Virtual Research Communities
Towards a Molecular Science VRC

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e-infrastructure

Summary

- Chemistry as HUC: state of the art
- On the way to build a Chemistry VRC
- Tools for an E-science environment
- Research activities

HUC in Chemistry: MMSC

- Molecular and Material Science Community
- Present since EGEE Project within the Computational Chemistry (CC) cluster forming global (pan-European) grid VOs

  - GAUSSIAN (CYFRONET) devoted to implementing and maintaining commercial codes

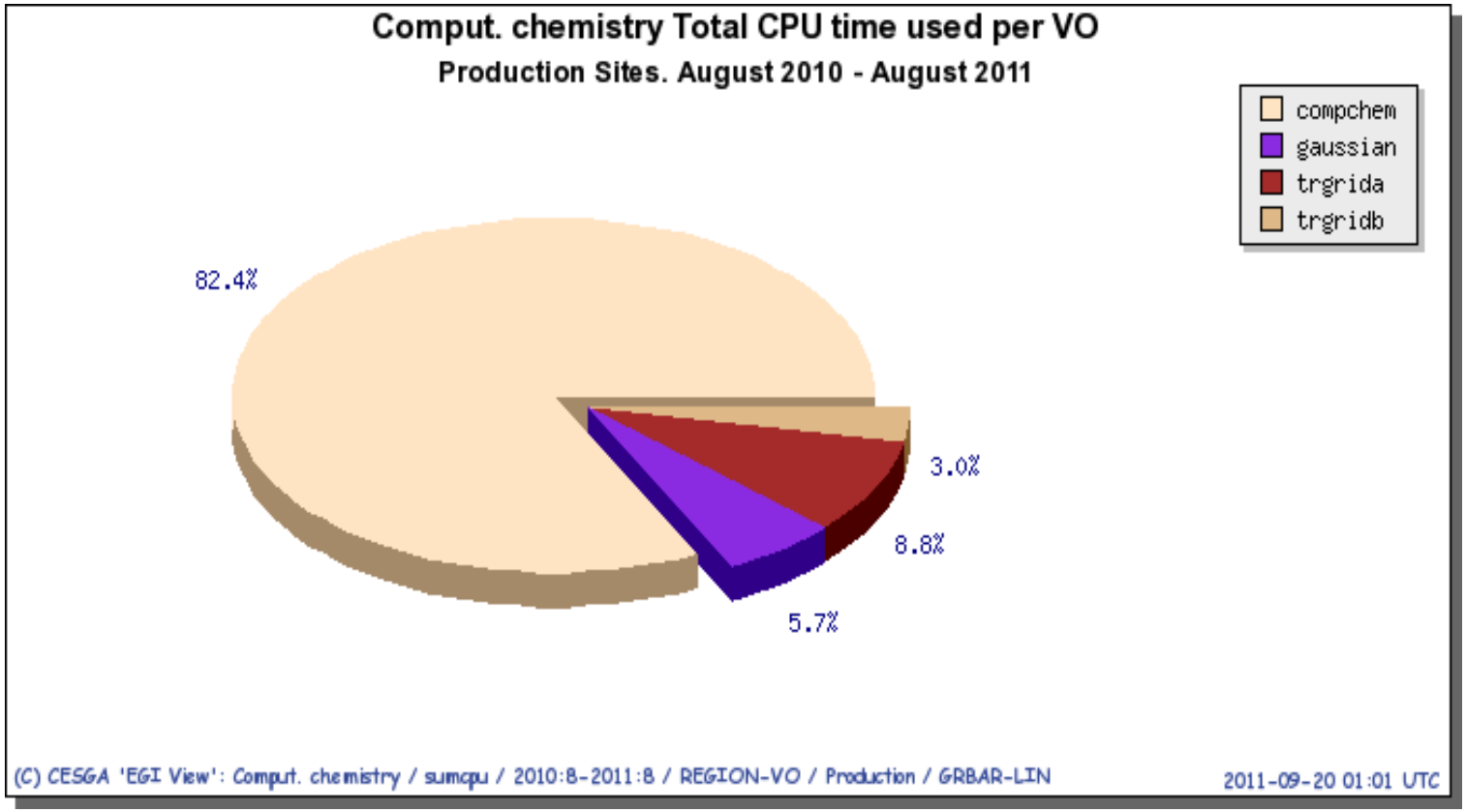
  - COMPCHEM (UNIPG) devoted to the implementation of non commercial codes

