

AID(2)E: AI-Assisted Detector Design at EIC



DE-FOA-0002785



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CUA, T. Horn
Duke, A. Vossen
JLab, M. Diefenthaler
W&M, CF (PI)

Cristiano Fanelli on behalf of AID(2)E



PI Exchange Meeting - Cristiano Fanelli - Dec 5, 2024

Team Members



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coPI



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consulting



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Expertise: medium energy nuclear physics, EIC, 3D hadron Imaging, calorimetry



coPI



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Expertise: Physics, PID and calorimetry for the EIC

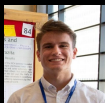


coPI



Cynthia Nunez, PhD

Expertise: Postdoc: physics, simulations



Connor Pecar, MS

Expertise: physics, PID and detector simulations for the EIC



Markus Diefenthaler, PhD

Expertise: ePIC Software & Computing Coordinator, EIC Science, Simulations



coPI



Makoto Asai, PhD

Expertise: Detector Simulations, Geant4



consulting



Cristiano Fanelli, PhD

Expertise: Data Science, Physics, MOO, Bayesian, Detectors, Artificial Intelligence, Computing



PI



Karthik Suresh PhD

Expertise: Postdoc - Data Science, Physics, MOO, Bayesian, Detectors, Distributed Computing



Hemalata Nayak, MS

Expertise: Physics, Data Science, Optimization, Reconstruction

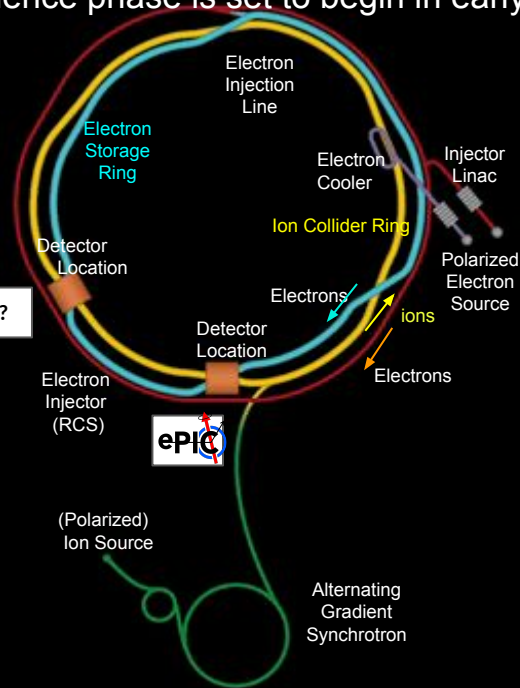


Electron Ion Collider

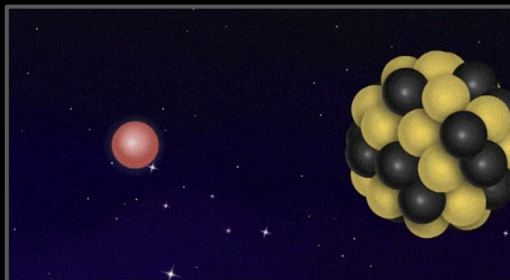
A US-led and international effort to build a precision machine to study the “glue” that binds us all. This will put the US at the frontier of nuclear physics research for the next 30 years.

The science phase is set to begin in early 2030.

polarized electron - polarized protons/ions



Detector 2?



CoM energy $\sqrt{s_{e-p}} \sim (20-140)$ GeV

High luminosity up to 10^{34} cm⁻²s⁻¹,
a factor $\sim 100-1000$ times HERA

Possibility of second detector in addition
to EIC Project Detector / ePIC.

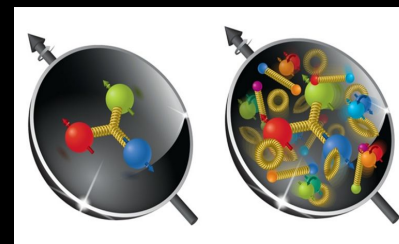
AI/ML will play a major role in optimizing
this complex operation

3 fundamental questions
(Nuclear Science Advisory Committee)

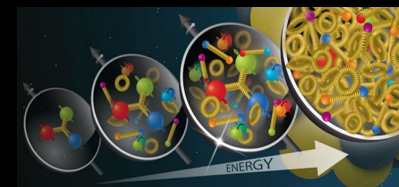
How does the mass of the nucleon arise?



How does the spin of the nucleon arise?

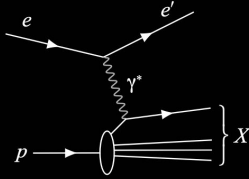


What are the emergent properties of
dense systems of gluons?

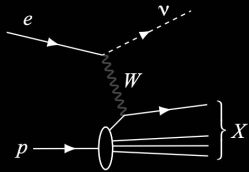


A Glimpse into EIC Physics

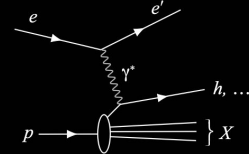
Neutral current
inclusive DIS



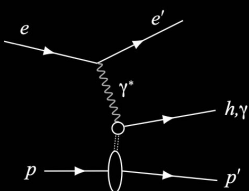
Charged current
inclusive DIS



Semi-inclusive DIS



Exclusive DIS



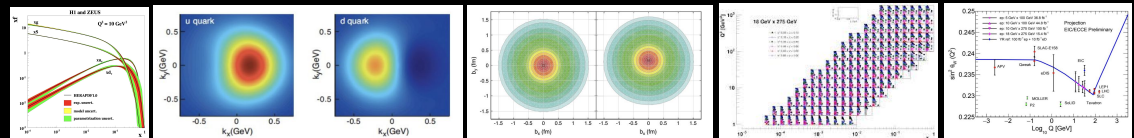
Detector requirements and design are tailored to optimize physics reach, guided by the EIC Yellow Report:

- Mass and Tomography
- Spin and Flavor Structure of the Nucleons and Nuclei
- Internal Landscape of Nuclei
- QCD at Extreme Parton Densities - Saturation
- etc

Important synergies with HL-LHC science program:

- Precision QCD studies with proton & nuclear targets α_s , quarkonia, quark exotica, jet physics in e-p collisions, ...
- Precision electroweak and BSM physics Weak mixing angle, LFV, ...
- etc

For more info in the [RAG-based EIC Chatbot](#)

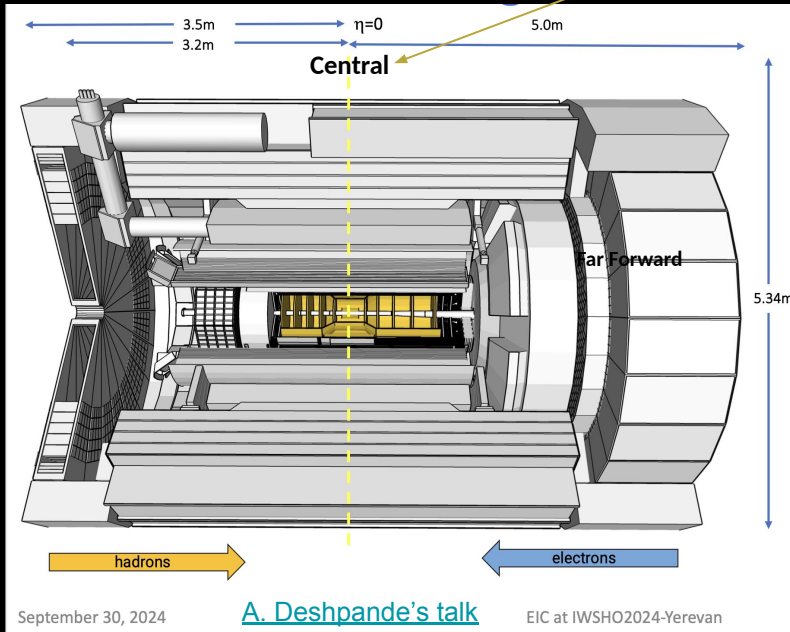


ePIC Detector



As of now, 171 institutions, 24 countries and 500+ participants

ePIC stands out as an **Integrated Detector** encompassing Central, Far-Forward, and Far-Backward regions, all crucial to access the EIC physics.



