Experience of HSF-India HEP Software Workshop at NISER, Bhubaneswar During 18-22 dec, 2023

https://indico.cern.ch/event/1328624/

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Thanks to Dr. Prolay Kumar Mal for accepting our participation.

Topics Covered during the workshop

- Scientific Python
- Parallel Programming with GPUs
- Basics of Machine Learning
- Simulation techniques in HEP

- First, We had an introduction to python language, using the syntax, declaring variables , defining functions.

Defining variables

In [3]:
```
E = 68.1289790
px = -17.945541
py = 13.1652603
pz = 64.3908386
```

Now we can use `E` , `px` , `py` , `pz` :

In [4]:
```
px
```

Out[4]: -17.945541

The syntax for defining a function is:

In [8]:
```
def euclidean(x, y, z):
    return (x**2 + y**2 + z**2)**(1/2)

def minkowski(time, space):
    return (time**2 - space**2)**(1/2)
```

- Learned about how to import the standard python libraries.
- started using numpy

```
In [ ]: import numpy
```

```
In [ ]: from hepunits import GeV
        from particle import Particle
```

```
In [ ]: muon = Particle.from_name("mu+")
        muon
```

- Learned about the data types in python

```
In [1]: type(1)
Out[1]: int
```

```
In [2]: type("2")
Out[2]: str
```

- Different types of collection type in python i.e list , dict . Fetching and updating data in collection.

```
In [8]: some_list = [0.0, 1.1, 2.2, 3.3, 4.4, 5.5, 6.6, 7.7, 8.8, 9.9]
        some_list
Out[8]: [0.0, 1.1, 2.2, 3.3, 4.4, 5.5, 6.6, 7.7, 8.8, 9.9]
```

```
In [9]: type(some_list)
Out[9]: list
```

In [10]:
```
some_dict = {"one": 1.1, "two": 2.2, "three": 3.3}
some_dict
```
Out[10]:
```
{'one': 1.1, 'two': 2.2, 'three': 3.3}
```

In [11]:
```
type(some_dict)
```
Out[11]:
```
dict
```

In [12]:
```
len(some_dict)
```
Out[12]:
```
3
```

In [13]:
```
some_list[3]
```
Out[13]:
```
3.3
```

In [14]:
```
some_dict["two"]
```
Out[14]:
```
2.2
```

A little data analysis

In [17]:
```
particles = [
    {"type": "electron", "E": 171.848714, "px": 38.4242935, "py": -28.779644, "pz": 165.006927, "charge": 1,},
    {"type": "electron", "E": 138.501266, "px": -34.431419, "py": 24.6730384, "pz": 131.864776, "charge": -1,},
    {"type": "muon", "E": 68.1289790, "px": -17.945541, "py": 13.1652603, "pz": 64.3908386, "charge": 1,},
    {"type": "muon", "E": 18.8320473, "px": -8.1843795, "py": -7.6400470, "pz": 15.1420097, "charge": -1,},
]
```

In [18]:
```
def particle_decay(name, particle1, particle2):
    return {
        "type": name,
        "E": particle1["E"] + particle2["E"],
        "px": particle1["px"] + particle2["px"],
        "py": particle1["py"] + particle2["py"],
        "pz": particle1["pz"] + particle2["pz"],
        "charge": particle1["charge"] + particle2["charge"],
    }
```

```
In [19]: z1 = particle_decay("Z boson", particles[0], particles[1])
         z1

Out[19]: {'type': 'Z boson',
          'E': 310.34997999999996,
          'px': 3.992874499999999,
          'py': -4.106605600000002,
          'pz': 296.871703,
          'charge': 0}
```

```
In [21]: z2 = particle_decay("Z boson", particles[2], particles[3])
         z2

Out[21]: {'type': 'Z boson',
          'E': 86.9610263,
          'px': -26.129920499999997,
          'py': 5.5252133,
          'pz': 79.5328483,
          'charge': 0}
```

```
In [22]: higgs = particle_decay("Higgs boson", z1, z2)
         higgs

Out[22]: {'type': 'Higgs boson',
          'E': 397.3110063,
          'px': -22.137045999999998,
          'py': 1.4186076999999981,
          'pz': 376.40455130000004,
          'charge': 0}
```

For loops and if branches

Python runs a program, one statement at a time, and `for` tells it to repeat an indented block for each value of a collection.

```
In [23]: for particle in particles:
             print(particle["type"], particle["charge"])

         electron 1
         electron -1
         muon 1
         muon -1
```

```
In [26]: for particle in particles:
             if particle["type"] == "electron":
                 print(particle)

         {'type': 'electron', 'E': 171.848714, 'px': 38.4242935, 'py': -28.779644, 'pz': 165.006927, 'charge': 1}
         {'type': 'electron', 'E': 138.501266, 'px': -34.451419, 'py': 24.6736384, 'pz': 131.864776, 'charge': -1}
```

