



CYBERINFRASTRUCTURE FOR HIGH-LEVEL SCIENCE GOALS

@KyleCranmer

New York University Department of Physics Center for Data Science Infrastructure Components

DASPOS AND DIANA

DASPOS and DIANA are two large projects funded by the U.S. National Science Foundation focusing on issues around software and data for high energy physics.

We are working closely with CERN Analysis Preservation (CAP) portal, INSPIRE, and HEPData to build infrastructure for High Energy Physics





FROM NSF

The SI2 program includes four classes of awards:

1. Scientific Software Elements (SSE): SSE awards are Software Elements. They target small groups that will create and deploy robust software elements for which there is a demonstrated need that will advance one or more significant areas of science and engineering.

2. Scientific Software Integration (SSI): SSI awards are Software Frameworks. They target larger, interdisciplinary teams organized around the development and application of common software infrastructure aimed at solving common research problems. SSI awards will result in sustainable community software frameworks serving a diverse community.

3. Scientific Software Innovation Institutes (S2I2): S2I2 awards are Software Institutes. They focus on the establishment of long-term hubs of excellence in software infrastructure and technologies that will serve a research community of substantial size and disciplinary breadth.

4. **Reuse**: In addition, SI2 provides support through a variety of mechanisms (including co-funding and supplements) to proposals from other programs that include, as an explicit outcome, reuse of software. Proposals that integrate with previously developed software, either by reference or inclusion, are encouraged. Proposals developing new software with an explicitly open design for reuse may also be considered. The purpose of the Reuse class is to stimulate connections within the broader software ecosystem. The class of reuse awards is currently being developed.



4

INFRASTRUCTURE FOR DATA AND ANALYSIS PRESERVATION





https://hepdata.net/search/?g=&collaboration=ATLAS&page=1



Interactive Plotting Library

HEPData Q Search HEP Data	Search			(€ About (© Help → Sign in		
Q Browse all 🔊 Aad, Georges et al.			Last upda	ted on 2016-04-08 15:56:50 🛄 Accessed 10 times		
Hide Publication Information Information	📩 Download All 🗸	Table 10		http://www.hepdata.net/r		
Charged-particle distributions in \sqrt{s} =13 TeV <i>pp</i> interactions measured	√ Filter 18 data tables	Extrapolated average transverse momentum i	n proton-proton collisions at a centre-of-m	ass energy of 13000		
with the ATLAS detector at the LHC	momentum for	particles >=1 having transverse momentum >500 MeV and absolute(pseudorapidity) <2.5.				
Aad, Georges, Abbott, Brad, Abdallah, Jalal, Abdinov, Ovsat, Abeloos, Baptiste, Aben, Rosemarie, Abolins,	Table 9 >	10.17182/hepdata.72205.v1/t10				
Maris, AbouZeid, Ossama, Abraham, Nicola, Abramowicz,	Data from Auxiliary Material 10.17182/hepdata.72205.v1/t9	observables	phrases	reactions		
ATLAS No Journal Information, 2016	Extrapolated charged-particle multiplicity distributions in proton-proton collisions at a centre-of-mass energy of 13000	PT	Inclusive Proton-Proton Scattering	S P P> CHARGED X		
http://dx.doi.org/10.17182/hepdata.72205 View paper in Inspire View old HepData	of	Showing 50 of 81 values	Show All 81 values	Visualize		
Additional Resources	Data from Auxiliary Material	ETARAP(P=3)	-2.5-2.5	1.30-		
Abstract (data abstract)	10.17182/hepdata.72205.v1/t10	Extrapolated to include strange baryons				
CERN-LHC. Measurements of charged particle distributions in proton-proton collisions at a centre-of-mass energy of 13	momentum in proton-proton collisions at a centre-of-mass	N(P=3)	>= 1	1.15 -		
TeV. A data sample of nearly 9 million events recorded by the ATLAS detector during a special LHC fill with low beam	energy of 13000 GeV as a function of the number	PT(P=3)	> 500 MEV	1.10 -		
currents, and thus giving a low expected mean number of interactions, is used. The charged-particle multiplicity, its	Table 11	RE	P P> CHARGED X	1.00 -		
dependence on transverse momentum and pseudorapidity and the dependence of the mean transverse momentum on	Data from F 5A	SQRTS(S)	13000.0 GeV	0.90 -		
the charged-particle multiplicity are presented. The measurements are performed with charged particles with	10.17182/hepdata.72205.v1/t11 Charged-particle multiplicities	N(P=3)	MEAN(NAME=PT(P=3)) [GEV]	0.85 -		
transverse momentum greater than 500 MeV and absolute pseudorapidity less than 2.5, in events with at least one	in proton-proton collisions at a centre-of-mass energy of 13000	0.50 - 1.50	0.7737 ±0.0008 stat ±0.0155 sys	20 40 60 80 100 120 140		
charged narticle satisfying these kinematic requirements	pseudorapidity for events with	1.50 - 2.50	0.7904 ±0.0007 stat ±0.0158 sys	N(P=3)		
	Table 12 >	2.50 - 3.50	0.809 ±0.001 stat ±0.008 sys	Sum errors 🧭 Log Scale (X) 🗌 Log Scale (Y) 🗌		
	Data from F 5B	3.50 - 4.50	0.8289 ±0.0006 stat ±0.0084 svs			

Open Data & Preservation

https://arxiv.org/abs/1205.4667



Table 3: Various preservation models, listed in order of increasing complexity.





A CASE STUDY WITH OPEN DATA

MIT-CTP 4890 V. ADVICE TO THE COMMUNITY

Jet Substructure Studies with CMS Open Data

Aashish Tripathee,^{1,*} Wei Xue,^{1,†} Andrew Larkoski,^{2,‡} Simone Marzani,^{3,§} and Jesse Thaler^{1,¶}

¹Center for Theoretical Physics, Massachusetts Institute of Technology, Cambridge, MA 02139, USA ²Physics Department, Reed College, Portland, OR 97202, USA ³University at Buffalo, The State University of New York, Buffalo, NY 14260-1500, USA

We use public data from the CMS experiment to study the 2-prong substructure of jets. The CMS Open Data is based on 31.8 pb^{-1} of 7 TeV proton-proton collisions recorded at the Large Hadron Collider in 2010, yielding a sample of 768,687 events containing a high-quality central jet with transverse momentum larger than 85 GeV. Using CMS's particle flow reconstruction algorithm to obtain jet constituents, we extract the 2-prong substructure of the leading jet using soft drop declustering. We find good agreement between results obtained from the CMS Open Data and those obtained from parton shower generators, and we also compare to analytic jet substructure calculations performed to modified leading-logarithmic accuracy. Although the 2010 CMS Open Data does not include simulated data to help estimate systematic uncertainties, we use track-only observables to validate these substructure studies.

