

Why the PharmaGRID Retreat ?

Chris Jones

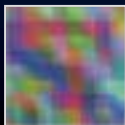
CERN

June 2003



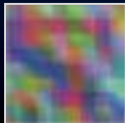
The Role of Computers

- Computers were invented in response to the need to **CALCULATE** numbers, floating point numbers
- which saved considerable effort over the previous electric or even hand cranked adding machines
- And this **ability to save time and effort** quickly became, beyond calculation, one of the computer's additional **MAJOR STRENGTHS**



The Role of Computers [cont.]

- For example their **early use to crack codes** where their strength was not just to accomplish the task much faster than before
- BUT thus **to make possible or practical something that was impossible or not sensible before**



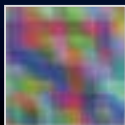
Computers and Networks

- The original **ARPA network** (1969 -) aimed to connect the compute power of a handful of distributed “supercomputers” (albeit only by remote job submission)
- But was used much more successfully for the original **electronic mail** service that the network made possible
- **Saving time and effort in communications between PEOPLE**



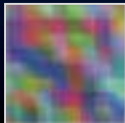
The Web

- Was a response to the needs of a **distributed collaborating community**
- And **saved time and effort in fetching information from other places**
- (it eliminated the effort e.g. to organise an account in a remote university, log-in, use an unfamiliar system in order to obtain info, contact info, telephone numbers, documents...)



The Web [cont.]

- Made sharing information so much easier
- That many **NEW things became possible**
- **Transparent access** to information
- Independent of and removing barriers of space and time



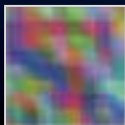
From Science to Society in 10 years

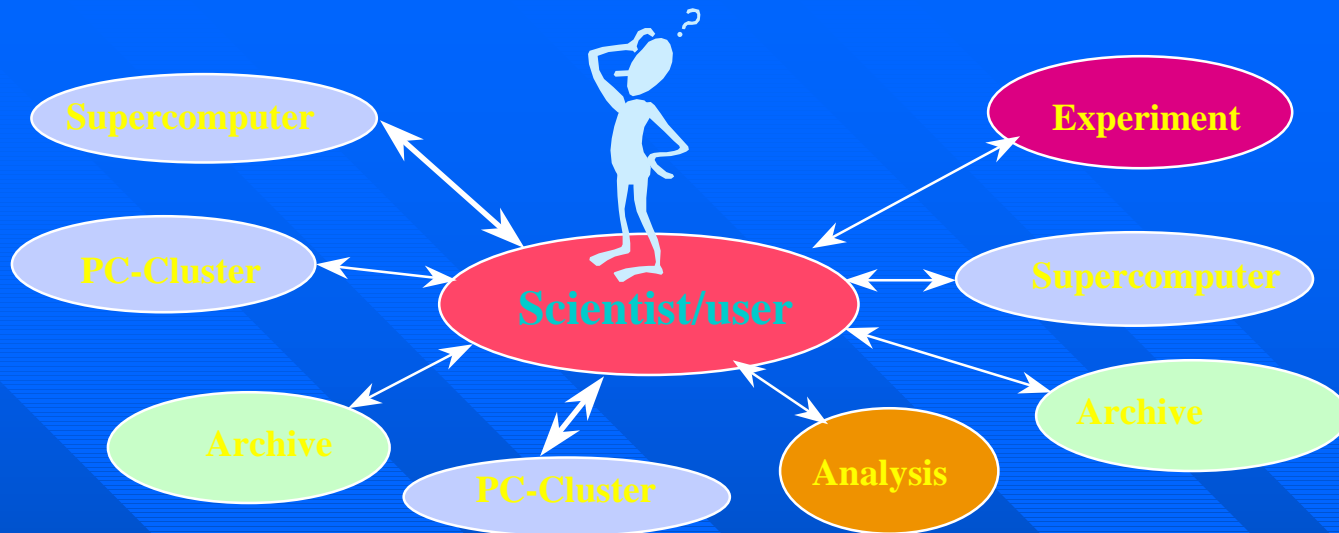
- **The Web** met the collaboration needs of particle physicists and was adopted quickly by other sciences and academia
- And spread to informatics-literate industry and to business, large and then small...and white vans
- And to pervasive commodity usage, internet cafés and homes
- A process of evolution which took 10 years from the original paper
- You had to chose the right time to get involved



