



### Computing Coordination Meeting Monday 2021-10-18

**The Software and Computing WG Conveners:** Andrea Bressan (University of Trieste and INFN), Dmitry Romanov (Jefferson lab), Sylvester Joosten (Argonne National Laboratory), Whitney Armstrong (Argonne National Laboratory), Wouter Deconinck (The University of Manitoba)



# Philosophy: Let's prepare for our future at the EIC!

- Build forward-looking team of developers to ensure the long-term success of the EIC scientific program in software & computing.
- Focus on modern scientific computing practices
  - Strong emphasis on modular orthogonal tools.
  - Integration with HTC/HPC, CI workflows, and enable use of data-science toolkits.
- Avoid "not-invented-here" syndrome, and instead leverage cutting-edge CERN-supported software components where possible.
  - Build on top of mature, well-supported, and actively developed software stack.
  - Externalize support burden where possible.
- Actively work with the EICUG SWG to help develop and integrate community tools for all collaboration.



# Software Stack In A Nutshell

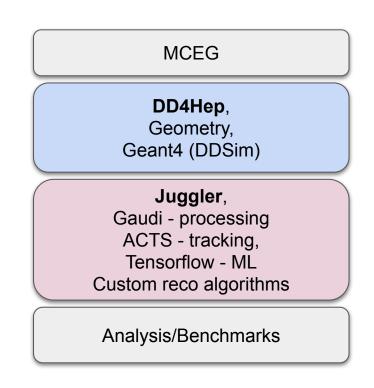
**DD4hep**: TGeo and Geant4 geometry definition, detector plugin library, wrappers to run Geant4.

**Juggler**: Digitization and reconstruction algorithms (based on Gaudi with Podio-based data model and genfit/ACTS for tracking).

**Gaudi**: Generic open project for building auto-scaling event processing frameworks. Enables task-based concurrent execution in a heterogeneous computing environment. Encourages efficient coding practices.

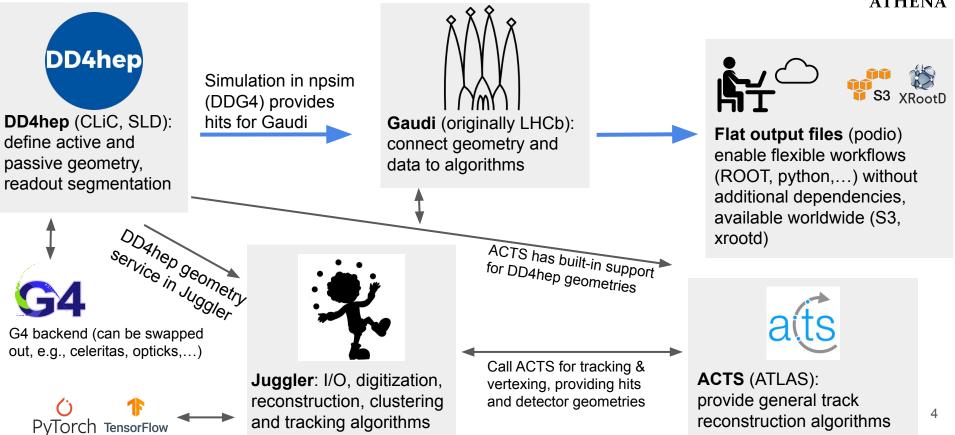
**ACTS**: Experiment-independent tracking toolkit (geometry constructed from DD4hep via plugin).

