NA4: Application Identification and Support

C. Loomis (CNRS), V. Floros (GRNET)

EGEE-II Final EU Review (CERN)
8-9 July 2008

www.eu-egee.org

Information Society and Media

Contents

- NA4: Application Identification and Support
- Adoption of Grid Technology
- Common APIs and Tools
- EGEE User Community
- Exploitation Plans
- Summary

- Presentation highlights important pointed raised in DNA4.2.2 and DNA1.2.2.
  - *Statistics broken down by date cover EGEE-II project.*
  - *Current status statistics are for June 2008.*

Goals & Organization

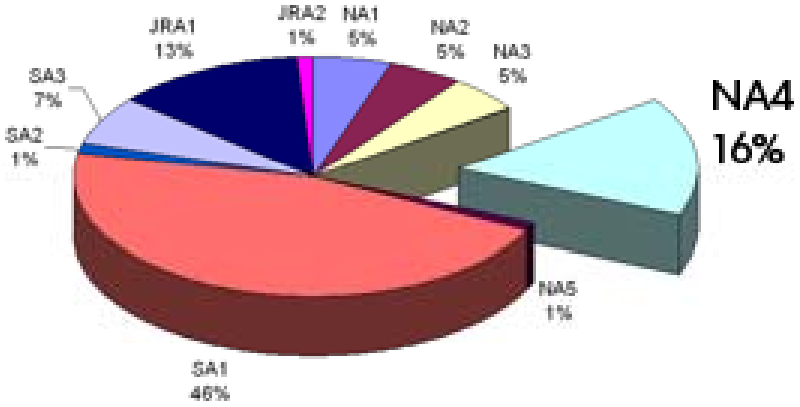
- **Expand use of EGEE infrastructure:**
  - **User**: Person exploiting EGEE services.
  - **Virtual Organization**: Unites individuals and organisations for common usage of the grid.
  - **Applications**: User codes, programs, and algorithms.
- **Ensure current users are satisfied.**

Steering Committee
Coordinator
Deputy Coordinator
VO Mgr. Group
NA4/NA1 Liaison
Astron. & Astrophysics
Comp. Chemistry.
Earth Science
Fusion
High-Energy Physics
Life Sciences
GILDA
GASuC

