Dynamic Applications on Grids

Computing ---> Data, Metadata, Networks

Ed Seidel

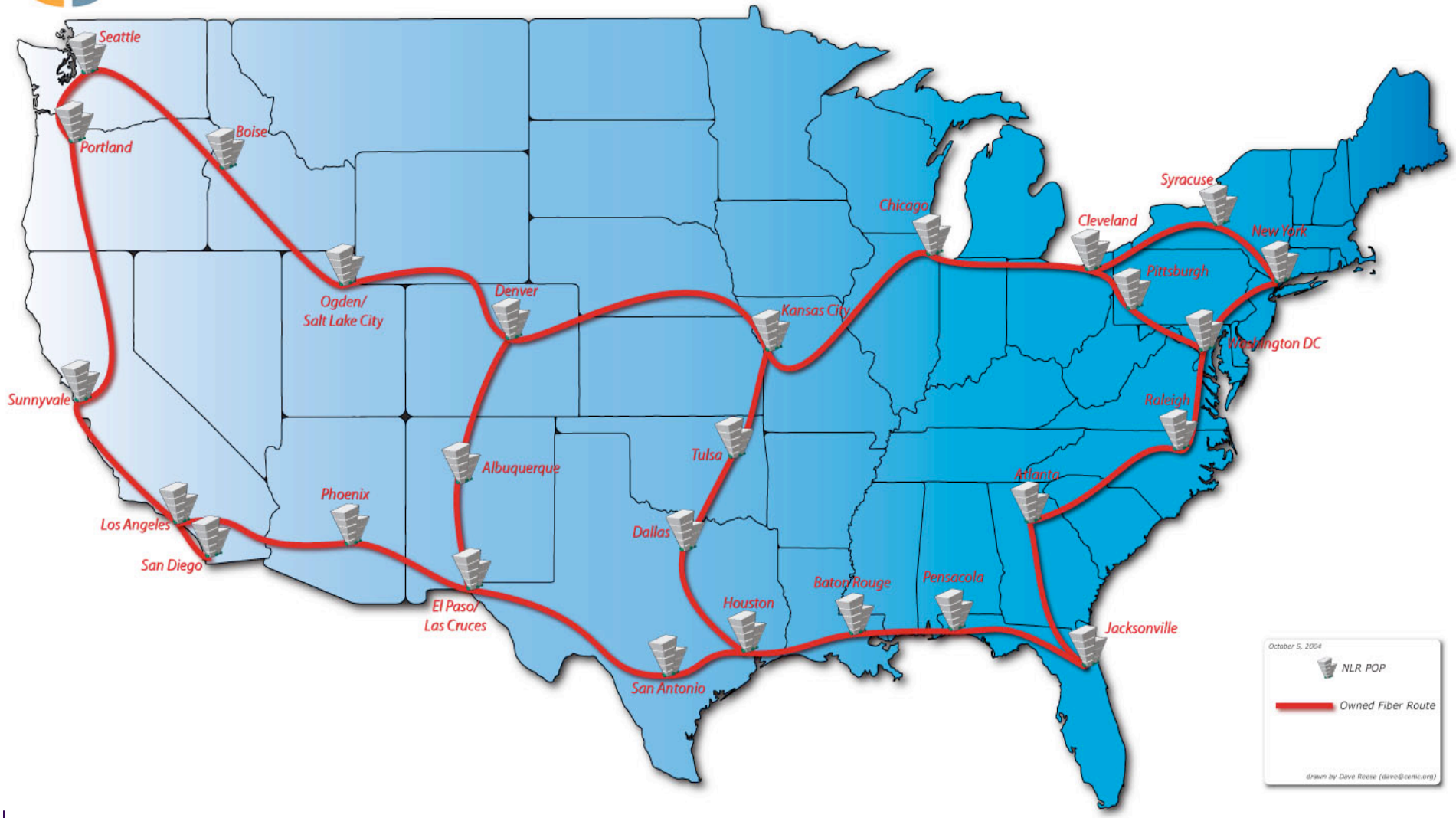
Center for Computation & Technology

Louisiana State University

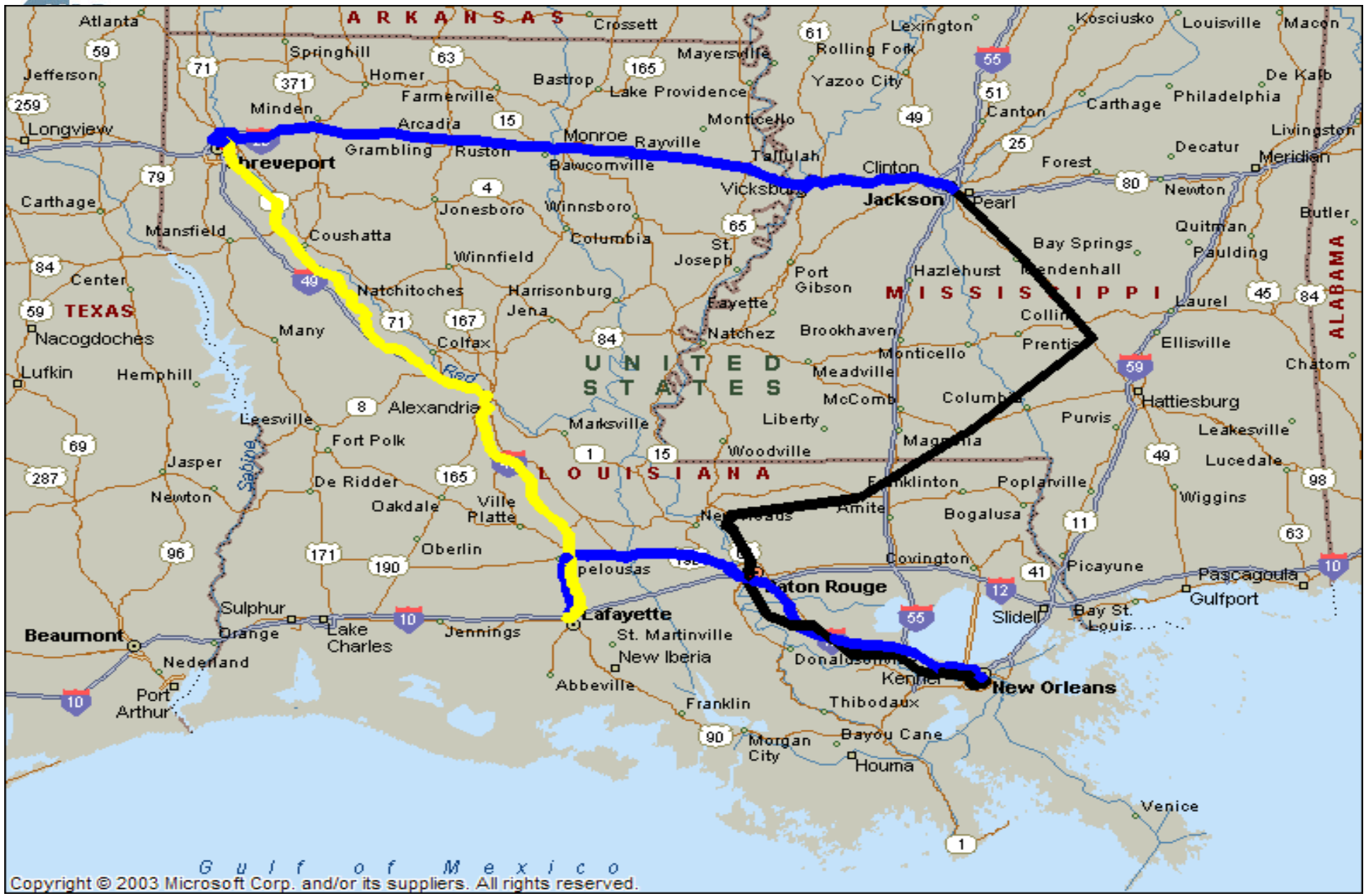
Optical Networks

- New technology for decade: 1000x faster than typical regional networks: Louisiana statewide network (LONI)
- National Lambda Rail
  - $100M USA Optical Network
  - Backbone for next gen. research
  - Locally funded!! No Federal $$
- Other countries: $100'sM
  - Canada, Poland, Holland, Czech, etc; linked!
- 2 dozen+ states committed
- Southern US states investing to be competitive for federal funding, industry

National LambdaRail Architecture



For more information regarding NLR see http://www.nlr.net or contact info@nlr.net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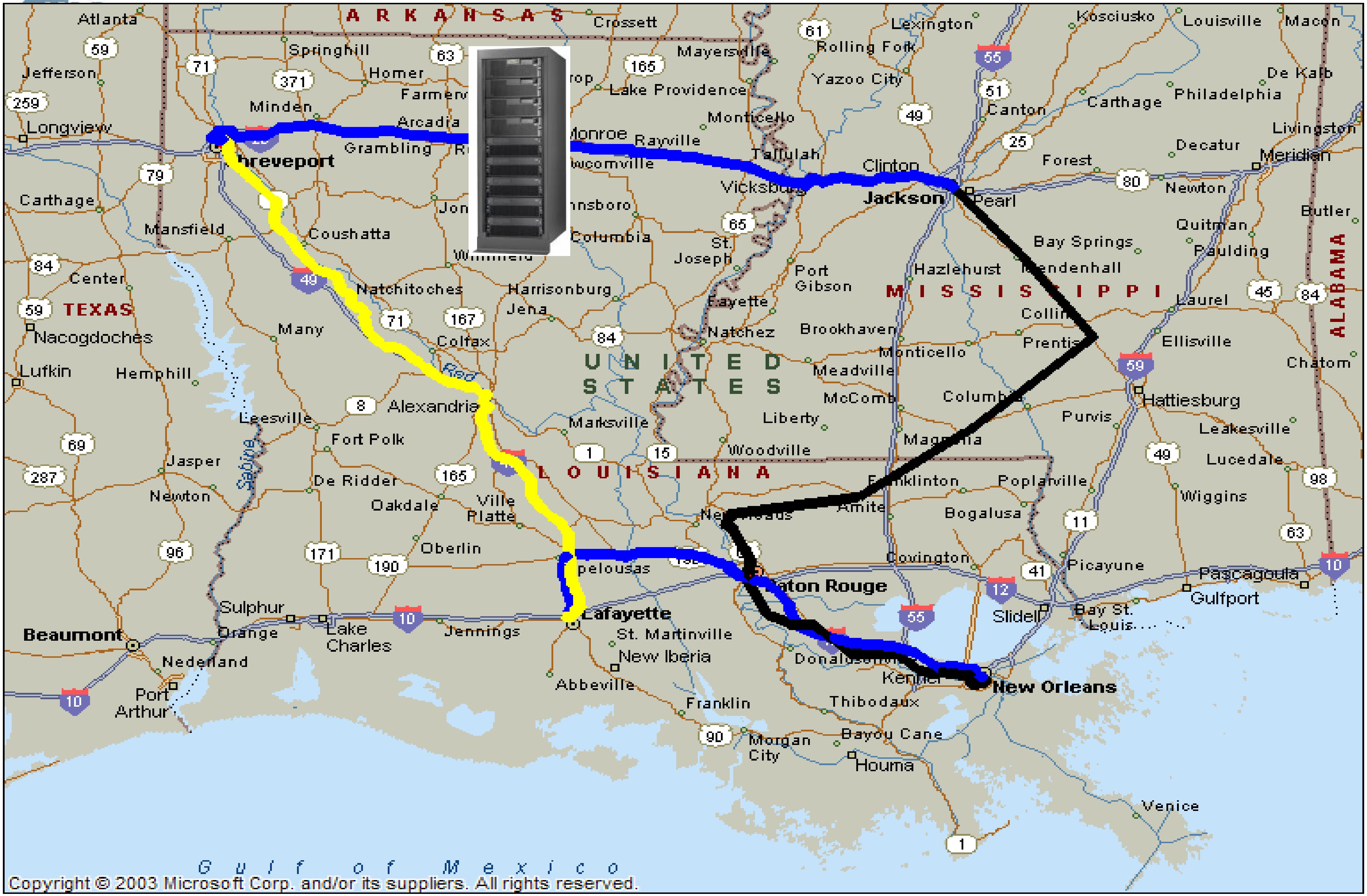
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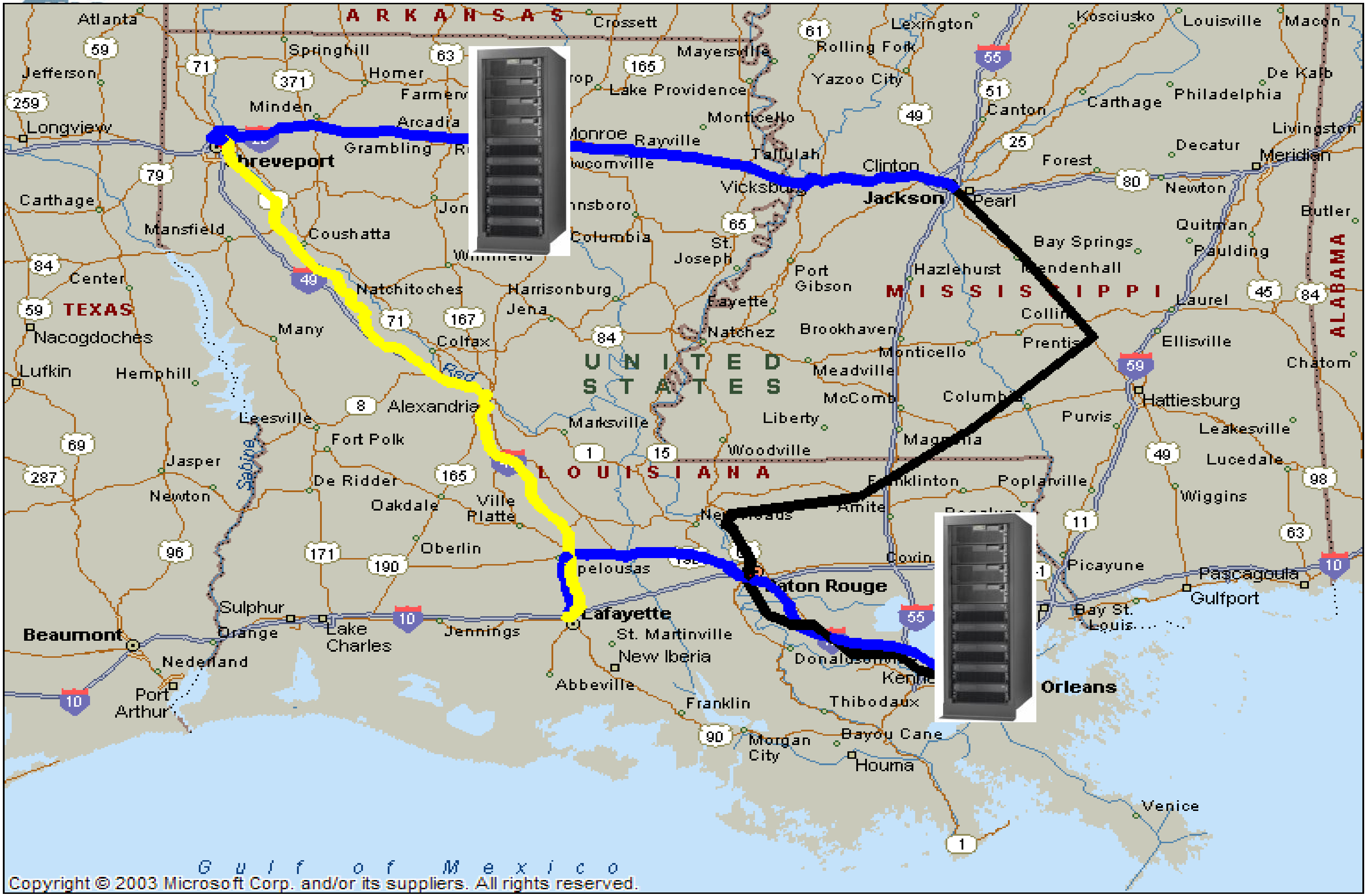
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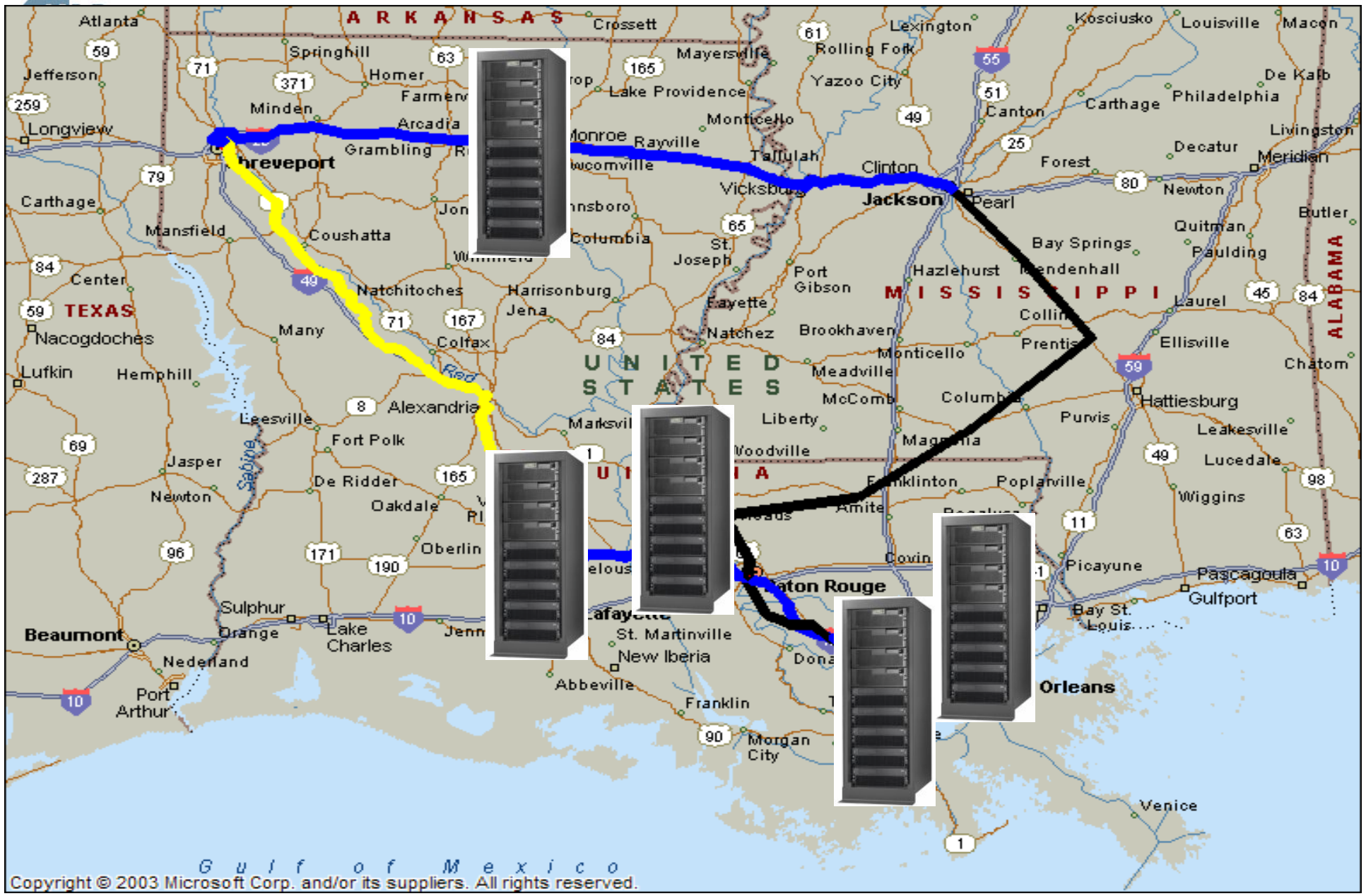
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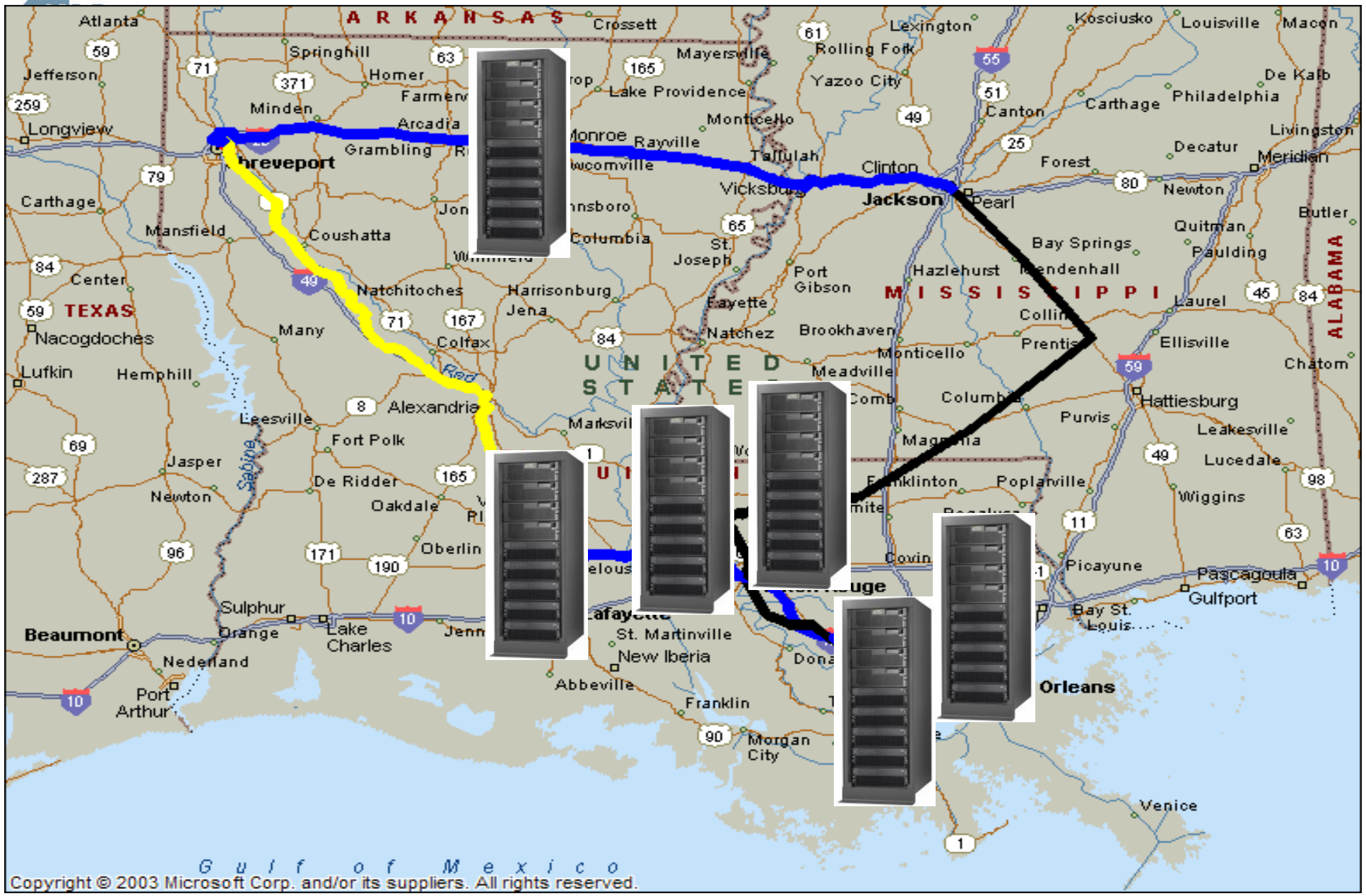

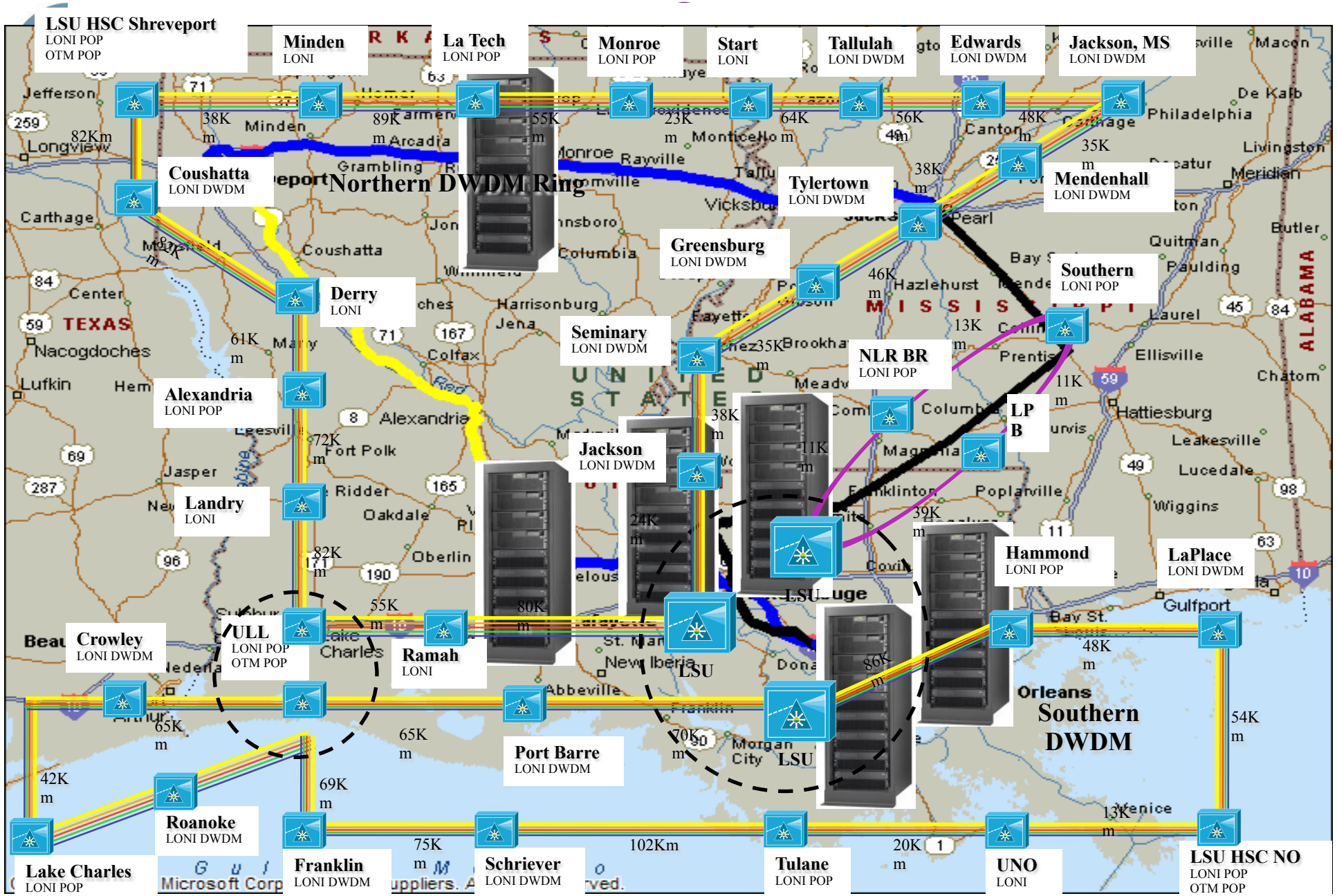
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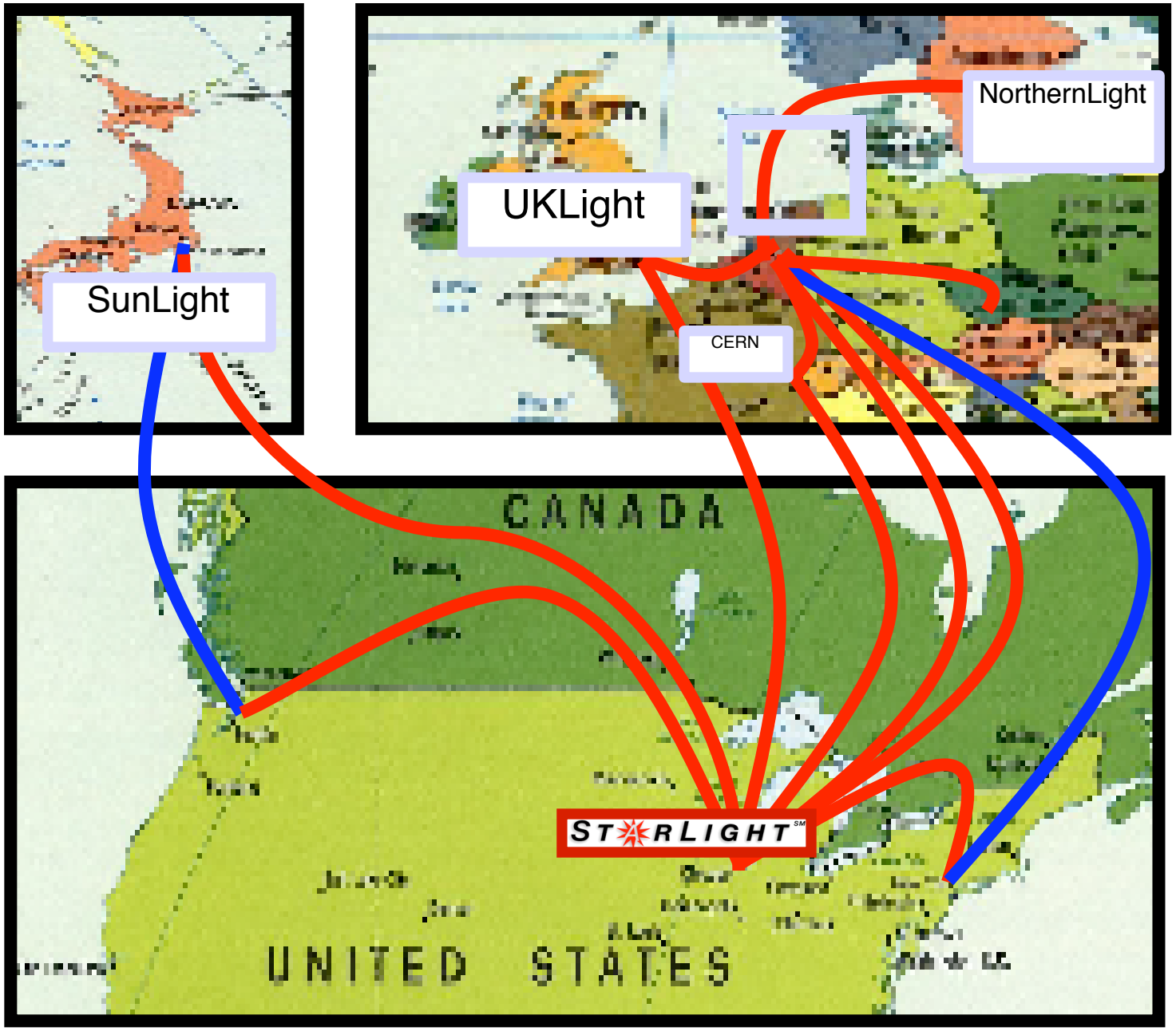
Microsoft Corp

