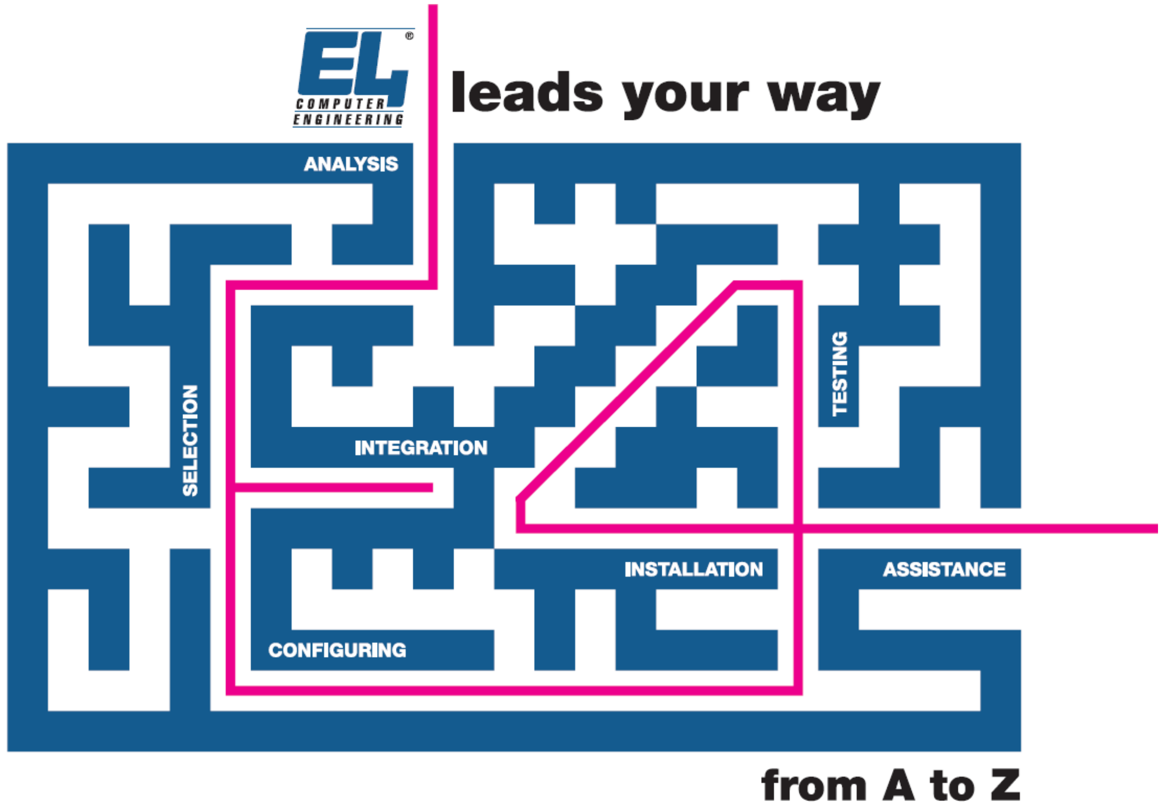
# EUROPAR 2010, Ischia

## When benchmarking makes the difference: simulation of pump and probe experiments, a practical case





***Piero Altoè***

*HPC Specialist (EMEA)*

# E4 Focus

## leading-edge & cost-effective
## *HPC solutions*

# E4 Products Portfolio

**Workstation** (deskside, desktop, TESLA)

**Server** (nodes, blades)

**Storage** (parallel, distributed file systems)

**SAN**

**Cluster** (with GPGPUs, FPGAs)

**Interconnect and switch**
(GigE, 10GigE, Infiniband, Myrinet)

**Scalable, Reliable, Advanced**

# E4 Services



**Assessment of the requirements**

**Benchmarking**

**Analysis of Alternatives**

**TCO, ROI analysis**

**Installation and start-up**

**Predictive and on-fault maintenance**

# Partners

intel

2008
Special Award to
**E4 Computer**



AMD, QLOGIC, areca, intel, dot HILL, SilverStorm Technologies, ASUS, PathScale, SUPERMICRO, RITTAL, Lex SYSTEM, ANSYS, APPRO HPC Cluster Solutions, Western Digital, Myrinet, NVIDIA, Raritan, Microsoft, redhat, adaptec, aethia, ENGIN SOFT, Seagate, panasas, TYAN, ORACLE, DataDirect Networks, CRAY, HITACHI, vmware, Chelsio Communications, DataCore Software, BLADE Network Technologies, CITRIX