Tracking

- New 1.7T solenoid
- Si MAPS Tracker
- MPGDs (μ RWELL/ μ Megas)

September 30, 2024

[A. Deshpande's talk](#)

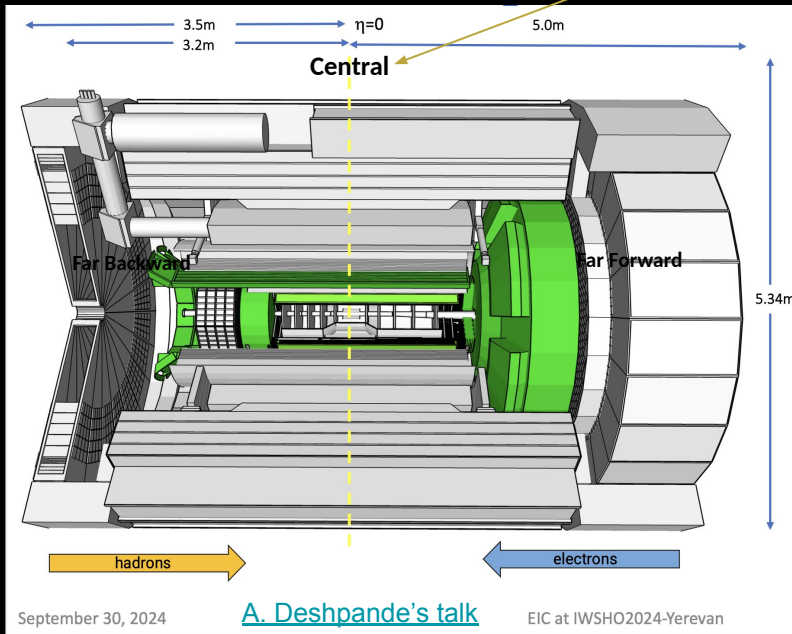
EIC at IWSHO2024-Yerevan

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PID

- hpDIRC
- pfRICH
- dRICH
- AC-LGAD (~ 30 ps TOF)

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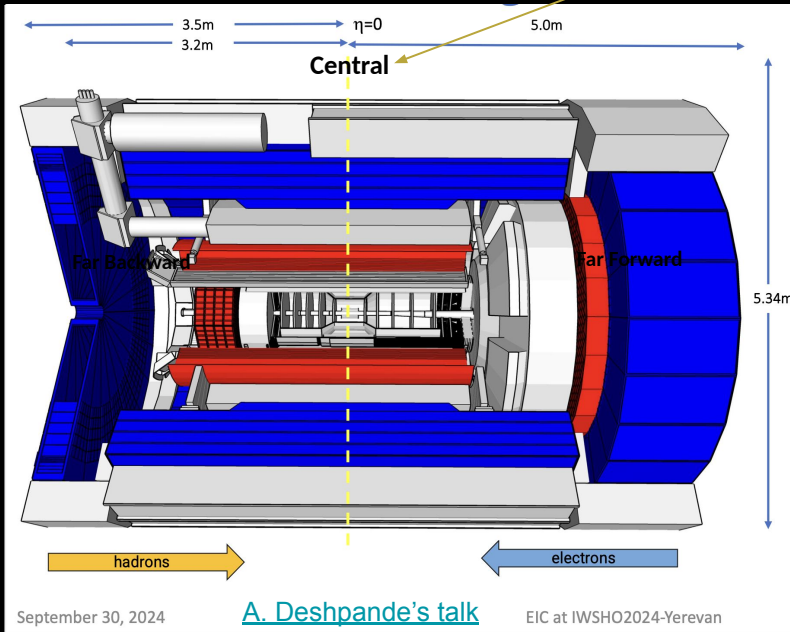


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Calorimetry

- Imaging Barrel EMCal
- PbWO₄ EMCal in backward direction
- Finely segmented EMCal +HCal in forward direction
- Outer HCal (SPHENIX re-use)
- Backwards HCal (tail-catcher)

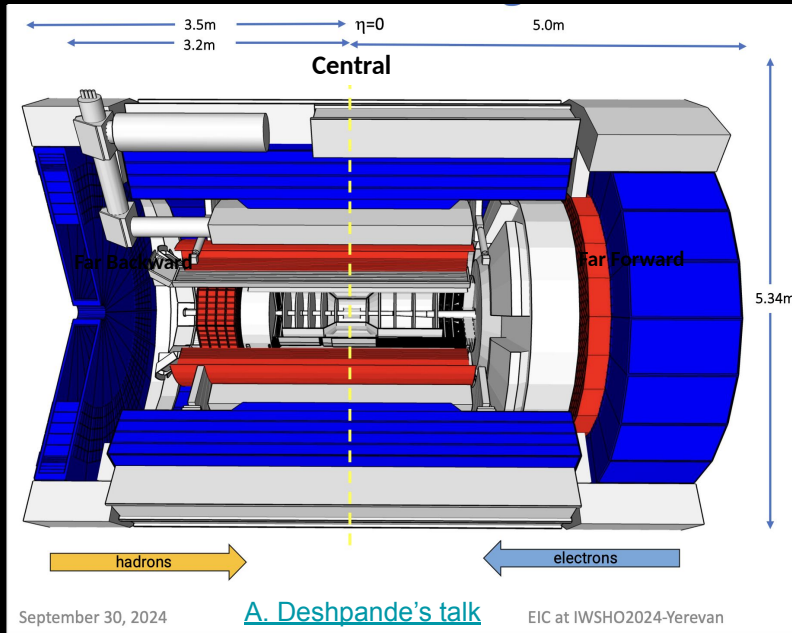
ePIC Detector



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ePIC extends across -35m to +35m.



Tracking

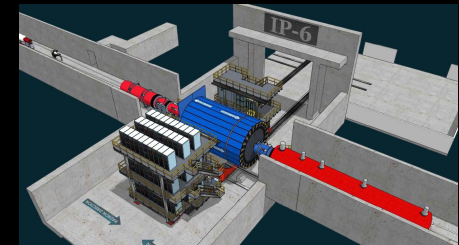
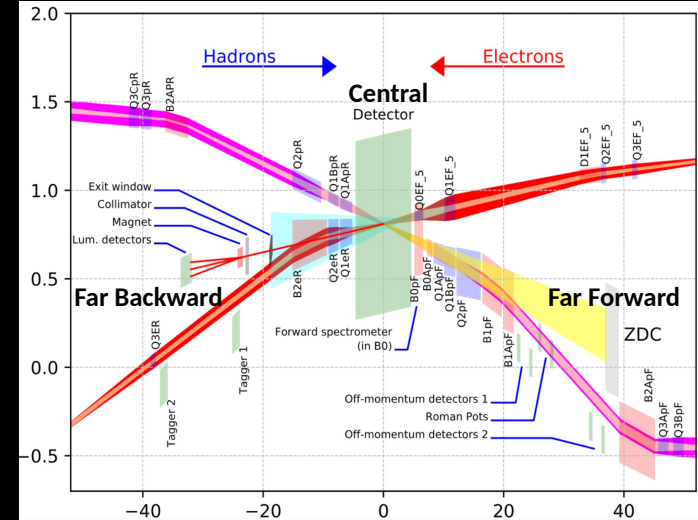
- New 1.7T solenoid
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Traditional Approach to Detector Design

- Sub-detector systems are **optimized individually**, using **single-objective criteria** per sub-detector, within the constraints of the overall detector design. This approach often leads to suboptimal solutions.
- Each combination of sub-detector choices creates a new overall detector design. **Accurate and reliable full simulation pipelines are required to reduce possible bias when exploring new designs**. Fast simulations may become unreliable in regions that have not been previously explored or validated.
- Large simulation campaigns are required, often leveraging containerized software and distributed computing (e.g., NIM-A: 1047 (2023): 167859):
 - Each "design point" (a new detector configuration) potentially needs a new simulation campaign.
 - Exploring multiple design points demands significantly more simulations, increasing computational costs and complexity.

Reconstruction and Simulation Times	Times based on current software on modern cores
Reconstruction event processing time with background [s]	2
Reconstruction algorithmic speedup factor 10yrs out	1.5
Simulation event processing time with background [s]	15
Full simu speedup factor 10yrs out	1.5
Combined time with background, with speedup [s]	11

- Current simulation campaigns produce up to 15-20 TB / month ([T. Britton, Oct 2024](#))
- Towards a quantitative computing model ([M. Diefenthaler, Sep 2024](#))

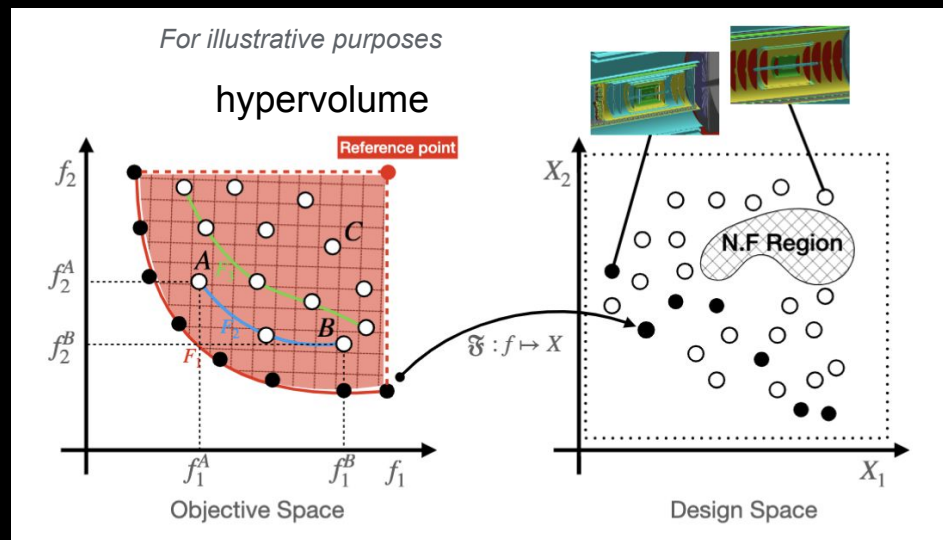
Simulating 5M charged particles for the tracker and PID system would require at least 15k CPU core hours. This requirement can grow significantly when accounting for additional particle types or extending the scope to include neutrals to design other sub-detector systems.



