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PSNC

Science Gateways over the last decade – lessons learned and best practices from the QCG middleware, applications and portal technologies

9th International Workshop on Science Gateways

19-21 June 2017

CRC
CENTER FOR RESEARCH COMPUTING

NSF

TCSC
IEEE

e-Infrastructure
Cyberinfrastructures

Scientific Use Cases

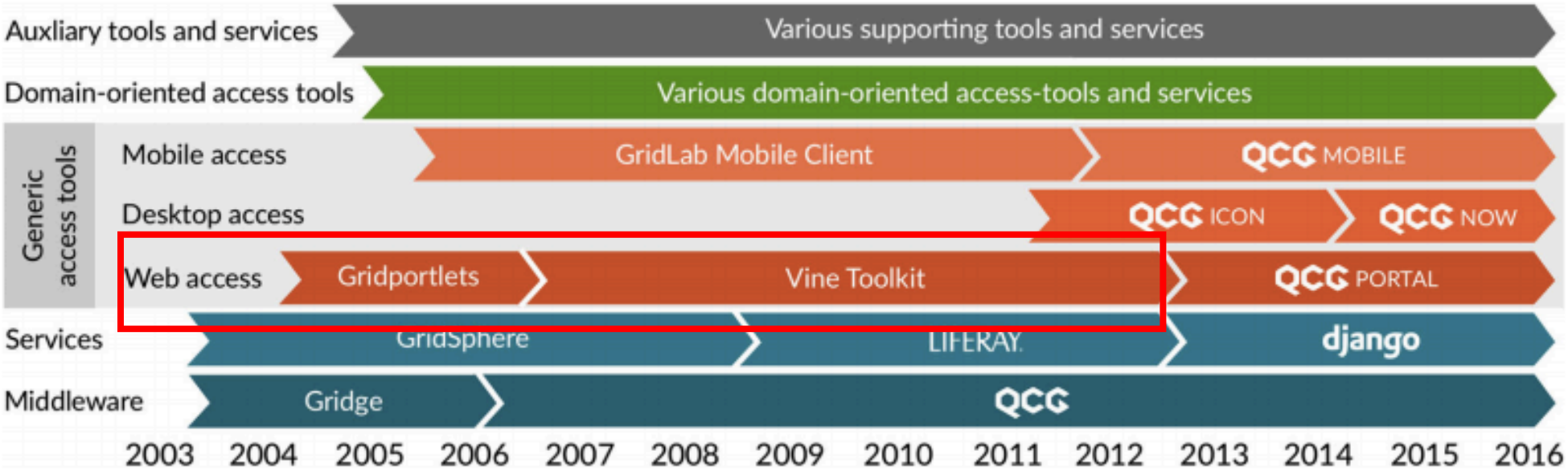
Scientific Use Cases II

Science Gateways

Components and platforms

Collaborative Science Gateways

Again a bit of history…



Some users questions…

How long do I have to wait for data analysis and visualization?

How can I check if computational resources are available?

Is real-time remote visualization possible today?

Can I use my/legacy GUI or I am forced to learn a new tool?

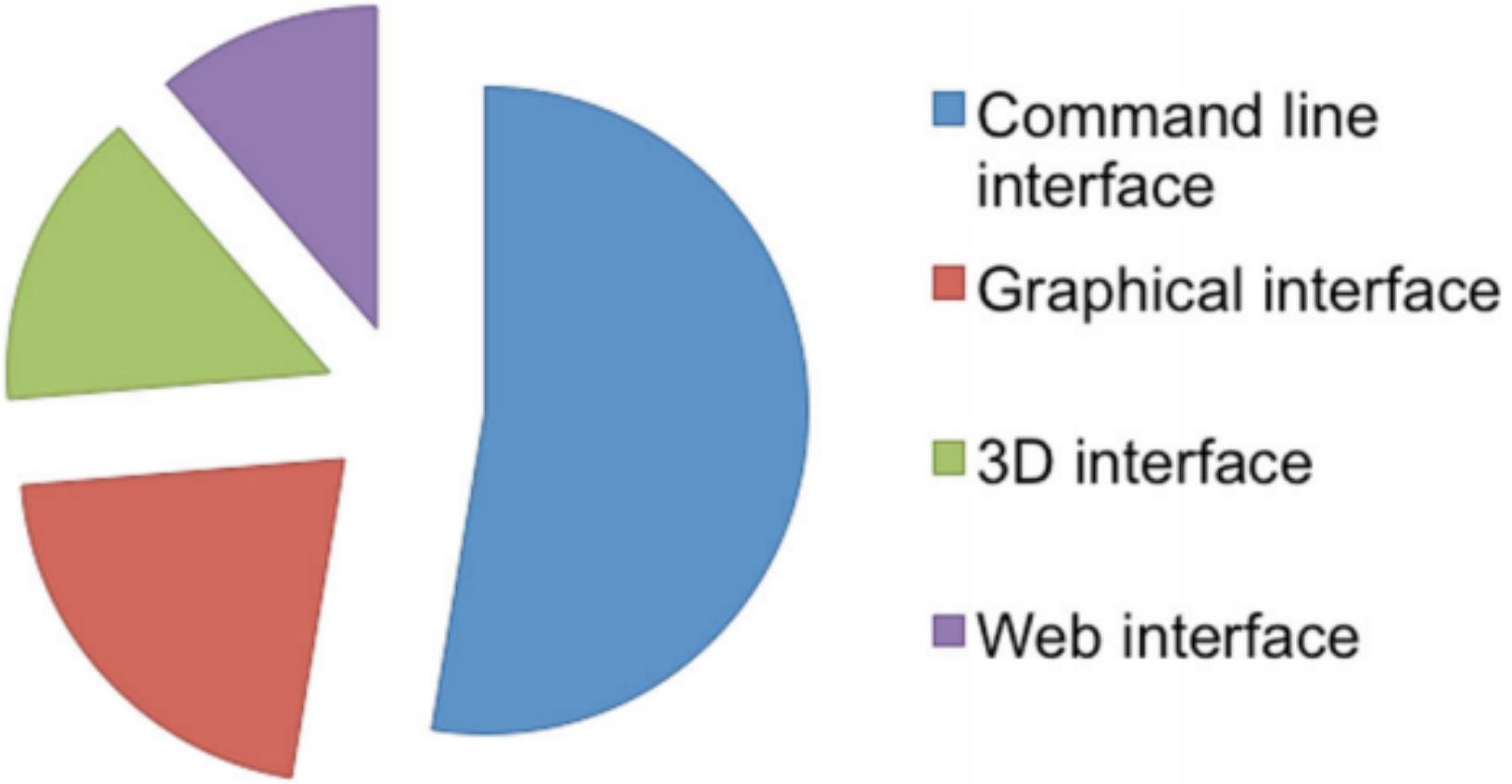
How can I share my results in an interactive way with other users?

Do I have to move my big data sources? Where?

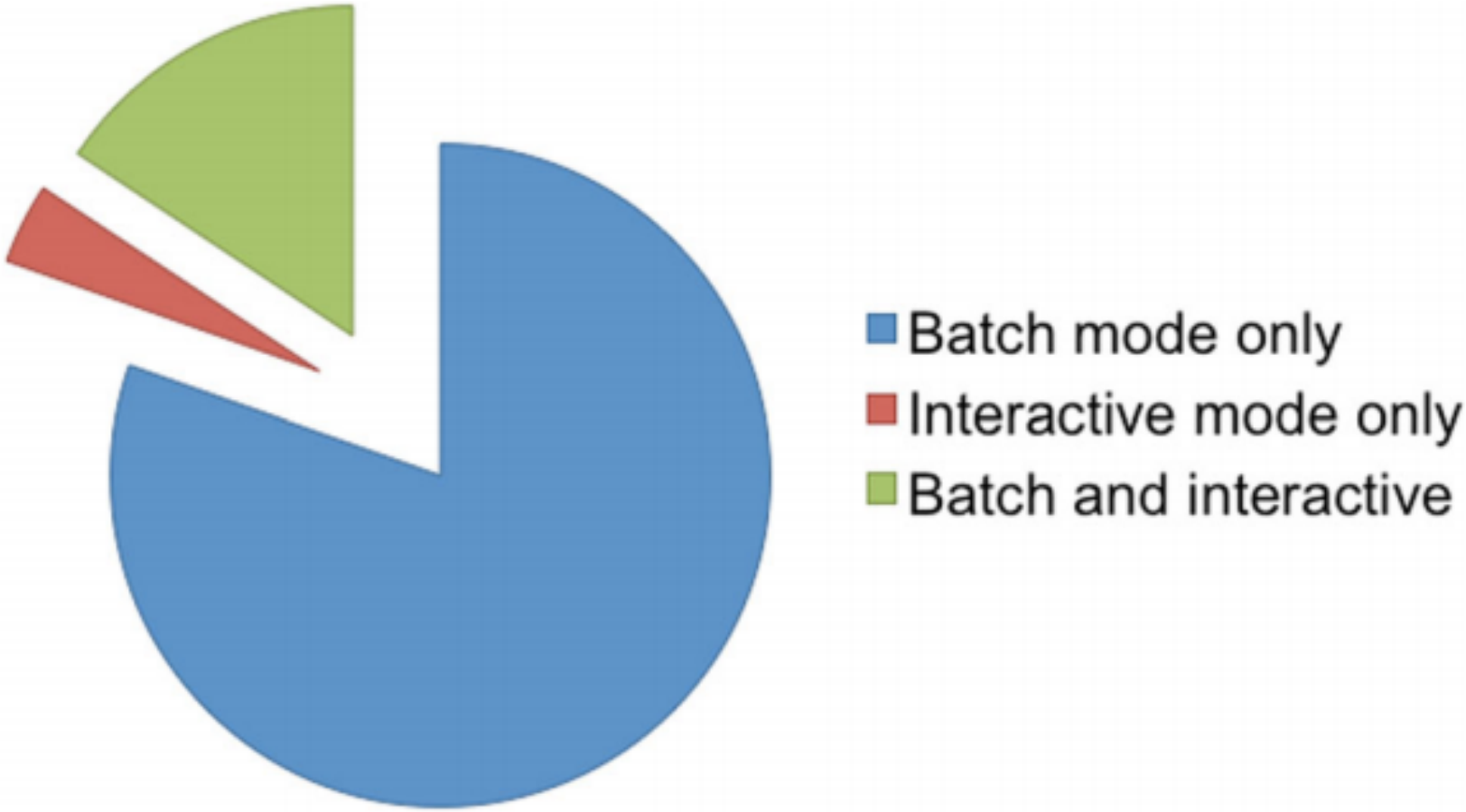
How can I steer my computations during run-time?

