Biosciences Working Group Update

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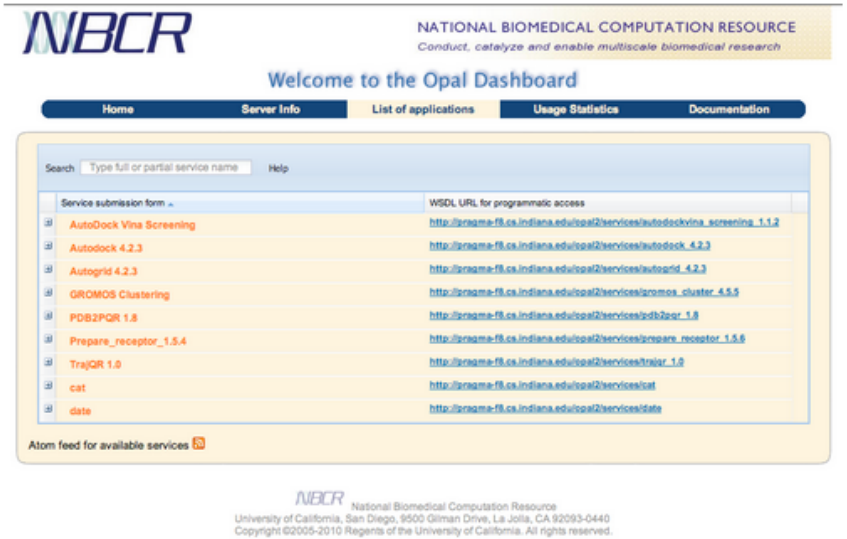
Hosted by Kasetsart University

