Engineering Simulation

done in NTUA's cloud enabled Computer Center

The system administrator's perspective

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NTUA's Computer Center

A brief history

- Founded in 1978. Hosted one of the first computer systems in Greece: The *Control Data Cyber 171/8* (1978–1992).
- During 1978–2010: from punch cards and ASCII terminals to *Silicon Graphics* systems and stand alone servers.
- The storage was unified in 2003 using *SGI* technology.
- Today:
  - 29 *SUN* Blades with a total of 568 cores and 2.2 TB of RAM.
  - Unified NAS and SAN storage of *EMC* and *Fujitsu*.
- Central procurement of specialized software for engineers (*ANSYS, SIMULIA, MSC,* etc).

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Administration challenges and the *Direct Access* vision

- 4 admins vs 10000+ potential users.
- As we administrer serious hardware and software infrastructure we should establish IAAS and SAAS services.
- Ultimate goal: Maximum infrastructure utilization with minimal administrative overhead.
- Regardless of location each and every NTUA member should have *Direct Access* to the CC's facilities and services.
- *Direct Access* should be as simple as possible: using a standard web browser.

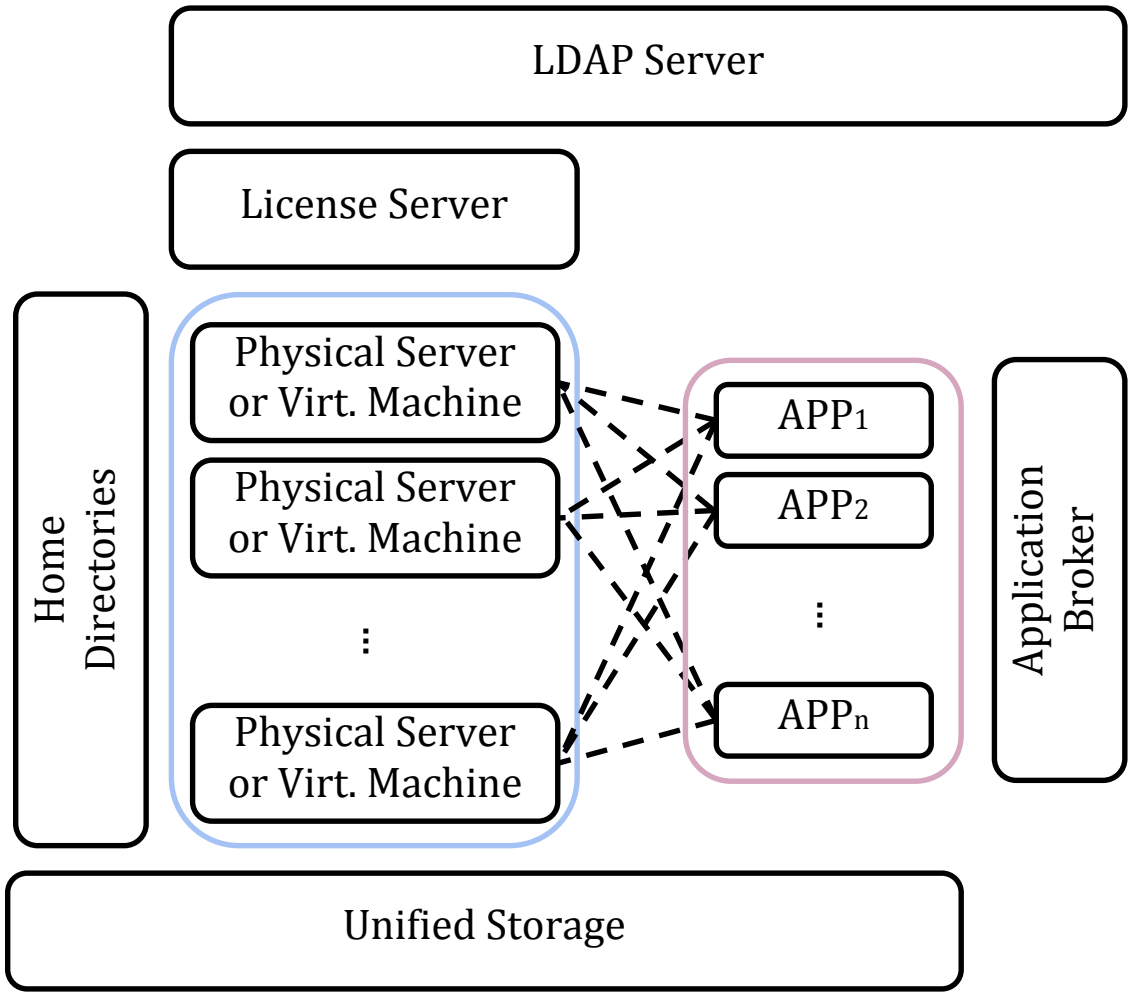
NTUA's *Central Cloud*

Our approach to IAAS and SAAS

- NTUA CC's facilities are integrated into a common environment: the *Central Cloud*:
  - Computing Power
  - Specialized software for engineers
  - General purspose software
  - Central storage
- Personalized and secure access to the Cloud environment through the *Central CloudFront* page.
- Automatic *Load Balancing* between the computing nodes.
- Increase the computing power by just adding blades and the storage capacity by just adding hard disks.

