Jefferson Lab

Summary of INT program (INT-24-2A)

Nobuo Sato

INT workshop: Inverse problems and uncertainty quantification in nuclear physics
Jul 9 2024

INSTITUTE for NUCLEAR THEORY

ABOUT PEOPLE PUBLICATIONS EVENTS JOBS VISITORS

Program Overview

INT PROGRAM INT-24-2A

QCD at the Femtoscale in the Era of Big Data

June 10, 2024 - July 5, 2024

ORGANIZERS

Julie Bessac
NREL
julie.bessac@nrel.gov

Ian Cloët
Argonne National Laboratory
icloet@anl.gov

Nobuo Sato
Jefferson Lab
nsato@jlab.org

Emil Constantinescu
Argonne National Laboratory
emconsta@mcs.anl.gov

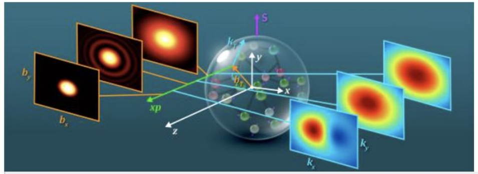


Image Courtesy of Argonne National Laboratory and Jefferson Lab

Challenge: process large scale data from JLab and EIC and solve fundamental questions in hadronic physics (spin, mass, imaging etc)

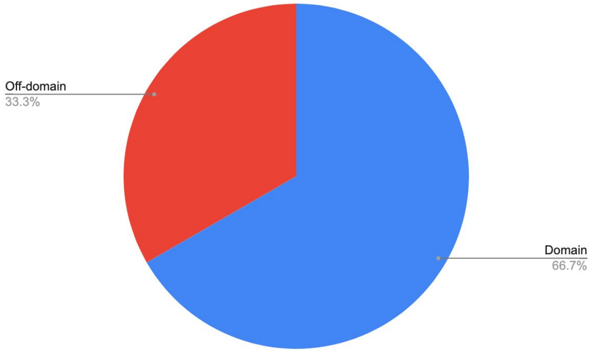
Opportunities: leverage expertise from applied math, stats, deep-learning and HPC experts

INT Workshop 24-2a In-Person Participants

QCD at the Femtoscale in the Era of Big Data

June 10 - July 5, 2024

Name	Institute
Ian Cloet	Argonne National Laboratory
Emil Constantinescu	Argonne National Laboratory
Nobuo Sato	Jefferson Lab
Daniel Adamiak	Jefferson Lab
Tareq Alghamdi	Old Dominion University
Patrick Barry	Argonne National Laboratory
Chiara Bissolotti	Argonne National Laboratory
Pi-Yueh Chuang	Virginia Tech
Anshu Dubey	Argonne National Laboratory
Abdullah Farhat	Jefferson Lab
Wu Feng	Virginia Tech
Adam Freese	Jefferson Lab
Leonard Gamberg	Penn State Berks
Yuxun Guo	Lawrence Berkeley National Lab
Sylvester Joosten	Argonne National Laboratory
Katie Keegan	Emory University
Shunzo Kumano	Japan Women's University / KEK
Yaohang Li	Old Dominion University
Vinicius Mikuni	LBNL
Pavel Nadolsky	Southern Methodist University
Jen-Chieh Peng	University of Illinois
Alexei Prokudin	Penn State University Berks
Nesar Ramachandra	Argonne National Laboratory
David Richards	Jefferson Laboratory
Felix Ringer	ODU/JLab
Niteya Shah	Virginia Tech
Andrea Simonelli	Jefferson Lab and ODU
Adam Szczepaniak	IU/JLab
Fernando Torales Acosta	LBNL
Marco Zaccheddu	Jefferson Lab



- **Domain**: QCD global analysis/pheno (PDFs, TMDs, GPDs), experimentalists (Epic, FNAL), HEP experimentalists (ML), LQCD, Spectroscopy.
- **Off-domain**: ML, numerical solvers, finite elements, hardware-software design for scientific problems

QCD theory

- Hadron structures: pdfs, tmds, gpds, soft factors/wilson lines, higher twist effects, tensor polarizations (QCFs: quantum correlation functions)
- Interpretation of QCFs, doppler effect, shock waves…
- Factorization
- Boundaries between physics and modeling
- Numerical methods for solving evolution equations: matrix multiplication, conformal moments
- QCD resummation

QCD pheno

- Global analysis: upol pdfs/tmds, gluon helicity, pion structure ..
- Modeling QCFs: simple parametrization, statistical model, ANN….
- New initiatives: event-level analysis
- Precision QCFs for BSM searches ..
- Uncertainty quantification for QCFs, reliability ..

Experiments

- Epic detector and challenges
- ML based unfolding, results for H1
- Diffusion models for particle physics

Data Science

- ANN regression
- Auto-encoders, latent space, tsne/PCA..

Math

- ODE/ASCR tools: eg. differential solvers,
- Error analysis in numerical implementations

HPC

- Numerical solutions vs hardware
- Regular programing
- Computer languages
- Abstraction of NP problem(s) and association to other fields to find solutions

Reproducibility

- Code standards
- (R)igor, (R) reproducibility, (R)igor
- How to avoid mistakes?
- Unitests
- Beyond unitests

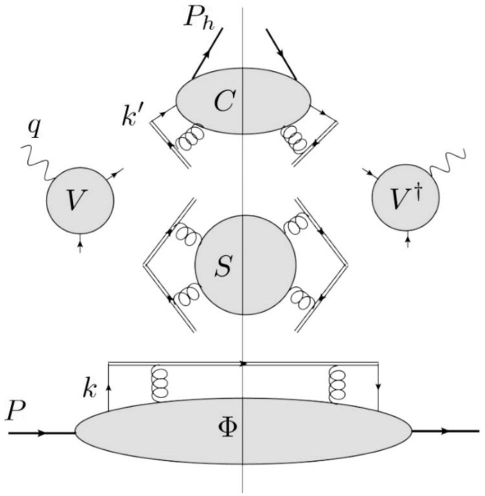
Afterthoughts

- Make friends: collective is more powerful than individuals
- Making friends with other silos.
- Abstraction of NP problem(s) and association to other fields to find solutions
- Role of AI: LLMs, co-pilots

"from gauge links to cpu flops"

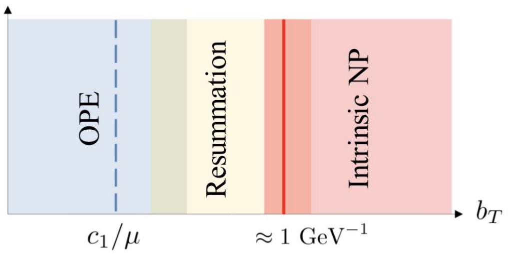
Talk by Simonelly

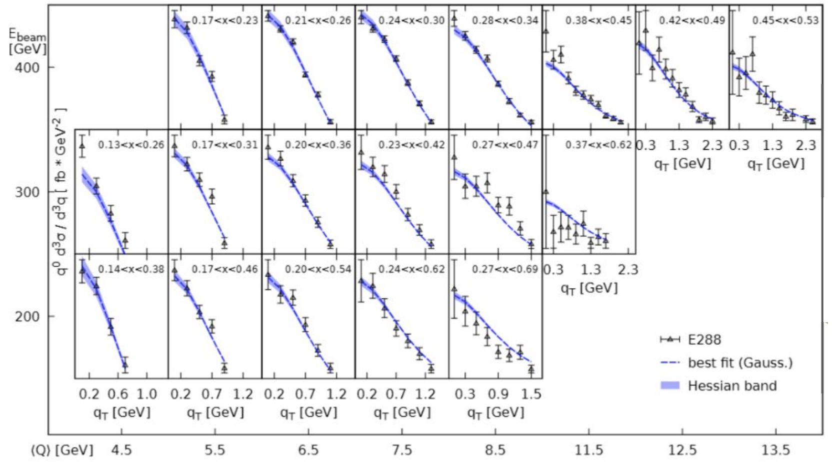
HSO (Hadron Structure Oriented)

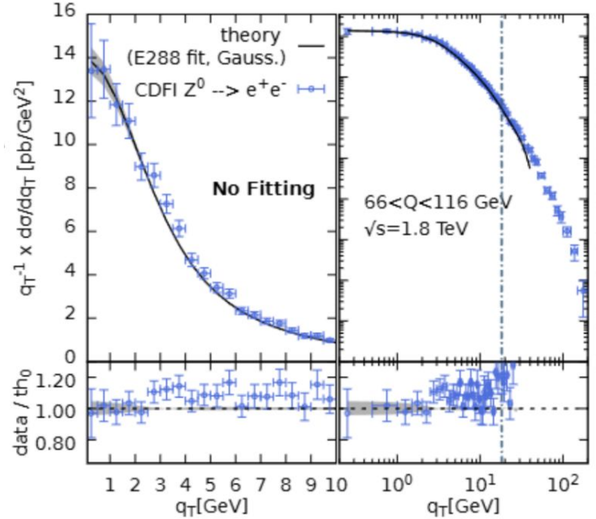


$$\frac{\partial \log \Phi_{\rm sqrt}}{\partial \log \sqrt{\zeta}} = K\left(a_S(\mu), \log\left(\frac{\mu b_T}{c_1}\right)\right)$$

$$\frac{\partial \log \Phi_{\rm sqrt}}{\partial \log \mu} = \gamma_\Phi\left(a_S(\mu); \log\left(\frac{\zeta}{\mu^2}\right)\right)$$







Talk by Gamberg

TMDs @ "twist-3 " NLP-the beginning?

