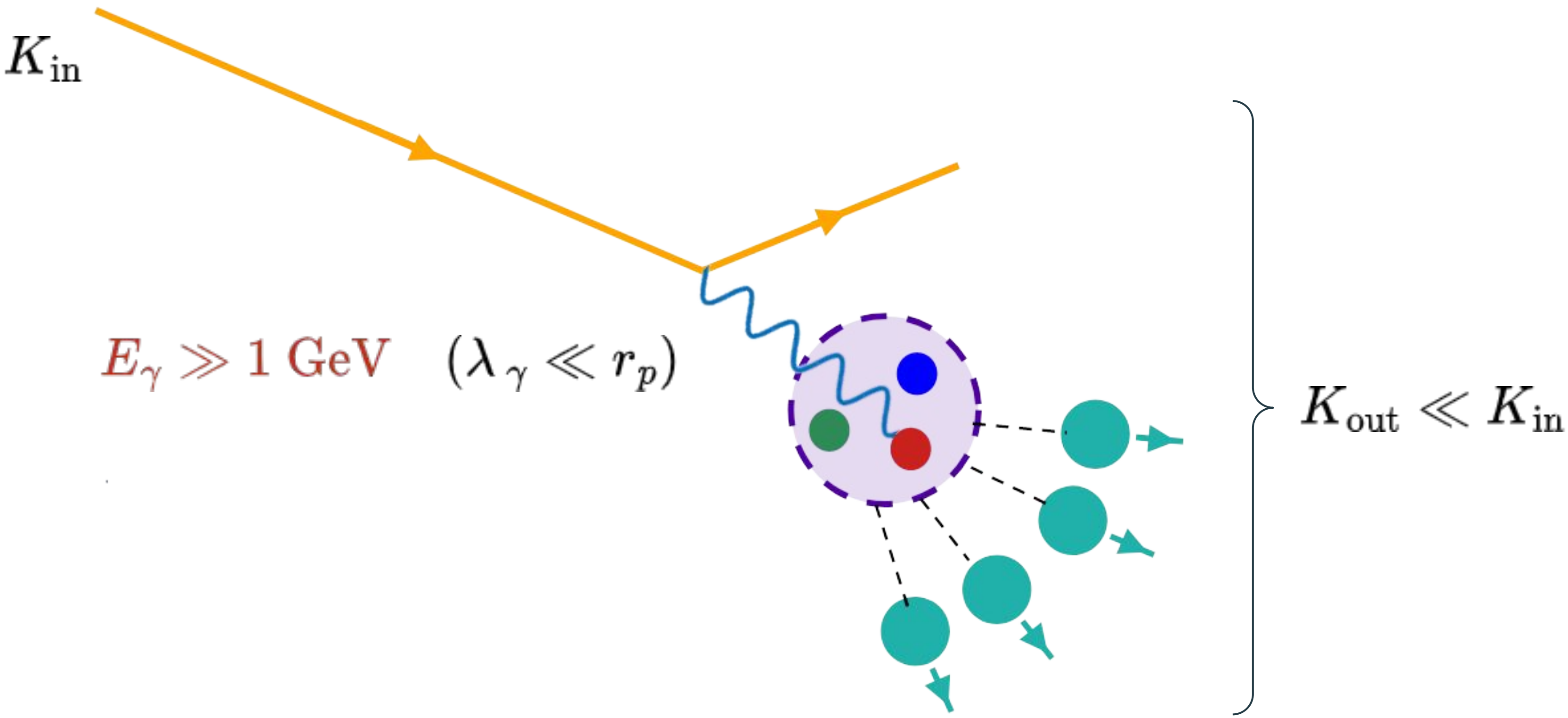
Electron-proton: inelastic

- Exchanged photon wavelength: $\lambda_\gamma = h/p_\gamma \approx hc/E_\gamma$



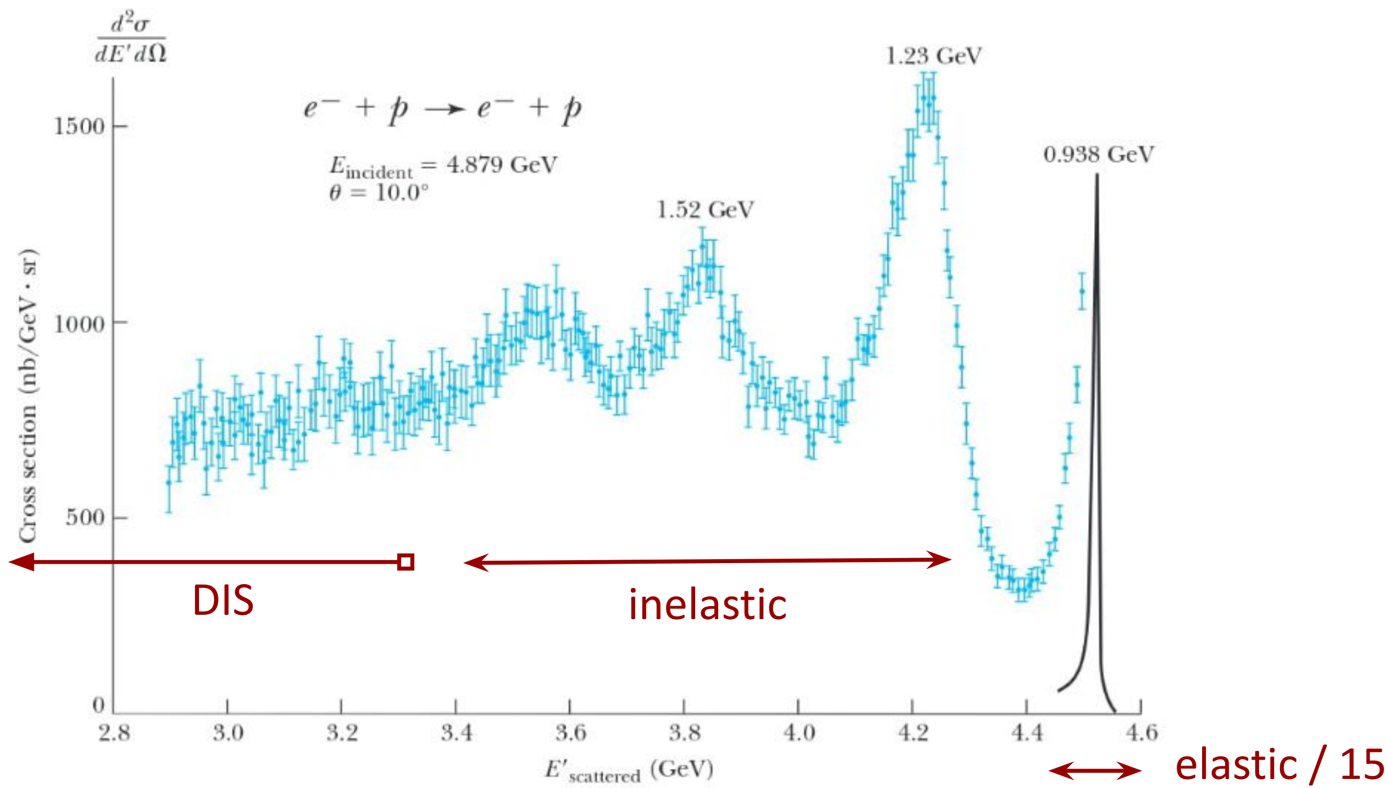
Electron-proton: deeply inelastic scattering (DIS)

- Exchanged photon wavelength: $\lambda_\gamma = h/p_\gamma \approx hc/E_\gamma$



Cross section

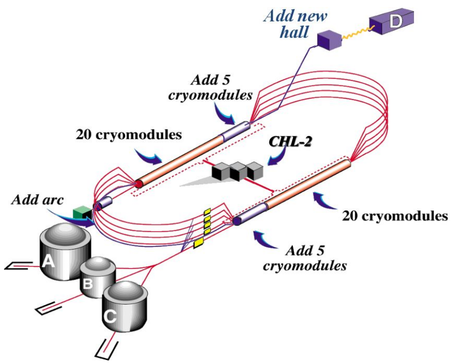
- Roughly, the probability that the electron hits the target



Bartel et al., Physics Letters B 28, 148 (1968)

