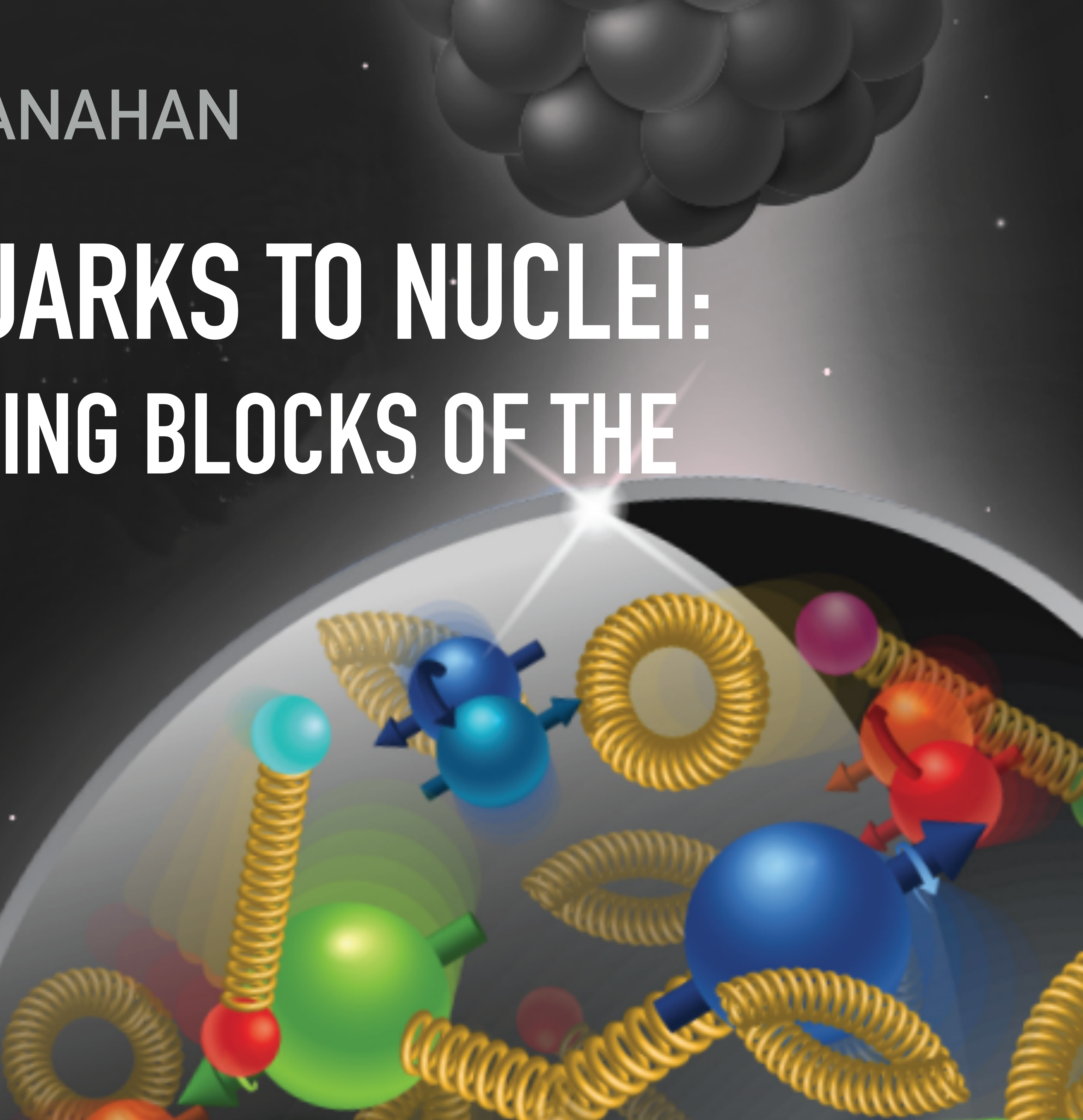
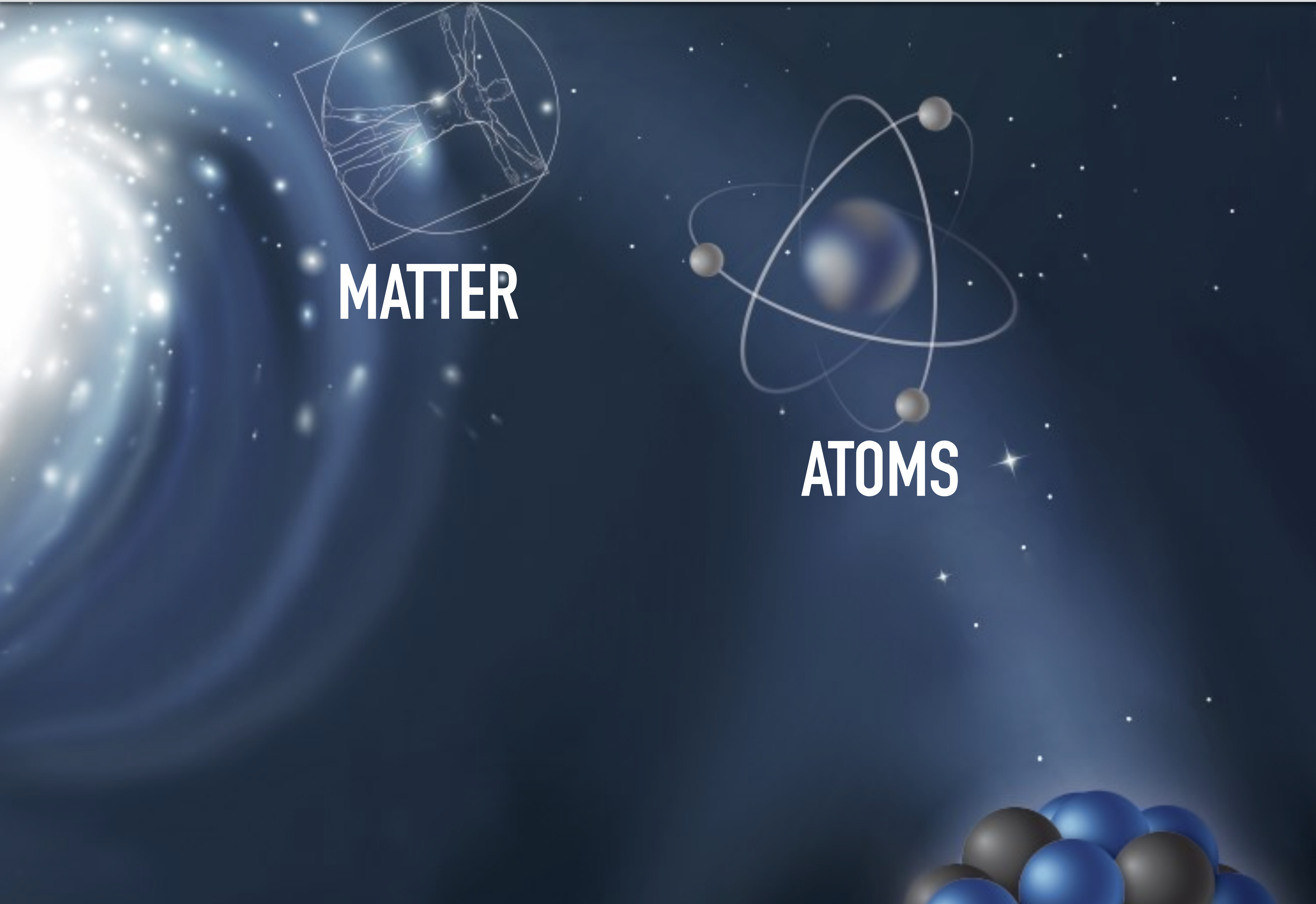
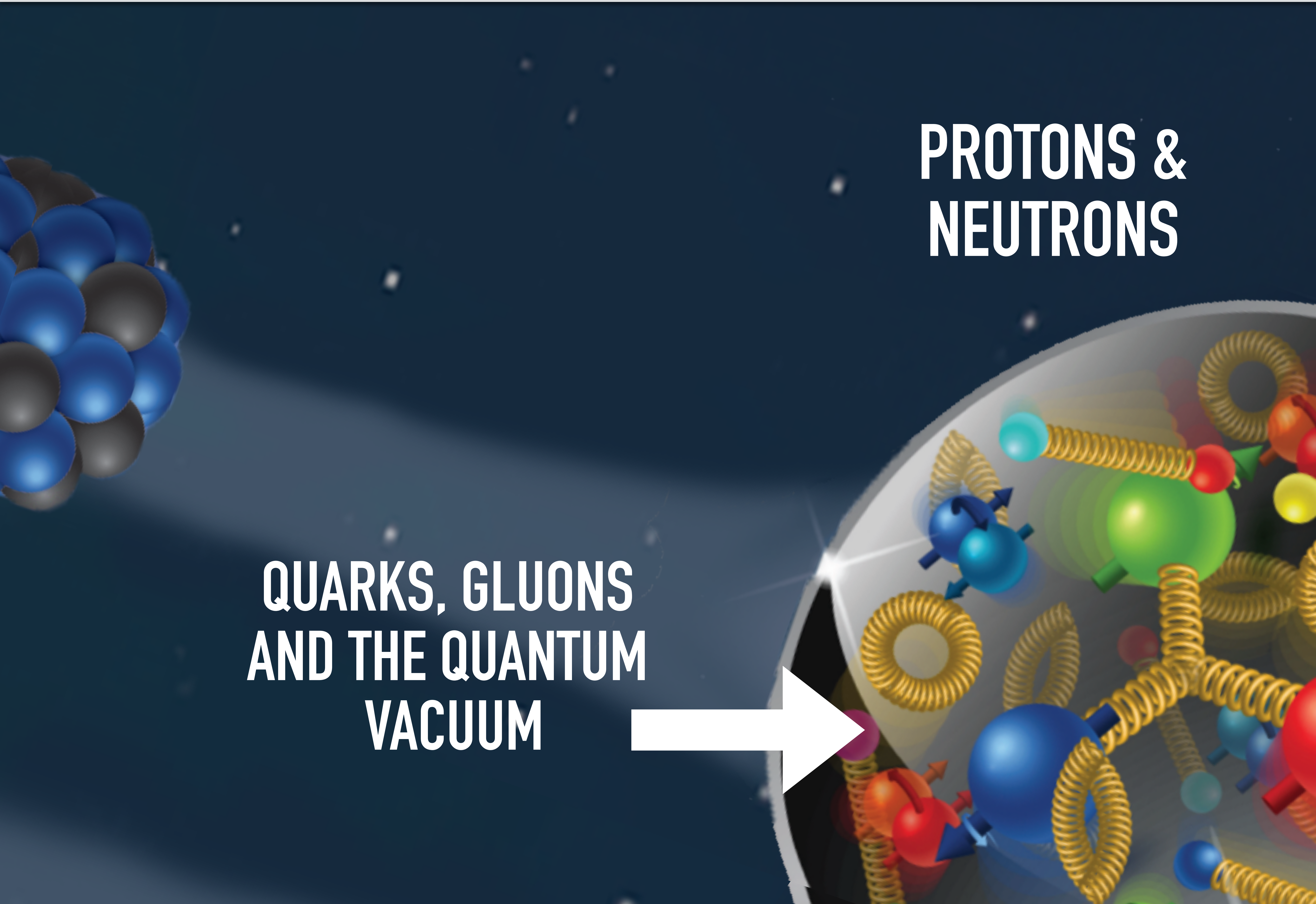
PHIALA SHANAHAN

FROM QUARKS TO NUCLEI:
THE BUILDING BLOCKS OF THE UNIVERSE



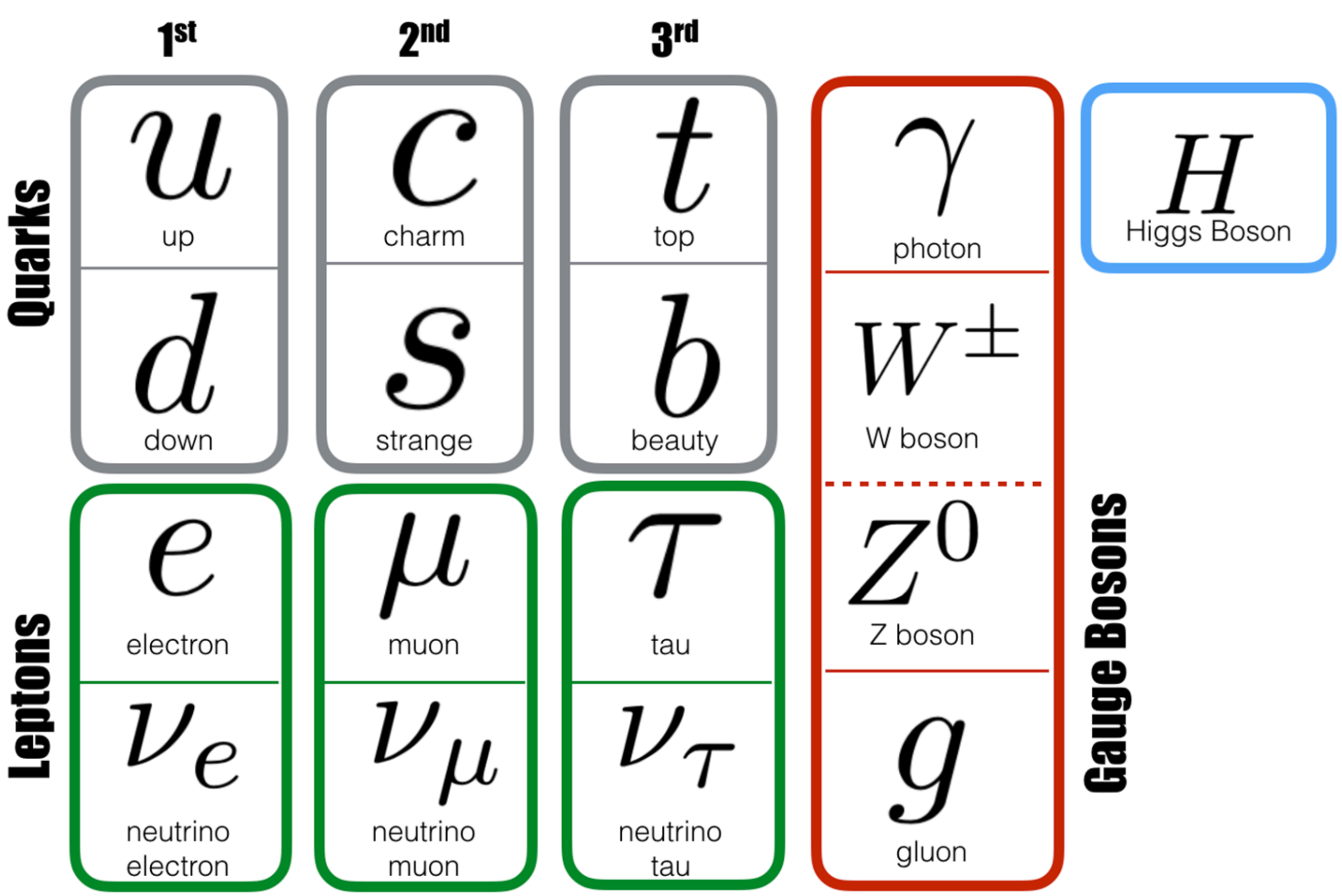
Massachusetts
Institute of
Technology

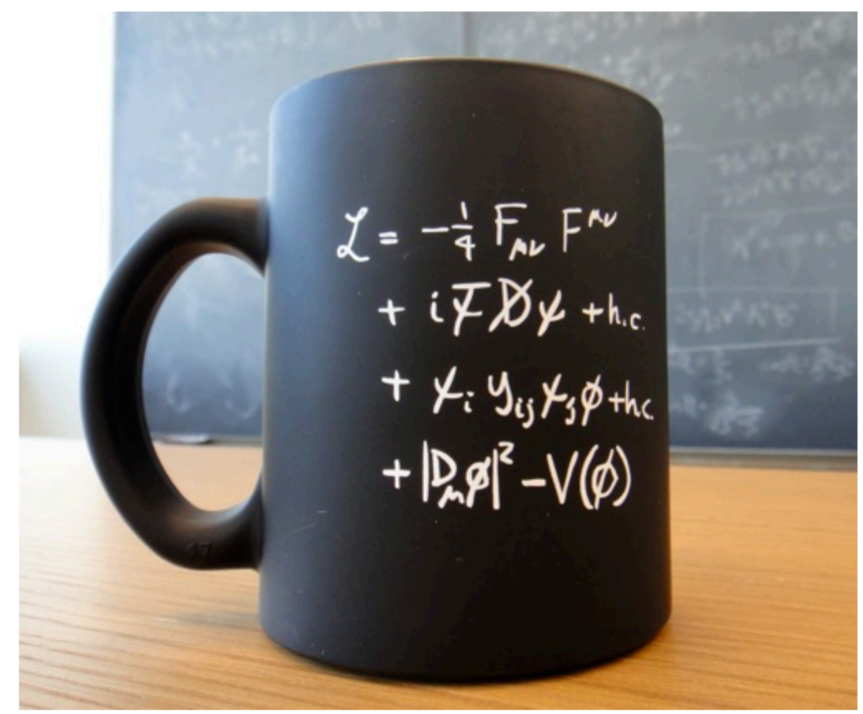

MATTER
ATOMS


PROTONS &
NEUTRONS
QUARKS, GLUONS
AND THE QUANTUM
VACUUM

The structure of matter

The Standard Model of nuclear and particle physics

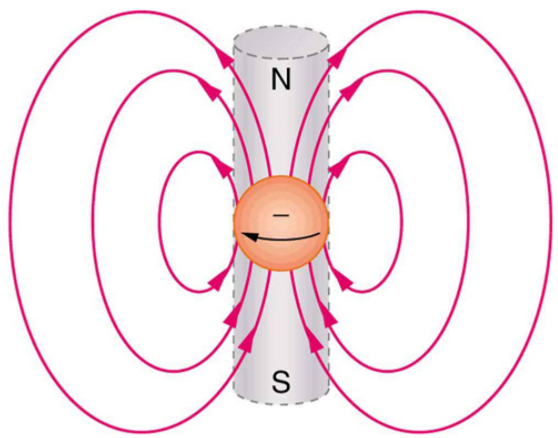




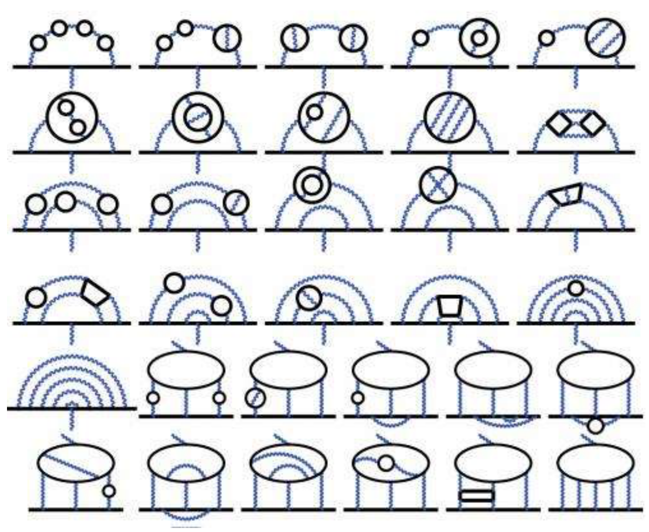
The structure of matter

The Standard Model is successful

Magnetic moment of the electron:
(torque an electron feels in a magnetic field) $a_e = (g-2)/2$



Most accurately verified prediction in the history of physics

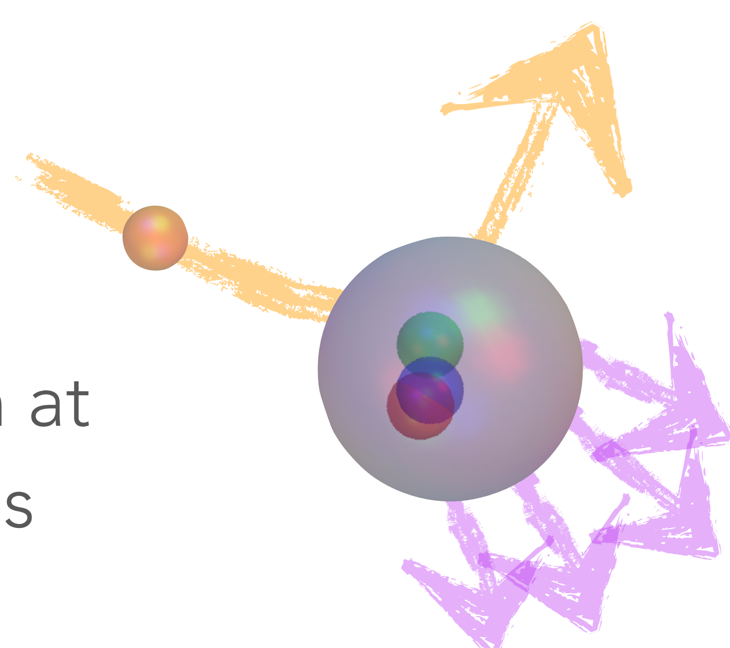


Theory	$a_e = 0.001159652181643(764)$
Exp.	$a_e = 0.00115965218073(28)$

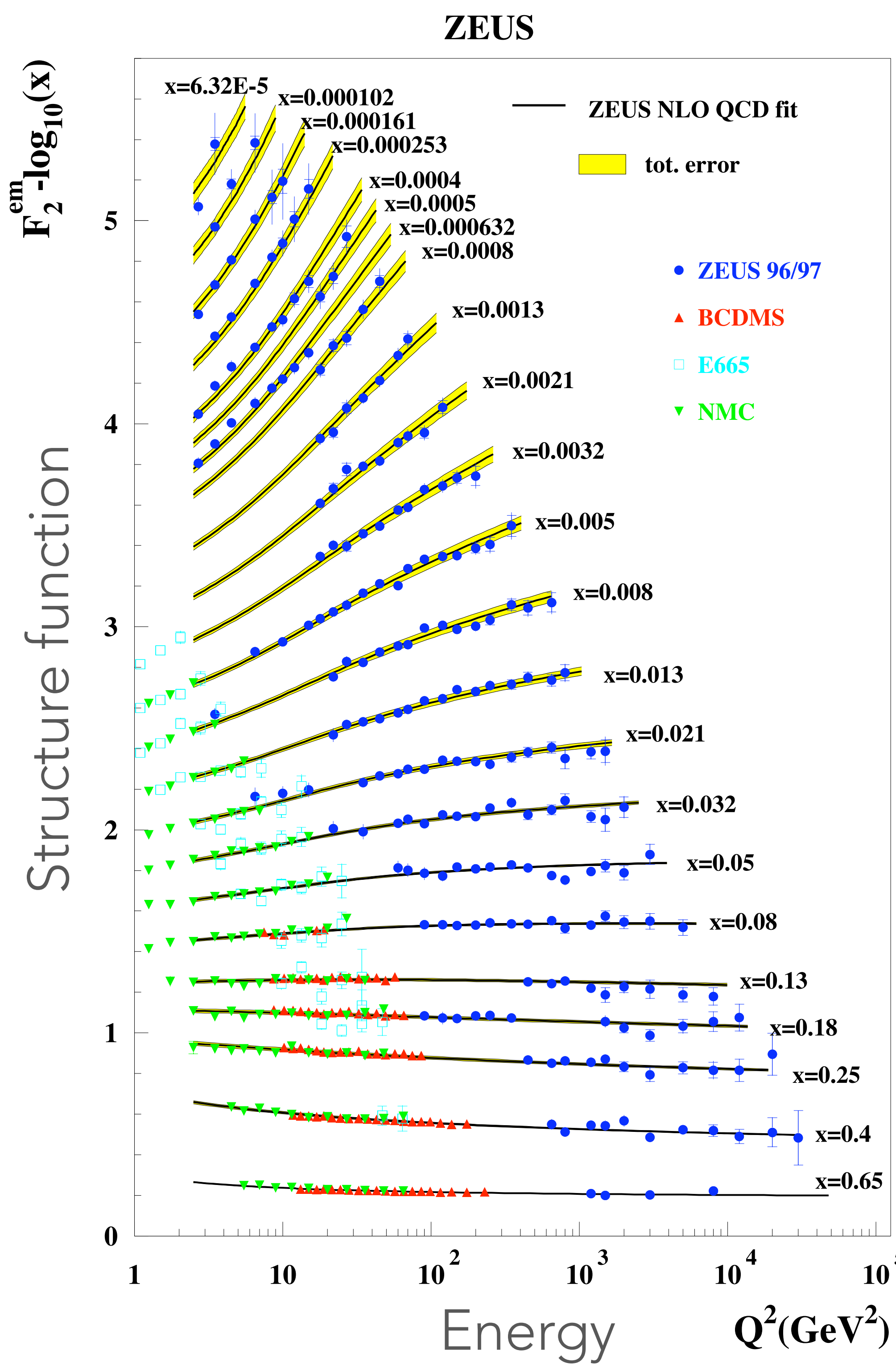
The structure of matter

The Standard Model
is successful

Deep inelastic scattering of electron on proton (hits and breaks proton apart)



