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GANANAM (गणनम्)

HIGH PERFORMANCE COMPUTING NEWSLETTER
INSTITUTE FOR PLASMA RESEARCH, INDIA



Quantum Computing: Opportunities for HPC Users to Test Quantum Algorithms

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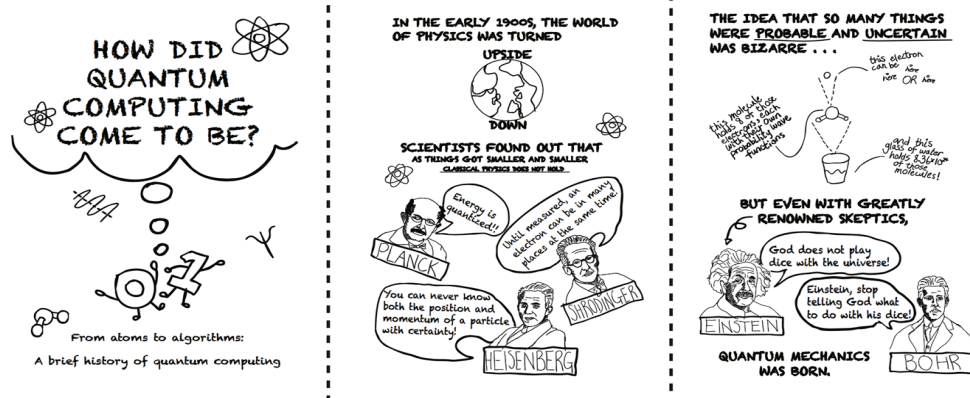
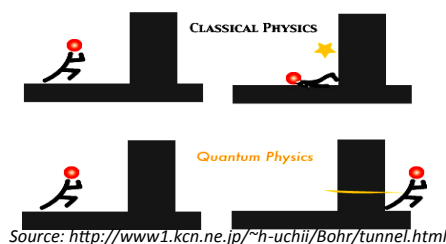


Figure 1: As a part of Enabling Practical-scale Quantum Computing (EPIQC) Expedition, University of Chicago's Diana Franklin has developed zines [1] that are comic-book like pamphlets accessible to a broad audience for education.

"Nature isn't classical, dammit, and if you want to make a simulation of nature, you'd better make it quantum mechanical, and by golly it's a wonderful problem because it doesn't look so easy"

- Richard Feynman

Quantum Computing explained through Figure 1 [1], is a revolutionary approach to algorithmic study that expands upon quantum mechanical phenomena, such as superposition, entanglement, and the tunneling effect, to the world of traditional computing. We often associate our understanding of the difference between classical and quantum physics with the tunneling effect explained below.



Source: <http://www1.kcn.ne.jp/~h-uchii/Bohr/tunnel.html>

The buzz around quantum computing is growing, with India recently joining the list of countries with a dedicated quantum mission. The National Quantum Mission (NQM) [2], announced on April 19, 2023, aims to develop intermediate scale quantum computers with 50-100 physical qubits within five years and 50-1000 physical qubits within eight years. As a classical high-performance computing (HPC) user, one may

"Quantum Computing is Coming!"

wonder why you should explore this radically new paradigm of computing, especially when classical HPC systems have already surpassed the exascale (10^{18}) barrier and can solve complex problems. However, the computational order of a problem, which measures the number of operations required to solve a problem as a function of the

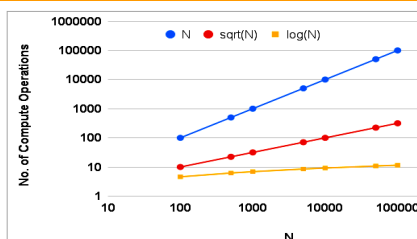
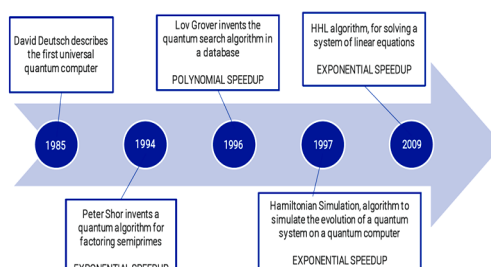


Figure 2: Exponential vs. Polynomial Speed up.

problem's size (N), is an essential factor to consider. Figure 2 demonstrates the number of compute operations needed to solve algorithms of different computational complexities. The various quantum algorithms developed timeline is shown below. To



Quantum Algorithms Timeline

get the gravity of the level of speedup which can be achieved with quantum algorithms, let us take the example of Shor's algorithm [3] where for a given number N, it finds the two prime numbers.

$$N = p \times q$$

Shor's algorithm can factor large prime numbers exponentially faster than classical algorithms, as shown in Figure 3. For instance, using ANTYA, it would take only 0.3 microseconds to factor a 300-digit number using Shor's algorithm.

