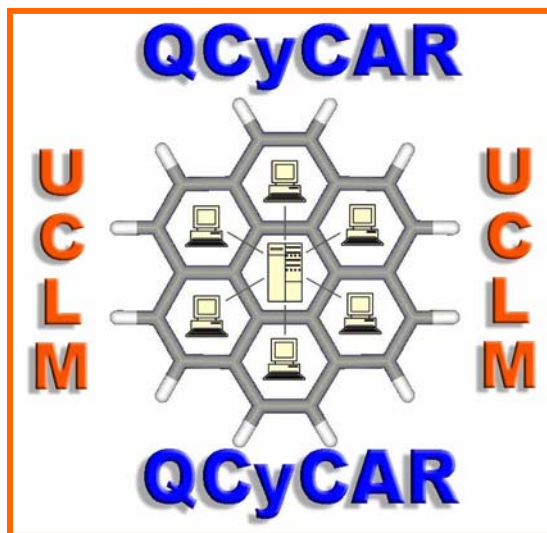


Organization of, and Experiences with, a Spain-Mexico Internet-Based Grid of Computers

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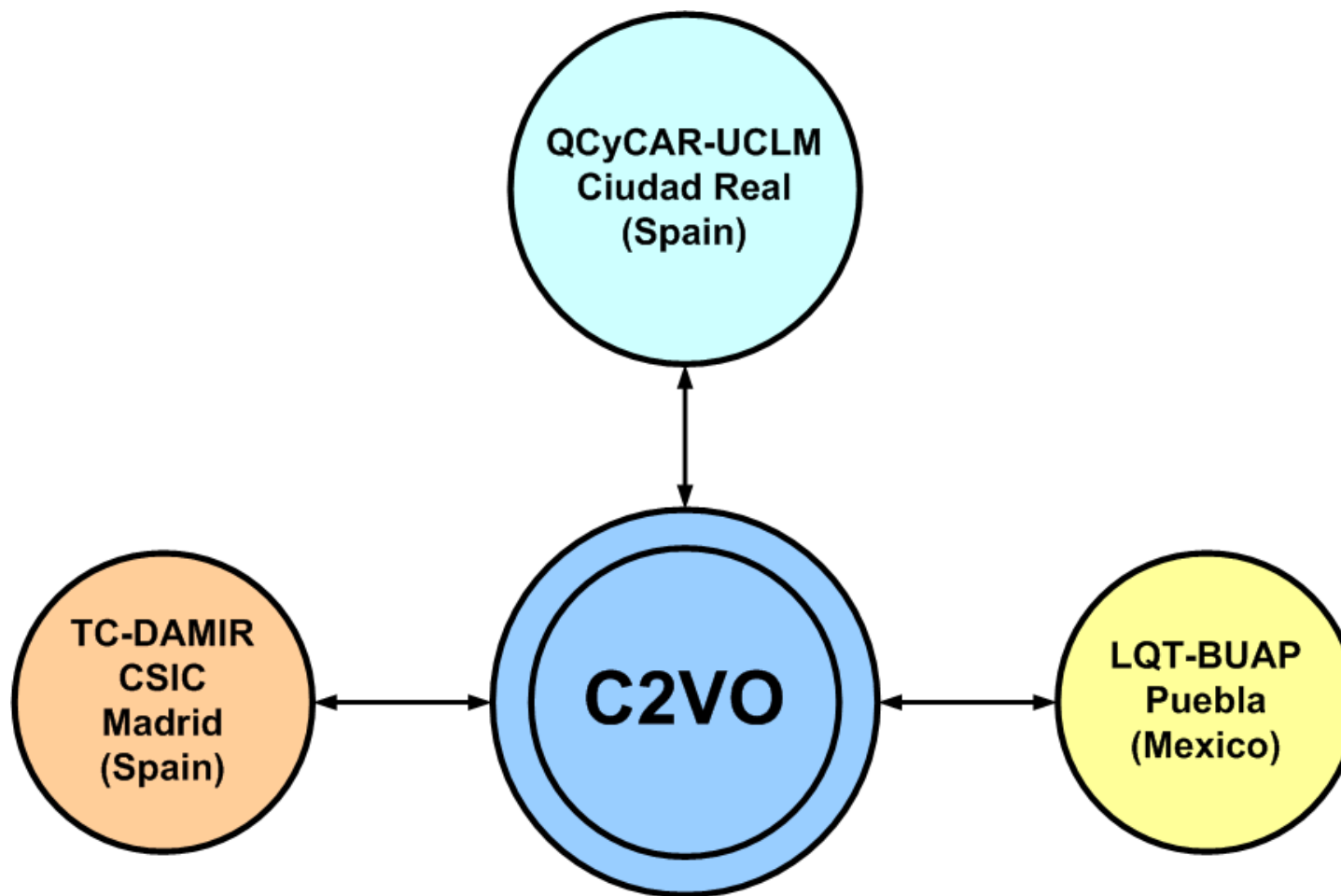
Outline

