FH SciComp Workshop 2024

Report of Contributions

https://indico.desy.de/e/44550

Contribution ID: **1** Type: **not specified**

DESY and the NFDI

Monday 1 July 2024 16:10 (15 minutes)

DESY plays a significant role in the German national research data infrastructure, with the PUNCH4NFDI and DAPHNE4NFDI consortia both being led by DESY scientists, and with strong contributions to their science goals. The NFDI consortia are now half-way through their first funding period of five years, and deliberations and discussions are commencing on the future setup of PUNCH4NFDI and DAPHNE4NFDI in a potential second funding period.
In this presentation, we give a short introduction to the NFDI and to PUNCH4NFDI as the consortium of particle, astroparticle, hadron&nuclear, and astrophysics, and we discuss potential future directions and projects. We also invite for discussion on and contributions to the shaping of a future programme for PUNCH4NFDI.

Authors: SCHNEIDE, Christiane (FTX (FTX Fachgruppe SFT)); SCHÖRNER, Thomas (DESY)

Presenter: SCHNEIDE, Christiane (FTX (FTX Fachgruppe SFT))

Session Classification: Scientific Computing I

Contribution ID: **2** Type: **not specified**

Belle II detector alignment with Millipede II

Monday 1 July 2024 16:25 (15 minutes)

The Belle II experiment at the SuperKEKB accelerator aims at precision measurements in B, tau and charm physic sectors. Many such measurements rely on high precision vertexing and thus precise alignment of the detection elements. A global alignment method utilizing Millepede II software package will be presented, which determines around sixty thousand alignment parameters simultaneously. Computational requirements as well as complex time-dependence of the alignment of the newly installed pixel sub-detector pose new challenges for future operation, which will be briefly discussed.

Author: BILKA, Tadeas (BELLE (BELLE Gruppe))

Presenter: BILKA, Tadeas (BELLE (BELLE Gruppe))

Session Classification: Scientific Computing I

Contribution ID: **3** Type: **not specified**

Solving the CMS High Granularity Calorimeter's Data Processing Challenges with Heterogeneous Computing

Monday 1 July 2024 16:40 (15 minutes)

CMS is upgrading its endcap detectors for the High-Luminosity LHC runs with a first-ever silicon/scintillator tracking calorimeter: HGCAL. It will allow to handle increased collision pile-up, improve the precision of measurements, and also enable completely new ways to search for new physics thanks to its particle-pointing and timing capabilities. However, these wonderful improvements come at a price - with over 6 million readout channels, processing the HGCAL's data becomes a significant challenge from the computing point of view. In this talk, I will introduce this future calorimeter of CMS, explain related computing challenges, as well as present how we are addressing them using heterogeneous computing.

Author: NIEDZIELA, Jeremi (DESY)

Presenter: NIEDZIELA, Jeremi (DESY)

Session Classification: Scientific Computing I

Contribution ID: **4** Type: **not specified**

Generative Machine Learning at CMS

Monday 1 July 2024 16:55 (15 minutes)

The CMS Generative Machine Learning Group will showcase three distinct projects, each utilizing point cloud-based generative models to advance particle physics research. The first project, "Attention to Mean Fields for Particle Cloud Generation", features an attention-based generative model that adeptly processes complex collider data represented as point clouds, demonstrating effectiveness on the JetNet150 and CaloChallenge datasets. The second project, "DeepTreeGAN", explores novel techniques for iterative up- and downscaling of point clouds, inspired by the tree-based development of particle showers. Finally, "CaloPointFlow" presents a generative model using normalizing flows.

