



Enabling Grids for E-science

NA4: Application Identification and Support

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8-9 July 2008*

www.eu-egee.org



- **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.*

- **Expand use of EGEE infrastructure:**
 - **User:** Person exploiting EGEE services.
 - **Virtual Organization:** Groups of users federating resources.
 - **Applications:** User codes, programs, and algorithms.

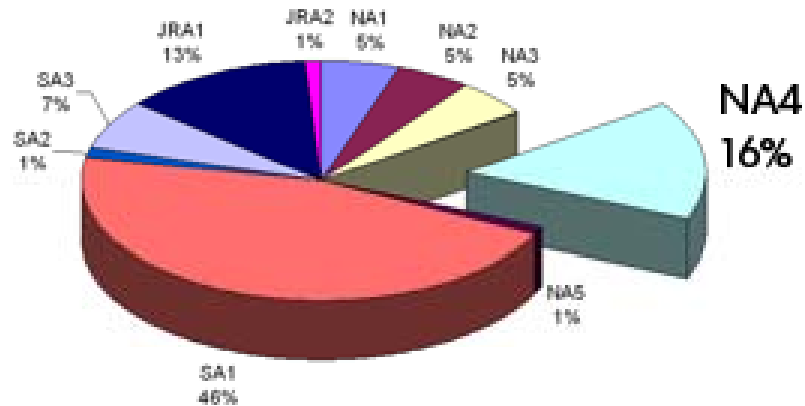
- **Ensure current users are satisfied.**

Steering Committee	
Coordinator	C. Loomis
Deputy Coordinator	V. Floros
VO Mgr. Group	F. Schaer
NA4/NA1 Liaison	F. Harris
Astron. & Astrophysics	C. Vuerli
Comp. Chemistry.	M. Sterzel
Earth Science	M. Petitdidier
Fusion	F. Castejon
High-Energy Physics	M. Lamanna
Life Sciences	C. Blanchet V. Breton J. Montagnat
GILDA	R. Barbera
GASuC	G. Sipos

