



**Exec Committee**

Pete Beckman

Jean-Yves Berthou

Jack Dongarra

Yutaka Ishikawa

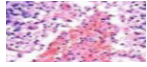
Satoshi Matsuoka

Philippe Ricoux

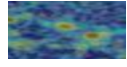
**BIG DATA *AND* EXTREME-SCALE COMPUTING**

# Science Communities

## Science Services



Digital Pathology Analysis



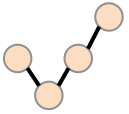
Cosmology Analysis / Image Server



Kbase Service

## Developed Services

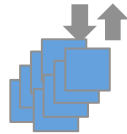
Workflow / Event Services



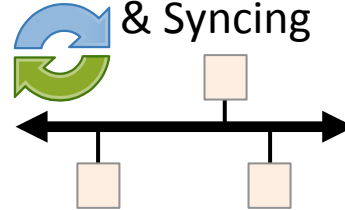
Data Services



Analysis/ Compute Services

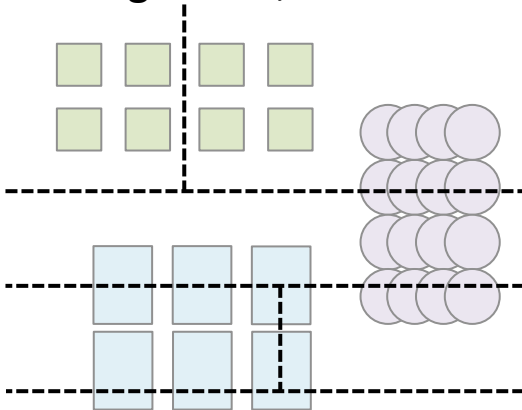


Data Moving & Syncing

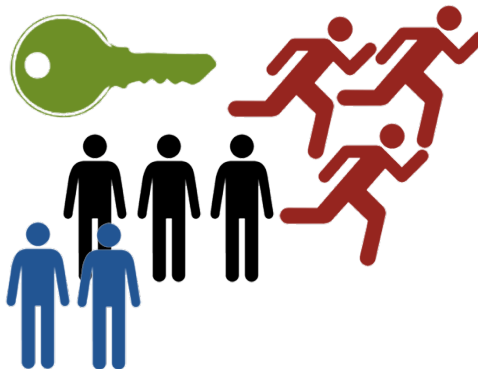


## Core Facility

Resource & Configuration Management, Resilience



Identity, Communities, Security



Core Software Tools, Services, & APIs



```
#!/usr/bin/python  
>>>
```

# Summary: New Ideas

(EC must change or be BD irrelevant)

- Resource Management
  - Elastic, Interactive, Reservations/co-scheduling
  - Economic models/cost, new incentive models, QoS
- System Complexity
  - Virtualization / BareMetal (encapsulation, elasticity)
  - Management tools
  - Machine learning & automation in operations
- Identity management & sharing / analysis
  - must move toward dropbox models
- Data sync/move/stream must be part of system

# ToDo (need more exploration):

- Workflow / execution model / programming
  - Still quite diverse, must create a few examples for discussion
- Archetypes for platforms, with quantitative measures & benchmarks
- Testbeds: Understand what we are missing, and how we can provide it
- Mini-apps: We need some real examples (with workflows) that the community can measure, re-code, explore
- Future tech that could help address BDEC
  - 100Gb networks, virtualization,

# Expectations

- ***Long term*** archival storage of science data is out of scope
- Looking at intersection of BD and EC

# Data Services

(2<sup>nd</sup> afternoon session)

James Ahrens, Chaitan Baru

- Beckman report
  - Report from database community about big data challenges
  - Recommending separation between storage layer and runtime layer.
- Propose a BDEC Workshop at VLDB 2015, Hawaii

- **Session 1: 90 Minutes**

- Describe what is needed in Common/Basic data services for BDEC system

- What are the most accepted (deployed) services?
    - What are the largest gaps for BDEC science communities?
    - What kinds of optimizations / specializations are required for science communities?

- **Report out during Plenary**

- **Session 2: 120 Minutes**

- Analyze and discuss the initial work of the other breakouts

- Describe:

- What is needed to support Federation, Provenance, and Curation?
    - What are the programming models needed?
    - What **basic services** should be included in BDEC facilities first?