2004 International Lambdas



European lambdas to US
–10Gb Amsterdam—Chicago
–10Gb London—Chicago
–3Gb CERN — Chicago

Canadian lambdas to US
–10Gb Chicago-Canada-NYC
–10Gb Chicago-Canada-Seattle

US lambda to Europe
–7Gb Chicago—Amsterdam

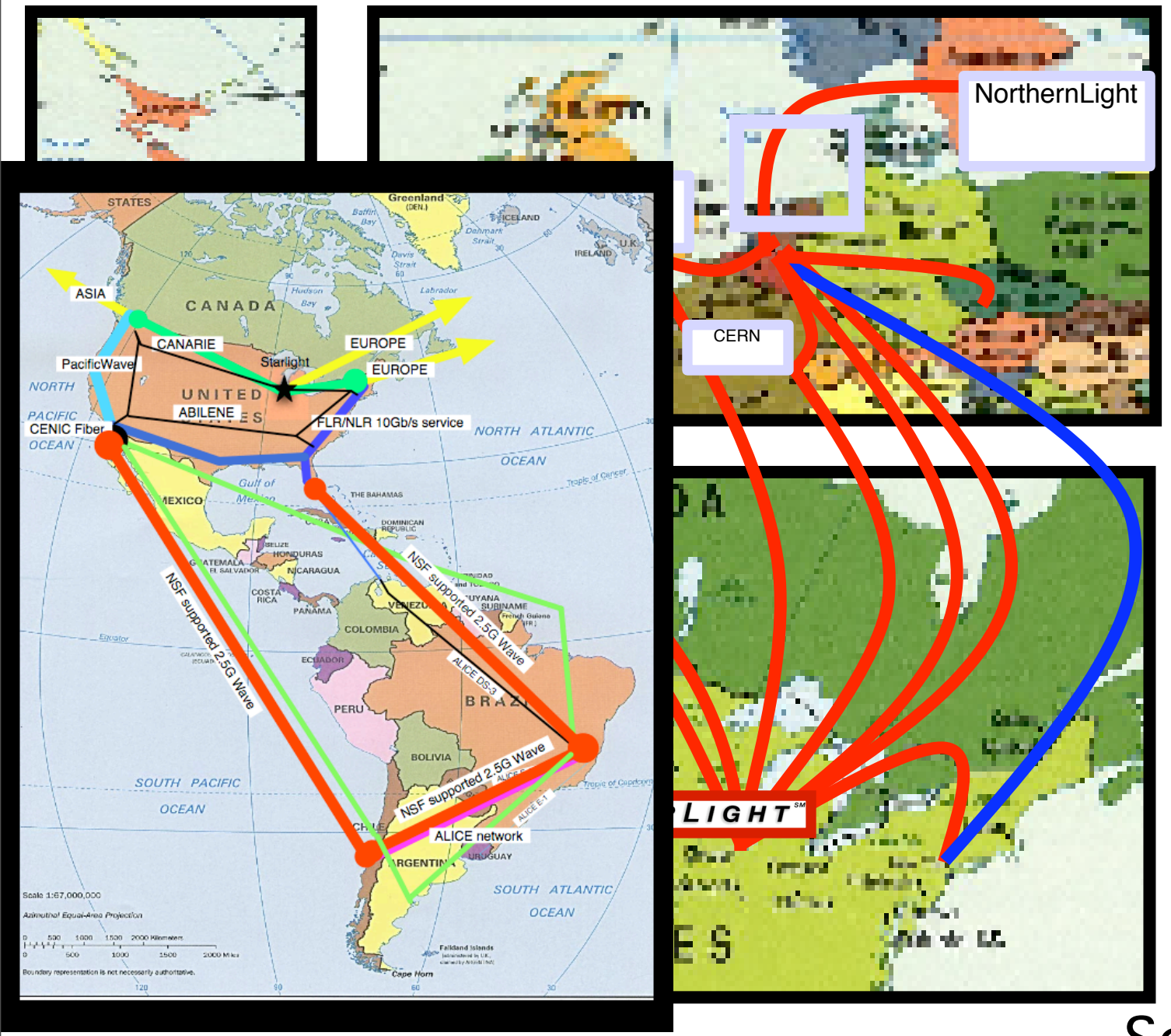
US/Japan lambda
–10Gb Chicago—Tokyo

European lambdas
–10Gb Amsterdam—CERN
–2.5Gb Prague—Amsterdam
–2.5Gb Stockholm—Amsterdam
–10Gb London—Amsterdam

IEEAF lambdas (blue)
–10Gb NYC—Amsterdam
–10Gb Seattle—Tokyo

Source: DeFanti

2004 International Lambdas



European lambdas to US
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–10Gb London—Chicago
–3Gb CERN — Chicago

Canadian lambdas to US
–10Gb Chicago-Canada-NYC
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–10Gb Amsterdam—CERN
–2.5Gb Prague—Amsterdam
–2.5Gb Stockholm—Amsterdam
–10Gb London—Amsterdam

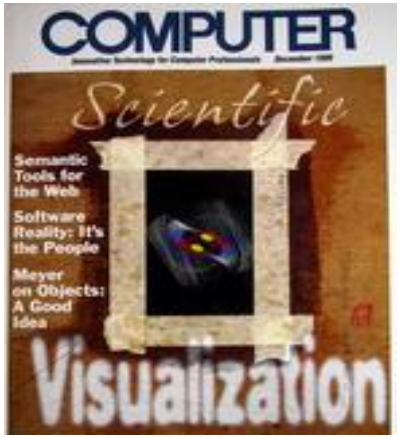
IEEAF lambdas (blue)
–10Gb NYC—Amsterdam
–10Gb Seattle—Tokyo

Source: DeFanti

What do we want to do with this?

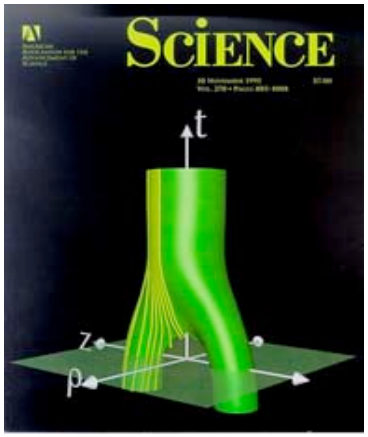
- Collaboration
  - Distributed communities share resources: GWEN, GEON, NEES, etc.
  - "Shared Cyberinfrastructure": data, code, tools, resources, simulations…
- "Standard Things"
  - Task Farming, Resource Brokering, Remote Steering, Managing Data (!)
- "New Scenarios"
  - Apps abstracted, become services
  - Dynamic apps decide their future, find their services (data, resources, applications, people): DDDAS
  - Apps distributed, spawned, task farmed, controlled, monitored with other apps/people

Collaborations for Complex Problems



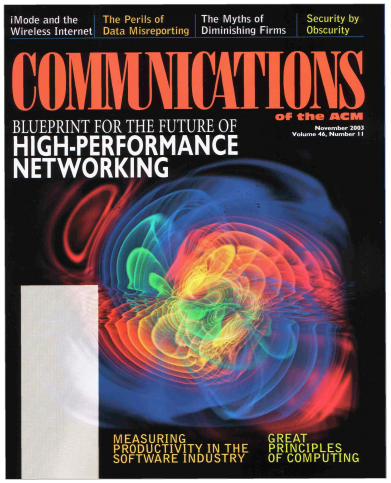
NASA Neutron Star Grand Challenge

- 5 US Institutions
- Attack colliding neutron star problem



NSF Black Hole Grand Challenge

- 8 US Institutions
- 5 years
- Attack colliding black hole problem



EU Astrophysics Network

- 10 EU Institutions
- 3 years
- Continue these problems

Examples of Future of Science & Engineering

- Require large scale data, simulations, beyond reach of any machine
- Require large geo-distributed cross-disciplinary collaborations
- Require Grid technologies

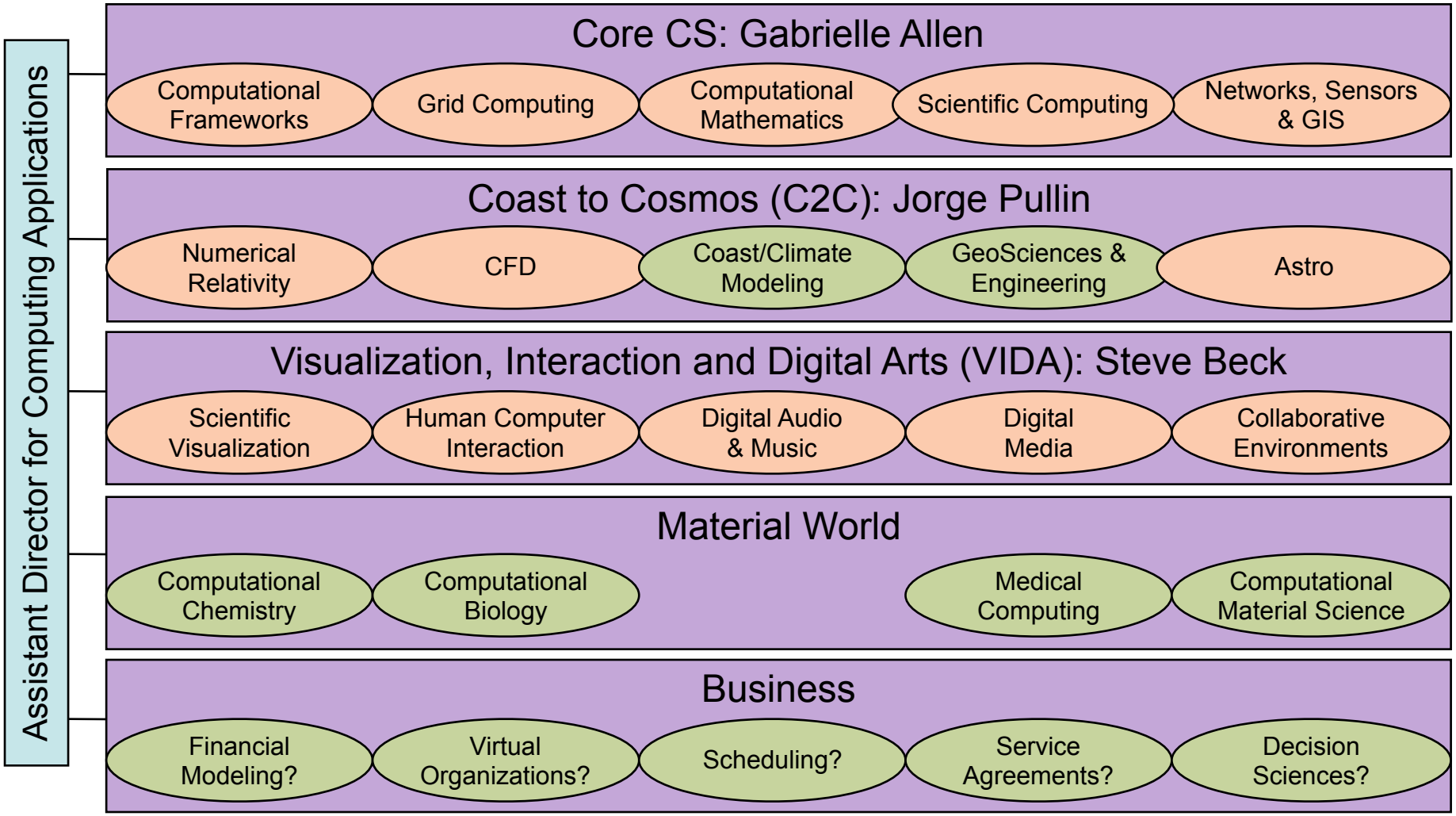
Recommendations from PITAC

- Universities must significantly change organizational structures: multidisciplinary & collaborative research to remain competitive in global science.
- Federal investments must rebalance to:
  - *Software*: create reliable, easy to use, scalable software that will enable scientists to focus on discovery: Software *Crisis*
  - *Hardware*: develop, prototype, evaluate new hardware architectures to deliver larger peak and sustained performance at the petaflop level for scientific apps
  - *Data*: focus on data-intensive solutions to address the coming data explosion with advances in sensors and sensor networks

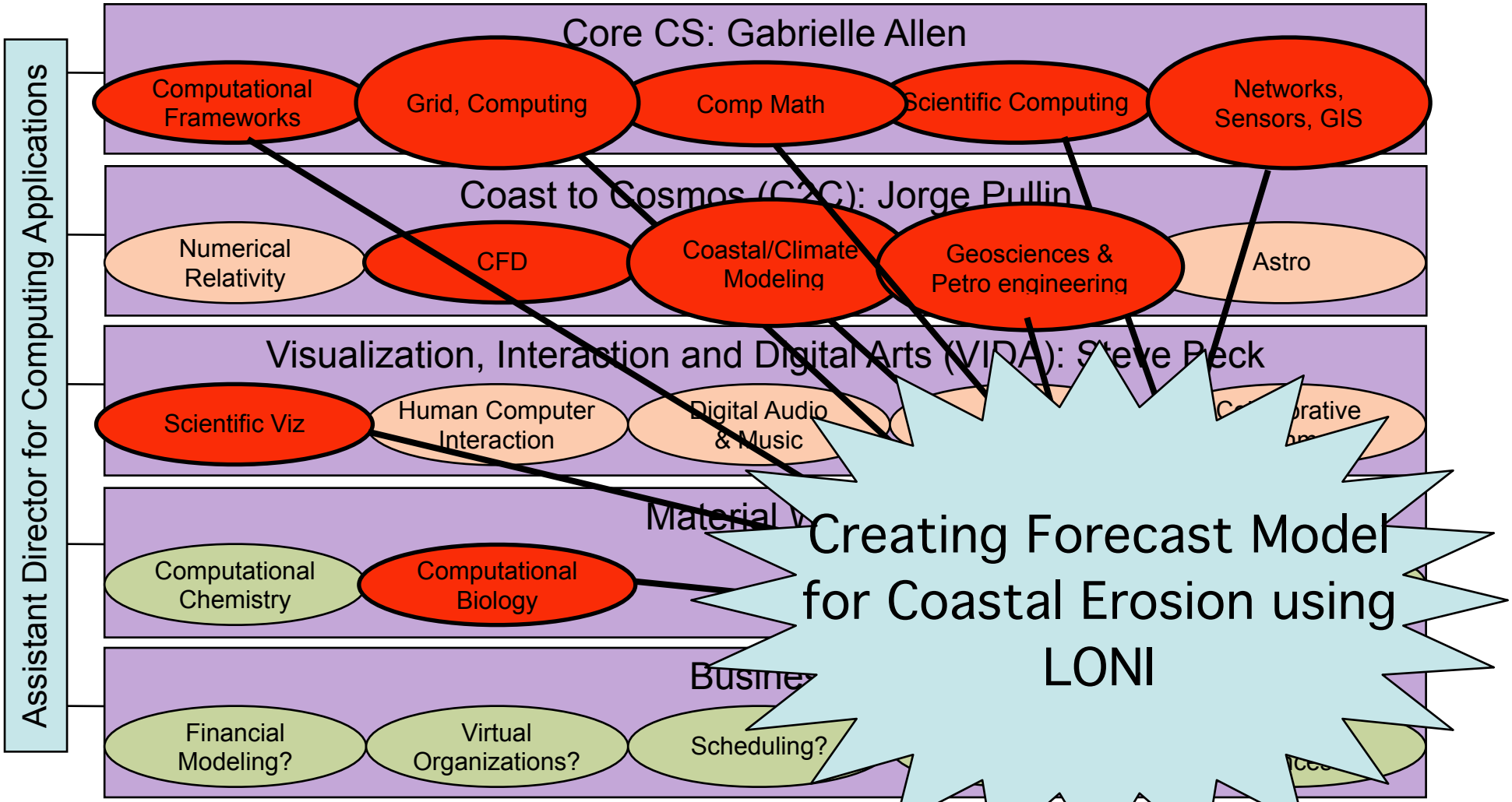
Source: President's Information Technology Advisory Committee

www.nitrd.gov/pitac

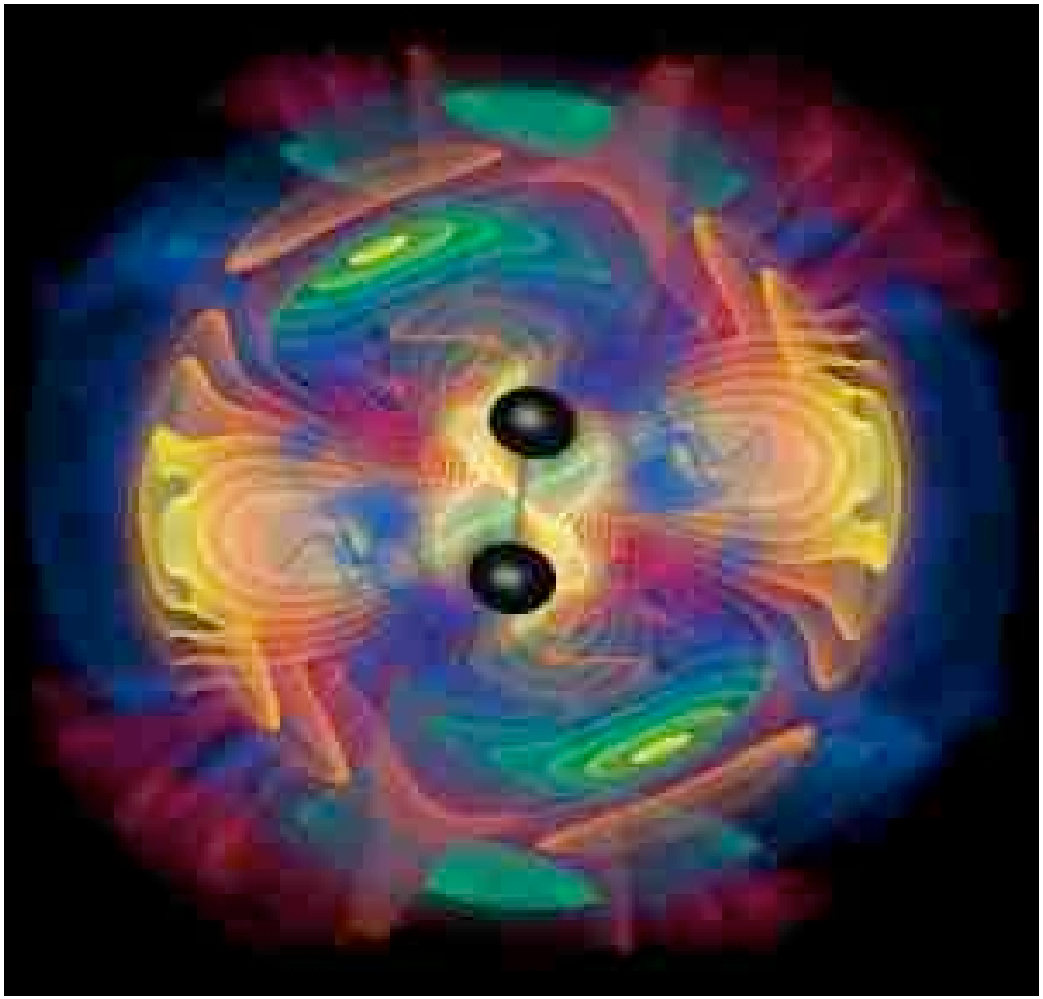
The NCSA-CCT Interdisciplinary Model



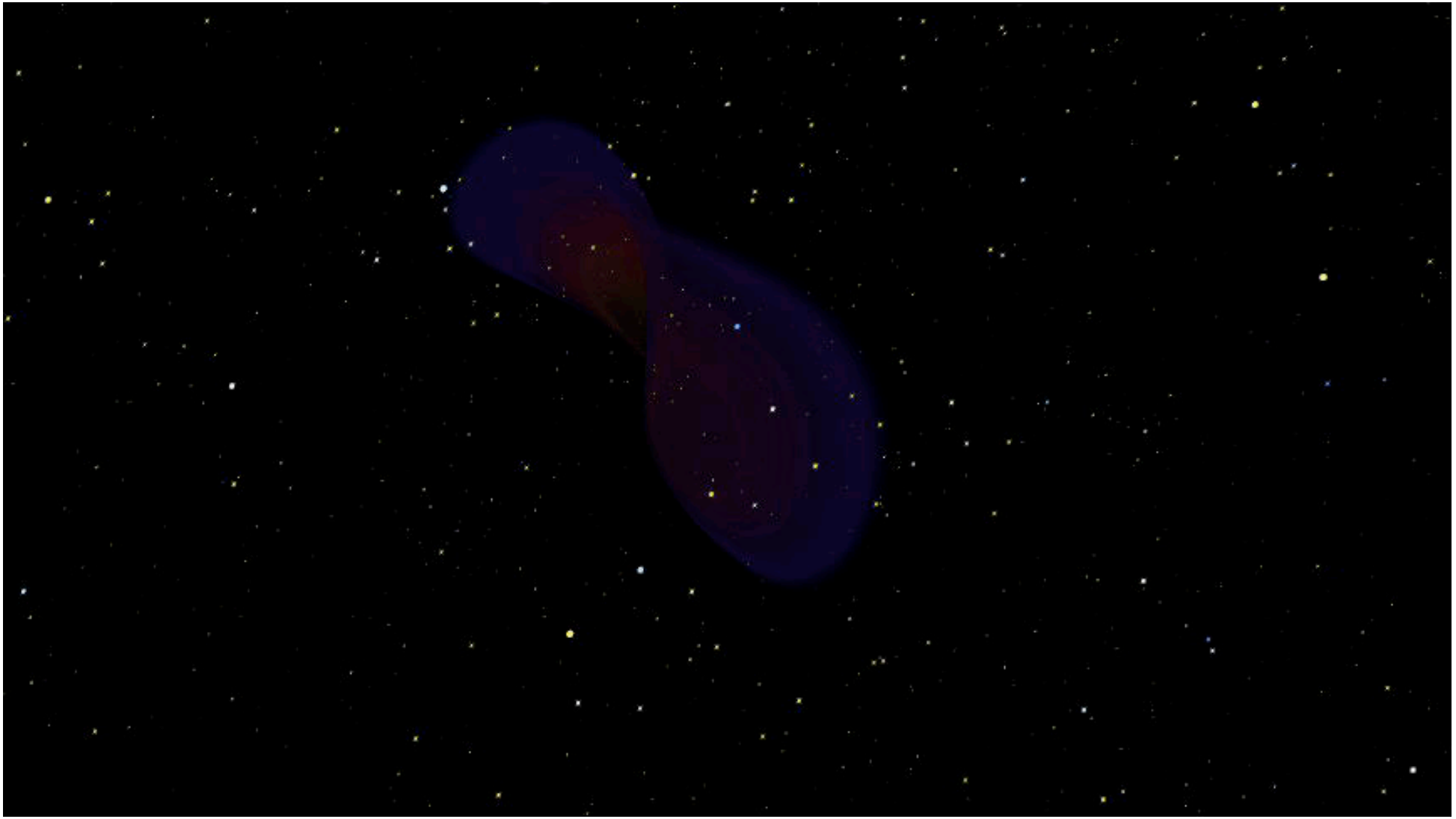
The NCSA-CCT Interdisciplinary Model



Huge Black Hole Collision Simulation



Huge Black Hole Collision Simulation



Issues for Complex Simulations

- Huge amounts of data needed/generated across different sites
  - Smarr: supercomputers are merely petabyte generators
  - How to retrieve, track, manage data across Grid? Data Archives! Metadata!
  - In this case, had to fly Berlin to NCSA, bring data back on disks!
- Many components developed by distributed collaborations
  - How to bring communities together?
  - How to find/load/execute different components?
- Many computational resources available
  - How to find best ones to start?
  - How to distribute work effectively?
- Needs of computations *change* with time!
  - How to adapt to changes?
  - How to monitor system?
- How to interact with experiments? Coming! Grids evolve: DDDAS
- Complex infrastructure accessed through common toolkits
  - Everyone should not reinvent the wheel (especially physicists)

Cactus Framework: Enabling User Communities in Advanced HPC
www.cactuscode.org

- Toolkit for HPC, Grid, Collaborative Applications
- Abstract interfaces for everything
  - Parallelism, I/O, AMR, elliptic solvers, etc
  - Other packages, toolkits (Grace, Petsc, Samrai, HDF, Carpet, etc)
- Advanced capabilities
  - Streaming data, communication, Viz
- Grid capabilities
  - Globus, GAT, Portals, etc
- Toolkits: Einstein Toolkit, CFD Toolkit, Bioinformatics Toolkit
- International developer/user base
  - We have openings for developers!!