Multi-Objective Optimization

MOO is needed to optimize a system of sub-detectors

- 3 Types of Objectives
 - **Intrinsic detector performance** (resolutions, efficiencies) for each sub-detector — Tracking, calorimetry, PID — noisy
 - **Physics-performance** — Multiple physics channels, equally important in the EIC physics program
 - **Costs** (e.g., material costs, provided a reliable parametrization)
- Objectives can be competing with each other
 - E.g. Better detector response come with higher costs; better resolutions may imply lower efficiencies; etc.



A generic MOO problem can be formulated as

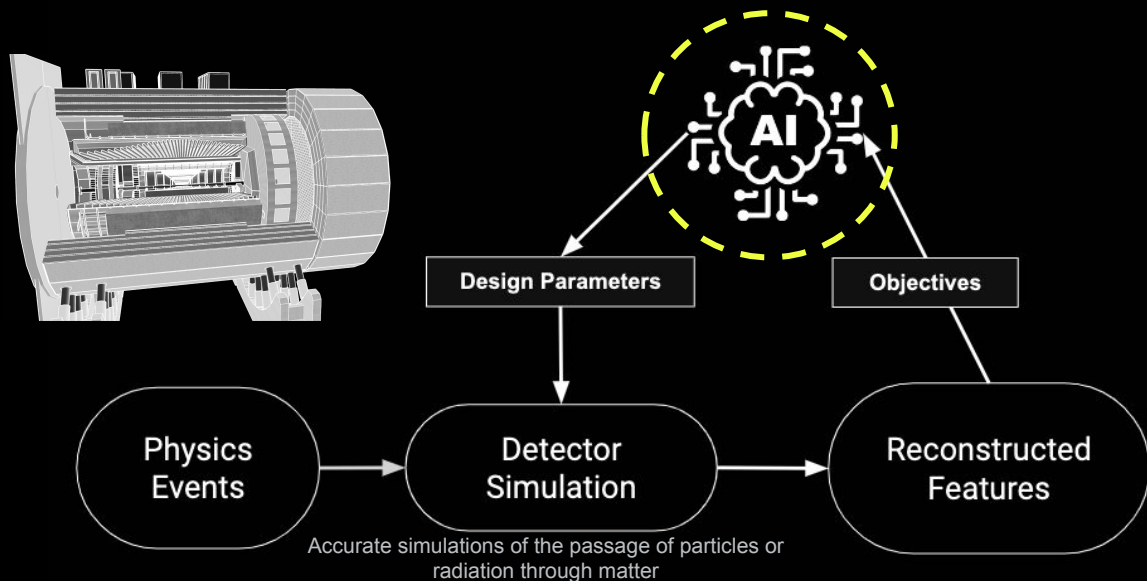
$$\begin{aligned} \min \quad & f_m(\mathbf{x}) & m = 1, \dots, M, & \text{objectives} \\ \text{s.t.} \quad & g_j(\mathbf{x}) \leq 0, & j = 1, \dots, J, & \text{constraints} \\ & h_k(\mathbf{x}) = 0, & k = 1, \dots, K, & \\ & x_i^L \leq x_i \leq x_i^U, & i = 1, \dots, N. & \text{ranges} \end{aligned}$$



AI-Assisted Detector Design at EIC



The AI-assisted design embraces all the main steps of the sim/reco/analysis pipeline...



- Benefits from rapid turnaround time from simulations to analysis of high-level reconstructed observables
- The ePIC SW stack offers multiple features that facilitate AI-assisted design (e.g., modularity of simulation, reconstruction, analysis, easy access to design parameters, automated checks, etc.)
- Leverages heterogeneous computing
- AI-assisted design started being used since proto-collaboration phase (NIM-A 1047 (2023): 167748)

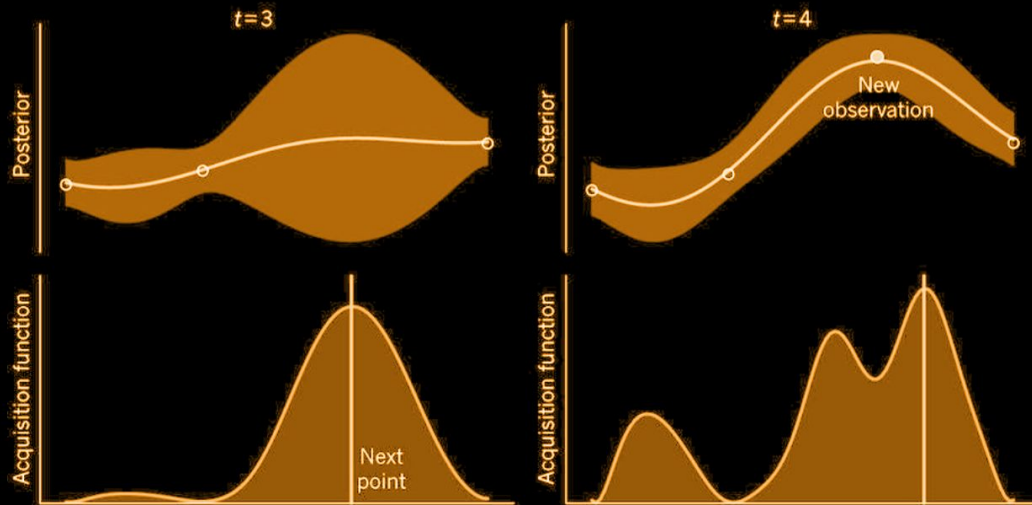
Provide a framework for an holistic optimization of the sub-detector system
A complex problem with (i) **multiple design parameters**, driven by (ii) **multiple objectives** (e.g., detector response, physics-driven, costs) subject to (iii) **constraints**

Those at EIC can be the first large-scale experiments ever realized with the assistance of AI



Bayesian Optimization in a nutshell

- BO is a sequential strategy developed for global optimization.
- After gathering evaluations we build a posterior distribution used to construct an **acquisition function**.
- This cheap function determines what is **next query point**.

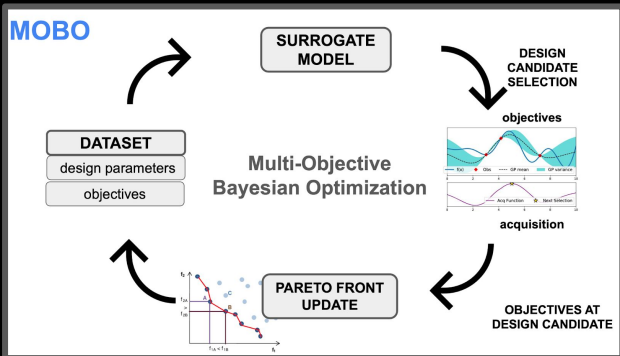


1. Select a Sample by Optimizing the Acquisition Function.
2. Evaluate the Sample With the Objective Function.
3. Update the Data and, in turn, the Surrogate Function.
4. Go To 1.