- **Report out during Plenary**



# Federation

- Federation: Needed to access data from different sources
- Need catalog services
- Load up large amounts of observational, remote sensing data, simulation data, etc into one place
  - Be able to access data from the cloud
- First problem: identify management
- Examples:
  - ESA Geohazard project: Combine ESA data with WHO data for malaria
  - AIST: GeoGrid project—remote sensing, in situ data.
  - Many agencies store their own data. Requires federated access.
  - NCI: Cancer Cloud initiative, 3PB cancer genomic data
- Need higher level analysis services with data
  - Should be able to run a toolbox in the cloud

# Provenance

- Provenance is a subset of the reproducibility problem, e.g. where did the data come from; who accessed it;
- Having good provenance information can help with reuse of data
  - Avoid re-computation; avoid replication (deduplication)
- If the data is in the cloud and we can monitor usage
  - Then easier to provide provenance on data
- Characterize/understand “Provenance preservation” between consecutive steps.
  - Provenance preservation is property of each transformation

# Curation

- Maintaining data for the long-term such that it is available for reuse and preservation
- Need to provide ready access to curated data
  - Need an architecture that allows you to easily access stored data
- How long do we keep the data?
  - Sensor data is precious—natural, observed phenomena; things that cannot be reproduced
- Unsure of how to sustain curation of data
  - Can industry assist: curation as a service?
  - Could they charge for the CPU for using the data?

# Programming Models

- Current models are not adequate for interacting with data
  - Declarative approaches are good
  - Need more abstractions; interact well with the runtime
  - Need an “explain” capability (debuggability)
  - Many users would like to have DSLs
- Support for resilience (tolerate faults)

# Basic services to include in BDEC first?

- Ability to specify and orchestrate workflows
  - On-demand access to compute and storage
- Virtualization (with hardware support)
- Analytics libraries at scale
  - Need to understand current performance and scaling characteristic of some of these packages, including GIS...
- Some runtime support, e.g. for data movement/caching, ...

# BDEC February 2014 Applications Breakout

Session 2

# The Desire for a Mini-App

- The complexity is in the data
  - Can you get a mini-data
  - Why isn't it so important in commercial analytics?

# Why is data movement so important

- Google moves the data once and keeps it
- Sensible designs do not require repeating the data movement over and over and over
- Is virtualization a need or is it an artifact of an assumption of how to run/allocate the system
- Domain-specific computing is an alternative that is likely to be more cost effective



# Work Flow Description

- Components
  - Algorithm
  - Compute pattern
  - Data size
  - Data access pattern
- Links – data transferred
- Data sources and sinks
- Coupling between compute and data
- Synchronous vs. asynchronous

# Spatio-temporal Sensor Integration, Analysis, Classification

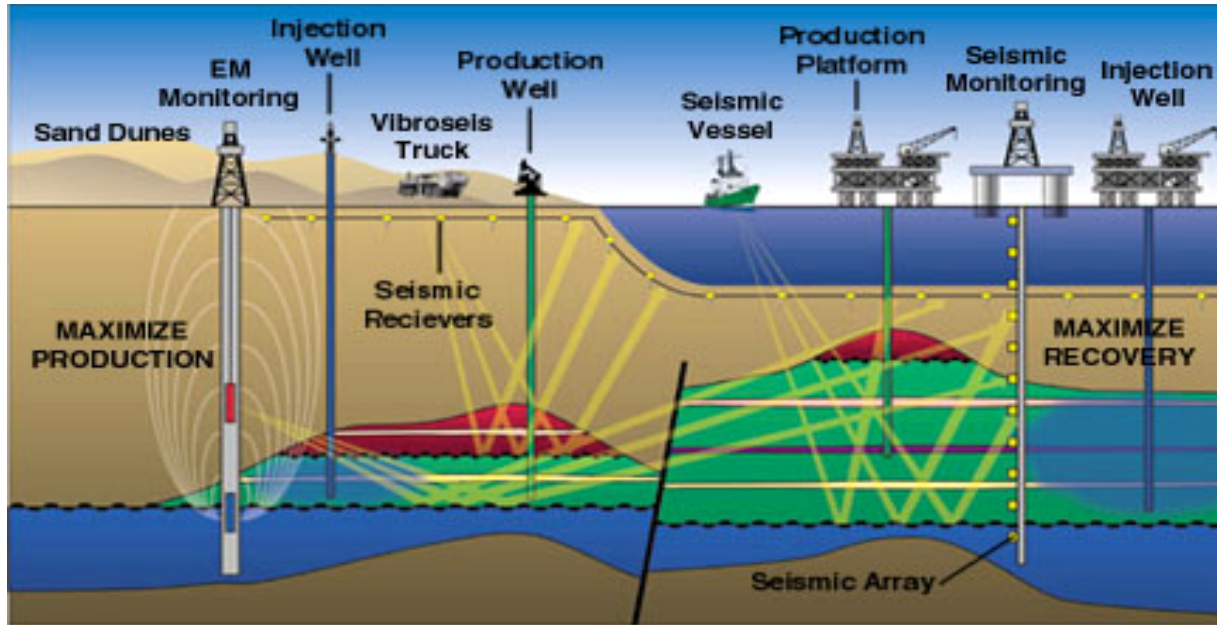
- Multi-scale material/tissue structural, molecular, functional characterization. Design of materials with specific structural, energy storage properties, brain, regenerative medicine, cancer
- Integrative multi-scale analyses of the earth, oceans, atmosphere, cities, vegetation etc – cameras and sensors on satellites, aircraft, drones, land vehicles, stationary cameras
- Digital astronomy
- Hydrocarbon exploration, exploitation, pollution remediation
- Aerospace – wind tunnels, acquisition of data during flight
- Solid printing integrative data analyses
- Autonomous vehicles, e.g. self driving cars
- Data generated by numerical simulation codes – PDEs, particle methods
- Fit model with data