  - TRGRID (ULAKBIM) Grid and HPC in Turkey

Statistics

11M of CPU hours ≈ 1.2 % of total CPU time*

*Used for production in EGI in the same period



On the way of a Chemistry VRC: CheMIST

* Develop a proper E-science environment

  - to build out of a HUC a VRC

  - to exploit the potentiality of the Grid

* Needs to develop a Chemistry VRC

  - Combination efforts between CC VOs and other Grid and non-Gird communities

  - Adoption (with appropriate adaptations) of Grid tools developed by other Grid Communities

  - Design, development and deployment of ad hoc tools

On the way of a Chemistry VRC: Sustainability

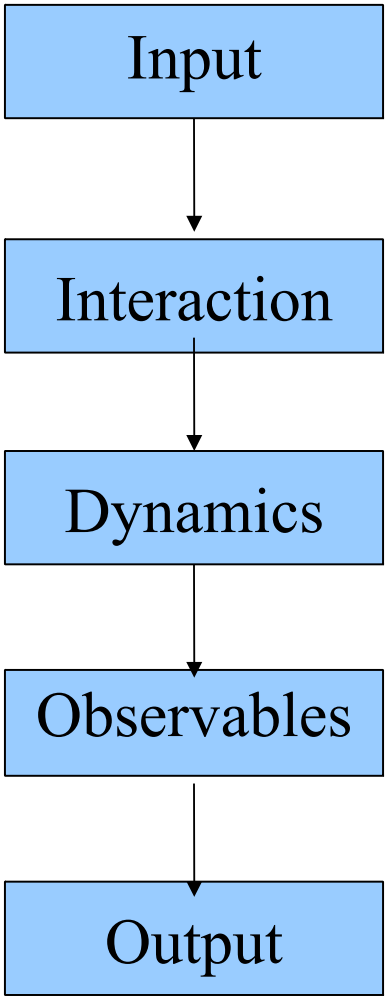
* Design, development and deployment of ad hoc tools
  - User-friendly interfaces
  - Easy access to different resources (Virtualization and HPC)
  - Visualization

* Design, development and deployment of ad hoc tools
  - credit based economy
  - QoU and QoS evaluation

