

# Bibliotheca Alexandrina Supercomputer Project



Mohammed Gaafar  
HPC System Administrator, BA Supercomputer Project.

Ain Shams University  
March 4<sup>th</sup> 2013

# Agenda

- What is High Performance Computing (HPC)?
- Why do We Need HPC?
- Characteristics of Problems Solved Using HPC.
- HPC Domain of Applications.
- HPC in The Real World.
  - Simulation of Car Crashes
  - Simulation of Molecular Interaction For New Drug Design
  - Case Study: Weather forecasting.

# Agenda (contd.)

- Supercomputer Project at BA (High Performance Computer).
- Hardware Specifications.
- Software Specifications.
- Scientific Packages available.
- Who Can Use BA HPC?
- How to Apply to Use BA HPC?
- Services and Resources Provided to BA HPC users.
- BA HPC Site Policy.
- Discussion.

# What is HPC?

- Computing resources that provide more computing power than is available to solve a problem in a reasonable amount of time.
- HPC systems range from workstations, up to the largest supercomputers.
  - The term Supercomputer refers to a powerful subset of high-performance computers.

# Why do We Need HPC?

- The great evolution in many fields of science has emerged many computational and simulation problems with large sizes.
- Unfortunately, the development of CPUs could not cope with the computational power needs of different fields of modern sciences.
- Parallel processing has emerged as an alternative to trying to make CPUs more faster.

# Why do We Need HPC?

- With scientific problems getting larger and more complicated, level of parallelization needed to be increased to provide the needed amount of computational power.
- With level of parallelization getting larger, more adequate, efficient and robust parallel environments became an essential need for scientific research.

# Why do We Need HPC?

- “Providing access to HPC infrastructure is necessary for all countries with ambitions towards science and innovation”, --Rene Belso from the Danish Center for Scientific Computing.

# Characteristics of Problems Solved Using HPC

- Takes long to compute its results (Need More compute power).
- Needs large quantity of resources (memory, disk, etc...).
- Requires large quantity of runs.
- Time critical.



# HPC Domain of Applications

- Finite element analysis.
- Medical Physics and Medicine.
- Chemistry and Biochemistry.
- Climate research.
- Biophysics and Bioinformatics
- Nanoscience
- And more ....

# HPC in The Real World

# Simulation of Vehicle Crashes

- A virtual recreation of a destructive crash test of a vehicle in order to examine the level of safety of the vehicle and its occupants.
- Data obtained indicate the capability of the vehicle body to protect the vehicle occupants during a collision against injury.
- Produces results without actual destructive of a new car model. Tests can be performed quickly and inexpensively.

# Simulation of Molecular Interaction For New Drug Design

- A drug is an organic molecule which activates the function of a biomolecule which in turn results in a therapeutic benefit to the patient.
- Drug design involves design of molecules that are complementary in shape and charge to the biomolecular target to which they interact and therefore will bind to it.

# Create Accurate Weather Forecasts

- Modern atmospheric model is a set of equations (primitive equations) used to predict the future state of the atmosphere.
- These equations, with the ideal gas law, are used to predict the atmospheric conditions.
- The equations are nonlinear partial differential equations which are impossible to be solved exactly through analytical methods, therefore numerical methods are used.

# Case Study: Weather Forecasting

- Simulating changes in the weather of Crete (A Greek Island).
- The area of the island = 8,336 km<sup>2</sup>
- The simulation is for the next 20 years.
- Simulation is performed using WRF software package.
- A simulation of 1 month running on 1 core took 75 hours.
- The complete simulation of the 20 years roughly would take 18000 hours = 25 months.
- Using BA HPC cluster, the simulation runs on 120 cores. The simulation of 1 month took 43 minutes, and the complete simulation took around 7 days, with a speedup around 100.



# Supercomputer Project at BA



4/3/2013

Bibliotheca Alexanrina Supercomputer Project

15

# Supercomputer Project at BA

- In mid 2009 the BA international school of information science (ISIS) of Alexandria, Egypt in partnership with the Egyptian ministry of telecommunication have placed a joint HPC in Bibliotheca Alexandrina.
- The vision of the project is to provide a modern, national HPC infrastructure in an international and competitive setting, and stimulate research in computational science.



# Supercomputer Project at BA

- The project serves the Egyptian computational science community by providing access to the infrastructure to individuals or groups involved in education and research at Egyptian universities and research institutes.

# Hardware Specifications

- Cluster Details.

Type	Number of nodes	Number of cores	CPU Type	Theoretical Peak	Total Memory	Total Shared Storage
Cluster	130	1040	Intel Xeon	~11.8 TFLOPS	~ 1.05 TBytes	36 TBytes

- Compute Nodes Details.

