Good Practices in HPC Management

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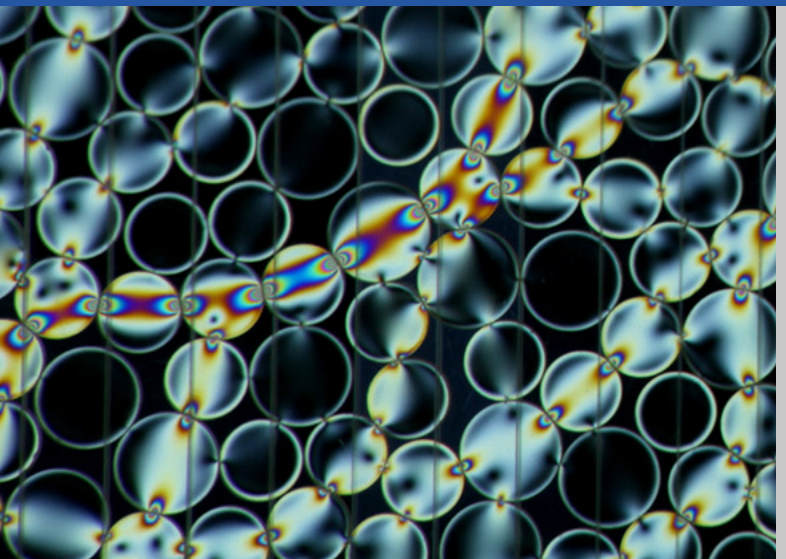


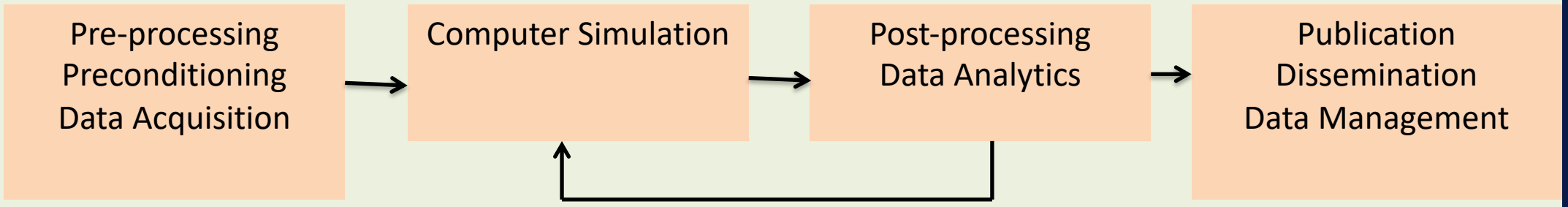
Sept 2023

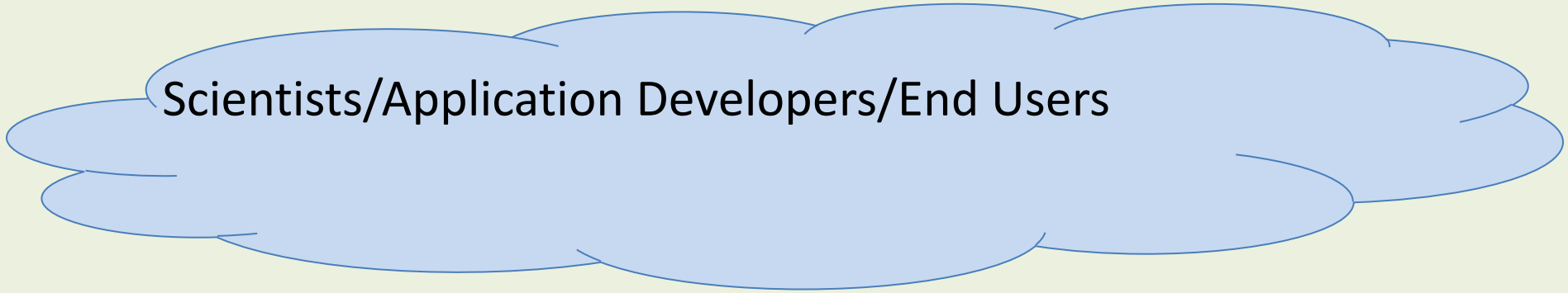
The Abdus Salam International Centre for Theoretical Physics

HPC is not IT !!

