Reaction Aware Dataframes Derek Glazier University of Glasgow

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Preamble

EXPERIMENTAL::

The point, for me, was to see if

RDataFrame could be used in complex analyses For example, in analysing multi-final state event generators

This could be made simple and "user friendly"

This could be extended to ePIC data

The point today is to encourage others to try out RDataFrame for ePIC analysis

Summary

- What are dataframes
- Why use a dataframe instead of a for loop in a large Root script ? Or a more Object Orientated approach
- How can I use a dataframe
	- Simple things
	- More complicated things : functions and functors
- What does "reaction aware" mean ?
- RAD with Pythia
- 3 RAD with benchmarking

What is ROOT RDataFrame

Some aspects particular to HEP

Input datasets are much larger than memory, entries are statistically independent.

Histograms, new ROOT files as common aggregations.

Collections are ubiquitous. The goal

 \Box

Ease of use, good performance and scaling from 1 to 1000+ cores out of the box. Extensibility.

Ergonomic support for common HEP use cases (systematics, working with collections, ...).

https://indico.fnal.gov/event/23628/contributions/241029/

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What is RDataFrame

Construct → Transform → Results

Use strings!

```
ROOT: : RDataFrame df("mytree", <math>{\lceil "f1.root", "f2.root" \rceil});
```

```
auto h = df.Finter("x > 0"). HistolD("x");
```
 $h\rightarrow$ Draw(); // the event loop is run here, upon first access to one of the results

Use modern C++!

// C++11 lambda expressions and C++ functions are also supported as filter expressions

```
auto filtered df = df.Filter([](float x) { return x > 0; }, {"x"});
```

```
auto hx = filtered df.HistolD("x");
```

```
auto hy = filtered df.HistolD("y");
```
 $hx \rightarrow Draw()$; // event loop is run here, both hx and hy are filled

RDataFrame Actions

ROOT::RDat event selection aset); www.www.www.on this (ROOT, CSV, ...) dataset auto $df2 = df.Filler("x > 0")$ derived quantities, object selections vents for which $x > 0$ df2.Snapshot("newtree", "out.root"); ………… write the skimmed data and r2 to a new ROOT file data aggregations Users can inject **arbitrary code** at all steps, which makes this

relatively simple API extremely versatile.

Plus lots of other stuff….

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For my analysis I want to take reconstructed data and create a TTree of high level physics info for my reaction

EIC Tutorial with Python (I)

```
# Open input file and define branches we want to look at with uproot
events tree = up.open(intile) ["events"]
# Get particle information# Get particle information
partGenStat = events tree["MCParticles.generatorStatus"].array()
partMomX = events tree["MCP articles.momentum.x"].array()
partMomY = events tree["MCParticles.momentum.y"].array()
partMomZ = events tree["MCParticles.momentum.z"].array()
partPdg = events tree["MCParticles.PDG"].array()
```
Get reconstructed track information

```
trackMomX = events tree["ReconstructedChargedParticles.momentum.x"].array()
trackMomY = events tree["ReconstructedChargedParticles.momentum.y"].array()
trackMomZ = events tree["ReconstructedChargedParticles.momentum.z"].array()
# Get assocations between MCParticles and ReconstructedChargedParticles
recoAssoc = events tree["ReconstructedChargedParticleAssociations.recID"].array()
simuAssoc = events tree["ReconstructedChargedParticleAssociations.simID"].array()
```
Define histograms below

partEta = ROOT.TH1D("partEta","Eta of Thrown Charged Particles;Eta", 100, -5, 5)

matchedPartEta = ROOT.TH1D("matchedPartEta","Eta of Thrown Charged Particles That Have Matching Track", 100, -5,5); matchedPartTrackDeltaR = ROOT.TH1D("matchedPartTrackDeltaR","Delta R Between Matching Thrown and Reconstructed Charg e Particle", 5000, 0, 5);

