

# United Devices

## Grid Computing in Life Sciences

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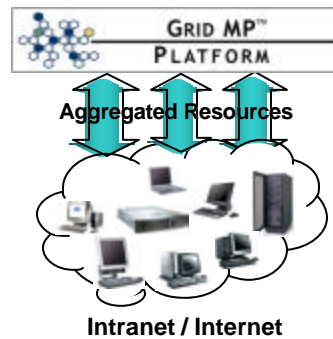
### Topics

- **The drive towards single, integrated Enterprise-wide Grids**
- **Growing application knowledge / leverage**
  - R & D
  - Clinical
  - Data Mining / Processing
- **UD perspective on running a 'large' grid**
  - Grid.org

## What does United Devices do?

### Business

- United Devices develops software for creating the largest grids in the world for:
  - Enterprises
  - Partners
  - The Public
- United Devices operates the largest public grid in the world dedicated to life science research @ [www.grid.org](http://www.grid.org)



### Vision

- Every device is part of an enterprise or global grid

## Enterprise Grid Architecture

## Our Vision of the Grid Driven Enterprise



### INFRASTRUCTURE TODAY

*Generally accepted that the average node's utilization is 5-10%, yet enterprises are constantly buying more infrastructure*

### INFRASTRUCTURE WITH UD

*Grid MP virtualizes access to infrastructure based on business priorities and policies with guaranteed service levels, generates huge ROIC while accelerating business processes*

### VALUE

*"We invested roughly \$400K in Grid software and figure we saved at least \$2 million" – Manuel Peitsch, Novartis*

### ENTERPRISE OPTIMIZATION

*Grid MP enables organizations to deploy an Enterprise-wide Grid across ALL compute infrastructure enabling IT professionals to manage and direct those resources for the first time*

## Application Drivers

## R & D

- **Applications**

- GOLD
    - GOLD Grid Monitor
  - FlexX
    - FlexX Grid Monitor
  - LigandFit / LigScore
    - LigandFit Grid Monitor
  - BLAST
  - HMMER
- Archimedes
  - Structure Checker
  - FLO
  - FRED
  - Glide
  - R
  - (...)



- **Large, successful production deployments**

- Johnson & Johnson
- Sanofi-Synthalabo
- Novartis
- GSK
- Galderma

- **Published results**

- Nature Drug Discovery '02
- Journal of Medicinal Chemistry '03

"[Jeff] Mathers (Director of the Research & Innovation group at Johnson & Johnson PRD) noted that when Johnson & Johnson was studying molecules used in drug development in computer simulations on a 32-way server, the processing time took about three months. After moving those simulations to a grid that uses several hundred computing resources, processing time was cut to about two weeks."

*Computerworld, May 2004*

## Clinical / Simulation

- **Applications**

- NONMEM
- NONMEM (JSP)
- Archimedes
- R (modules)
- SPSS (modules)
- SAS (modules - caveats apply!)

- **Large, successful production deployments**

- American Diabetes Association
- Johnson & Johnson
- Sanofi-Synthalabo
- Novartis
- Kaiser Permanente
- GSK

- **GSK Case Study**

- Published Q2 '04
- See me for copies

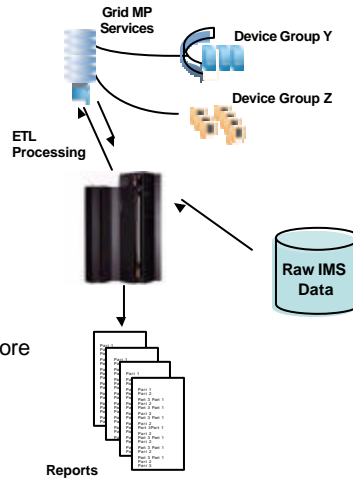


"The Grid MP platform keeps track of all the data related to our job runs – where the job was executed, what type of machine, how long it took. So not only does the grid save us time, but in automating this function it allows us to define a validated process for job execution. That goes a long way toward achieving FDA compliance."