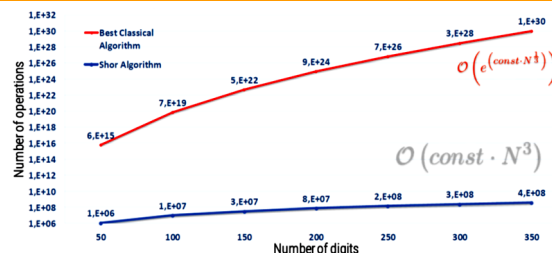


Figure 3: Shor's algorithm vs. the best classical factorization algorithm.

Opportunities for HPC users: How can classical HPC users test quantum algorithms? Cloud-based quantum computing platforms, such as IBM Quantum (<https://quantum-computing.ibm.com/>), offer the opportunity to run quantum algorithms on actual quantum hardware with up to 5 free qubits. Additionally, open-source software like Qiskit (<https://qiskit.org/>) allows users to simulate quantum algorithms on HPC systems like ANTYA, exploring the potential of quantum computing without the need for a physical quantum computer. This experience can help users prepare for the future and stay ahead of the curve in the field of quantum computing.

In summary, HPC users can start exploring quantum algorithms using cloud-based platforms or simulators. The future of computing is quantum, and it is time to dive in and start testing the quantum wave.

References:

1. Zines under EPIQC, <https://www.epiqc.cs.uchicago.edu/zines>
2. National Quantum Mission (NQM), <https://pib.gov.in/PressReleaseFramePage.aspx?PRID=1917888>.
3. P. Shor, Polynomial-Time Algorithms for Prime Factorization and Discrete Logarithms on a Quantum Computer, 1996, <https://arxiv.org/pdf/quant-ph/9508027.pdf>.

Installing Packages/Applications with Spack in User Environment on ANTYA

In the last issue, we have introduced about Spack and how it and its installed applications/libraries can be availed on ANTYA. This article will demonstrate how Spack can be used by the users to easily install, build, and maintain a wide range of software packages and libraries in their own environments.

Why to Use Spack in Your Own Environment?

Spack can be useful for installing multiple versions of the same package having a complex set of dependencies. It also provides a variety of build options, which allow users to customize the installation process to their specific needs while resolving the dependencies in the background.

How to Use on ANTYA?

On ANTYA, if a user need to install anything with Spack, it needs to be first installed in user account. Once the Spack is installed, a user can install packages with different compiler options as demonstrated below to install a version of **OpenMPI**.

Installing Spack first in User Environment

```
# Clone the latest spack repo.
[user@login1 ~]$ git clone https://github.com/spack/spack
[user@login1 ~]$ cd spack
[user@login1 ~]$ git fetch origin releases/latest:latest
[user@login1 ~]$ git checkout latest
# The following will enable spack in your environment
[user@login1 ~]$ source spack/share/spack/setup-env.sh
# To check if installed correctly
[user@login1 ~]$ which spack
Your_dir/spack/bin/spack
```

To check the availability of OpenMPI and its Versions

```
# To list the availability of OpenMPI
[user@login1 ~]$ spack list openmpi
openmpi
==> 1 packages
# To check different versions of OpenMPI and their detailed information
[user@login1 ~]$ spack info openmpi
# This will show a long list of different versions of openmpi
with their links and various other useful details.
```

Installing latest version of OpenMPI

```
# Before installing, it is recommended to check how the package will be installed and what
are the dependencies which will be installed along with it. To check use the following command
[user@login1 ~]$ spack spec -I openmpi
# This will list out various dependencies along with the compiler
which will be installed along with OpenMPI.

# For installing OpenMPI, by default if you do not specify the version, it will automatically
take the latest version. However you can specify the version as well using the following
command:
[user@login1 ~]$ spack install openmpi@4.1.4
# This will install openmpi-4.1.4 in your home environment.
```

Finding/Loading Spack Installed Packages

```
# Find the package and its location
[user@login1 ~]$ spack find openmpi
[user@login1 ~]$ spack location -I openmpi
# To load the installed openmpi package as a module in your environment
[user@login1 ~]$ spack load openmpi@4.1.4
[user@login1 ~]$ which mpirun
```

ANTYA UPDATES AND NEWS

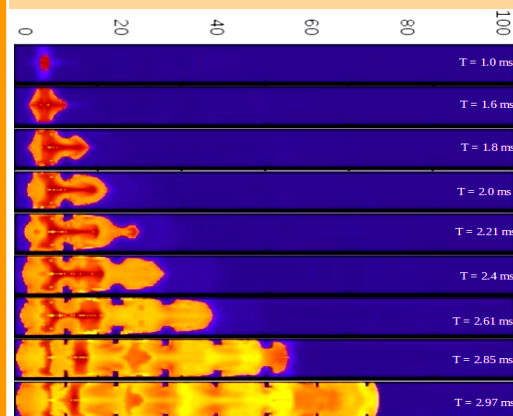
1. New Packages/Applications Installed

⇒ **Spack package manager installed modules**

- Pumi-2.2.7
- Paraview-5.10.1
- netCDF-4.9.0
- Petsc-3.15.5
- Openmpi-4.0.2
- Texlive