- **Scientific applications are in constant development**
- **Scientific applications are mostly written by rookie developers (i.e. PhD students, post-docs)**
- **Scientific application are composed of multipule etherogenous components expected to work at full speed**
- **IT is for standardized SW, HPC is for scientific computing!**

HPC INFRASTRUCTURE





SW Workflow & Parallel Applications

Compilers/Libraries/Debugging & Profiling

HW/Resource Management/File System/...

HPC ecosystem (HD + SW + Science)

- **ICTP experience**
  - **scientists looking for resources**
  - **HPC managers reporting about empty and/or disused infrastructures**

How to: ensure technology is not the limiting factor of scientific progress

- **understand your target domain of users**
- **(beginners, average, experts)**
- **make available HW that fits their needs**
- **make available SW that can enable scientific production**

Example of the ICTP Scenario

- **Example of the ICTP Scenario**
  - **Experts users -> CINECA/PRACE (EuroHPC)**
  - **Average users -> Argo/CINECA**
  - **Beginners users -> Argo + Training**

- **ICTP goal of building HPC ecosystem for scientific research in dev-countries: the ICSC**

An International Consortium for Scientific Computing

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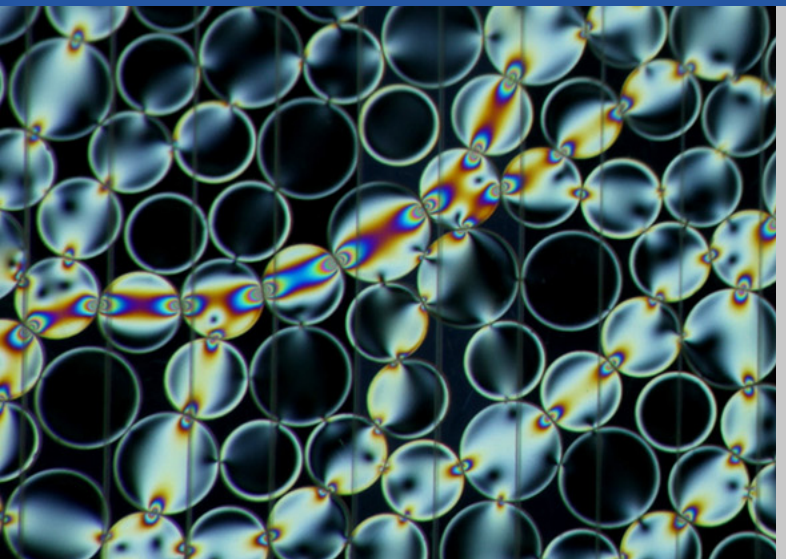