Bangkok, Thailand March 20-22, 2012

Rocks BioApp

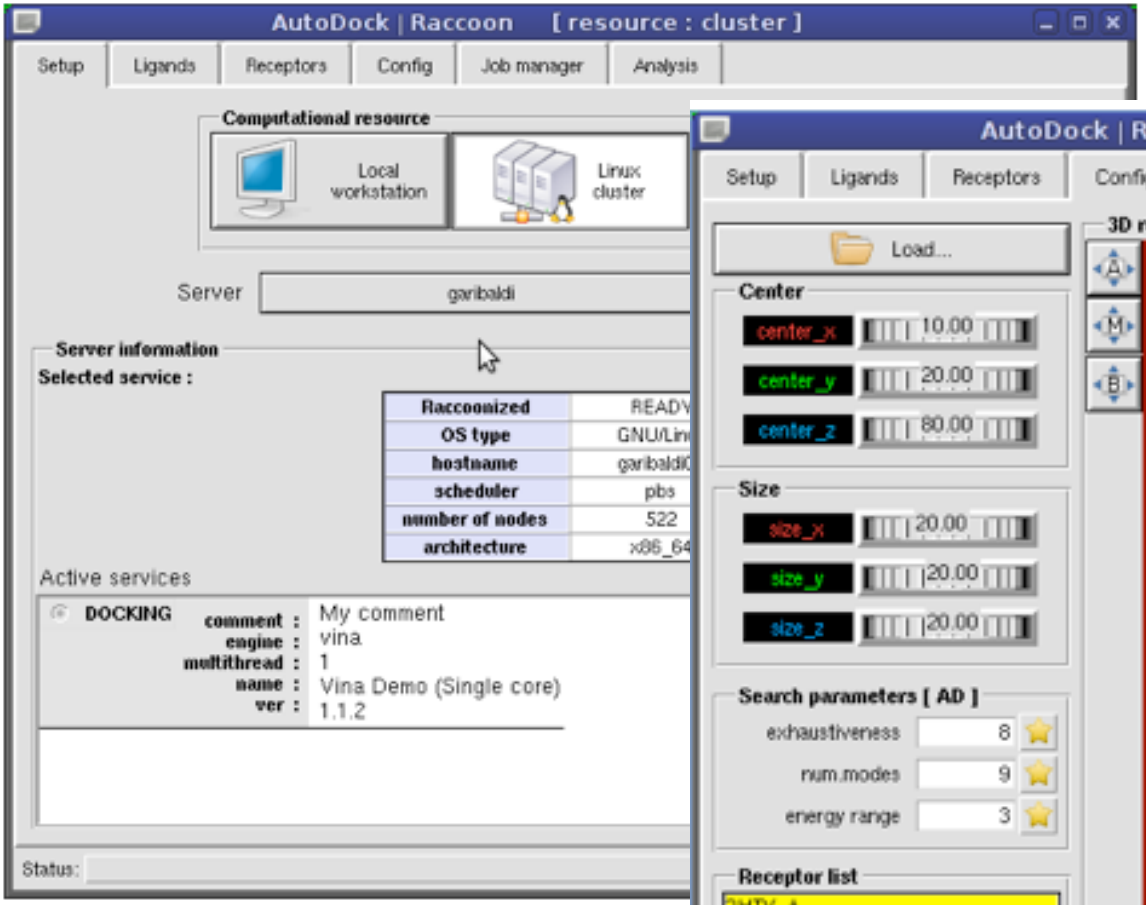


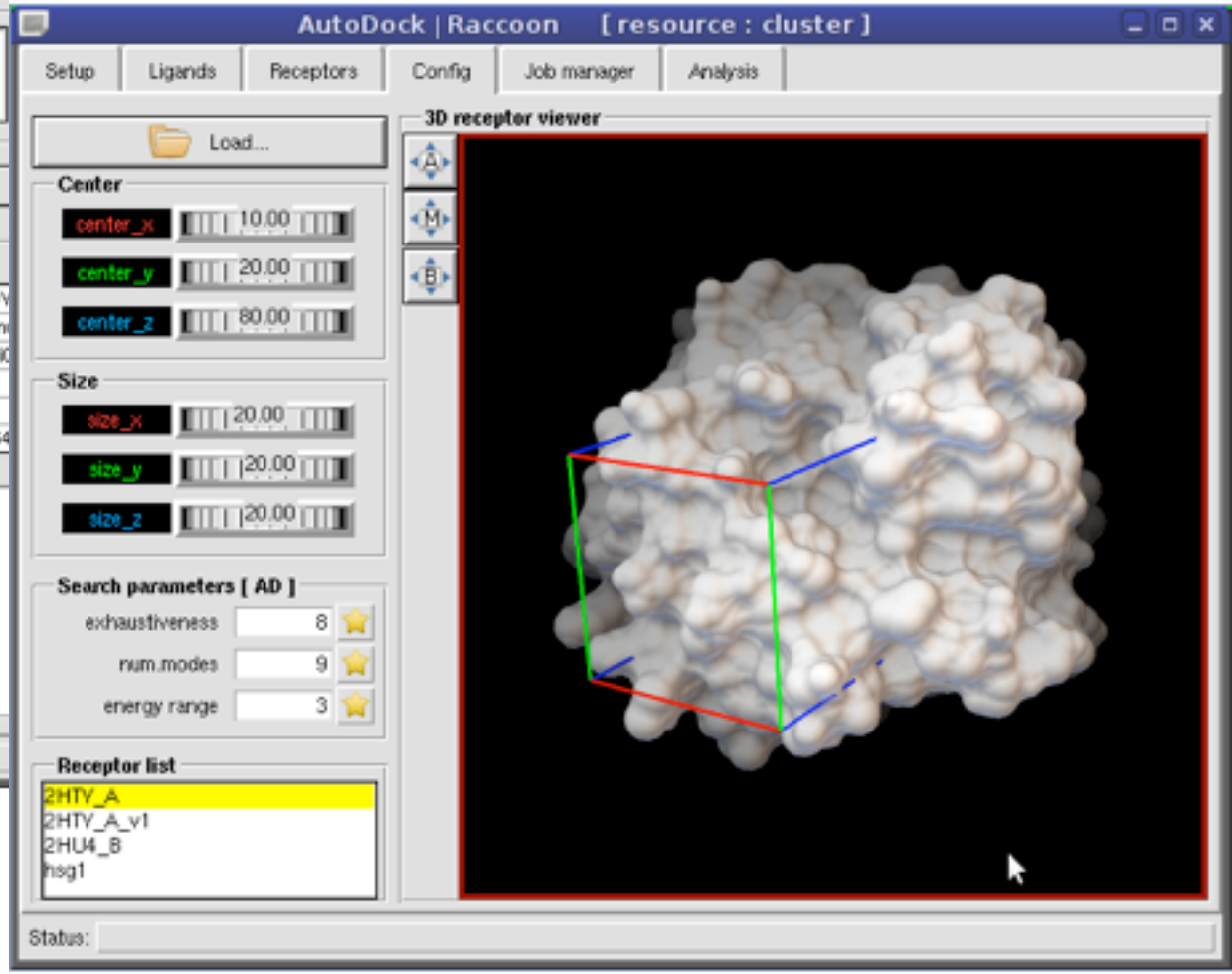
- Originated as a toolkit to deploy scientific application as web services using the SOAP protocol
  - Developed by S. Krishnan
- Released as Opal toolkit
- Now available as Rocks 5 VM
- Applications:
  - AutoDock
  - AutoDock Vina
  - PDB2PQR
  - MEME
  - …
- Contact: Nadya Williams