EIC Tutorial with Python (II)

```
# Add main analysis loop(s) below
for i in range (0, len(events tree)): # Loop over all events
    for \mathbf i in range (0, len (partGenStat[i])): # Loop over all thrown particles
        if partGenStat[i][j] == 1: # Select stable particles
            p dq = abs(partPdq[i][i]) # Get PDG for each stable particle
            if (pdq == 11 or pdq == 13 or pdq == 211 or pdq == 321 or pdq == 2212):
                trueMom = ROOT.TVector3(partMomX[i][j], partMomY[i][j], partMomZ[i][j])
                trueEt = trueMom.PseudoRapidity()truePhi = trueMom, Phi()partEta. Fill (trueEta)
                for k in range (0, len (simuAssoc[i])): # Loop over associations to find matching ReconstructedChargedP
articleif (simuAssoc[i][k] == i):
                        recMom = ROOT.TVector3(trackMomX[i][recoAssoc[i][k]], trackMomY[i][recoAssoc[i][k]], trackMo
mZ[i][recoAssoc[i][k]]delta = trueEt = recMom.PseudoRapidity()deltaPhi = TVector2. Phi mpi pi(truePhi - recMom.Phi())
                        delta = math.sqrt((delta * delta) + (delta * delta)matchedPartEta. Fill (trueEta)
                        matchedPartTrackDeltaR.Fill(deltaR)
```
EIC Tutorial with RDataFrame

ROOT:: RDataFrame df ("events", infile);

// Define histograms

= df1.HistolD({"partEta", "Eta of Thrown Charged Particles; Eta", 100, -5., 5.}, "filtMCEt auto partEta anticontrolleri a controlleri a controlleri a controlleri a controlleri a controlleri a controller

$a^{\prime\prime}$);

auto matchedPartEta = df1.HistolD({"matchedPartEta", "Eta of Thrown Charged Particles That Have Matching Tr ack", 100, -5., 5. }, "accoMCEta") ;

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ROOT::RVec<>

Basically wrapper for std::vector<> ROOT gives some additional utiltities

- implicit looping (like numpy arrays)

RAD gives some more

<https://github.com/dglazier/rad/blob/master/include/RVecHelpers.h>

ePIC data in RDataFrame will be contained in RVecs These will be the arguments given to functions

```
//calculate magnitude for all entries in vecs
 RVec<double> ThreeVectorMag(const RVec<double> &x,
                           const RVec<double> &y, const RVec<double> &z){
    return sqrt(x * x + y * y + z * z);
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Note best to pass in const references (&)
Keeps data safe and prevents unecessary copy
```
Don't use TLorentzVector

https://root.cern.ch/doc/master/classTLorentzVector.html

Attention

TLorentzVector is a legacy class. It is slower and worse for serialization than the recommended superior alternative ROOT::Math::LorentzVector. ROOT provides specialisations of the ROOT::Math::LorentzVector template which offer superior runtime performance, i.e.:

- ROOT::Math::PtEtaPhiMVector based on pt (rho),eta,phi and M (t) coordinates in double precision
- ROOT::Math::PtEtaPhiEVector based on pt (rho),eta,phi and E (t) coordinates in double precision
- ROOT::Math::PxPyPzMVector based on px,py,pz and M (mass) coordinates in double precision
- ROOT::Math::PxPyPzEVector based on px,py,pz and E (energy) coordinates in double precision
- ROOT::Math::XYZTVector based on x,y,z,t coordinates (cartesian) in double precision (same as PxPyPzEVector)
- ROOT::Math::XYZTVectorF based on x,y,z,t coordinates (cartesian) in float precision (same as PxPyPzEVector but float)

More details can be found in the documentation of the Physics Vectors package.

Main user difference using external functions not class methods $auto cmBoost = cm.BoostToCM();$ PxPyPzMVector CMTar=boost(tar, cmBoost);

