

EGI Community Forum 2014 - Helsinki

Tuesday, 20 May 2014

EGI and XSEDE Tools and Common Needs for the Computational Chemistry, Molecular Modeling and Materials Science Community - Room 10 (11:00 - 12:30)

-Conveners: Antonio Lagana; Alessandro Costantini

time	[id] title	presenter
11:00	[304] Introduction	LAGANA, Antonio
11:10	[202] XSEDE for extreme computing in science	M. RYNGE
11:20	[203] WS-PGRADE for Molecular sciences and XSEDE	J. KRUGER P. KACSUK
11:30	[204] The CMMST VRC of EGI	A. COSTANTINI
11:40	[205] Quality Evaluation on the Grid and Requirements	C. MANUALI
11:50	[206] Usecase 1: quantum reactive scattering	G. PARKER
12:00	[207] Usecase 2: direct classical and semiclassical dynamics calculations	W. HASE
12:10	[208] Discussion	