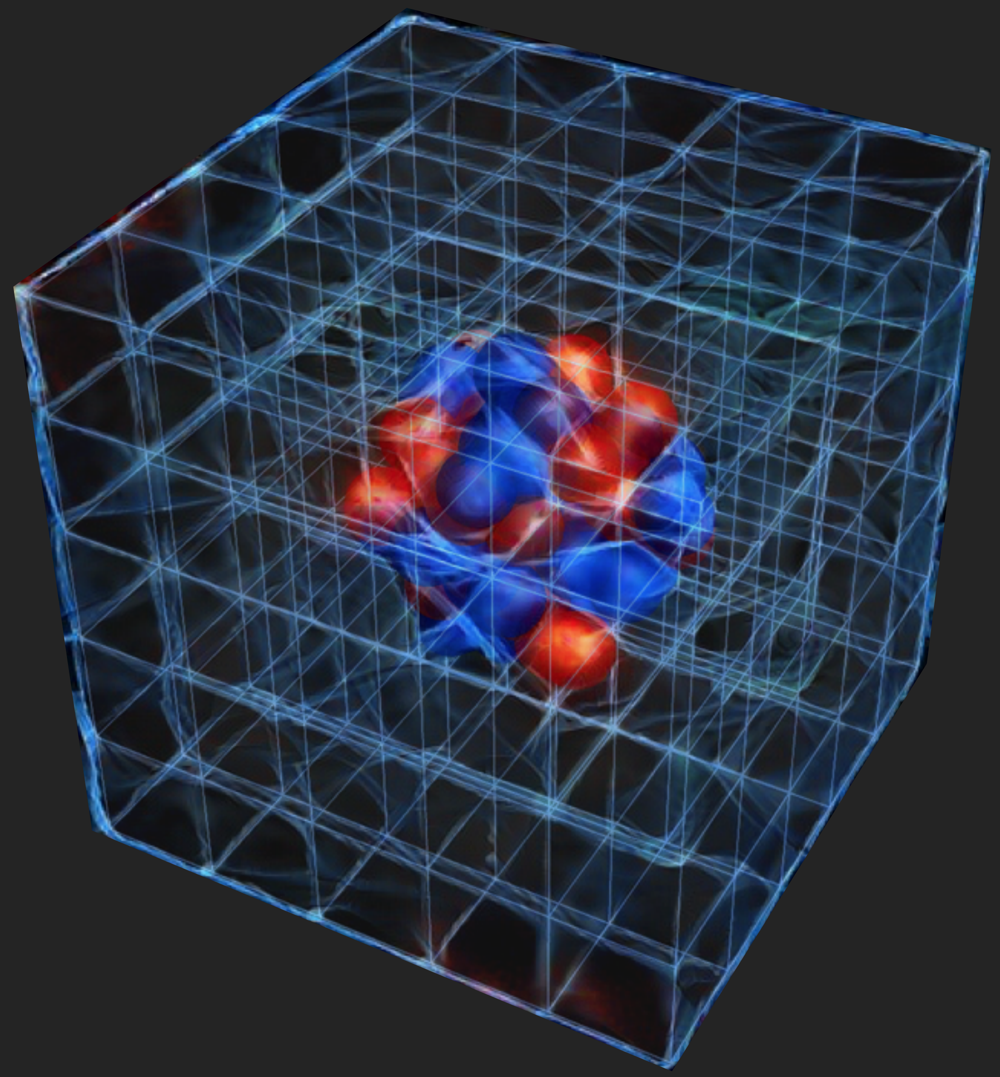
Machine Learning for Lattice Field Theory



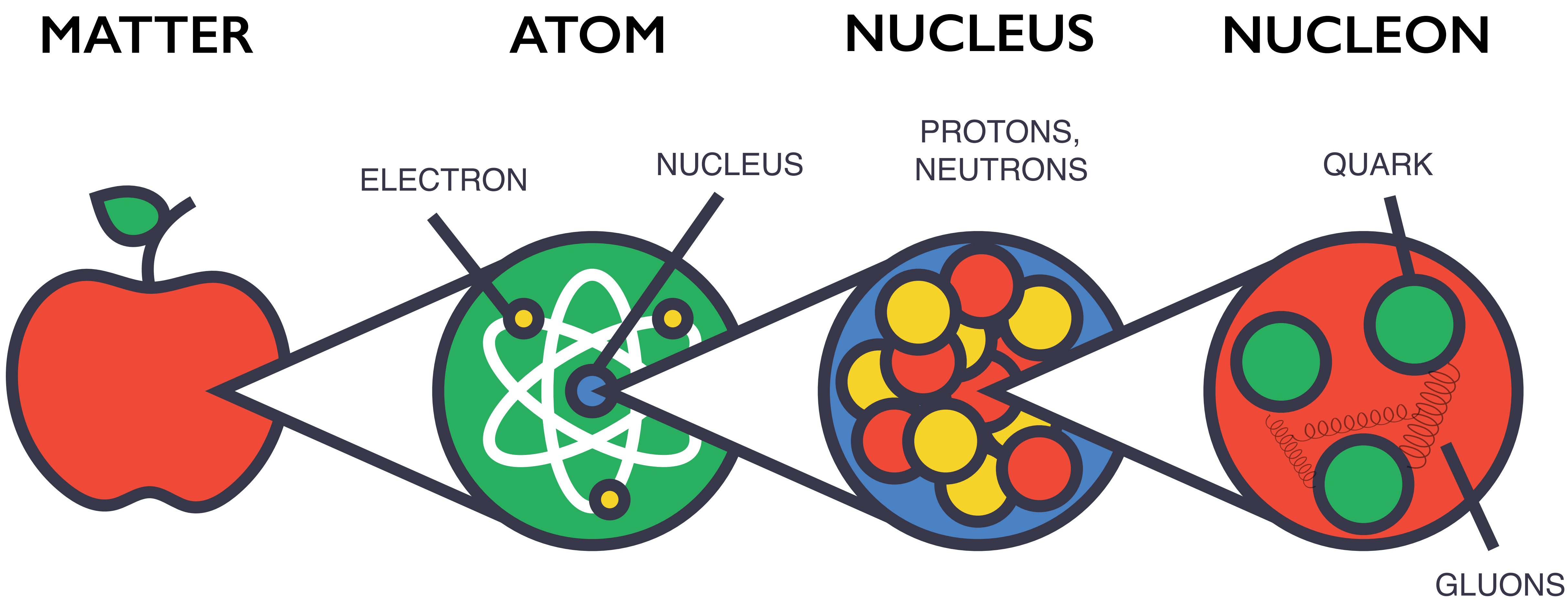
Phiala Shanahan

Massachusetts Institute of Technology

The structure of matter

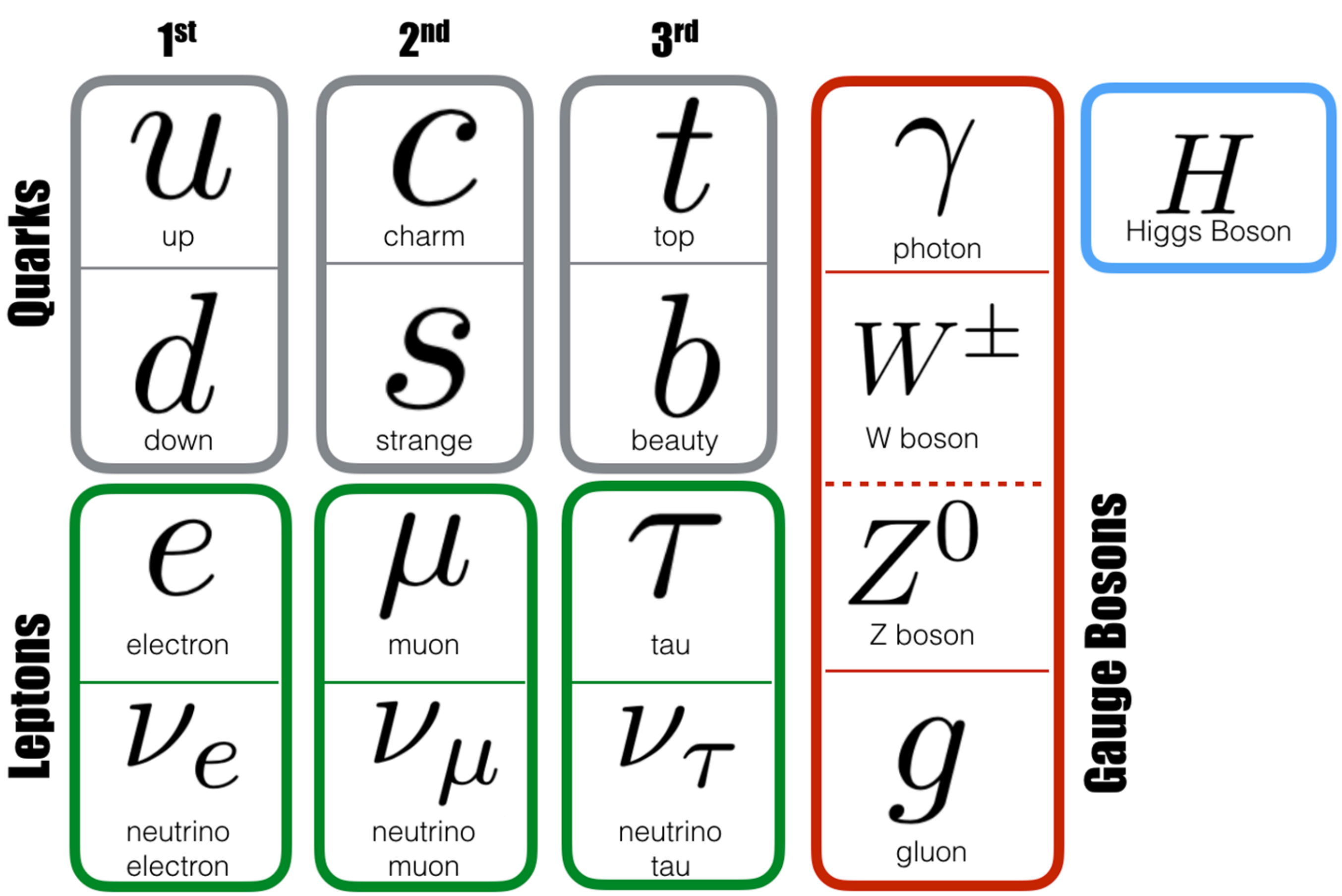
What is everything made of?

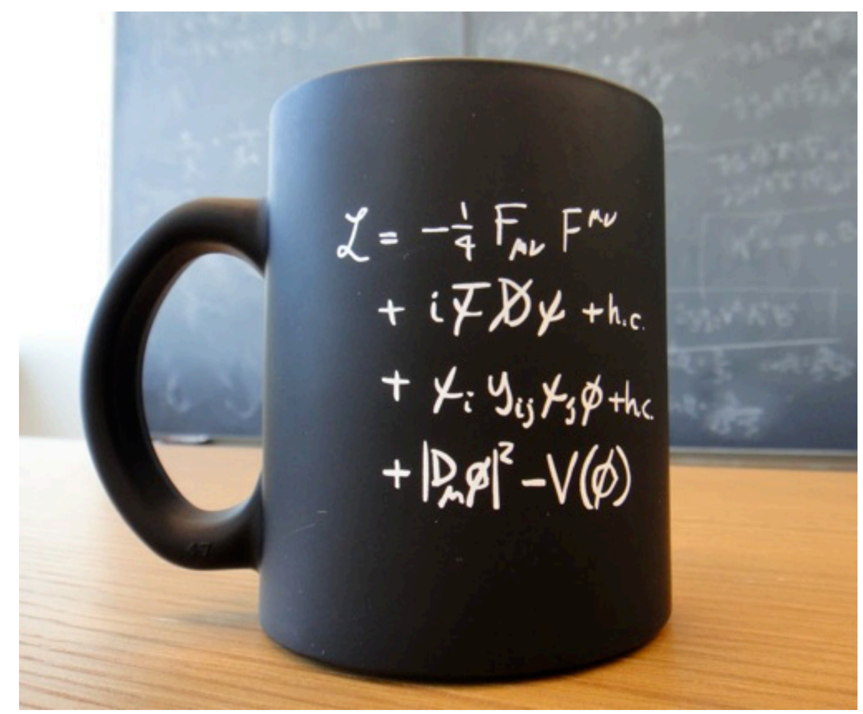
What laws describe the properties of matter?



The structure of matter

The Standard Model of nuclear and particle physics



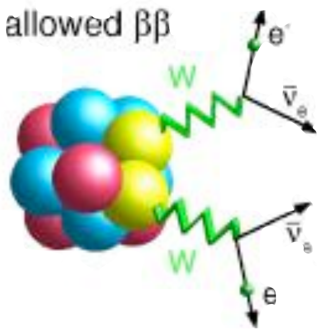


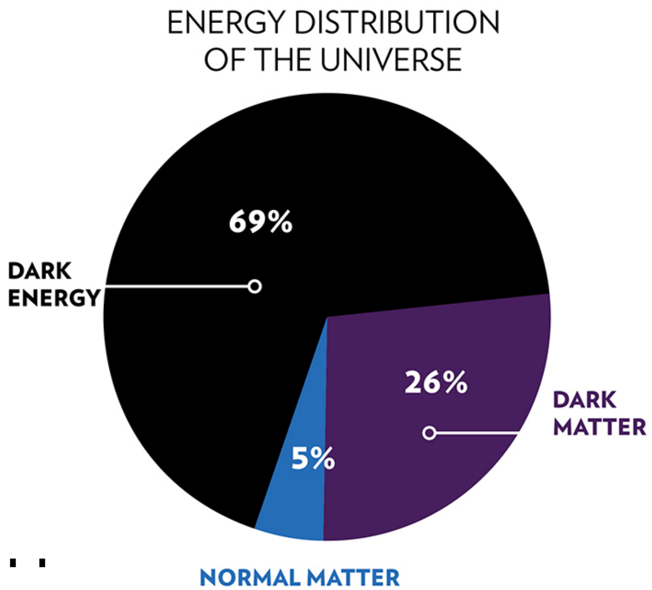
The search for new physics

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…





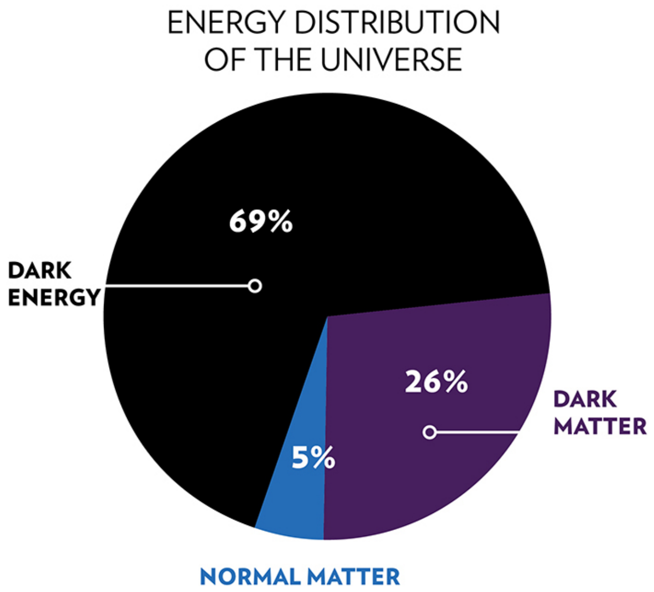
The search for new physics

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 NUCLEI

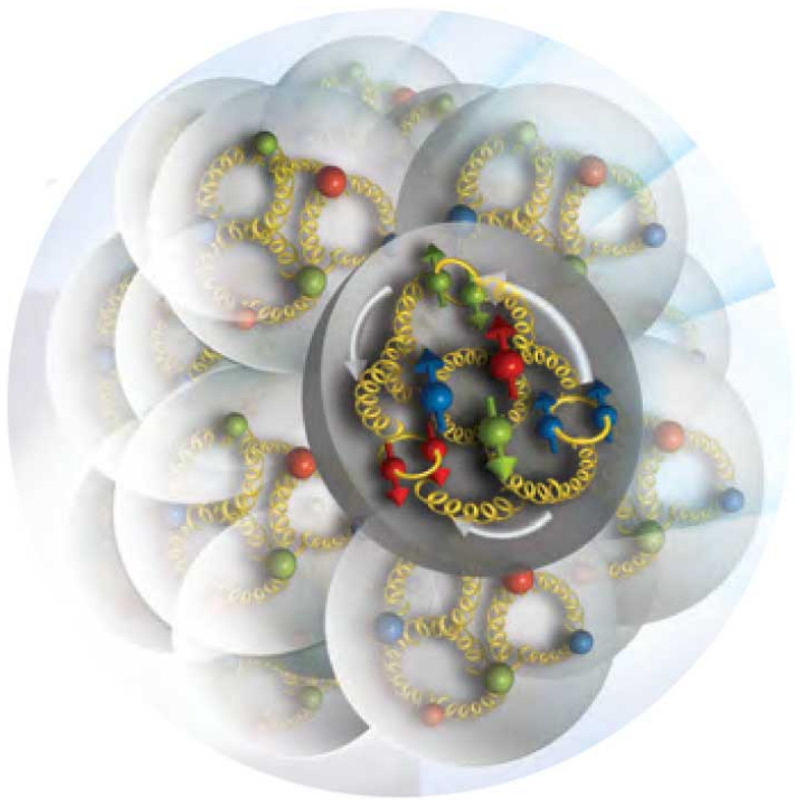


The structure of matter

Nuclear structure from the Standard Model

Emergence of complex structure in nature

Backgrounds and benchmarks for searches for new physics

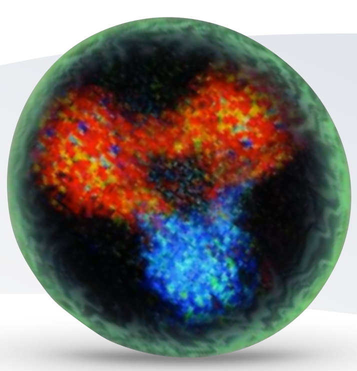


Strong interactions

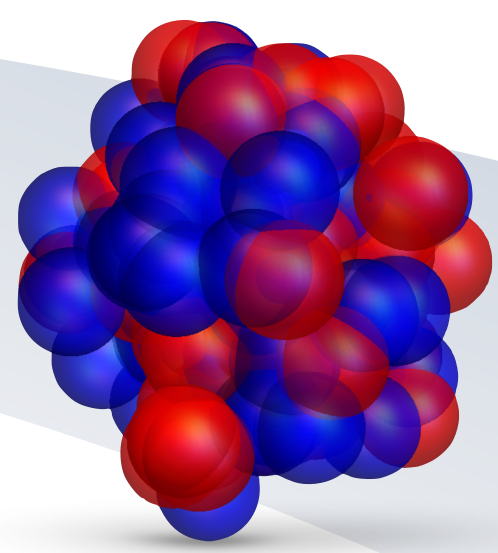
Study nuclear structure from the strong interactions