- Related Projects:
- Opal OP
  - Developed by K. Ichikawa
- Contact: Jason Haga, Susumu Date

http://goc.pragma-grid.net/wiki/index.php/Using_Bioapp

NBCR CADD Expedition





http://mgltools.scripps.edu

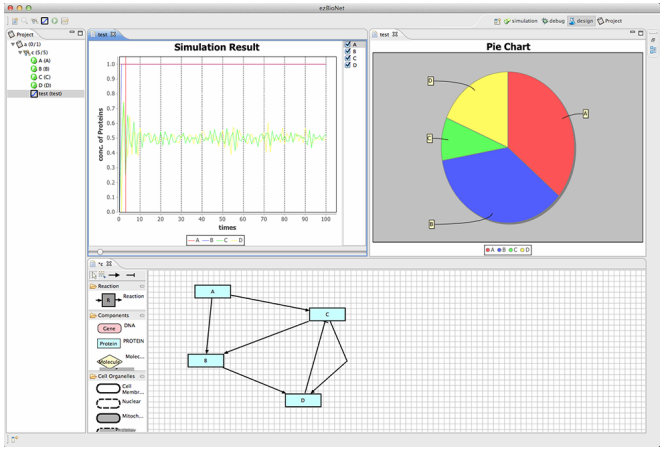
Other Bio-related VM

- NAMD, Species Simulation – Rocks 6, Bio1
  - Contact: Zhang Yang, Lanzhou University (LZU)
- Fmotif - Ezilla
  - Contact: Weicheng Huang – NCHC/NARL
- Lifemapper Project – VC
  - Contact: Aimee Stewart – Kansas U.
- Galaxy VM—workflow for NGS
  - Contact: Seok Jung Yu – KISTI

Source: PRAGMA GOC

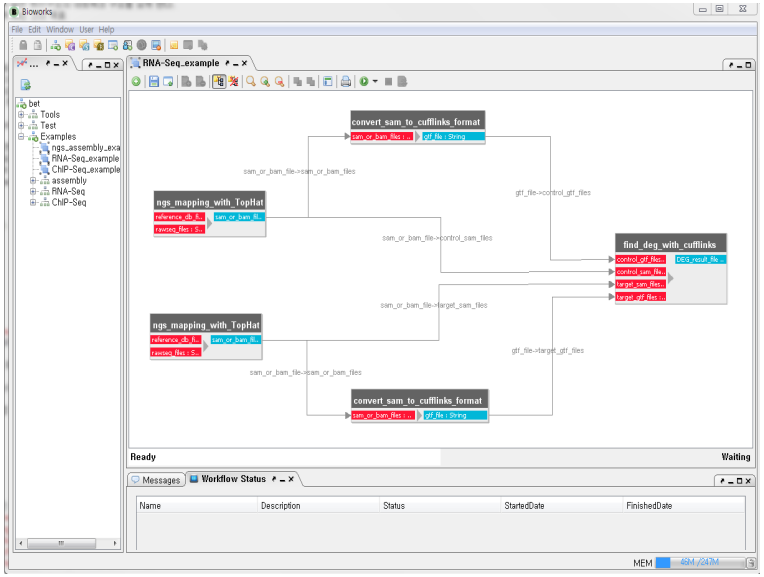
Recent Developments - KISTI

- KISTI – Dr. Seok Jong Yu
  - insilicoCell system
    - Implements the VCellSim (a simulation system) for biological reaction on the KISTI cluster.
    - Making a client software (ezBioNet) for modeling tool for biological reactions.
    - OPAL was setup and enhanced the job monitoring module.

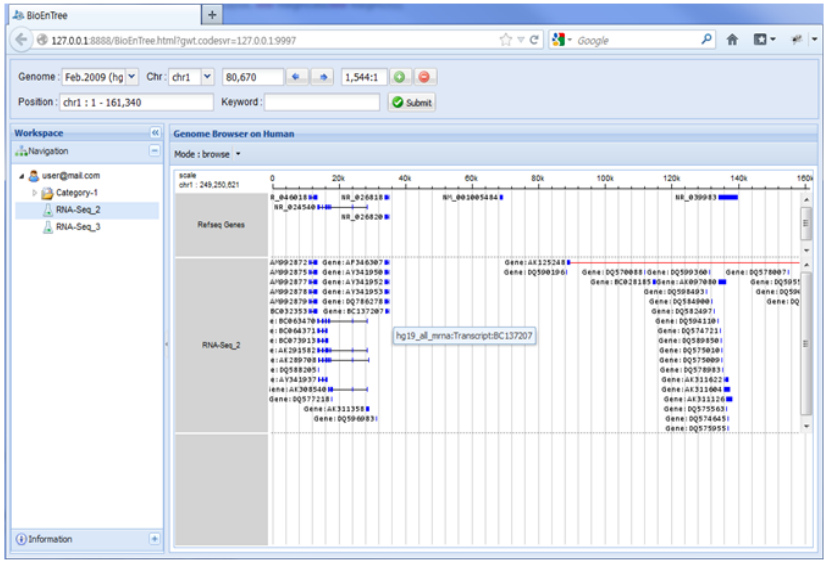


– Bioworks for NGS analysis

- Developing a workflow system for NGS analysis process
- Currently, have made a workflow for RNA-seq analysis.