$$W_{\mu\nu} = \frac{1}{(2\pi)^4} \sum_X \int d^4x\, e^{-iqx} \langle P | J^\dagger_\mu(0) | h, X \rangle \langle h, X | J_\nu(x) | P \rangle$$

$$\frac{d\sigma}{dx_H\, dy\, dz_H\, d^2P_T} := \mathcal{A} + \mathcal{B}\cos\phi + \mathcal{C}\cos 2\phi + \mathcal{D}\sin\phi + \mathcal{E}\sin 2\phi$$

$$J_\mu(x) = J^{(2)}_\mu(x) + J^{(3)}_\mu(x)$$

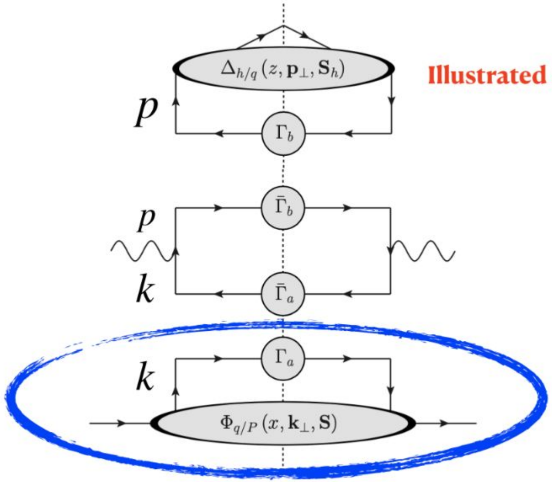
Pert. QCD

$$\langle \cos\varphi \rangle_{ep} = -\frac{\alpha_s}{2} \kappa \sqrt{1-z}\, \frac{(2-y)\sqrt{1-y}}{1+(1-y)^2}$$

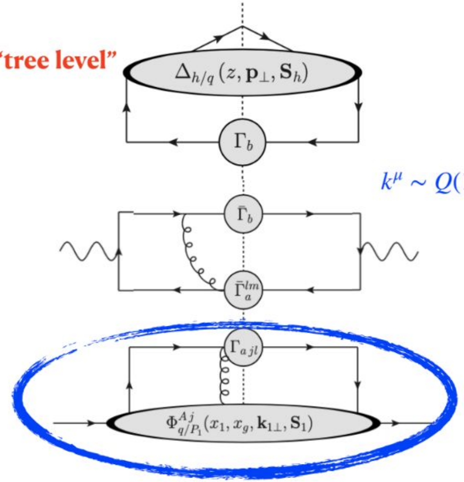
NLP

$$\langle \cos\phi \rangle_{ep} = -\left[\frac{2p_\perp}{Q}\right] \frac{(2-y)\sqrt{1-y}}{1+(1-y)^2}$$

Factorization at sub-leading power ... revisit Tree level



Illustrated at "tree level"



$k^\mu \sim Q(1,$

Talk by Kumano

TMD correlation functions for spin-1 hadrons

Correlation functions

$$\Phi_{ij}(k,P,T) = \int \frac{d^4\xi}{(2\pi)^4} e^{ik\cdot\xi} \left\langle P,T \left| \bar{\psi}_j(0) W(0,\xi) \psi_i(\xi) \right| P,T \right\rangle$$

$$W(0,\xi) = P\exp\left[-ig\int_0^\xi d\xi \cdot A(\xi)\right]$$

Spin vector: $S^\mu = S_L \frac{P^+}{M}\bar{n}^\mu - S_L \frac{M}{2P^+} n^\mu + S_T^\mu$

Tensor: $T^{\mu\nu} = \frac{1}{2}\left[\frac{4}{3}S_{LL}\frac{(P^+)^2}{M^2}\bar{n}^\mu\bar{n}^\nu + \frac{P^+}{M}\bar{n}^{\{\mu}S_{LT}^{\nu\}} - \frac{2}{3}S_{LL}\left(\bar{n}^{\{\mu}n^{\nu\}} - g_T^{\mu\nu}\right) + S_{TT}^{\mu\nu} - \frac{M}{2P^+}n^{\{\mu}S_{LT}^{\nu\}} + \frac{1}{3}S_{LL}\frac{M^2}{(P^+)^2}n^\mu n^\nu\right]$

Tensor part (twist-2): Bacchetta, Mulders, PRD 62 (2000) 114004

$$\Phi(k,P,T) = \left(\frac{A_{13}}{M}I + \frac{A_{14}}{M^2}\not{P} + \frac{A_{15}}{M^2}\not{k} + \frac{A_{16}}{M^3}\sigma_{\rho\sigma}P^\rho k^\sigma\right)k_\mu k_\nu T^{\mu\nu} + \left[A_{17}\gamma_\nu + \left(\frac{A_{18}}{M}P^\rho + \frac{A_{19}}{M}k^\rho\right)\sigma_{\nu\rho} + \frac{A_{20}}{M^2}\varepsilon_{\tau\nu\rho\sigma}P^\rho k^\sigma\gamma^\tau\gamma_5\right]k_\mu T^{\mu\nu}$$

Tensor part (twist-2, 3, 4): n^μ dependent terms are added for up to twist 4.

[For the spin-1/2 nucleon: Goeke, Metzand, Schlegel, PLB 618 (2005) ,90; Metz, Schweitzer, Teckentrup, PLB 680 (2009) 141.]

Kumano-Song-2021, for the details see PRD 103 (2021) 014025

$$\Phi(k,P,T\,|\,n) = \left(\frac{A_{13}}{M}I + \frac{A_{14}}{M^2}\not{P} + \frac{A_{15}}{M^2}\not{k} + \frac{A_{16}}{M^3}\sigma_{\rho\sigma}P^\rho k^\sigma\right)k_\mu k_\nu T^{\mu\nu} + \left[A_{17}\gamma_\nu + \left(\frac{A_{18}}{M}P^\rho + \frac{A_{19}}{M}k^\rho\right)\sigma_{\nu\rho} + \frac{A_{20}}{M^2}\varepsilon_{\tau\nu\rho\sigma}P^\rho k^\sigma\gamma^\tau\gamma_5\right]k_\mu T^{\mu\nu}$$

Bacchetta -Mulders (2000)

$$+\left(\frac{B_{21}M}{P\cdot n}k_\mu + \frac{B_{22}M^3}{(P\cdot n)^2}n_\mu\right)n_\nu T^{\mu\nu} + i\gamma_5\varepsilon_{\mu\tau\rho\sigma}P^\rho\left(\frac{B_{23}}{(P\cdot n)M}k^\tau n^\sigma k_\nu + \frac{B_{24}M}{(P\cdot n)^2}k^\tau n^\sigma n_\nu\right)T^{\mu\nu}$$

$$+\left[\frac{B_{25}}{P\cdot n}\not{n}\not{k}k_\mu k_\nu + \left(\frac{B_{26}M^2}{(P\cdot n)^2}\not{n} + \frac{B_{28}}{P\cdot n}\not{P} + \frac{B_{30}}{P\cdot n}\not{k}\right)k_\mu n_\nu + \left(\frac{B_{27}M^4}{(P\cdot n)^3}\not{n} + \frac{B_{29}M^2}{(P\cdot n)^2}\not{P} + \frac{B_{31}M^2}{(P\cdot n)^2}\not{k}\right)n_\mu n_\nu + \frac{B_{32}M^2}{P\cdot n}\gamma_\mu n_\nu\right]T^{\mu\nu}$$

$$-\left[\varepsilon_{\mu\tau\rho\sigma}\gamma^\tau P^\rho\left(\frac{B_{34}}{P\cdot n}n^\sigma k_\nu + \frac{B_{33}}{P\cdot n}k^\sigma n_\nu + \frac{B_{35}M^2}{(P\cdot n)^2}n^\sigma n_\nu\right) + \varepsilon_{\lambda\tau\rho\sigma}k^\lambda\gamma^\tau P^\rho n^\sigma\left(\frac{B_{36}}{P\cdot nM^2}k_\mu k_\nu + \frac{B_{37}}{(P\cdot n)^2}k_\mu n_\nu + \frac{B_{38}M^2}{(P\cdot n)^3}n_\mu n_\nu\right)\right]\gamma_5 T^{\mu\nu}$$

$$+\varepsilon_{\mu\tau\rho\sigma}k^\tau P^\rho n^\sigma\left(\frac{B_{39}}{(P\cdot n)^2}k_\nu + \frac{B_{40}M^2}{(P\cdot n)^3}n_\nu\right)\not{n}\gamma_5 T^{\mu\nu}$$

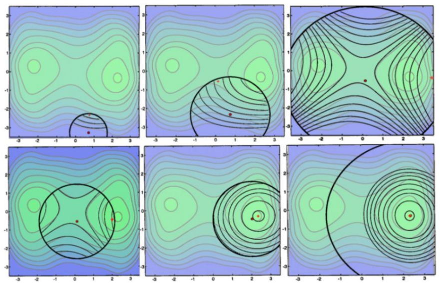
$$+\sigma_{\rho\sigma}\left[P^\rho k^\sigma\left(\frac{B_{41}}{(P\cdot n)M}k_\mu n_\nu + \frac{B_{42}M}{(P\cdot n)^2}n_\mu n_\nu\right) + P^\rho n^\sigma\left(\frac{B_{43}}{(P\cdot n)M}k_\mu k_\nu + \frac{B_{44}M}{(P\cdot n)^2}k_\mu n_\nu + \frac{B_{45}M^3}{(P\cdot n)^3}n_\mu n_\nu\right)\right]T^{\mu\nu}$$

$$+\sigma_{\rho\sigma}\left[k^\rho n^\sigma\left(\frac{B_{46}}{(P\cdot n)M}k_\mu k_\nu + \frac{B_{47}M}{(P\cdot n)^2}k_\mu n_\nu + \frac{B_{48}M^3}{(P\cdot n)^3}n_\mu n_\nu\right)\right]T^{\mu\nu} + \sigma_{\mu\sigma}\left[n^\sigma\left(\frac{B_{49}M}{P\cdot n}k_\nu + \frac{B_{50}M^3}{(P\cdot n)^2}n_\nu\right) + \left(\frac{B_{51}M}{P\cdot n}P^\sigma + \frac{B_{52}M}{P\cdot n}k^\sigma\right)n_\nu\right]T^{\mu\nu}$$

New terms in our paper (2021)

From this correlation function, new tensor-polarized TMDs are defined in twist-3 and 4 in addition to twist-2 ones.