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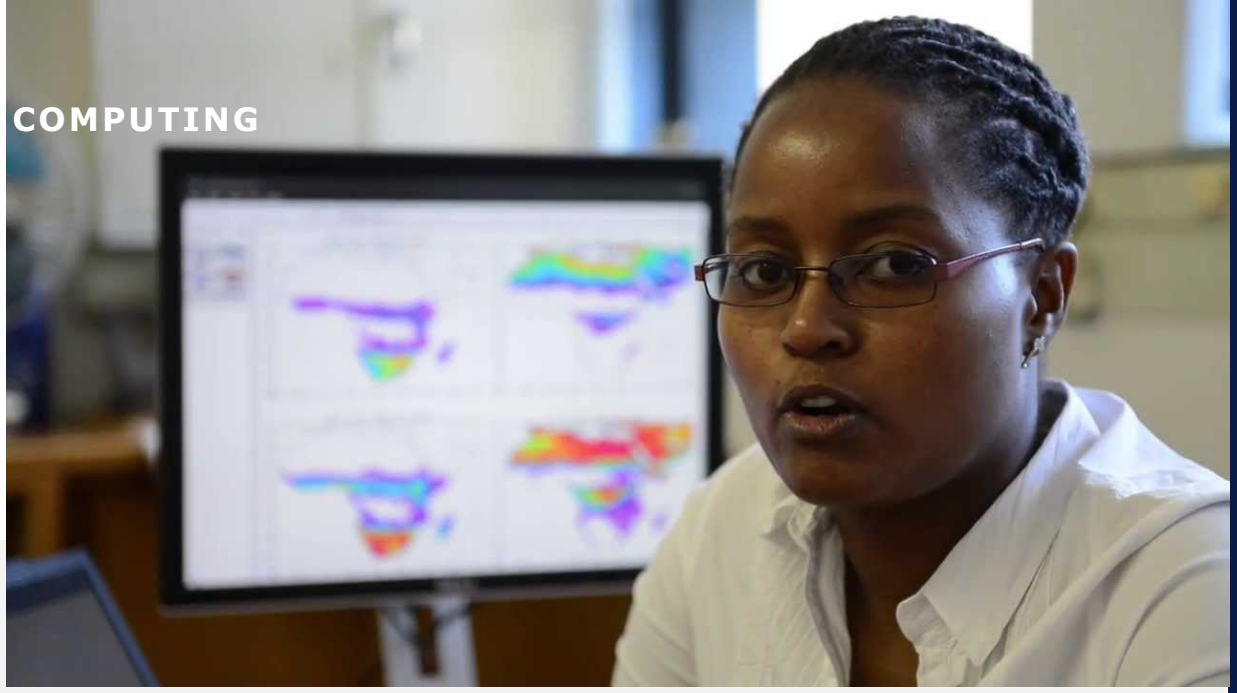
Mary-Jane's dream



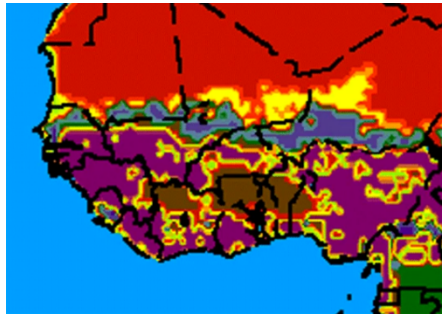
Prof. Mary-Jane Bopape,

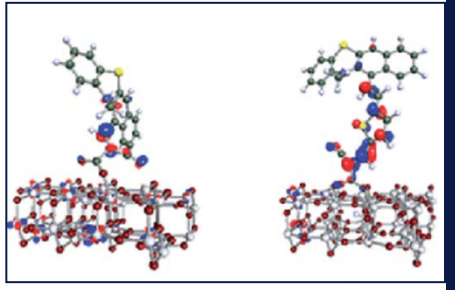
meteorologist, South Africa

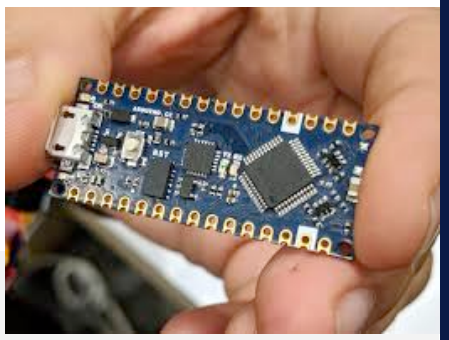
Climate modelling is key for the provision of actionable information for use in impact, vulnerability and adaptation assessments and policies (agriculture, water resources, natural hazards, etc)

Mary-Jane's dream: to develop a ultra-high resolution (~1 km) regional climate model for Southern Africa