From a physics perspective, our experience with the CMS Open Data was fantastic. With PFCs, one can essentially perform the same kinds of four-vector-based analyses on real data as one would perform on collisions from parton shower generators. Using open data has the potential to accelerate scientific progress (pun intended) by allowing scientists outside of the official detector collaborations to pursue innovative analysis techniques. We hope that our jet substructure studies have demonstrated both the value in releasing public data and the enthusiasm of potential external users. We encourage other members of the particle physics community to take advantage of this unique data set.

From a technical perspective, though, we encountered a number of challenges. Some of these challenges were simply a result of our unfamiliarity with the CMSSW framework and the steep learning curve faced when trying to properly parse the AOD file format. Some of these challenges are faced every day by LHC experimentalists, and it is perhaps unreasonable to expect external users to have an easier time than collaboration members. Some of these challenges (particularly the issue of detectorsimulated samples) have been partially addressed by the 2011A CMS Open Data release [215]. That said, we suspect that some issues were not anticipated by the CMS Open Data project, and we worry that they have deterred other analysis teams who might have otherwise found interesting uses for open data. Therefore, we think it is useful to highlight the primary challenges we faced, followed by specific recommendations for how potentially to address them.

A. Challenges

Here are the main issues that we faced in performing the analyses in this paper.

• Slow development cycle. As CMSSW novices, we often needed to perform run-time debugging to figure out how specific functions worked. There were two elements of the CMSSW workflow that introduced a considerable lag between starting a job and getting debugging feedback. The first is that, when using the XROOTD interface, one has to face the constant overhead (and inconstant network performance) of retrieving data remotely. The second is that, as a standard part of every CMS analysis, one has to load configuration files into memory. Loading FrontierConditions_GlobalTag_cff (which is necessary to get proper trigger prescale values) takes around 10 minutes at the start of a run. For most users, this delay alone would be too high of a barrier for using the CMS Open Data. By downloading the AOD files directly and building our own MOD file format, we were able to speed up the development cycle through a lightweight analysis framework. Still, creating the MODPRODUCER in the first place required a fair amount of trial, error, and frustration.

- Scattered documentation. Though the CMS Open Data uses an old version of CMSSW (v4.2 compared to the latest v9.0), there is still plenty of relevant documentation available online. The main challenge is that it is scattered in multiple places, including online TWIKI pages, masterclass lectures, thesis presentations, and GITHUB repositories. Eventually, with help from CMS insiders, we were able to figure out which information was relevant to a particular question, but we would have benefitted from more centralized documentation that highlighted the most important features of the CMS Open Data. Centralized documentation would undoubtably help CMS collaboration members as well, as would making more TWIKI pages accessible outside of the CERN authentication wall.
- Lack of validation examples. When working with public data, one would like to validate that one is doing a sensible analysis by trying to match published results. While example files were provided, none of them (to our knowledge) involved the complications present in a real analysis, such as appropriate trigger selection, jet quality criteria, and jet energy corrections. Initially, we had hoped to reproduce the jet p_T spectrum measured by CMS on 2010 data [263], but that turned out to be surprisingly difficult, since very low p_T jet triggers are not contained in the Jet Primary Dataset, and we were not confident in our ability to merge information from the MinimumBias Primary Dataset. (In addition, the published CMS result is based on inclusive jet p_T spectra, while we restricted our analysis to the hardest jet in an event to simplify trigger assignment.) Ideally, one should be able to perform event-by-event validation with the CMS Open Data, especially if there are important calibration steps that could be missed.¹³
- Information overload. The AOD files contains an incredible wealth of information, such that the majority of official CMS analyses can use the AOD format directly without requiring RAW or RECO information. While ideal for archival purposes, it is an overload of information for external users, especially because some information is effectively duplicated. The main reason we introduced the MOD

21

¹³ In the one case where we thought it would be the most straightforward to cross check results, namely the luminosity study in Fig. 2, it was frustrating to later learn that the AOD files contained insufficient information.

Excerpts from Symposium



REACHING FOR THE HORIZON



LONG RANGE PLAN

for NUCLEAR SCIENCE

NUCLEAR PHYSICS IN A DECADE

DONALD GEESAMAN Argonne National Laboratory

luclear Physics Computing



The 2015

Future Trends in Nuclear Physics Computing May 2, 2017

IN MOST CASES, IT WILL BE JOINT PROGRESS BETWEEN THEORY AND EXPERIMENT THAT MOVES US FORWARD, NOT IN ONE SIDE ALONE

Does the structure of the proton and the forces between nucleons change in nuclear matter (beyond n-body force effects)?

This has been an active subject since the dawn of the EMC effect. The problem is we have just had "toy" models that fit systematics for one observable but gave us little insight into others.

In ten years I expect lattice QCD calculations of nuclei to be able to properly ask this question and tell us what measurements will confirm it. I think we will have the measurements in hand.



SUMMARY

- It will be joint progress and theory and experiment that moves us forward, not in one side alone
- Continued rapid progress in Nuclear Physics Computing is imperative.
 - · Challenge in handling the raw data
 - · Challenge in analyzing the data
 - · Challenge in simulating real detectors
 - Theory challenge in calculating the physics right
 - Nuclear structure
 - Hadron structure
 - Astrophysical environments

Argonne 🛆

GLOBAL COLLABORATION

All of this is in the context of more globalization of the research effort.

There will be an emphasis on

- Common Tools
- Common Structures
- Remote collaboration

but on diverse architectures and with diverse short range goals.

8

Argonne 🛆



Synergies of Computing and the Next Generation of Nuclear Physics Experiments

Rolf Ent (Jefferson Lab)

With acknowledgement to Amber Boehnlein, Markus Diefenthaler and Graham Heyes for their help

Future Trends in Nuclear Physics Computing May 2, 2017



Interplay of data and theory



Comparison to:

- analytical calculations
- Monte Carlo (MC) simulations
- Lattice-QCD calculations

Data-theory comparison: relies on

- open access to data-theory tools
- standardization of data-theory tools
- comparison tools for quick turnaround

MC event generator:

- faithful representation of QCD dynamics
- based on QCD factorization and evolution equations

Usage by experimentalists:

- detector corrections
- analysis prototyping
- comparing to theory

Usage by theoreticians:

- easy off-the-shelf state-of-the-art tool that looks like data
- validate against and investigate theoretical improvements





Developments of analysis environments:

- new projects starting (JLab 12 GeV) and on the horizon (EIC)
- likely explosion of data even at the small nuclear experiments
- think about the next generation(s) of analysis environments that will maximize the science output

LHC experiments: tremendous success in achieving their analysis goals and producing results in timely manners

Lesson learned at LHC experiments:

- as the complexity and size of the experiments grew
- the complexity of analysis environment grew
- time dealing with the analysis infrastructure grew

Anecdote from LHC

a typical LHC student or post-doc spends up to 50 % of his/her time dealing with computing issues





Targeting the theory/experiment interface

ATLAS POLICY DOCUMENT

Level-1. Published results

All scientific output is published in journals, and preliminary results are made available in Conference Notes. All are openly available, without restriction on use by external parties beyond copyright law and the standard conditions agreed by CERN.

