Intro to High Performance Computing and its Applications

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CHPC
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The CHPC

- South African National supercomputing facility, started 2007
- 40 staff, 16 researchers supporting >500 users in many fields (>140 active research programmes)
- Over 32 000 cores + 5 large memory machines (1 TB)
  Test-bed facilities including GPUs FPGA, MIC
  Petabyte storage facility
- Training & development

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HPC, my view

HPC hardware = many computers linked together with fast networking + storage

HPC = using HPC hardware to do useful research

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The CHPC – applications

CHPC in South Africa has users in many fields:

- Health
- Mining
- Construction
- Energy
- Weather, Oceans, Climate change
- Film & media
- Finance
- Astronomy

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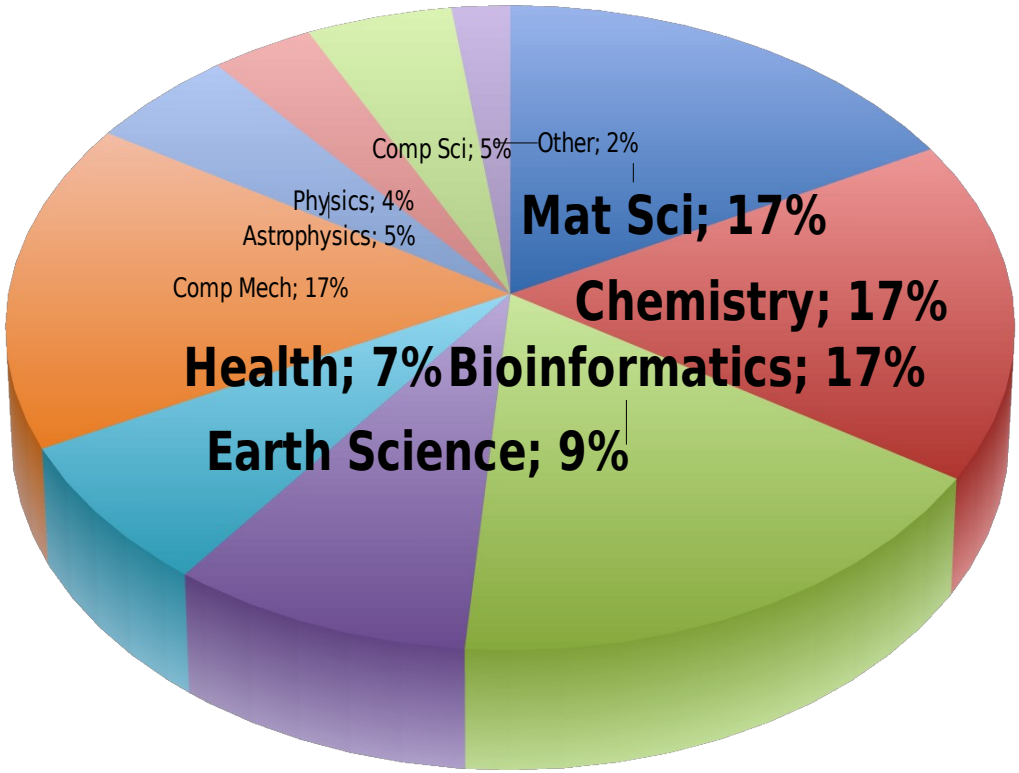
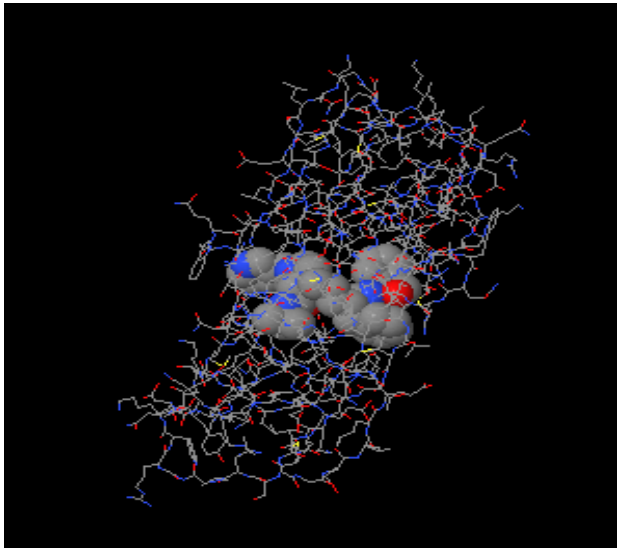
The CHPC – applications