Quantum Chromodynamics (QCD)

Strongest of the four forces in nature

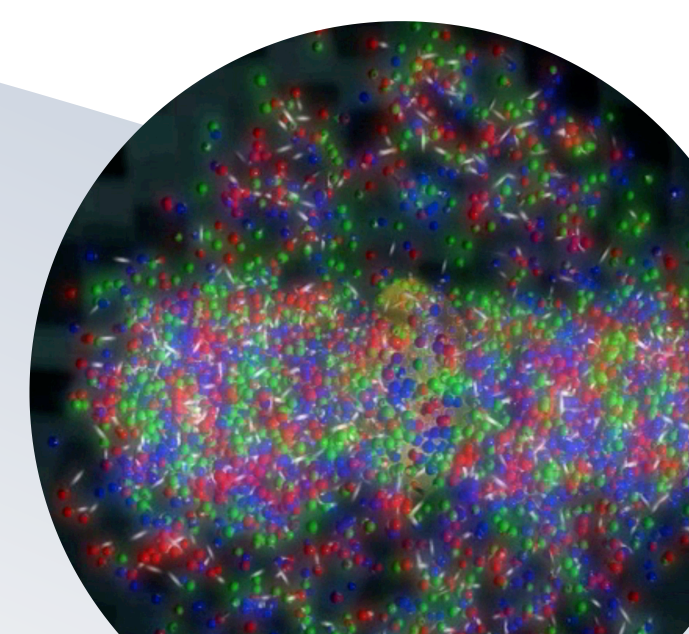


Binds quarks and gluons into protons, neutrons, pions etc.



Binds protons and neutrons into nuclei

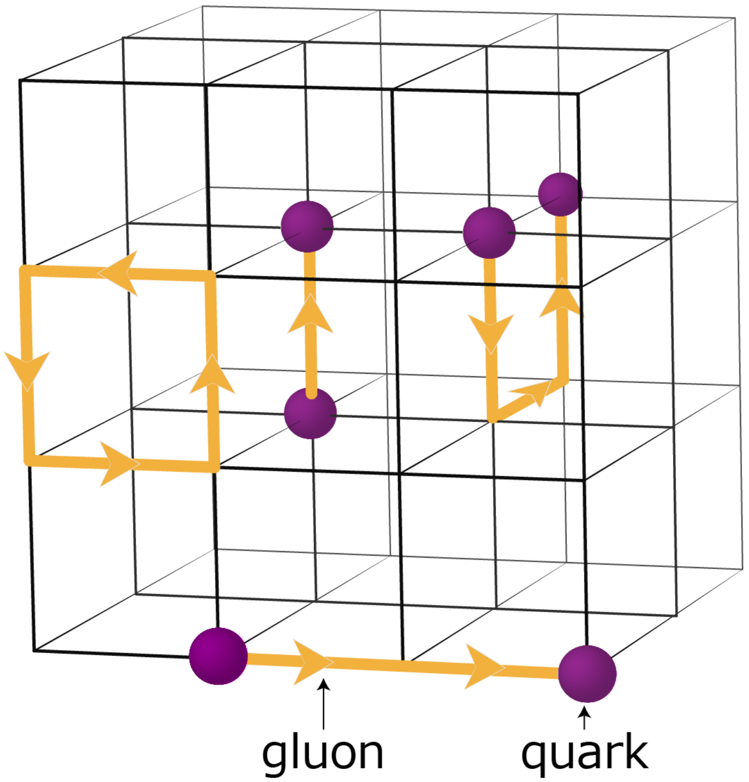
Forms other types of exotic matter e.g., quark-gluon plasma



Lattice QCD

Numerical first-principles approach to
non-perturbative QCD

- Discretise QCD onto 4D space-time lattice
- Approximate QCD path integral using Monte-Carlo methods and importance sampling
- Run on supercomputers and dedicated clusters
- Take limit of vanishing discretisation, infinite volume, physical quark masses



Lattice QCD

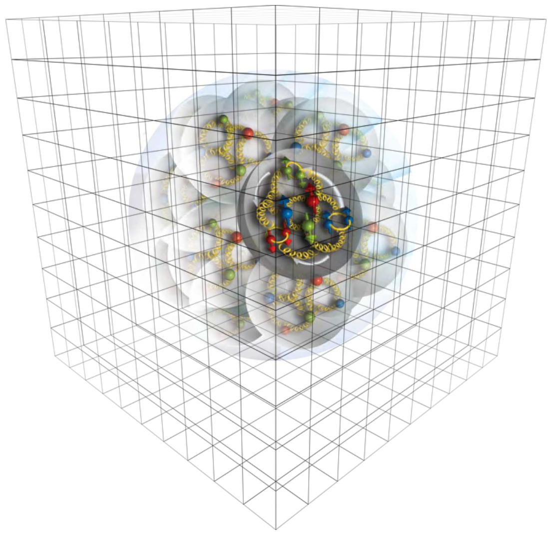
Numerical first-principles approach to non-perturbative QCD

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 Y, or f_π or Ω mass

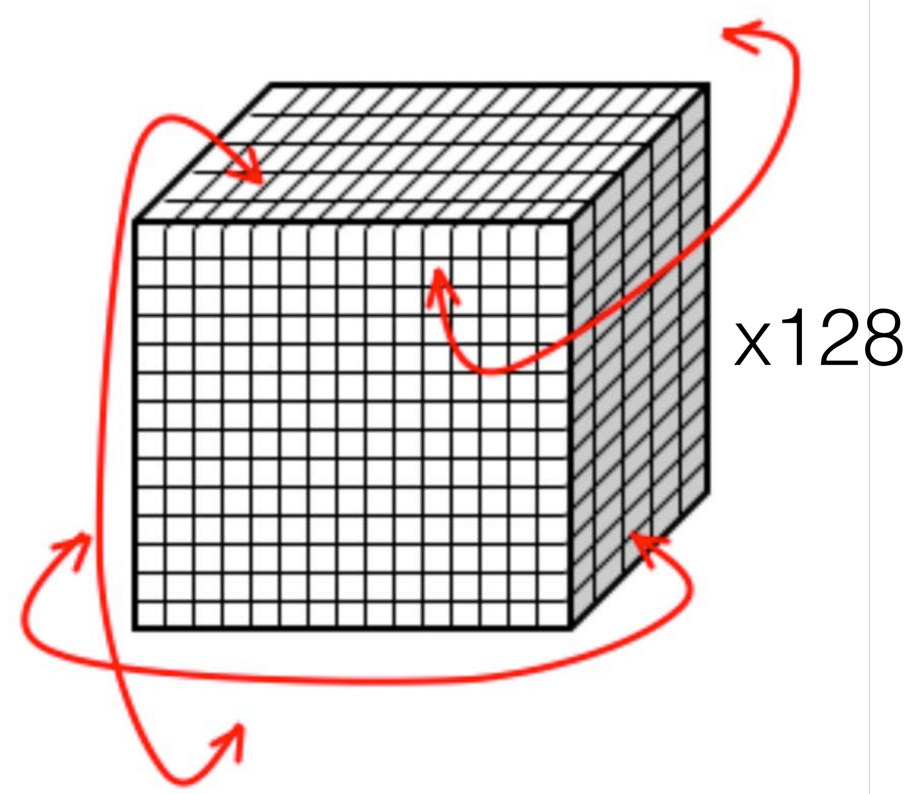
OUTPUT

Calculations of all other quantities are QCD predictions



Lattice QCD

- Numerical first-principles approach to non-perturbative QCD
- Euclidean space-time $t \to i\tau$
  - Finite lattice spacing a
  - Volume $L^3 \times T \approx 32^3 \times 64$
  - Boundary conditions
- Some calculations use larger-than-physical quark masses (cheaper)



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

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

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

Lattice QCD

Workflow of a lattice QCD calculation

1 Generate configurations via Hybrid Monte Carlo

- Leadership-class computing
- ~100K cores or 1000GPUs, 10's of TF-years
- O(100-1000) configurations, each ~10-100GB

2 Compute propagators

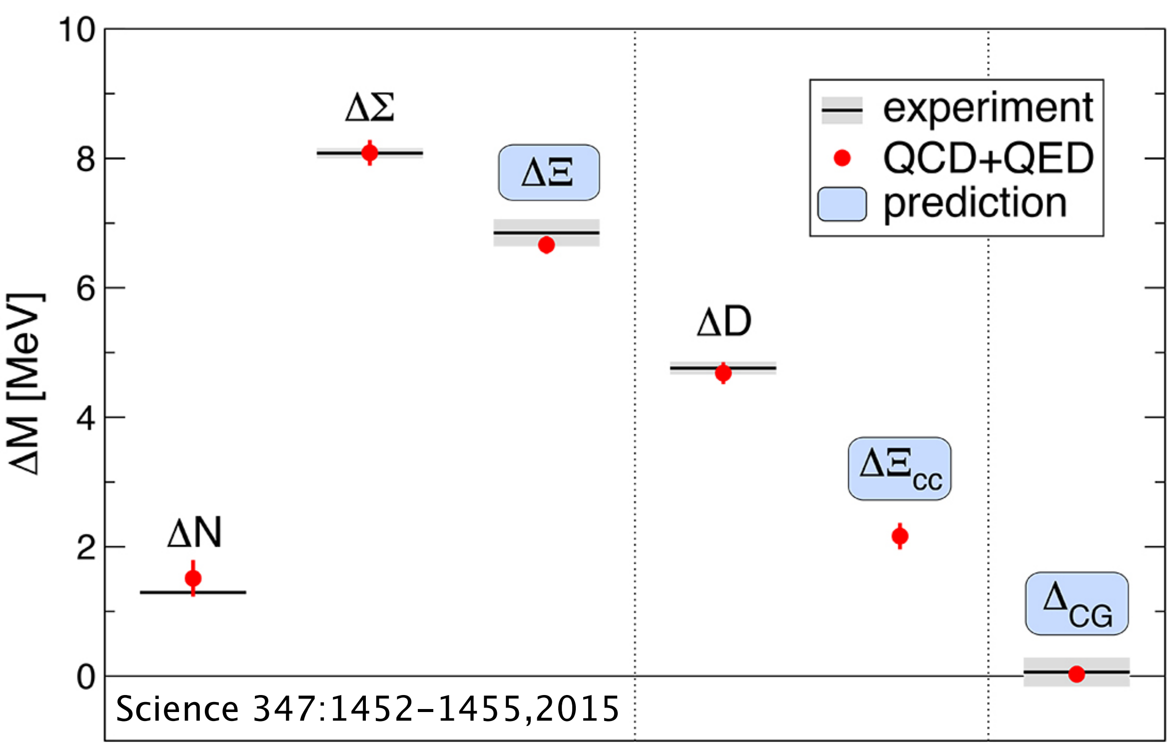
- Large sparse matrix inversion
- ~few 100s GPUs
- 10x gauge field in size, many per config

3 Contract into correlation functions

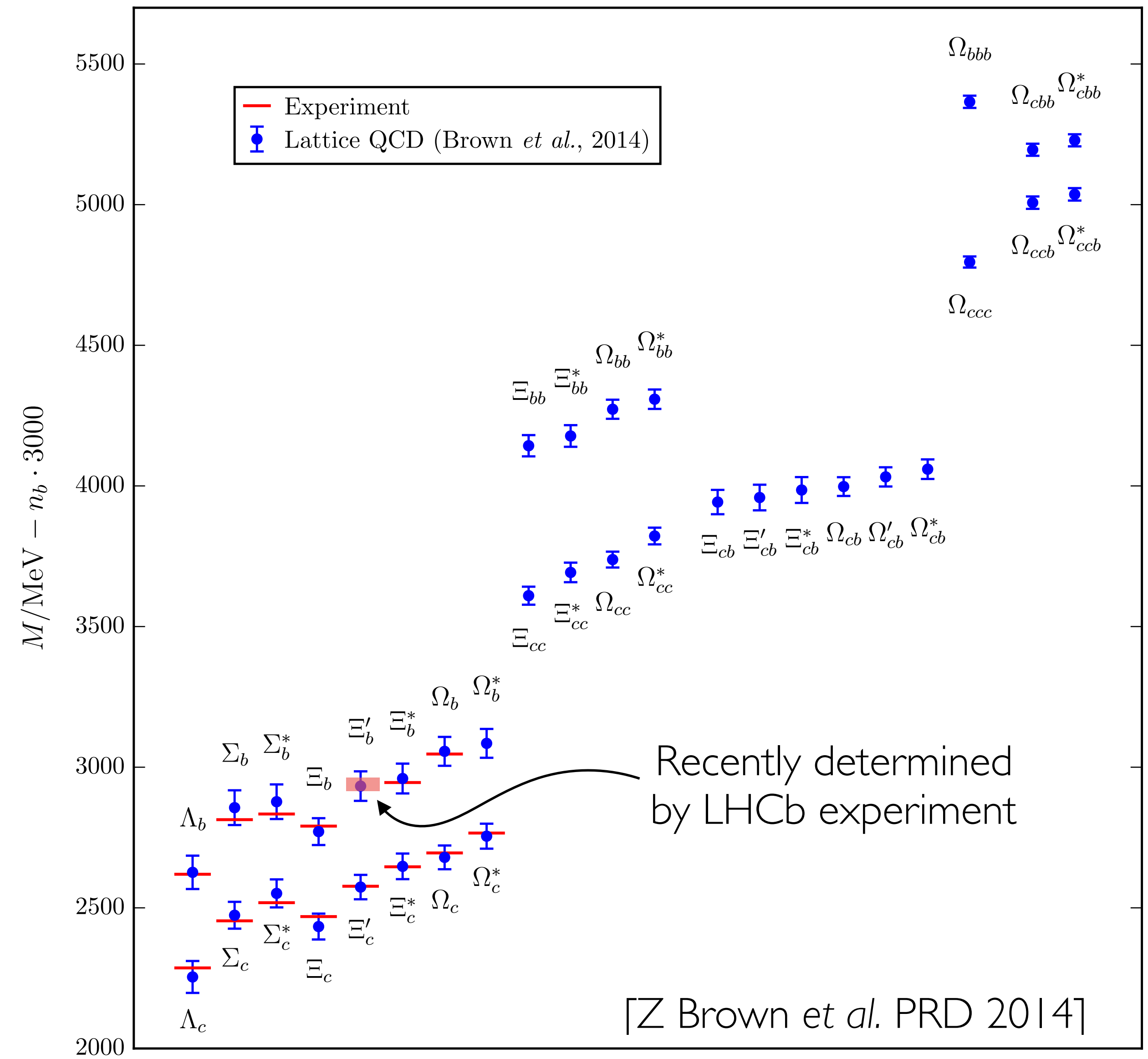
- ~few GPUs
- O(100k-1M) copies

Lattice QCD works

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



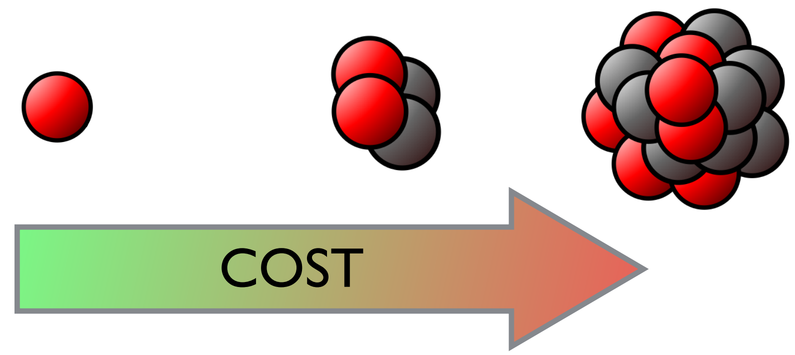
- Predictions for new states with controlled uncertainties