Terms associated with $n = \frac{1}{\sqrt{2}}(1,\ 0,\ 0,\ -1)$



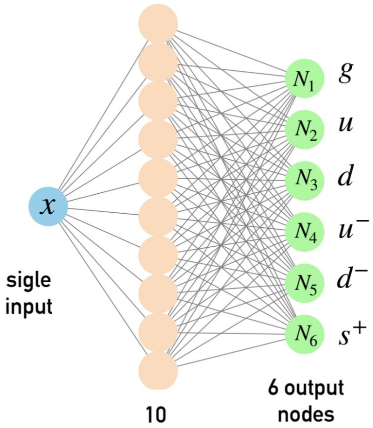
minimization carried out by **ceres-solver**

trust region
Levenberg–Marquardt
combines the gradient-descent algorithm to the Gauss-Newton method

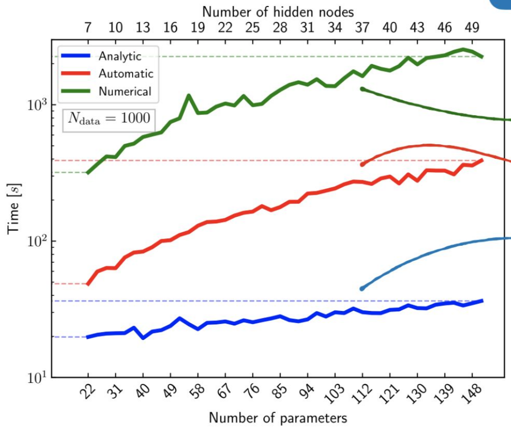
need the knowledge of the derivatives of the χ^2 with respect to the parameters θ

analytic derivatives provided by **NNAD**

Talk by Bissolotti

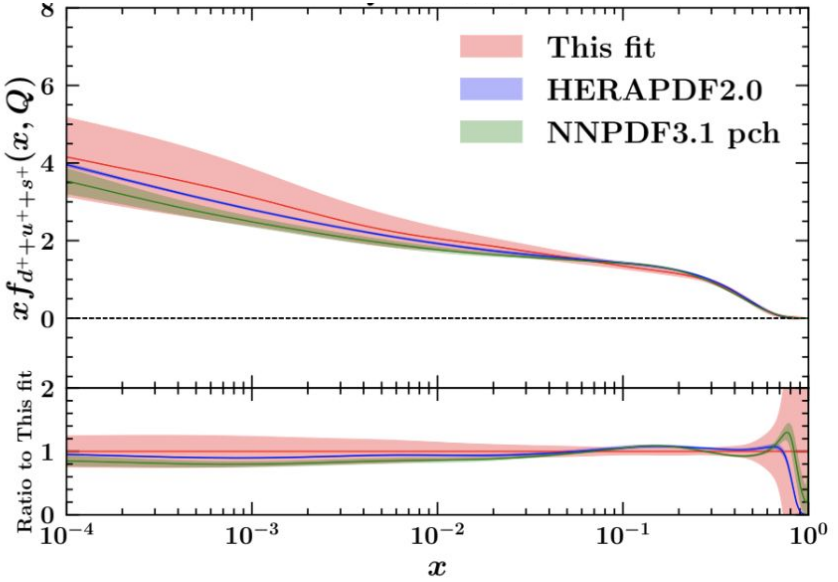


performance advantage



differentiation methods as implemented in ceres-solver

NNAD
analytic back-propagation formula



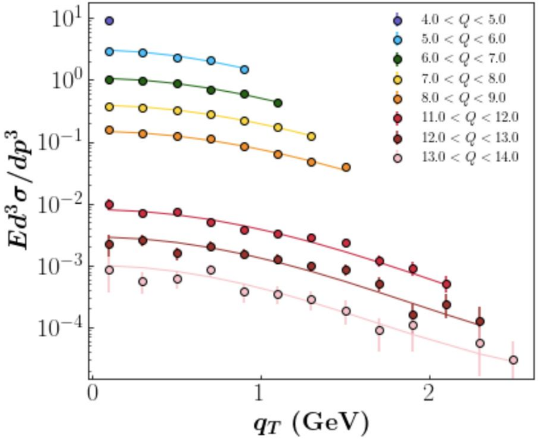
Talk by Barry

$$\frac{d\sigma}{dQ^2\,dy\,dq_T^2} = \frac{4\pi^2\alpha^2}{9Q^2 s}\sum_{j,j_A,j_B} H^{\rm DY}_{j\bar{j}}(Q,\mu_Q,a_s(\mu_Q)) \int \frac{d^2\boldsymbol{b}_T}{(2\pi)^2} e^{i\boldsymbol{q}_T\cdot\boldsymbol{b}_T}$$
$$\times\, e^{-g_{j/A}(x_A,b_T;b_{\max})} \int_{x_A}^1 \frac{d\xi_A}{\xi_A} f_{j_A/A}(\xi_A;\mu_{b_*})\, \tilde{C}^{\rm PDF}_{j/j_A}\left(\frac{x_A}{\xi_A}, b_*;\mu_{b_*}^2,\mu_{b_*},a_s(\mu_{b_*})\right)$$
$$\times\, e^{-g_{\bar{j}/B}(x_B,b_T;b_{\max})} \int_{x_B}^1 \frac{d\xi_B}{\xi_B} f_{j_B/B}(\xi_B;\mu_{b_*})\, \tilde{C}^{\rm PDF}_{\bar{j}/j_B}\left(\frac{x_B}{\xi_B}, b_*;\mu_{b_*}^2,\mu_{b_*},a_s(\mu_{b_*})\right)$$
$$\times\, \exp\left\{-g_K(b_T;b_{\max})\ln\frac{Q^2}{Q_0^2} + \tilde{K}(b_*;\mu_{b_*})\ln\frac{Q^2}{\mu_{b_*}^2} + \int_{\mu_{b_*}}^{\mu_Q}\frac{d\mu'}{\mu'}\left[2\gamma_j(a_s(\mu')) - \ln\frac{Q^2}{(\mu')^2}\gamma_K(a_s(\mu'))\right]\right\}$$

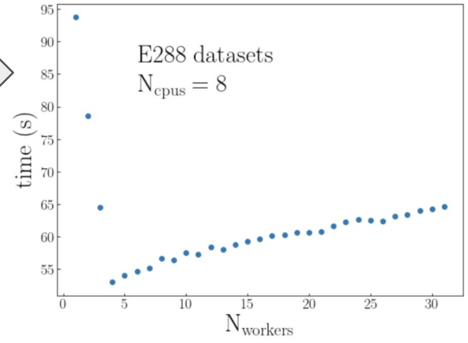
Perturbative pieces

Non-perturbative pieces

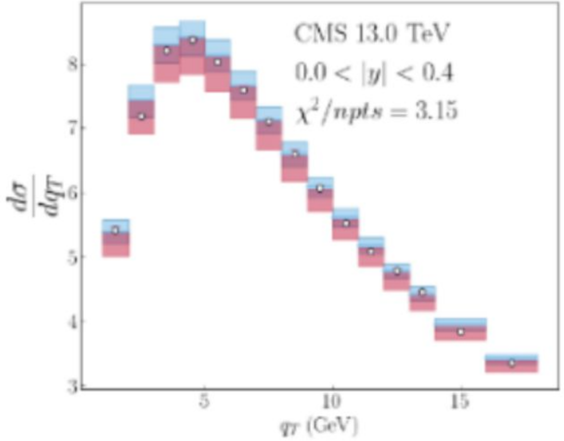
Non-perturbative piece of the CS kernel



Computational cost



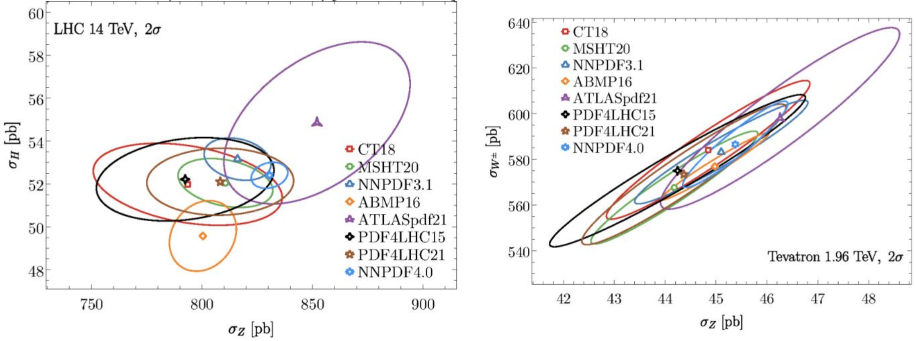
Very precise data as in LHC requires precise numerical calculations



The tolerance puzzle

Why do groups fitting similar data sets obtain different PDF uncertainties?

Precision PDFs (Snowmass 21 WP) [2203.13923v2]



The answer has direct implications for high-stake experiments such as 3D femtography, W boson mass measurement, tests of nonperturbative QCD models and lattice QCD, high-mass BSM searches, etc.

Statistics with many parameters is different!

1. Epistemic uncertainties may dominate when other uncertainties are suppressed

More often than not, the realistic 1σ PDF uncertainty does not correspond to $\Delta\chi^2 = 1$.

2. Common estimations of systematic uncertainties are incomplete because…
   - a. **There is no single global minimum of** χ^2 (or another cost function)
   - b. **The law of large numbers may not work**
   - – uncertainty may not decrease as $1/\sqrt{N_{rep}}$, leading to the **big-data paradox** [Xiao-Li Meng, 2018]:

The bigger the data, the surer we fool ourselves.

Complexity and PDF tolerance

- **Bad news:** The tolerance puzzle is *intractable* in very complex fits
  - In a fit with N_{par} free parameters, the minimal number of PDF replicas to estimate the expectation values for $\forall\ \chi^2$ function grows as $N_{min} \geq 2^{N_{par}}$
  - Example: $N_{min} > 10^{30}$ for $N_{par} = 100$

[Sloan, Wo´zniakowski, 1997]
[Hickernell, MCQMC 2016, 1702.01487]

Good news: expectation values **for typical QCD observables** can be estimated with fewer replicas by reducing dimensionality of the problem or a targeted sampling technique.

