The Abdus Salam
International Centre
for Theoretical Physics

United Nations Educational, Scientific and Cultural Organization

IAEA International Atomic Energy Agency

2494-16

Workshop on High Performance Computing (HPC) Architecture and Applications in the ICTP

14 - 25 October 2013

The management aspect

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The management aspect

Experience based on ICTP's HPC during the last 3 years

Ulrich Singe - ICTP

The Abdus Salam International Centre for Theoretical Physics

UNESCO

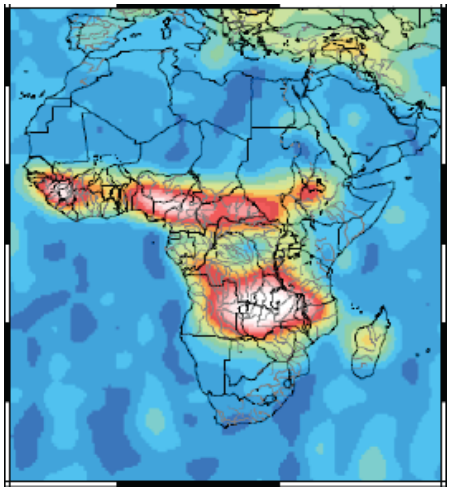
IAEA International Atomic Energy Agency

ICTP initiatives in High Performance Computing (HPC)

Computational Sciences is one of the three new research areas identified in 5-yr strategic plan (2010)

Excerpts from the 5-yr plan:

- “Computational sciences mirror the role that theoretical physics played when ICTP was founded”
- “A local cluster of computers would provide a world-class facility for the Centre’s scientists and visitors”
- “Access to the SISSA building is essential for all these expansion plans”



HPC at ICTP

Strong in house research activities in computational modeling

- ESP: Climate modeling (RegCM model)
- CMSP: Computational materials science (Quantum-Espresso)

Outreach and training activities

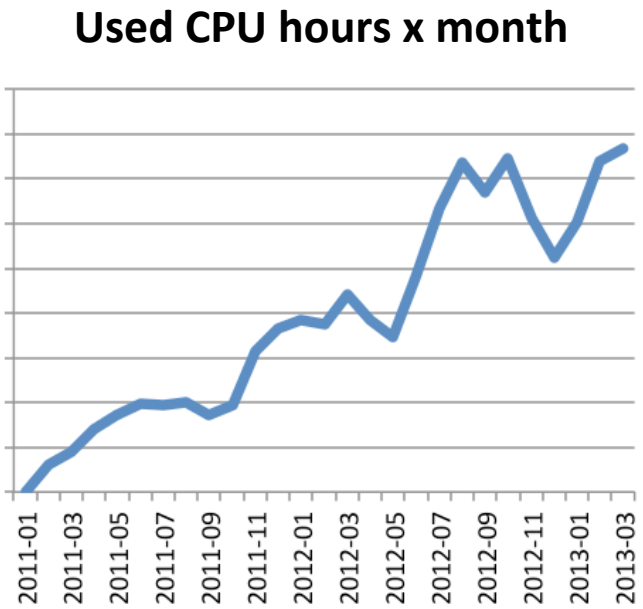
- Advanced schools at ICTP and elsewhere

HPC usage at ICTP

The scientific user community uses various resources:

- **ICTP HPC cluster**
- **SISSA/ICTP cluster (to be operational in 2014)**
- **CINECA (~14M CPU hours in 2013 BG/Q)**
- **PRACE**
- **Data center Karlsruhe**
- **INFN clusters**

