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Painless computational chemistry in the cloud with SCIGRESS

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Why bother with computations?

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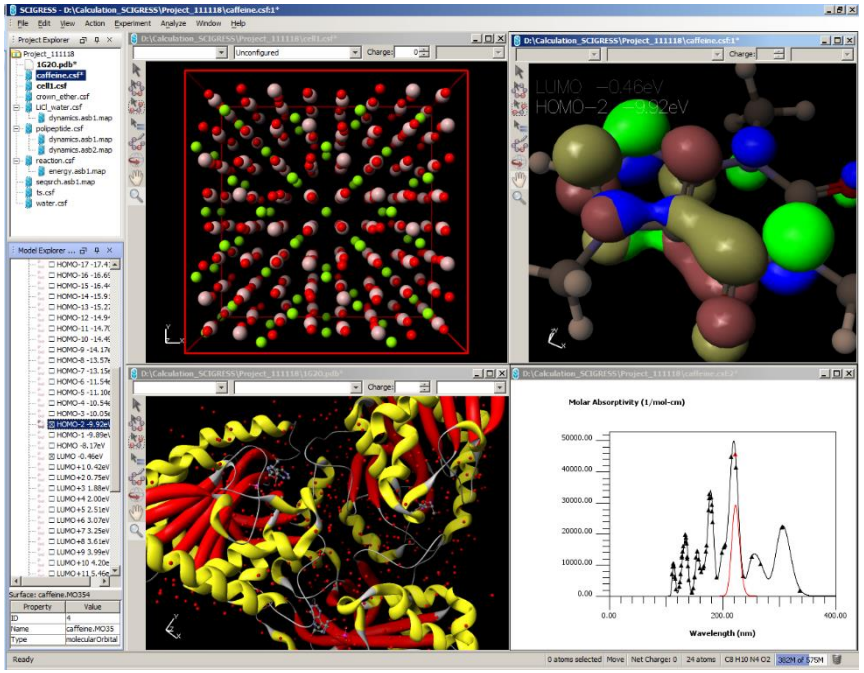
- Main objectives
  - **Aid everyday chemist's work**
  - **Reduce costs**
  - Speed up research
  - Limit environmental harm
  - Make new discoveries
  - Break less glassware ;)

"To the electron -- may it never be of any use to anybody." *-- JJ. Thomson's favorite toast*

SCIGRESS at a glance

- Molecular Modeling & Molecular Dynamics Suite for Windows, Linux and Mac
- Fully integrated GUI, predefined computational procedures
- Builders for a range of systems
- Integrated engines MM to DFT
- Can run ADF, GAMESS, GAUSSIAN,LAMMPS, MOPAC 2012
- Quantum docking
- Batch calculations