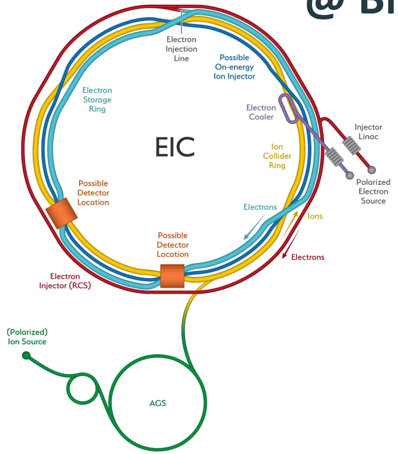
Modern particle accelerators

JLab 12 GeV



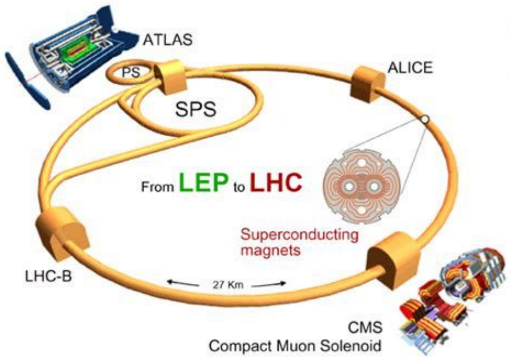
e (12 GeV) ⟶ proton

Electron-Ion Collider @ BNL



e (10 GeV) ⟶ ⟵ (275 GeV) p

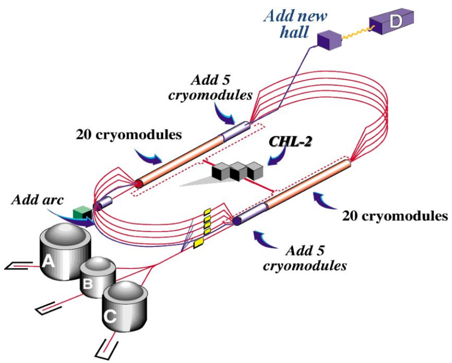
Large Hadron Collider @ CERN



p (7000 GeV) ⟶ ⟵ (7000 GeV) p

Modern particle accelerators

JLab 12 GeV



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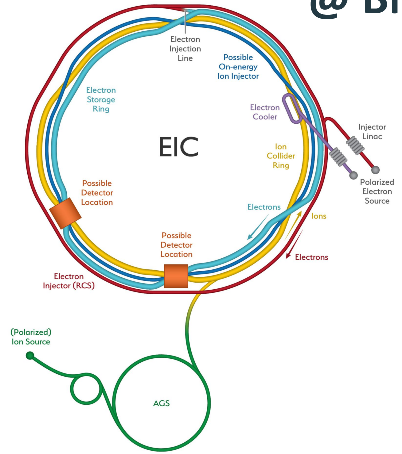
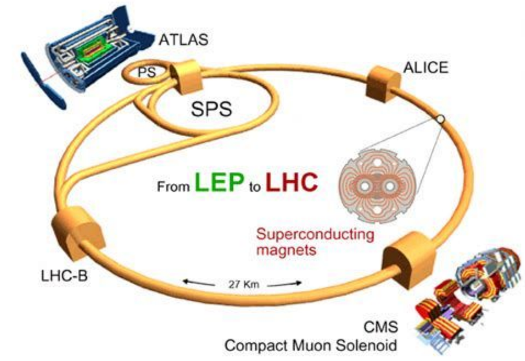
Electron-Ion Collider @ BNL

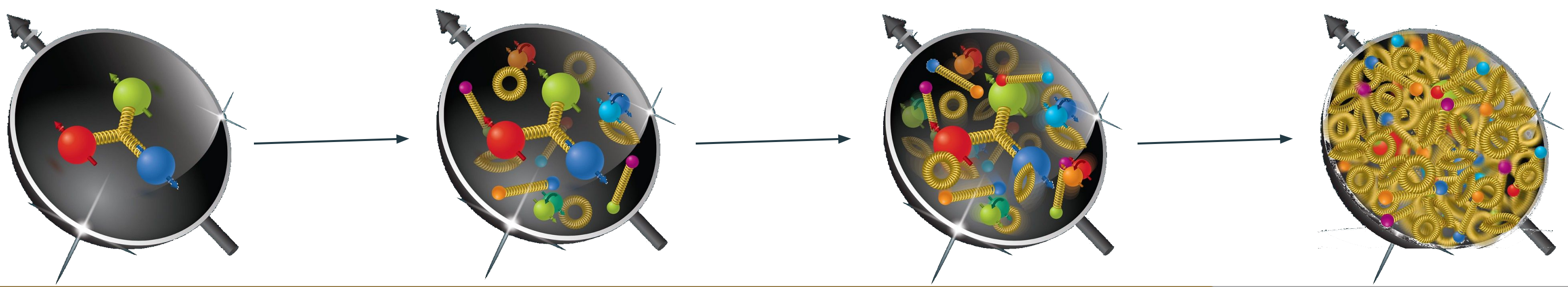


e (10 GeV) ⟶ ⟵ (275 GeV) p

Large Hadron Collider @ CERN

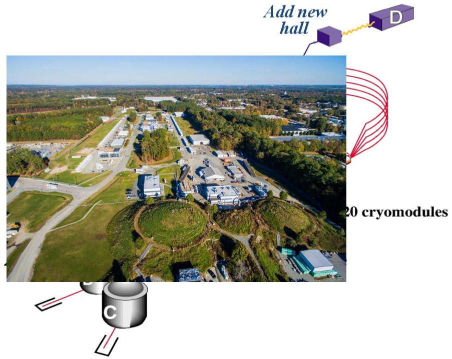


p (7000 GeV) ⟶ ⟵ (7000 GeV) p



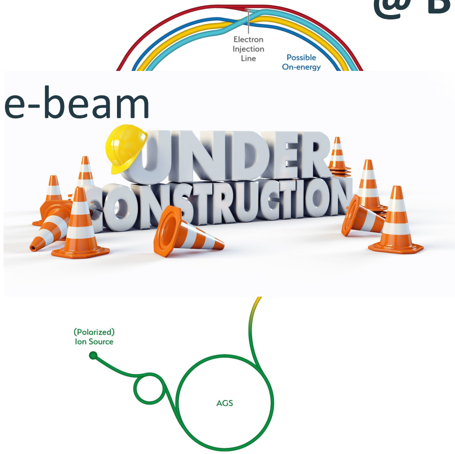
Modern particle accelerators

JLab 12 GeV



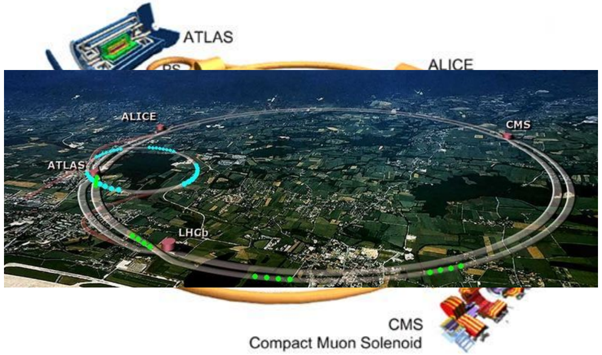
e (12 GeV) ⟶ proton

Electron-Ion Collider @ BNL

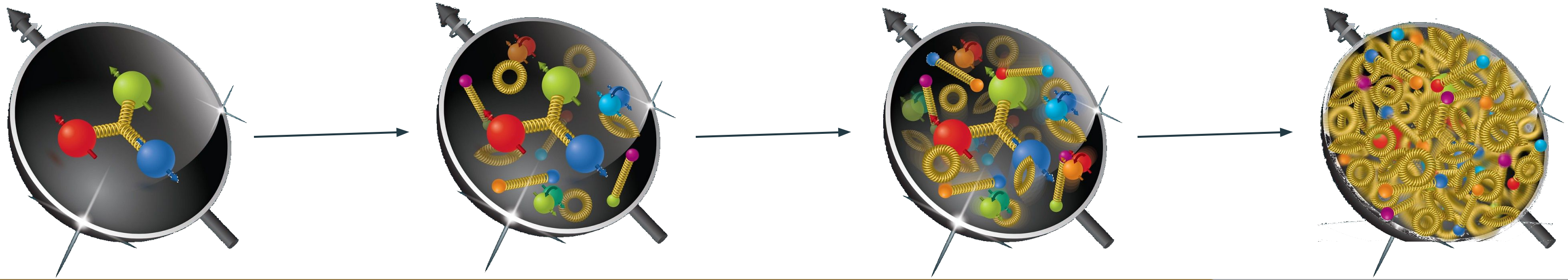


e (10 GeV) ⟶ ⟵ (275 GeV) p

Large Hadron Collider @ CERN

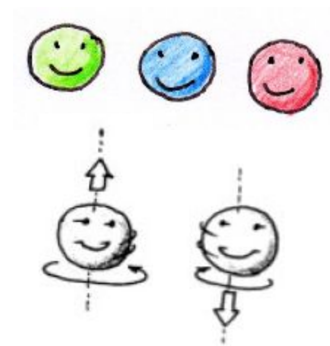


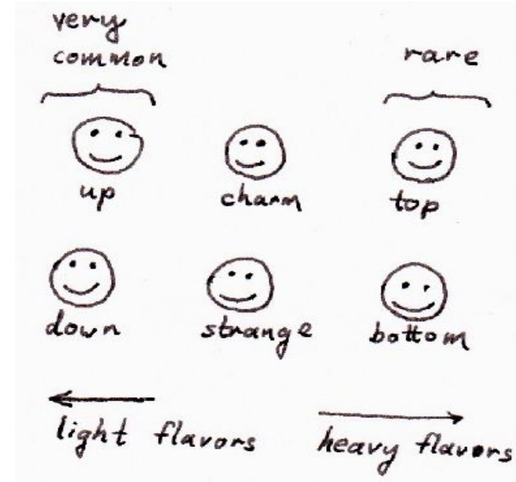
p (7000 GeV) ⟶ ⟵ (7000 GeV) p



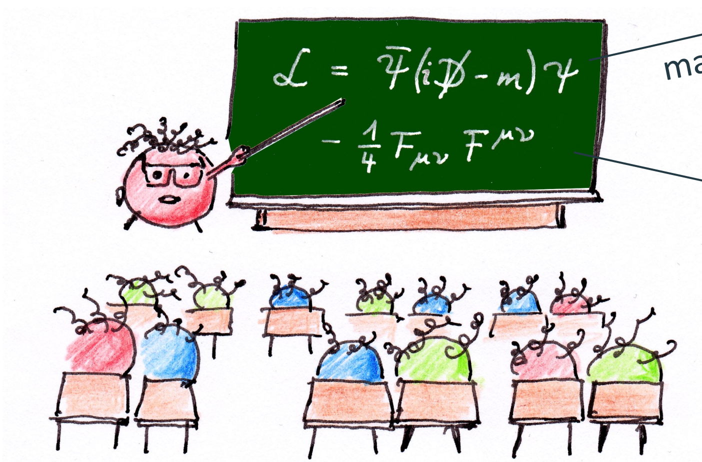
Quantum Chromodynamics (QCD)

- **Simple rules**
  - **Matter** = quarks + antiquarks:
    ⟶ 3 colors, 6 flavors, spin = ± ½
  - **Interaction** = exchange of gluons





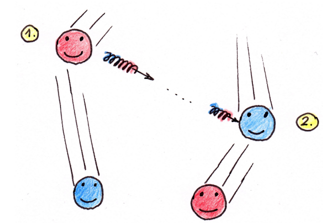
- **“Lagrangian”:** contains the theory

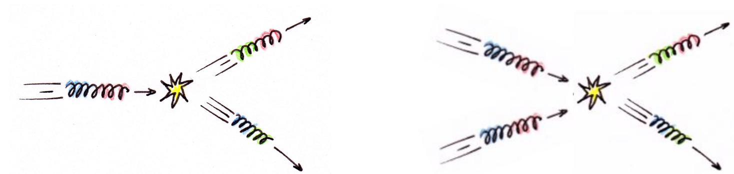


matter: $\psi, \bar{\psi}$

interactions: $\not{D}$

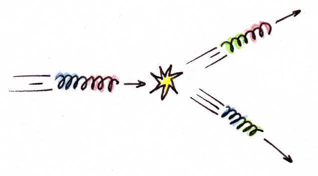
$F_{\mu\nu}$

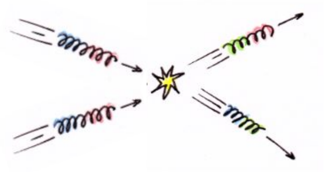




Unlike any other fundamental theory!