Contributions

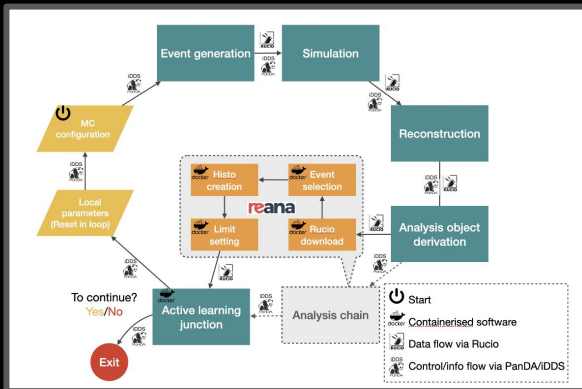
The AID2E Collaboration, “AI-assisted detector design for the EIC”, [2024 JINST 19 C07001](#)

Multi-Objective Optimization



(i) Contributing to advance state of the art MOO complexity (e.g., Multi-Objective Bayesian Optimization) to accommodate a large number of objectives. AID2E supports also other methods (e.g., MOGA) and explores usage of physics-inspired approaches

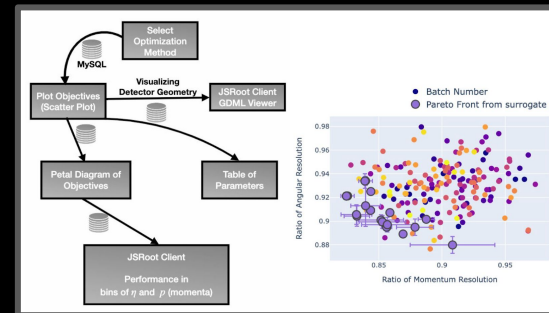
Distribution and Workload Management



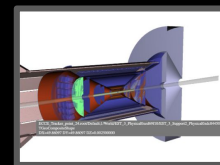
(ii) Will leverage cutting-edge workload management systems capable of operating at massive data and handle complex workflows

<https://github.com/aid2e>

Human-in-the-loop: interactive Pareto navigation



(iii) Development of suite of data science tools for interactive navigation of Pareto front (multi-dim design with multiple objectives). Point are determined with uncertainties.



<https://ai4eicdetopt.pythonanywhere.com/>

<https://wandb.ai/scheduler/AID2E-Closure-1>

Benefits of AID2E

- Integrating holistic, multi-objective optimization into detector design marks a significant paradigm shift, with AI-assisted methods poised to profoundly impact large-scale NP projects such as at the EIC.
 - AI provides quantifiable insights into complex design and objective spaces, enabling a comprehensive evaluation of various tradeoff design solutions.
- A fractional improvement in the objectives translates to a more efficient use of beam time which will make up a majority of the cost of the EIC over its lifetime.
- Examining solutions on the Pareto front of EIC detectors at different values of the budget can have great cost benefits.
- Implementing AI-assisted, multi-objective optimization accelerates the design process, quantifies trade-offs between design points, and produces designs that optimize both performance and cost. This approach will also be valuable during construction, accommodating new constraints as they arise.
- Possibility of extending this framework to other computational intensive tasks such as calibrations and alignment of detectors.



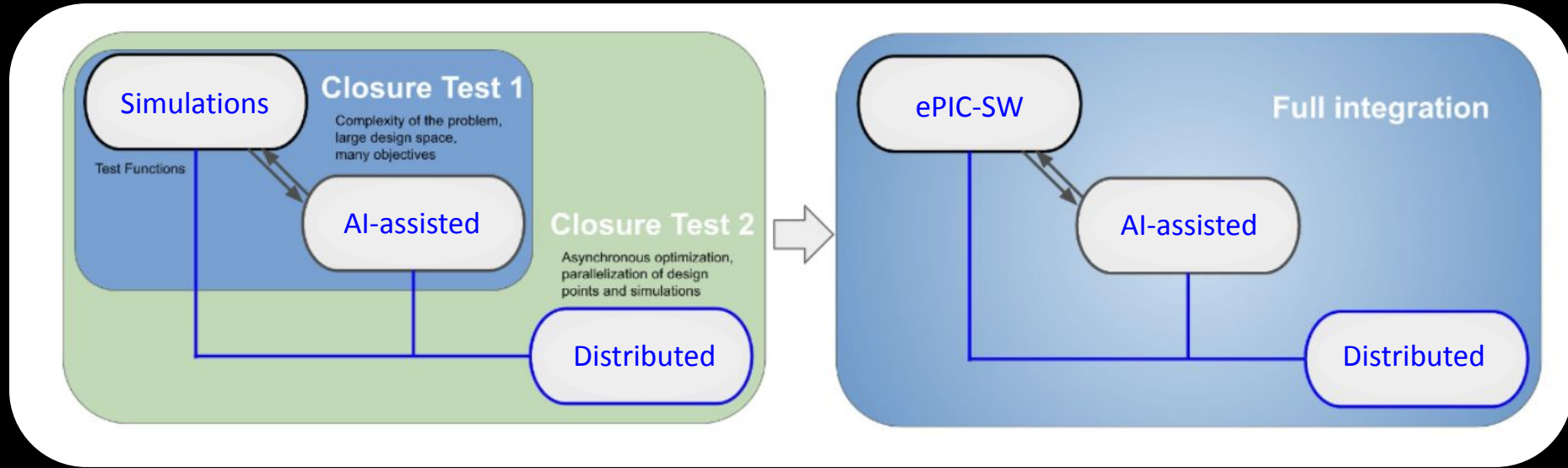
Deliverables and Staffing (estimated at start of project)

Deliverables	Fiscal Quarter After Award							
	FY24				FY25			
	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
Closure test 1 — MOBO framework (ePIC complexity)	■							
Closure test 2 — Distributed MOBO		■						
ePIC design parametrization — cont. integr.	■							
Objectives/constraints — cont. integr.	■							
Performance analysis (detector, physics, costs)					■			
Interface AI-assisted/distributed — V&V, API for grid jobs	■							
AI-assisted design — coupling MOBO to ePIC SW			■					
Deployment of AI-optimization pipelines				■				
Distributed ePIC simulations		■						
Full integration				■				
Deployment of distributed AI-optimization pipelines						■		

- All deliverables for FY24 met.
- In the following I will provide more details on the accomplished work.



AID2E Closure Tests and Workflow



(Rationale)

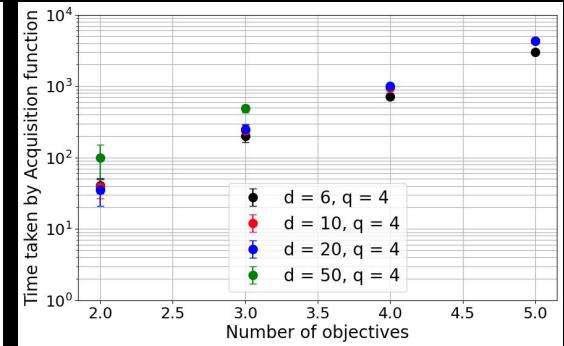
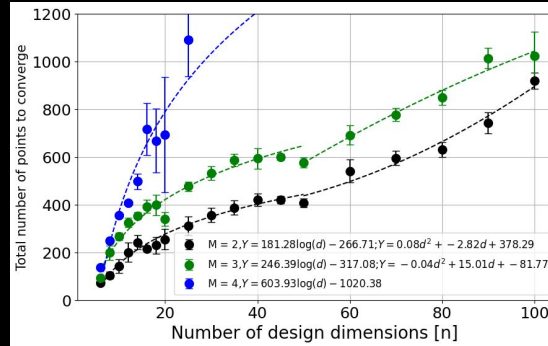




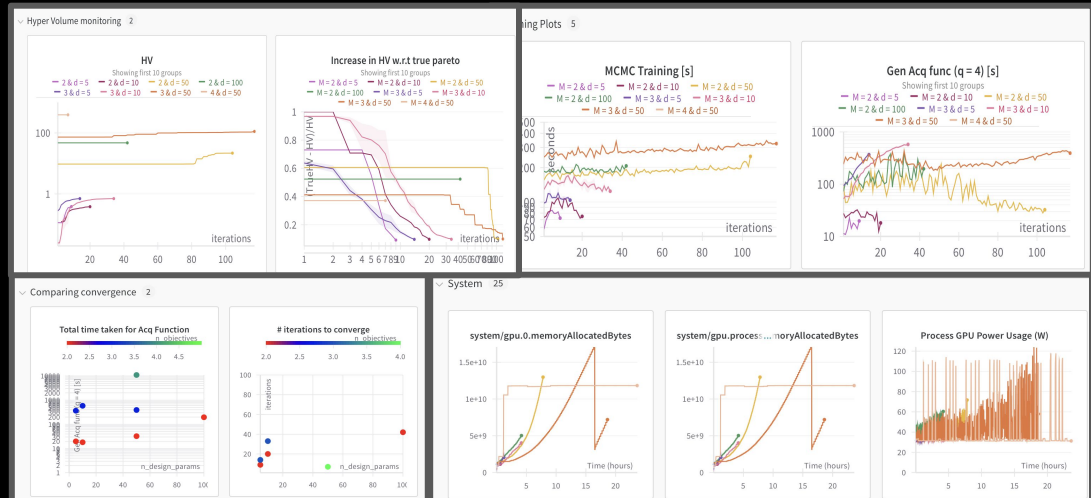
Closure Test 1

Goals:

- Utilize test functions to evaluate proximity to known Pareto front
 - Accuracy of optimization, convergence properties, compute resources
- Characterization of Complexity
 - Stress-testing for problems with increased complexity