http://www.scigress.com chemistry@fqs.pl

The problem

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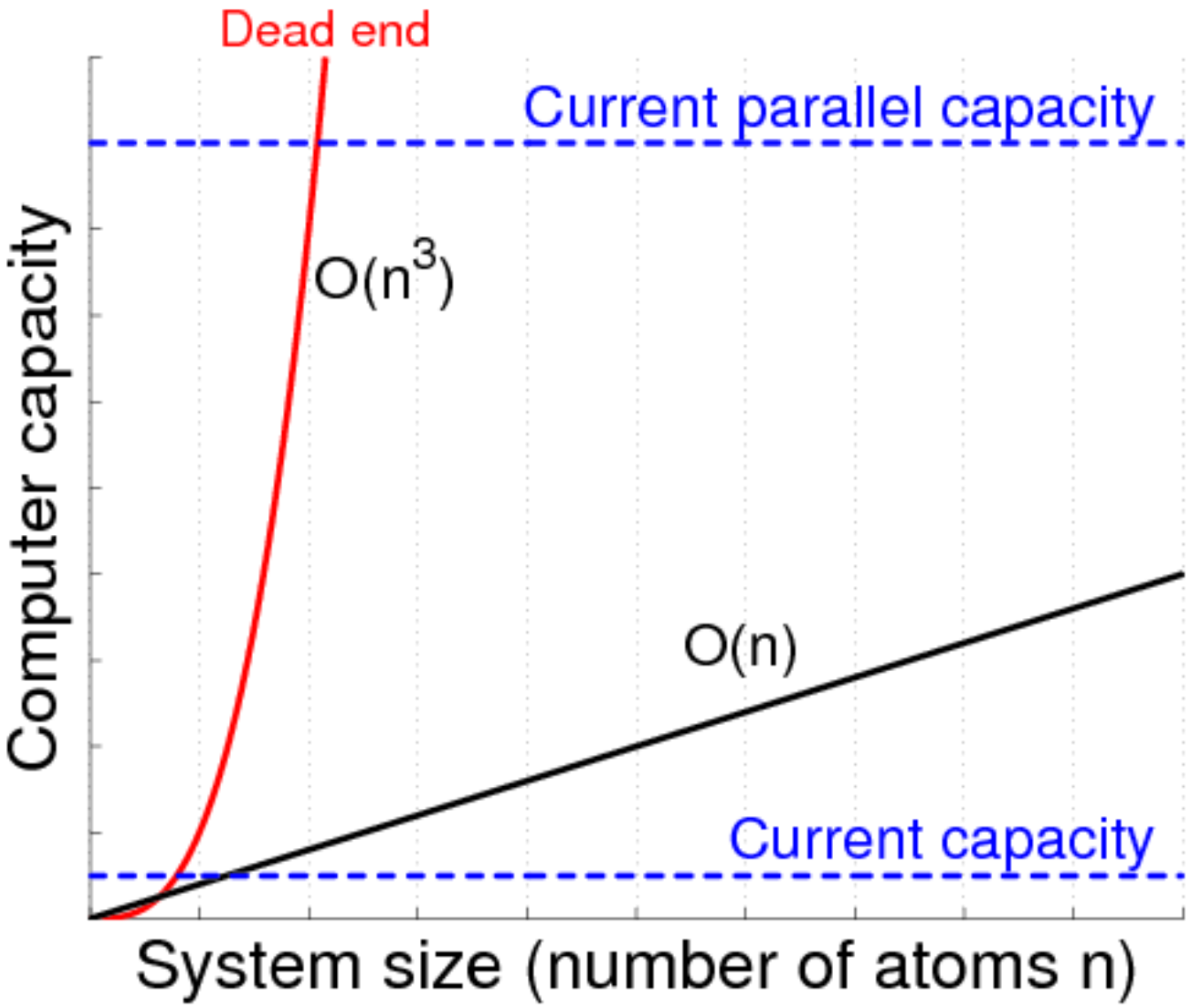

Solving basic needs by public providers

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The cloud

Google Actual Cloud Platform, one of the company's April Fool's Day 2015 gags. Google

Where is the technological change?

Our solution?