Bioworks



Genome map Viewer

- Bio-Cloud service using Galaxy on PRAGMA Cloud
  - Creating a virtual image for NGS analysis on Galaxy system.

University of Indonesia Bio-WG

- **Member :**
  - Prof. Heru Suhartanto, Ph.D (High Performance and Numerical Computing)
  - Dr. Arry Yanuar (Pharmaceutical Chemistry)
  - Alhadi Bustamam, Ph.D. (GPU Computing)
  - Dr. Abdul Mun'im (Phytochemistry)
- **Student:**
  - Rezi Riadhi Syahdi, MSc.

University of Indonesia Bio-WG

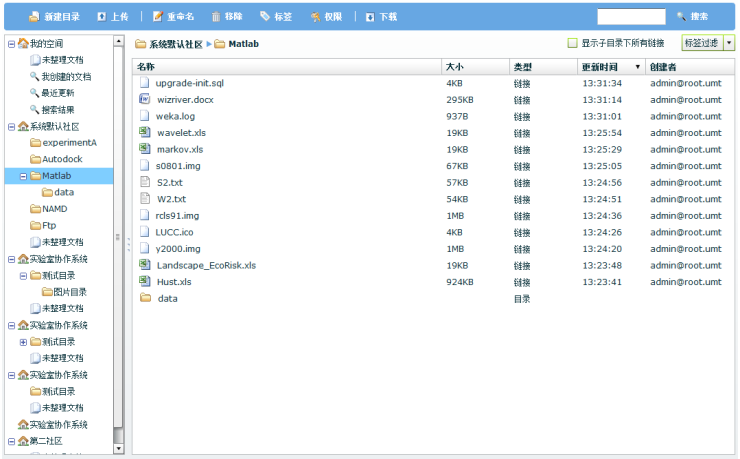
- **On progress Research Activities**
  - High performance computing Simulation process as part of infectious disease drug discovery based on Indonesian grown medical plants,
  - Virtual Screening and *invitro* activity of Compounds from Medicinal Plants Database in Indonesia for targeting HIV-1 and Malaria.

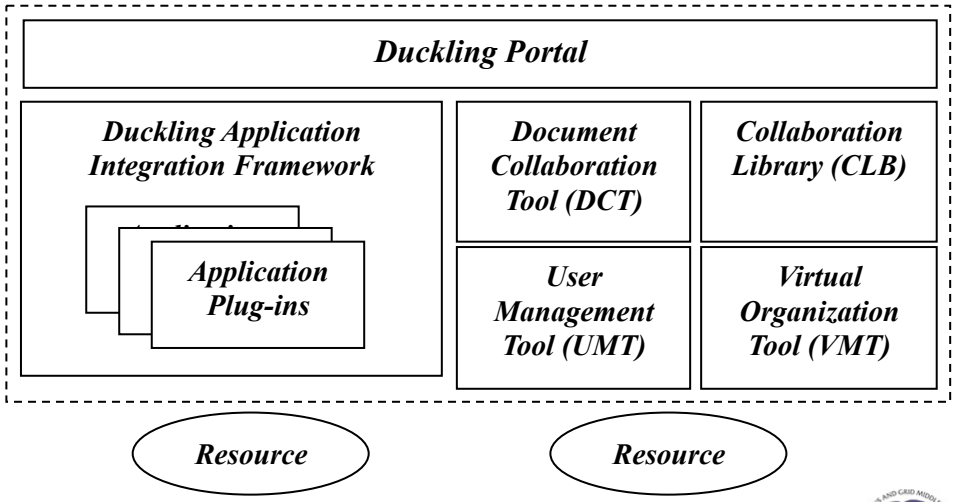
University of Indonesia Bio-WG

- **Publication**
  - Hayun; Hudiyono, S. , Hanafi, M., and **Yanuar, A**., **Synthesis and COX-2 Inhibitory Activity of 4-[(E)-2-(4-Oxo-3-phenyl-3, 4-dihydroquinazolin-2-yl) ethenyl] benzene-1-sulfonamide and Its Analogs**, Pharmaceuticals 2012, 5(12) 1282-1290; doi:10.3390/ph5121282
  - Syahdi, RR., Mun'im, A., Suhartanto, H., **Yanuar, A**. **Virtual Screening of Indonesian Herbal Database as HIV-1 Reverse Transcriptase Inhibitor**, Bioinformation 2012, 8(24) 1201-1210,

CNIC – Duckling Collaboration Library

- CLB - Collaboration Library
  - A component of Duckling, an open-source toolkit developed by the CNIC, Chinese Academy of Sciences (CAS)
  - Used by all Duckling applications as the Data Repository