NA4 in Numbers

40 (42) Partners, 25 (27) Countries

EGEE-II Budget



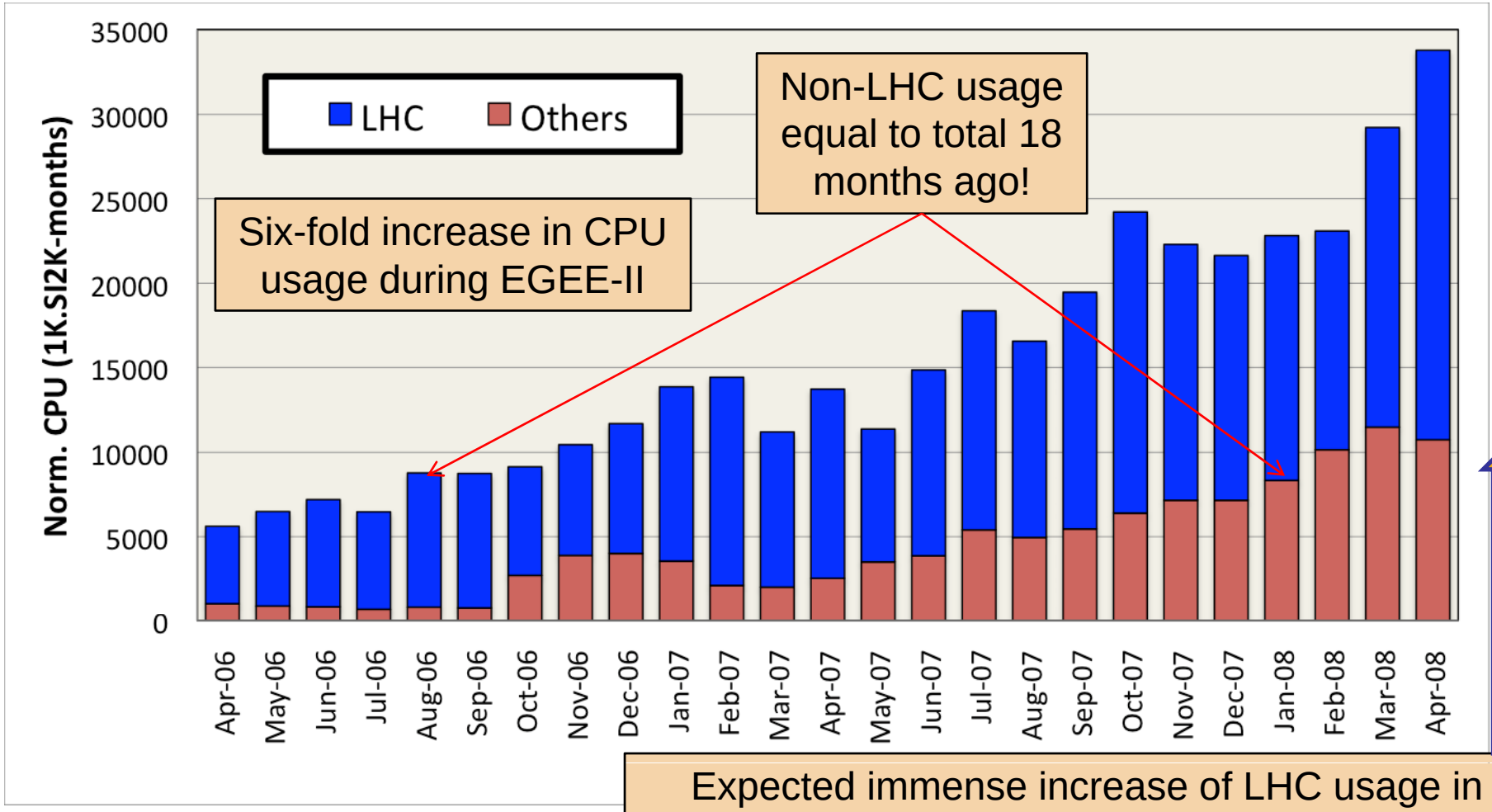
Federation	FTE	People
Cent. Europe	6	51
CERN	12	18
FR	16	93
DE/CH	3	17
IT	18	54
N Europe	3	31
Russia	2	6
SE Europe	5	79
SW Europe	11	29
UK/IRE	1	4
Asia	0	4
US	0	0
Total	77	386

27%

Adoption of Grid Technology

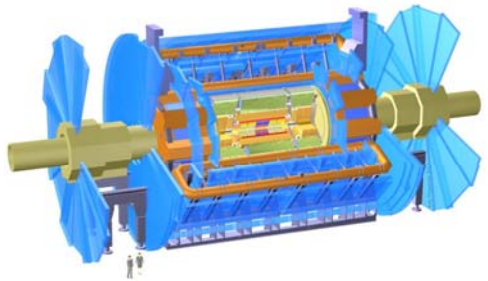
CPU Utilization

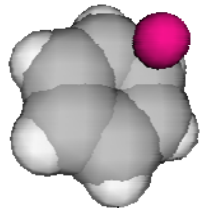
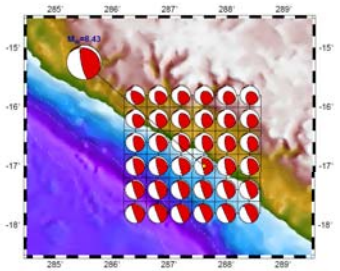
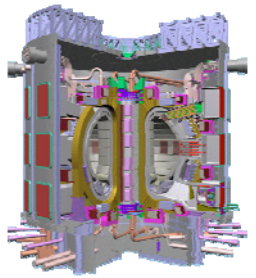
- **Recent level equal to ~32000 CPUs in continuous use.**



Reported Applications

- **1st year**
  - Growth in reported apps.
- **2nd year**
  - Transition: prototype to production