**Podio**: Robust data model definition to cross the boundaries between tools, independent of file format.



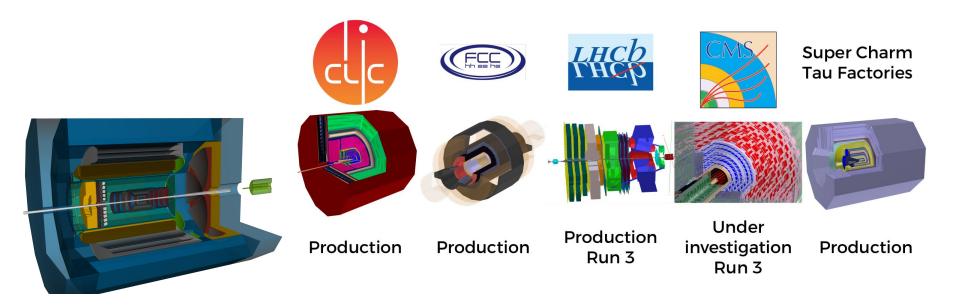


# ATHENA Software Ecosystem: Emphasis On Modularity



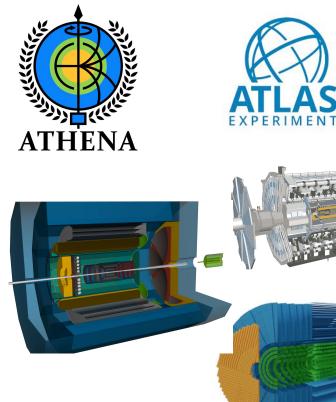
# The DD4hep community

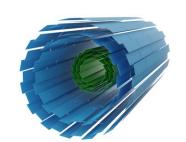




"framework for providing a complete solution for full detector description (geometry, materials, visualization, readout, alignment, calibration, etc.)"

# The ACTS community

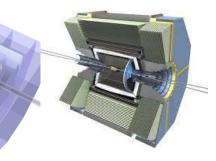


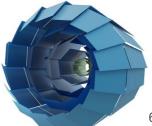


SPHENIX









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# Automated Workflows at eicweb



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### GitLab server (eicweb.phy.anl.gov)

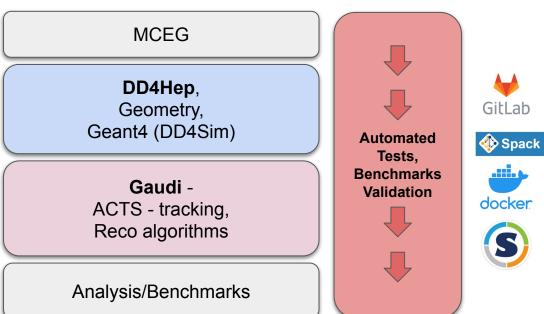
- mirrored on github.com/eic
- continuous integration
- dedicated build cluster

Runs automatically on each user commit, executing workflows running multiple tests, benchmarks and analysis

### **Automated containers**

Both Docker and Singularity images are created nightly or on demand (commit) providing:

- reproducibility,
- production level images
- latest updates for those working locally



### Why use a custom GitLab server?

- CI system loses benefits with shared, queued jobs
- Our collaboration controls users, yet access to HPC

## Automated Workflows at eicweb



### **High Level Requirements**

- Failures should show up in minutes, but benchmarking may take longer.
- Merge request cannot be held up by checks for more than ~two hours.
- Modular framework with large dependencies (root, geant4, ACTS) results in large containers, which must be distributed efficiently to CI nodes.
- Access for new users at institutions without MOU/NPUA (e.g. EIC India) without a lengthy approval process.
- Compliance with data management, export controls (private repositories).

### Infrastructure at ANL

- Dedicated servers with 384 job slots to run ~10-minute to 3-hour long CI pipelines of ~50 to ~100 individual steps for commits and merge requests. (Github free tier: 2k mins / month)
- Docker build server of 128 cores and high bandwidth to distribute to nodes with modified gitlab-runners running unprivileged singularity containers.
- Integrated development environment with kubernetes for container shells.
- Full control over users accounts, no lab account required.