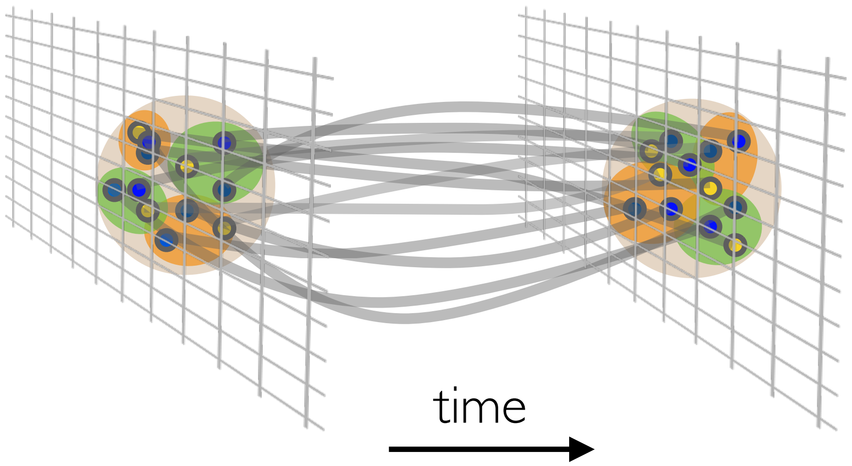
Nuclear physics from LQCD

Nuclei on the lattice: HARD

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



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



Calculations possible for A<5 (unphysically heavy quark masses)

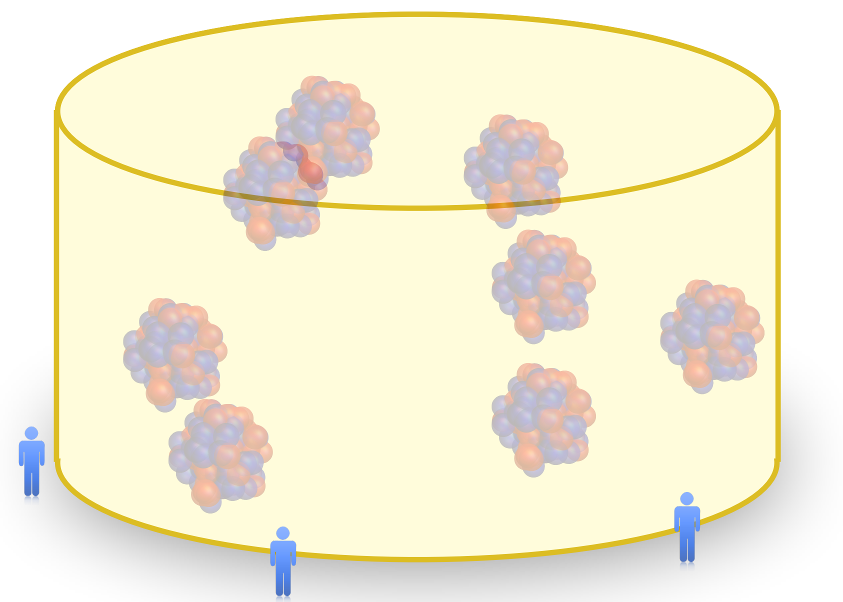
Dark matter

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

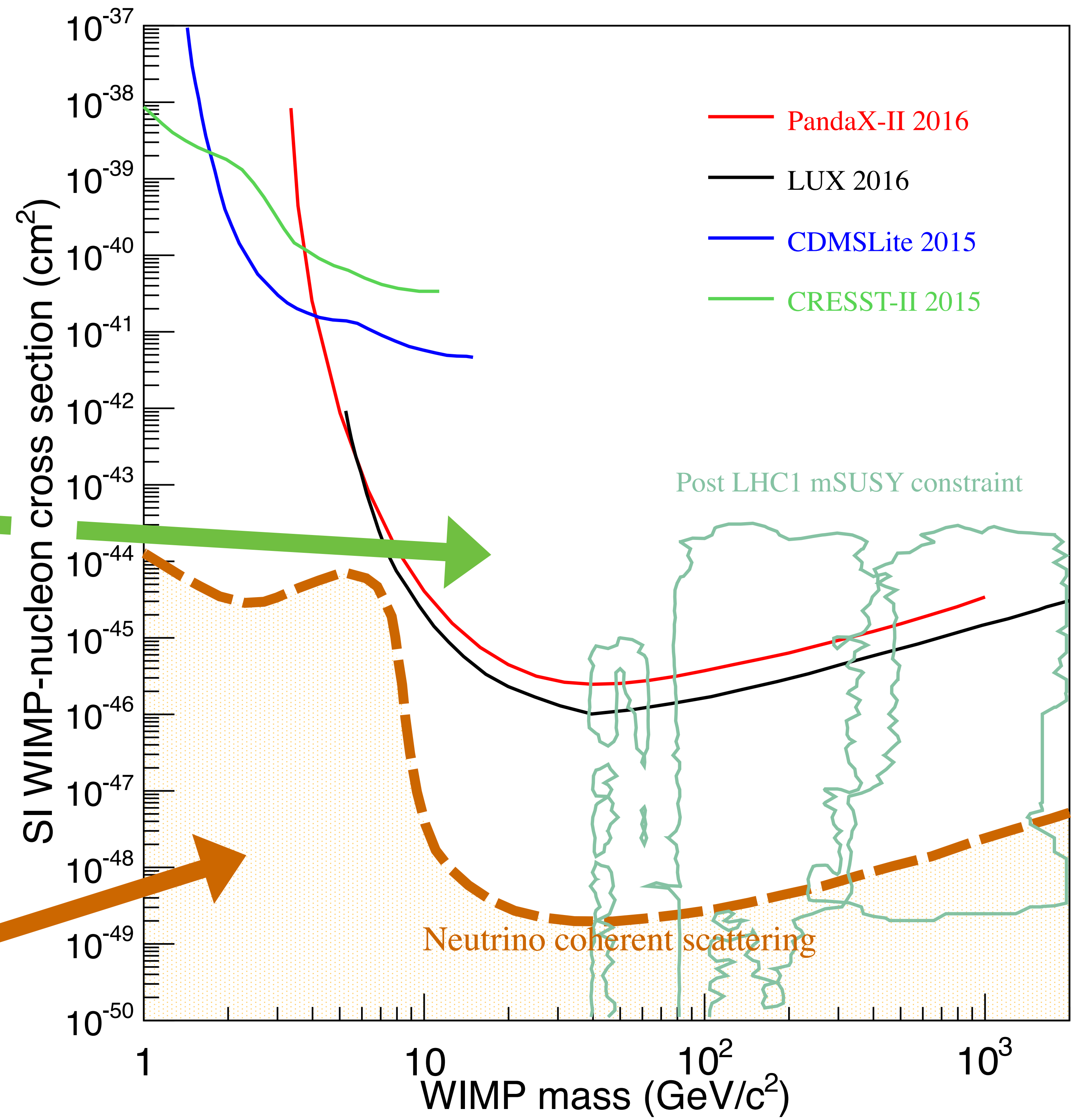
- Dark matter properties
- Probability for interaction with nucleus

Dark matter direct detection

Limits on WIMP-nucleon interaction from direct detection experiments

Ruled out above the solid lines

Background



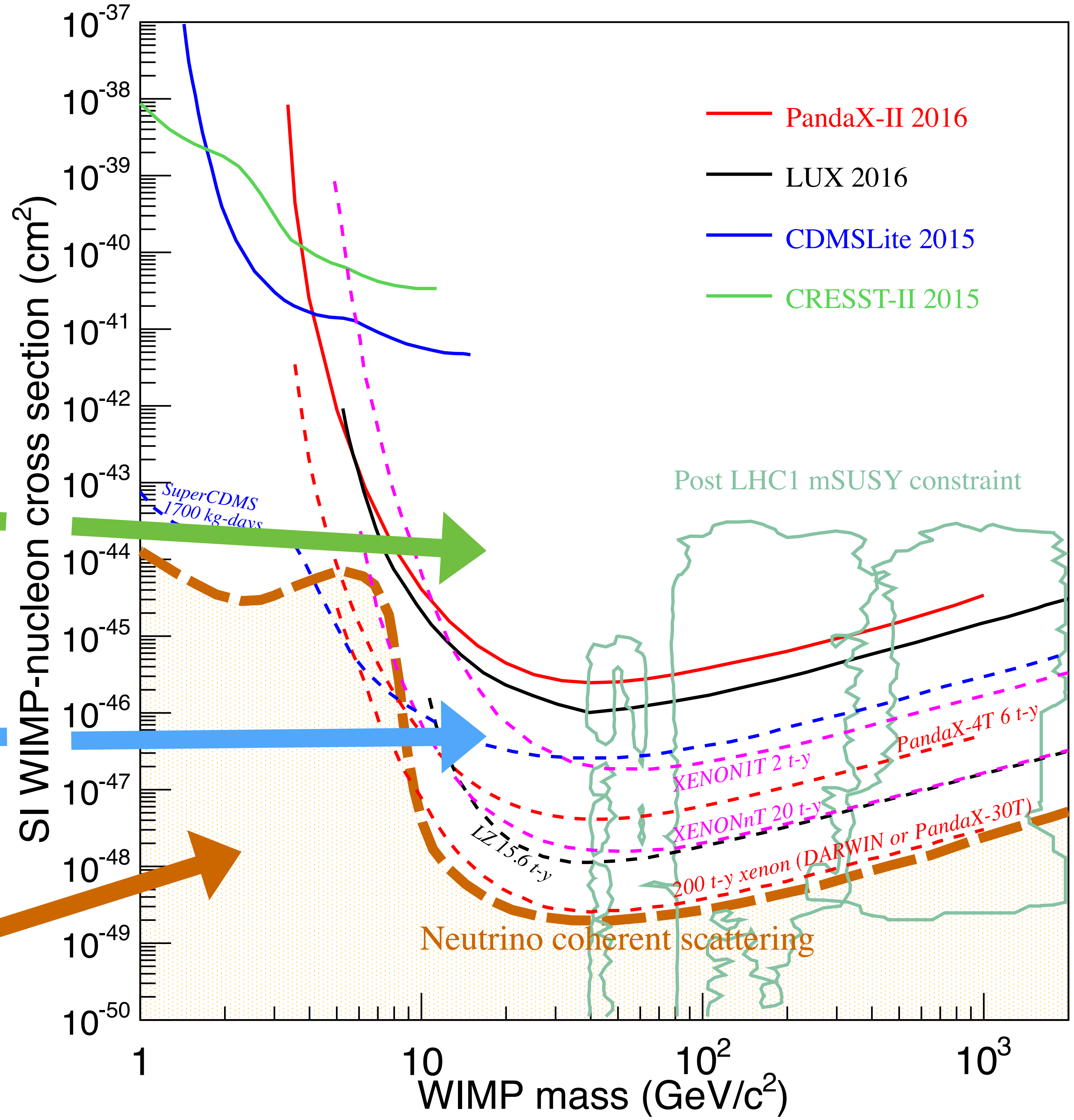
Dark matter direct detection

Limits on WIMP-nucleon interaction from direct detection experiments

Ruled out above the solid lines

Projected limits from future experiments

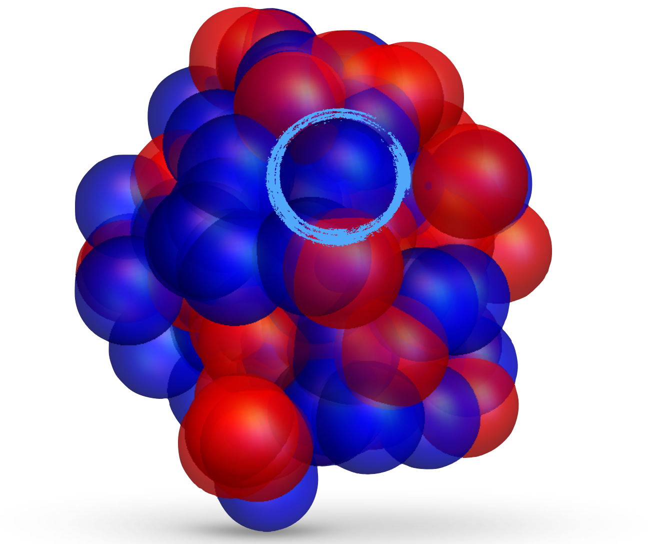
Background



Dark matter

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

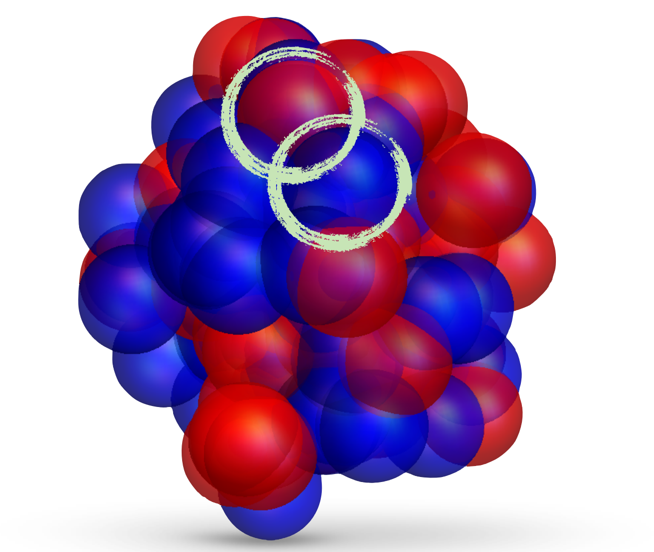
- Born approximation – interacts with a single nucleon



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

known from LQCD

- Interacts non-trivially with multiple nucleons

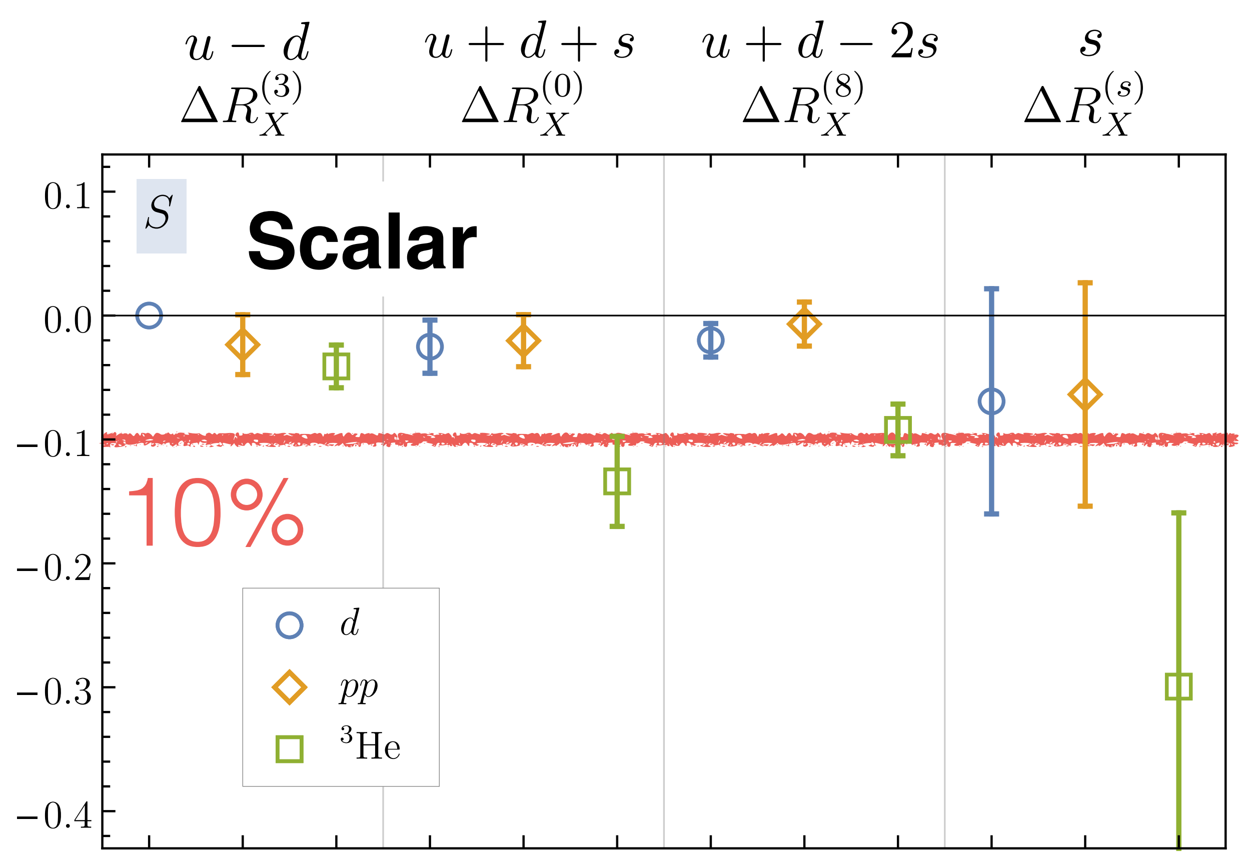


$$\sigma \sim |A \langle N|DM|N\rangle + \alpha \langle NN|DM|NN\rangle + \ldots|^2$$

poorly known!