Cactus Framework: Enabling User Communities in Advanced HPC

www.cactuscode.org

Numerical Relativity/Astrophysics

AEI numrel
WashU
UNAM
Soton
RIKEN
Goddard
Monash
Thessaloniki
Pitt
PSU
Tübingen
TAC
SISSA
Portsmouth
UT
EU Astrophysics Network
NASA
Arizona
Caltech
Brownsville
S. Africa
LSU
UNAM
Garching

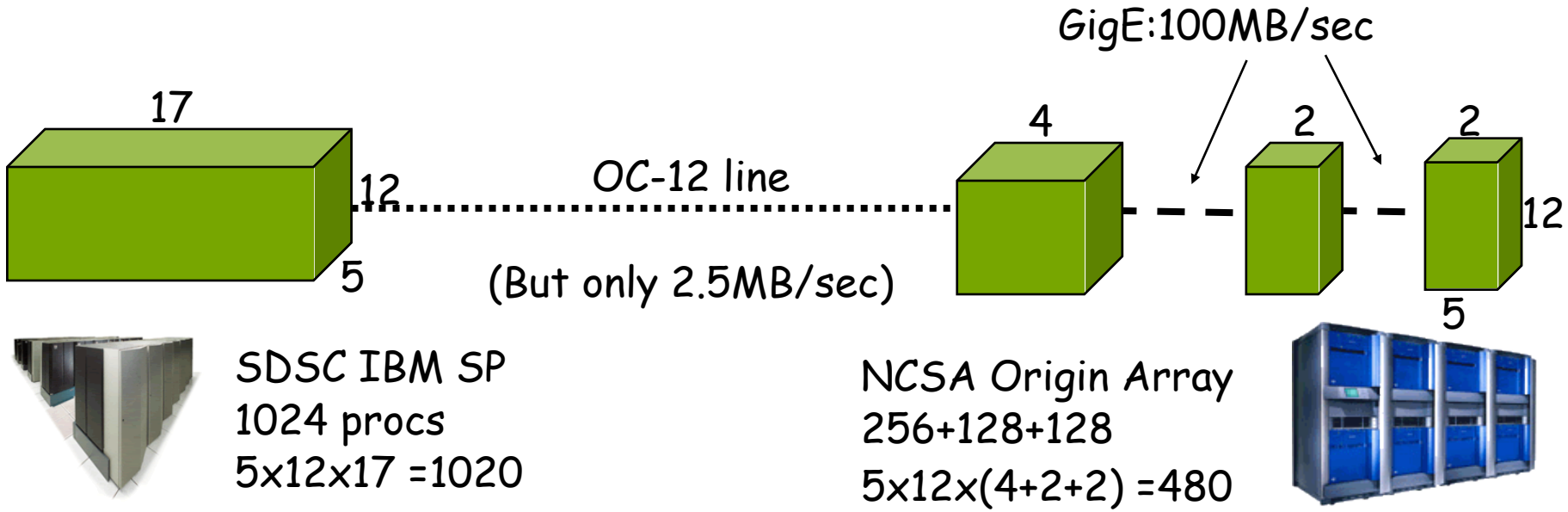
Other Applications

Chemical Engineering (U.Kansas)
Climate Modeling (NASA,Utrecht)
Bio-Informatics (Chicago)
CFD (KISTI, LSU)
Early Universe (LBL)
Benchmarking
CS groups worldwide
Plasma (Princeton)
Astrophysics (Zeus/Innsbruck)

Dynamic Adaptive Distributed Computation

(T.Dramlitsch, with Argonne/U.Chicago)

GridLab



SDSC IBM SP
1024 procs
5x12x17 =1020

NCSA Origin Array
256+128+128
5x12x(4+2+2) =480

These experiments:

- Einstein Equations (but could be any Cactus application)

Achieved:

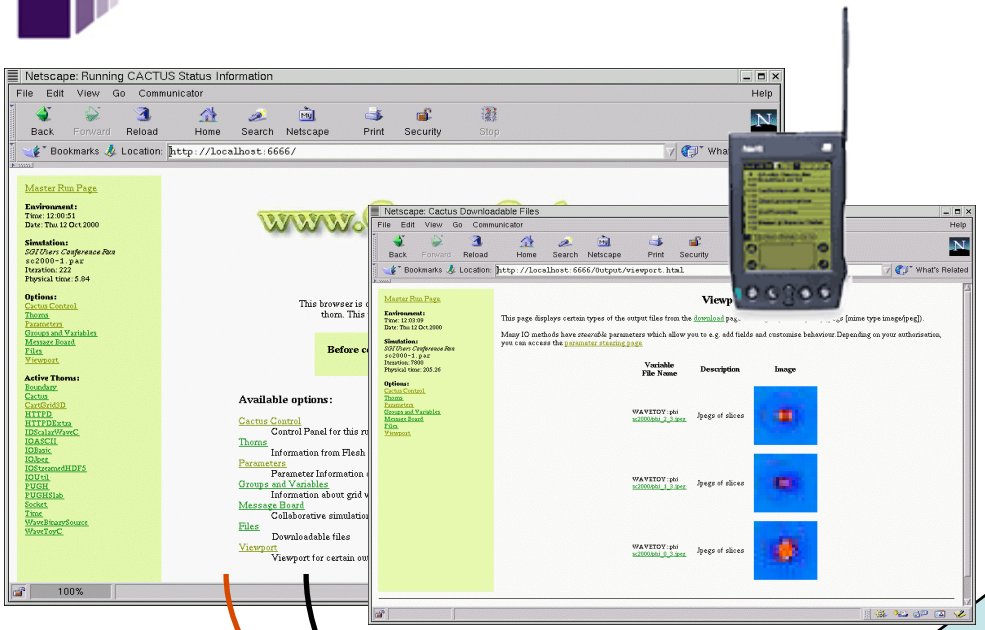
- First runs: 15% scaling
- With new techniques: 70-85% scaling, ~ 250GF

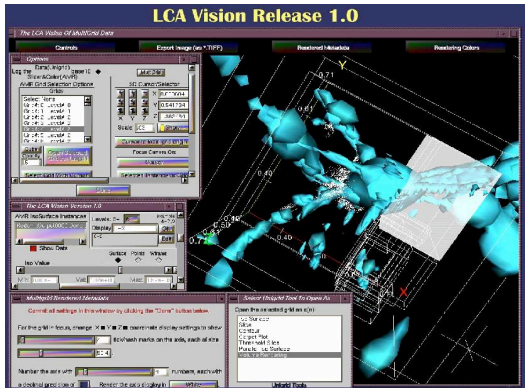
Dynamic Adaptation: Number of ghostzones, compression, …

Won

"Gordon Bell Prize" (Supercomputing 2001, Denver)

Interacting with Jobs using Cactus





Any Viz Client:

LCA Vision, OpenDX

Changing any steerable parameter

- Parameters
- Physics, algorithms
- Performance

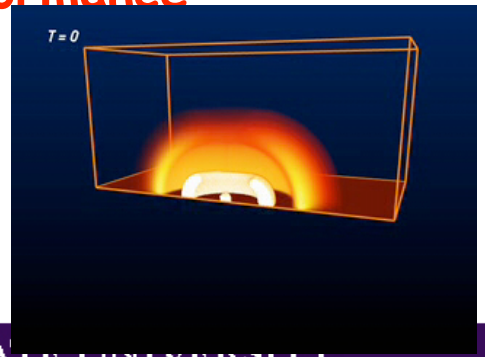
Remote Viz data

Streaming HDF5

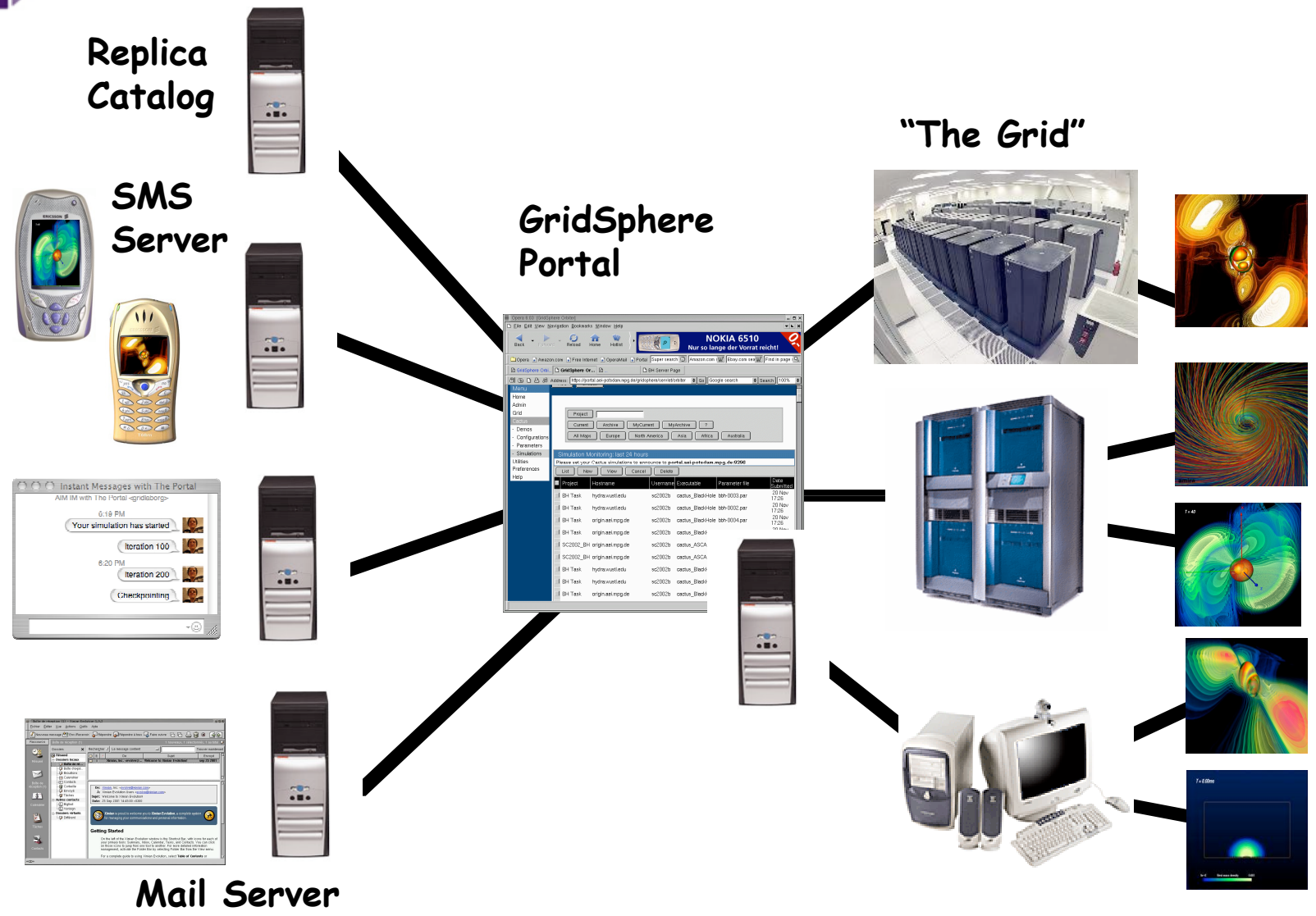
Autodownsample

Remote Viz data

Amira

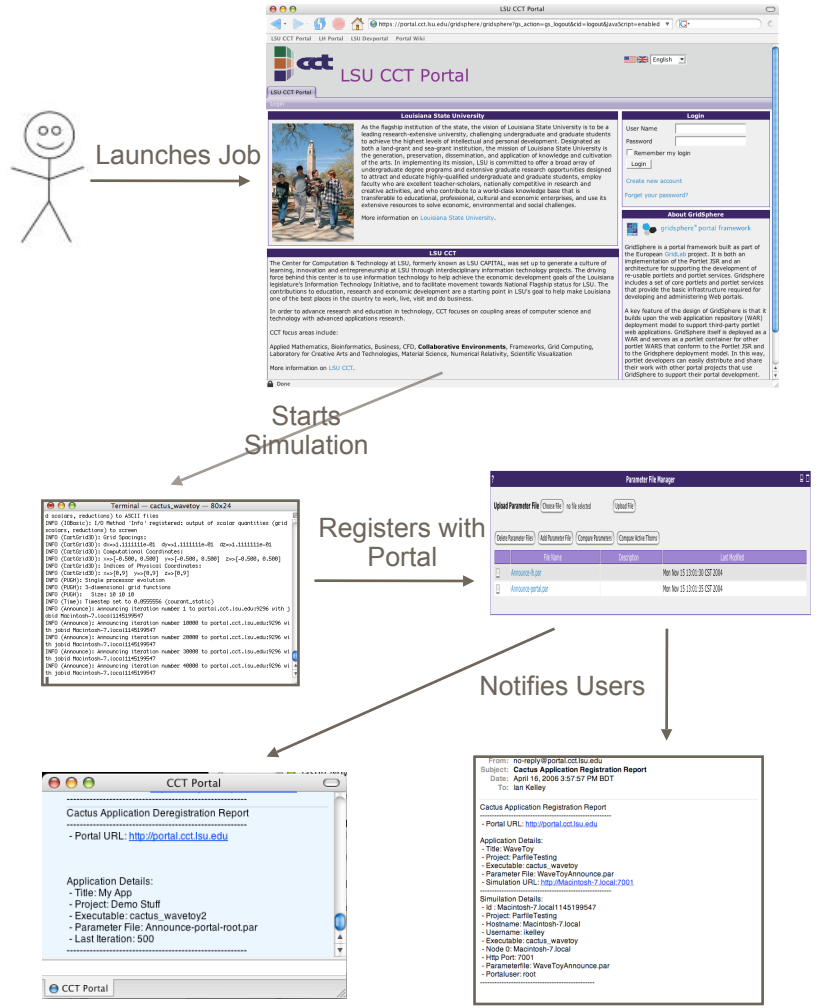


Notification and Information



Cactus Portal

- **GridSphere**-based, JSR 168 compliant portal.
- Monitors Cactus applications by sending metadata to the portal at application *startup*, *shutdown*, and regular *user-defined intervals*
- Keeps users updated through *instant messages* and/or *e-mail*
- Has facilities for *sharing*, *viewing*, *editing* and *comparing* parameter files.
- Modular design, allowing new Cactus (or other) applications to easily customize metadata.



Computers as Petabyte Generators

(Black holes and more…)

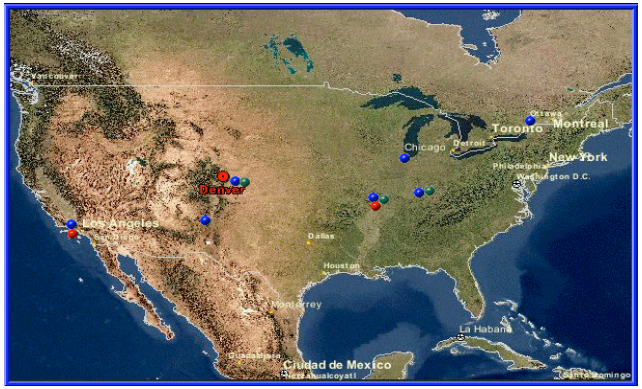
- Crude vacuum BH collisions today
  - 10^{15} Flops, Tbytes output, vastly downsampled!
- Desired BH, NS scenarios in few years
  - 10^{20} Flops, multiple orbits, adaptive meshes, hydro, 1 day on 50TF machine, 25TB+ output per run
  - May be physically distributed due to grid activities
- Need metadata to describe simulations
- Real time scheduling across multiple resources for distributed computing
  - Lambda provisioning on demand: spawning (analysis, steering), migration, interactive viz from distributed collaborations
- Parameter Space! 10^3 - 10^6 simulations!

New Grid Applications: be creative

- Intelligent Parameter Surveys, Monte Carlos
  - May control other simulations!
- Dynamic Staging: move to faster/cheaper/bigger machine ("Grid Worm")
  - Need more memory? Need less?
- Multiple Universe: clone to investigate steered parameter ("Gird Virus")
- Automatic Component Loading
  - Needs of process change, discover/load/execute new component somewhere
- Automatic "Look Ahead", convergence testing
  - spawn off and run coarser resolution to predict future, study convergence
- Spawn Independent/Asynchronous Tasks
  - send to cheaper machine, main simulation carries on
- Routine Profiling
  - best machine/queue, choose resolution parameters based on queue
- Dynamic Load Balancing: inhomogeneous loads, multiple grids
- DDDAS: injecting data into the above, feed back to experiment
- Model-Model coupling: very important in DDDAS

Already did a lot of this! Spawning on ARG Testbed

Main Cactus BH Simulation starts here



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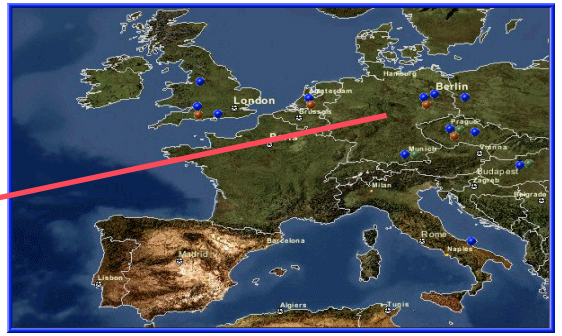

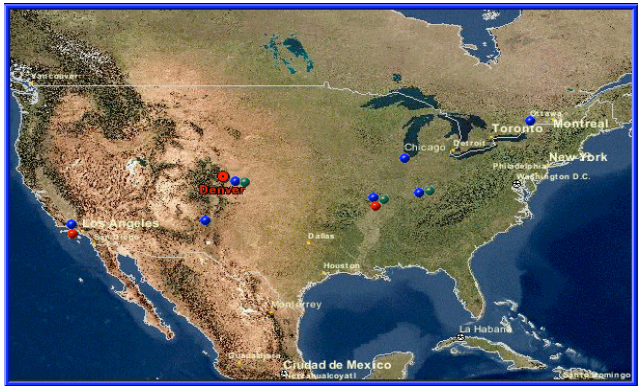

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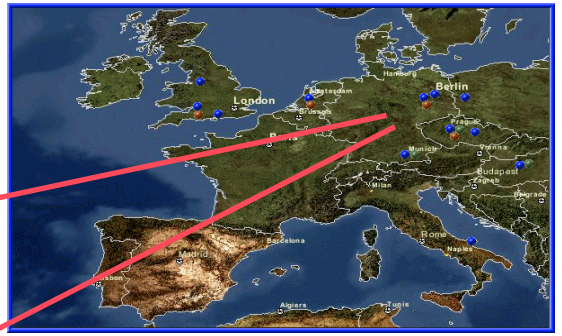

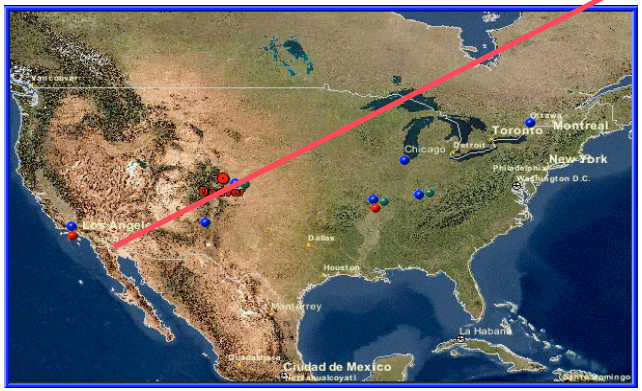

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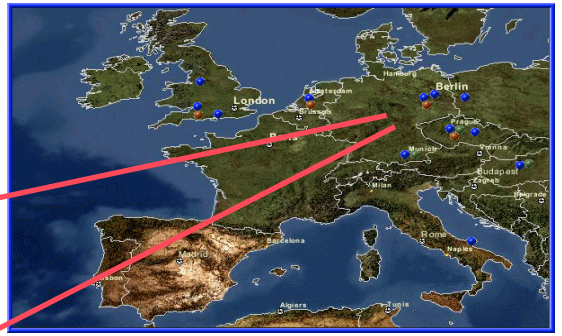

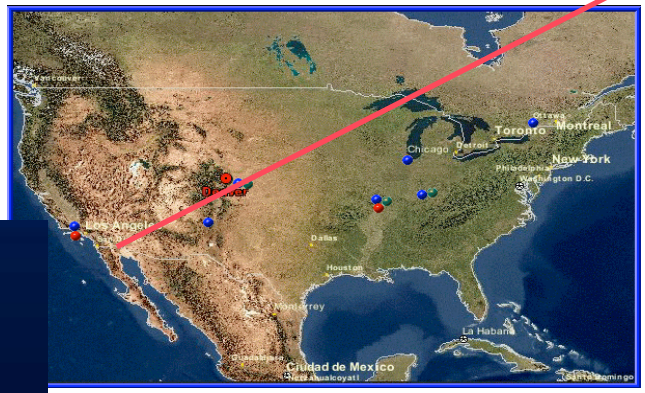

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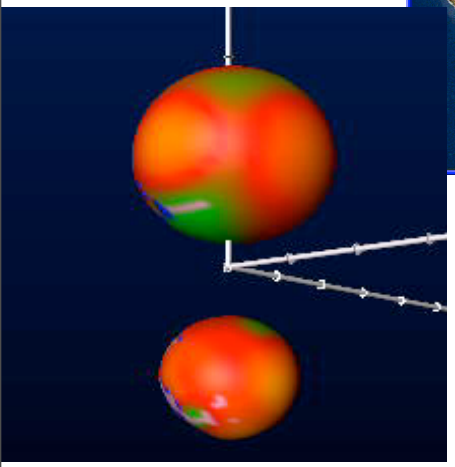

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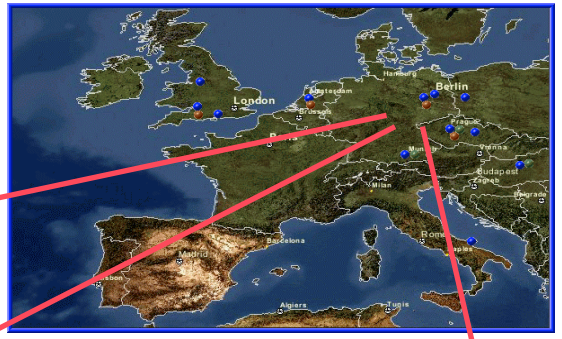

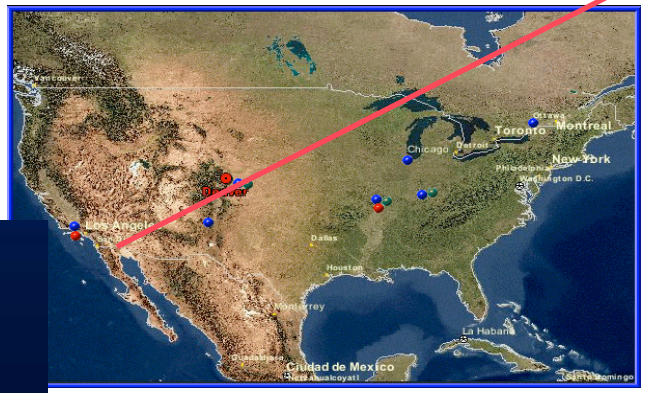

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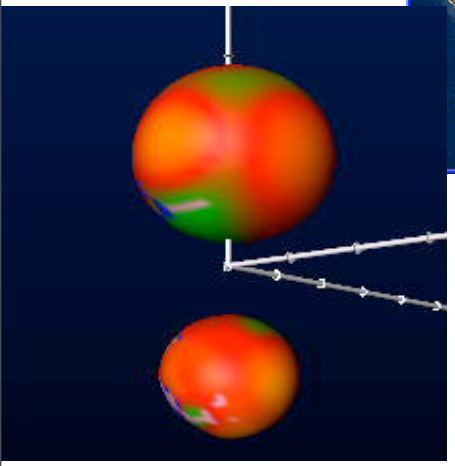

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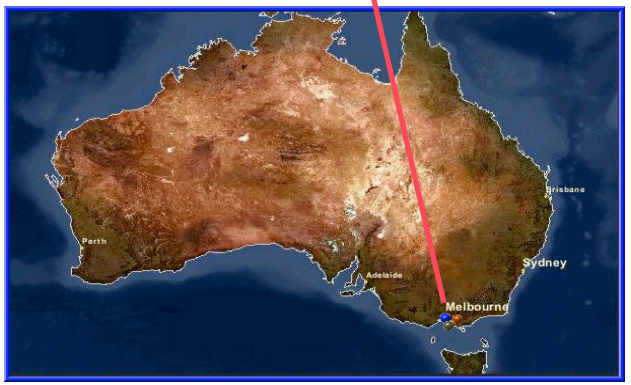

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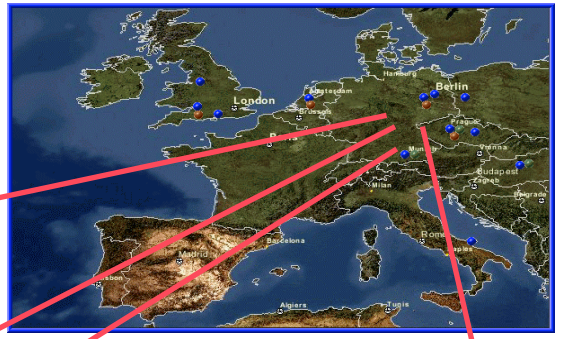

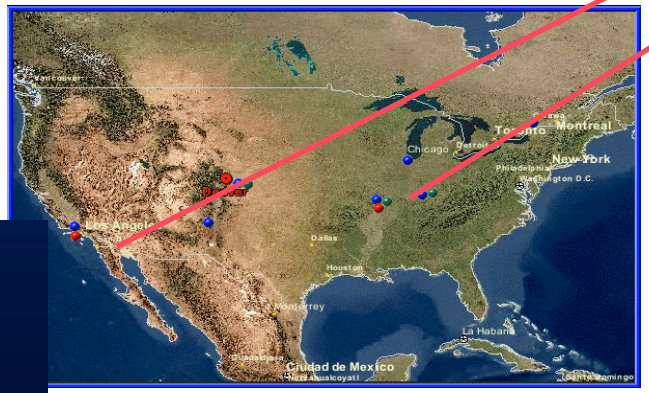

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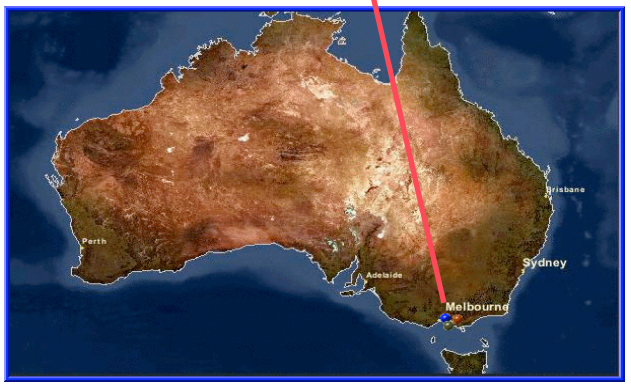