Challenges and Solutions



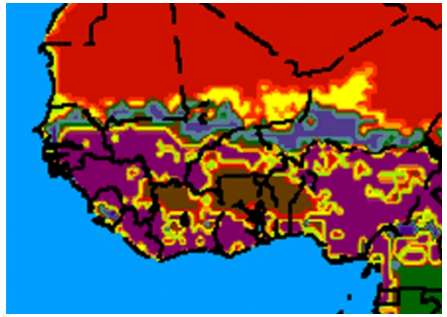


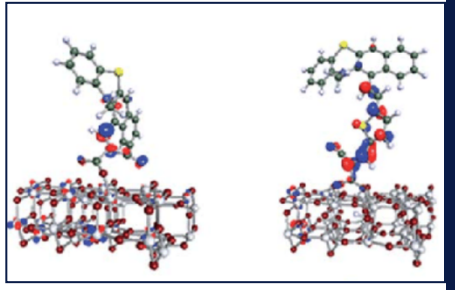


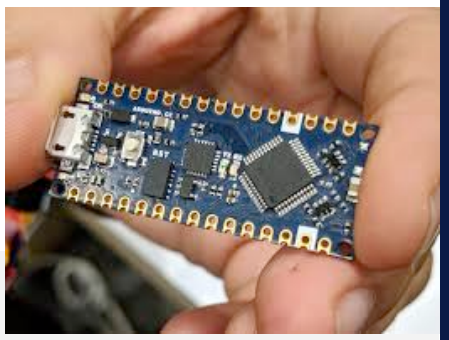
Challenges:

- Lack of international collaborations & research ecosystems
- Limited «human capacity» in emerging fields (AI & Data Science)
- Computational infrastructures (LATAM's top facility for research 173th in Top500)
- Growing «divide» between developed and developing world

Challenges and Solutions





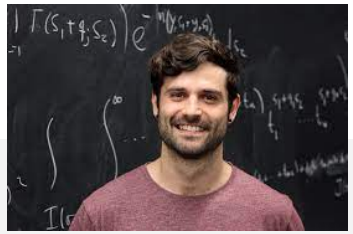


The **International Consortium for Scientific Computing** will:

- ✓ Create a shared platform to seize the opportunities offered by new algorithms (ML, AI, BigData) and new hardware architectures
- ✓ Offer access to large-scale computational facilities
- ✓ Strengthen training programs and tie them to scientific collaborations & access to computer time
- ✓ Tackle selected scientific grand challenges (with impact on SDGs)

Current Status at ICTP

Climate Models (RegCM)



ERC Starting Grant ML/Data-Science Theory

Molecular/Materials Modeling
(e.g. Quantum Espresso)
Cosmology
Many-body Physics
…

HPC in-house experts
I. Girotto (HPC)
G. Giuliani (Climate)
S. Di Gioia (Astro)

Schools

MHPC Master in High Performance Computing — **SISSA**

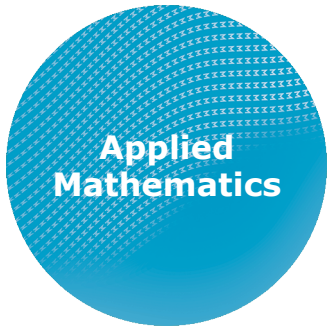
DATA SCIENCE & SCIENTIFIC COMPUTING — **Univ Trieste**

CINECA, CHPC, NItheCS
(South Africa)

ARGO
(in-house cluster)

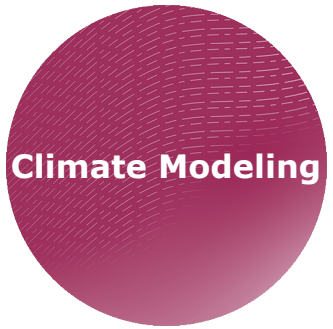
INTERNATIONAL CONSORTIUM FOR SCIENTIFIC COMPUTING