The GRID

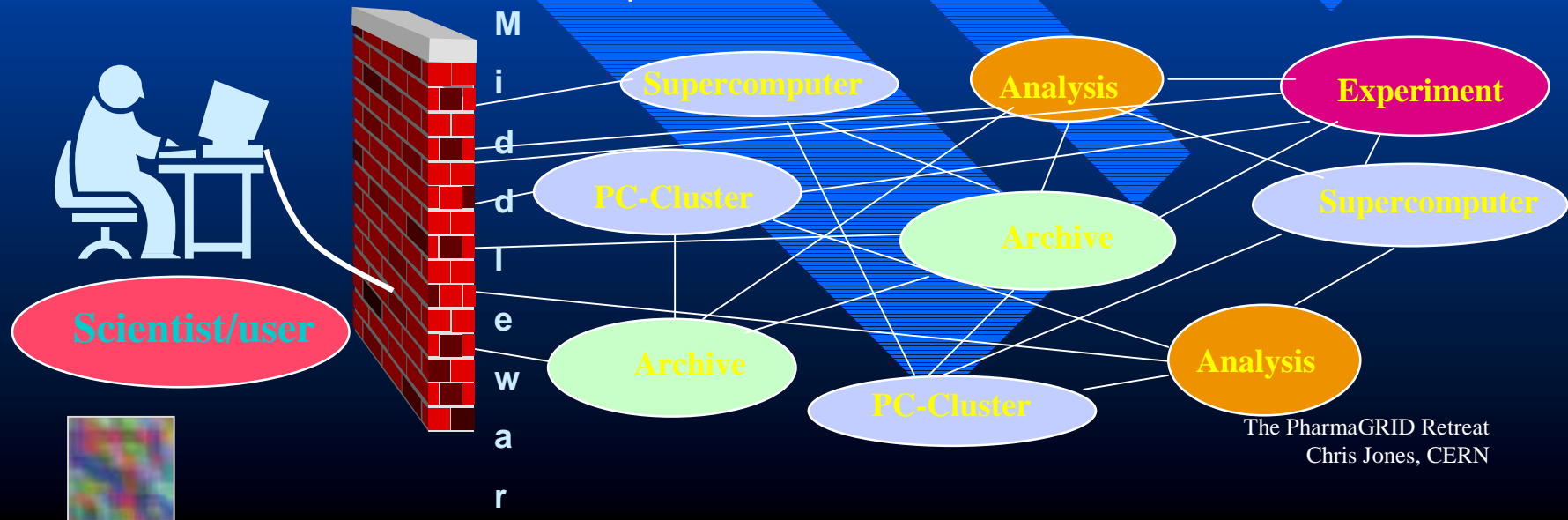
- (As we will see) **Combines many of these themes**
- It started with ideas to link supercomputers
- And spread to linking all major computational resources
- And massive distributed data
- In a **worldwide GRID of resources**
- **Made transparently available**
- In a “one stop shopping” - John Taylor





