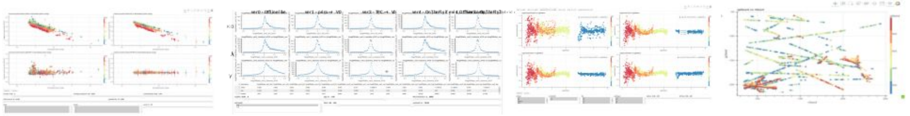
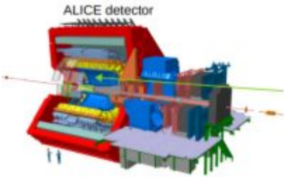
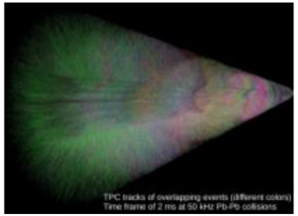
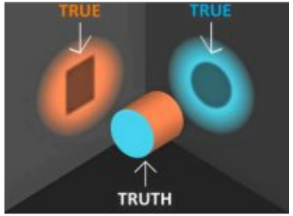
# RootInteractive expert tool for multidimensional statistical analysis, machine learning and analytical model validation.

Marian Ivanov (GSI Darmstadt), Marian Ivanov (UK Bratislava)
On behalf of ALICE collaboration



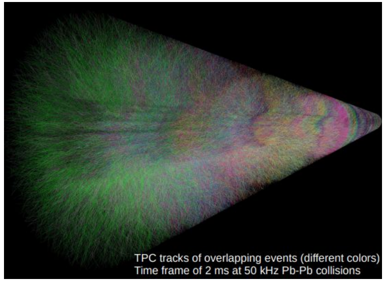



https://github.com/miranov25/RootInteractive

# Alice Run 3 - goals and challenges

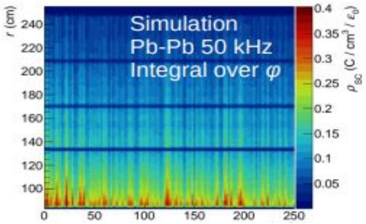



**Record large pp and Pb-Pb minimum bias sample**

- Continuous readout at 50 kHz Pb-Pb collisions and 500kHz-1Mhz pp collisions
- Unknown collision time
- Events overlapping in TPC ⟶ substantial higher occupancy (~5 PbPb collisions, 100 pp collisions)

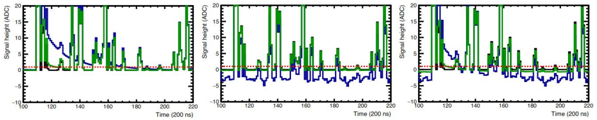
**Tracking challenge: space charge in TPC detector distorting trajectories**

- Non-uniform space-charge distorting E field
- Large space point distortions O(5 cm) and Distortion fluctuations O(5 %) ~ 0.2 cm
- To be calibrated to σ ~100 µm with space granularity O($10^6$) in space O(1-5 ms) in time