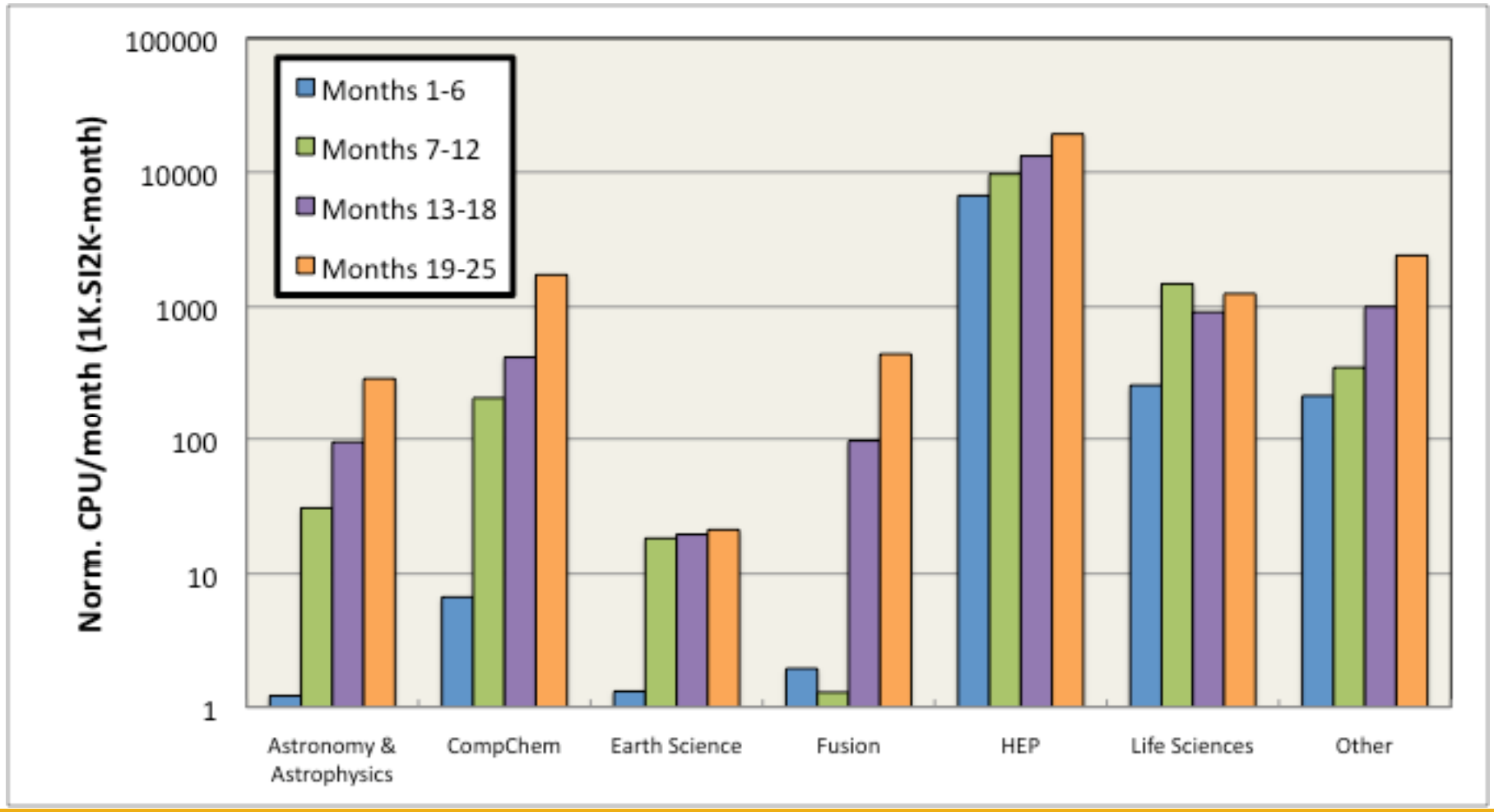




	6/2006	2/2007	1/2008
Astron. & Astrophysics	2	8	9
Comp. Chemistry	6	27	21
Earth Science	16	16	18
Fusion	2	3	4
High-Energy Physics	9	11	7
Life Sciences	23	39	37
Others	4	14	21
Total	**62**	**118**	**117**

Condensed Matter Physics
Comp. Fluid Dynamics
Computer Science/Tools
Civil Protection

Maturing User Communities

- **Continued strong use in developed disciplines.**
- **Prototyping to production for younger disciplines.**