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No change *

* From user's perspective

Run remote calculations just as local ones

PLGrid - computational infrastructure for Polish science

Computing resources

- 3,6+ PTFLOPS
- 90 000+ cores

Scientific Software

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

Storage

- 20+ PB
- fast scratch
- distributed access

Tools for collaboration

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

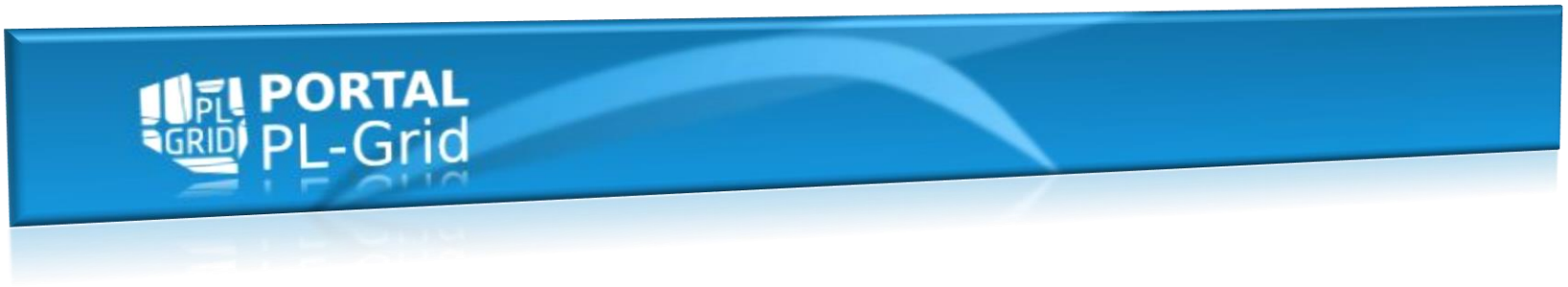
Computational Cloud

- PaaS based on OpenStack

ci task · WCSS · CYFRONET · icm · PCSS

PLGrid - computational infrastructure for Polish science

- 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

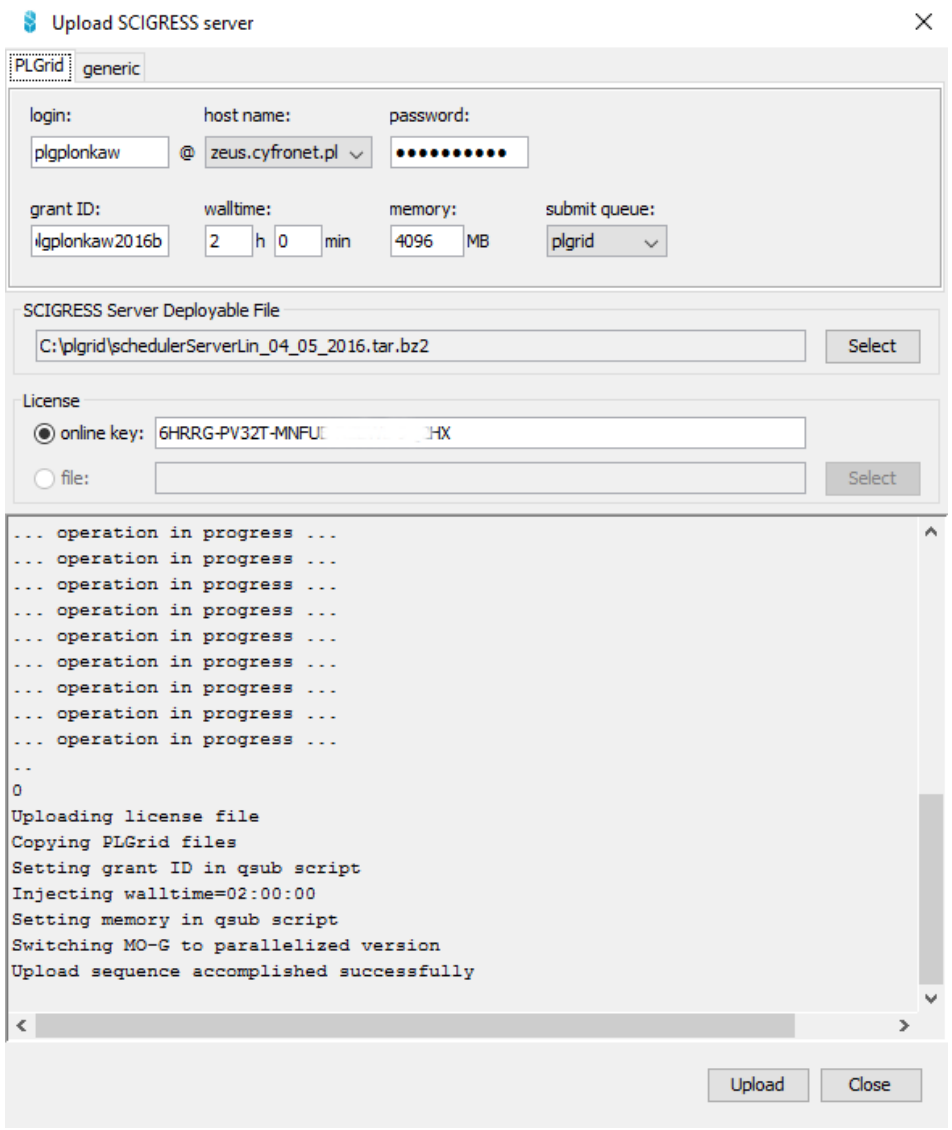
Access to all PLGrid resources through **one account** and **one passphrase** (or grid certificate)