- **Lengau Total # Research Programmes (1 Apr 2016 - 30 Nov 2017): 193**

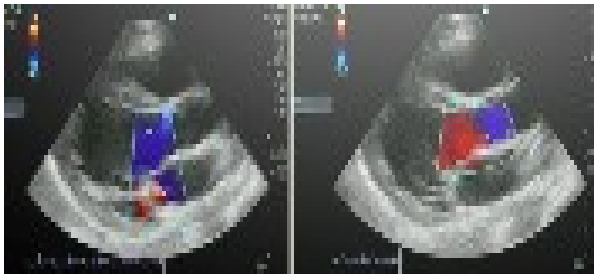


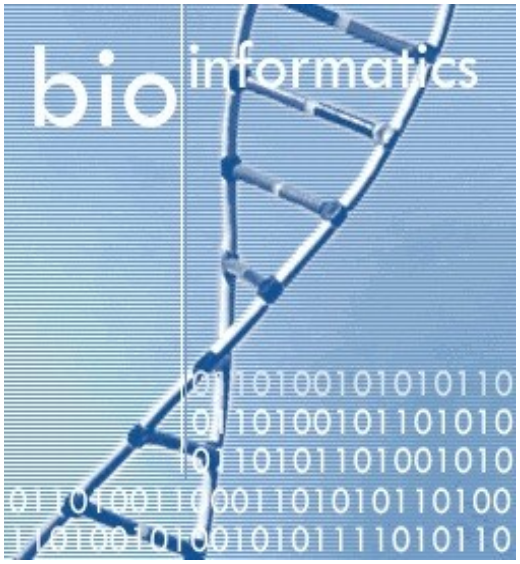
The CHPC - applications

Health → drug design, heart image processing, genetics



GPU + data portal





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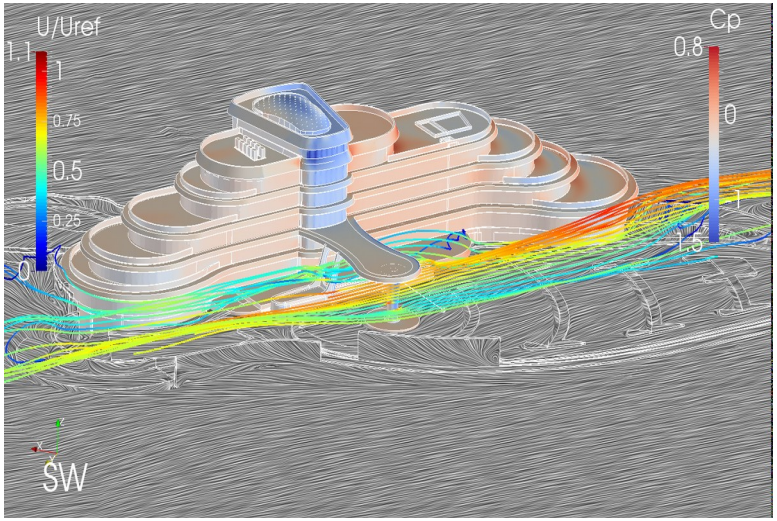
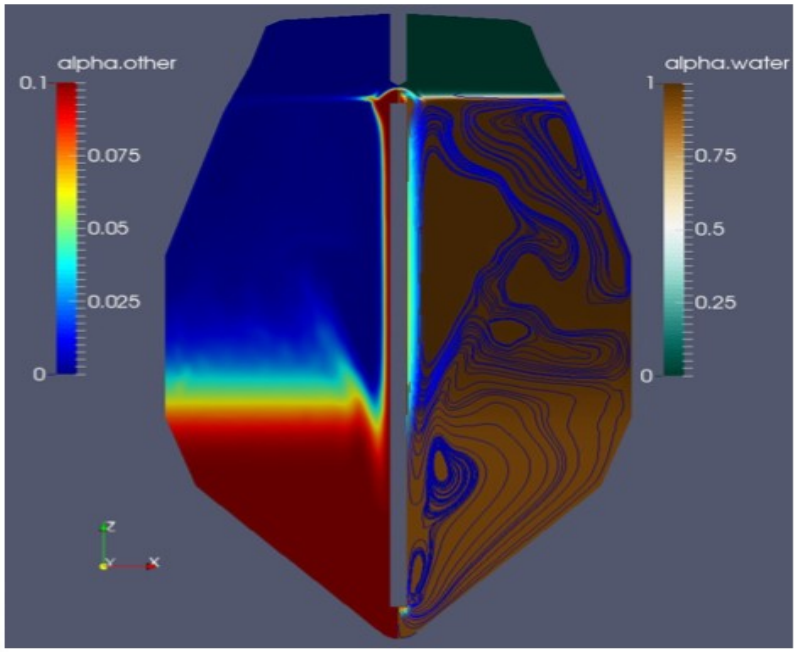
The CHPC - applications