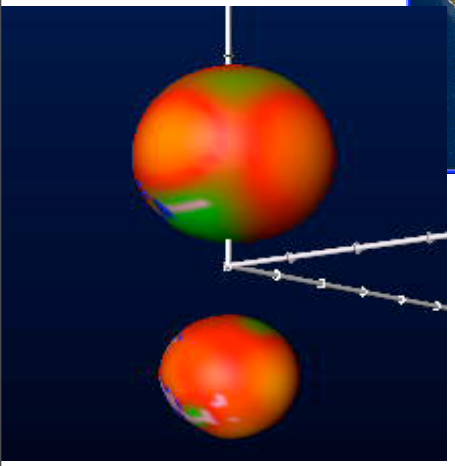

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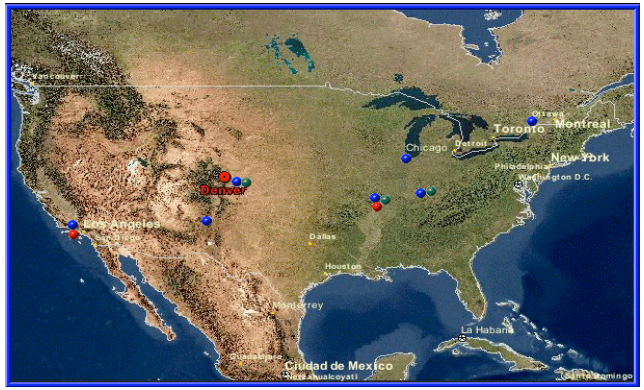
Task Farming, Spawning & Migration



Task Farming, Spawning & Migration

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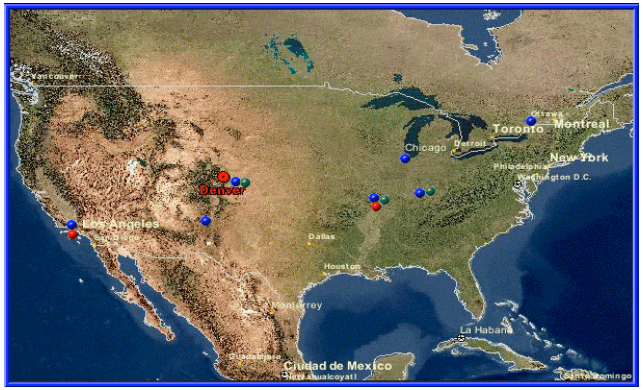

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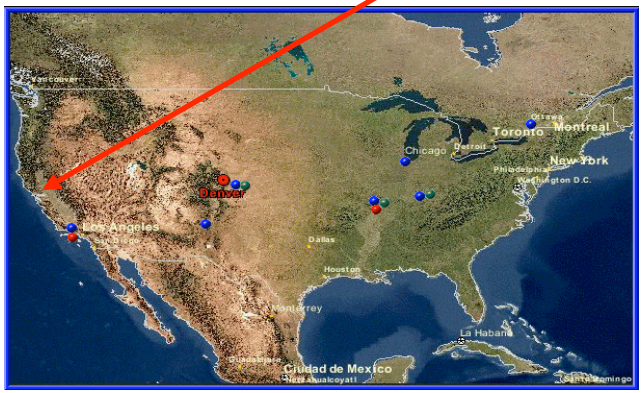

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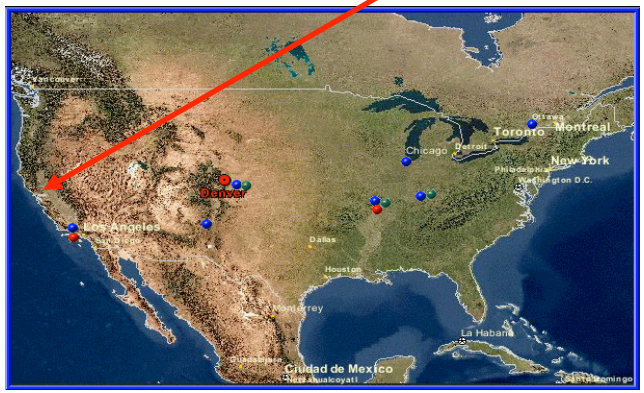

Dozens of small jobs sent out to test parameters

Task Farming, Spawning & Migration

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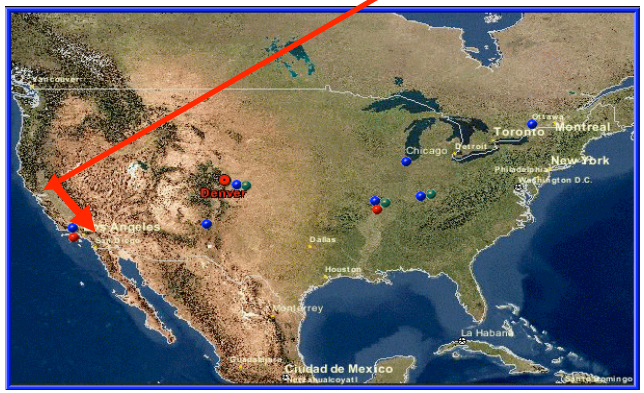

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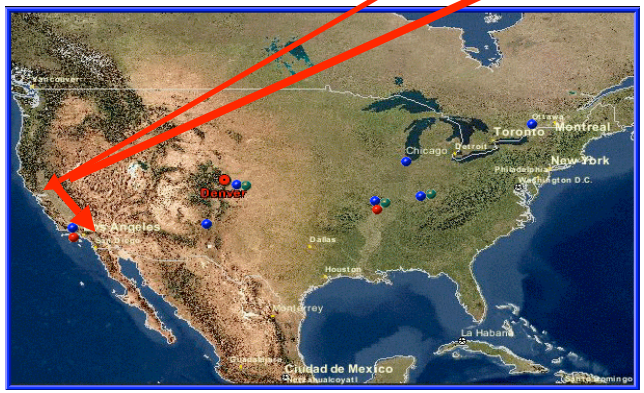

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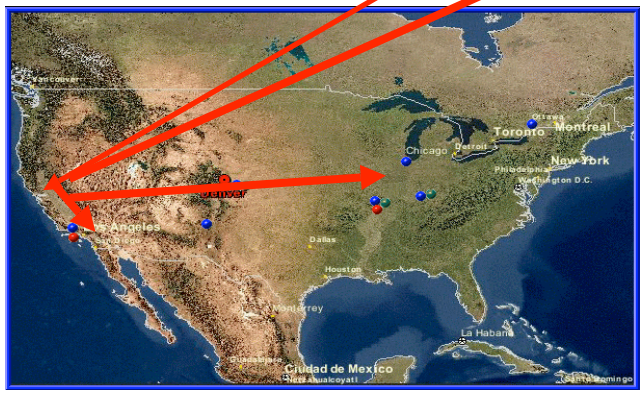

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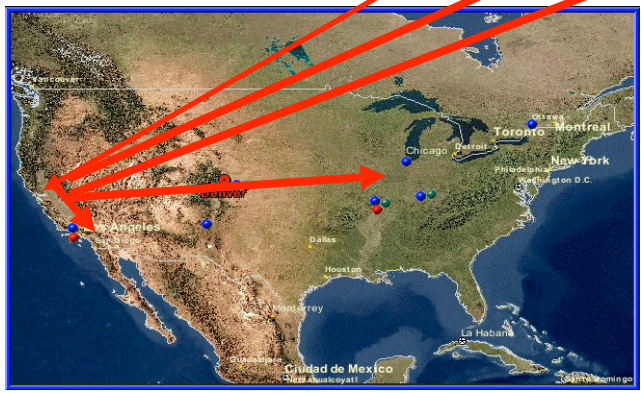

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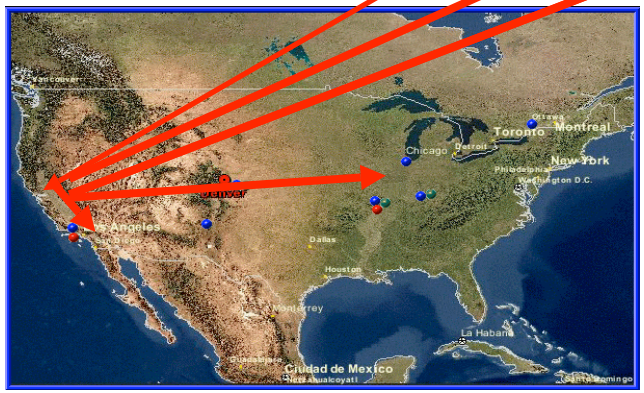

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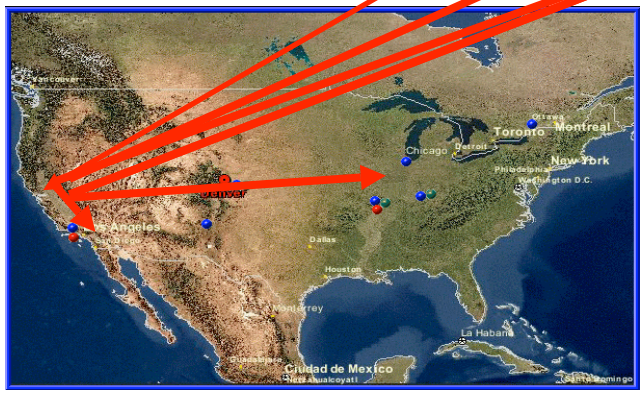

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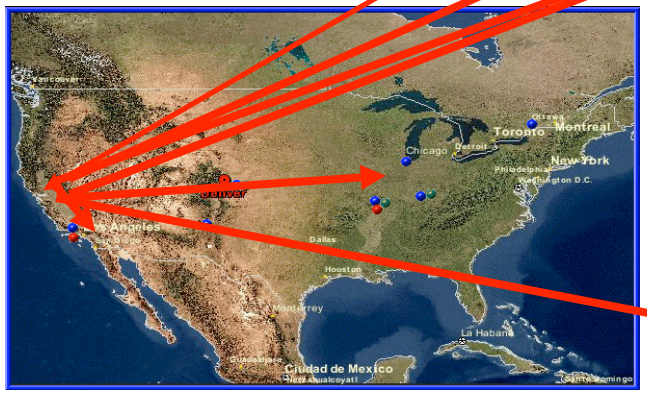

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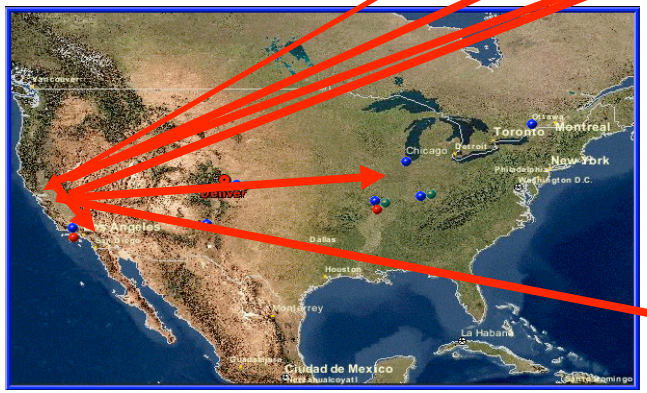

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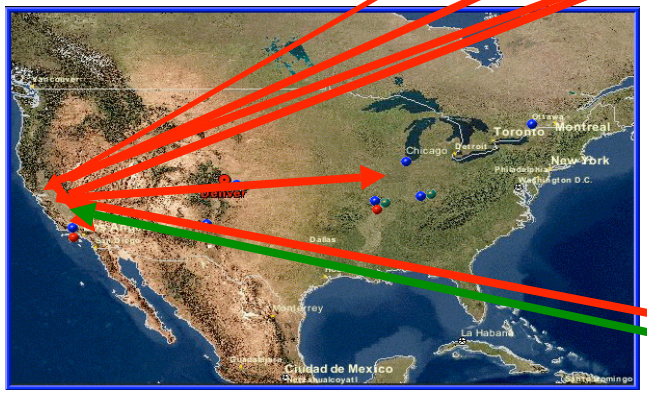

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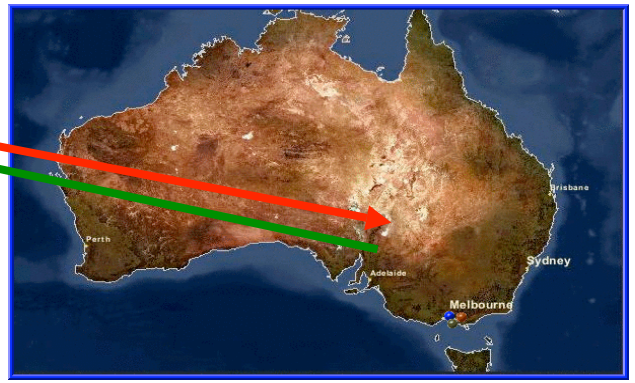

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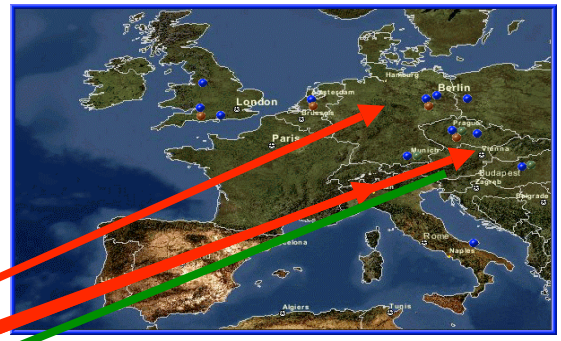

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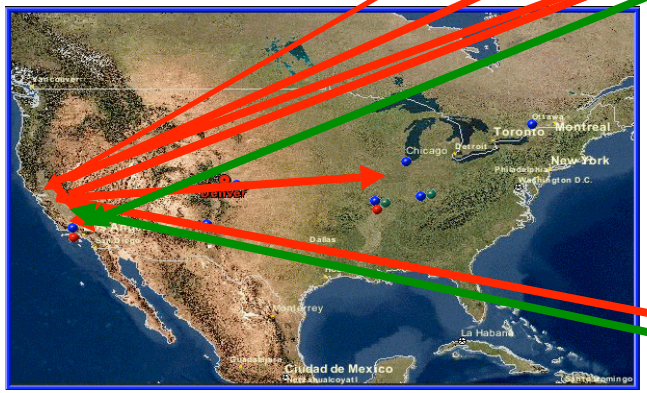

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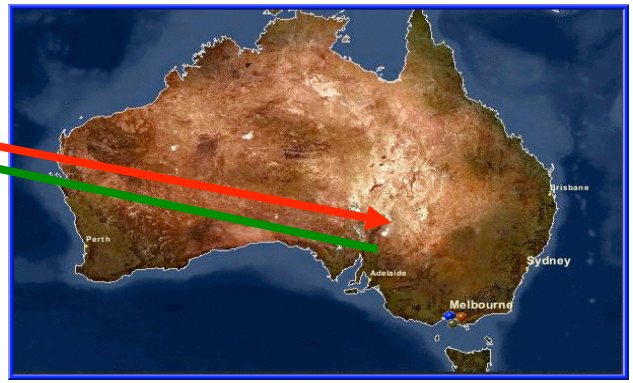

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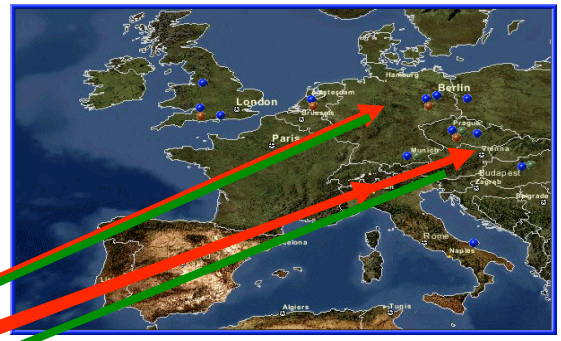

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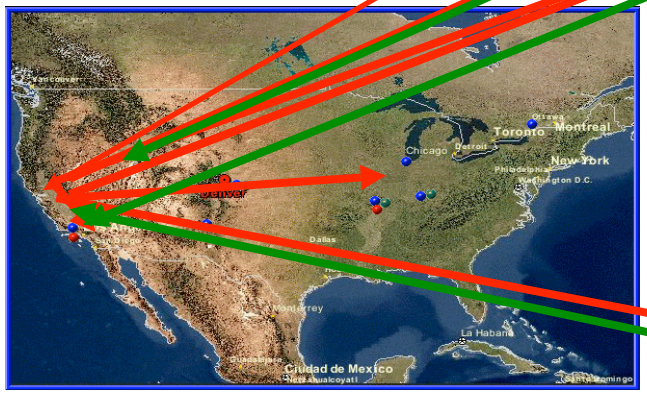

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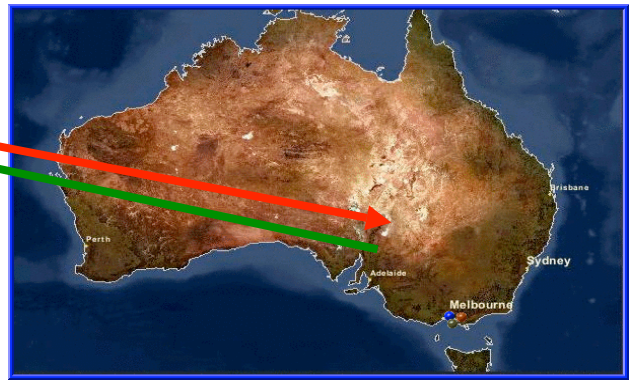

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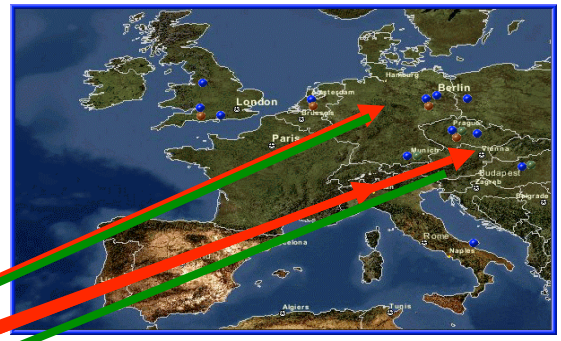

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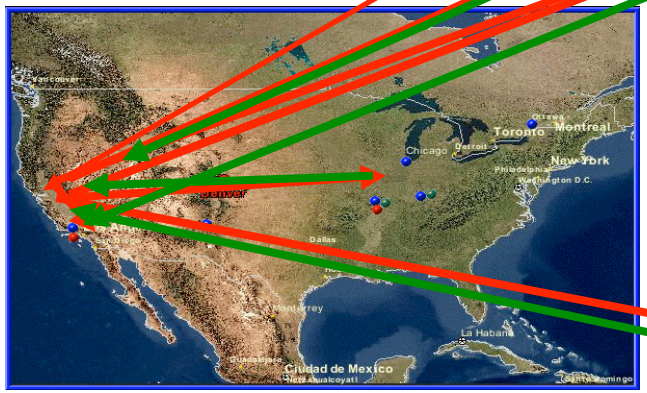

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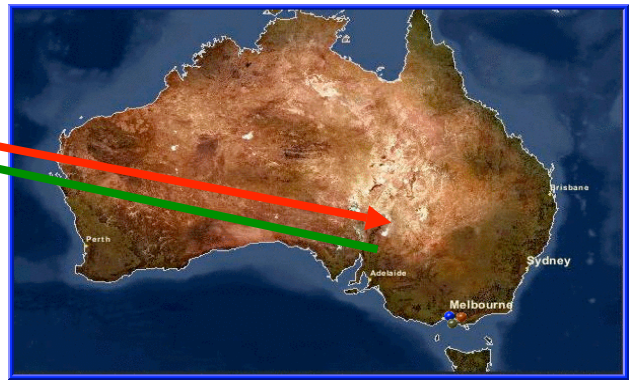

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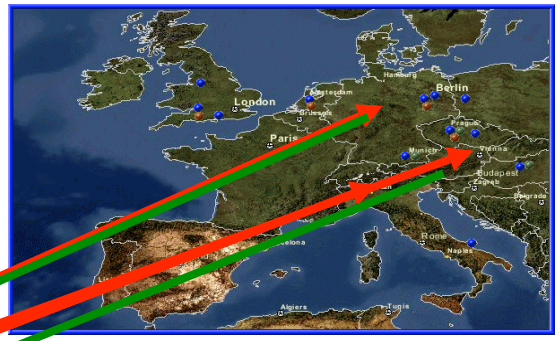

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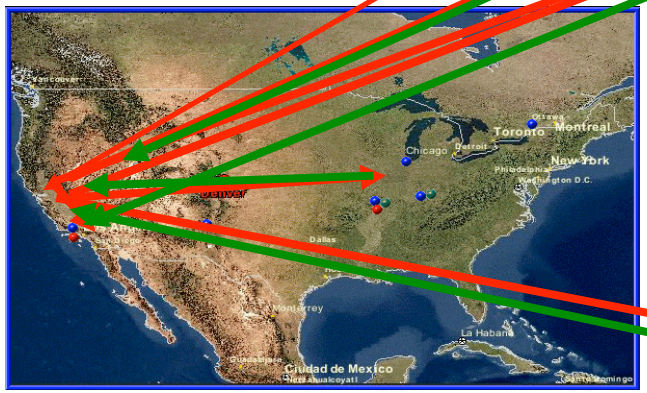

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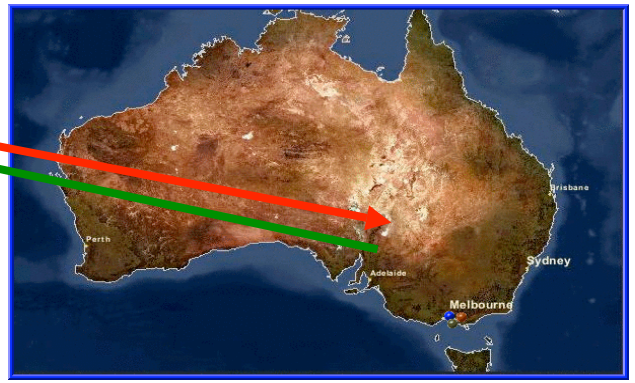

Huge job generates remote data to be visualized in Baltimore

Task Farming, Spawning & Migration

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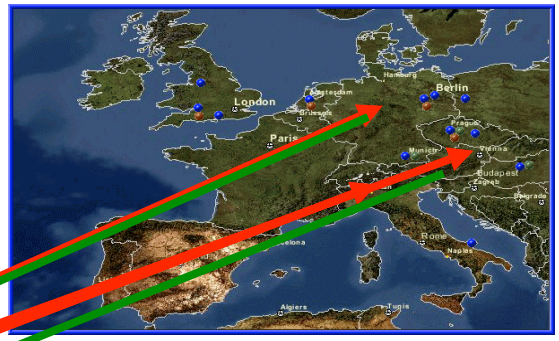

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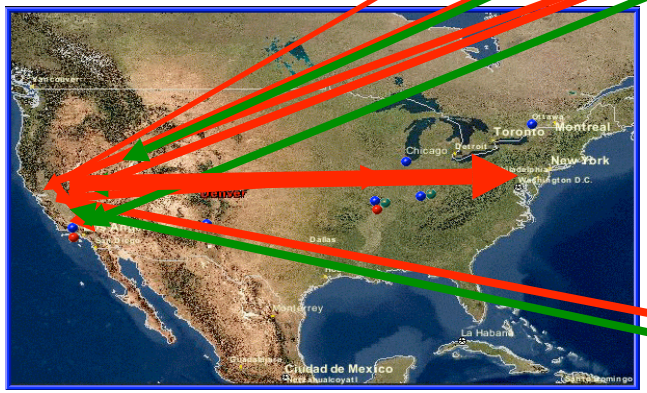

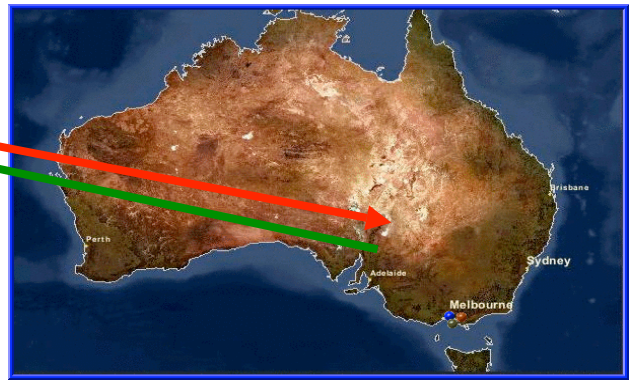

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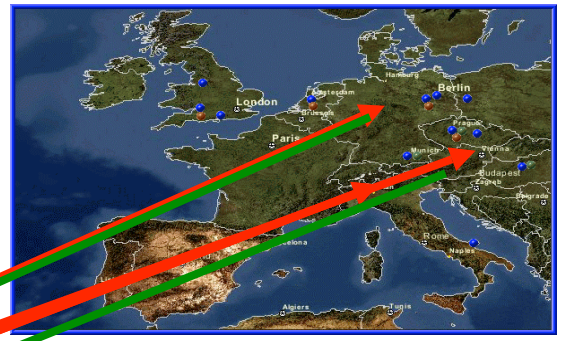

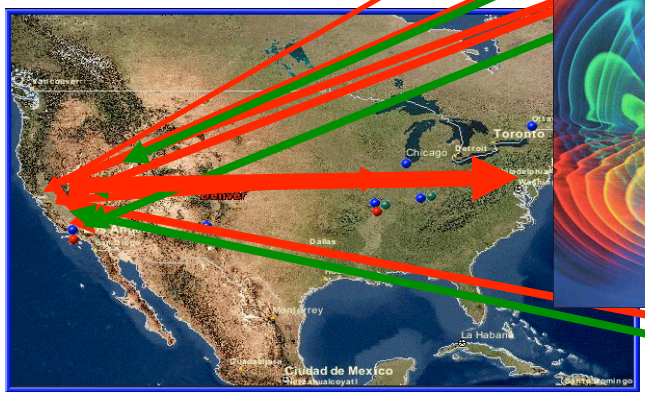

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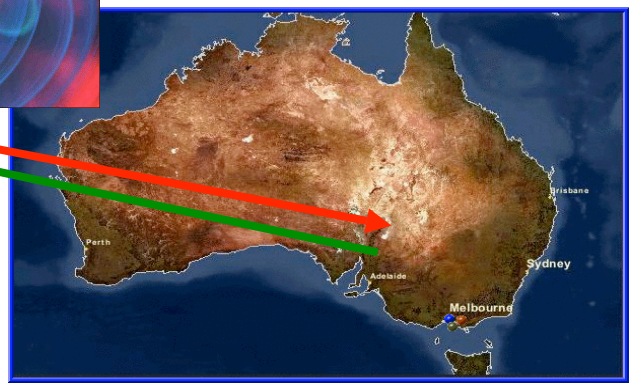

