## HPC Cloud Interactive User support

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**Big** Grid the dutch e-science grid

### SARA Project involvements





HPC Cloud Philosophy

#### HPC Cloud Computing:

#### Self Service Dynamically Scalable Computing Facilities

# Cloud computing is not about new technology, it is about new uses of technology







# Our starting point for BiG Grid HPC Cloud

- Easy & standard(familiar) access protocol
  - name&password (or x509 certificates)
  - Support ad hoc collaborations
  - Support Cloud standards (OCCI, OVF, CDMI, WebdDAV)
- Zero client software install
  - Standard browser with java applets & javascript enabled
  - Additional tools optional: VNC viewer, ssh/putty etc
- User has free choice
  - Operating System & applications
  - Root rights in VM and on private network
  - Configuration of private cluster
  - Anything goes: Multi core, multi node, long running (services, databases)
- It doesn't have to be optimal, great is good enough
  - Virtualization overhead acceptible, only thousands of users not millions, only terabytes not petabytes

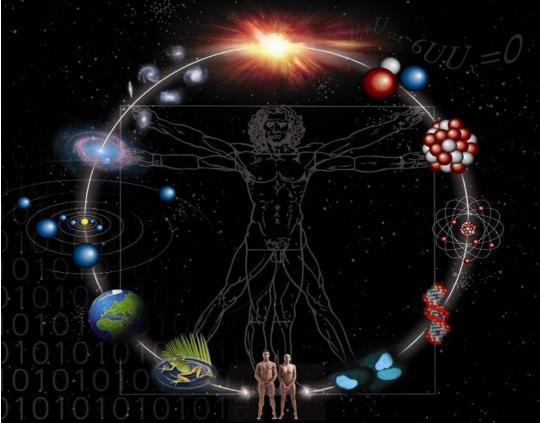


# Users of Scientific Computing

- High Energy Physics
- Atomic and molecular physics (DNA);
- Life sciences (cell biology);
- Human interaction (all human sciences from linguistics to even phobia studies)
- from the big bang;
- to astronomy;
- science of the solar system;
- earth (climate and geophysics);
- into life and biodiversity.

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Slide courtesy of prof. F. Linde, Nikhef

# Users in pilot and beta phase

- From the start at least 50% in use
- Currently between 70-80%
- 50 user groups
  - 30 % from lifesciences (bio-informatics)
  - Psychology
  - Geography
  - Linguistics
  - Econometrists
- Currently 19 requests on waitinglist (!)
- Festive Launch at 4 th October in Amsterdam (www.sara.nl → Agenda)

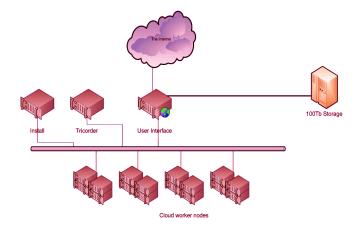


# The product: Virtual Private HPC Cluster

#### • We offer:

- Fully configurable HPC Cluster (a cluster from scratch)
- Fast CPU
- Large Memory (256GB/32 cores)
- High Bandwidth (10Gbit/s)
- Large and fast storage (400Tbyte)
- Users will be **root** inside their own cluster
- Free choice of OS, etc
- And/Or use existing VMs: Examples, Templates, Clones of Laptop, Downloaded VMs, etc
- **Public** IP possible (subject to security scan)

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Platform and tools:

- Redmine collaboration portal
- Custom GUI (Open Source)
- Open Nebula + custom add-ons
- CDMI storage interface