# Typical Computational/Analysis Tasks

Spatio-temporal Sensor Integration, Analysis, Classification

- Data Cleaning and Low Level Transformations
- Data Subsetting, Filtering, Subsampling
- Spatio-temporal Mapping and Registration
- Object Segmentation
- Feature Extraction
- Object/Region/Feature Classification
- Spatio-temporal Aggregation
- Diffeomorphism type mapping methods (e.g. optimal mass transport)
- Particle filtering/prediction
- Change Detection, Comparison, and Quantification

Coupled data acquisition, data analysis, modeling, prediction and correction – data assimilation, particle filtering etc.



Detect and track changes in data during production

Invert data for reservoir properties

Detect and track reservoir changes

Assimilate data & reservoir properties into  
the evolving reservoir model

Use simulation and optimization to guide future production

# Soft real time and streaming Sensor Data Analysis, Event Detection, Decision Support

- Integrated analyses of patient data – physiological streams, labs, mediations, notes, Radiology, Pathology images, mobile health data feeds
- High frequency trading, arbitrage
- Real time monitoring earthquakes, control of oilfields
- Control of industrial plants, aircraft engines
- Fusion – data capture, control, prediction of disruptions
- Internet of things
- Twitter feeds
- Intensive care alarms

# Typical Computational Analysis Tasks

Streaming Sensor Data Analysis, Event Detection, Decision Support

- Prediction algorithms – Kalman, particle filtering
- Machine learning algorithms on aggregated data to develop model, use of model on streaming data for decision support
- Searching for rare events
- Statistical algorithms to distinguish signal from noise
- On the fly integration of multiple complementary data streams

# “omics”

- Sequence assembly
- Metagenomics – identification/characterization of populations of organisms based on DNA/RNA sequencing
- Phylogenetics, genetic based population biology, cancer mutation landscaping
- Pathway modeling using integrated sequence, expression, epigenetics, protein, glycans
- Genetic/genomic based design of organisms with specific properties

# Typical Computational/Analysis Tasks “omics”

- Discrete algorithms – hashing, searching, sorting, comparisons, dynamic programming, indexing, similarity search
- Compression
- Statistical algorithms to distinguish biological signal from experimental artifacts/noise
- Graph construction, traversal, partial/sub graph matching, graph partitioning
- Statistical methods on graphs e.g. Bayesian networks



# Population and Social Network Analyses

- Aggregated electronic health data to predict likelihood of disease onset, treatment response, likelihood of re-hospitalization etc
- Predict demand for products, target advertising, store shelf placement
- Characterize influence in social networks

# Typical Computational/Analysis Tasks

## Population and Social Network Analyses

- Structural properties of graphs – PageRank, diameter, radius, connected component
- Graph spectral analysis
- Graph mining
- Machine learning, cluster analysis
- Statistical modeling and analyses
- Natural language processing

# Approach

- Detailed example workflows led by application experts
- Key cases involve interplay between simulation and data acquisition – “data assimilation”
- Scenarios involving current and future state associated with origin and movement of data between workflow stages
- Definition of workflow components

