

# ICT & e-Science

Cees de Laat

GLIF.is & CineGrid.org founding member

SURFnet  
BSIK  
NWO  
EU

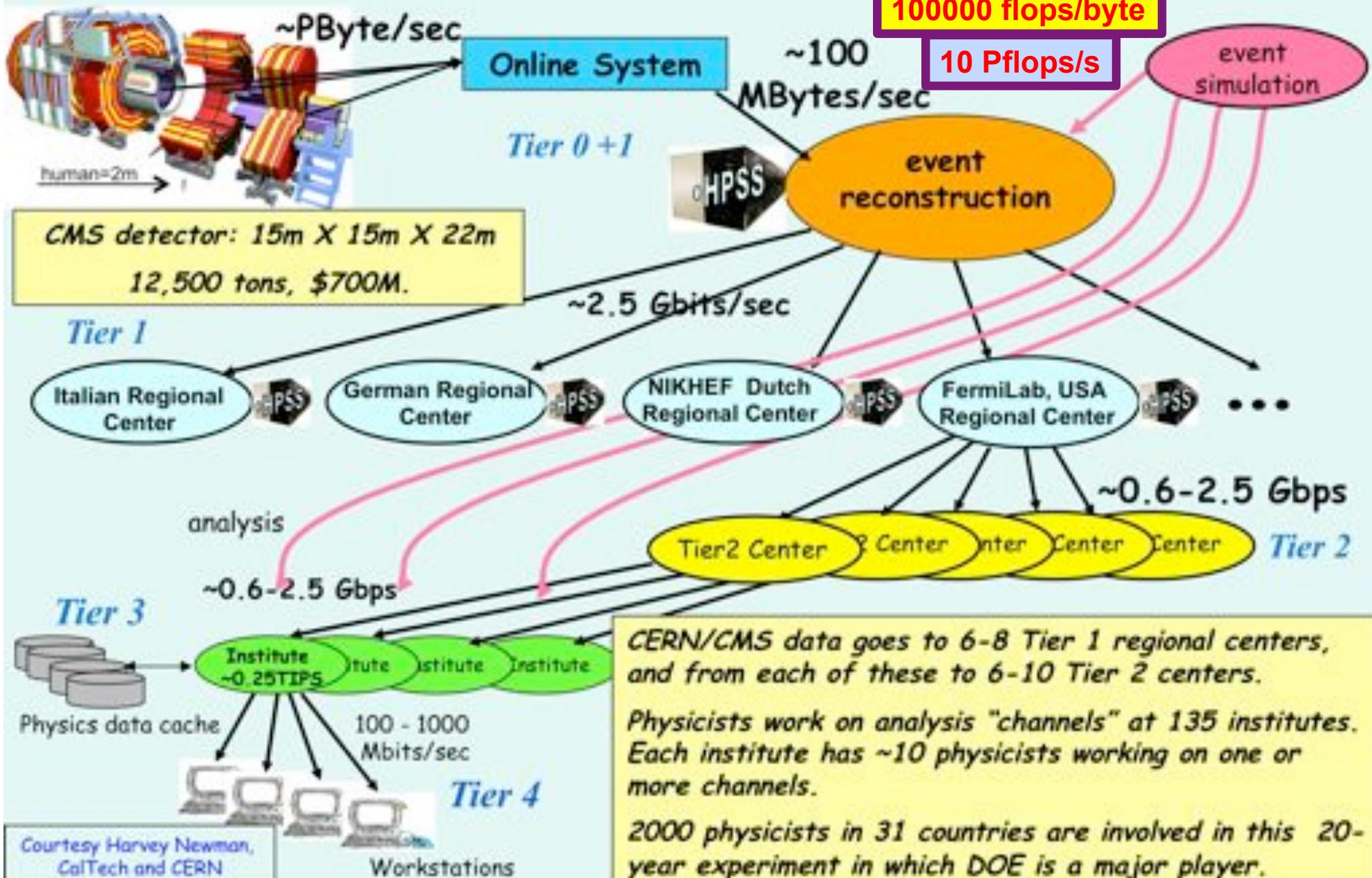
University of Amsterdam





# LHC Data Grid Hierarchy

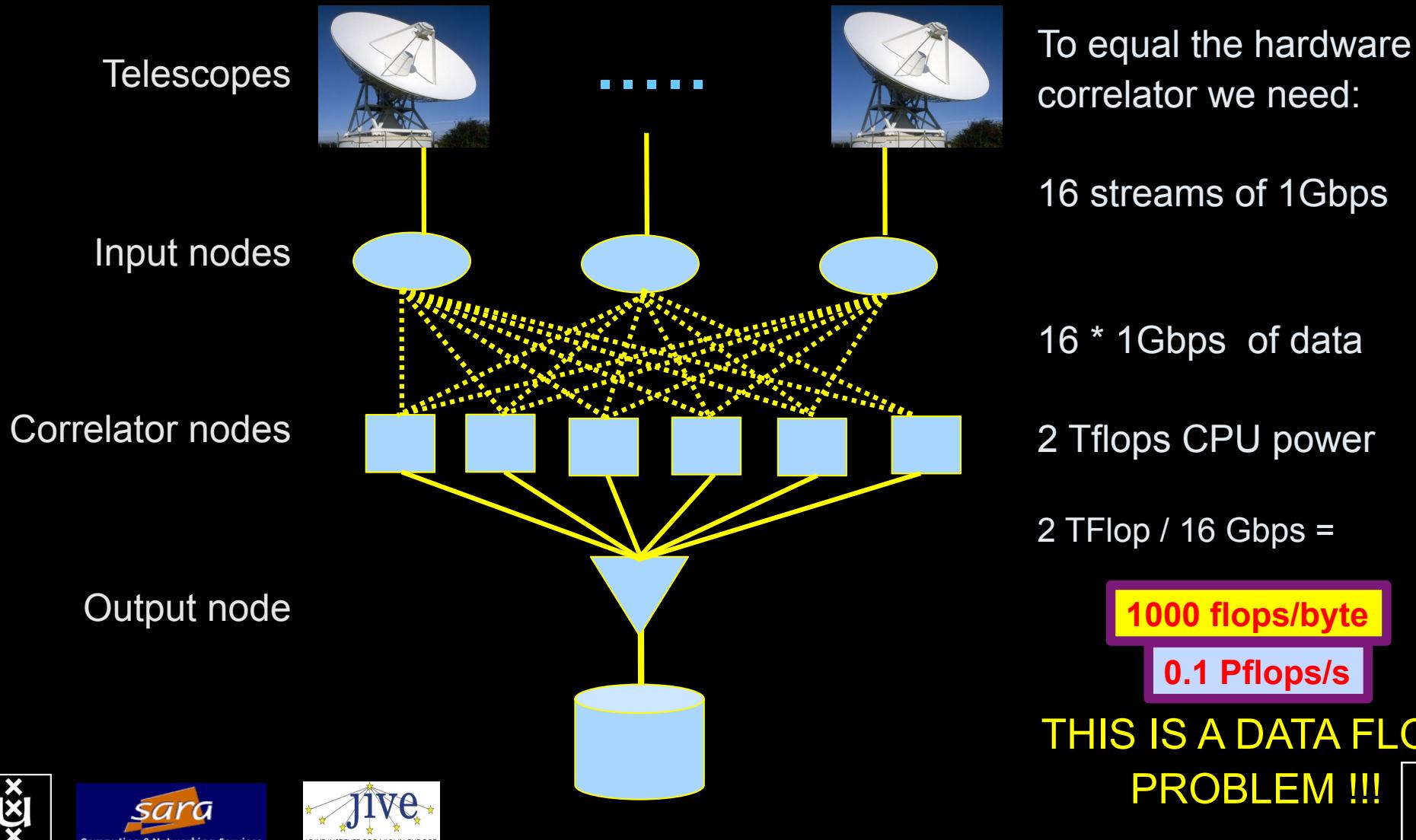
CMS as example, Atlas is similar



# The SCARIE project

**SCARIE:** a research project to create a Software Correlator for e-VLBI.

**VLBI Correlation:** signal processing technique to get high precision image from spatially distributed radio-telescope.



# LOFAR as a Sensor Network

**20 flops/byte**



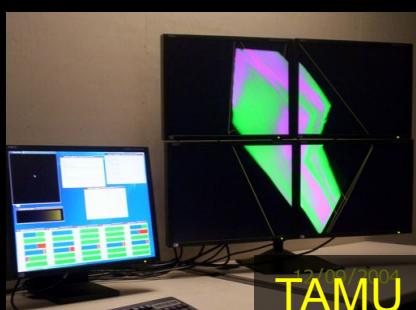
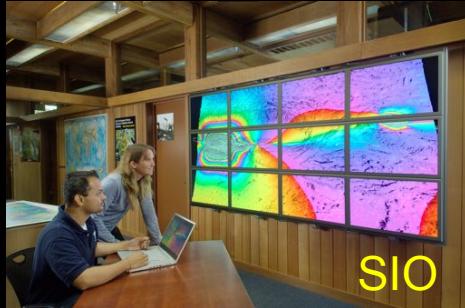
- LOFAR is a large distributed research infrastructure:

**2 Tflops/s**

- Astronomy:
  - >100 phased array stations
  - Combined in aperture synthesis array
  - 13,000 small “LF” antennas
  - 13,000 small “HF” tiles
- Geophysics:
  - 18 vibration sensors per station
  - Infrasound detector per station
- >20 Tbit/s generated digitally
- >40 Tflop/s supercomputer
- innovative software systems
  - new calibration approaches
  - full distributed control
  - VO and Grid integration
  - datamining and visualisation



# US and International OptIPortal Sites



Real time, multiple 10 Gb/s



# The “Dead Cat” demo

1 Mflops/byte

Real time issue



SC2004,  
Pittsburgh,  
Nov. 6 to 12, 2004  
iGrid2005,  
San Diego,  
sept. 2005

Many thanks to:

AMC  
SARA  
GigaPort  
UvA/AIR  
Silicon Graphics,  
Inc.  
Zoölogisch Museum

M. Scarpa, R.G. Belleman, P.M.A. Sloot and C.T.A.M. de Laat, "Highly Interactive Distributed Visualization",  
iGrid2005 special issue, Future Generation Computer Systems, volume 22 issue 8, pp. 896-900 (2006).