Authors: KAECH, Benno (CMS (CMS Fachgruppe Searches)); KRUECKER, Dirk (CMS (CMS Fachgruppe Searches)); MELZER-PELLMANN, Isabell (Deutsches Elektronen-Synchrotron DESY); BORRAS, Kerstin (DESY and RWTH Aachen University); SCHAM, Moritz (CMS (CMS Fachgruppe Searches)); SCHNAKE, Simon Patrik (CMS (CMS Fachgruppe Searches))

Presenter: SCHNAKE, Simon Patrik (CMS (CMS Fachgruppe Searches))

Session Classification: Scientific Computing I

Contribution ID: **5** Type: **not specified**

Quantum algorithms for charged particle track reconstruction in the LUXE experiment

Monday 1 July 2024 18:00 (15 minutes)

We investigate the potential of quantum computers for pattern recognition in track reconstruction at LUXE, based on a quadratic unconstrained binary optimisation and a quantum graph neural network.

Authors: KROPF, Annabel (DESY); SPATARO, David (FTX (FTX Fachgruppe SLB)); MELONI, Federico (ATLAS (ATLAS SM and Beyond)); YAP, Yee Chinn (FTX (FTX Fachgruppe SLB))

Presenter: YAP, Yee Chinn (FTX (FTX Fachgruppe SLB))

Session Classification: Scientific Computing I

Contribution ID: **6** Type: **not specified**

4D track reconstruction with quantum algorithms

Tuesday 2 July 2024 10:00 (15 minutes)

We investigate the use of quantum algorithms to reconstruct charged particle trajectories from 4D tracker measurements.

Authors: SPATARO, David (FTX (FTX Fachgruppe SLB)); MELONI, Federico (ATLAS (ATLAS SM and Beyond)); YAP, Yee Chinn (FTX (FTX Fachgruppe SLB))

Presenter: SPATARO, David (FTX (FTX Fachgruppe SLB))

Session Classification: Scientific Computing II

Contribution ID: **7** Type: **not specified**

Summary of Scientific Research and Innovation Group (IT-RIC) activities

Tuesday 2 July 2024 09:30 (30 minutes)

I would like to report on activities of the IT-RIC group in supporting DESY scientific domains. This includes but is not limited to our work on:

- using Artificial Intelligence for advancing imaging in scientific applications;
- providing an open science platform including a catalogue for open data at DESY;
- providing a Helmholtz-wide Scientific IT Infrastructure, in collaboration with other Helmholtz Centers, for sharing compute and storage resources;
- providing Data Transfer and Data Orchestration Solutions to connect to Sciences in Europe based on WLCG technologies including access to European HPC centres.

Author: FUHRMANN, Patrick (IT (Research and Innovation in Scientific Co))

Presenter: FUHRMANN, Patrick (IT (Research and Innovation in Scientific Co))

Session Classification: Scientific Computing II

Contribution ID: **8** Type: **not specified**

CNNs and GNNs for tagging anomalous showers with ATLAS

Tuesday 2 July 2024 11:00 (15 minutes)

This talk will discuss recent work towards developing a ML (CNN/GNN) tagger to distinguish anomalous showers caused by the decays of long-lived particles from QCD jets with the ATLAS detector

Authors: MELONI, Federico (ATLAS (ATLAS SM and Beyond)); BAUCKHAGE, Lukas (ATLAS (ATLAS Upgrade))

Presenter: BAUCKHAGE, Lukas (ATLAS (ATLAS Upgrade))

Session Classification: Scientific Computing III

Contribution ID: **9** Type: **not specified**

Helmholtz Imaging Support Team in DESY-IT/RIC

The Helmholtz Imaging Support Team exploits and develops a broad spectrum of deep learning architectures, to a variety of challenges as they occur along the scientific imaging pipeline. The tasks include classification, segmentation, registration, generation, denoising, reconstruction and more. The most commonly used architectures in the team are CNNs, VAEs, GANs, MLPs, Autoencoder/Decoder and LLMs.

