



# Virtual Research Communities Towards a Molecular Science VRC

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e-infrastructure



21/09/11 EGI-InSPIRE RI-261323

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



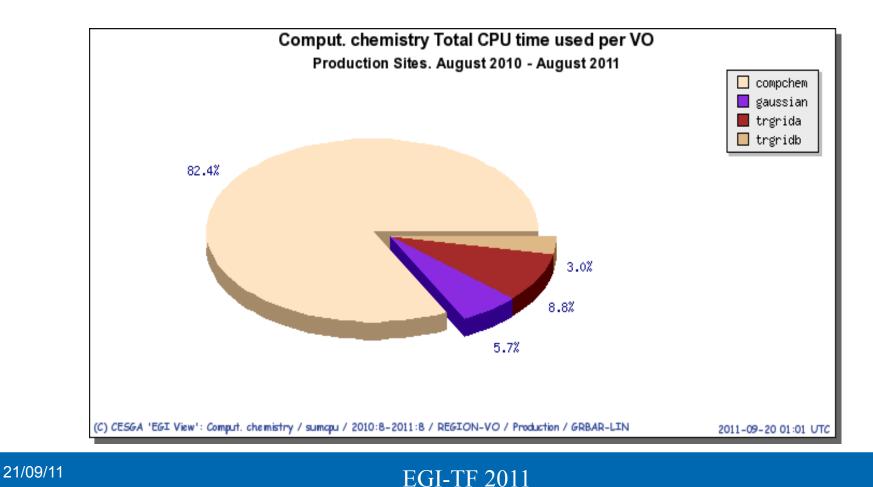
- Molecular and Material Science Community
- Present since EGEE Project within the Computational Chemistry (CC) cluster forming global (pan-European) grid VOs
  - GAUSSIAN (CYFRONET) devoted to implementing and maintaining commercial codes
  - COMPCHEM (UNIPG) devoted to the implementation of non commercial codes
  - TRGRID (ULAKBIM) Grid and HPC in Turkey



#### **Statistics**

# 11M of CPU hours $\approx 1.2$ % of total CPU time\*

#### \*Used for production in EGI in the same period



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## 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

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## On the way of a Chemistry VRC: Sustainability

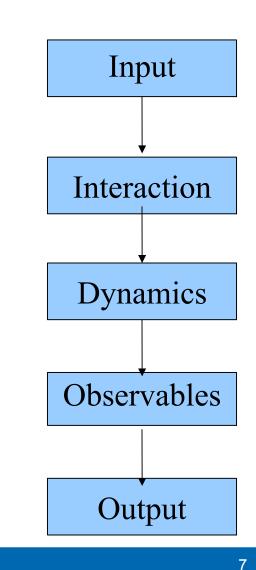
\* Design, development and deployment of ad hoc tools

- 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



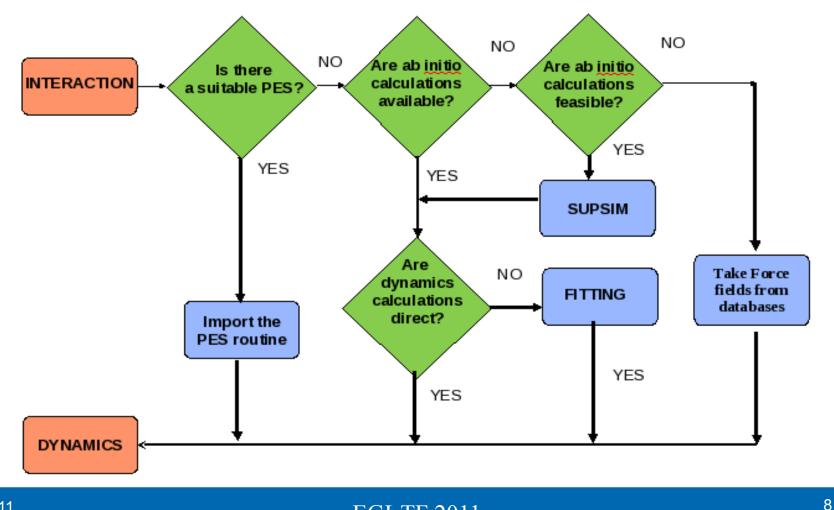
- Specialized in quantum reactive scattering and MD problems
- Structured as a workflow and divided in three blocks
  - INTERACTION
  - DYNAMICS
  - OBSERVABLES





**Structure of GEMS** 

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





# Tools for an E-science environment: Porting

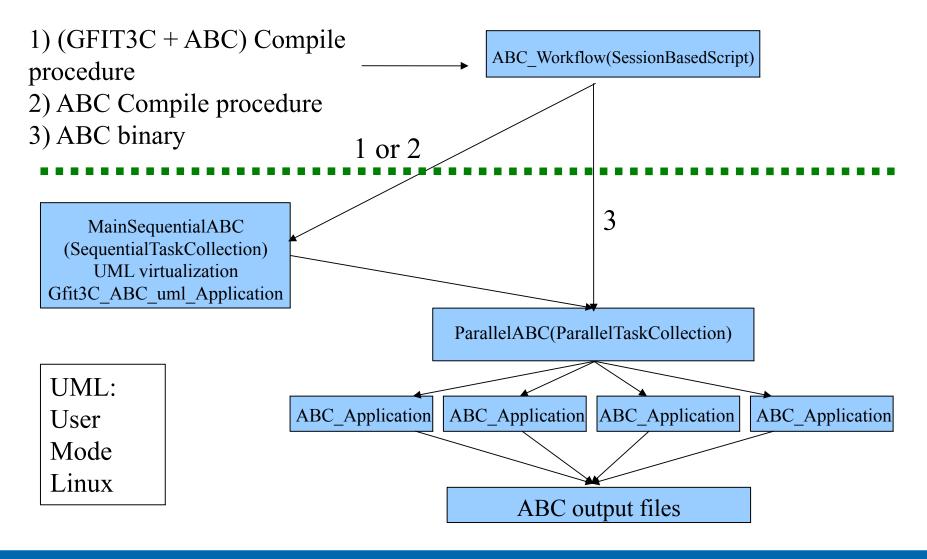
- P-GRADE Grid Portal
  - Open source tool (java)
  - Collect Grid resources
  - The generic application structure is a workflow
  - Specific graphical tools can be added

