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High Performance Heterogeneous Computing for Quantum Computing Simulations for Training the Quantum Workforce

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ABSTRACT

World over Industry is reporting about Quantum breakthroughs. Similarly, Scientists and Engineers from Research Institutes are claiming the hurdles surpassed in realizing the most talked about Technology of this Millennium i.e., QUANTUM COMPUTING. To take forward this Quantum Revolution, there will be need to nurture Super Quantum Engineer skills in human resource that will form the core of the Quantum Technologies Ecosystem.

This article describes High Performance Heterogeneous Computing for Quantum Computing Simulations for Training the Quantum Workforce to meet the challenges from Disruptive Technologies within a dynamic Academic curriculum framework through Internships to sustain careers in rapidly changing Technology landscapes.

Quantum Workforce Training sole objective is making technology accessible to stake holders in academic, research, industry/consulting and government institutions. Competencies imparted through Quantum Workforce Training aims to accelerate the fundamental and applied research and developing Quantum Computing aware human resource.

Quantum Workforce Training will enable dynamic response to technological changing scenarios to develop Super Quantum Engineer skill sets for sustainable future career of students.

The main highlights of High Performance Heterogeneous Computing for Quantum Computing Simulations for Training the Quantum Workforce are as follows: (I) Theoretical Conceptual Frameworks (II) Classical Computing Hardware Frameworks (III) Scientific Computing Programming Language Frameworks

Need for Quantum Workforce Training

➔ Futureproof Desirable Skills for Mechanical Engineers [1]

Simulation
Quantum
Energy

➔ Futureready Disruptive Skills in demand for Technology Firms [2]

Quantum Computing
Parallel Computing
Cloud Technologies
Software Development Methodologies
AI and Machine Learning

Connected Technologies
Fintech
Natural Language Processing
Proactive Security
IT Automation

It is quite evident that there is skills shortage as there are far less quantum trained workforce with undergraduate qualification. Academic Research Internships [3] are the gateway to introducing and providing opportunities to students at undergraduate engineering schools [4 - 6] worldwide.

Scientific Computing changing Landscapes [9]

Technology Used	*Paradigm Old*	*Paradigm Shift – Integration, Convergence, Synergy and Accessible*
Accelerating Numerical Computations	CPU High Performance Computing	GPU, FPGA, ASIC, TPU, NPU, QPU High Performance Computing
Computing	Classical	Quantum, Biological, Analog, Reversible
HPC Resources	Centralized Cloud	Decentralized Blockchain
Simulation Data Interpretation Visualization	Off line	Real time

Software	Bare metal	Containerized
Programming Language	Compiled	Interpreted, Interpreted+Compiled
Heterogenous HPC Hardware	Fixed configuration and energy inefficient	Reconfigurable and energy efficient
Electronic Design	Moore's Law	Thermodynamic Limited
Computing Architecture	Incognitive	Neural Brain inspired
Entropy	Minimize disorder	Order from Disorder – Self organized
Programming Algorithms	Serial	Inherently parallel
Computer Memory	Separate	Unified
Industrial Revolution	Industry 1.0, 2.0, 3.0	Industry 4.0
Manufacturing	Substractive	Additive

High Performance Computing TFLOPS Workload	Off Line Cloud Computing	Real Time Edge Computing