J. Barbier (ERC)
+ 1 staff



ADVANCED
COMPUTING
CORE
THRUST

ACCT



E. Coppola
F. Kucharski
F. Giorgi
A. Tompkins
R. Farneti
+ 1 staff

R. Gebauer
N. Seriani
N. Binggeli
S. Scandolo
+ 1 staff

I. Girotto
G. Giuliani
S. Di Gioia
+ 1 staff

A. Hassanali (ERC)
+ 1 staff

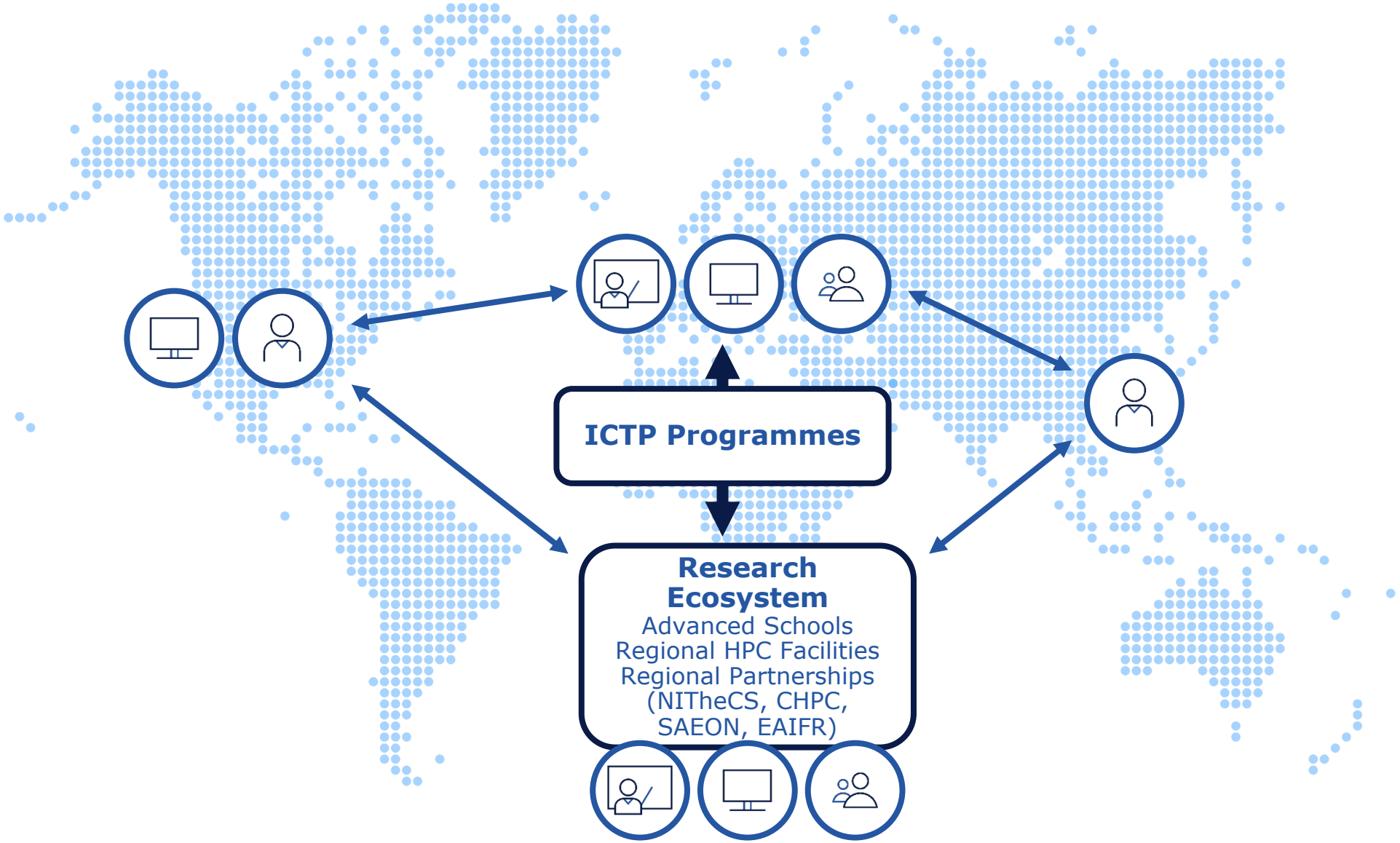
Scientific Advisory Board (external)