How can I benefit from high-speed network?

Users preferences



Reality


Batch mode only
Interactive mode only
Batch and interactive

PSNC POZNAŃ SUPERCOMPUTING AND NETWORKING CENTER

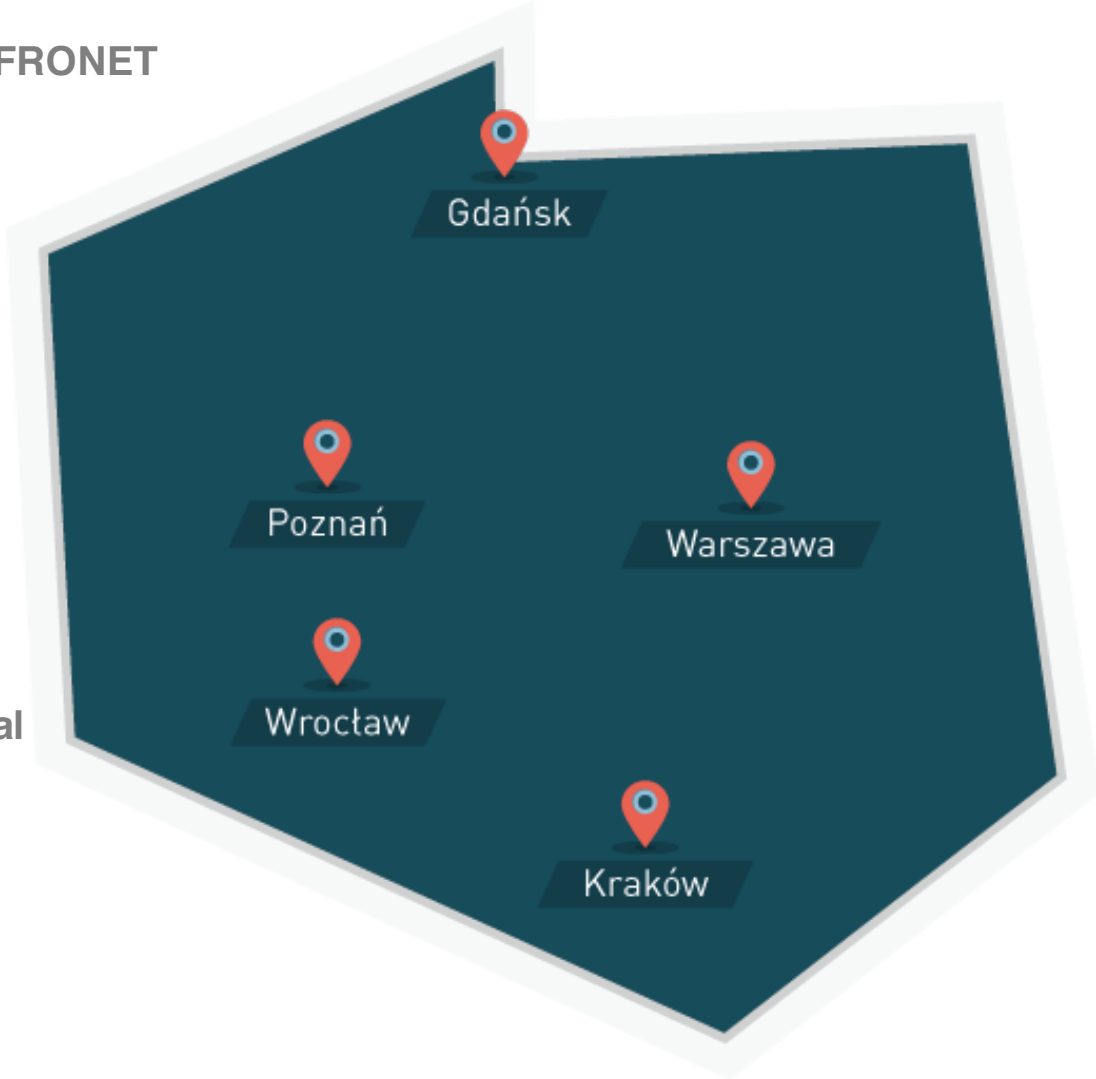
Academic Computer Centre CYFRONET AGH, Kraków (Coordinator)

Tricity Academic Computer Centre, Gdańsk

Poznan Supercomputing and Networking Center, Poznań

Interdisciplinary Centre for Mathematical and Computational Modelling, Warszawa

Wroclaw Centre for Networking and Supercomputing, Wrocław



Computing resources

- 5+ PTFLOPS
- 90 000+ cores

Scientific Software

- 500+ applications, tools, libraries
- apps.plgrid.pl

PL GRID

Storage

- 20+ PB
- fast scratch
- distributed access

Tools for collaboration

- project tracking (JIRA)
- version control (Git)
- teleconferencing (Adobe Connect)

Computational Cloud

- PaaS based on OpenStack

ci task WCSS CYFRONET icm PCSS

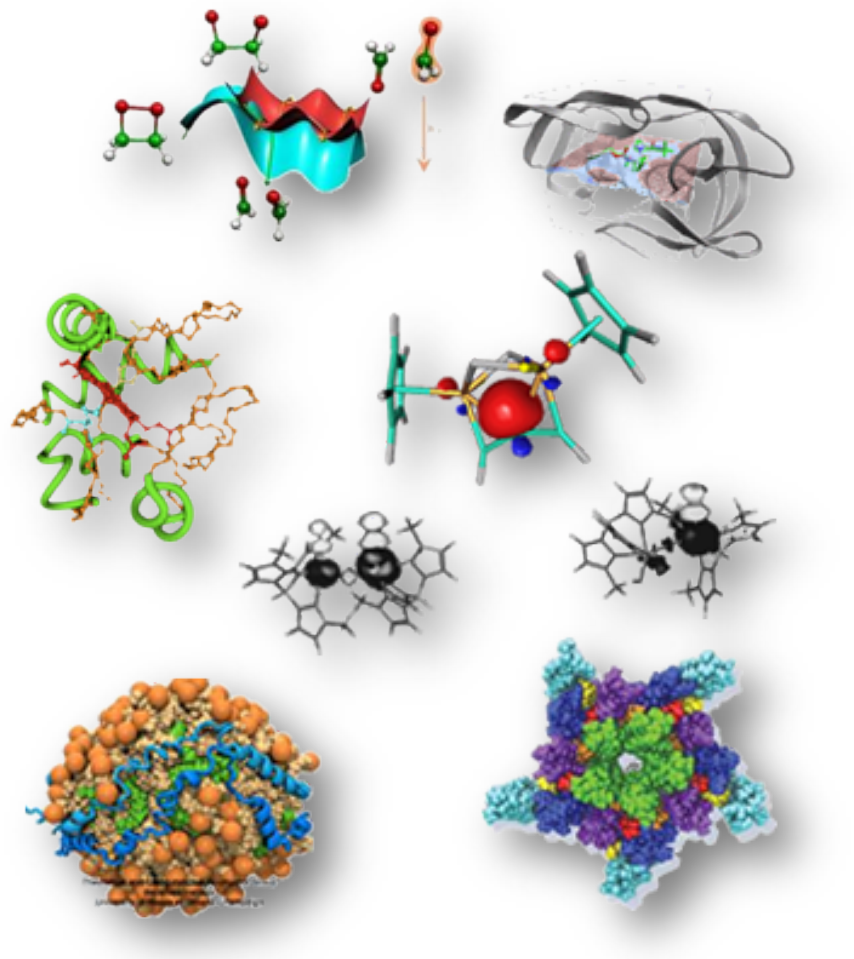
- The PLGrid Infrastructure is available free of charge for Polish researchers and all those engaged in scientific activities in Poland
- On-line registration through PLGrid Users' Portal - portal.plgrid.pl
- User verification based on Polish Science Database - www.nauka-polska.pl