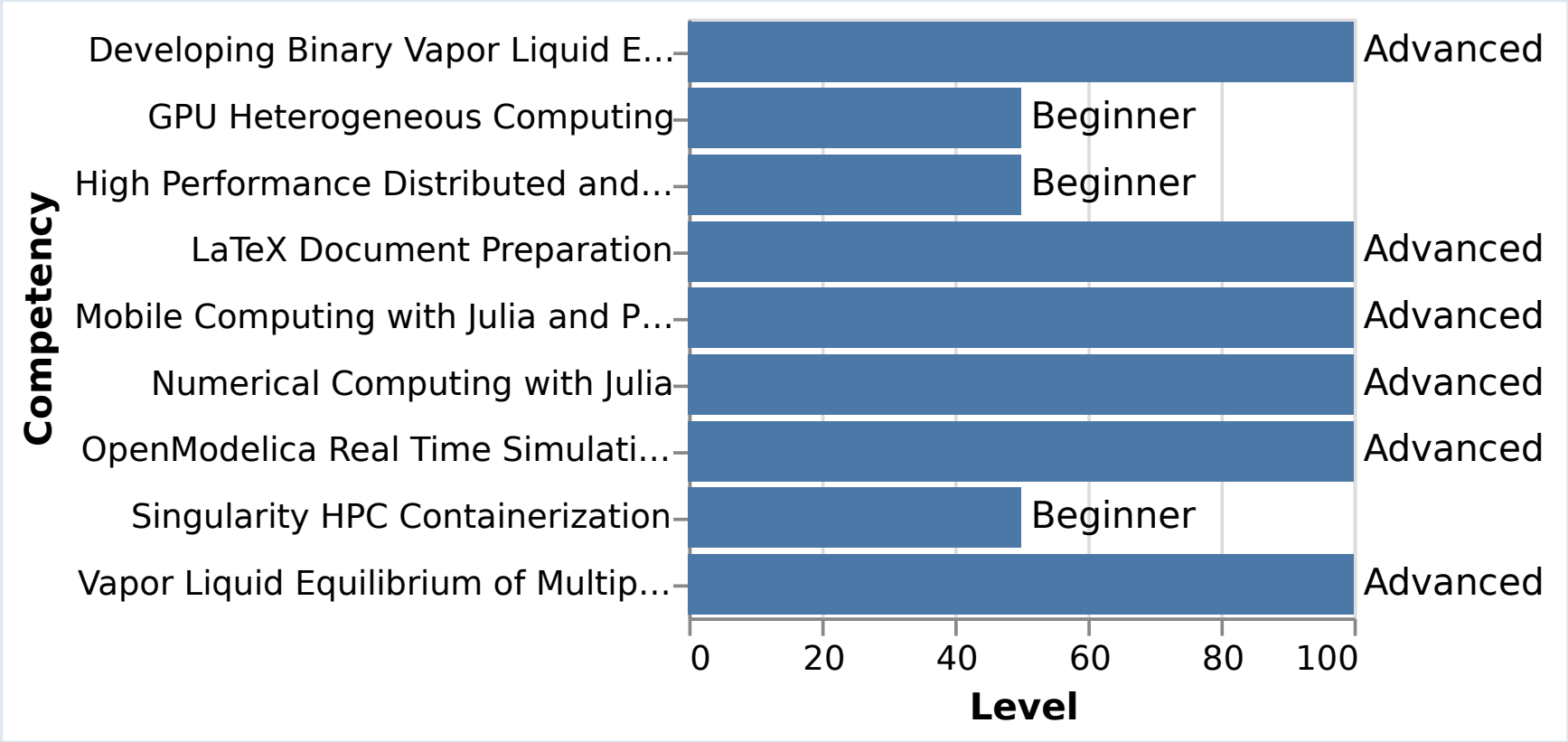
Skills and Competency Learning changing Landscapes [9]

Technology Used	*Paradigm Old*	*Paradigm Shift – Integration, Convergence, Synergy and Accessible*
Learning	Classroom	Online
Skill Sets	Discipline specific	Multi talented
Lectures	Seminar	Webinar
Recruitment	In Campus	Off Campus
Experience	Real	Portfolio