- Introduction
- Grid Organization
- Use Cases
- Experiences
- Acknowledgements

Introduction



Computational Chemistry Virtual Organization (C2VO)



Grid Organization



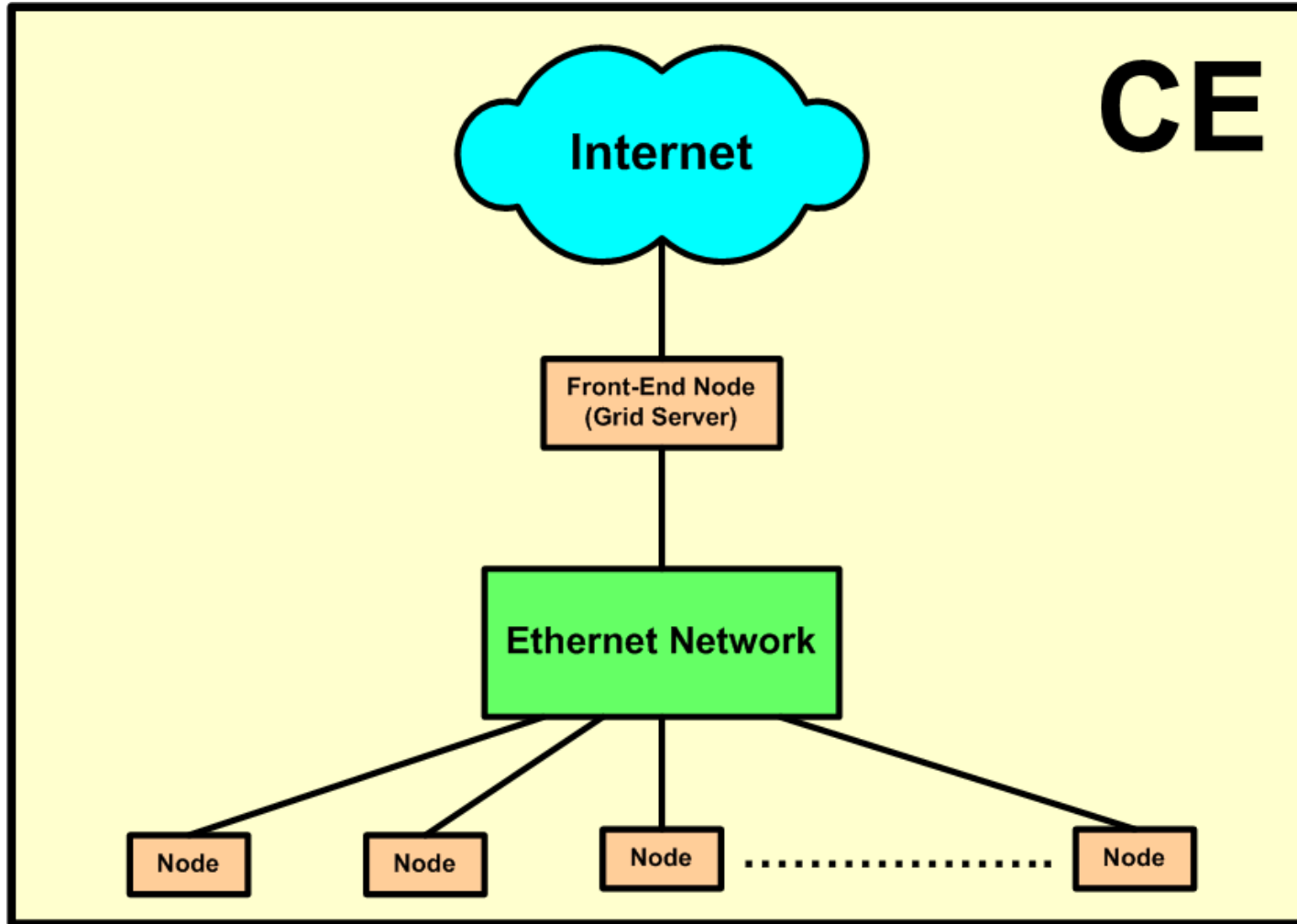
Computational Chemistry Virtual Organization (C2VO)