IJKDIJK

300000 \* 60 kb/s \* 2 sensors (microphones) to cover all Dutch dikes



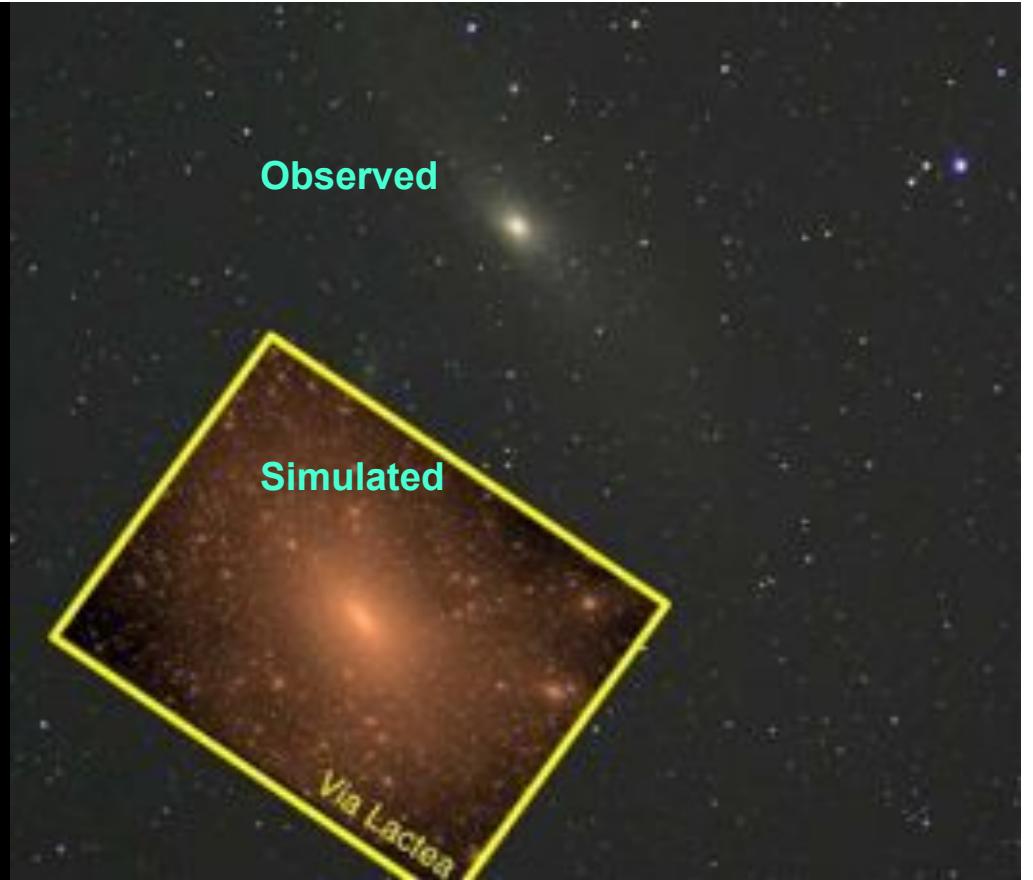
# Sensor grid: instrument the dikes

First controlled breach occurred on sept 27th '08:



# CosmoGrid

- Motivation:  
**previous simulations found >100 times more substructure than is observed!**
- Simulate large structure formation in the Universe
  - Dark Energy (cosmological constant)
  - Dark Matter (particles)
- Method: Cosmological N-body code
- Computation: Intercontinental SuperComputer Grid



# The hardware setup

10 Mflops/byte  
1 Eflops/s

- 2 supercomputers :
  - 1 in Amsterdam (60Tflops Power6 @ SARA)
  - 1 in Tokyo (30Tflops Cray XD0-4 @ CFCA)
- Both computers are connected via an intercontinental optical 10 Gbit/s network



# Auto-balancing Supers



# CosmoGrid

## Supercomputing Grid across Continents and Oceans

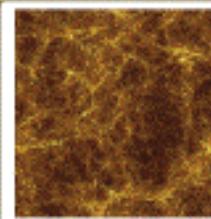
And yes,  
it works!

### Application

We originally developed MPWide to manage the long-distance message passing in the CosmoGrid project. This is a large-scale cosmological project whose primary goal is to perform a dark matter simulation using supercomputers on two continents. In this simulation, we use the cosmological A Cold Dark Matter model<sup>1</sup> to simulate the dark matter particles using a parallel tree/particle-mesh N-body integrator, TreePM. This requires relatively little communication between different sites after each timestep. The integrator calculates the dynamical evolution of 2048<sup>3</sup> (8.5 billion) particles. More information about the parameters used and the scientific rationale can be found in <sup>2,3</sup>.

The integrator can be run as a single MPI application, or as two separately launched MPI applications on different supercomputers.

- <sup>1</sup> Portegies Zwart et al., 2009; IEEE Computer (submitted)
- <sup>2</sup> Geha, 1991; Physical Review D
- <sup>3</sup> Yoshikawa and Fukushige, 2005; PASJ

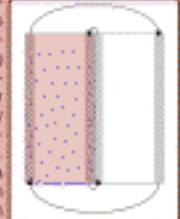


A snapshot of the CosmoGrid simulation. The central dense areas form a cosmic web structure.

### Motivation

We use MPWide to manage the wide area communications in the CosmoGrid project, where cosmological N-body simulations run on grids of supercomputers connected by high performance optical networks. To take full advantage of the network light paths in CosmoGrid, we need a message passing library that supports the ability to use customized communication settings (e.g. custom number of streams, window sizes) for individual network links among the sites. The supercomputers we use vary both in hardware architectures and software setup.

Many supercomputers have a recommended MPI implementation which has been optimized for the network architecture of that particular machine. Installing and optimizing a homogeneous MPI implementation on multiple supercomputer platforms is a task that may be politically difficult to initiate, and requires considerable effort and man hours to complete. This has led us to develop MPWide, a light-weight communication library which connects two applications, each of them running with the locally recommended MPI implementation.



After each computation step, the data in grey regions is transferred to the other supercomputer.

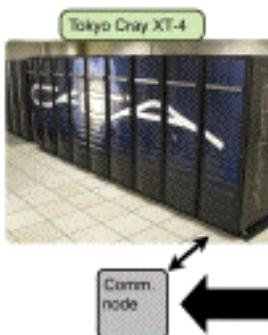
## MPWide

A communication library for distributed supercomputing

Derek Groen<sup>1,2</sup>, Steven Rieder<sup>1,2</sup>,  
Paola Grosso<sup>2</sup>, Simon Portegies  
Zwart<sup>1</sup> and Cees de Laat<sup>2</sup>

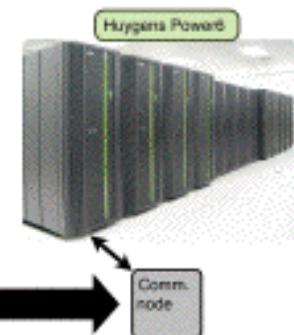
<sup>1</sup>Lorentz Observatory, Leiden, The Netherlands

<sup>2</sup>University of Amsterdam, Amsterdam, The Netherlands



Comm.  
node

10 Gbps light path



Comm.  
node

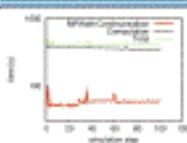
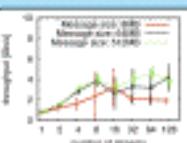
### Benchmarks

We measured the performance of MPWide between two nodes on different supercomputers, one located in The Netherlands, the other in Finland. These supercomputers are connected with a 10 Gbps interface. The round trip time for this network is 37.6 ms.

Each test consists of 100 two-way message exchanges, where we record the average throughput and the standard error. We performed the tests over a shared network with frequent background traffic.

Our tests show increased performance when using more streams, especially for longer message sizes.

We also tested MPWide in a production environment, during a CosmoGrid run. In this run, we used the Huygens supercomputer in Amsterdam and the Cray supercomputer in Tokyo. In this run, the calculation time dominated the overall performance, with the communication time constituting about one eighth of the total execution time.

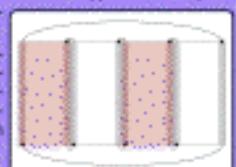


### Related work and future

The MPI implementation most closely related to our work is the PACX-MPI implementation. Like MPWide, this implementation connects different machines, while making use of the vendor MPI library on the system. The main difference between PACX-MPI and MPWide lies in the fact that MPWide supports a de-centralized startup, where PACX-MPI does not. For CosmoGrid, support for this is required, as it is not possible to start the simulation on all supercomputers from one site.

Other implementations of MPI, like Open MPI and MPIICH-G2, differ further from MPWide, and do not support manual specification of the network topology, required by CosmoGrid.

In the near future, we will expand the CosmoGrid simulation to run on four supercomputer sites, and we will implement support for this in MPWide.