- 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

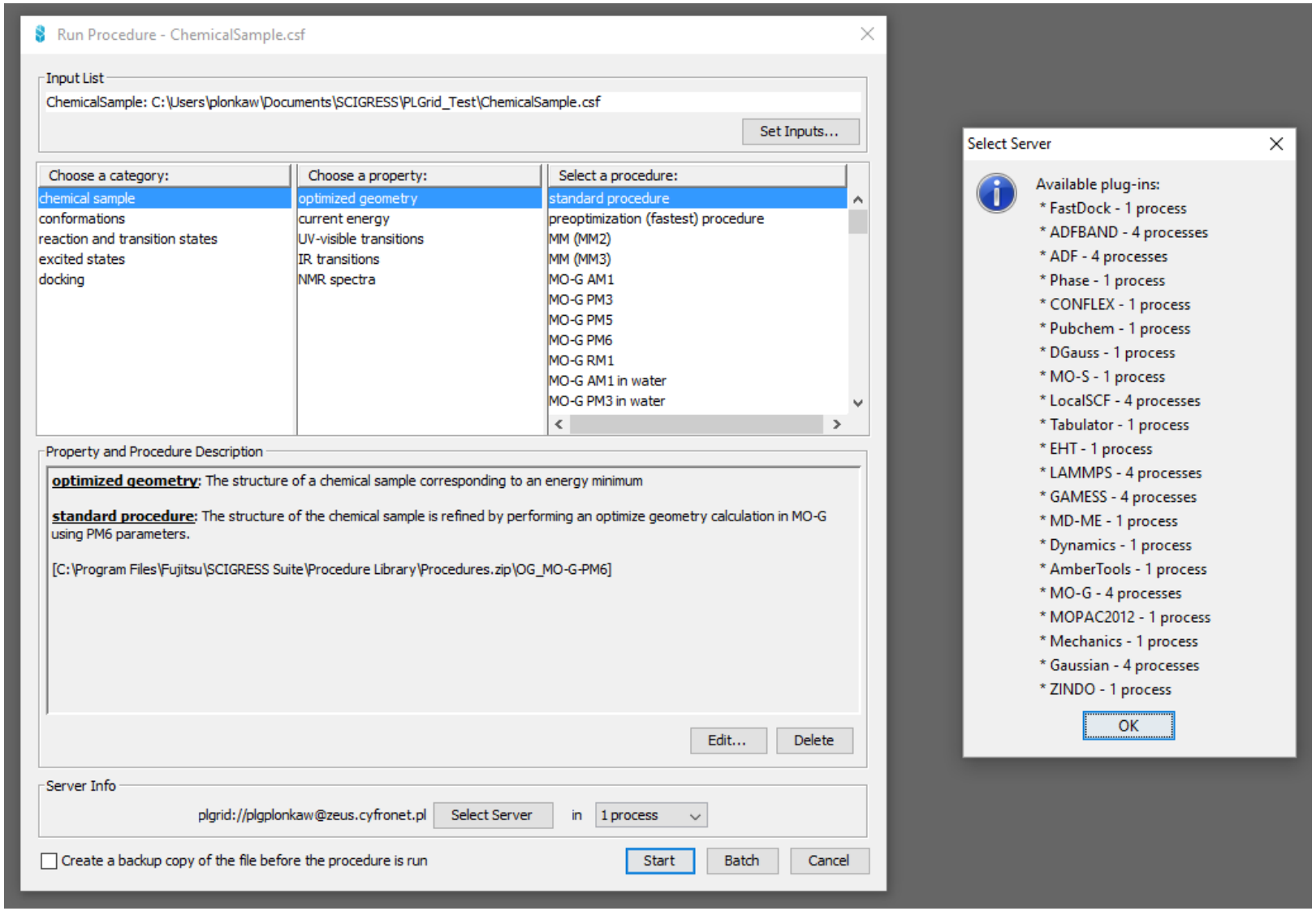
- PLG-Data team
  - easy access to data through web browser or other tools
  - data.plgrid.pl
  - team:
    - Tomasz Gubała

The installation

- Minimal IT knowledge
- PLGrid credentials & Grant ID required
- Fully automated process
- Nothing to do for sysadmins