- QCD is analogous to electromagnetism, but:
  - **gluons can split…**
  - **…and bang on each other**
    (no linear superposition principle!!)

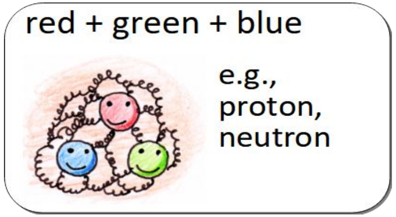


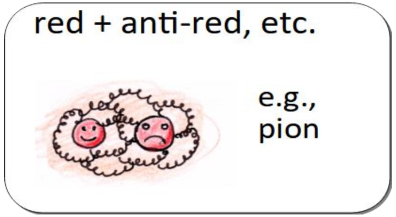


- This happens so often that quarks are always surrounded by a dense network of gluons that holds together a group of several quarks

- Quarks form particles that are **always "color-neutral"** as a whole:

Color is *confined* inside hadrons!





  - Not your everyday charge…

Mysteries

- **Gluon binding energy provides most of the proton mass:**

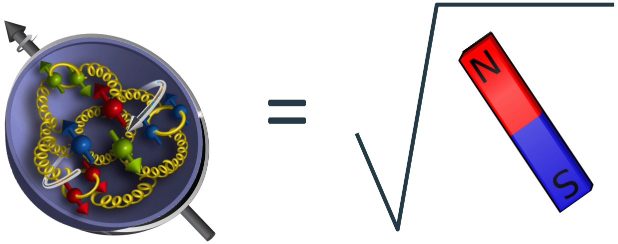
$$m_{\text{proton}} = 1\ \text{GeV}/c^2$$

vs.

$$m_u + m_u + m_d \approx 0.015\ \text{GeV}/c^2$$

  - Are we actually made of a force field??

- **Why is the spin of proton = ½ ?**
  An unlikely way of combining:
  - the spin of (many) quark and gluons
  - and their orbital angular momentum!

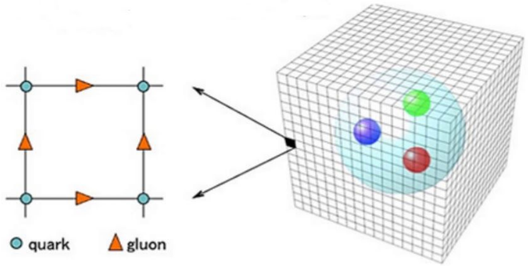


- In fact, **why isn't there any free quark??**

Color confinement

- Only "color neutral" particles have ever been (can ever be?) observed

- **Why??**
  - **Mathematical explanation from QCD Lagrangian**
    - ⟶ I attempted one a long time ago (1996-1998) – my first scientific love!
    - ⟶ $1M "millennium prize" from the Clay Institute!!
  - **Lattice QCD** – computational explanation
    - ⟶ But "black box"...



  - **Look at the effects of confinement**
    - ⟶ Dynamical mass generation
    - ⟶ Parton Distribution Functions at the "edge of confinement"

my research!

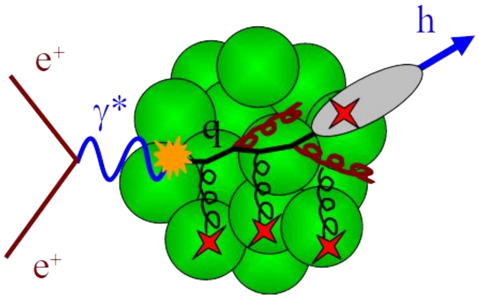
Dynamical mass generation:

how do massive hadrons emerge from nearly massless quarks?

Parton propagation and fragmentation

Review: Accardi et al., *Riv. Nuovo Cim. 032 (2010)*

- **Nuclei as femtometer-scale detectors**



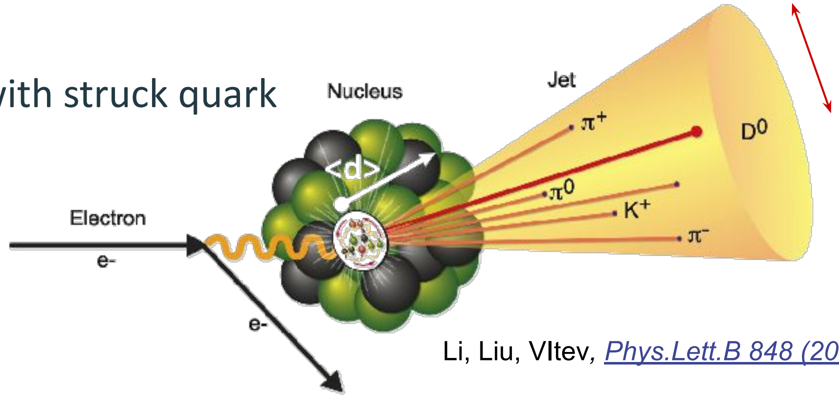
Transverse momentum broadening

$$\Delta p_T^2 = \langle p_T^2 \rangle_A - \langle p_T^2 \rangle_D$$

Hadron attenuation

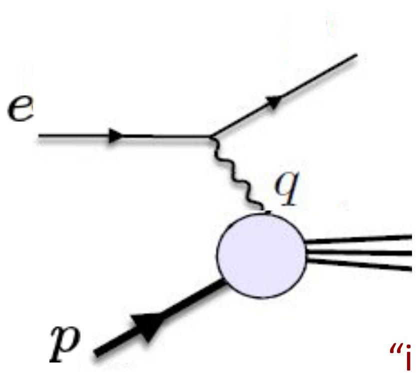
$$R_M = (N^h/N^e)_A/(N^h/N^e)_D$$

- **At the Electron-ion collider**
  - Higher energy
  - "Jets" of particles aligned with struck quark



Li, Liu, Vitev, *Phys.Lett.B 848 (2024) 138354*

“Inclusive jets” in vacuum

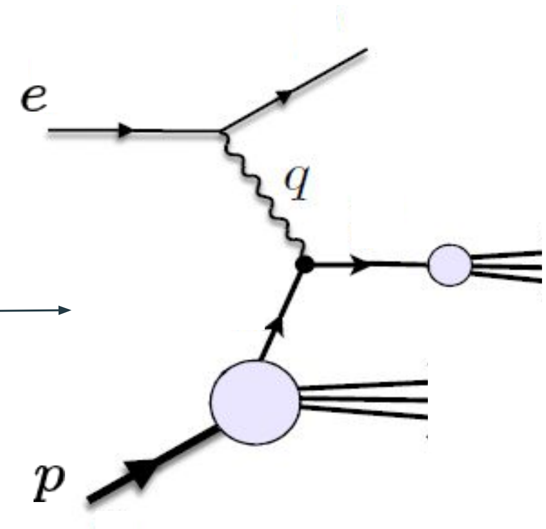


$$(p+q)^2 \longrightarrow M^2$$

“invariant” mass

proton mass

the difference is the (relativistic) energy available for particle production



aligned with scattered quark

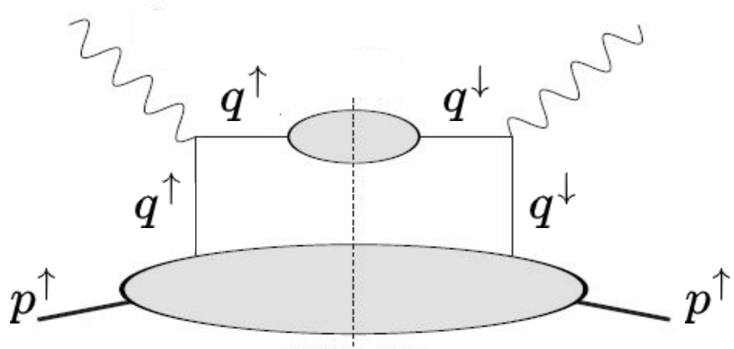
A self-made jet!