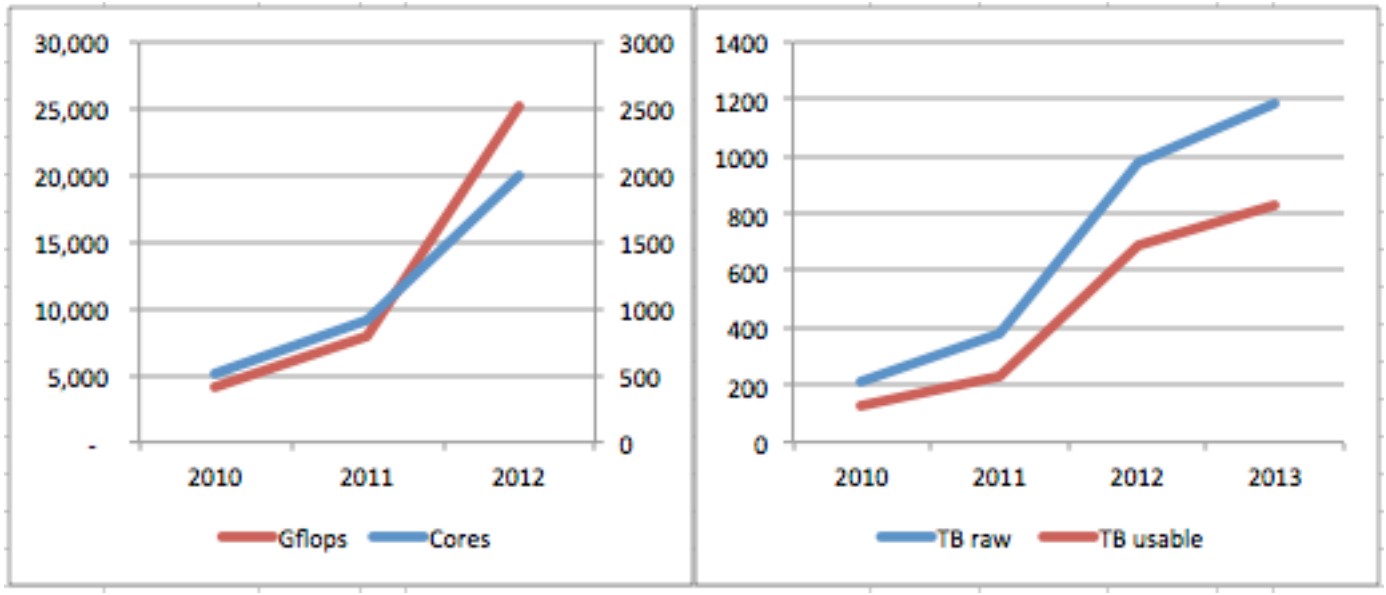
HPC facilities at ICTP



HPC cluster “ARGO”

- Processors: 1910 cores – Intel based
- Theoretical calculation power: 25 teraFLOPS and 2 teraFLOPS via accelerators (GPUs)
- Storage: ~1,150TB raw (high speed and archive)

HPC facilities at ICTP



HPC cluster “ARGO”

- Balance calculation power and storage
- Storage: high speed and archive

HPC facilities at ICTP

	€ x Gflop*	# cores	Watt	Watt/core	Watt/Gflop
2009 Nehalem		4	80	20.0	2.20
2010 Westmere	100%	4	80	20.0	2.08
2011 Westmere	129%	6	95	13.3	1.39
2012 Sandybridge	79%	6	95	15.8	0.99
2013 Ivybridge	64%	10	115	11.9	0.60

* depends on memory

- Price per Gflop is decreasing dramatically due to multi-core concept
- Power consumption is also decreasing
- Importance to enable applications/programs to run on multi-core platforms is increasing dramatically