W&B dashboard for monitoring



Shown here:

- Test function: DTLZ
- Technique: MOBO





Closure Test 1: MOBO Complexity

n: number of design points
d: design dimensionality (each point)
M: objectives

Gaussian Process
 $O(n^3)$

Bayesian Sampling
from posteriors
NUTS – $O(Md^{5/4})$ NUTS

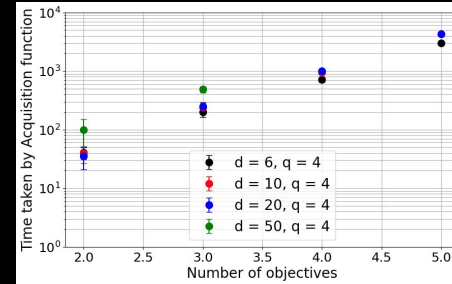
Acquisition function
qNEHVI – $O(Md(n + i)^M)$ q

Complexity Studies

- Surrogate model.
- SAAS¹¹ priors have been proven to be successful up to 388 design dimensions
- Assumes several design variables has increased importance compared to others
- Computational expensive as iteration increases
- Benefit from GPU hardware acceleration

- Sample L points from the posterior distribution
- HMC is a popular algorithm, NUTS is a variant
- Mainly depends on the number of objectives and design space dimensions
- Has minimal dependence on iteration.
- GPU acceleration through JAX backend.

- Captures HV improvement
- A "cheaper" function to evaluate as a proxy for the black box function
- Scales nonlinearly with iteration, total points explored, design space and objective space.
- Partially benefitted by GPU acceleration.



- Benefitting from GPU acceleration
- With sufficient parallelization, if possible, the time associated to the MOBO part at some point becomes dominant (bottom plot shown at 15th iteration with number of points between ~70-160)

q: batch size

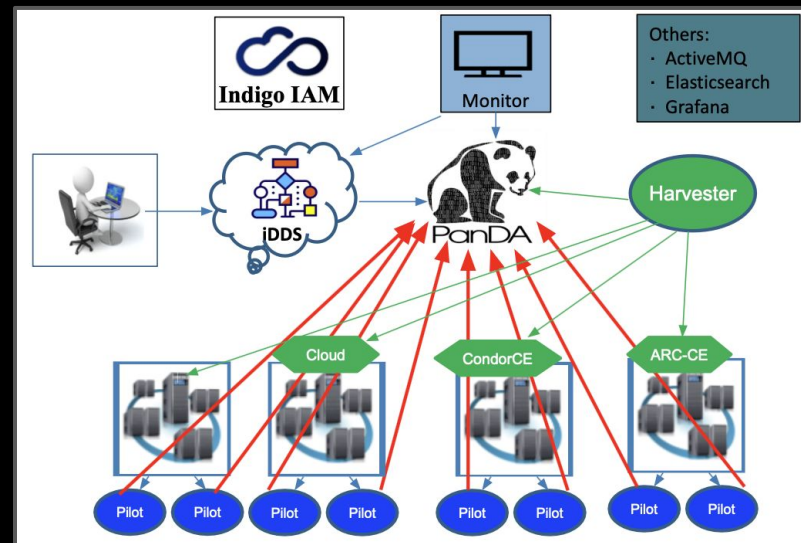




Closure Test 2: PaNDA/iDDS

Goals:

- **Enhance Workflow Management for Design Optimization:** Adapt [PanDA/iDDS](#) AI/ML services to support a Function-as-a-Task workflow management for design optimization with MOO
- **Ensure System Scalability and Robustness:** Stress-testing scalability, robustness across distributed resources
- **Assessing Consistency:** Compare results against the closure test to evaluate consistency.



PanDA (Production and Distributed Analysis system):

- Distributed Workload Management
 - General interface for users, one authentication for all sites
 - Integrate different resource providers(Grid, Cloud, k8s, HPC and so on), hide the diversities from users, large scale

iDDS (intelligent Data Delivery Service):

- Workflow Management Orchestration
 - [CHEP2023 Talk: T. Maeno, et al. Utilizing Distributed Heterogeneous Computing with PanDA in ATLAS](#)
 - [CHEP2023 Talk: W.Christian, et al. Distributed Machine Learning with PanDA and iDDS in ATLAS](#)



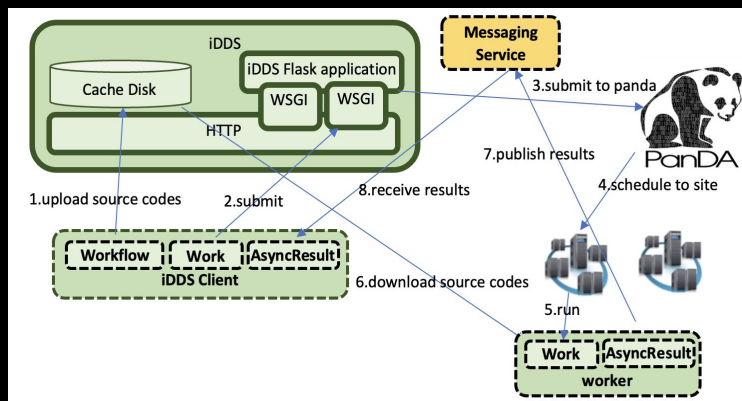
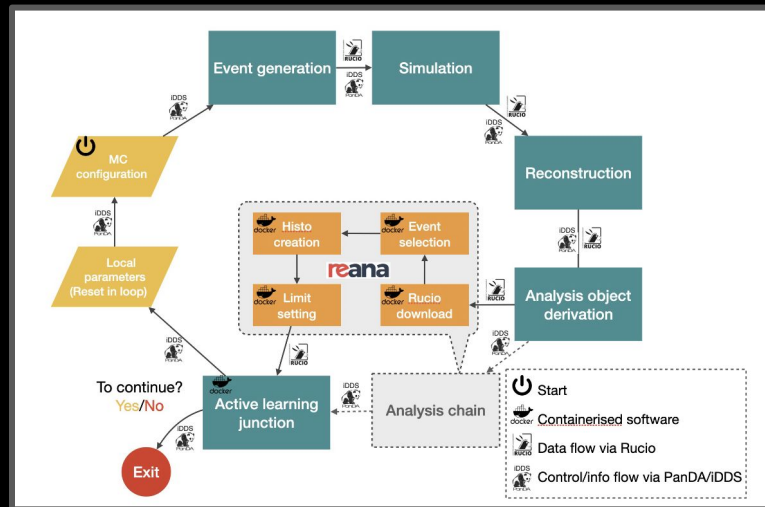


Closure Test 2: PaNDA/iDDS

Bayesian optimisation based active learning with Panda/iDDS

PanDA/iDDS supported complex workflow managements; different use cases in production:

- Fine-grained Data Carousel for **LHC ATLAS**
- DAG management for **Rubin Observatory** to sequence data processing
- Distributed HyperParameter Optimization (HPO)
- Monte Carlo Toy based Confidence Limits
- Active Learning assisted technique to boost the parameter search in New Physics search space