(no particle is detected)

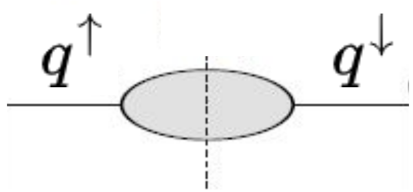
Quantum mechanically

- **Polarized electron+proton scattering:**

$$\sigma(\vec{e} + p^{\uparrow} \to X) \sim \mathcal{M}\mathcal{M}^{*} \sim$$



measurable!
In “inclusive LT asymmetries”



$$= \int \mu\, \rho_1(\mu^2)\, d\mu^2 \sim \langle \mu \rangle$$

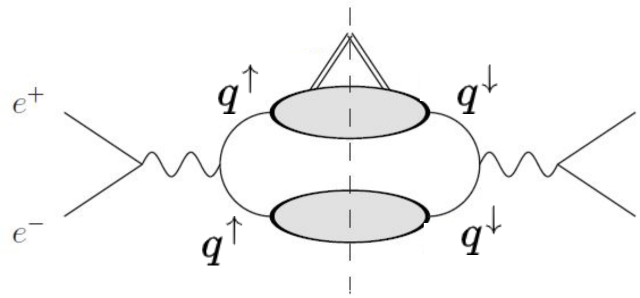
“Spectral function”: prob. distrib. of produced mass

calculable:
lattice QCD / Dyson-Schwinger

Quantum mechanically

- Polarized electron+positron scattering:

$$\sigma(\vec{e}^{\,-} + \vec{e}^{\,+} \to \vec{\Lambda}) \sim$$



- We are looking also for observables in proton-proton collisions

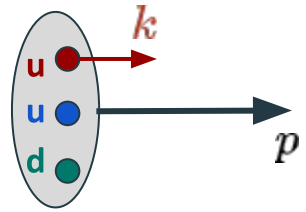
- **Many observables → can think of a "global analysis"** (see later)

Parton Distributions
at the “edge of confinement”

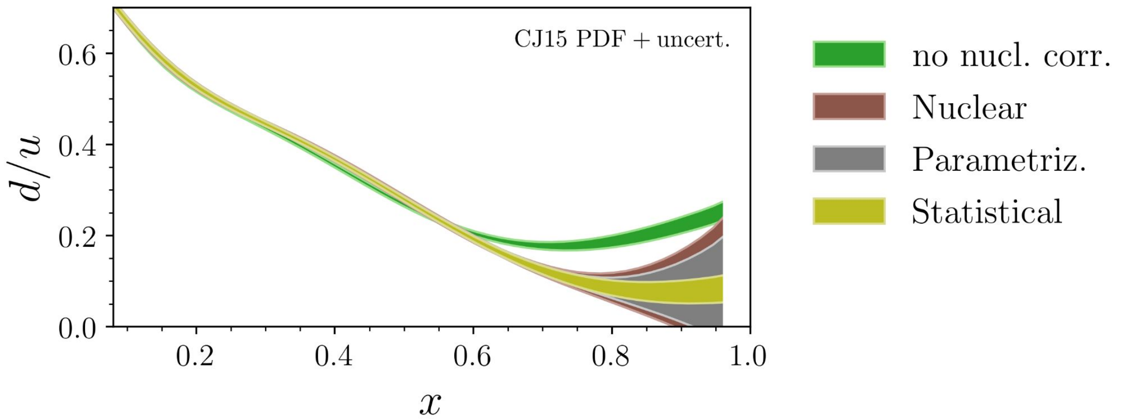
What happens when a single quark contributes most of the proton’s momentum?

Parton Distribution Functions

- **PDF** = probability distribution for a parton (quark or gluon) inside a proton to have momentum fraction $x = \frac{k}{p}$



- **Large** $x \to 1$
  - The proton "is" a single quark – up or down
  - Confinement most directly determines the behavior of the d/u ratio



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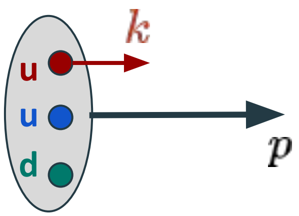

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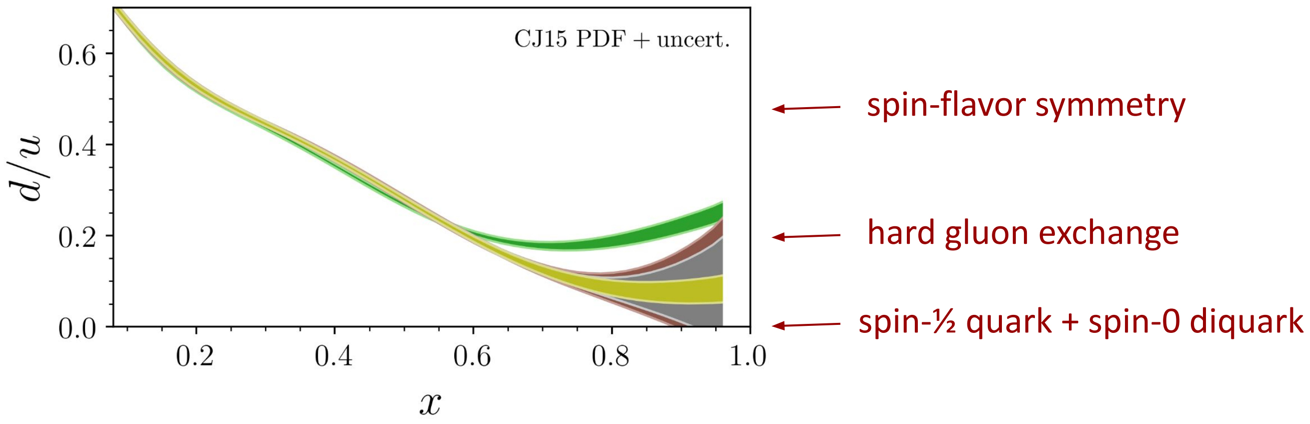
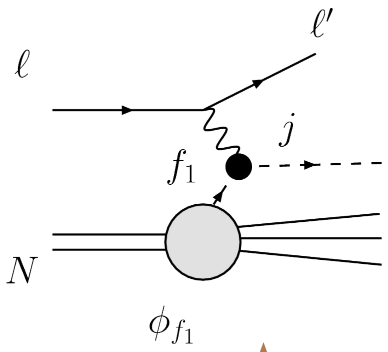


How to measure the PDFs?



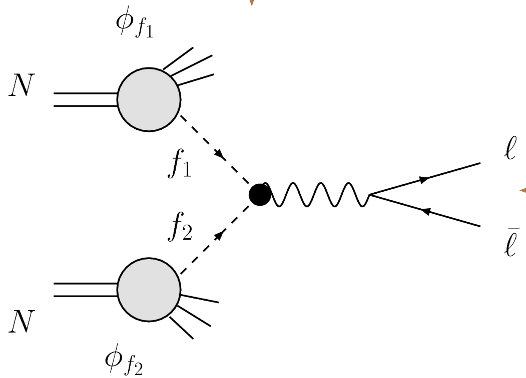
- **QCD factorization**
  of short and long distance interactions

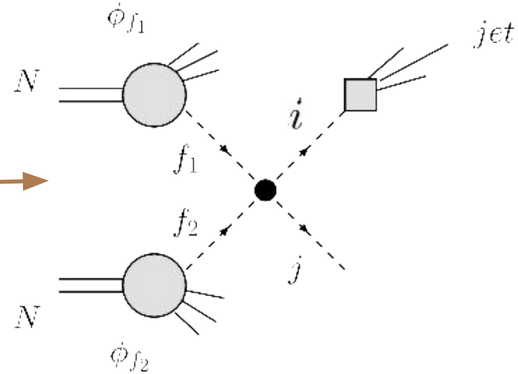
perturbative. QCD calc.

$$d\sigma_{\text{hadron}} = \sum_{f_1,f_2,i,j} \phi_{f_1} \otimes \hat{\sigma}^{f_1 f_2 \to ij}_{\text{parton}} \otimes \phi_{f_2}$$

PDFs

- **Universality:** same PDFs for many processes





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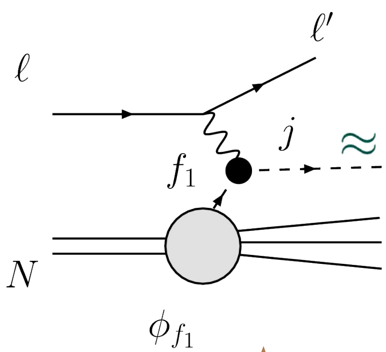


$$\approx \sum_q e_q^2 q(x, Q^2)$$

- **QCD factorization**

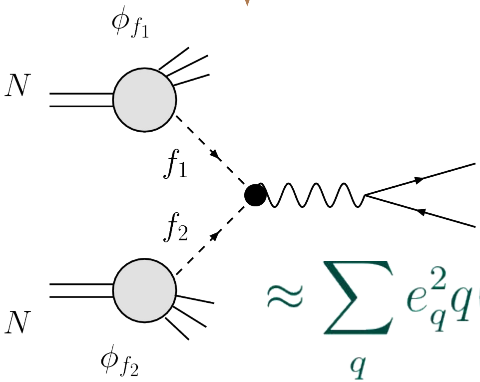
  of short and long distance interactions

perturbative. QCD calc.

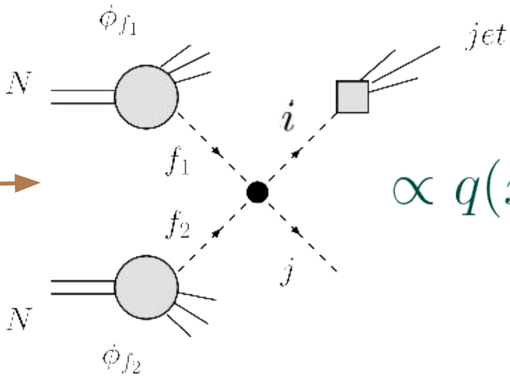
$$d\sigma_{\text{hadron}} = \sum_{f_1,f_2,i,j} \phi_{f_1} \otimes \hat{\sigma}^{f_1 f_2 \to ij}_{\text{parton}} \otimes \phi_{f_2}$$