<http://www.lns.leidenuniv.nl/research/pace/maar>

7.6 Gb/s

Real time issue

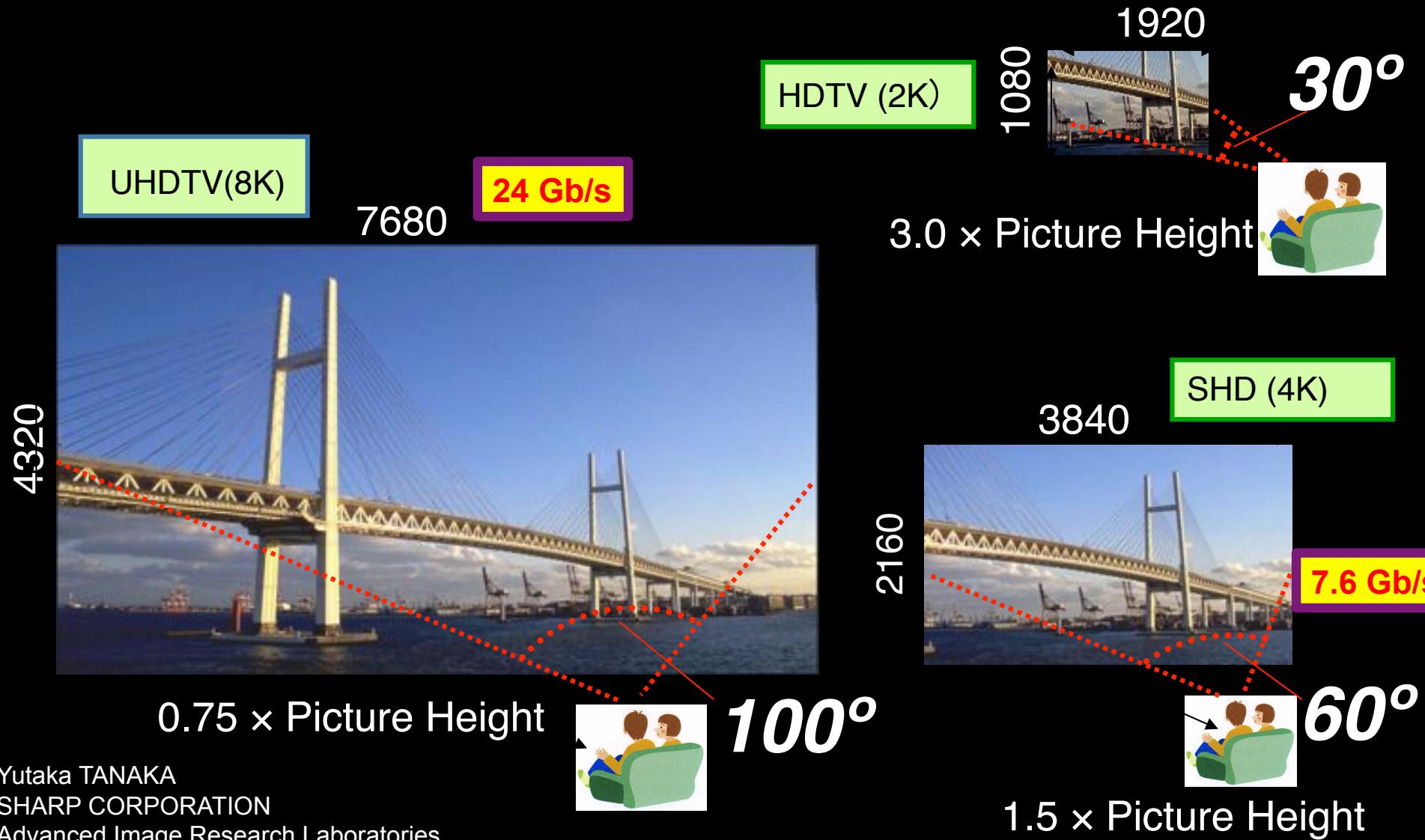


**CineGrid @ Holland Festival 2007**



# Why is more resolution is better?

1. More Resolution Allows Closer Viewing of Larger Image
2. Closer Viewing of Larger Image Increases Viewing Angle
3. Increased Viewing Angle Produces Stronger Emotional Response



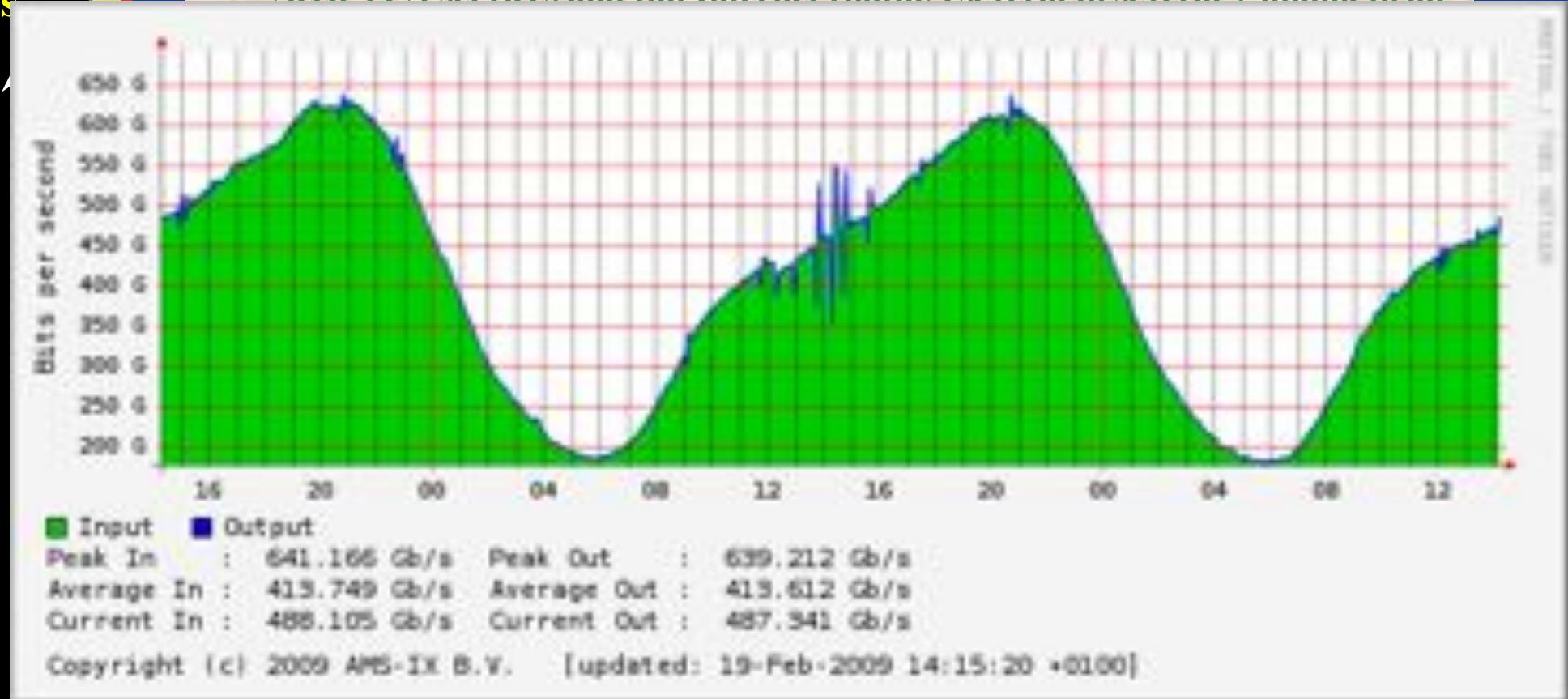
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## A. Lightweight users, browsing, mailing, home use

Need full Internet routing, one to all

## B. Business/grid applications, multicast, streaming, VO's, mostly LAN

Need VPN services and full Internet routing, several to several + unlinked to all



B

C

ADSL (12 Mbit/s)

BW GigE

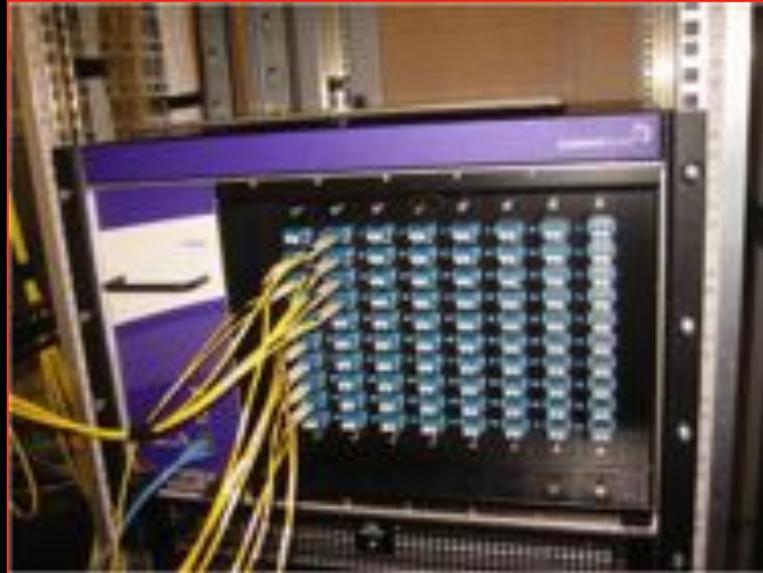
Ref: Cees de Laat, Erik Radius, Steven Wallace, "The Rationale of the Current Optical Networking Initiatives"  
iGrid2002 special issue, Future Generation Computer Systems, volume 19 issue 6 (2003)



# Towards Hybrid Networking!

- Costs of photonic equipment 10% of switching 10 % of full routing
  - for same throughput!
  - Photonic vs Optical (optical used for SONET, etc, 10-50 k\$/port)
  - DWDM lasers for long reach expensive, 10-50 k\$
- Bottom line: look for a hybrid architecture which serves all classes in a cost effective way
  - map A -> L3 , B -> L2 , C -> L1 and L2
- Give each packet in the network the service it needs, but no more !