Data associated with journal publications are also made available: tables and data from plots (e.g. cross section values, likelihood profiles, selection efficiencies, cross section limits, ...) are stored in appropriate repositories such as HEPDATA[2]. ATLAS also strives to make additional material related to the paper available that allows a reinterpretation of the data in the context of new theoretical models. For example, an extended encapsulation of the analysis is often provided for measurements in the framework of RIVET [3]. For searches information on signal acceptances is also made available to allow reinterpretation of these searches in the context of models developed by theorists after the publication. ATLAS is also exploring how to provide the capability for reinterpretation of searches in the future via a service such as RECAST [4]. RECAST allows theorists to evaluate the sensitivity of a published analysis to a new model they have developed by submitting their model to ATLAS.





DIGITAL PUBLISHING STATISTICAL MODELS



COLLABORATIVE STATISTICAL MODELING



$$\mathbf{f}_{\text{tot}}(\mathcal{D}_{\text{sim}}, \mathcal{G} | \boldsymbol{\alpha}) = \prod_{c \in \text{channels}} \left[\text{Pois}(n_c | \nu_c(\boldsymbol{\alpha})) \prod_{e=1}^{n_c} f_c(x_{ce} | \boldsymbol{\alpha}) \right] \cdot \prod_{p \in \mathbb{S}} f_p(a_p | \alpha_p)$$

COLLABORATIVE STATISTICAL MODELING





Not possible for others to reproduce results from paper.



Not possible for others to reproduce results from paper.



What info and how to retrieve it

Through collaboration with theoretical community, we were able to identify a targeted form of data sharing that balanced generality &



These data are directly linked to the paper in INSPIRE and have been cited:



LIKELIHOODS ON HEPDATA

Reproducing derived results from original paper!



Reinterpretation & Reusability



FOLDING VS. UNFOLDING





RECASTING / REINTERPRETATION



It's the difference between if you had airplanes where you threw away an airplane after every flight, versus you could reuse them multiple times.

– Elon Musk

ATLAS analysis ATLAS analyses

It's the difference between if you/had airplanes where you threw away an airplane after every flight, versus you could reuse them multiple times.

checking one theory

– Elon Musk

DEMAND

>50 requests from theorists within ~2 months



About this site

RECAST is a framework for extending the impact of existing analyses performed by highenergy physics experiments.

- 1. Anyone can add *analyses* to the Analysis Catalog
- 2. Anyone can upload alternative signals in the LHE format and *request* that any given analysis is "recast" for their alternative model (Note: this is a request, there is no obligation for the experiments to respond.)
- Anyone can *subscribe* to an analysis to be informed of activity associated with the analysis
- 4. Experimentalists can accept the request, process these alternative signals with the full simulation, reconstruction, and analysis selection. If they are authorized by their collaboration, then they can respond with an authoritative *result* for the selection efficiency and cross-section limits for the alternative signal. Note, anyone can provide a non-authoritative result, for instance one based on fast simulation.

Latest Requests

Search

Request	Analysis	Model	Status
1603.0045	Search for massive supersymmetric particles decaying to many jets using the ATLAS detector in pp collisions at $\sqrt{s} = 8$ TeV	asdafa	Incomplete
1505.0044	Search for massive supersymmetric particles decaying to many jets using the ATLAS detector in pp collisions at $\sqrt{s} = 8$ TeV	stealth supersymmetry	Incomplete
1408.0043	Search for direct third-generation squark pair production in final states with missing transverse momentum and two b-jets in $\sqrt{s}= 8$ TeV pp collisions with the ATLAS detector	3-body decay of sbottom into b- quark and two invisible final states	Active
1408.0042	Search for direct top-squark pair production in final states with two leptons in pp collisions at sqrt(s)=8TeV with the ATLAS detector	3-body decay of stop into top and two invisible final states	Active
1408.0041	Search for direct pair production of the top squark in all-hadronic final states in proton-proton collisions at $\sqrt{s}=8$ TeV with the ATLAS detector	3-body decay of stop into top and two invisible final states	Active
	Search for direct third-generation squark pair	3-body decay of	

PHENO RECASTING SOFTWARE

- Several tools being developed by phenomenologists to address the need for an organized approach to recasting (but using unofficial and/or approximate methods.
 - ATOM
 - FastLim
 - MadAnalysis
 - Gambit
 - SModelS
 - XQCAT
 - CheckMate
 - unofficial contributions to Rivet



• As I'll show, it is possible to interface RECAST infrastructure with these unofficial pheno recasting tools.

REINTERPRETATION FORUM

TWiki > LHCPhysics Web > LHCPhysics > InterpretingLHCresults (2017-03-02, SabineKraml)



Forum on the Interpretation of the LHC Results for BSM studies

The quest for new physics beyond the Standard Model is arguably the driving topic for Run 2 of the LHC. Indeed, the LHC collaborations are pursuing searches for new physics in a vast variety of channels. While the collaborations typically provide themselves interpretations of their results, for instance in terms of simplified models, **the full understanding of the implications of these searches requires the interpretation of the experimental results in the context of all kinds of theoretical models.** This is a very active field, with close theory-experiment interaction and with several public tools being developed.

With this forum, we want to provide a platform for continued discussion of topics related to the BSM (re)interpretation of LHC data, including the development of the necessary **public** RecastingTools and related infrastructure.

If you have questions or want to contribute, contact Sabine Kraml, sabine.kraml@gmailNOSPAMPLEASE.com, or any of the topical contacts given below.

Meetings

Meetings of this forum

- 2nd workshop 2, 12-14 Dec 2016 at CERN
- Kick-off workshop: (Re)interpreting the results of new physics searches at the LHC 2, 15-17 June 2016 at CERN

Other workshops, potentially interesting for our forum

- The Les Houches PhysTev2017 workshop will have a strong activity on interpreting LHC results; the BSM session in LH is taking place 14-23 June 2017.
- 2nd LHC Long-Lived Particle workshop 2, CERN, 24-26 April 2017, "to address the status and future of beyond-the-Standard Model LLP searches at the ATLAS, CMS, and LHCb experiments, as well as auxiliary LHC detectors and projects".
- 6th edition of the workshop "Implications of LHCb measurements and future prospects ?", CERN, 12-14 October 2016. NB participation is restricted to the members of the LHCb Collaboration, and of interested theorists.