PDFs

- **Universality:** same PDFs for many processes



$$\approx \sum_q e_q^2 q(x_1) \bar{q}(x_2)$$



$$\propto q(x_1) g(x_2)$$

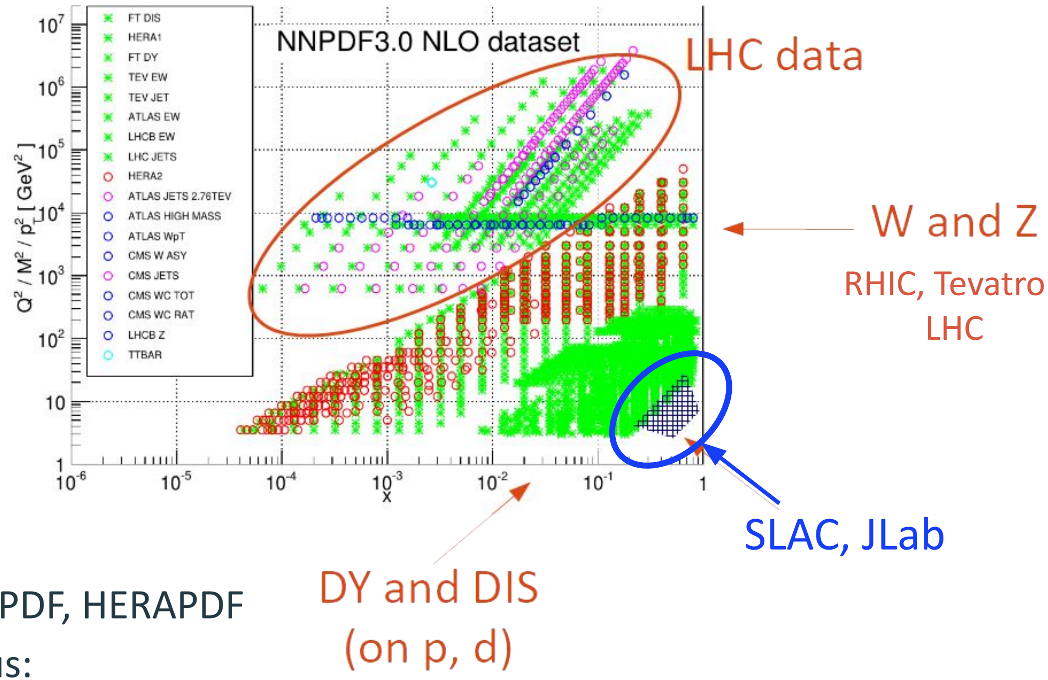
Global QCD fits

$$d\sigma_{\text{hadron}} = \sum_{f_1,f_2,i,j} \phi_{f_1} \otimes \hat{\sigma}^{f_1 f_2 \to ij}_{\text{parton}} \otimes \phi_{f_2}$$

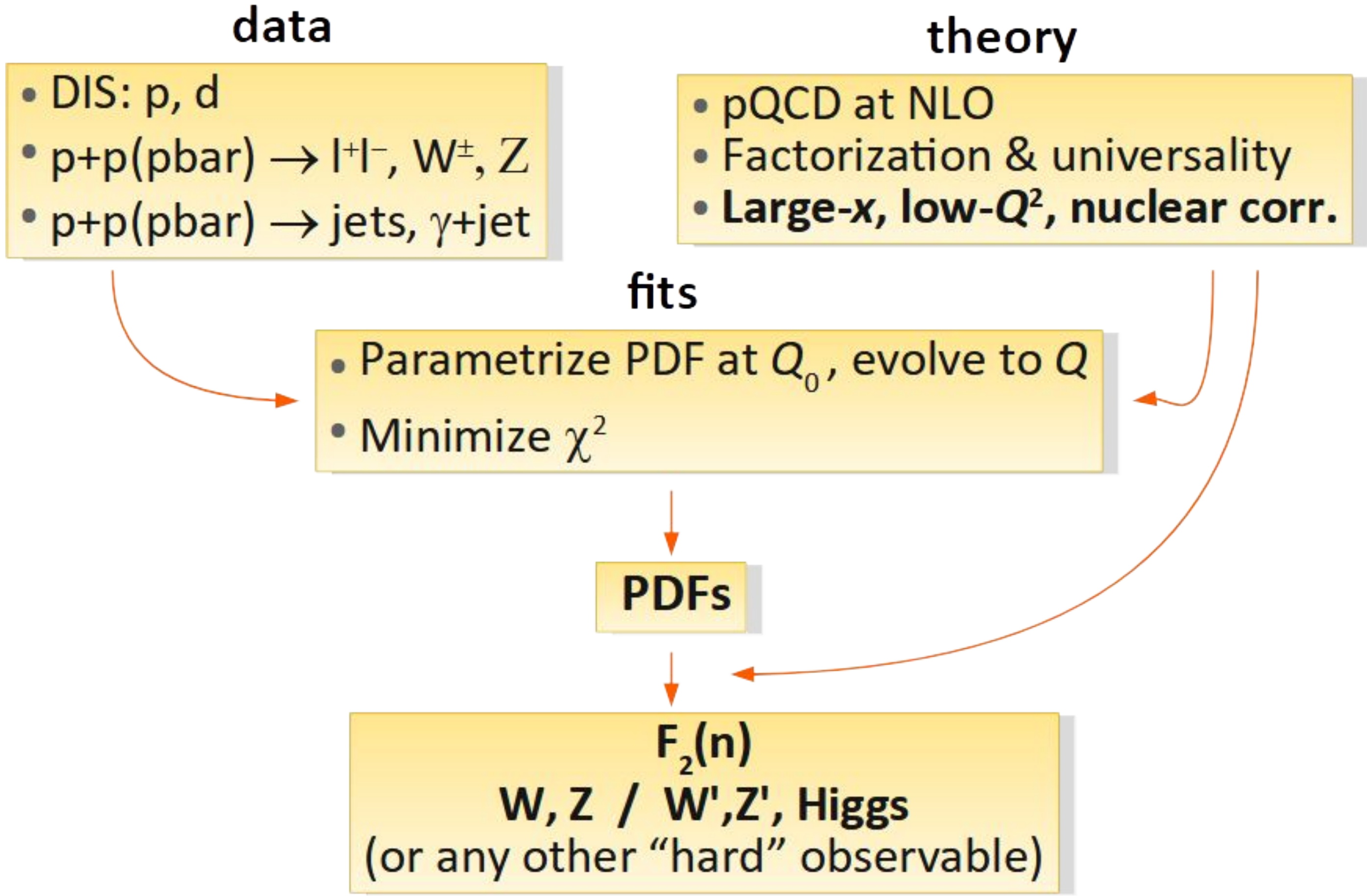
pert. QCD calc.

PDFs

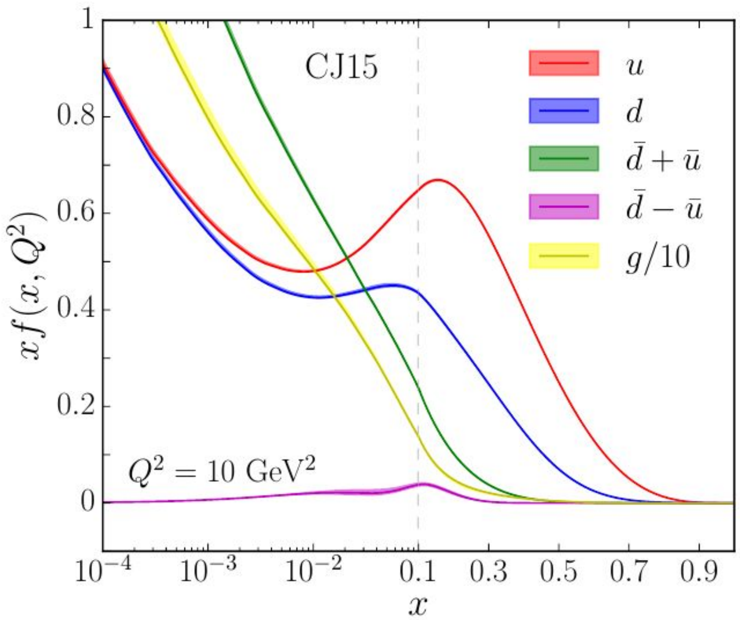
- **QCD factorization & universality:**
  can fit PDFs to a variety of hard scattering data
  - Hadron-hadron collisions
    - ⟶ Jets
    - ⟶ Electro-weak boson production
  - Electron-proton DIS
  - Electron-Deuteron DIS
- **>1000's data points**
- **40+ years of experience,**
  - "High-energy" fitters:
    - ⟶ CTEQ-TEA, MMHT, NNPDF, HERAPDF
  - Lower-energy / nuclear focus:
    - ⟶ **CTEQ-JLab,** AKP, JAM