- CE1 Popocatepetl
- CE2 Aristoteles
- CE3 Hermes
- CE4 Tales
- CE5 Carrasca

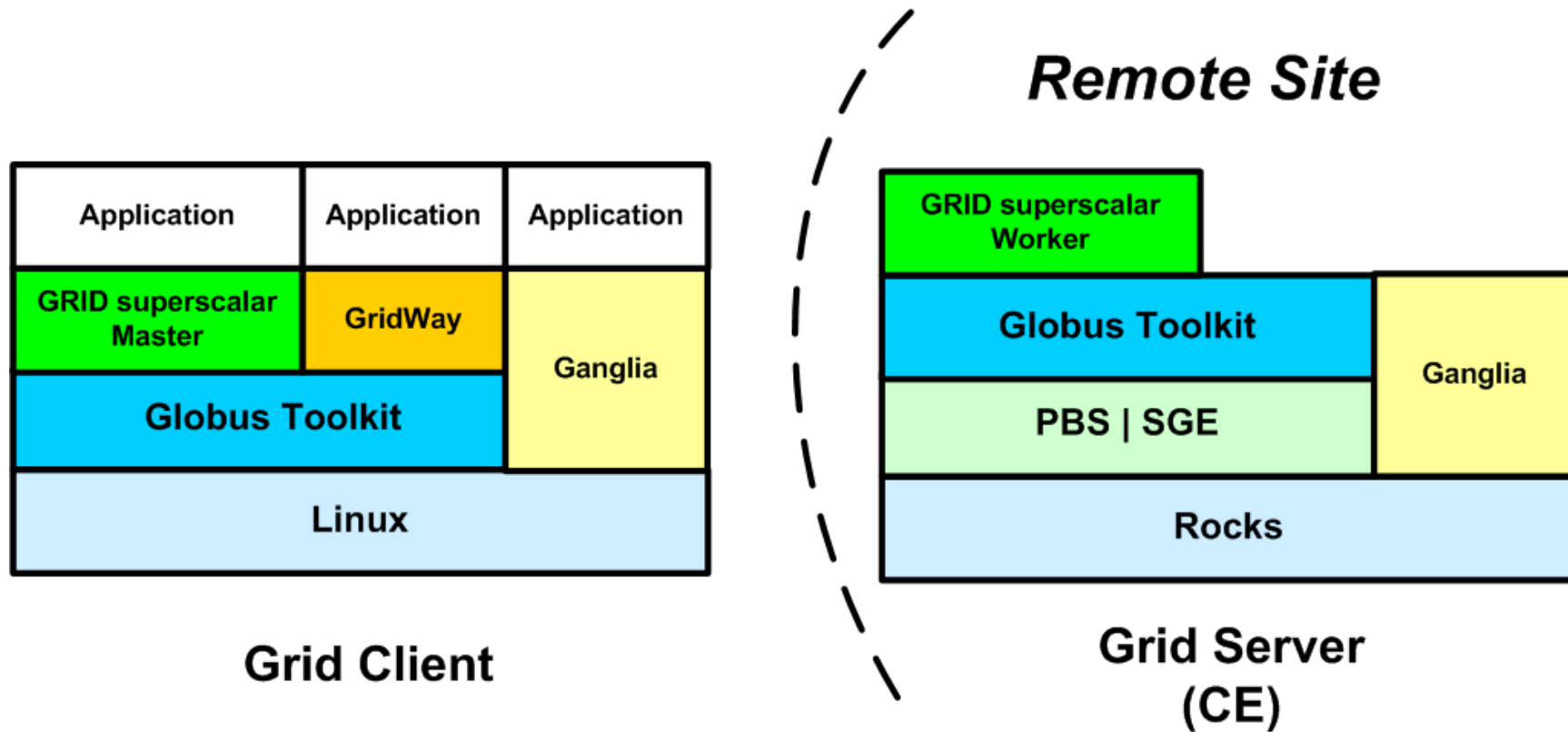