Choose what & where to compute



Data transfer happens automagically

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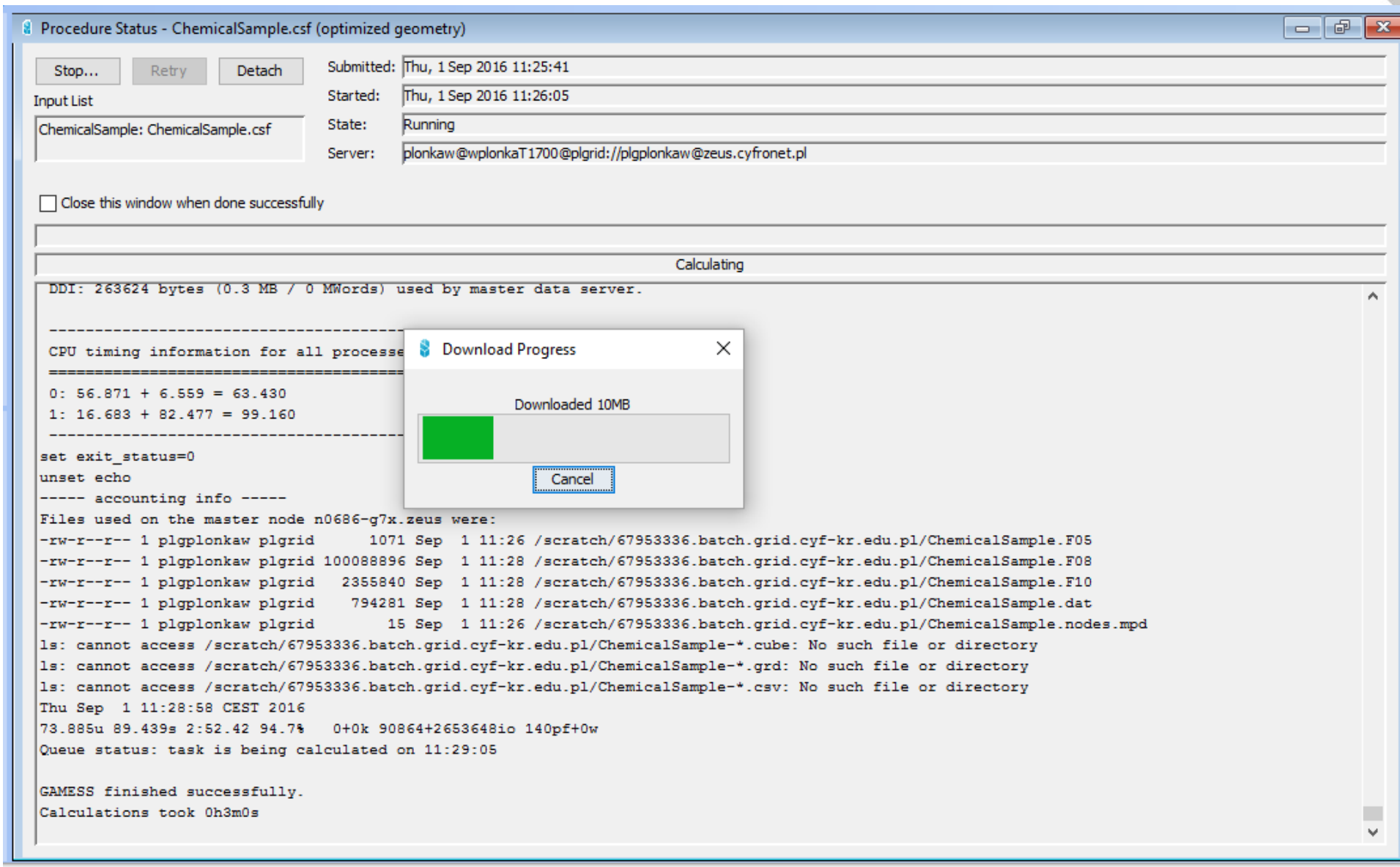