Mailing list

- CERN e-group: info-LHC-interpretation@cernNOSPAMPLEASE.ch

A FLEXIBLE WORKFLOW MODEL

Ynin Xwar - command 1) read/export json X. ... Xn L-line AX, ·· SXn 2) interactive shell N. ... Wn I - interface 3) projection (3×3×33 ->1×3 3×4×5×6 -> 4×5×6 4) dimension reduction 3×4×5×6 -> 3×2×5×6 5) rebin one dimension 6) interpolation TMD 7) merging X-Sec mains mypioncalc 8) Visulazion program ms. load ("SF1") 9) random & generator (Y... Y.) produce ms.get (BFI", Q?, ms.load ("SF3") ms.get ("XSEG").set Bin (ms.create (7, ...) 10) event generator c'in ? x, y, R, B, Y, Y, S Q?, Y, X, PT, xs). X, Y, RM_FP, Q, Q

A FLEXIBLE WORKFLOW MODEL

A workflow composed of sub-workflows that run Rivet, Delphes, and ATLAS analyses in parallel on the same input



Technical Solution:

Workflow (i.e. logic which steps to run in which order: reconstruction \rightarrow analysis \rightarrow fit)

- in easy to write / read text based format (YAML)
- generic workflow language "yadage" based on graphs. No assumption on how you
 run your analysis. Should be able to accommodate your workflows.
- integrated into CERN Analysis Preservation.
- re-run workflow using tool that interprets info stored in CAP







Front-End: public facing collects requests

Recast All Analyses All Requests

Recast Control Center An Analysis Reinterpretation Framework

Introduction

This is an early prototype for the RECAST control center. While the RECAST front-end at <u>http://recast.per/meterinstitute.ca</u> is used to gather requests for analysis reinterpretation from the community, this web application is used to launch jobs for different back-ands that actually perform the reinterpretation.

It supports CERN SSO authentication which will allow for fine-grained control over which users are able to launch the reinterpretation jobs and/or upload the results to the front-end. This web application provides a plugin model for analyses. Currently, we have a template plugin for Rivet analyses that runs quickly. We are working with CERN IT's analysis preservationproduct to provide a template plugin for reinterpretation basedon the full simulation, reconstruction, and event selection.

For convenience, one can initiate a request directly from the control center, which will be uploaded to the front-end.

Instructions

- To test the RECAST service, click on the All Analyses link in the navigation above. Select the analyses that you want to recast. Alternatively you can also create a request on the RECAST front-end (currently the development instance)
- Once you have chosen the analysis you want to recast, create a new request by clicking the New RECAST Request button and fill out the form. After you created the request you can click through to the page describing your new request
- 3. On the request page you can now upload simulated events for specific parameter points in the Les Houche

Control Center: not public, uses CERN auth., oversees processing of jobs on back-end



CERN Analysis Preservation: Stores workflows, provides back-end computing resources

front-end (open)

Home » Analyses Catalog » D	emo with working riv	vet-based ba	ack-end »	List Re	quests » t	test for UCI	
View Edit Edit C	Contact Requester	Show Re	sults	Devel			
^T 1. request	initiated	, k					
Analysis:	Demo with worki	ng rivet-bas	ed back-	end			
Status:	Completed						
Requester:	lheinric	E ro				منامل	
Recast Audience:	all	ɔ. re	spo	nse	e pr		
Model Name:	CMSSM						
Selected Subscriber(s):	lheinric, cranmer						
Mon, 02/02/2015 - 14:20 Wed, 02/04/2015 - 03:0	6 - Activated 6 - Completed						
Request Description and	d Potential						
Reason for request: because we can Additional Informatio No information available	n:						

control center (closed to experiment)

Request Details			
analysis status model-type uuid new-model-information title predefined-model reason-for-request requestor audience	Demo with working rivet-based 1 None 4cdc558c-8f4a-eab4-fdbf-cd91 None test for UCI CMSSM because we can Iheinric None	back-end a34db4b2	
subscribers additional-information	None 4. UPIC	Jad respons	se
		2	
		Z. proc	ess reques
	Copioad to RECAST		
Parameter Des	ciption Number of Eve	nts Cross-Section	
		3. r	eview resu
Results for I	request 4cdc558c	-8f4a-eab4-fdbf-cd91a3	4db4b2 - parameter-0
Results for I	request 4cdc558c	-8f4a-eab4-fdbf-cd91a3	4db4b2 - parameter-0
Results for I	request 4cdc558c	-8f4a-eab4-fdbf-cd91a3	4db4b2 - parameter-0



Home » Analyses Catalog » Demo with working rivet-based back-end » List Requests » test-upload-2 » Show Results » Recast Response for Request #test-upload-2

Recast Response for Request #test-upload-2

View Edit Devel

Submitted by Iheinric on Sun, 01/18/2015 - 09:54

Request: test-upload-2 ROOT file with TH1: 1 20150118095414b5872ab0-1a2b-10a4-c154-5cead413bc8f.zip Status: Completed Abstracting the Problem for the Machine Learning Community



- NP has some computations that require exponential time on a classical computer - quantum computer?
- Microsoft, Google, IBM indicate ~50 qubit QC's up within a year
- NP could start exploring

Quantum Testbeds Stakeholder Workshop



Machine Learning

- · Already in use in HEP expt at some level
- · Sophisticated pattern recognition correlations in data
- Nonlinear regression on steroids+epo
- · Some NP engagement, and much more, would likely be valuable





THE PLAYERS



The Forward Model

$$\mathcal{L}_{SM} = \underbrace{\frac{1}{4} \mathbf{W}_{\mu\nu} \cdot \mathbf{W}^{\mu\nu} - \frac{1}{4} B_{\mu\nu} B^{\mu\nu} - \frac{1}{4} G^a_{\mu\nu} G^{\mu\nu}_a}_{a}$$

kinetic energies and self-interactions of the gauge bosons

$$+ \bar{L}\gamma^{\mu}(i\partial_{\mu} - \frac{1}{2}g\tau \cdot \mathbf{W}_{\mu} - \frac{1}{2}g'YB_{\mu})L + \bar{R}\gamma^{\mu}(i\partial_{\mu} - \frac{1}{2}g'YB_{\mu})R$$

kinetic energies and electroweak interactions of fermions

+
$$\frac{1}{2} \left| (i\partial_{\mu} - \frac{1}{2}g\tau \cdot \mathbf{W}_{\mu} - \frac{1}{2}g'YB_{\mu})\phi \right|^2 - V(\phi)$$