Verification at many scales

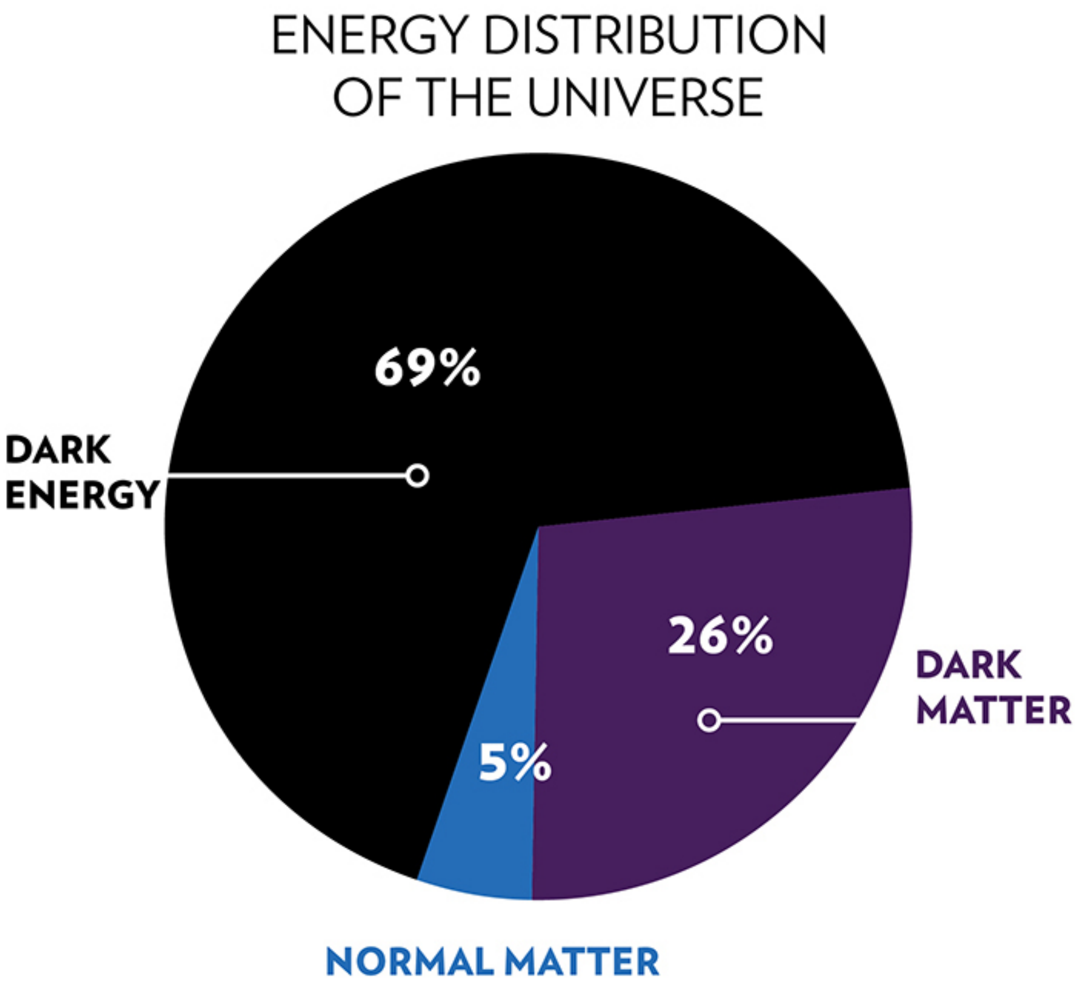


The structure of matter

BUT The Standard Model isn't everything

Example:
Dark matter

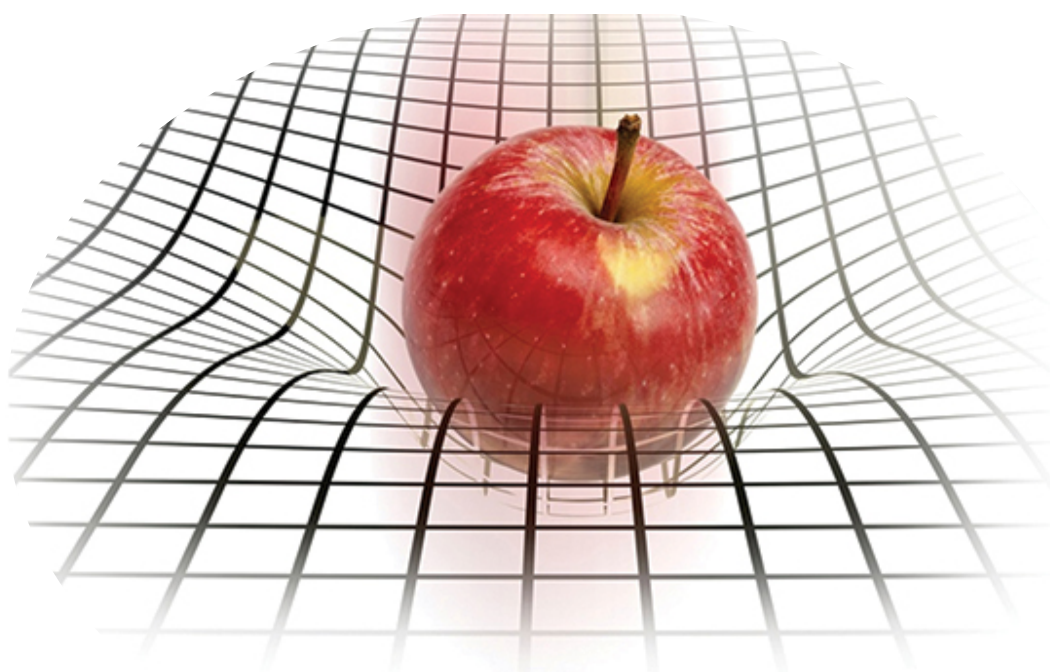
Despite the success of the Standard Model, most of the matter in the universe is something else!



The structure of matter

BUT The Standard Model isn't everything

- Dark matter and dark energy
- Neutrino masses
- Matter–antimatter asymmetry
- Gravity
- Naturalness problems
- …

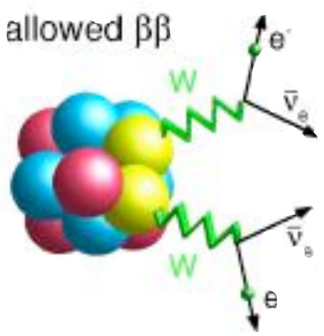


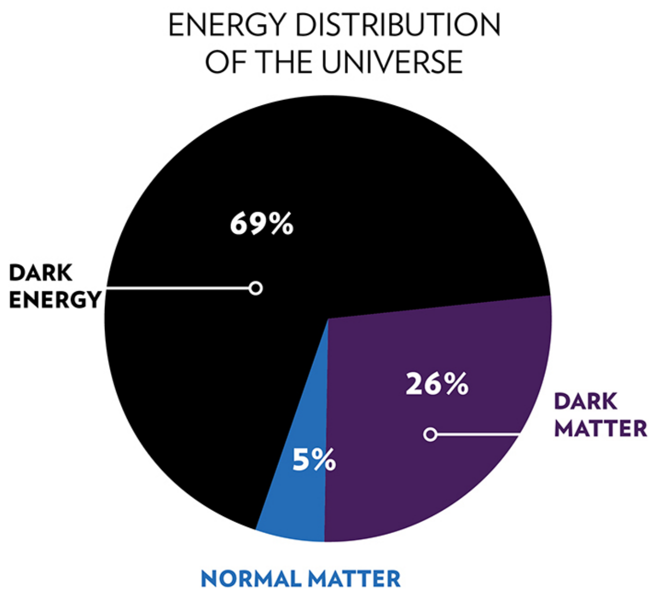
The search for new physics

Precise experiments seek new physics at the "Intensity Frontier"

- Sensitivity to probe the rarest Standard Model interactions
- Search for beyond—Standard-Model effects

- Dark matter direct detection
- Neutrino physics
- Charged lepton flavour violation, ββ-decay, proton decay, neutron-antineutron oscillations…





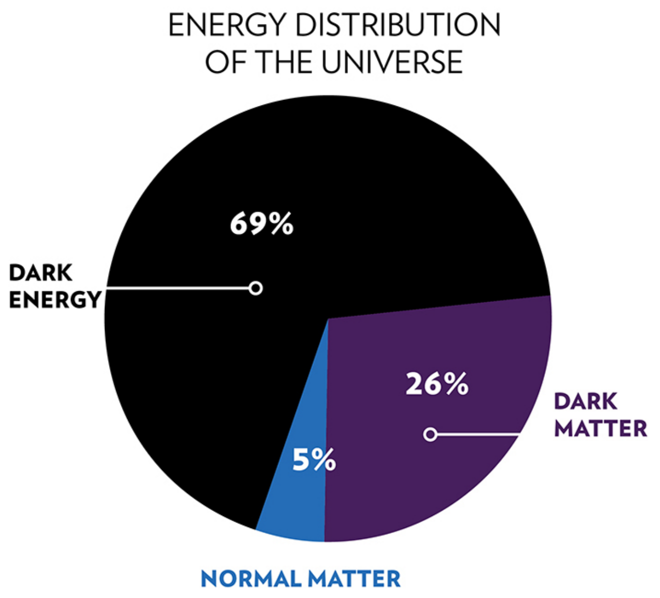
The search for new physics

Precise experiments seek new physics at the "Intensity Frontier"

- Sensitivity to probe the rarest Standard Model interactions
- Search for beyond—Standard-Model effects

EXPERIMENTS USE NUCLEAR TARGETS

NEED TO UNDERSTAND STANDARD MODEL PHYSICS OF PROTONS & NUCLEI

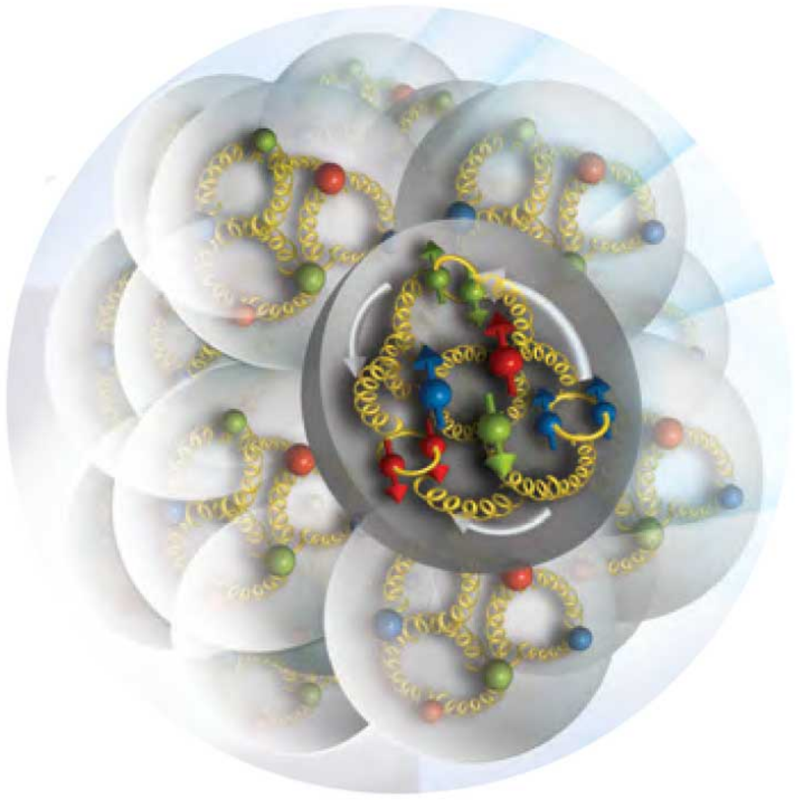


The structure of matter

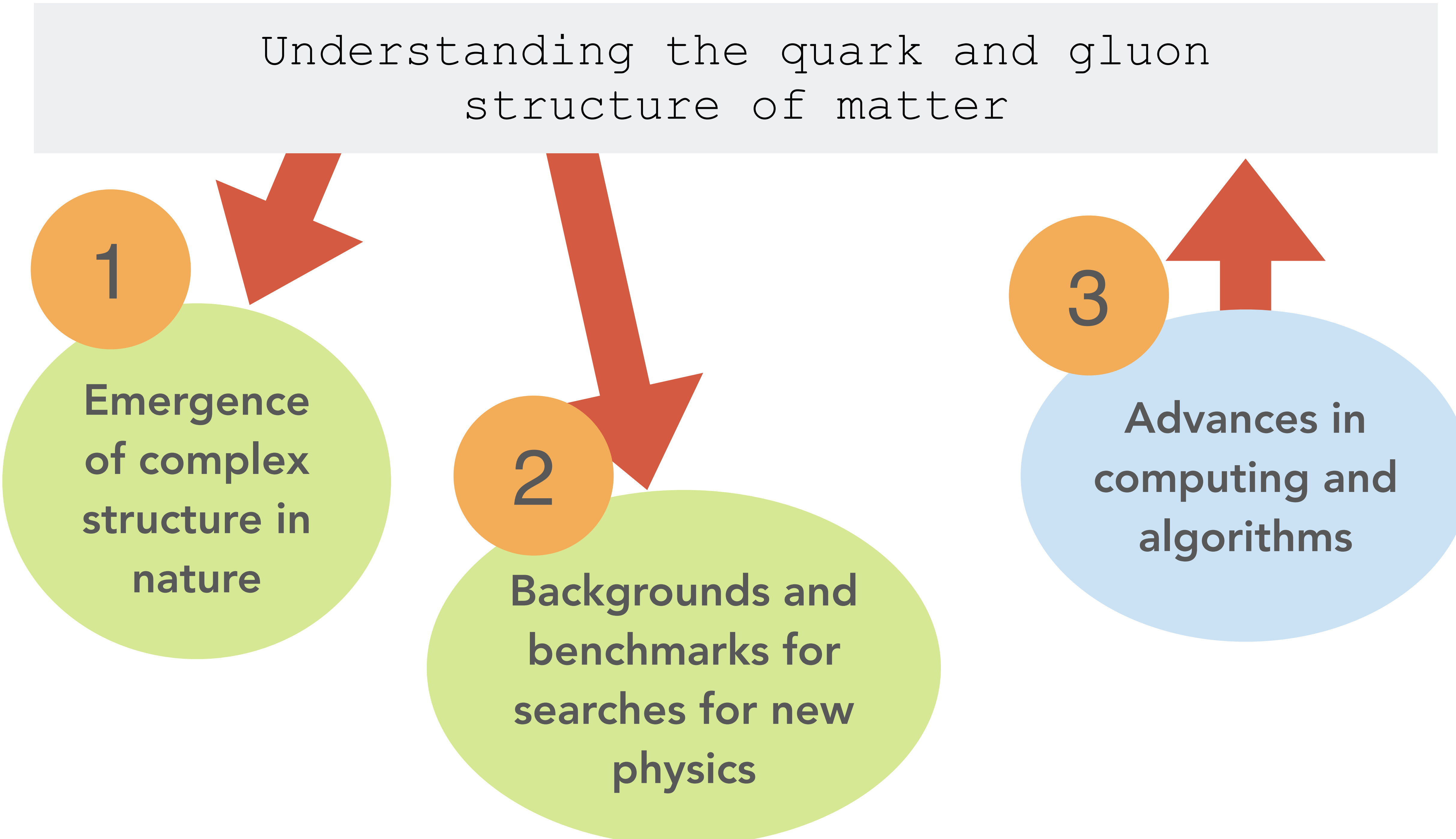
Understanding the quark and gluon structure of matter

Emergence of complex structure in nature

Backgrounds and benchmarks for searches for new physics



The structure of matter

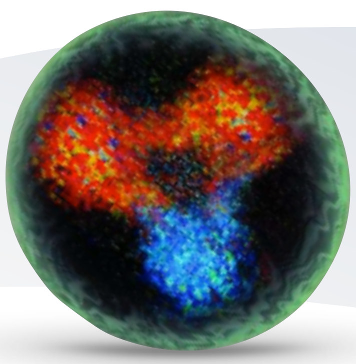


Strong interactions

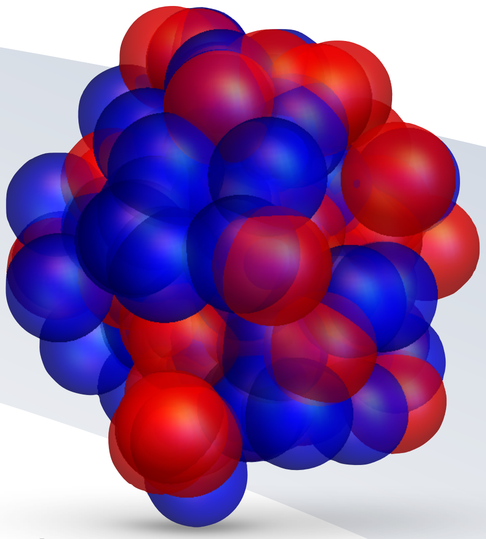
Study nuclear structure from the strong interactions

Quantum Chromodynamics (QCD)

Strongest of the four forces in nature

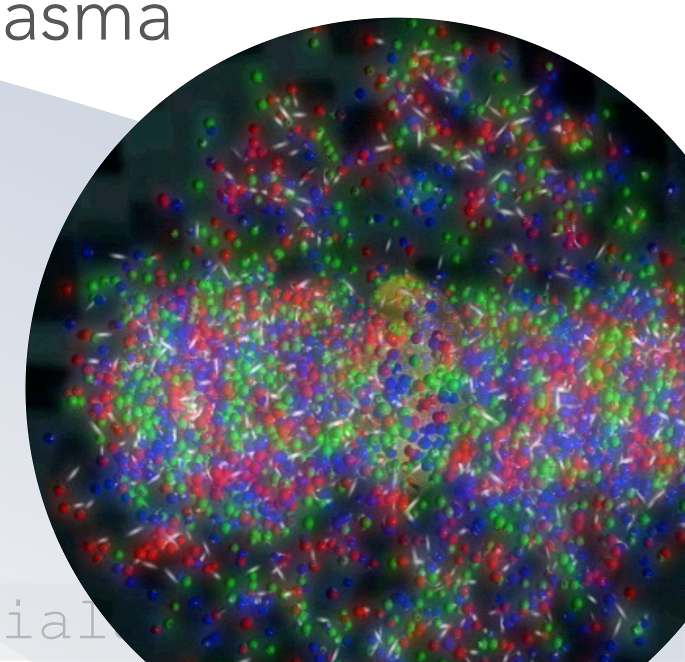


Binds quarks and gluons into protons, neutrons, pions etc.



Binds protons and neutrons into nuclei

Forms other types of exotic matter e.g., quark-gluon plasma



Strong interactions

Interaction strength depends on energy

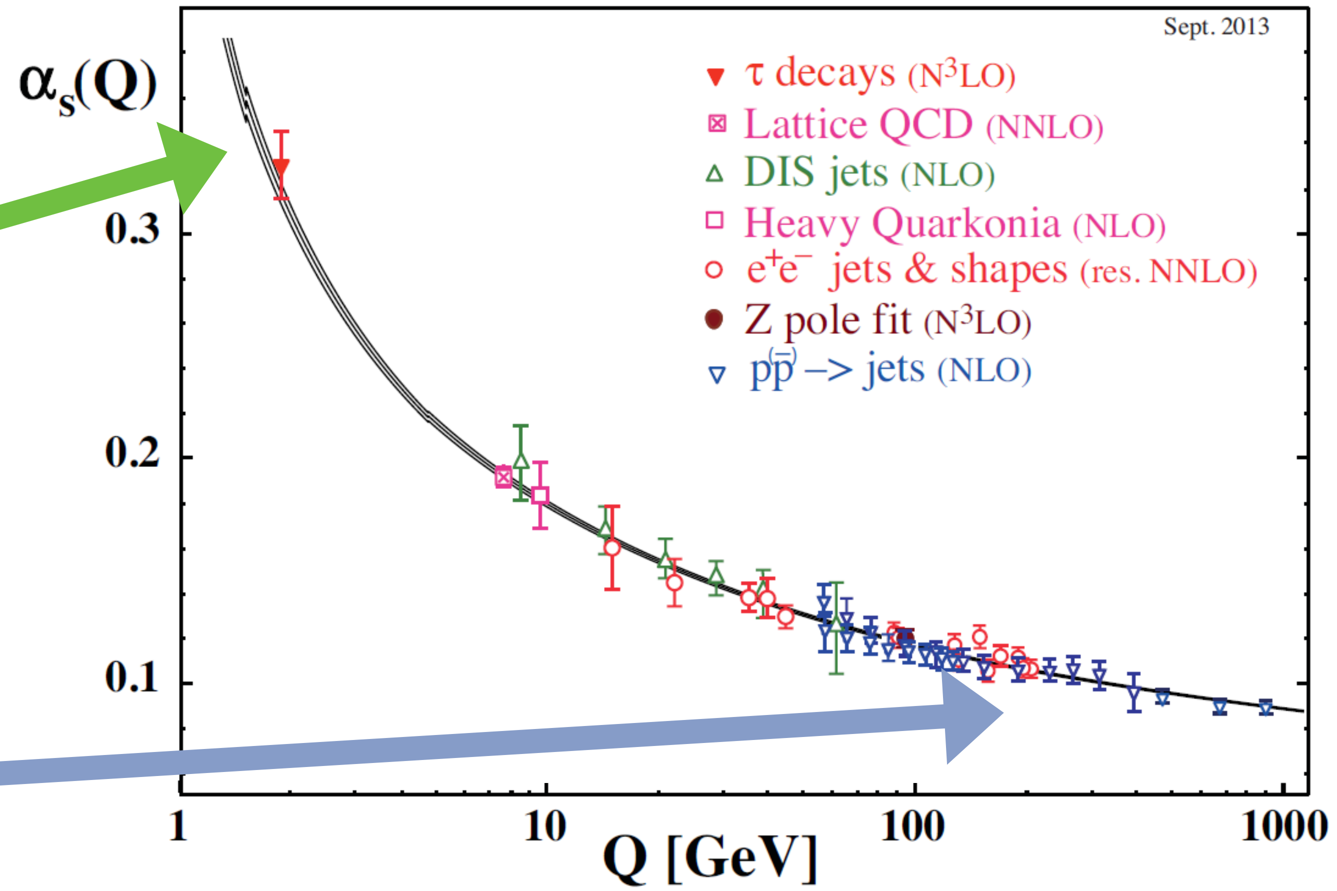
[Gross, Politzer, Wilczek, Nobel 2004]

Low-energy QCD is non-perturbative

Perturbation theory at high energies

$$\mathcal{O}_{\text{exact}} = \mathcal{O}_0 + \mathcal{O}_1\alpha_s + \mathcal{O}_2\alpha_s^2 + \ldots$$

Strong coupling

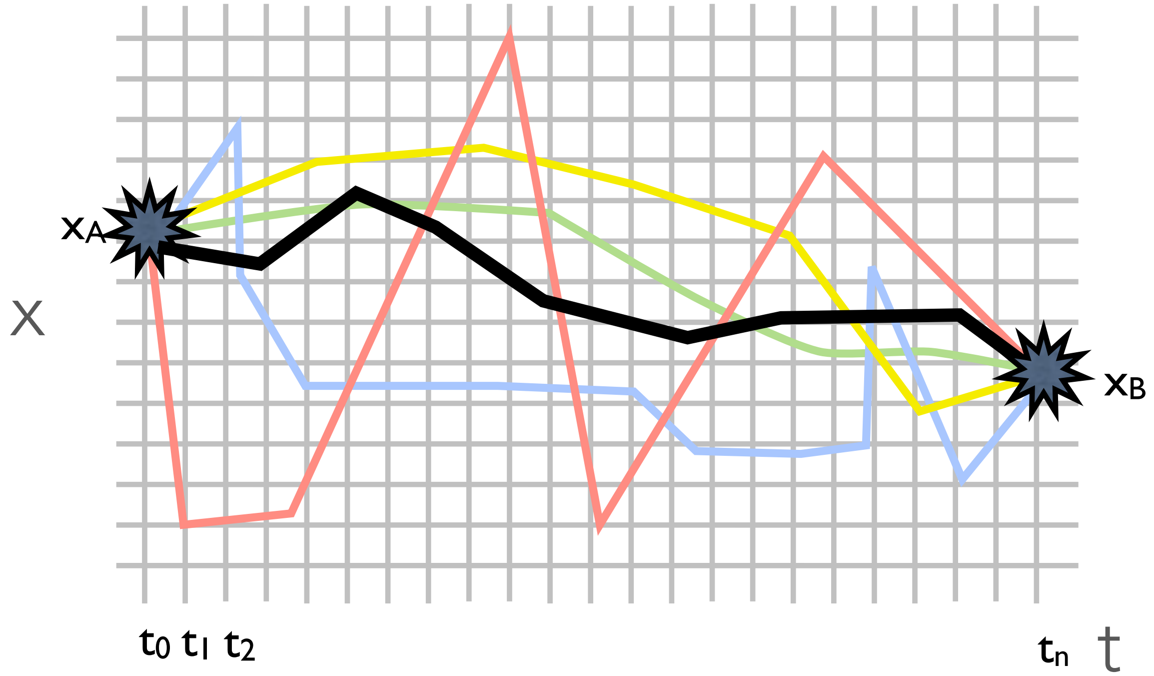


Energy

Lattice QCD

Numerical first-principles approach to non-perturbative QCD

- QCD equations ⟷ integrals over the values of quark and gluon fields on each site/link (QCD path integral)
- ~10^{12} variables (for state-of-the-art)

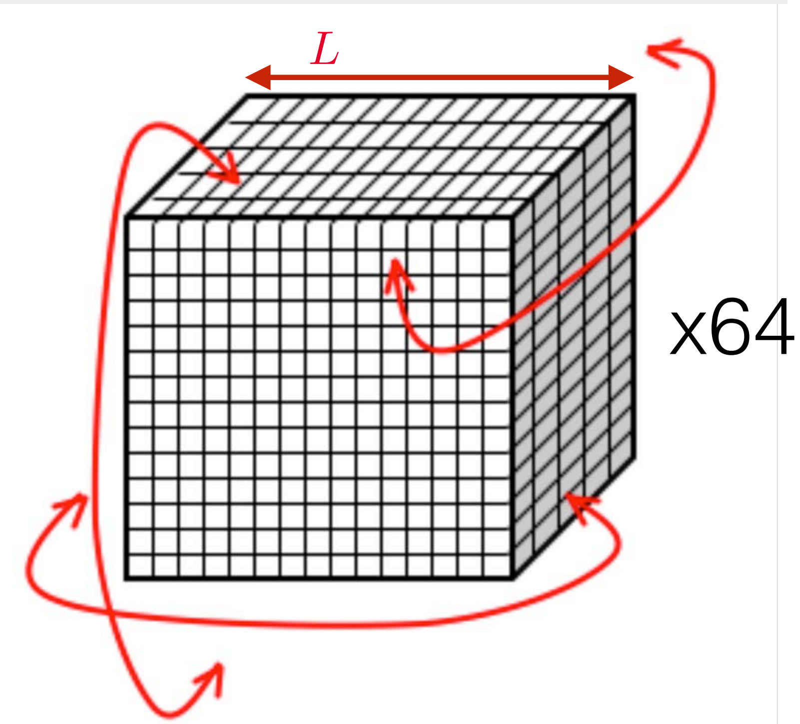


- Evaluate by importance sampling
- Paths near classical action dominate
- Calculate physics on a set (ensemble) of samples of the quark and gluon fields

Lattice QCD

Numerical first-principles approach to non-perturbative QCD

- Euclidean space-time
  - Non-zero lattice spacing a
  - Volume $L^3 \times T \approx 32^3 \times 64$
- Some calculations use larger-than-physical quark masses (cheaper)