Services and Consulting

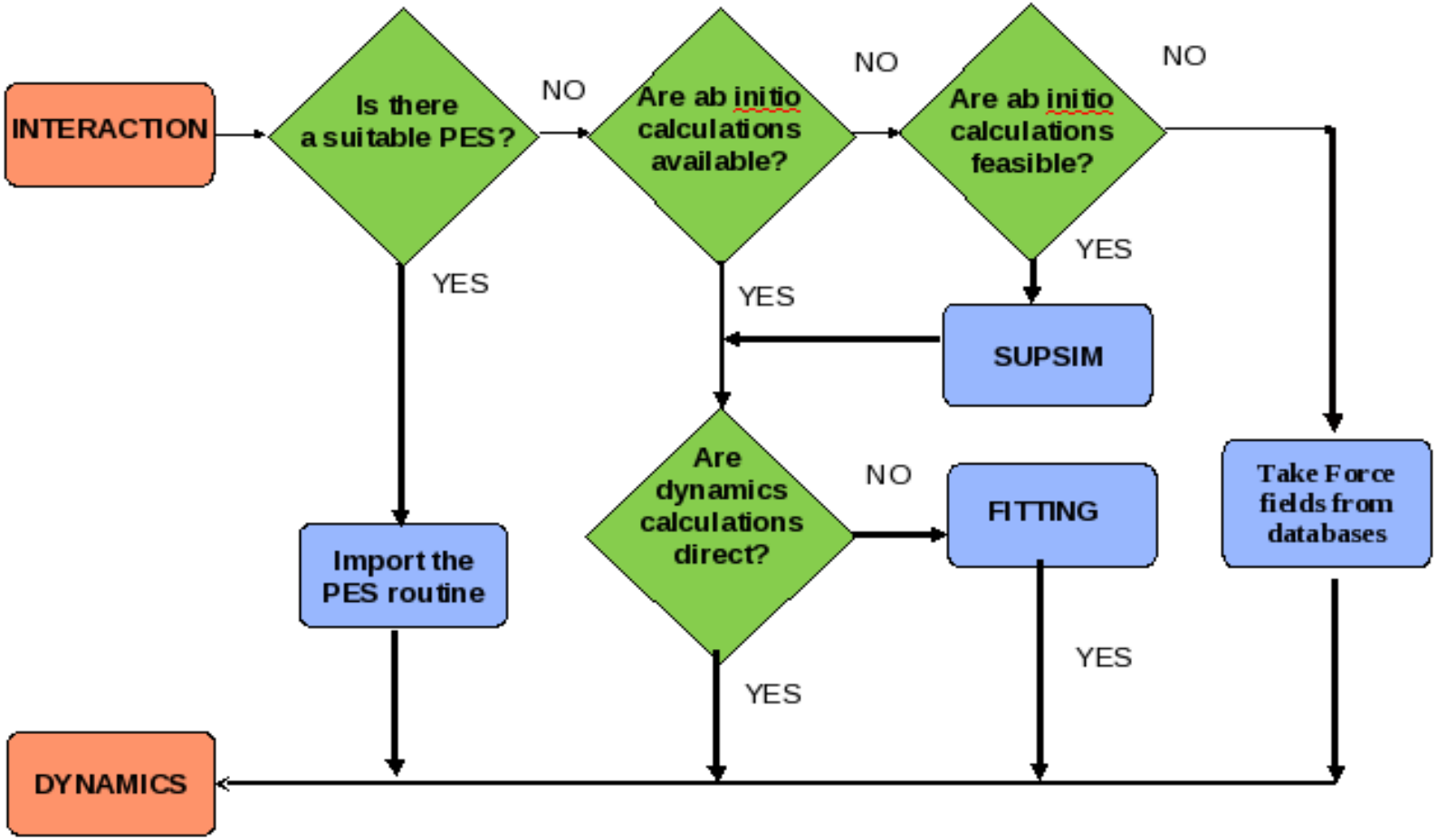
Grid Enabled Molecular Simulator

- Specialized in quantum reactive scattering and MD problems
- Structured as a workflow and divided in three blocks
  - INTERACTION
  - DYNAMICS
  - OBSERVABLES