On PLGrid Users Portal user can

- apply for access to tools and services
- monitor utilization of resources
- manage their computational grants and grid certificates

Access to all PLGrid resources through **one account** and **one passphrase** (or grid certificate)

- **Chemistry & Biology:** ADF, AMBER, CFOUR, CP Dalton, GAMESS, Gaussian, Molcas, Molpro, MOPAC, NWChem, Open Babel, TURBOMOLE, AutoDock/AutoGrid, BLAST, Clustal, Siesta, Quantum Espresso, VASP (user's own license required), CPMD, Gromacs, NAMD
- **Physics:** FLUENT, Meep, OpenFOAM
- **Nanotechnology:** ABINIT, Quantum Espresso, NAMD
- **Multipurpose:** Mathematica, MATLAB
- **Development:** Intel, PGI, GNU compilers, MKL, CUDA, MPI, OpenMP, Alinea, Python, R, Ruby
- **Databases**
- **Sequential, Parallel (MPI, OpenMP), interactive runs possible**
- **Users' own licences could be used**



https://apps.plgrid.pl/

- Rimrock – Robust Remote Process and Job Controller
  - ease jobs submission and management on remote servers
  - submit.plgrid.pl
  - team:
    - Daniel Harężlak
    - Marek Kasztelnik
    - Maciej Pawlik

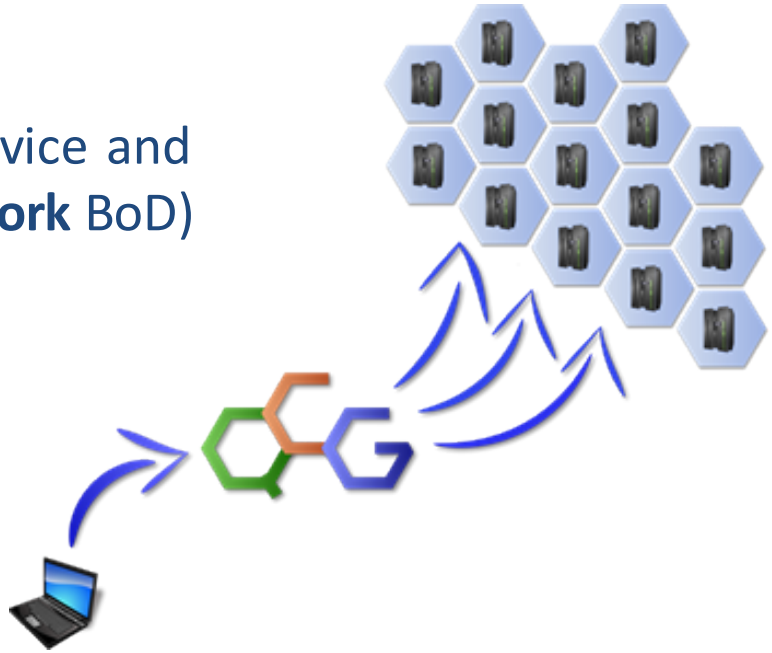
- PLG-Data team
  - easy access to data through web browser or other tools
  - data.plgrid.pl
  - team:
    - Tomasz Gubała

PLG-Data

Quality in Clouds & Grids (QCG) middleware

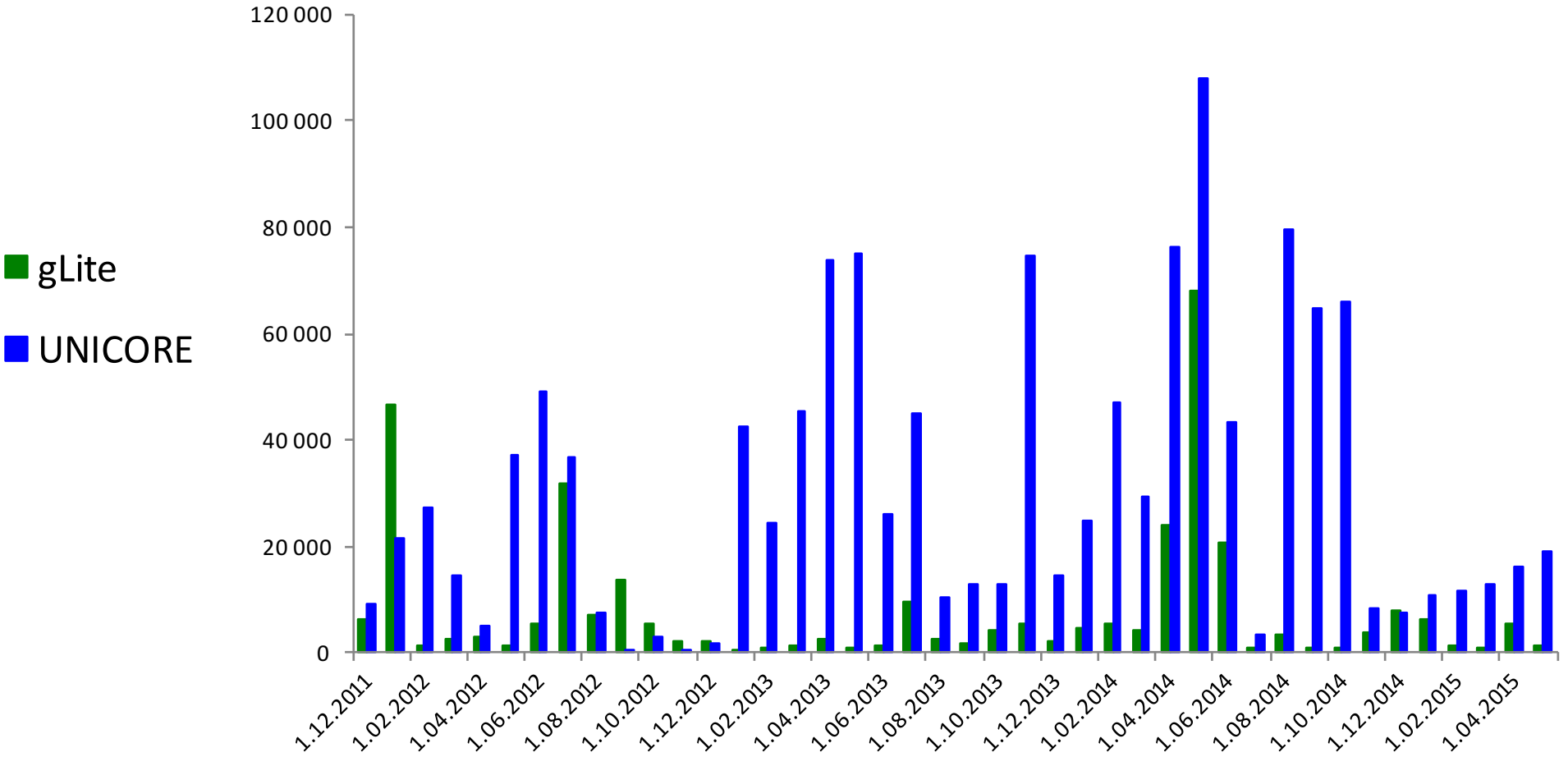
www.qoscosgrid.org

- A set of **integrated lightweight services and user tools** for **job management & steering** in various **HPC/HTC** and **Cloud** (work in progress) environments.
- **Advance reservation** capabilities (Quality of Service and co-allocation of **computing resources** and **network** BoD)
- Dynamic application **progress monitoring** and multi-protocol (SMTP, XMPP, SOAP, JSON) **notifications** capabilities + **Python SDKs**
- External **in-situ visualization apps** and **web tools** available