Note on usage

```
//standard rdataframe usage :
                                                                     Returns Rnode (df1)
    auto df1 = df.Define("Mass0", "MassCalc(px[0], py[0], pz[0], e[0]))with define
                 . Define("Mass1","MassCalc(px[1],py[1],pz[1],e[1])");
                                                                     applied
    //equivalent to :
    auto df0 = df.Define("Mass0", "MassCalc(px[0], py[0], pz[0], e[0]))");
    auto df1 = df0.Define("Mass1", "MassCalc(px[1], py[1], pz[1], e[1])");1/and in rad :
    rad.Define("Mass0", "MassCalc(px[0],py[0],pz[0],e[0])");rad.Define("Mass1", "MassCalc(px[1], py[1], pz[1], e[1])");\frac{1}{2} //or if rdf interface defined :
    rad: \text{rdf::Mass(rad,"Mass0", "<math>\{0\}')</math>);* I prefer thisrad: rdf::Mass(rad,"Mass1", "{1}");Rad keeps the last defined RNode as a datamember
Can be accessed with rad.CurrFrame()
    auto df0 = epic.CurrFrame();12 auto hW = df0.Histo1D({"W","W",100,0,20.},"tru_W");
```
PODIO Data Format

Plain-Old-Data I/O, aka PODIO avoid deep-object hierarchies

To both improve runtime performance and simplify the implementation

Support for inter-object relations

For Example HepMC3 root file shows :

particles.pid : Int_t pid[particles_] particles.status : Int_t status[particles_] particles.mass : Double_t mass[particles_] particles.momentum.m_v1 : Double_t m_v1[particles_] particles.momentum.m_v2 : Double_t m_v1[particles_]

...

ePIC Data Format

O(4000) branches !

ReconstructedParticles.energy : Float_t energy[ReconstructedParticles_] ReconstructedParticles.momentum.x : Float_t x[ReconstructedParticles_] ReconstructedParticles.charge : Float_t charge[ReconstructedParticles_] ReconstructedParticles.mass : Float_t mass[ReconstructedParticles_]

ReconstructedParticleAssociations.recID : UInt_t recID[ReconstructedParticleAs_] ReconstructedParticleAssociations.simID : UInt_t simID[ReconstructedParticleAs_]

```
MCParticles.momentum.x : Float_t x[MCParticles_]
MCParticles.charge : Float_t charge[MCParticles_]
MCParticles.mass : Double_t mass[MCParticles_]
```
And many more ...

Injecting algorithms

Functions and functors

If your calculation depends on event data use a function These can be defined in some header or in a C++ lambda Event data is passed in as arguments

If your calculation also depends on some parameters use a functor

A functor is an instance of a class with a function and parameters kept as data members

ePIC truth matching

Optional analysis strategy :

Use ReconstructedParticles and MCParticles branches Map these to "rec" and "tru" types of variables Filter tru indices for gen stat $== 1$ (removes a lot!) Loop over tru, look for rec and link to tru index Filter/reorder all other columns to sync with new tru

Can now operate on real matched reaction when reconstructed particles exist Calculations automatically performed for both rec and tru Resolutions can be determined for all variables

Installation

Header only Compilation at run-time via standard ROOT scripting(cling)

Download from github (CURRENTLY NOT STABLE)

git clone <https://github.com/dglazier/rad>

Add the include directory to you ROOT INCLUDE PATH

setenv ROOT INCLUDE PATH /to/where/is/rad/include

Structure : Some classes to configure RAD dataframes Some functions/functors to calculate stuff

Reaction Aware

To analyse a reaction in general we need to :

- Identify final state particles (Filter)
- Associate them with Top and Bottom vertices (Define)
- Calculate Photon Kinematics
- Calculate Production Kinematics
- Calculate Top/Bottom Intermediate states
- Calculate Top/Bottom Decay Kinematics

How is it Reaction Aware

The method is to identify the indices of each particle in the data vector

These are then stored in a reaction Map This can change event-to-event Given an index helper functions create 4-vectors etc. Can then be used in standarised kinematic calculations

//Analysing HepMC or MCMatched data **I know my pion is 2nd** epic.setParticleIndex("idxPi".2): **In particle listCan use any complicated algorithm** //Analysing reconstrcuted, with no matching epic.setParticleIndex("idxPi", rad::indice::useNthOccurance(1,211), {"ReconstructedParticles.PDG"});

From indices to 4-vectors

User code :