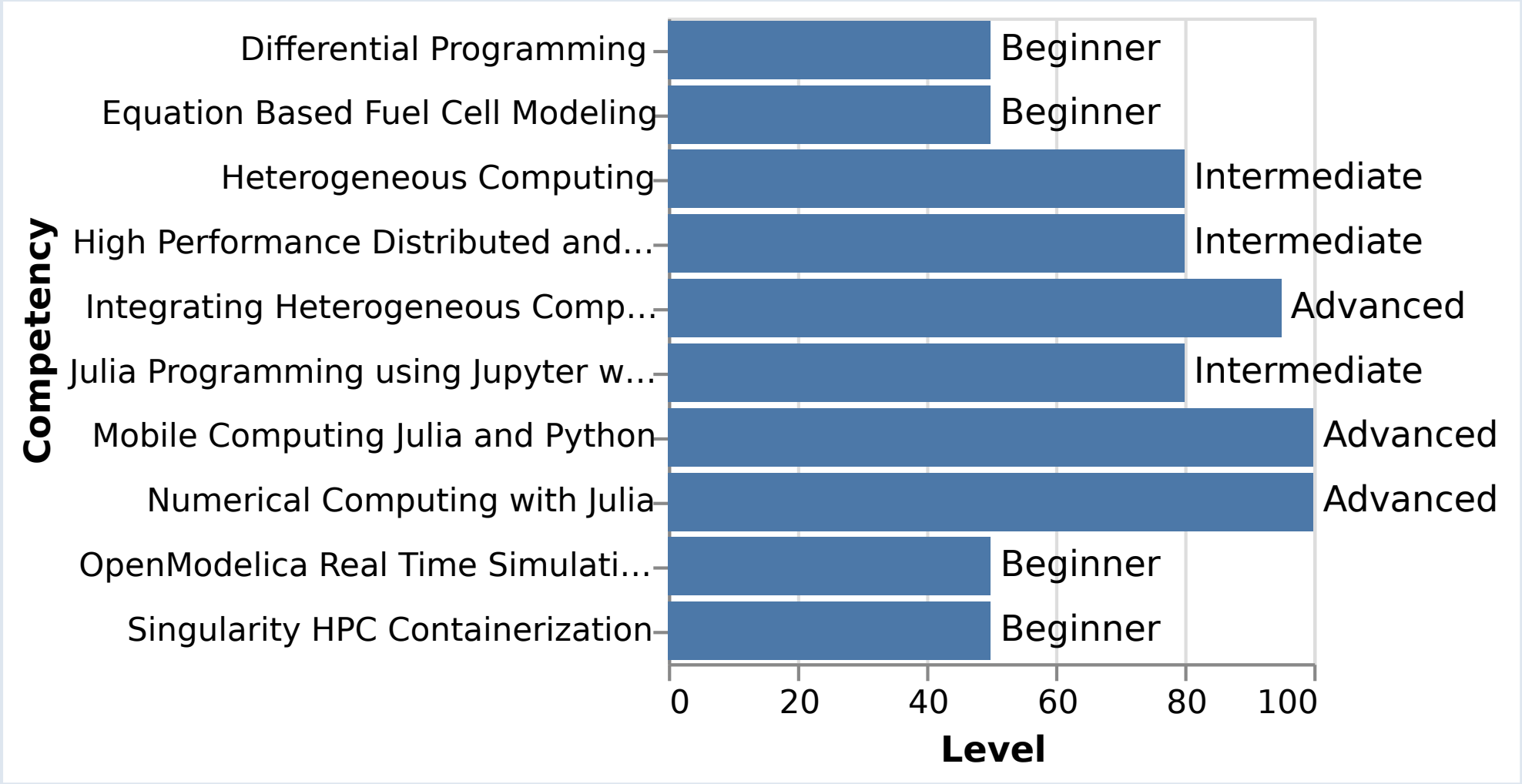
Curriculum development	Static and obsolete	Dynamic and futureready – Preempt the future, update pedagogy and includes Professional Development
Training	Rigid and inflexible	Adaptable and seamless transition
Job functions	Predefined	Evolves with time and flexible
Workplace	Corporate Office	Remote Working
Professional Skill Sets	Remain Competitive	Future Ready and Future Proof

Academic Research Internships and Professional Development Courses - Skills and Competency Imparted [5, 10]

Summer Academic Research Internships - Industrial Cryogenics for Quantum Technology and Preparatory Training on Industry 4.0 Certification



Professional Development Courses - Hands on Practice Scientific Machine Learning and AI for Energy Technology and Engineering and Hands on Practice Electric, Hybrid, Fuel Cell Vehicle and Autonomous Transport



Elements of Academic Research Internship for Training the Quantum Workforce

Quantum Workforce Training envisaged here uses grounds up methodology with the following key highlights

- ➔ *Theoretical Conceptual Frameworks*
- ➔ *Classical Computing Hardware Frameworks*
- ➔ *Scientific Computing Programming Language Frameworks*

Frameworks Detail of Academic Research Internship

I Theoretical Conceptual Frameworks
Linear Algebra Mathematics: Quantum Computation can be described in terms of elementary Linear Algebra with vectors, matrices and their properties and familiarity with Dirac notation for vectors and matrices
Quantum Mechanics: Quantum computing is based on principles of Quantum Mechanics that governs a quantum phenomena characterized by particle and wave nature, discrete, probabilistic, non local and sub atomic scales postulated by Max Planck, Albert Einstein, Werner Heisenberg, Louis de Broglie, Erwin Schrodinger, Wolfgang Pauli, John von Neumann, Paul Dirac, Niels Bohr, William Hamilton, David Hilbert and Max Born and