Global QCD fits



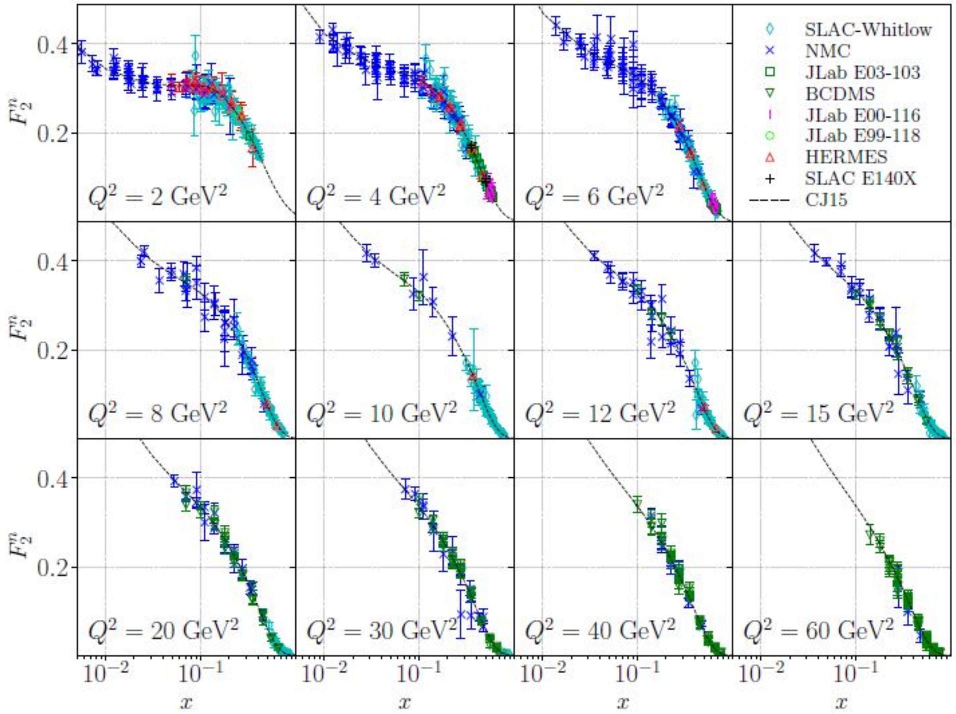
The CJ15 PDFs



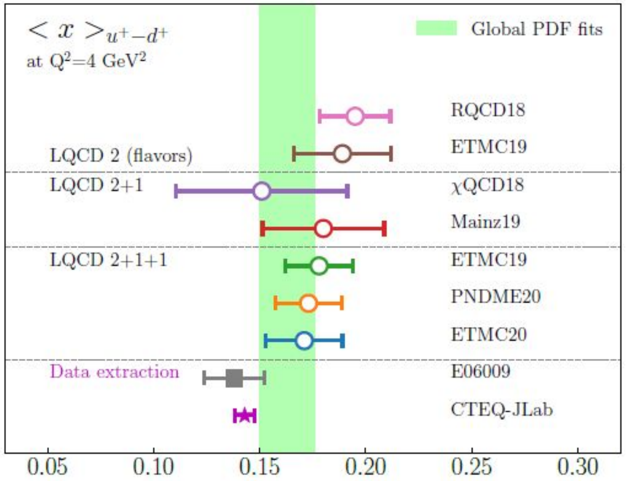
- Fitted with χ^2 = 1.04 / datum
- Propagation of exp. errors
  - Hessian analysis
  - Correlated errors used if available
- "PDF error band" for $\Delta\chi^2$ = 2.71
  - → 90% c.l. in a perfect world
  - Many alternative methods
    - See review by Kovarik et al.
- Theoretical systematics more difficult
  - Recent effort by fitting community

Neutron structure function extraction

- **There is no free neutron target**
  - Use (fitted) nuclear correction model
  - Confine model dependence in deuteron / free p + n correction ratio



Apply data:
→ e.g. to benchmark lattice QCD

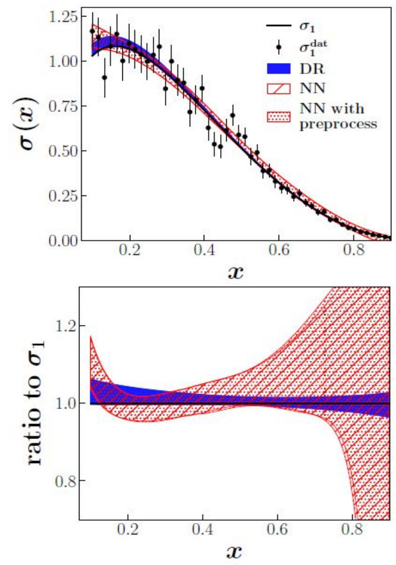


(Some of the) challenges

- **Very large data set**:
  - Need to: modernize code, speed up calcs!

- **Need fit flexibility → many parameters, highly correlated**
  → numerical instability in Hessian matrix
  - Increase numerical robustness?
  - Use neural networks?
    - → But: Cross Valid. leads to likelihood deformation!
  - Better parametric methods
    - → (iterative) bootstrap?
    - → Fully Bayesian methods (MCMC, …)?

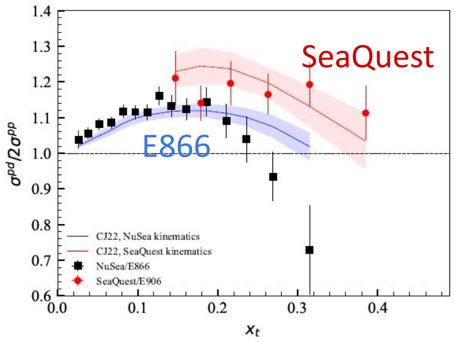
- **Visualization tools / information compression**



CJ22

(Some of the) challenges

- **Incompatible data sets**
  - Increase "tolerance": blow up errors
  - More solid (Bayesian) treatment
    - ⟶ E.g., multi-Gaussian mixtures
      [K. Mohan @ DIS 2023]



CJ22

- **How can AI/ML help?**

To conclude…

Summary and Perspective

- **What are we made of?**
  - Study the effects of confinement
  - 2 intertwined research lines

- **Global QCD analysis**
  - Many new data & better precision in near future
  - Needs matching uncertainty determination
    - ⟶ **Interdisciplinary challenge**
    - ⟶ **Expanded CTEQ-JLab collaboration**

- **Dynamical mass generation**
  - Theory: factorization with inclusive jet functions
  - New observables
    - ⟶ **Novel global analysis**
    - ⟶ PDFs + i-JFN ⟶ mass generation

Summary and Perspective

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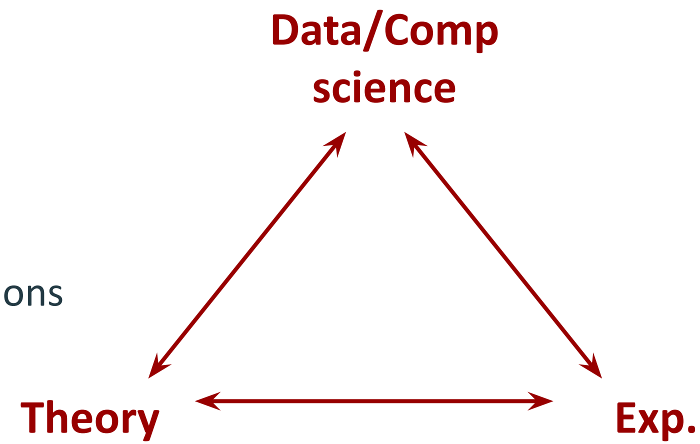


Thank you!

Backup #1:

Evidence for quarks and gluons

Evidence for quarks and gluons - a whirlwind tour

- **Baryon spectroscopy – light sector (*u*, *d*, *s*), ground state**
  - J=3/2⁺: $|q_1\uparrow, q_2\uparrow, q_3\uparrow\rangle$
  - J=1/2⁺: $|q_1\uparrow, q_2\uparrow, q_3\downarrow\rangle$

totally symmetric w.fn.

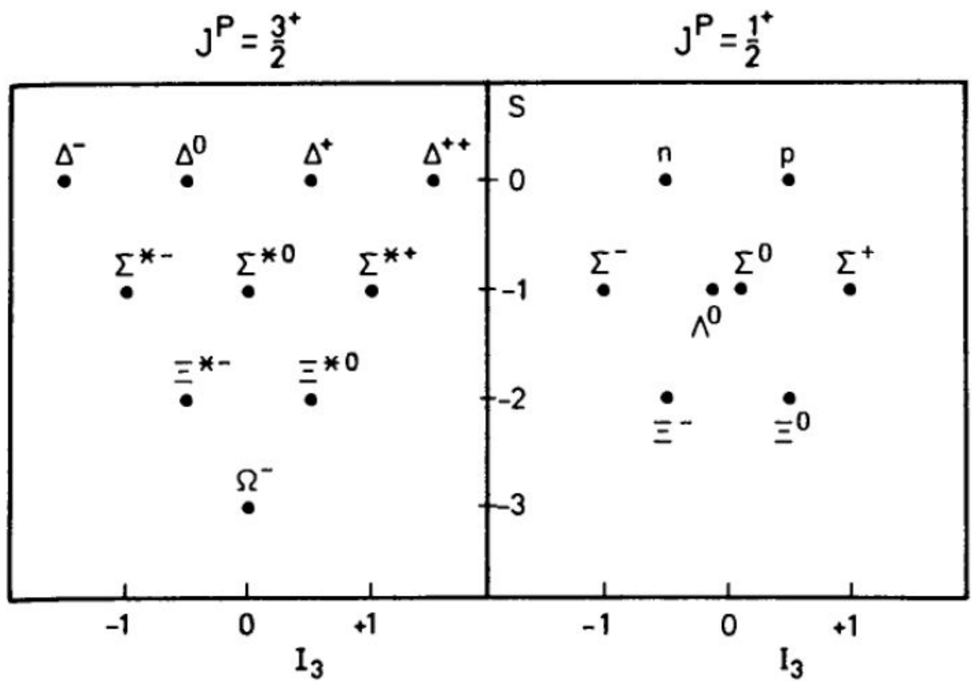


Fig:
[from Povh et al.]

Evidence for quarks and gluons - a whirlwind tour

- **Baryon spectroscopy – light sector (*u, d, s*), ground state**
  - $J=3/2^+$: $|q_1\uparrow,q_2\uparrow,q_3\uparrow\rangle$ spin symmetric, color antisymmetric
  - $J=1/2^+$: $|q_1\uparrow,q_2\uparrow,q_3\downarrow\rangle$ spin antisymmetrics, color symmetric