Changes **may** come faster than expected

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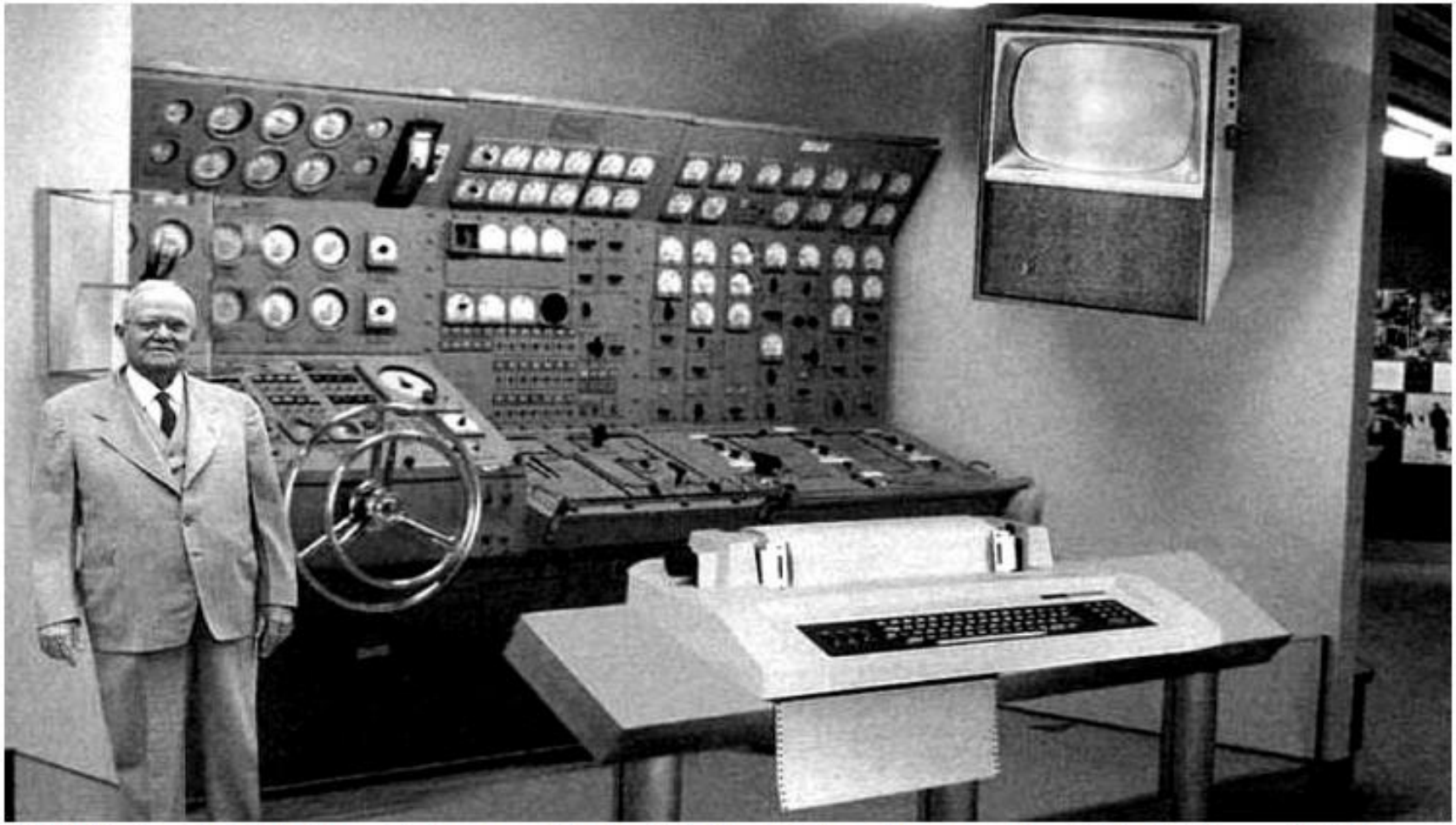
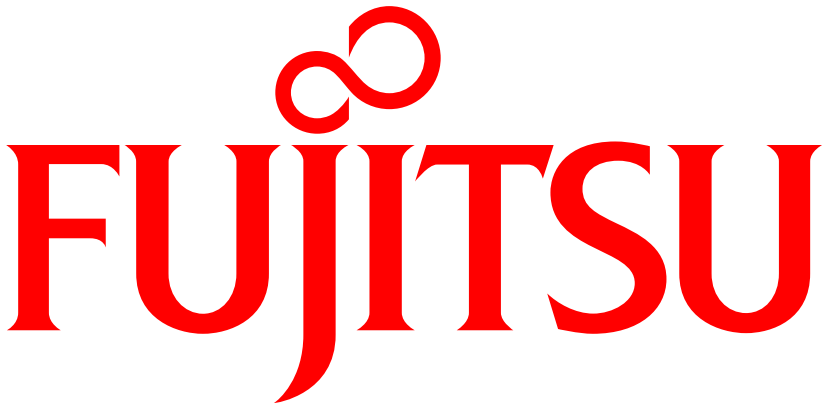


"Scientists from the RAND Corporation have created this model to illustrate how a home computer might look in the year 2004. However, the needed technology will not make it economically affordable for the average home. Also the scientists readily admit that the home computer will require not yet invented technology to actually work, but 50 years from now scientific progress is expected to have solved these problems. With teletype printer output and the Fortran langauge to program desired instructions, this computer will be easy to use."



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