$L1 \approx 2-3 \text{ k\$/port}$



$L2 \approx 5-8 \text{ k\$/port}$



$L3 \approx 75+ \text{ k\$/port}$



# Hybrid computing

Routers



Supercomputers

Ethernet switches



Grid & Cloud

Photonic transport



GPU's

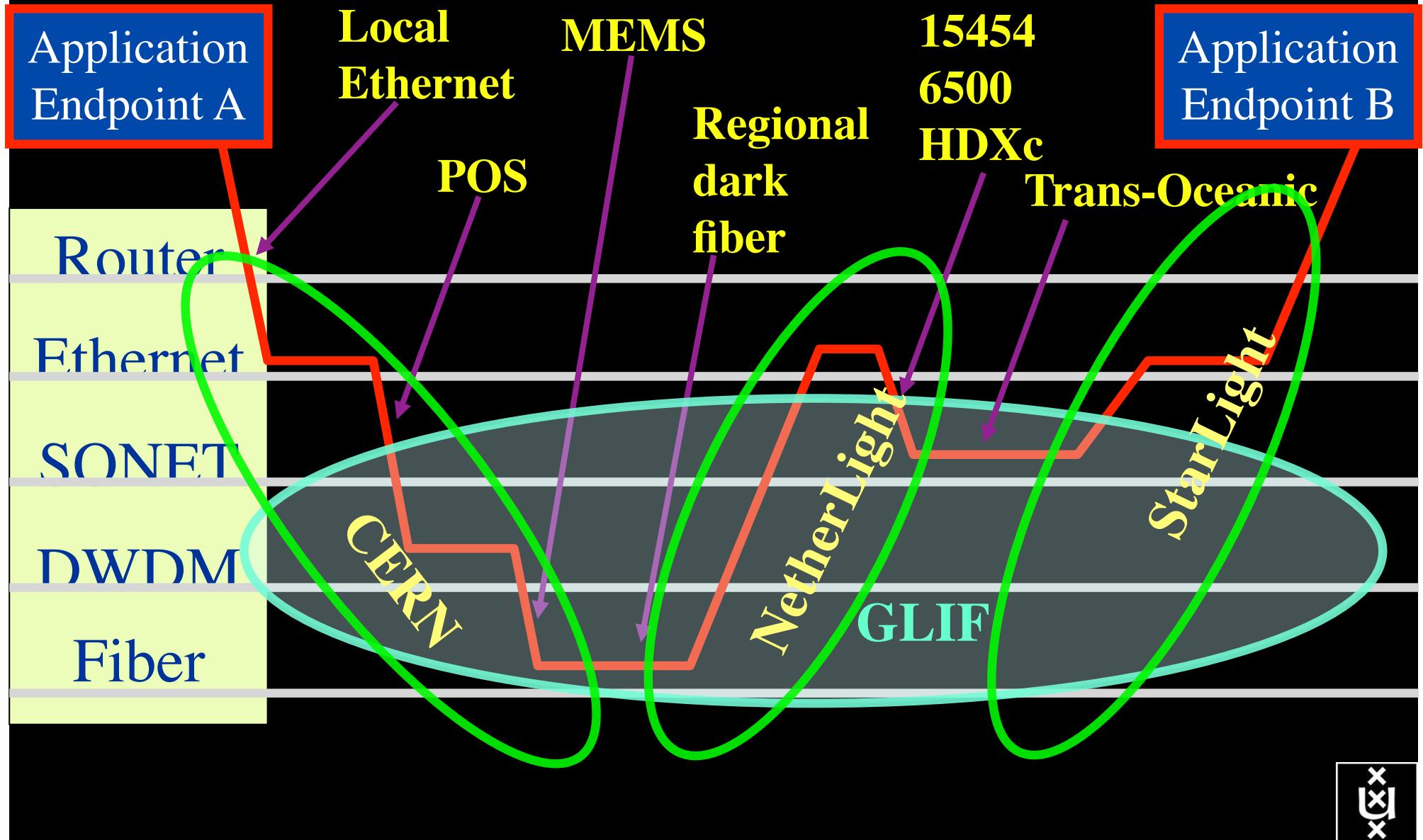
What matters:

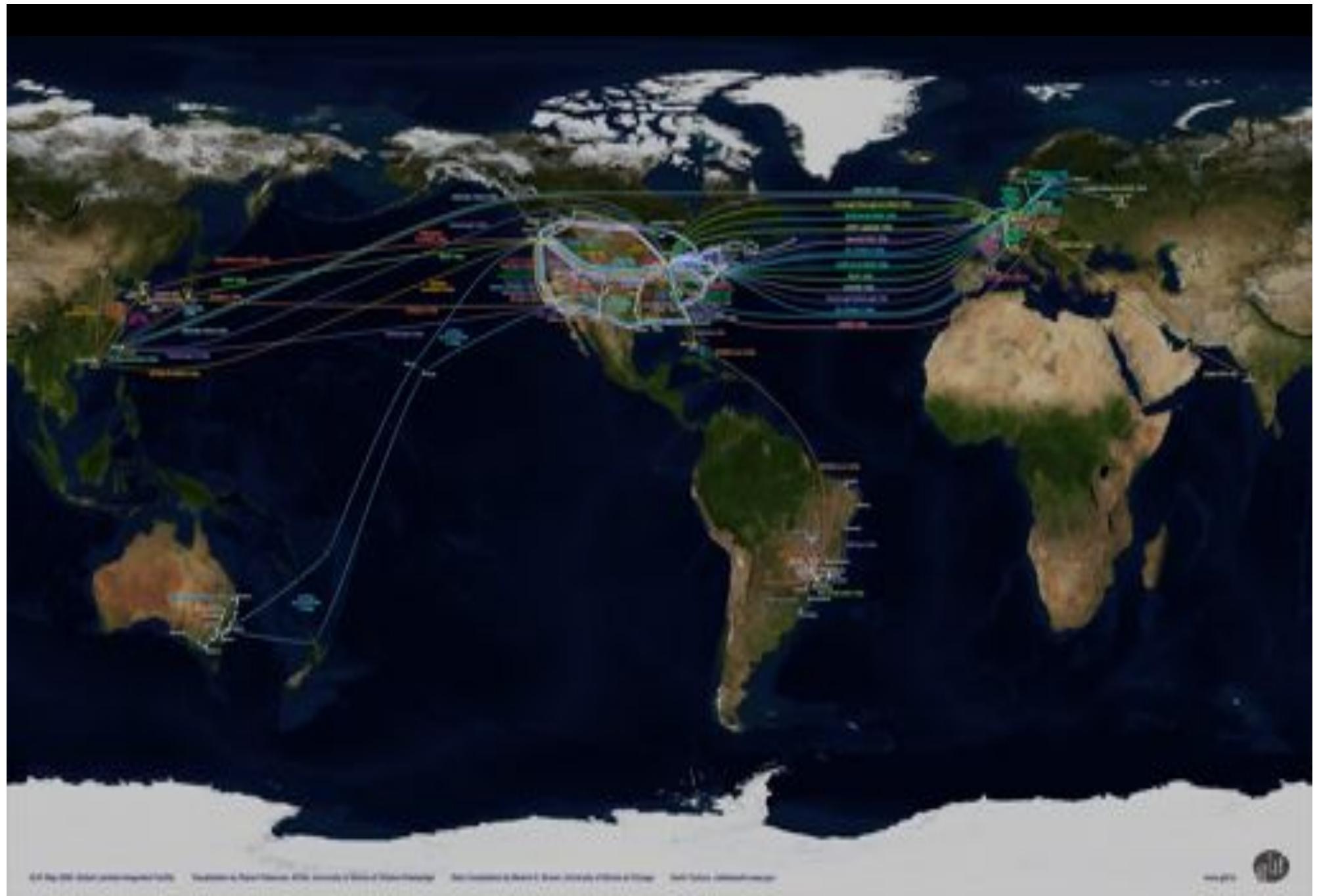
Energy consumption/multiplication

Energy consumption/bit transported



# How low can you go?

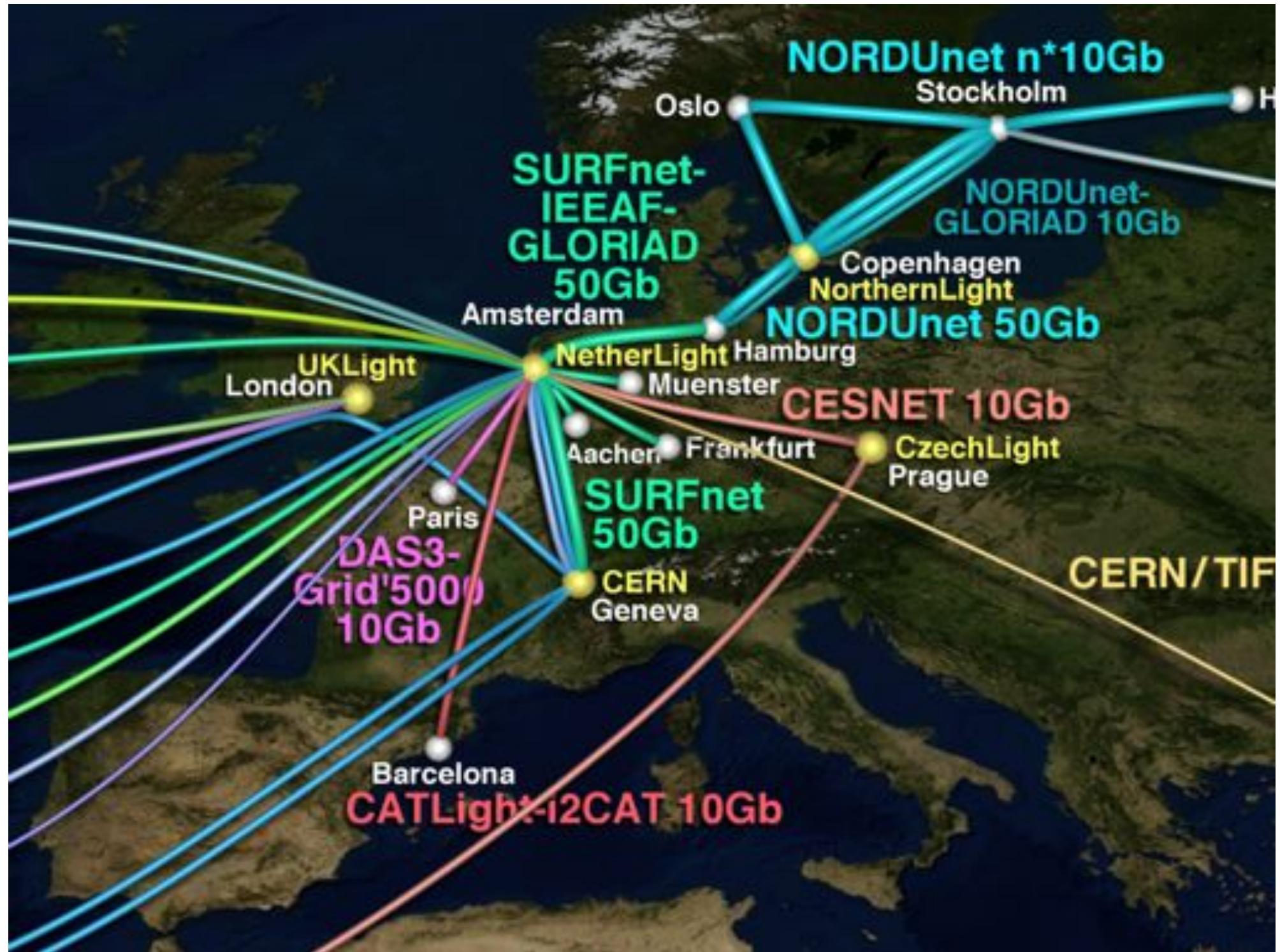


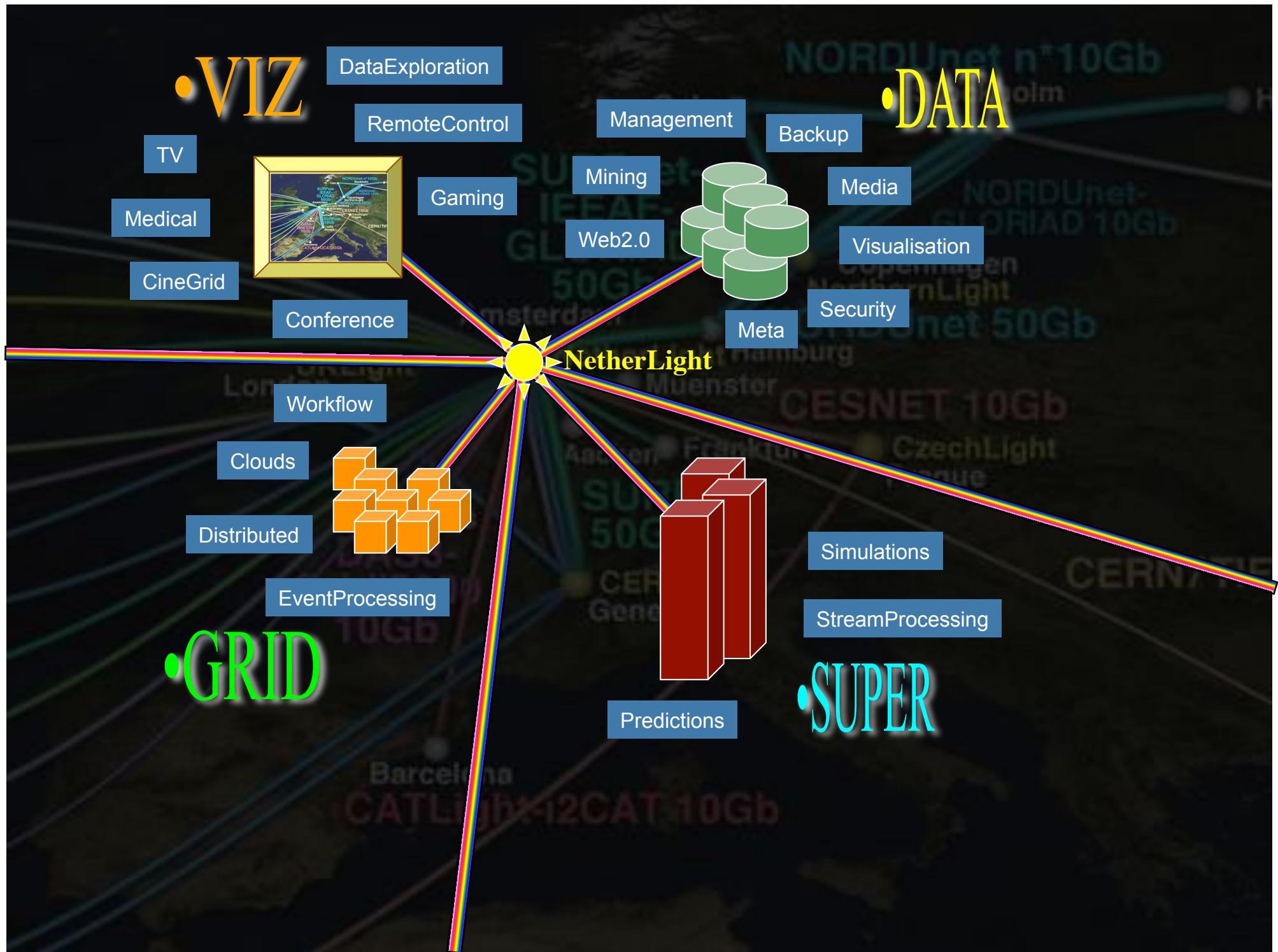


GLIF 2008

Visualization courtesy of Bob Patterson, NCSA  
Data collection by Maxine Brown.









In The Netherlands SURFnet connects between 180:

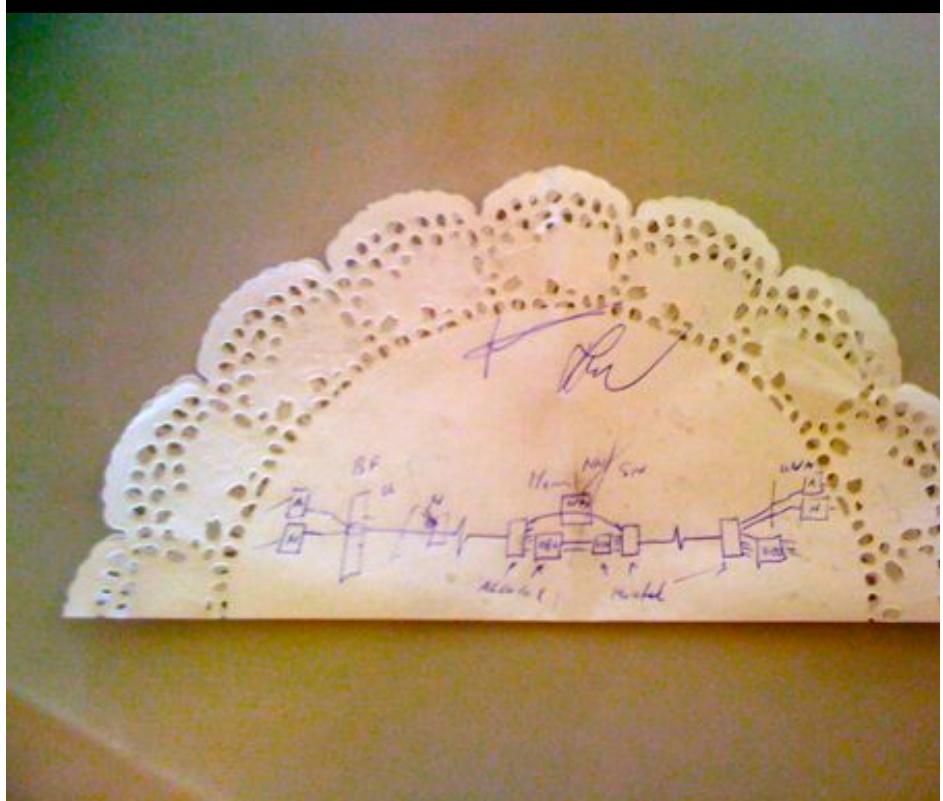
- universities;
- academic hospitals;
- most polytechnics;
- research centers.

with an indirect ~750K user base

~ 8860 km  
scale  
comparable  
to railway  
system



# Alien light From idea to realisation!



## 40Gb/s alien wavelength transmission via a multi-vendor 10Gb/s DWDM infrastructure



### Alien wavelength advantages

- Direct connection of customer equipment<sup>[1]</sup>  
→ cost savings
- Avoid OEO regeneration → power savings
- Faster time to service<sup>[2]</sup> → time savings
- Support of different modulation formats<sup>[3]</sup>  
→ extend network lifetime

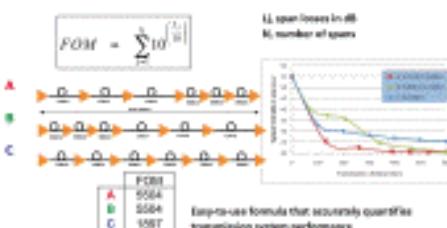
### Alien wavelength challenges

- Complex end-to-end optical path engineering in terms of linear (i.e. OSNR, dispersion) and non-linear (FWM, SPM, XPM, Raman) transmission effects for different modulation formats.
- Complex interoperability testing.
- End-to-end monitoring, fault isolation and resolution.
- End-to-end service activation.

In this demonstration we will investigate the performance of a 40Gb/s PM-QPSK alien wavelength installed on a 10Gb/s DWDM infrastructure.

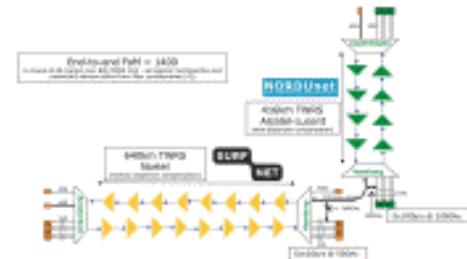
### New method to present fiber link quality, FOM (Figure of Merit)

In order to quantify optical link grade, we propose a new method of representing system quality: the FOM (Figure of Merit) for concatenated fiber spans.

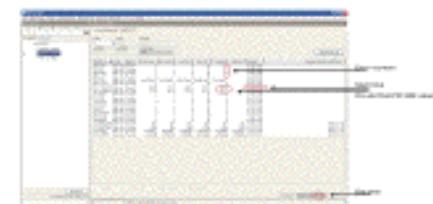


### Transmission system setup

JOINT SURFnet/NORDUnet 40Gb/s PM-QPSK alien wavelength DEMONSTRATION.