Structure of GEMS

- Devoted to the building of the eigensolutions of the electronic system



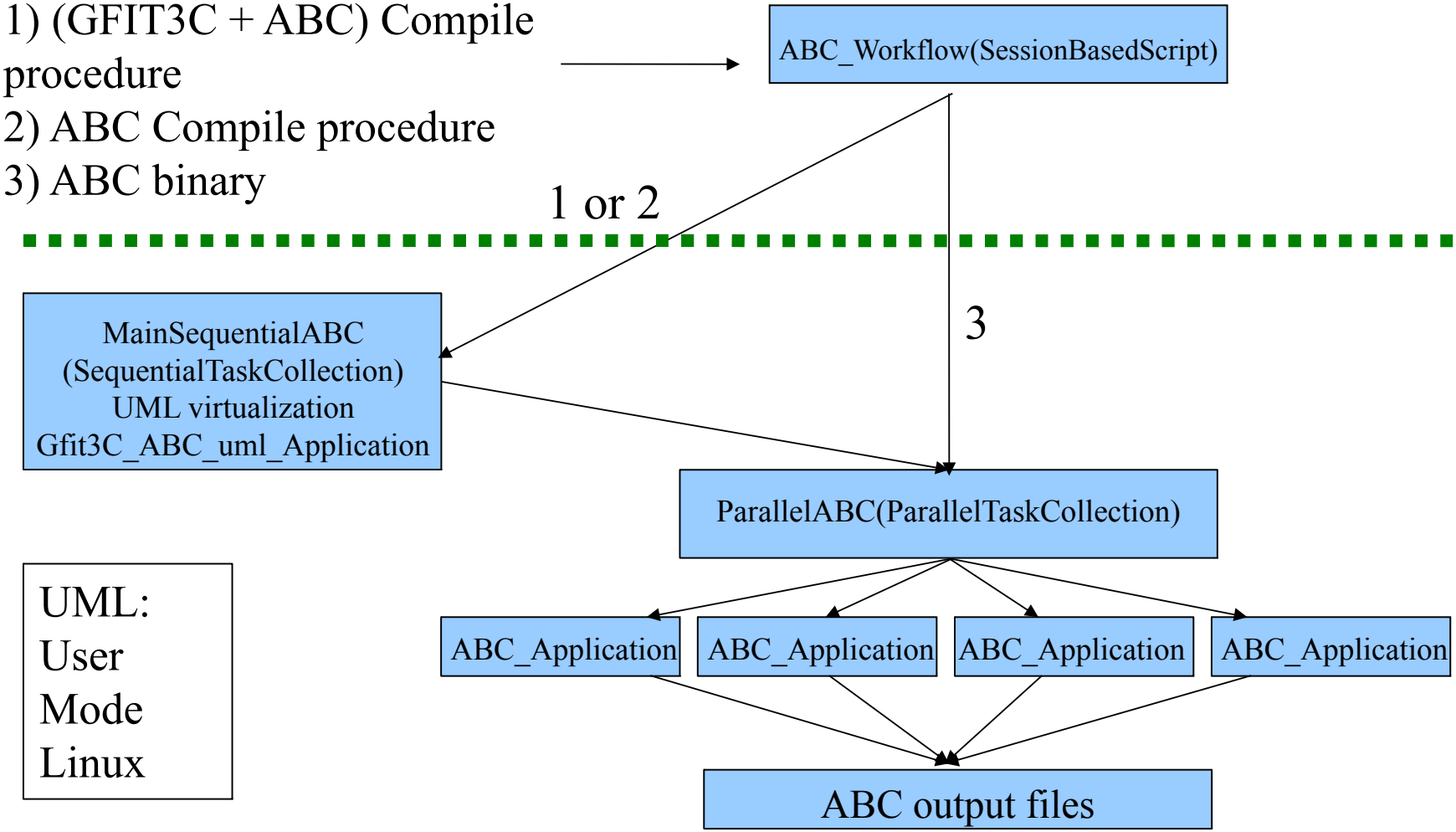
Tools for an E-science environment: Porting

- P-GRADE Grid Portal
  - Open source tool (java)
  - Collect Grid resources
  - The generic application structure is a workflow
  - Specific graphical tools can be added

- GC3Pie (booth SwiNG)
  - Developed from GC3 group @ UZH (sergio.maffioletti@gc3.uzh.ch)
  - Open Source Tool in Python
  - Collects grid (arc, gLite), distributed (cluster) and local resources
  - Provides building blocks for developing dynamic workflows

