NSF: AI Institute for Artificial Intelligence and Fundamental Interactions

IAIFI (“eye+φ”)

Philip Harris
Experimental Physics coordinator

With Much Help from
Jesse Thaler and Mike Williams

NSF: National AI Research Institutes

5 Inaugural Institutes:

NSF AI Institute for Research on Trustworthy AI in Weather, Climate, and Coastal Oceanography

NSF AI Institute for Foundations of Machine Learning

NSF AI Institute for Student-AI Teaming

NSF AI Institute for Molecular Discovery, Synthetic Strategy, and Manufacturing

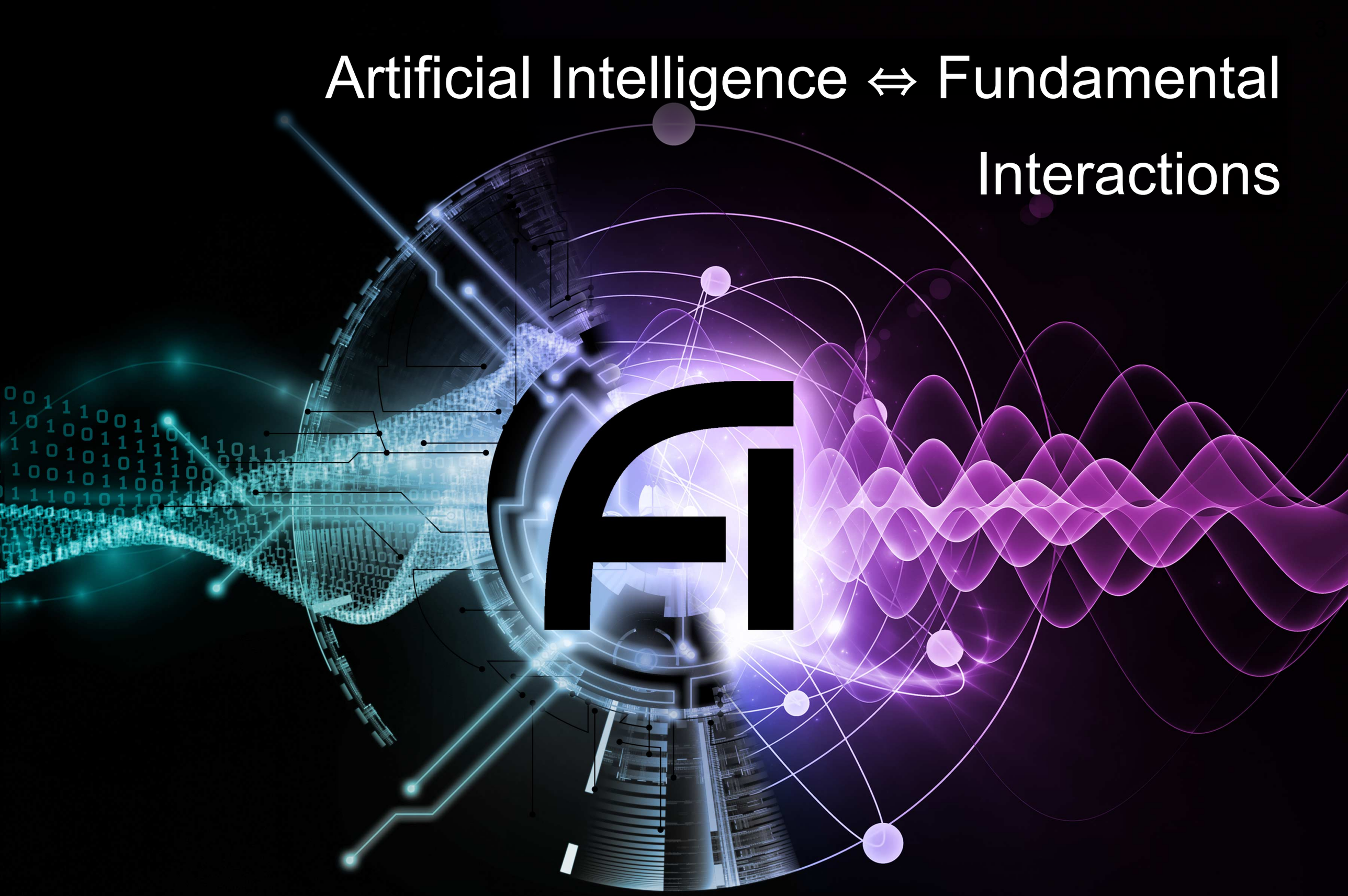
NSF AI Institute for Artificial Intelligence and Fundamental Interactions

8 Themes for Next Round:

AI Institute in Dynamic Systems
AI-Augmented Learning
AI to Advance Biology
AI-Driven Innovation in Agriculture and the Food System
Human-AI Interaction and Collaboration
AI Institute for Advances in Optimization
AI and Advanced Cyberinfrastructure
Advances in AI and Computer and Network Systems

[NSF Announcement, August 26, 2020; Call for New Proposals]

Artificial Intelligence ⇔ Fundamental Interactions



[http://iaifi.org/, MIT News Announcement]

The NSF AI Institute for Artificial Intelligence and Fundamental Interactions (IAIFI)

"I-φ"

Senior Investigators: 20 Physicists + 7 AI Experts
Junior Investigators: ≈20 PhD Students, ≈7 IAIFI Fellows in steady state

Pulkit Agrawal
Lisa Barsotti
Isaac Chuang
William Detmold
Bill Freeman
Philip Harris
Kerstin Perez
Alexander Rakhlin
Phiala Shanahan
Tracy Slatyer
Marin Soljacic
Justin Solomon
Washington Taylor
Max Tegmark
Jesse Thaler
Mike Williams
Demba Ba
Edo Berger
Cora Dvorkin
Daniel Eisenstein
Doug Finkbeiner
Matthew Schwartz
Yaron Singer
Todd Zickler
James Halverson
Brent Nelson
Taritree Wongjirad

Boston Area: Critical Mass for Transformative Ab Initio AI Research

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Advisory Board
(External advisory board)
To be appointed

SI Board
(Represents interests of all SIs)
All SIs have equal voting rights
Ratifies Management proposals

Institute Board
(Internal advisory board)
Bill Freeman (MIT)
Cora Dvorkin (Harvard)
James Halverson (Northeastern)
Taritree Wongjirad (Tufts)
ex-officio: ECEC Chair,
CB Chair, MIT-LNS Director,
Management Team

Management
(Executive body)
Director: Jesse Thaler (MIT)
Deputy Director: Mike Williams (MIT)
Institute Manager: To be hired

ECEC
(Early Career & Equity)
Chair: Tracy Slatyer (MIT)
5 members, including post-docs
and grad students

Coordination Board
(Coordinates all ₵AIFI activities)
Chair: Matthew Schwartz (Harvard)

Ab Initio AI for Theory Calculations:	Phiala Shanahan (MIT)
Ab Initio AI for Experiments:	Philip Harris (MIT)
Ab Initio AI for Advancing AI:	Demba Ba (Harvard)
Outreach:	Brent Nelson (Northeastern)
Education & Workforce Development:	Isaac Chuang (MIT)
Knowledge Transfer:	Todd Zickler (Harvard)
Post-doc Fellows:	Marin Soljačić (MIT)
Community Building:	Max Tegmark (MIT)
Resources:	William Detmold (MIT)

ex-officio: ECEC Chair, Management Team

₵AIFI Outputs

Director:
Jesse Thaler
Deputy:
Mike Williams

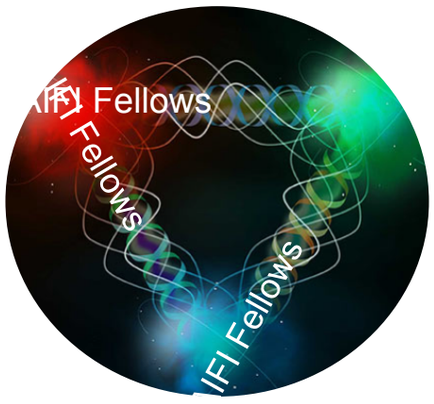
Boston Area: Critical Mass for Transformative Ab Initio AI Research

The NSF AI Institute for Artificial Intelligence and Fundamental Interactions (IAIFI)

"I-φ"

Advance physics knowledge — from the smallest building blocks of nature to the largest structures in the universe — and galvanize AI research innovation

Physics Theory



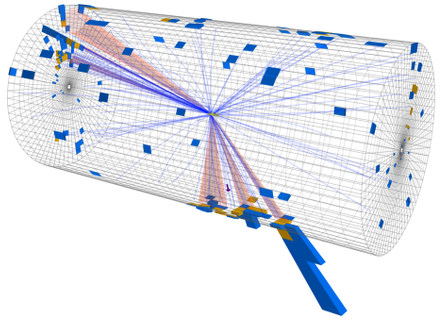
Physics Experiment

AI Foundations

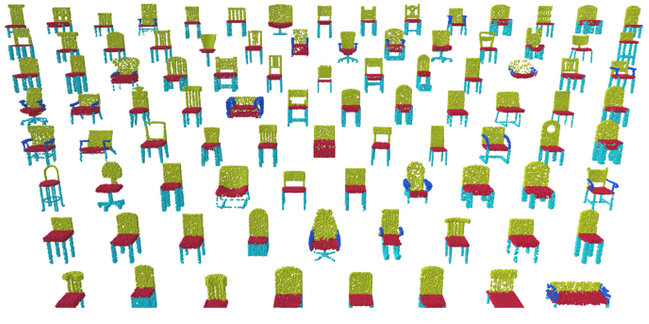
E.g.

Training, education & outreach at Physics/AI intersection
Cultivate early-career talent (e.g. IAIFI Fellows)
Foster connections to physics facilities and industry
Build strong multidisciplinary collaborations
Advocacy for shared solutions across subfields

Analyzing Collisions ⇔ Geometric Data Processing



[Harris, Schwartz, JDT, Williams]



[Wang, Sun, Liu, Sarma, Bronstein, Solomon, TOG 2019]

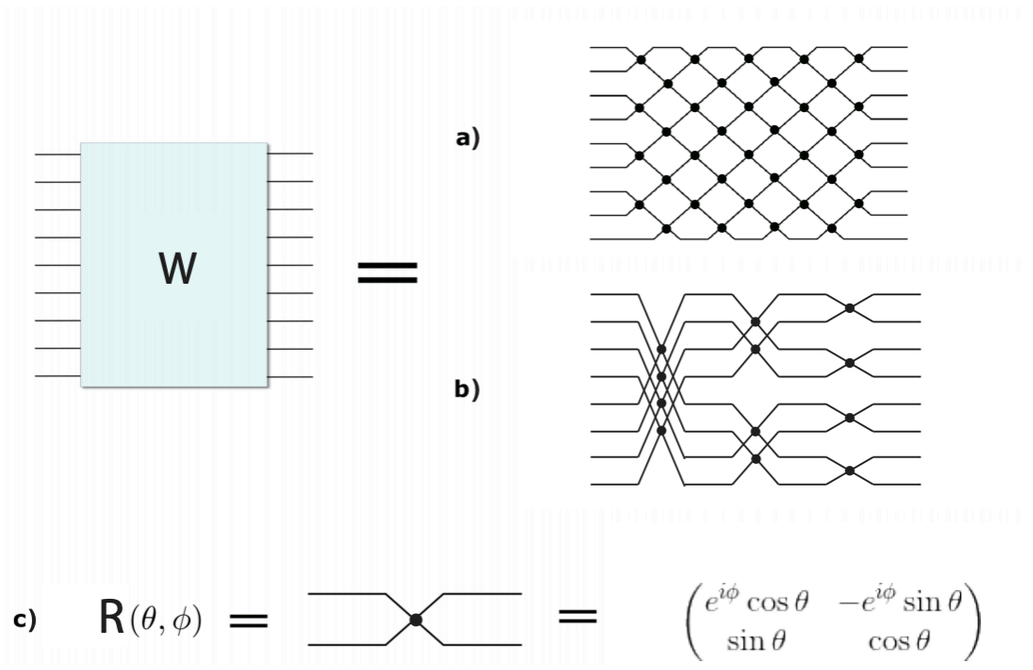
“What is Ab Initio Artificial Intelligence?”