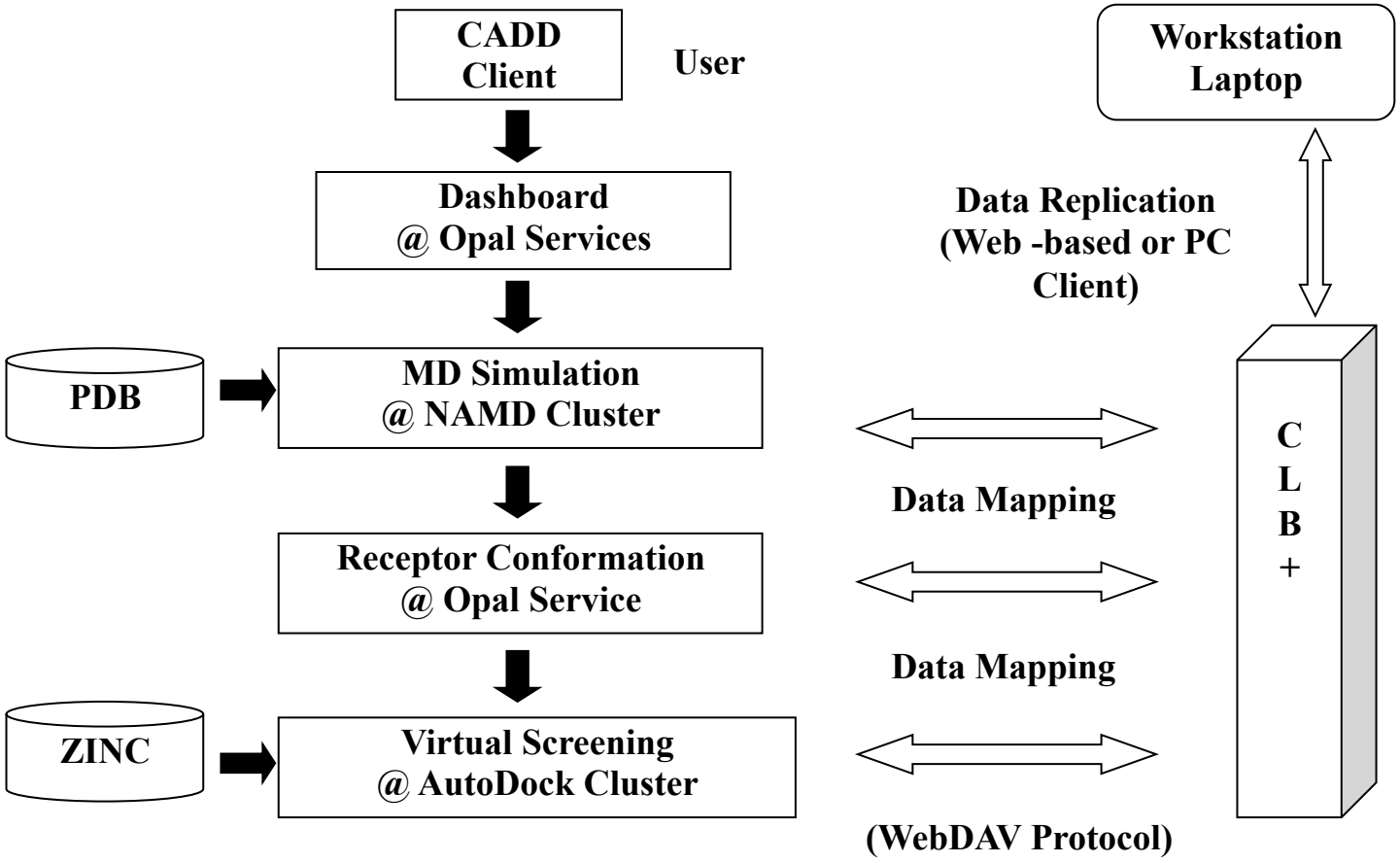




Key Features

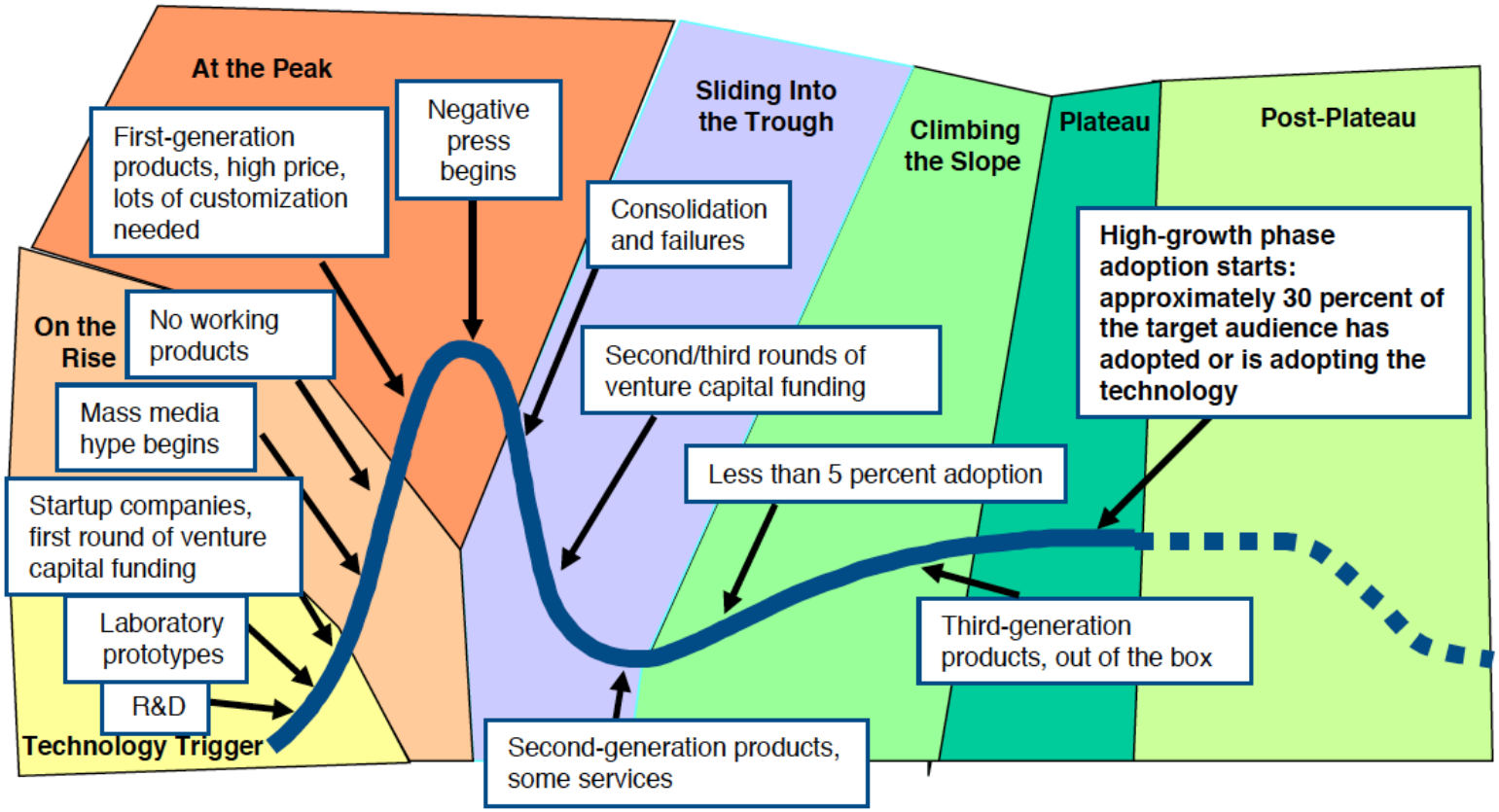
- Cloud-based Data Repository
  - Means offering a robust and scalable data cloud service. Researchers do not need to worry about where the data is stored or whether it is backed up or not.
- Ease of Access
  - Stands for the data accessibility from most experimental environments. Scientists can access the data from their desktop, servers and mobile devices on demand.
- Data Life Cycle Management