*Mark Sale  
Global Director of Research Modeling and Simulation  
GlaxoSmithKline*

## Data Mining / Processing

- **Applications**
  - Syncsort
  - SAS
  - Text Mining (various)
- **Small, promising deployments**
- **Example - ETL**
  - ETL = Extraction, Translation & Load
  - A data processing step typically run before data is input into a data warehouse
  - Often the bottleneck in front of report generation
  - Can be critical for business functions in Pharma



Reports returned in hours vs. days

## The Grid Driven Enterprise is Happening Now

"If you look at dedicated clusters versus a more flexible [grid] environment where you can take advantage of both new acquisitions and existing systems through a single tool, it's just a better way to invest your money." J&J's grid technology of choice is the Grid MP platform from United Devices Inc., Austin, Texas. **"By going with the United Devices tool, we can have a single tool that can both do a virtual cluster and also take advantage of CPU harvesting off of the existing equipment that we already have.** That was one of the big reasons we picked United Devices over other ways of providing HPC capabilities."

"[Our grid] is a mixture of devices. Back-end servers, NPI devices—It's a way of taking a set of resources and treating them as if they were a cluster... **The United Devices tool gives us the ability to have all of these resources in the grid and through profiling and policy settings use them in different ways.**"

*Johnson & Johnson*



September, 2004



# Grid.org

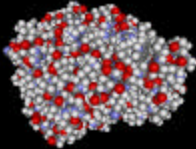
**LigandFit**
computational chemistry

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LIFE SCIENCES

Currently working on:  
generating energy grid

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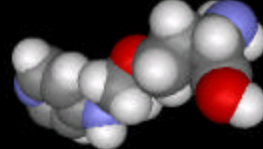
Current Protein Target




Legend:


● Carbon	● Hydrogen	● Iron
● Oxygen	● Phosphorus	● Iodine
● Nitrogen	● Sodium	● Other

Current Prospective Ligand 3D Structure: 168 hits




22 of 30 ligands processed







MEET DR. RICHARDS  
WWW.NFCR.ORG



IBM  
life science solutions



# Grid.org is...



- > 2.5M Nodes
- > 191+ Countries




- > A worldwide public phenomenon




- > Fully hosted, scalable
- > In production for over 3 years

Grid.org  
Total CPU Hours

2,147,483,647

- > Proven
- > Powerful

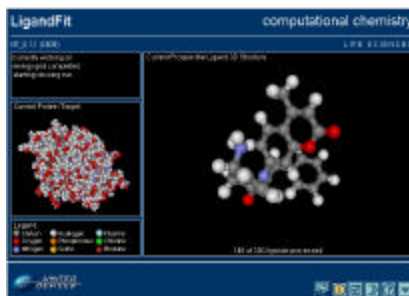


Intel said the software's security is "robust end to end". Barrett said he was going to allow it to be run inside his company.

- > Secure
- > Trusted by the public and the world's leading institutions

## The Cancer Project

- **Goal**
  - Exhaustive screen of 12 targets identified in multiple cancers using the world's largest molecular library
- **Challenge**
  - Massive computational power was required to realize Oxford's vision
- **Solution Highlights**
  - Built a working Public Grid dedicated to Life Science research
  - Accomplished the initial stage of the project in less than 12 months
- **Results**
  - Over 2.5M nodes from around the world are part of Grid.org
  - Total CPU time for project was over 190,000 years
  - Results published in Nature Drug Discovery



## Biodefense Projects

- **Anthrax Toxin Project**
  - First pass completed in 5 days
  - Screening time reduced from years to weeks
- **Smallpox Research Grid Project**
  - 11 active sites examined vs. 35M+ compounds
  - 44 lead molecules identified and turned over to USAMRIID

"These results are unprecedented. Had we done this using traditional methods, it would have taken years instead of less than 4 weeks."

Dr. Graham Richards, Chairman of the Chemistry Department at Oxford University and the Director of the Centre for Computational Drug Design.



Dr. Graham Richards, Chairman of the Chemistry Department at Oxford University, discussing the Smallpox Project at the hand-over event held at the British Embassy September 30<sup>th</sup>, 2003.

**Recipient of ComputerWorld's 2004 21st Century Achievement Award**

***"Judged best IT application in the world in Medicine."***