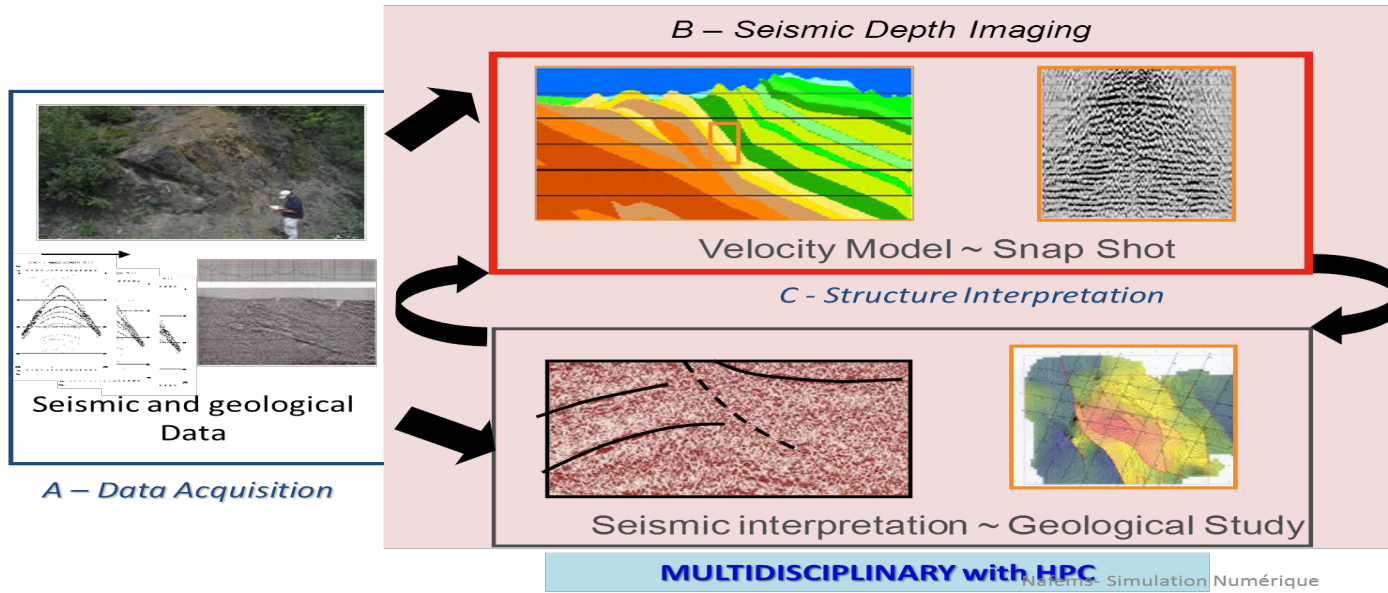
# Follow up

- Yutaka Akiyama– Metagenomics
- Geoffrey Fox – Components
- Jean-Claude Andre – Climate
- Philippe Ricoux – Oil exploration/reservoir management
- Joel Saltz – Medical imaging

# Oil Exploration

- Seismic data acquisition – 20PB
- Transport by plane
- Extract 400TB, load to HPC center
- Obtain complementary datasets – EM, gravimetry and conductivity by network
- Use model to analyze at HPC center
- Generate 3D image (3TB)
- Analysts examine, modify model, modify extraction