Tools for an E-science environment: Porting

1) (GFIT3C + ABC) Compile procedure
2) ABC Compile procedure
3) ABC binary



UML:
User
Mode
Linux

Tools for an E-science environment: Efficient Grid submission

GriF: a collaborative tool for grid empowered computational applications

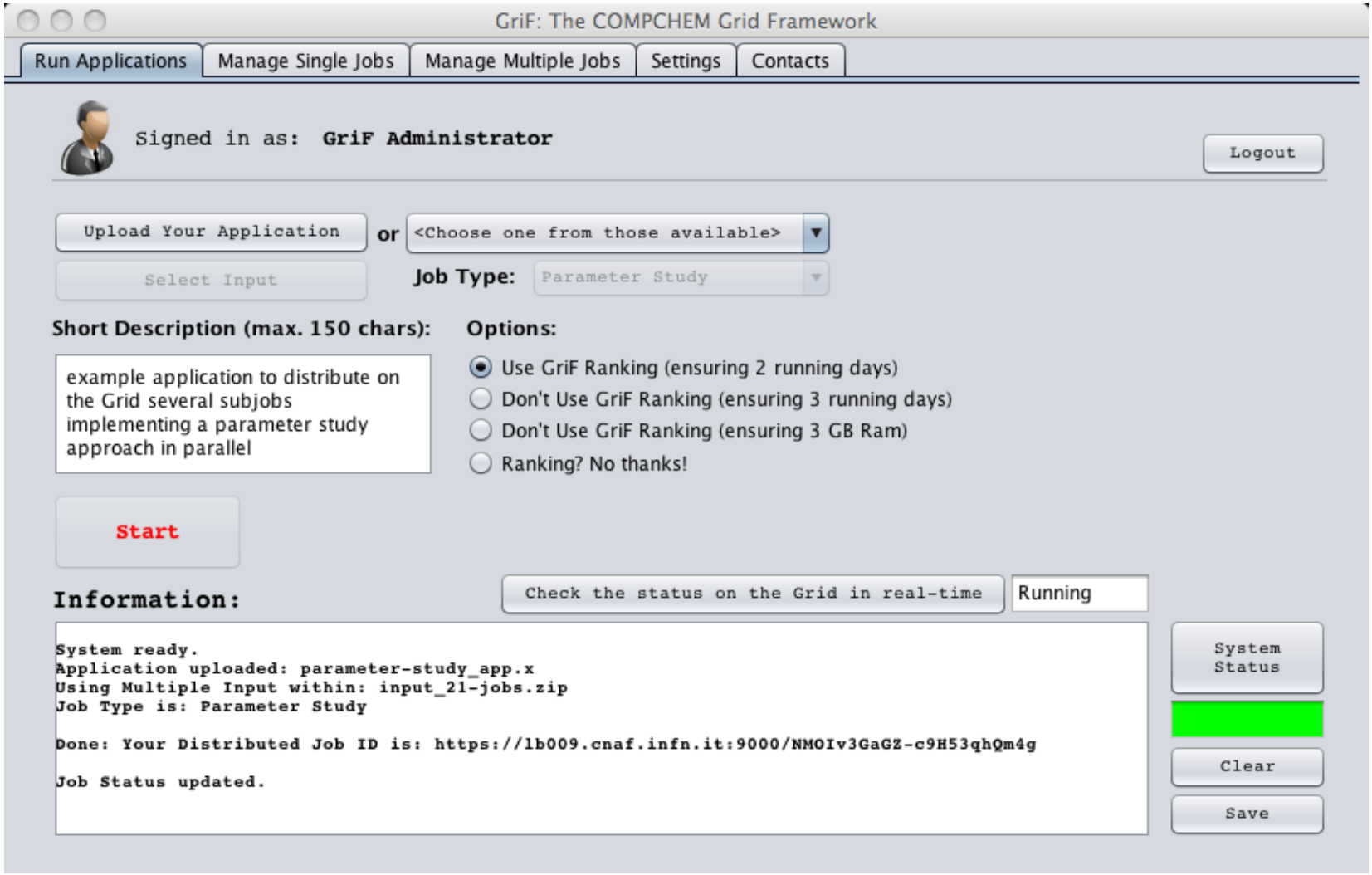
– Easy submission over the Grid

– Optimized distributions of tasks

– Java based framework

– Support single and multiple job submission

Tools for an E-science environment: Efficient Grid submission



Tools for an E-science environment: Credit system

GCreS: a credit system to reward member

– Use Grid sensors to evaluate services provided
– Use Grid sensors to evaluate user activities
– Introduce a metric in the VO
– Implement a credit system and cost of services