Non-Equilibrium and Quantum Thermodynamics: Quantum Thermodynamics study rebuilds Thermodynamics from the laws of Quantum Mechanics and useful for exploring the link between information and thermodynamics as established by Landauer in quantum regime and predicting the thermodynamic resources required to generate/sustain quantum phenomena
Industrial Cryogenics: Use of Quantum Fluid Dilution Refrigeration in Quantum and Cryogenic Computing

II Classical Computing Hardware Frameworks

High Performance Distributed and Parallel Computing: High Performance Computing includes Computations in parallel over lots of compute elements (CPU, GPU), using a very fast Network to connect between the compute elements using Programming model of Message Passing Interface (MPI)

GPU Heterogeneous Computing: GPUs are currently being used to accelerate resource heavy computing in Real Time Design requiring moderate Programming effort

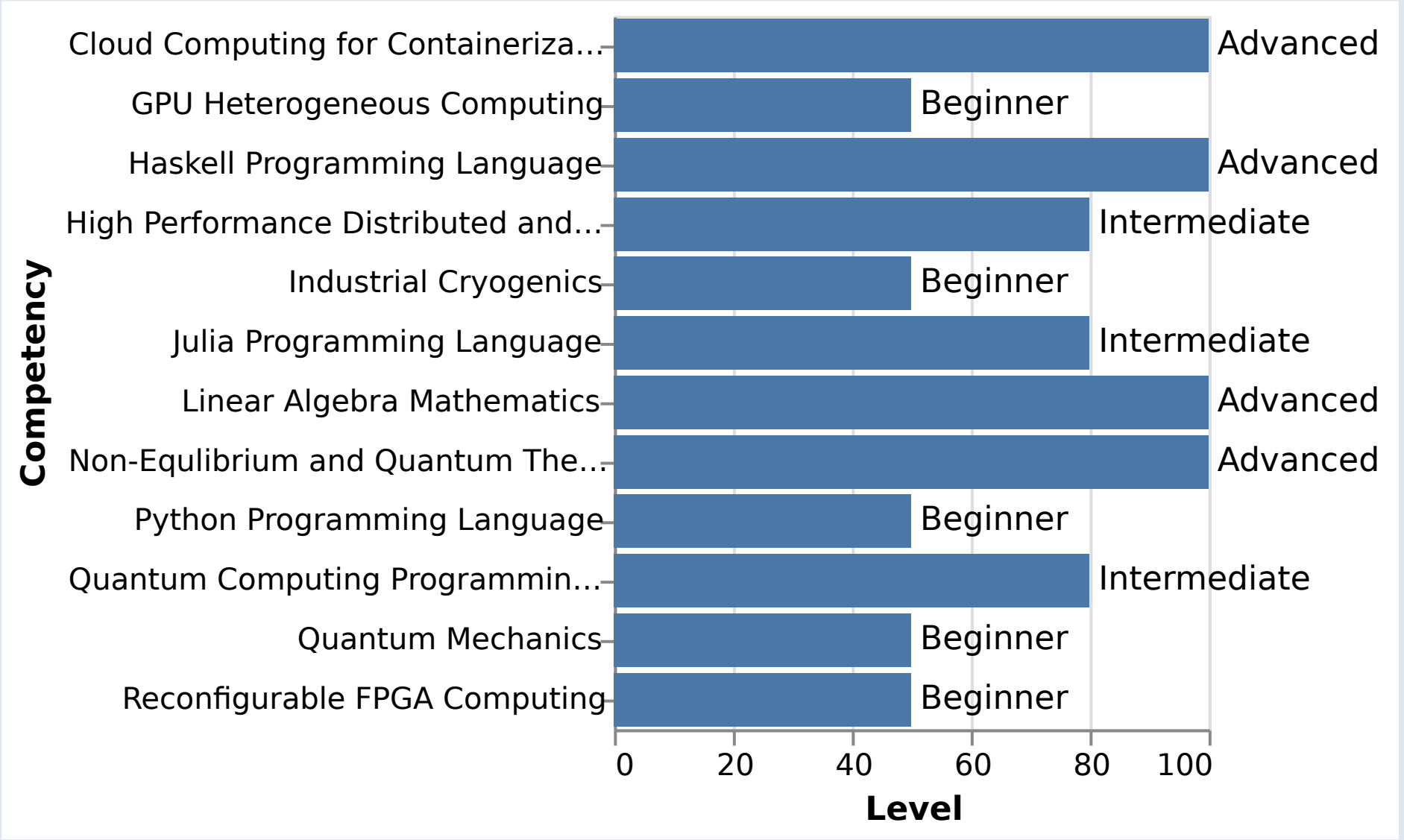
Reconfigurable FPGA Computing: Extremely Fast Real Time Processing in Parallel with limited Programming Flexibility but better performance