Authors: SCHWARTZ, David (IT (Research and Innovation in Scientific Co)); EREN, Engin (DESY / Helmholtz Imaging); AHRENS, Jennifer (IT (Informationstechnik)); HEUSER, Philipp (DESY/Helmholtz Imaging)

Presenter: HEUSER, Philipp (DESY/Helmholtz Imaging)

Session Classification: Scientific Computing II

Contribution ID: **10** Type: **not specified**

Tracker alignment of the CMS detector with Run 3 data

Tuesday 2 July 2024 10:15 (15 minutes)

The tracking system of the CMS experiment is the world's largest silicon tracker with its 1856 and 15148 silicon pixel and strip modules, respectively. To accurately reconstruct trajectories of charged particles the position, rotation and curvature of each module must be corrected such that the alignment resolution is smaller than, or comparable to, the hit resolution. This procedure is known as tracker alignment and will be described in the context of this talk with a focus on performance during the start of Run 3 data-taking.

Author: Dr PETERSEN, Henriette (CMS (CMS Fachgruppe TOP))

Presenter: Dr PETERSEN, Henriette (CMS (CMS Fachgruppe TOP))

Session Classification: Scientific Computing II

Contribution ID: **11** Type: **not specified**

Automation of the flavour tagging calibration software in the ATLAS experiment

Tuesday 2 July 2024 12:00 (15 minutes)

Particle cascades originating from quarks and gluons decays (jets) are omnipresent in proton-proton collisions at the LHC. The identification of jet flavours is essential for many physics searches at the ATLAS experiment. This is achieved using machine learning algorithms (taggers) which combine tracks and jets information to determine the flavour of the jets (b-jets, c-jets and light jets). These taggers are trained with simulated Monte Carlo events and, due to simulations imperfections, their performance need to be measured in data in order to extract correction factors for the simulation predictions. ATLAS developed a set of calibration techniques for different jets flavours to correct, then the correction factors need to be re-derived every time a new tagger is deployed. Automating the calibration workflow significantly accelerates the calibration cycle and makes it less prone to manual mistakes. We present the first automated calibration framework in ATLAS using REANA platform. The results are compared with the official results using 36.2 fb^{-1} of 13 TeV collisions data from ATLAS, and a new set of calibration results with a customised setup is also included. The same method can be applied in other contexts to reduce the amount of time and resources needed to achieve the scientific goals.

Author: BARAKAT, Marawan (Z_ATLAS (Experiment ATLAS))

Presenter: BARAKAT, Marawan (Z_ATLAS (Experiment ATLAS))

Session Classification: Scientific Computing III

Contribution ID: **12** Type: **not specified**

Precise Quantum Angle Generator Designed for Noisy Quantum Devices

Tuesday 2 July 2024 09:00 (15 minutes)

The Quantum Angle Generator (QAG) is a new quantum machine learning model designed to produce precise images on current Noise Intermediate Scale (NISQ) Quantum devices. The QAG model uses variational quantum circuits as its core, and multiple circuit architectures are evaluated.
This study explores the QAG model's noise robustness through an extensive quantum noise study. The results indicate that the model, when trained on a quantum device, can learn the hardware noise behavior and produce excellent outcomes. When simulated quantum hardware noise is included, the model's results remain stable until approximately 1.5% of noise during inference and almost 3% in training. However, running the noise-less trained model on real quantum hardware leads to a decrease in accuracy. If the model is trained on hardware, it can learn the underlying noise behavior, where the same precision is achieved by the noisy simulator. Additionally, the training showed that the model can recover precision even with significant hardware calibration changes during training with an increase of noise up to 8% for one qubit.
This work demonstrates the QAG model's ability to learn hardware noise behavior and deliver accurate results in the presence of realistic noise levels expected in real-world quantum hardware. The QAG model is utilized on simulated calorimeter shower images, which are employed in high-energy physics simulations to determine particle energies and to identify unknown particles at CERN's Large Hadron Collider.