 W^{\pm}, Z, γ , and Higgs masses and couplings

+
$$\underbrace{g''(\bar{q}\gamma^{\mu}T_aq)G^a_{\mu}}_{\mu}$$
 + $\underbrace{(G_1\bar{L}\phi R + G_2\bar{L}\phi_c R + h.c.)}_{\mu}$

interactions between quarks and gluons

fermion masses and couplings to Higgs

1) We begin with Quantum Field Theory

The Forward Model

$$\mathcal{L}_{SM} = \underbrace{\frac{1}{4} \mathbf{W}_{\mu\nu} \cdot \mathbf{W}^{\mu\nu} - \frac{1}{4} B_{\mu\nu} B^{\mu\nu} - \frac{1}{4} G^a_{\mu\nu} G^{\mu\nu}_a}_{\text{kinetic energies and self-interactions of the gauge bosons}} \\ + \underbrace{\bar{L} \gamma^{\mu} (i\partial_{\mu} - \frac{1}{2} g\tau \cdot \mathbf{W}_{\mu} - \frac{1}{2} g' Y B_{\mu}) L + \bar{R} \gamma^{\mu} (i\partial_{\mu} - \frac{1}{2} g' Y B_{\mu}) R}_{\text{kinetic energies and electroweak interactions of fermions}} \\ + \underbrace{\frac{1}{2} \left| (i\partial_{\mu} - \frac{1}{2} g\tau \cdot \mathbf{W}_{\mu} - \frac{1}{2} g' Y B_{\mu}) \phi \right|^2 - V(\phi)}_{W^{\pm}, Z, \gamma, \text{and Higgs masses and couplings}}$$

+
$$\underbrace{g''(\bar{q}\gamma^{\mu}T_aq)G^a_{\mu}}_{\mu}$$
 + $\underbrace{(G_1\bar{L}\phi R + G_2\bar{L}\phi_c R + h.c.)}_{\mu}$

interactions between quarks and gluons

fermion masses and couplings to Higgs

1) We begin with Quantum Field Theory





hierarchical: $2 \rightarrow O(10) \rightarrow O(100)$ particles

The Forward Model

$$\mathcal{L}_{SM} = \underbrace{\frac{1}{4} \mathbf{W}_{\mu\nu} \cdot \mathbf{W}^{\mu\nu} - \frac{1}{4} B_{\mu\nu} B^{\mu\nu} - \frac{1}{4} G^a_{\mu\nu} G^{\mu\nu}_a}_{\text{kinetic energies and self-interactions of the gauge bosons}}$$

+
$$\underbrace{\bar{L}\gamma^{\mu}(i\partial_{\mu}-\frac{1}{2}g\tau\cdot\mathbf{W}_{\mu}-\frac{1}{2}g'YB_{\mu})L}_{\mathbf{V}} + \bar{R}\gamma^{\mu}(i\partial_{\mu}-\frac{1}{2}g'YB_{\mu})R}_{\mathbf{V}}$$

kinetic energies and electroweak interactions of fermions

+
$$\frac{1}{2} \left| (i\partial_{\mu} - \frac{1}{2}g\tau \cdot \mathbf{W}_{\mu} - \frac{1}{2}g'YB_{\mu})\phi \right|^{2} - V(\phi)$$

 $W^{\pm}, Z, \gamma,$ and Higgs masses and couplings

+
$$\underbrace{g''(\bar{q}\gamma^{\mu}T_aq)G^a_{\mu}}_{\mu}$$
 + $\underbrace{(G_1\bar{L}\phi R + G_2\bar{L}\phi_c R + h.c.)}_{\mu}$

interactions between quarks and gluons

fermion masses and couplings to Higgs

1) We begin with Quantum Field Theory



hierarchical: $2 \rightarrow O(10) \rightarrow O(100)$ particles

THE FORWARD MODEL

$$\mathcal{L}_{SM} = \underbrace{\frac{1}{4} \mathbf{W}_{\mu\nu} \cdot \mathbf{W}^{\mu\nu} - \frac{1}{4} B_{\mu\nu} B^{\mu\nu} - \frac{1}{4} G^a_{\mu\nu} G^{\mu\nu}_a}_{\text{kinetic energies and self-interactions of the gauge bosons}}$$

+
$$\underbrace{\bar{L}\gamma^{\mu}(i\partial_{\mu}-\frac{1}{2}g\tau\cdot\mathbf{W}_{\mu}-\frac{1}{2}g'YB_{\mu})L}_{\mu}+\bar{R}\gamma^{\mu}(i\partial_{\mu}-\frac{1}{2}g'YB_{\mu})H$$

kinetic energies and electroweak interactions of fermions

+
$$\frac{1}{2} \left| (i\partial_{\mu} - \frac{1}{2}g\tau \cdot \mathbf{W}_{\mu} - \frac{1}{2}g'YB_{\mu})\phi \right|^2 - V(\phi)$$

 W^{\pm}, Z, γ , and Higgs masses and couplings

+
$$\underbrace{g''(\bar{q}\gamma^{\mu}T_aq)G^a_{\mu}}_{\mu}$$
 + $\underbrace{(G_1\bar{L}\phi R + G_2\bar{L}\phi_c R + h.c.)}_{\mu}$

interactions between quarks and gluons

1) We begin with Quantum Field Theory



hierarchical: $2 \rightarrow O(10) \rightarrow O(100)$ particles



3) The interaction of outgoing particles with the detector is simulated.

>100 million sensors

THE FORWARD MODEL

$$\mathcal{L}_{SM} = \underbrace{\frac{1}{4} \mathbf{W}_{\mu\nu} \cdot \mathbf{W}^{\mu\nu} - \frac{1}{4} B_{\mu\nu} B^{\mu\nu} - \frac{1}{4} G^a_{\mu\nu} G^{\mu\nu}_a}_{\text{kinetic energies and self-interactions of the gauge bosons}} \\ + \bar{L} \gamma^{\mu} (i\partial_{\mu} - \frac{1}{2} g\tau \cdot \mathbf{W}_{\mu} - \frac{1}{2} g' Y B_{\mu}) L + \bar{R} \gamma^{\mu} (i\partial_{\mu} - \frac{1}{2} g' Y B_{\mu}) R$$

kinetic energies and electroweak interactions of fermions

+
$$\frac{1}{2} \left| (i\partial_{\mu} - \frac{1}{2}g\tau \cdot \mathbf{W}_{\mu} - \frac{1}{2}g'YB_{\mu})\phi \right|^2 - V(\phi)$$

 W^{\pm}, Z, γ , and Higgs masses and couplings

+
$$\underbrace{g''(\bar{q}\gamma^{\mu}T_aq)G^a_{\mu}}_{\mu}$$
 + $\underbrace{(G_1\bar{L}\phi R + G_2\bar{L}\phi_c R + h.c.)}_{\mu}$

interactions between quarks and gluons

fermion masses and couplings to Higg

We begin with Quantum Field Theory



hierarchical: $2 \rightarrow O(10) \rightarrow O(100)$ particles



The interaction of outgoing particles with the detector is simulated.

>100 million sensors

Finally, we run particle identification and feature extraction algorithms on the simulated data as if they were from real collisions.