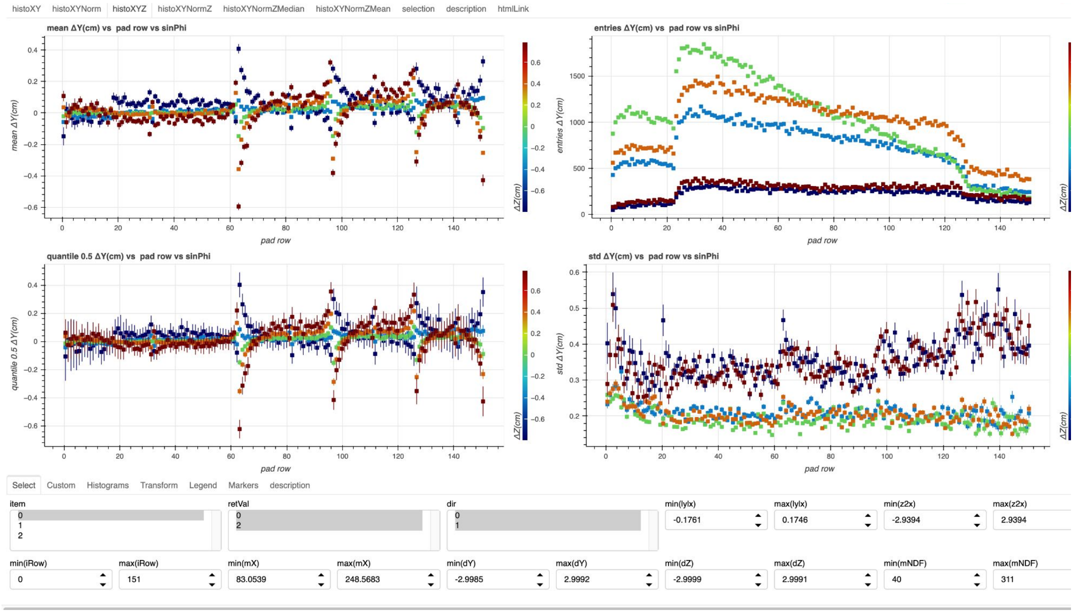

**PID challenge: Significant baseline bias and fluctuation**

- Online digital signal processing to recover baseline (in FPGA)
- To be corrected below internal noise level



*A high interaction rate environment, pile-up, distortions fluctuation, etc. ... necessitates the use of advanced methods of data analysis. Experts and highly customisable tools are needed*

# RootInteractive project




*Seeing is believing*

*Querying/Iterative*

*Interacting/predicting is understanding*

Reconstruction/distortion monitoring example
$10^7$ points x 50 attributes (space points,track, MC predictions)

- https://github.com/miranov25/RootInteractive#readme

Multi-Dimensional interactive analysis - ML, fits, histograming, data aggregation on server (Jupyter notebook, python scripts) and on clients O($10^6$-$10^7$ rows, $10^8$ entries rows x columns) (browser)

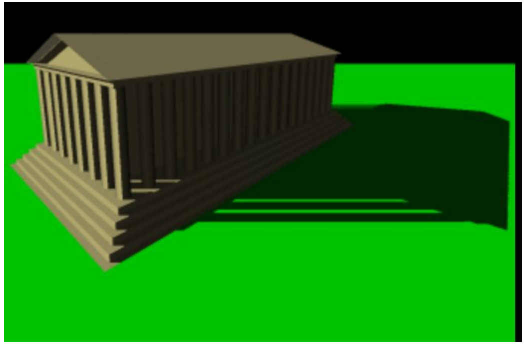
# RootInteractive - current ALICE expert projects

- Run3 alignment & space point distortion calibration
- Run3 digital signal processing
- Run2, Run3 track reconstruction optimization, validation
- MC/data mapping & TPC data volume studies
- Run2, (Run3) expert differential QA/QC , performance parameterization, performance web pages

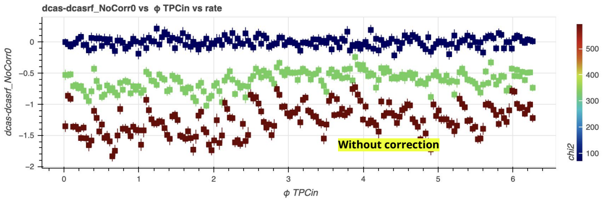
- Run3 (4D) reconstruction development - trackCombinator - V0, Cascade, Kink, cosmic finder
- Fast simulation - fastMCkalman for detector and reconstruction optimization (Run3,Alice3)
- Expert data representative sampling/skimming
- PID calibration/validation and dEdx optimization
- High dEdx,spallation tracking (collaboration with DUNE experiment)
- Magnetic monopole reconstruction

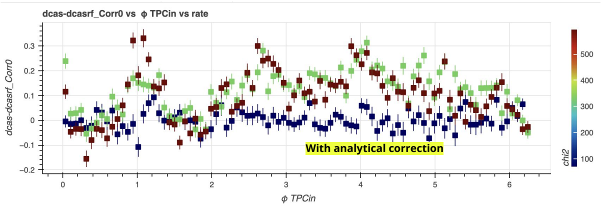
- Particle production - MC generators parameter scan
- Particle production as function of event properties

# Multi-dimensional analysis vs shadow projections



**Track DCA bias due space charge distortion contribution before and after correction**
**Reference-ML prediction at low rate without SC**