Authors: KRUECKER, Dirk (CMS (CMS Fachgruppe Searches)); Dr REHM, Florian (CERN); BORRAS, Kerstin (DESY and RWTH Aachen University); Dr GROSSI, Michele (CERN); MONACO, Saverio (CMS (CMS Fachgruppe Searches)); VALLECORSA, Sofia (CERN)

Presenter: MONACO, Saverio (CMS (CMS Fachgruppe Searches))

Session Classification: Scientific Computing II

Contribution ID: **13** Type: **not specified**

Event Generators for Future Colliders

Monday 1 July 2024 14:00 (20 minutes)

Author: REUTER, Juergen (DESY)

Presenter: REUTER, Juergen (DESY)

Session Classification: Scientific Computing for Future Colliders

Contribution ID: **14** Type: **not specified**

Discussion

Monday 1 July 2024 14:20 (10 minutes)

Session Classification: Scientific Computing for Future Colliders

Contribution ID: **15** Type: **not specified**

Key4hep - Core, Sim and Rec Tools for Future Colliders

Monday 1 July 2024 14:30 (20 minutes)

Author: MADLENER, Thomas (FTX (FTX Fachgruppe SFT))

Presenter: MADLENER, Thomas (FTX (FTX Fachgruppe SFT))

Session Classification: Scientific Computing for Future Colliders

Contribution ID: **16** Type: **not specified**

Discussion

Monday 1 July 2024 14:50 (10 minutes)

Session Classification: Scientific Computing for Future Colliders

Contribution ID: **17** Type: **not specified**

Applying Machine Learning to Future Colliders

Monday 1 July 2024 15:00 (20 minutes)

Author: GAEDE, Frank (FTX (FTX Fachgruppe SFT))

Presenter: GAEDE, Frank (FTX (FTX Fachgruppe SFT))

Session Classification: Scientific Computing for Future Colliders

Contribution ID: **18** Type: **not specified**

Discussion

Monday 1 July 2024 15:20 (10 minutes)

Session Classification: Scientific Computing for Future Colliders

Contribution ID: **19** Type: **not specified**

The SciComp Platform - Mandate, Mission, and Activities

Monday 1 July 2024 16:00 (10 minutes)

Author: WISSING, Christoph (DESY)

Presenter: WISSING, Christoph (DESY)

Session Classification: Scientific Computing I

Contribution ID: **20** Type: **not specified**

Open Data and Infrastructure Portal for DESY and HIFIS

Tuesday 2 July 2024 11:45 (15 minutes)

Following FAIR principles, we are setting up portals for access to Open Data and the corresponding infrastructure to explore the published data sets. The open datasets and their metadata are available in a Scicat instance to everyone interested and can either be downloaded directly or accessed through an open infrastructure portal called VISA upon reasonable request.
In the short talk I will present and architecture overview and short interaction examples with regard to the portals. A blueprint architecture of this setup will be available later this year in a comprehensible form for the scientific community.

Authors: FUHRMANN, Patrick (IT (Research and Innovation in Scientific Co)); WETZEL, Tim (IT (Research and Innovation in Scientific Co))

Co-authors: MILLAR, Alexander Paul (IT (Research and Innovation in Scientific Co)); AGGARWAL, Anjali (FS-EC (Experimente Control)); REPPIN, Johannes (IT (IT Information Fabrics)); PITHAN, Linus (FS-EC (Experimente Control)); Dr JANDT, Uwe (HIFIS / IT (Research and Innovation in Computing, RIC))

Presenter: WETZEL, Tim (IT (Research and Innovation in Scientific Co))

Session Classification: Scientific Computing III

Contribution ID: **21** Type: **not specified**

From testing cosmological inflation models to solving PDEs – dNNsolve: an efficient NN-based PDE solver

Monday 1 July 2024 17:25 (15 minutes)

!!!Please place me into the Monday afternoon 4:30 pm - 6 pm session!!!