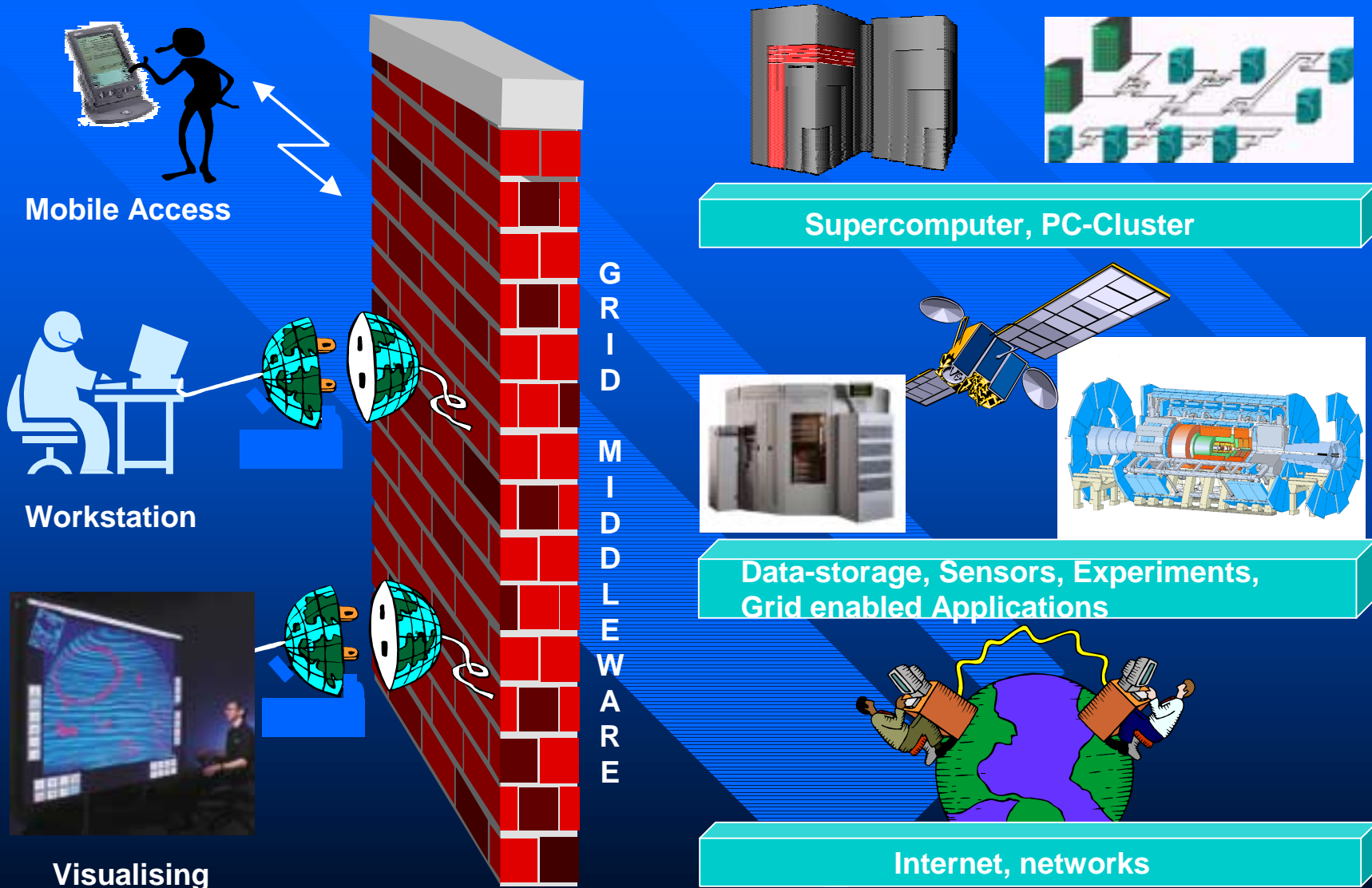
Often monolithic, "vertical", proprietary solutions

Through open, standard interfaces: flexible, adaptable, interchangeable, multiple vendor solutions



The PharmaGRID Retreat
Chris Jones, CERN

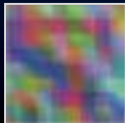
The "One-Stop Shopping" view of the GRID