### Test results



### Conclusions

- We have investigated experimentally the all-optical transmission of a 40Gb/s PM-QPSK alien wavelength via a concatenated native and third party DWDM system that both were carrying live 10Gb/s wavelengths.
- The end-to-end transmission system consisted of 1056 km of TWRS (TrueWave Reduced Slope) transmission fiber.
- We demonstrated error-free transmission (i.e. BER below 10<sup>-12</sup>) during a 23 hour period.
- More detailed system performance analysis will be presented in an upcoming paper.



#### REFERENCES

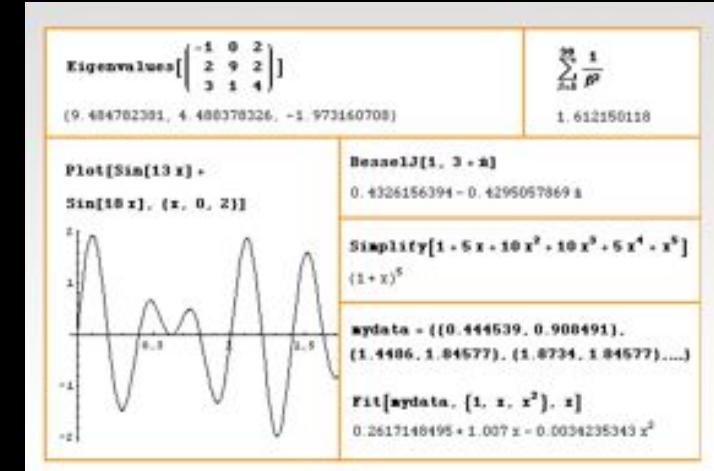
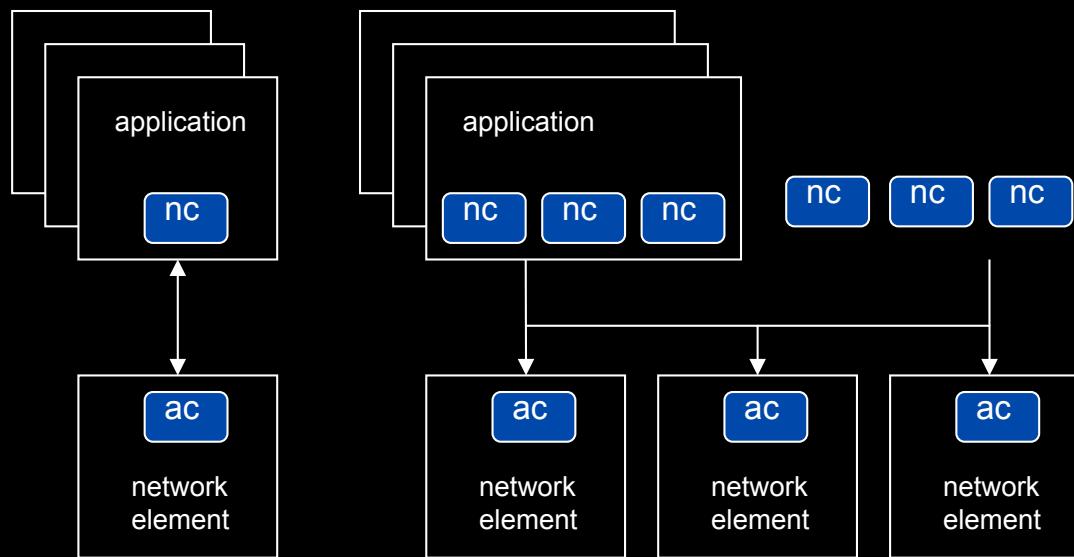
#### ACKNOWLEDGEMENTS

- [1] "INTEGRATIONAL SOLUTIONS FOR AN OPTICAL NETWORK", G. GENTILETTI et al., DOCUMENT I, DIAZETAL OPTICAL TRANSMISSION SYSTEM, BANBURY, U.K., 2001
- [2] "FACT SHEET OF ALL-OPTICAL CORE NETWORKS", ANDREW LIND AND CARL HEDBERG, DOCUMENT I, 3G ALL-OPTICAL CORE NETWORK, COMMUNICATIONS IN A 3G ENVIRONMENT, 2001
- [3] ANY CREDITS TO NORDUnet FOR PROVIDING AN END SPANNING TRIO. THEIR CONTRIBUTION TO THIS EXPERIMENT AND ALSO FOR THE SUPPORT AND ASSISTANCE DURING THE EXPERIMENT IS HIGHLY APPRECIATED. THANK YOU AND BEST REGARDS, KURT HETZEL IS NORDUnet DIRECTOR AND MEMBER OF THE SUPPORT TEAM.

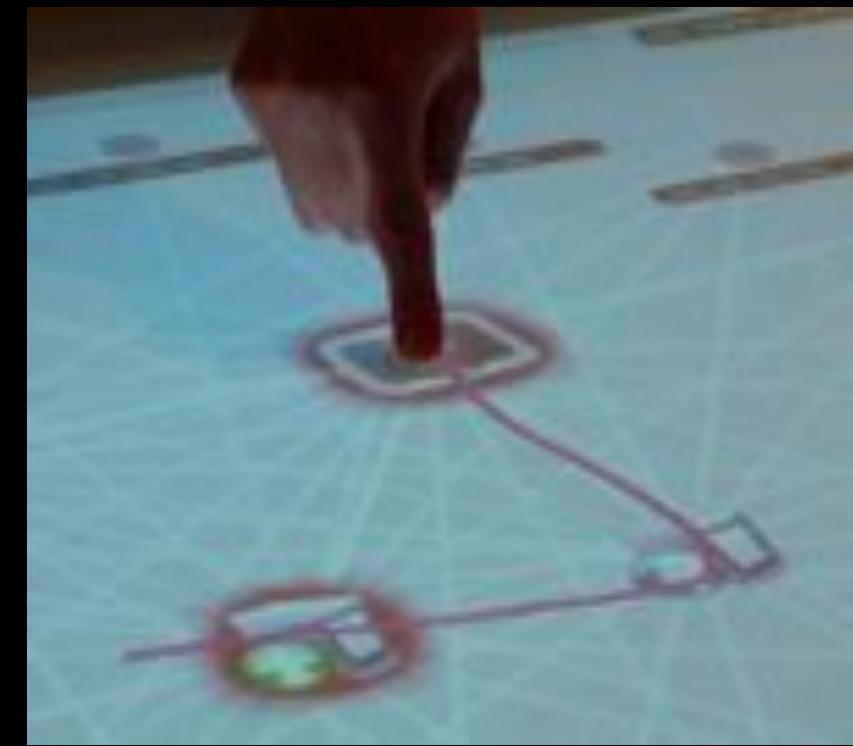


# User Programmable Virtualized Networks allows the results of decades of computer science to handle the complexities of application specific networking.

- The network is virtualized as a collection of resources
- UPVNs enable network resources to be programmed as part of the application
- Mathematica, a powerful mathematical software system, can interact with real networks using UPVNs



# TouchTable Demonstration @ SC08



# Interactive programmable networks



# Applications and Networks become aware of each other!

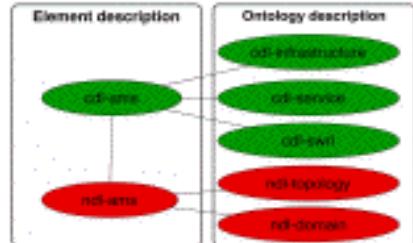
## CineGrid Description Language

CineGrid is an initiative to facilitate the exchange, storage and display of high-quality digital media.

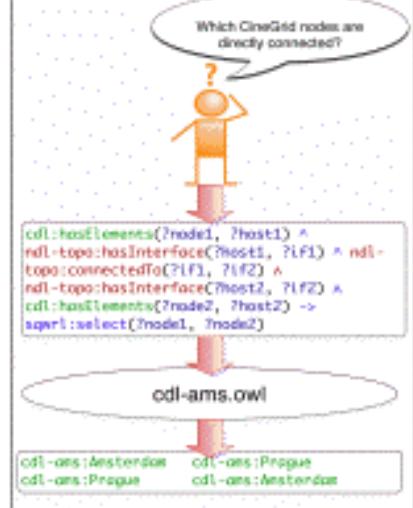
The CineGrid Description Language (CDL) describes CineGrid resources. Streaming, display and storage components are organized in a hierarchical way.

CDL has bindings to the NDL ontology that enables descriptions of network components and their interconnections.

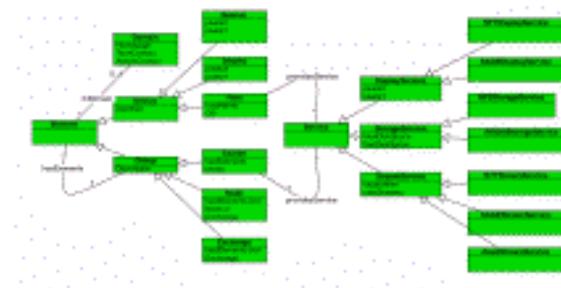
With CDL we can reason on the CineGrid infrastructure and its services.



SQWRL is used to query the Ontology.