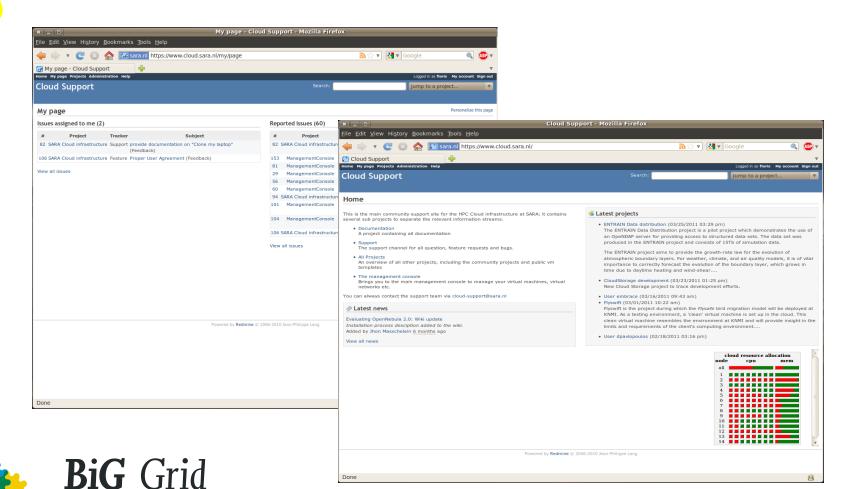
# HPC Cloud, what is it good for?

- Interactive applications
- High Memory, Large data
- Same data, many different applications (Cloud reduces porting efforts!)
- Dynamic, fast changing and complicated applications
- Clusters with Multi Operating Systems
- Collaboration
- Flexible and Versatile
- System architecture is expandable and scalable

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### **User collaboration Portal**

#### Redmine (www.redmine.org)



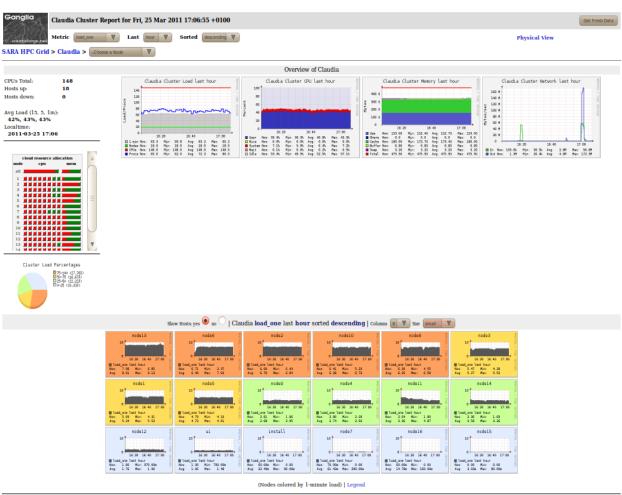
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## Self Service GUI

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#### Monitoring workload





Gangla Web Frontend version 3.1.7 Check for Updates. Gangla Web Backend (ometad) version 3.1.7 Check for Updates Downloading and parsing gangla's XML tree took 0.0288s. Images created with RRDTool version 1.3.1. Pages generated using TemplatePower version 3.0.1.

# Advantages of HPC Cloud

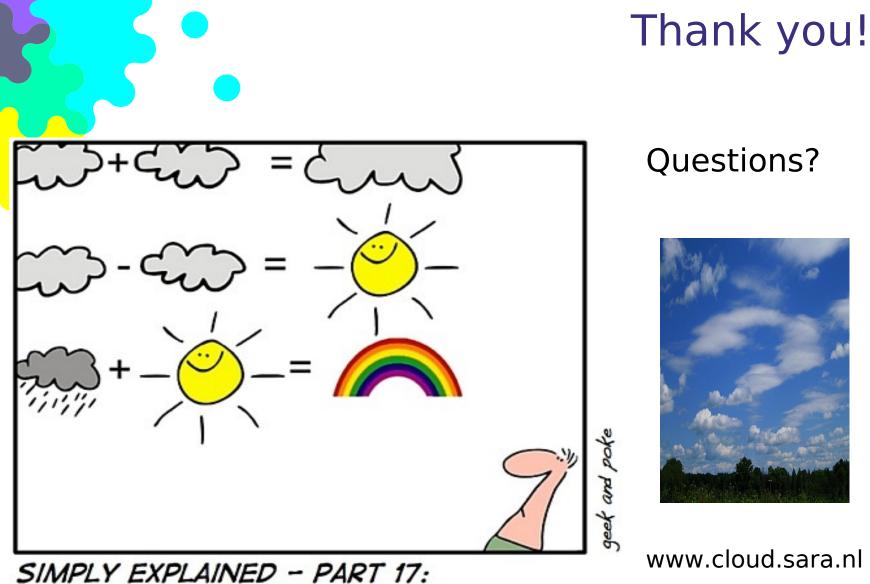
- Only small overhead from virtualization (5%)
- easy/no porting of applications
- Applications with different requirements can coexist on the same physical host
- Long running services (for example databases)
- Tailored Computing
- Service Cost shifts from manpower to infrastructure
- Usage cost in HPC stays Pay per Use
- Time to solution shortens for many users