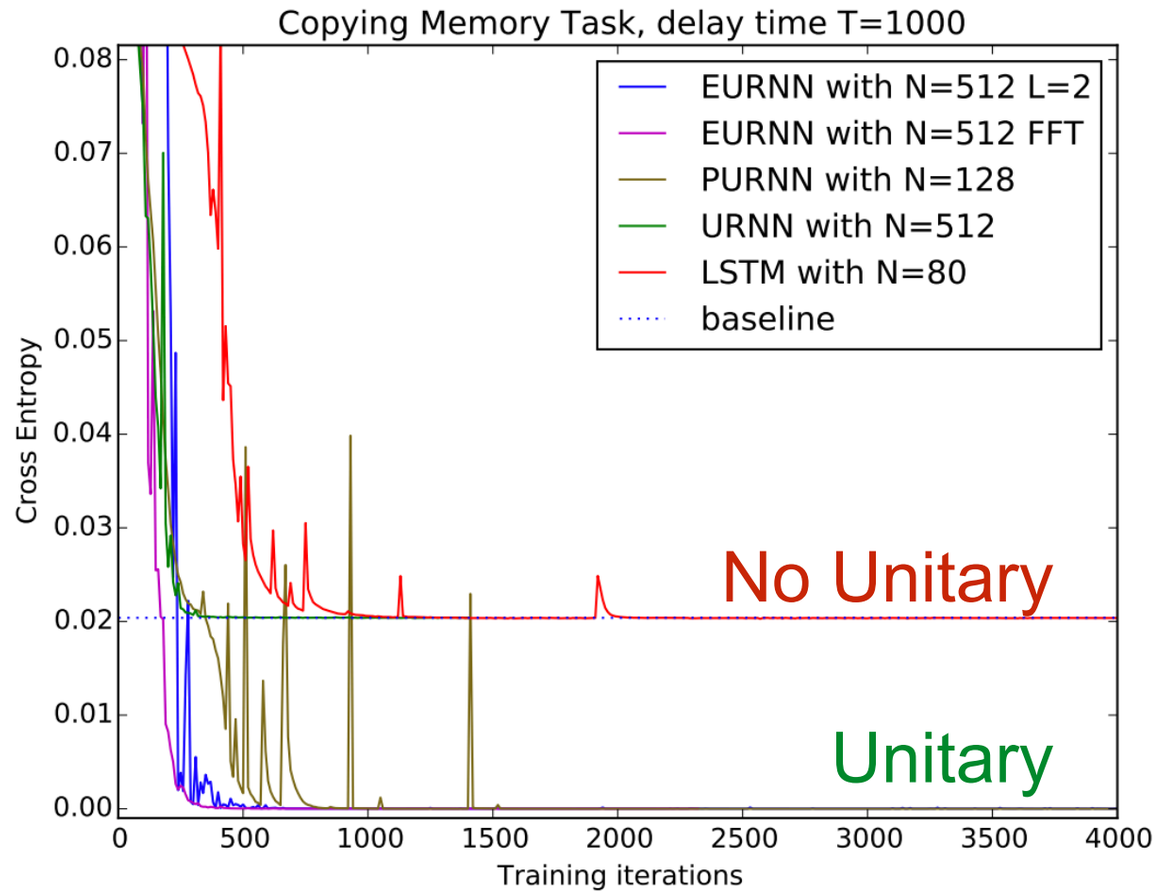
Machine learning architectures that incorporate
first principles, best practices, and domain knowledge
from fundamental physics

Physics going back to AI

Reconstruct dense matrices with unitary rotations

Eliminates the potential for unstable minimum





Tunable Efficient Unitary Neural Networks (EUNN) and their application to RNNs

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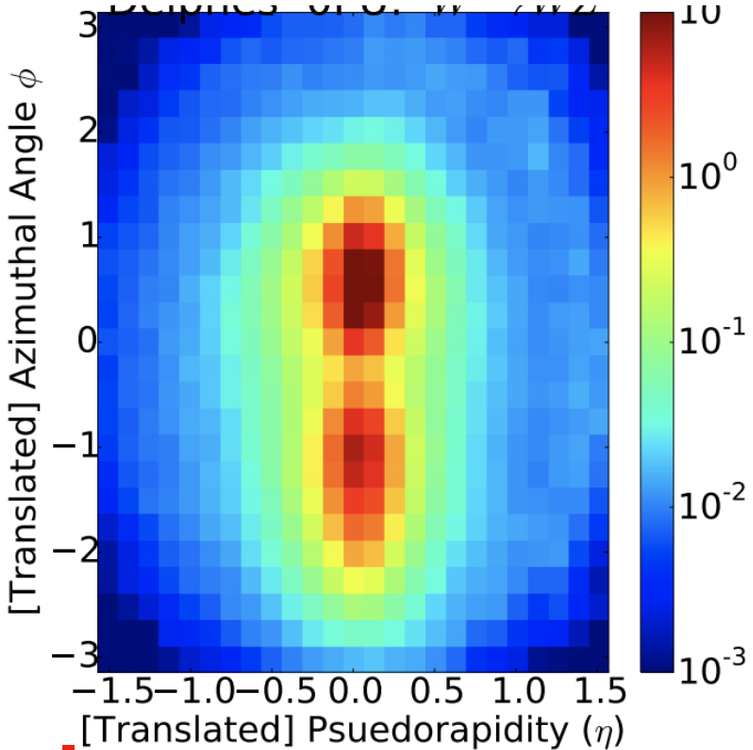
Li Jing [*1] **Yichen Shen** [*1] **Tena Dubcek** [1] **John Peurifoy** [1] **Scott Skirlo** [1] **Yann LeCun** [2] **Max Tegmark** [1]
Marin Soljačić [1]

https://arxiv.org/pdf/1612.05231.pdf

AI going back to physics

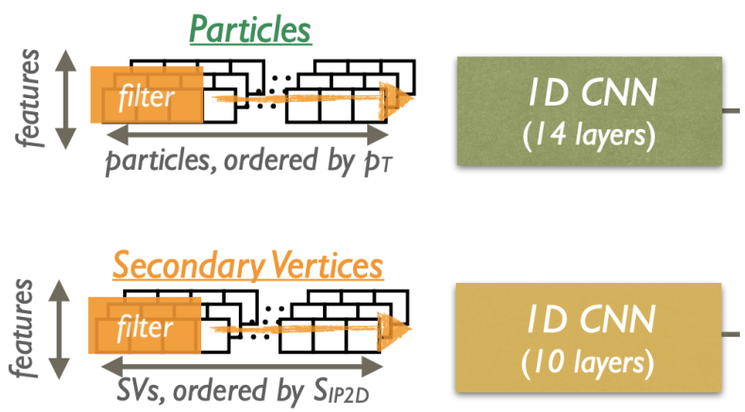
Aim to incorporate physics fundamentals into AI

2016



Images
(not lorentz invariant)

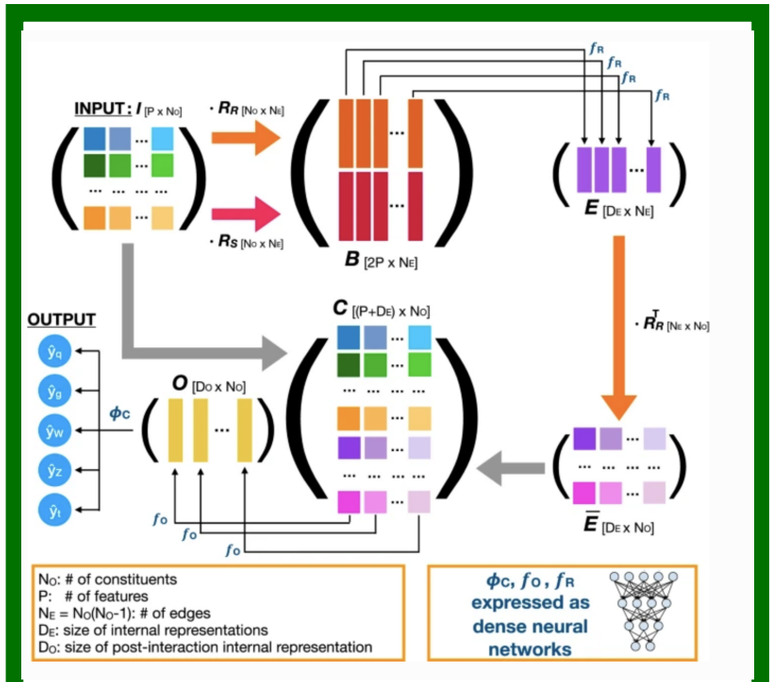
2018



Particles and SVs
with 4-vectors+features

Particles
(limited correlations)

2020



Graphs
(Particles+correlations)

Current collaboration results

Progressively moving towards use of more info

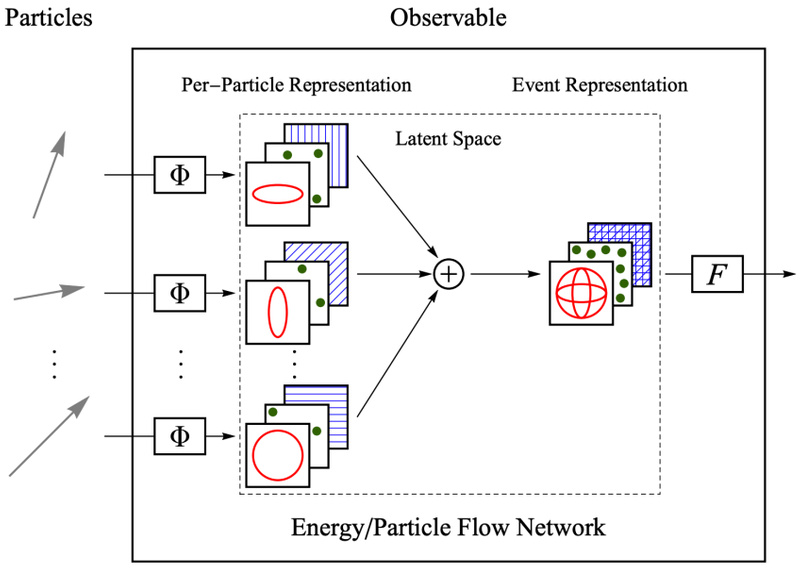
AI²: Ab Initio Artificial Intelligence

Symmetries, conservation laws, scaling relations, limiting behaviors, locality, causality, unitarity, gauge invariance, factorization, unit tests, exactness, systematic uncertainties, …

ML incorporates first principles, best practices, and domain knowledge from physics

Images: Convolutional Neural Networks Translational Equivariance
Momentum Conservation

Particle Level Energy Flow Networks ⇔ Identical Particles (QM)
Infrared/Collinear Safety (QFT)