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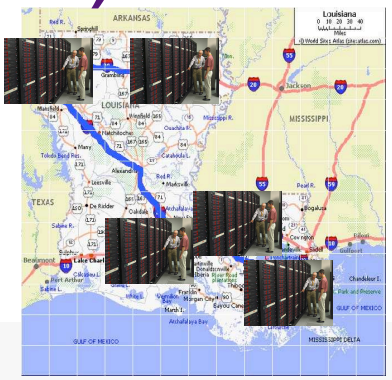
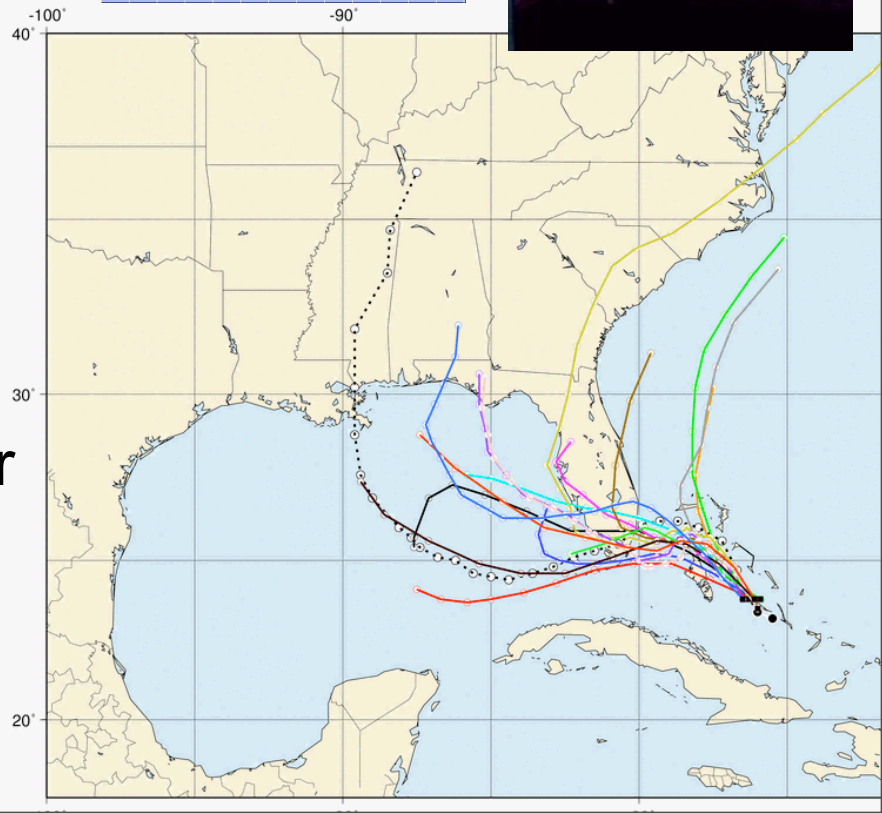
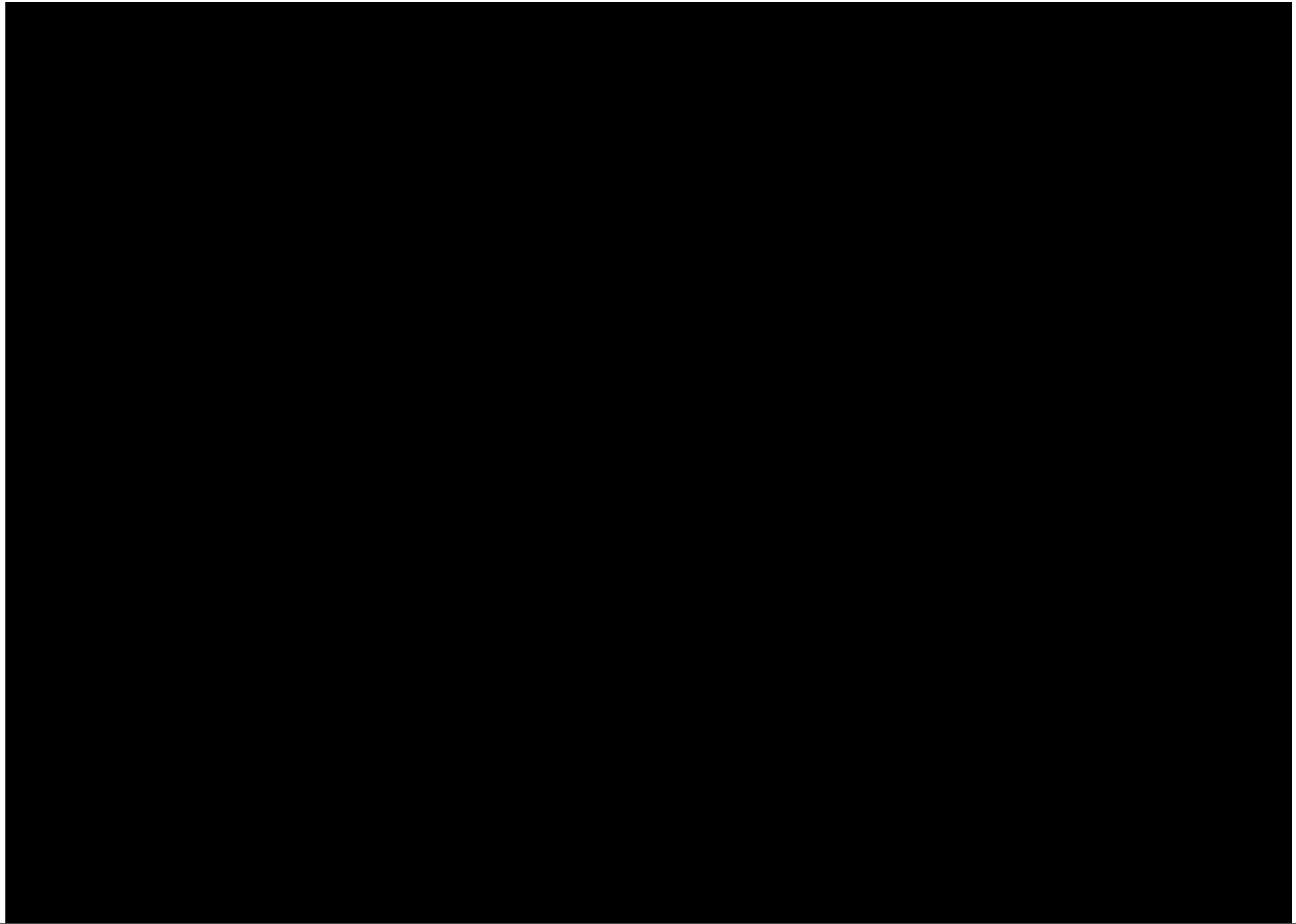
Huge job generates remote data to be visualized in Baltimore

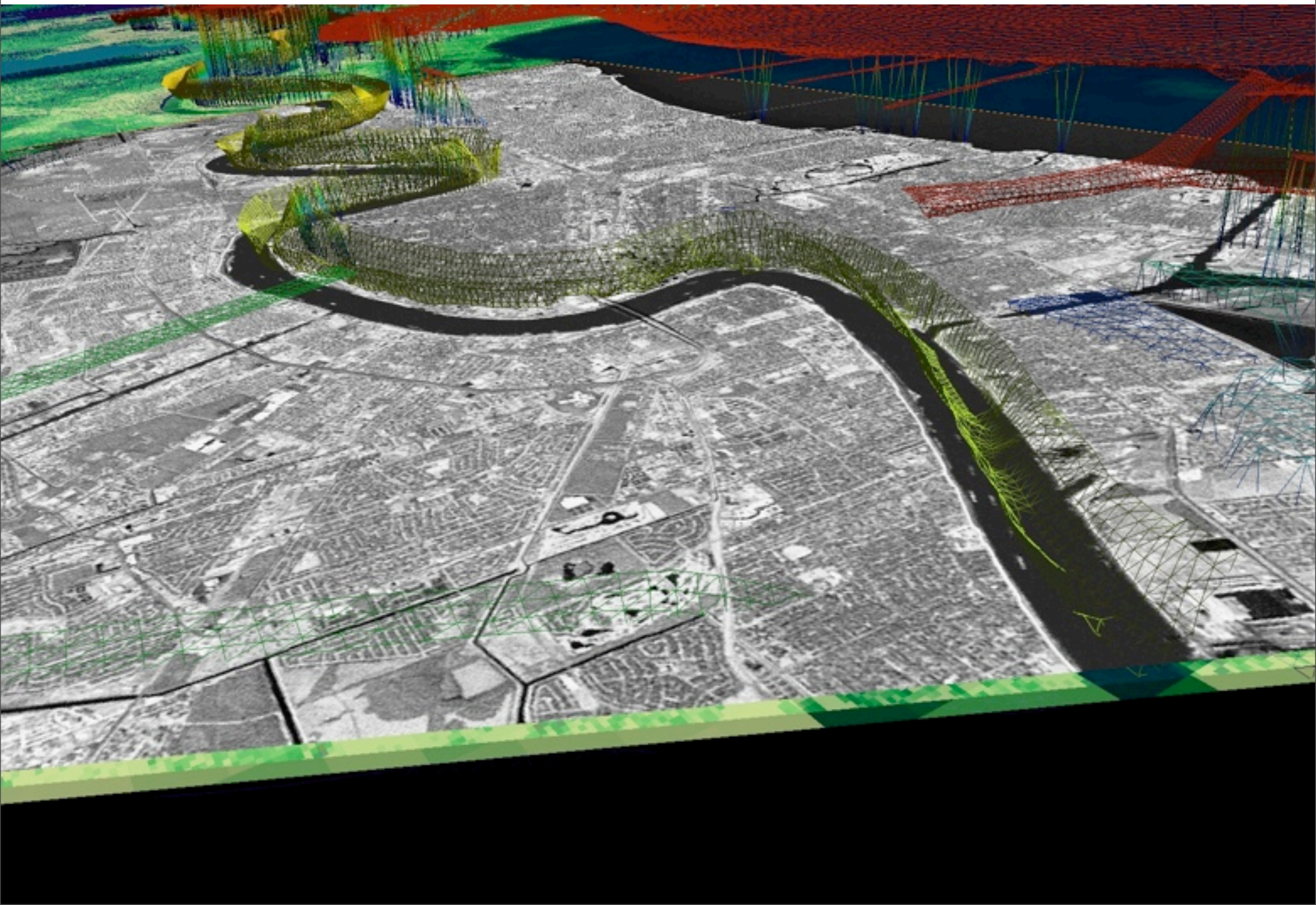
DDDAS Scenarios (Gabrielle Allen)

- UCoMS (Petroleum Engineering)
  - Deploy sensor networks across Gulf
  - Data collected to provide input to simulations, tasks farmed out
  - Results collected (transmitted back)
  - http://www.ucoms.org
- SCOOP, DynaCode (Coastal Modeling)
  - Data coming in from sensors all over Gulf Realtime Operational Grid
  - Feeds in to models on Grid sites
  - Algorithms invoked dynamically

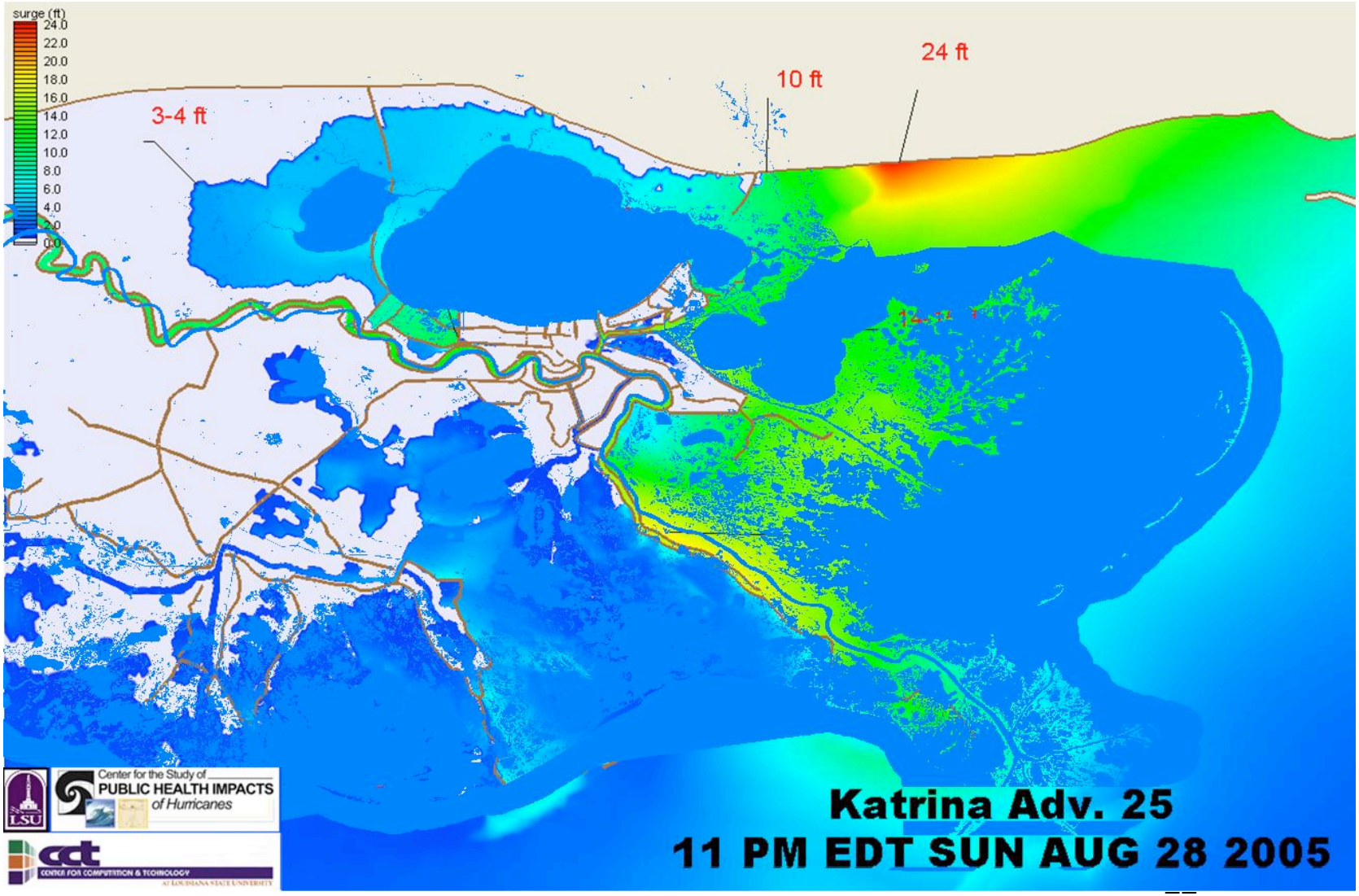




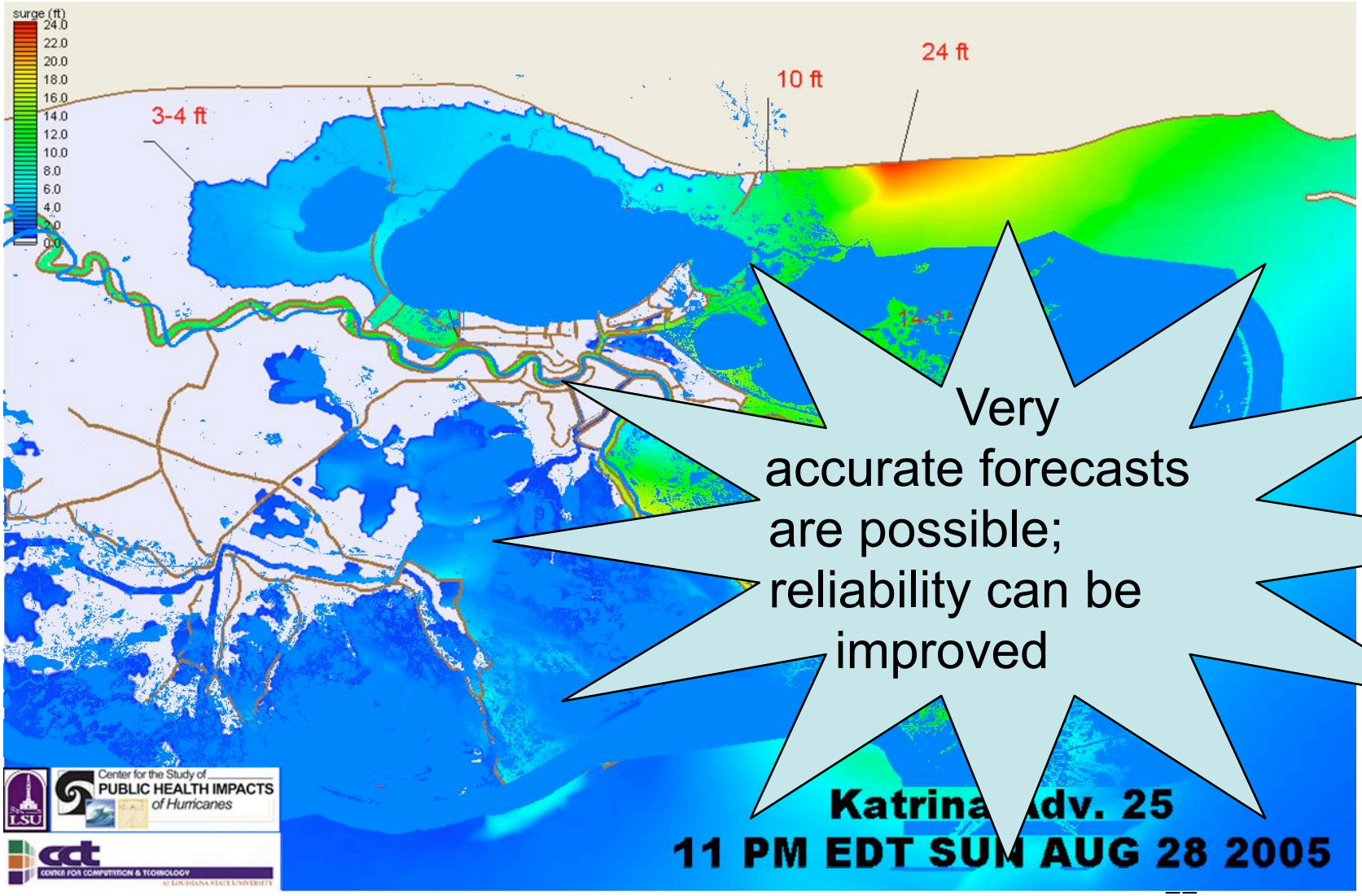




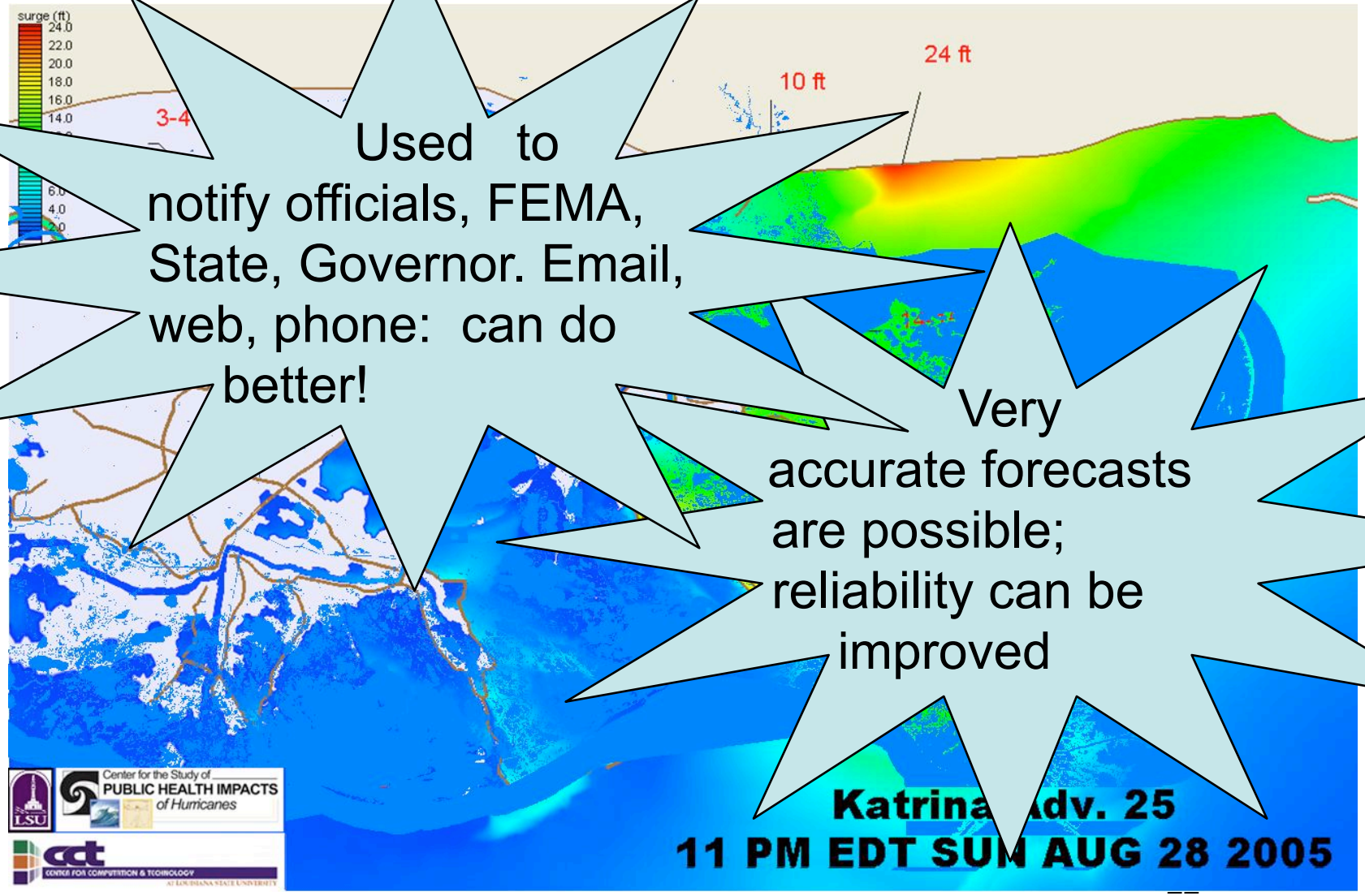
Emergency Forecast



Emergency Forecast

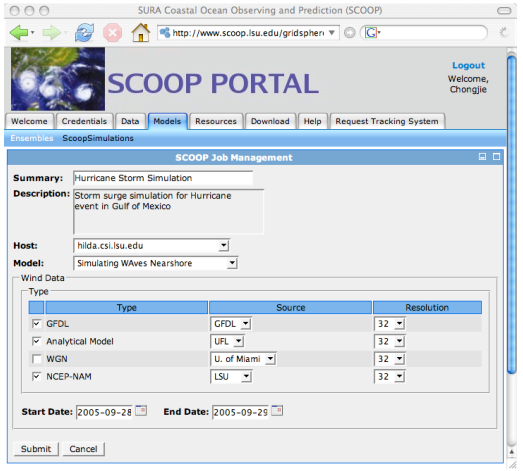


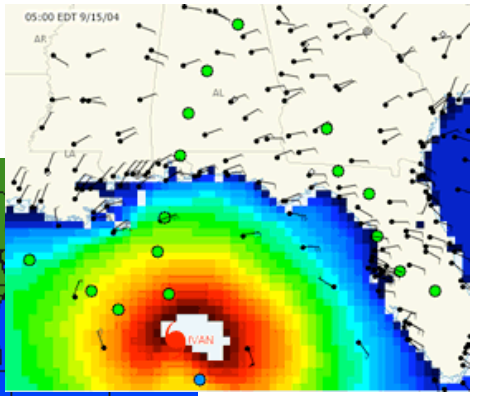
Emergency Forecast



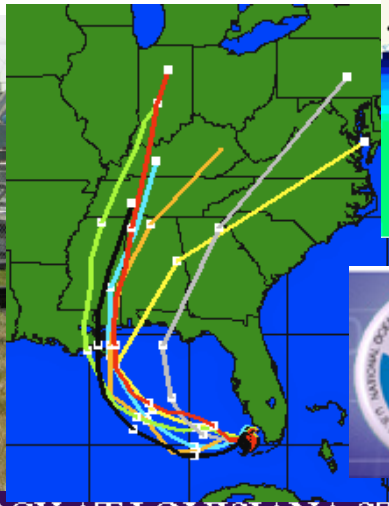
SURA Coastal Ocean Observing Program (SCOOP)

- Integrating data from regional observing systems for realtime coastal forecasts in SE
- Coastal modelers, computer scientists
  - couple models
  - provide data solutions
  - deploy ensembles of models on the Grid
  - assemble realtime results with GIS



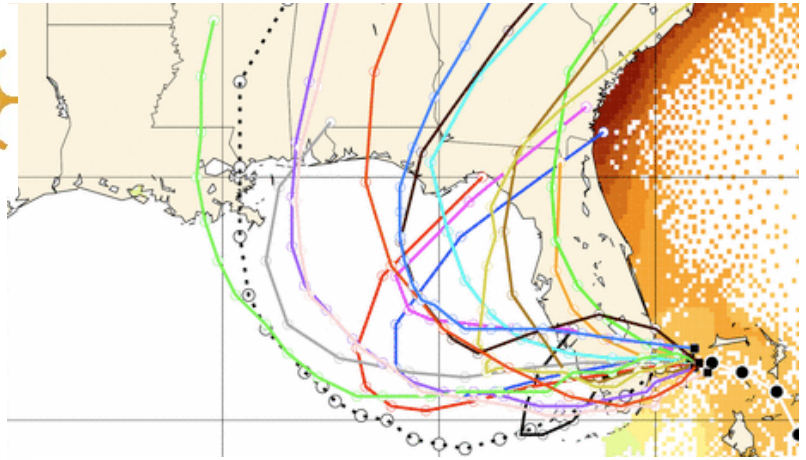


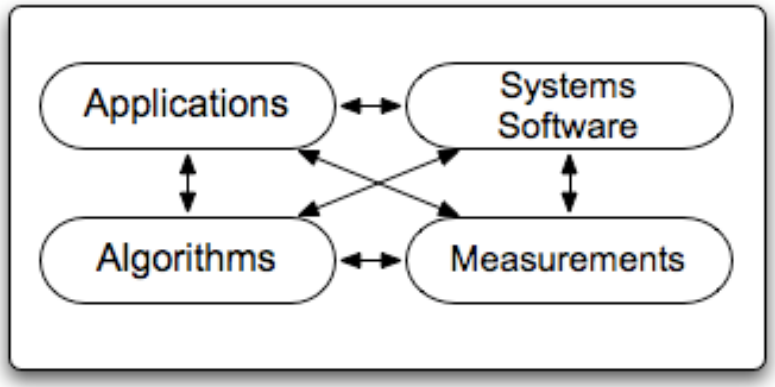
University of Alabama at Huntsville, University of Florida, GoMOOS, Louisiana State University, University of Miami, University of Maryland, University of North Carolina, Texas A&M, Virginia Inst of Marine Sciences



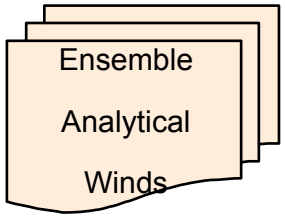
DynaCode

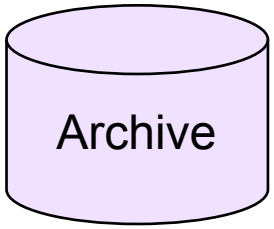
- Focus on scenarios:
  - Hurricane ensemble modeling
    - Coupling ocean circulation, storm surge, wave generation models for the Gulf
    - Notifications from NHC trigger customized ensemble hurricane models (surge/wind/wave), sensors verify, guide dynamic ensembles
    - Event driven, dynamic component framework with algorithm selection, optimization tools, workflow, data assimilation, result validation with sensor/satellite.
  - Ecological restoration and control
    - Breton Sound diversion, control structure to allow Mississippi to flow into wetlands
    - Coupled models (hydrodynamic, salinity, geomorphic, sediment) control diversion, sensors/wind fields inject real time data.