Construction



Water Treatment



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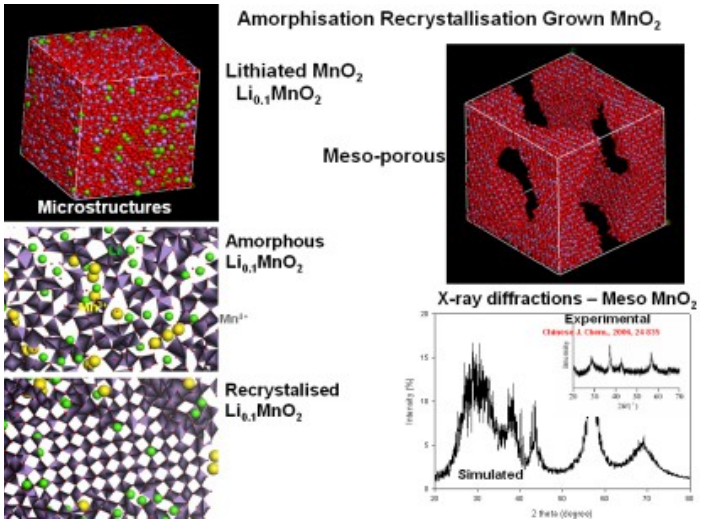
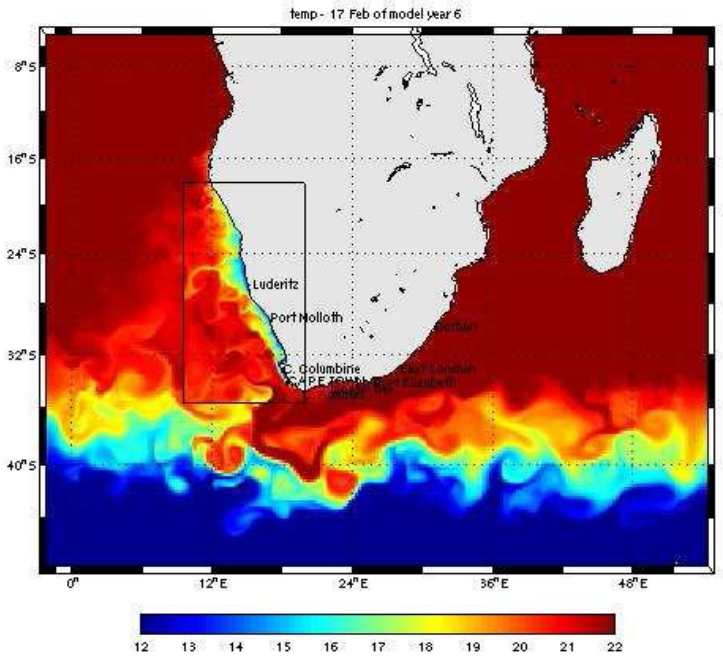
Energy:

Battery materials
Smelting



Oceans & Climate Change



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The CHPC - applications

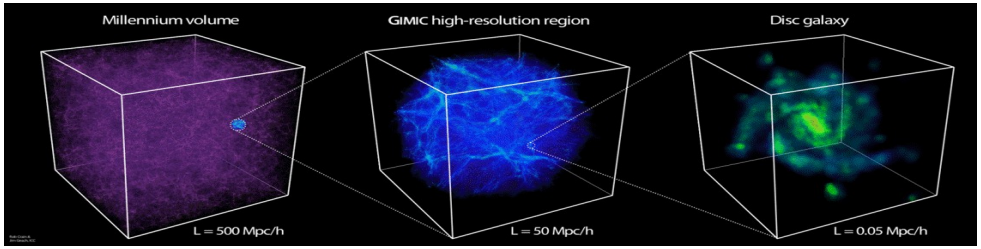
Astronomy

Theoretical calculations (exotic cosmologies)

Sean February

Galaxy Evolution Simulation

Matthew Cawood



Probing Dark Matter & Dark Energy using light from early universe

Data Mining

Israel Tshililo

Measuring expansion rate of universe at half age of universe

Model fitting and Statistics + own data from SA Large Telescope)

Ando Ratsimbazafy - Madagascar

Relating dark matter to luminous matter

Data mining and model fitting

Vijay Chumroo - Mauritius

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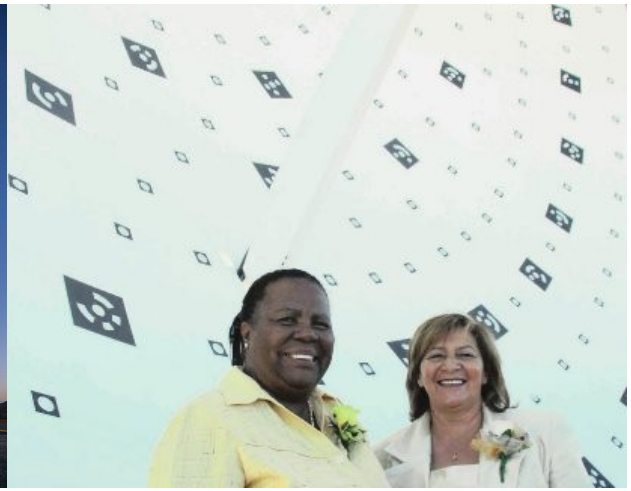
The Square Kilometer

Billion dollar radio telescope for 2020+

Phase 1: 200 dishes in SA + array in Australia

Phase 2: Antennae in 9 African countries including Kenya



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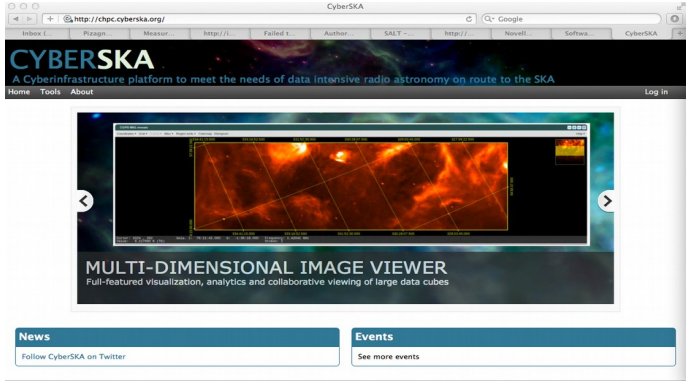
SKA → HPC, Big Data

SKA data more than 10x current global internet traffic

Many levels of data crunching

* Hardware accelerators: FPGA, GPU
* Calibration and Imaging of data → image processing, visualisation
* Detecting sources like radio galaxies in HUGE multidimensional data
* Statistical analysis of resulting catalogs of galaxies
* Comparison of models with data → stats, N-body simulation