AI × AI = AI²

Tools to identify physics

Understanding of AI architectures

Cross-cutting AI across Physics

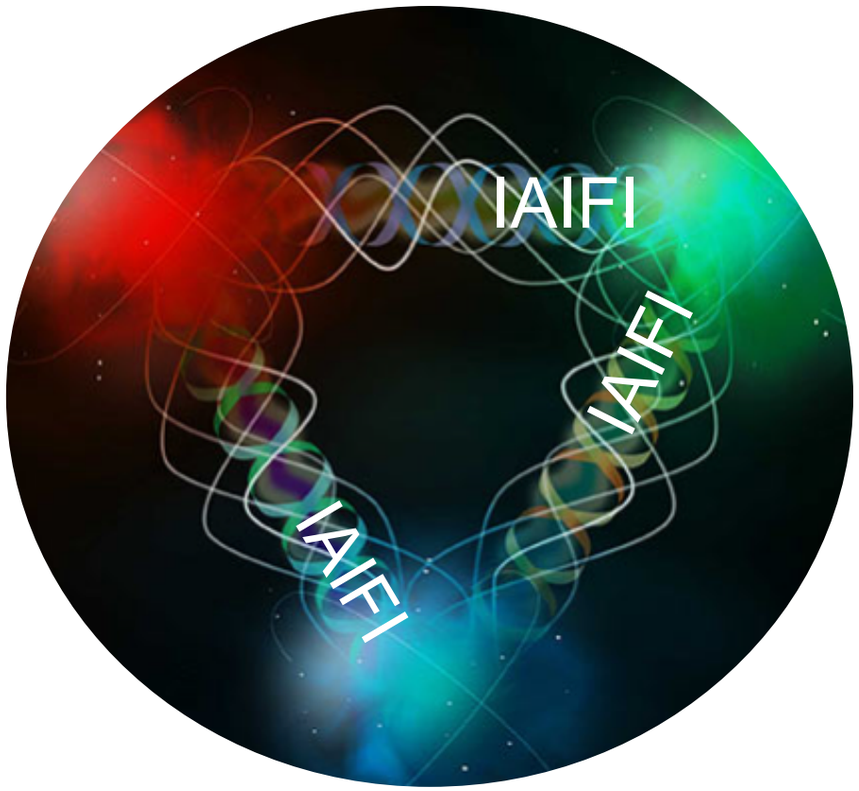
https://arxiv.org/abs/1810.05165

IAIFI Research Highlights, Proposed Activities & Synergies

IAIFI Postdoctoral Fellowships

Recruit/train a talented and diverse group of early-career researchers
Spark interdisciplinary, multi-investigator, multi-subfield collaborations

Physics Theory



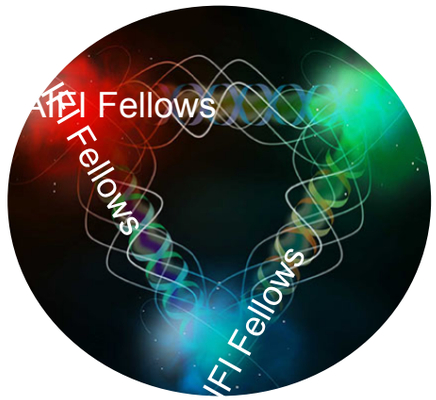
Physics Experiment

AI

2021–2024 application deadline: *October 20, 2020*

[https://iaifi.org/fellows.html; https://academicjobsonline.org/ajo/jobs/16695]

IAIFI Research Plan



AI² for Theoretical Physics

Standard Model of Nuclear & Particle Physics
String Theory & Physical Mathematics
Astroparticle Physics
Automated Discovery of Physics Models

AI² for Experimental Physics

Particle Physics Experiments
Gravitational Wave Interferometry
(Multi-Messenger) Astrophysics

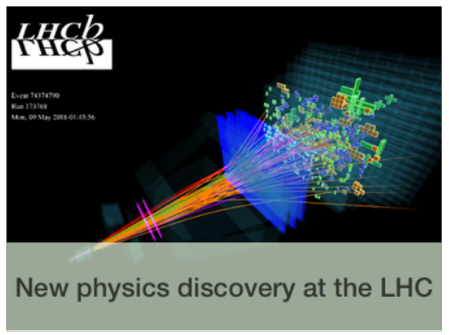
AI² for Foundational AI

Symmetries & Invariance
Speeding up Control & Inference
Physics-Informed Architectures
Neural Networks Theory

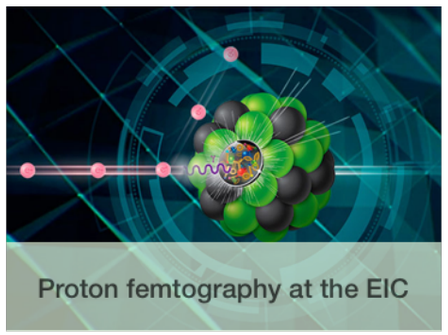
AI² for Theoretical Physics

E.g. Lattice Field Theory for Nuclear/Particle Physics

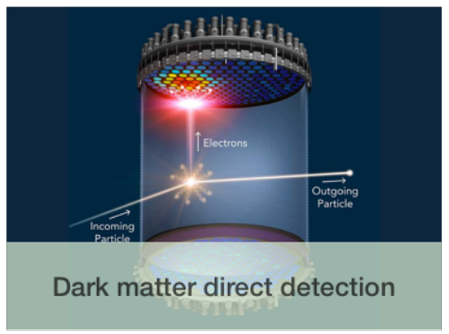
Equations governing the strong nuclear force are known, but precision computations are extremely demanding (>10% of open supercomputing in US)



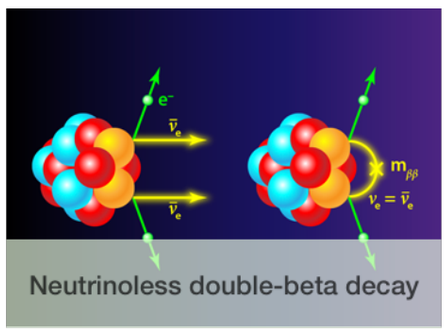
New physics discovery at the LHC



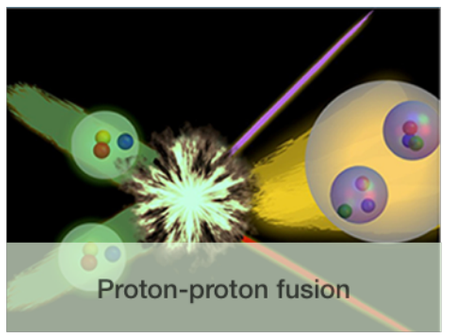
Proton femtography at the EIC



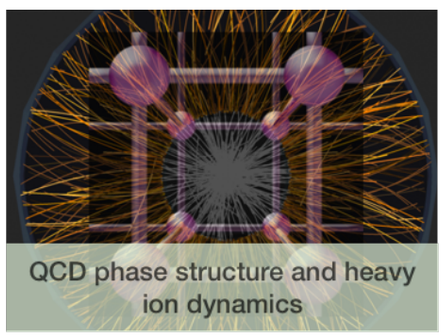
Dark matter direct detection



Neutrinoless double-beta decay



Proton-proton fusion



QCD phase structure and heavy ion dynamics

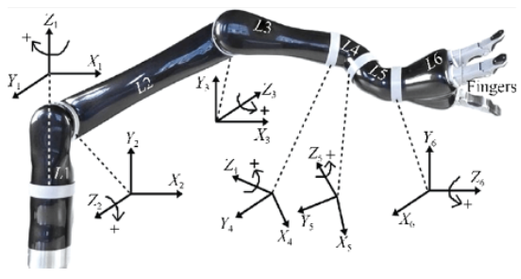
Industry collaboration to develop custom AI tools

Google DeepMind Massachusetts Institute of Technology

Custom generative models based on normalizing flows achieve 1000-fold acceleration while preserving symmetries & guaranteeing exactness

Tools designed for physics find interdisciplinary applications

Robotics



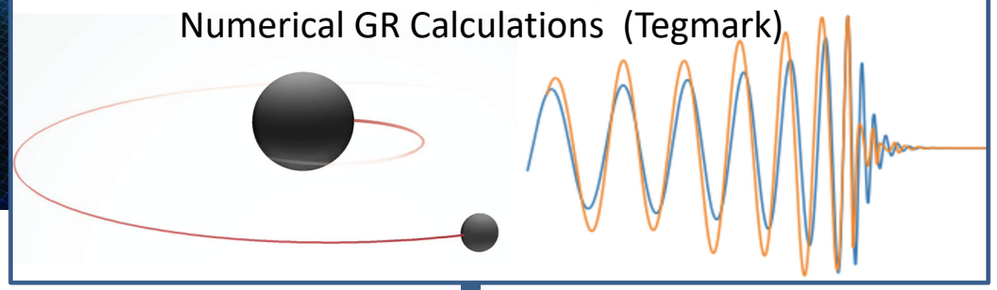
[Kanwar, Albergo, Boyda, Cranmer, Hackett, Racanière, Rezende, **Shanahan**, arXiv 2020]

AI² for Experimental Physics

E.g. Gravitational Wave Interferometry at LIGO

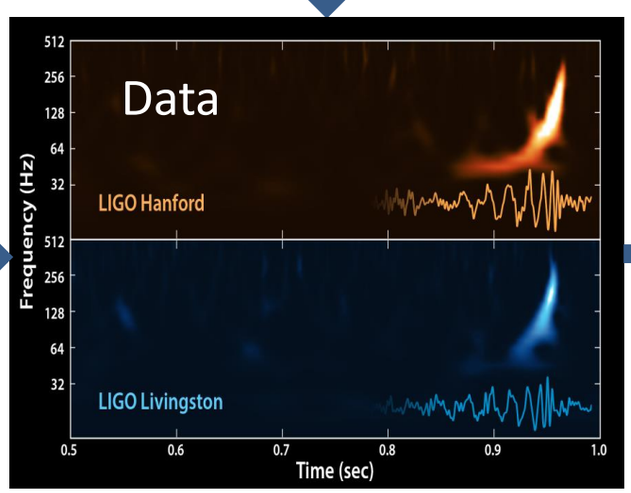
Potential to enhance the physics potential of flagship experiments via improved calibrations, better quantification of uncertainties, enhanced interpretability, and sub-microsecond inference

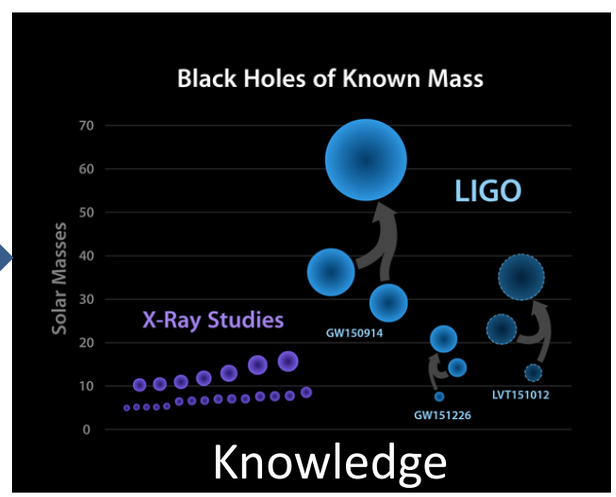
Theory Inputs: AI² to Speed Up Numerical GR Calculations (Tegmark)



LHC Fast-ML to speed up multi-messenger astrophysics (Harris)

Autoencoders improve LIGO's sensitivity by 20% [2005.06534]