<b>Memory</b>	8GB memory
<b>CPU</b>	2 Intel Xeon Quad Core E5440, 2.83 GHz (8 cores)
<b>Interconnect</b>	4x DDR Infiniband Switch 10Gbit
<b>Management Nodes</b>	2 batch, 2 login, 1 backup, 1 monitoring
<b>Filesystem</b>	2 Meta Data Servers, 2 Object Storage Servers
<b>Tape Library</b>	48 Tapes, each 400GB/800GB flat/compressed
<b>Power Consumption</b>	90KW

# Software Specifications

- Management Software

<b>Operating System</b>	RHEL 5.2
<b>Cluster Management</b>	ROCKS
<b>Queuing/Scheduling System</b>	Open Grid Scheduler
<b>Filesystem Software</b>	Lustre Filesystem
<b>Backup Software</b>	Symantec Veritas Netbackup
<b>User Environment</b>	Modules
<b>Default Size of Home Directory</b>	100 MB
<b>Max. Job Runtime</b>	24 Hrs
<b>Max. Number of Cores/job</b>	50%

# Software Specifications

- **Compilers and MPI.**

Software	Version
Intel Compiler	11.0
GCC	4.1.2
Intel MPI	3.1 and 3.2
MPICH	1.4
MVAPIC	1.8a
OpenMPI	1.2.7

- UNIT 1.0 performance analysis framework is available for performance analysis, parallel programs debugging, performance profiling, performance tracing, etc.

# Scientific Packages Available

<b>Software</b>	<b>Version</b>
FFTW	2.1.5, 3.2.2, and 3.3
OpenFOAM	1.6 and 2.1.0
NAMD	2
FERRET	6.67
Geant4	4.9.5
GROMACS	4.5.4, and 4.5.5
LAMMPS	3Jul2012
Metis	4.0.3, and 5.0.2
ParMetis	3.2.0, and 4.0.2
NetCDF	3.6.2, and 4.2.1.1
Octopus	4.0.1
PETSC	3.1, and 3.2

# Scientific Packages Available

<b>Software</b>	<b>Version</b>
Quantum-espresso	4.2, and 5.0.1
Root	5.0.1
WRF	3
SuperLU	2.0, 2.5, and 4.1
R	2.13.0
TopC	2.5.2
TCL	8.4
ParaView	3.10.0
BLAS	
GoToBLAS	1.13
GSL	1.15
ccp4	6.3.0

# Who Can Use BA HPC?

- 40% of the available computational resources are available for the scientific use from Egyptian Governmental Universities and Institutes.
- Any researchers in an Egyptian governmental research institution can apply to use the resources for free.

# How to Apply to Use BA HPC?

- Initiating a contact with BA Supercomputer team by sending and email to [supercopmuter@bibalex.org](mailto:supercopmuter@bibalex.org)
- The applicant will receive a welcome email, attached to this email two forms to fill.
- The “*Application Form*” should be filled by the applicant and stamped by his college stamp.
- The “*Proposal Form*” should be filled by the user specifying the resources he needs and the scientific case of the project.
- We will be more than happy to provide to help in filling the forms.



# How to Apply to Use BA HPC?

- The two forms should be filled and resent to BA HPC team.
- The two forms will be reviewed by BA Supercomputer Reviewing Committee.
- A reply is sent to the applicant with the committee decision.
- Once the application is accepted by the committee the technical preparation starts.

# How to Apply to Use BA HPC?

- The applicant is granted remote access to BA HPC through SSH connection.
- In order to setup the SSH connection the user should provide the following.
  - A Public static IP(s) that will be used to connect to BA HPC.
  - SSH private keys.
  - Desired username.

# Provided Resources

- Each project is granted the following resources.

Resource	Value
Core Hours	10,000
Home Disk Quota	100MB
Scratch Storage Quota	100GB
Access Duration	6 Months

- Those are the default resources and they can be renewed upon user request.

# Provided Services

- BA Supercomputer team provides 2 hours kick-off training for system usage upon user request.
- The training can be provided online using Skype or on-site (at BA).
- BA Supercomputer team provides all aspects of user support starting from helping with Linux commands and job submission to performance analysis and software optimization.

# BA HPC Site Policy

- Do not ever run heavy jobs on Login nodes (Only code development, compilation and data transfer).
- All jobs should be submitted through OGS scheduler.
- Each user can run maximum of 30 processes on login nodes.
- Each user can run 5 jobs simultaneously on the compute nodes.
- Each user can use simultaneously 50% of the available number of cores.

# BA HPC Site Policy

- 1 Node is the accounting unit. Jobs should use 8 cores or multiples of 8.
- The maximum runtime for a job is 24 hours.
- The limit on the runtime of a job is related to the number of cores it uses and it can be calculated using the following formula.

$$\text{Max\_Job\_Runtime} = \text{Max\_Available\_Cores} / \text{Requested\_Cores}$$

# Questions and Discussion.

Thank You !