

### **Cloud Computing for Research**

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### Introduction

- Happy to be here at a HealthGrid event
- Still remember the start of this initiative in the early 2000's at the same time we started EU DataGrid and CrossGrid
- Interesting evolution of a self-sustained infrastructure, leveraging DCI in Europe, mostly EU supported
- Interesting critical mass of well organized scientific user communities with a common focus to Health and Well Being
- Important to understand and develop longer term sustainability
- Important to review technology evolution and current trends in DCI



### The Cloud

- A model of computation and data storage based on "pay as you go" access to "unlimited" remote data center capabilities
- A cloud infrastructure provides a framework to manage scalable, reliable, on-demand access to applications
- A cloud is the "invisible" backend to many of our mobile applications
- Historical roots in today's Internet apps
  - Search, email, social networks
  - File storage



## The Cloud is built on massive data centers

- Range in size from "edge" facilities to megascale.
- Economies of scale
  - Approximate costs for a small size center (1K servers) and a larger, 100K server center.



| Technology     | Cost in small-sized<br>Data Center | Cost in Large Data<br>Center    | Ratio |                                   |
|----------------|------------------------------------|---------------------------------|-------|-----------------------------------|
| Network        | \$95 per Mbps/<br>Month            | \$13 per Mbps/<br>month         | 7.1   | Each data center is<br>11.5 times |
| Storage        | \$2.20 per GB/<br>Month            | \$0.40 per GB/<br>month         | 5.7   | the size of a football field      |
| Administration | ~140 servers/<br>Administrator     | >1000 Servers/<br>Administrator | 7.1   |                                   |

### Microsoft Advances in DC Deployment

Conquering complexity.

- Building racks of servers & complex cooling systems all separately is not efficient
- Package and deploy into bigger units







http://www.microsoft.com/showcase/en/us/details/36db4da6-8777-431e-aefb-316c

#### DCs vs Grids, Clusters and Supercomputer Apps

- Supercomputers
  - High parallel, tightly synchronized MPI simulations
- Clusters
  - Gross grain parallelism, single administrative domains
- Grids
  - Job parallelism, throughput computing, heterogeneous administrative domains
- Cloud
  - Scalable, parallel, resilient web services



### Changing the way we do research

#### • The Rest of Us

- Use laptops
- Got data, now what?
- And it is really is about data, not the FLOPS...
  - » Our data collections are not as big as we wished
  - » When data collection does grow large, not able to analyze
- Tools are limited, must dedicate resources to build analysis tools
- Paradigm shifts for research
  - The ability to marshal needed resources on demand
    - » Without caring or knowing how it gets done...
  - Funding agencies can request grantees to archive research data in common public repositories
  - The cloud can support very large numbers of users or communities in a flexible way



## Focus Client + Cloud for Research

#### Seamless interaction

- Cloud is the lens that magnifies the power of desktop
- Persist and share data from client in the cloud
- Analyze data initially captured in client tools, such as Excel
  - Analysis as a service (think SQL, Map-Reduce, R/MatLab)
  - Data visualization generated in the cloud, display on client
  - Provenance, collaboration, other 'core' services...







# The Clients+Cloud Platform

- At one time the "client" was a PC + browser Now:
  - The Phone
  - The laptop/tablet
  - The TV/Surface/Media wall

#### And the future:

- The instrumented room
- Aware and active surfaces
- Voice and gesture recognition
- Knowledge of where we are
- Knowledge of our health





# The Future: an Explosion of Data















# Changing Nature of Discovery

Complex models

- Multidisciplinary interactions
- Wide temporal and spatial scales Large multidisciplinary data
  - Real-time steams
  - Structured and unstructured

Distributed communities

- Virtual organizations
- Socialization and management Diverse expectations
  - Client-centric and infrastructure-centric



#### The FOURTH PARADIGM DATA-INTENSIVE SCIENTIFIC DISCOVERY

http://research.microsoft.com/en-us/collaboration/fourthparadigm/

### The Cloud Landscape

- Infrastructure as a Service (IaaS)
  - Provide a data center and a way to host client VMs and data.
- Platform as a Service (PaaS)
  - Provide a programming environment to build a cloud application
  - The cloud deploys and manages the app for the client
- Software as a Service (SaaS)
  - Delivery of software from the cloud to the desktop



# Some examples based on MSR ongoing Cloud Research Engagements



## AzureBLAST\*

#### **Seamless Experience**

- Evaluate data and invoke computational models from Excel.
- Computationally heavy analysis done close to large database of curated data.
- Scalable for large, surge computationally heavy analysis.
- Test local, run on the cloud.