Approximate the QCD path integral by **Monte Carlo**

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \mathcal{D}A \mathcal{D}\overline{\psi} \mathcal{D}\psi \mathcal{O}[A, \overline{\psi}\psi] e^{-S[A,\overline{\psi}\psi]} \rightarrow \langle \mathcal{O} \rangle \simeq \frac{1}{N_{\mathrm{conf}}} \sum_{i}^{N_{\mathrm{conf}}} \mathcal{O}([U^i])$$

with field configurations U^i distributed according to $e^{-S[U]}$

Lattice QCD

Numerical first-principles approach to non-perturbative QCD

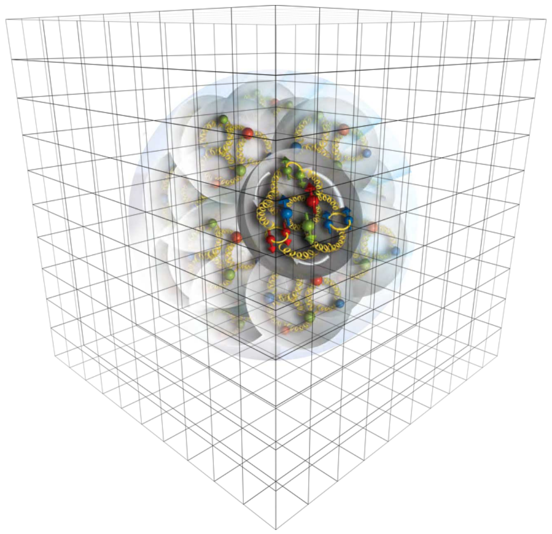
INPUT

Lattice QCD action has same free parameters as QCD: quark masses, α_S

- Fix quark masses by matching to measured hadron masses, e.g., π, K, D_s, B_s for u, d, s, c, b
- One experimental input to fix lattice spacing in GeV (and also α_S), e.g., $2S$-$1S$ splitting in Υ, or f_π or Ω mass

OUTPUT

Calculations of all other quantities are QCD predictions



Lattice QCD

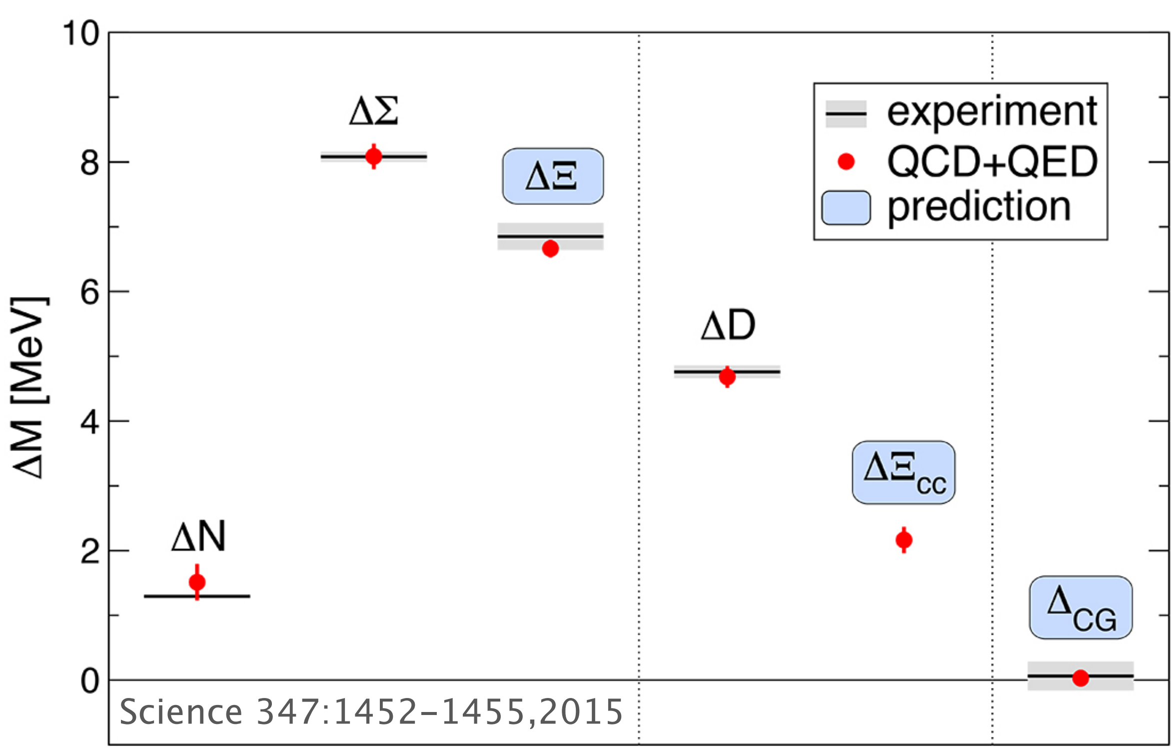
Numerical first-principles approach to non-perturbative QCD

Calculations use world's largest computers

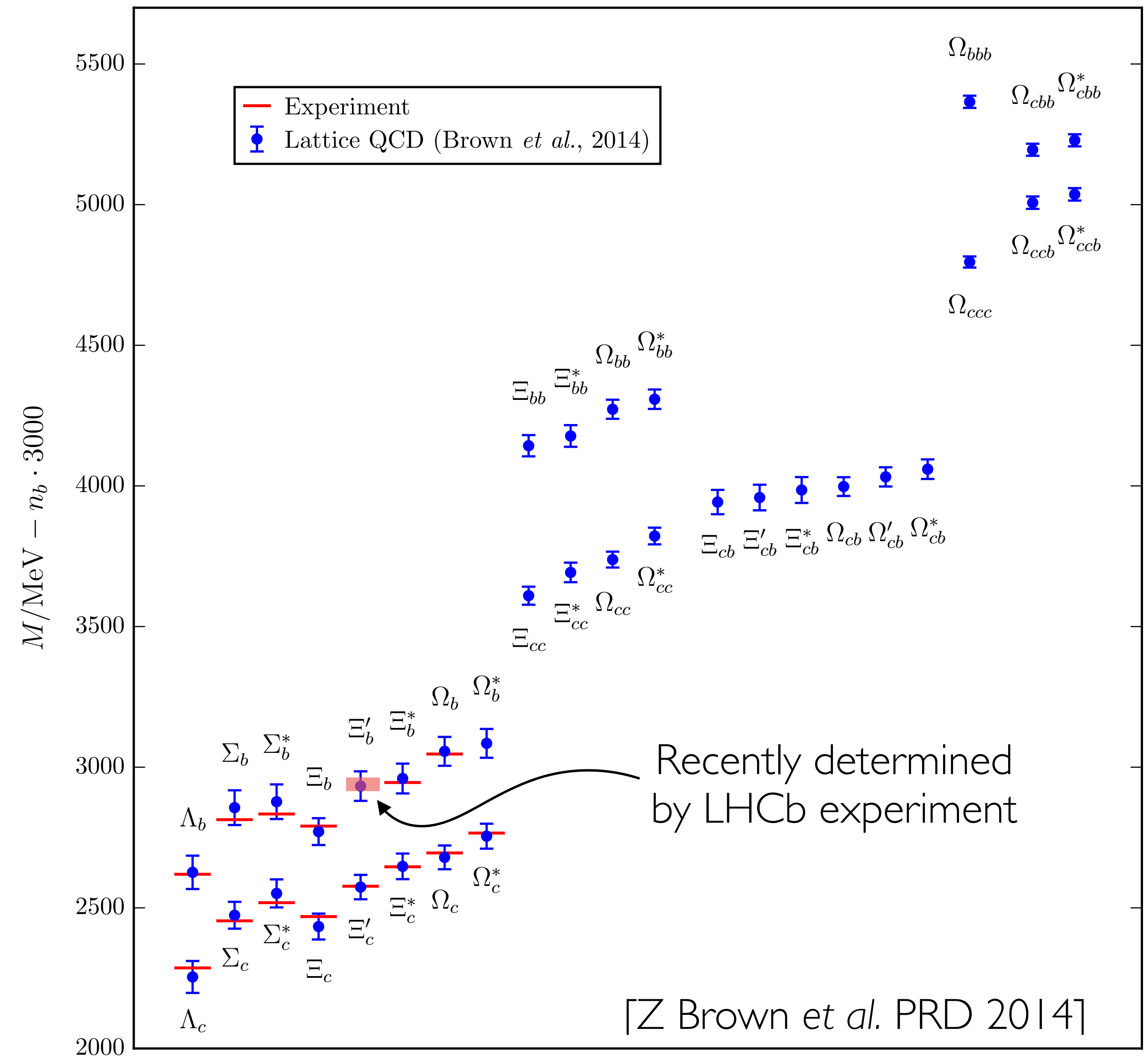
- Many millions of CPU/GPU hours
- Specifically designed processors for QCD

Lattice QCD works

- Ground state hadron spectrum reproduced
- p-n mass splitting reproduced
- …



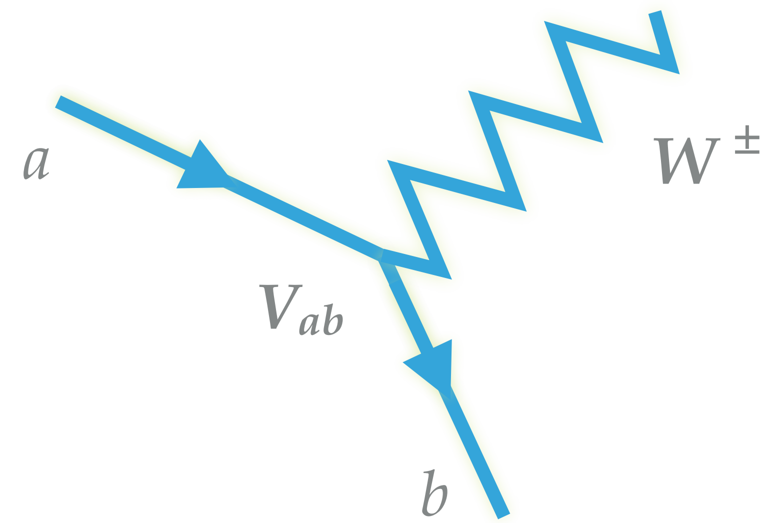
- Predictions for new states with controlled uncertainties



Lattice QCD works

Essential input for flavour physics by constraints on CKM matrix

- CKM matrix determines strength of weak interactions between quark flavours

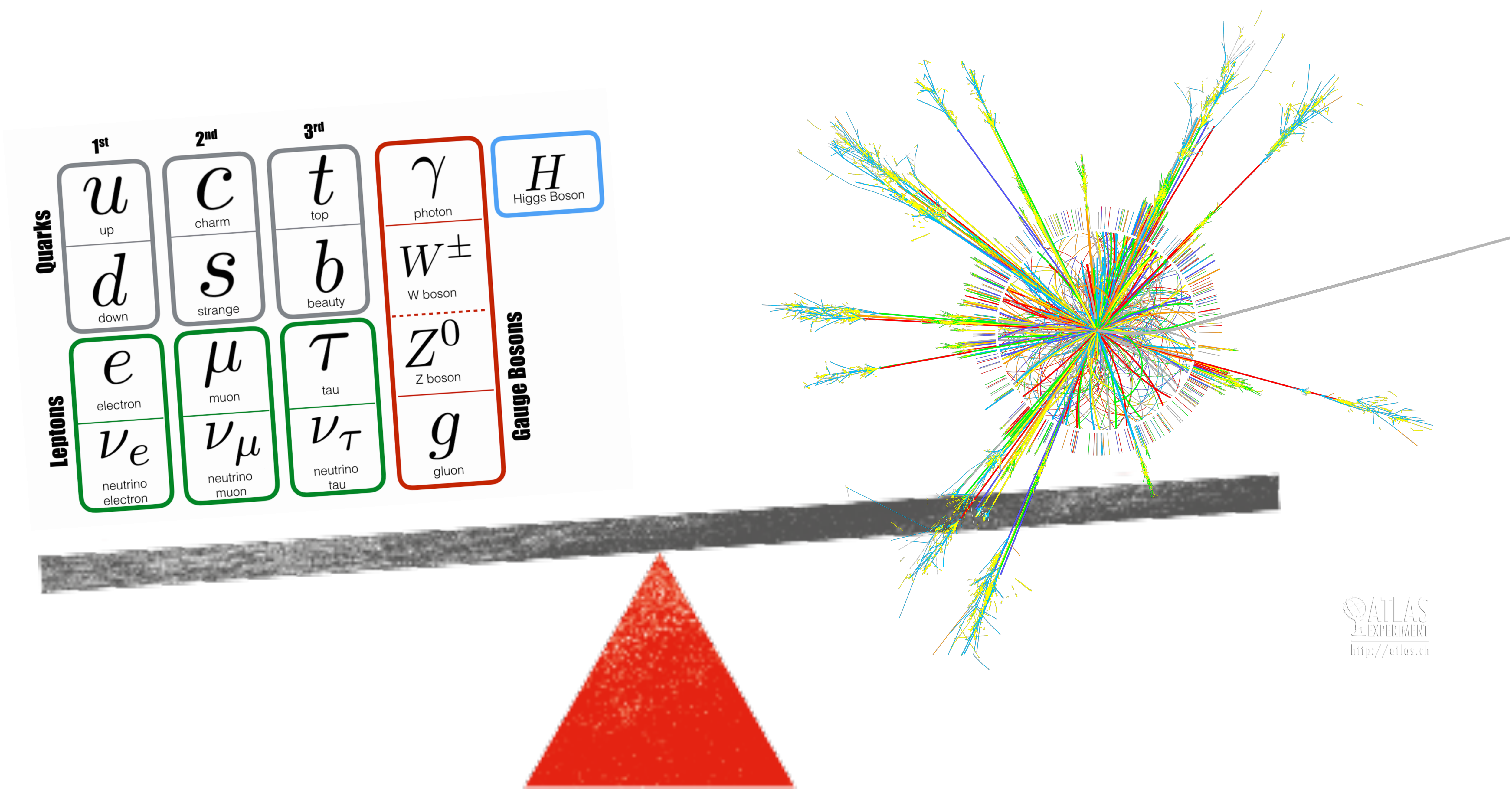


- Parameters are inputs to Standard Model
  → overdetermining CKM tests Standard Model

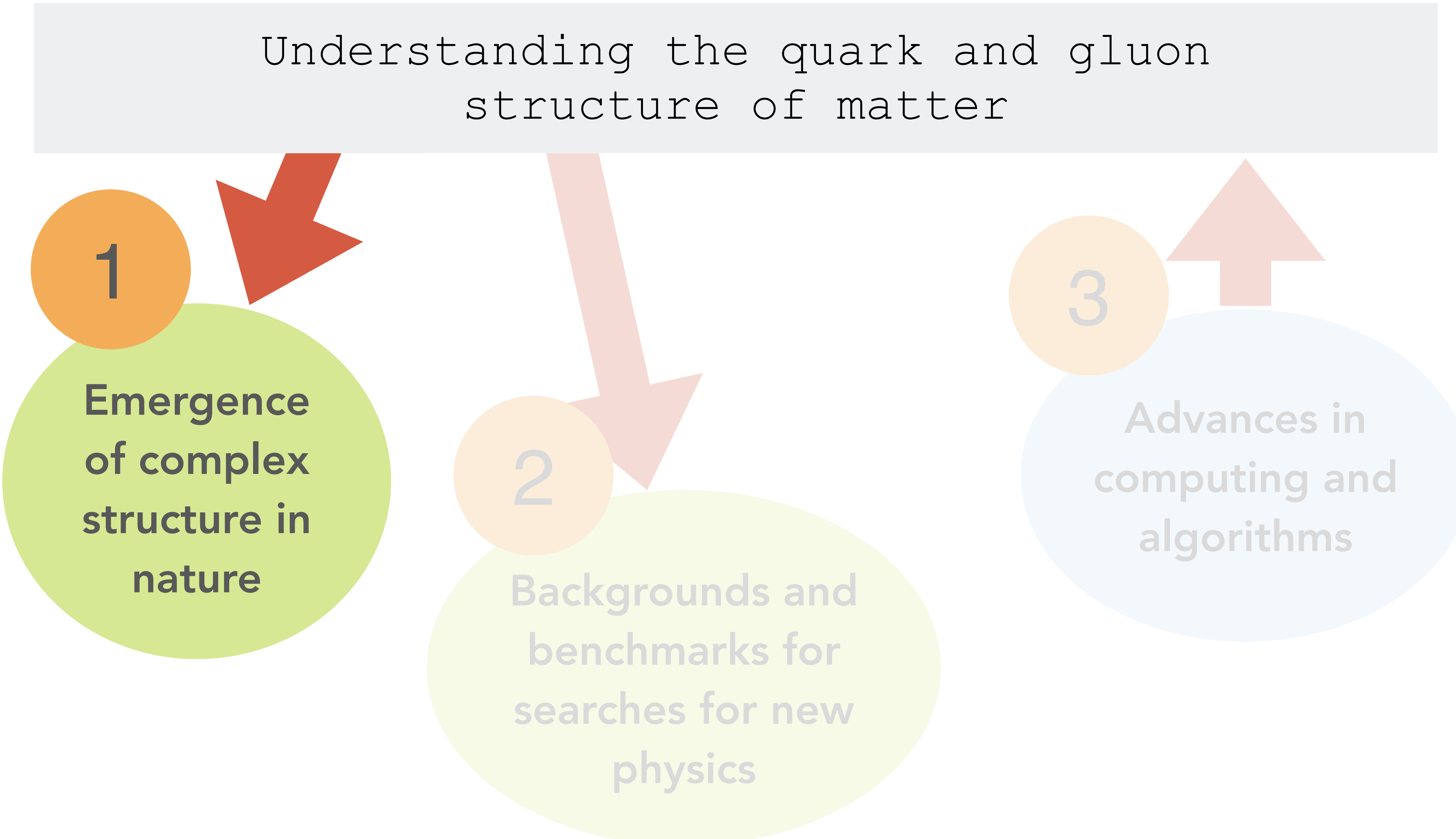
- LQCD critical to extraction of all but V_{td}: a synergy between theory and experiment

[experiment] = [known] x [CKM] x [hadronic matrix element]

Theory complements experiment



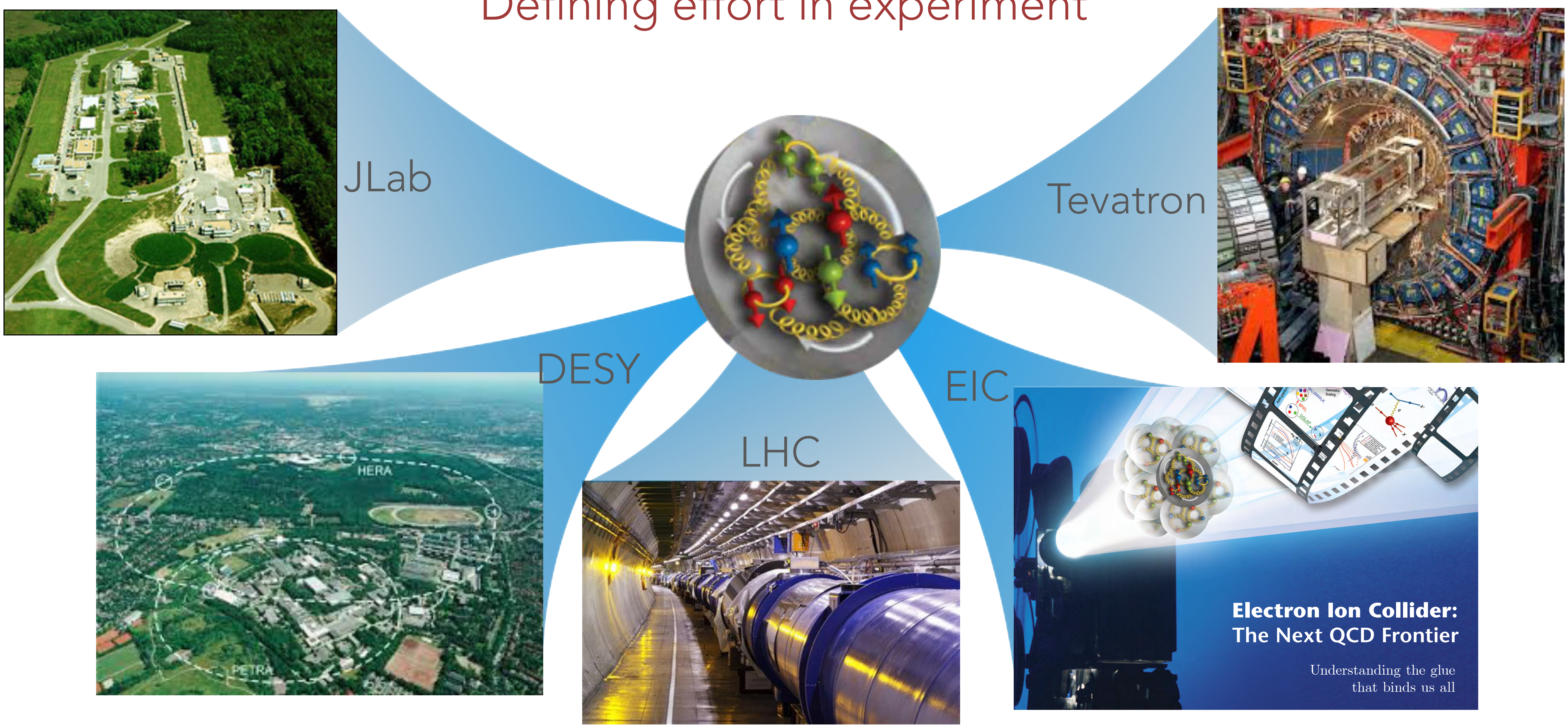
The structure of matter



The structure of matter

Understanding the quark and gluon structure of matter

Defining effort in experiment

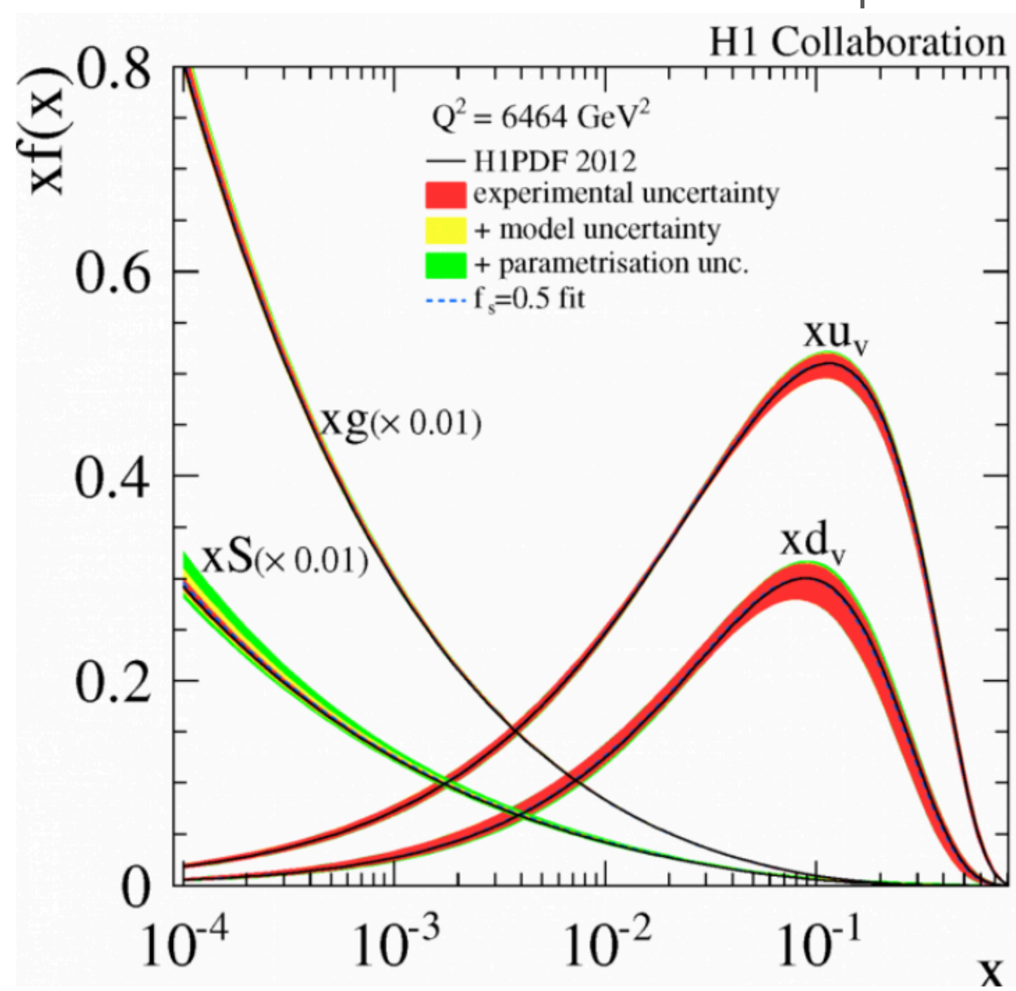


The gluon structure of the nucleon

Gluons offer a new window on proton/nuclear structure

- Past 60+ years: detailed view of quark structure of nucleons
- Gluon structure also important
  - Unpolarised gluon parton distribution function dominant at small longitudinal momentum fraction
- Other aspects of gluon structure relatively unexplored