Scalar matrix elements

- Spin-independent scattering of many WIMP candidates governed by scalar matrix elements
- Lattice QCD calculation shows 10% nuclear effects! (CAVEAT: still significant systematics, computation limited)



$$\frac{\textbf{ME}}{\textbf{Nucleon ME}} - \textbf{naive expectation}$$

“Multiply up” nucleon expectation

Scalar matrix elements

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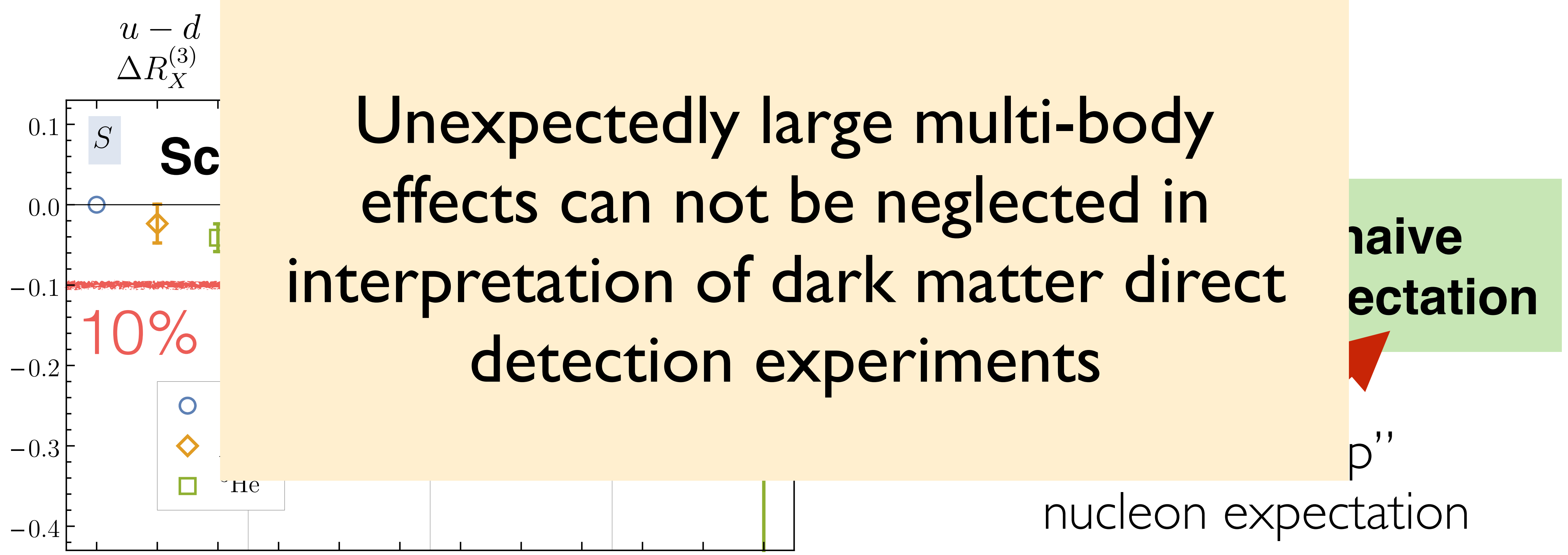


Unexpectedly large multi-body effects can not be neglected in interpretation of dark matter direct detection experiments

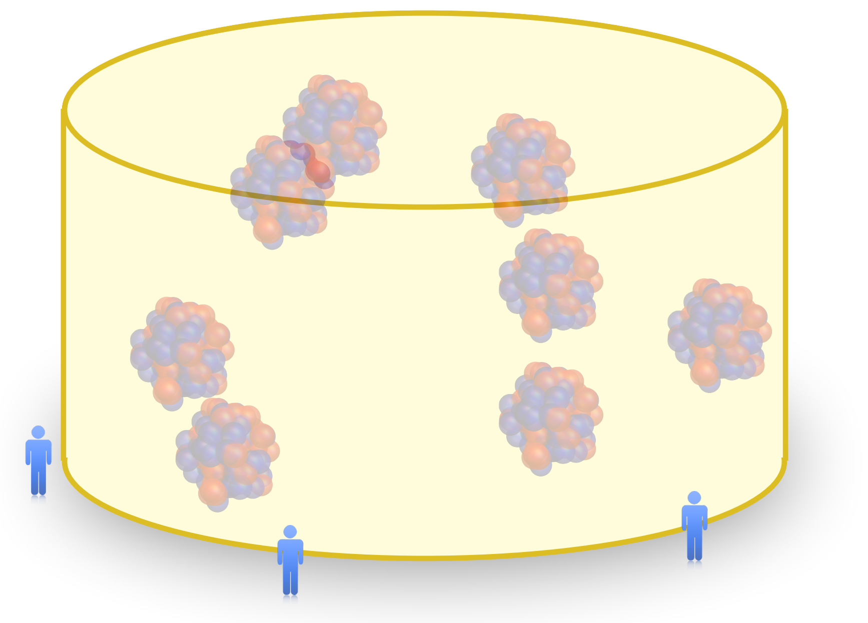
Motivation: ML for LQCD

First-principles nuclear physics beyond A=4

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

Interpretation of intensity-frontier experiments

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



Exponentially harder problems → Need exponentially improved algorithms

Machine learning for LQCD

APPROACH

Machine learning as ancillary tool for lattice QCD

- Accelerate gauge-field generation
- Optimise extraction of physics from gauge field ensemble

} Will need to accelerate all stages of lattice QCD workflow to achieve physics goals

- **ONLY apply where quantum field theory can be rigorously preserved**

Generate QCD gauge fields

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

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

Molecular dynamics

Classical motion with

conjugate

$$H = \sum_x \frac{\pi^2(x)}{2} + S[\phi(x)]$$

- Reversible
- Volume-preserving

BUT

- Energy non-conservation for numerical integrators

Markov Chain Monte Carlo

Propose update using integrated molecular dynamics trajectory

Accept/ reject with probability

$$\alpha = \min(1, e^{(-S[\phi'(x)]+S[\phi(x)])})$$

- Numerical error corrected by accept/reject

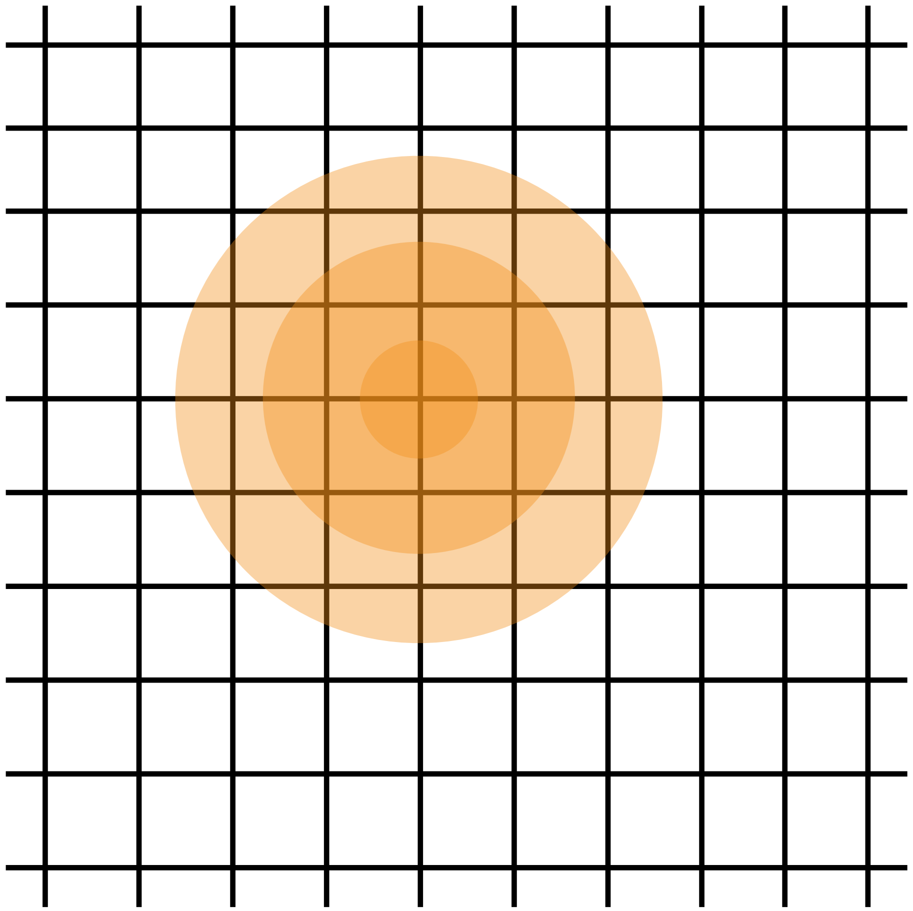
BUT

- Short trajectories for high acceptance

Accelerating HMC: action matching

QCD gauge field configurations sampled via

Hamiltonian dynamics + Markov Chain Monte Carlo



Updates diffusive

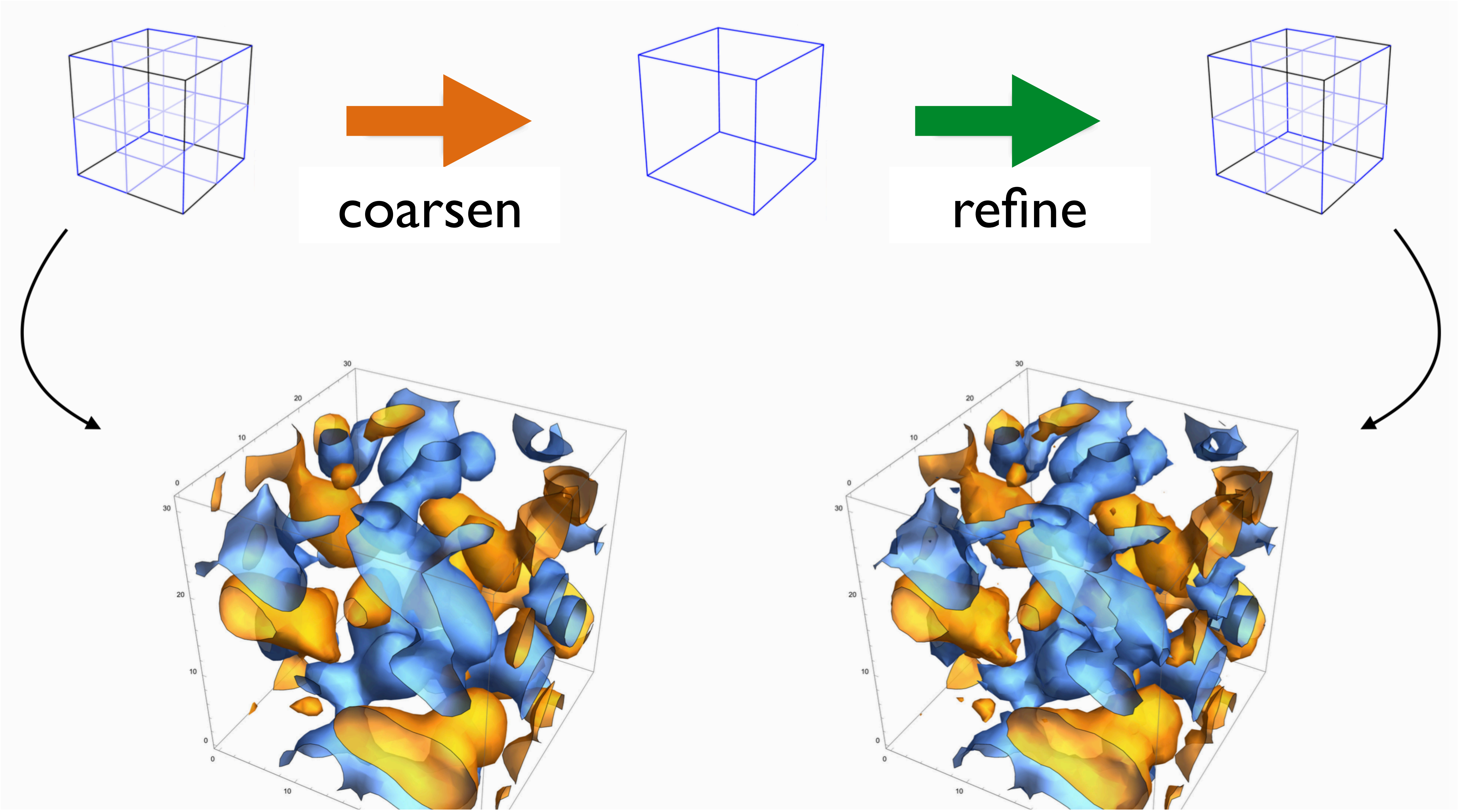
Lattice spacing → 0

Number of updates to change fixed physical length scale → ∞

"Critical slowing-down" of generation of uncorrelated samples

Multi-scale HMC updates

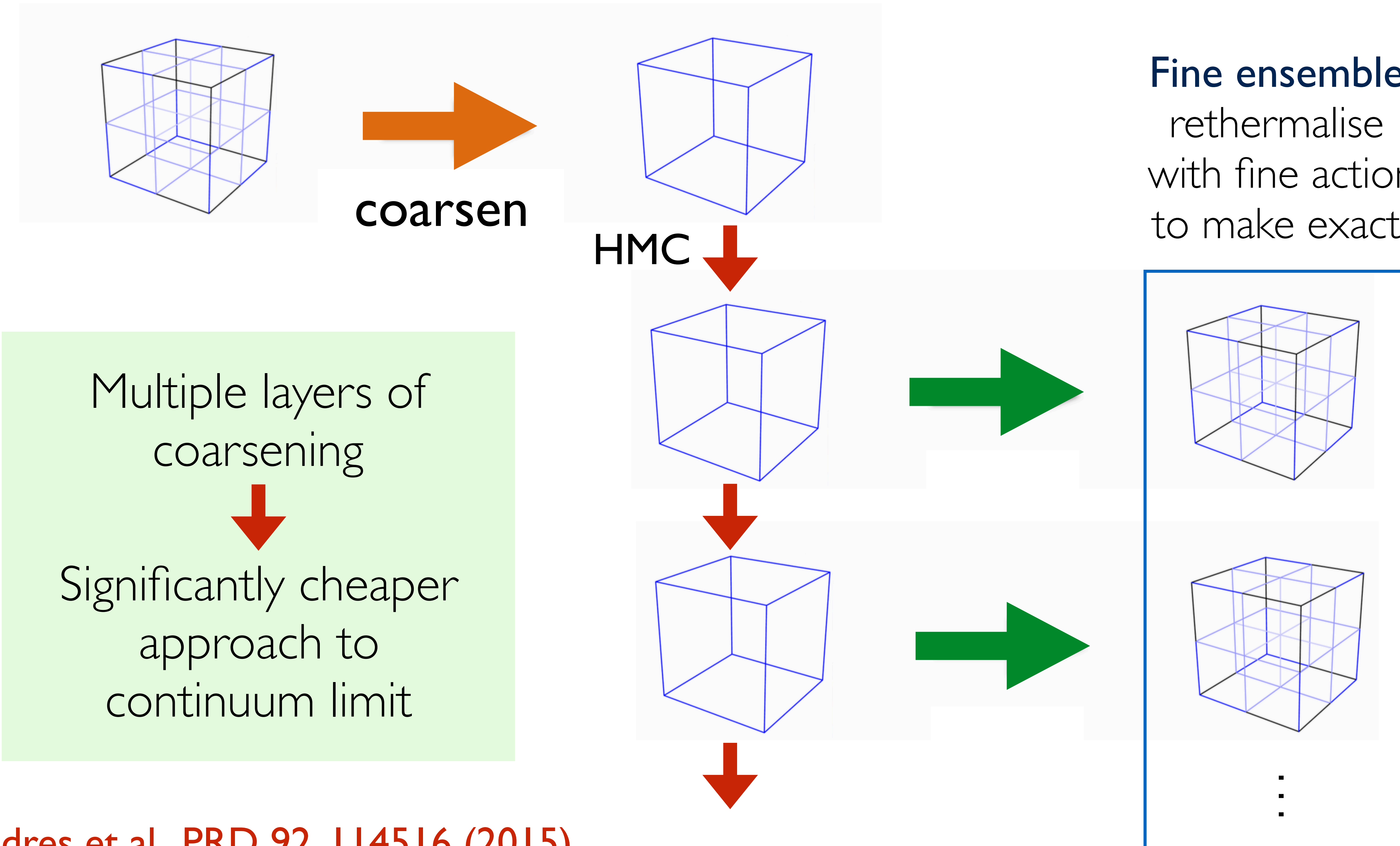
Given coarsening and refinement procedures…



Endres et al., PRD 92, 114516 (2015)

Multi-scale HMC updates

Perform HMC updates at coarse level



Multiple layers of coarsening

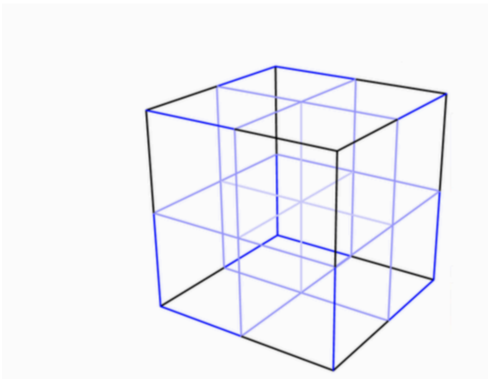
↓

Significantly cheaper approach to continuum limit

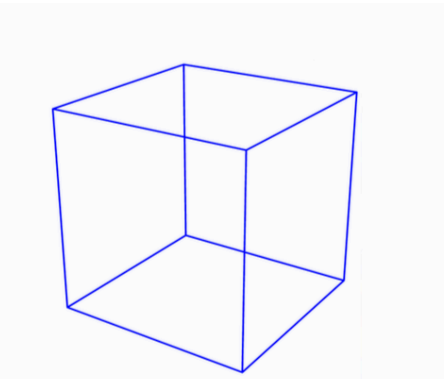
Endres et al., PRD 92, 114516 (2015)

Multi-scale HMC updates

Perform HMC updates at coarse level



encode same long-distance physics



MUST KNOW
parameters of coarse QCD action that reproduce ALL physics parameters of fine simulation

Map a subset of physics parameters in the coarse space and match to coarsened ensemble

OR

Solve regression problem directly: "Given a coarse ensemble, what parameters generated it?"