40 (42) Partners, 25 (27) Countries



EGEE-II Budget

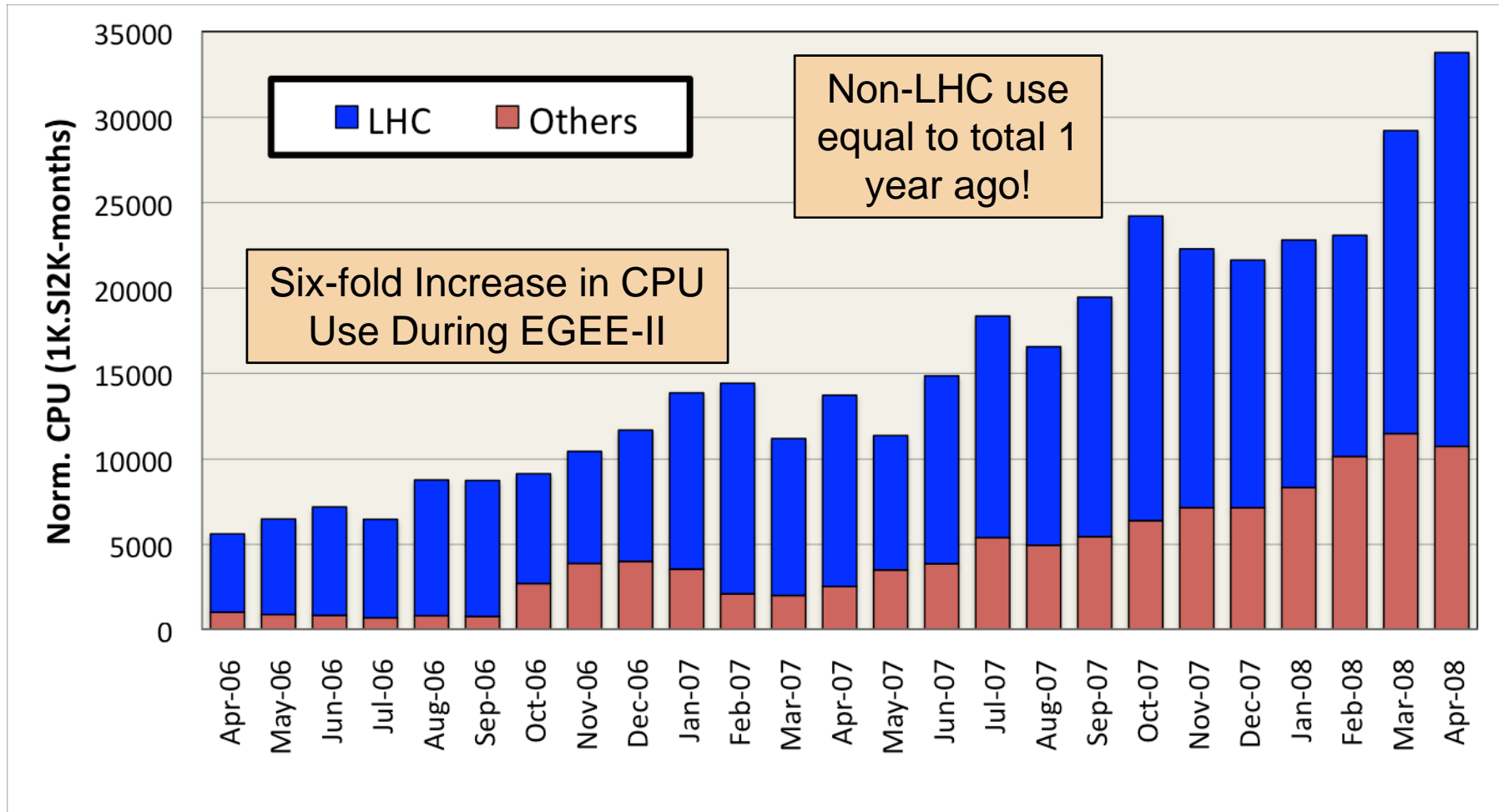


Federation	FTE	People
Cent. Europe	6	51
CERN	12	18
FR	16	93
DE/CH	3	17
IT	18	54
N Europe	3	31
Russia	2	6
SE Europe	5	79
SW Europe	11	29
UK/IRE	1	4
Asia	0	4
US	0	0
Total	77	386

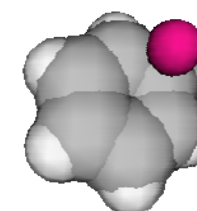
27%

Adoption of Grid Technology

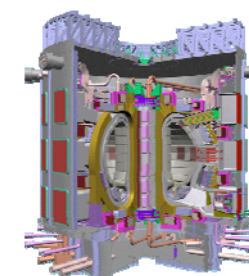
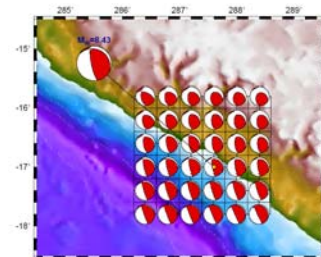
- Recent level equal to ~32000 CPUs in continuous use.