~10-30 features describe interesting part

DETECTOR SIMULATION

Conceptually: Prob(detector response | particles)

Implementation: Monte Carlo integration over micro-physics

Consequence: evaluation of the likelihood is intractable



DETECTOR SIMULATION

Conceptually: Prob(detector response | particles)

Implementation: Monte Carlo integration over micro-physics

Consequence: evaluation of the likelihood is intractable

This motivates a new class of algorithms for what is called **likelihood-free inference**, which only require ability to generate samples from the simulation in the "forward mode"

A COMMON THEME

ABC	
resources on approximate Bayesian computational methods	
P Search	
Home	

Home

This website keeps track of developments in approximate Bayesian computation (ABC) (a.k.a. likelihood-free), a class of computational statistical methods for Bayesian inference under intractable likelihoods. The site is meant to be a resource both for biologists and statisticians who want to learn more about ABC and related methods. Recent publications are under Publications 2012. A comprehensive list of publications can be found under Literature. If you are unfamiliar with ABC methods see the Introduction. Navigate using the menu to learn more.

ABC in Montreal ABC in Montreal (2014)

ABC in Montreal

Approximate Bayesian computation (ABC) or likelihood-free (LF) methods have developed mostly beyond the radar of the machine learning community, but are important tools for a large and diverse segment of the scientific community. This is particularly true for systems and population biology, computational neuroscience, computer vision, healthcare sciences, but also many others.

Interaction between the ABC and machine learning community has recently started and contributed to important advances. In general, however, there is still significant room for more intense interaction and collaboration. Our workshop aims at being a place for this to happen.

NIPS 2016

BARCELONA · SPAIN · DECEMBER 5 - 10, 2015 | http://nips.cc/

TUTORIALS

Deep Reinforcement Learning Through Policy Optimization Pieter Abbeel (OpenAI, UC Berkeley) and John Schulman (OpenAI)

Large-scale Optimization: Beyond Stochastic Gradient Descent and Convexity Francis Bach (INRIA, ENS) and Suvrit Sra (MIT)

Variational Inference: Foundations and Modern Methods David Blei (Columbia), Shakir Mohamed (Google Deepmind) and Rajesh Ranganath (Princeton)

Natural Language Processing for Computational Social Science Cristian Danescu-Niculescu-Mizil (Cornell) and Lillian Lee (Cornell)

Generative Adversarial Networks Ian Goodfellow (OpenAI)

Theory and Algorithms for Forecasting Non-stationary Time Series Vitaly Kuznetsov (Google) and Mehryar Mohri (Courant Institute, Google Research)

Deep Learning for Building Al Systems Andrew Ng (Baidu, Stanford University)

ML Foundations and Methods for Precision Medicine and Healthcare Suchi Saria (Johns Hopkins) and Peter Schulam (Johns Hopkins)

Crowdsourcing: Beyond Label Generation Jenn Wortman Vaughan (Microsoft Research)

INVITED SPEAKERS

Reproducible Research: the Case of the Human Microbiome Susan Holmes (Stanford University)

Dynamic Legged Robots Marc Raibert (Boston Dynamics)

Intelligent Biosphere Drew Purves (Google DeepMind)

Predictive Learning Yann LeCun (Facebook and New York University)

Machine Learning and Likelihood-Free Inference in Particle Physics Kyle Cranmer (New York University)

Learning About the Brain: Neuroimaging and Beyond Irina Rish (IBM T.J. Watson Research Center)

Engineering Principles From Stable And Developing Brains Saket Navlakha (The Salk Institute for Biological Studies)

SYMPOSIA

Recurrent Neural Networks and other Machines that Learn Algorithms Alex Graves (Google DeepMind) Juergen Schmidhuber (IDSIA) Rupesh Srivastava (IDSIA) Sepp Hochreiter (Johannes Kepler University)

Deep Learning Navdeep Jaitly (Google) Roger Grosse (University of Toronto) Yann LeCun (New York University & Facebook)

Machine Learning and the Law Adrian Weller (Cambridge, Alan Turing Inst.) Conrad McDonnell (Gray's Inn Tax Chambers) Jatinder Singh (University of Cambridge) Thomas Grant (University of Cambridge)

ORGANIZING COMMITTEE

General Chairs: Daniel D Lee (University of Pennsylvania) Masashi Sugiyama (The University of Tokyo)

Program Chairs: Ulrike von Luxburg (University of Tübingen) Isabelle Guyon (Clopinet)

Tutorials Chair: Joelle Pineau (McGill University) Hanna Wallach (Microsoft)

Workshop Chairs: Ralf Herbrich (Amazon)

Demonstration Chair: Raia Hadsell (Google DeepMind)

ANA AND DOLODAL

Publications Chair & Electronic Proceedings Chair: Roman Gamett (Washington University)

Program Managers: Krikamol Muandet (Mahidol University and MPI) Rohit Babbar, Behzad Tabibian (MPI for Intelligent Systems)

PROGRAM COMMITTEE

Emmanuel Abbe, Princeton Univ. Alekh Agarwal, Microsoft Anima Anundkumur, UC Irvine Chloé-Agathe Azenoct, MINES ParisTech Shai Ben-David, Univ. Waterloo Alina Boygétzimer, Yahoo Research Jeff Bitmes, Univ. of Watshington, Seattle Gilles Blanchard, Univ. of Potsdam Matthew Blaschko, KU Leuven Tamara Broderick, MIT

 Sebastien Bubeck, Princeton
 Finale Doshi-Vel

 Alexandra Carpentier, Univ. Potsdam
 Ran El-Vank, Te

 Miguel Carreira-Perpinan, UC Merced
 Hugo Jair Escalu

 Kamtalika Chavethuri, UC San Diego
 Sergio Escalera

 Gal Chechik, Googie, Bar-Ilan Univ.
 Maryam Fazel, I

 Azoro Couville, Univ. of Montreal
 Rob Fergues, Ne

 Koby Crammer, Technion
 Xiacli Fern, Oreg

 Florence d'Alché-Buc, Tolecom Paris Tech
 Surya Ganguli, S

 Arnak Dalalyan, ENSAE ParisToch
 Surya Ganguli, S

 Marc Deisenroth, Ingerial College London
 Peter Gehler, Ur

 Francesco Dinuzzo, Amazon
 Claudo Gentie, C

Finale Doshi-Velez, Harvard Ran El-Yaniv, Technion Hugo Jair Escalante, INACE Sergio Escalera, Univ. of Barcelona Maryam Fazel, Univ. of Barcelona Asas Feragon, Univ. of Gopenhagen Rob Fergus, New York Univ. Xiaoli Fern, Oregon State Univ. Francois Flauret, Idiap Research Institute Surya Gangui, Stanford Peter Gehler, Univ. of Tübingen Claudo Gentle, DISTA, Universita dell'Insubria