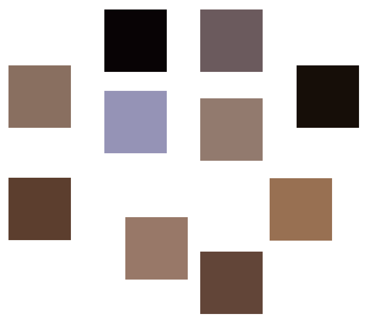
Machine learning LQCD

Neural networks excel on problems where

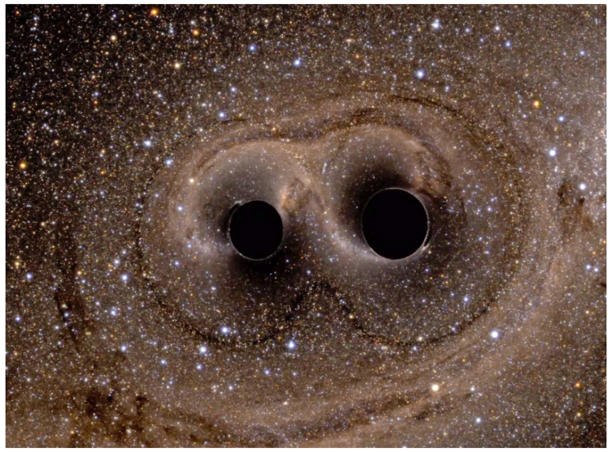
Basic data unit has little meaning ⟷ Combination of units is meaningful

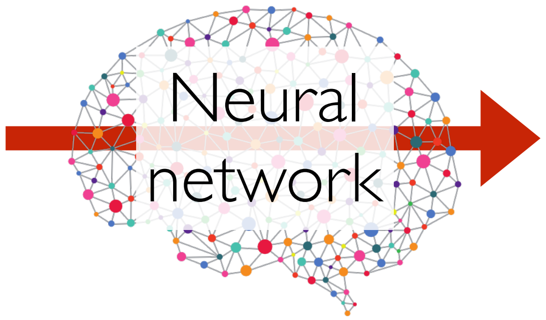
Image recognition

Pixel



Image





Label

"Colliding black holes"

Machine learning LQCD

Neural networks excel on problems where

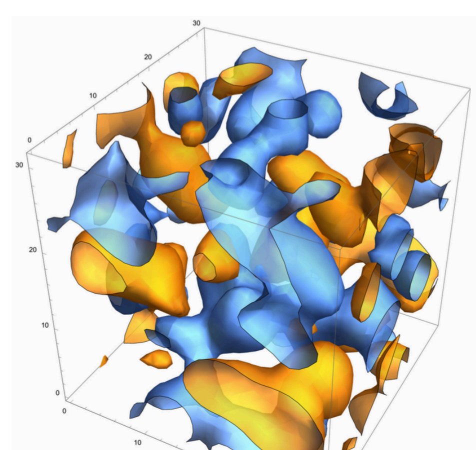
Basic data unit has little meaning	⟷	Combination of units is meaningful

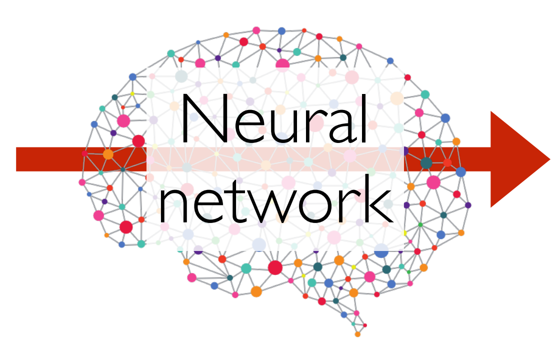
Parameter identification

Element of a colour matrix at one discrete space-time point

0 6 7 3 5 2 8 4 1 6

Ensemble of lattice QCD gauge field configurations





Label

Parameters of action

Machine learning LQCD

CIFAR benchmark image set for machine learning

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

Ensemble of lattice QCD gauge fields

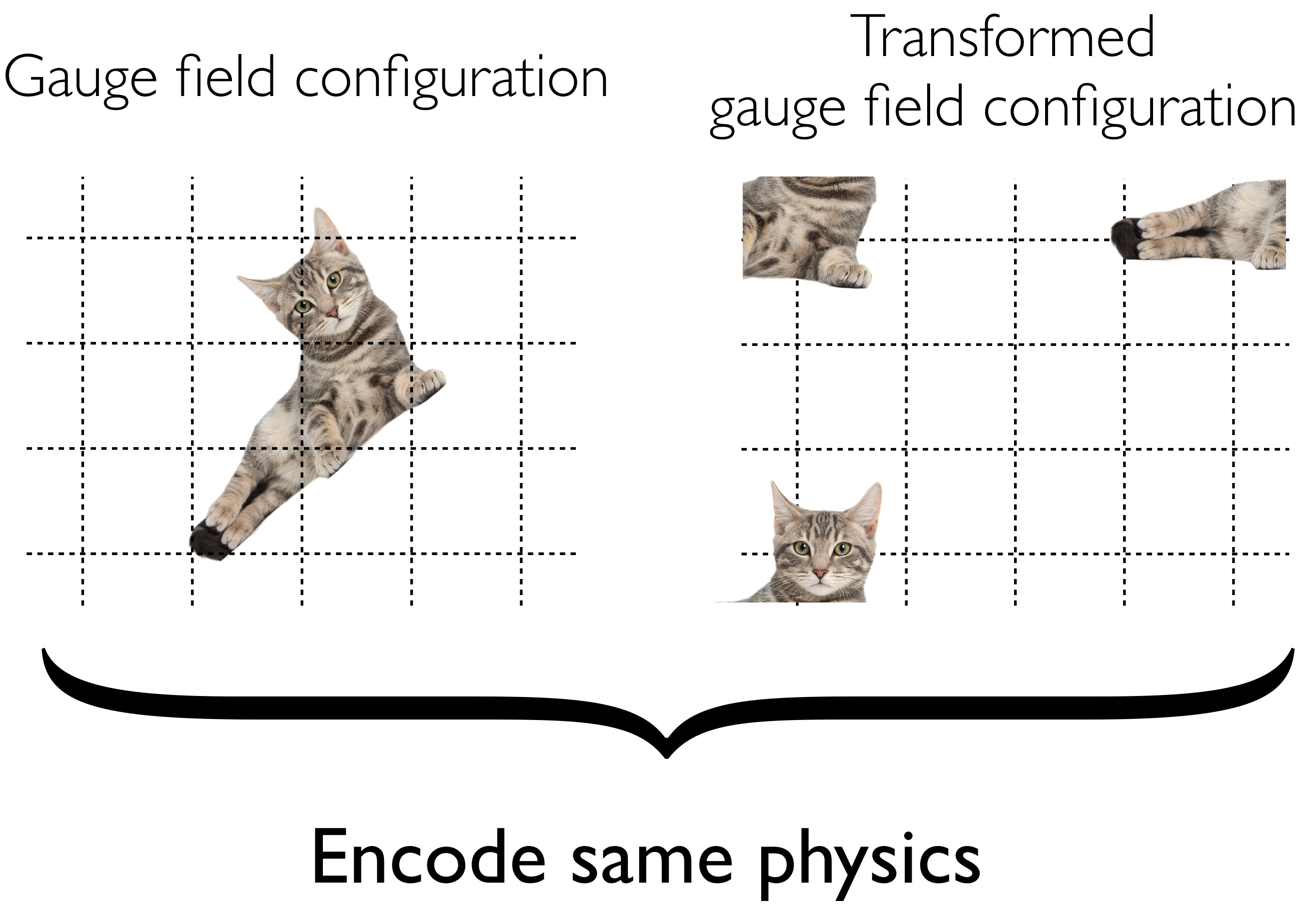
- $64^3 \times 128 \times 4 \times N_c^2 \times 2 \simeq 10^9$ numbers
- ~ 1000 samples
- Ensemble of gauge fields has meaning
- Long-distance correlations are important
- Gauge and translation-invariant with periodic boundaries

Symmetries of LQCD gauge fields

Physics encoded by lattice QCD gauge fields
is invariant under specific field transformations

- **Rotation (4D)**
- **Translation**

with periodic
boundary conditions

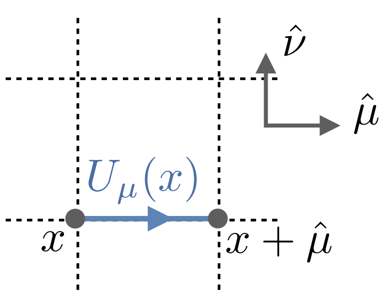


Symmetries of LQCD gauge fields

Physics encoded by lattice QCD gauge fields
is invariant under specific field transformations

Gauge transformation

Separate group transformation of each link matrix $U_\mu(x)$

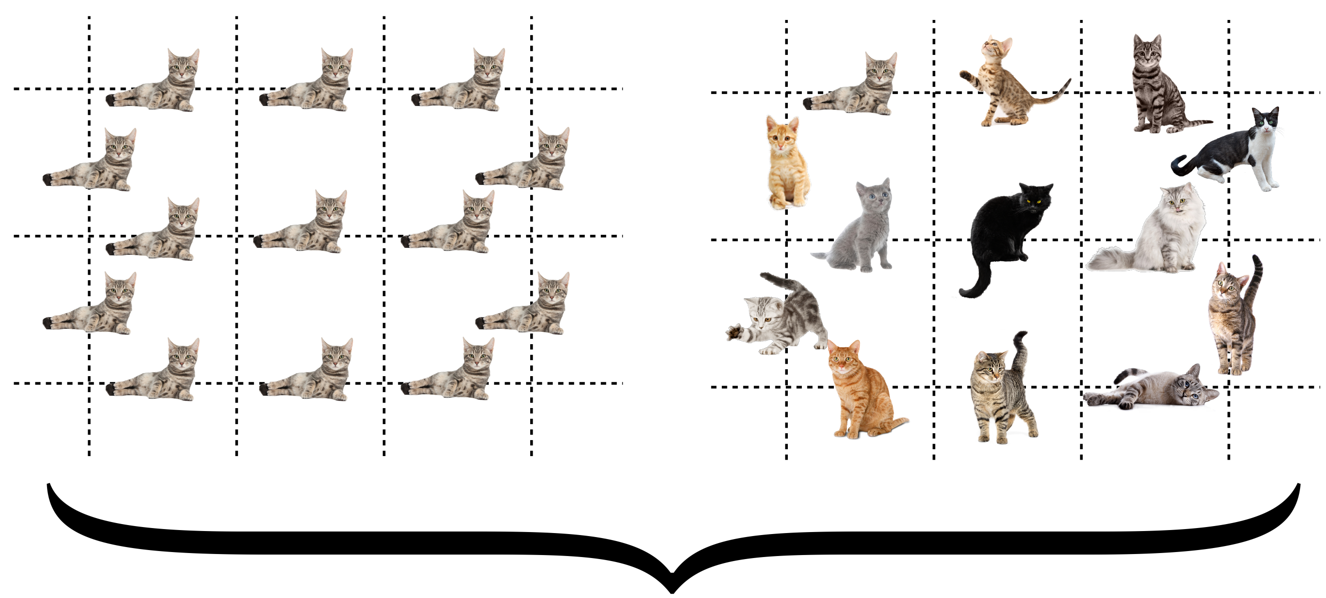


$$U_\mu(x) \to U'_\mu(x) = \Omega(x) U_\mu(x) \Omega^\dagger(x+\hat{\mu})$$

$$\text{for all } \Omega(x) \in \mathrm{SU}(3)$$

Gauge field configuration

Transformed
gauge field configuration



Encode same physics

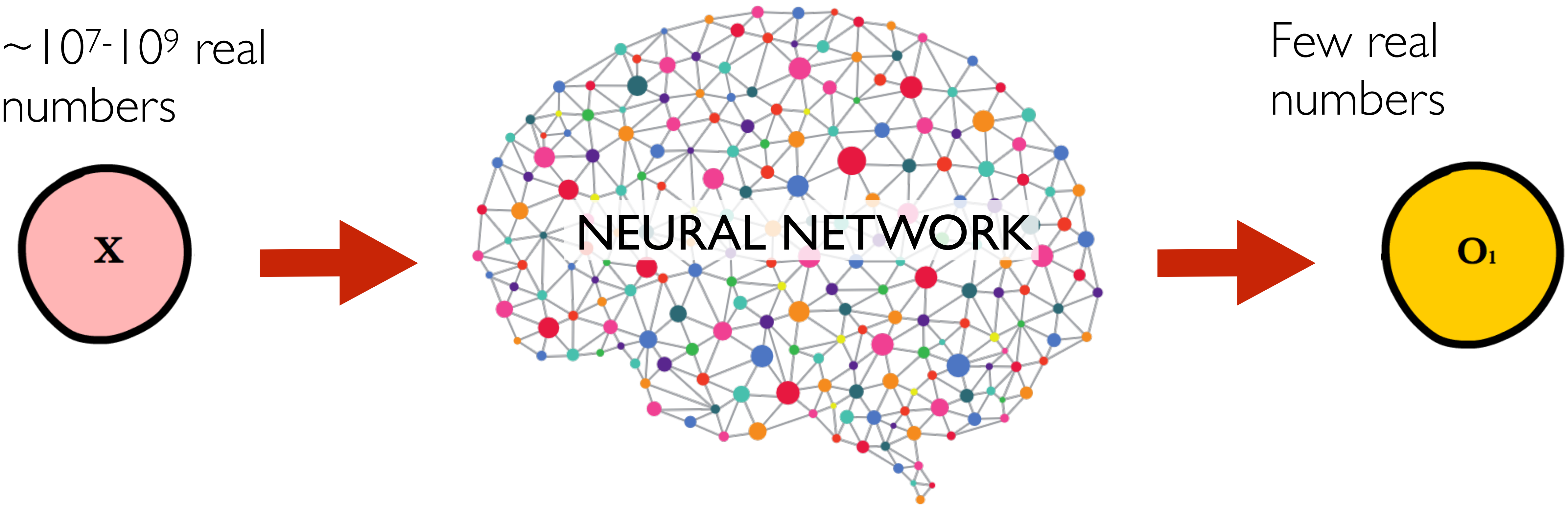
Regression by neural network

Lattice QCD gauge field

~10^7-10^9 real numbers

Parameters of lattice action

Few real numbers



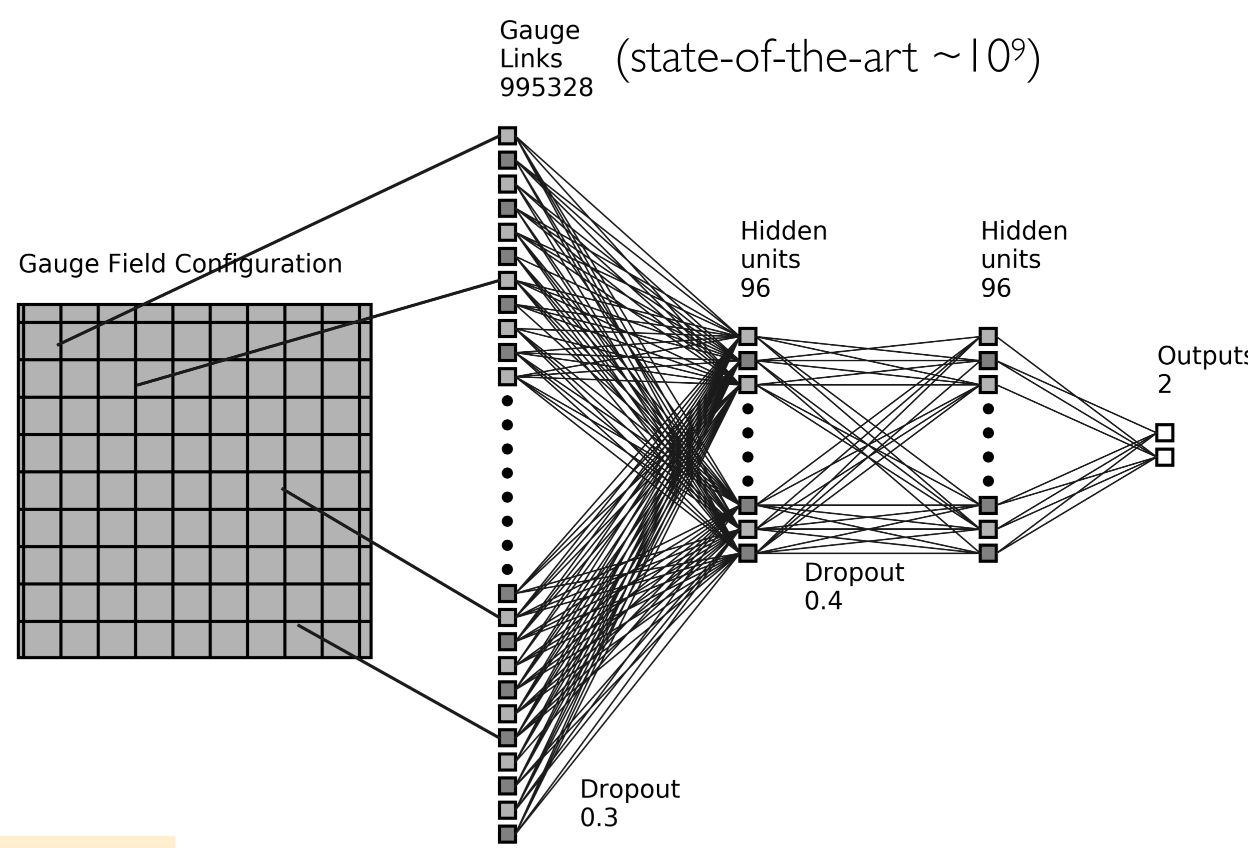
- **Complete:** not restricted to affordable subset of physics parameters
- **Instant:** once trained over a parameter range