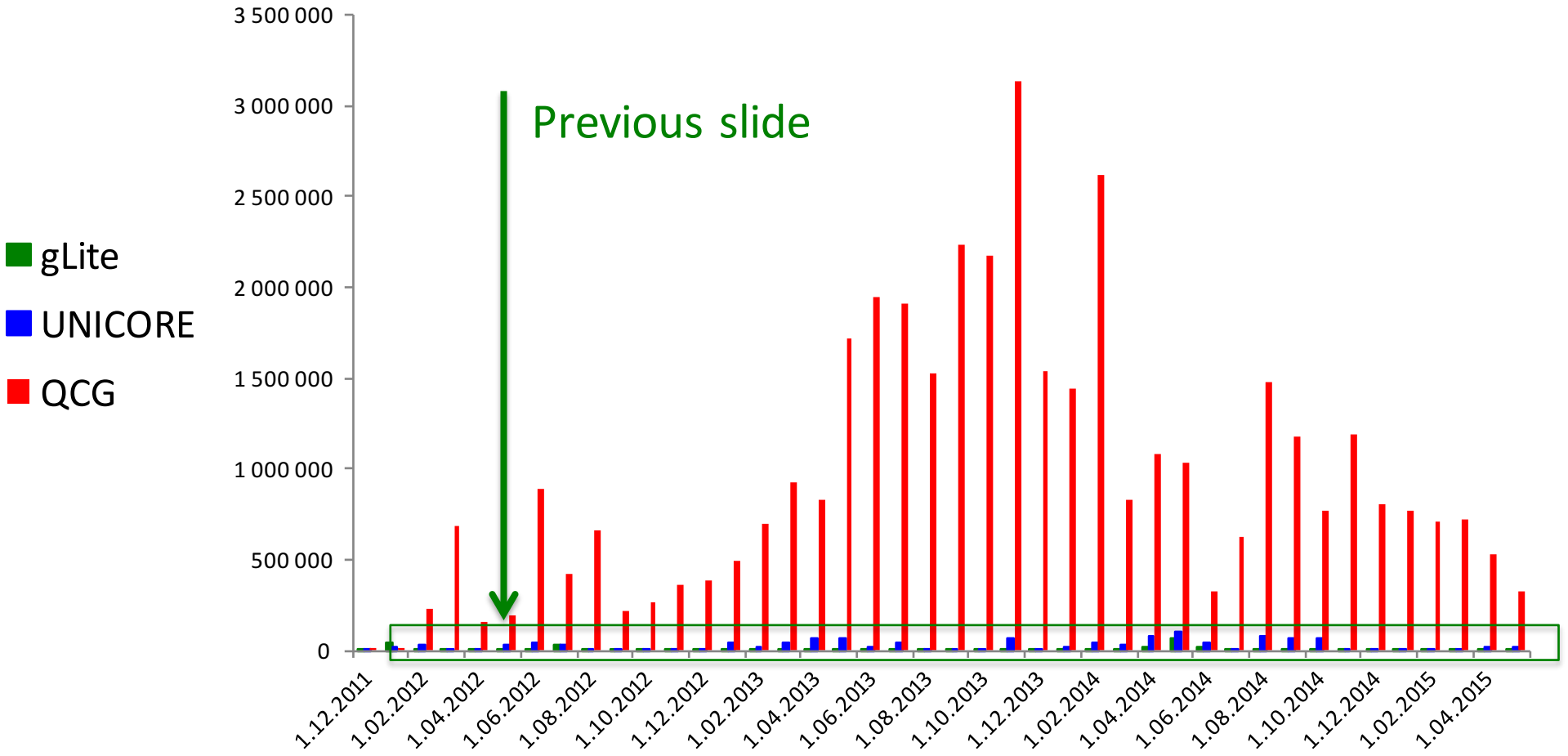


QCG quality in cloud and grid

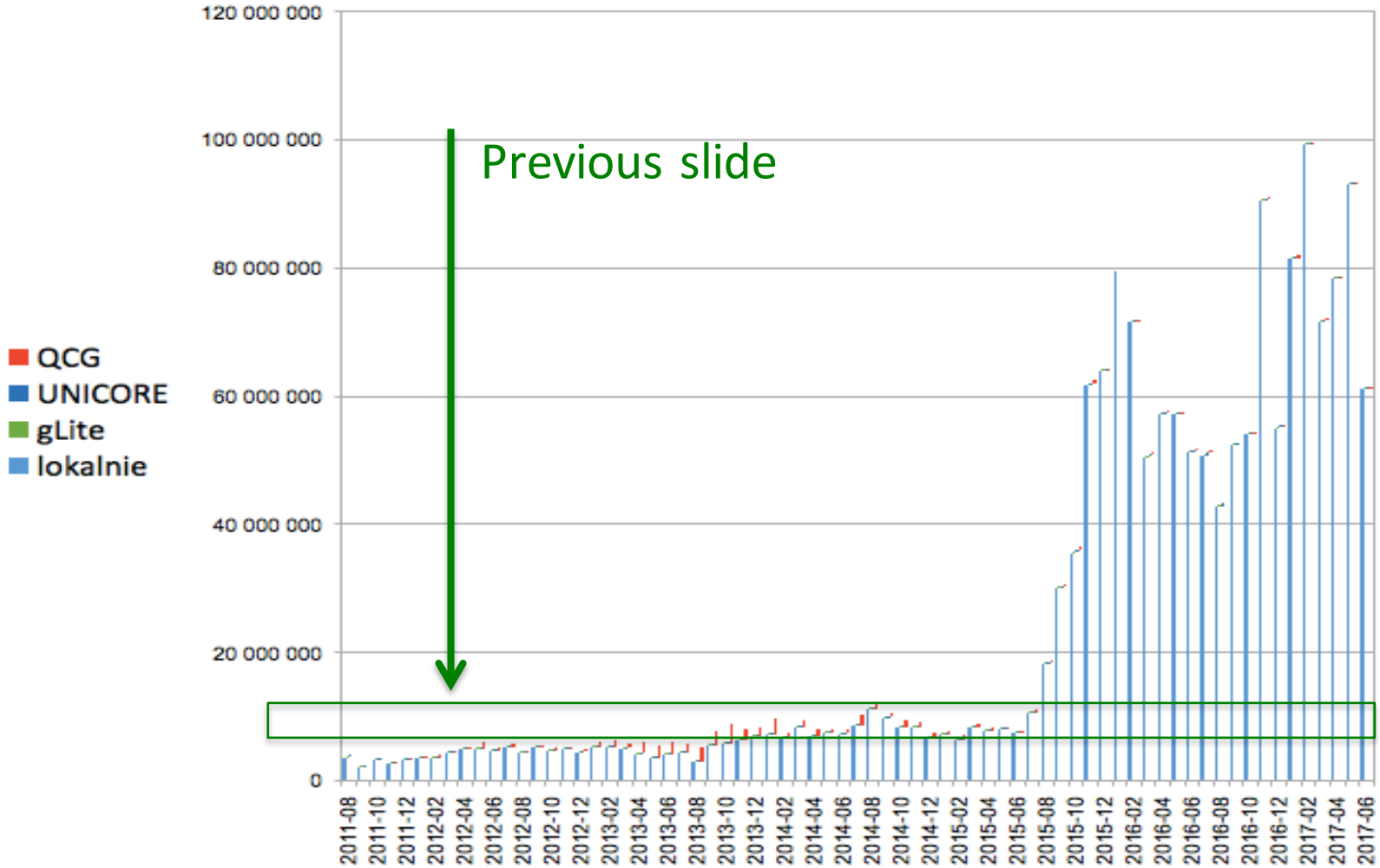
PL-Grid statistics [CPUhours]



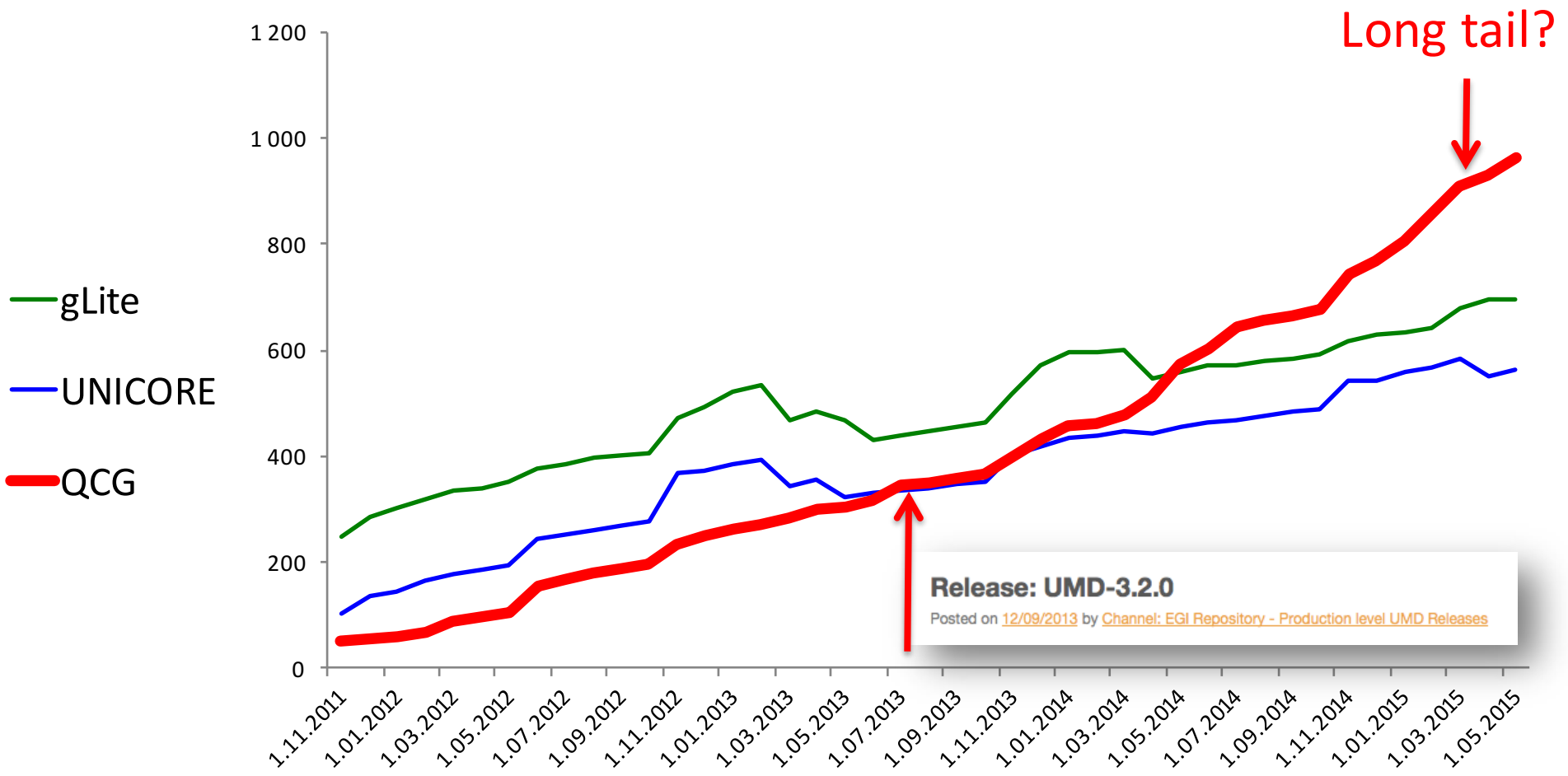
PL-Grid statistics with QCG [CPUhours]