Examples of Scientific Results

- **Earth Science**
  - Seismic noise calculation.
- **Fusion**
  - Ion kinetic transfer
  - Simulation of wall interactions
  - Stellarator optimization

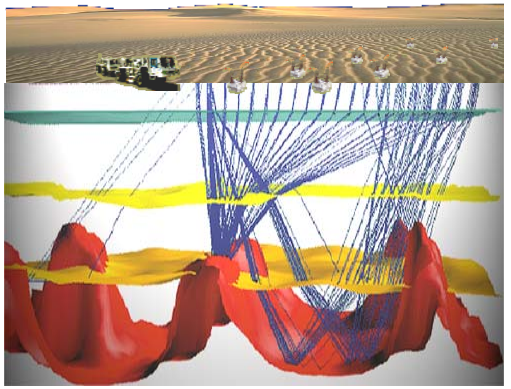
EGEE has been the driving force for achieving these scientific results by
- **Providing access to large amount of reliable computing resources**
- **Helping the establishment of new collaborations**

- **Drug Discovery (WISDOM)**
  - Malaria: 6/30 compounds similar or better than PepstatinA
  - Avian flu: 20% of compounds better than Tamiflu
  - Ongoing tests with compounds from later calculations.

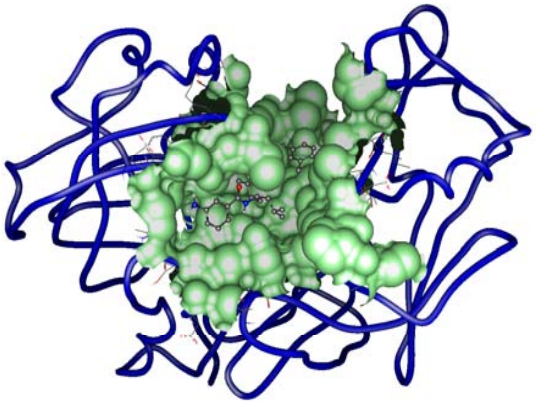
Industrial Participation

- **Collaboration with industry in NA4:**
  - Discuss with industry how to port applications to grid.
  - Network restrictions apply to commercial traffic.

- **Geocluster (CGGVeritas)**
  - Geoscience software package, used for example in petroleum search.
  - Made available to researchers on EGEE grid infrastructure.



- **WISDOM**
  - Collaboration with BioSolveIT.
  - Provided free licenses for docking calculation on EGEE.



License Models

- **Expanding community needs commercial software on the grid. Working to find good license models (focus on academic licenses):**
  - VO License Model
    - Used for comp. chemistry packages Gaussian and Turbomole.
    - Puts burden of enforcement on VO manager.
    - Inflexible and poorly adapted to workflow.
  - Client/Server License Model
    - Used by MATLAB Parallel Computing Toolkit.
    - Allows separate licenses for client and server.
    - More flexible and allows sites to provide a “resource”.
    - Currently in process of running a trial with EGEE users.
- **Collaboration with MathWorks:**
  - Shows EGEE becoming target platform for software vendors.
  - Jointly written technical report is evidence on engagement on both sides (http://doc.cern.ch//archive/electronic/egee/tr/egee-tr-2008-001.pdf).

Common APIs and Tools

Middleware

- **Middleware critical for success of NA4:**
  - gLite provides important core services.
  - Application-level code and services supplements those services.

- **NA4 contributions:**
  - Improvements to gLite and gLite deployment.
  - Development of high-level services.
  - Identification of external services and packages.

Middleware

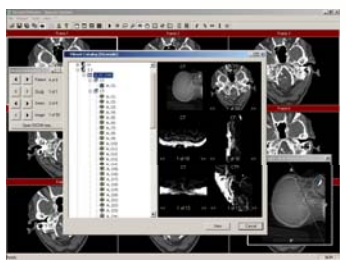
- **Extensive testing of services**
  - HEP and life science communities leaders in this area
  - Recent work with gLite WMS indicative of positive results.
  - Advanced testing of prototypes, like Hydra for data encryption.

- **Collaborate through targeted working groups:**
  - MPI, SDJ, MDM etc.
  - *Issue: Ensure recommendations are acted upon.*

Development

Direct development has usually resulted in generic service used by several scientific communities.