Naive neural network

Simplest approach ⟷ Ignore physics symmetries

Train simple neural network on regression task

- Fully-connected structure
- Far more degrees of freedom than number of training samples available

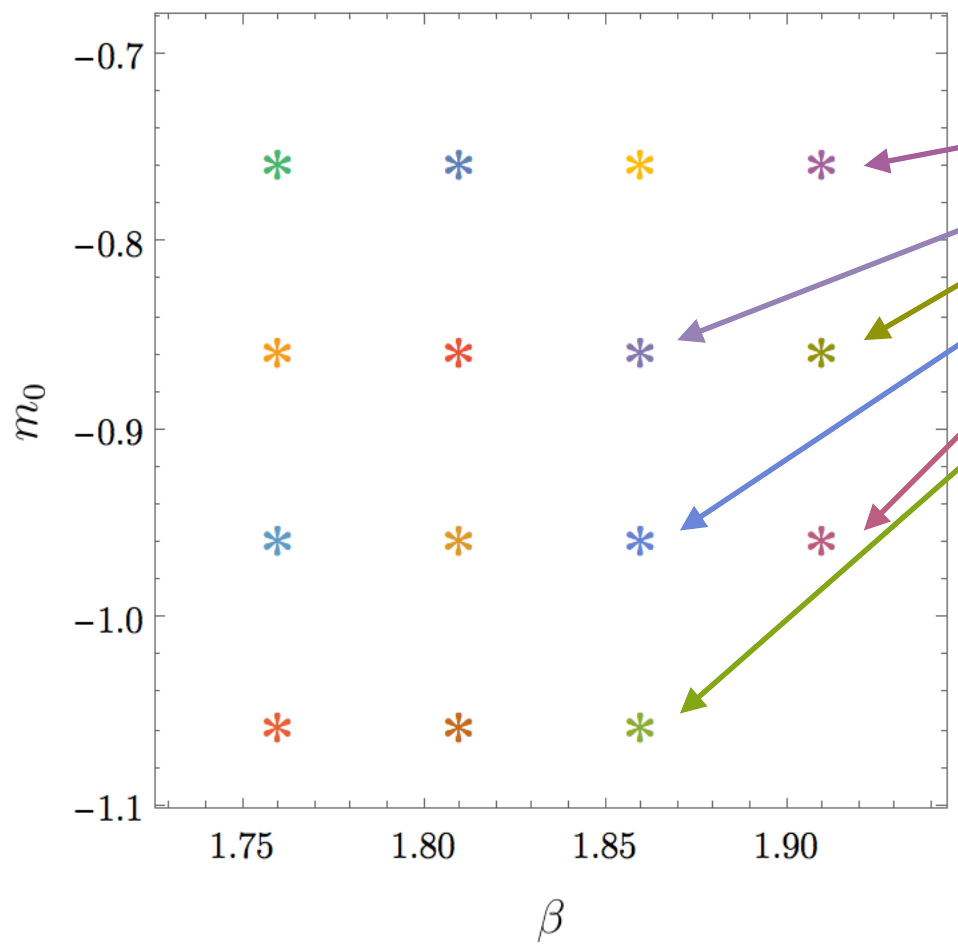


"Inverted data hierarchy" → Recipe for overfitting!

Naive neural network

Training and validation datasets

Quark mass parameter



Parameter related to lattice spacing

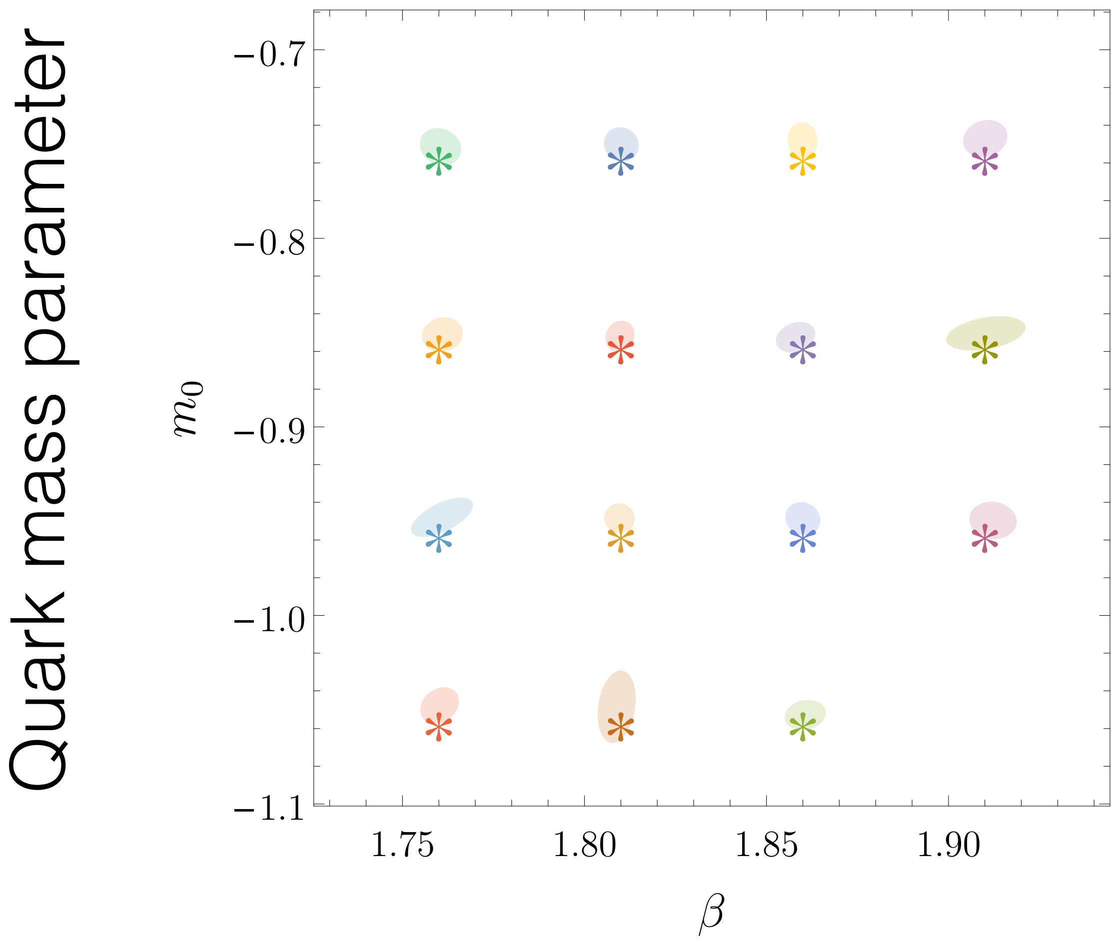
* Parameters of training and validation datasets

- O(10,000) independent configurations generated at each point
- Validation configurations randomly selected from generated streams

Spacing in evolution stream >> correlation time of physics observables

Naive neural network

Neural net predictions on validation data sets



Parameter related to lattice spacing

* True parameter values

Confidence interval from ensemble of gauge fields

SUCCESS?

No sign of overfitting

- Training and validation loss equal
- Accurate predictions for validation data

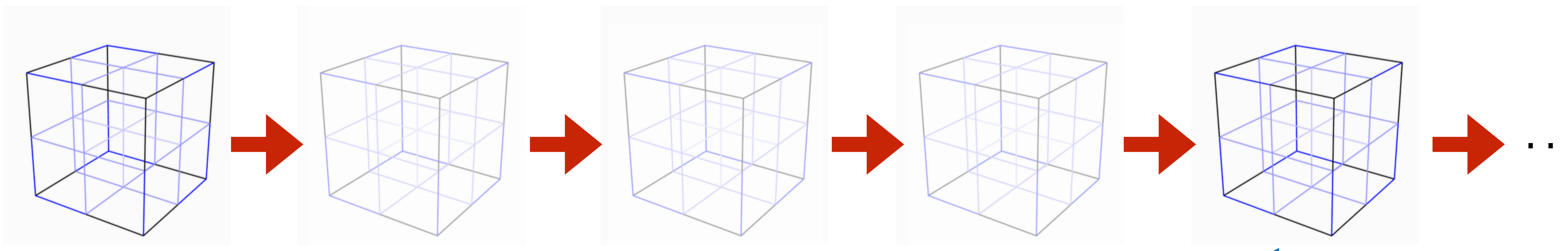
BUT fails to generalise to

- Ensembles at other parameters
- New streams at same parameters

NOT POSSIBLE IF CONFIGS ARE UNCORRELATED

Naive neural network

Stream of generated gauge fields at given parameters



Training/validation data selected from configurations spaced to be decorrelated (by physics observables)

- Network succeeds for validation configs from same stream as training configs
- Network fails for configs from new stream at same parameters

} **Network has identified feature with a longer correlation length than any known physics observable**

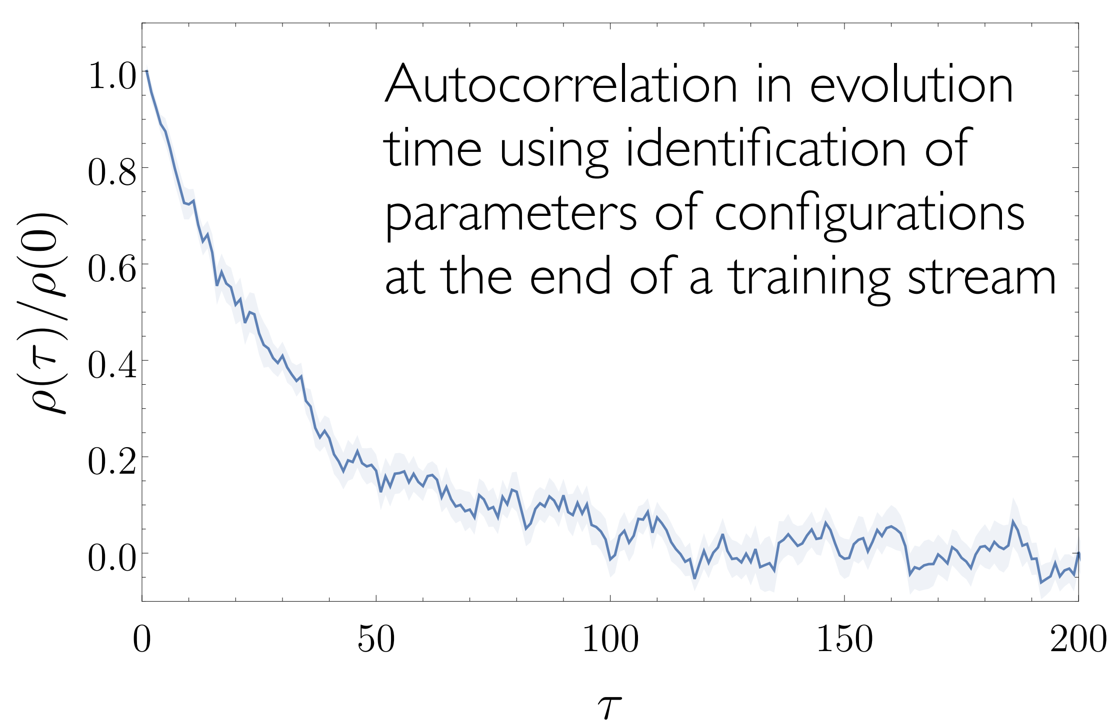
Naive neural network

- Naive neural network that does not respect symmetries fails at parameter regression task

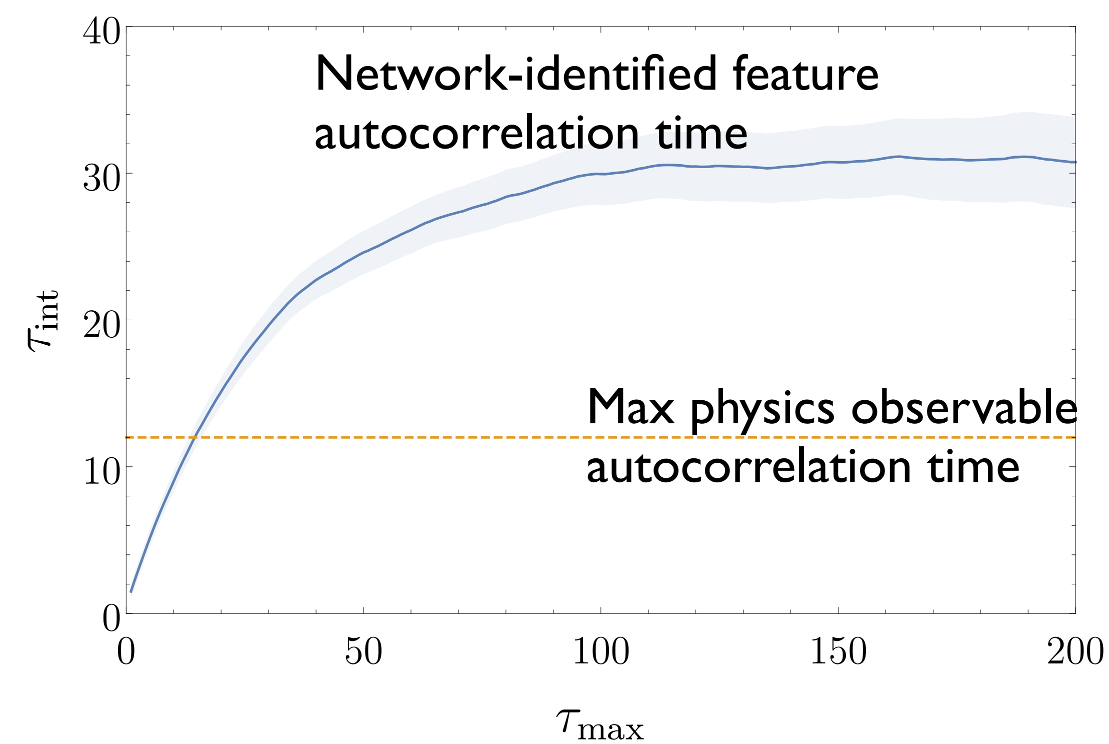
BUT

- Identifies unknown feature of gauge fields with a longer correlation length than any known physics observable

Network feature autocorrelation



$$\tau_{\text{int}} = \frac{1}{2} + \lim_{\tau_{\max}\to\infty} \frac{1}{\rho(0)} \sum_{\tau=0}^{\tau_{\max}} \rho(\tau)$$



Regression by neural network

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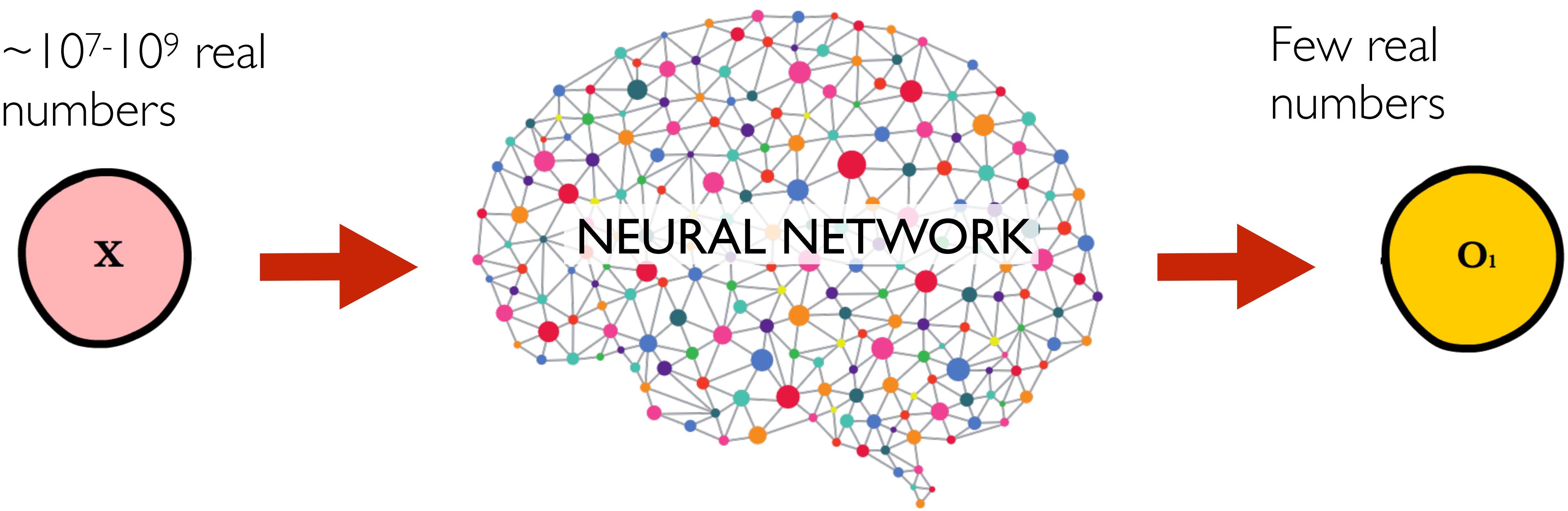

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Regression by neural network

Lattice QCD gauge field

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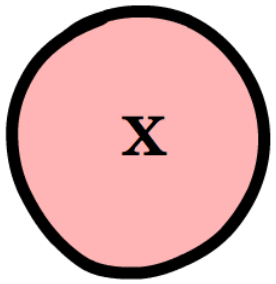
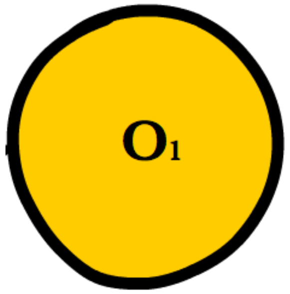