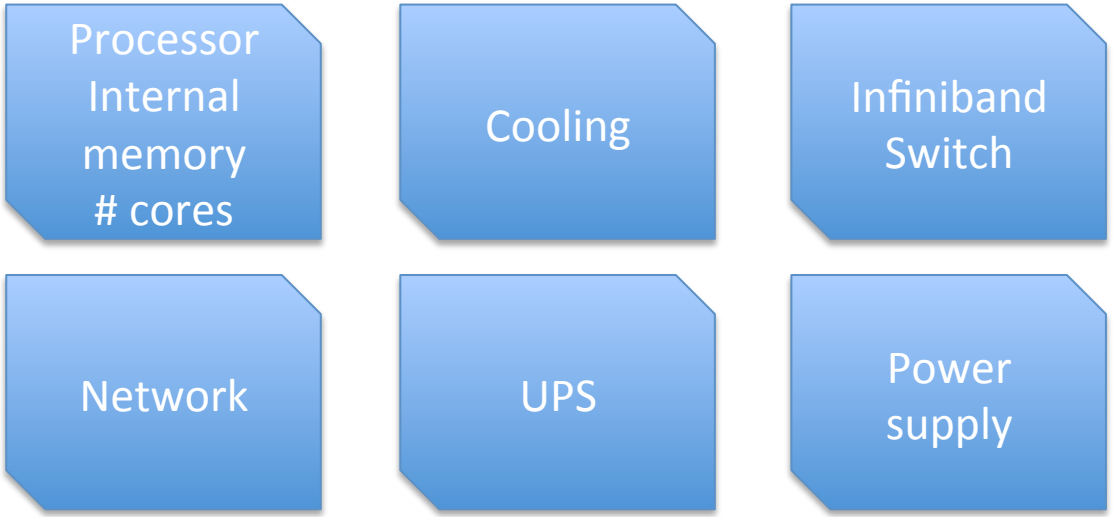
HPC facilities at ICTP

12GB quad-core twin node Nehalem
12GB quad-core twin node Westmere
24GB quad-core twin node Westmere
24GB six-core twin node Westmere
32GB six-core twin node Sandybridge
32GB eight-core twin node Sandybridge
20GB ten-core twin node IvyBridge

Changes in time

- After almost each extension, there is a change in technology
- After 4 years, ICTP has 4 different processor family types
- The amount of memory per core depends on the actual needs and cost
- Same technologies are often grouped in separate queues

HPC facilities at ICTP



Changes in time

- Processors: see previous slide
- Cooling doubled
- Different switches and compatibility issues with Infiniband switches/servers
- Fast network connection (1GB/s) for users of data intensive applications
- Separate UPS installed for the cooling system
- 2nd generator was installed
- Power supply doubled

HPC facilities at ICTP

Advantage to have a local HPC cluster:

- Access control policies can be defined by ICTP
  - Provide access to scientists in developing countries based on our mission
  - Fast process and full control
- Ability to provide a platform with the installation of all relevant software installed for the specific user communities
- Provide the required calculation and storage facilities to ESP
- Keep and develop in-house knowledge of system administration

HPC facilities at ICTP

Earth System Physics (~35 users)	General (> 200 users)	Condensed Matters and Statistical Physics (~30 users)

Management aspects:

- Keep your focus on the satisfaction of the user groups
- Cluster structure mirrors the user group structure
- Finance aspects
  - Extensions partially paid by groups => all contribute, all feel part of ARGO
  - Centrally designed and purchased by IT
- Users with different needs
  - Different queues
  - Treat each user group separately and let them decide their own part
  - Focal points should be assigned within each user group
  - Focal Points should approve each individual access
  - IT is also accountable to the success of the scientific groups

HPC facilities at ICTP

Other management aspects:

- Monitoring in order to ensure a reliable service and to have facts:
  - Ganglia (usage)
  - Nagios (warnings and error messages)

- IT user support team needs to cover the following areas:
  - Access support
  - User support via ticket system (RT)
  - System Admin support
  - Application support (in particular with respect to the multi-core usage)
  - Enabling Scientific Application on High-End Systems

HPC facilities at ICTP

Other management aspects:

- Maintenance strategies
  - Introduce changes only when it is necessary

- Extensions
  - Old machines will be shifted to regular servers (email, web, administrative applications etc.)
  - Focus on price, as technology is changing fast and prices are decreasing always in a short period
  - Donation of old equipment fails normally due to operational cost (power consumption etc.)

HPC education

Workshops / activities:

- Addis Ababa: Workshop on GPU computing (2012). Support to the HPC Master students
- Cartagena, Colombia: Joint ICTP-TWAS Caribbean School on Electronic Structure Fundamentals and Methodologies
- AUST:
  - Presentation at the AUST Seminar Series “HPC Specialization and Opportunities for Graduate Studies and Research”.
  - Workshop on "Cluster installation and management and performance tuning of the Quantum-ESPRESSO package.”
- Nairobi (Kenya): Workshop ESP at ICPAC Centre
- Abidjan (Ivory Coast): Workshop on ESP
- Jakarta: HPC workshop (Dec 2013)

Other meetings/collaborations:

- Meeting with the South African Centre for High Performance Computing (CHPC)

Joint SISSA/ICTP HPC academic program

Joint SISSA/ICTP HPC academic program: HPC Master Program

- Objective: provide HPC expertise and insights for scientists in academia and industrial R&D
- MSc programme will start in fall 2013 (Pre-lectures started)
- Lecturers/staff from Trieste (ICTP, SISSA) and external specialists
- Duration: 18 months
- Program:

Part I: 6 months	Part II: 3 months	Part III: 6-9 months
Introduction to HPC Advanced and parallel programming, software design and management, numerical analysis, data management, computer hardware and administration	**Building Blocks for HPC in Science and Technology** Fundamental algorithms and strategies common to many scientific HPC applications	**Practical HPC Experience** An HPC project contributing to an ongoing research effort