\*The Basic Local Alignment Search Tool (BLAST) finds regions of local similarity between sequences. The program compares nucleotide or protein sequences to sequence databases

### Making Excel the user interface to the cloud



#### AzureMODIS – Azure Service for Remote Sensing Geoscience



### **Project JUNIOR**

Newcastle University, UK -Paul Watson

- Investigating applicability of commercial clouds for scientific research
- Build a working prototype for use-cases in chemo-informatics
- Uses Microsoft technologies to build science-related services (Windows Azure, Silverlight...)
- Exploits Azure and Amazon Clouds

Built initial proof-of-concept

- Silverlight UI for basic Quantitative Structure-Analysis Relationship (QSAR) modeling
- Demonstrated ability to scale QSAR computations in Windows Azure



# Dynamic shared state

 multiplayer games, virtual worlds, social networks, clinical tests

New modalities of collaboration







#### Reaching Out: Azure Research Engagement project

#### In the U.S.

Memorandum of Understanding with the National Science Foundation

- Provide a substantial Azure resource as a donation to NSF
- NSF will provide funding to researchers to use this resource

#### In Europe

- We interested in direct engagement with the thought leaders in the U.K., France and Germany
- EC engagements where possible (VENUS-C to start off)

#### In both we provide our engagement team

 We provide workshops, tutorials, best practices and shared services, learn from this community, shape policy...

#### In Asia

- We wish to explore possibilities.

# **VENUS-C**



#### Virtual multidisciplinary EnviroNments USing Cloud infrastructures

**Funding Scheme:** Combination of Collaborative Project and Coordination and Support Action: Integrated Infrastructure Initiative (13)

**Program Topic:** INFRA-2010-2 1.2.1. Distributed Computing Infrastructures



# Consortium

| 1 (co) | Engineering Ingegneria Informatica S.p.a.                             | ENG      | IT |
|--------|---|----------|----|
| 2      | European Microsoft Innovation Centre                                  | EMIC     | DE |
| 3      | European Charter of Open Grid Forum                                   | OGF.eeig | UK |
| 4      | Barcelona Supercomputing Center – Centro Nacional de Supercomputación | BSC-CNS  | ES |
| 5      | Universidad Politecnica de Valencia                                   | UPV      | ES |
| 6      | Kungliga Tekniska Hoegskolan  | КТН      | SE |
| 7      | University of the Aegean  | AEG      | GR |
| 8      | Technion  | TECH     | IL |
| 9      | Centre for Computational and Systems Biology                          | CoSBi    | IT |
| 10     | University of Newcastle   | NCL      | UK |
| 11     | Consiglio Nazionale delle Ricerche                                    | CNR      | IT |
| 12     | Collaboratorio  | COLB     | IT |



# Goals

- 1. Create a platform that enables user applications to leverage cloud computing principles and benefits.
- 2. Leverage the state of the art to on-board early adopters quickly, incrementally enable interop with existing DCI and push the state of the art where needed to satisfy on-boarding and interop
- 3. Create a sustainable infrastructure that enables the cloud computing paradigms for the user communities inside the project, the one from the call for applications, as well as others.

### Supporting multiple basic research disciplines

- **Biomedicine:** Integrating widely used tools for Bioinformatics (UPV), System Biology (CosBI) and Drug Discovery (NCL) into the VENUS-C infrastructure
- **Civil Protection and Emergency:** Early fire risk detection (AEG), through an application that will run models on the VENUS-C infrastructure, based on multiple data sources.
- **Civil Engineering:** Support complex computing tasks on Building Information Management for green constructions (provided by COLB) and dynamic building structure analysis (provided by UPV).

**D4Science:** Integrating computing through VENUS-C on data repositories (CNR). In particular focus will be on Marine Biodiversity through Aquamaps.

### Open Call for 20 e-Science Applications

- 20K€ funding each (in addition to Azure Compute , Storage and Network Resources)
- -> porting applications to the cloud
- -> education and traning
- -> scalability tests



### Thanks for your attention