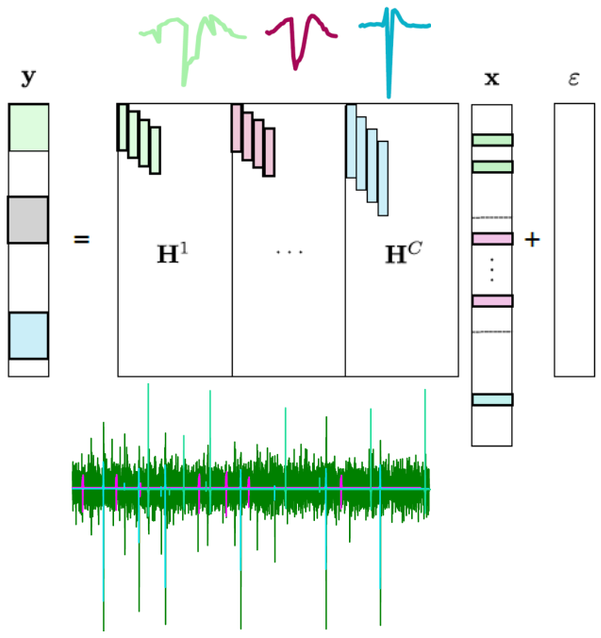
Propose using RL for Noise Reduction (Barsotti, Rakhlin)

AI² for Foundational AI

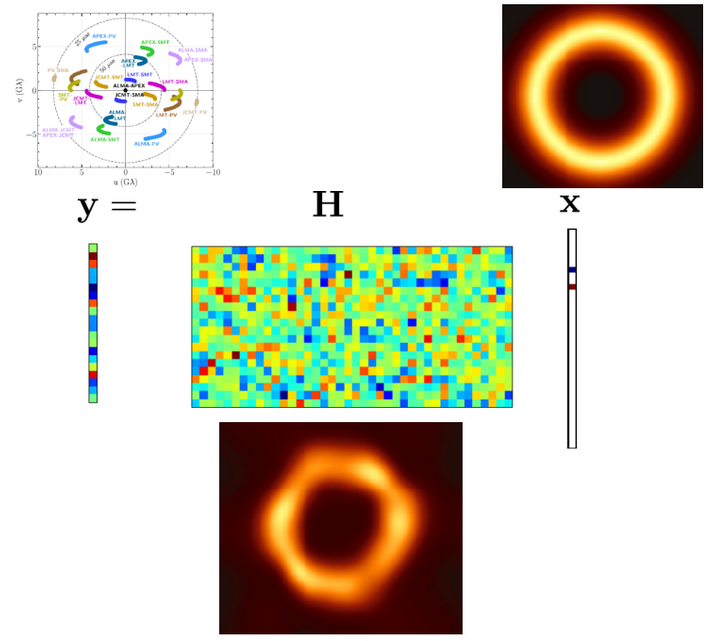
Deconvolution Across Disciplines

The unique features of physics applications and the power of physics principles offer compelling research opportunities to advance the field of AI research itself

Sparse Coding Networks and Neuronal Source Separation (Ba)



Event Horizon Telescope and Black Hole Imaging (Freeman)



Capitalize on physics priors and interpretability for improved robustness
Leverage tools from physics to explain ability of networks to generalize

IAIFI For experimental Physics
+ Computing challenges

William Detmold
Philip Harris
Phiala Shanahan
Kerstin Perez
Tracy Slatyer
Washington Taylor
Jesse Thaler
Mike Williams

Lisa Barsotti
Isaac Chuang
Marin Soljacic
Max Tegmark

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Daniel Eisenstein
Doug Finkbeiner
Matthew Schwartz

Demba Ba
Yaron Singer
Todd Zickler

James Halverson
Brent Nelson

Taritree Wongjirad

Experimentalist Theorist Computing Other physics

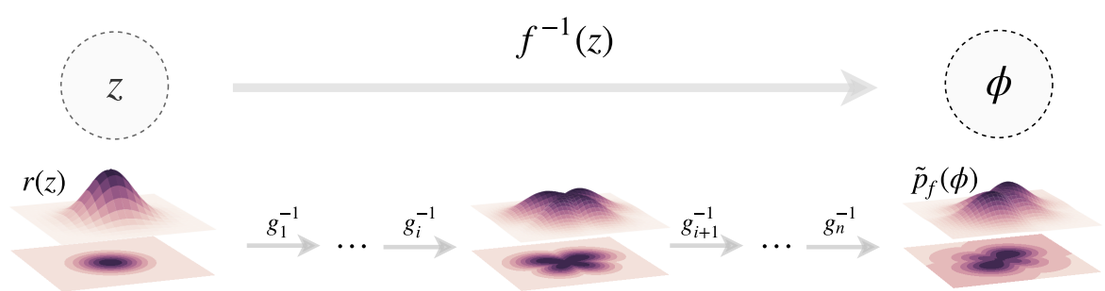
Major Computing Challenges

A number of computing challenges are present within AIFI

Large Scale distributed GPUs

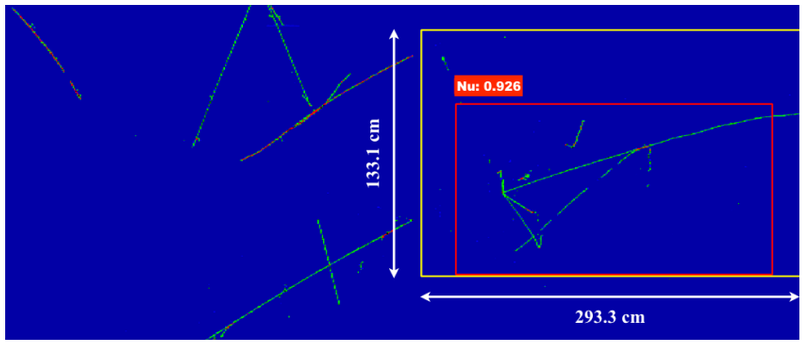
Adaptive Sampling for Lattice QCD

[Albergo, Kanwar, **Shanahan**, PRD 2019; Rezende, Papamakarios, Racanière, Albergo, Kanwar, **Shanahan**, Cranmer, arXiv 2020]



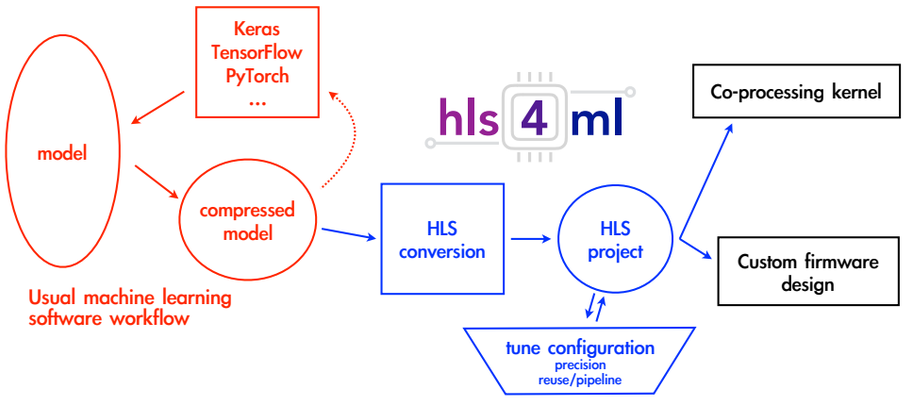
LArTPC Object Classification

[MicroBooNE collaboration (incl. **Wongjirad**), JINST 2017]



Sub-Microsecond LHC Inference

[Duarte, Han, **Harris**, Jindariani, Kreinar, Kreis, Ngadiuba, Pierini, Rivera, Tran, Wu, JINST 2018]



Processing of LHC/Neutrino Data

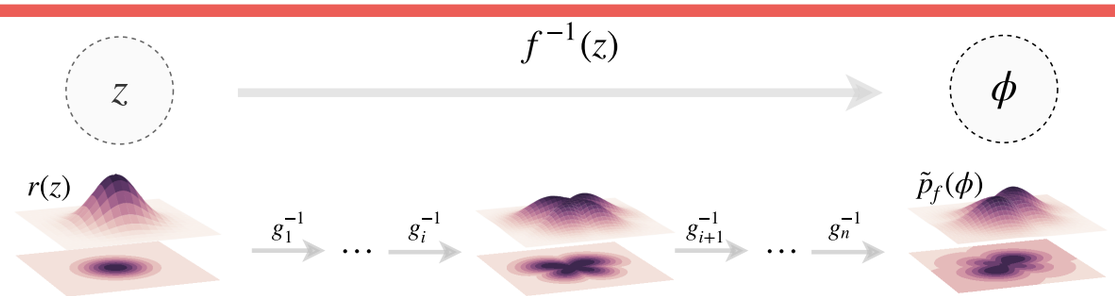
Major Computing Challenges

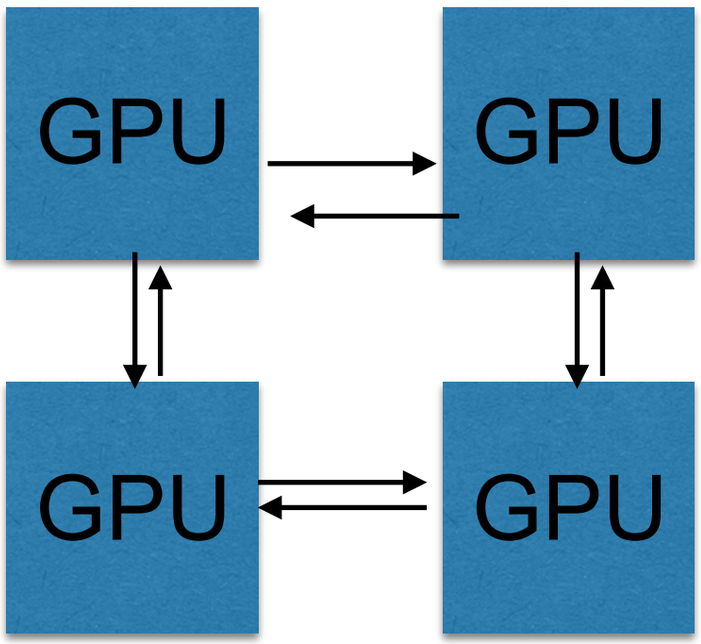
A number of computing challenges are present within AIFI