Example: a "**hopscotch scan**", see 2205.10444

Strategy for the GPD global analysis

Talk by Guo

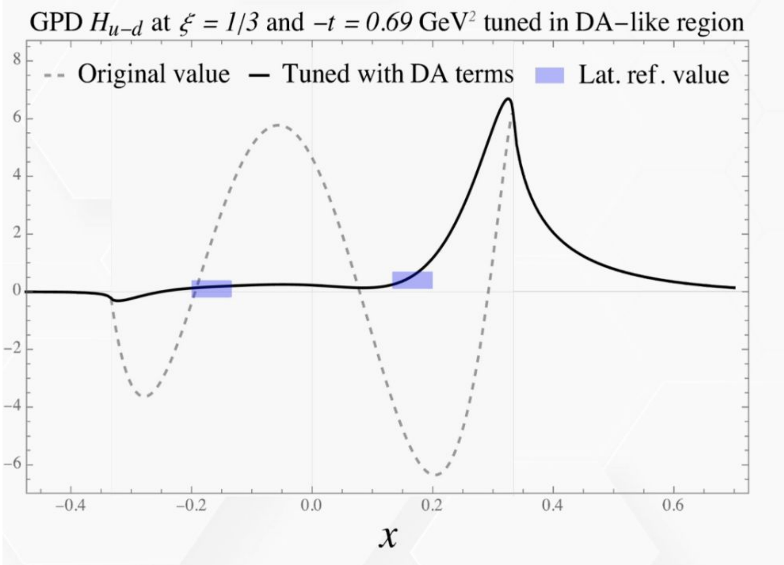
Experimental data and constraints

- ❑ Polarized and unpolarized PDFs from global analysis
  - Alternatively, one can fit to (polarized) DIS directly
- ❑ Neutron/ Proton charge form factors from global analysis
- ❑ Deeply virtual Compton scattering data at JLab/HERA
- ❑ Deeply virtual meson productions data at HERA

Lattice QCD simulations

- ❑ Lattice simulations of nucleon generalized form factors
- ❑ Lattice simulations of unpolarized and helicity GPDs at zero and non-zero ξ (skewness)

Sequential fit as first step to accelerate the convergence



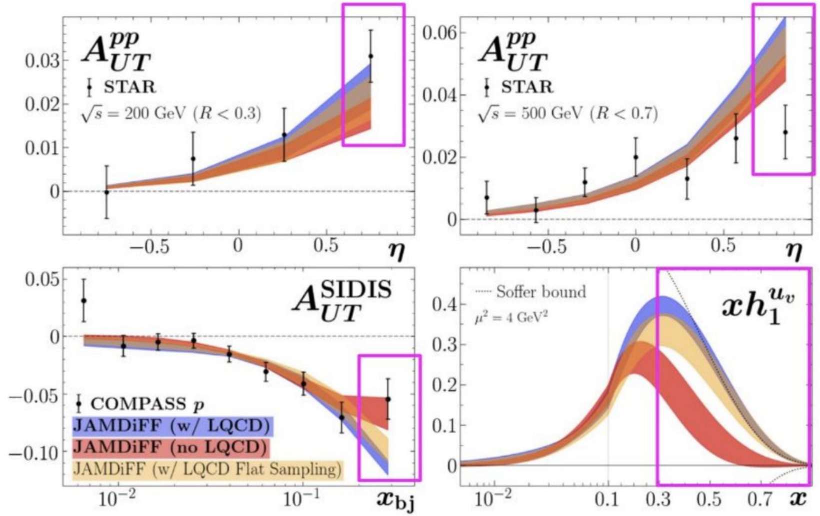
- JAM (2022) PDF global analysis results
- Globally extracted electromagnetic form factors (*Z. Ye et al* 2018)
- Lattice GPDs (*Alexandrou et al* 2020) and form factors (*Alexandrou et al* 2022)

DVCS measurements from JLab (*CLAS* 2019 & 2021, *Hall A* 2018 & 2022) and HERA (*H1* 2010)

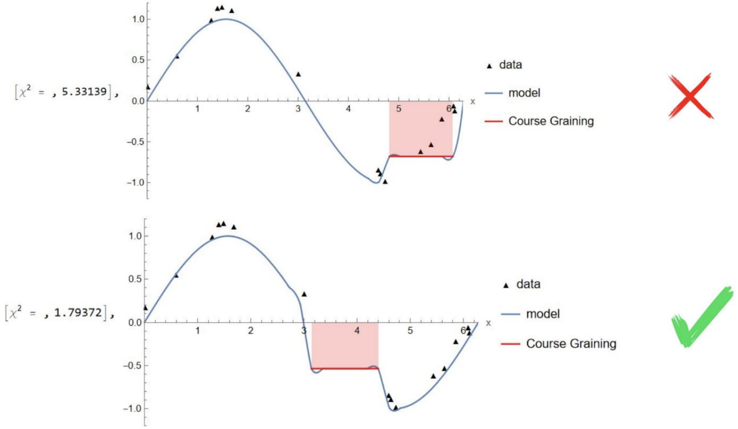
Discrete representation of PDFs

Talk by Adamiak

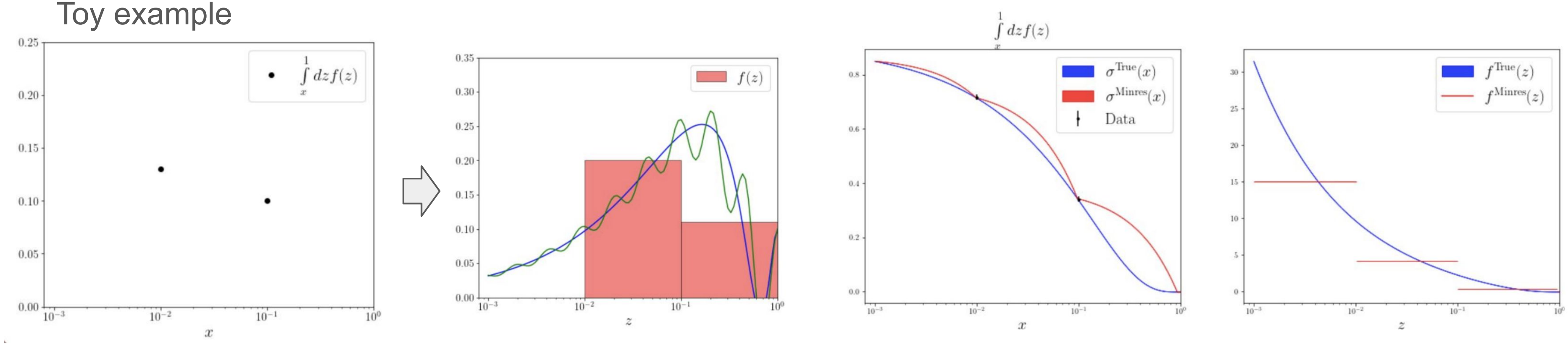
Motivations (see talk by Pitonyak)



Reject the Bucket if it Harms the Chi^2



Toy example



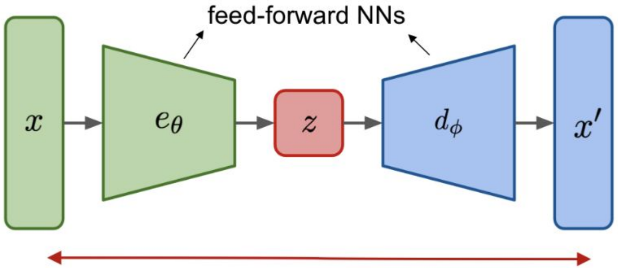
Developments in Interpretable and Explainable AI/ML for PDFs

or, can we understand what ML models are actually doing in the quest to quantify PDFs and their uncertainties...

DALL-E: "A confused, despondent robot painted in the style of Matisse."

PDF reconstruction: autoencoder

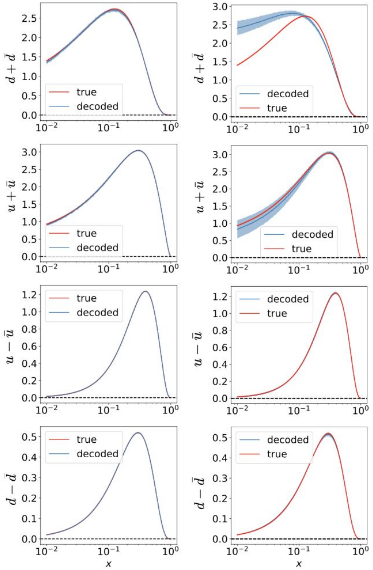
- basic structure: *encoder* takes input space, *x*, to latent vector, *z*
  → corresponding *decoder* maps latent, z, to decoded output, *x*'



$$\mathcal{L} = \|x - d_\phi(e_\theta(x))\|_2^2$$

- *undercomplete* network structure
  → latent space of lesser dimensional size than input (dimensionality reduction)

trained model performance: VAIM

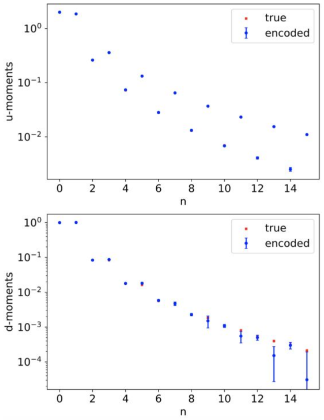


- as default, illustrate for VAIM: consistently robust reconstructions

nb, open questions in UQ; ensembling [left] vs latent sampling [right];

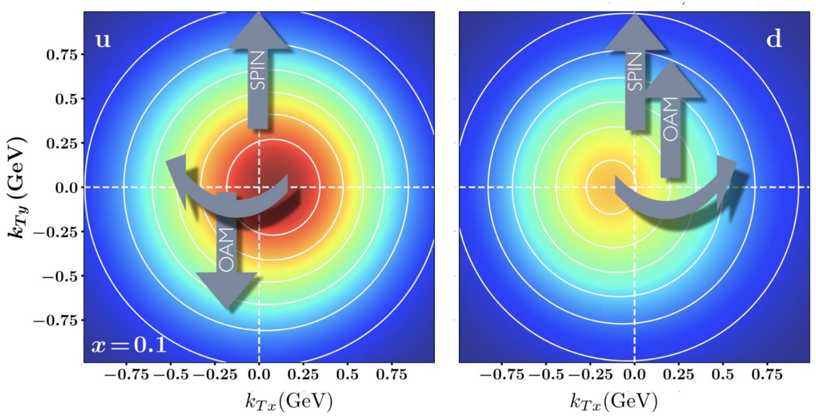
(more in later study)

moment reconstructions, by order



NUCLEON TOMOGRAPHY

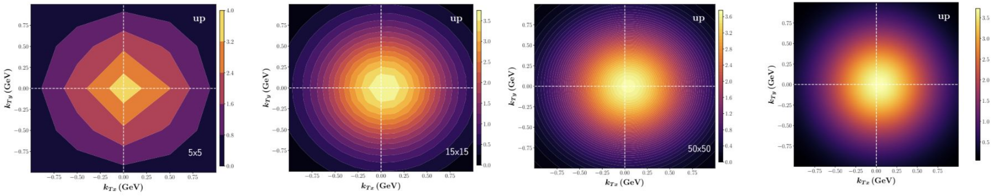
Talk by Prokudin



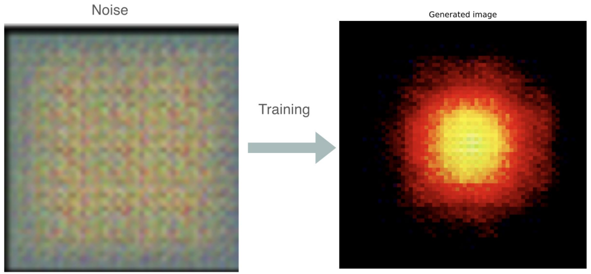
$$\rho_{1;q\leftarrow h^\uparrow}(x, \boldsymbol{k}_T, \boldsymbol{S}_T, \mu) = f_{1;q\leftarrow h}(x, k_T; \mu, \mu^2) - \frac{k_{Tx}}{M} f_{1T;q\leftarrow h}^{\perp}(x, k_T; \mu, \mu^2)$$