Cloud Computing for Containerization and Virtualization: A Cloud offers classical computing as well as quantum computing environment, providing the way for executing quantum algorithms and to ease

the difficulty to install and run Quantum Algorithm Libraries on different computing architectures, containerization is used to make this process easier

III Scientific Computing Programming Language Frameworks
Julia Programming Language: Julia takes advantage of different computing architectures while reducing the programmer's burden and notably Parallel computing features was introduced from start in Julia
Python Programming Language: Python is widely used in all popular Quantum Algorithms Libraries and building quantum circuit, simulating qubit operations
Haskell Programming Language: Haskell is a functional programming for simulating quantum computations with haskell functions
Quantum Programming Language: Silq is a high level quantum programming language for quantum computers which optimizes the programming of quantum computers with shorter code

providing both read and write ease



Implementation Methodology

Sample Methodology for Competency on "High Performance Distributed and Parallel Computing"
Brief Steps described for a Ethernet/WiFi Network Switch based Distributed Memory Computing
1. Use Linux Mint Live 2. In the live mode install openmpi and openssh-server in Machine-1 3. In the live mode install openmpi and openssh-server in Machine-2 4. Configure for password less ssh on Machines 1 and 2 5. Establish password less remote login from Machines 1 to 1, 1 to 2, 2 to 2 and 2 to 1 6. Run the mpitest executable for Distributed Memory Computing

Sample Methodology for Competency on "Singularity HPC Containerization"
Installing and Running WineHQ (Installing and Running Windows Programs in Linux) inside a Ubuntu Singularity container
mkdir ADCOMB cd ADCOMB/ wget http://fchartsoftware.com/assets/downloads/ad_comb.exe sudo singularity build --sandbox ~/ubuntu_latest.sif docker://ubuntu:latest sudo singularity exec -w ~/ubuntu_latest.sif apt update sudo singularity exec -w ubuntu_latest.sif apt install wine sudo singularity exec -w ~/ubuntu_latest.sif /bin/bash dpkg --add-architecture i386 apt-get update exit sudo singularity exec -w ~/ubuntu_latest.sif apt install wine32 singularity exec --home $PWD -w ~/ubuntu_latest.sif wine ad_comb.exe

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Past Professional Development Courses:

[1] ***Python for Mechanical Engineering with applications from Applied Thermodynamics, MEMS & Micro-Nano Fluidics, Non-Equilibrium & Quantum Thermodynamics and Biological Thermodynamics***, Professional Development Course PDC02_200, Pondicherry Engineering College, Pondicherry, 2018.

[2] Auro Ashish Saha, ***Project Management for Industrial Energy and Engineering Projects***, Professional Development Course PDC02_198, Pondicherry Engineering College, Pondicherry, 2018.

[3] Auro Ashish Saha, ***Quantum Biology for Engineers***, Professional Development Course PDC02_XXX, Pondicherry Engineering College, Pondicherry, 2019.

[4] Auro Ashish Saha, ***Quantum Machine Learning using Non-Equilibrium and Quantum Thermodynamics Framework for Quantum Technology Applications***, Professional Development Course PDC02_XXX, Pondicherry Engineering College, Pondicherry, 2020.

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[6] Auro Ashish Saha, ***Skills for Industry 4.0***, Professional Development Course PDC02_XXX, Pondicherry Engineering College, Pondicherry, 2020.

[7] Auro Ashish Saha, ***Advances in Seawater Desalination Technology Practice***, Professional Development Course PDC02_XXX, Pondicherry Engineering College, Pondicherry, 2020.

[8] Auro Ashish Saha, ***Hands on Practice Computational Biological Thermo-Fluid Mechanics***, Professional Development Course PDC02_XXX, Pondicherry Engineering College, Pondicherry, 2020.

Past Academic Research Internships:

[1] **High Performance Heterogeneous Computing for Quantum Computing Simulation**

[2] **Preparatory Training on Energy Auditor and Energy Manager Certification**