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```
epic.setParticleIndex("idxEl",0,11);
epic.setParticleIndex("idxPo",1,-11);
epic.setParticleIndex("idxPi",2,211);
epic.setParticleIndex("idxN",3,2112);
```
Index known as MCmatched

epic.setMesonParticles({"idxEl","idxPo","idxPi"});

Inside RAD function definition :

Returns 4-vector sum of e-, e+, π+ //Get meson (Top) 4-vector $auto$ meso=FourVector(react[names::MesonsIdx()], px, py, pz, m);

react \rightarrow the reaction map, stores particle indices MesonsIdx is the position in react where meson indices are stored

Inside RAD Kinematic Function

///\brief return 4 momentum transfer squared of "in particles" - "out particles" on top vertex

```
Uses react for beam and 
                           scattered e- indicesVectors of momentum
//Get photon 4-vector
                                                         components
auto phot=PhotoFourVector(react,px,py,pz,m);
//Get meson (Top) 4-vector
auto meso=FourVector(react[names::MesonsIdx()], px, py, pz, m);
//subtract
auto psum = phot-meso;//return t
return - (psum.M2());
```
react \rightarrow the reaction map, stores particle indices

MesonsIdx is the position in react where meson indices are stored

Inside RAD Kinematic Function

```
///\brief return 4 momentum transfer squared of "in particles" - "out particles" on top vertex
template<typename Tp, typename Tm>
Tp TTop(const config::RVecIndexMap& react,
       const RVec<Tp> &px, const RVec<Tp> &py, const RVec<Tp> &pz, const RVec<Tm> &m){
                                                             Vectors of momentum
 //Get photon 4-vector
                                                            componentsauto phot=PhotoFourVector(react,px,py,pz,m);
 //Get meson (Top) 4-vector
 auto meso=FourVector(react[names::MesonsIdx()], px, py, pz, m);
 //subtract
 auto psum = phot-meso;//return t
 return - (psum.M2());
```
React \rightarrow the reaction map, stores particle indices

MesonsIdx is the position in react where meson indices are stored

Particle Creator

As well as reconstructed particles, we also need to manipulate intermediate or missing particle 4-vectors

ParticleCreator adds these momentum components to the reconstructed components vectors and generates index for the new particle

Sum – sum 4-vector of given particles Diff – subtract 4-vector of given indices Beam – define a fixed 4-vector for beam particle Miss – subtract given particles from sum of beams

User code configure stage

rad::config::ePICReaction epic{"events","ipac z3900 10x100.root"}: epic.SetBeamsFromMC();

//epic.AliasColumnsAndMC(): epic.AliasColumnsAndMatchWithMC();

//Assign particles names and indices epic.setScatElectronIndex(4); **e-'** epic.setParticleIndex("idxEl".0.11); **e** $epic.setParticleIndex("idxPo", 1, -11);$ $e+$ **Final state particles π** epic.setParticleIndex("idxN",3,2112); n

//Create some intermediate particles **decaying states** epic.Particles().Sum("idxJ",{"idxEl","idxPo"}); **J/ψ → e- + e+** epic.Particles().Sum("idxZ",{"idxPi","idxJ"});
New name{Particles to sum} Z → J/ψ + π

//Group particles into top and bottom vertices epic.setMesonParticles({"idxEl","idxPo","idxPi"}); //can also add missing particles**Missing particle : n = beams- e'-Z**
epic.Particles().Miss("idxCalcN",{rad::names::ScatEle().data(),"idxZ"}); $epic.setBaryonParticles({"idxCalcN"})$;

//must call this after all particles are configured $epic.makeParticleMap()$;

User code kinematics stage

Call predefined rad::rdf functions for kinematics