Internet-Based Grid Infrastructure



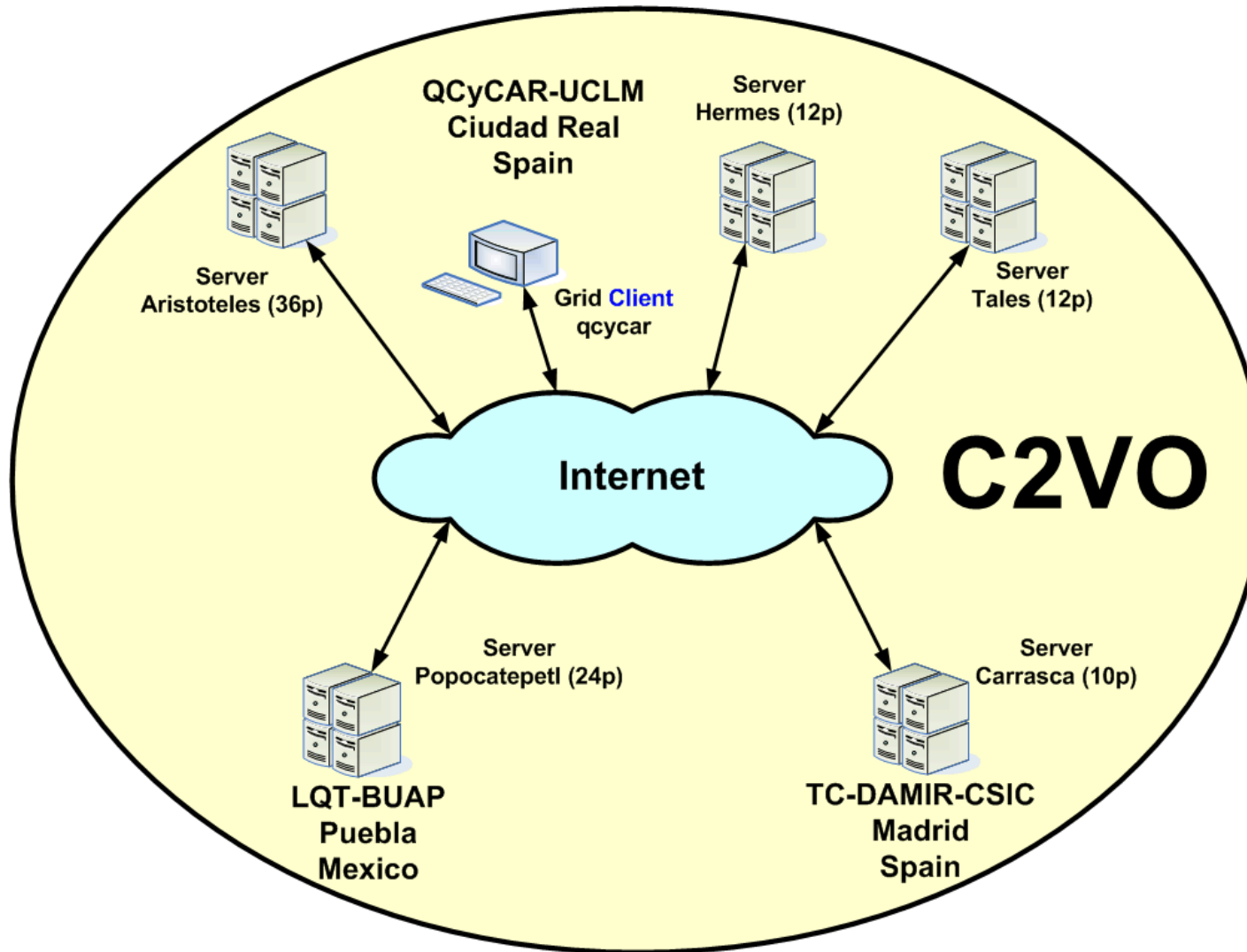
Structure



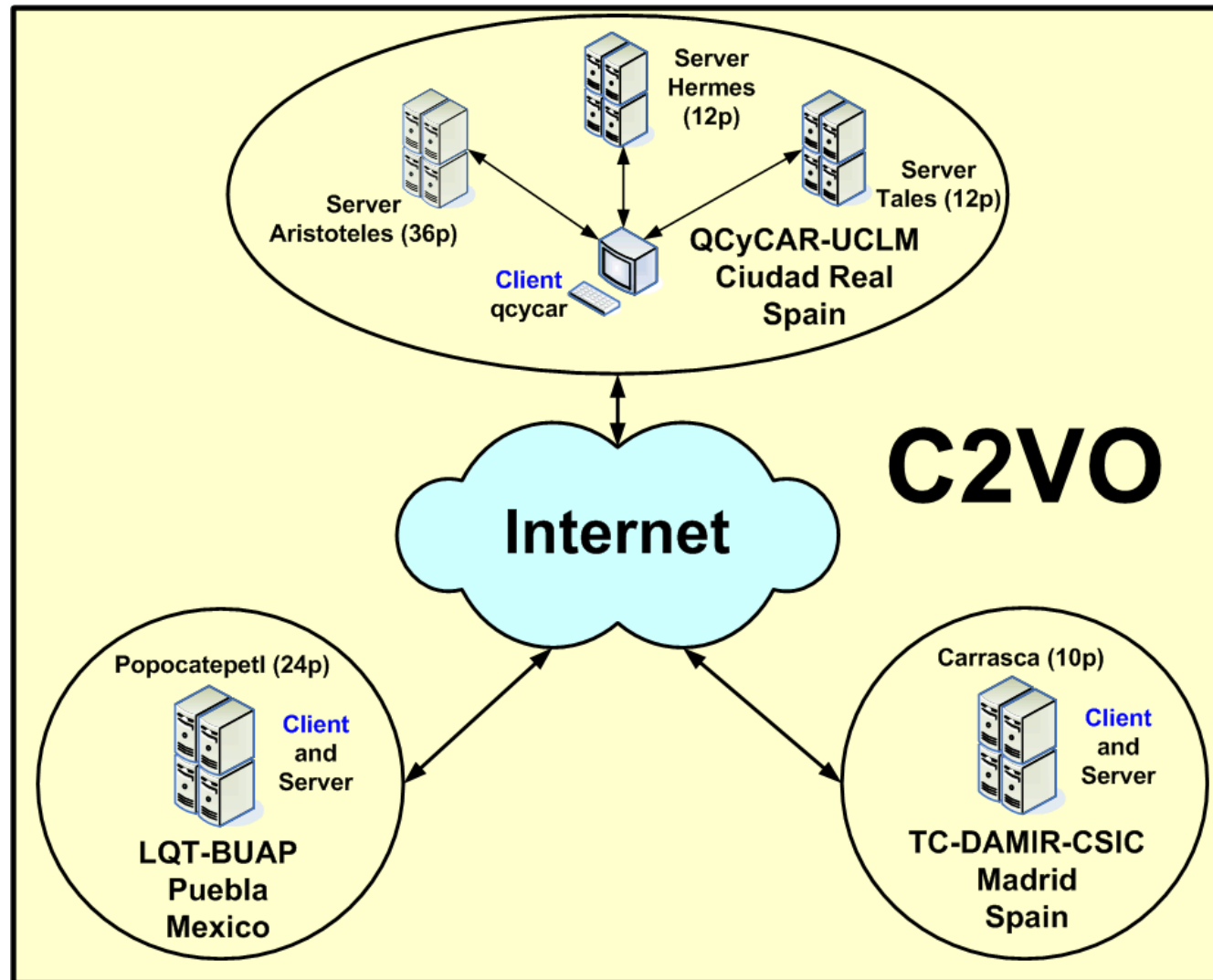