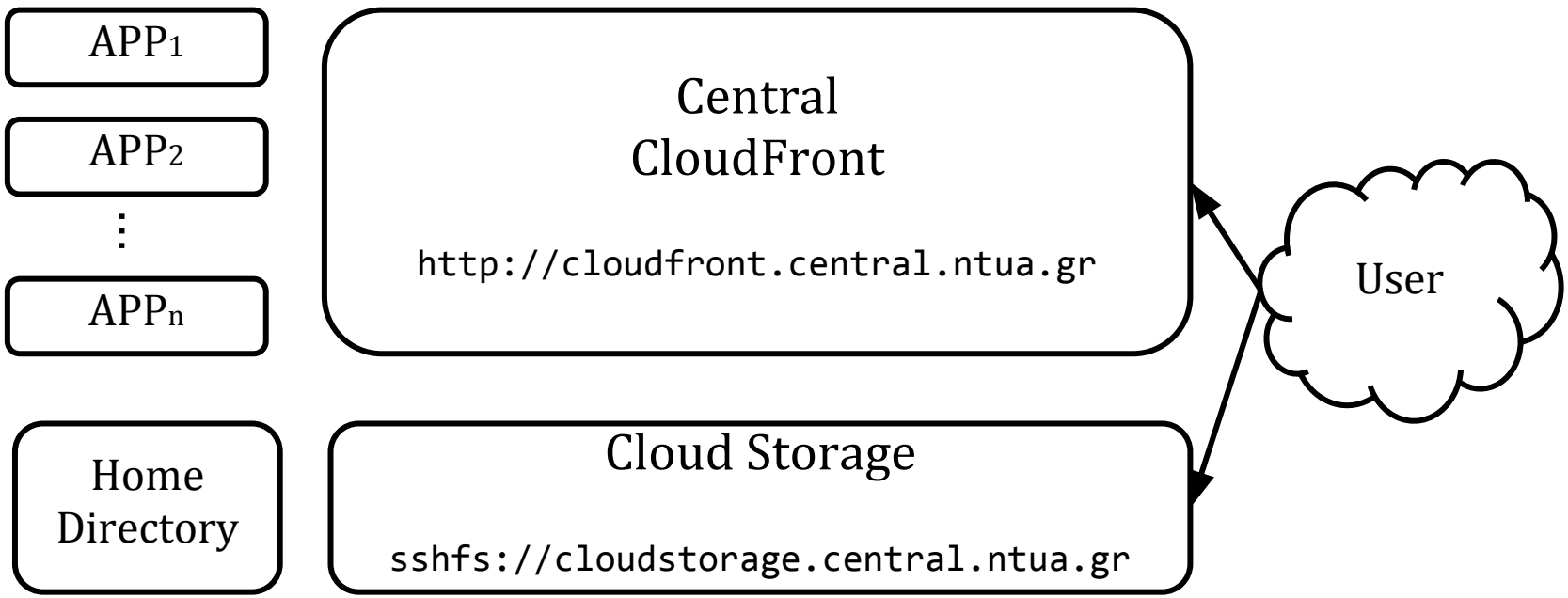
NTUA's *Central Cloud*

A bird's eye view of the implemented architecture



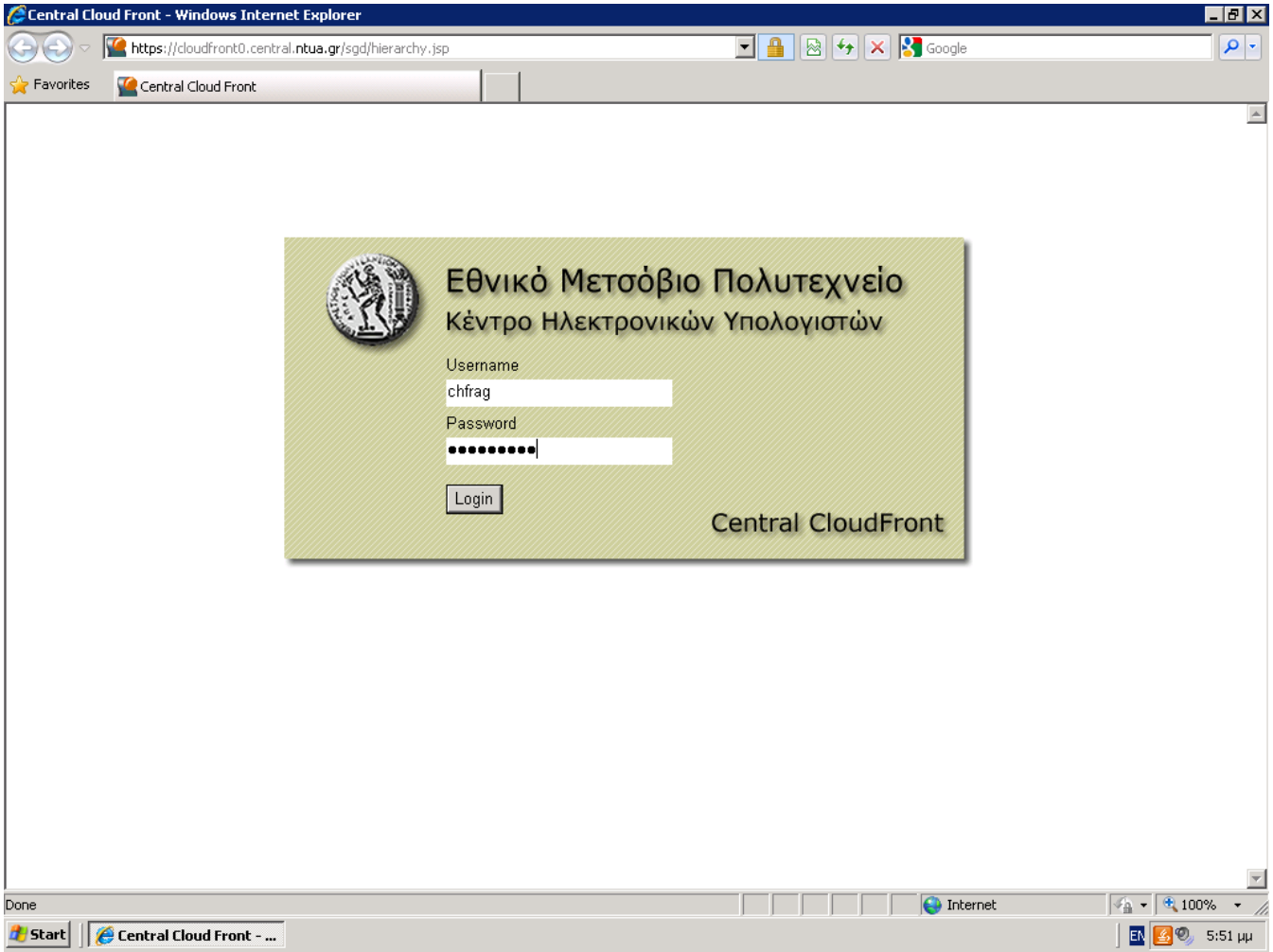
NTUA's *Central Cloud*

The user's experience: transparent technical details



Central CloudFront

http://cloudfront.central.ntua.gr



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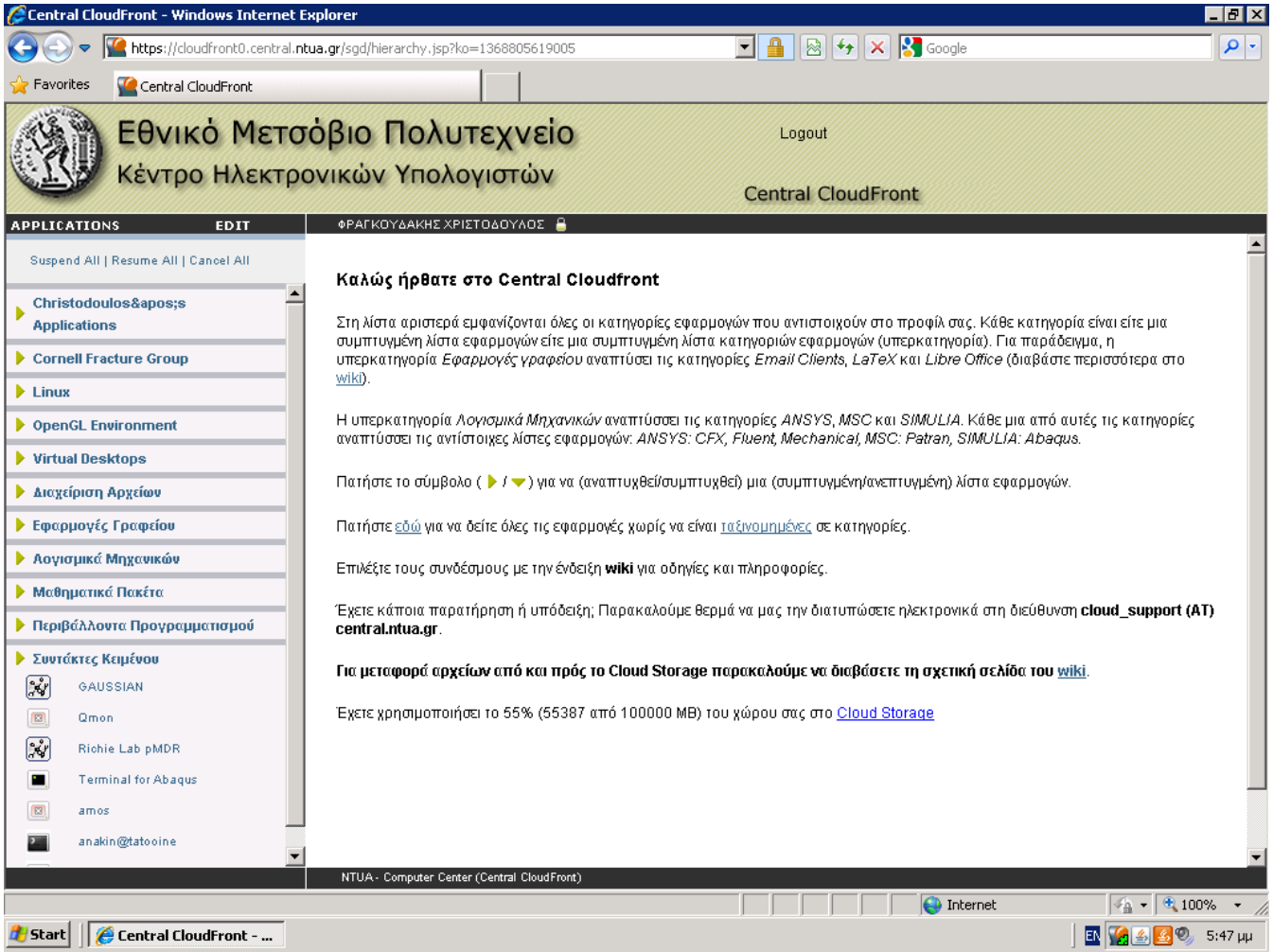
The Webtop