Parton distributions in the proton



Longitudinal momentum fraction carried by parton

The gluon structure of the nucleon

How much do gluons contribute to the proton's

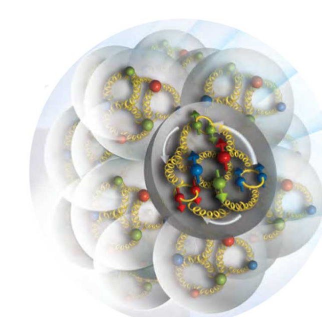
- Momentum
- Mass
- Spin
- D-term

What is the 3D gluon distribution of a proton

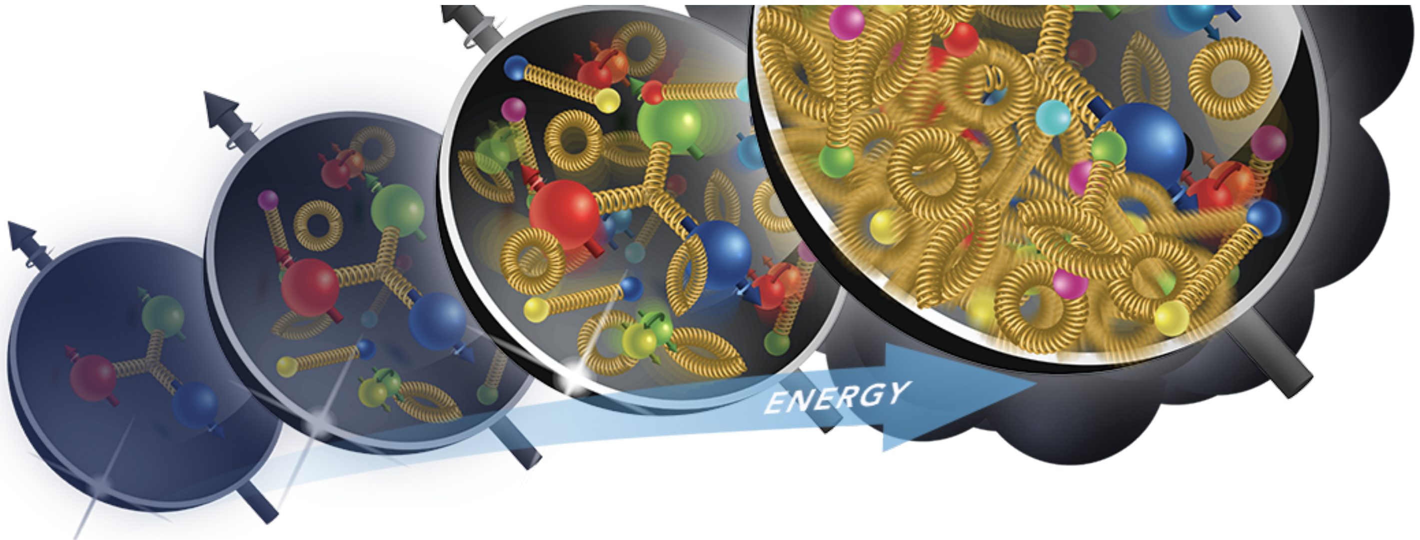
- Encoded in gluon distribution functions and form factors
- Pressure distribution

How is the gluon structure of a proton modified in a nucleus

- Gluon 'EMC' effect
- Exotic glue



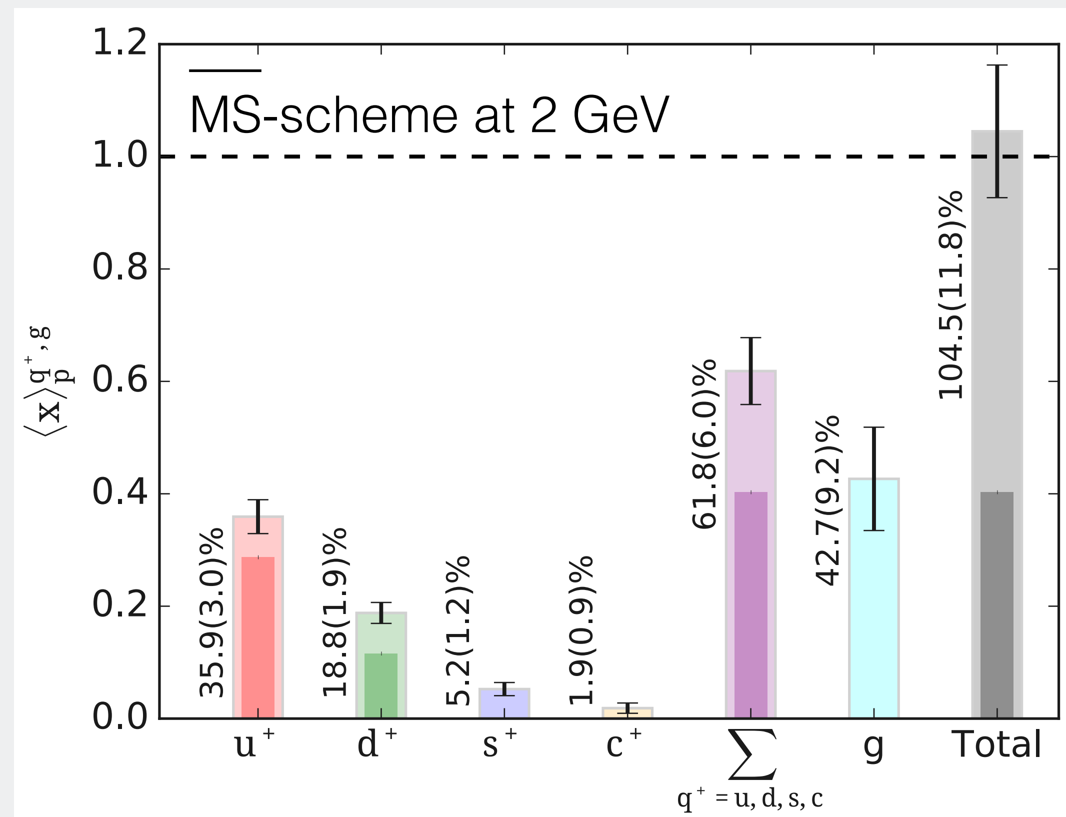
Decomposition of proton momentum



State-of-the-art calculations for simple quantities have:

- Fully-controlled systematic uncertainties competitive with or better than experiment for some quantities
- Separate contributions from
  - Strangeness and light flavours
  - Gluons

2020 Highlight: All terms of proton momentum decomposition calculated



[C. Alexandrou et al., PRD 101 (2020)]

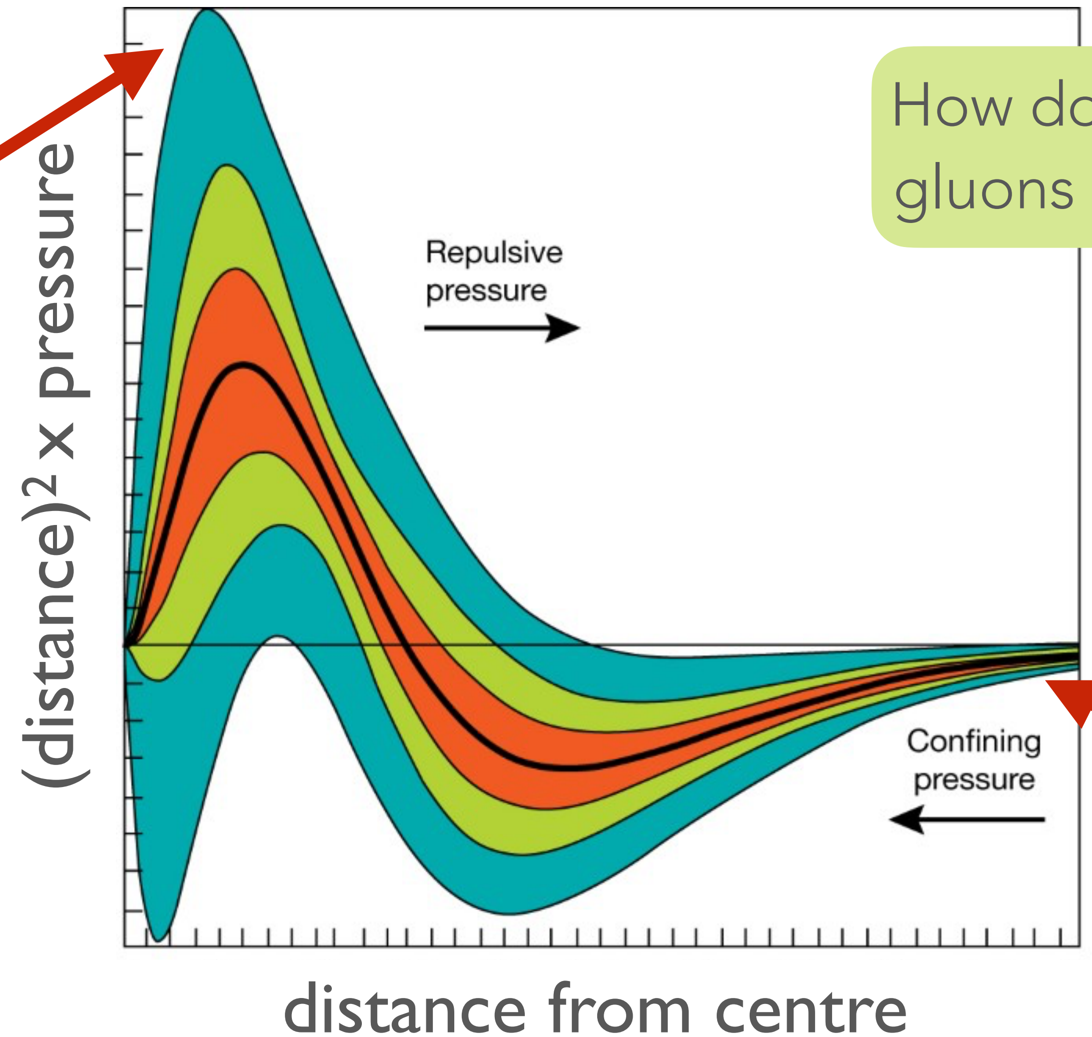
Pressure inside the proton

Quarks are confined inside protons

→ compressive forces must cancel expanding force for stability

What is the peak pressure?

Bike tyre ~10^5 Pa
Ocean floor ~10^8 Pa
Neutron star ~10^{34} Pa
Proton ~??



How do quarks and gluons contribute?

What is the radial extent of the pressure distribution?

Pressure inside the proton

Recent experimental extraction of proton's pressure distribution

[V. D. Burkert et al, Nature 557, 396 (2018)]

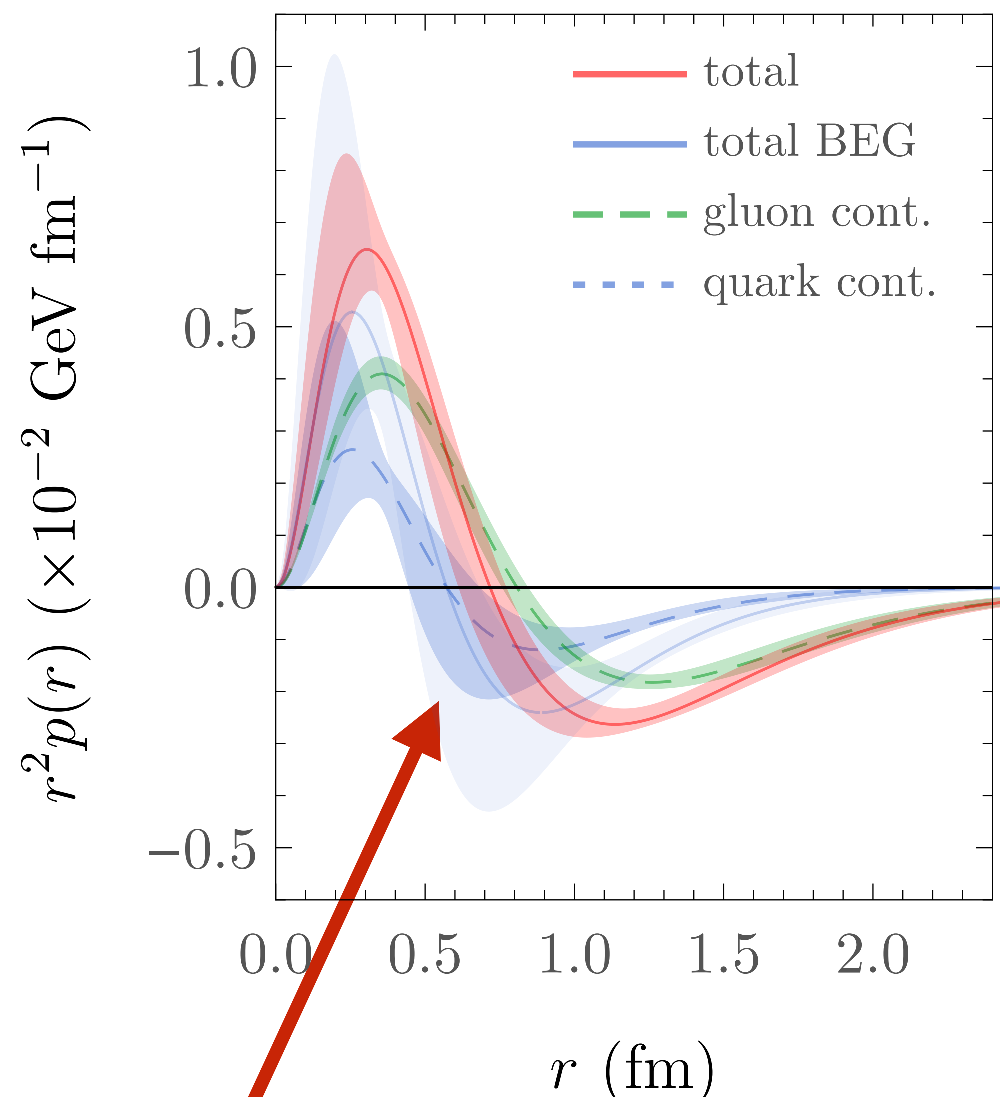
- Peak pressure near the centre ~1035 Pascal > pressure estimated for neutron stars
- Experiment only sensitive to quark contributions, not to gluons

EXPERIMENT + LQCD

[Shanahan, Detmold PRL 122 072003 (2019)]

- First complete pressure determination
- Gluons change the picture!
- Explore kinematics needed in future experiments

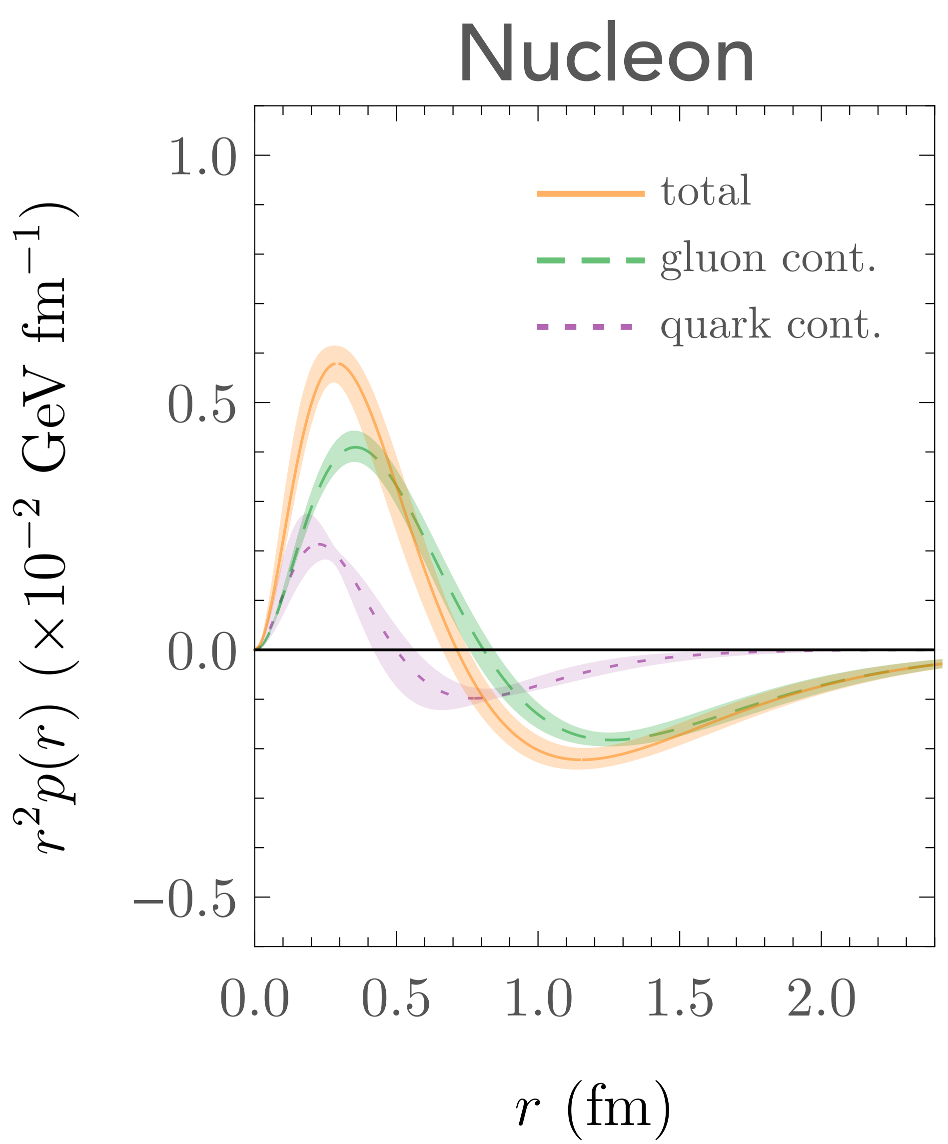
Radial pressure distribution

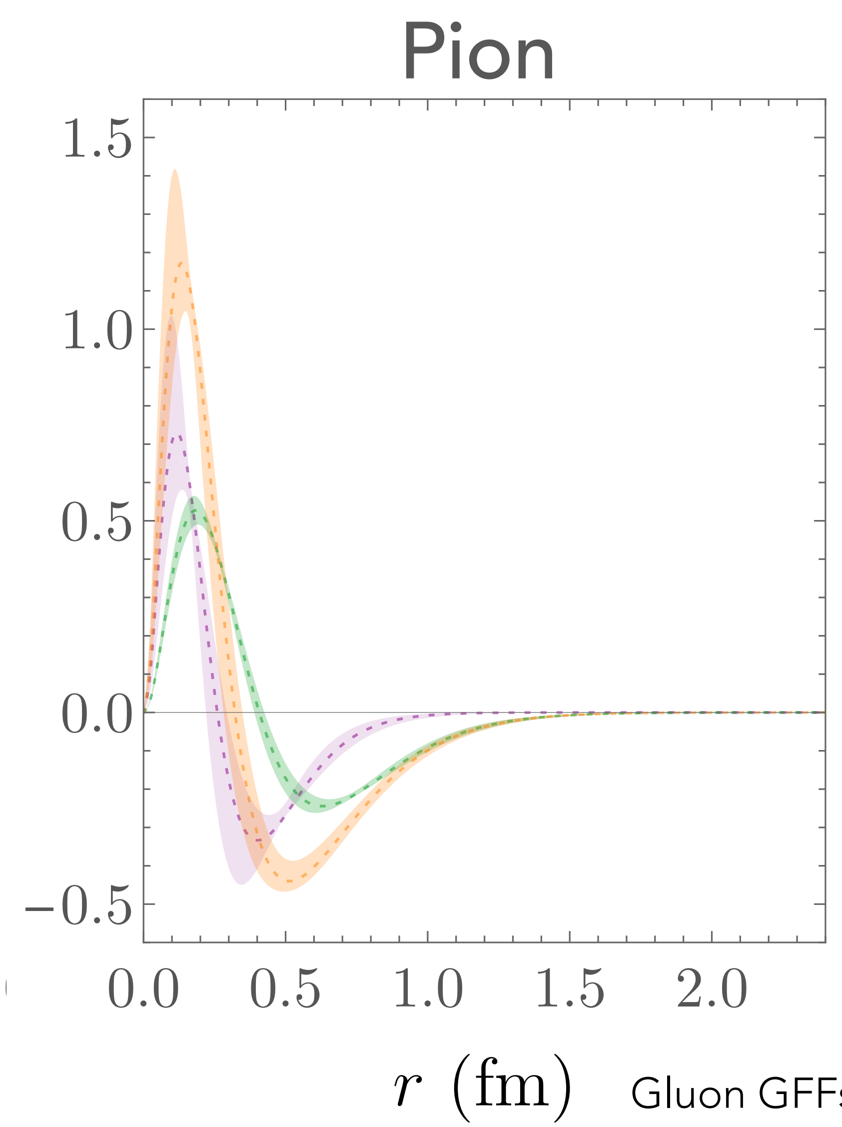


Blue → Red:
gluon contribution shifts peaks, extends region over which pressure is non-zero

Next: pressure distribution in nuclei

Pressure in light nuclei c.f. pressure in the nucleon?





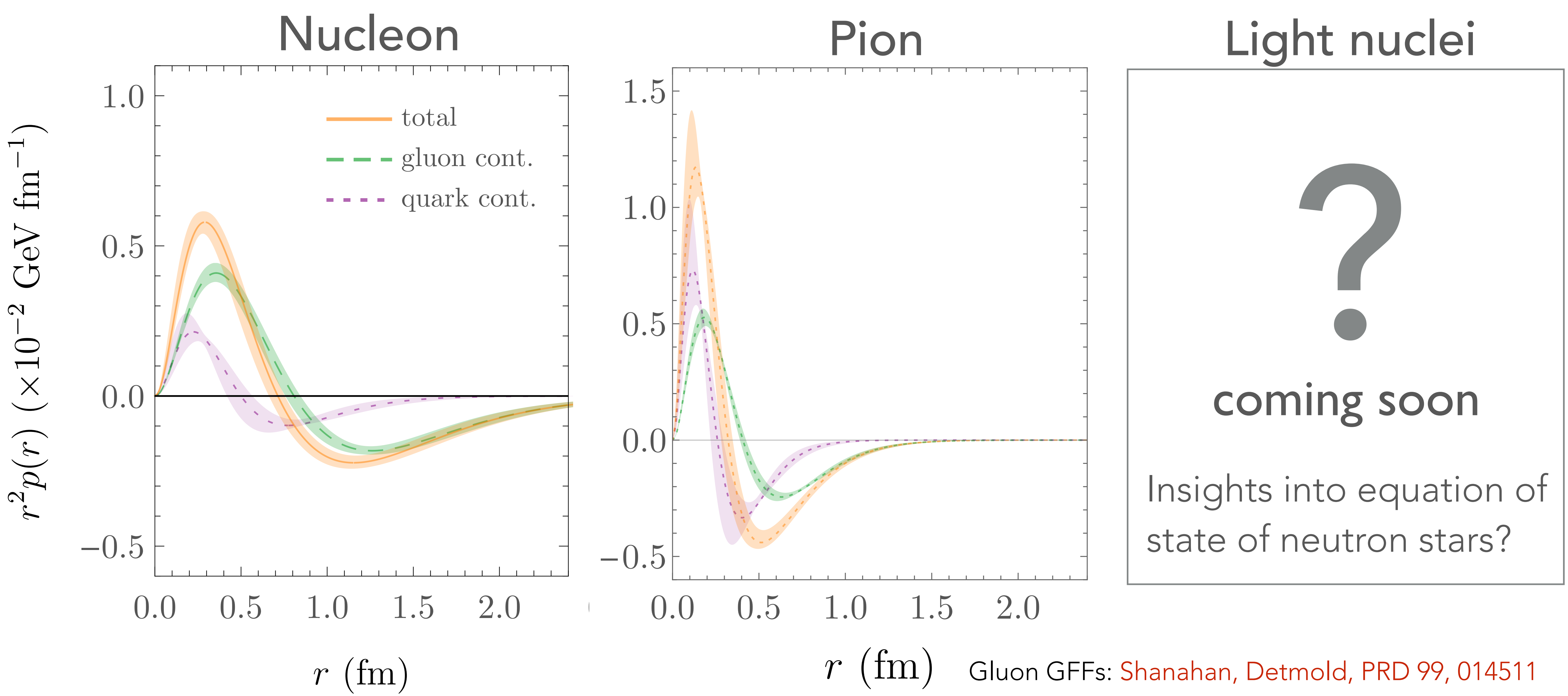
Pion & Nucleon quark and gluon momentum fractions consistent within uncertainties, but very different pressure distributions

Gluon GFFs: Shanahan, Detmold, PRD 99, 014511

Quark GFFs: P. Hägler et al. (LHPC), PRD77, 094502 (2008)

Next: pressure distribution in nuclei

Pressure in light nuclei
c.f. pressure in the nucleon?