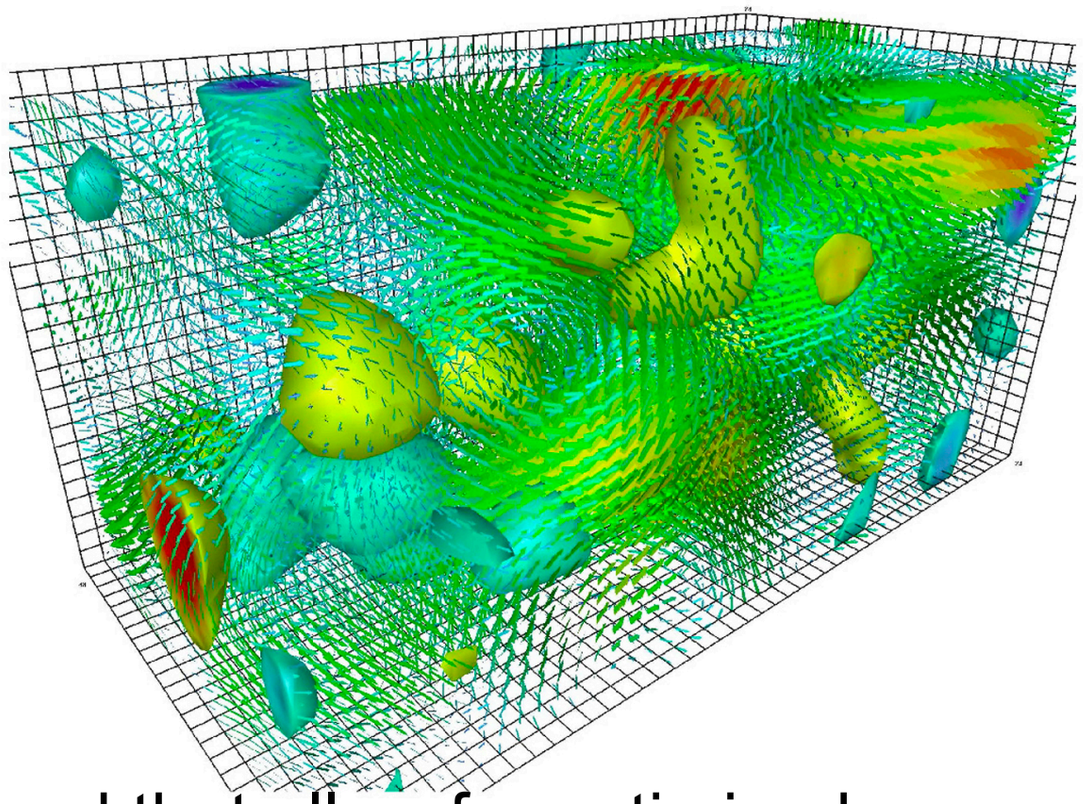
Large Scale distributed GPUs

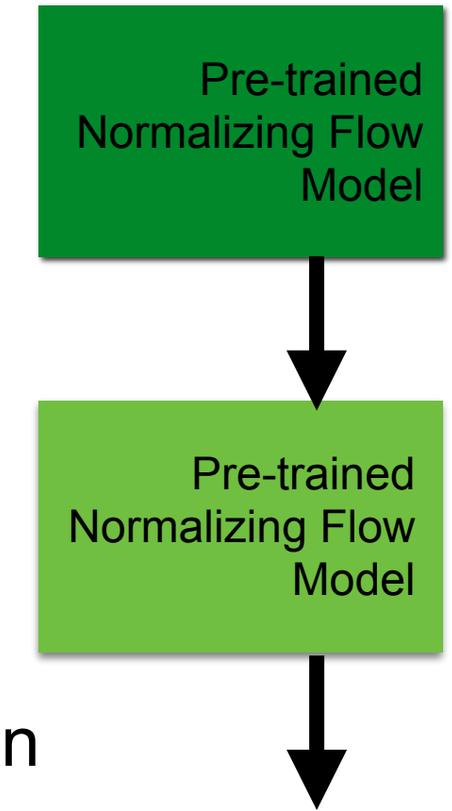
Adaptive Sampling for Lattice QCD

[Albergo, Kanwar, **Shanahan**, PRD 2019; Rezende, Papamakarios, Racanière, Albergo, Kanwar, **Shanahan**, Cranmer, arXiv 2020]





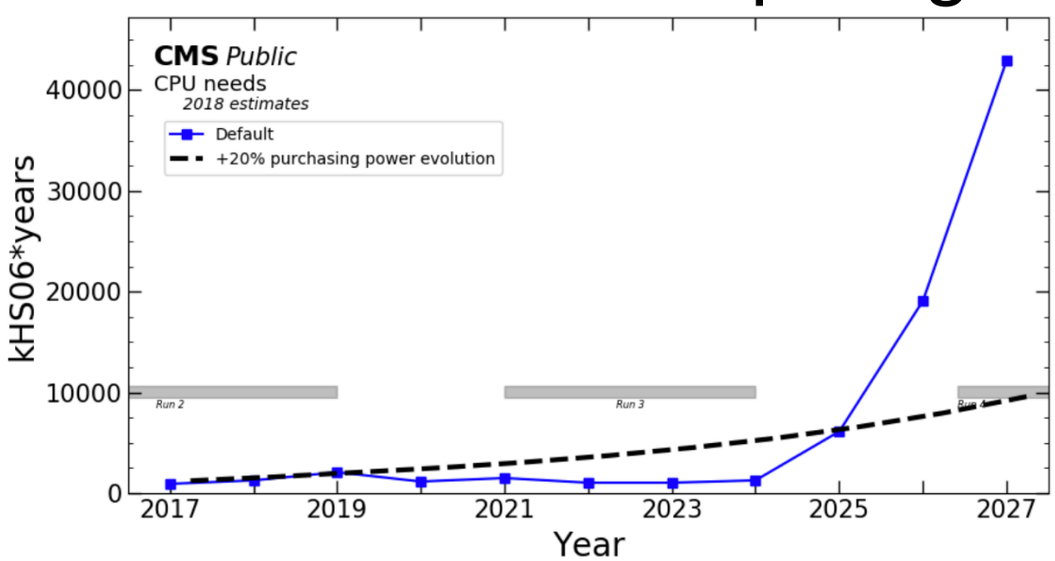




New ideas have emerged that allow for optimized computation

Major Computing Challenges

A number of computing challenges are present within AIFI

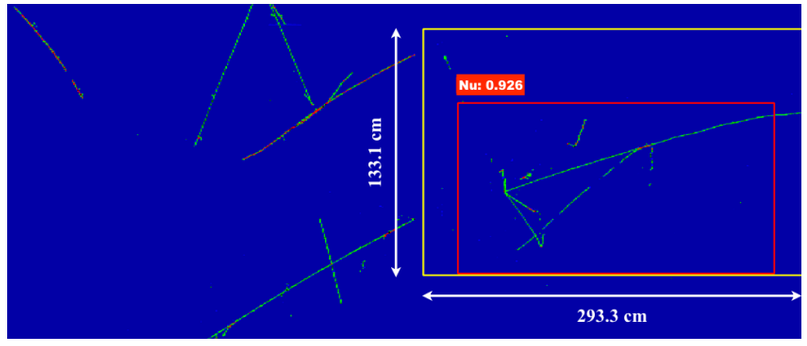


Demands at the LHC require significantly more computing power

AI + coprocesors is a solution

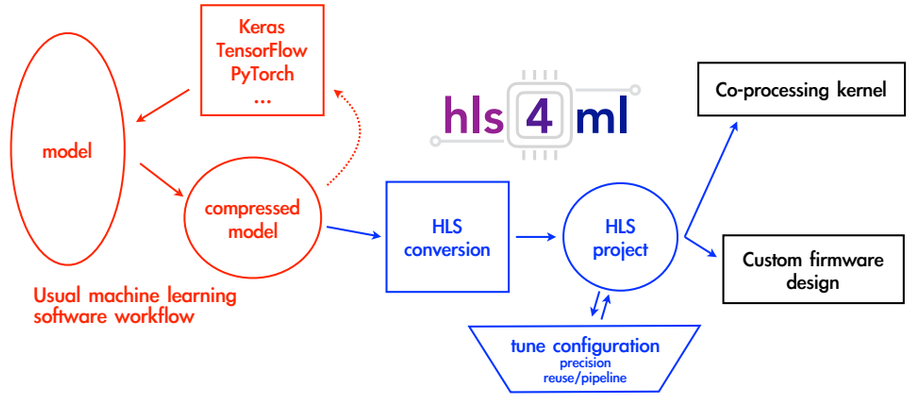
LArTPC Object Classification

[MicroBooNE collaboration (incl. Wongjirad), JINST 2017]



Sub-Microsecond LHC Inference

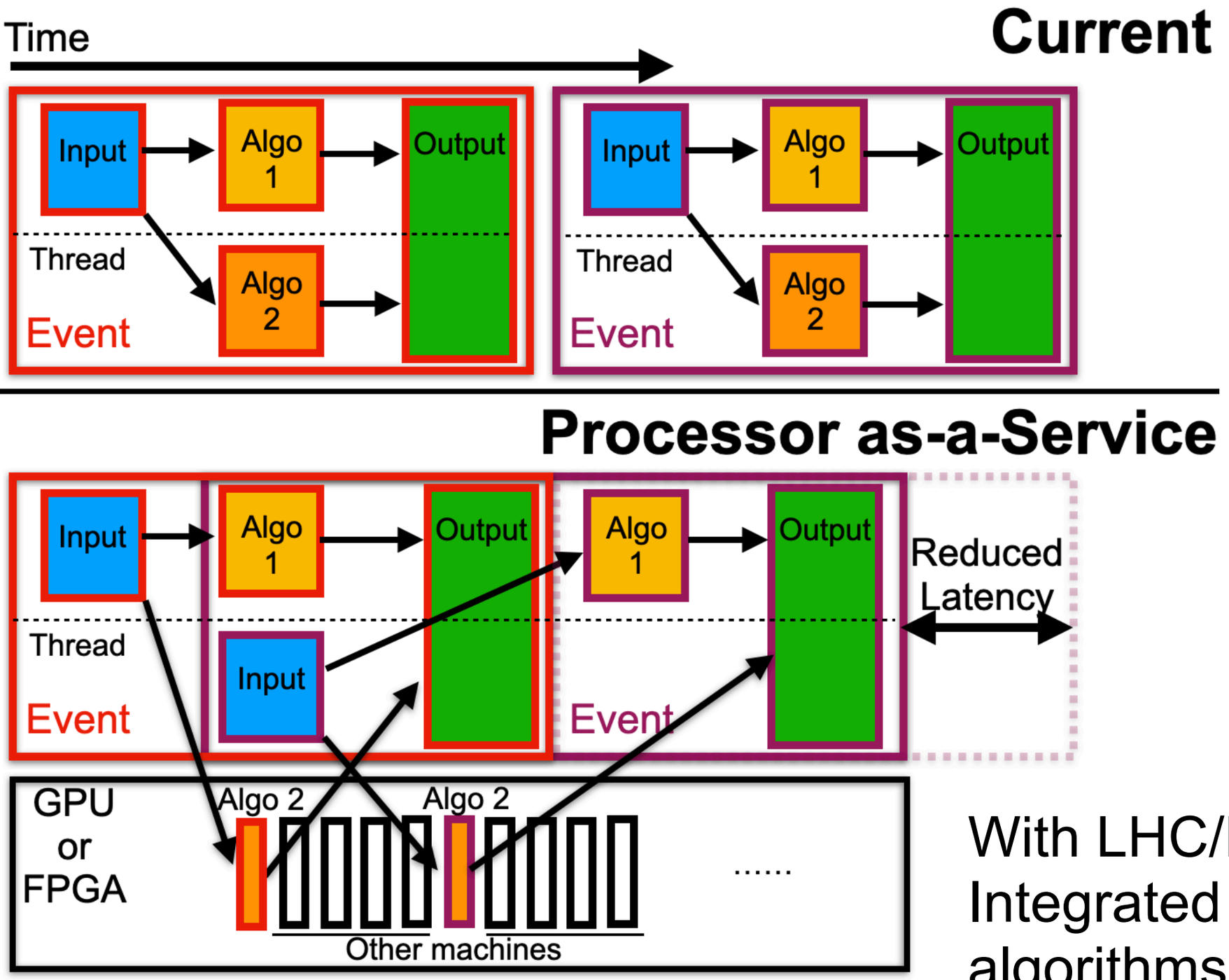
[Duarte, Han, Harris, Jindariani, Kreinar, Kreis, Ngadiuba, Pierini, Rivera, Tran, Wu, JINST 2018]