# This infrastructure was not available on short notice at either BNL or JLab.











# Automated Workflows: Local Environment Access



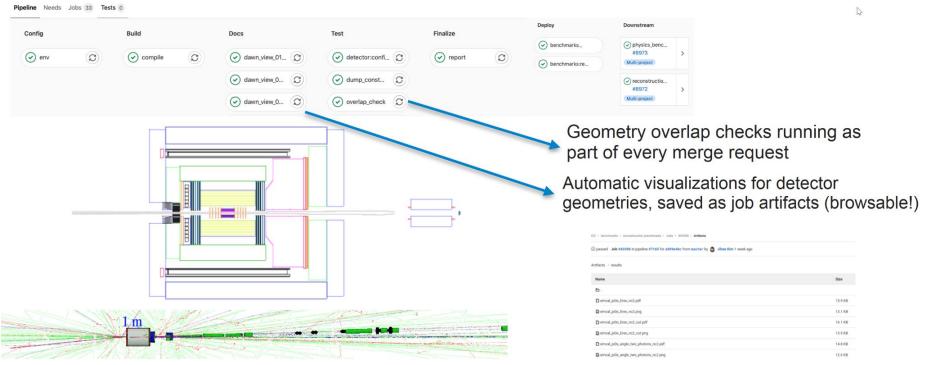
curl -L get.athena-eic.org | bash

• Uses images on /cvmfs when available, downloads singularity sifs otherwise.

• Basis of scalable computing on OSG: same containers are used everywhere.