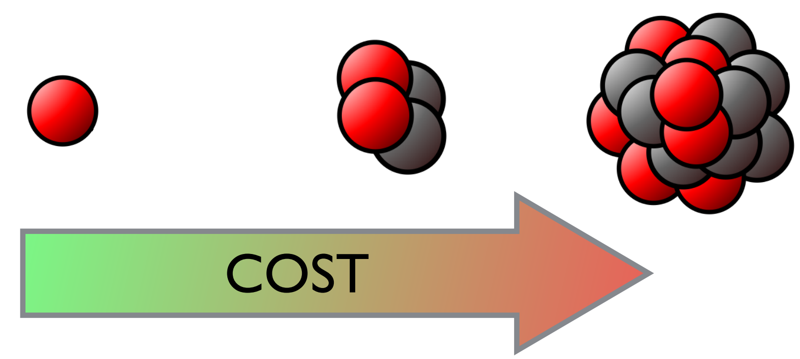


Gluon GFFs: Shanahan, Detmold, PRD 99, 014511

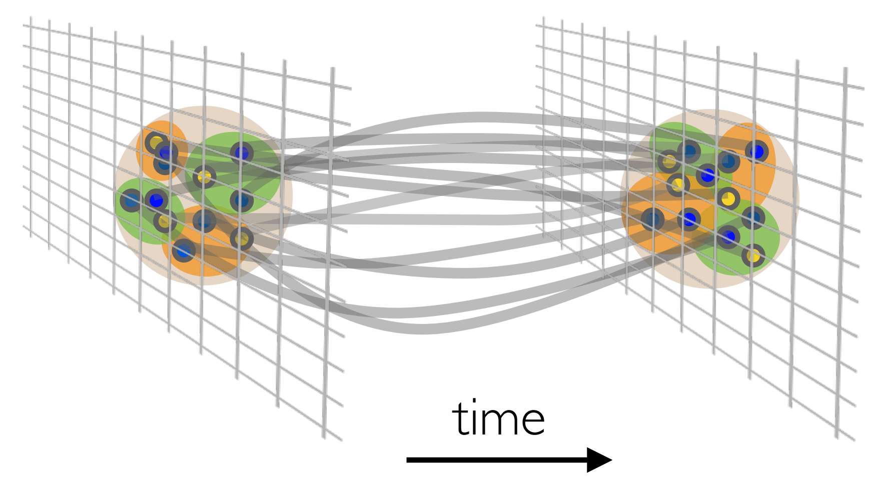
Quark GFFs: P. Hägler et al. (LHPC), PRD77, 094502 (2008)

Nuclear physics from lattice QCD

Nuclei on the lattice are HARD



- **Noise:**
  Statistical uncertainty grows exponentially with number of nucleons



- **Complexity:**
  Number of contractions grows factorially

Calculations possible for A<5

Nuclear physics from lattice QCD

- Nuclear physics from lattice QCD Collaboration

- Nuclei with A<5 unphysical quark masses
- First calculation of spectrum of light nuclei in 2013

Other lattice studies of nuclei:

PACS-CS e.g. ,Yamazaki et al, Phys.Rev.D 92 (2015);

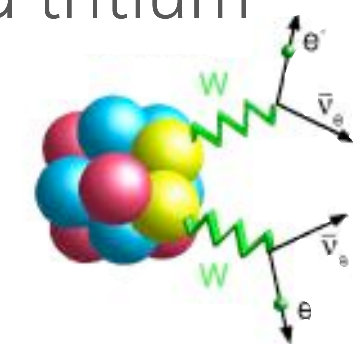
Callatt e.g., E Berkowitz et al, Phys.Lett.B 765 (2017) 285

Mainz e.g., A. Francis et al, Phys.Rev.D 99 (2019)

HALQCD e.g., Ishii et al, Phys.Rev.Lett. 99 (2007) (potential approach)

Recent highlights

- Proton-proton fusion and tritium β-decay
  [PRL 119, 062002 (2017)]

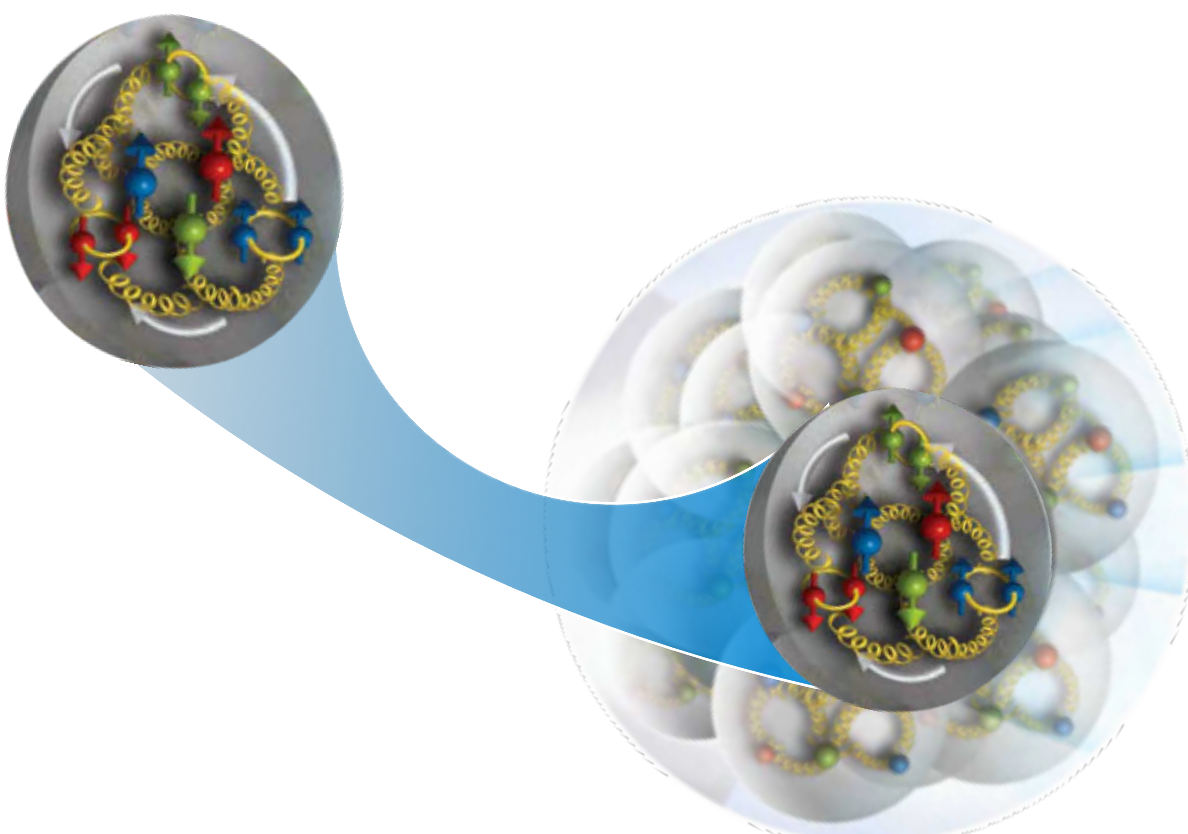


- Double β-decay
  [PRL 119, 062003 (2017), PRD 96, 054505 (2017)]
- Gluon structure of light nuclei
  [PRD 96 094512 (2017)]
- Scalar, axial, tensor MEs
  [PRL 120 152002 (2018)]
- Baryon-baryon interactions, including QED
  [2003.12130, 2009.12357]
- EMC-type effects in light nuclei
  [2009.05522]

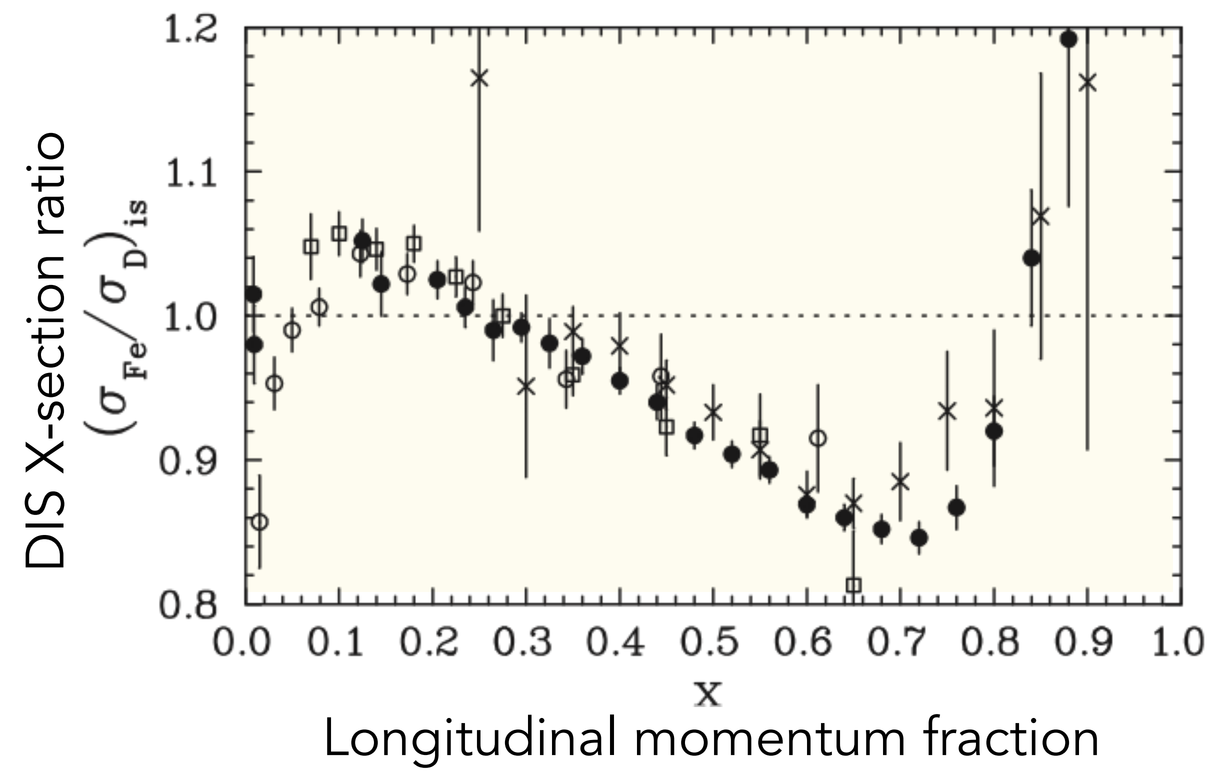
The structure of matter

Understanding the quark and gluon structure of matter

How is the partonic structure of nucleons modified in nuclei?



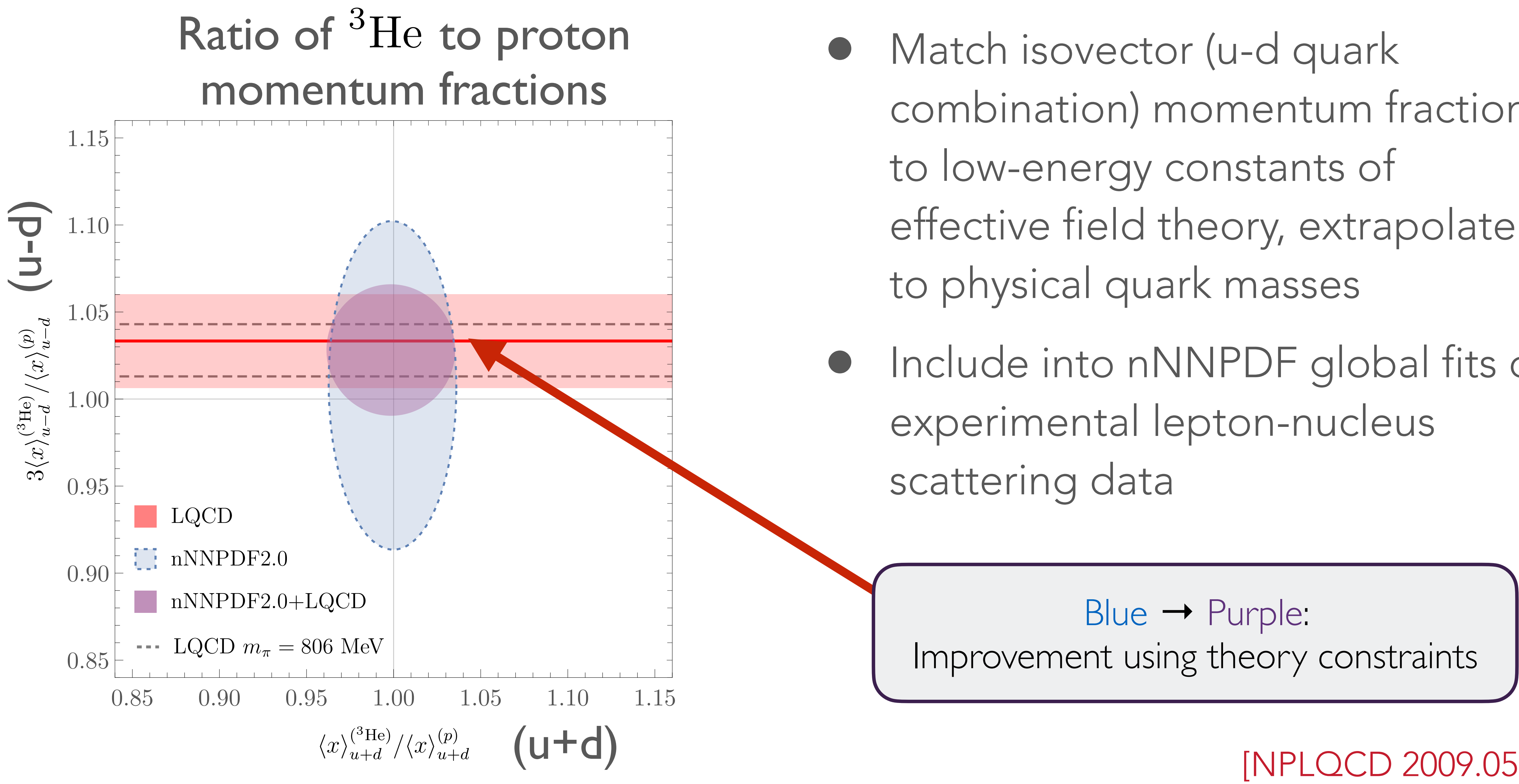
Encoded in EMC-type effects



(EMC: Aubert et al., 1983)

Momentum fraction of ^{3}He

Study nuclear effects in the breakdown of momentum carried by quarks in nuclei



- Match isovector (u-d quark combination) momentum fraction to low-energy constants of effective field theory, extrapolate to physical quark masses
- Include into nNNPDF global fits of experimental lepton-nucleus scattering data

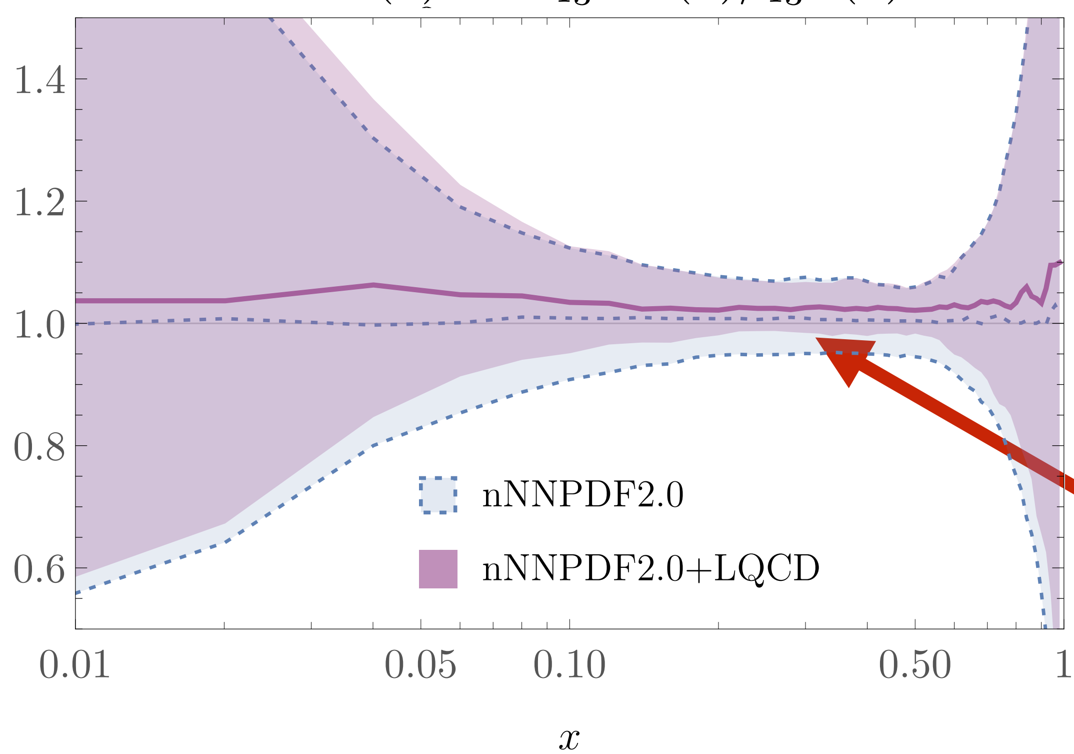
[NPLQCD 2009.05522 (2020)]

Momentum fraction of ^{3}He

Study nuclear effects in the breakdown of momentum carried by quarks in nuclei

Ratio of ^{3}He to proton parton distributions

$$R^{(^3\text{He})}(x) = 3q_3^{(^3\text{He})}(x)/q_3^{(p)}(x)$$



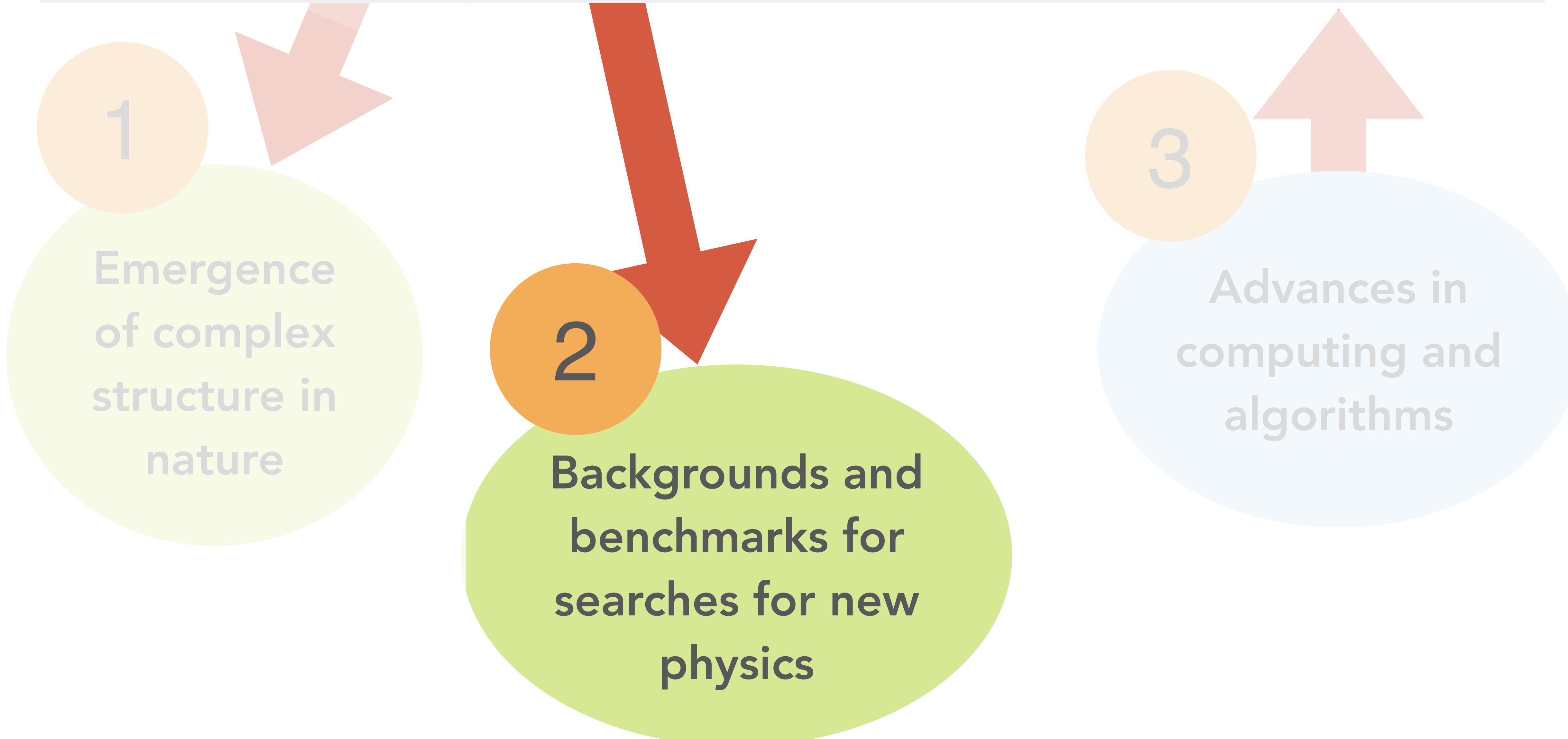
- Match isovector (u-d quark combination) momentum fraction to low-energy constants of effective field theory, extrapolate to physical quark masses
- Include into nNNPDF global fits of experimental lepton-nucleus scattering data

Blue → Purple:
Improvement using theory constraints

[NPLQCD 2009.05522 (2020)]

The structure of matter

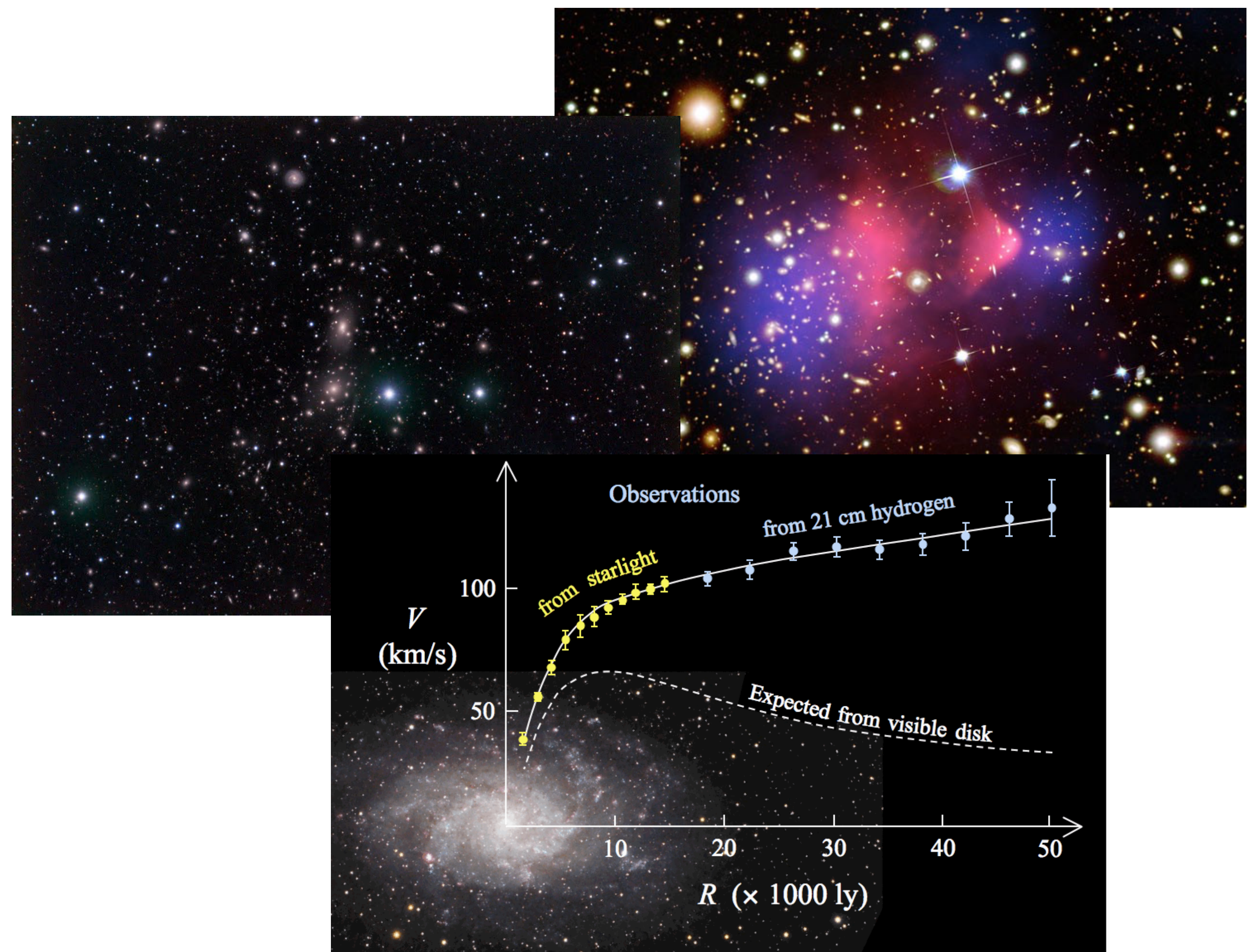
Understanding the quark and gluon structure of matter



The structure of matter

Compelling evidence for dark matter

- Rotation curves
- Lensing
- Structure formation
- Cosmic microwave background

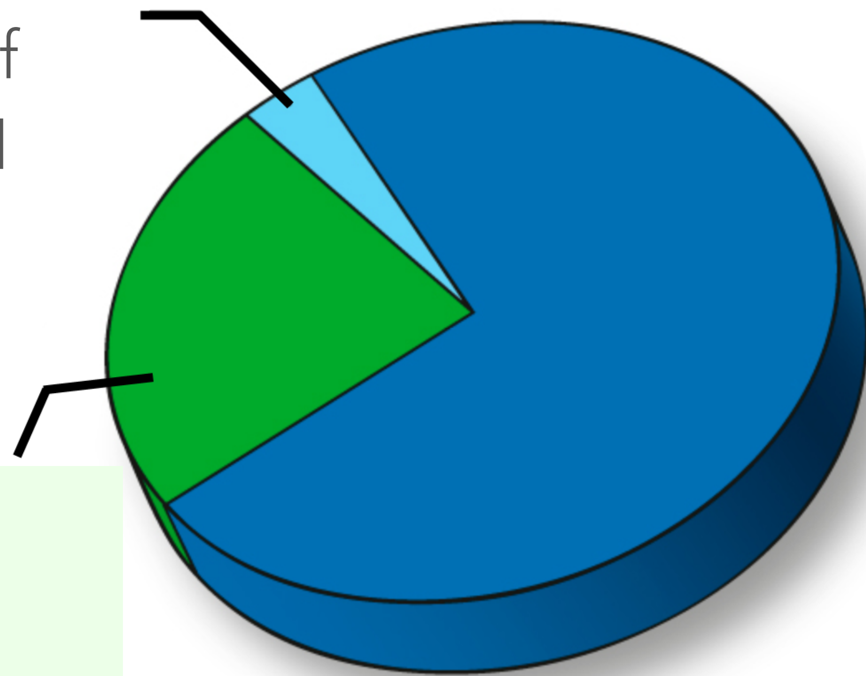


Dark matter

5%

Normal matter

The building blocks of stars and planets (and everything on Earth).



69 %

Dark energy

Something that we don't understand… but it's not matter.

Responsible for the accelerating expansion of the universe

26 %

Dark matter

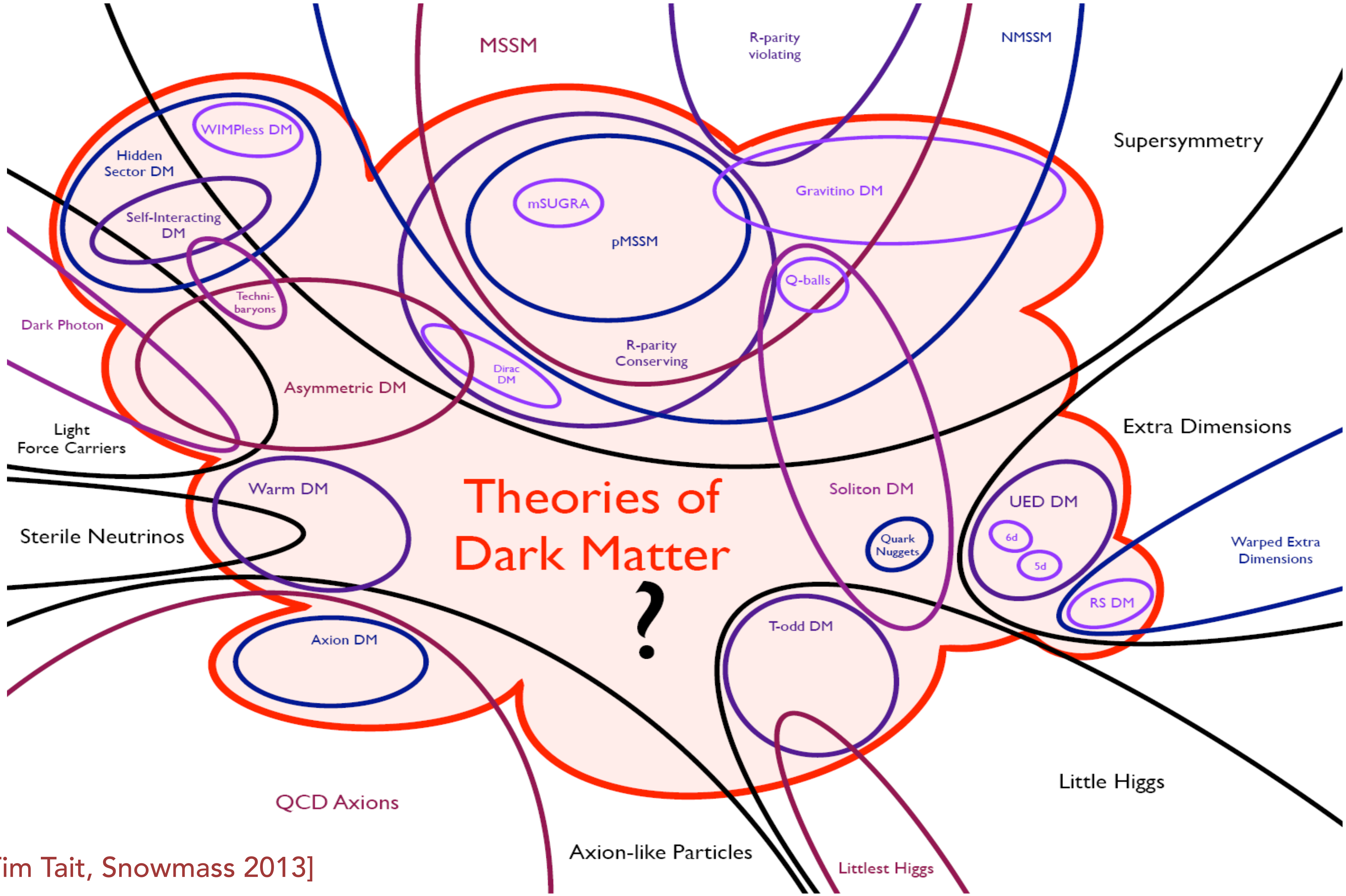
Matter that we don't understand.