Processing of LHC/Neutrino Data

IAIFI for Experimental Physics

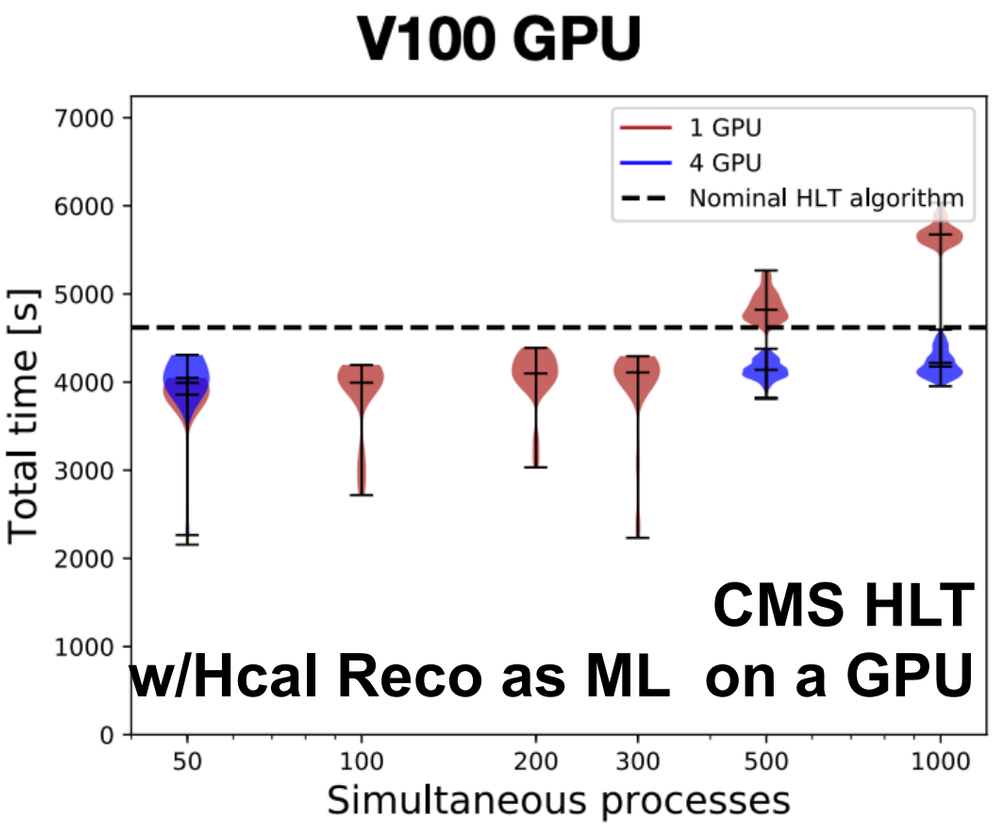
Performing Deep Learning as a service

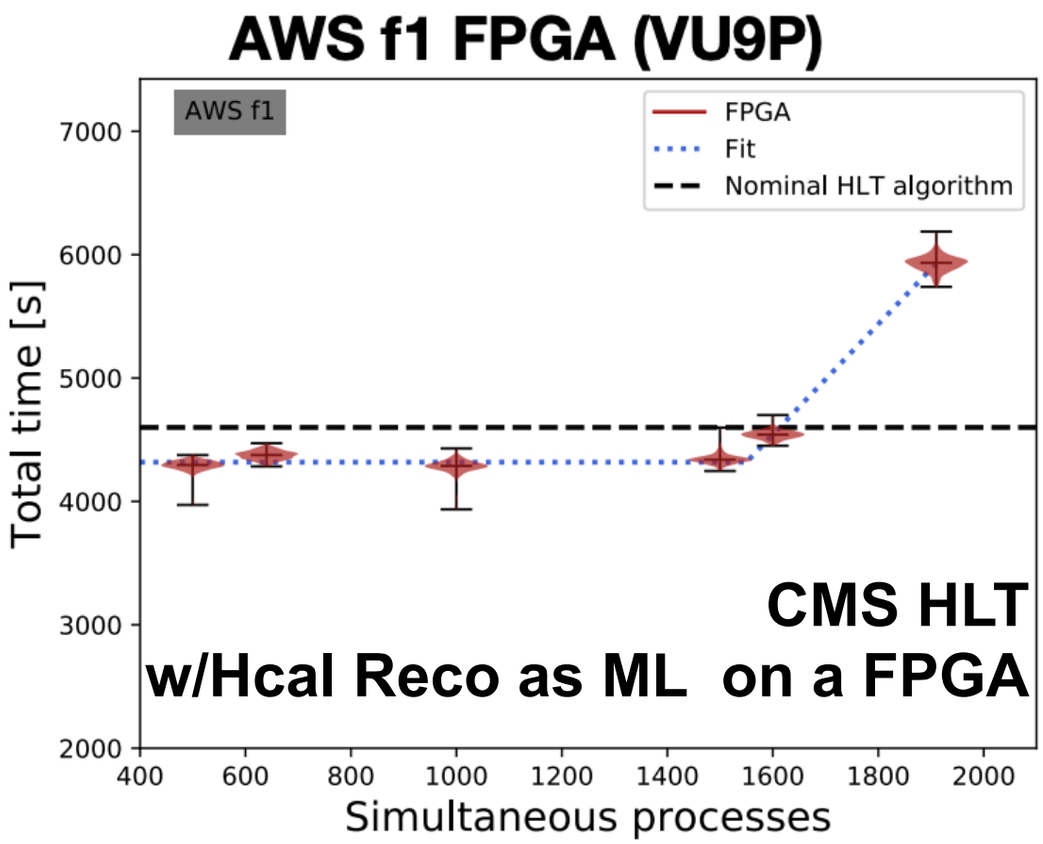


With LHC/Dune workflows
Integrated ability to offload algorithms to a coprocessor

IAIFI for Experimental Physics

Recent results with High Level Trigger





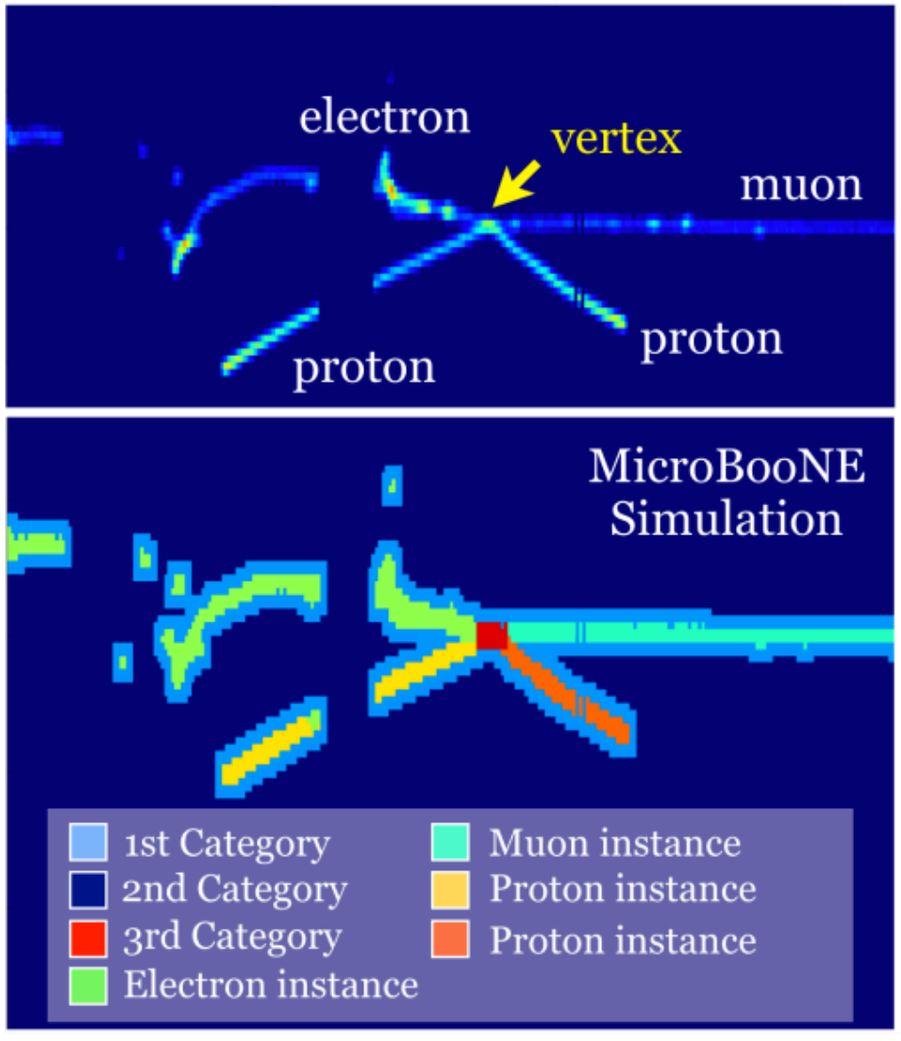
GPU/FPGA aaS	***Gain w.r.t. CPU***
2 ms (GPU) 0.2 ms (FPGA)	**8x (GPU)** **80x (FPGA)**
0.1 ms (GPU) in progress (FPGA)	**750x**
1-2 ms (GPU/FPGA)	**500x**

Constructing tools to integrate Deep Learning algorithms into LHC workflows….
Along with exploration of Algos

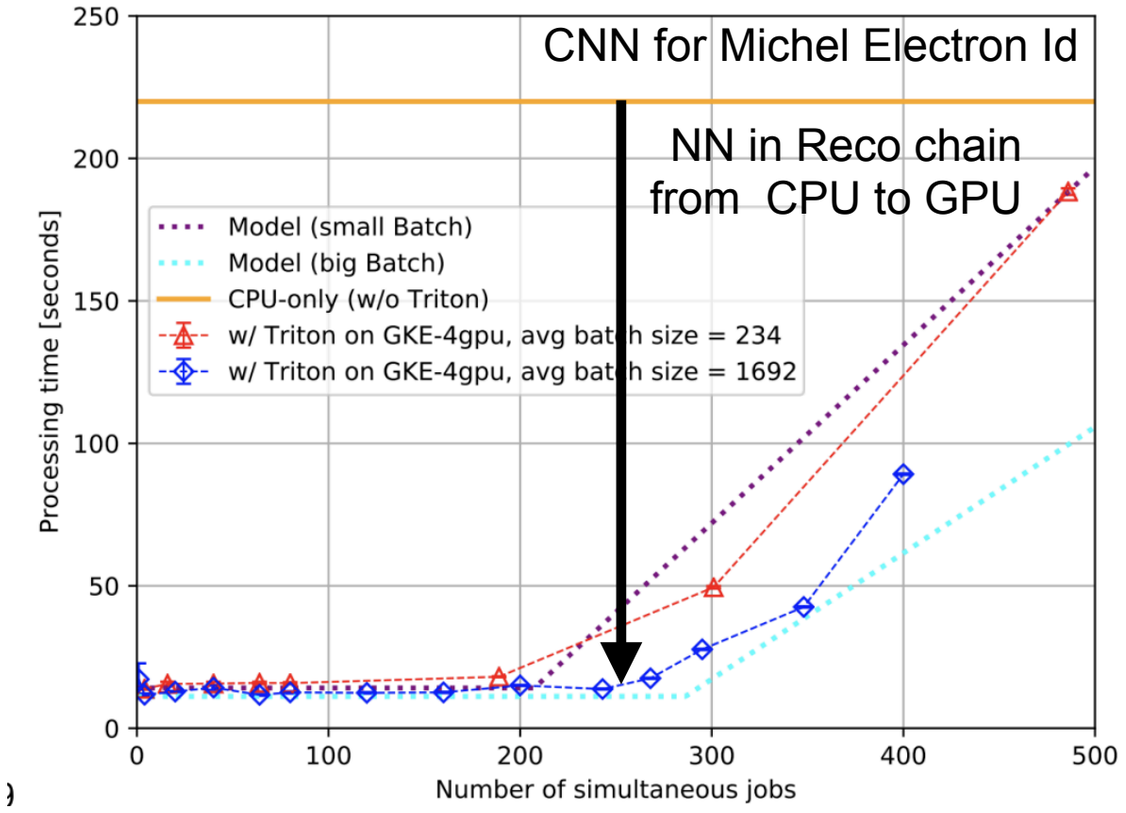
IAIFI for Experimental Physics

AI with Neutrino reconstruction

T. Wongjirad



UResNet and other related CNN models have led to improved reconstruction in neutrinos