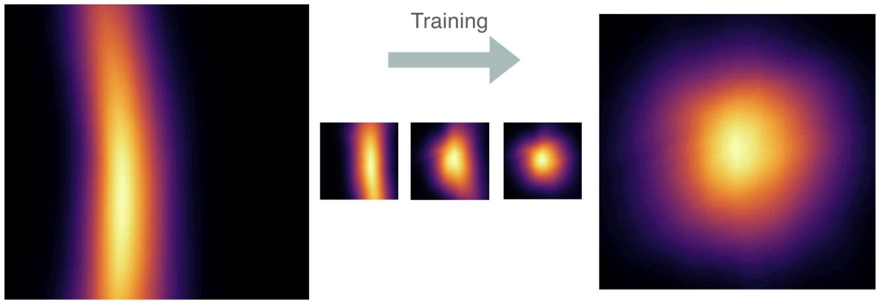
WHY DO WE WANT IT?

- We would like to not know how fuzzy the image is and what impact new measurements will have on it.
- We would like to harness rapidly evolving methods of the Artificial Intelligence and Machine Learning
- We would like to contribute to fostering new generations of nuclear scientists and of the digital literate workforce
- Last but not least, we would like to open new avenues of studies of the nucleon structure



Generative models

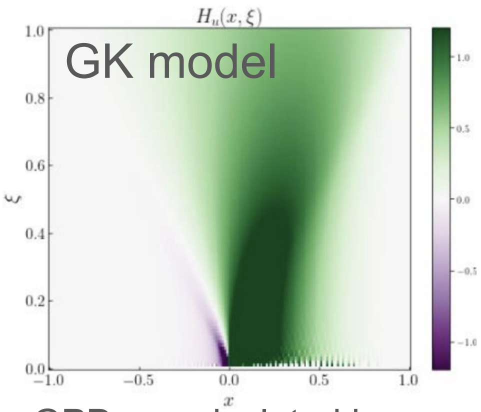




Extracting GPDs from CFFs with NN

Talk by Zaccheddu

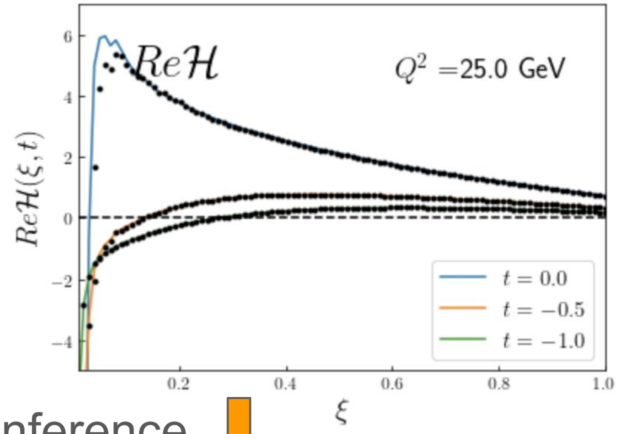
$$H^q(x,\xi,t) \;=\; \int d\beta\, d\alpha\, \delta(x-\beta-\xi\alpha)(f^q(\beta,\alpha,t)$$



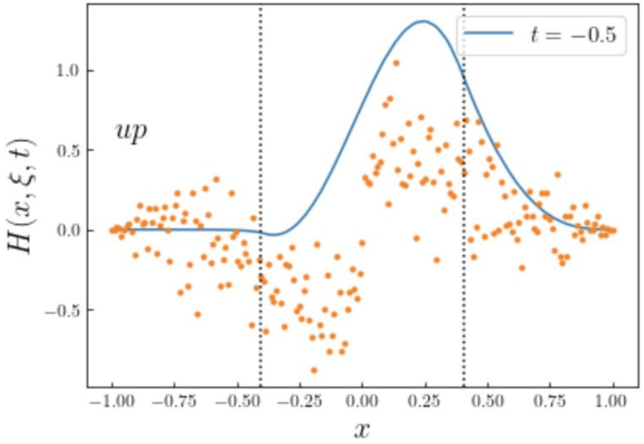
GPDs as pixelated images

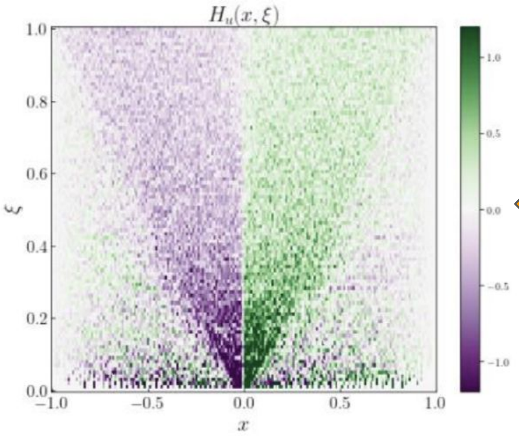
simulation

DVCS observable



inference



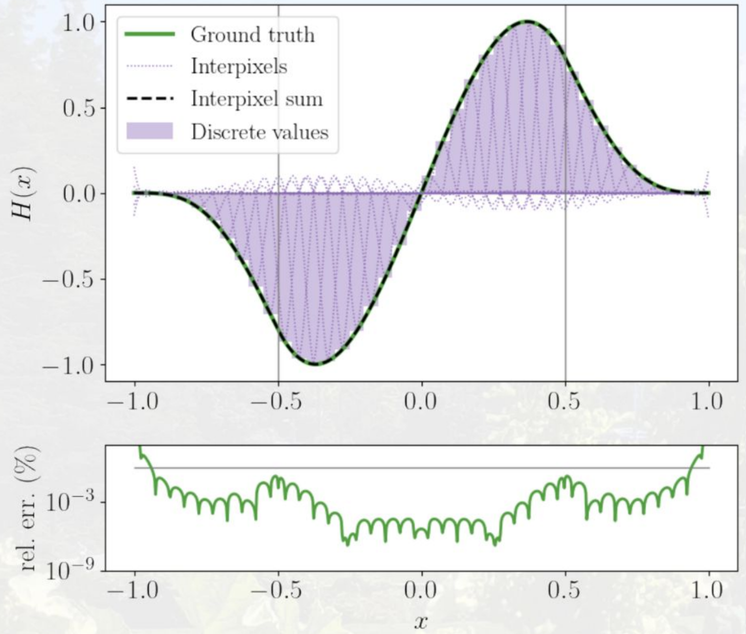


- **Inverse problem:** difficult to reconstruct GPDs from DVCS -> shadow GPDs
- **Additional data is needed:** LQCD "prios", other observables

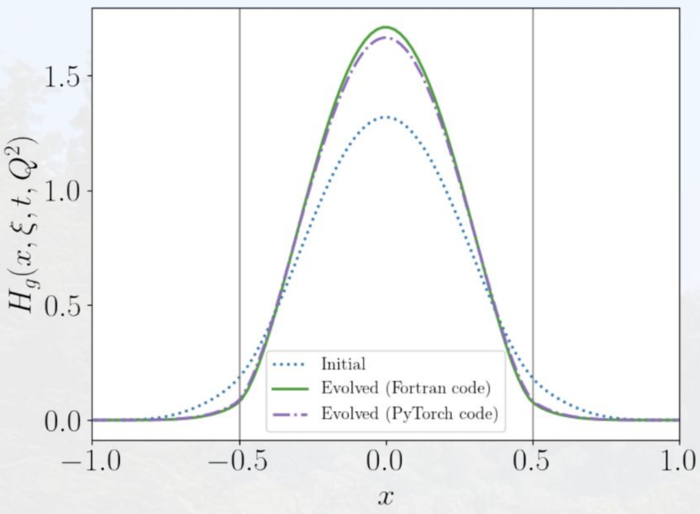
Talk by Freese

Ultra-fast x-space evolution for generalized parton distributions

$$\frac{\mathrm{d}H(x,\xi,t,Q^2)}{\mathrm{d}\log(Q^2)} = \int_{-1}^{+1} \mathrm{d}y\, K(x,y,\xi,Q^2)H(y,\xi,t,Q^2)$$

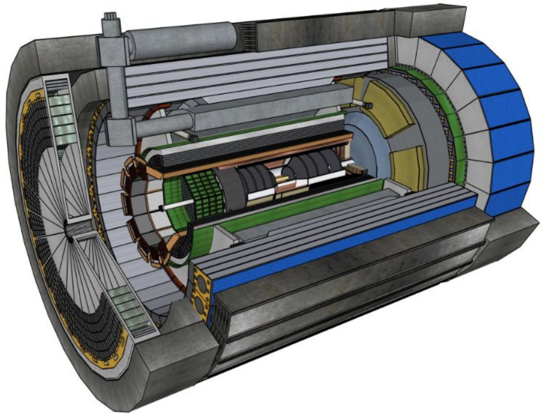


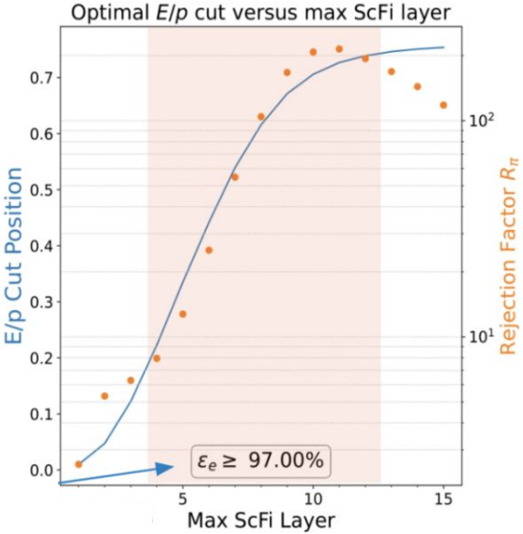
"Kernel based method"