Neural Networks (NNs) can be used to solve Ordinary and Partial Differential Equations (ODEs and PDEs) by redefining the question as an optimization problem. The objective function to be optimized is the sum of the squares of the PDE to be solved and of the initial/boundary conditions. A feed forward NN is trained to minimise this loss function evaluated on a set of collocation points sampled from the domain where the problem is defined. A compact and smooth solution, that only depends on the weights of the trained NN, is then obtained. This approach is often referred to as PINN, from Physics Informed Neural Network. Despite the success of the PINN approach in solving various classes of PDEs, an implementation of this idea that is capable of solving a large class of ODEs and PDEs with good accuracy and without the need to finely tune the hyperparameters of the network, is not available yet. In this paper, we introduce a new implementation of this concept - called dNNsolve - that makes use of dual Neural Networks with different activation functions to solve ODEs/PDEs. We show that dNNsolve is capable of solving a broad range of ODEs/PDEs in 1, 2 and 3 spacetime dimensions, without the need of hyperparameter fine-tuning.

Author: WESTPHAL, Alexander (T (Cosmology))

Presenter: WESTPHAL, Alexander (T (Cosmology))

Session Classification: Scientific Computing I

Contribution ID: **22** Type: **not specified**

MUSICS

Tuesday 2 July 2024 12:15 (15 minutes)

The main objectives of the project are to to develop a user friendly service via which users will be able to publish open data following the FAIR principles and also to find these published data again and access them in a convenient and performant way. The service shall be operable via a large language model based user interface so that users would be able to ‘’talk” to the service requesting the required actions. Behind the scenes the requests would be translated into search commands to the metadata catalogue and the results can be confirmed by the user. After the URL to the storage infrastructure has been given an automatic redirect to the corresponding storage infrastructure would be provided and the data are being served. This can be accomplished by combining the already existing components at DESY with the locally developed distributed storage middleware ‘’dCache” being in the centre of it. Further major components are the SciCat based metadata catalogue, the Helmholtz Authentication and Autorisation infrastructure as well as an easy to use landing page as user interface and for binding the components together.

Author: Dr SCHWARZ, Kilian (IT (IT Scientific Computing))

Co-authors: Prof. HUMM, Bernhard (Hochschule Darmstadt); STANITZKI, Marcel (FTX (FTX Fachgruppe TBT)); KARSTENSEN, Sven (FTX (FTX Fachgruppe AST))

Presenter: Dr SCHWARZ, Kilian (IT (IT Scientific Computing))

Session Classification: Scientific Computing III

Contribution ID: **23** Type: **not specified**

CaloClouds: Fast Geometry-Independent Highly-Granular Calorimeter Simulation with Diffusion Point Clouds

Tuesday 2 July 2024 12:30 (15 minutes)

A novel approach for fast simulation of energy depositions in high-granular detectors, essential for upcoming high-luminosity collider experiments.

Author: KOROL, Anatolii (FTX (FTX Fachgruppe SFT))

Presenter: KOROL, Anatolii (FTX (FTX Fachgruppe SFT))

Session Classification: Scientific Computing III

Contribution ID: **24** Type: **not specified**

Infrastructures for scientific computing & sutainability at DESY-IT

Monday 1 July 2024 17:40 (20 minutes)

Within the EU-Project RF2.0, DESY focus on sustainable scientific computing infrastructure splitted into more classical/obvious directions like, new architectures, longer system lifetimes, software efficiencies etc. and the model to operate a decent amount of compute resources with variable power consumption coupled to 'true RE power' availability at DESY location by steering the compute load - with dependencies amongst them. Beside these core technical challenges, which we believe are manageable within the project team, the true effective GHG emission reduction strongly depends on user acceptance. In other words - assume that will all be done and works, you will see job completion times extended (vary) and shifted job starting times (even if compute resources are available) due to unavailable RE power:
- what will be the motivation for each user to accept that ?
- i.e. bonus, directorate directive, being a good citizen, …

Authors: VOSS, Christian (DESY); GASTHUBER, Martin (IT (IT Scientific Computing)); KEMP, Yves (IT (IT Systems))