Data Portals: large international collaborations



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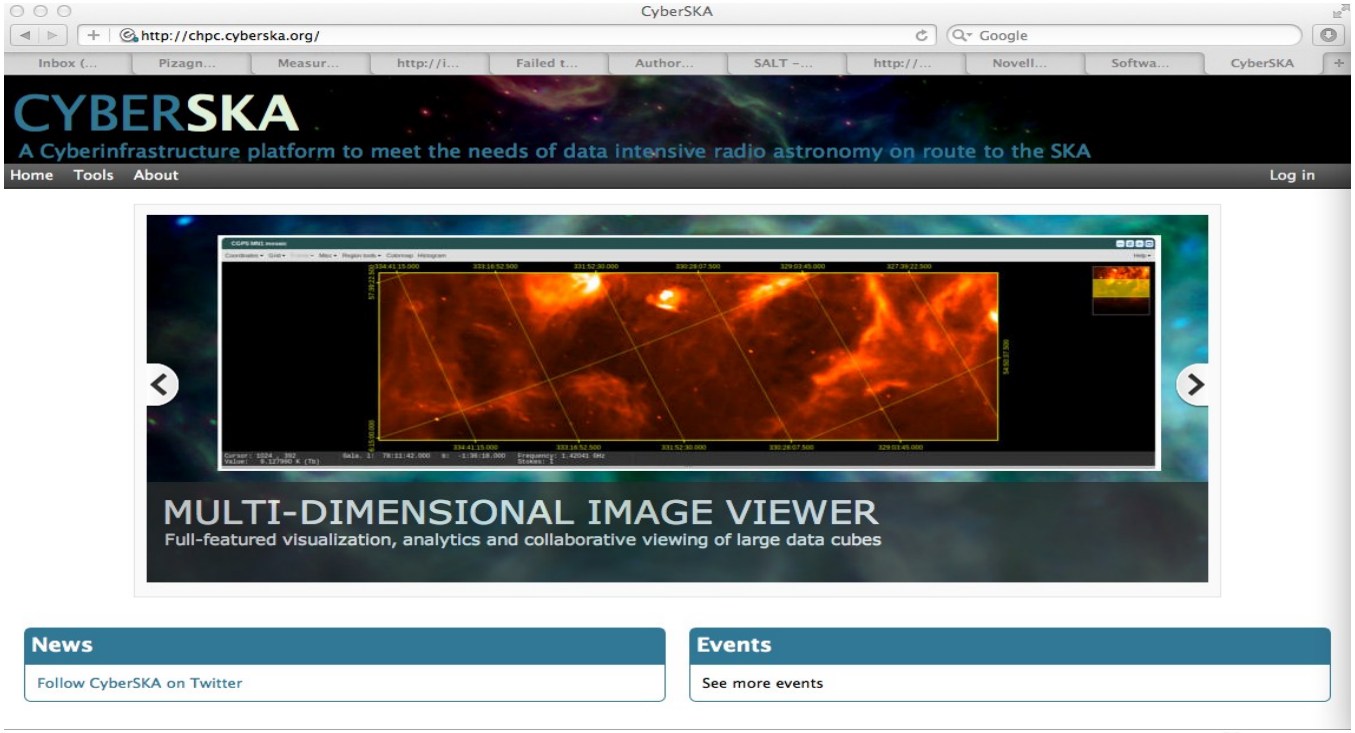
SKA → HPC, Big Data

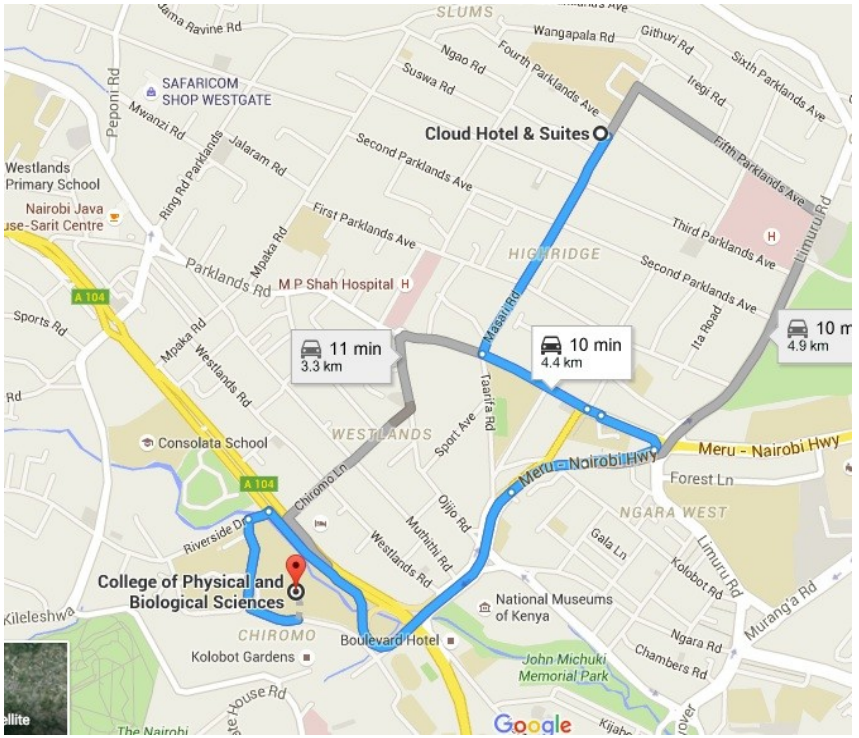
Needs for large global teams to collaborate
CyberSKA data portal