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

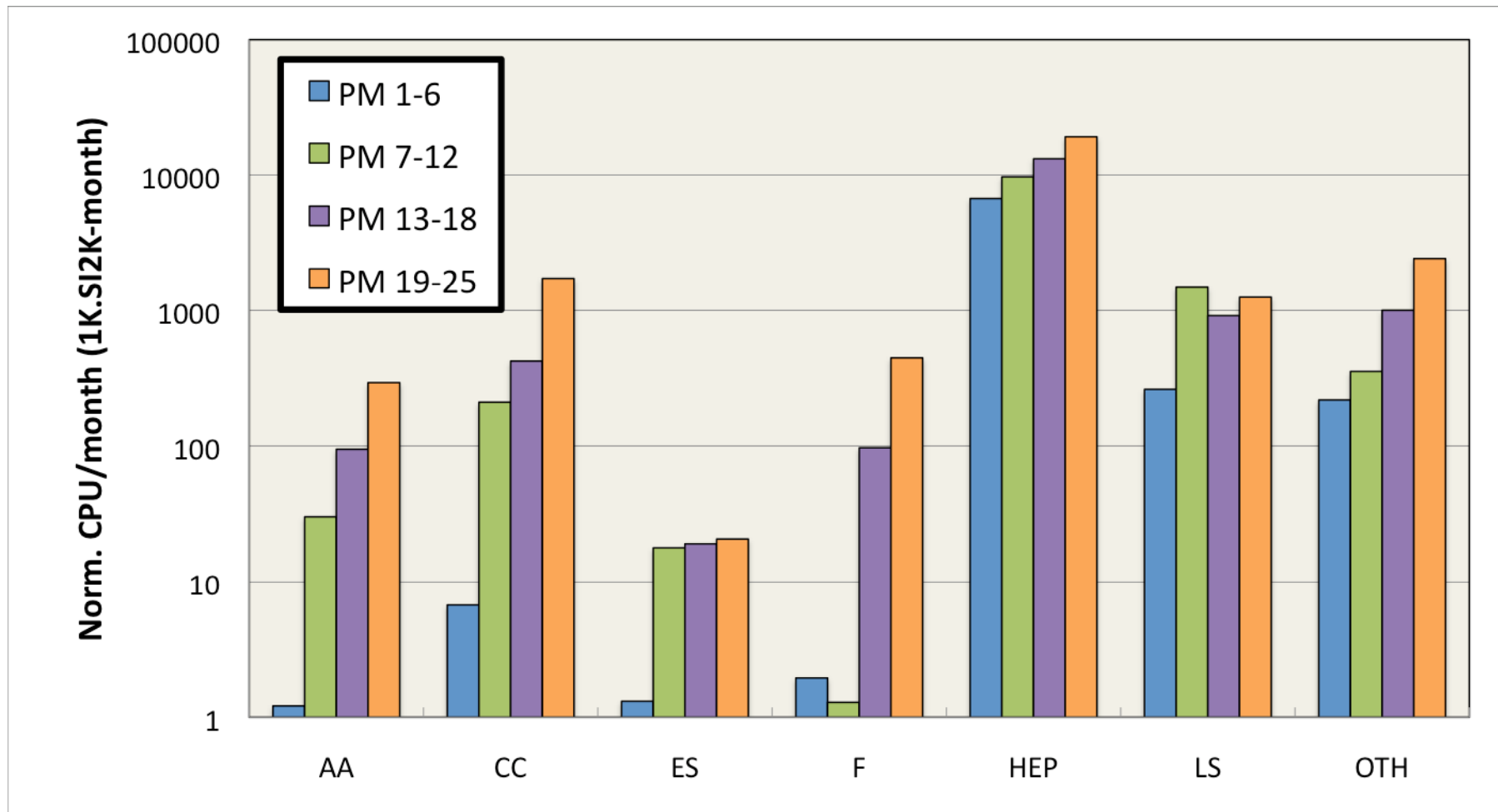


	6/2006	2/2007	1/2008
Astron. & Astrophysics	2	8	9
Comp. Chemistry	6	27	21
Earth Science	16	16	18
Fusion	2	3	4
High-Energy Physics	9	11	7
Life Sciences	23	39	37
Others	4	14	21
Total	62	118	117



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

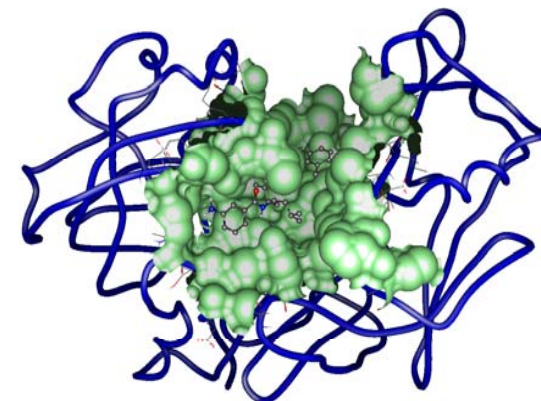
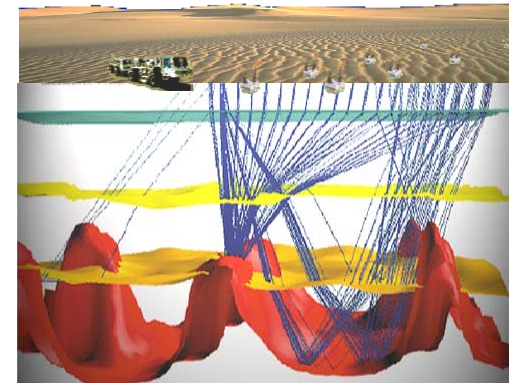
- Continued strong use in developed disciplines.
- Prototyping to production for younger disciplines.