- **AMGA: Metadata catalog.**
- **Ganga: Job submission framework.**
- **DIANE: Master/slave task manager.**
- **Dashboard: VO and user-level monitoring.**
- **MOTEUR: Workflow engine.**
- **MDM: Medical Data Management**



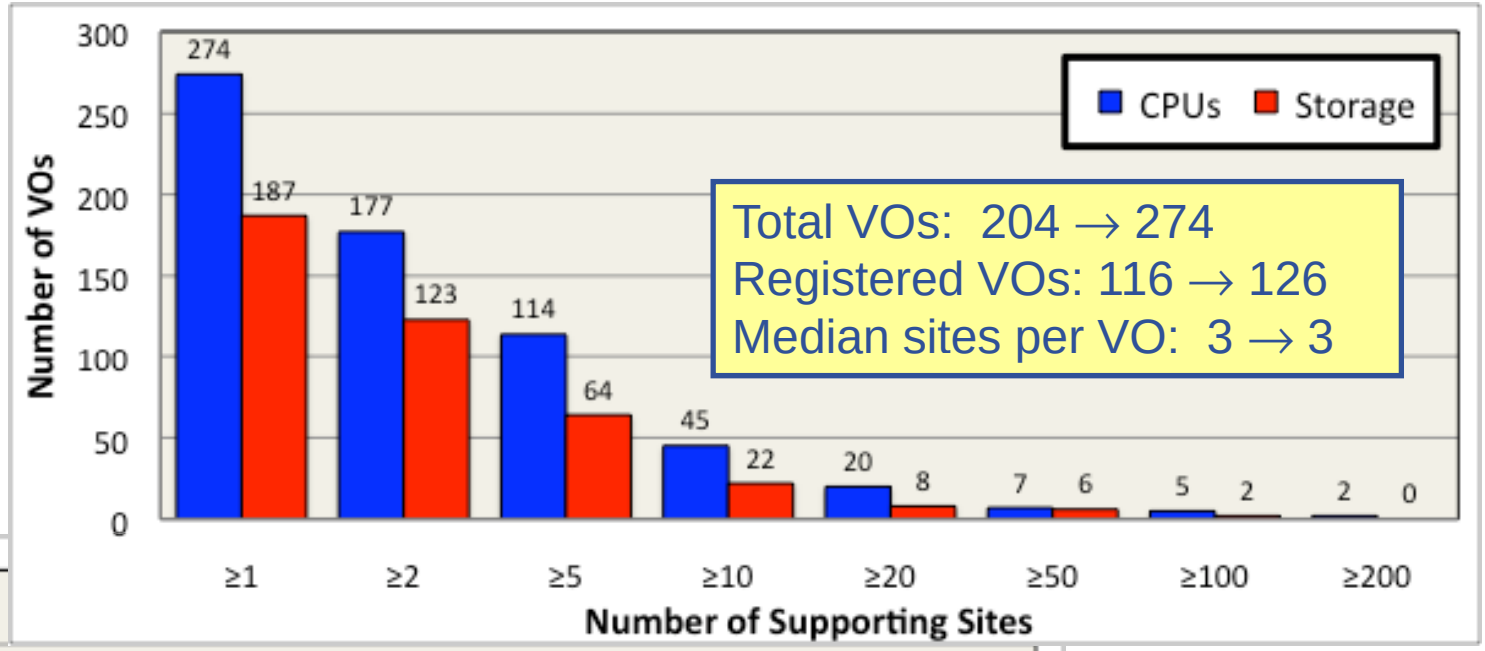
RESPECT

- **Rec. External Software Pkgs. for the EGEE Community**
  - Identify useful, 3rd-party software that works with gLite.
  - Make people aware of that software to avoid duplicated efforts.
  - http://egeena4.lal.in2p3.fr/index.php?option=com_content&task=view&id=71&Itemid=63
- **Current packages:**
  - GridWay: Grid metascheduler.
  - P-GRADE Portal: Workflow oriented graphical environment.
  - Ganga: Job submission framework.
  - DIANE: Master/slave task manager.
  - i2glogin: Interactive login to grid nodes.
  - *GReIC*: Database access and management.
- **Discussing with int.eu.grid to add more of their products to the RESPECT program.**