Big Data Impact

Example:

Google Maps:
Real time navigation,
Incredible detail



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Astronomy → Data Scientists

McKinsey: By 2018, shortage of over 150000 data scientists.

Astronomers/Physicists often data scientists

Data Science courses:
Statistical Analysis
Modelling
Visualisation
Machine learning
HPC & parallelisation
Databases and SQL
Security & governance

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SKA Computing development in Africa

* Zambia:
hardware up and running, workshops run

* Mauritius, Madagascar, Namibia
hardware shipped, projects underway

* Botswana
hardware in place

* Kenya
Negotiation on hardware, projects initiated

* Ghana
AVN, existing computer infrastructure

* Mozambique
Initial discussions

ACCESS TO CHPC

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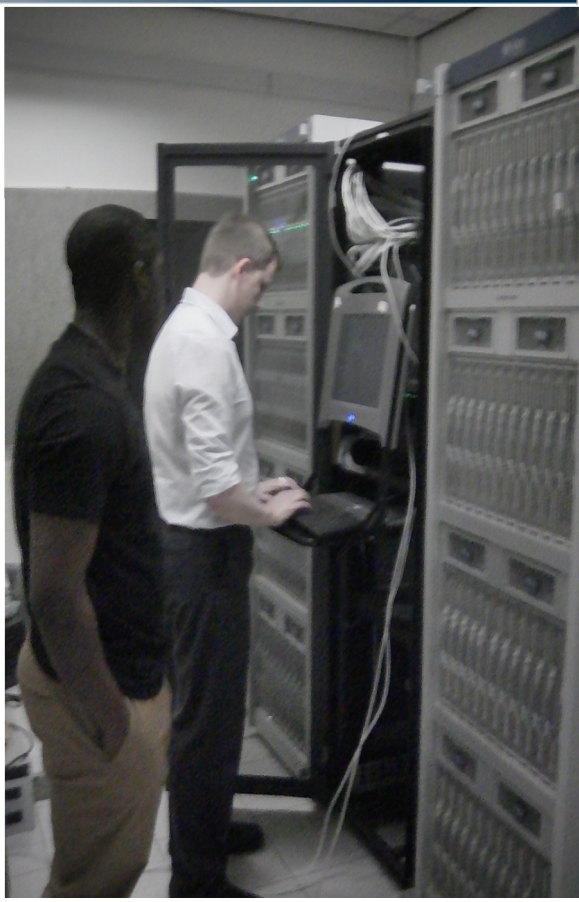
eg. Botswana's



Used hardware donated by Texas ACC
4 racks
rack has 4 chassis
chassis has 12 nodes
node: 4 quad-cores = 16 cores

16x12x4x4= 3072 cores
Only power-up a fraction of these (2x192?)

Users?:
Atmospheric Physics, Chem/Phys:
eg Catalysis, Bioinformatics, Geophysics (eg seismology)

CHPC Computing development in Africa

Twelve visits (22 trips funded)
Over 200 contacts in database

	SysAdmin	User ID (staff)	User Workshops	Visit Dates
Botswana	30	10UB+3 (BIUST)	20+15	8Jul16, 15-22Oct16
Namibia		3		25Jun16
Zambia	3	4CBU+5UZAM	50+20+20	23-30Sept15
Madagascar	3	4UA+5	20+30	14-26 Nov15, 20-31Aug16
Mauritius		3		1-10Jul13
Mozambique		3	50+20	16-23Mar16
Kenya		6	30+30	6Jul15, 5-14Jun16
Ghana				21-22Nov13

CHPC Computing development in Africa

Priorities:

1. User development
   - people on the ground – in Astronomy and other fields
   - need projects in useful fields eg agric, health, mining, tourism
   - view to jobs & commerce → data science business?: ML etc.