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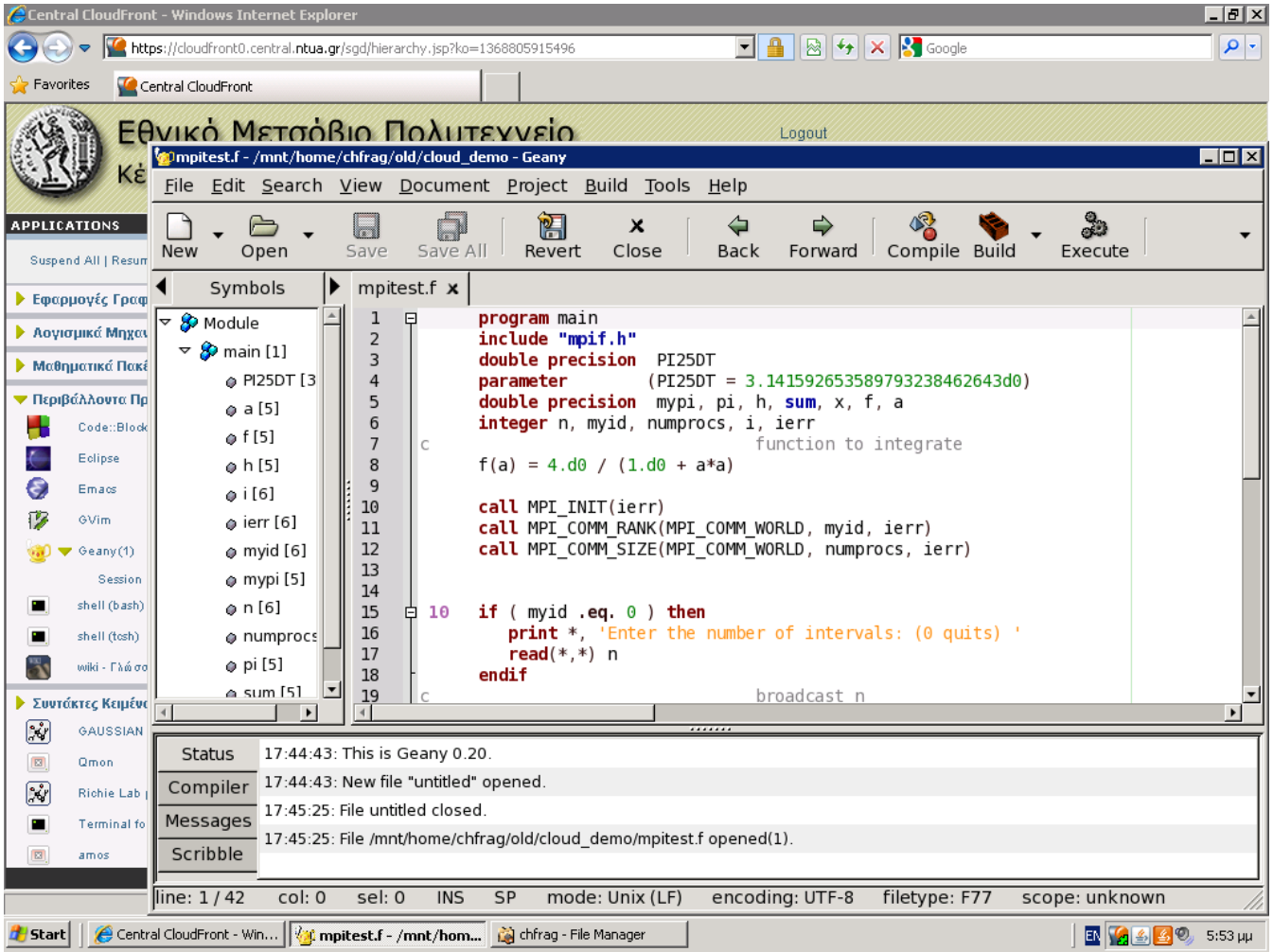
Programming courses



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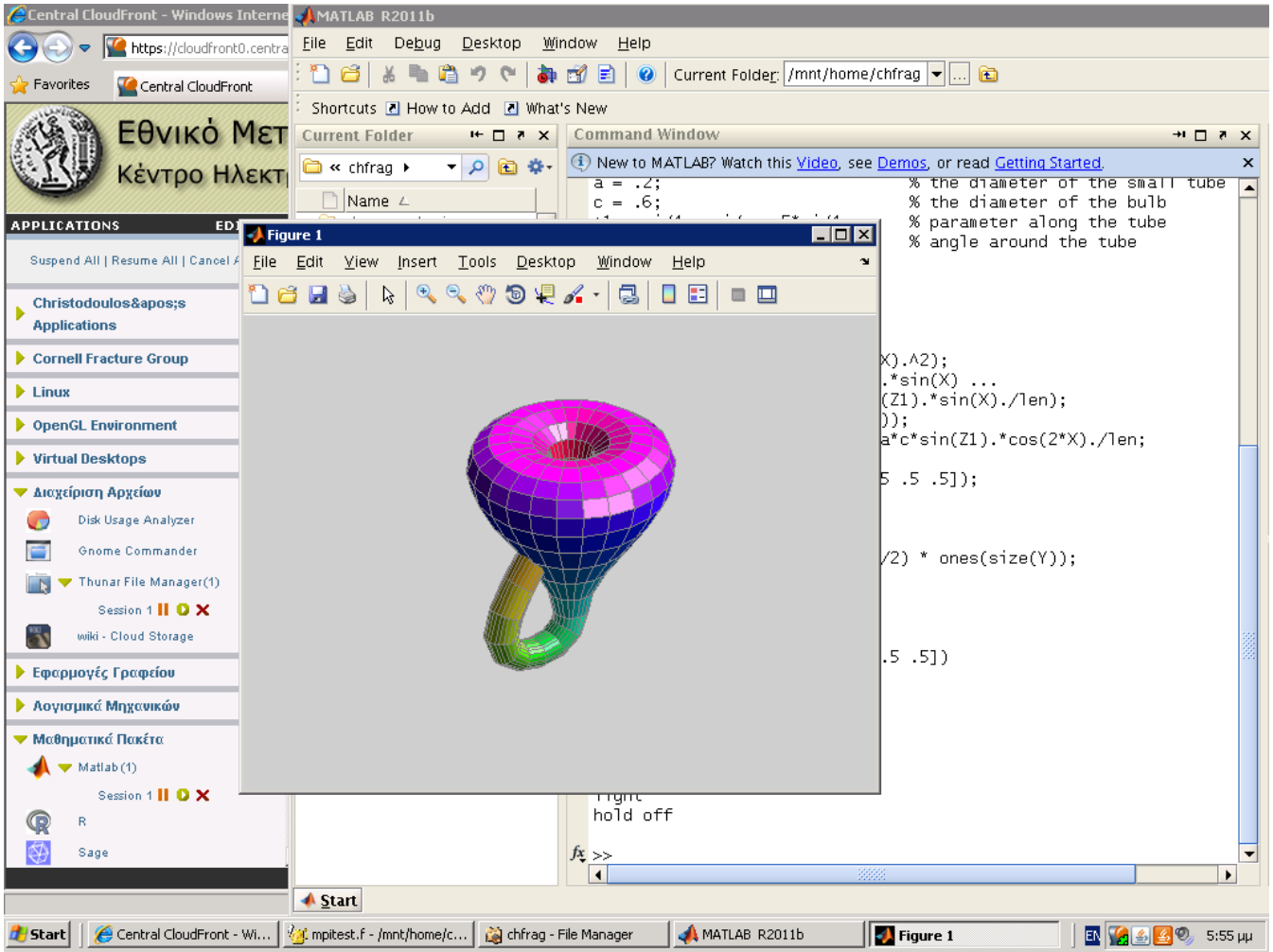
Mathematical Software



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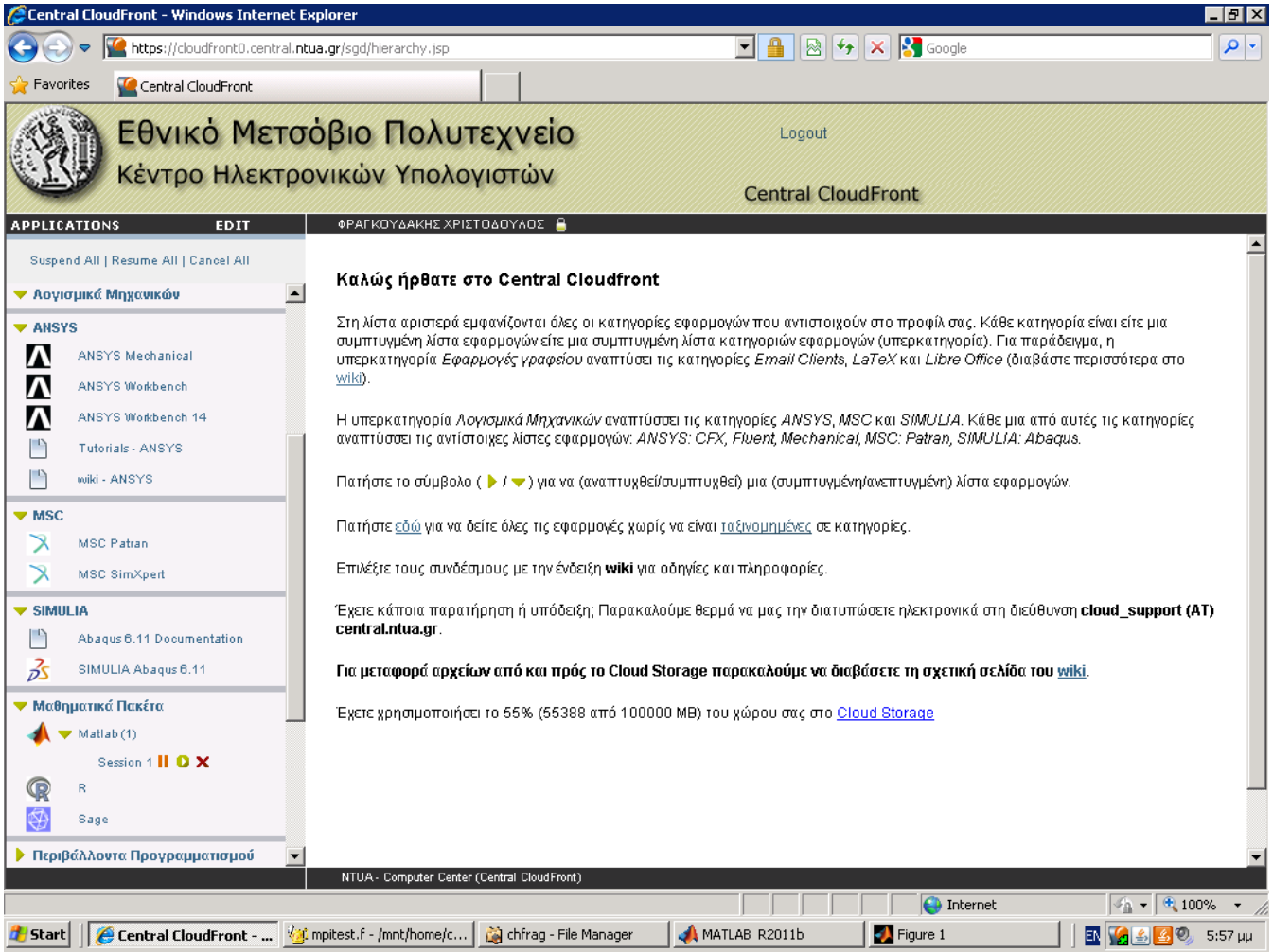
Engineering Simulation Packages