Schema of how a workflow executes a function at remote distributed resources



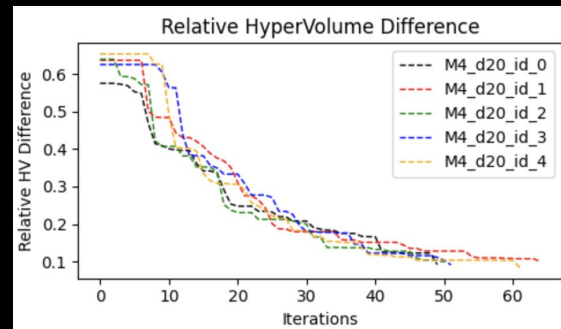
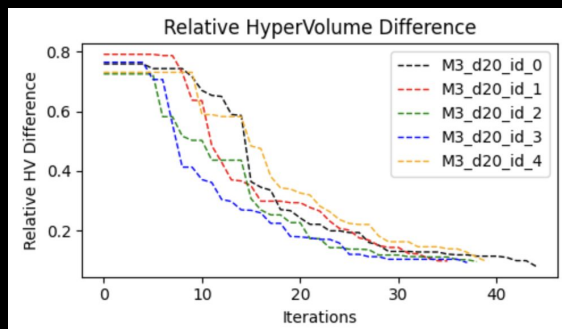
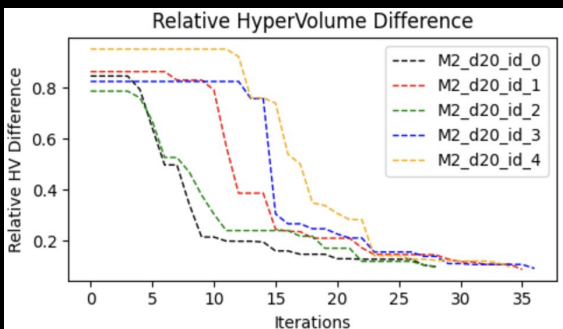
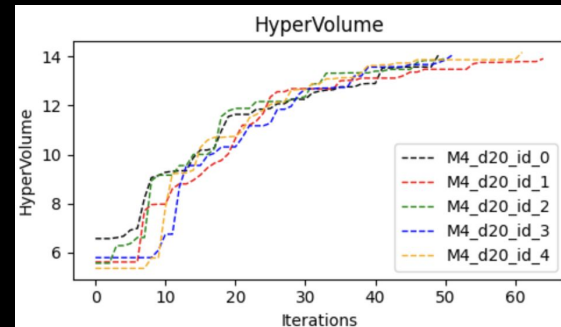
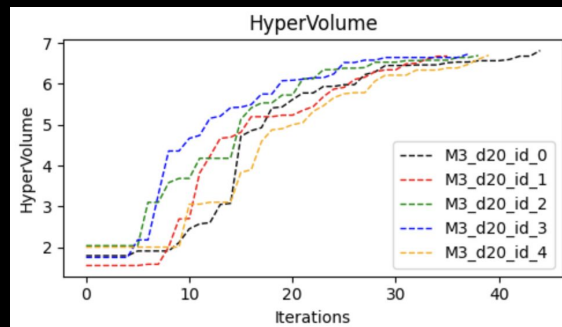
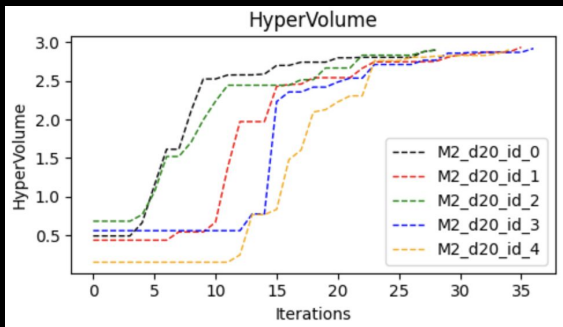
Closure Test 2:
obtaining convergence on Pareto fronts using test functions and distributed computing





Closure Test 2: Results

Examples of optimization pipelines run using PanDA



- Relative **HyperVolume Difference** = $(HVol_{pareto} - HVol) / HVol_{pareto}$
When reaches the tolerance (0.1 here), stops the training
- HVol_pareto: HyperVolume of Pareto Front

Recent tests covered:

- d=50 and M=3

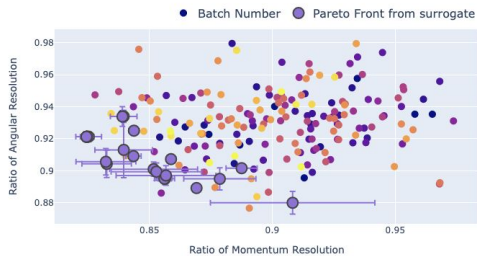




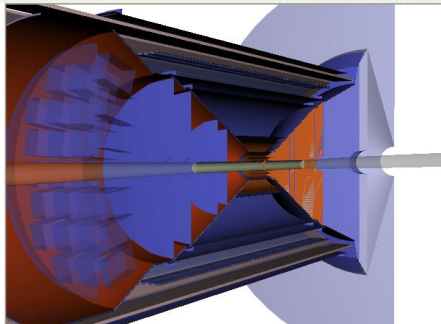
Interactive Pareto Front Navigation

C.Fanelli et al, NIM A, 2023, 167748

Multi Objective Bayesian Optimization

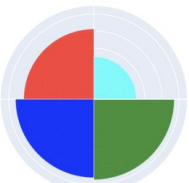


GEANT4 Visualization of the design



Click on petals for finer evaluations

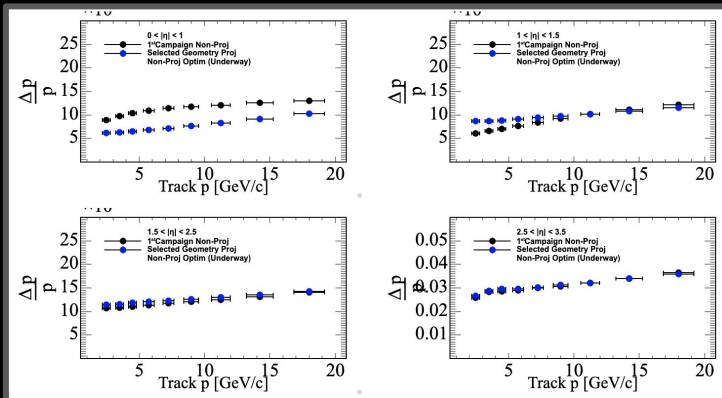
Performance of the Chosen Design Solution



■ Momentum res ■ Theta res
■ Phi res ■ KF InEff

Design Parameters Table

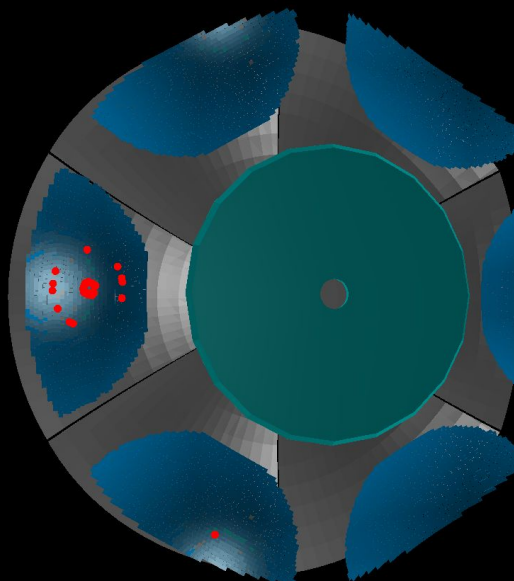
Parameter Name	Parameter Value
Angle of cone [deg]	25.00
Radius of uRweil-1 [cms]	32.47
z E-TTL [cms]	171.00
z F-TTL [cms]	157.60
z EST-1 [cms]	40.39
z EST-3 [cms]	85.09
z FST-1 [cms]	35.03
z FST-3 [cms]	83.78
z FST-5 [cms]	131.27





Integration with ePIC SW: ePIC dRICH

Considering all the constraints as ePIC is in the process of finalizing engineering designs, we can select those sub-detectors that still have tunable parameters



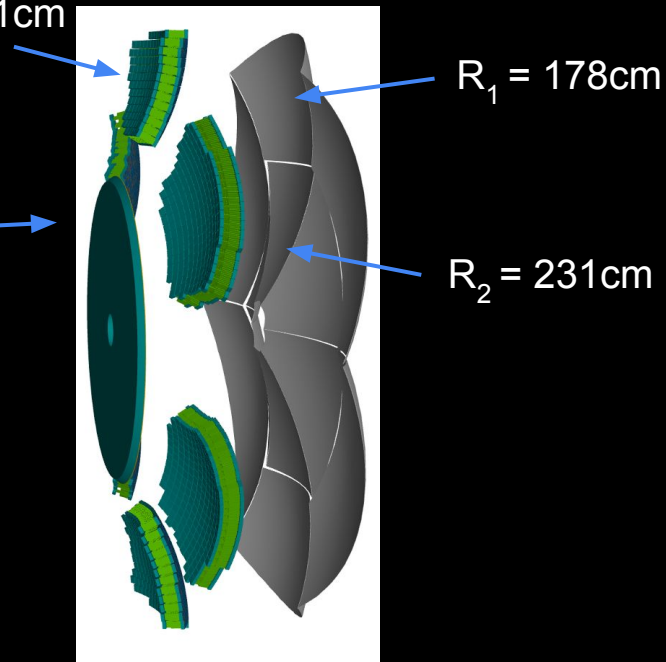
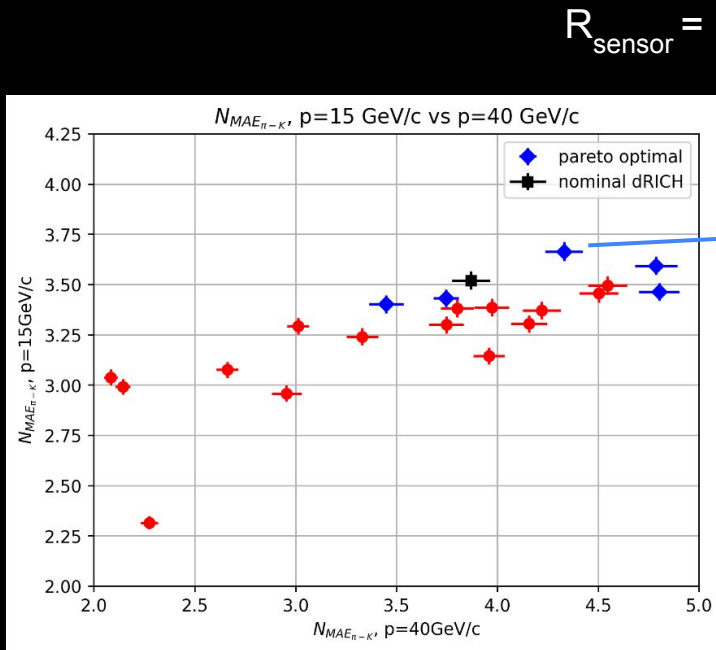
dual-RICH