Management board (internal)

Actions:

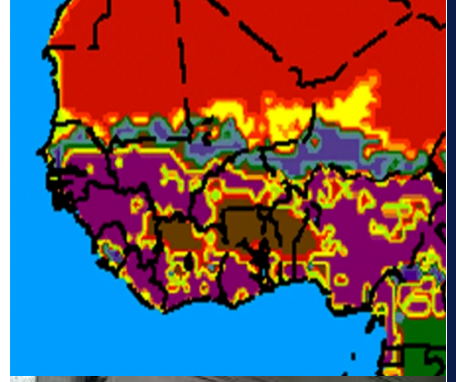
- 5 projects / area to be defined with help from Sci. Adv. Board
- Consolidation of ACCT
- "Acquisition" of computer time
- Partnerships and fund raising
- 5 extra staff members

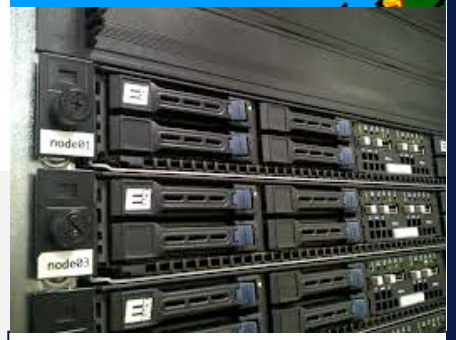
Example: Regional Climate Model for Southern Africa

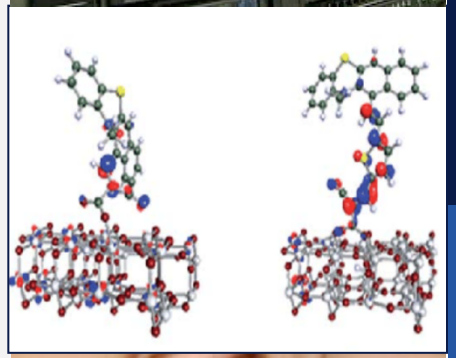


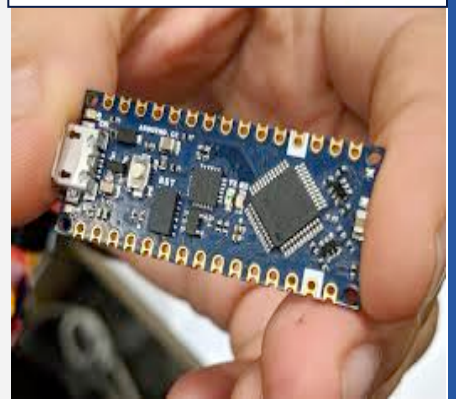
Expected Outcomes

- To operate as an **incubator of scientific research collaborations** open to scientists from all over the world.
- To leverage the fundamental components of modern research (education, resources, technical skills and scientific insight) towards the **creation of ecosystems** for advanced computing that will advance scientific research in the developing world and contribute to **close the growing divide between North and South** in fields that are crucial for the sustainable development of these regions.
- To **fight the brain drain** of high-level technical experts in strategic areas of economic development.









Review by Experts

Reviewers:

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N. Carriero (Flatiron Institute)

J.M. Gutiérrez (U. Cantabria)

H. Sithole (NICIS, S. Africa)

F. Ricci-Tersenghi (Roma)

Comments:

- expand scientific case, identify scientific challenges in each field
- consider extension to observational cosmology (SKA, etc)
- ask letters of support from partners
- include scientists from developing countries as advisors