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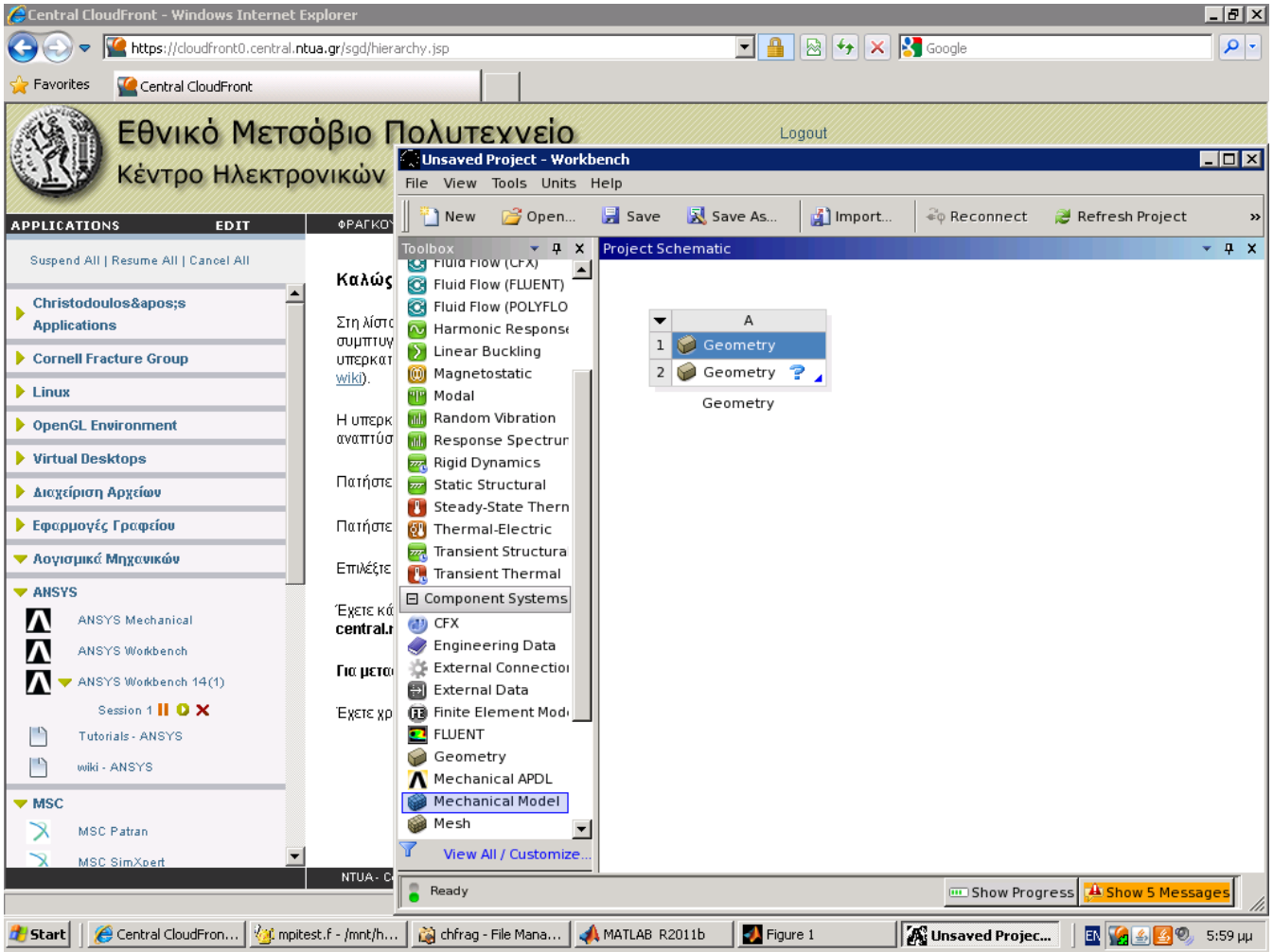
ANSYS Workbench



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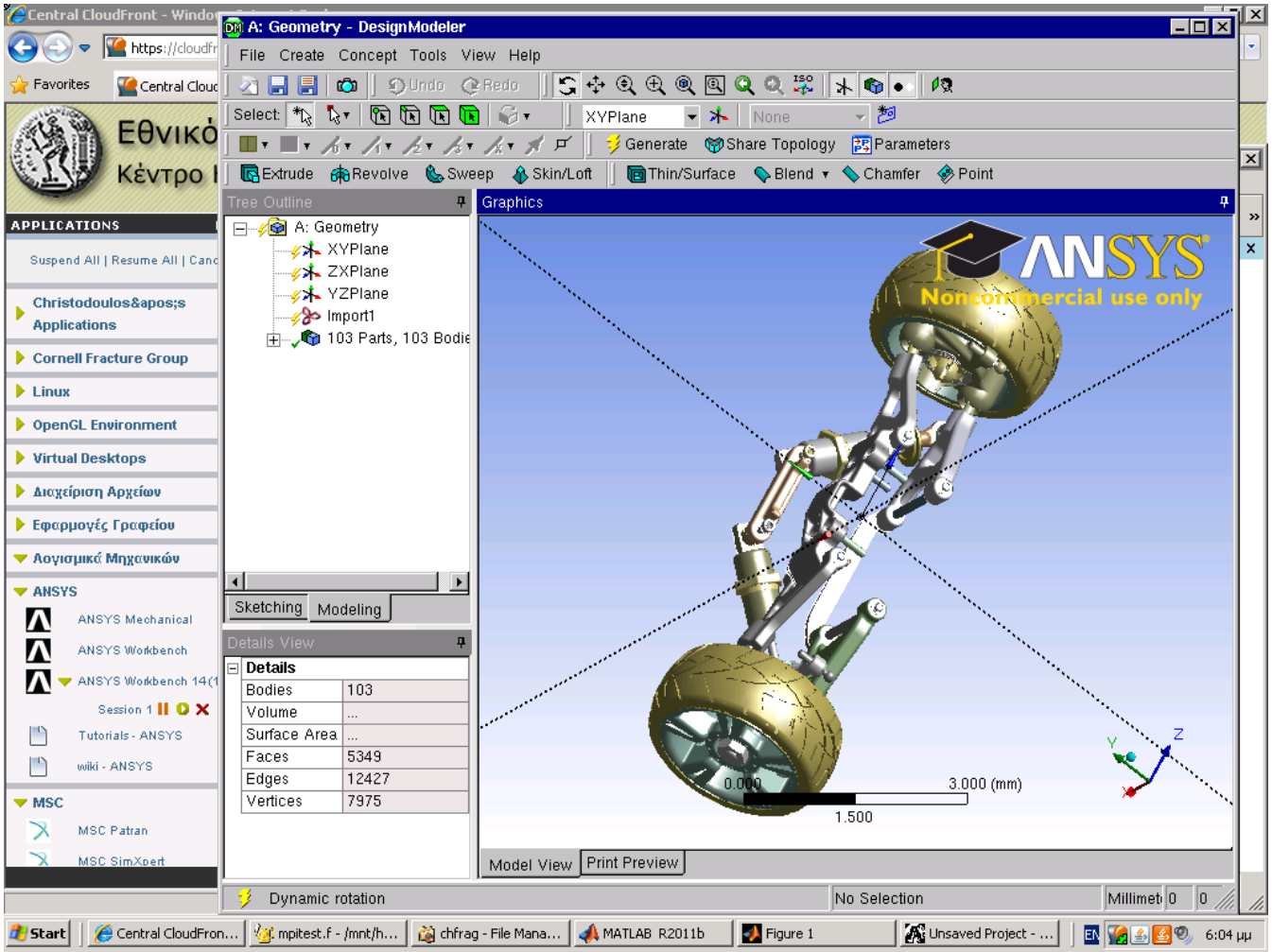
ANSYS Design Modeler