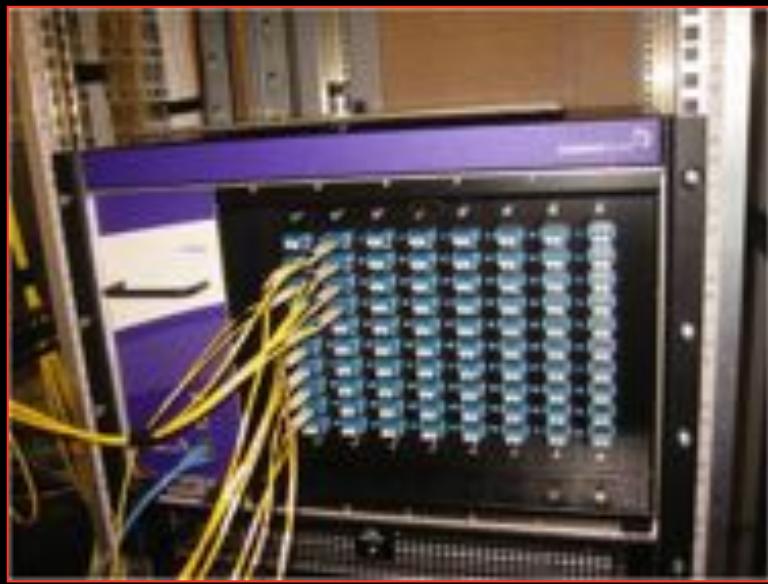
### UML representation of CDL



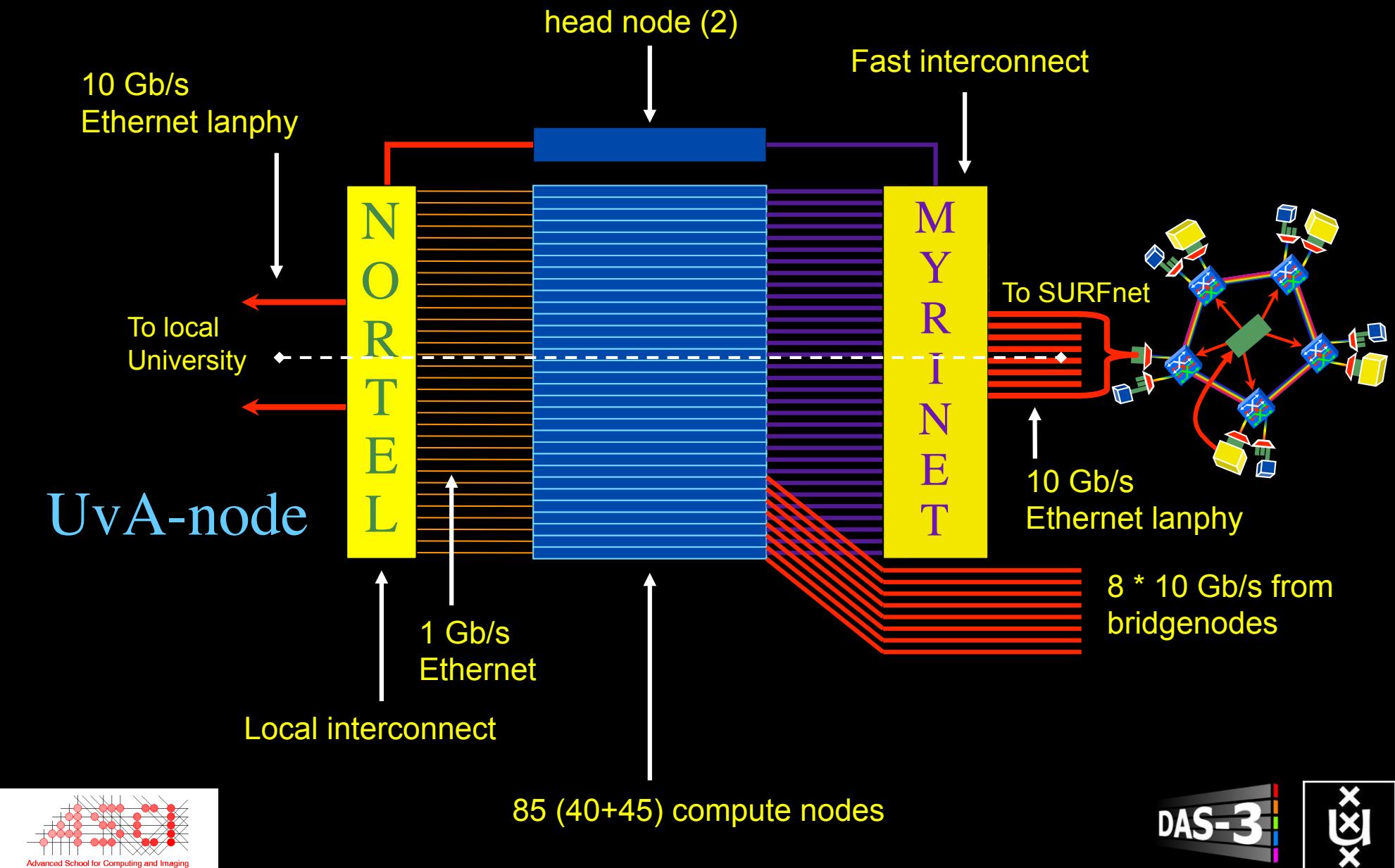
CDL links to NDL using the `owl:SameAs` property. CDL defines the services, NDL the network interfaces and links. The combination of the two ontologies identifies the host pairs that support matching services via existing network connections.