Lise Getoor, UC Santa Cruz Mark Girotami, Imporial College London Amir Globerson, Tol Aviv Univ. Yoav Gokberg, Bar Ilan Univ. Manuel Gomiz, Max Planck Institute Yves Grandviet, Univ. of Compigne & CNRS Moritz Grosse-Wentrup, MPI Zaid Harchaoui, Univ. of Washington Mortz Hatt, Google Matthias Hein, Skartland Univ. Philipp Hennig, MPI IS Tübingen Frank Hubr, Univ. of Freiburg

Pratoek Jain, Microsoft Research Navdeep Jaity, Google Brain Stefanie Jegeka, MIT Samuel Kaski, Aato Univ. Koray Kavukcuoglu, Google DeepMind Jens Kober, TU Deith Samory Kpotufe, Princeton Univ. Sarby Kpotufe, Princeton Univ. Sarby Kwok, Hong Kong Univ. Simon Lacoste-Julion, U. of Montreal Christoph Lampert, IST Austria Hugo Larochello, "Witter Francois Laviolette, L'Université Laval Honglak Lee, Univ. et Michigan Christoph Lippert, Human Longevity Po-Ling Loh. UNV-Madison Phil Long, Sersteint Technologies Jakob Macke. Caesar Bonn Julien Mairat, Innia Shie Mannor, Technion Manna Meila, Univ. et Washington Claire Monteleoni, George Washington Univ. Guilaume Obozinski, Ecole Paris Mehro Cheng Seon Ong, DataB1 and ANU Rusla Francesco Orabona, Stony Brook U. Purna Fernando Perez-Cruz, Universidad Fei St Carlos III de Madrid, Bel Labs (Nokia) Jonathan Pilow, Princeton Univ. Jonati Doina Precup, MGBI Montreal David Alain Rukotomamonjy, Univ. of Rouen Masuel Rodriguez, Max Planck Inst. Romer Rosales, Linkedin Bhara Lorenzo Rosasco, U. of Genova, MIT Penns Sivan Sabato, Ben-Gurion Univ. Enk S

Mehreen Saeed, FAST, Univ of CES Cr Rustan Salakhudsinov, CMU G Purnamvta Sarkar, Univ. T. Austin Ar Fei Sha, USC Ru Ohad Shami Weizmann, Inst of Science Br Jonathon Shlens, Google Brain Je David Sontag, New York Univ. Br Suvit Sra, MiT Je Karthik Sridharan, Cornell Univ. Mi Bharath Sriperumbudur, Li Pennsyivania State Univ. Ku Enk Sudderth, Brown Univ.

Csaba Szepesvari, Univ. of Alberta Graham Taylor, Univ. of Gueiph Ambuj Tewari, Univ. of Michigan Ruth Urner, MPI Tübingen Benjamin Van Roy, Starford Jean-Philipo Ven, MNES ParisTech Bob Williamson, Data61 and ANU Jeonider Wortman, Vaughan Microsoft Research Lin Xiao, Microsoft Research Kun Zhang, CMU

REFE

Conclusions

CONCLUSIONS

A large portion of the scientific process involves interaction between theory and experiment

- The scientific process does not end when the results of an analysis are published in a paper!
- this requires a different type of infrastructure
- often neglected or addressed post-facto

I recommend targeted approach to theory/experiment interface

- An open-ended approach often gets bogged down
- start by identifying problems of scientific value with limited scope

Reusable & composable workflows are incredibly helpful and recent technology from industry makes it possible

Backup

EXAMPLE RECAST → HEPDATA / ZENODO

After re-running analysis on new physics model, experiments might want to push result of new interpretation to HEPData. Technically we can do this with Zenodo. Discussing with HEPData and INSPIRE to have API connection to upload result. Both are based on Invenio, so should be easy.

• this allows for new results to get a DOI and be associated with the original analysis publication



"NETFLIX FOR MONTE CARLO"

Lukas has prototyped a web service called Aretha that encapsulates Monte Carlo tools and wraps them as a web service.

- Specific version of "cards" configuring Monte Carlo generator
- specific installation (stored in a docker container) that ensures version of generator and other dependencies (compiler etc.)



In recent years, the idea of regarding computing infrastructure as a service has quickly changed the standard procedures among IT specialists to provision end deploy networked applications. Among others, Google and Amazon provide these laaS (infrastructure as a Service) services that are the backbone of may resource intensive applications. This change in perspective on computing resources allows us to revisit the traditional \emph{modi operandi} within both the experimental and phenomenological high-energy physics communities. A main interface between these sub-field are the Monte-Carlo generators used to produce simulated particle collisions. Among the leading software products here are SHERPA, Herwig, or MadGraph. Conventionally, these codes are used to produce collisions, that can be optionally written out in several standardized file formats, most often the HepMC event format. These events are then, for example, analyzed directly e.g. with tools such as Rivet or used by high-energy physics experiments such as those at the LHC, to serve as input into the detector simulation to produce fully-simulated particles collisions, which can be then compared to data https://github.com/aretha-hep/aretha-doc

- ideally, give DOIs to the generator cards and docker container
- can generate more consistent MC on demand

LIKELIHOOD FREE INFERENCE

DeepMind and OpenAI releasing simulators to train advanced machine learning models

Similarly, HEP could / should release simulation tools and analysis workflows to produce training data for ML.

Also, new "likelihoodfree" inference techniques (like Approximate Bayesian Computation) require running the simulation Observations





A sample of Universe game environments played by human demonstrators.

http://beta.briefideas.org/ideas/ff0489d51bdb17359cef823c1d6b7029

Create standalone simulation tools to facilitate collaboration between HEP and machine learning community

By Pierre Baldi, Peter Sadowski, Daniel Whiteson, <u>Christian Lorenz</u> <u>Müller</u>, Michael Williams, Lukas Heinrich, Steven Schramm, Maurizio Pierini, Sergei Gleyzer, Amir Farbin, jean-roch vlimant, Tim Head, Juan Pavez, Peter Elmer, Balázs Kégl, Andrey Ustyuzhanin, Vladimir Gligorov, Gilles Louppe, Kyle Cranmer

dslhc machinelearning datascience open data simulation

Discussions at recent workshops have made it clear that one of the key barriers to collaboration between high energy physics and the machine learning community is access to training data. Recent successes in data sharing through the HiggsML and Flavours of Physics Kaggle challenges have borne much fruit, but required significant effort to coordinate.

While static simulated datasets are useful for challenges, in the course of investigating new machine learning techniques it is advantageous to be able to generate training data on demand (e.g. Refs. 1, 2, 3).