Co-author: Dr SCHWARZ, Kilian (IT (IT Scientific Computing))

Presenters: VOSS, Christian (DESY); GASTHUBER, Martin (IT (IT Scientific Computing)); KEMP, Yves (IT (IT Systems))

Session Classification: Scientific Computing I

Contribution ID: **25** Type: **not specified**

KAI-Project: Self Adaptive dCache

Tuesday 2 July 2024 11:15 (15 minutes)

dCache is a storage system for scientific institutions that manages large amounts of data in a distributed system. Although the dCache code base already has self-regulating mechanisms, there are still situations in daily operation, in which the storage system is overloaded. The challenge of the project is to identify indicators, which can be used to reliably identify the times and causes of overload. The focus here is on the identification and manipulation of relevant system parameters.

Authors: Mr DICHTE, Daniel; Mr CHRISTIANS, Felix; Mr SUDEIKAT, Jan; Mr SCHWARZ, Kilian; Mr GEBHARDT, Luca; Mr MANSOUR, Lukas; KÖHLER-BUSSMEIER, Michael; GRIZZO, Sandro (IT (IT Scientific Computing)); Mr MKRTCHYAN, Tigran; Mr PRIES, Tim

Presenter: GRIZZO, Sandro (IT (IT Scientific Computing))

Session Classification: Scientific Computing III

Contribution ID: **26** Type: **not specified**

ASAPO: A high-speed streaming framework to support an automated data-processing pipeline.

Monday 1 July 2024 17:10 (15 minutes)

Modern scientific experiments often generate large amounts of data, posing challenges for real-time processing and analysis. ASAPO, a high-performance streaming framework developed at DESY, addresses these challenges by providing a robust solution for online and offline data processing. Leveraging TCP/IP and RDMA over Ethernet and Infiniband, ASAPO facilitates high-bandwidth communication between detectors, storage systems, and analysis processes.

ASAPO offers user-friendly interfaces for C/C++ and Python on all major platforms, streamlining the development of data processing pipelines. A high-level Python library reduces boilerplate code and enables the creation of complex analysis workflows with ease. Key features include automatic retransfer, trivial parallelization on a per-image basis, support for multi-module detectors, and web-based monitoring capabilities.

Several experimental facilities at Petra III already benefit from ASAPO, employing it in various data-processing pipelines. Examples include azimuthal integration of X-ray scattering data, peak finding, and indexing of diffraction patterns. These applications demonstrate ASAPO's versatility and effectiveness in accelerating scientific discovery.

Authors: GASTHUBER, Martin (IT (IT Scientific Computing)); KARNEVSKIY, Mikhail (IT (IT Scientific Computing)); SCHOOF, Tim (DESY)

Presenter: KARNEVSKIY, Mikhail (IT (IT Scientific Computing))

Session Classification: Scientific Computing I

Contribution ID: **27** Type: **not specified**

Monte Carlo algorithms for lattice QCD simulations

Tuesday 2 July 2024 11:30 (15 minutes)

In this talk, I will discuss the basic ideas of Monte Carlo algorithms for computing correlation functions and how to extract physical information from them. In particular, I will discuss our recent use of advanced algorithms to reduce the statistical errors.

Author: BARCA, Lorenzo (Z_ZPPT (Zeuthen Particle PhysicsTheory))

Presenter: BARCA, Lorenzo (Z_ZPPT (Zeuthen Particle PhysicsTheory))

Session Classification: Scientific Computing III

Contribution ID: **30** Type: **not specified**

Quantum computing @ Scientific Computing

Tuesday 2 July 2024 09:15 (15 minutes)

An overview of my ongoing research projects with CQTA Zeuthen and a brief overview of where QC could be used in SC in the future.

Author: MANSOUR, Lukas (DESY IT Dual)

Presenter: MANSOUR, Lukas (DESY IT Dual)

Session Classification: Scientific Computing II