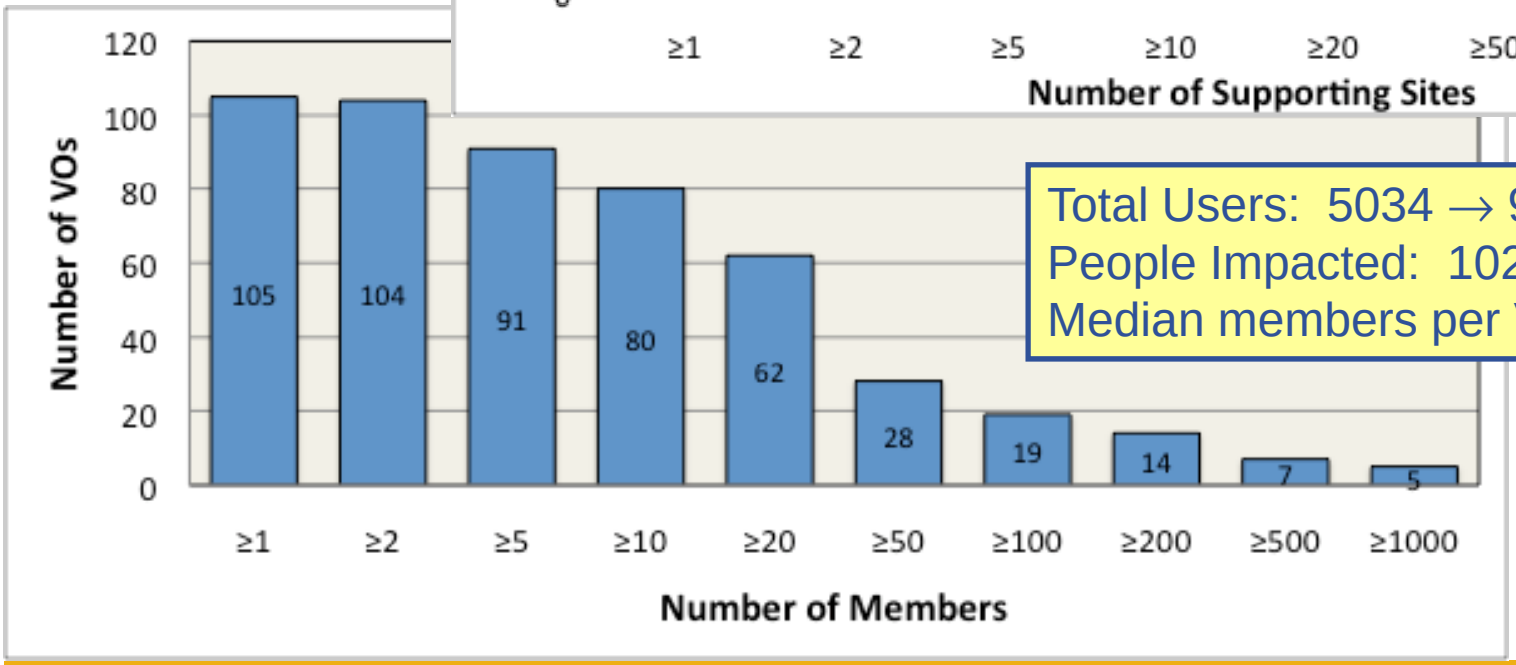
EGEE User Community

Virtual Organizations

EGEE is an open infrastructure; not all VOs register with the project.



Total VOs: 204 → 274
Registered VOs: 116 → 126
Median sites per VO: 3 → 3



Total Users: 5034 → 9000
People Impacted: 10200 → 14000+
Median members per VO: 18 → 21

Support Services

- **EGEE has comprehensive and efficient support system.**

- **Support from other activities:**
  - GGUS (SA1), Training (NA3), Middleware (JRA1)

- **Support activities within NA4:**
  - Administrative support: OAG, VO Mgrs. Group
    - Improved relations between VOs and operations.
    - http://cic.gridops.org/index.php?section=home&page=volist
  - User support: UIG, NA4 Portal
    - Improved documentation.
    - http://egee-uig.web.cern.ch/egee-uig/production_pages/UIGindex.html
  - Application porting support: GILDA, GASuC

Previous Support Issues

All of these issues have been resolved in EGEE-III via structural changes to the NA4 activity and tasks.