Doesn't emit or absorb light. Interacts through gravity.

Many models for dark matter!

BUT few constraints

Dark matter



[Tim Tait, Snowmass 2013]

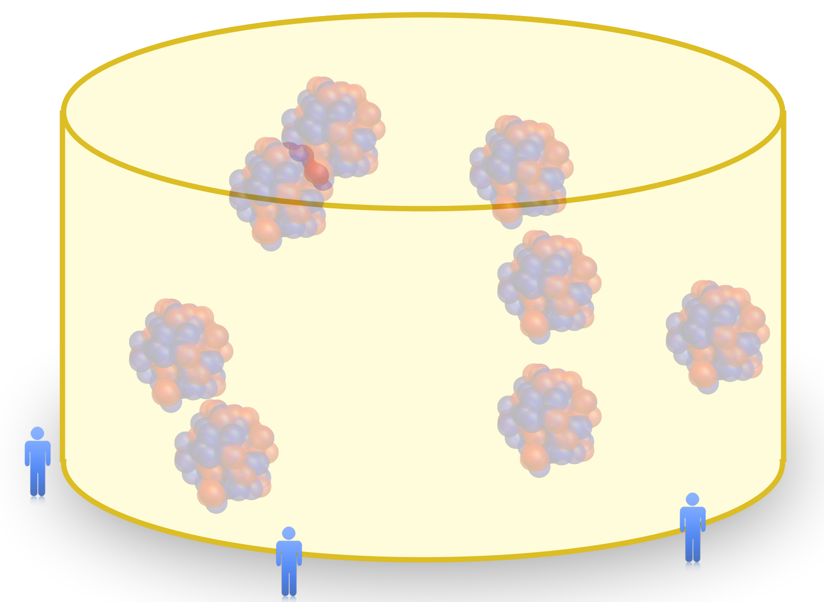
Dark matter

How do we find dark matter?

- Dark (does not interact with light)
- Interacts through gravity

WIMP
Weakly-interacting massive particles

Direct detection
Wait for DM to hit us



Detection rate depends on

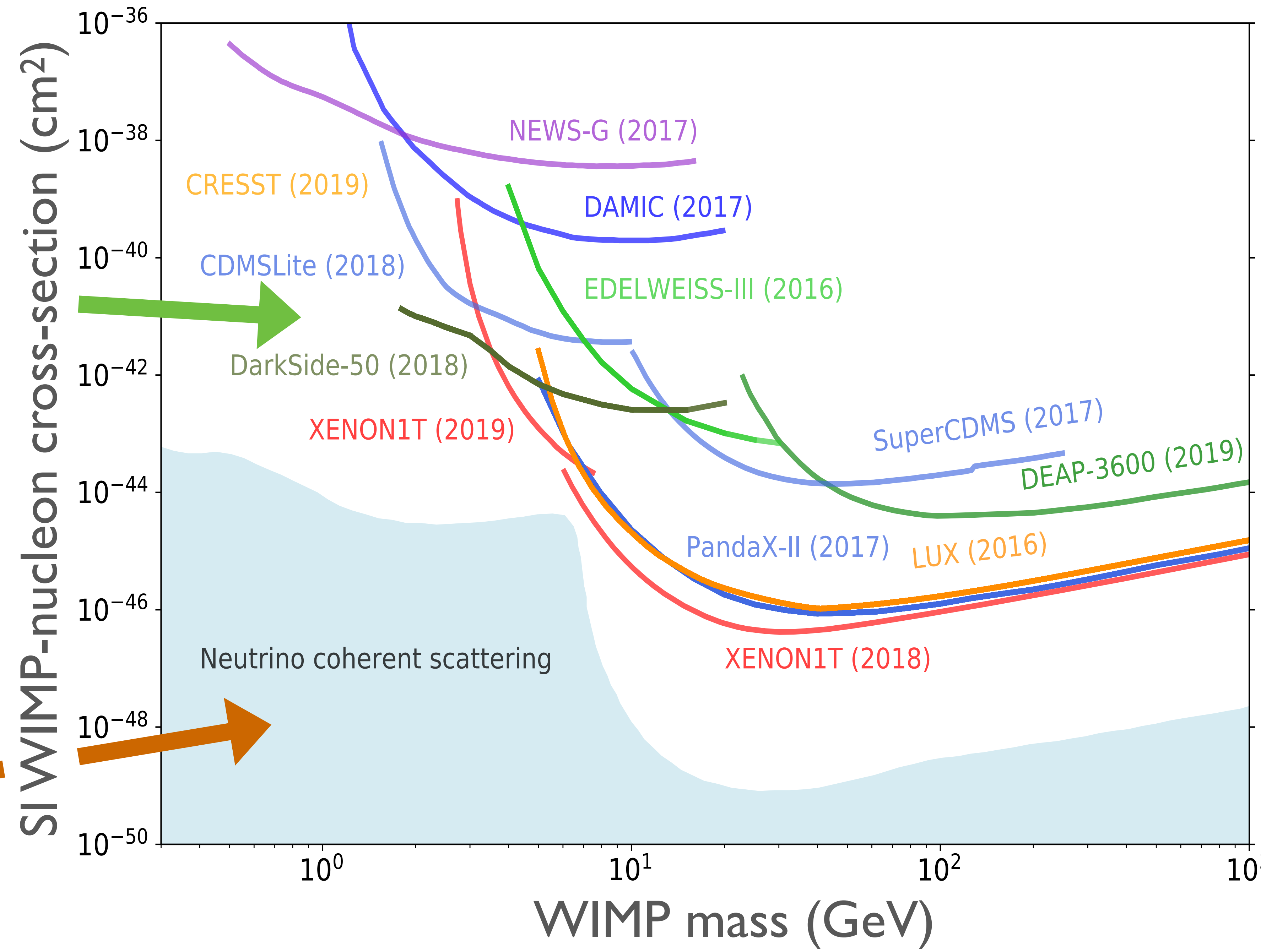
- Dark matter properties
- Probability for interaction with nucleus

Dark matter direct detection

Limits on WIMP-nucleon interaction from direct detection experiments

Ruled out above the lines

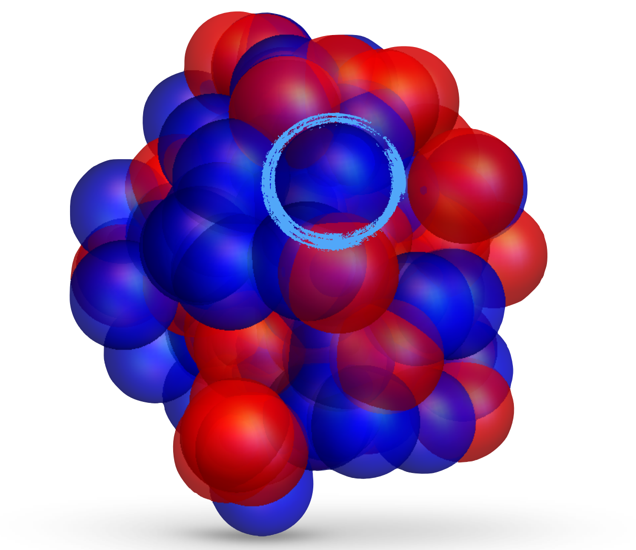
Background



Dark matter direct detection

Direct detection experiments use nuclear targets e.g., Xenon

Determine interaction cross-section (with nucleus) for a given dark matter model



- Born approximation – interacts with a single nucleon

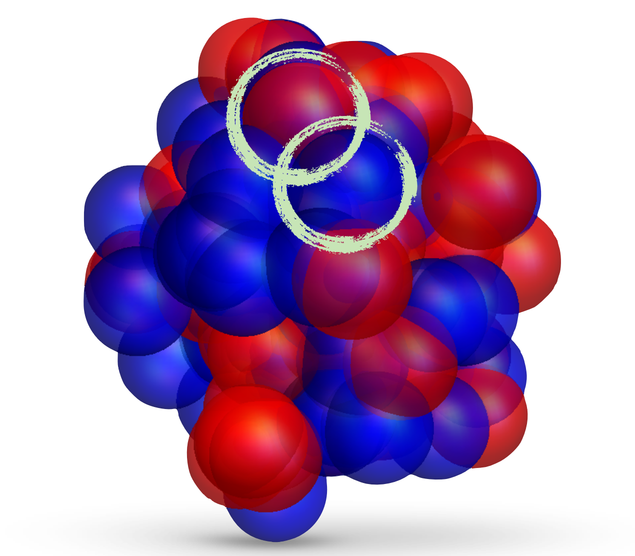
$$\sigma \sim |A \langle N|DM|N\rangle|^2$$

known from lattice QCD

- Interacts non-trivially with multiple nucleons

$$\sigma \sim |A \langle N|DM|N\rangle + \alpha \langle NN|DM|NN\rangle + \ldots|^2$$

Not known!

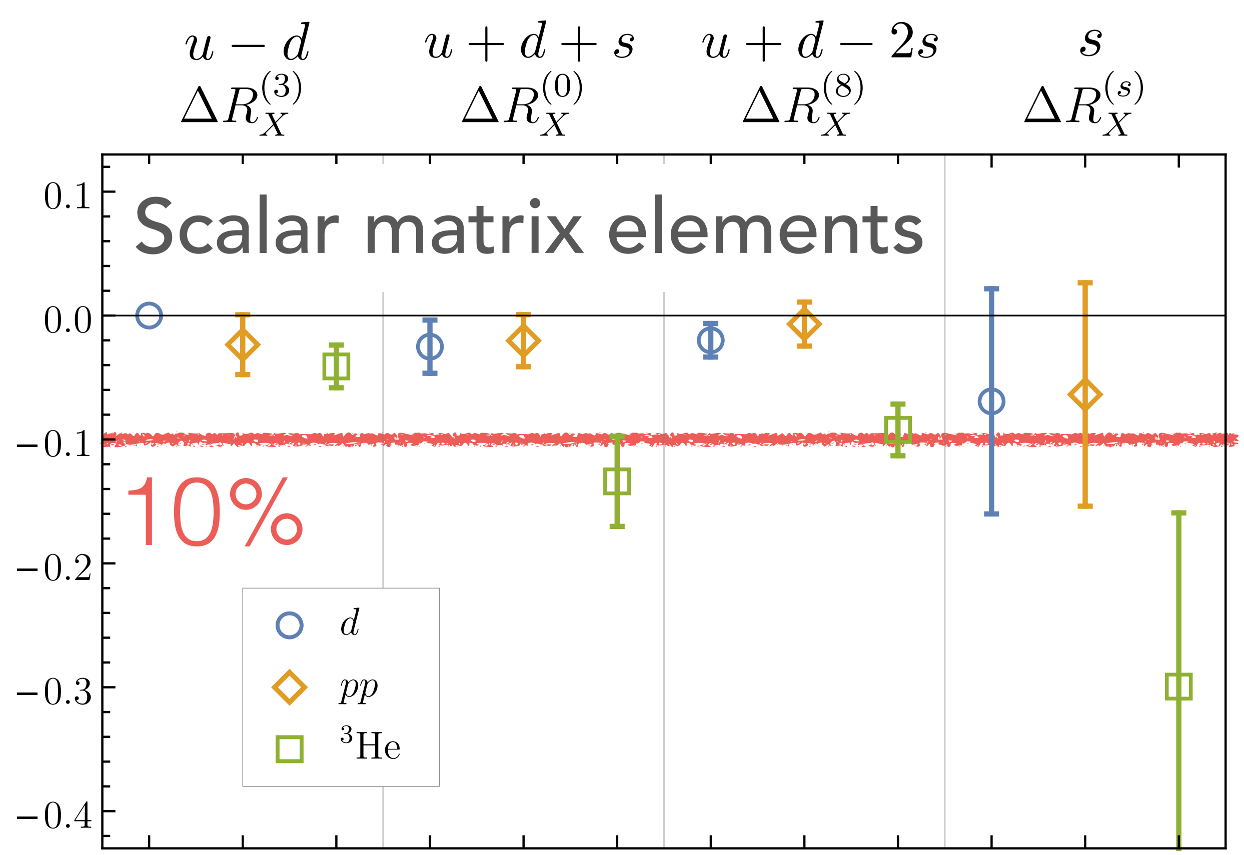


Second term may be significant!

Dark matter direct detection

Spin-independent scattering of WIMP candidates is governed by scalar matrix elements

- Lattice QCD calculation with m_π~800 MeV shows 10% nuclear effects in ^{3}He ➡ potentially very significant effects in e.g., Xenon
- Same calculation gives axial and tensor nuclear effects around ~1%



[NPLQCD PRL120 (2018), 152002]

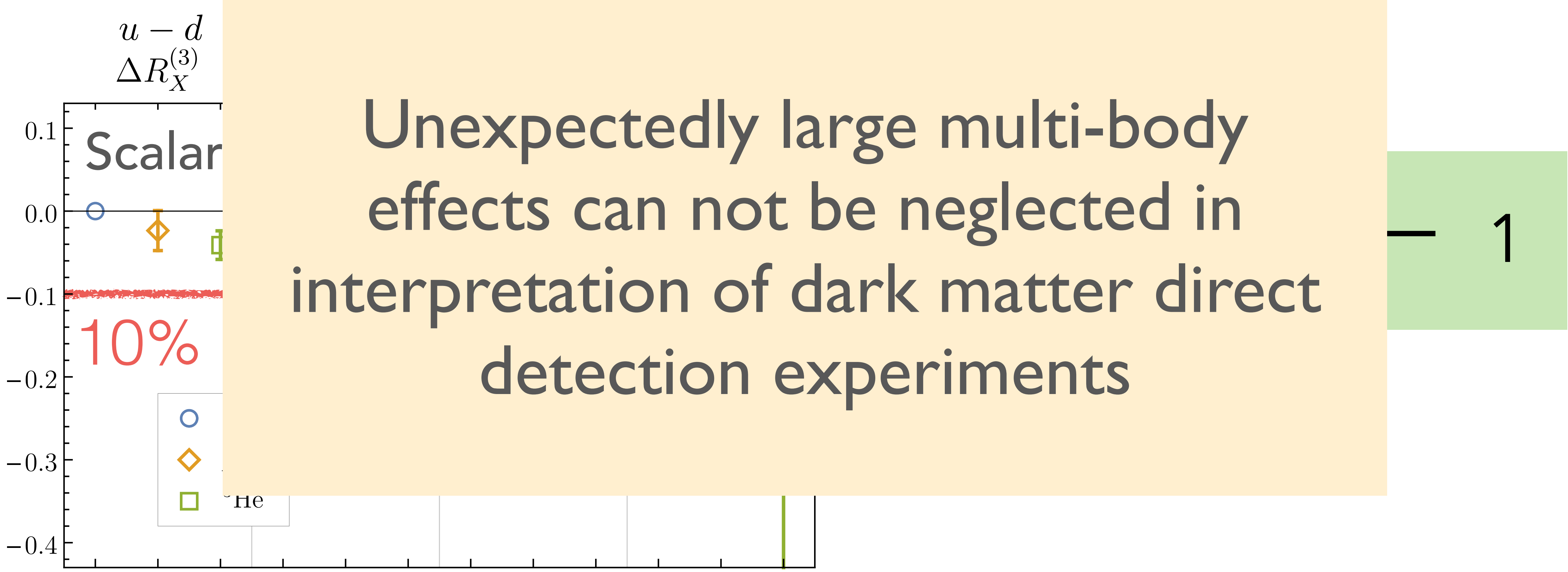
$$\frac{\text{ME}}{\text{A(Nucleon ME)}} - 1$$

Isolate "nuclear effect"

Dark matter direct detection

Spin-independent scattering of WIMP candidates is governed by scalar matrix elements

- Lattice QCD calculation with m_π~800 MeV shows 10% nuclear effects in ^{3}He → potentially very significant effects in e.g., Xenon
- Same calculation gives axial and tensor nuclear effects around ~1%



Unexpectedly large multi-body effects can not be neglected in interpretation of dark matter direct detection experiments

[NPLQCD PRL120 (2018), 152002]

Dark matter direct detection

Spin-independent scattering of WIMP candidates is governed by scalar matrix elements

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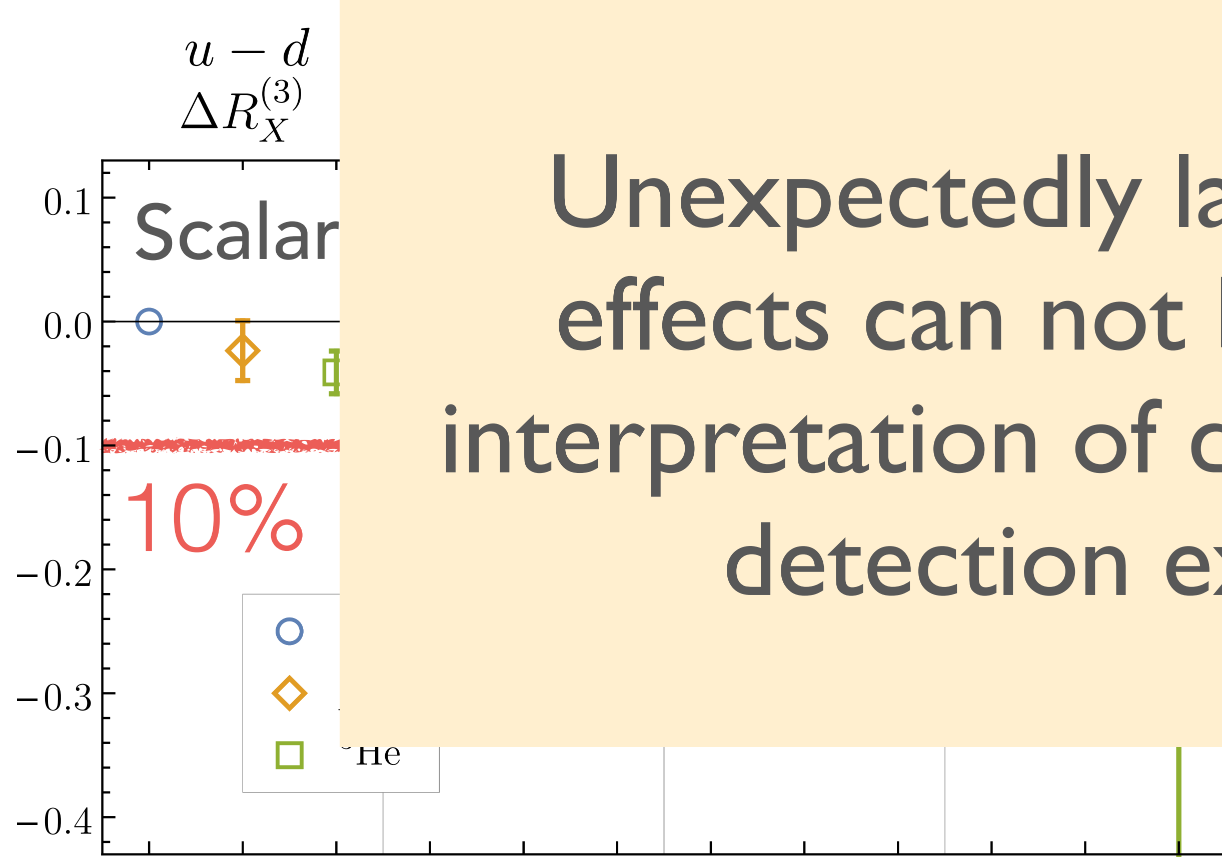
- Same calculation gives axial and tensor …



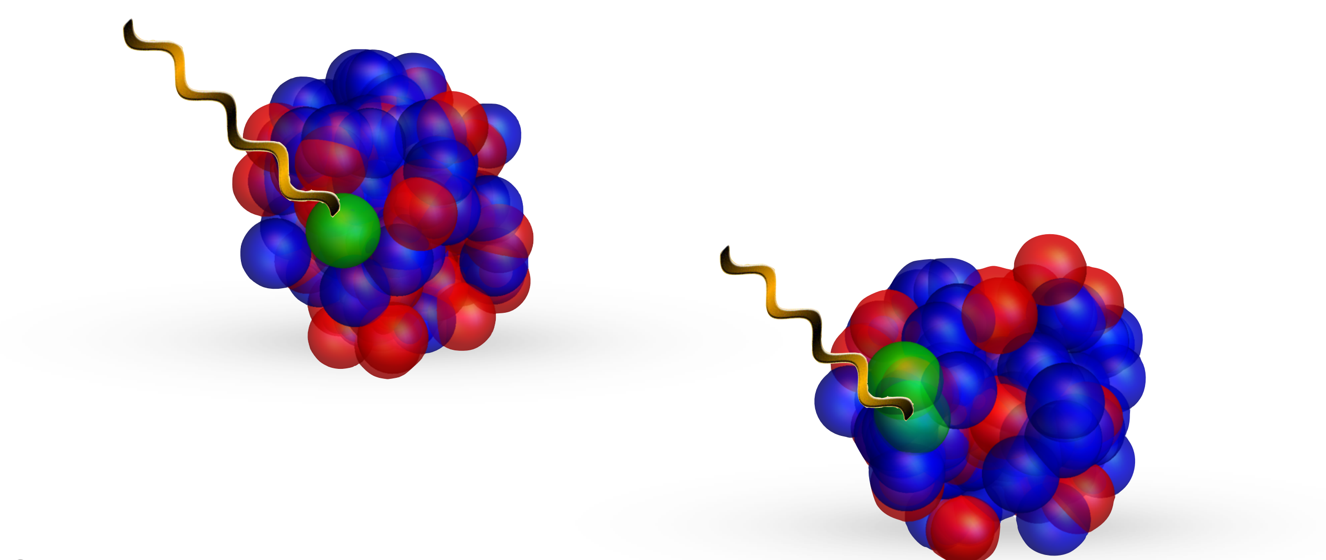
[NPLQCD PRL120 (2018), 152002]

Unexpectedly large mul… effects can not be neglected in interpretation of dark matter direct detection experiments

Calculation at ~physical quark masses in progress
Stay tuned!

Larger nuclei

What about larger (phenomenologically-relevant) nuclei?



- Nuclear effective field theory:
  - 1-body currents are dominant
  - 2-body currents are sub-leading *but non-negligible*
- Determine one body contributions from single nucleon
- Determine few-body contributions from A=2,3,4...
- Match effective theory and many body methods to lattice results to make predictions for larger nuclei

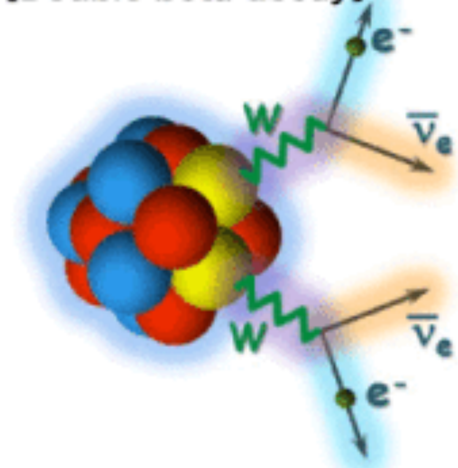
Pushing the boundaries

Will we ever achieve first-principles nuclear physics beyond A=4?