#### **BiG** Grid the dutch e-science grid



- Usage: Scientific programmer prepares environment, Scientist uses
- Several "heterogenic clusters" Microsoft Instances combined with Linux
- Modest parallelism (maximum 64)
- User wishlist: Possibility to share a collection of custom made virtual machines with other users
- Added value: support by your trusted HPC centre.
- HPC Cloud on HPC hardware is necessary addition to a complete HPC eco-system
- Interactive support works (some users do read tickets and documentation)





SIMPLY EXPLAINED - PART 17: CLOUD COMPLITING

www.cloud.sara.nl

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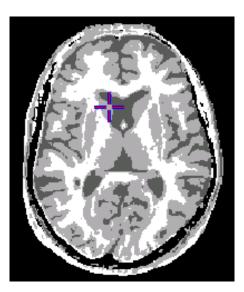
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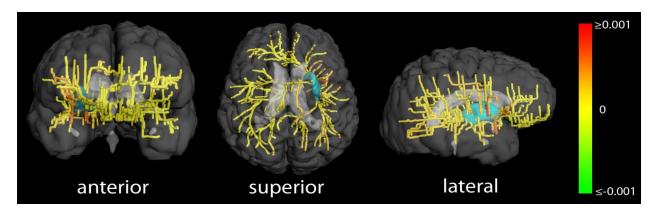
# Example Project 1

- Medical data MRI Image processing pipeline
  - Cluster with custom imaging software
  - Dynamic scaling up depending on the load
  - Added 1 VM with web service for user access, data upload and download

**BiG** Grid

es from H. Vredne duter of science grid





#### Example project 2 MR spectroscopy: Virtual Cing by J. Doreleijers

With NMR spectroscopy the 3D structure of biomolecules such as proteins and DNA are solved in solution. It thus provides a structural view of the chemical reactions that underly most diseases.

NMR structure determination needs a solid validation of the experimental data in relation to the resulting 3D coordinates because the process in many labs has not and often -can- not be automated fully. A virtual machine called VirtualCing (VC for short) interfaces to the best 24 NMR validation programs, together with CING's internal unique checks. VC was developed because installing the external programs on a traditional grid would take too long in development and would be cumbersome to maintain. We were able to validate all the 8,000+ structures currently available in the worldwide database Protein Data Bank (wwPDB) in just a week. The same strategy is applied to recalculate, improve and validate several thousand protein structures in a new project named NMR\_REDO.

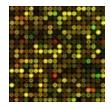
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## **User Experience**

#### (slides from Han Rauwerda, transcriptomics UVA)

**Microarray analysis**: Calculation of F-values in a 36 \* 135 k transcriptomics study using of 5000 permutations on 16 cores. Over 10 week period **30.000** core-hours Data analysis using R (statistical analysis) with specialized plugin



#### Ageing study - conditional correlation

- dr. Martijs Jonker (MAD/IBU), prof. van Steeg (RIVM), prof. dr. v.d. Horst en prof.dr. Hoeymakers (EMC)
- 6 timepoints, 4 tissues, 3 replicates and 35 k measurements + pathological data
- Question: find per-gene correlation with pathological data (staining)
- Spearman Correlation conditional on chronological age (not normal)
- p-values through 10k permutations (4000 core hours / tissue)

#### Co-expression network analysis

- 6k \* 6k correlation matrix (conditional on chronological age)
- calculation of this matrix parallellized. (5.000 core hours / tissue)

Development during testing period (real life!)

#### Conclusions

- Many ideas were tried (clusters with 32 64 cores)
- worked out of the box (including the standard cluster logic)
- no indication of large overhead
- Cloud cluster: like a real cluster
- Virtually no hick-ups of the system, no waiting times
- User: it is a very convenient system

# BiG Grid

the dutch e-science grid