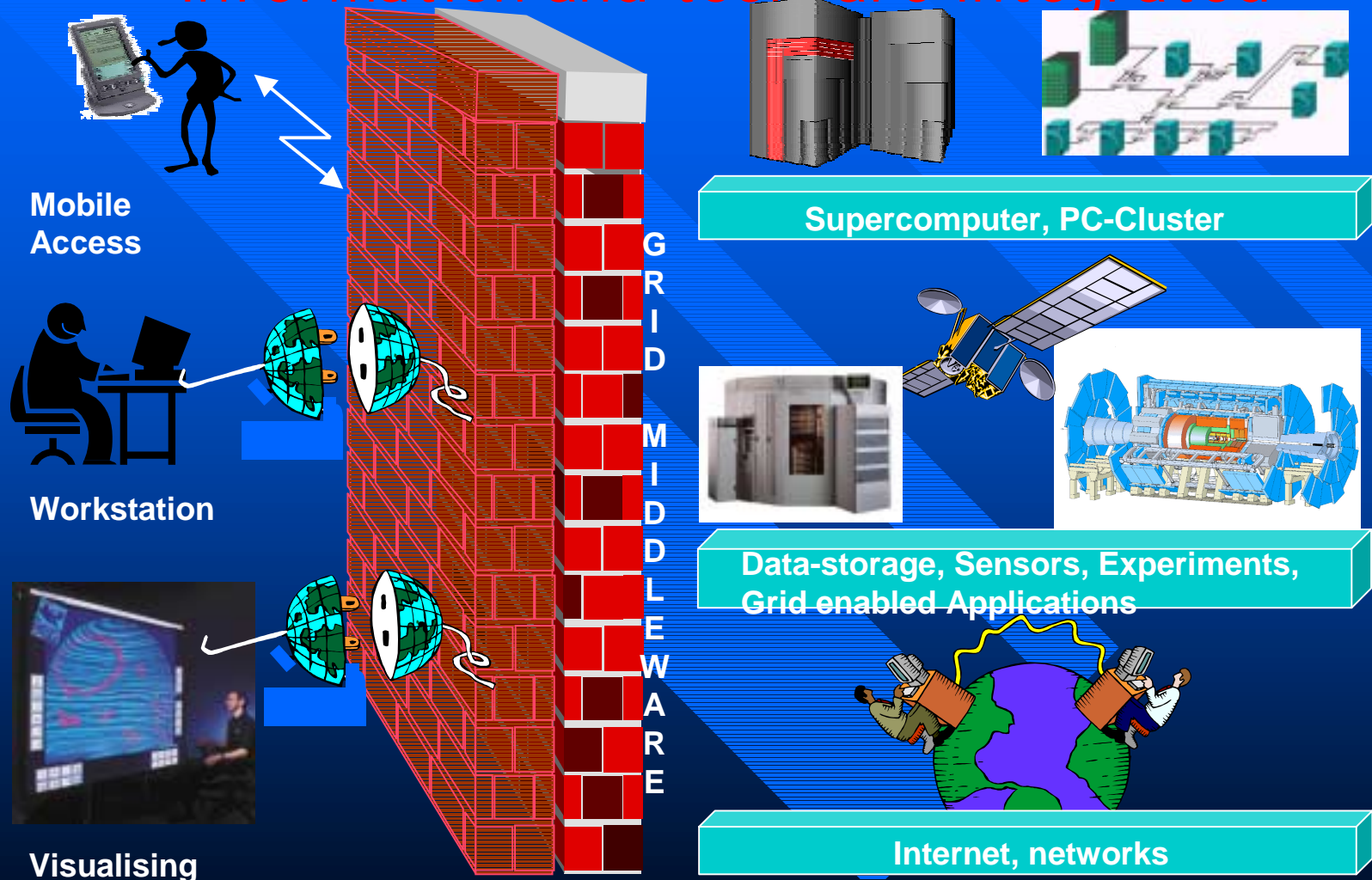
Hoffmann, Putzer, Reinefeld

The GRID evolves

- Thinking about The GRID is evolving to encompass not just computational and data resources but
- All sources of services and resources that one needs: information of all types (including e.g. medical records), databases of all forms, data, simulations, applications...
- In a transparent fashion independent of location and time
- Strong support for work in HealthGRIDs, and in Grids for Complex Problem Solving Environments