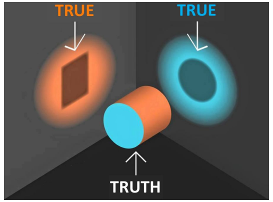




$$\sigma_{\vec{A}\ominus\vec{A}_{ref}} \leq \sigma_{\vec{A}}(+)\sigma_{\vec{A}_{ref}}$$

**Object and reference objects (models/reference models, MC/Data,Data/ref. data), should be compared optimally in the full relevant multi-dimensional space.**

- Shadow projection → Assumptions, imagination and rhetorical art in describing data needed
- Comparison statements to be based on invariants or on normalized data - e.g. the difference between the object and the reference object
  - After projection impossible
- In many typical cases variance $\sigma_{A-Aref}$ is very often smaller by orders of magnitude
  - For example, the rms value of the difference between ionic currents and scaled average values can be used as an alarm criterion. We cannot use the ion current itself
- Differential approach - possibility to decompose and understand the data e.g. distortion due space charge, and alignment in figure above

# RootInteractive general purpose tool for multi-dimensional statistical analysis




**By oversimplifying in analysis level, the explanations tends to be more complex resp. wrong**

Our goal to provide a tool to deal with multidimensional problem simplify data analysis in many dimensions :

- Fit and visualise N-dimensional functions including their uncertainties and biases
- **Easy to validate assumptions, numerically evaluate approximations, differentially compare models**
- Enable simple **functional composition** for (non-parametric, analytical/parametric) functions and error propagation
- Very fast feedback from day one - seconds instead of weeks, to allow interactive expert communication
- **Multidimensional parametric optimization**
- Easily configurable visualization of unbinned and binned data, interactive multidimensional histogramming/projection and derived **aggregate information extraction** on the server (Python/C++) and **client (Javascript)**
- **Client side application (standalone HTML document) without necessity to install additional software**

*A detailed differential understanding of the detector system, MC and reconstruction/calibration performance is a prerequisite for the successful application of Machine learning in physical analysis*

# Consideration: symmetries, alarms and invariants

**Aggregation/projections of normalized data e.g. (data-model), (MC-Data), (data-symmetry) in multiple dimensions :**

- RMS spread is much smaller
- Alarms/Outlier tagging with statistical significance - e.g. (data-model) > N σ , or likelihood
- **Invariance/symmetries**
    - in-variance in time (using e.g. reference/average run), in-variance in space (e.g. rotation, mirror symmetry)
    - B field symmetry
    - data - non parametric/parametric analytical model
    - smoothness resp. local smoothness

*In RootInteractive supported mostly comparing data with reference "symmetric regression" and "template support" automatic comparison to reference data*

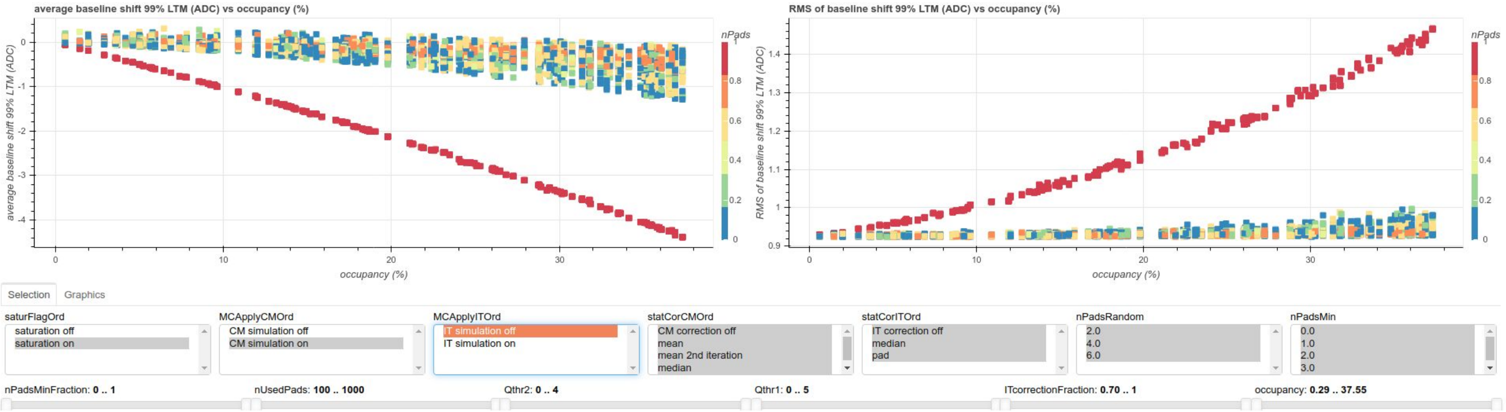
# Multidimensional parameter optimization example - ALICE digital signal processing