Architecture



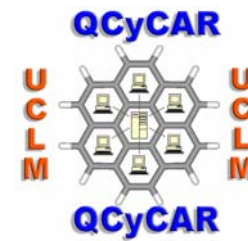
Centralized Topology



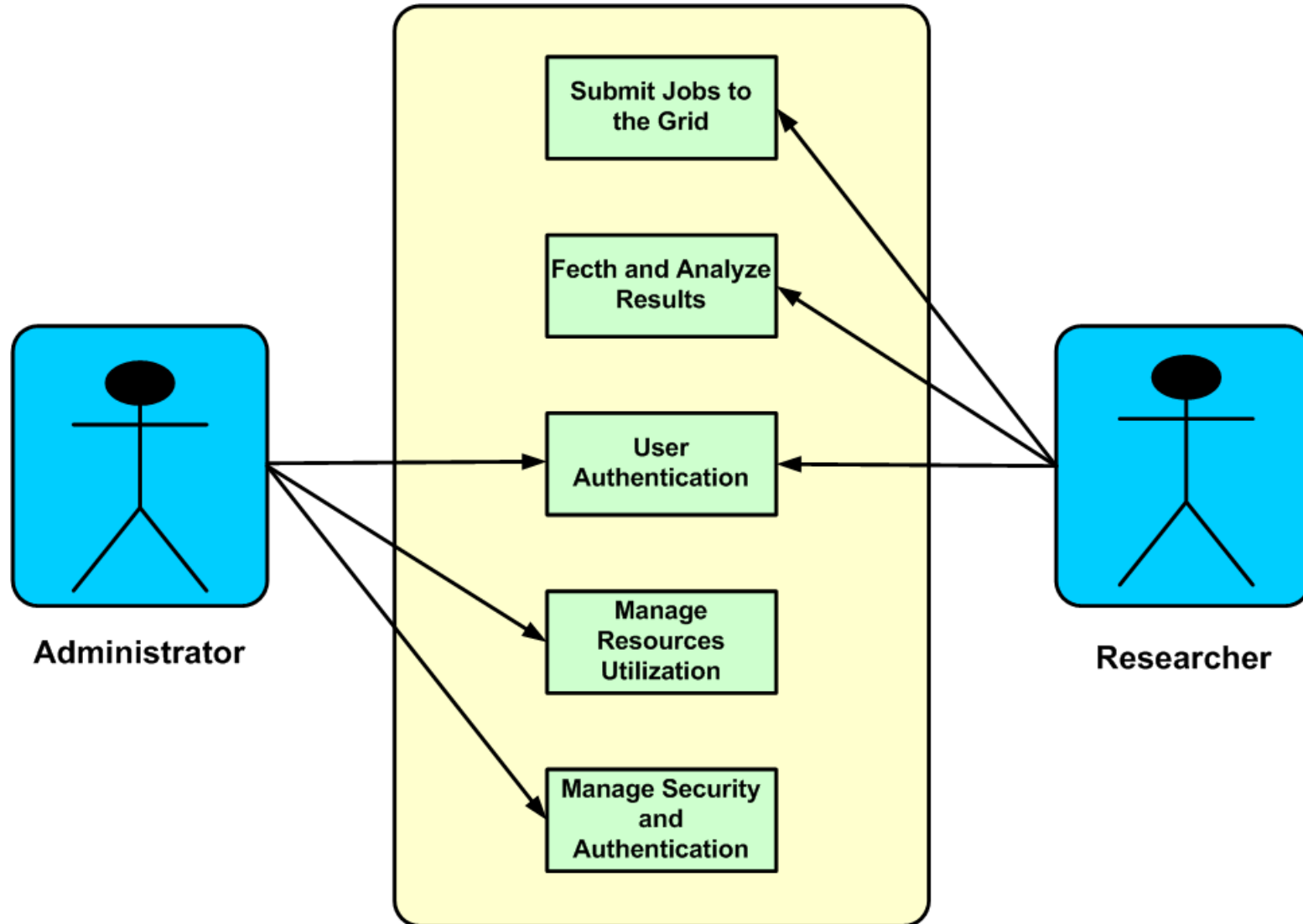
Decentralized Topology



Use Cases



Use Cases (I)



Use Cases (II)

■ **Electronic Structure Packages**

- Dalton, Gamess, Gaussian, ...