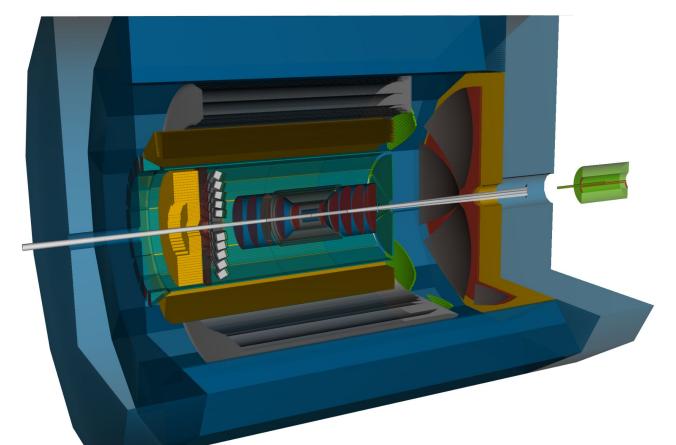


# Benchmarks, Documentation, Containerization



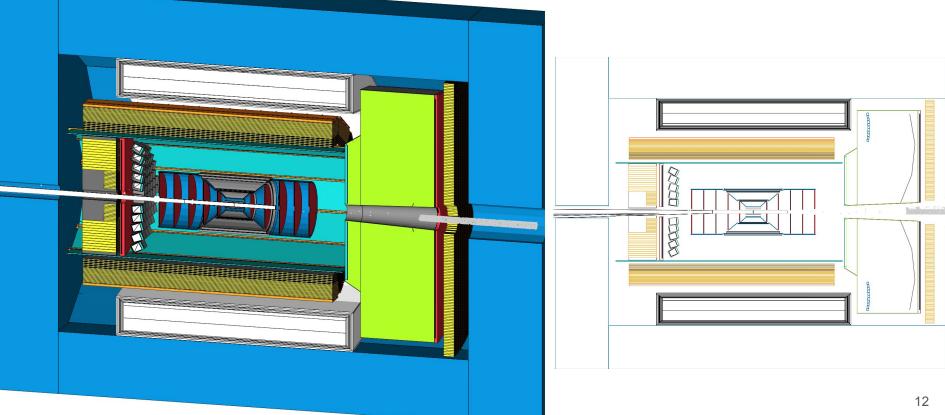
# ATHENA

### Automatic Visualization



### Automatic Visualization







### **Development Boards on eicweb**

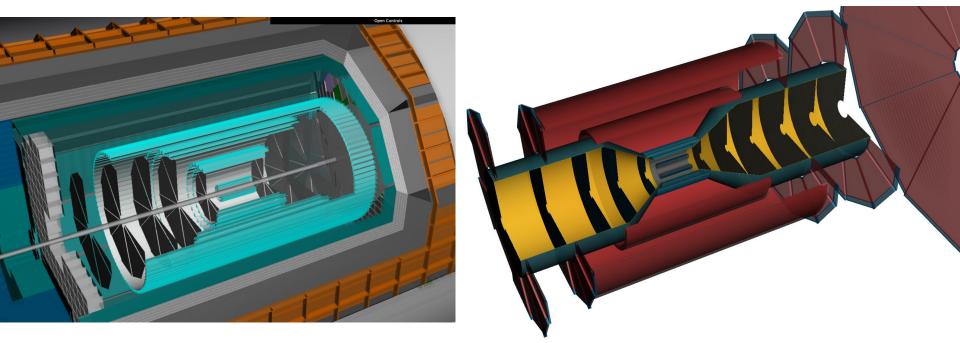
- <u>https://eicweb.phy.anl.gov/groups/EIC/-/boards</u>
- Working to polish/integrate task list to make it easier for people to find/check out a task

> Open D 154 +	> Doing D 2 + Q	> important D 14 + Ø	> critical D 8 + O	> priority D 5 + 🌣	Closed □ 375
DVMP process benchmark (DVM2) exclusive process (new benchmark ElC/benchmarks/physics_benchmarks#2	Optimize Barrel EM Calo geometry ElC/detectors/topside#24	Add some basic usage examples (documentation) EIC/eicd#2	Fix juggler options file EIC/benchmarks/physics_benchmarks#19	Beampipe Smultion EIC/detectors/ip081	Implement WSCFi for the hadron endcap endersy EIC/detectors/athena#10
Detailed tracker space frame and servcies EIC/detectors/athena#5	HCal clustering benchmark centisal) cenhascement, priorty ctatus update needed EIC/benchmarks/reconstruction_benchmarks#31	Triggering large simulations discussion (framework) (simulation)	Benchmarks for sampling calorimetry with reference detector ElC/benchmarks/detector_benchmarks#6	First RICH Detector Benchmark	Material scan benchmark EIC/benchmarks/detector_benchmarks#54
Fill the documentation to presentable state EIC/documentation/athena#2		EIC/benchmarks/reconstruction_benchmarks#4	Discussion: Large output files.	EIC/benchmarks/reconstruction_benchmarks#8	MRICH: Add frame behind the entire system to stand in for support structure
		Eta -2.5 to -2.0: Energy resolution for e/gamma	EIC/benchmarks/physics_benchmarks#7	HCal clustering benchmark	EIC/detectors/athena#86
DIS benchmark (deep inelastic scattering) new benchmark EIC/benchmarks/physics_benchmarks#3		PodioInput to PodioOutput	Update B0 magnet design Nack-a-thon cimulation	Status update needed	$\begin{array}{ll} \mbox{MRICH: electronics/material budget} \\ \mbox{EIC/detectors/athena#91} & \overline{\tilde{t}}_{1-2}^{-1} \end{array}$
Implement ffi_NEG_TRK		bug::major event processing framework ELC/juggler#10	EIC/detectors/ip6#4	Forward Endcap dimentions for dRHIC/TRD/CAL, etc	mRICH alternative implementation EIC/detectors/athena#96
hack-a-thon low priority EIC/detectors/reference_detector#29		Forward track reconstruction.	Energy resolution as a function of E  Dec 23, 2020  EIC/benchmarks/reconstruction_benchmarks#11	EIC/detectors/athena#67 🕸	Change number of imaging layers in Barrel ECAL
First SIDIS benchmark SIDIS new benchmark semi-inclusive process		EIC/juggler#15 🛱 Jul 28, 2020 🜘	Clean up found track output	Negative endcap ECAL breaks parametrization EIC/detectors/athena#69	EIC/detectors/athena#97
EIC/benchmarks/physics_benchmarks#4		4.0 to 5.0: Neutron Detector and hadron calorimeter	EIC/juggler#18 🛱 Dec 23, 2020 👰		Flip dawn top views EIC/detectors/athena#99
Conic part of ECal barrel hack-a-thon low priority simulation		EIC/benchmarks/reconstruction_benchmarks#15	Material mapping		Simplify switching imaging layer number for
EIC/detectors/reference_detector#46		MRich optics EIC/detectors/athena#48	EIC/NPDet#76 💾 May 20		Barrel ECAL EIC/detectors/athena#100
Detailed Magnet and Field Map hackathon EIC/detectors/reference_detector#4		3.5 to 5.0: Far forward tracking EIC/benchmarks/reconstruction_benchmarks#16	HCal clustering benchmark (Deing) (enhancement) (priority) (status update needed) ElC/benchmarks/reconstruction_benchmarks#31		Beampipe reduced by 5 mm for ACTS geometry bug:minor (priority) (reconstruction) (tracking) EIC/detectors/tp6#38
Implement fi_B0_EMCAL		Eta 1.0 - 3.0: Forward detector PID			Fix DD contor position