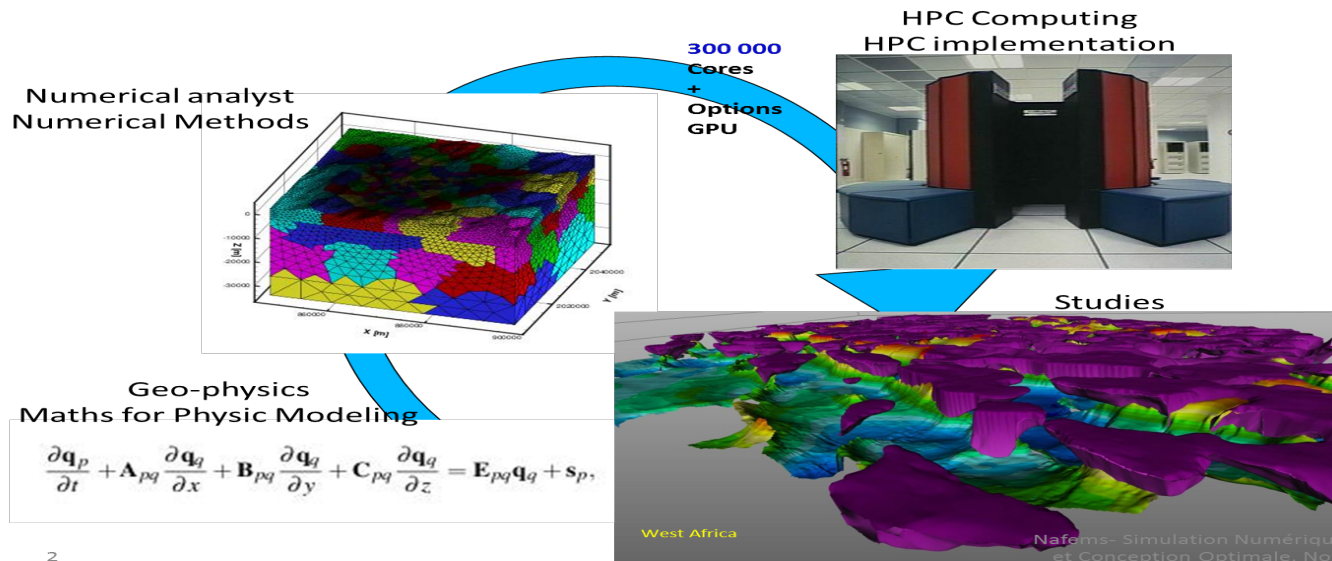
# Seismic Imaging and geological structures