- Then we were introduced to classes and Object Oriented Programming

```
In [ ]: class Electron:
            def __init__(self, E, px, py, pz):
                self.E = E
                self.px = px
                self.py = py
                self.pz = pz

            def __repr__(self):
                return f"<Electron E={self.E} px={self.px} py={self.py} pz={self.pz}>"

            def draw(self, ax):
                ax.plot([0, self.px], [0, self.py], [0, self.pz], c="blue")
```

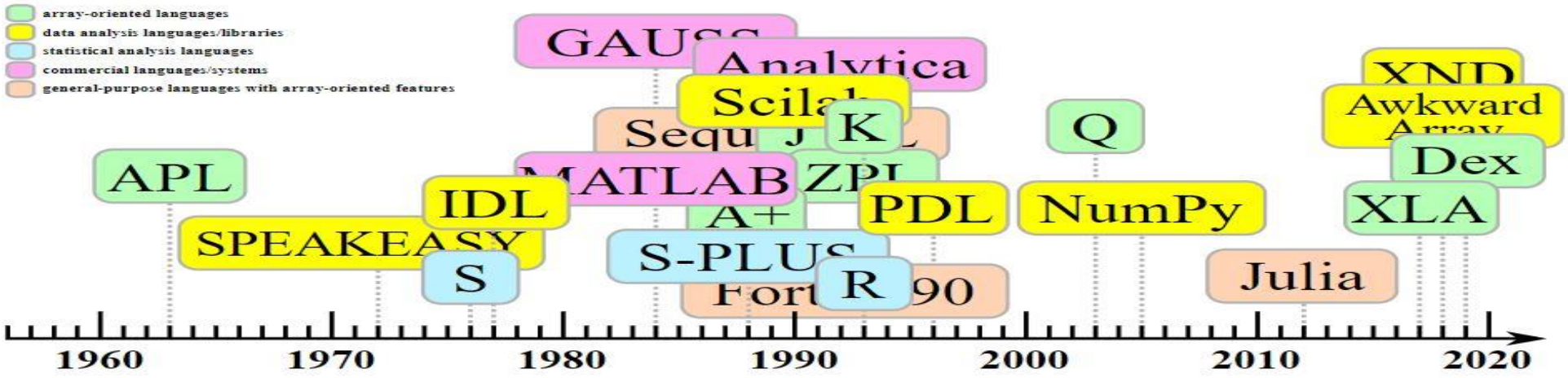
- Then Array Oriented Programming

In array-oriented programming, the primary data type is an array, and most functions perform one operation on all the elements of the array.

```
In [2]: input_data = np.array([1, 2, 3, 4, 5, 6, 7, 8, 9])
        output_data = np.array([0, 0, 0, 0, 0, 0, 0, 0, 0])

        for i in range(len(input_data)):            # explicitly specifies an order of execution
            output_data[i] = input_data[i]**2       # user says what happens to each element

        output_data

Out[2]: array([ 1,  4,  9, 16, 25, 36, 49, 64, 81])
```

What is array-oriented programming good for?

All of the languages/major libraries that emphasize array-oriented programming (that I know of):



Almost all of them are intended as *interactive data-analysis* environments.

(Fortran-90 is the only one that is not interactive.)

- Then using some operations over numpy array like arrange, sum , cumsum

```
In [5]: np.arange(10)
Out[5]: array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])
```

```
In [6]: np.sum(np.arange(10))
Out[6]: 45
```

```
In [7]: np.cumsum(np.arange(10))
Out[7]: array([ 0,  1,  3,  6, 10, 15, 21, 28, 36, 45])
```

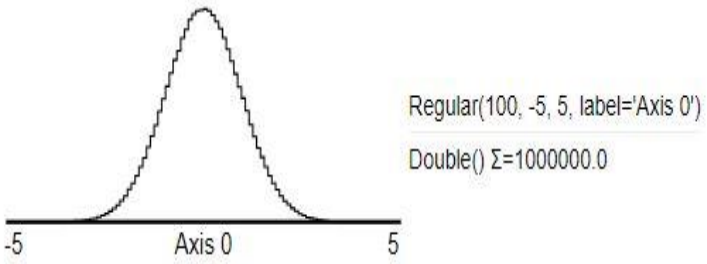
- Then we learned to use Histograms.

```
In [9]: from hist import Hist  # histogram library
```

```
In [10]: dataset = np.random.normal(0, 1, 1000000)  # one MILLION data points
```

```
In [11]: Hist.new.Reg(100, -5, 5).Double().fill(dataset)
```

Out[11]:



- Then we had an introduction to awkward arrays.
- Library for Array Oriented Programming like Numpy, but for arbitrary data structures.

```
In [6]: import awkward as ak
```

- Then done some operations like multidimensional indexing, basic slicing, advance slicing and reductions.
- Introduction to uproot and its operations.