#### - 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





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



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#### **Tools for an E-science environment: Efficient Grid submission**

GriF: The COMPCHEM Grid Framework					
un Applications Manage Single Jobs	Manage Multiple Jobs	Settings	Contacts		
Signed in as: GriF Ad	<b>ministrator</b> <choose from="" one="" th="" tho<=""><th>se availa</th><th>uble&gt; 🔻</th><th></th><th>Logout</th></choose>	se availa	uble> 🔻		Logout
Select Input	Job Type: Parameter	Study	T		
Short Description (max. 150 chars example application to distribute on the Grid several subjobs implementing a parameter study approach in parallel	<ul> <li>Use GriF Ranki</li> <li>Don't Use GriF</li> <li>Don't Use GriF</li> <li>Ranking? No the</li> </ul>	Ranking (e Ranking (e anks!	nsuring 3 ru	nning days) 8 Ram)	
Information:	Check the	status or	the Grid	in real-time Running	3
System ready. Application uploaded: parameter-study_app.x Using Multiple Input within: input_21-jobs.zip Job Type is: Parameter Study Done: Your Distributed Job ID is: https://lb009.cnaf.infn.it:9000/NMOIv3GaGZ-c9H53qhQm4g Job Status updated.					System Status Clear
					Save



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** 

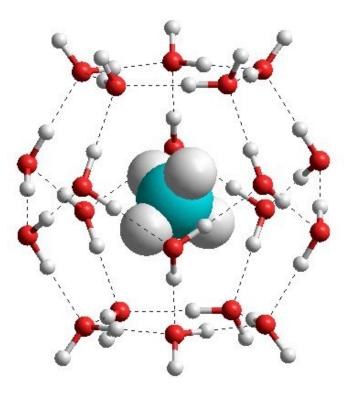
- DISTRIBUTED REPOSITORIES OF LEARNING **OBJECTS (G-LOREP) AND VIRTUAL CAMPUS**
- DISTRIBUTED ELECTRONIC SELF ASSESSMENT TESTS
- -VIRTUAL LABORATORY TO SUPPORT EUROMASTER AND EURODOCTORATE
- SCHOOLS AND TUTORIAL (BASIC AND AVANCED) FOR GRID USERS



#### **Methane Hydrates**

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

- Cl<sub>2</sub>
- H<sub>2</sub>S
- **CO**<sub>2</sub>
- **CH**<sub>4</sub>
- **H**<sub>2</sub>
- *etc*.





#### **Methane Hydrates**

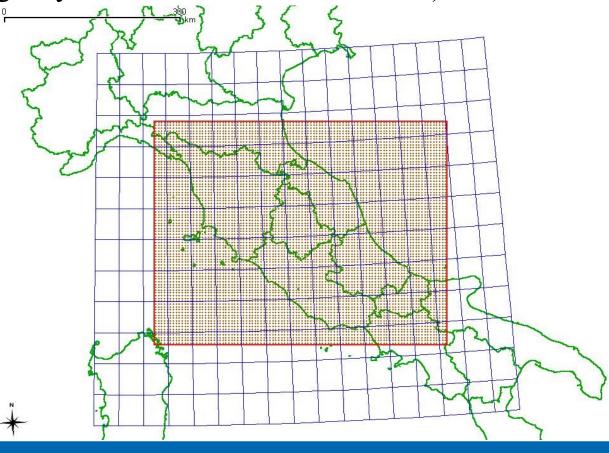
## APPEARANCE: ice like CAPTURING AND RELEASING: energetically cheap SAFETY: no risks UTILIZED TECHNOLOGIES: consolidated





# **Atmospheric Modeling: CHIMERE**

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



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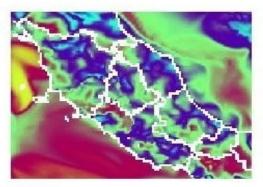
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#### **Atmospheric Modeling: CHIMERE**

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

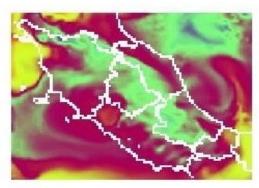


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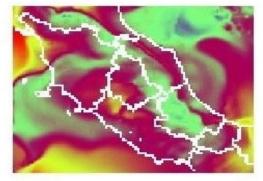
O3 (15.7 to 82.9 ppb)



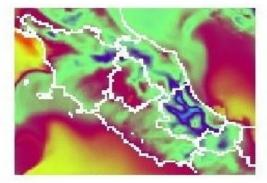
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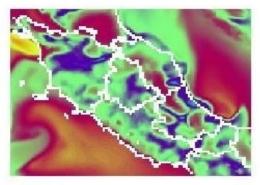
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