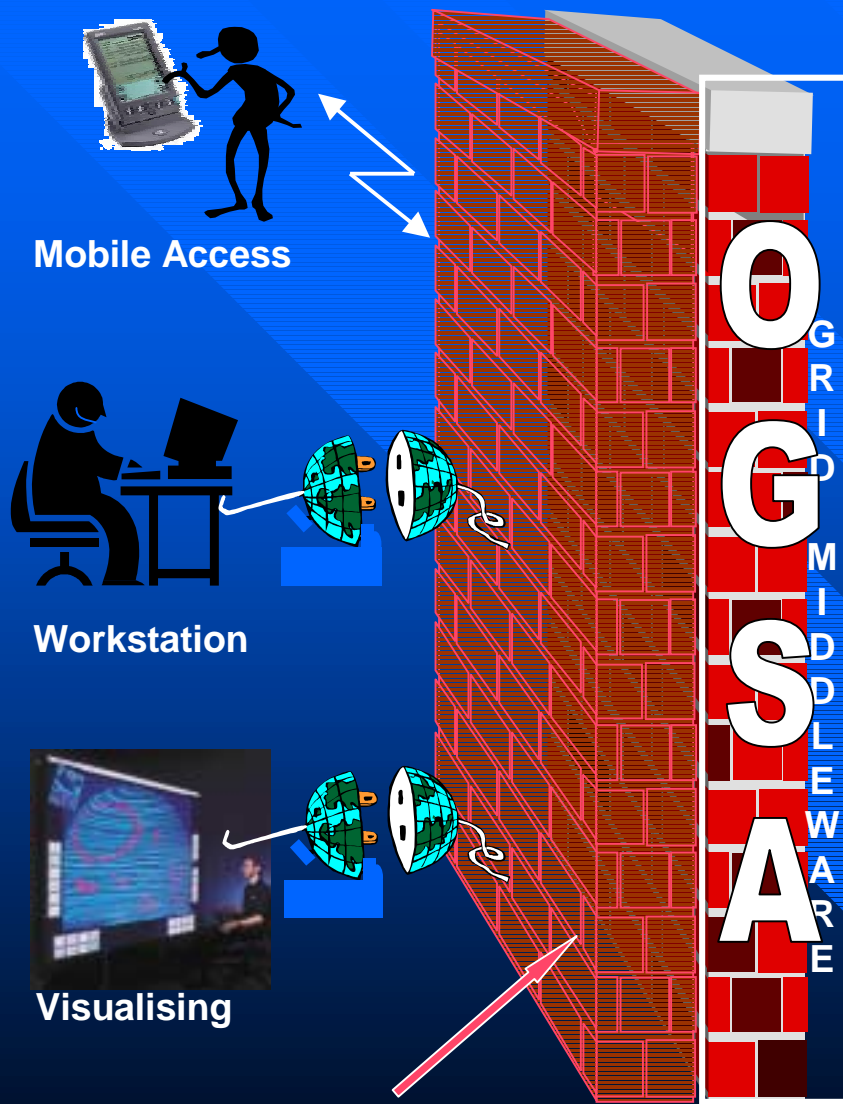


Life Sciences and Health need more middleware for tailored environments in which all relevant information and tools are integrated

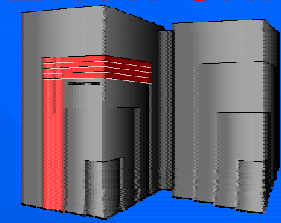


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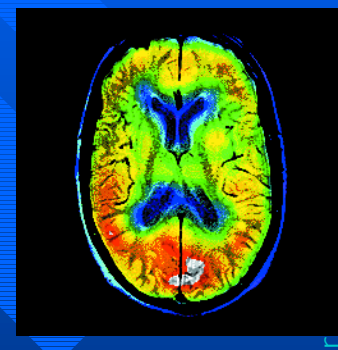
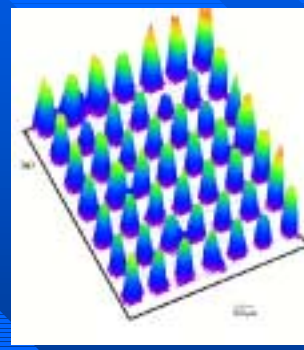
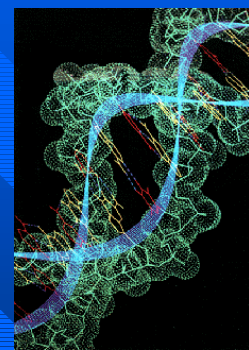
The User connects to his "Virtual Laboratory" or "Workbench Environment"



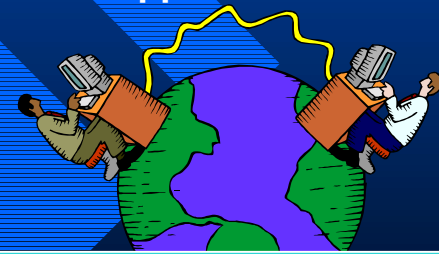
Integrating framework middleware and Virtual Laboratory



Supercomputer, PC-Cluster



Data-storage, Sensors, Experiments, Grid enabled Applications

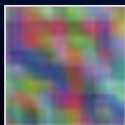


Internet, networks

Hoffmann, Putzer

Its all about Distributed Computing

- “Distributed computing is where a machine that I’ve never even heard of FAILS – and I can’t get my work done”
- The GRID is about doing this better



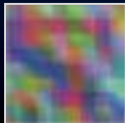
E-Science, e-Health, e-everything...e-Pharma

- The GRID is an evolving enabling technology that will permit transparent access to much more information, services and computing resources than currently available
- That will allow new ways of working, enhanced science, enhanced healthcare, enhanced drug discovery etc.
- And this will evolve, as did the Web, beyond science into other areas of society



e-Pharma Remarks

- It is in the nature of the relationship of the Pharma industry and IT to be conservative
- And focused on delivery
- Yet Pharma's involvement with GRIDS has **enormous opportunities**
- And Pharma has to **consider its relationship with standardization activities, leading academic projects and primary providers of GRID software and services**



Concluding Remarks

- Paradoxically...
- The Pharma Industry has as much to gain as any industry from the enabling technology represented by the GRID
- It needs education and discussion
- Hence this PRISM Forum Retreat on the potential of “PharmaGRID”