PL-Grid statistics with QCG [CPUhours]



PL-Grid statistics [Users]



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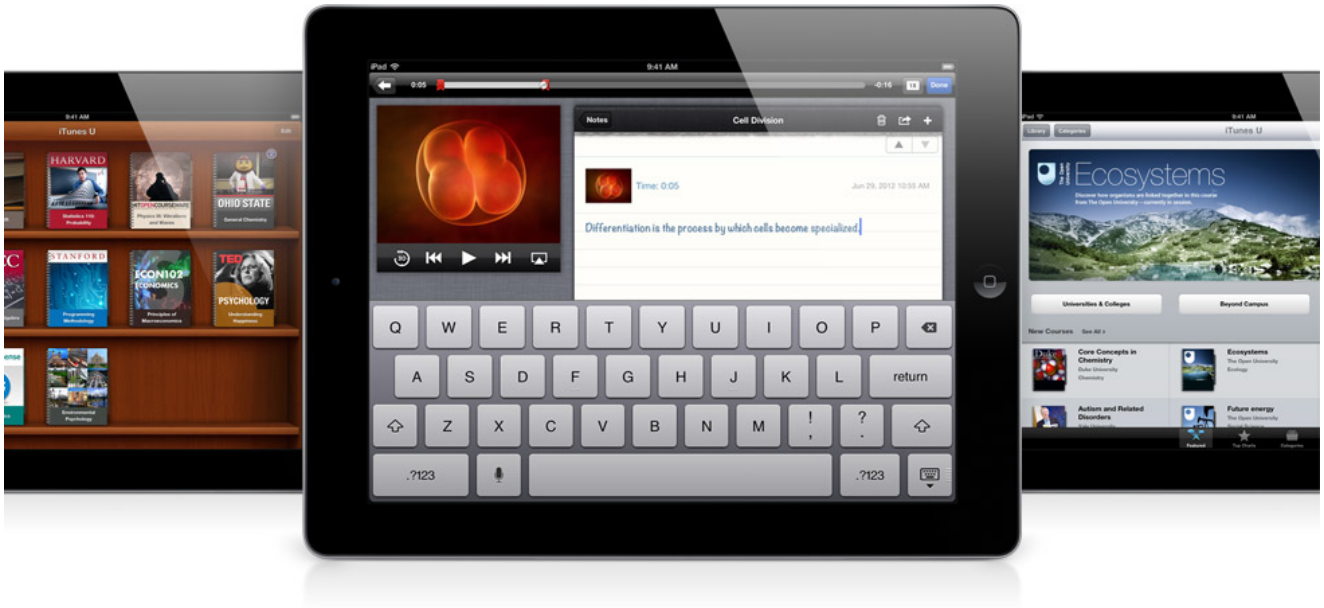
QCG-Now
A desktop tool for HPC management

E-textbooks & OERs pillar

- **62 complete e-textbooks for K12**: pre-, primary, secondary schools on 14 main subjects in Polish
- **2500+** additional educational high-quality OERs Completed and delivered to users in September 2015
- All e-textbooks have been **officially approved** by Ministry of Education in January 2016
- **40%** of teachers and K12 students in Poland should be ready to use open educational resources from tablets, smartphones, PCs, readers, etc.

Subjects

- Early education
- Polish language
- History
- Biology
- Geography
- Physics
- Chemistry
- Mathematics
- Informatics
- Computer classes
- Education for safety
- Civics



creative commons

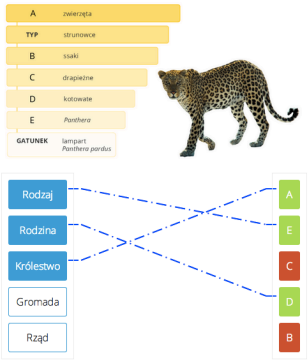
open source

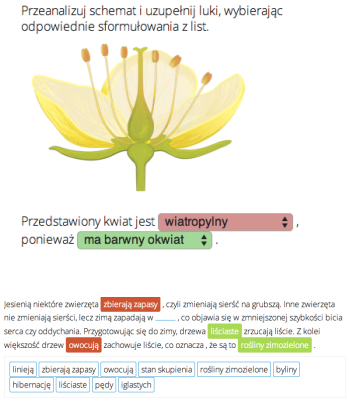
KEY STAGE	AGES	SUBJECTS	HOURS OF CONTENT
I	6-9	Early Education	1150 h
II	10-12	Polish language History Biology Mathematices Computer Classes	510 h 130 h 290 h 385 h 95 h
III	13-15	Polish language History Civics Geography Biology Chemistry Physics Education for safety Mathematices Informatics	450 h 190 h 65 h 130 h 130 h 130 h 130 h 30 h 385 h 65 h
IV	16-18	Polish language History Cicics Geography Biology Chemistry Physics Education for safety Mathematices Informatics	360 h 60 h 30 h 130 h 30 h 30 h 30 h 30h 300 h 30 h

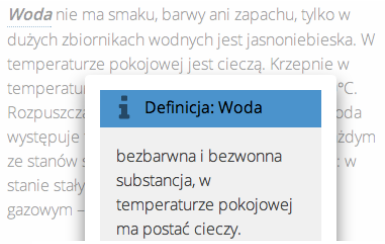
Variety of OERs in e-textbooks

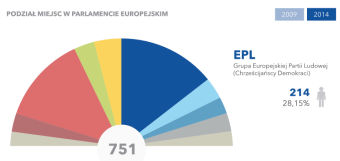










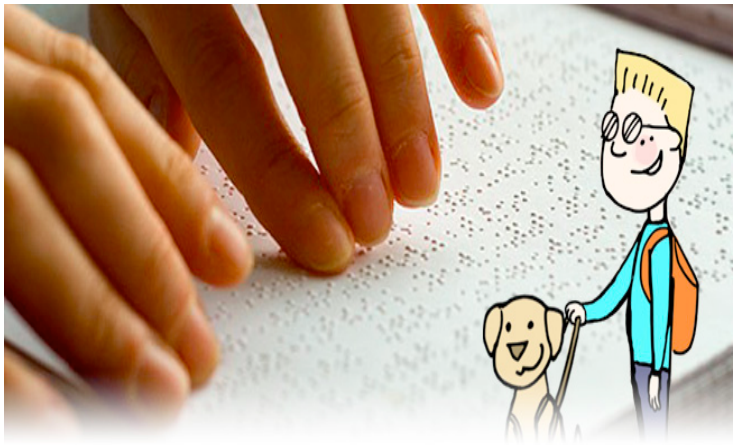


www.epodreczniki.pl platform

- **HTML5/JS/CSS3** for cross-platform support, no software to install and maintain
- Tested in various **web browsers** and HW
- Additional **native apps** for Android, iOS and Windows to synchronize on/off-line e-textbooks and personal notes
- **Different data formats** available and will be supported in the future
- Extensions possible through **APIs** to various edu service and cloud providers (e.g. e-diary school systems for SSO)