```
//masses column name. {+ve particles}. {-ve particles}
rad::rdf::MissMass(epic."W"."{scat ele}"):
rad::rdf::MissMass(epic."MissMass"."{scat ele.idxN.idxZ}"):
rad::rdf::Mass(epic,"Whad","{idxPi,idxEl,idxPo,idxN}");
rad::rdf::Mass(epic,"JMass","{idxJ}");
rad::rdf::Mass(epic,"ZMass","{idxZ}");
rad::rdf::Mass(epic,"MissNMass","{idxCalcN}");
                                                        //Define histograms
//t distribution, column name
                                                    auto df0 = epic.CurrFrame();rad::rdf::TTop(epic, "t qZ"):
rad::rdf::TBot(epic,"t pn");
                                                    auto hW = df0.HistolD({'W", "W", 100, 0, 20.}, "tru W");rad::rdf::TPrimeBot(epic,"tp pn");
                                                    auto hWhad = df0.Histo1D({'Whad",''Whad",100,0,20.},''truWhad'');rad: rdf: TPrimeTop(epic, "tp qZ")auto hMesonMass = df0.HistolD({\{}}"MesonMass", M(e-,e+, #pi) [GeV]", 100,.3,5.}, "tru ZMass");auto hMissMass = df0.HistolD({\lceil}MissMass","Mmiss \lceil GeV\rceil", 1000, -10, 10},"tru MissMass");
                                                    auto hJMass = df0.Hist01D({T'JMass", "M(e-,e+) [GeV]", 100,.3,5.}, "tru JMass");//CM production angles
                                                    auto htpn = df0.Histo1D({"tpn","t(p,n) [GeV^{2}]",100,-2,5},"tru_t_pn");
rad::rdf::CMAngles(epic,"CM");
                                                    auto htgZ = df0.Histo1D({"tgZ","t(g,Z) [GeV^{2}]",100,-2,5},"tru t gZ");
                                                    auto htprimepn = df0.Histo1D({'tprimepn", "t'(p,n) [GeV^{2}]", 100,-2,5}, "tru_tp_pn");auto htprimeqZ = df0.HistotD({'tprimeqZ", 't'(p,n) [GeV^{-2}]", 100,-2,5}, 'tru tp qZ');auto hthCM=df0.Histo1D({"cthCM","cos(#theta {CM})",100,-1,1},"tru CM CosTheta");
                                                    auto hphCM=df0.Histo1D({"phCM","#phi {CM})".100.-TMath::Pi(),TMath::Pi()},"tru CM Phi");
```
More complicated functor

class UndoAfterBurn

```
public:
 UndoAfterBurn(PxPyPzMVector p beam,PxPyPzMVector e beam,Float t angle=-0.025): crossAngle{angle}{
   //calculate and store current boosts and rotations
   RotsAndBoosts(p beam.e beam):
 template<typename Tp, typename Tm>
 void operator()(RVec<Tp> &px,RVec<Tp> &py,RVec<Tp> &pz, const RVec<Tm> &m) const
   //apply to all particles
                                                      Functors need operator()auto n parts = m.size():
   for(uint i=0; i<n parts; ++i){
     undoAfterburn(i.px.pv.pz.m):
private:
 //Determine transformations
 void RotsAndBoosts(PxPvPzMVector p beam, PxPvPzMVector e beam):
 //change momentum for a particle as per prescription
 template<typename Tp, typename Tm>
 void undoAfterburn(uint idx, RVec<Tp> &px, RVec<Tp> &py, RVec<Tp> &pz, const RVec<Tm> &m) const;
 // Objects for undoing afterburn boost
 Float t crossAngle{-0.025}; // Crossing angle in radians
 RotationX _rotAboutX;
 RotationY rotAboutY;
 MomVector vBoostToCoM;
                                                                           automatically
 MomVector vBoostToHoF:
```
Undo ePIC afterburner Applied to each particle

Going further : multiple reactions

Maximise efficiency : 1 data read, multiple reactions Become less read bound

- Make the most of multi-core processing
- Just need ROOT::EnableImplicitMT(8);

Difficult to do in a single script for loop

Here relatively simple : Prior to indicing take copies of the RAD frame Configure each for their own reaction and observables Lazy execute all at once!

* note : currently tree snaphot is not lazy so this only works for histogramming type analysis

Automation : ReactionChannel

Utility class to do the index configuration - just requires meson and baryon indices

Can use to analyse Pythia data, HepMC or ePIC

e.g $M \rightarrow \pi-\pi+\beta$ B \rightarrow p π 0 ReactionChannel channel{rad, {211, -211}, {2212, 22, 22}}; RAD dataframe

Multiple channels code

//identify a number of final states by pdg code auto mesons= $\{211, -211\}$, $\{-211\}$, $\{113\}$, $\{211, 111, -211\}$; auto baryons={{2212}, {2212,211},{2212},{2212} };