1

Nafems- Simulation Numérique et Conception Optimale, Nov. 2013

## HPC for Depth Imaging : 3 fundamental steps



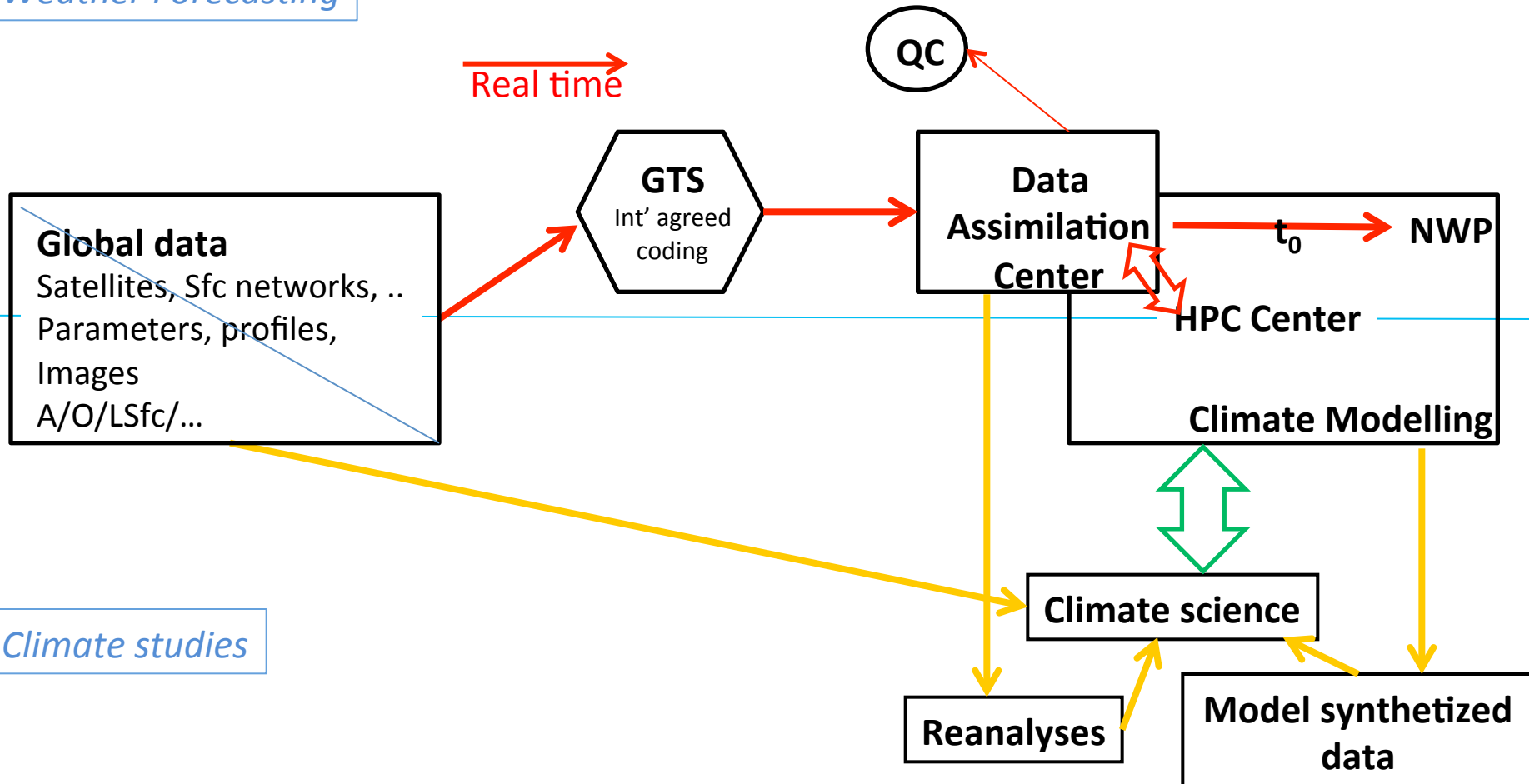
2

Nafems- Simulation Numérique et Conception Optimale, Nov. 2013

# A simplified (?) view of workflows for weather and climate

*Weather Forecasting*

Real time



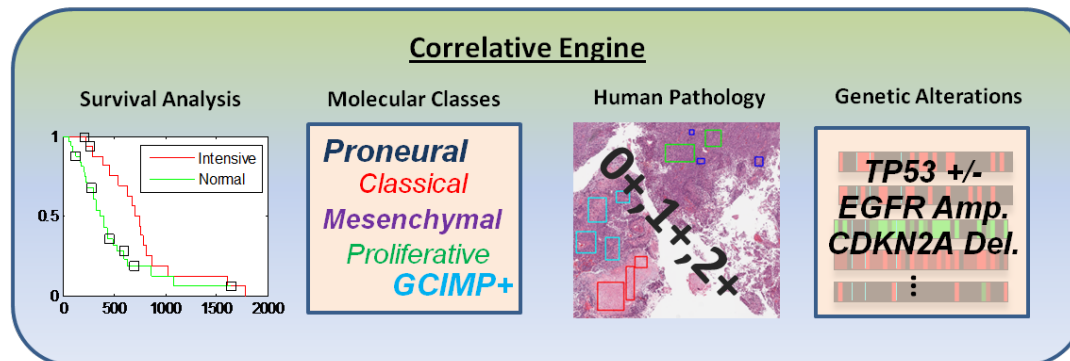
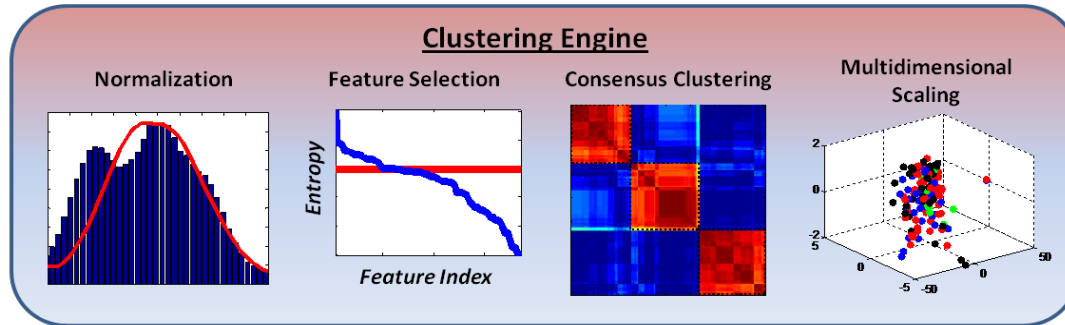
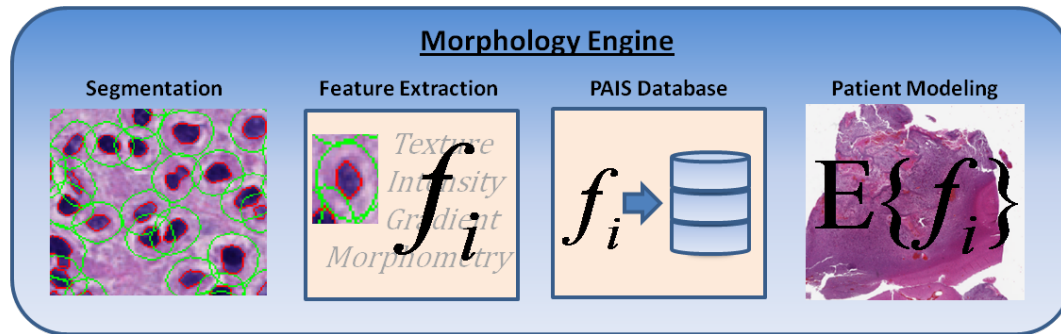
*Climate studies*