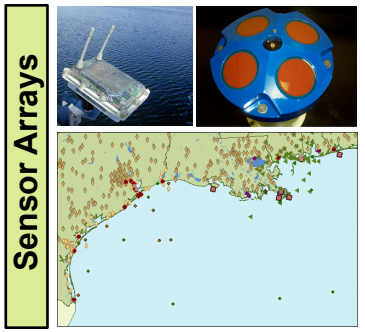
Dynamic, Event Driven Computing





Application Manager

Data Assimilator



Dynamic, Event Driven Computing

Event Driven!

Ensemble

Analytical

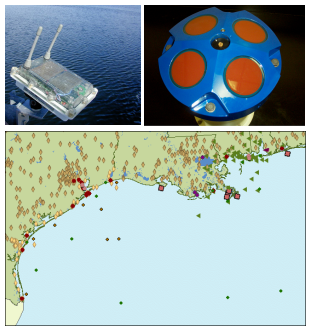
Winds

Archive

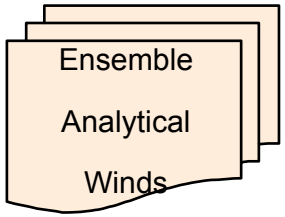
Application Manager

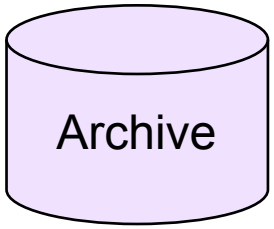
Data Assimilator

Sensor Arrays



Dynamic, Event Driven Computing





Application Manager

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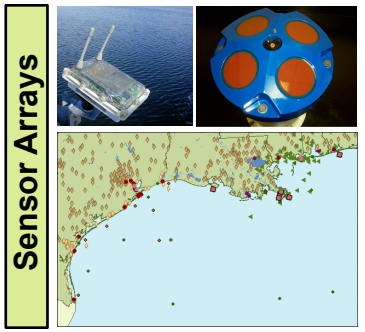

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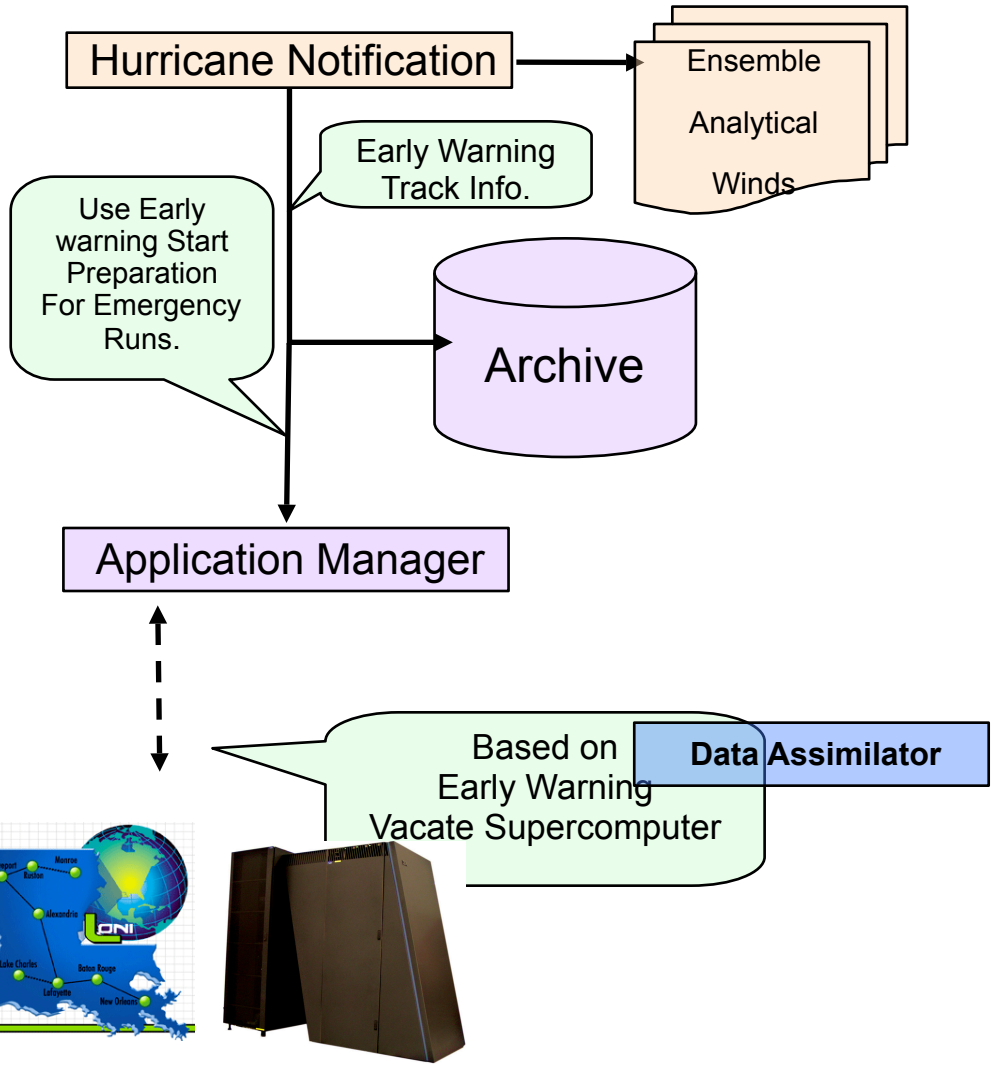
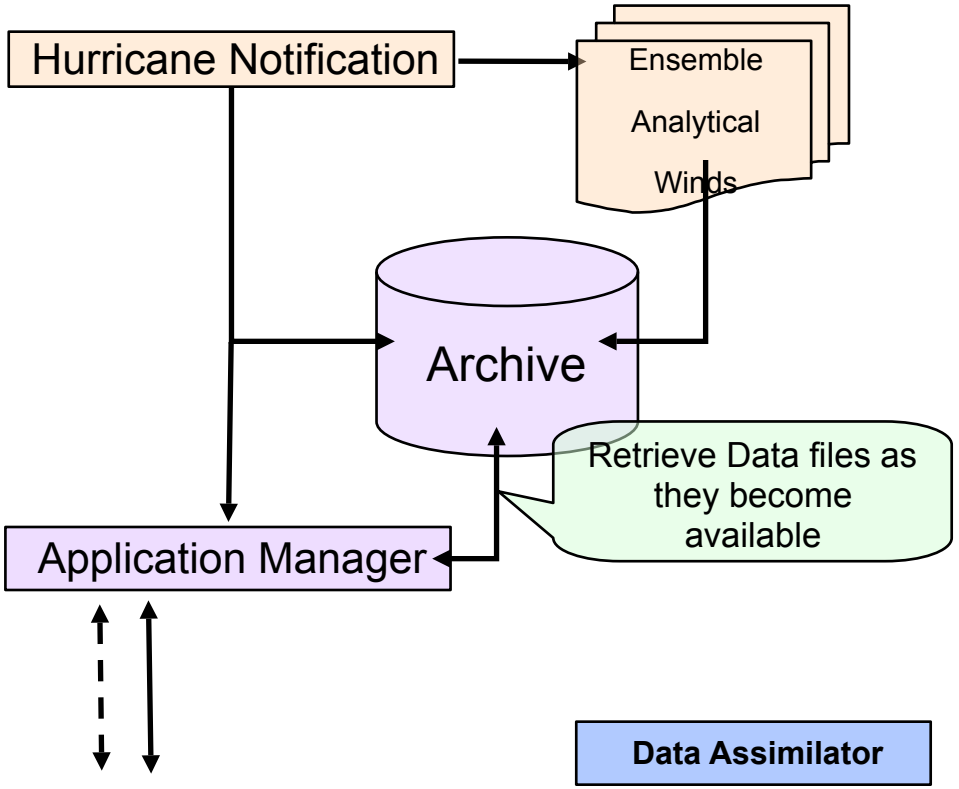
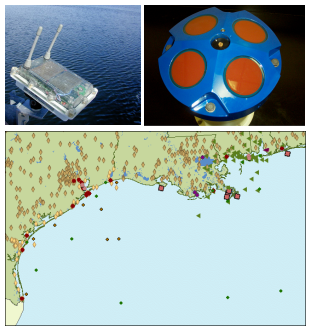


Dynamic, Event Driven Computing



Data Assimilator

Sensor Arrays



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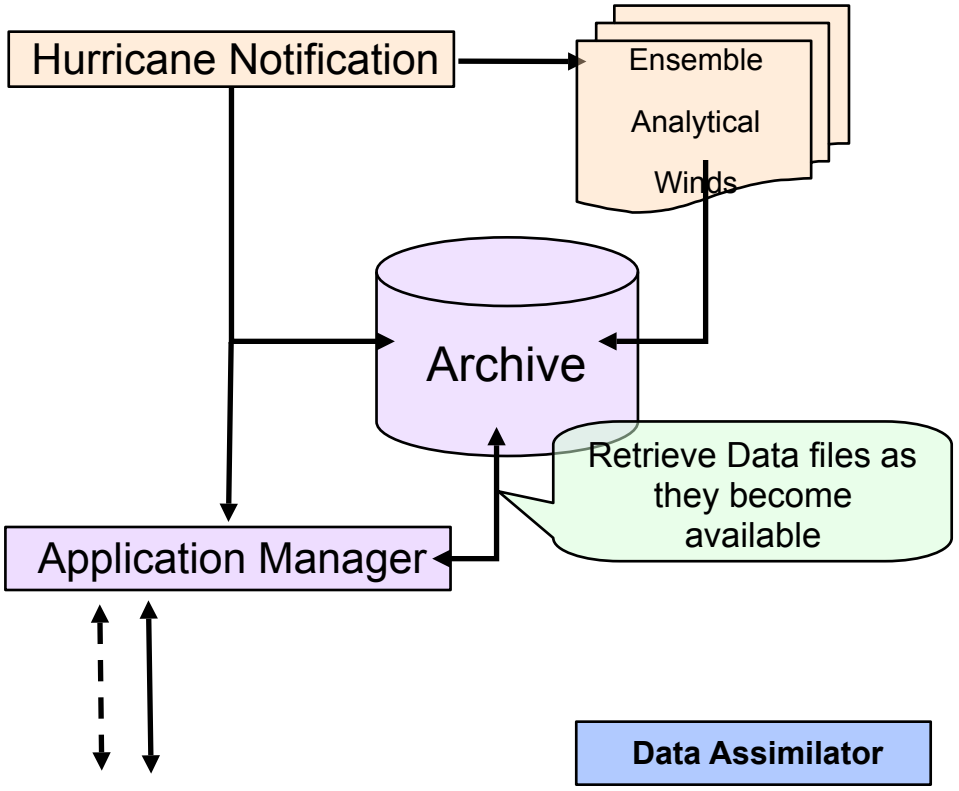

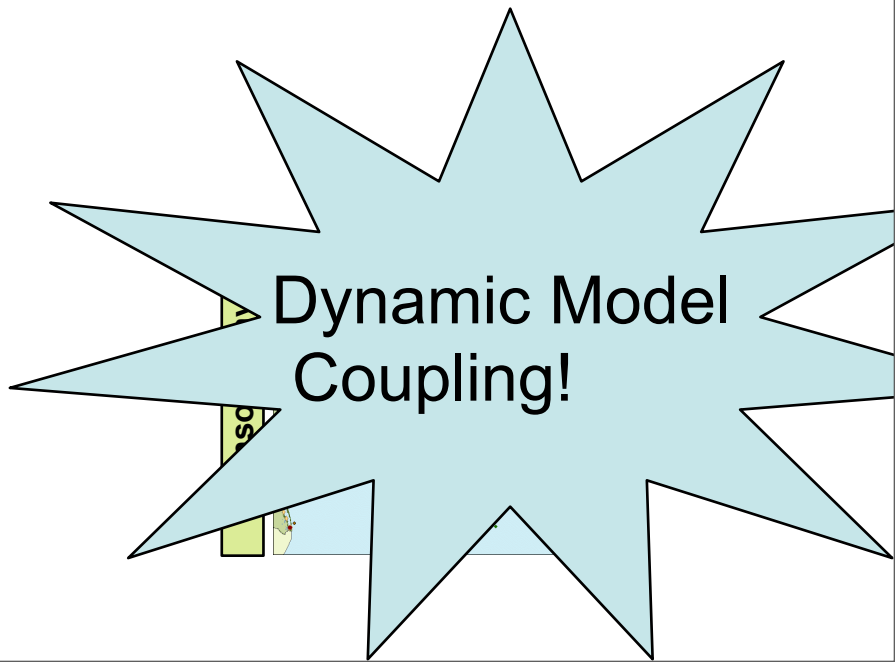

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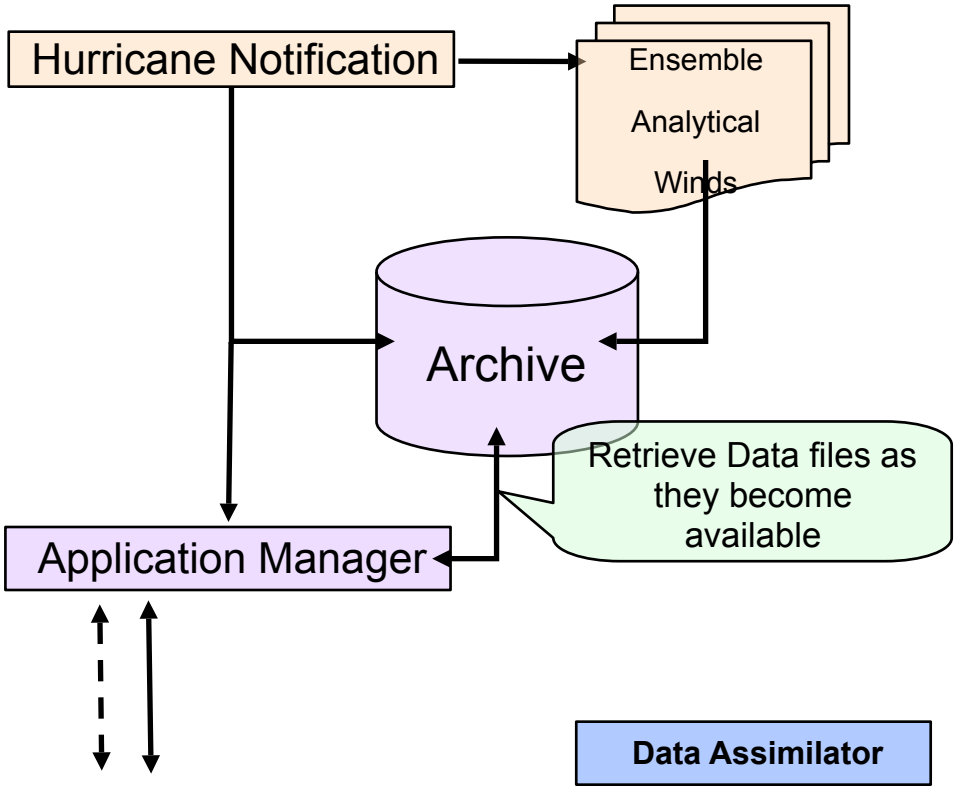

Data Assimilator

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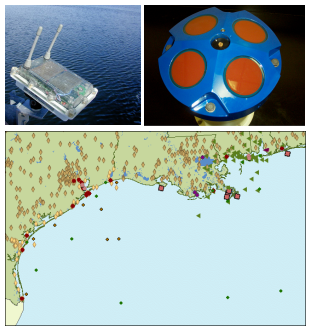

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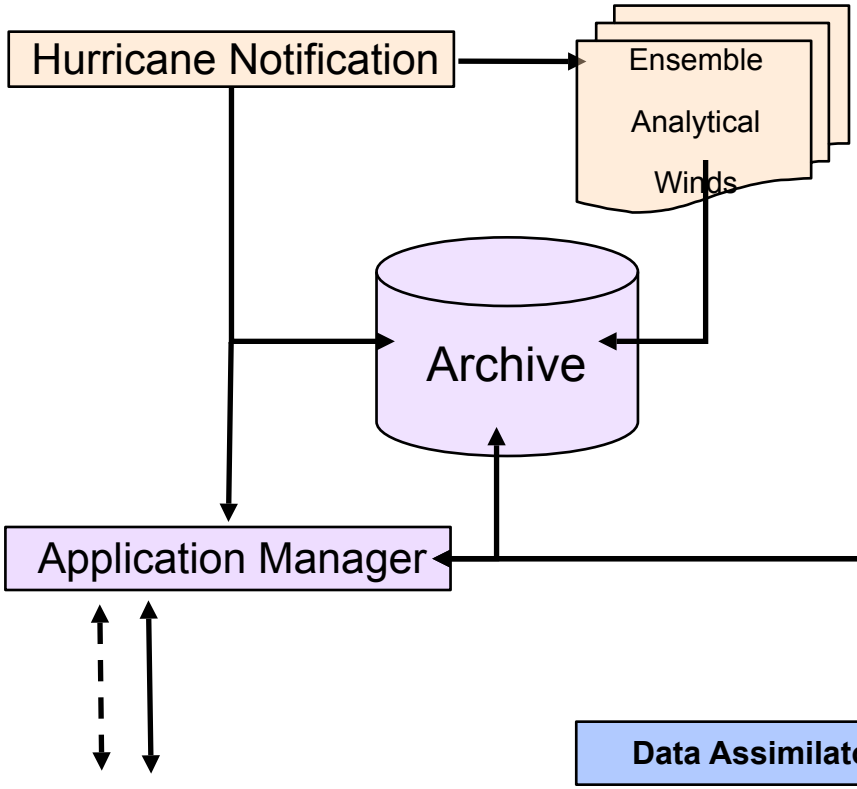
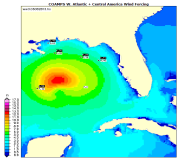
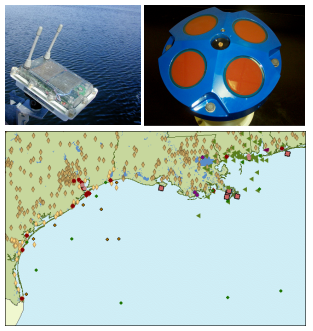




Data Assimilator

Sensor Arrays



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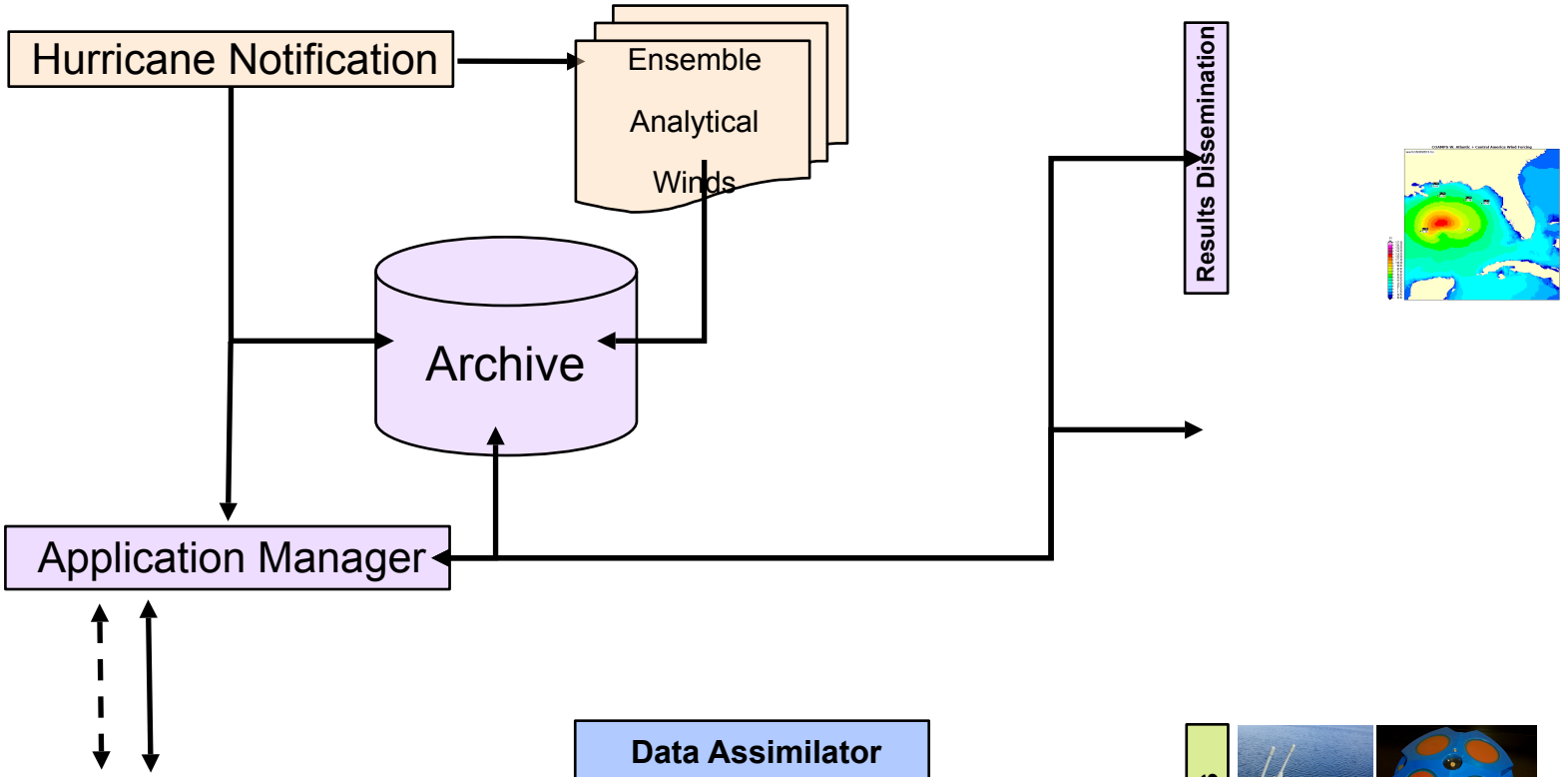

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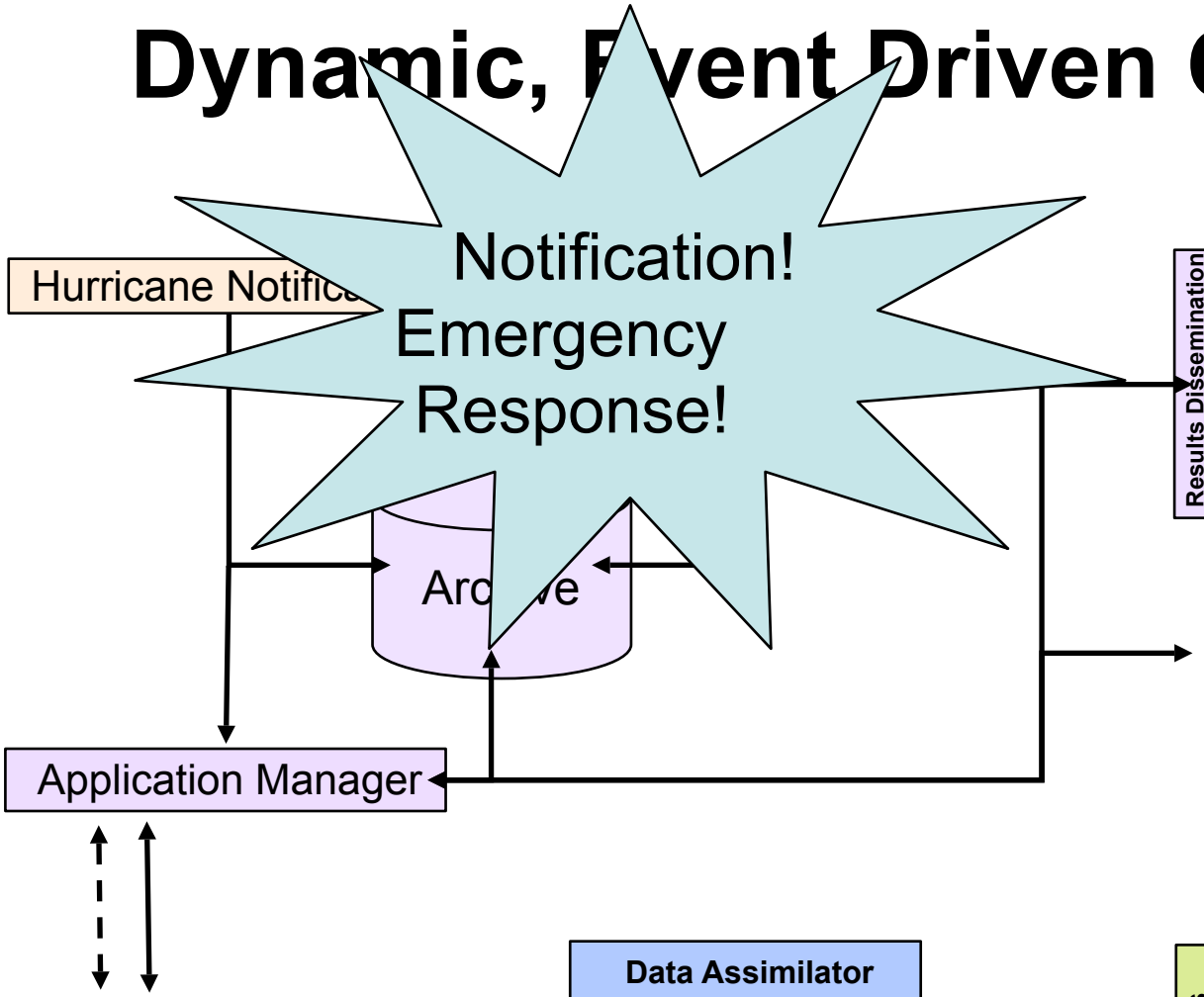
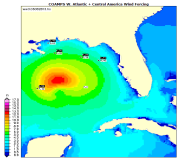
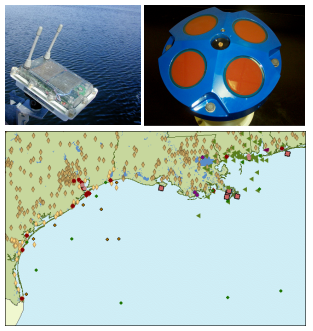