Interpretation of intensity-frontier experiments

- Axial form factors of Argon A=40
  DUNE long-baseline neutrino expt.
- Double-beta decay rates of Calcium A=48
- Scalar matrix elements in A=131
  XENON1T dark matter direct detection search

[Double beta decay]



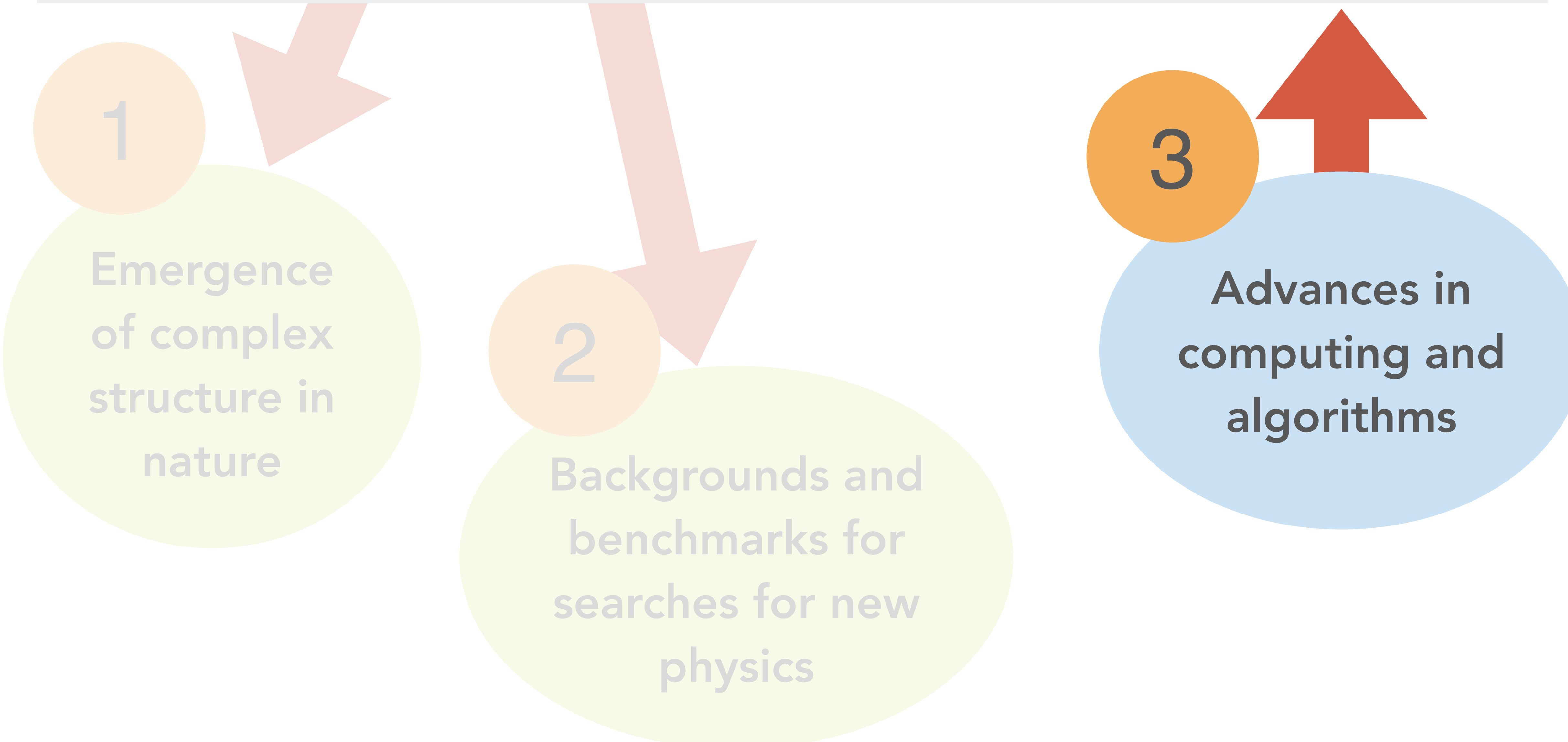
Double beta decay which emits anti-neutrinos

How finely tuned is the emergence of nuclear structure in nature?

Exponentially harder problem → Need exponentially improved algorithms

The structure of matter

Understanding the quark and gluon structure of matter

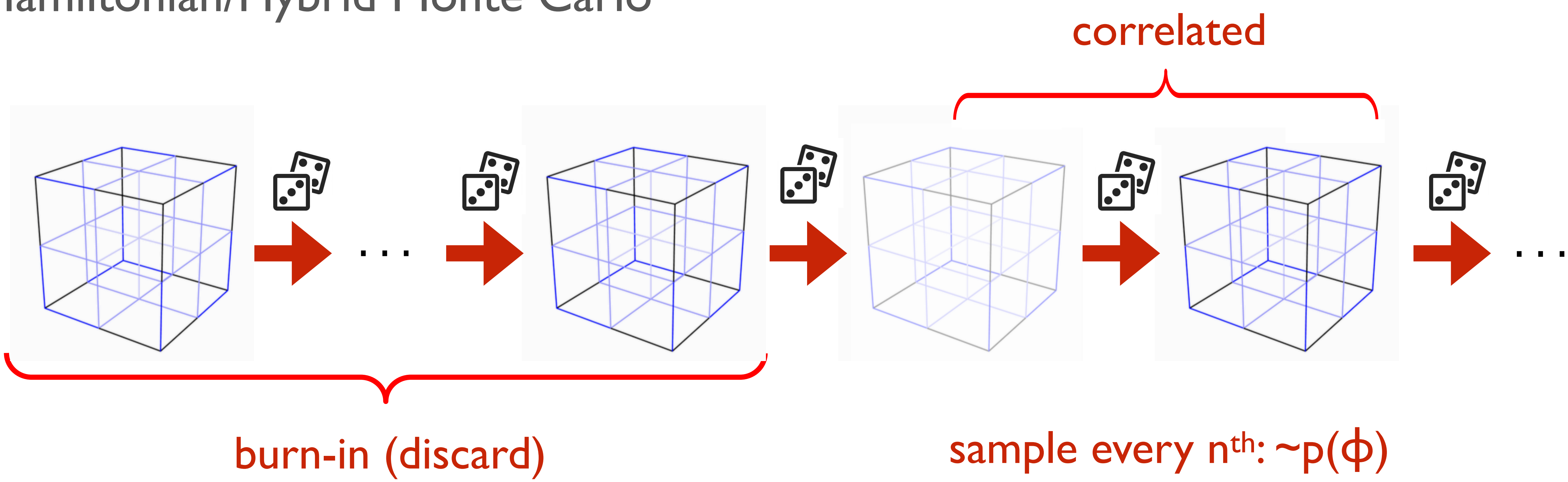


Generate QCD gauge fields

Generate field configurations $\phi(x)$ with probability

$$P[\phi(x)] \sim e^{-S[\phi(x)]}$$

Hamiltonian/Hybrid Monte Carlo

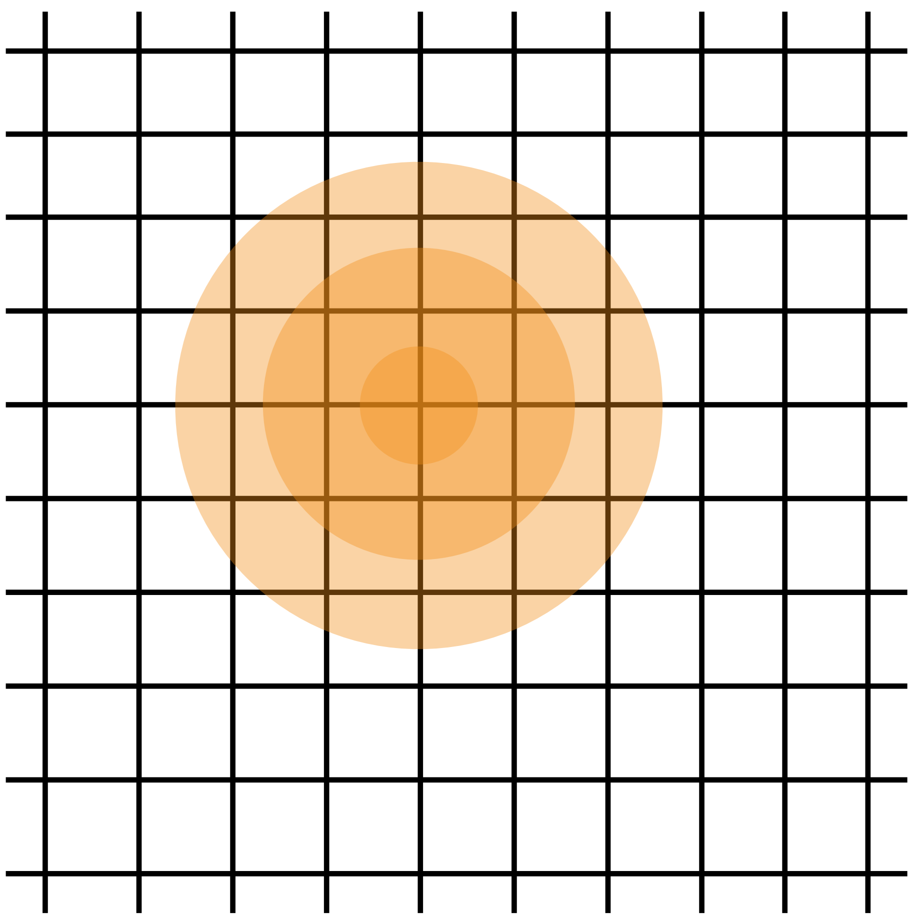


Burn-in time and correlation length dictated by Markov chain ‘**auto-correlation time**’: shorter autocorrelation time implies less computational cost

Generate QCD gauge fields

QCD gauge field configurations sampled via

Hamiltonian dynamics + Markov Chain Monte Carlo



Updates diffusive

Lattice spacing → 0

Number of updates to change fixed physical length scale → ∞

"Critical slowing-down" of generation of uncorrelated samples

Generate QCD gauge fields

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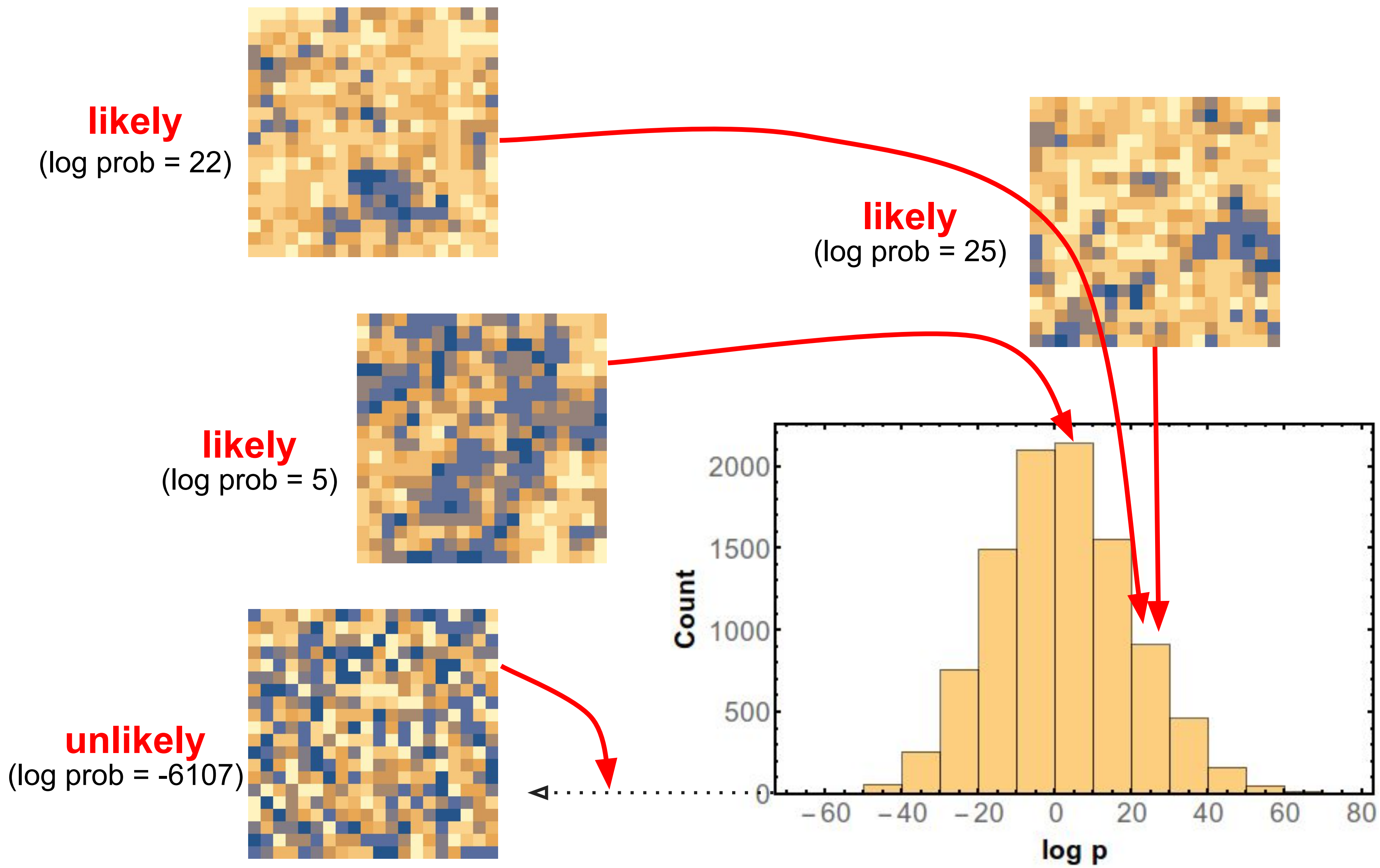
$$P[\phi(x)] \sim e^{-S[\phi(x)]}$$



Generate QCD gauge fields

Generate field configurations $\phi(x)$ with probability

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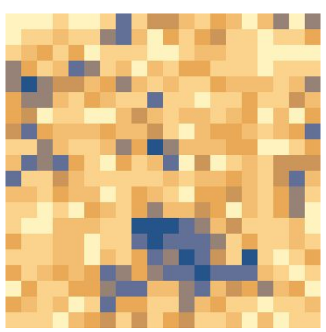
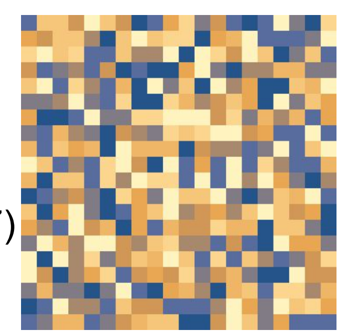
Parallels with image generation problem

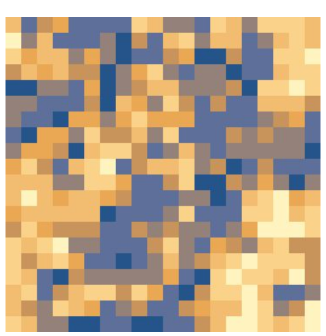
likely
(log prob = 22)



unlikely
(log prob = -6107)



likely
(log prob = 5)



likely

[Karras, Lane, Aila / NVIDIA 1812.04948]

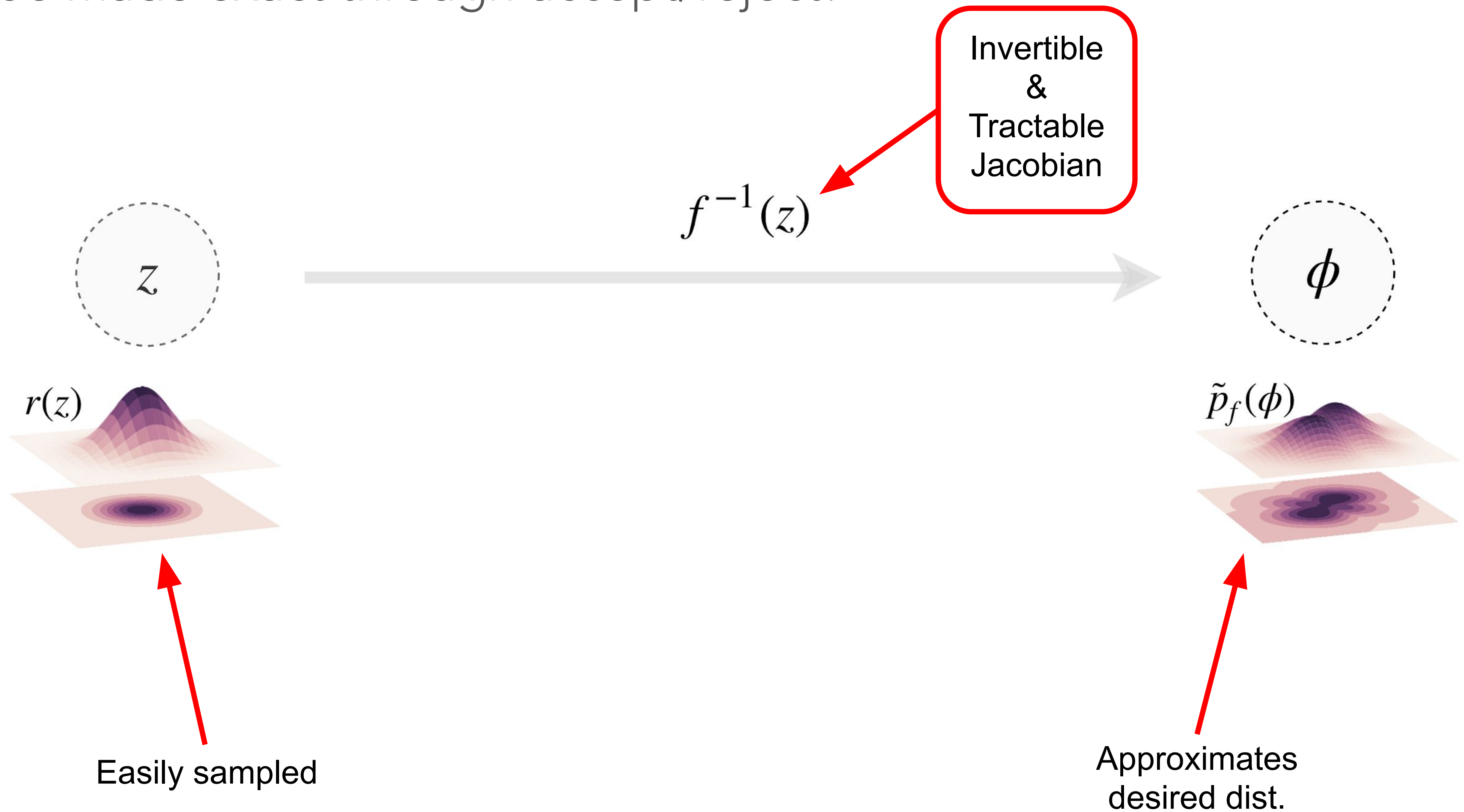
likely

unlikely

Generative flow models

Flow-based models learn a change-of-variables that transforms a known distribution to the desired distribution [Rezende & Mohamed 1505.05770]

Can be made exact through accept/reject!



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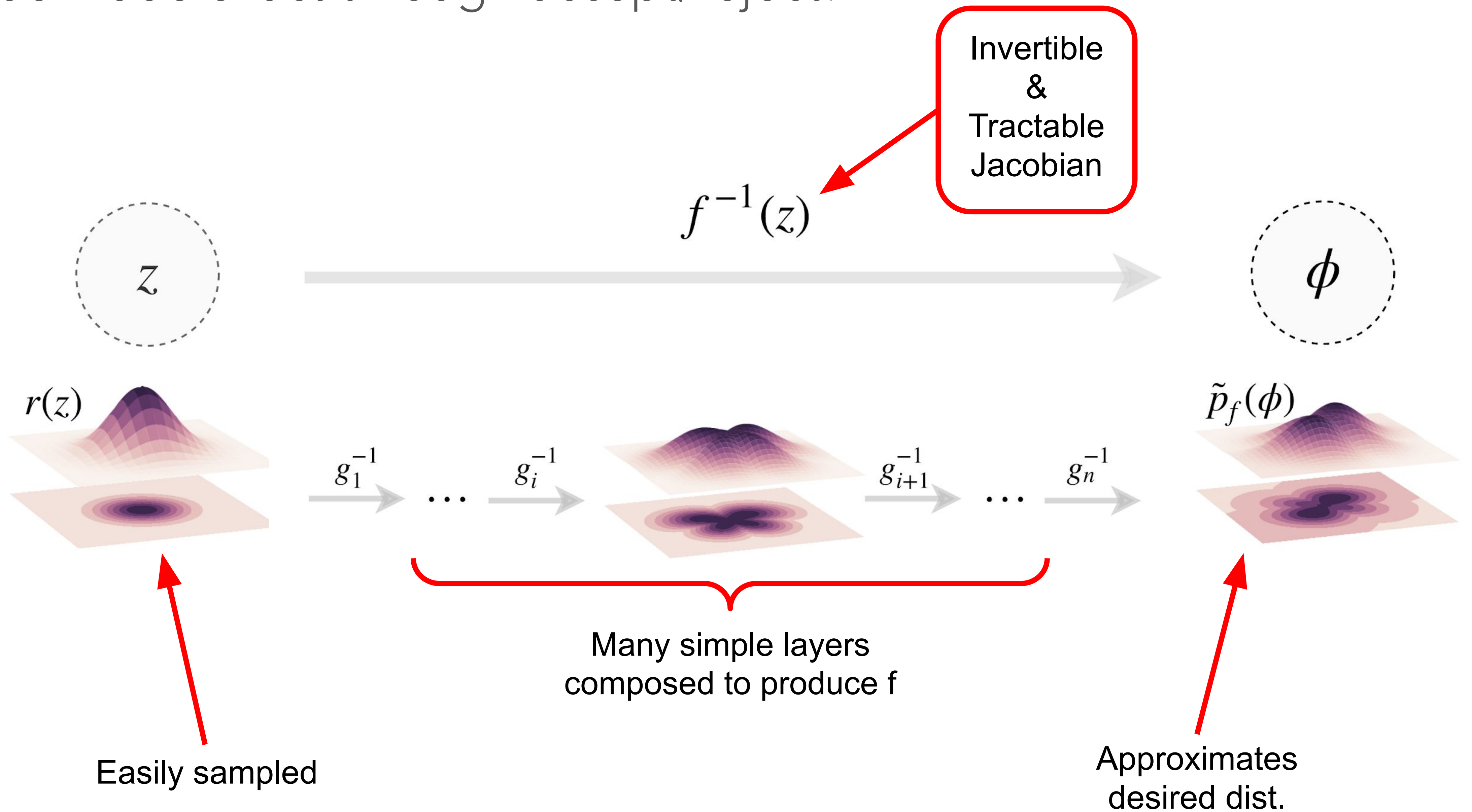


Machine learning QCD

Ensemble of lattice QCD gauge fields

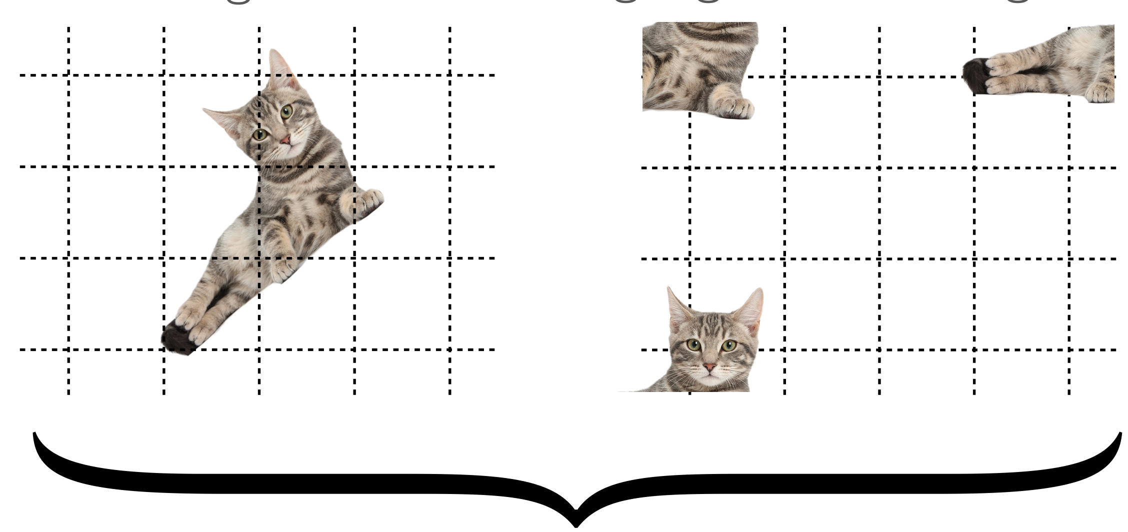
- $64^3 \times 128 \times 4 \times N_c^2 \times 2$ $\simeq 10^9$ numbers
- ~1000 samples
- Ensemble of gauge fields has meaning
- Long-distance correlations are important
- Gauge and translation-invariant with periodic boundaries

Physics is invariant under specific field transformations

- **Rotation, translation (4D), with boundary conditions**

Gauge field configuration

Transformed gauge field configuration



Encode same physics

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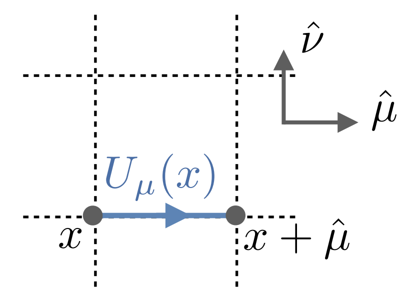
Physics is invariant under specific field transformations

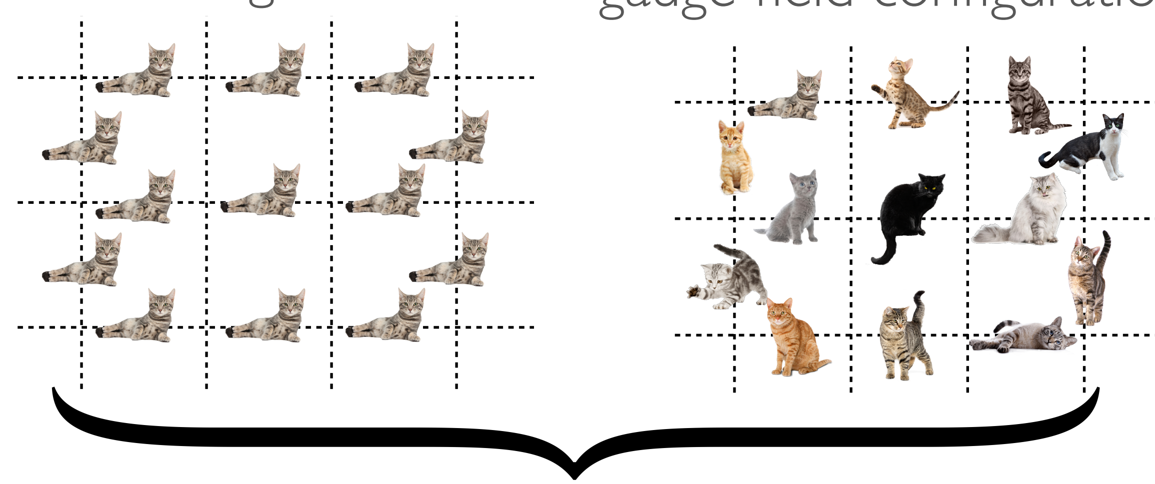
- **Gauge transformation**



$$U_\mu(x) \to \Omega(x) U_\mu(x) \Omega^\dagger(x+\hat{\mu})$$
$$\text{for all } \Omega(x) \in \mathrm{SU}(3)$$