# Bottleneck

- Long term storage for simulation data - 10-30 PB/year
- Access to facilities to analyze



# Direct Study of Relationship Between **Image Features** vs **Clinical Outcome, Response to Treatment, Molecular Information**



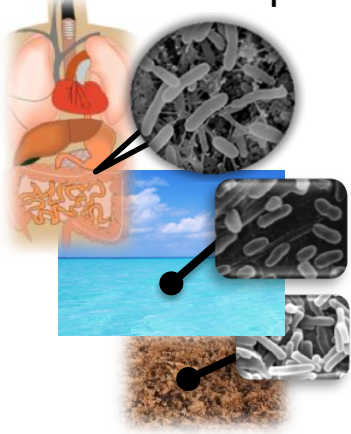
# Future State

- 100K – 1M pathology slides/hospital/year
- 2GB compressed per slide
- 1-10 slides used for Pathologist computer aided diagnosis
- 100-10K slides used in hospital Quality control
- Groups of 100K+ slides used for clinical research studies -- Combined with molecular, outcome data

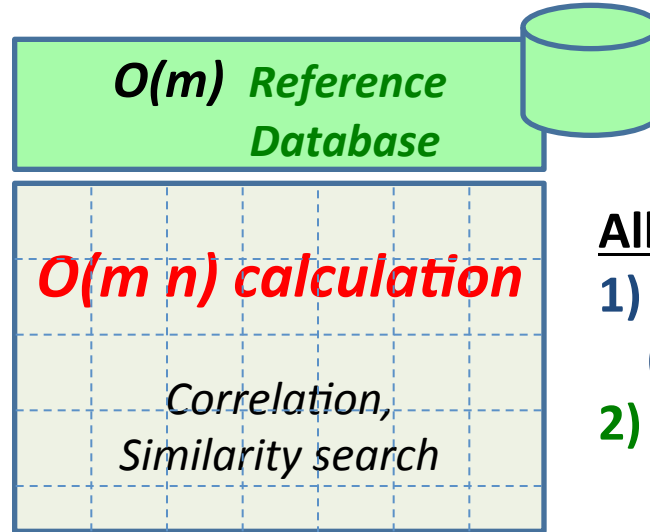
# Metagenome Analysis

Direct sequencing of uncultured microbiomes in a target environment

1TB/run at Year 2012 and  
300% increase per year



$O(n)$   
Meas.  
data



Allocation on nodes:

- 1) Measured data (transient)
- 2) References DB (resident)

Thousands of sequencers will  
work every day on **Year 2015**

**Year 2010**



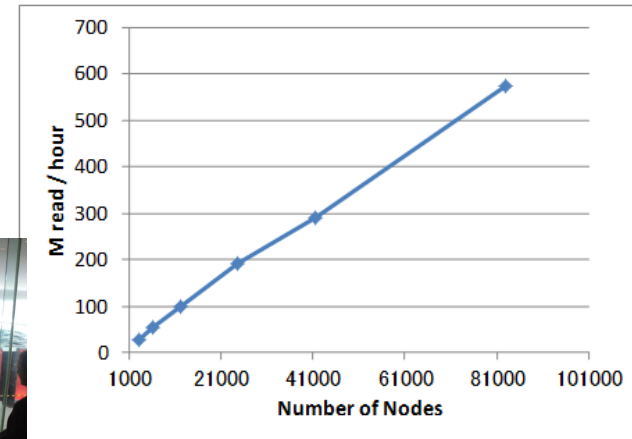
0.18 M Reads / hour  
144core Xeon Cluster

3000-fold  
speed-up  
achieved

**GHOST-MP**  
OpenMP / MPI



**Year 2012**



573 M Reads / hour with  
82944 node **K-computer**

# Marine Phage Sequencing Project

Marine Phage Sequencing Project: Home

www.broadinstitute.org/annotation/Viral/Phage/Home.html

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What is Broad News and Publications For the Scientific Community