  - Indicates that the cloud repository can be used to store and track all processes and data generated by experiments, especially for workflow-based jobs, by the means of data versioning, which is crucial for experimental data collaboration.

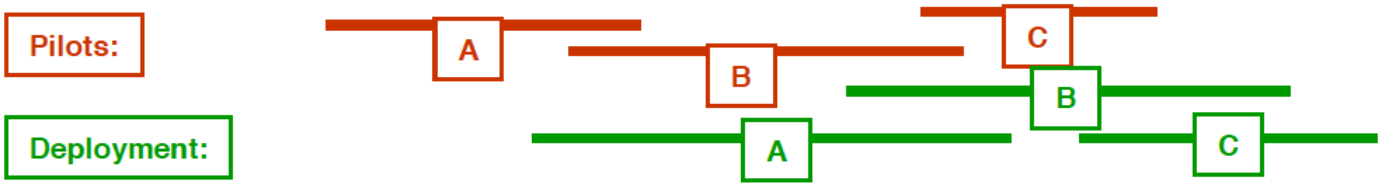
Use Case Scenario



Breakout Sessions

- Presentations
  - Kevin Dong, Cloud Environment for biomedical case studies, Duckling collaboration library
  - Seok Jong Yu, Bio-Cloud services
- Training
  - NBCR Summer Institute 2013, Aug 5-9, 2013
- Workshop, Conferences
  - PRAGMA 25, 10/16-18/2013
  - IEEE e-Science 2013, 10/23-25/2013