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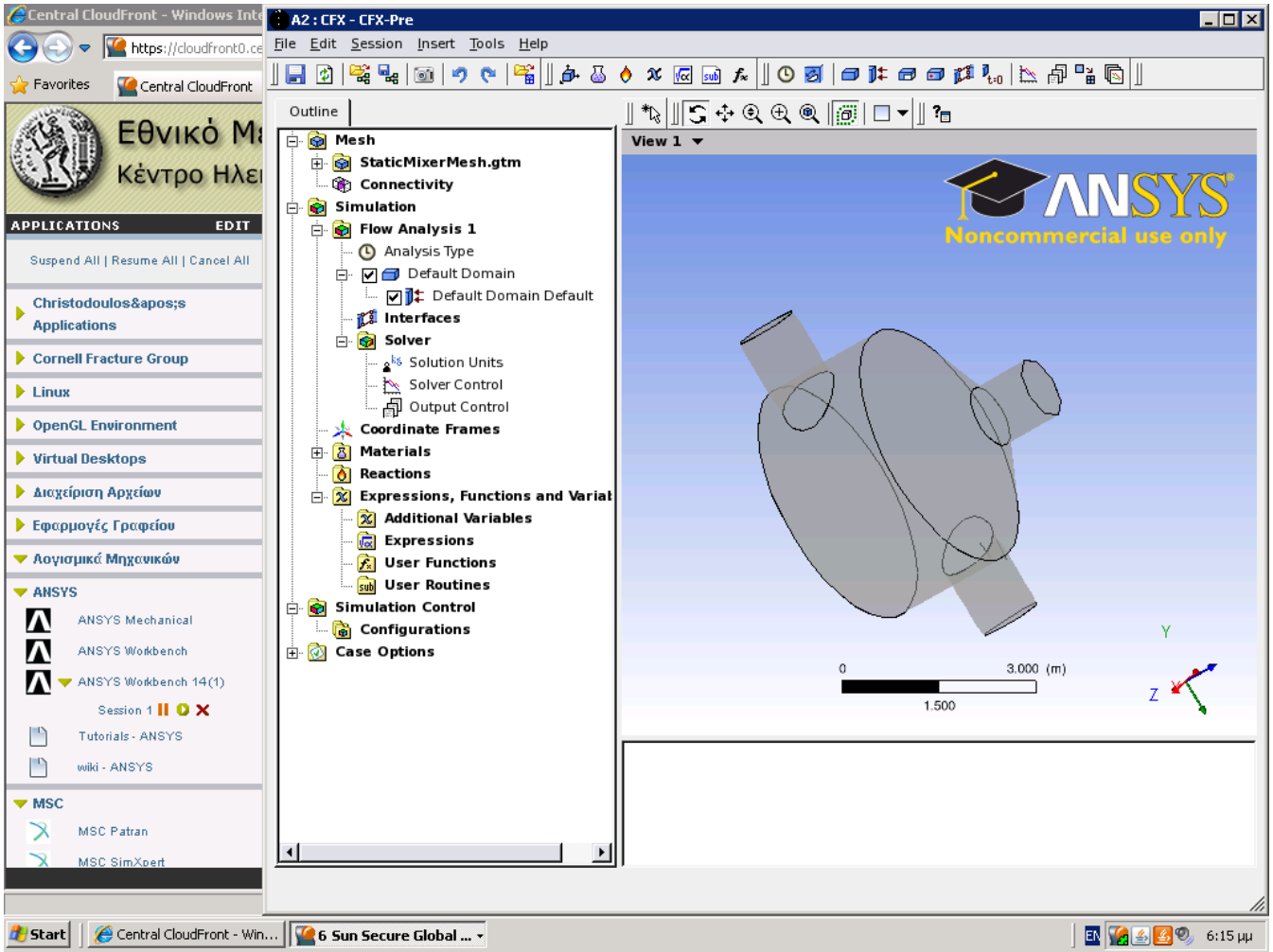
ANSYS CFX Preprocessor



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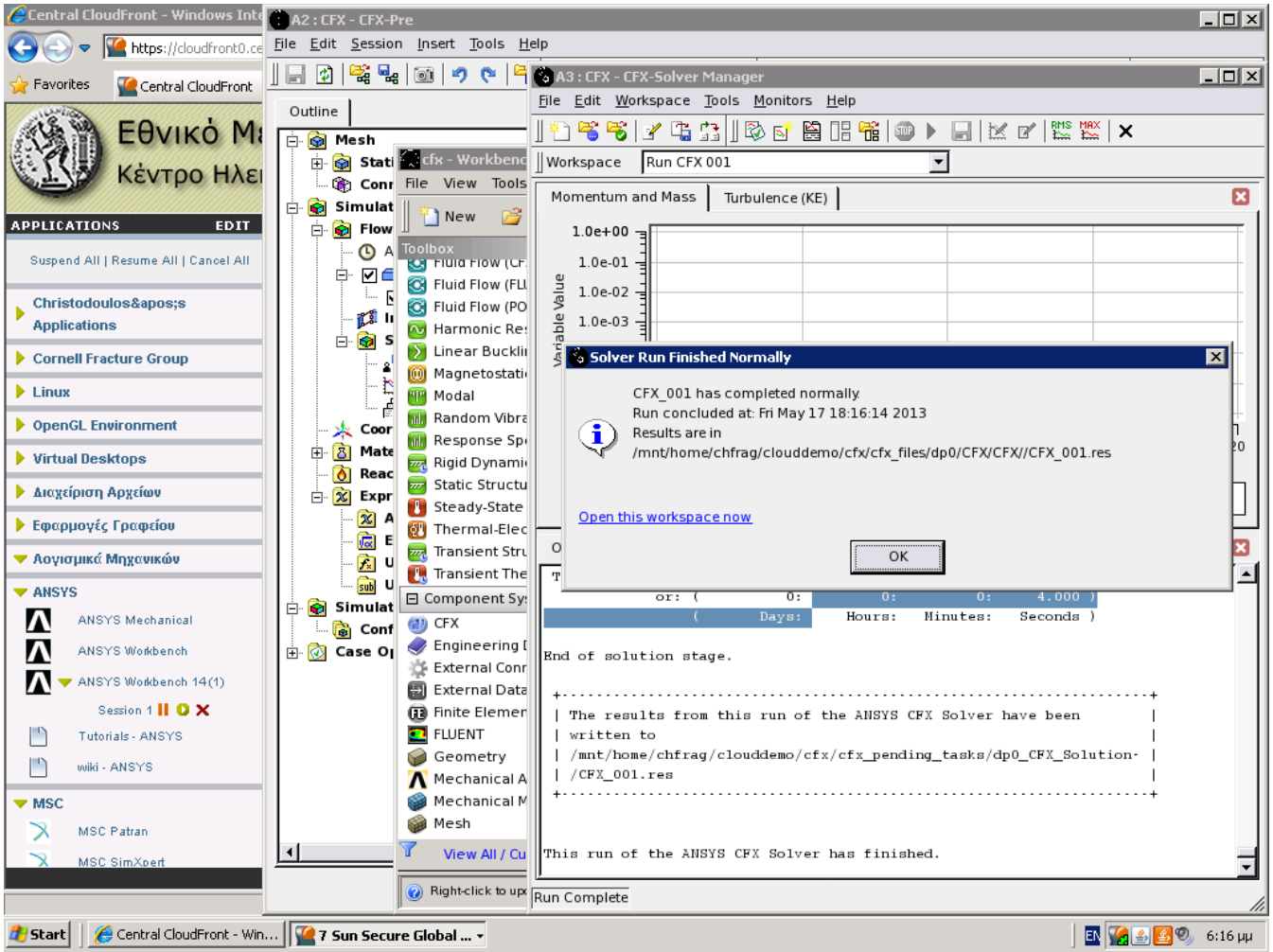
ANSYS CFX Solver