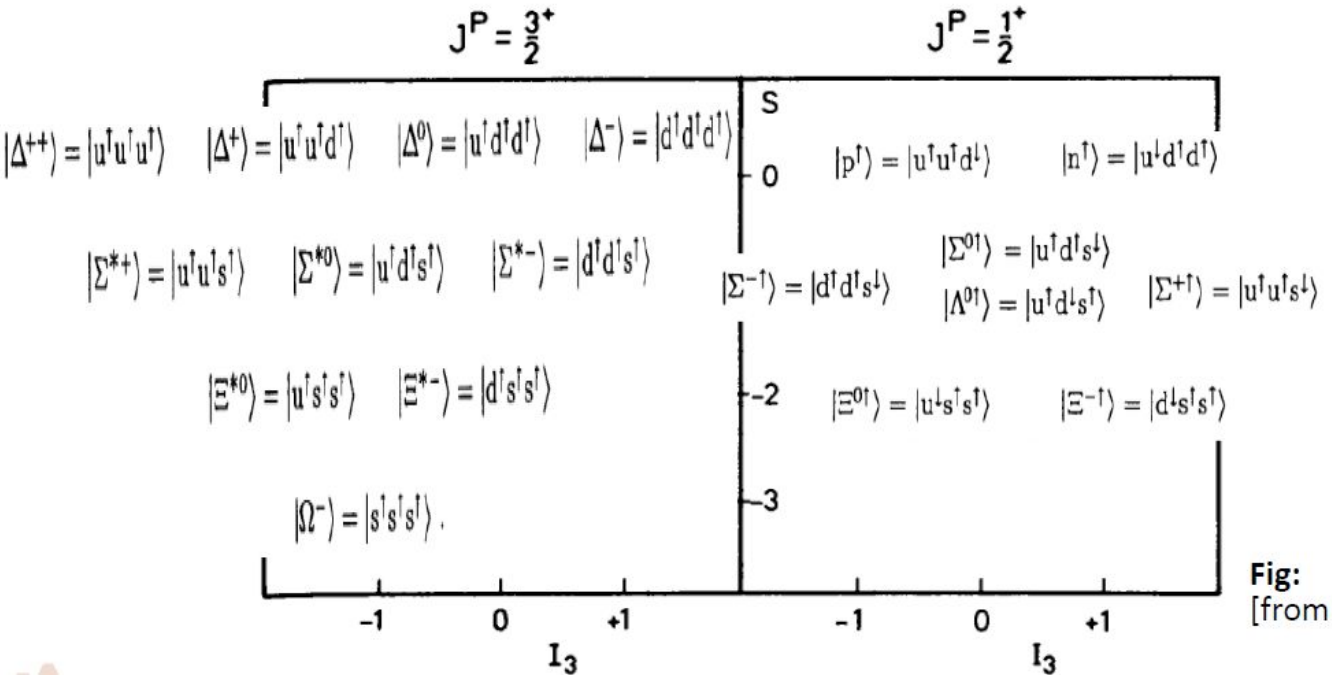
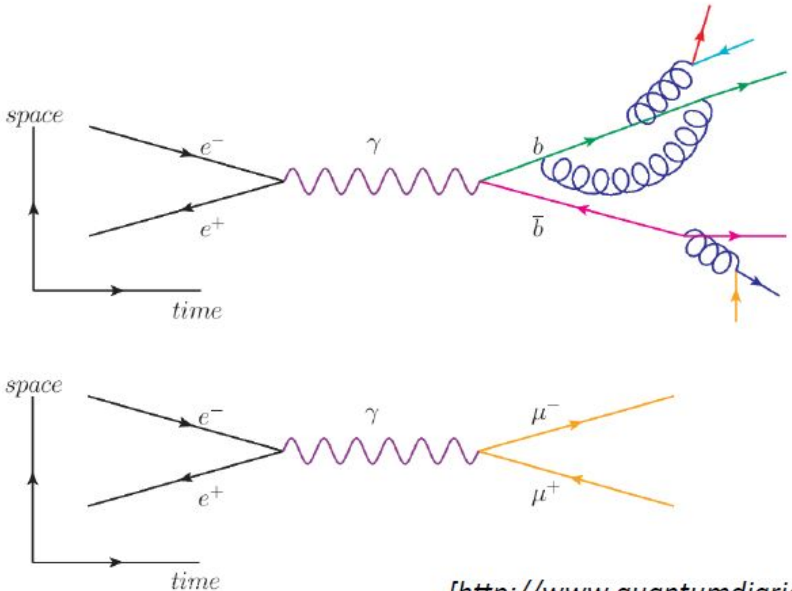


Fig:
[from Povh et al.]

Evidence for quarks and gluons - a whirlwind tour

- $e^+ + e^-$ **annihilation into hadrons**
  - quark-mediated process $e^+ + e^- \to q + \bar{q} \to hadrons$

$$R = \frac{\sigma(e^+e^-hadrons)}{\sigma(e^+e^-\mu^+\mu^-)} = N_{colors}\sum_q e_q^2$$



[http://www.quantumdiaries.org/author/richard-ruiz/]

Evidence for quarks and gluons - a whirlwind tour

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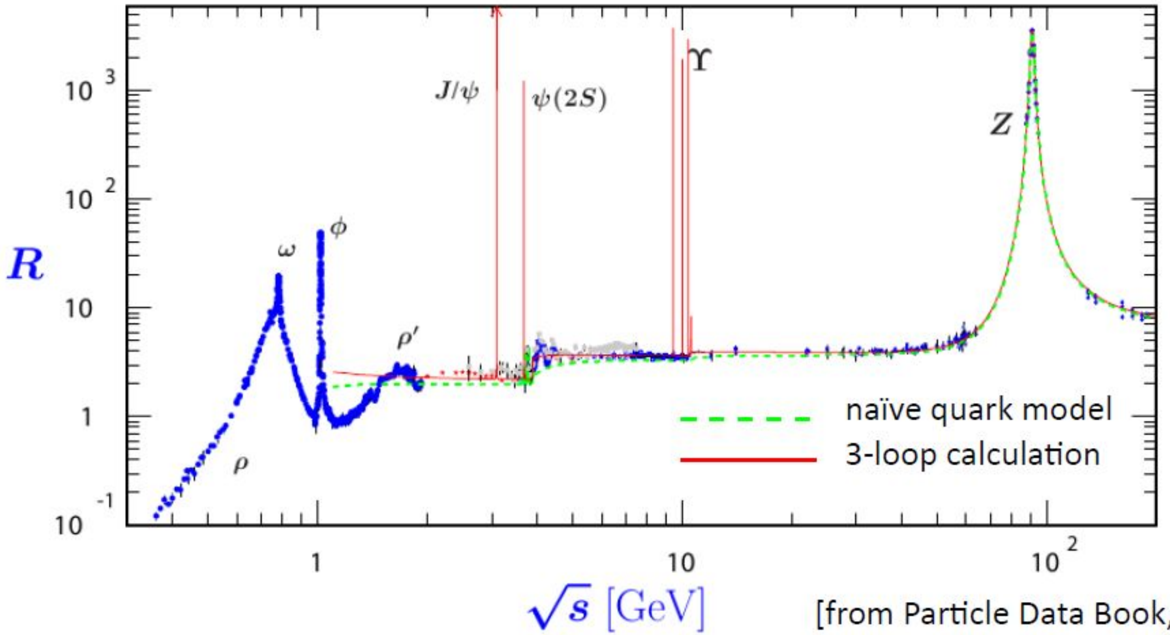


[from Particle Data Book, pdg.lbl.gov]

Evidence for quarks and gluons - a whirlwind tour

- **Jets in high-energy $e^+ + e^-$ collisions**
  - Hadron produced in 2, 3, … N, high-energy collimated "jets"
  - Evidence of common origin from a parton

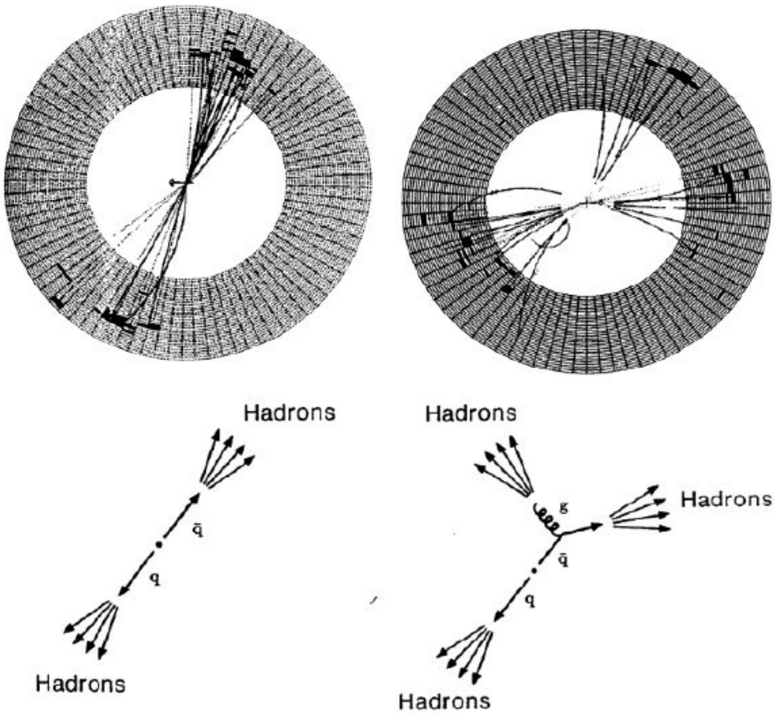


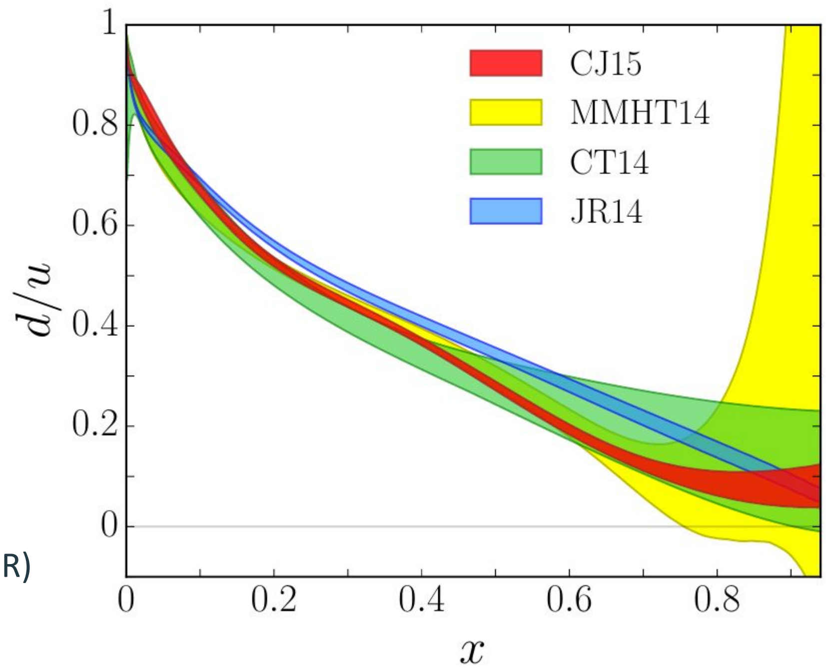
Fig.: 2- and 3-jet events observed by the JADE detector at PETRA [from Povh et al.]