Source: Gartner Research (May 2003)


PRAGMA24 Workshop
March 20-22, 2013
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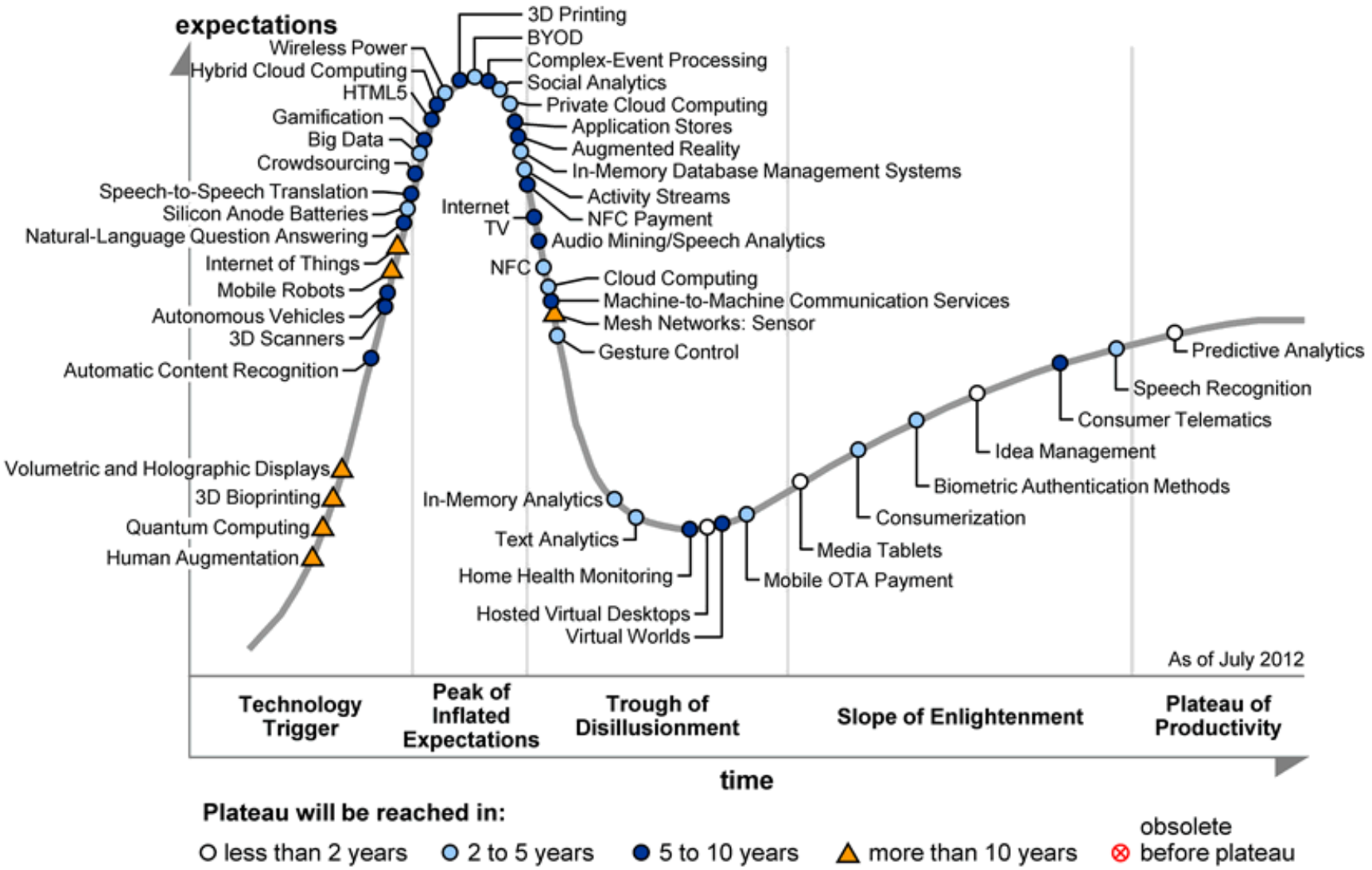
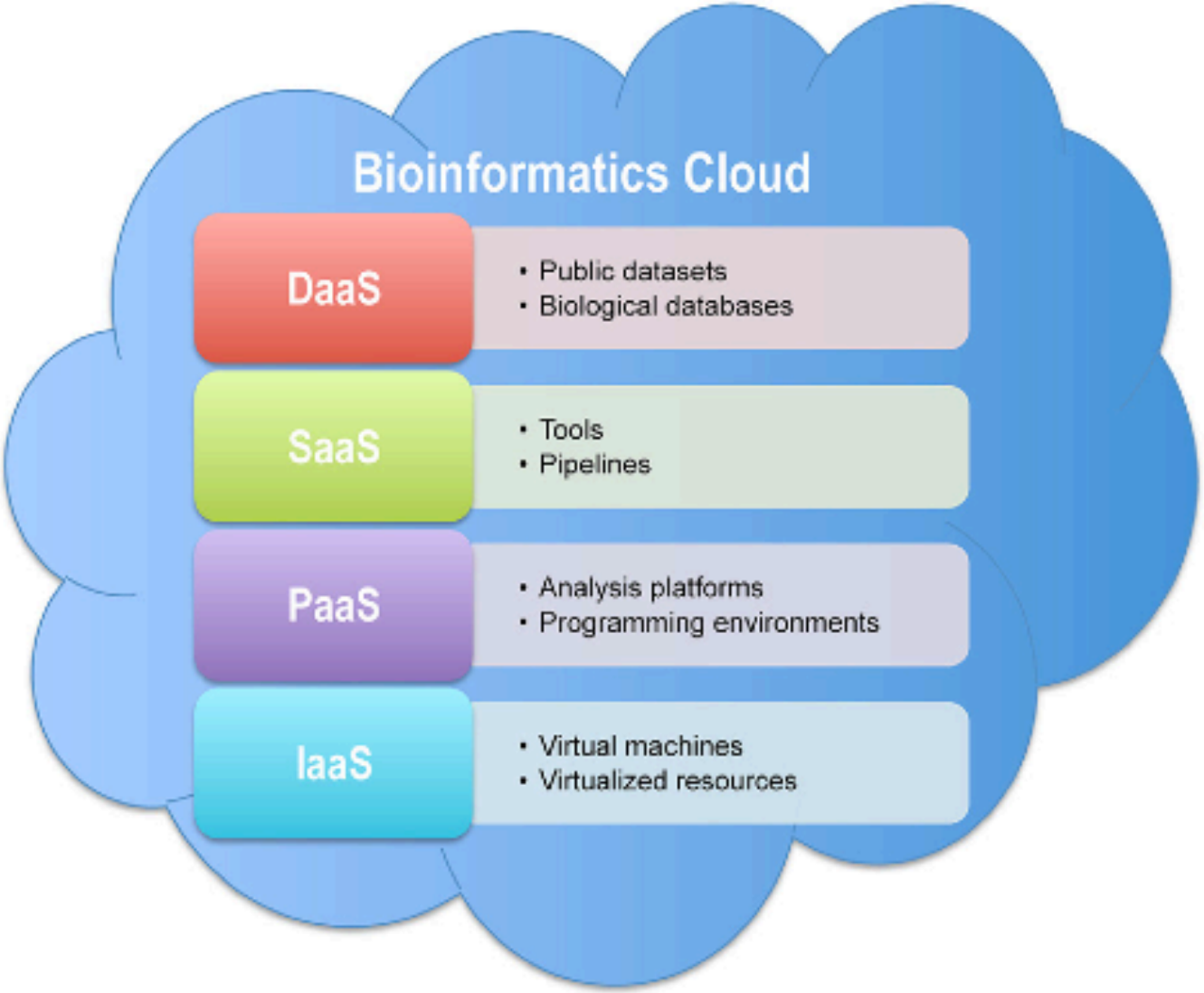