Digital signal processing (13 parameters in example) needed for particle identification and data volume optimization. **O(200000) parameter settings simulated/generated on server**

- parameters: effects (On/Off), algorithm (different version), parameters of individual algorithms

Simulation and visualization/aggregation (NDPipeline+RootInteractive ) done by bachelor student, fully solving optimization problems of DSP (several attempts before failed)

- Dashboard to answer “all questions”, FEEDBACK time for follow up questions O(seconds)
- Standalone dashboards, others could reproduce result based on the instruction in presentation, movie instruction
- **Interactive expert use-case discussion within ONE meeting. DSP understand and solved. Project DONE.**




**Presentation, notebook, interactive dashboard and movie in RootInteractive tutorial:**

- https://indico.cern.ch/event/1135398/contributions/4764024/subcontributions/370740/attachments/2402507/4114272/CMITSimulGEMTPC_RootInteractiveTutorial10032022.pdf
- https://gitlab.cern.ch/alice-tpc-offline/alice-tpc-notes/-/blob/master/JIRA/ATO-559/parameterScan.ipynb
- https://indico.cern.ch/event/1073883/contributions/4588170/attachments/2334149/3986420/simulScan_02112021.html
- https://indico.cern.ch/event/1135398/contributions/4764024/subcontributions/370740/attachments/2402507/4109039/CMITSimulationsGEMTPC.mp4

# Machine learning in RootInteractive - differential validation of MC/data and ML models

## Using external models:

- E.g comparing the U-Net for the distortion correction with simple data driven Machine learning using Random Forest
- Parameter optimization in respect to different cost functions

## RootInternactive extensions wrappers to scikit-learn and xgboost

- Fast approximation of functions  and local PDFs

## Interactive validation in RootInteractive on client O($10^6$-$10^7$) points

- Unbinned predict
- Aggregated information for further postaggragation
    - Local mean, median, STD - unbinned predict
    - Local kernel regression parameters -aggregated information on the mesh
        - Usually statistical properties of predict- value, resp. Mash of 1D histograms
- Generalized kernel linear regression on client (ND groupby+rolling+kernel)
- Predict on client (wasm+ONNX) in queue

# Generalized linear (kernel) regression in RootInteractive - client side

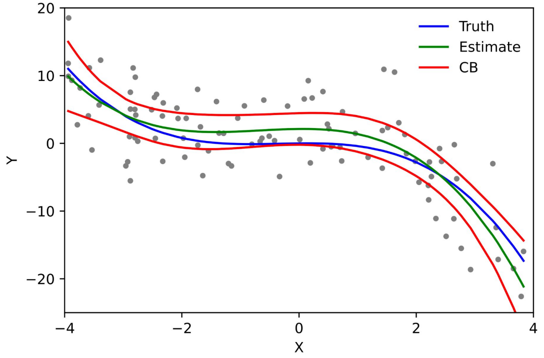
**Example, declaring generalized linear kernel regression**

```
regressionArray=[
    {"name":"regre1", "varX":["x1","x2"...,"xn"], "varY":"y1", "weights":"w"}
    {"name":"regreAgg1", "varX":["x1","x2"...,"xn"], "varY":"y1", "weights":"w"
    "varAgg":["xagg1","xagg2"...,"xaggn"],"nbinsAgg":[...],"rollingAgg":[...]}
]
```

- **Scikit-learn like user interface**
  - https://scikit-learn.org/stable/modules/generated/sklearn.linear_model.LinearRegression.html
  - Using fit and predict
  - Regression predict new data source can be used as an alias function
- Pol0 group-by regression, mean, median,quantiles, RMS
- **Pandas groupby + ND-rolling/sliding kernel + Linear regression**
  - Interface as in the C++ code in original ND pipeline
  - Using fit and predict on the grid
  - Prediction of values and derived variables (using local fit parameters, e.g local derivatives)
  - Predict is new data source
  - **Work in progress**

- https://en.wikipedia.org/wiki/Linear_regression
- https://en.wikipedia.org/wiki/Kernel_regression

**Linear regression** is a linear approach for modelling the relationship between a scalar response and one or more explanatory variables




Example of a cubic polynomial regression, which is a type of linear regression. Although *polynomial regression* fits a nonlinear model to the data, as a statistical estimation problem it is linear, in the sense that the regression function E(*y* | *x*) is linear in the unknown parameters that are estimated from the data. For this reason, polynomial regression is considered to be a special case of multiple linear regression.

