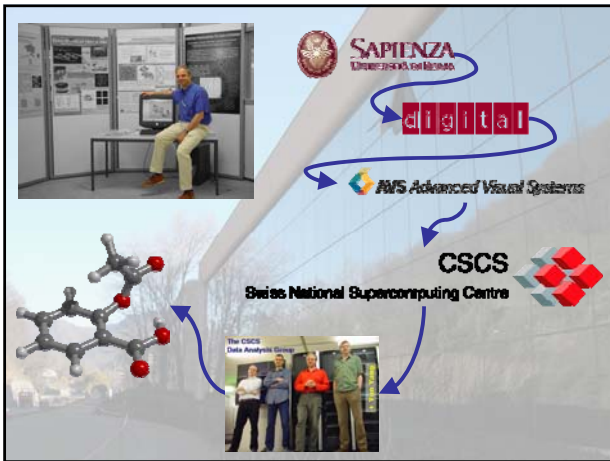
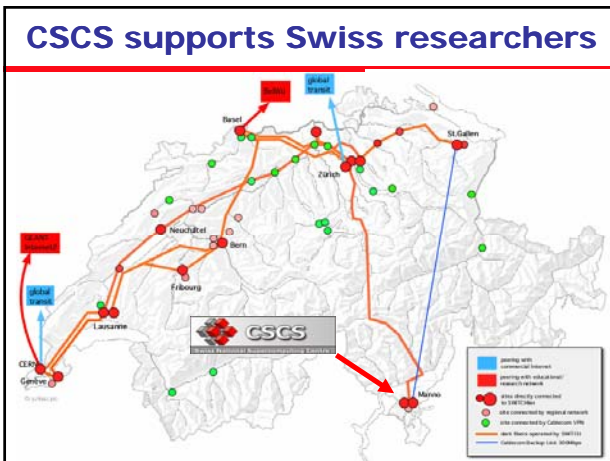


CSCS
Swiss National Supercomputing Centre

Ing. Mario Valle
CSCS Data Analysis Group

Chemistry visualization using the STM4 visualization toolkit





CSCS - not only computing power



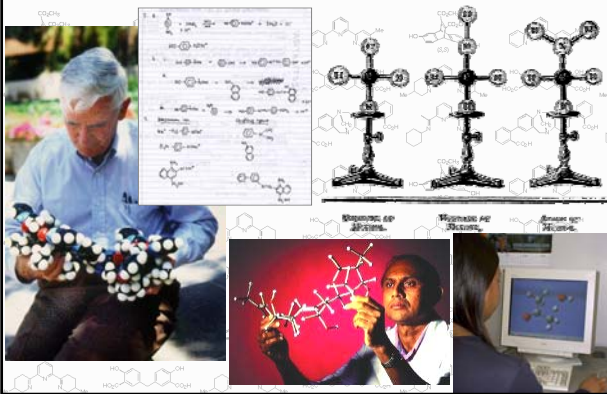
High impact science at CSCS

Publication	Impact factor	Principal investigator	Application field
Opagava J.R. & Das S. (2008) Transition and exponential solutions for a quasi-periodic phase of MgPb. <i>arXiv:0812.4026</i>	20.145	A.R. Opagava	Flam Science/Molecular Dynamics
Pfister C., Hülber D., Füllkrug D., Füllkrug C., Haber G., Singer M. & Apperholdt G. (2008) The role of increasing temperature variability for European summer heat waves. <i>Nature</i> , 467 , 292-295. doi:10.1038/nature07200	20.098	C. Guter	Atmosphere/Ocean
Van Daeleghem M., Lemaire M., Allouet A.L. (2009) Binary stellar merger resulting in a super-Earth. <i>Nature</i> , 462 , 385-388	17.831	E. V. Rosenberg	Planet Science/Molecular Dynamics
Qin Q., Wang Y., Puchner G., Gollner F., Pohlmann W., Hübner N. & Schmittner J. (2010) Climate reproduction with regional resolution: A new high-resolution climate model on the Mechanism of Climate. <i>Nature Geosci.</i> , 3 , 515-519	15.783	Ulrich/Verbits	Biochemistry/Molecular Dynamics
Opagava J.R., Das S. (2008) New high precision phase of diamond and implications for Earth's core. <i>Proc. Natl. Acad. Sci.</i> , 105 , 13330-13333	10.452	A. H. Opagava	Earth Science/Molecular Dynamics
Allegre C., Brunetti G., Duvolski A., Simon J., & others for the entire team. <i>Science</i> , 307 , 1208-1211. doi:10.1126/science.1145201	9.747	Verbits	Geochemistry/Molecular Dynamics
Guo X., Liang Q., Sun M. & Lichtenhan J. (2010) Linear Classifier Consistent with High-Dimensional Models of Quantum States. <i>Phys. Rev. Lett.</i> , 105 , 190404-05	8.101	L. Lichtenhan	Quantum/Molecular Dynamics

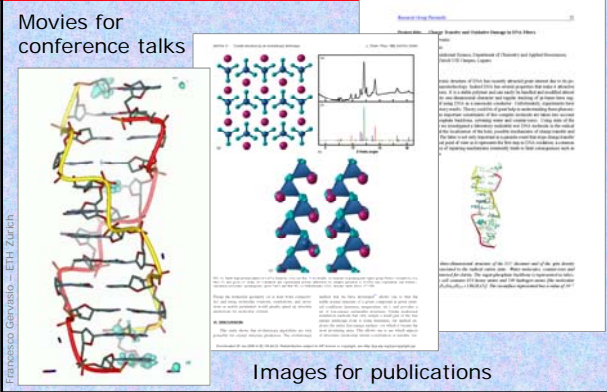
Chemists are visual people



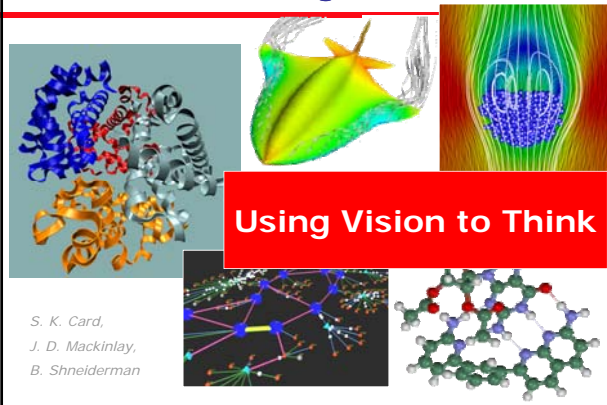
Chemistry is a visual science



Often limited to postprocessing



But with much higher ambitions



Agenda