www.epodreczniki.pl platform

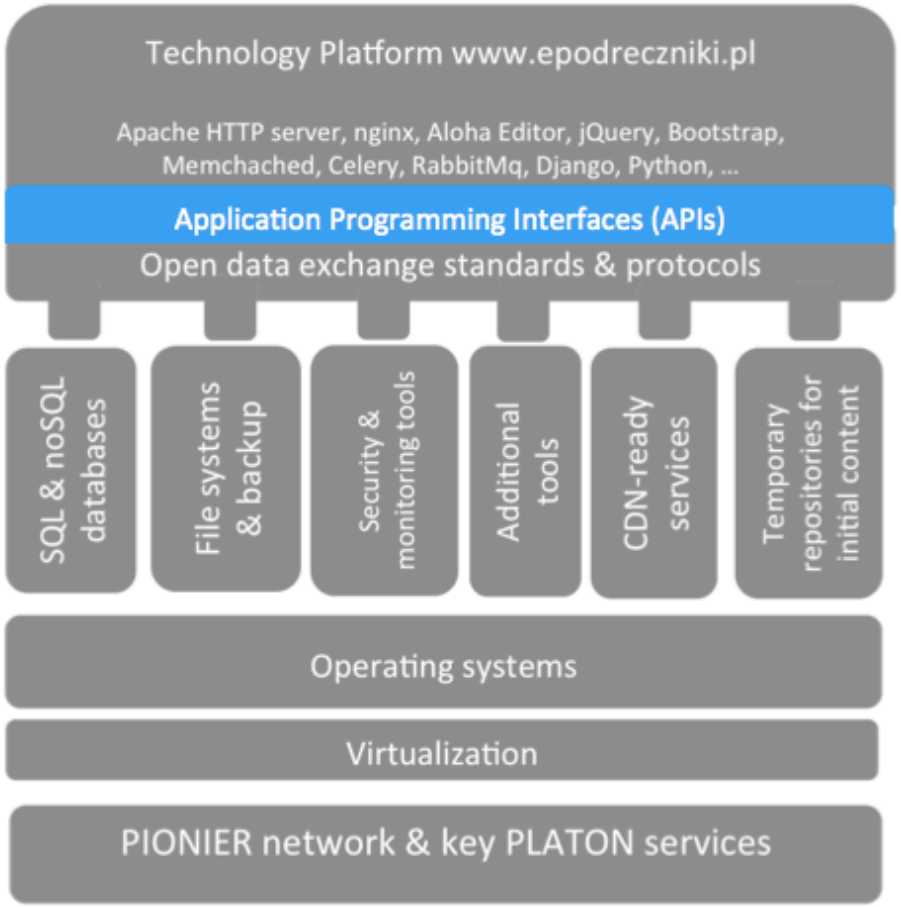
- Improved accessibility thanks to XML/XSLT schemas and transformations (based on **open standards - cnx.org**)
- Metadata already provided for Geant **eduOER hub**
- **Many schools just put links to OERs in their websites, moodle spaces, LMS, …**
- **Modular** approach taken
- Additional metadata and alternative descriptions for the collected edu content to meet WCAG2.0 requirements



www.epodreczniki.pl platform

- OERs are available now (in polish) at www.epodreczniki.pl
- Basic technical documentation (english) http://dev.epodreczniki.pl
- UNESCO report on OERs in Poland