# Data preparation - RDataFrame <-> awkward (new interface)

**Defining RDataFrame**

```
ROOT::RDataFrame df(nTracks);
auto rdf = df.Define("qVector", "getQVector(160)")
             .Define("logqVector", "ROOT::VecOps::log(qVector)")
             .Define("qStd", "StdDev(qVector)")
             .Define("qMean", "Mean(qVector)")
             .Define("qlStd", "StdDev(logqVector)")
             .Define("qlMean", "Mean(logqVector)")
             .Define("qMedian", "TMath::Median(qVector.size(), qVector.data())")
             .Define("qlMedian", "TMath::Median(qVector.size(), logqVector.data())")
             .Define("qTrunc", "truncate(qVector);")
             .Define("logqTrunc", "ROOT::VecOps::log(qTrunc);");
```

**Loading awkward array**

```
In [7]:
%%time
array = ak.from_rdataframe(
        rdf,
        columns=(
            "logqTrunc",
            "logqVector",
            "qMean",
            "qMedian",
            "qStd",
            "qTrunc",
#            "qVector",
            "qlMean",
            "qlMedian",
            "qlStd",
        ),
    )

CPU times: user 1min 44s, sys: 884 ms, total: 1min 45s
Wall time: 10.2 s
```

## dEdx optimization example

- Defining the data and derived function (C++) with native data representation
- loading the data → awkward array
- Execution scaling with number of cores (32 used in example)
- ML training/prediction → RDataFrame ()

*Significant performance increase with parallel "RDataFrame ↔ awkward" in respect to previously used direct Tree queries interface. Used extensively, e.g. in fastMCKalman (distortion simulation/correction) and in trackCombinator (V0,cascade,cosmic,loop finder) prototyping use case studies*

# RootInteractive/Multi-Interactive project preparation and presentation

## Expert data preparation

- Agreement on data  to collect and aggregate
- Data sources
- Variables to import  - asking questions
- Symmetries,  invariances and possible alarms
- Pre-aggregation
- Data sampling
- Machine learning models
- Underlying Analytical models if exist
- Re-iteration

## Data presentation:

- **Agenda: presentation, notebook, dashboard+ (optional)movie)**
- Goal
- **Data preparation explained**
- **Variables description**
- Observation highlights with snapshot from dashboard
- Domain experts, participants in the  meeting should be able to participate in decisions, resp. be able to interact with dashboard  data based on description in presentation

*The data is presented in a multidimensional way. The aim is to answer all questions within one meeting/session.  If the information is not sufficient, new data sources to be agreed on.*

# RootInteractive pad map dashboard declarations

**User defined RootInteractive properties are required to get the html output (explained in next slides)**

- **Alias array for derived variable/function definition - e.g defining status bitmask**
  - aliasArray=[("IDC0_OK","(0x2*(abs(IDC0_MeanRF0_LRatio)<sigmaRFCut0))|(0x4*(abs(IDC0_MeanRFL_LRatio)<sigmaRFCutL))"),..]
- **Variable array**
- **Parameter array - to control parameterized functions, selection and variable selection for ND histograms**
- **Widget descriptionArray**
- **Widget layout dictionary**
- **Histogram array**
- **Figure array**
- **Figure layout dictionary**

*aliasArray, variables, parameterArray, widgetParams, widgetLayoutDesc, histoArray, figureArray, figureLayoutDesc = getDefaultVarsDiff()*

*Simplification of using interface using set of predefined parameterizable templates to define standard layouts, extending only user defined widget control.*
*Templates focussed mostly on comparison of data and reference data, resp comparison of their distributions for user defined selection*