Gauge field configuration

Transformed gauge field configuration



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- Ensemble of gauge fields has meaning
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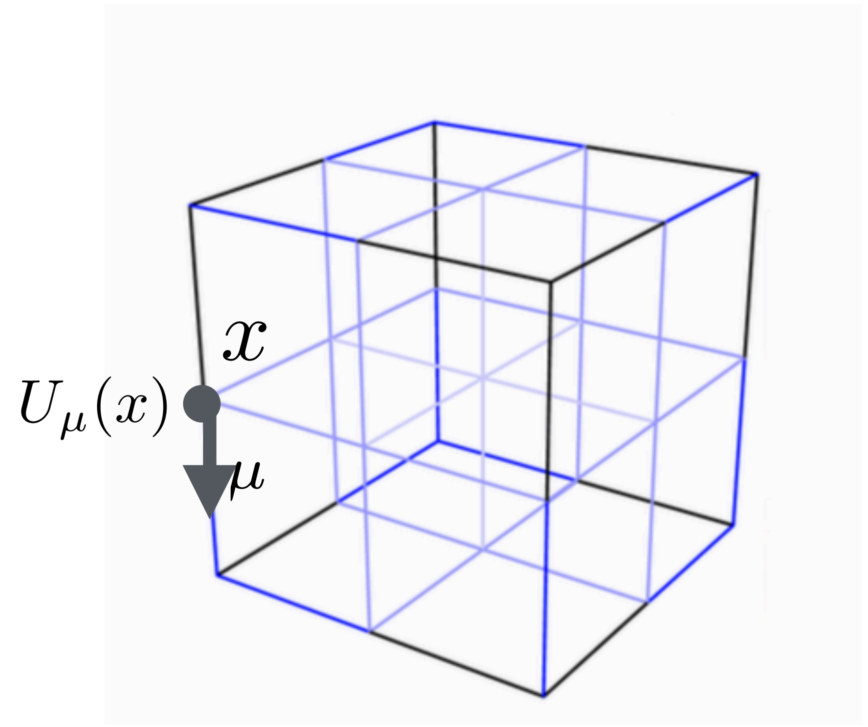
CIFAR benchmark image set for machine learning

- 32 x 32 pixels x 3 cols $\simeq 3000$ numbers
- 60000 samples
- Each image has meaning
- Local structures are important
- Translation-invariance within frame

Incorporating symmetries

Gauge field theories

- Field configurations represented by links $U_\mu(x)$ encoded as matrices
- e.g., for Quantum Chromodynamics, SU(3) matrices (3x3 complex matrices M with $det[M] = 1$, $M^{-1} = M^\dagger$)
- Group-valued fields live not on real line but on compact manifolds
- Action is invariant under group transformations on gauge fields



1. Flows on compact, connected manifolds
2. Incorporate symmetries: gauge-equivariant flows

[2008.05456 (2020), PRL 125, 121601 (2020), 2002.02428 (2020)]

Incorporating symmetries

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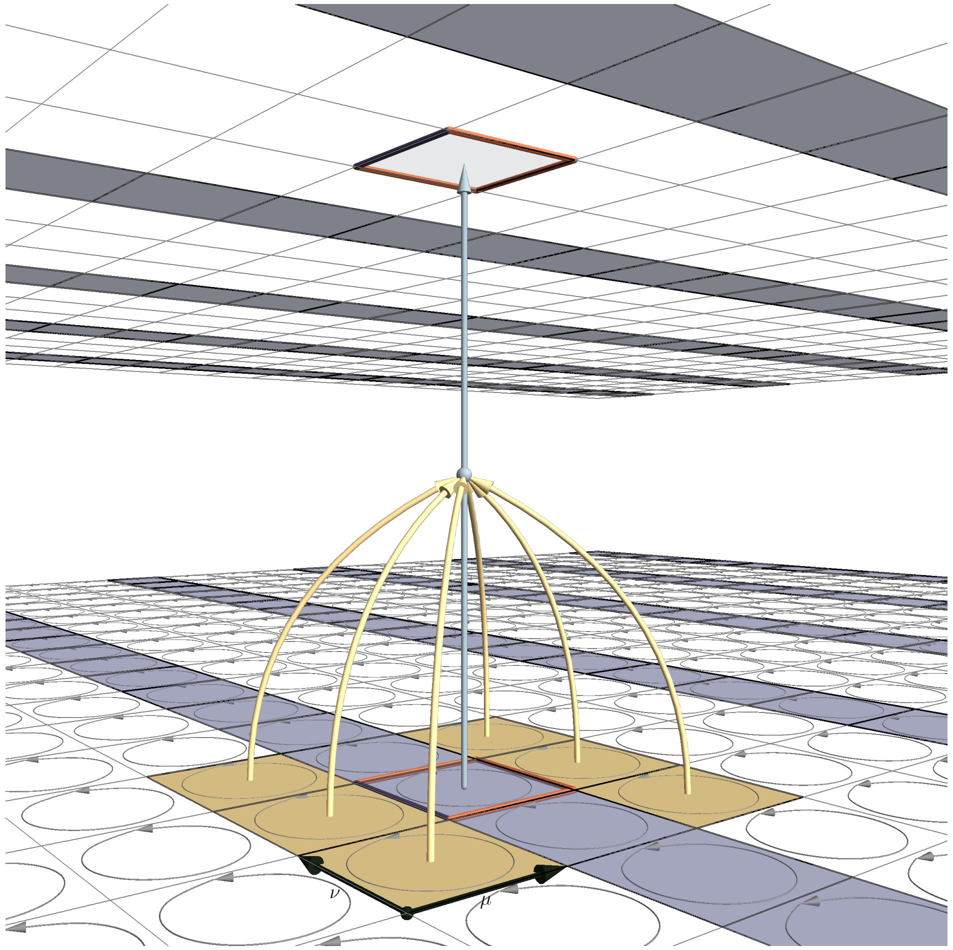


1. Flows on compact, connected manifolds
2. Incorporate symmetries: gauge-equivariant flows

[2008.05456 (2020), PRL 125, 121601 (2020), 2002.02428 (2020)]

Application: U(1) field theory

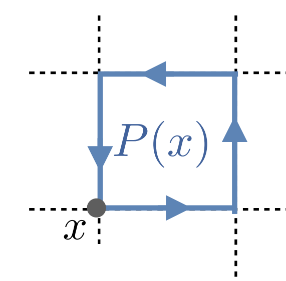
First gauge theory application: U(1) field theory

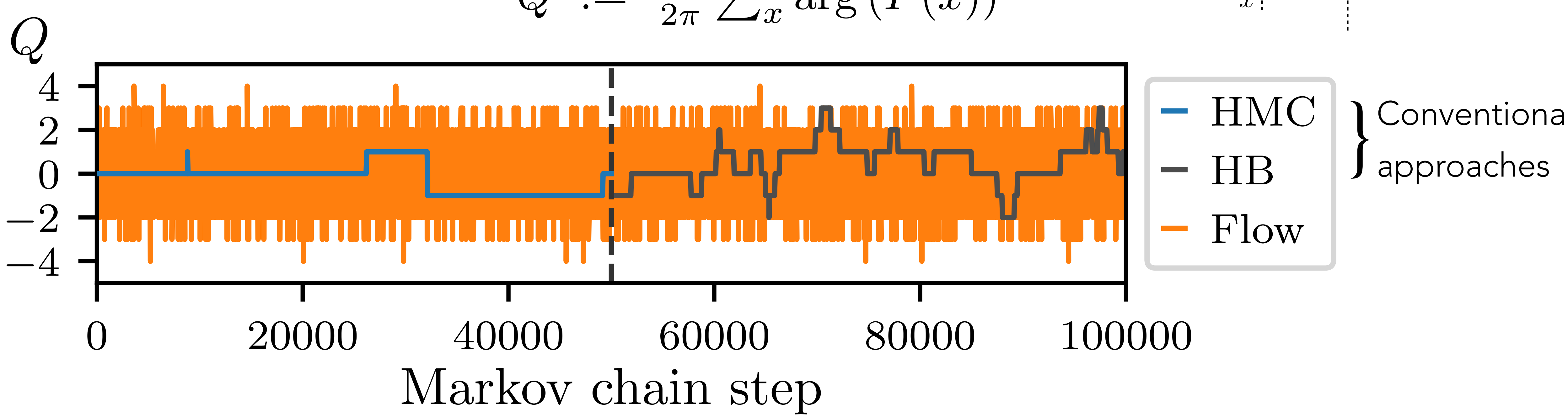
Success: Critical slowing down is significantly reduced

Cost: Up-front training of the model

Sampling of the topological charge

$$Q := \frac{1}{2\pi} \sum_x \arg\left(P(x)\right)$$





2D, L=16, β=6

[2008.05456 (2020), PRL 125, 121601 (2020), 2002.02428 (2020)]

Application: U(1) field theory

First gauge theory application: U(1) field theory

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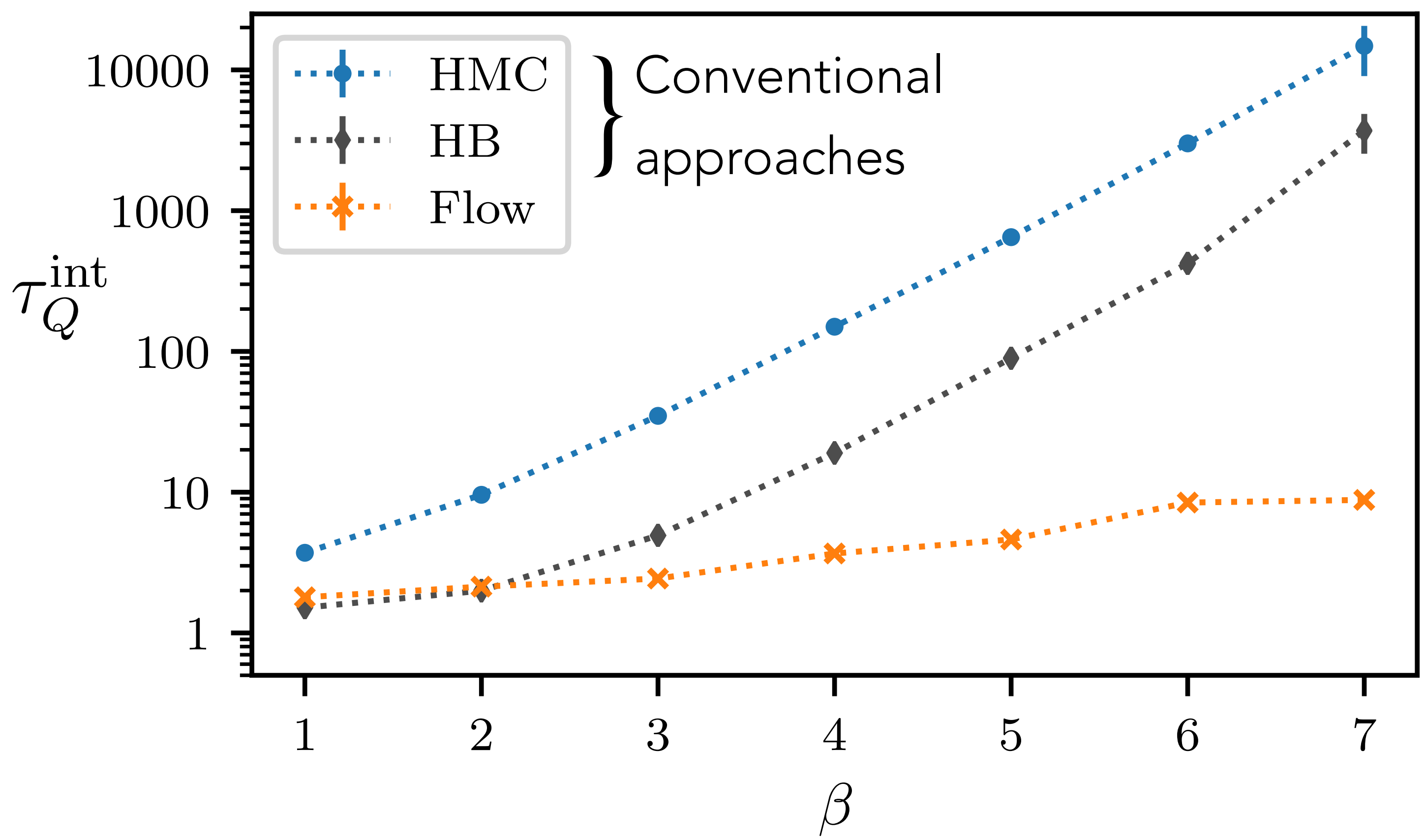
Cost per independent sample



2D, L=16

[2008.05456 (2020),
PRL 125, 121601 (2020),
2002.02428 (2020)]

Application: U(1) field theory

First gauge theory application: U(1) field theory

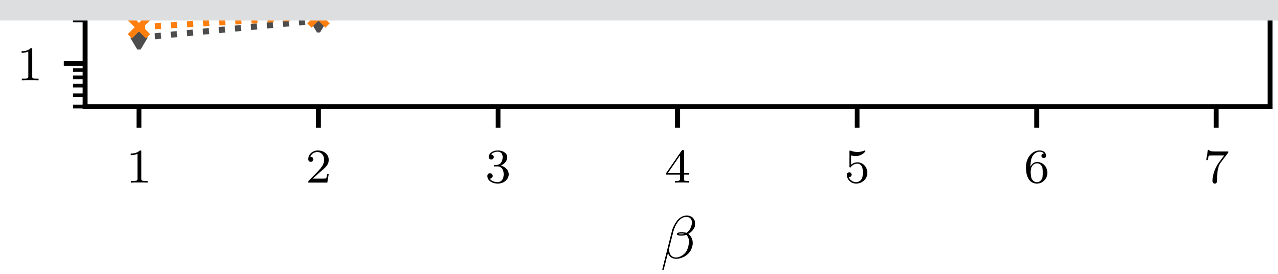
Succe… ed

Cost:

SUCCESS!

Proof-of-principle of efficient, exact, ML algorithm for LQFT

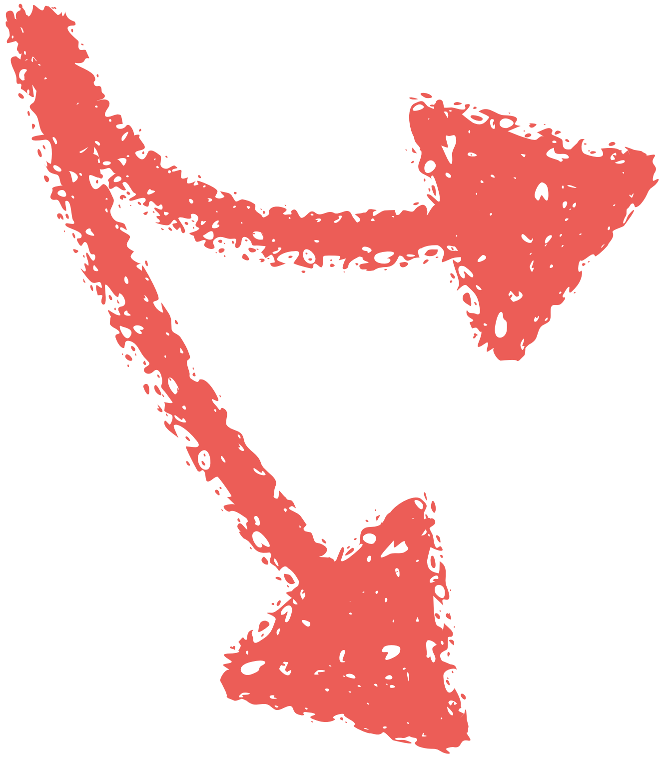
Already extended to SU(N).
Significant work required to scale to state-of-the-art



[2008.05456 (2020),
PRL 125, 121601 (2020),
2002.02428 (2020)]

2D, L=16

Interdisciplinary applications



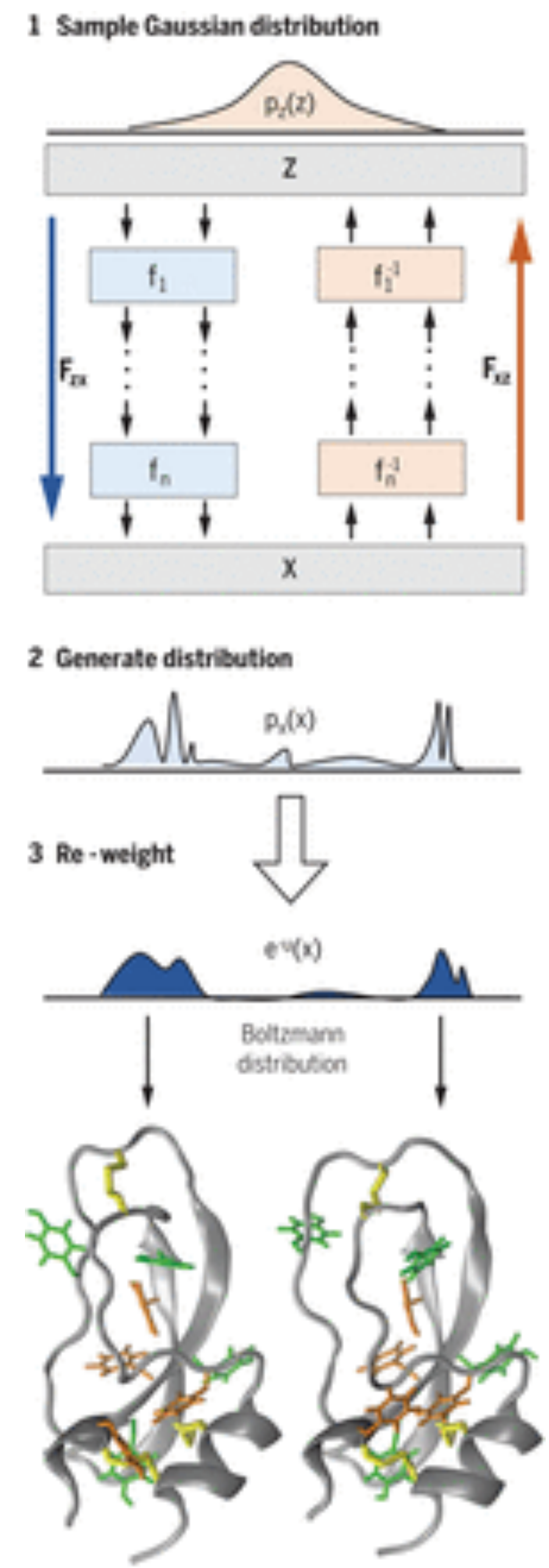
Molecular genetics and drug design

RESEARCH ARTICLE SUMMARY

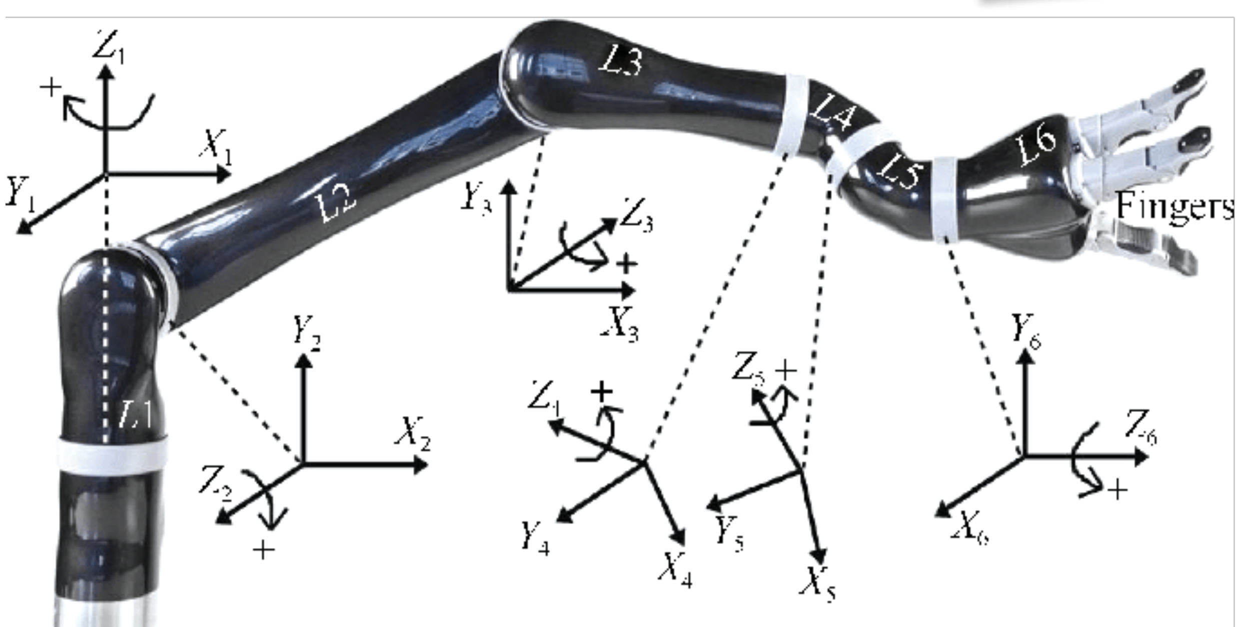
MACHINE LEARNING

Boltzmann generators: Sampling equilibrium states of many-body systems with deep learning

Frank Noé*†, Simon Olsson*, Jonas Köhler*, Hao Wu



Robotics



H. Application: Multi-Link Robot Arm

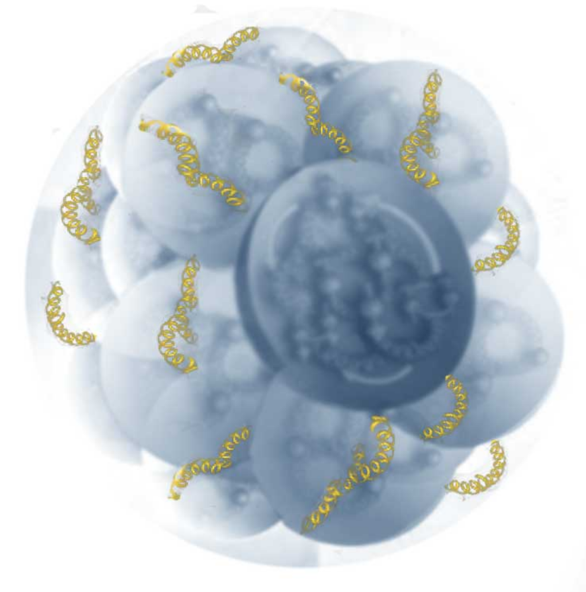
As a concrete application of flows on tori, we consider the problem of approximating the posterior density over joint angles $\theta_{1,\ldots,6}$ of a 6-link 2D robot arm, given (soft) constraints on the position of the tip of the arm. The possible configurations of this arm are points in $\mathbb{T}^6$. The position r_k of a joint $k = 1, \ldots, 6$ of the robot arm is given by

$$r_k = r_{k-1} + \left(l_k \cos\left(\sum_{j\le k} \theta_j\right), l_k \sin\left(\sum_{j\le k} \theta_j\right)\right),$$

Nuclear physics from the Standard Model

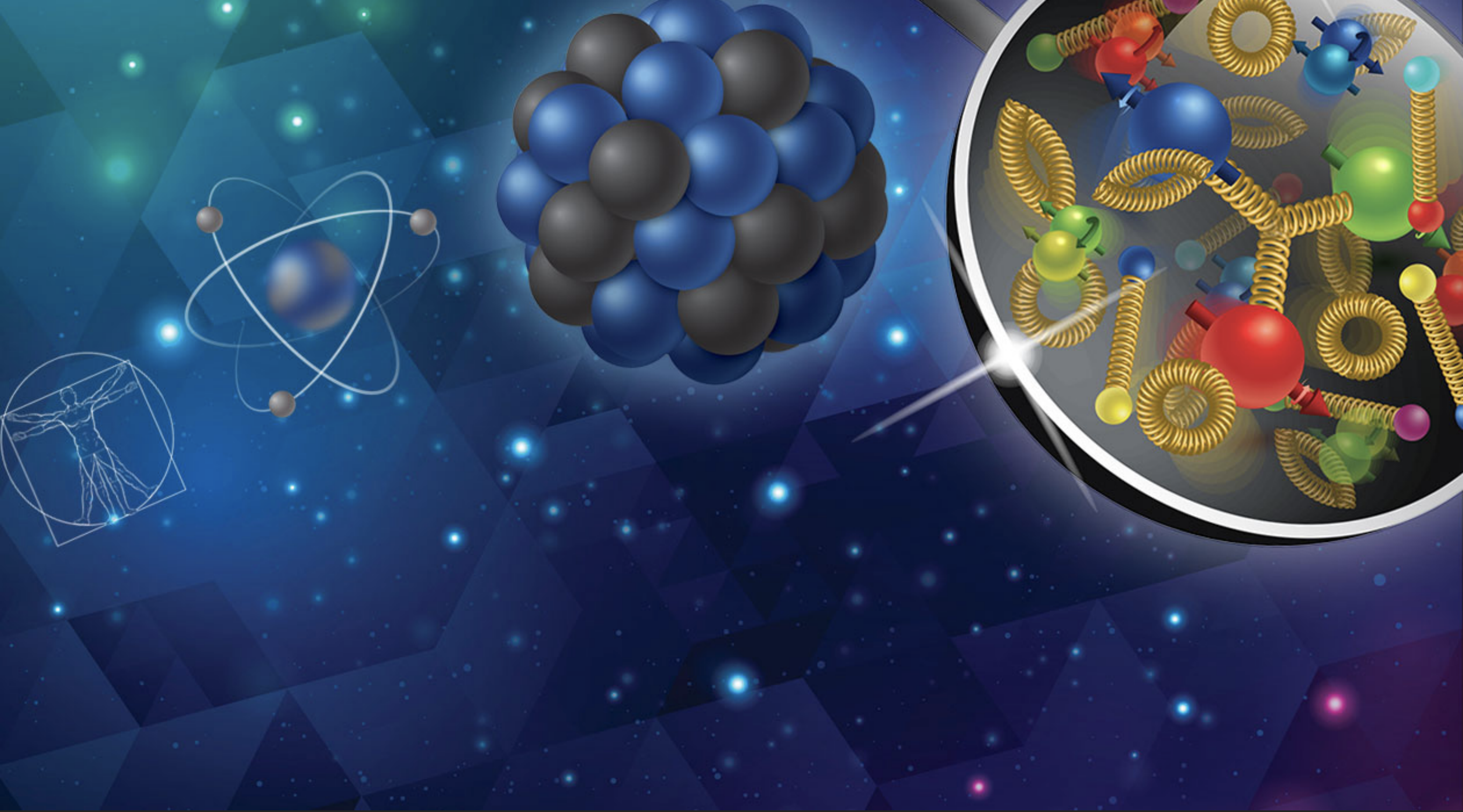
1 **New insights into proton and nuclear structure**

First-principles QCD calculations to reveal nuclear structure and provide benchmarks for BSM searches



2 **Beyond the frontiers with ML**

- Reaching nuclei with A>4
- Provably-exact physics-informed machine learning algorithms



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