2. “last mile” networking

3. Online community development – courses together, data science

BIG DATA AFRICA FELLOWSHIP PROGRAM

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CHPC user support

Over 500 users on system – not all active
Over 150 different research programs

Each program has Principal Investigator(PI) + team
PI = permanent staff member with publication record from South Africa or SKA partner country
Team = students, postdocs, foreign members
Each program allocated research scientist at CHPC

User database, resource allocation
Wiki
Training
National conference – www.chpcconf.co.za
Flagship projects

Do I need CHPC?

Scenario 1:

Student:
“my code runs to too slowly on my laptop, I need HPC”

Supervisor:
“I can't/won't code – contact the CHPC”

HPC not necessarily the answer
But possibly support for code improvement from CHPC staff

Do I need CHPC?

HPC:

1. Many computers linked together + fancy networking
2. One computer with many cores, large shared memory (1TB)

(3. not really at CHPC: GPUs)

Before considering HPC:

1. Can I improve my code so it runs faster on my laptop?
   Excessive I/O? Unnecessary loops? code profiler? Compiler?
2. How can I break down my problem into smaller pieces?
   Run many instances at same time? Which parts parallelize?
3. Do I have huge files that need to be open in memory?

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Do I need CHPC?

HPC vs Big Data

HPC used to be focussed on maximising number of operations possible
Now need more thought about large I/O → Big Data

CHPC vs Cloud services eg Amazon etc
No GPUs on production cluster (future?) → machine learning?

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Do I need CHPC?

At CHPC:

Main cluster
1 node has 24 cores, 128 GB mem (360nodes have 64GB)
1368 nodes => ~32000 cores

'Fat nodes'
56 cores, 1 TB each

You will need to rewrite code to run in parallel
Eg. MPI4Py

Do I need CHPC?

Scenario 2:

I want to store large amounts of data (many TB) for long periods

→ CHPC does not provide storage for long periods

→ Contact DIRISA (another part of SA CyberInfrastructure)