# Functions on client - derived variables and functional composition

Predefined parametric  javascript function

```
# here we can define derived variables -  to define some invariances eg abs(XX_Mean/XXXMedain)<
aliasArray=[
#     ("","dNprimdx*padLength"),     # ionization over pad
    ("Unit","1+roc*0"),
    ("phi","arctan2(gy,gx)"),
    ("QMax_Clusters_OK","(0x1*(NClusters_Clusters_Mean>minEntries))|(0x2*(abs(QMax_Clusters_MeanRF0_LRatio)<sigmaRFCut0))|(0x4*(abs(QMax_Clusters_MeanRFL_LRatio)<sigmaRFCutL))"),
    ("QMax_Digits_OK","(0x1*(NClusters_Digits_Mean>minEntries))|(0x2*(abs(QMax_Digits_MeanRF0_LRatio)<sigmaRFCut0))|(0x4*(abs(QMax_Digits_MeanRFL_LRatio)<sigmaRFCutL))"),
    ("SAC0_OK","(0x2*(abs(SAC0_MeanRF0_LRatio)<sigmaRFCut0))|(0x4*(abs(SAC0_MeanRFL_LRatio)<sigmaRFCutL))"),
    ("IDC0_OK","(0x2*(abs(IDC0_MeanRF0_LRatio)<sigmaRFCut0))|(0x4*(abs(IDC0_MeanRFL_LRatio)<sigmaRFCutL))"),
    #("IDC0_OK","1+(abs(IDC0_RMS/IDC0_Mean)<0.5)"),
    ("IDC0_MeanOK","0x1*(IDC0_RMS<5) |0x2*(IDC0_MeanLxCut)")
]
```

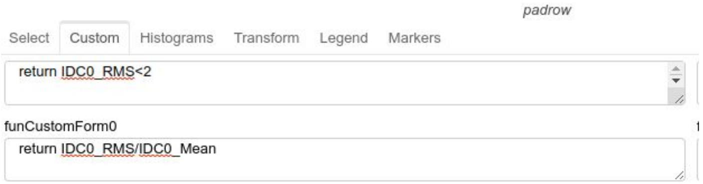
Anonymous function  (used for example  in ND histograms as weights or variable)


```
{
    "name": "histoXYNormZData",
    "variables": ["varX","varY/varYNorm","varZ"],
    "nbins":["nbinsX","nbinsY","nbinsZ"], "axis":[1,2],"quantiles": [0.35,0.5],"unbinned_projections":True,
},
{
    "name": "histoXYZNormData",
    "variables": ["varX","varY","varZ/varZNorm"],
    "nbins":["nbinsX","nbinsY","nbinsZ"], "axis":[1,2],"quantiles": [0.35,0.5],"unbinned_projections":True,
},
```

Figure axis transformation


Custom javascript function (javascript function  as a text)

```
# defining custom java script function to query  (used later in varaible list)
aliasArray+=[{
        "name": "funCustom0",
        "variables": [i for i in variables if  "ustom" not in i ],
        "func":"funCustomForm0",
    },
    {
        "name": "funCustom1",
        "variables": [i for i in variables if   "ustom" not in i],
        "func":"funCustomForm1",
    },
    {
        "name": "funCustom2",
        "variables": [i for i in variables if   "ustom" not in i],
        "func":"funcCustomForm2",
    },
]
```



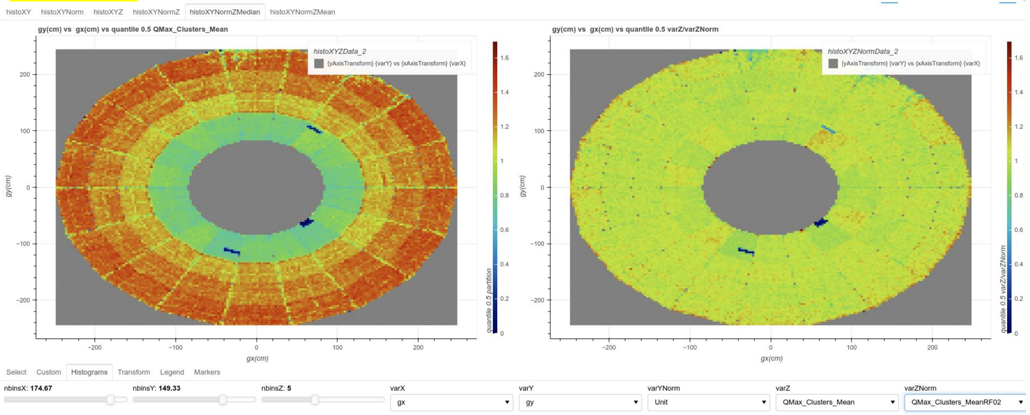

*Many different ways to define derived variables and functional composition.*
*Dependency trees to resolve functional and data source dependencies.*