- **Resource Allocation:**
  - *Issue: No EGEE computing and storage resources to allocate to new virtual organizations as bridge to production use.*
  - Solution: Create seed resources for new communities.
- **Application Porting Support:**
  - *Issue: Porting support is most efficient "in person". How to finance travel for unfunded people?*
  - Solution: Fund to partially finance travel to GASuC.
- **Direct User Support:**
  - *Issue: Providing user support to "outside" users.*
  - Solution: Team within NA4 to provide this type of support.

Application Porting Support

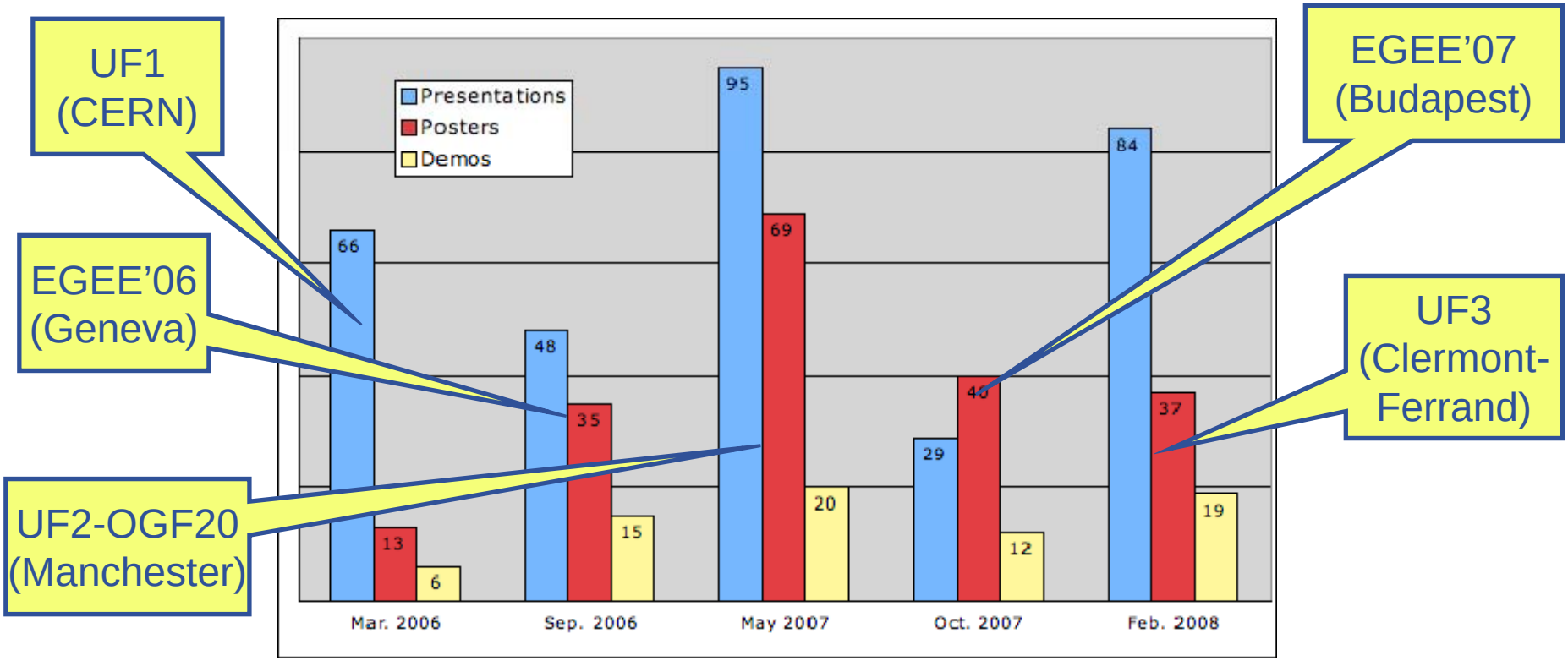
- **Porting an application to the grid usually requires expertise that new virtual organizations do not have.**

- **Grid usage can start either on training or production infrastructure**
  - Training infrastructure (with NA3):
    - https://gilda.ct.infn.it/
    - GILDA team advises new users on EGEE grid technology.
    - t-infrastructure provides resources for testing new applications.
  - Porting to production service:
    - http://www.lpds.sztaki.hu/gasuc/
    - Some prefer porting directly to production service.
    - GASuC (SZTAKI/Hungary) now offers hands-on consulting to do this.