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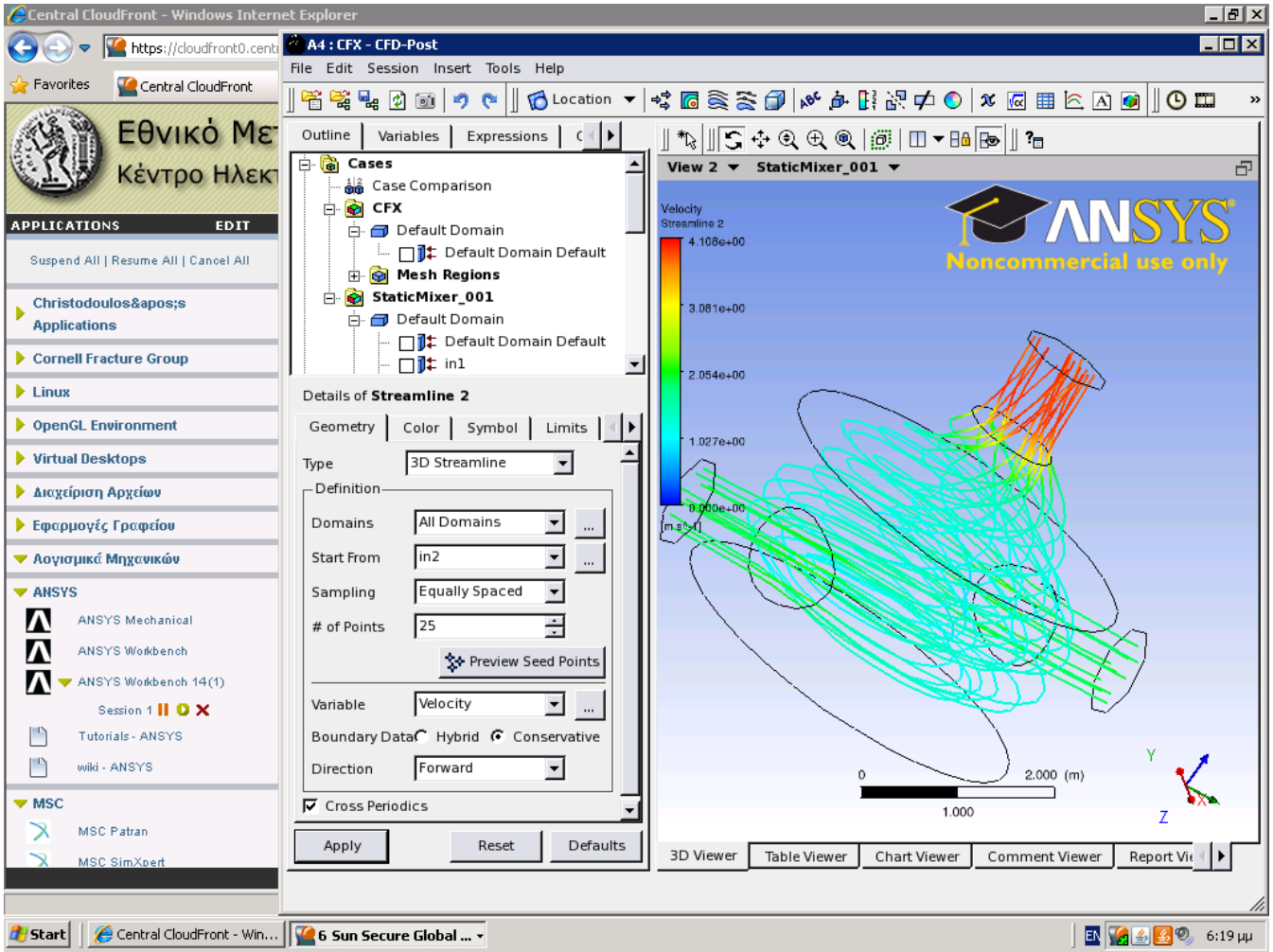
ANSYS CFX Post Processor



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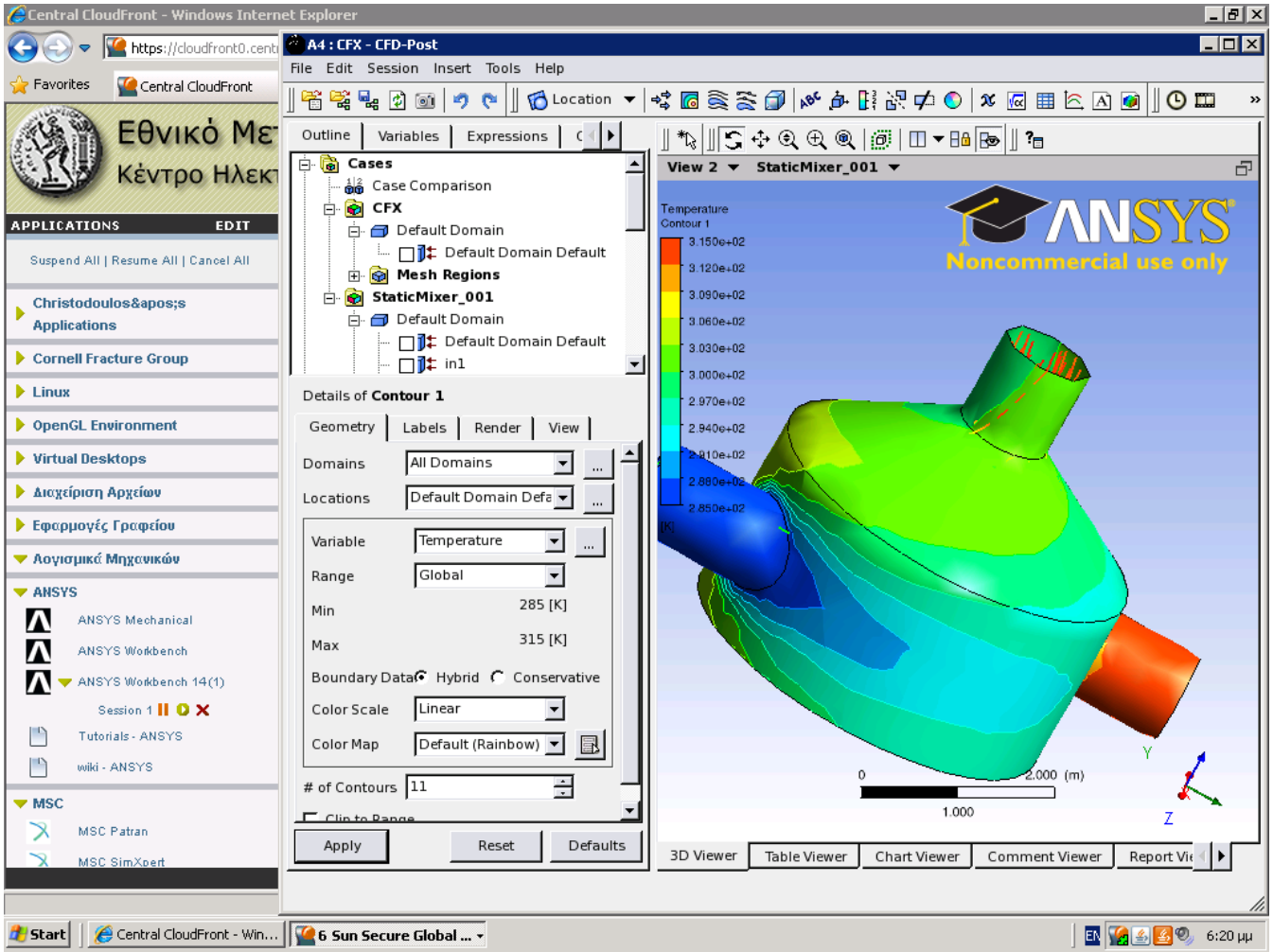