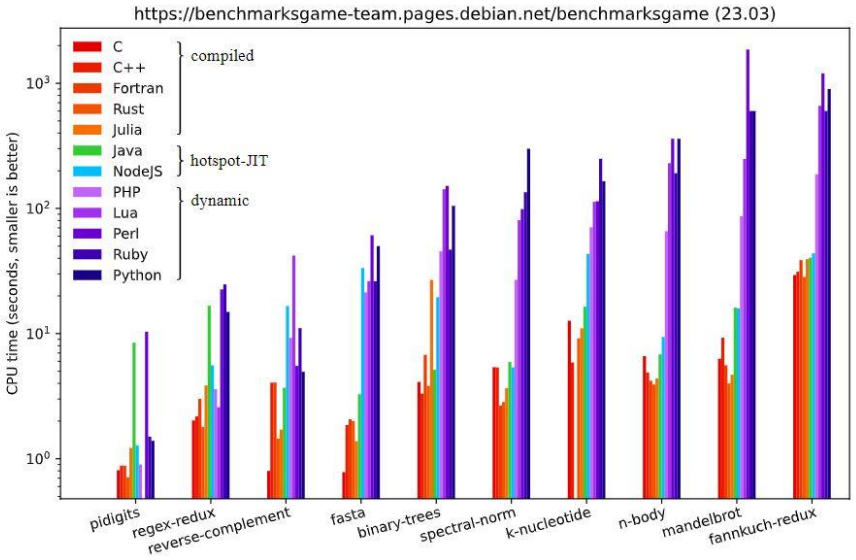
```
In [15]: import uproot

         file = uproot.open("../data/SMHiggsToZZTo4L.root")
         file
```

```
Out[15]: <ReadOnlyDirectory '/' at 0x01fac72bf050>
```

```
In [16]: tree = file["Events"]
         tree
```

```
Out[16]: <TTree 'Events' (32 branches) at 0x01fac80b9590>
```

As shown in the below picture Python is slower among most of the languages.



Overview

- Hardware accelerators and heterogeneous computing
- The GPU
- GPU applications in HEP
- The CUDA programming model

- Devices built for executing specific tasks more efficiently compared to running on the standard computing architecture of a CPU.

- Example : GPUs / FPGAs / TPUs

- Central Processing unit(CPU), how CPU work, principal components of CPU like ALU, CU,
- How exactly hardware accelerators used, introduction to heterogeneous computing
- Some types of hardware accelerators like GPU, FPGA, ASIC, TPU etc.
- Multicore vs Many core architectures.
- Nvidia GPU architecture.
- The Streaming Multiprocessor(SMs).
- Overview of main differences between CPU and GPU
- Computing needs in HEP, how GPUs can help.
- Introduction to CUDA, CUDA programming model

- Had some hands on like showing the device information

nvidia-smi

nvidia-smi: NVIDIA System Management Interface program

- Command line utility
- Aids in the management and monitoring of NVIDIA GPU devices

Lets try this out!

Click on the following link to access a GPU

https://binderhub.ssl-hep.org/v2/gh/research-software-collaborations/courses-hsf-india-december2023/gpu_onlycudagpu_true

Click on the Terminal icon (will look like this → )

Then type the following in the terminal:

```
nvidia-smi
```

What do you see ? Let's now try running a small utility script :

```
cd hsf-india-gpus
nvcc deviceInfo.cu -o deviceInfo
./deviceInfo
```