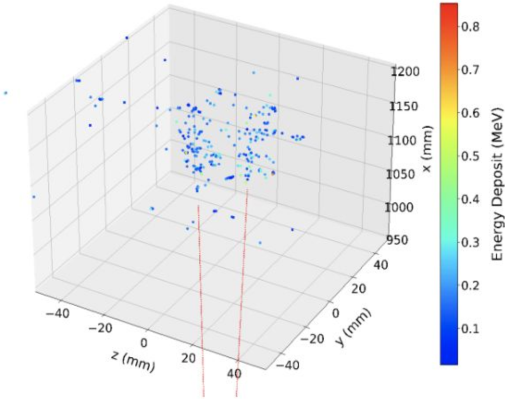


- **PyTorch code:**
  - on **GPU** (JLab farm): 10.8 s
  - on CPU (JLab farm): 19.7 s
- **Fortran code**
  - on CPU (JLab farm): 26.3 s
  - on CPU (my laptop): 54 s

EIC Experimental considerations







THE EPIC BARREL IMAGING CALORIMETER

Optimized for electron-pion separation by combining a high-performance sampling calorimeter with inexpensive silicon sensors for shower profiling

Challenging goal: at least 90% electron purity everywhere

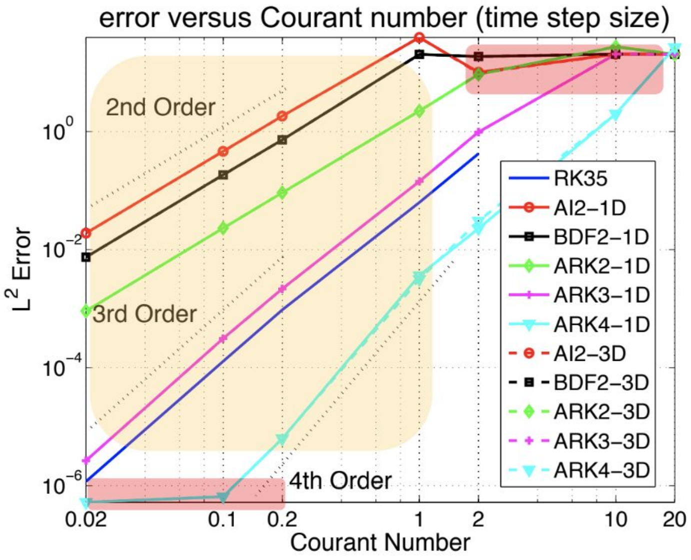
However, this means there are regions were 10% of our “electrons” are really pions!

Not all of these will be problematic (i.e. reconstruct as the most likely primary electron), but some effects unavoidable.

Modern Evolution Algorithms

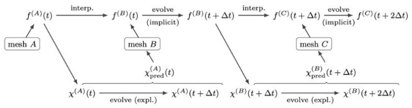
Overview – What is Modern (3)

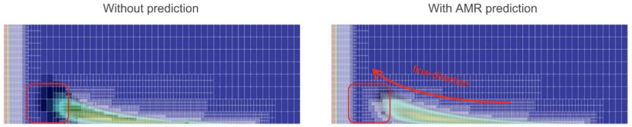
- The Runge-Kutta 4 (RK4) method was developed between 1895-1901, a few years before vacuum tubes were invented
- The BDF-2 method was developed in 1952, one year before the first transistor was used in a device



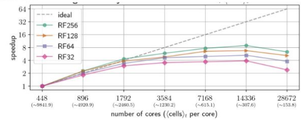
Scalable Implicit Solvers with Dynamic Mesh Adaptation for a Relativistic Drift-Kinetic Fokker-Planck-Boltzmann Model

Algorithm for dynamic AMR with prediction. The evolution of an auxiliary function χ is evolved in time separately, indicating where to adapt the mesh





Refinement levels of the dynamically adapted mesh (white lines) without prediction vs. AMR with prediction. Note the refined mesh ahead of the flow



Frontera strong scaling – preliminary results

ANL: Johann Rudi, Max Heldman, Emil Constantinescu
LANL: Qi Tang, Xianzhu Tang

Solvers' Ecosystems

Talk by Constantinescu

- Solvers available in small packages addons (Python, Jax, …) are limited/not sophisticated
- Matlab/Julia solvers are well-tested and developed but do not scale
- DOE software libraries can be used for prototyping and scaling
  - PETSc – Argonne solver library provides a hundreds of solvers; scale to HPC
  - Trilinos (developed at Sandia)
  - SUNDIALS (and extensions) developed at Livermore
  - All provide access to many sophisticated methods
- Adaptive meshing:
  - P4est (Parallel AMR on Forests of Octrees)
  - ParMETIS (Parallel Graph Partitioning and Fill-reducing Matrix Ordering)
  - FLASH <- Paramesh (see Anshu's talk)

Reliability of Modern-Day High-Performance Scientific Computing (How) Can I Trust It?

Talk by Chuang

r/PhD • 3 yr. ago
JLane1996

Do any other PhD students who code worry about all their code being wrong?

"All software has bugs." ~~ True

"It's usually not a huge deal as long as you're honest about it and you do your best to correct it." ~~ True

Can we trust any computing result in academia?

Can we still trust the 1st image of a black hole?

"Good unit tests resolve the issue." ~~ **What?????? Not really…**

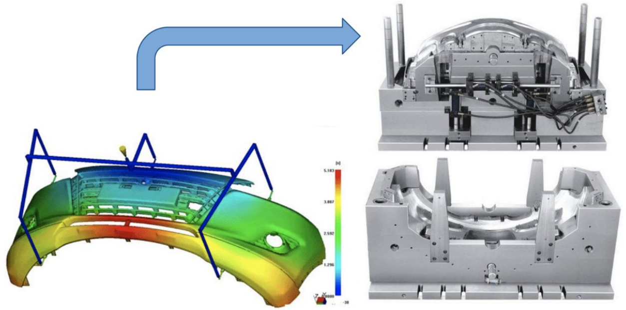
Story 1: Plastic Injection Molding (2012)

<u>Loss</u>

$1M

<u>Cause</u>

Forgot to update the version on the cluster after a local bug fix.



This is from SciPy... one of the most used Python packages now

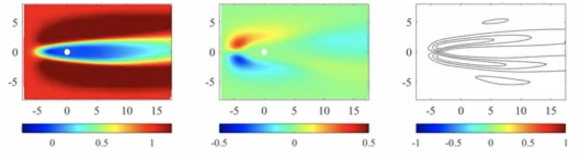
BUG: wrong weights of the 7-point gauss rule in QUADPACK: dqk15w.f #14807

Closed adamadanandy opened this issue on Oct 4, 2021 · 26 comments

40+ year old Fortran library

How many people know that their numerical library is using another library that had a long-standing bug, which was fixed only in 2021?

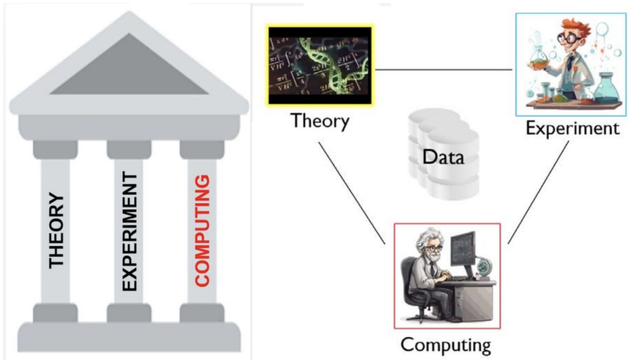
Story 5: AI-Predicted Impossible Cylinder Flow



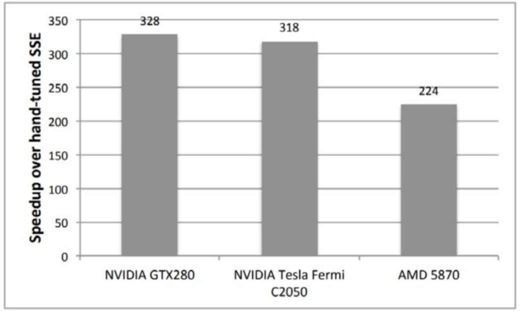
Cause: ~~Exaggeration~~ Projection without Validation.

- We showed his "novel method" could not solve flow over a cylinder
- He was extremely angry... and showed us "working" videos and plots
- And we found apparent errors in these videos and plots

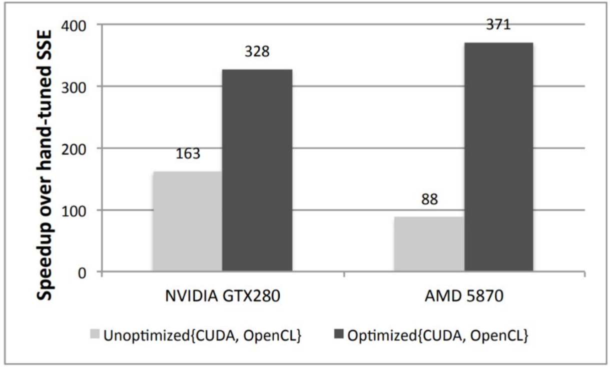
The Three Pillars of Science



Takeaway #2: Synergistic co-design of algorithms, software, and hardware can massively accelerate discovery, e.g., rational drug design