❖ **GridWay**

■ **Grid Applications**

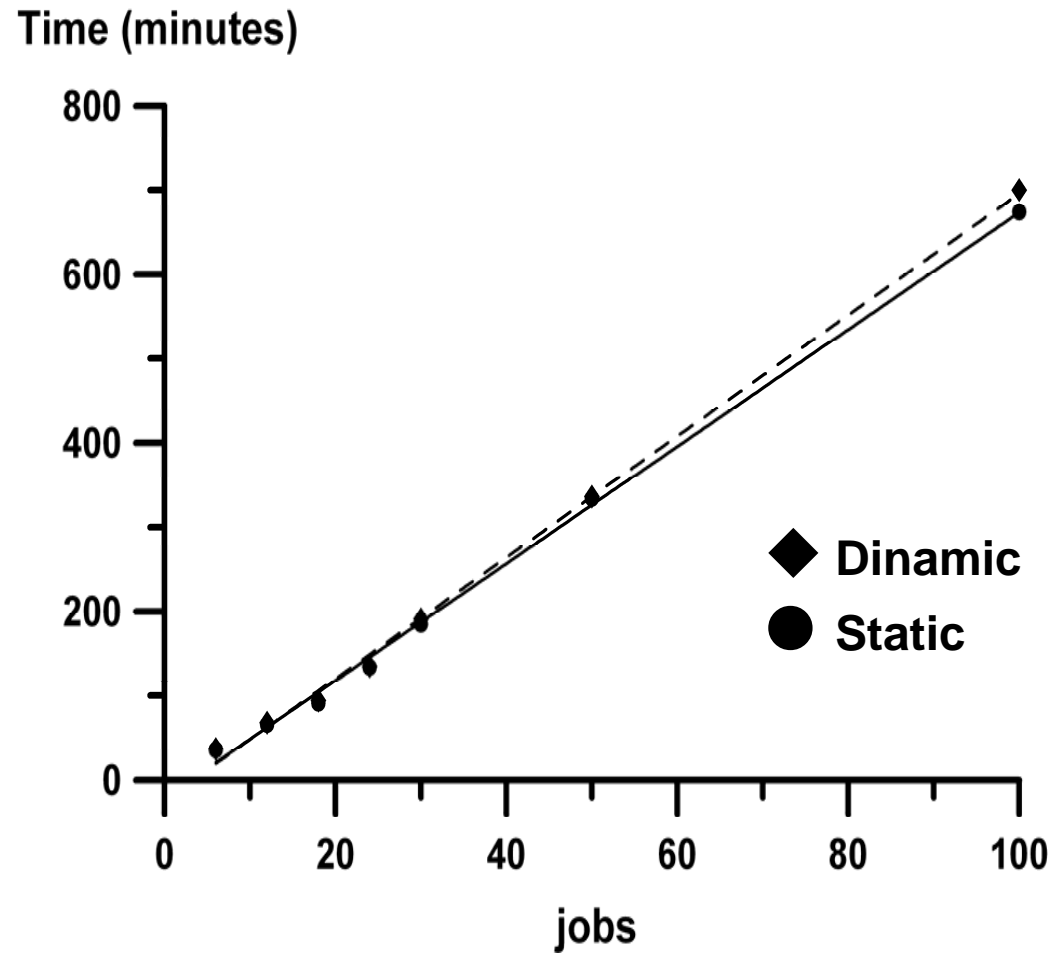
- Mapping of molecular potencial energy hypersurfaces.

❖ **GRID superscalar**

Experiences



TestBed Resources Discovery



TestBed

Potencial Energy Hypersurfaces

	# Structures	# Processors	Time	Distribution
Acetone	1120	64	17 hours	QCyCAR (22); LQT-BUAP (14); BSC-CNS (28).
H₂COH⁺	45385	92	3 days 13 hours	QCyCAR (24); LQT-BUAP (16); BSC-CNS (36); CESGA (16).

Aknowledgements



■ Organisms

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- Departamento de Tecnologías y Sistemas de Información de la UCLM

■ Institutions



Thank you for your attention

For further information:

<http://qcy-car.inf-cr.uclm.es>