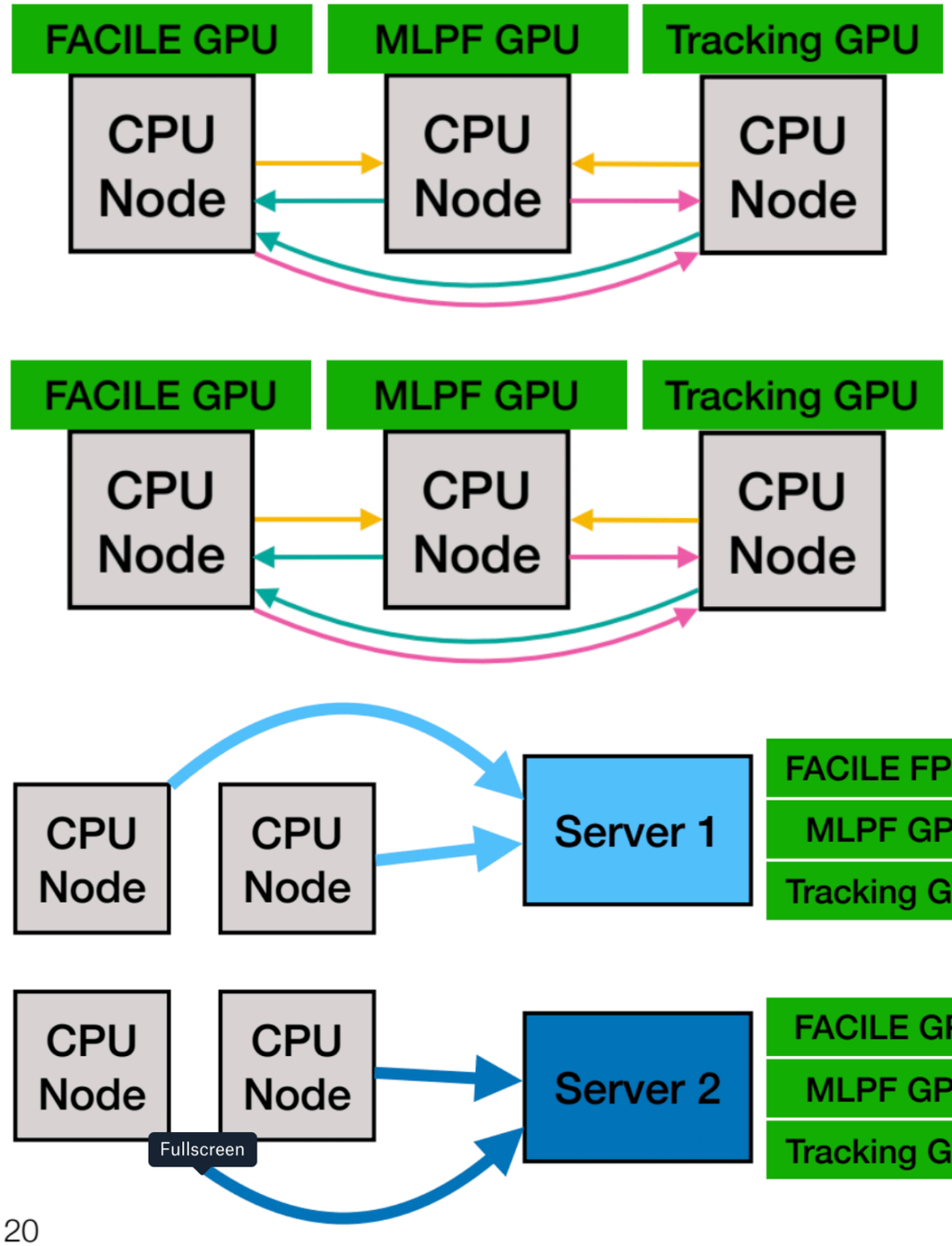


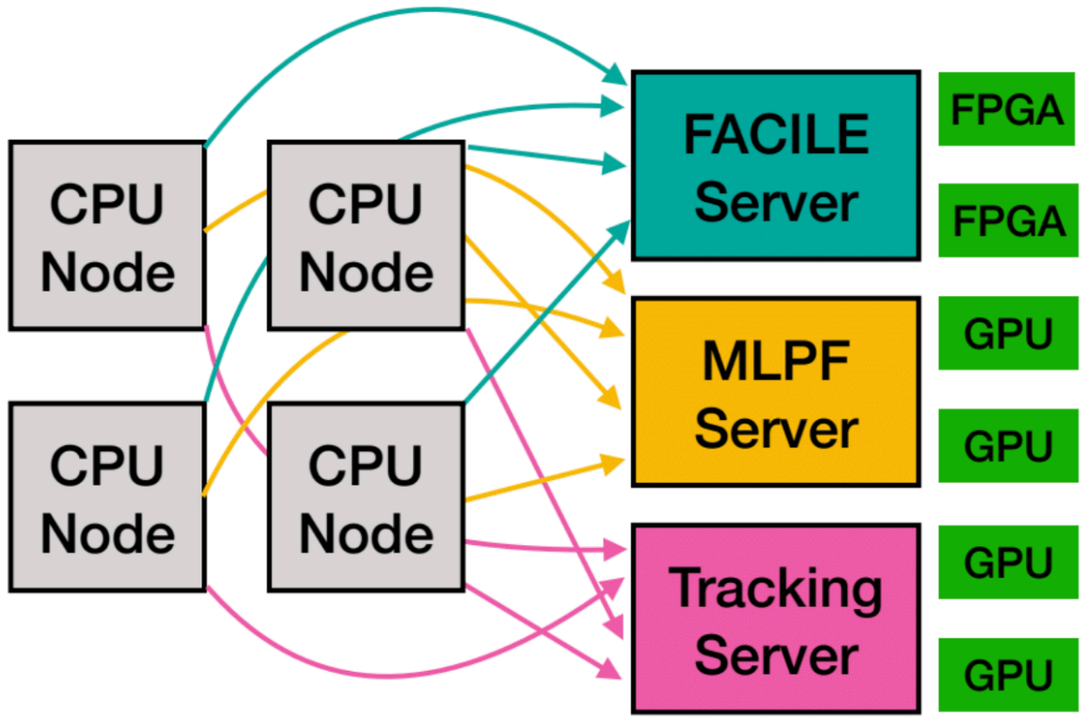
Integrating ML with GPU based tools can lead to significant speedups

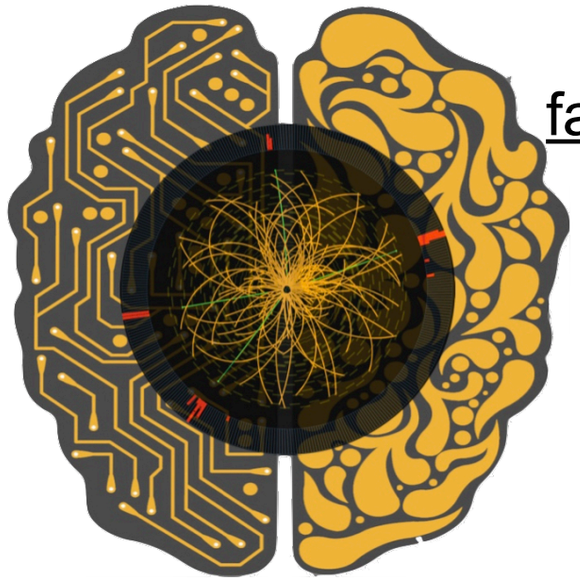
Provided network performs optimized speed ups

IAIFI for Experimental Physics

With the tools in FastML (a broad range of functionality)
How to integrate 3 different ML Algos in HLT?







fastmachinelearning.org
Work Done as part of Fast ML

Similar studies For L1 Trigger

Building on these ideas

With Experimental component :

- AI^2 focus is to ensure AI is solving problems
- A critical component of that is to ensure this goes to experiment
- With AIFI:
  - Aim to develop networks with physics principles
  - Algorithms are intended for use in Physics or AI community

- With Fast ML :
  - Aim is to deploy precepts of algorithm design to opmize algo
    - Exploiting symmetries
    - Also exploiting bit precision and NAS
  - Aim is to ensure algorithms can be sped up significantly
    - Put the infrastructure in place to do this

IAIFI Activities & Synergies

Research Engagement

- Regular Internal Meetings
- External Seminar Speakers
- Long-term Visitor Program
- IAIFI Affiliates
- Annual IAIFI Workshop (Summer 2022)

Workforce Development

- IAIFI Postdoctoral Fellowship (Fall 2021)
- Cross-Disciplinary Mentoring
- Interdisciplinary PhD Program
- Annual PhD Summer School (Summer 2022)

Digital Learning

- Online Physics/AI Course Modules
- Expansion of MITx MicroMasters Program

Outreach

- IAIFI Podcasts
- K-12 Engagement
- Festivals & Museums

Broadening Participation

- Early Career & Equity Committee
- Summer Research Program
- MicroFellowship Program

Knowledge Transfer

- Summer Internship Placement
- Joint Research Initiatives

IAIFI Activities & Synergies

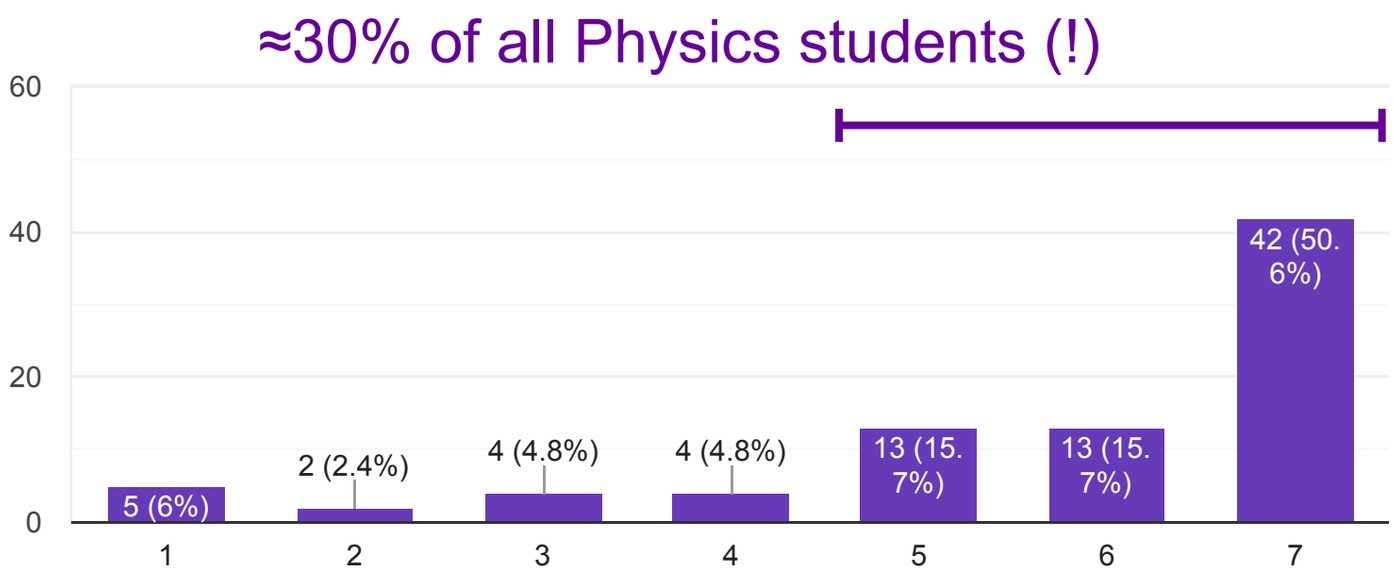
Interdisciplinary PhD in Physics, Statistics & Data Science

MIT Physics

MIT STATISTICS + DATA SCIENCE CENTER

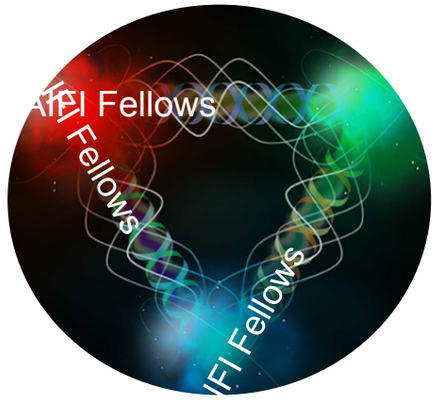
This interdisciplinary degree would have a number of requirements, in addition to the standard requirements for the MIT Physics PhD. How interested would you be in submitting and defending a PhD thesis that uses statistical methods in a substantial way?