# Detailed geometry implementation

EXAMPLE: Tracking Systems





# **Computing Philosophy**



### **Encourage Upstream Contributions**

- Requirements of well-formed HepMC as input has resulted in real improvements to multiple MCEGs used by EIC community.
- Various upstream contributions to DD4hep, ACTS, Spack, uproot,...

### **Encourage Social Coding**

- CI platform provides the incentive for developers to commit code frequently: achieving data management and analysis preservation goals.
- Merge request reviews ensure higher quality code and build developer skills.

### **Enable Access Without Restrictions**

- ATHENA collaboration members include INFN, EIC India, LBL, ANL,...
- Data 'publicly' available through BNL S3 and publicly available through JLab xrootd.
- Flat data structures (i.e. could be a csv), stored as ubiquitous ROOT trees without need for data structure libraries.
- Support for uproot using numpy library (awkward not needed).

### **Under Evaluation**

- Rucio for data management
- Reana for analysis workflows

# Anatomy Of ATHENA Jobs



- 1. HepMC3 files generated by physics working groups (or internal single particle generator):
  - a. Pythia8: full beam crossing angle and divergence effects included in hepmc3
  - b. Other generators: hepmc3-to-hepmc3 afterburner to boost head-on collisions (independent of ATHENA: contribution to the EIC community)
- 2. CI analysis of HepMC3 files (produces csv artifacts):
  - a. Running test, smoke tests, sanity checks, time-per-event determination
- 3. Job submission (identical syntax for slurm and condor systems)
  - a. Automatic retrieval of csv artifacts, automatic job strategy determination
  - b. No user code is needed: all submission support is available on /cvmfs
- 4. Job progression on node (entirely inside on container on /cvmfs)
  - a. S3 download of HepMC3 file
  - b. Run full simulation (downloads additional artifacts as needed)
  - c. S3 upload of full simulation podio output
  - d. Several reconstruction strategies (downloads additional artifacts as needed)
  - e. S3 upload of reconstruction podio outputs
- 5. Mirroring from S3 to xrootd

# **Operational Benefits of OSG Jobs**



#### Running at JLab (capacity 25k job slots, 14% for EIC) Running on OSG (capacity 50k) osgsub1.sdcc ifarm job node /volatile/eic /work/eic S3/ATHENA dtn1902 OSG job node S3/ATHENA .bnl.gov start condor submit start request hepmc3 request hepmc3 retrieve hepmc3receive hepmc3 sbatch local hepmc3 copy copy full simulation output copy full simulation copy reconstruction output copy reconstruction copy logging output copy logging output copy condor logs mirror reconstruction output copy reconstruction output mirror logging output copy logging output mirror full output copy full output

Now 500 TB each on /work/eic{2,3}; larger EIC xrootd service

Also mirroring S3 to xrootd at JLab



# Questions?