Data Assimilator

Sensor Arrays



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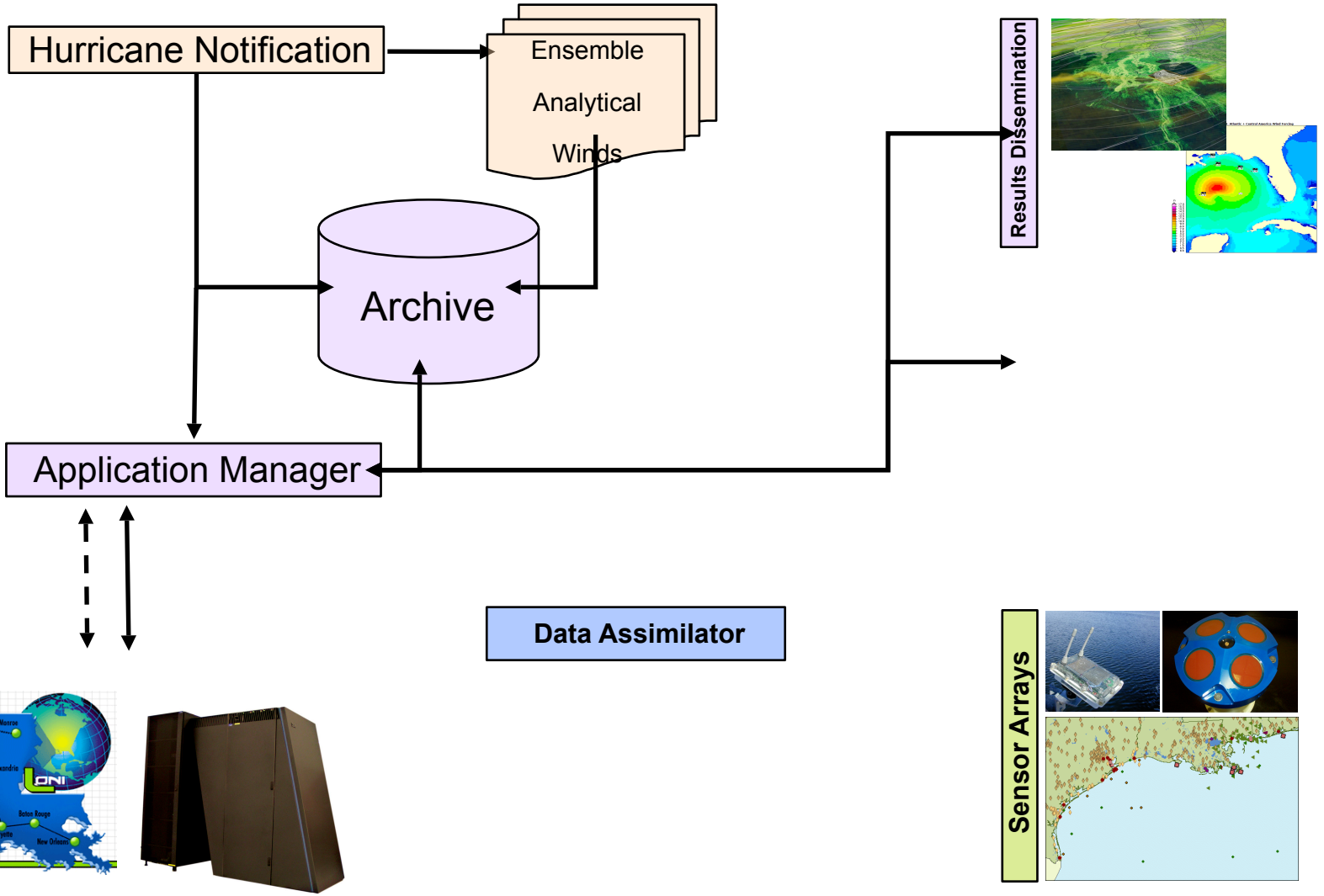

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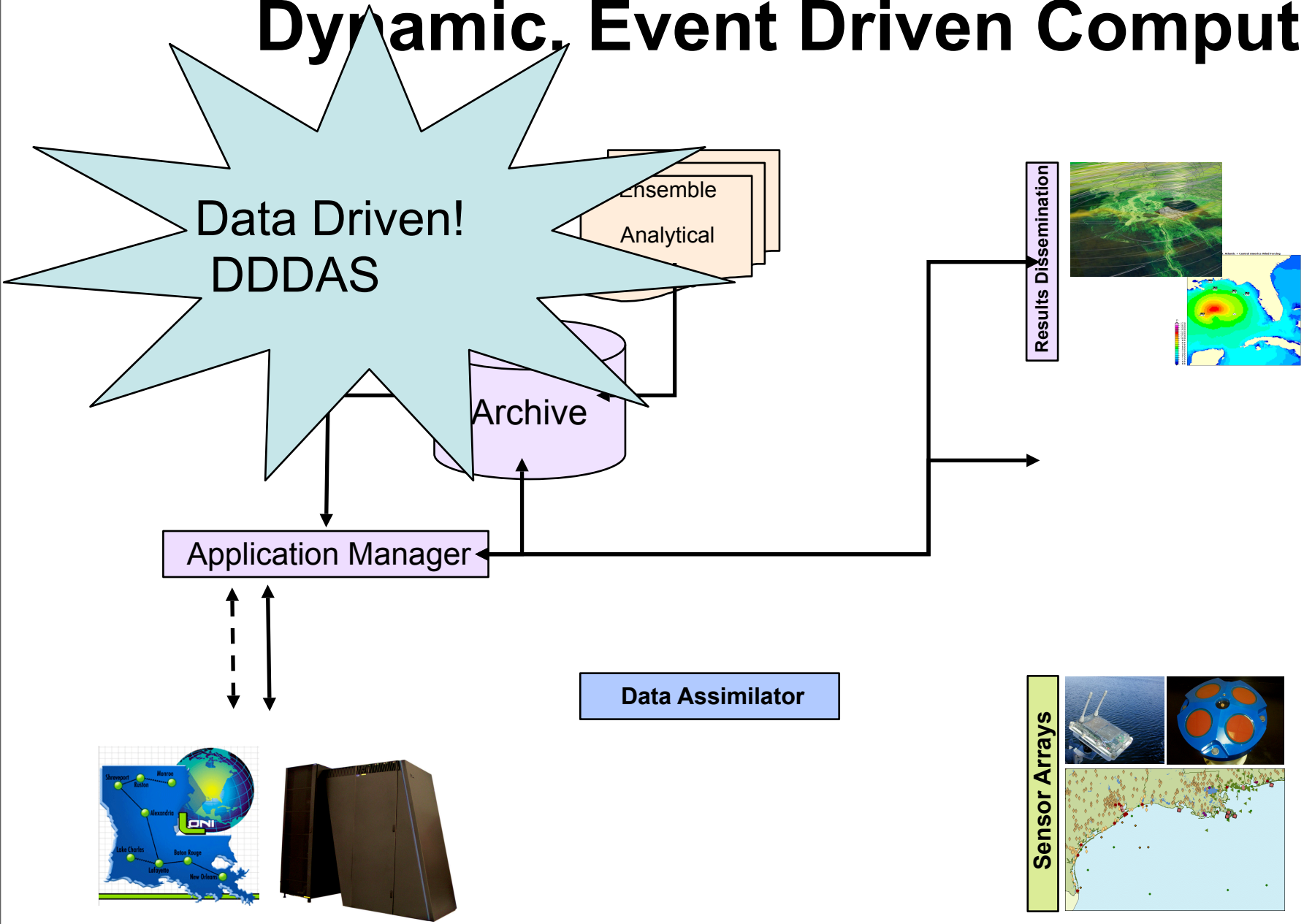
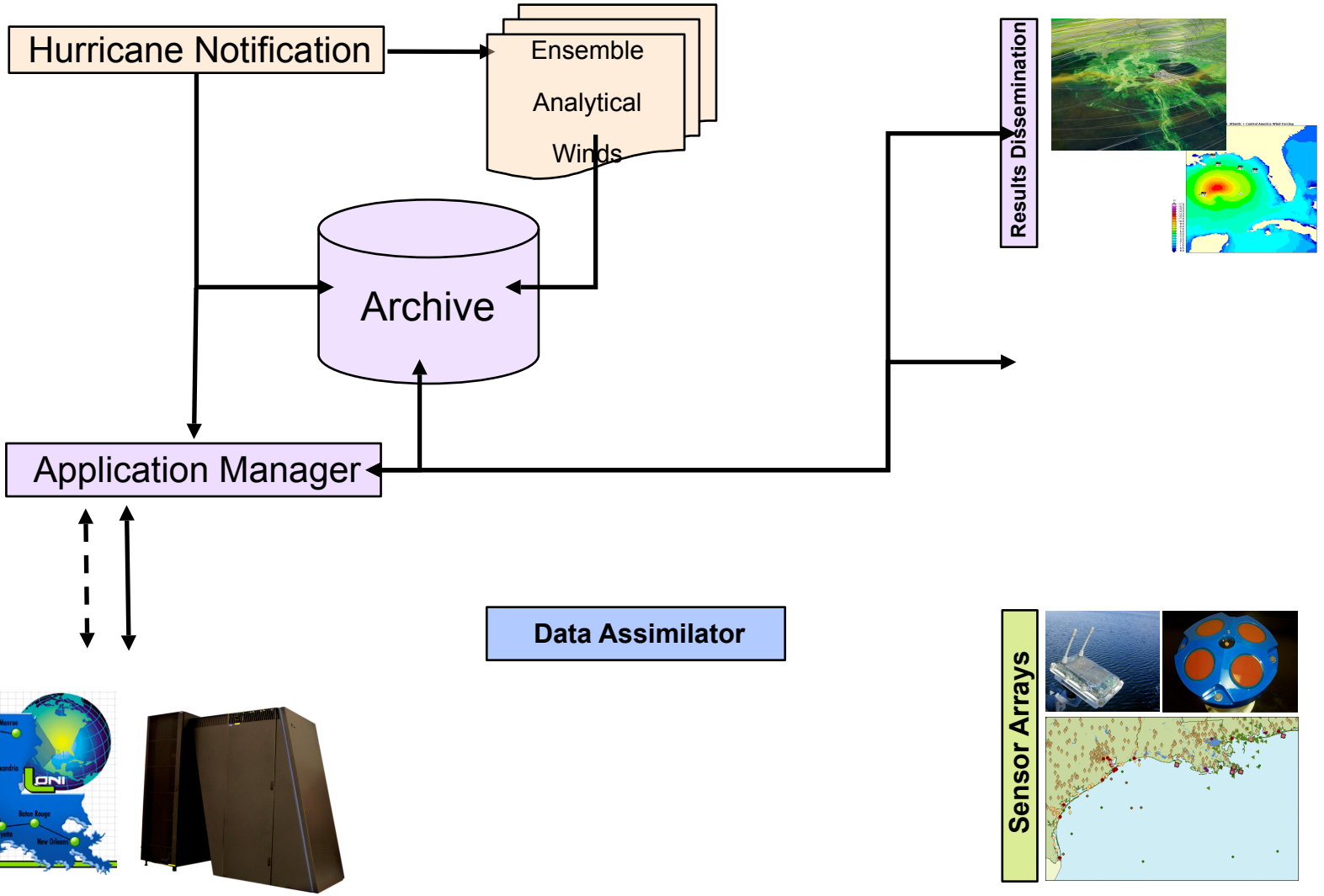


Dynamic, Event Driven Computing



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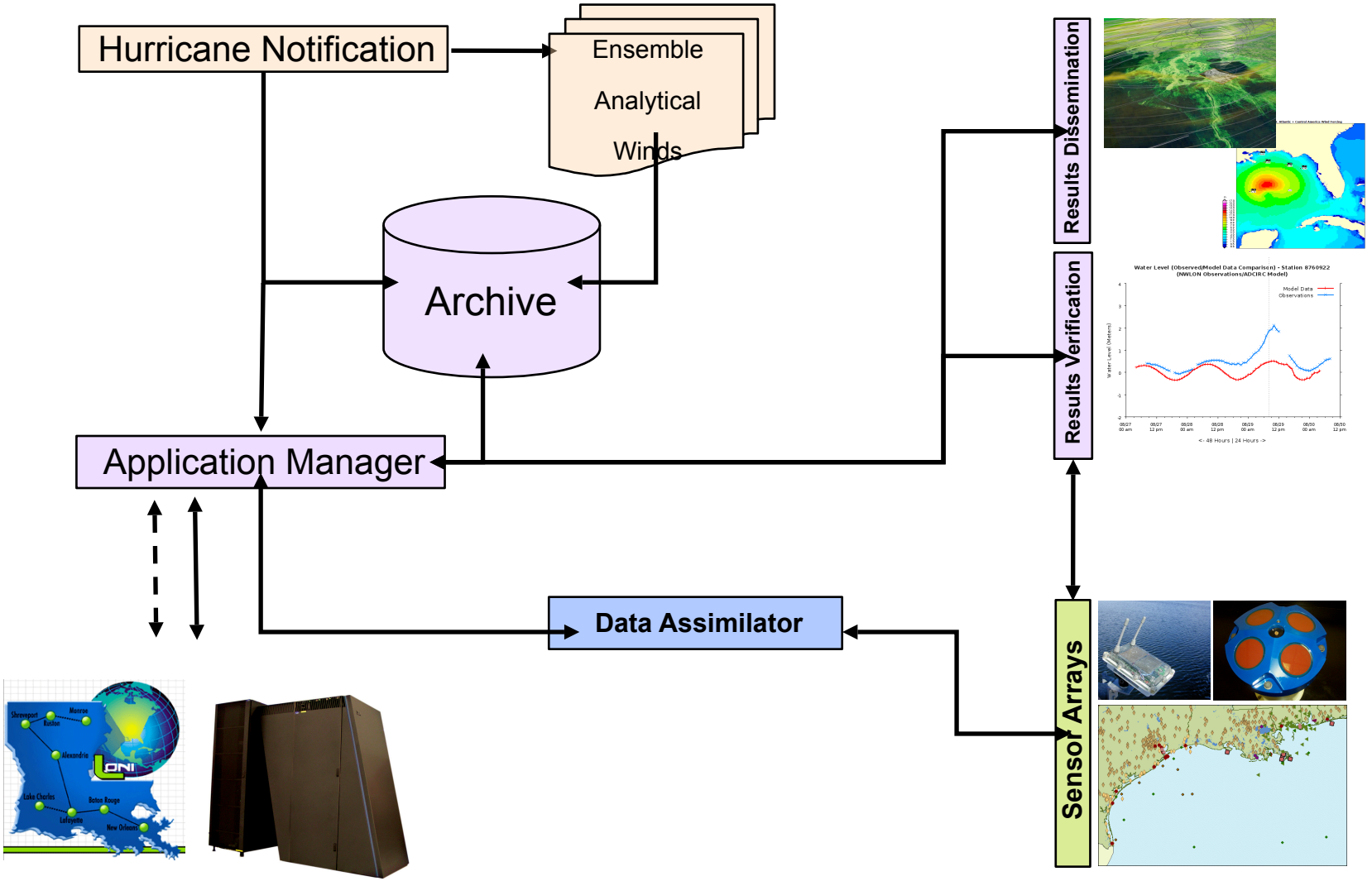
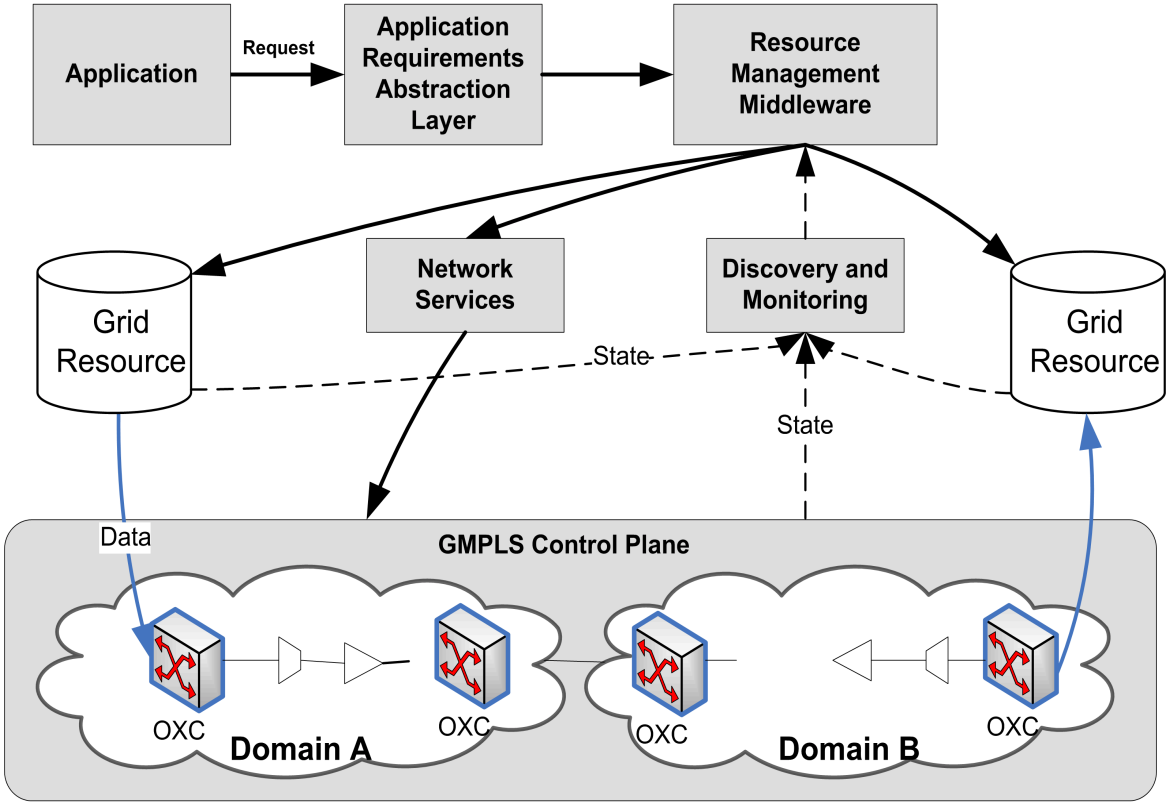


enλIGHTened computing

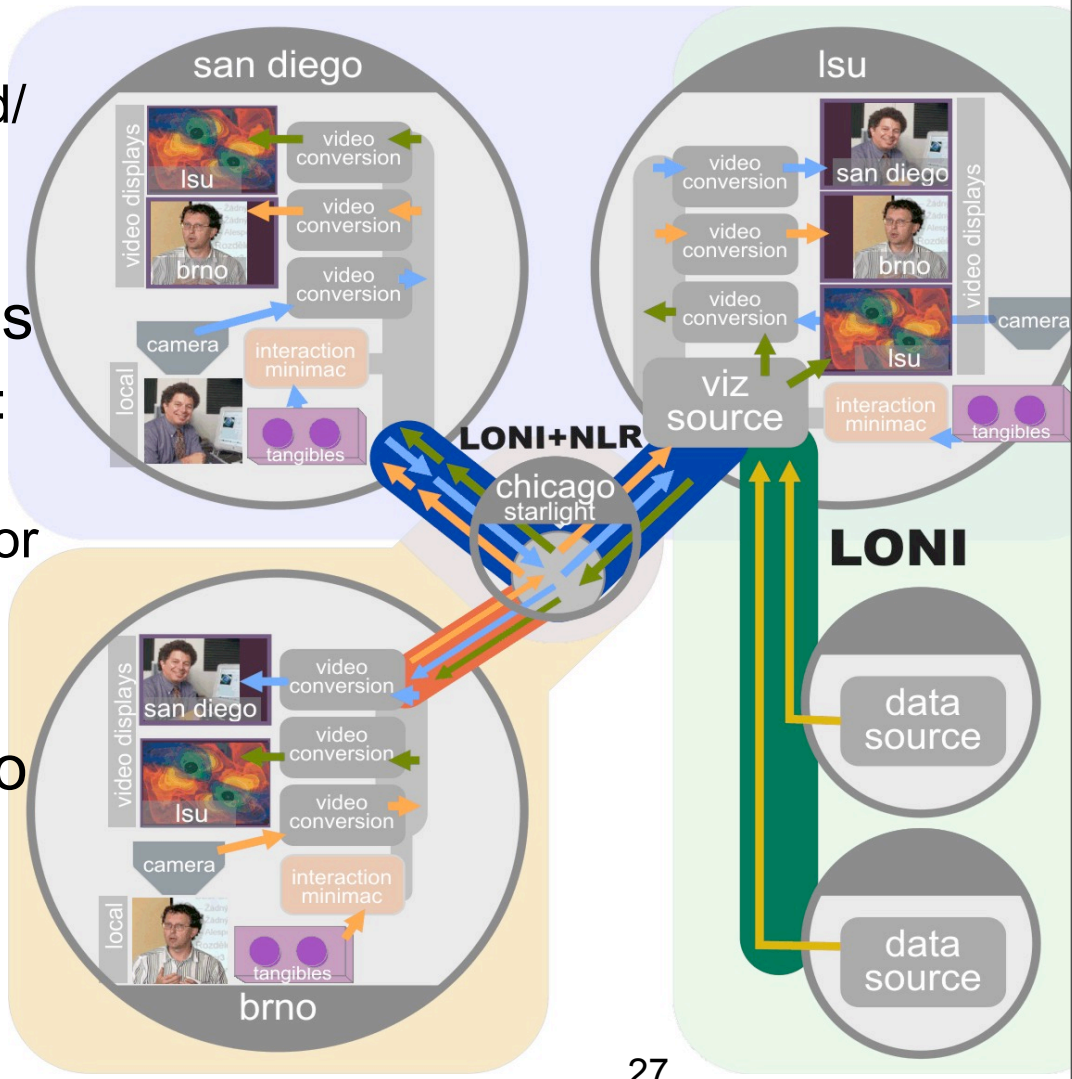
- Coordinated use of compute and network resources
- Define the network through the set of services that it can offer

- MCNC (lead), LSU, RENCI, NCSU, Cisco, AT&T, Calient Networks
- 10Gig capacity testbed running over LONI and NLR



iGrid 2005
Distributed, Collaborative, Viz

- Scenario
  - TBs data, must be interactively viz'd/ analyzed by international collaboration
- Distributed Data and Viz Services
  - Data larger than memory, disk slow: streaming data servers
  - Co-scheduling machines, network for collaborative event
  - Lambda Provisioning
- High Resolution: not science w/o details, analysis
  - Uncompressed HD stream: near latency-free remote viz at 1.5Gbit
  - Video for colleagues

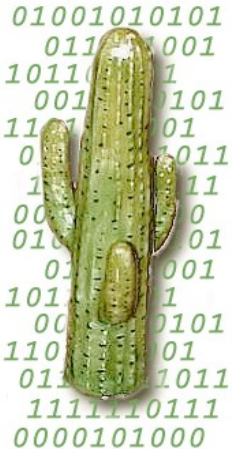


All Require a Common Infrastructure

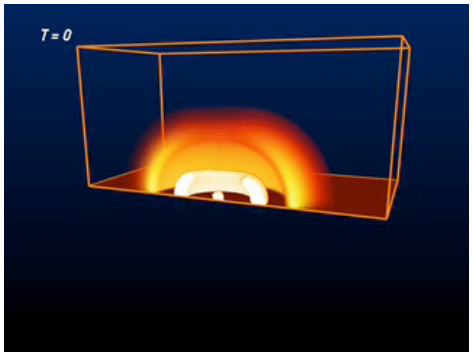
- Common Needs Driven by the Science/Engineering
  - Large Number of Sensors / Instruments
  - Daily Generation of Large Data Sets
  - Data is on Multiple Length and Time Scales
  - Automatic Archiving in Distributed Federated Repositories
  - Large Community of End Users
  - Multi-Megapixel and Immersive Visualization
  - Collaborative Analysis From Multiple Sites
  - *Complex Simulations Needed to Interpret Data*
- Will need Optical Networks
  - Communications → Dedicated Lambdas
  - Data → Large Peer-to-Peer Lambda Attached Storage
  - FAQ: Will usage policies allow scientists to use them?

Source: Smarr

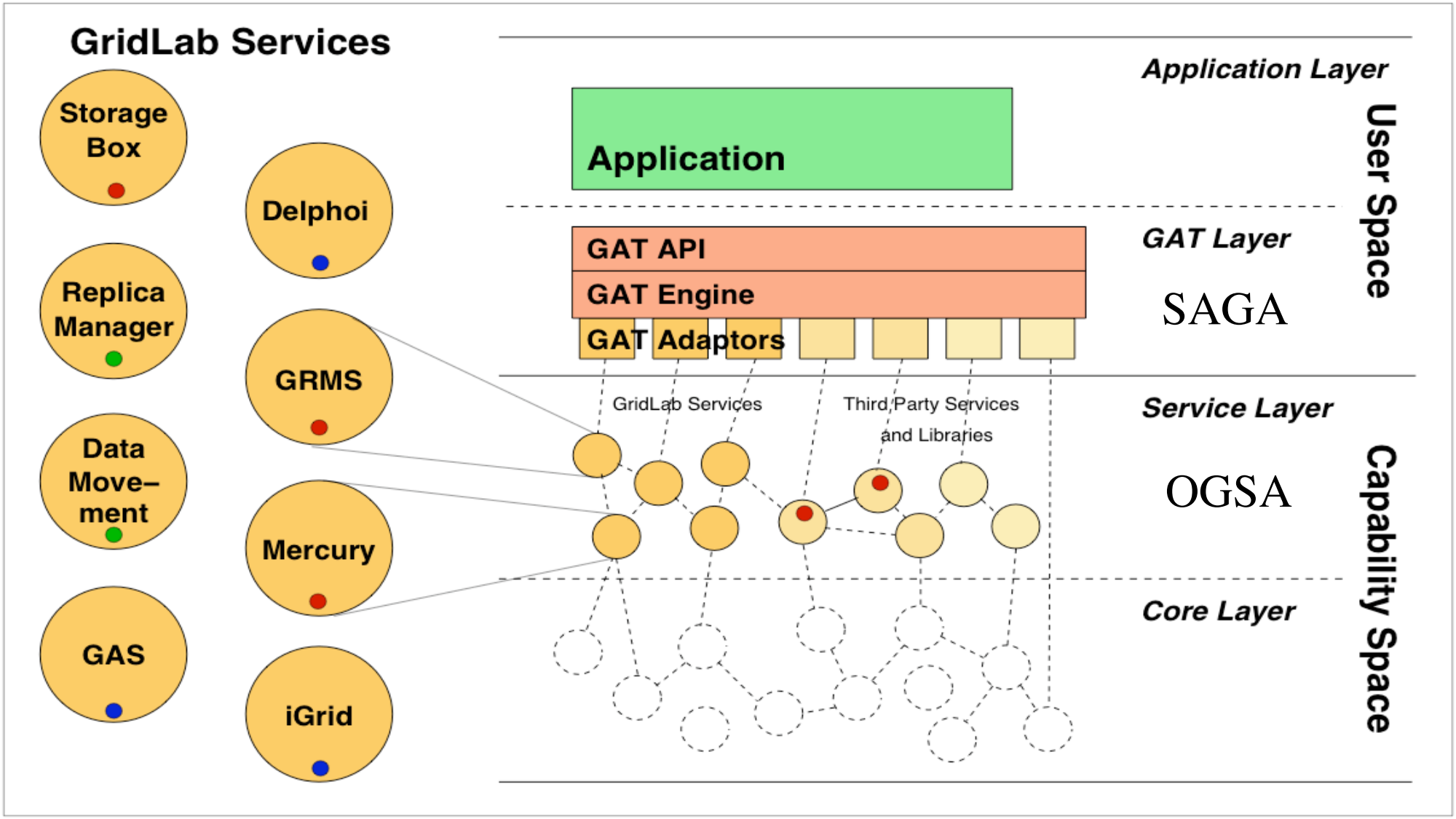
Developing Advanced Applications on Grids