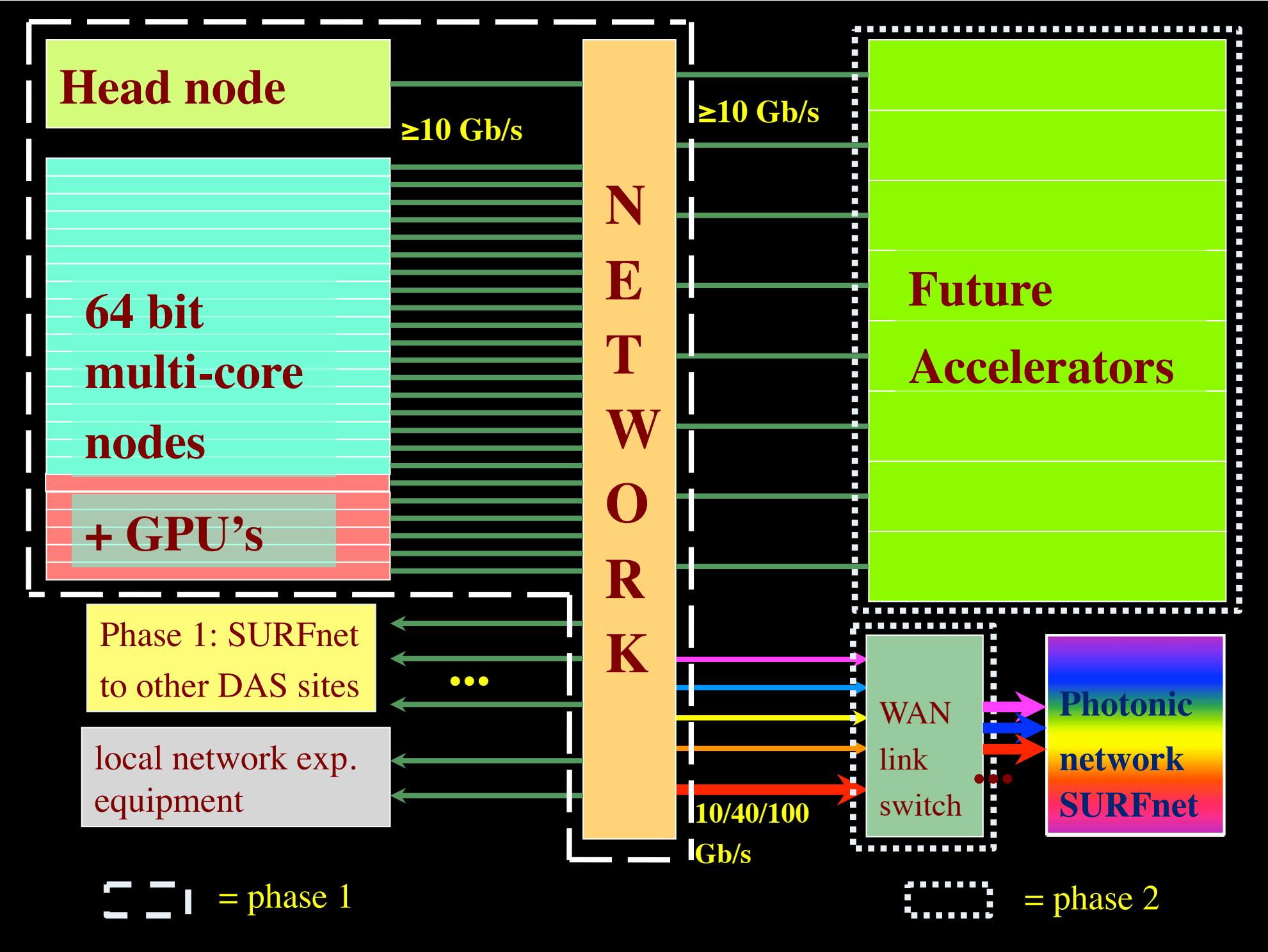


# Our Christmas Trees 😊

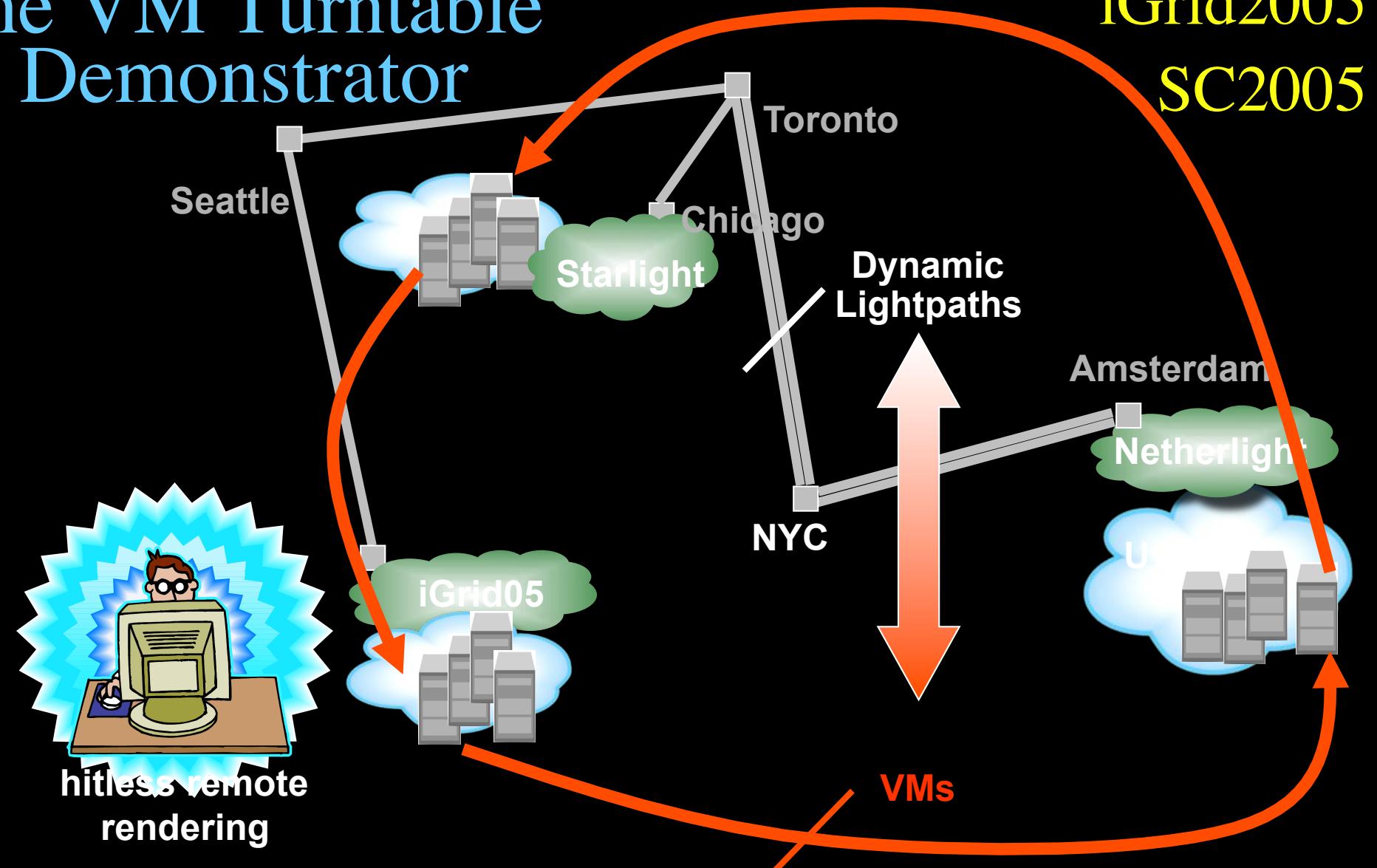


# DAS-3 Cluster Architecture



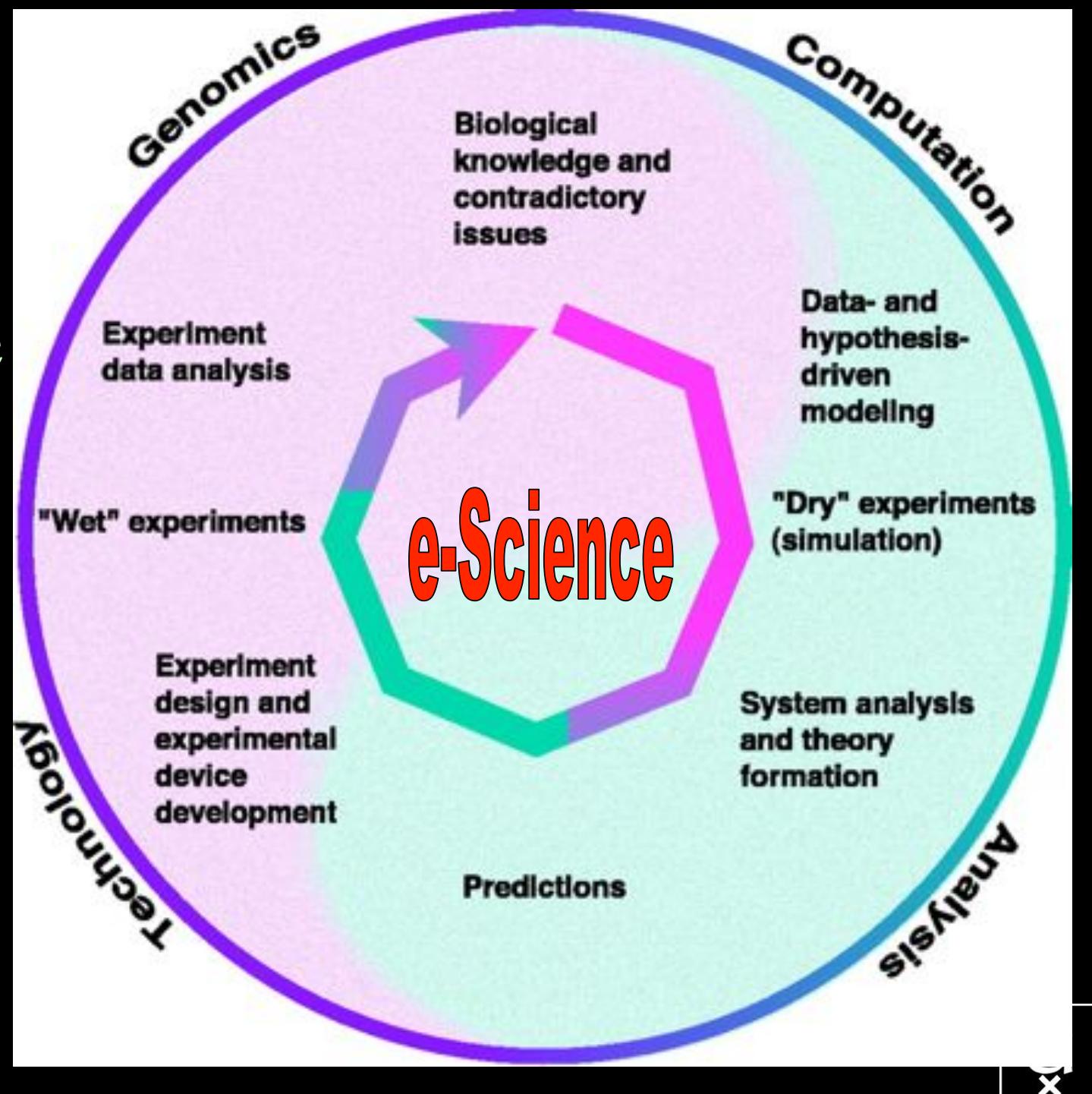


# The VM Turntable Demonstrator



**The VMs that are live-migrated run an iterative search-refine-search workflow against data stored in different databases at the various locations. A user in San Diego gets hitless rendering of search progress as VMs spin around**

# e-Science toegepast in biologie



# Waarom e-Science?

- ICT probleem voor wetenschap, Industrie en maatschappij
  - Er wordt heel veel data verzameld
    - LOFAR, CERN, Life Sciences, Earth sciences, etc
  - Er wordt heel veel data gegenereerd
    - Klimaatmodellen, watermanagement, drugdesign, etc
    - Simulaties van ‘catastrofes’ die niet experimenteel getoetst kunnen worden i.v.m. Veiligheid, complexiteit, capaciteit en/of kosten
  - Nieuwe vormen van wetenschap
    - Interdisciplinair: Impact van High Throughput techniques (sequencing) in biologie, MRI in medische wetenschappen en farmacie
    - Science 2.0
- Nu Inefficiënt: ieder domein (biologen, chemici, etc.) vindt het wiel opnieuw uit.
  - Geen kennisoverdracht op gebied van techniek en methoden
  - Te beperkte interdisciplinair onderzoek
  - Te weinig professionele ICT support waardoor er kostbare ‘science’ tijd verloren gaat
  - Door te weinig gebruik van ICT in onderzoek kunnen we, op een aantal gebieden, de aansluiting bij de wereld gaan missen.



# Problemen

- Coördinatie activiteiten
- Te weinig interdisciplinaire samenwerking
- Gekwalificeerd personeel
- Financiering
  - NWO etc zijn klassiek discipline georganiseerd
  - Nationale infrastructuur vereist nationale fondsen
  - Structureel geld en niet alleen impuls (core)
- Status. Science of Engineering?
- Mensen, met kennis van Science en ICT.
  - > Zijn belangrijker dan Computers!



# Themes for next years

- 40 and 100 Gbit/s
  - Network modeling and simulation
  - Cross domain Alien Light switching
  - GreenLight - GreenSonar
  - Network and infrastructure descriptions & WEB2.0
  - Reasoning about services
  - Cloud Data - Computing
  - Web Services based Authorization
  - Network Services Interface (N-S and E-W)
  - Fault tolerance, Fault isolation, Monitoring
  - eScience integrated services
  - Data and Media specific services
-  → Smart e-Infrastructure

# Progress

- Kilobit/s       $\leftarrow \rightarrow$  keyboard
- Megabit/s       $\leftarrow \rightarrow$  process ques / rpc's
- Gigabit/s       $\leftarrow \rightarrow$  discs, screens
- Terabit/s       $\leftarrow \rightarrow$  GPU

# Onwards!

- We aim for extreme [comp,data,net,viz] experiments!
- Computer & Computational & e- Science needs open and unrestricted environments for experimentation with ICT!
- Our laboratory must be very well connected!
- Our laboratory must be easy accessible and nearby!
- Participation in master education.
- We need participation from IC to build & operate & utilize our laboratory!
- We need to be able to break things!

If we never broke something we did not try hard enough!



# Networks

- Make sure we couple to the SURFnet hybrid services
  - Routed plus lightpaths implemented as NGE
  - Go to 100 Gb/s in next 5 years
- Create a scalable dwdm photonics layer
- Limit routers to the minimum (2)
- Use some form of Layer2 for traffic transport& aggregation
  - MPLS-TE or PBT, PLSB, etc.
- Make sure it is controllable & manageable
  - and ultimately partly by users & applications



# *Questions ?*

Thanks: Paola Grosso & Henri Bal & Hans Dijkman & Bob Hertzberger  
& Jeroen vd Ham & Freek Dijkstra & team for several of the slides.