- **Collaboration with industry in NA4:**
 - Discuss with industry how to port applications to grid.
 - Network restrictions discourage direct collaboration on infrastructure.

- **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.



- **Expanding community needs commercial software on the grid.**
Working to find good license models:
 - 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 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.



- **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: improve parallel job support on grid
 - SDJ: reduce scheduling latencies for quasi-interactive apps.
 - MDM: mgt. of medical data on the grid
 - Priority: provide mechanisms to define VO-level job priorities
 - Portal: define best practices for grid portals
 - VO Config.: improve sharing via simpler VO configuration
 - DB Access: improve database access from grid
 - *Issue: Ensure recommendations are acted upon.*

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

- AMGA: Metadata catalog.



- Ganga: Job submission framework.



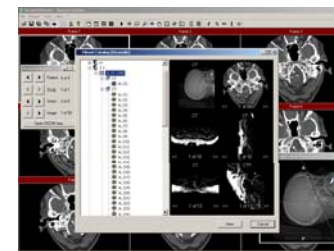
- DIANE: Master/slave task manager.



- Dashboard: VO and user-level monitoring.



- MOTEUR: Workflow engine.

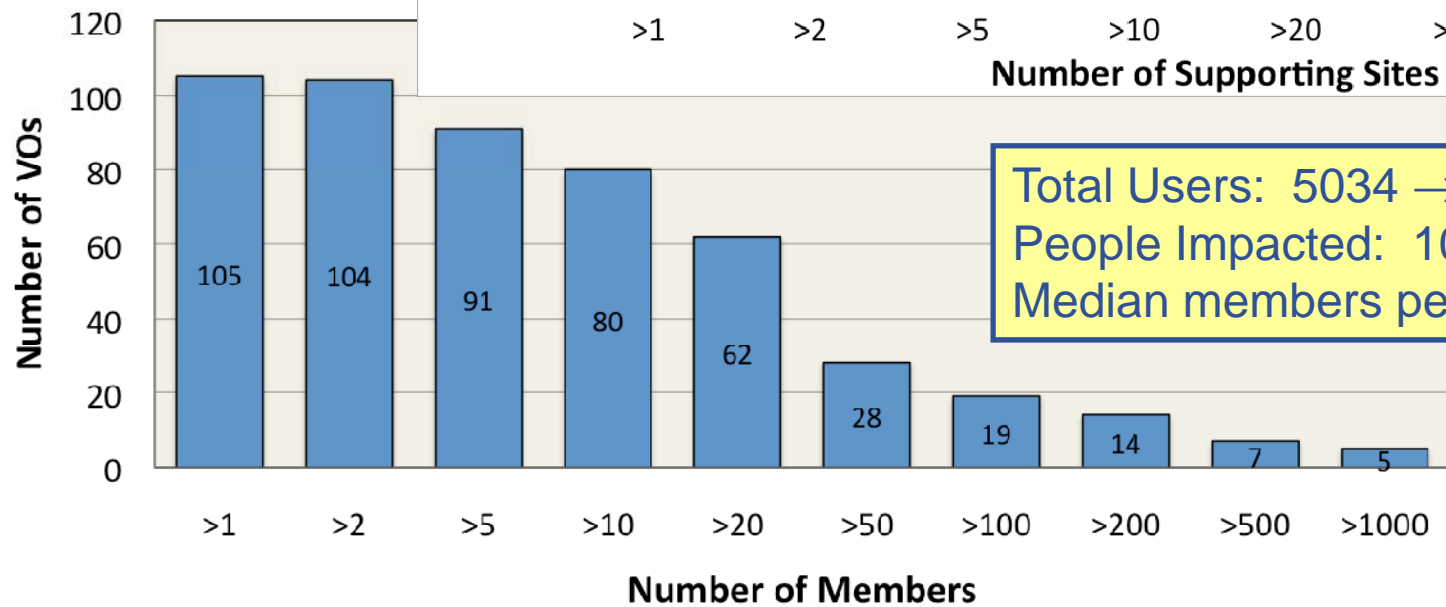
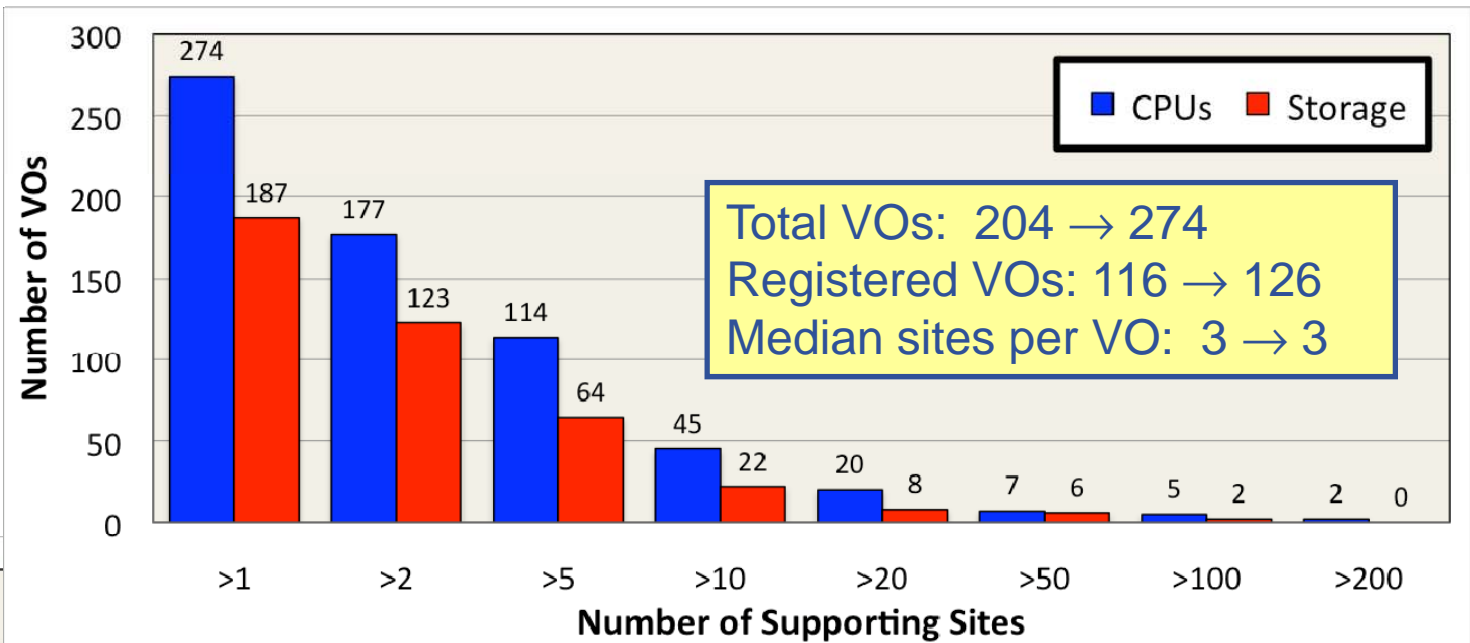


- MDM: Medical Data Management

- **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.
 - GRe/C: Database access and management.
- **Discussing with int.eu.grid to add more of their products to the RESPECT program.**