```
//create base RAD object
rad::config::ePICReaction epic{"events","pythia.edm4eic.root"};
```

```
for(auto ipy = 0; ipy<mesons.size() ; ++ipy){
  //copy from base dataframe to allow lazy execution
  //on all final states
   auto rad = epic;
```
//create a reaction channel which is defined in terms of the //meson and baryon decay products rad::config::ReactionChannel channel{rad,mesons[ipy],baryons[ipy]};

```
//Define all kinematics we are interested in
rad::rdf::MissMass(rad,"W","{scat_ele}");
rad::rdf::MissMass(rad,"MissMassMeson","{scat_ele,idxMeson}");
rad::rdf::MissMass2(rad,"MissMassMeson2","{scat ele,idxMeson}");
rad::rdf::MissMass2(rad,"MissMassBaryon2","{scat ele,idxBaryon}");
```
ePIC Benchmarking

I need to make some benchmark tests for the lowQ2 Tagger

- Use the Pythia ReactionChannel Framework
- Use ePIC common benchmark format https://eicweb.phy.anl.gov/EIC/benchmarks/common_bench

```
Need to produce a json file :"tests": \Gamma"description": "Resolution benchmark for Q2",
               "name": "02".
               "quantity": "Resolution",
               "result": "pass","taret": "0.004645738386922428","title": "Q2",
               "value": 0.0030971589246149523.
               "weight": 1.0
```
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ReactionBenchmarks

Class to automate benchmarking with RAD Requires truth matching

User defines histograms for observables For each observable ReactionBenchmarks :

- generates tru and rec distributions
- generates acceptance histograms
- generates resolutions histograms
- produces plots on configurable canvases
- writes common_benchmark tests in json

Supplement : common benchmark/benchmark against.h

- Defines test target to be result from previous analysis

Coding ReactionBenchmarks

```
//create a copy of rad dataframe so we can apply different cuts etc
auto rad tagger=rad;
//cut on Low02 Tagger acceptance region
rad tagger. Filter("tru theta [scat ele]>3.12", "tagger cut");
```
ReactionBenchmarks incTaggHists{"IncTagger",mesons[ipy],baryons[ipy]}; //Set output directory for saving plots and tests incTaggHists.SetOutDir(out dir): //define canvas formatting as 2 by 2 plots $array.$ $exists. push_back({2, 2})$;

```
//Define each variable we wish to benchmark with histogram model
incTagqHists.AddVar("Q2", {'Q2", "Q2", 500000, 0, 1});incTaggHists.AddVar("W", ["W", "W", 500, 0, 1.1*WMax});
incTaggHists.AddVar("MissPzMeson",{"MissPz","MPz",1200,-10,110});
incTaggHists.AddVarElement("scat_ele","pmag", {"epmag",
                            "Scattered Electron momentum", 130, -1, 12});
```
//Now declare all the histograms, add some cuts incTaggHists.Declare(rad tagger, channel.CutParticleCondition("rec_pmag",">0.05")+ "&&rec_pmag[scat_ele]>0.1&&rec_theta[scat_ele]>3.1");

//assign to my vector of reaction benchmarks allIncHists.push back(incTaggHists);

```
Take rad dataframe
From slide 28
```

```
Create benchmark
Store final state pdgs
```
Must use previously defined variables

Can use particle momentum

```
Let ReactionBenchmarks
Create all histograms
Store in vector for now
Must create all 
reactions and benchmarks 
first to use parallel 
lazy execution
```
Distributions

Efficiencies

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Resolutions

common_benchmarks

Conclusions

RDataFrame offers a appealing framework for data analysis

Collaborations can build a common scheme on top of this - for example using edm4hep, edm4eic

Here we only use ROOT dependencies (simple to install)

We make the dataframe "Reaction Aware" by defining indices User coding is minimised Kinematic functions are reusable Truth Matching is automated Many reactions can be run in parallel on multi-cores

 But the code behind the scenes is complicated and difficult to develop...

Title