Tools for an E-science environment
E-learning and education

- DISTRIBUTED REPOSITORIES OF LEARNING OBJECTS (G-LOREP) AND VIRTUAL CAMPUS

- DISTRIBUTED ELECTRONIC SELF ASSESSMENT TESTS

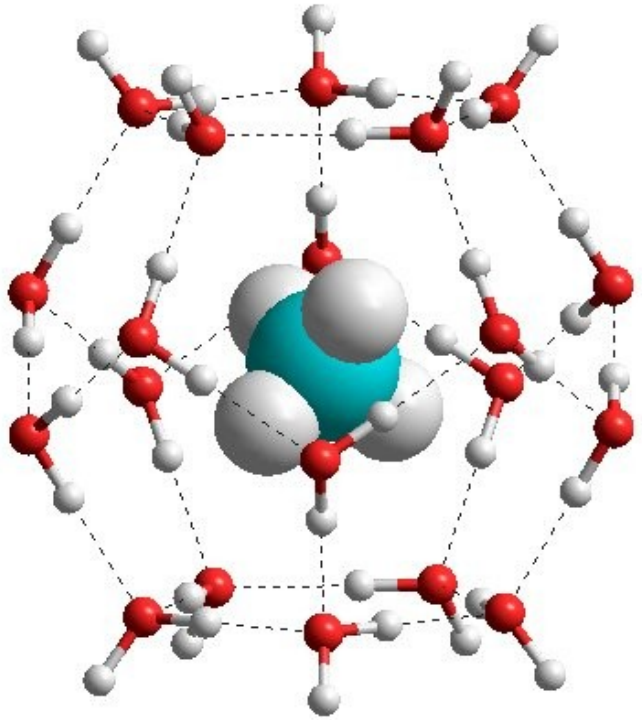
-VIRTUAL LABORATORY SUPPORT TO EUROMASTER AND EURODOCTORATE