Science Data Software

Home > Science > Data > Marine Phage Sequencing Project > Home

## Marine Phage, Viruses and Viromes

The Gordon & Betty Moore Foundation's Marine Microbiology Initiative (MMI) aims to generate new knowledge about the composition, function, and ecological role of the microbial communities that serve as the basis of the ocean's food webs and that facilitate the flow of nitrogen, carbon, and energy in the ocean. Phage and viruses play a critical role in shaping microbial diversity, abundance and evolution and in this capacity have a significant impact on atmospheric composition and ecosystem function. In an effort to understand the ecology and evolution of marine phage and viruses and to explore the diversity and ecological roles of entire phage/viral communities through metagenomics, the Broad Institute is collaborating with MMI and research groups whose sequencing nominations were chosen by

**News**

- 2010.12.20: Sequencing, Assembly, and Annotation for all samples completed; all project data available from CAMERA
- Project status updates are [here](#)
- Audio of assembly, annotation, and file format tutorial is available

Marine Phage Sequencing Project

- Home
- Project Info
- Protocols
- Links
- Contact

Genomic Sequencing Center for Infectious Disease

# Earth Microbiome Project

Earth Microbiome Project

www.earthmicrobiome.org

earth microbiome project

Home Defining the Tasks Getting Involved EMP Protocols and Standards Affiliations Publications Meetings EMP Logo No categories

The Earth Microbiome Project is a systematic attempt to characterize the global microbial taxonomic and functional diversity for the benefit of the planet and mankind

Constructing the Microbial Biomap for Planet Earth

The Earth Microbiome Project is a proposed massively multidisciplinary effort to analyze microbial communities across the globe. The general premise is to examine microbial communities from their own perspective. Hence we propose to characterize the Earth by environmental parameter space into different biomes and then explore these using samples currently available from researchers across the globe. We will analyze 200,000 samples from these communities using metagenomics, metatranscriptomics and amplicon sequencing to produce a

SEARCH

Meetings

There are currently no EMP centric meetings planned, however we will update this space as soon as the next meeting is organized.

News

Neil Hall highlights the now-stabilizing price of sequencing and how the EMP and others have

# Home Microbiome Study

Home Microbiome Study

home microbiome.com

HOME ANNOUNCEMENTS RESULTS ABOUT

## HOME MICROBIOME STUDY

The Home Microbiome Study

Published February 24, 2012 - No Comments

Most of us are aware of the bacteria on the surfaces we come in contact with. The doorknob for the bathroom, coins and paper currency in our pockets, handrails in subway cars, computer keyboards and mice at the library... the list of built environments on which microbes thrive is nearly on ...

read more

Microbial Biodiversity of Cell Phones and Shoes

Published February 24, 2012 at 4:55 am - No Comments

The results are in! So, what lives on reporters' cell phones and shoes, you ask? As you can see from the graph at left, quite a lot! Each vertical bar is one shoe or cell phone and each color represents a different

The Home Microbiome Study

Published February 24, 2012 at 2:58 am - No Comments

Most of us are aware of the bacteria on the surfaces we come in contact with. The doorknob for the bathroom, coins and paper currency in our pockets, handrails in subway cars, computer keyboards and mice at the

Latest Articles

Latest Articles from the Blog

- GSC13 Presentation
- Published June 12, 2012 at 2:41 pm
- Microbial Biodiversity of Cell Phones and Shoes
- Published February 24, 2012 at 4:55 am

# Hospital Microbiome Project

Hospital Microbiome Project

hospitalmicrobiome.com

Home Goals Overview Design Timeline Consortium Findings Affiliations

## Hospital Microbiome

This study aims to collect microbial samples from surfaces, air, staff, and patients from the University of Chicago's new hospital pavilion in order to better understand the factors that influence bacterial population development in healthcare environments.

Study Design

# General Structure/Features/Components

- **Data Gathering**
  - Blocked or Real Time (Streaming)
  - Interval = Month(Seismic, Remote sensing) -- Day (genomic) – seconds
- **Storage**
  - Type SQL NoSQL Files etc
  - Style: Dedicated or Permanent or Transient
  - Possible static databases of other data for comparison
- **Process (Analytics, Visualization)**
  - Analytics algorithm: Pattern recognition, Clustering, Blast, Collaborative Filtering, learning network, outlier detection ....
  - Pleasingly parallel or not
  - Flops per I/O byte
  - Communication/Interconnection needs
- **Produce output**
  - Often output much lower size
- Then possibly *iterate process* by further analysis of produced output
- Possibly *share data* from different sources