http://iite.unesco.org/pics/publications/en/files/3214727.pdf



www.epodreczniki.pl statistics

59
e-podręczników

5599
Modułów

18322
Obiekty interaktywne

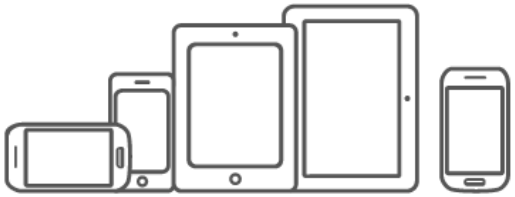
2123
Filmy

485
Nagrań

20949
Ilustacji

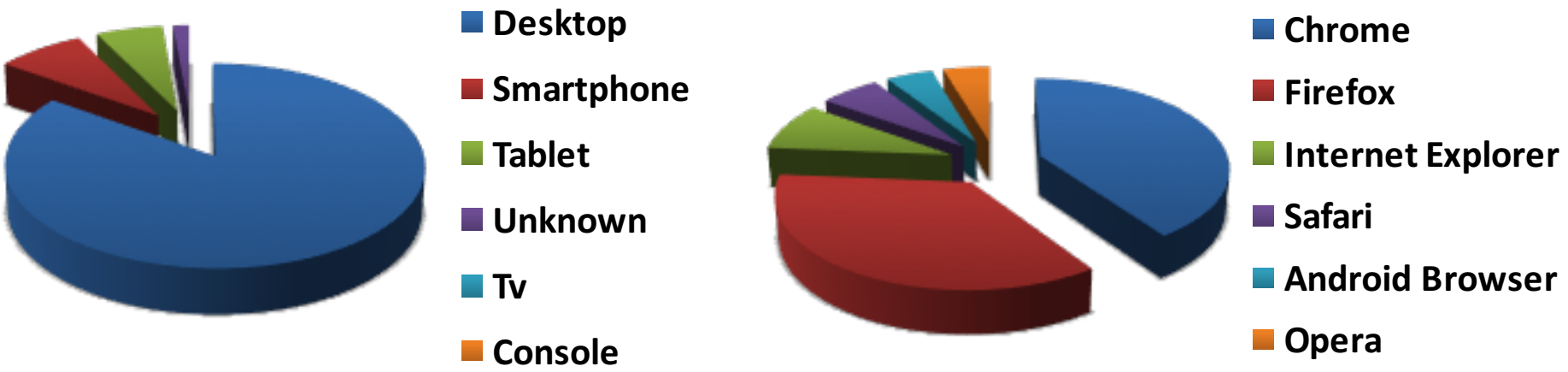
3166
Zasobów dodatkowych

92%



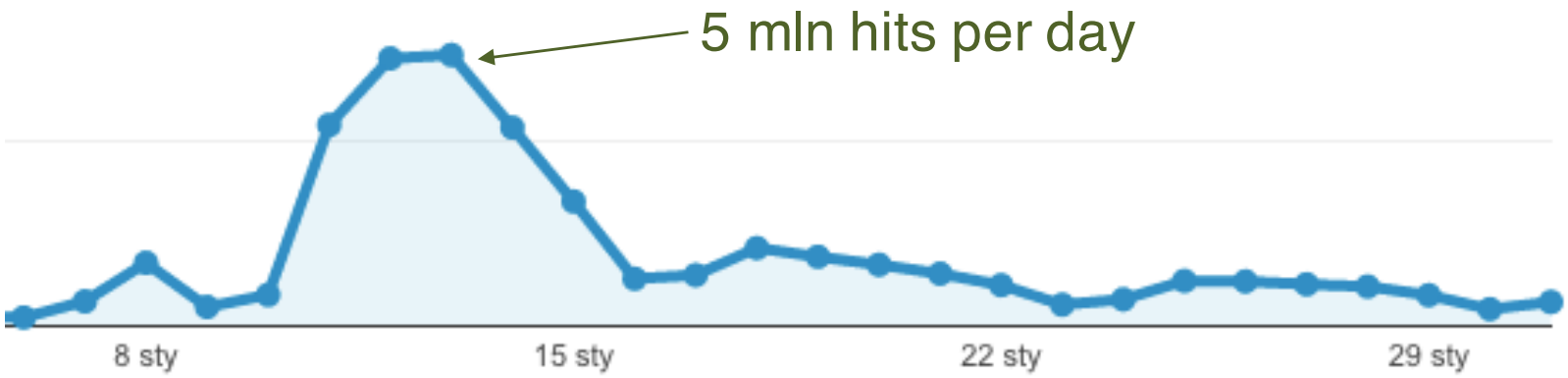
8%

www.epodreczniki.pl statistics

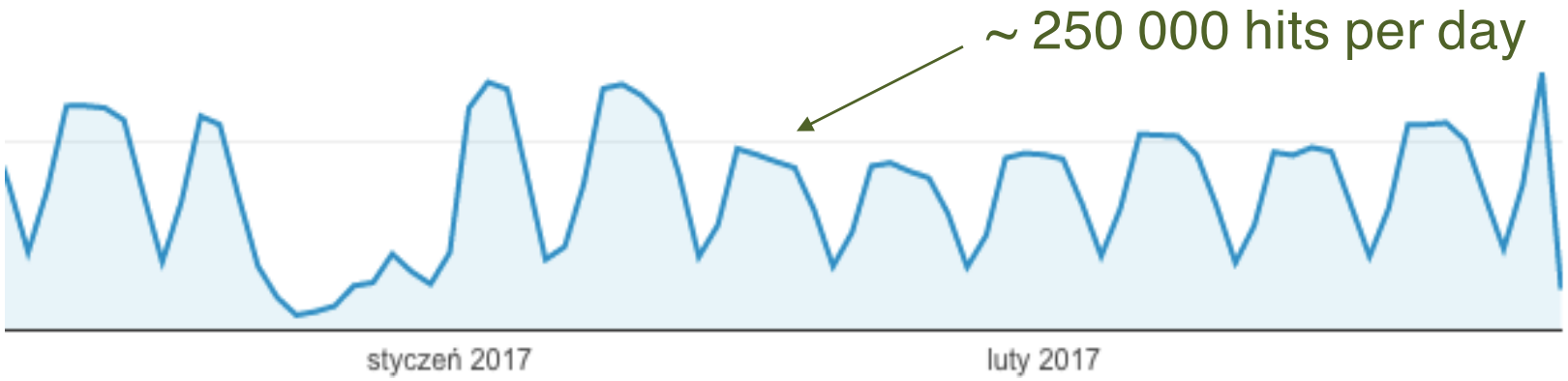


www.epodreczniki.pl statistics

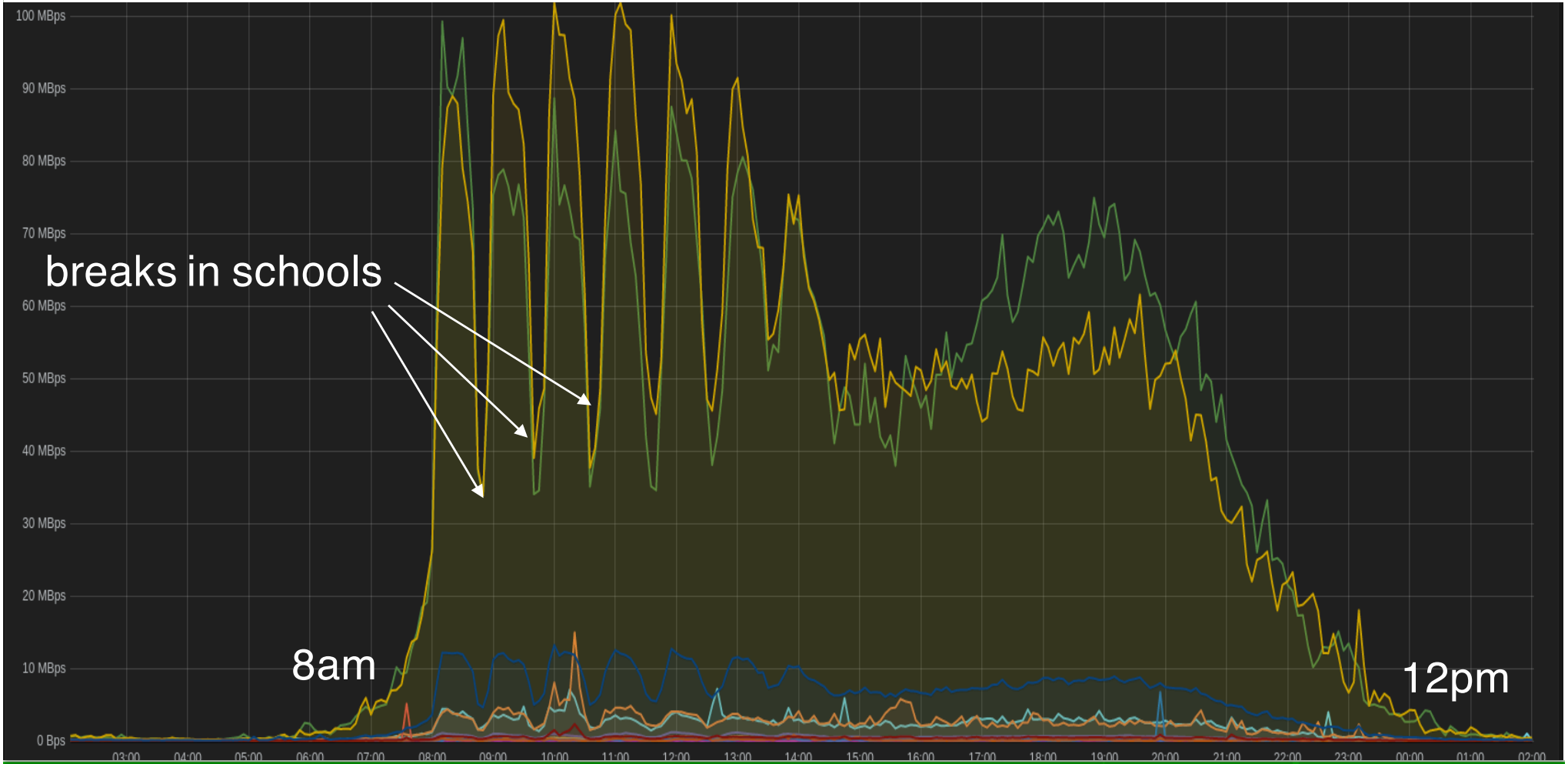
2016



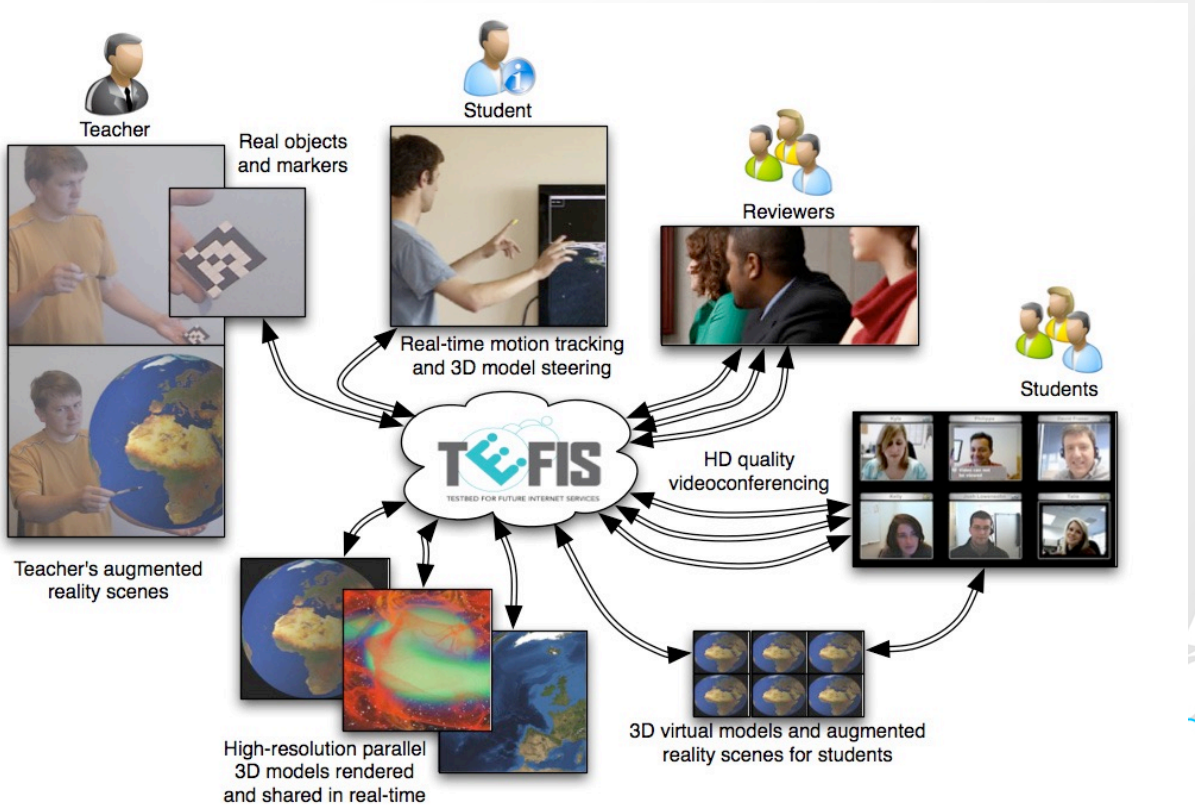
2017

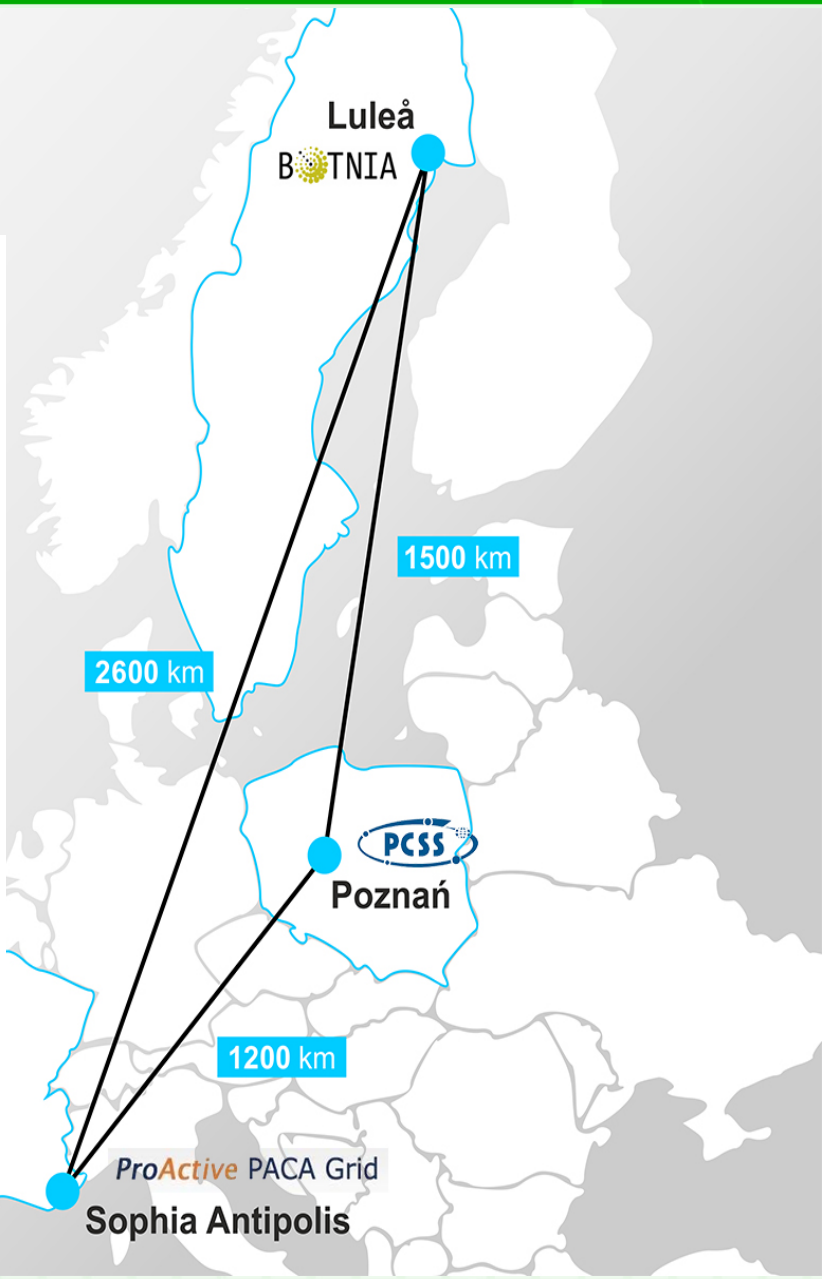


www.epodreczniki.pl statistics



Use cases


Teacher
Real objects and markers
Student
Real-time motion tracking and 3D model steering
Reviewers
Students
TEFIS
HD quality videoconferencing
Teacher's augmented reality scenes
High-resolution parallel 3D models rendered and shared in real-time
3D virtual models and augmented reality scenes for students

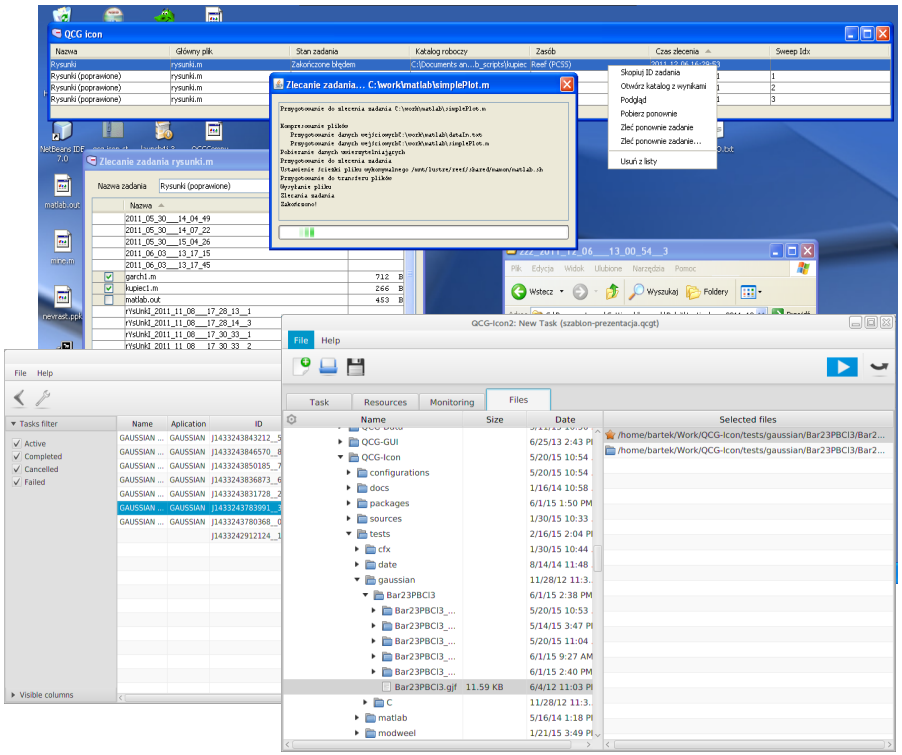

Luleå
BOTNIA
1500 km
2600 km
PCSS
Poznań
1200 km
ProActive PACA Grid
Sophia Antipolis


TEFIS
TEEPOL
NTED REALITY COLLABORATIVE WORKSPA
RE INTERNET VIDEOCONFERENCING PLA
R REMOTE EDUCATION AND LEARNING
EMOTE BIOLOGY IN ENGLISH LESSON

QCG users tools (QCG-Icon and QCG-Vis)

- QCG-Icon/Vis are simple desktop applications integrated tightly with operating systems (systray, context menu, etc. + **C++/Java/Python SDKs**)
- Available for Windows, Mac OSX and Linux
- Supported applications on many HPC systems:
  - MATLAB
  - R
  - Mathematica
  - Gaussian (integrated with Gaussview)
  - GAMESS
  - Molpro
  - plus any bash script!
- Demo movies:

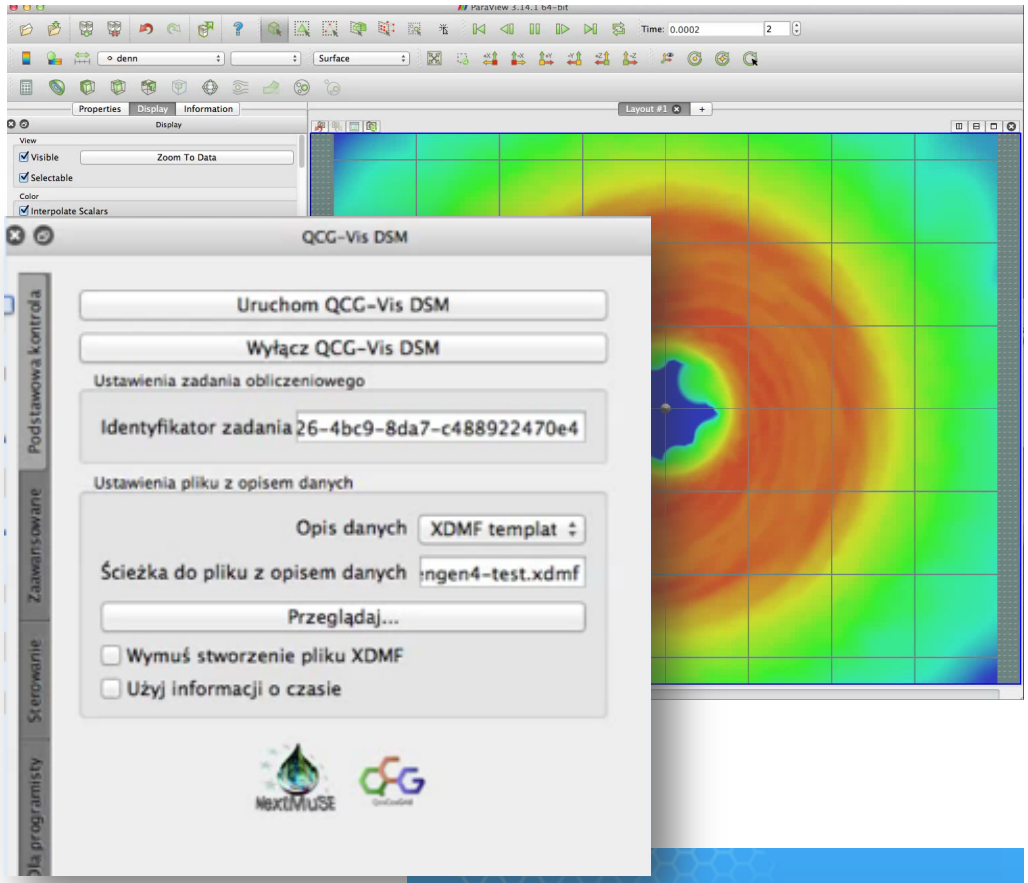
http://www.qoscosgrid.org/trac/qcg-icon



ParaView + QCG-Vis

Visual data discovery environment

- Open-source, multi-platform data analysis and visualization application
- Tailored towards Computational Fluid Dynamics community (but not limited to)
- Capable of handling big datasets
- Advanced 3D visualization possible
- **Integrated with QCG middleware for a transparent connection between a user and remote visualization processes**
- **Integrated with ICARUS – plugin for remote in-situ visualization**



ParaView

QCG quality in cloud and grid

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Where we are… (1617's perspective)

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Poznań University of Technology
Adam Mickiewicz University in Poznań
Poznań University of Economics
Poznan University of Medical Sciences
Poznań University of Life Sciences
The Eugeniusz Piasecki University School of Physical Education in Poznań
The Ignacy Jan Paderewski Academy of Music in Poznań
University of Arts in Poznań
Collegium da Vinci
Poznan College of Communications and Management
Poznan School of LogisticsPoznań Trade and Commerce College
Poznan University College of Business
University of Social Sciences and Humanities (USWPS)
WSB University in Poznań


PSNC
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