expectations
Wireless Power
Hybrid Cloud Computing
HTML5
Gamification
Big Data
Crowdsourcing
Speech-to-Speech Translation
Silicon Anode Batteries
Natural-Language Question Answering
Internet of Things
Mobile Robots
Autonomous Vehicles
3D Scanners
Automatic Content Recognition
Volumetric and Holographic Displays
3D Bioprinting
Quantum Computing
Human Augmentation
3D Printing
BYOD
Complex-Event Processing
Social Analytics
Private Cloud Computing
Application Stores
Augmented Reality
In-Memory Database Management Systems
Activity Streams
NFC Payment
Internet TV
Audio Mining/Speech Analytics
NFC
Cloud Computing
Machine-to-Machine Communication Services
Mesh Networks: Sensor
Gesture Control
In-Memory Analytics
Text Analytics
Home Health Monitoring
Hosted Virtual Desktops
Virtual Worlds
Media Tablets
Mobile OTA Payment
Consumerization
Biometric Authentication Methods
Idea Management
Consumer Telematics
Speech Recognition
Predictive Analytics
As of July 2012
Technology Trigger
Peak of Inflated Expectations
Trough of Disillusionment
Slope of Enlightenment
Plateau of Productivity
time
Plateau will be reached in:
less than 2 years
2 to 5 years
5 to 10 years
more than 10 years
obsolete before plateau

Cloud computing for Biosciences



Dai et al. Biology Direct 2012, 7:43