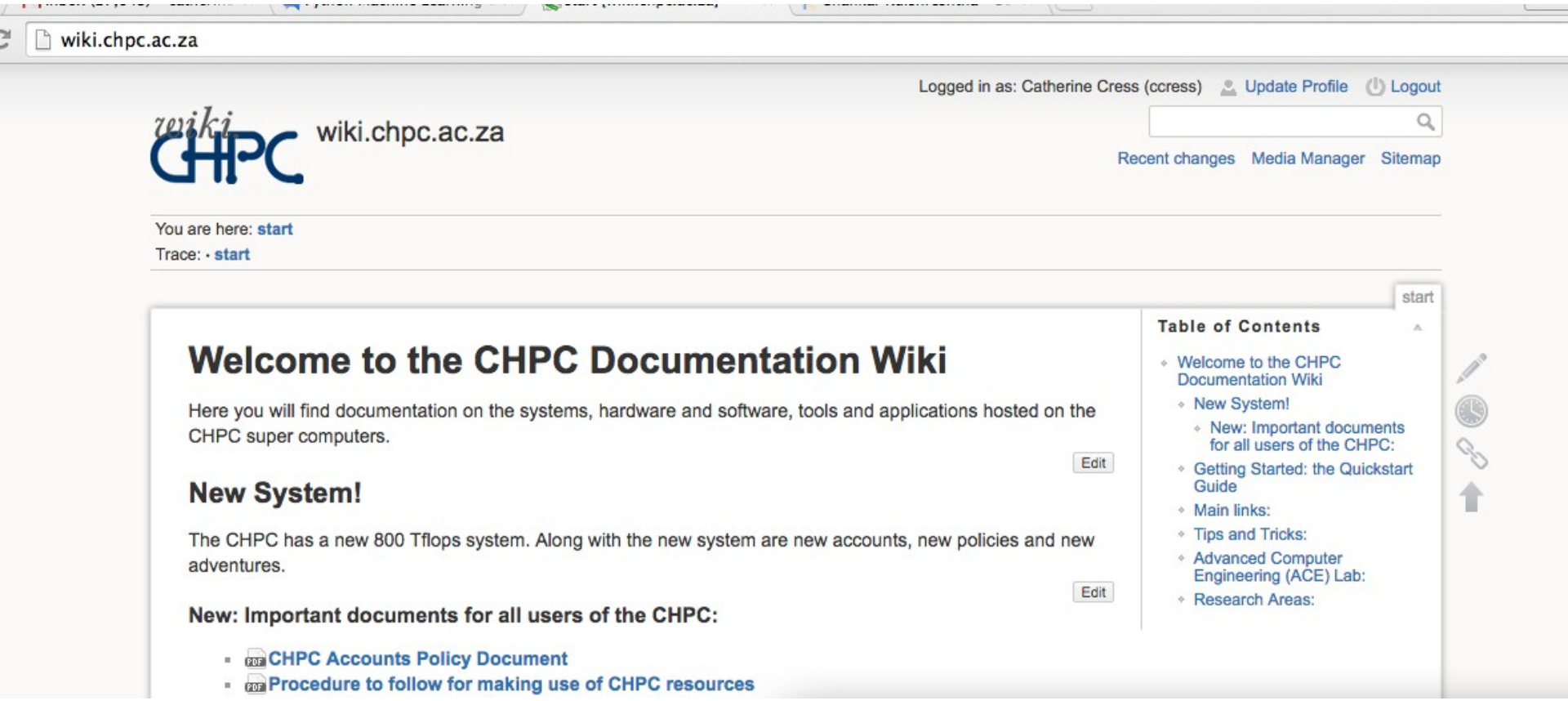
CHPC user support - database

Principal Investigator (PI) : permanent staff member at SA university/institute, with PhD & publications

PI applies, once approved, creates research project then adds team members (students etc)

Amolo, George	gamolo	georgeamolo862@gmail.com	University of Eldoret	Properties of Materials for Green Energy Harnessing
Anand, Krishnan	kanand	organicanand@gmail.com	Durban University of Technology	Combined kinetics,quantum-chemical investigation of reaction mechanisms involving catalysts
Anandjiwala, Rajesh	ranandi	ranandjiwala@nmmu.ac.za	Council for Scientific and Industrial Research	Mechanics of Flexible Fibrous Assemblies
Anderson, Matthew	None	andersmw@indiana.edu	0 Other	
Andeve, Calvin	candeve	215082608@stu.ukzn.ac.za	University of KwaZulu-Natal	IN SILICO EVALUATION OF NANO DRUG DELIVERY SYSTEMS
Andriambelaza, Noeliarinala Felana	None	arinala.f@gmail.com	University of Pretoria	
Andriambeloson, Joely	jandriambeloson	andyjoely@gmail.com	Stellenbosch University	Radio Frequency Interference Measurement, Monitoring and Mitigation for MeerKAT and SKA

CHPC user support - wiki



CHPC training

- Intro to Linux and python → data science
- Parallel programming
- Applications courses (usually at december conference)
- Research Scientist help

- **Student Cluster Competition:**
  Students compete to make best compute cluster
  S.African team won 3 times! (vs Chinese,Germans etc)

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Cloud at the CHPC

Cloud for HPC Project
Virtual Clusters
- HPC Software Evaluation and R&D
- Clusters for training courses
- Support users with special computing needs
- Hybrid Clouds
- Clusters for the Student Cluster Competition

Public Cloud Prototype
Exploring OpenStack further
- New features, Docker integration, GPUs

Summary

Centre for High Performance Computing in South Africa:
> 500 users: chem, materials, climate, fluid engineering, film

Involved in SKA project: Astronomy driving tech dev → HPC, Big Data
Astrophysics projects: Nature of dark matter and dark energy?
Data, simulation, theory → Data science

Computing development in African SKA partner countries
old hardware in some places – few users

Who should use HPC?

→ User support at CHPC → training, in-house researchers, wiki, slack