Custom network structures (or data preprocessing)

- Respects gauge-invariance, translation-invariance, boundary conditions
- Emphasises QCD-scale physics
- Range of neural network structures find same minimum

Parameters of lattice action

Few real numbers

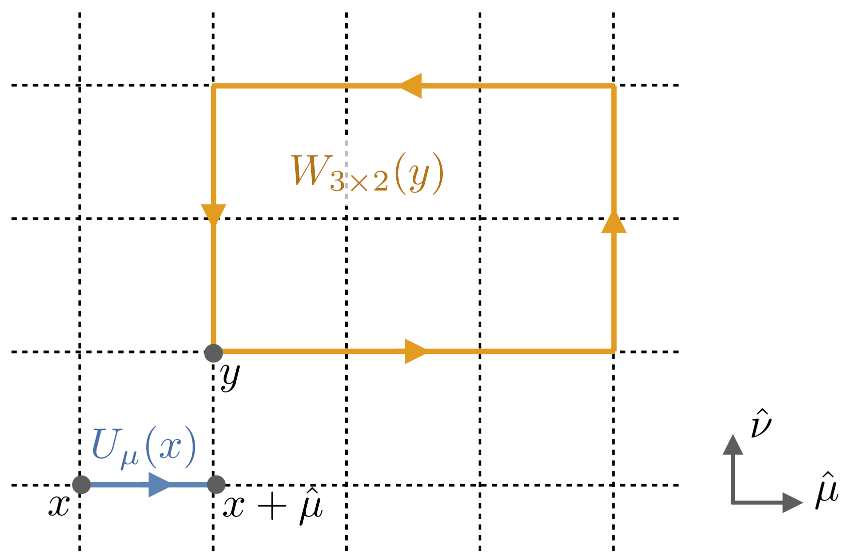


- **Complete:** not restricted to affordable subset of physics parameters
- **Instant:** once trained over a parameter range

Symmetry-preserving network

Network based on symmetry-invariant features

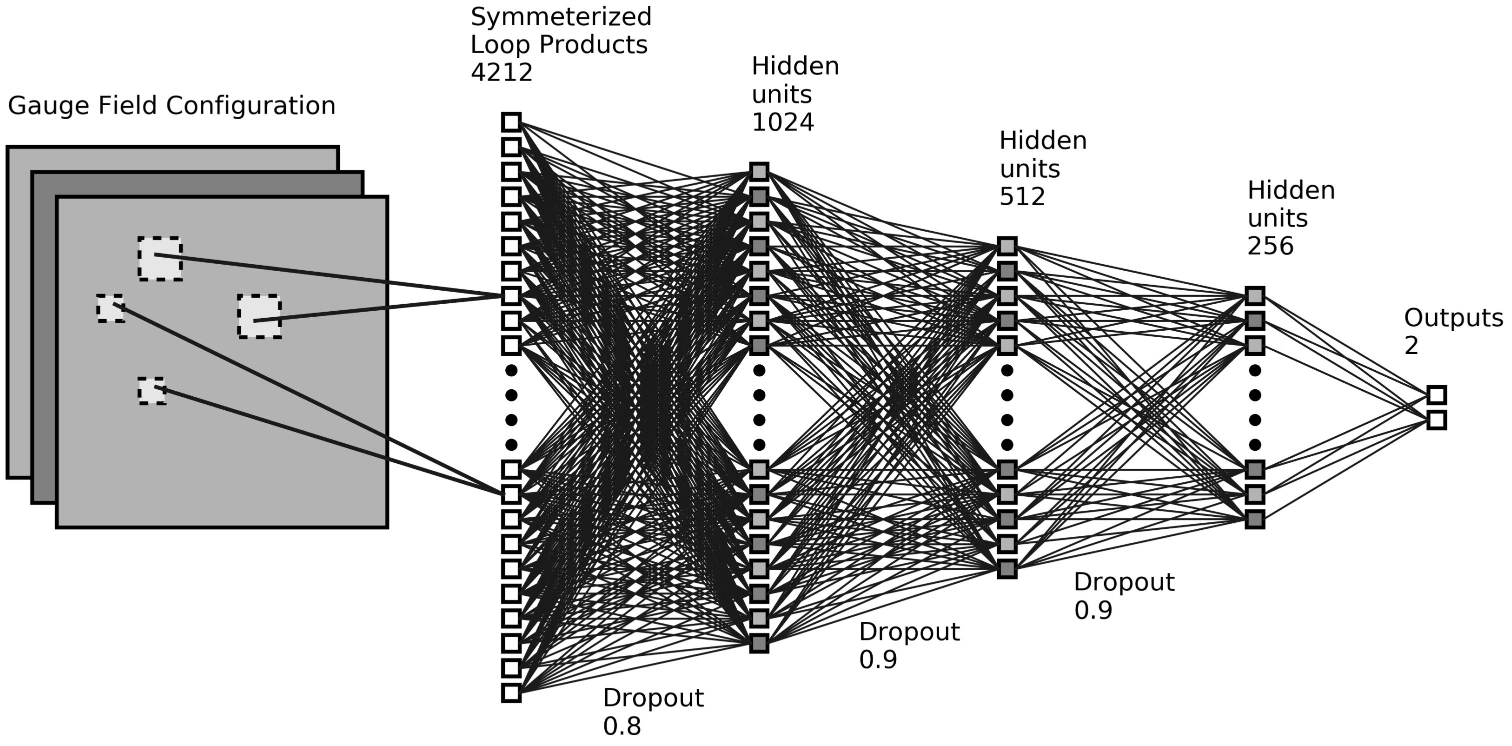
Closed Wilson loops
(gauge-invariant)



- Loops
- Correlated products of loops at various length scales
- Volume-averaged and rotation-averaged

Symmetry-preserving network

Network based on symmetry-invariant features



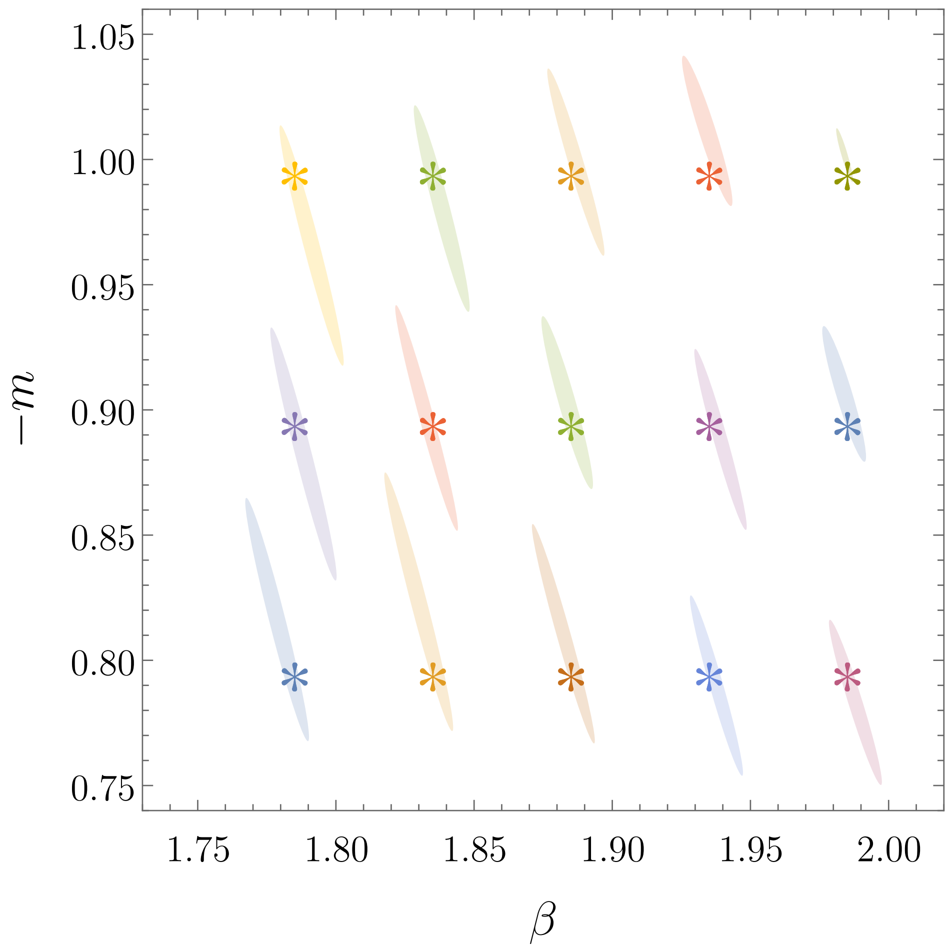
- Fully-connected network structure
- First layer samples from set of possible symmetry-invariant features

Number of degrees of freedom of network comparable to size of training dataset

Gauge field parameter regression

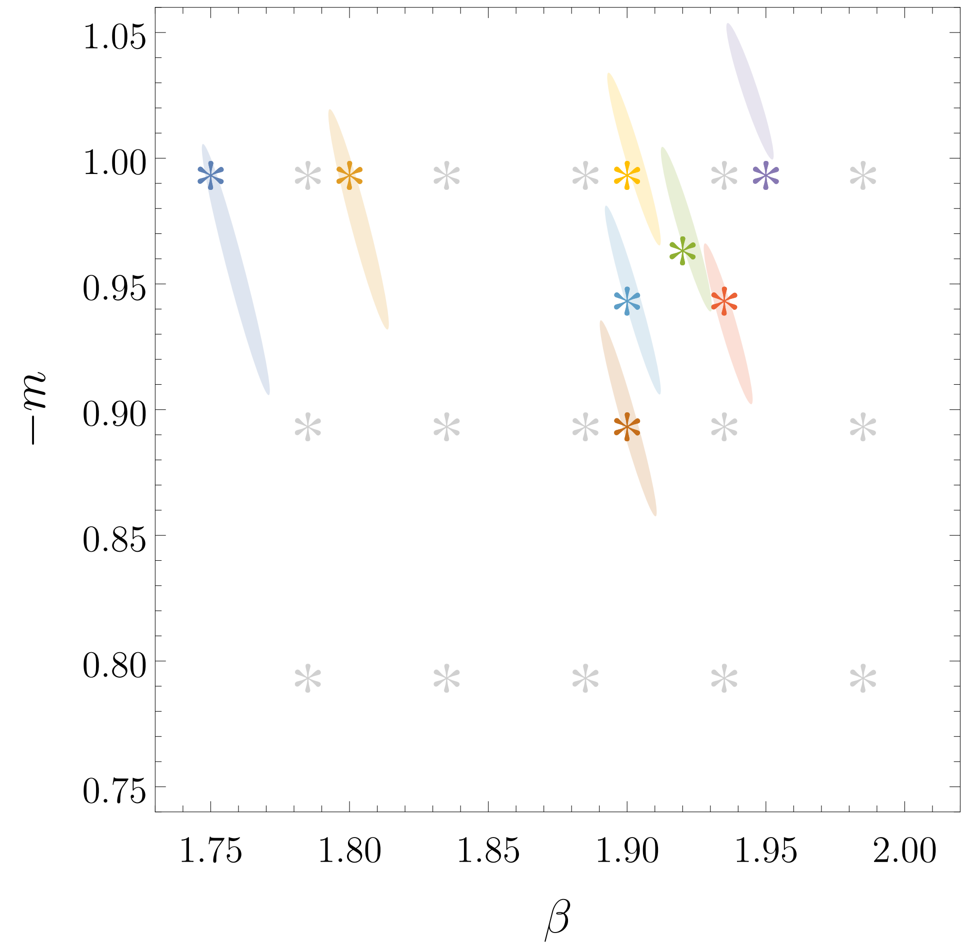
Neural net predictions on validation data sets

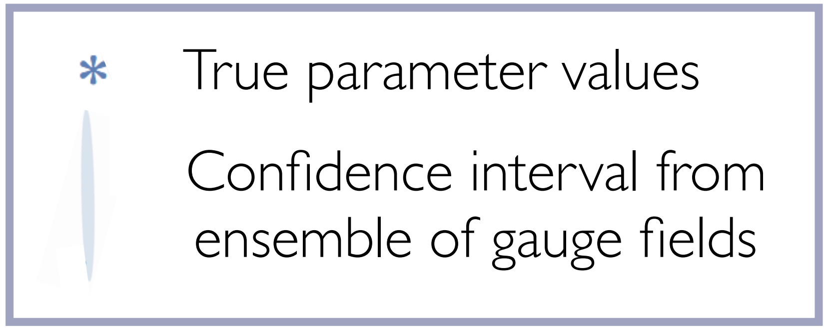
Quark mass parameter



Parameter related to lattice spacing

Predictions on new datasets

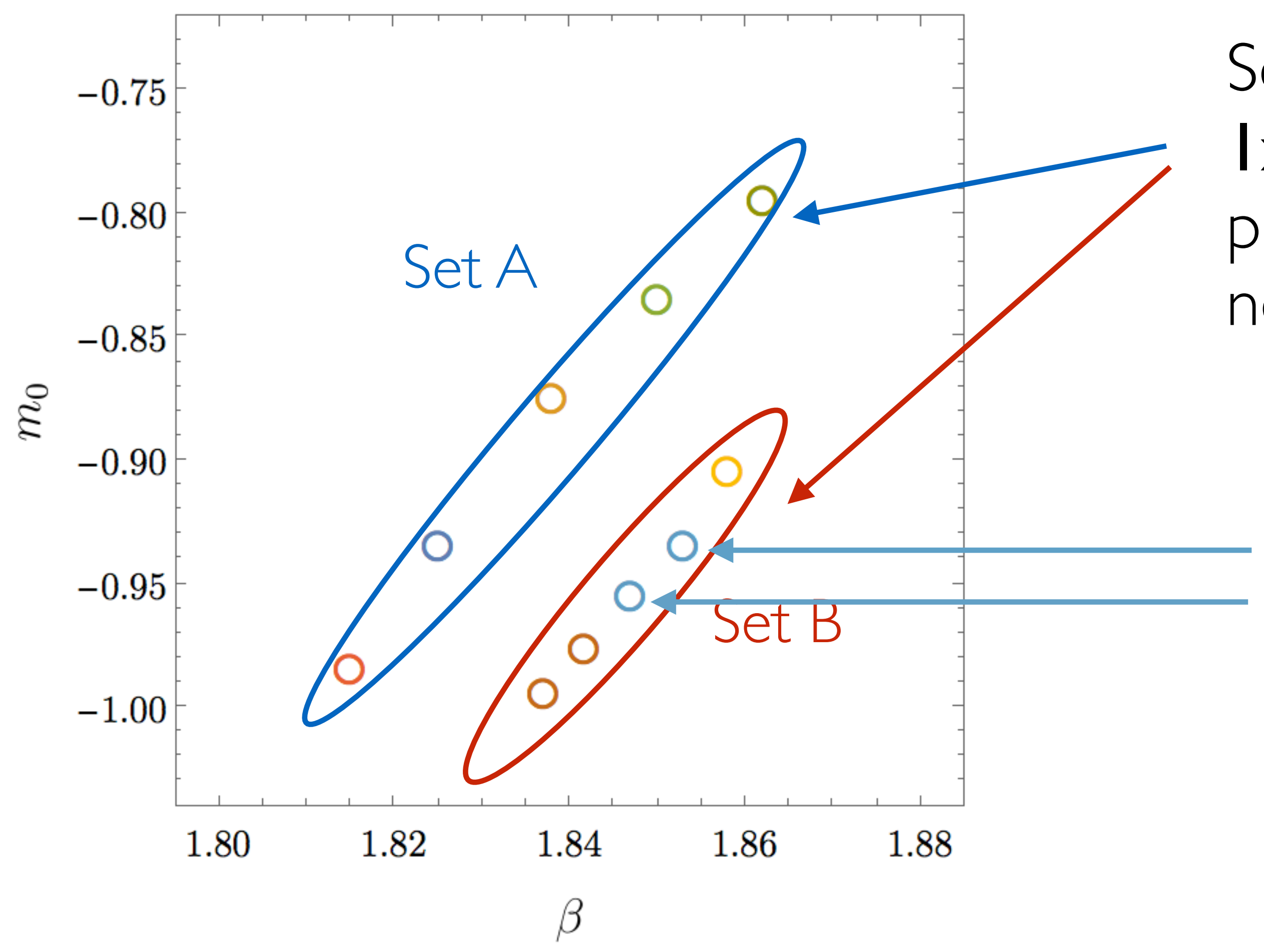




Tests of network success

How does neural network regression perform compared with other approaches?