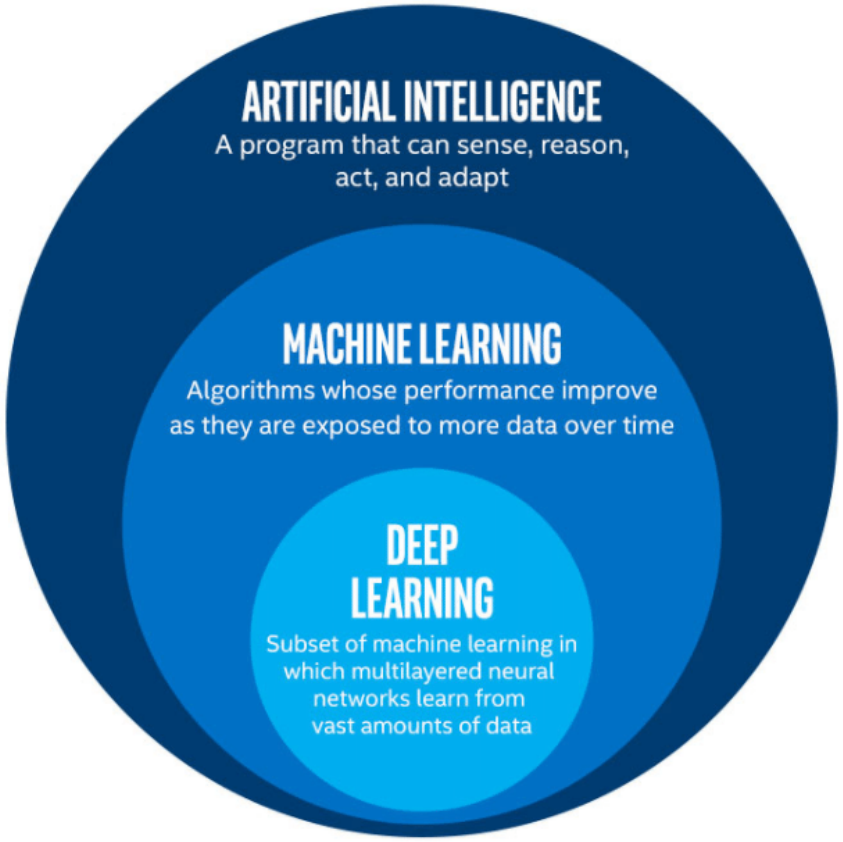
What do you see now?

HSF-India HEP Software workshop - Introduction to GPU programming - Charis Kleio Koraka - December 20th 2023 39

- Detailed introduction on threads and blocks. Indexing using blockIdx and threadIdx.
- CUDA Kernel, CUDA Functions declarations, launching CUDA kernels, memory management, synchronization, atomic operations.
- Then there were some hands on sessions.

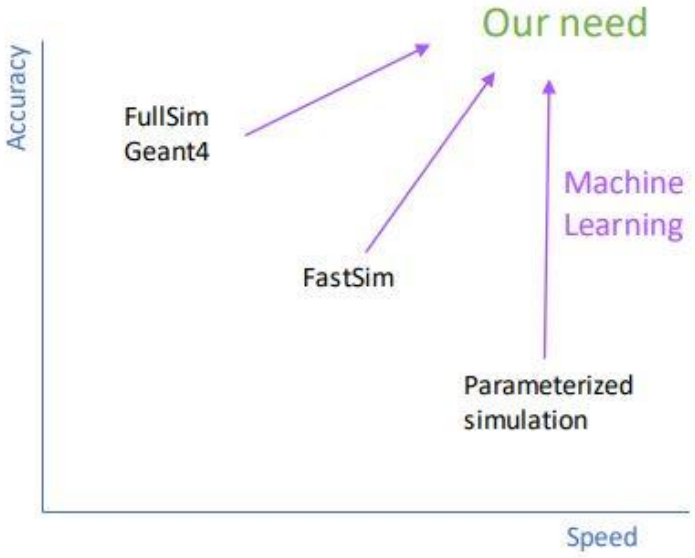
Basics of Machine Learning by Gordon Watts (University of Washington (US))

- What is artificial intelligence and machine learning
- Why to use python for deep learning , machine learning purpose
- Support vector machine(SVM)
- Decision Tree example
- BDT example
- Using the popular BDT library xgboost
- Introduction to neural networks
- Training of neural networks
- Approaches to learning i.e supervised learning, unsupervised learning, semi supervised learning
- Short introduction to Convolutional Neural Network(CNN), Recurrent Neural Network(RNN)



Simulation Techniques in HEP By Rafael Coelho Lopes De Sa (University of Massachusetts (US))

- How to use ML with simulation where primary goal is to increase the speed with preserving the accuracy as well as preserving speed with increasing accuracy.
- Introduction to Generative Adversarial Network(GAN) its upside and downside
- Had some hands on using Pytorch and scikit-learn



GEANT4 By Sunanda Banerjee (University of Wisconsin Madison (US))

- There was a full 90 minutes session on GEANT4
- How GEANT4 works.

Modern C++ Techniques By David Lange (Princeton University (US))

- Started with declaring variables, showing their range.
- Declaring arrays , using loops.
- Using Standard Template Library(STL) to reduce code complexity.
- How should we loop over vectors with the recent language improvements to increase the readability and performance.
- C++ memory management
- Pointers
- Use of unique_ptr, shared_ptr
- Different types of C++ compilers and what they do
- Code formatting using clang-format
- Then some hands on session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Thank You