# Histogram declaration - calibration QA browser

Set of the 2D, 3D (ND) histograms declared ()

```
histoArray=[
    {
        "name": "histoXYData",
        "variables": ["varX","varY"],
        "nbins":["nbinsX","nbinsY"], "axis":[1],"quantiles": [0.35,0.5],"unbinned_projections":True,
    },
    {
        "name": "histoXYNormData",
        "variables": ["varX","varY/varYNorm"],
        "nbins":["nbinsX","nbinsY"], "axis":[1],"quantiles": [0.35,0.5],"unbinned_projections":True,
    },
    {
        "name": "histoXYZData",
        "variables": ["varX","varY","varZ"],
        "nbins":["nbinsX","nbinsY","nbinsZ"], "axis":[1,2],"quantiles": [0.35,0.5],"unbinned_projections":True,
    },
    {
        "name": "histoXYNormZData",
        "variables": ["varX","varY/varYNorm","varZ"],
        "nbins":["nbinsX","nbinsY","nbinsZ"], "axis":[1,2],"quantiles": [0.35,0.5],"unbinned_projections":True,
    },
    {
        "name": "histoXYZNormData",
        "variables": ["varX","varY","varZ/varZNorm"],
        "nbins":["nbinsX","nbinsY","nbinsZ"], "axis":[1,2],"quantiles": [0.35,0.5],"unbinned_projections":True,
    },
]
```

QA example mean charge: left - raw values(varZ) , right-normalized to "expectation" (varZNorm)




Anonymous function (used for example in ND histograms as weights or variables)


Parameterized histograms:

- Variables and weights could be any variable from data source (column, derived functions, anonymous function)
  - In the QA/calibration browser variables defined by user selecting (varX,varY, varZ)
  - Binning controlled by parameters (nbinsX, …)
- Derived aggregated data exported as new data source
  - Declaring quantiles and projections
  - Projection could be binned (fast) and unbinned

**Customizable Ndimensional histograms and projection. Example**:

- X,y median profile of cluster charge map (left) and normalized to phi symmetric RF prediction

# Webasm interface - under development

New functions/transformations/data sources using wasm:

- Fast Fourier transform
- Convolution, deconvolution
  - Numpy like interface (binned data)
  - Functional interface (unbinned kernel function)
- ONNX interface
- Based on benchmark transformation of the older javascript numerical code to wasm

https://webassembly.org/

# RootInteractive - conclusion

RootInteractive is used extensively and successfully in many ALICE use cases for multidimensional analysis