Backup #2:

Experimental uncertainties
or
“ Why do different global fits give different PDF uncertainties? ”

Global fits are not created equal…

- **Uncertainty determination**
  - Hessian (JR)
  - Hessian + “Tolerance” (*)
    - ⟶ T ~ 10 (CT14)
    - ⟶ T ~ 5-7 (MMHT14)
    - ⟶ T = 1.646 (CJ15)
  - Data Resampling (JAM)
  - DR + Cross Validation (NNPDF)
- **Parametrization**
  - $x^a (1-x)^b P(x)$ – most groups
  - d-quark:
    - ⟶ extended (CJ, CT) or std (MMHT, JR)
  - Neural Nets – NNPDF
- **Data choice and coverage, …**
  - Can use SLAC, JLab only if considering TMC, HT corrections
  - Highest *x* reach for d/u on proton if using reconstructed W asymmetries (vs. decay lepton asymmetries)
  - …



(*) CJ vs. CT comparison on “equal” footing:
Accardi, Hobbs, Jing, Nadolsky, EPJC 81 (2021) 7

Bayesian estimators

- **Bayes theorem** $p(a|m) = \frac{1}{Z}\, p(m|a)\, p(a)$

  with "evidence" $Z = \int \mathrm{d}a\; p(m|a)\, p(a)$

  and "likelihood" $p(m|a) = \mathcal{N} \exp\left[-\frac{1}{2}\chi^2(a,m)\right]$

  Typical choice in PDF analyses

- **Algorithms for sampling of likelihood $\longrightarrow$ probability density in $\{a_k\}$**
  - **HMC**: Hamiltonian Monte Carlo (an example of Markov-Chain MC methods)
  - **NS**: Nested Sampling, primarily aimed at estimating the evidence

    $\longrightarrow$ Samples the likelihood as a byproduct

- **Expectation values** $E_{\rm Bayes}\{\mathcal{O}(a)\} = \frac{1}{n}\sum_{k=1}^{n} \mathcal{O}(a_k)\,,$

  and variance $V_{\rm Bayes}\{\mathcal{O}(a)\} = \frac{1}{n}\sum_{k=1}^{n} \left[\mathcal{O}(a_k) - E_{\rm Bayes}\{\mathcal{O}(a)\}\right]^2$

Generalized Hessian Approximation

Hunt-Smith et al., PRD 106 (2022) 036003

- **Start as usual:**
  - Find minimum of likelihood
  - Diagonalize Hessian $\longrightarrow \boldsymbol{e}_k$ eigenvectors, w_k eigenvalues
- **Change variables:** $a(t) = a_0 + \sum_{k=1}^{n_{\rm par}} t_k \frac{e_k}{\sqrt{w_k}}$ **, then** $p(a|m) \to p(t|m)$
- **Assume likelihood factorized along Hessian eigendirection, then**

$$E_{\rm Hess}\{\mathcal{O}(a)\} = \int d^n t \; p(t|m)\, \mathcal{O}(a(t)) \approx \mathcal{O}(a_0)$$

$$V_{\rm Hess}\{\mathcal{O}(a)\} \approx \sum_k T_k^2 \left(\frac{\partial \mathcal{O}(a(t))}{\partial t_k}\Big|_{a_0} \right)^2$$

- **Here** $T_k^2 = \int dt_k \; p_k(t_k|m)\, t_k^2$ **is the "tolerance" :**
  - T_k = 1 where likelihood is Gaussian;
  - Approximates well the likelihood in non-Gaussian directions
  - Maintains a "68%" or "1σ" kind of meaning also when ≠ 1

CT, MSTW $\longrightarrow$ T=5-10

- **Often T_k determined "ad hoc" to account for statistical inconsistency of data**

Data resampling

- **Data Resampling (DR) approximates Bayes' posterior using frequentist logic**
    - Assume some prior (typically "flat")
    - Reshuffle data within data uncertainty (Gaussian distribution)
    - Maximize likelihood
    - Repeat n_{rep} times $\longrightarrow \{\boldsymbol{a}_k\}$

- **Estimate**

$$E_{\text{freq}}\{\mathcal{O}(a)\} = \frac{1}{n_{\text{rep}}} \sum^{n_{\text{rep}}} \mathcal{O}(a_{\text{rep}}),$$

$$V_{\text{freq}}\{\mathcal{O}(a)\} = \frac{1}{n_{\text{rep}}} \sum^{n_{\text{rep}}} \left[\mathcal{O}(a_{\text{rep}}) - E_{\text{freq}}\{\mathcal{O}(a)\}\right]^2$$

- **Good in parameter space region well constrained by data**

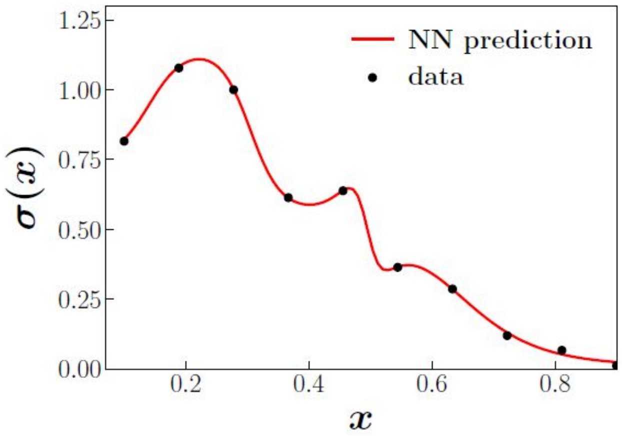
Neural Networks and overfitting

- **Neural networks provide:**
  - Efficient, very flexible parametrizations
  - Hundreds of parameters
  - Essentially a parameter free functional form ("nonparametric method")

- **Use Data Resampling and aims at maximizing the same likelihood function**

$$p(m|a) = \mathcal{N} \exp\left[-\tfrac{1}{2}\chi^2(a,m)\right]$$

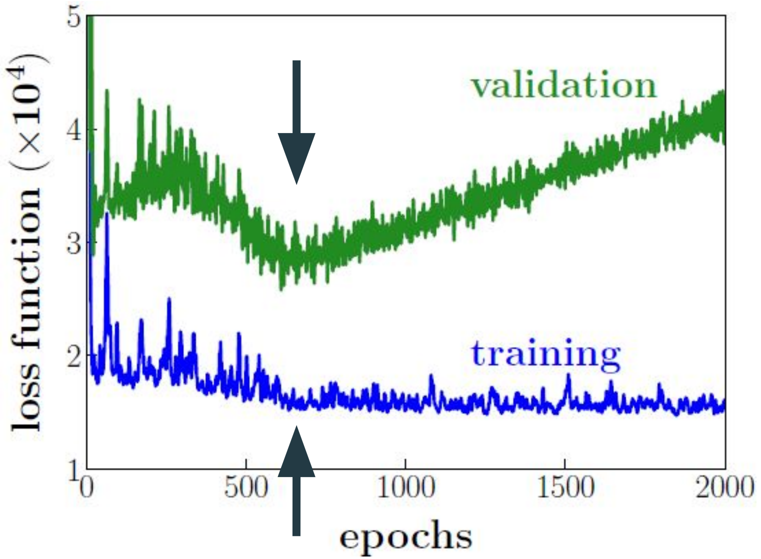
- **Without intervention, will overfit the data**
  - The plot shows an extreme example



Cross-validation (CV) and stopping

- **Needs a "stopping criterion"**
  - to avoid fitting statistical noise instead of physics
- **Randomly separate the data into 2 groups, say**
  - 70% ⟶ training (T)
  - 30 % ⟶ validation (V)
- **Fit the training, calculate χ^2(T) and χ^2(V)**
- **Resample data, repeat**
- **"Stop" training when χ^2(V) is minimum:**

$$\sigma = E[\sigma_{\text{fit}}]$$
$$\delta\sigma = V[\sigma_{\text{fit}}]$$



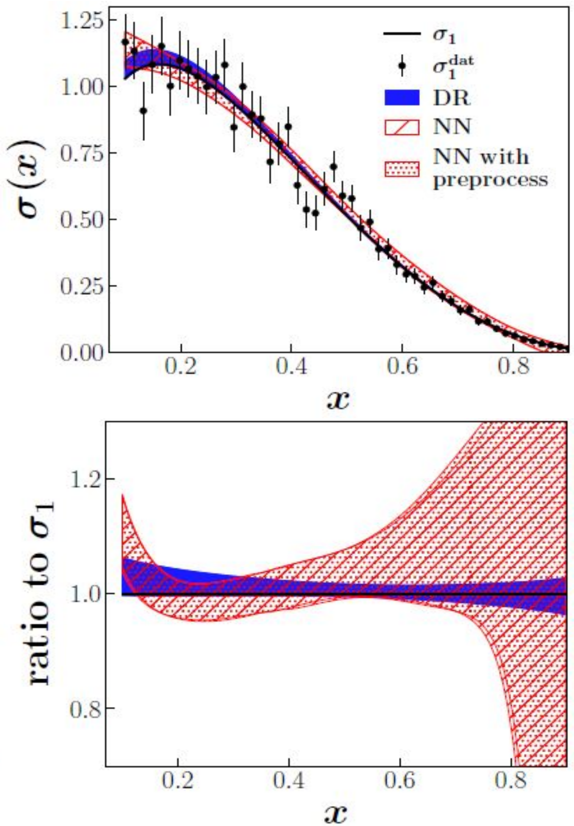
Statistical uncertainties

- **The method can effectively modify the likelihood!**
  - Even with perfectly compatible (toy) data!

N. Hunt-Smith et al., PRD 106 (2022) 036003

- **Bayesian Methods**
  (Markov Chain MC, Nested Sampling)
  - Explore the likelihood function
  - Well approximated by
    $\longrightarrow$ Hessian, Data Resampling (**DR**)

- **Cross Validation, NN-based fits**
  - Inflate the uncertainties
  - Deform the likelihood



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[N. Hunt-Smith et al., PRD 106 (2022) 036003]

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