HPC PICTURE OF THE MONTH

Transition of Subsonic Flames into Supersonic Detonations



Pic Credit: **Sunil Bassi**

When ignited by conventional spark plugs, fuel-air mixture burns initially in subsonic combustion mode called deflagrations. As the flame interacts with obstructions and walls of the tube, it gets accelerated and gets into supersonic regime called detonations. The figure shows flame visualized by temperature plots at various time frames. Time of flight calculations are used to measure the speed of flame front and observed that initial time frames flame speed are small compared to later time frames where flame front covers more distance in less time.

The simulations are performed by solving navier-strokes equations coupled with chemical reaction models with in-house modified Conchas-Spray CFD code. The serial code runs approximately 1 day for one run and image is plotted using gnuplot.

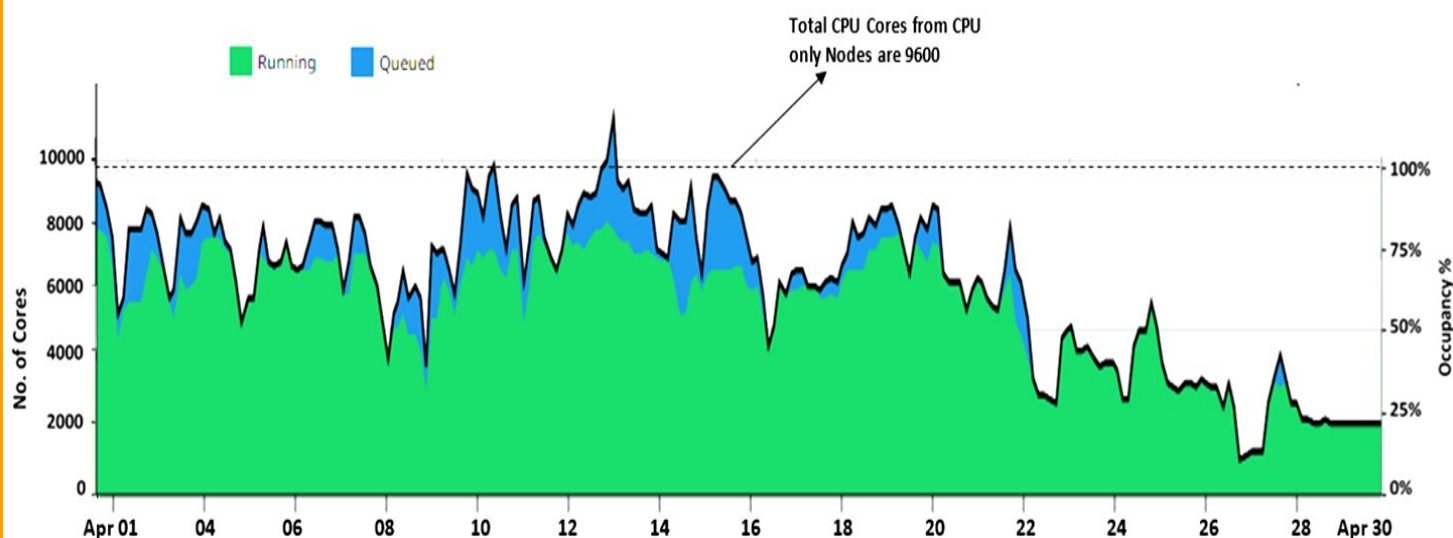
TIP OF THE MONTH

Resolving the paths of various libraries needed for the execution of an executable is one of the important thing that the users need to take care. “ldd” is a simple Linux command that displays the shared library dependencies of an executable.

```
[user@login1 ~]$ ldd a.out
# This will list out all the required shared libraries of a.out.
```

ANTYA Utilization: APRIL 2023

ANTYA Daily Observed Workload



Other Recent Work on HPC (Available in IPR Library)

Design and development of Hydrogen Isotopes Extraction System at IPR	Rudreksh Bhratbhai Patel
MD Simulation of Stably Stratified Plane-Couette Flow in 3D Yukawa Liquids	Suruj Jyoti Kalita
Shear dynamo action in non-helical base flows	Shishir Biswas

ANTYA HPC USERS' STATISTICS—

APRIL 2023

◆ Total Successful Jobs — **2485**

◆ Top Users (Cumulative Resources):

- CPU Cores **Amit Singh**
- GPU Cards **Suruj Kalita**
- Walltime **Lucky Saikia**
- Jobs **Someswar Dutta**

Acknowledgement

The HPC Team, Computer Division IPR, would like to thank all Contributors for the current issue of **GANANAM**.

On Demand Online Tutorial Session on HPC Environment for New Users Available
Please send your request to hpcteam@ipr.res.in.

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