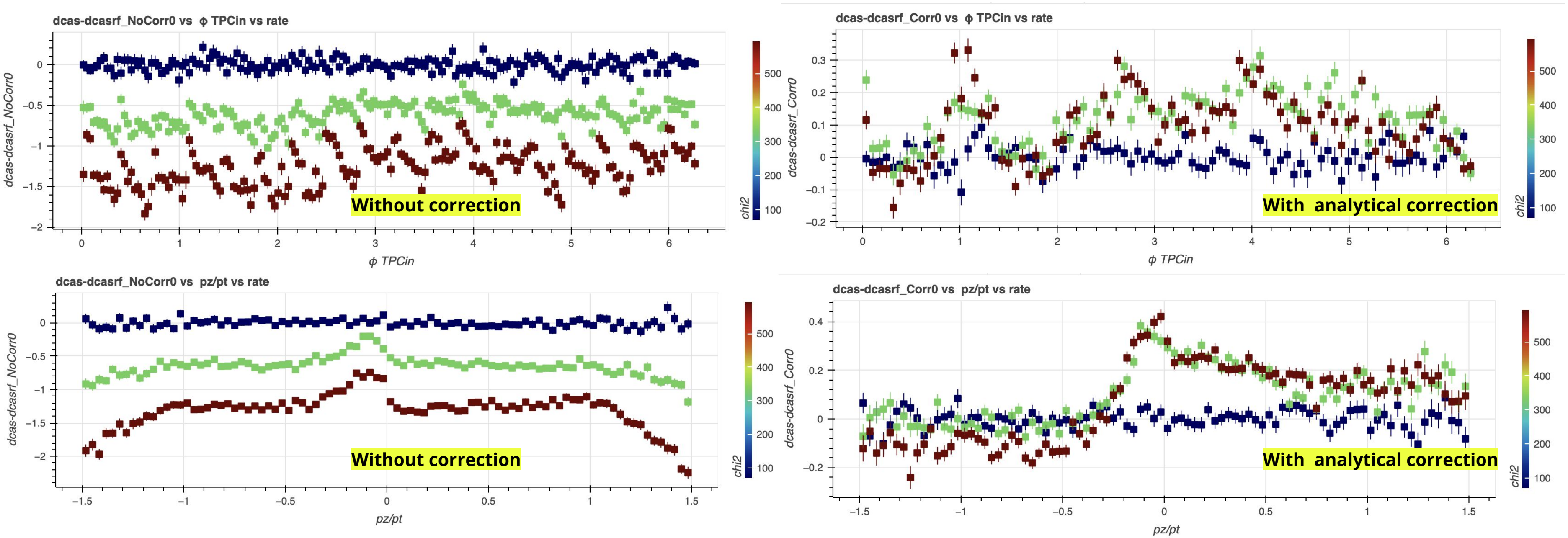
- Most important expert tools for the many use cases - .e.g. distortion calibration, reconstruction and dEdx optimisation, preparation of a new reconstruction algorithm (trackCombiantor)

Current use cases, now mainly related to detector(calibration, simulation, QA) and global reconstruction (RUN3, RUN2 as reference, Alice 3)

Pilot N-dimensional physical analysis with sampled/skimmed data is in the queue

# Backup

# DCA-DCA0 bias - rate evolution (4,330 kHz, 660 kHz)




**DCA bias in phi direction** strongly eliminated - residuals O(2 mm) **comparable with intrinsic resolution** of the tracks in vertex O(0.2 cm). New analytical fits - fitting also density profile

**DCA bias in theta direction** strongly eliminated. Remaining bias due charge up on C side - to add up in the analytical fit version (IFC and OFC fit). Charging up rate and time dependent (see Run1,Run2 studies)

# RootInteractive usage in ALICE

in following slides code snippet with user code declaration shown for illustration
without further discussion

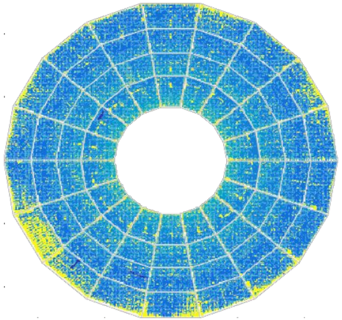
# Machine learning - derived variables - RF regression - per channel QA example

```
statDictionary={"mean":None,"median":None, "std":None}

varListG=["lx","ly","GainMap","A_Side"]
varListLocal=["lx","ly","GainMap","roc"]
vars=[
   "NClusters_Clusters_Mean",'NClusters_Digits_Mean',
   'QMax_Clusters_Mean', 'QMax_Digits_Mean',
   'IDC0_Mean','SAC0_Mean'
]
statOut=miErrPDF.predictStat(dfK0[variableX],statDictionary)
```

**Per channel QA and example derived QA variables for NClusters_Clusters:**

- **NClusters_Clusters_Mean**
- NClusters_Clusters_MeanRF0,
- NClusters_Clusters_MeanRF0,
- NClusters_Clusters_MeanRFL,
- NClusters_Clusters_MeanRFL_Med
- NClusters_Clusters_MeanRFL_Std



## Defining models:

- varying parameter of models, input variables  and local statistics

**Global (varListG)** and **local regression (varListLocal)** extracting for basic calibration and QA properties of ALICE TPC calibration and QA variables

- global **φ symmetric** model, local model **without φ symmetry**
- **Automatic alarms - data "out of range "|data-prediction|<nσ"  without "reason" (other calibration, masking known problems)**

Robust local statistics - median and local std estimator for the outlier tagging and PDF description