(a) Speedup on GPU Platforms with NVIDIA-Specific Optimizations

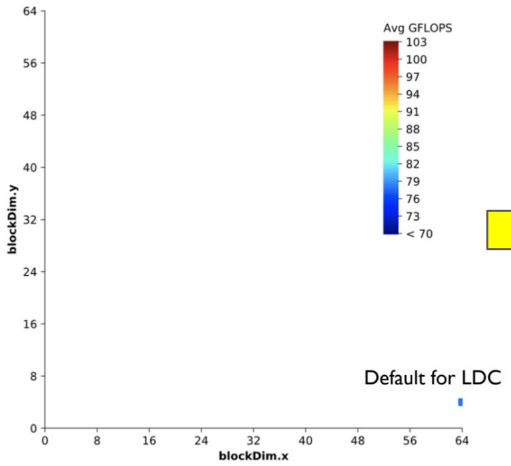


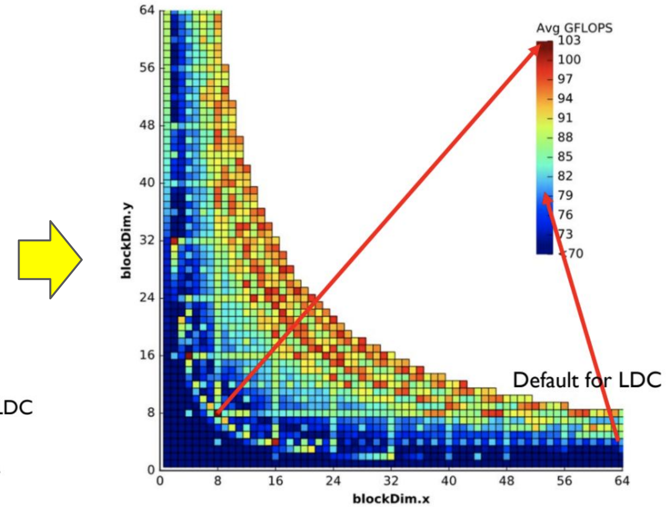
Talk by Feng

- **Problem**

  Many parameters to tune to achieve best performance
  - ✓ Thread block size
  - ✓ # streams
  - ✓ Register usage
  - ✓ Compiler optimization flags
  - ✓ *… and so on*

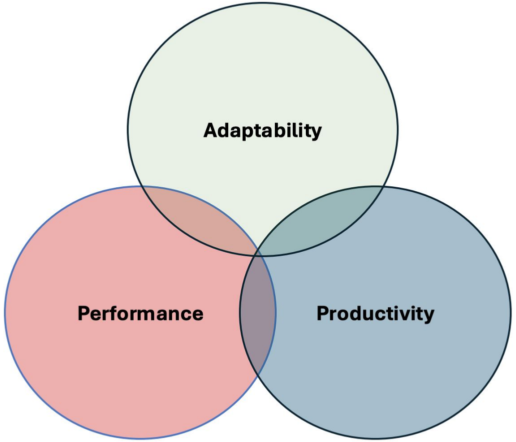
  O(millions)* potential software configurations for the *same code
- Our Focus
  - ✓ ***Thread block size***
- Example
  - ✓ Lid-driven cavity (LDC) code with varying GPU thread block size (NVIDIA K20m GPU)





The HPC Balancing Act

Talk by Shah



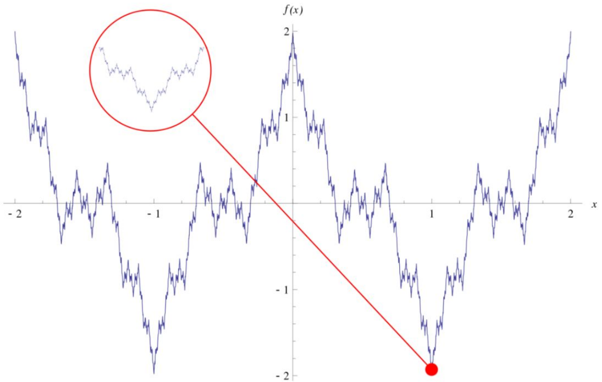
The Battle of the Languages

Pytorch isn't Magic

I see this get thrown around a lot

> "We are using Pytorch because we want [Something] to be differentiable"

$$\text{Pytorch}\left(\sum_{n=1}^{\infty} \frac{\sin(n^2 x)}{n^2} \right)$$



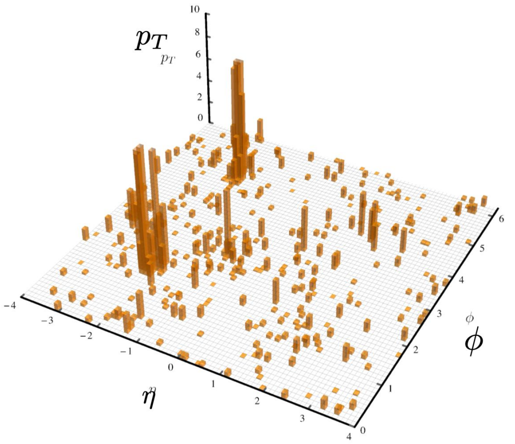
- A derivative of a function at a point exists or doesn't
- A library can't change that
  - A library can make it **simpler** to find out the derivative

Generative models for EIC events

Talk by Ringer

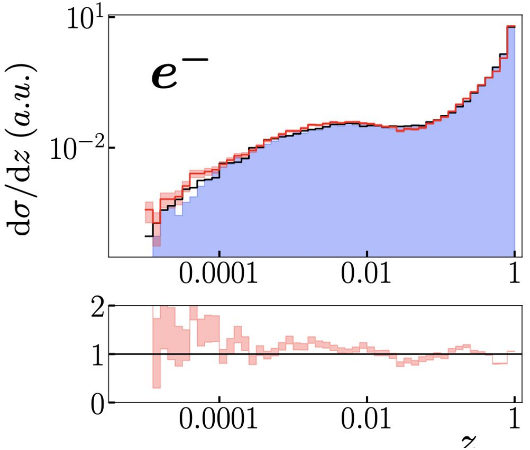
- Surrogate models
- Searches of physics beyond the Standard Model
- Event-level data analysis (differentiable)
- Development of MC event generators

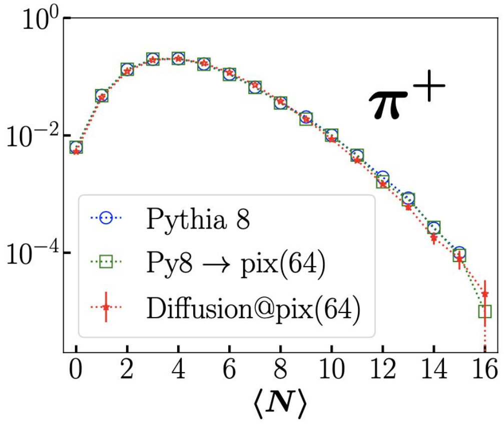
GANs e.g. Lai, Neill, Ploskon, FR `20



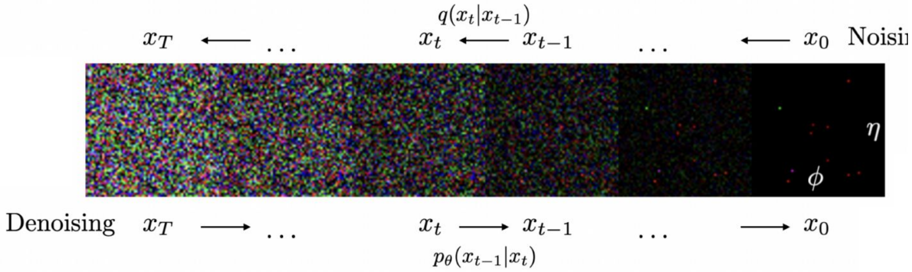
$$\tilde{z}_i = \frac{2M_{Ti}}{\sqrt{s}} \cosh y_i$$

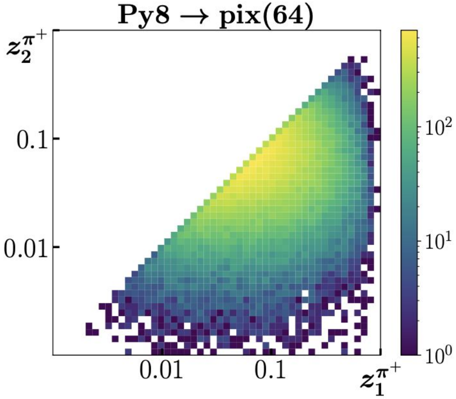
Devlin, Qiu, FR, Sato `23

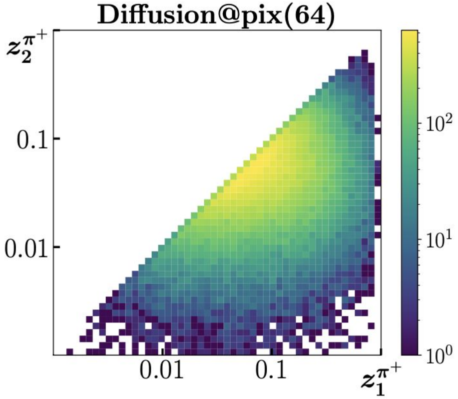




Diffusion models

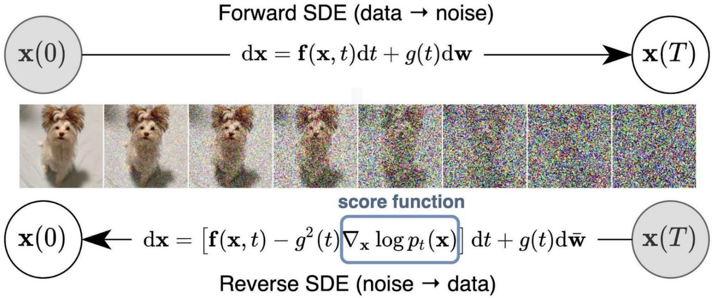






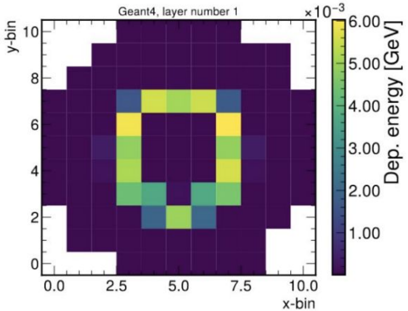
Represent events as images (pixelated)