83 responses



Respondent #11: "I think ML is the most important thing happening in the world right now and should be incorporated into any STEM degree."

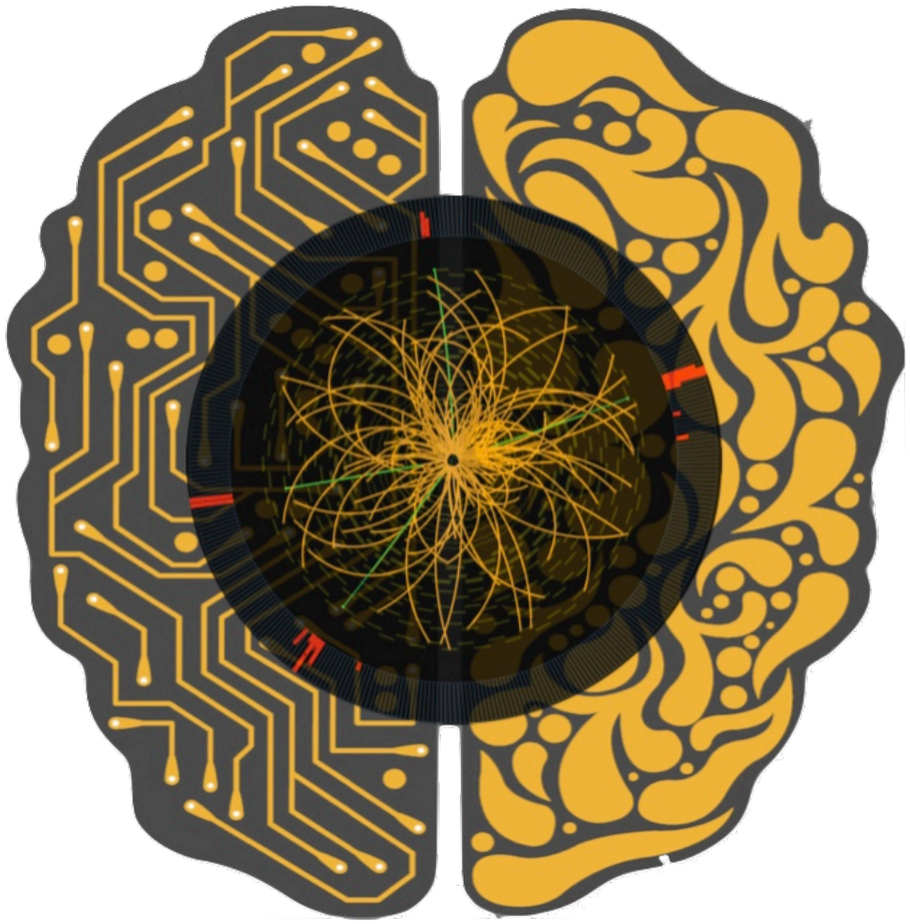
IAIFI Outreach Plan

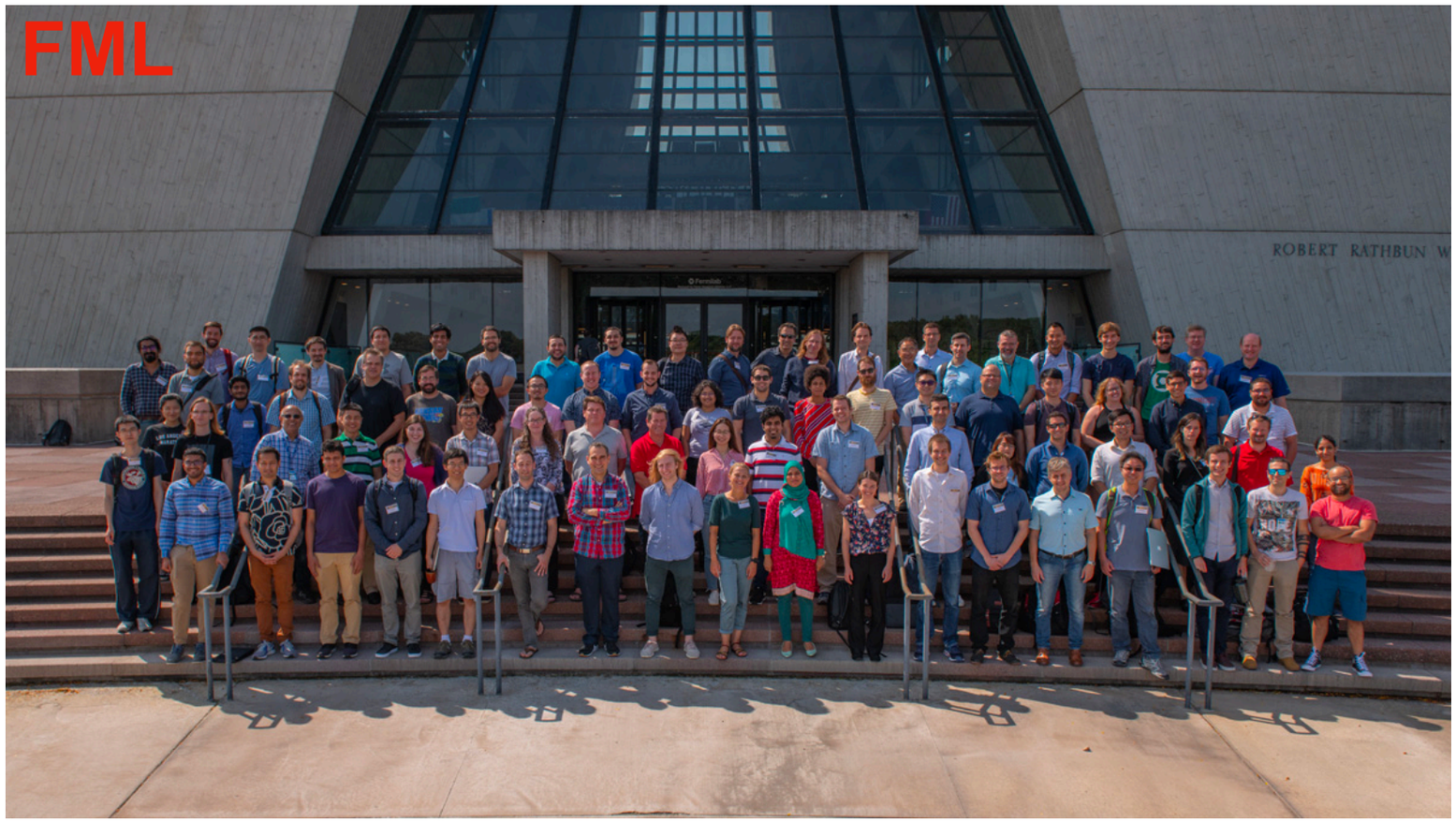


Training, education & outreach at Physics/AI intersection
Cultivate early-career talent (e.g. IAIFI Fellows)
Foster connections to physics facilities and industry
Build strong multidisciplinary collaborations
Advocacy for shared solutions across subfields

Backup

FastMachineLearning.org





Group Founded by P. Harris and N. Tran (FNAL)https://indico.cern.ch/event/822126/

- Project now covers some LHC, DUNE, LIGO, Materials science….
- Collaboration is now > 40 members at 10 institutes (2 years old)
- Our aim : bring the fastest machine learning to science

IAIFI for Experimental Physics

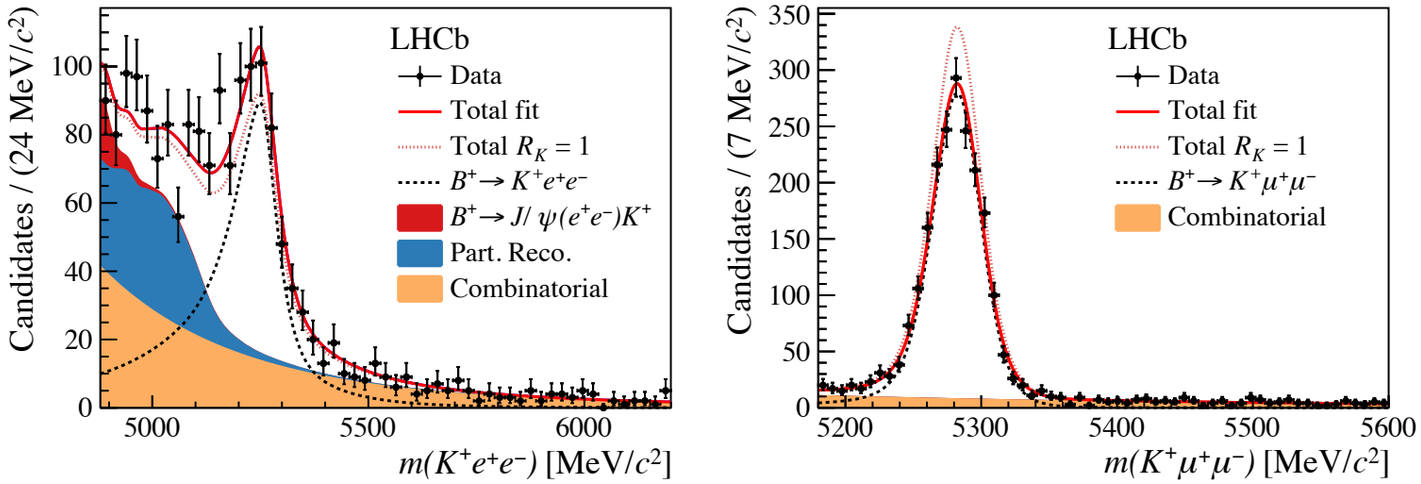
Strategy for experimental physics is about taking AI to data

E.g. Tests of Lepton Universality using the LHCb Software Trigger

[LHCb collaboration, PRL 2019]

[using Gligorov, Williams, JINST 2013; Likhomanenko, Ilten, Khairullin, Rogozhnikov, Ustyuzhanin, Williams, JPCS 2015]

Interpretable AI is enabling reliable real-time event selection at LHCb



type	$\varepsilon_{4-\text{body}}$ (%)	$\varepsilon_{5-\text{body}}$ (%)	instability (%)	
cuts	63.2 ± 0.5	55.3 ± 0.5	9 ± 3	Traditional Cuts
BDT	76.9 ± 0.4	68.1 ± 0.5	55 ± 4	Traditional AI
BBDT	73.8 ± 0.4	68.9 ± 0.5	10 ± 3	Interpretable AI