- SCHOOLS AND TUTORIAL (BASIC AND AVANCED) FOR GRID USERS

Methane Hydrates

***Gas hydrates (Clathrates)**: water hydrogen bonded structures caging gas molecules*

- Cl_2
- H_2S
- CO_2
- CH_4
- H_2
- *etc.*



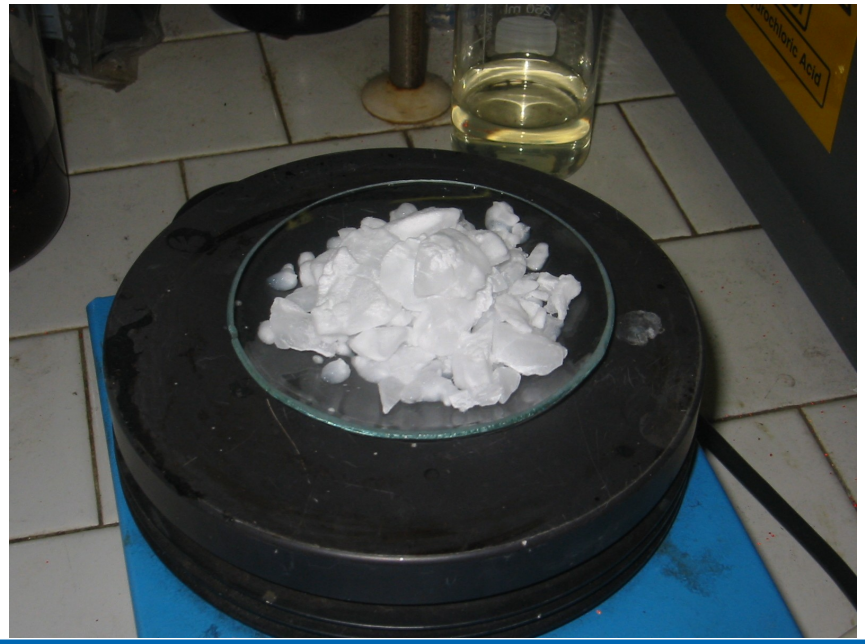
Methane Hydrates

APPEARANCE: ice like

CAPTURING AND RELEASING: energetically cheap

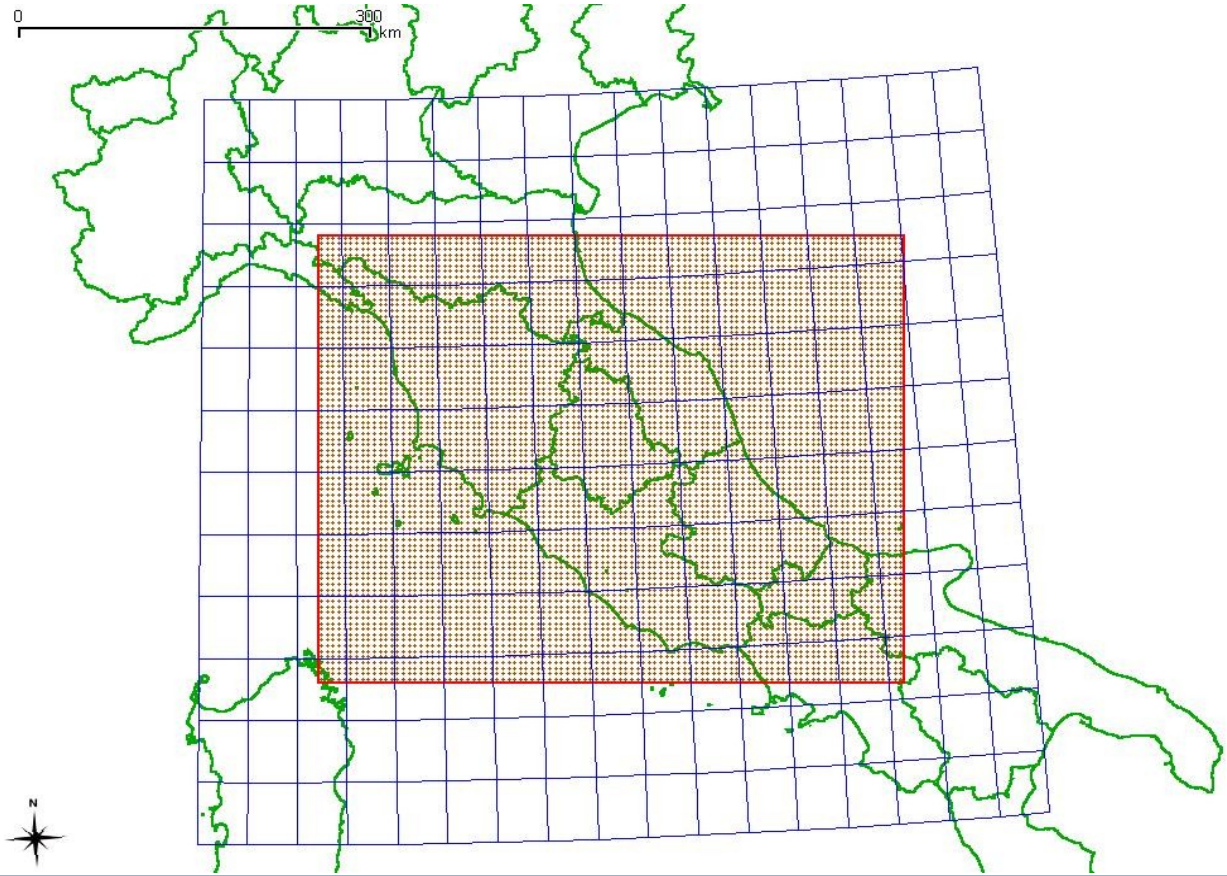
SAFETY: no risks

UTILIZED TECHNOLOGIES: consolidated



Atmospheric Modeling: CHIMERE

- Simulated Center Itlay domain
- Service for simulations of pollutants (in collaboration with Regional Agency for Environment Protection)



Atmospheric Modeling: CHIMERE

- Daily prevision of gas phase pollutant (Ozone) on Center Italy domain