- *dual-RICH: two radiators for wide momentum coverage ($\sim 3\text{GeV}/c$ - $60\text{GeV}/c$), $1.5 < \eta < 3.5$*
- *Simultaneously focus all η regions, gas and aerogel rings*
- *Mirror, sensor placement and radii, gas, mirror material (lower cost material)...*
- *PID performance, costs, ...*





Integration with ePIC SW: ePIC dRICH



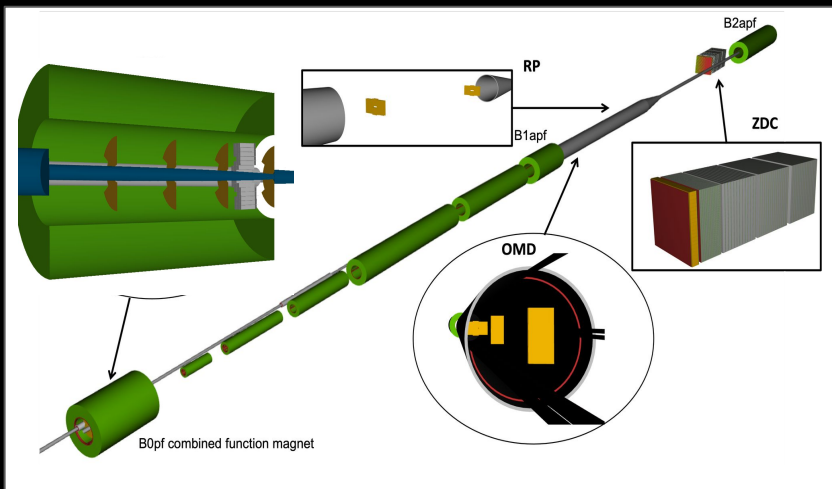
- Three-objective optimization: π -K separation at 15 GeV/c, 40 GeV/c, and fraction of tracks with > 5 photons
- Work ongoing with ePIC to refine two-mirror reconstruction algorithm, finalize optimization





Integration with ePIC SW: Far-Forward

Far-Forward detectors

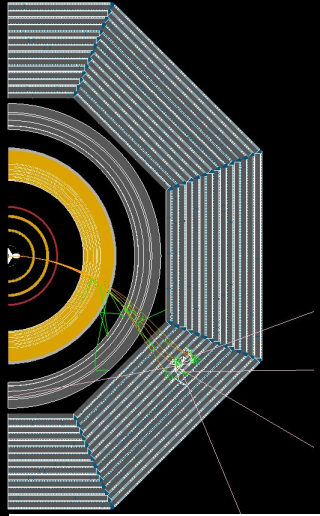


- *B0 subsystem*
 - *Tracker (AC-LGAD)*
 - *Crystal Calorimeter*
 - *Proton tagging critical for Forward Physics*
- *Magnetic Field is inhomogeneous & Mechanical constraints restrict detector real estate (entire length of B0 fixed)*
- *Tracking layers, ECAL crystals & tiling of crystals*
- *Objectives: Tracking resolution and detector acceptance.*

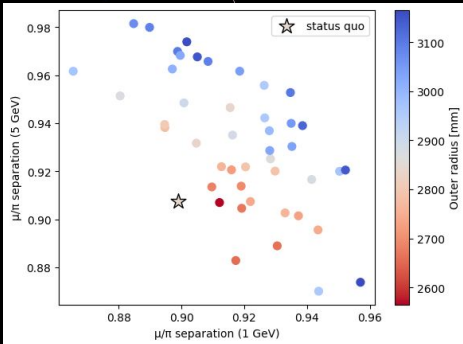
Ongoing discussion with the ePIC working group to consolidate optimization



Spin-off: Detector2 μ Id/HCAL



- Physics Motivation: Muon channels (J/Psi DDVCS), cost effective HCAL
- Iron/Scintillator sandwich integrated in flux return
 - Longitudinal segmentation for better h/μ ID, energy reconstruction with ML
 - R&D on fast scintillator (readout) ($\mathcal{O}(50ps)$) for ToF ongoing
 - Possible solution for endcap HCAL of ePIC
- **Pilot project:**
 - Optimize μ ID performance @1 & 5 GeV
 - Parameters: number of layers, thickness of passive iron layers
- **Activities to pursue in the future:**
 - Optimize μ ID and ToF/ σ_E concurrently \rightarrow competing requirements Active/passive detector ratio
 - Explore complex configurations (e.g. nonlinear layer thickness), parameters
 - Holistic optimization of magnet/detector geometry \rightarrow explore physics impact and complementarity to project detector



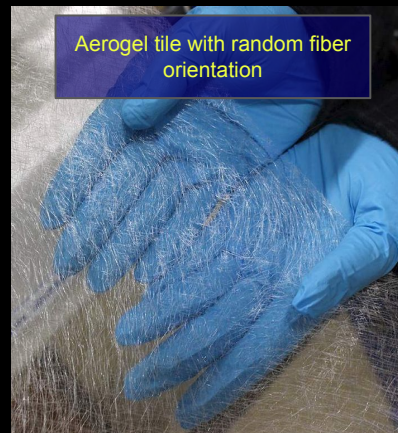
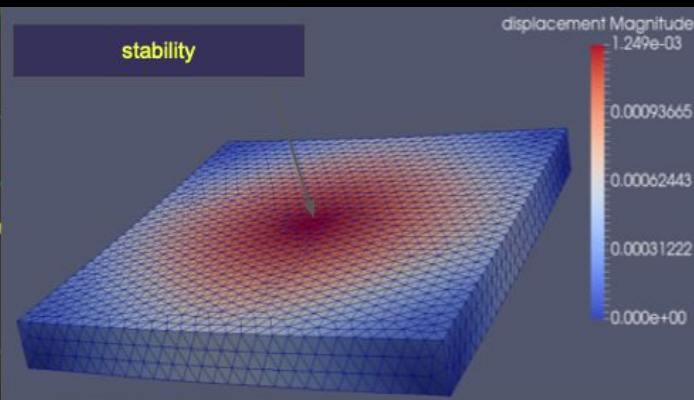
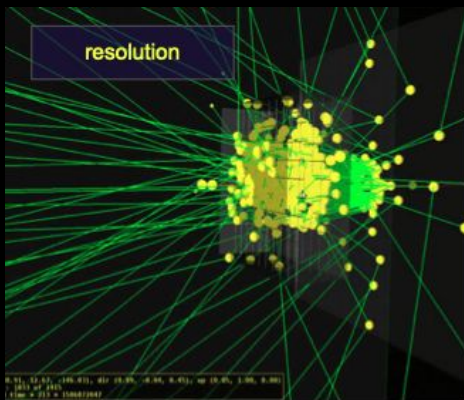
Spin-off: Material Design

Reinforced novel aerogel material with fibers

Software Stack

Simple Ring Imaging CHerenkov Geant4 based simulation
Aerogel + Optical Fibers

Gmsh - define geometry and produce mesh
ElmerGrid - convert the gmsh mesh to elmer compatible mesh
ElmerSolver - do modeling (solve linear and nonlinear equation)
Paraview - visualize Elmer Solver and provide a python interface to automate



Publication in preparation



Documentation and Outreach

- GitBook and/or other knowledge sharing platforms will be part of the initiatives related to documentation and outreach
- Offering opportunities for experiential learning with easy access for beginners
 - 1 week summer bootcamp
 - Final Projects
- The first AID2E bootcamp took place in July 2024
 - <https://aid2e.github.io/boot-camp-2024/intro.html>



A screenshot of a web browser displaying the AID2E bootcamp 2024 website. The page is titled "Schedule" and lists various topics and exercises. The navigation menu on the left includes sections for "Introduction to git", "Introduction to High Performance Computing (HPC)", "Using VS-Code", "Day 2 - Introduction to Optimization", "Day 3 - Multi Objective Evolutionary Algorithm", and "Day 4 - Bayesian Optimization". The main content area shows a detailed list of topics and exercises, including "Introduction to git", "Introduction to High Performance Computing (HPC)", "Using VS-Code", "Day 2 - Introduction to Optimization", "Day 3 - Multi Objective Evolutionary Algorithm", and "Day 4 - Bayesian Optimization".