- **Direct support from NA4 partners:**
  - Motivated to port “local” applications.

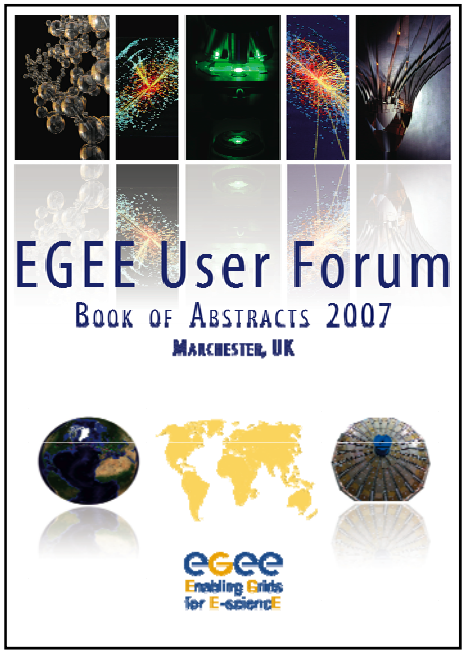
Community Building

- **Meetings for specific scientific disciplines.**
- **Strong participation in technical working groups.**
- **User Forums & EGEE Conferences.**



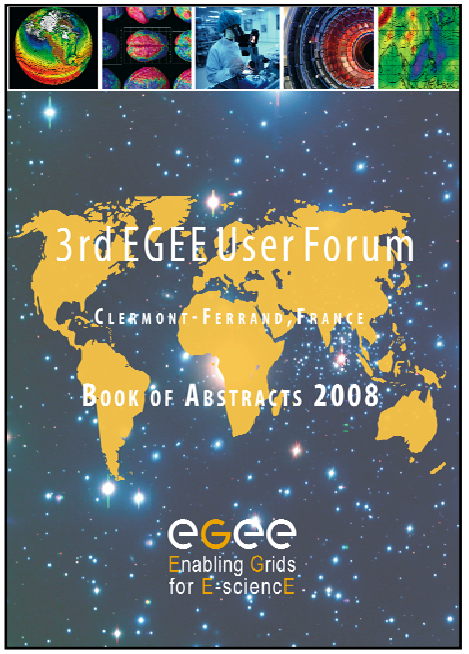
User Forum Results

- **Rich scientific program.**
- **Some contributions submitted to referred journals.**



ISBN: 978-92-9083-303-1

http://indico.cern.ch/conferenceDisplay.py?confId=7247



ISBN 978-92-9083-310-9

http://indico.cern.ch/conferenceDisplay.py?confId=22351

Collaborating Projects

- **Community building is also pursued through interaction with various collaborating projects**
  - Share resources among communities
  - Re-user application software
  - Transfer scientific results and applications between projects
- **Liaise via EGEE Conferences and User Forums**
- **In EGEE-III collaborations are formalized through MoUs**

Exploitation Plans

- **Detailed exploitation plans for each sector given in final periodic report. Generally, plans are to expand number, size, and complexity of ported applications.**

- **EGEE-III**
  - Provides grid infrastructure for next two years.
  - EGEE-II experience improved NA4 structure in EGEE-III.
  - All current disciplines will continue into EGEE-III.
  - Add Grid Observatory activity.

- **Future exploitation depends on having a stable, production platform available for the long-term.**

Summary

- **Adoption of grid tech. and growth of user community:**
  - 6x increase in CPU utilization over life of project
  - Use by a set of diverse VOs and scientific disciplines.
- **Work on common APIs and tools:**
  - Improvement of gLite itself through testing and enhancements.
  - Direct development of tools.
  - Identification of third-party tools via RESPECT.
- **Scientific disciplines continue with EGEE-III:**
  - Expand number, size, complexity of ported applications.
  - Structural and task changes should address previous issues.
  - Challenge: Effectively support large and growing community.
  - Strong participation from people not financially supported by EGEE.