Consider very closely-spaced validation ensembles at new parameters



Sets along lines of **constant 1x1 Wilson loop** (most precise feature allowed by network)

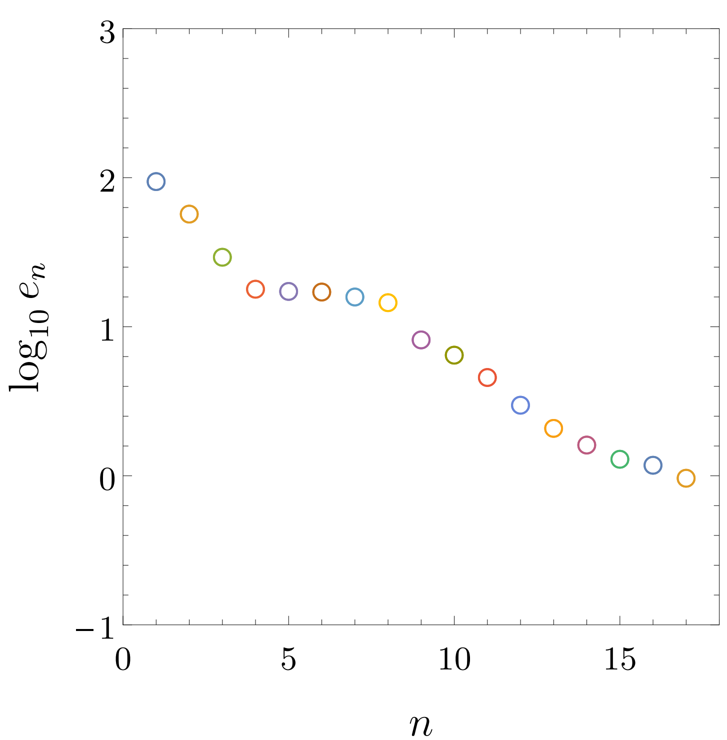
Much closer spacing than separation of training ensembles

Tests of network success

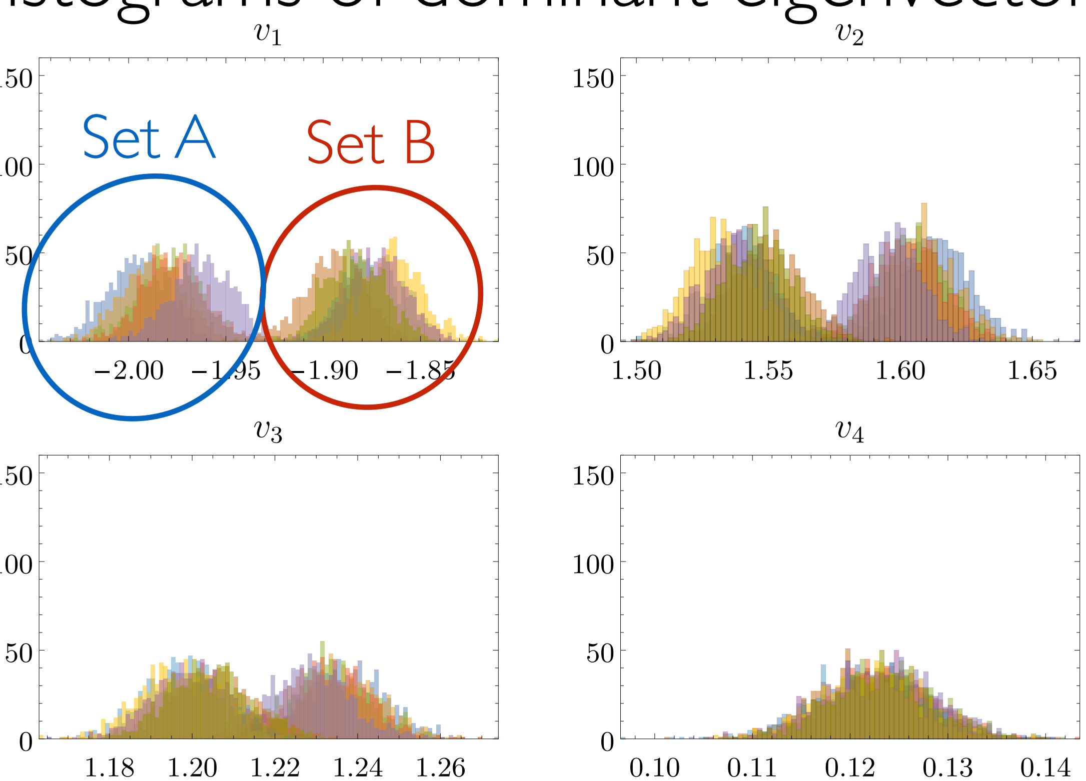
How does neural network regression perform compared with other approaches?

Consider very closely-spaced validation ensembles at new parameters: **not distinguishable to principal component analysis in loop space**

Eigenvalues



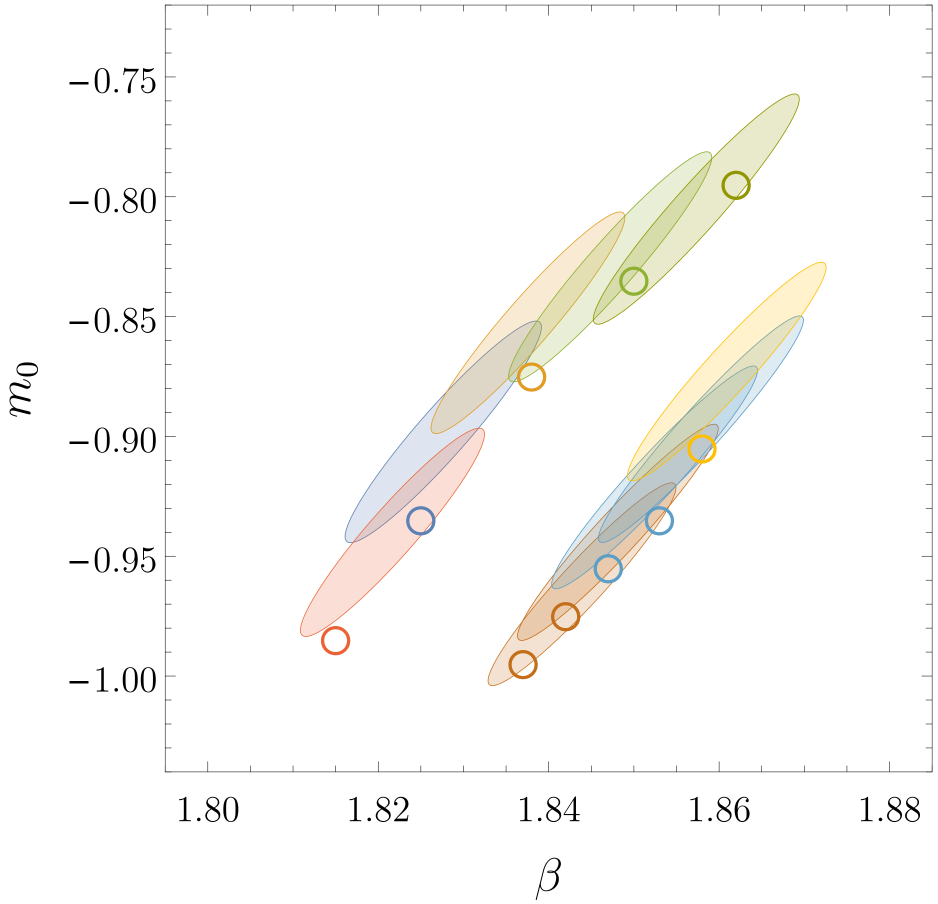
Histograms of dominant eigenvectors



Tests of network success

How does neural network regression perform compared with other approaches?

Consider very closely-spaced validation ensembles at new parameters: **distinguishable to trained neural network**

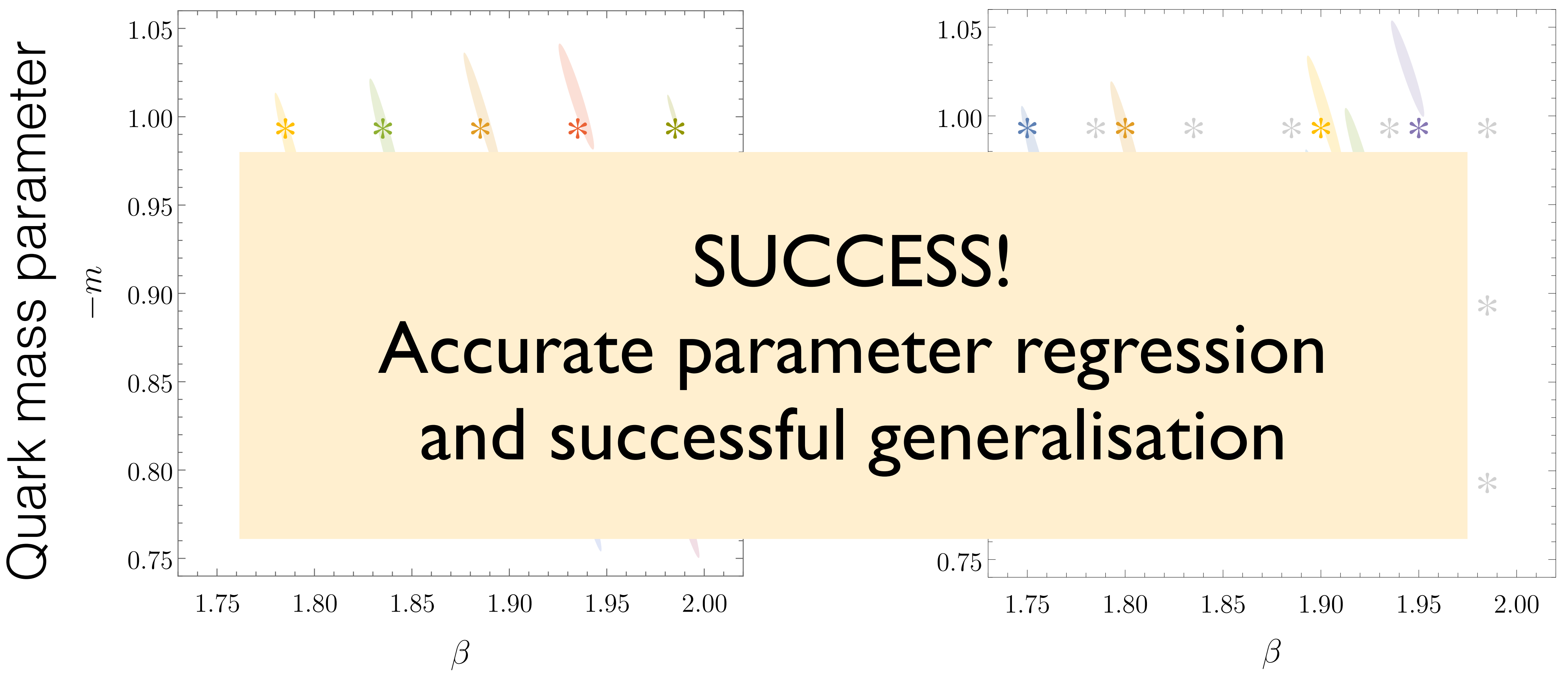


- Correct ordering of central values
- Accurate regression differences even at very fine resolution

Gauge field parameter regression

Neural net predictions on validation data sets

Predictions on new datasets



SUCCESS!
Accurate parameter regression and successful generalisation

Parameter related to lattice spacing

* True parameter values

Confidence interval from ensemble of gauge fields

Gauge field parameter regression

PROOF OF PRINCIPLE

Step towards fine lattice generation at reduced cost

1. Generate one fine configuration
2. Find matching coarse action
3. HMC updates in coarse space
4. Refine and rethermalise

Accurate matching minimises cost of updates in fine space

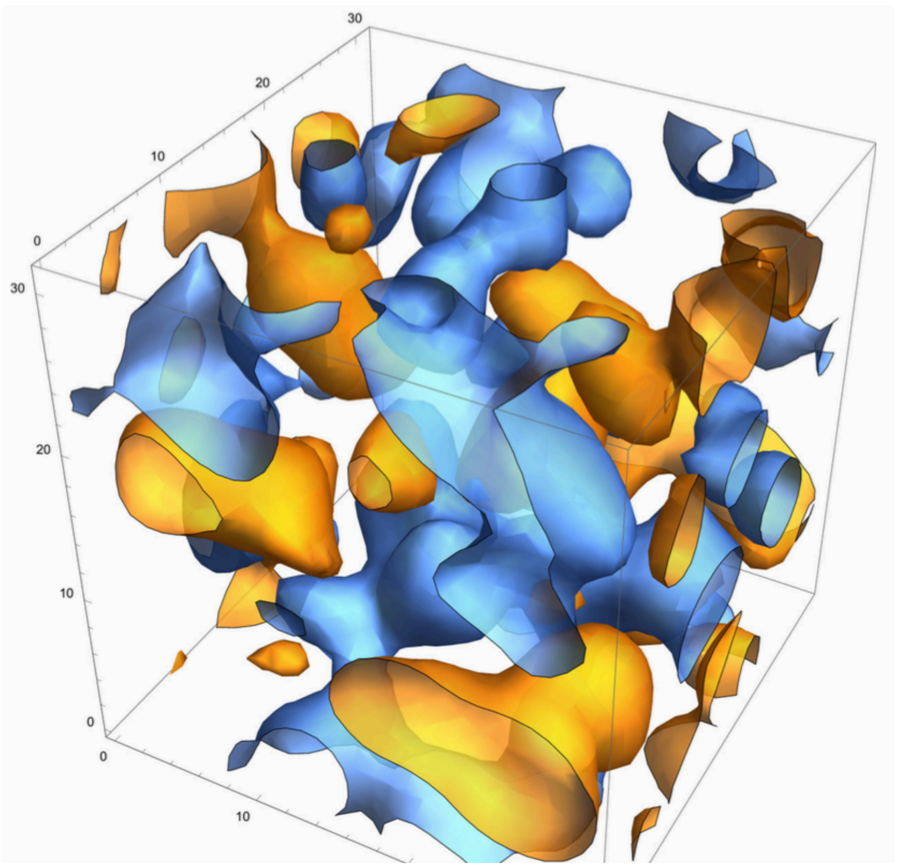
Guarantees correctness ✓

Shanahan, Trewartha, Detmold, PRD (2018) [1801.05784]

Machine learning QCD

Accelerate gauge-field generation

- Multi-scale matching PROOF OF PRINCIPLE ✓
- Generative models to replace expensive HMC IN PROGRESS
- Learn parameters of a complicated pure-gauge action (cheap) to reproduce action with dynamical fermions (expensive)

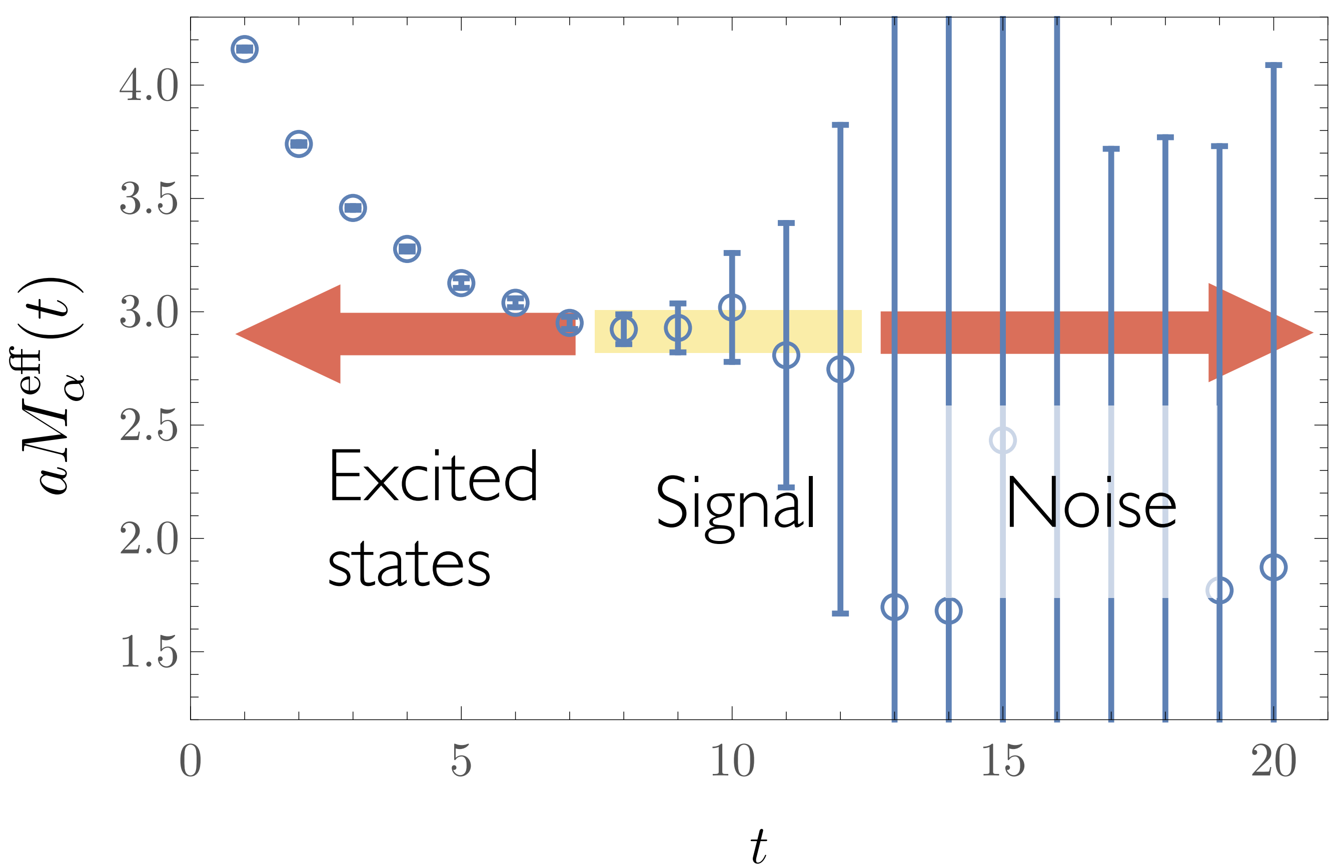


Machine learning QCD

Optimise extraction of physics from gauge fields

- Optimise source operator construction
  → beat down excited states
- New analysis approaches to maximise signal-to-noise
  → beat down noise

EXPONENTIAL IMPROVEMENTS



Huge potential to enable first-principles nuclear physics studies