Conclusions

The EIC could feature the first large-scale experiments designed and optimized with the aid of Artificial Intelligence.

- We completed coupling of different MOO techniques to the ePIC SW, closure tests and other FY24 deliverables that demonstrated effective distribution and expected scalability.
- We are on track to deliver a framework that can optimize holistically a large-scale detector:
 - Shown ongoing activities with detector subsystems (dRICH, far-forward) in ePIC.
 - The ePIC design is in progress with CD-2 not before end of 2025.
 - Optimization studies of Detector II subsystems and magnet could provide valuable insights on complementarity with ePIC.
- In detector projects, most changes happen during the construction phases (e.g., changes in the available material or budget). AID2E will be an ideal tool to optimize design changes with objectives (e.g., reduce cost).
- This framework inherently offers broader impacts, as it can be adapted for use in various experiments and is suitable for a wide range of compute-intensive applications that necessitate MOO (e.g., calibrations, alignments, novel material design, etc)








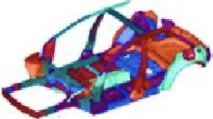




Spares



Multi-Objective Optimization: Example

Vehicle Design Optimization:

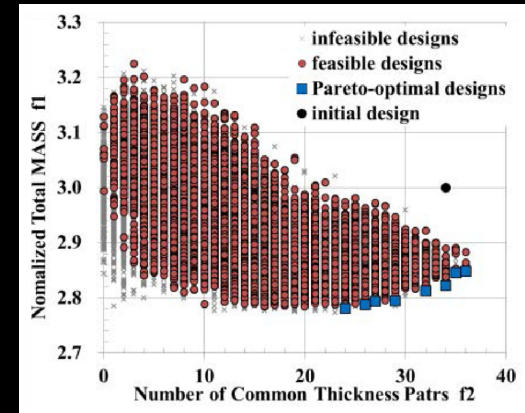
222 parameters + 2 objectives + 54 constraints

Car Type	SUV	Constraint Conditions	Frontal 40% Offset Impact	Full Frontal Impact	Longitudinal Bending Mode	Torsion Mode
						
Design Variables			Side Impact	Rear 70% Offset Impact	Lateral Bending	Torsion Stiffness
						

T. Kohira et al. Proposal of benchmark problem based on real-world car structure design optimization. GECCO 2018

Objectives:

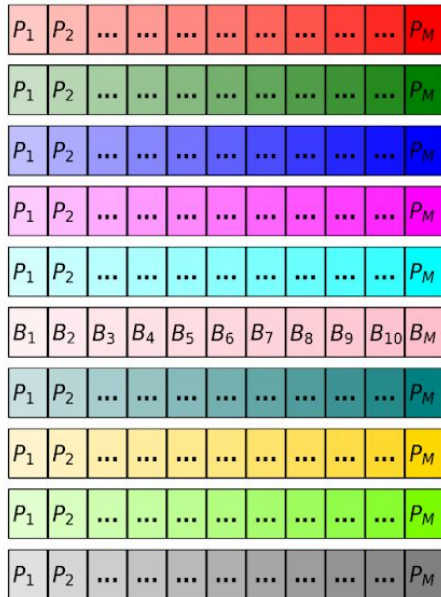
- minimize total vehicle mass of three vehicles (Mazda 3, 6, CX-5)
- maximize number of parts shared across vehicles



MOGA Pipeline

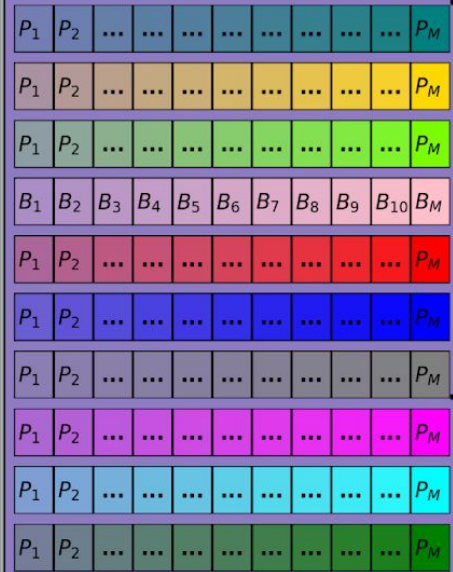
Initial population creation (N_pop)

Inject baseline Genes
Faster convergence



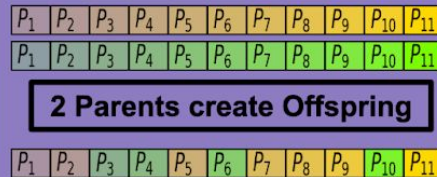
The Evolution Cycle

Rank & sort - NSGA2 (Objs)

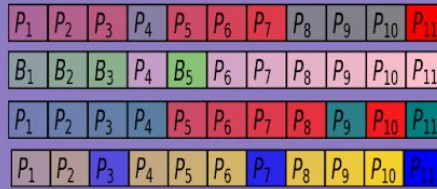


Healthy Design points

Genetic Evolution of designs



N_Offsprings for next call

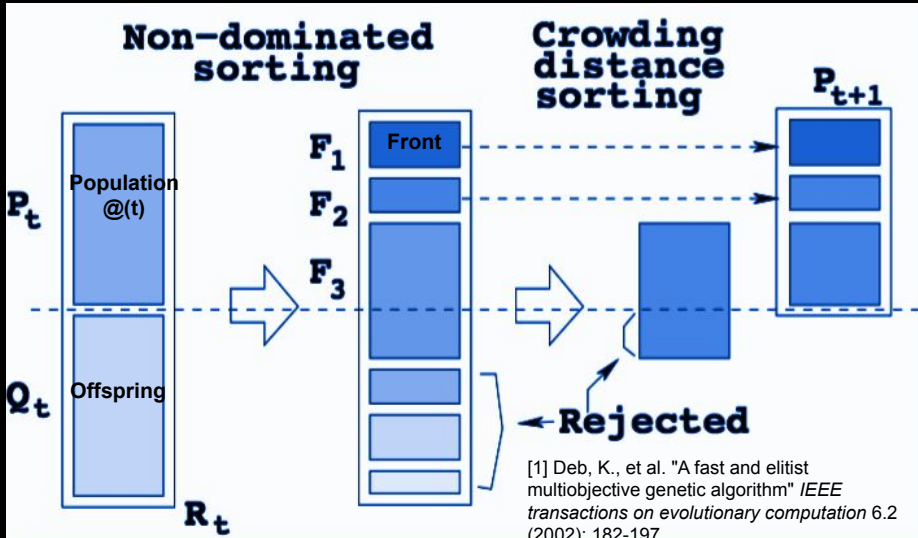


ePIC dd4hep Sim + eic-recon

Yields Performance of the design.
Objectives that decide evolution



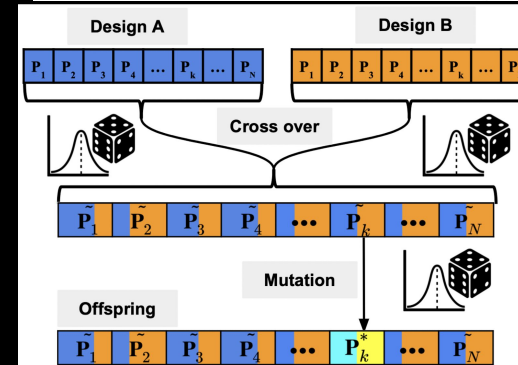
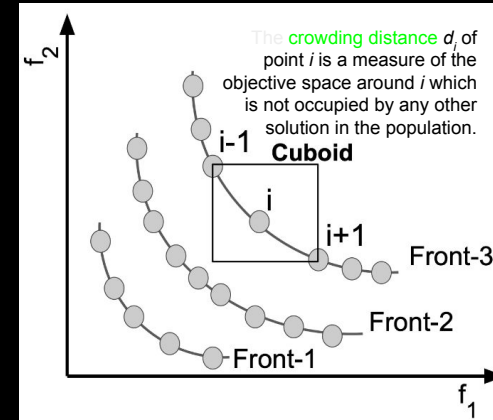
Non-Dominated Sorting Genetic Algorithm



This is one of the most popular approach (>35k citations on google scholar), characterized by:

- Use of an elitist principle
- Explicit diversity preserving mechanism
- Emphasis in non-dominated solutions

The population R_t is classified in non-dominated fronts. Not all fronts can be accommodated in the N slots of available in the new population P_{t+1} . We use **crowding distance** to keep those points in the last front that contribute to the highest diversity.



This is to illustrate Binary Crossover