Therefore we recommend efforts be made to produce the ingredients required to facilitate such collaboration:

- Specific challenges for HEP experiments should be fully specified such that minimal domain-specific knowledge is required to attack them.
- Stand-alone simulators should be made open source. They should be developed to be easy to use without domain-specific expertise, while still being representative of real experimental challenges. Such a simulation will permit non-HEP researchers to generate realistic HEP datasets for training and testing. These simulators could range from truth-level simulation of a hard scattering to fast simulation like Delphes, to full GEANT4 simulation of sensor arrays.
- Performance metrics (objective functions) and operational constraints should be defined to evaluate proposed solutions.



Actions



Authors

Pierre Baldi, Peter Sadowski, Daniel Whiteson, Christian Lorenz Müller, Michael Williams, Lukas Heinrich, Steven Schramm, Maurizio Pierini, Sergei Gleyzer, Amir Farbin, jean-roch vlimant, Tim Head, Juan Pavez, Peter Elmer, Balázs Kégl, Andrey Ustyuzhanin, Vladimir Gligorov, Gilles Louppe, Kyle Cranmer

Metadata

DOI 10.5281/zenodo.46864

Published: 26 Feb, 2016



ENCAPSULATING THE SIMULATION



https://github.com/lukasheinrich/weinberg-test

E README.md

Run HEP workflows from the web.

by Kyle Cranmer and Lukas Heinrich

An example notebook on how to generate simulated high energy physics collision events using the generator package MadGraph. Simulated datasets obtained from this notebook can then be used to train and evaluate the performance of generative models for physics.

Usage:

This repository has been equipped with a Dockerfile to encapsulate its software environment. It can be used with the mybinder service to launch an ephemeral jupyter notebook server to run the notebook.

Click on the below badge and open the notebook adage.ipynb.

launch binder

$$\begin{split} \mathcal{L}_{SM} = & \underbrace{\frac{1}{4} \mathbf{W}_{\mu\nu} \cdot \mathbf{W}^{\mu\nu} - \frac{1}{4} B_{\mu\nu} B^{\mu\nu} - \frac{1}{4} G^a_{\mu\nu} G^{\mu\nu}_a}_{\text{kinetic energies and self-interactions of the gauge bosons}} \\ & + \underbrace{\bar{L} \gamma^{\mu} (i \partial_{\mu} - \frac{1}{2} g \tau \cdot \mathbf{W}_{\mu} - \frac{1}{2} g' Y B_{\mu}) L + \bar{R} \gamma^{\mu} (i \partial_{\mu} - \frac{1}{2} g' Y B_{\mu}) R}_{\text{kinetic energies and electroweak interactions of fermions}} \\ & + \underbrace{\frac{1}{2} \left| (i \partial_{\mu} - \frac{1}{2} g \tau \cdot \mathbf{W}_{\mu} - \frac{1}{2} g' Y B_{\mu}) \phi \right|^2 - V(\phi)}_{W^{\pm}, Z, \gamma, \text{and Higgs masses and couplings}} \\ & + \underbrace{\frac{g''(\bar{q} \gamma^{\mu} T_a q) G^a_{\mu}}_{\text{interactions between quarks and gluons}} + \underbrace{(G_1 \bar{L} \phi R + G_2 \bar{L} \phi_c R + h.c.)}_{\text{fermion masses and couplings to Higgs}} \end{split}$$







Analysis as a function mapping data and models to results



collision data from LHC detector

EW YORK UNIVERSITY

Analysis Preservation: two-step process

Modern HEP analysis:

• Multiple steps/code-bases, possibly developed by independent teams, with differing software requirements. Example: one team developing the event selection, another team developing the statistical analysis

Need to capture:

1. Individual processing steps

- code bases
- software environments
- identify binaries, scripts in code base
- templates how to run binaries (semantic description of arguments, naming etc..)
- description of step output, what are the relevant data fragments

2. How to connect these steps

- How to wire individual steps together
- What outputs of which steps, are used as inputs for other steps, ...

Goal: capture all this with least amount of work for analysis teams, preferably *while analysis is being developed. Should not take make than a few days*

How to preserve $f_{\text{analysis}}(\cdot)$?

1. Problem: Preserve Individual Processing Steps

(Example: Run Detector Simulation + Reconstruction on MC events)

Example:

process:

```
process_type: 'string-interpolated-cmd'
cmd: 'DelphesHepMC {delphes_card} {outputroot} {inputhepmc}'
publisher:
    publisher_type: 'frompar-pub'
    outputmap:
        rootfile: outputroot
environment:
    environment_type: 'docker-encapsulated'
    image: lukasheinrich/root-delphes
```

python package: "packtivity"

- executes packtivities according to JSON spec for given parameters
- cli tool and python bindings
- multi-host / remote execution ready via e.g. Docker Swarm

CLI tool



How to preserve $f_{\text{analysis}}(\cdot)$?

2. Problem: Preserve Parametrized Workflow



Natural Data Model: directed acyclic graphs (DAGs)

- nodes: individual steps
- edges: dependency relations

Two place where parametrization enter:

- individual steps parametrized: covered by "packtivities" graph topology may *depend on the parameters* of the analysis and only emerge during run-time
- 2. Examples:
 - variable number of created files during execution,
 - conditional choices (if/else)/flags do enable/disable steps, e.g. run systematics / not



How to preserve $f_{\text{analysis}}(\cdot)$?

2. Problem: Preserve Parametrized Workflow

Therefore: Sequentially build up graph, as sufficient information becomes available, using a number of stages that add nodes and edges step 1 To capture analysis workflow, capture the stages. **Example: Parametrized** step 2 step 3 **Map-Reduce** step 4 step 5 step 6

Stage 1: unknown number of files. e.g. download & unpack archive with a priori unknown # of files

Stage 2: for each file in the archive, add node to process it (only possible after first node done)



Stage 3:

add a node that merges results of the map nodes node/edge can be added before execution of map nodes



NEW YORK UNIVERSITY

Technical Solution:

Preserve Software using industry standard Linux Containers (Docker)

- industry backed (Google, Amazon, ...) solution for reproducible software environments. Like a VM, but boots in milliseconds.
- complete freedom for analysis team on software choices. Makes no assumption on how you run your code ("snapshot your work directory")
- can capture using a script or in an interactive session :

```
lxplus> docker run ... #start snapshot session
container> svn co ...
container> make ...
lxplus> docker commit ... #save snapshot of workdir
```









Many people contributing now. Contributions from CERN, DASPOS, DIANA, GitHub, Moore-Sloan Data Science Environment at NYU, Notre Dame, Nebraska, ...

Using **yadage** and **packtivity** JSON schemas developed by Lukas Heinrich and described in draft DASPOS technical report for packaging realistic LHC analyses

CERN Analysis Portal (CAP) is able to store and serve up analysis workflows stored in this format.

New front-end webpage thanks to Christian Bora (Nebraska, DASPOS) and Eamonn Maguire (CERN)