EGEE User Community

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



- **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

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:**

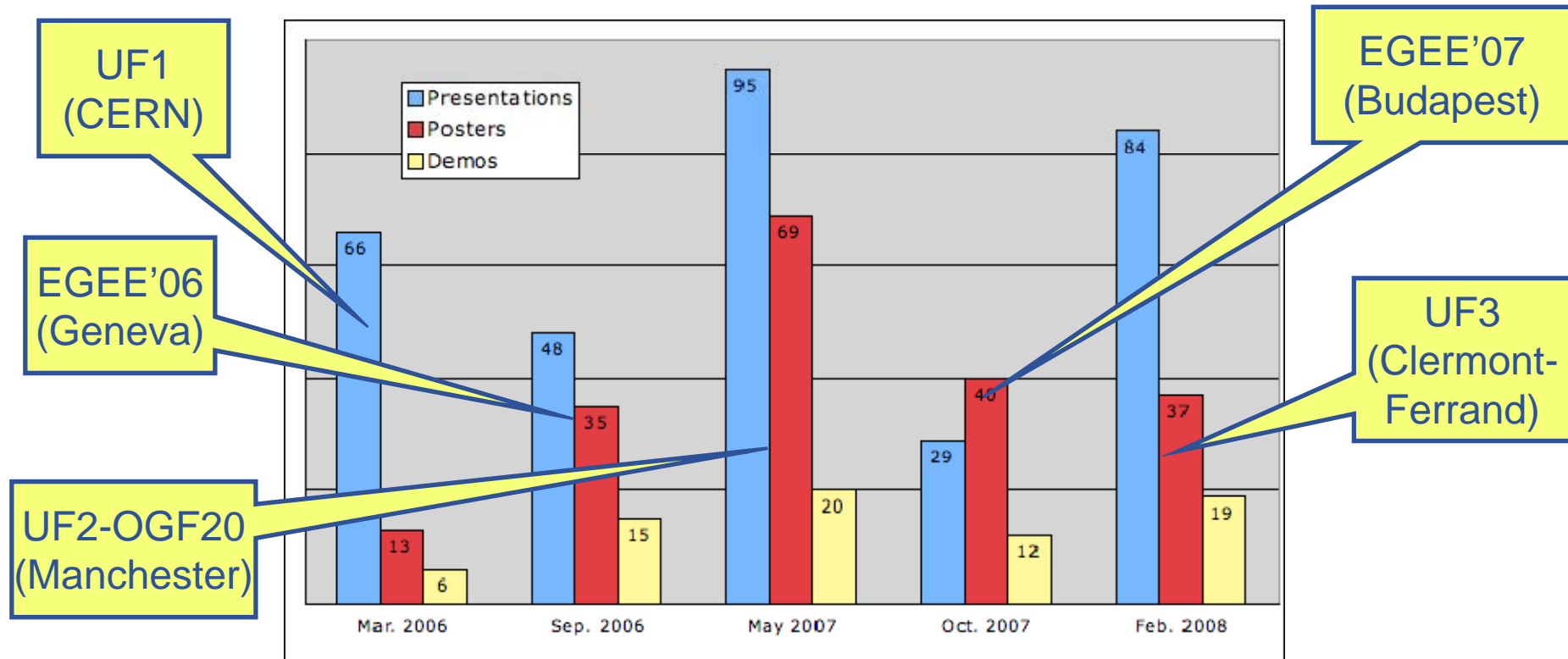
- *Issue: Porting support is most efficient “in person”. How to finance travel for unfunded people?*
- Solution: Fund to partially finance travel to GASuC.

- **Direct User Support:**

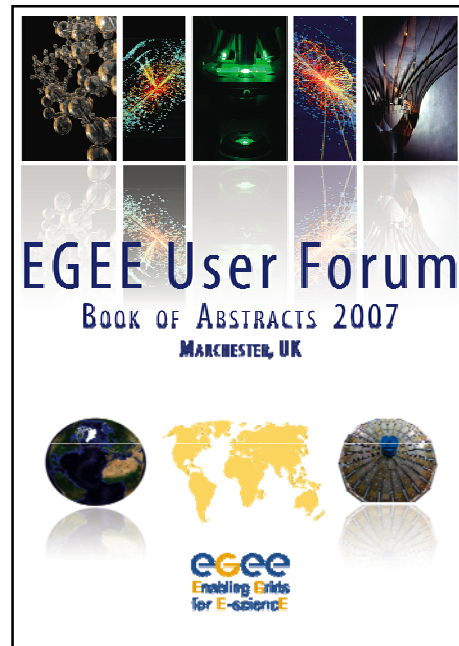
- *Issue: Providing user support to “outside” users.*
- Solution: Team within NA4 to provide this type of support.

- **Porting an application to the grid usually requires expertise that new virtual organizations do not have.**
- **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) now offers hands-on consulting to do this.
- **Direct support from NA4 partners:**
 - Motivated to port “local” applications.

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



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



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



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

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

- **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**

- **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.
- **Long-term exploitation depends on having a stable, production platform available.**

- **Adoption of grid tech. and growth of user community:**
 - 6x increase in CPU utilization over life of project
 - Use by diverse set of 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.