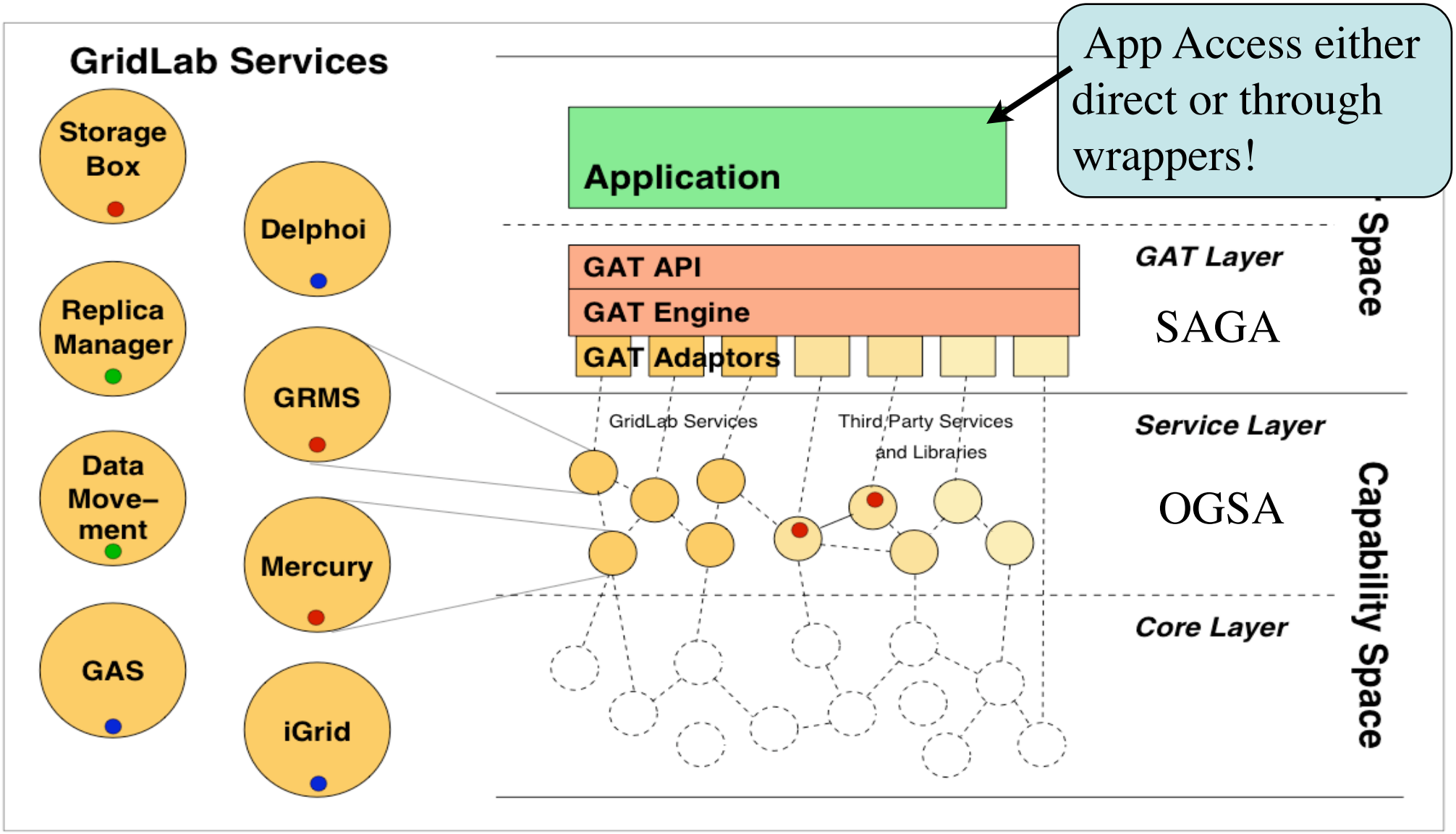
GridLab



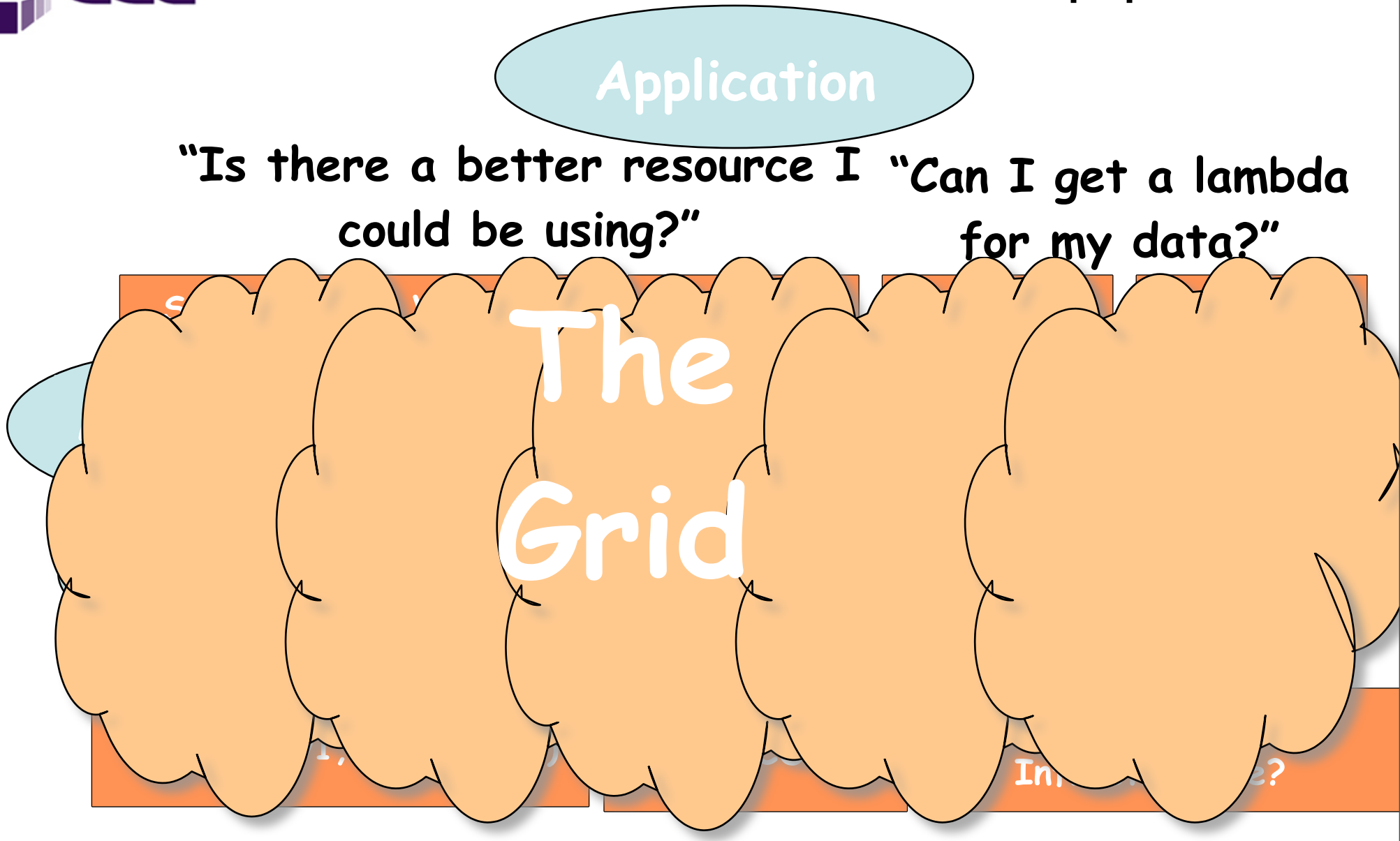
GridLab Architecture



GridLab Architecture



How to build Grid Apps?



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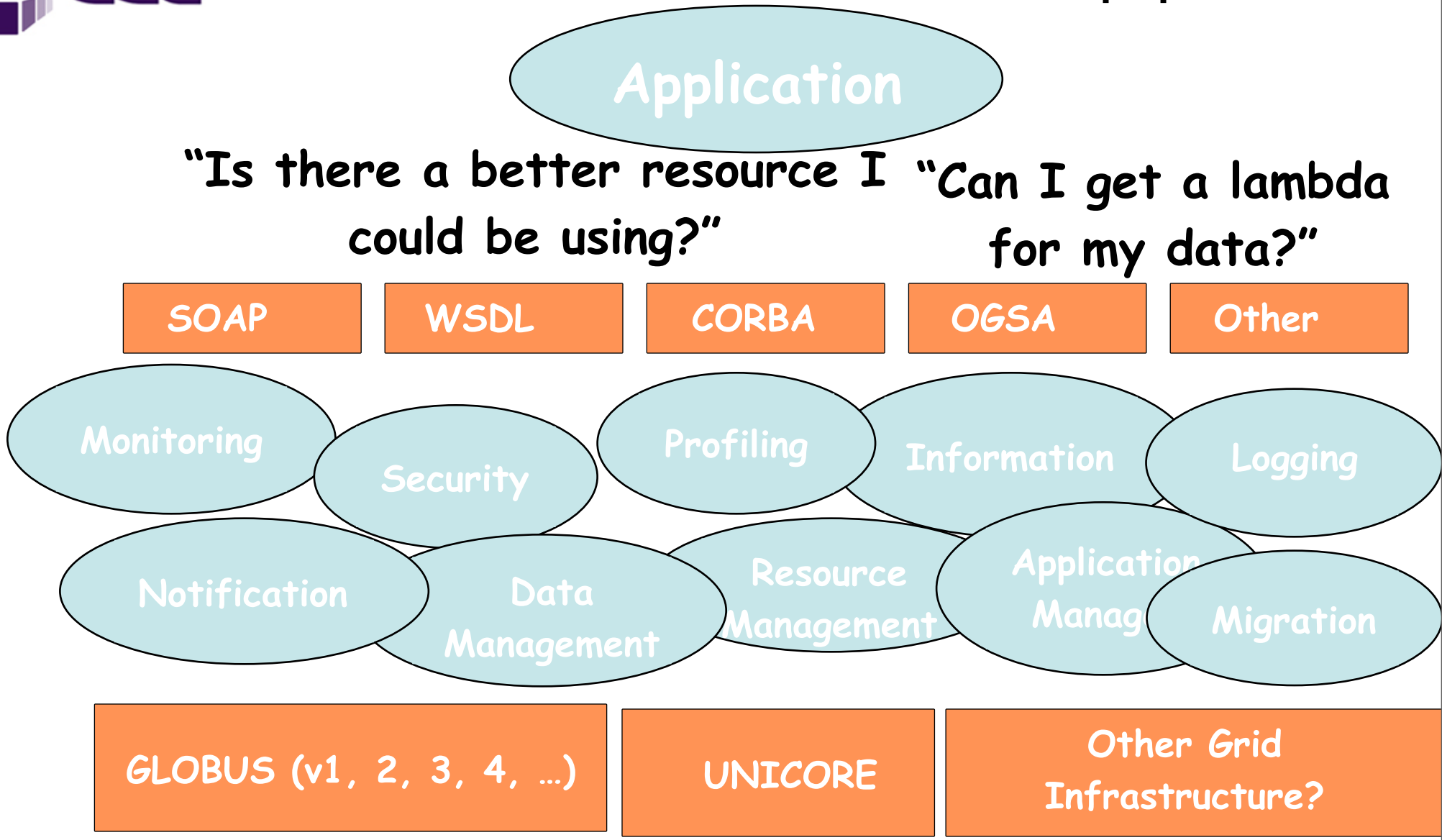
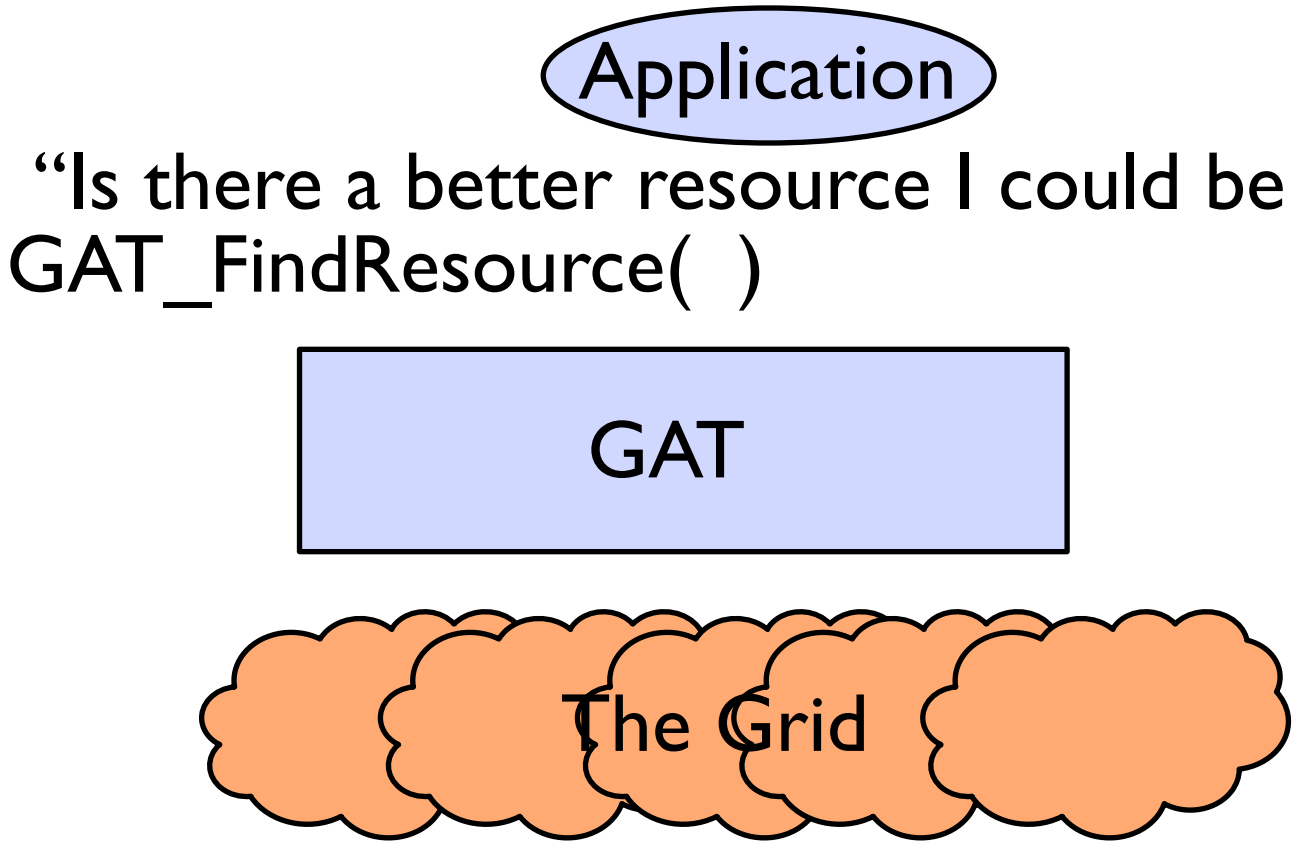
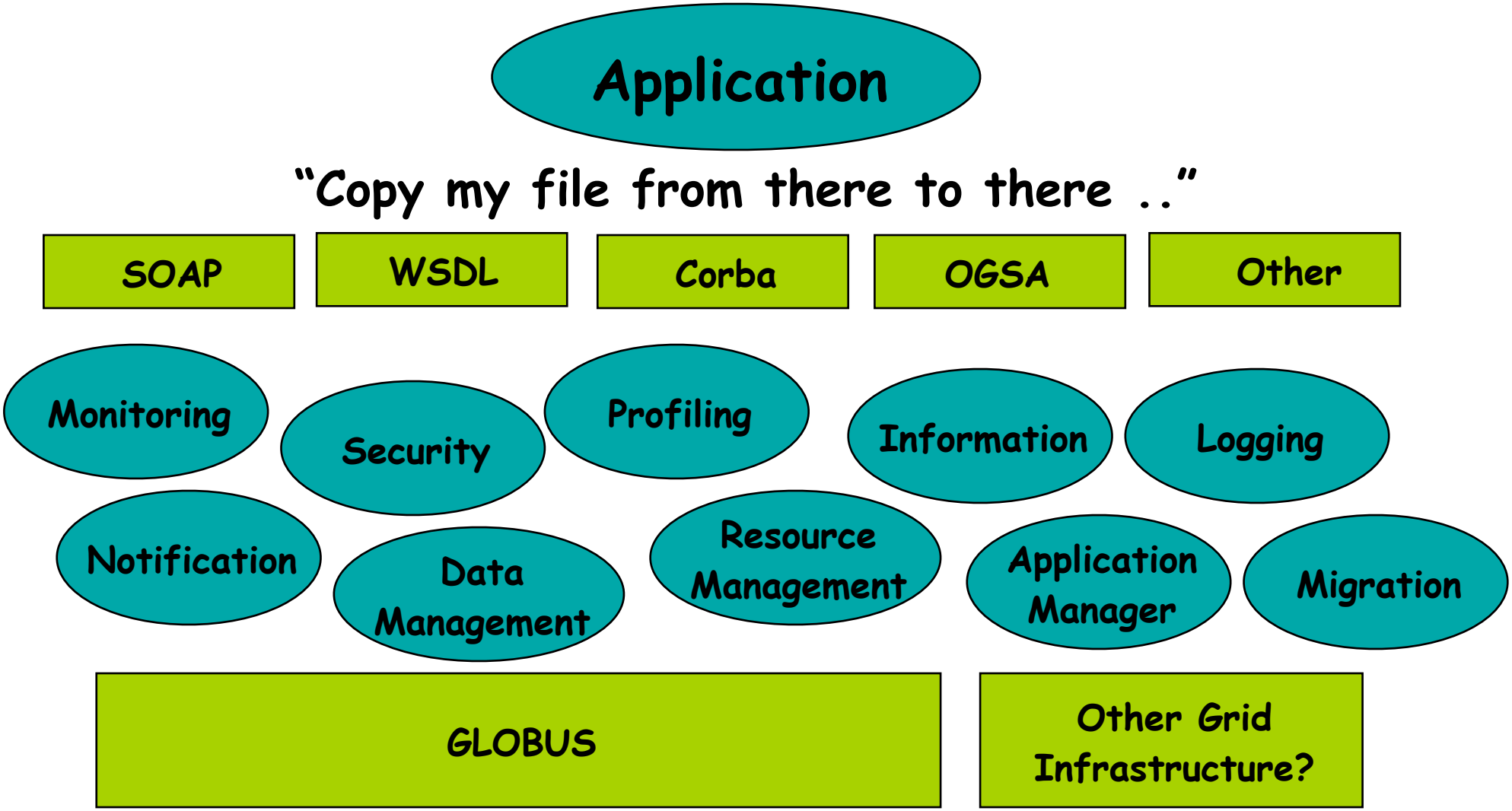


Hiding Complexity with Toolkits



Example: Remote File Copying



Copy a File: GASS

```
int RemoteFile::GetFile (char const* source,
                         char const* target) {
globus_url_t                        source_url;
globus_io_handle_t                  dest_io_handle;
globus_ftp_client_operationattr_t   source_ftp_attr;
globus_result_t                     result;
globus_gass_transfer_requestattr_t  source_gass_attr;
globus_gass_copy_attr_t             source_gass_copy_attr;
globus_gass_copy_handle_t           gass_copy_handle;
globus_gass_copy_handleattr_t       gass_copy_handleattr;
globus_ftp_client_handleattr_t      ftp_handleattr;
globus_io_attr_t                    io_attr;
int                                 output_file = -1;

if ( globus_url_parse (source_URL, &source_url) != GLOBUS_SUCCESS ) {
  printf ("can not parse source_URL \"%s\"\n", source_URL);
  return (-1);
}

if ( source_url.scheme_type != GLOBUS_URL_SCHEME_GSIFTP &&
     source_url.scheme_type != GLOBUS_URL_SCHEME_FTP    &&
     source_url.scheme_type != GLOBUS_URL_SCHEME_HTTP   &&
     source_url.scheme_type != GLOBUS_URL_SCHEME_HTTPS  ) {
  printf ("can not copy from %s - wrong prot\n", source_URL);
  return (-1);
}
globus_gass_copy_handleattr_init  (&gass_copy_handleattr);
globus_gass_copy_attr_init        (&source_gass_copy_attr);

globus_ftp_client_handleattr_init (&ftp_handleattr);
globus_io_fileattr_init           (&io_attr);

globus_gass_copy_attr_set_io      (&source_gass_copy_attr, &io_attr);
                                   &io_attr);
globus_gass_copy_handleattr_set_ftp_attr
                                  (&gass_copy_handleattr,
                                   &ftp_handleattr);
globus_gass_copy_handle_init      (&gass_copy_handle,
                                   &gass_copy_handleattr);

if (source_url.scheme_type == GLOBUS_URL_SCHEME_GSIFTP ||
    source_url.scheme_type == GLOBUS_URL_SCHEME_FTP    ) {
  globus_ftp_client_operationattr_init (&source_ftp_attr);
  globus_gass_copy_attr_set_ftp (&source_gass_copy_attr,
                                 &source_ftp_attr);
}
else {
  globus_gass_transfer_requestattr_init (&source_gass_attr,
                                         source_url.scheme);
  globus_gass_copy_attr_set_gass(&source_gass_copy_attr,
            &source_gass_attr);
}

output_file = globus_libc_open ((char*) target,
              O_WRONLY | O_TRUNC | O_CREAT,
              S_IRUSR  | S_IWUSR | S_IRGRP |
              S_IWGRP);
if ( output_file == -1 ) {
  printf ("could not open the file \"%s\"\n", target);
  return (-1);
}
/* convert stdout to be a globus_io_handle */
if ( globus_io_file_posix_convert (output_file, 0,
                                   &dest_io_handle)
     != GLOBUS_SUCCESS) {
  printf ("Error converting the file handle\n");
  return (-1);
}

result = globus_gass_copy_register_url_to_handle (
         &gass_copy_handle, (char*)source_URL,
         &source_gass_copy_attr, &dest_io_handle,
         my_callback, NULL);
if ( result != GLOBUS_SUCCESS ) {
  printf ("error: %s\n", globus_object_printable_to_string
          (globus_error_get (result)));
  return (-1);
}
globus_url_destroy  (&source_url);
return (0);
}
```

Copy a File: CoG/RFT

```
package org.globus.ogsa.gui;

import java.io.BufferedReader;
import java.io.File;
import java.io.FileReader;
import java.net.URL;
import java.util.Date;
import java.util.Vector;
import javax.xml.rpc.Stub;
import org.apache.axis.message.MessageElement;
import org.apache.axis.utils.XMLUtils;
import org.globus.*
import org.gridforum.ogsi.*
import org.gridforum.ogsi.holders.TerminationTimeTypeHolder;
import org.w3c.dom.Document;
import org.w3c.dom.Element;

public class RFTClient {
 public static void copy (String source_url, String target_url) {
  try {
   File requestFile      = new File (source_url);
   BufferedReader reader = null;
   try {
     reader = new BufferedReader (new FileReader (requestFile));
   } catch (java.io.FileNotFoundException fnfe) { }
   Vector requestData = new Vector ();
   requestData.add (target_url);
   TransferType[] transfers1      = new TransferType[transferCount];
   RFTOptionsType multirftOptions = new RFTOptionsType ();

   multirftOptions.setBinary          (Boolean.valueOf  (
         (String)requestData.elementAt (0)).booleanValue ());
   multirftOptions.setBlockSize       (Integer.valueOf  (
         (String)requestData.elementAt (1)).intValue     ());
   multirftOptions.setTcpBufferSize   (Integer.valueOf  (
         (String)requestData.elementAt (2)).intValue     ());
   multirftOptions.setNotpt           (Boolean.valueOf  (
         (String)requestData.elementAt (3)).booleanValue ());
   multirftOptions.setParallelStreams (Integer.valueOf  (
         (String)requestData.elementAt (4)).intValue     ());
   multirftOptions.setDcau(Boolean.valueOf(
          (String)requestData.elementAt (5)).booleanValue ());

 int i = 7;
 for (int j = 0; j < transfers1.length; j++)
 {
   transfers1[j] = new TransferType ();

   transfers1[j].setTransferId     (j);
   transfers1[j].setSourceUrl      ((String)requestData.elementAt (i++));
   transfers1[j].setDestinationUrl ((String)requestData.elementAt (i++));
   transfers1[j].setRftOptions     (multirftOptions);
 }

 TransferRequestType transferRequest = new TransferRequestType ();
 transferRequest.setTransferArray (transfers1);

 int concurrency = Integer.valueOf
                 ((String)requestData.elementAt(6)).intValue();

 if (concurrency > transfers1.length)
 {
   System.out.println ("Concurrency should be less than the number"
                       "of transfers in the request");
   System.exit (0);
 }
 transferRequest.setConcurrency (concurrency);

 TransferRequestElement requestElement = new TransferRequestElement ();
 requestElement.setTransferRequest (transferRequest);

 ExtensibilityType extension = new ExtensibilityType ();
 extension = AnyHelper.getExtensibility (requestElement);

 OGSIServiceGridLocator factoryService = new OGSIServiceGridLocator ();
 Factory factory = factoryService.getFactoryPort (new URL (source_url));
 GridServiceFactory gridFactory = new GridServiceFactory (factory);

 LocatorType locator = gridFactory.createService (extension);
 System.out.println ("Created an instance of Multi-RFT");

 MultiFileRFTDefinitionServiceGridLocator loc
                     = new MultiFileRFTDefinitionServiceGridLocator();
 RFTPortType rftPort = loc.getMultiFileRFTDefinitionPort (locator);
   ((Stub)rftPort)._setProperty (Constants.AUTHORIZATION,
                                 NoAuthorization.getInstance());
   ((Stub)rftPort)._setProperty (GSIConstants.GSI_MODE,
                                 GSIConstants.GSI_MODE_FULL_DELEG);
   ((Stub)rftPort)._setProperty (Constants.GSI_SEC_CONV,
                                 Constants.SIGNATURE);
   ((Stub)rftPort)._setProperty (Constants.GRIM_POLICY_HANDLER,
                                 new IgnoreProxyPolicyHandler ());

   int requestid = rftPort.start ();
   System.out.println ("Request id: " + requestid);

  }
  catch (Exception e)
  {
   System.err.println (MessageUtils.toString (e));
  }
 }
}
```

Copy a File: GAT/C++

```
#include <GAT++.hpp>

GAT::Result RemoteFile::GetFile (GAT::Context context,
                                 std::string source_url,
                                 std::string target_url)
{
  try
  {
    GAT::File file (context, source_url);
    file.Copy      (target_url);
  }
  catch (GAT::Exception const &e)
  {
    std::cerr << "Some error: " << e.what() << std::endl;
    return e.Result();
  }
  return GAT_SUCCESS;
}
```

GGF SAGA-WG

A. Merzky, T. Goodale. S. Newhouse, et al

- GAT evolves into GGF standard
  - Numerous attempts to address: GAT most ambitious, but also CoG, DRMAA, GridRPC, GridCPR, many others
- SAGA: Simple API for Grid Applications
  - Bringing all these efforts together through single API spec
  - Chicago, Berlin, Brussels, LSU, Berkeley, Seoul, Chicago, Boston
- GGF focussing now on standardization
  - SAGA API spec done
  - Much momentum in SAGA now

Finally

- Optical Networks, Grids promise new ways of computing
  - More than computing: Network, Data services critical
- Complex applications require comprehensive services
  - Event Driven: many examples. Hurricanes, earthquakes, tornados, explosions, ...
  - DDDAS: http://www.nsf.gov/cise/cns/dddas/2006_Workshop/exec_summ.pdf
  - Much of this can work now as prototypes
- Standards developing
  - 15 years ago: parallel computing drove interconnects, HPF, MPI
  - Now: 2 levels...OGSA grid services, SAGA for apps
- Cactus Computational Toolkit: *www.cactuscode.org*
- GGF "Simple API for Grid Applications" (SAGA)