Diffusion Generative Models for EIC Simulations

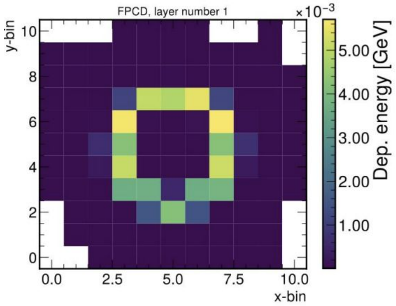


Calorimeter Simulation

Full Simulation



Diffusion point cloud

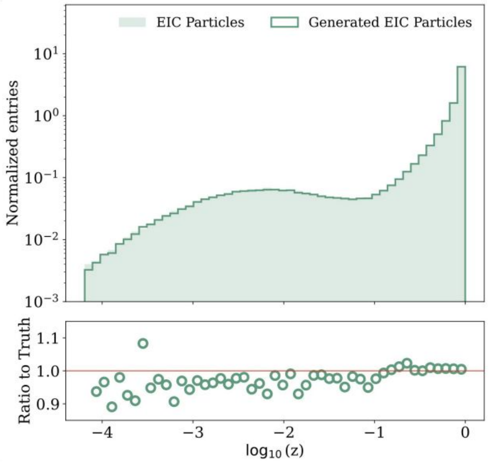


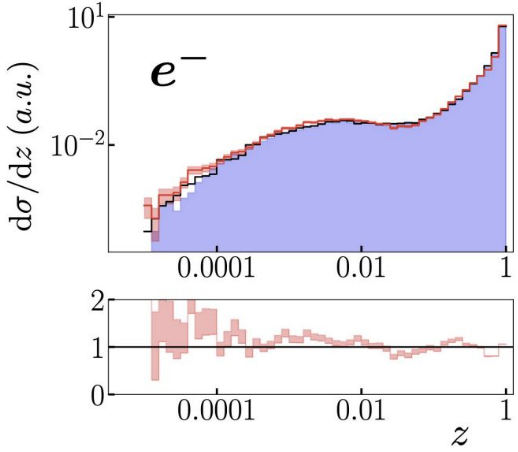
Point cloud model also requires less disk space and is faster to generate

Talk by Mikuni

Model	# Parameters	Disk Size (Full)	Sample Time
Image	2,572,161	1016 MB (62 GB)	8036.19 s
Point Cloud	620,678	509 MB	2631.41 s

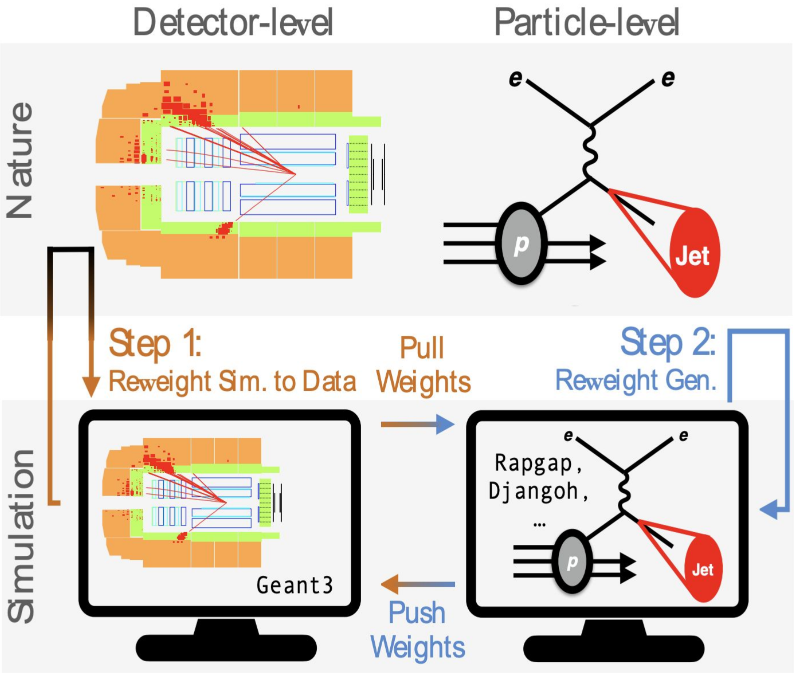
Point Cloud Description of the data





Unfolding Measurements at H1 using Machine Learning

OmniFold

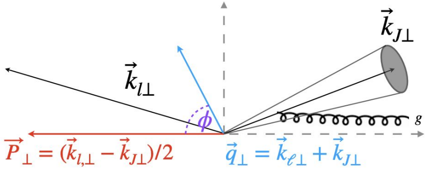


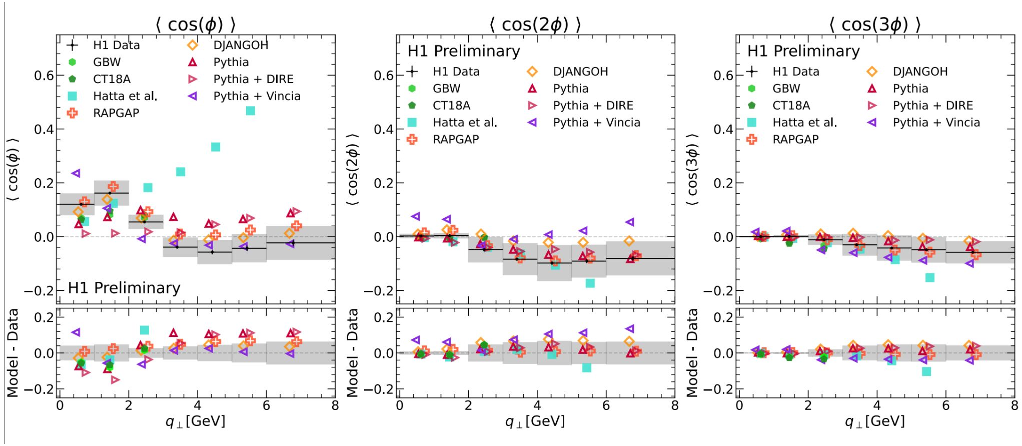
Talk by Torales Acosta

Multifold already used to unfold:

$p_x^e, p_y^e, p_z^e, p_T^{jet}, \eta^{jet}, \phi^{jet}, \Delta\phi^{jet}, q_T^{jet}/Q$

1. Probes soft gluon radiation $S(g)$
   - Soft gluon radiation can be the primary contribution to asymmetry
   - 10.1103/PhysRevD.104.054037
2. Asymmetry is perturbative
   - Opportunity to compare to unfolded H1 data
3. May represent a vital reference for other signals, in particular TMD PDF measurements
   - Factorize contributions TMD PDFs and Soft gluon radiation
4. Observable is sensitive to gluon saturation phenomena, possibly measurable at the EIC
   - 10.1103/PhysRevLett.130.151902





FOUNDATION MODELS FOR PHYSICS

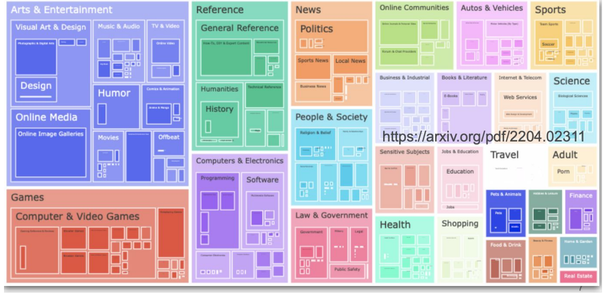
Talk by Ramachandra

Transformer blocks are the fundamental blocks, self-attention is essential functionality

"Attention is all you need"

https://arxiv.org/abs/1706.03762

LLM-ASSISTED RESEARCH: TEXT ONLY

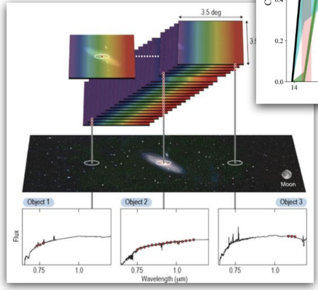


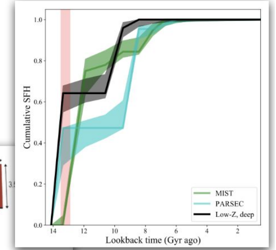
BENCHMARKING FOR AURORA-GPT

- Benchmark development may be crucial for a Science-focussed GPT comparison with existing LLMs.
- Benchmarking team at the Aurora-GPT collaboration has released a web-form to collect science questions of interest — with real-time evaluation from multiple LLMs.
- Goal is to collect O(1000) questions across scientific fields — **HELP needed! (and potential collaboration opportunities)**
  - High-quality.
  - Should represent what the science community wants out of an LLM.
  - Should not be exposed to current LLMs.

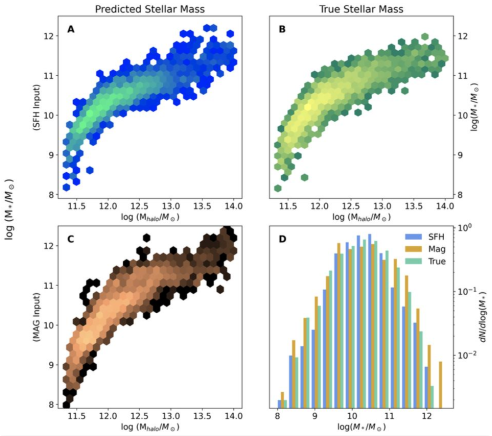
BEYOND-TEXT: FULL MODEL BUILDING

- Training is general purpose, deployment is task-specific.
- Flexibility in deployment: queries dictate latent space access.
- Compatibility wrto datasets in multiple domains
- DFMs can be joined with existing LLMs for contexts along with knowledge base access





Azton Wells, NR, Salman Habib, in prep



Summary & Outlook

- There is a lot that one can learn by gathering domain people and off domain (math, stats, data science,...)
- There are important lessons to learn on reproducibility in scientific computing from off domain people
- Hardware and software awareness is critical
- AI is opening new opportunities…need to effectively embrace new paradigms for science

Next steps

- Summary document of the program will be presented "snapshot"
- We plan to follow up with shorter workshop bringing domain+off domain to updated the document

INSTITUTE for NUCLEAR THEORY

ABOUT PEOPLE PUBLICATIONS EVENTS JOBS VISITORS

Program Overview

INT PROGRAM INT-24-2A

QCD at the Femtoscale in the Era of Big Data

June 10, 2024 - July 5, 2024

ORGANIZERS

Julie Bessac
NREL
julie.bessac@nrel.gov

Ian Cloët
Argonne National Laboratory
icloet@anl.gov

Nobuo Sato
Jefferson Lab
nsato@jlab.org

Emil Constantinescu
Argonne National Laboratory
emconsta@mcs.anl.gov

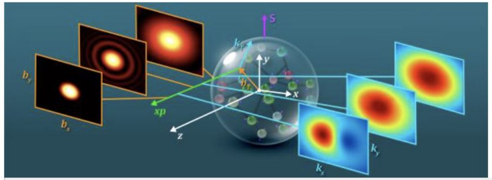


Image Courtesy of Argonne National Laboratory and Jefferson Lab