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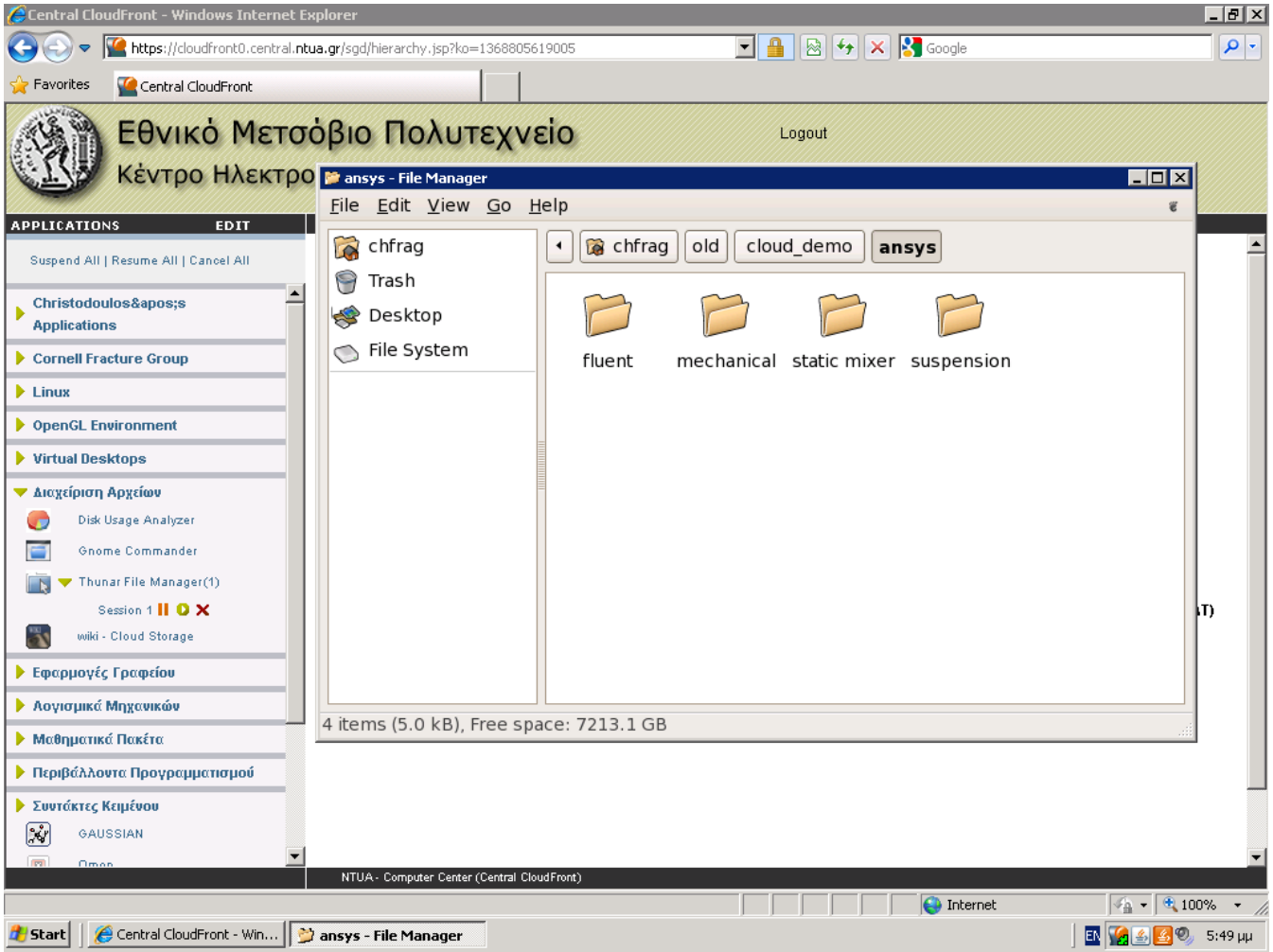
Cloud Storage



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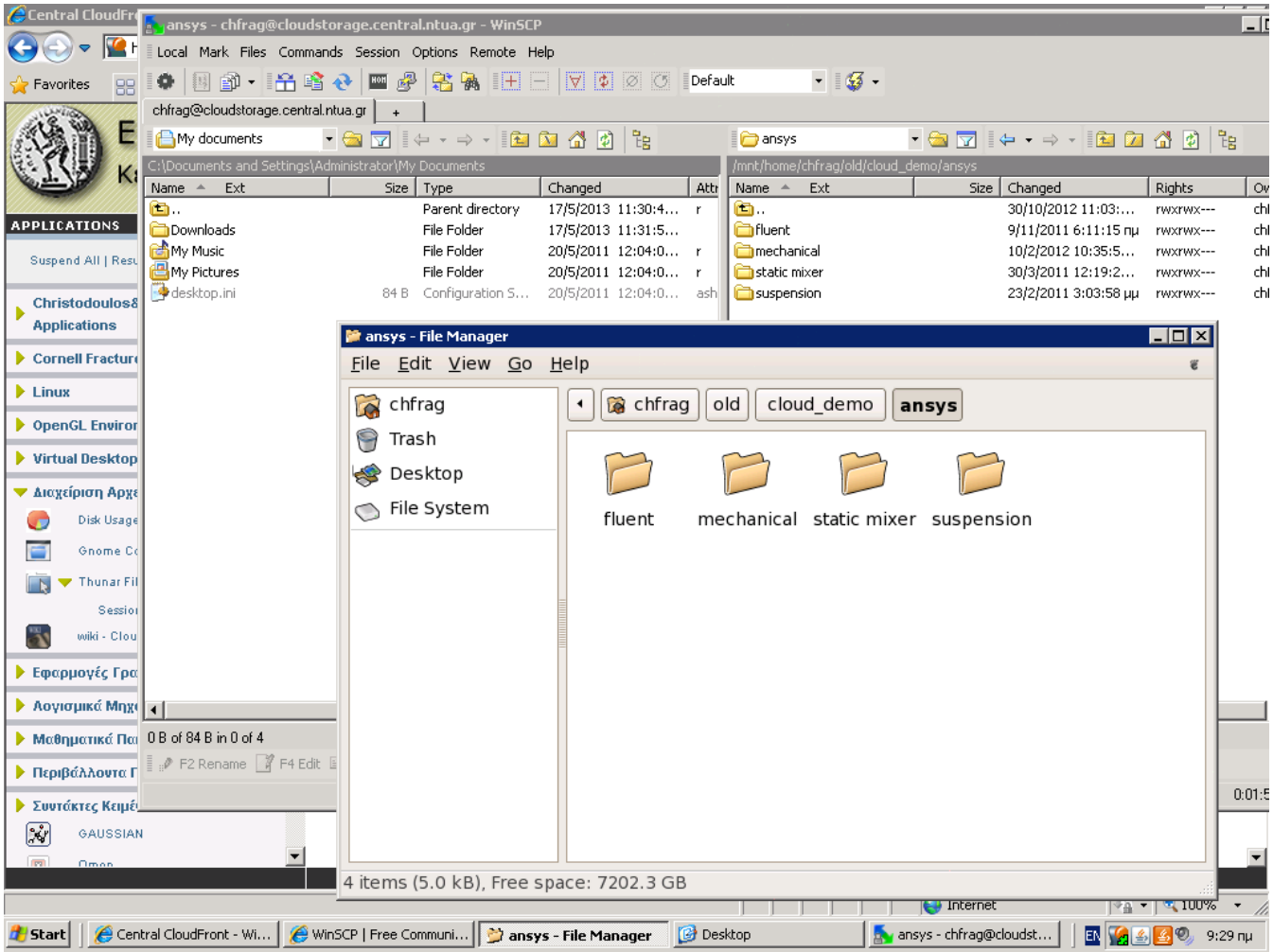
Moving/Coping files to/from Cloud Storage



Central Cloud

Minimization of local administrative burden

- Preparation for Philonnet seminars:
  - the traditional way: install ANSYS on *each and every* computer in the lab during non-working hours.
  - the *Central Cloud* way: install *ANSYS on the Cloud* only once during working hours.
  - Obsolete hardware in NTUA's labs are at least capable to connect to the Central Cloud. *Thin Client* technology could be incorporated.

Central Cloud

Economy of Scale

- Economy of scale:
  - If NTUA provides to each newcomer a very limited version of a certain commercial mathematical package:

    $$2.000 \times 40 € = 80.000 €$$

  - On the contrary, if 250 network licenses for the *FULL* package are incorporated into the Central Cloud the cost is:

    $$40.000 € \text{ initially and } 10.000 € \text{ per year}$$

  - The package will be available for **EVERY NTUA member.**

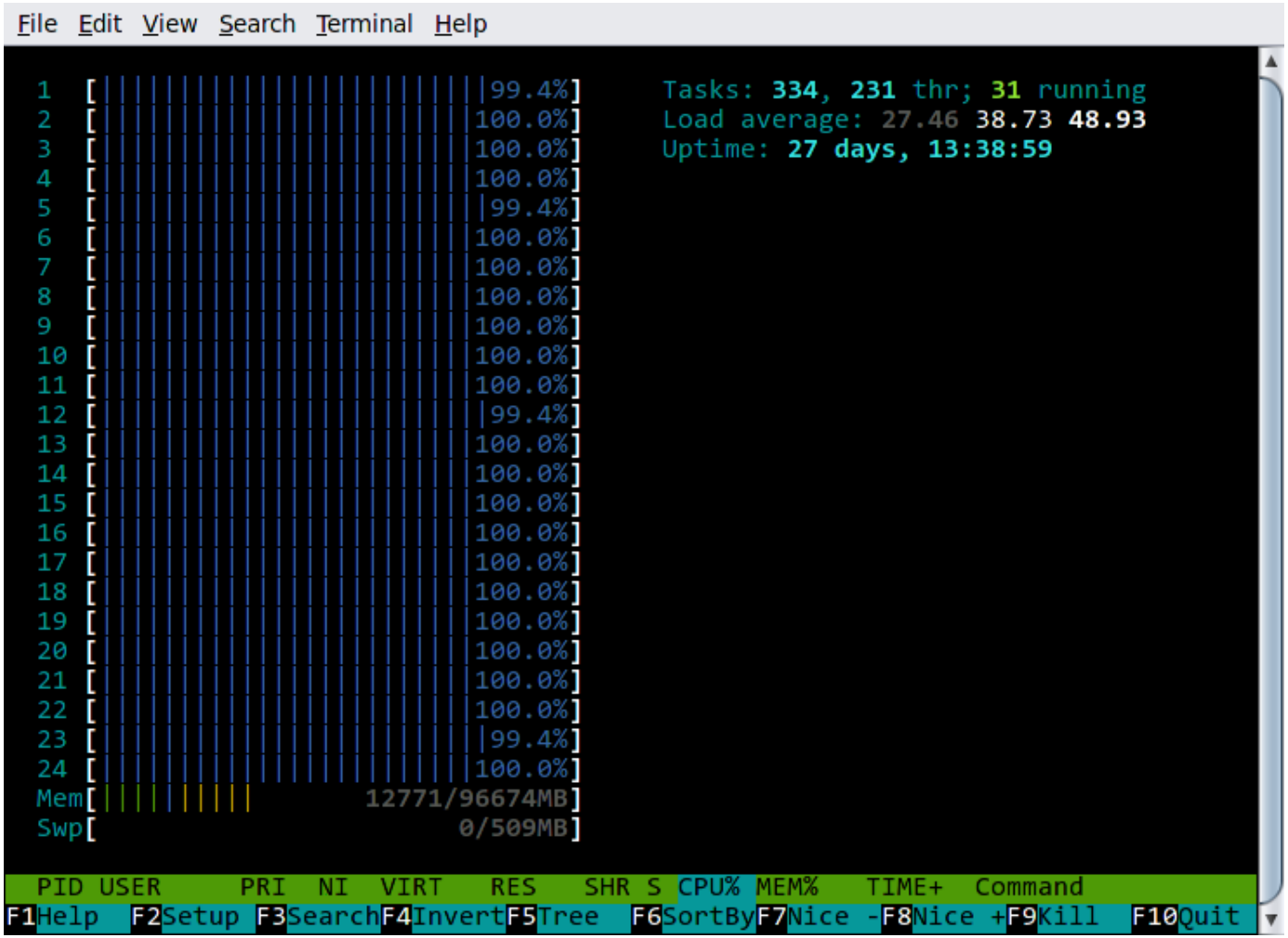
Central Cloud

Special advandages for NTUA schools and faculty members

- Faculty members or schools can utilize the Central Cloud's infrastructure by plugging their own blades or disks in the available empty slots:
  - Low cost: no chassis, power supplies, networking, etc.
  - Zero administration.
  - Security: behind enterprise class firewalls.
  - UPS, Power Generator, Air Conditioning.
  - Guaranteed dedicated usage.

Central Cloud

Problem: Users fight each other for resources



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Need for a batch job system

- The demand usually exceeds resources.
- Provide different *queues* for different types of jobs (serial, parallel, . . .).
- Attempt to keep load on machines as high as possible.
- Try to schedule submitted jobs by evaluating the needed resources.
- Users should provide as much information as possible (memory, wall clock time, . . .).

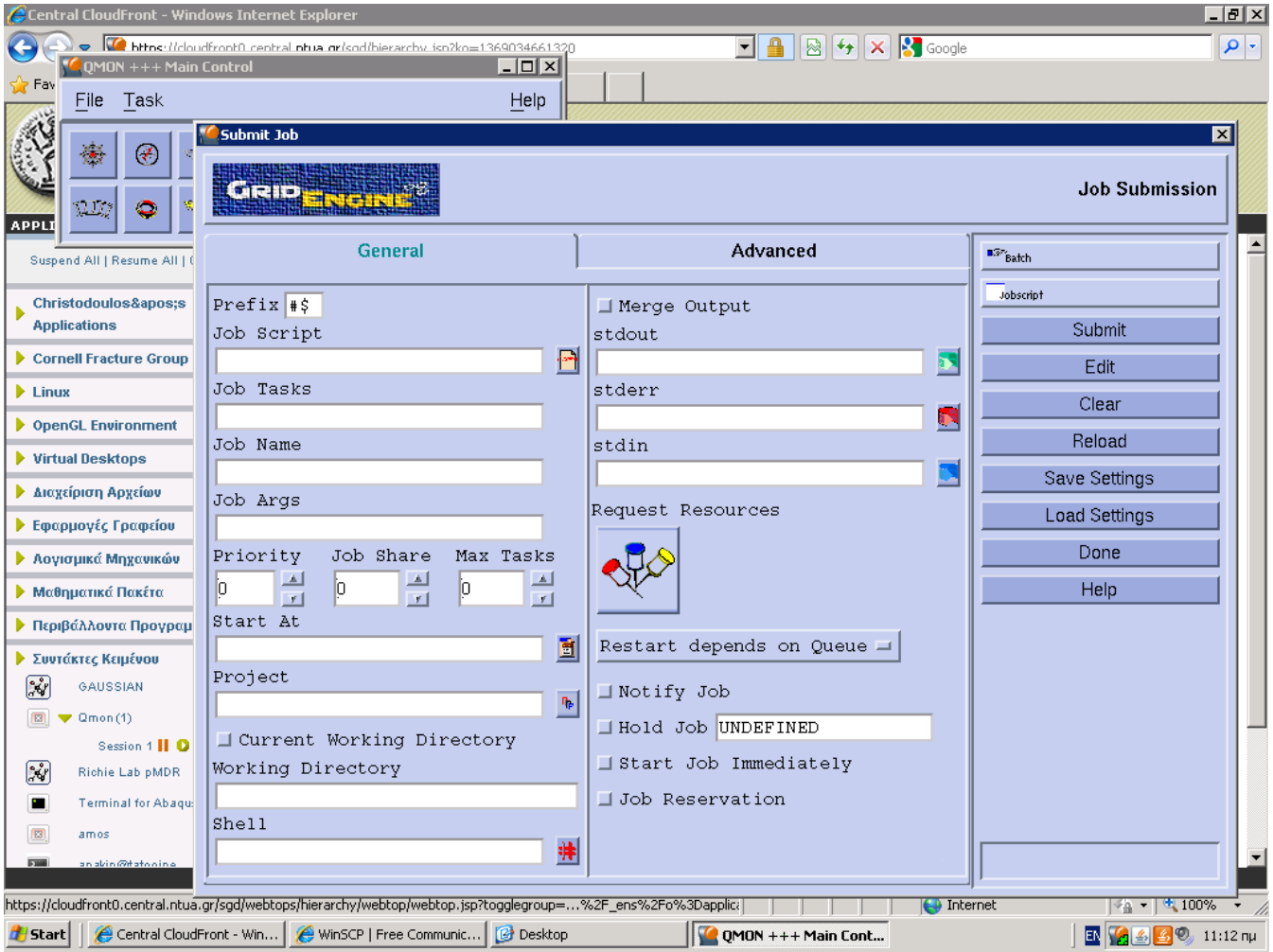
Grid Engine

What it is and what it does

- A set of computer hosts that work together with a single point of access.
  - Accepts jobs from the outside world. Jobs are users requests for computer resources.
  - Puts jobs in a holding area until the jobs can be run.
  - Sends jobs from the holding area to the an execution device.
  - Manages running jobs.
  - Logs the record of job execution when the jobs are finished
- A GUI front end of SGE, namely Qmon is available in Central CloudFront.

Central CloudFront

Launching Qmon and submiting a script



Grid Engine

ANSYS CFX example

```
#!/bin/bash
#$ -S /bin/bash
#$ -M chfrag@central.ntua.gr
#$ -m bae
#$ -l h_rt=24:00:00m h_vmem=1G
#$ cfx5solve -def file.def -double
   -start-method "MPICH Local Parallel"
    -part 16 -size 2 -sizepar 2
```

due to Ioannis Karathanassis

- CFX parallel (MPICH) job.
- Double precission.
- 16 processors.
- Heavy job (doubles allocated memory).
- Wall clock limit of 1 day.
- Maximum total memory of 1G.
- Sending email upon starting, aborting and finishing.

Grid Engine

Suggested usage

- What you need to know:
  - Don’t worry about queues or specific machines.
  - All you need to do when submitting a job is describe the resources your job will need to run successfully.
  - Grid Engine will take care of the rest.

My observation: NTUA’s researchers are having a hard time defining the required resources for their jobs. Most of the times they just want to “click solve”.

NTUA's Central Cloud

Recent acknowledgments

In "International Journal of Thermal Sciences":

- I.K. Karathanassis, E. Papanicolaou, V. Belessiotis, G.C. Bergeles, *Three-dimensional flow effects on forced convection heat transfer in a channel with stepwise-varying width*, 2013.

In "International Journal of Heat and Mass Transfer":

- I.K. Karathanassis, E. Papanicolaou, V. Belessiotis, G.C. Bergeles, *Effect of secondary flows due to buoyancy and contraction on heat transfer in a two-section plate-fin heat sink*, 2013.

Thank you!

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