E4 Computer Engineering

# Customer References

INFN

ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE

ALMA MATER STUDIORUM UNIVERSITÀ DI BOLOGNA

INAF

arpa

CERN

Scuola Internazionale Superiore di Studi Avanzati

- ma per seguir virtute e conoscenza -

Scientific Computing Laboratory

ENEA

CRS4

CASPUR

issia

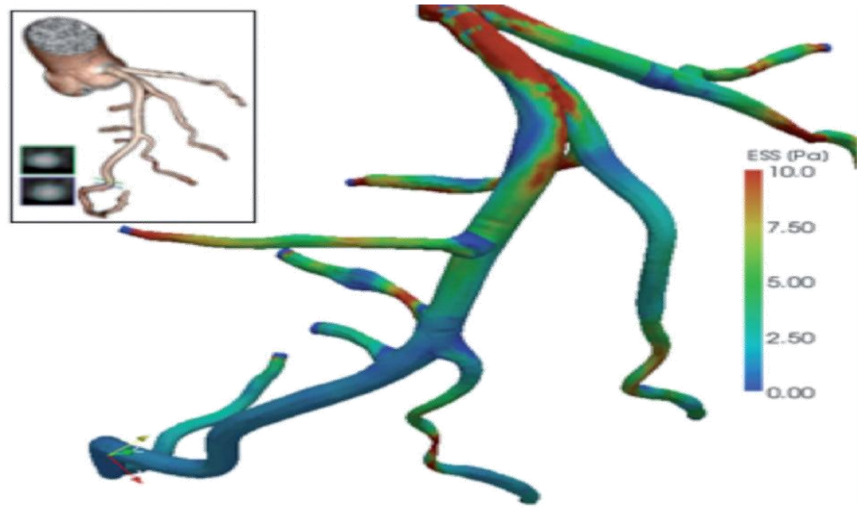
EL COMPUTER ENGINEERING

# A successful deployment

ÉCOLE POLYTECHNIQUE
FÉDÉRALE DE LAUSANNE

Laboratory of Multiscale Modelling of Materials (LMMM)

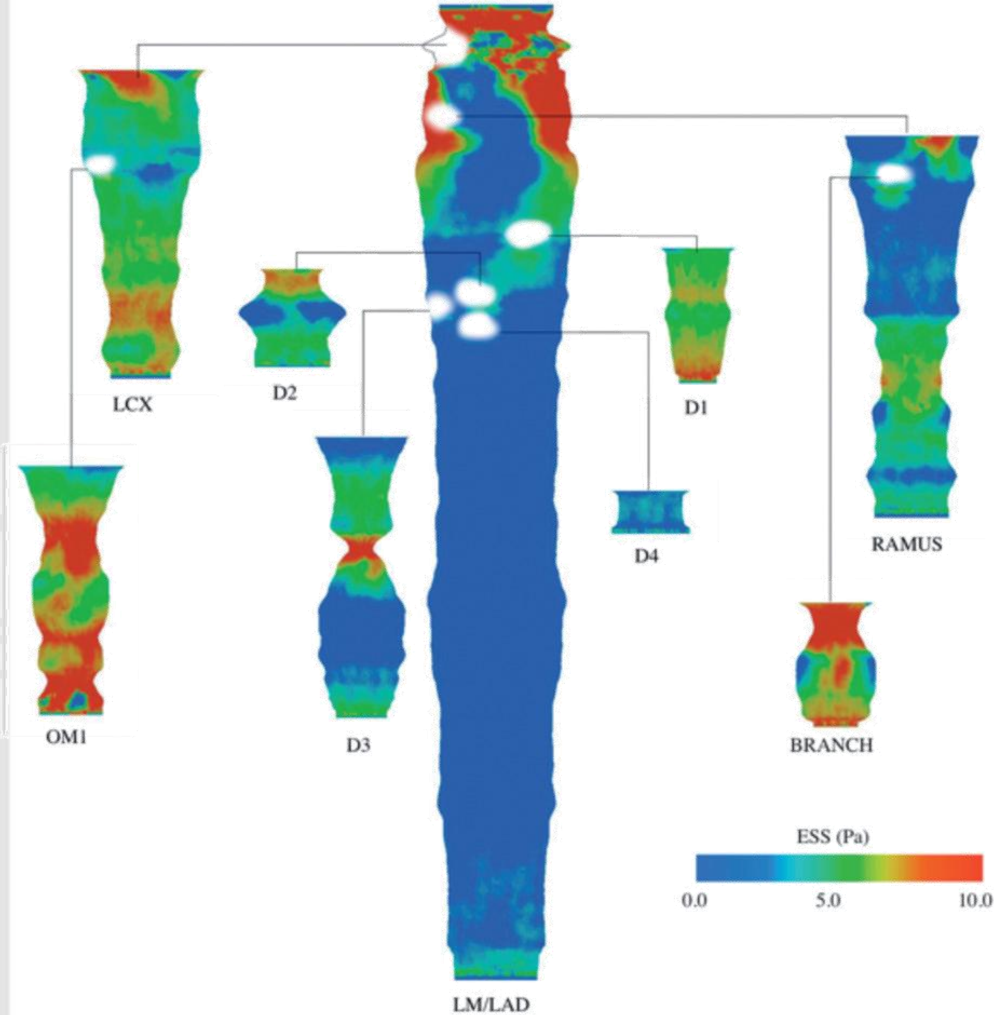
**Prof. Efthimios Kaxiras**




**Major applications:**

- computational method for clinical cardiovascular diagnosis
- combination of microscopic Molecular Dynamics (MD) with a hydrokinetic Lattice Boltzmann (LB) method
- hydrodynamic interactions among the suspended bodies and the surrounding fluid
- modelling blood flows in extended coronary arteries

# A successful deployment




Diagrammatic ESS map eliciting the connectivity of the vessels, the attachment points, and the longitudinal (vertical axis) and azimuthal (horizontal axis) modulation of ESS, indicated by the color scheme shown at the bottom.

The horizontal direction is proportional to the artery local diameter and labels indicate the conventional naming of coronary vessels. The white compact regions on the ESS map represent attachment regions on the mother vessel, where proper surface points are locally absent.

# A successful deployment

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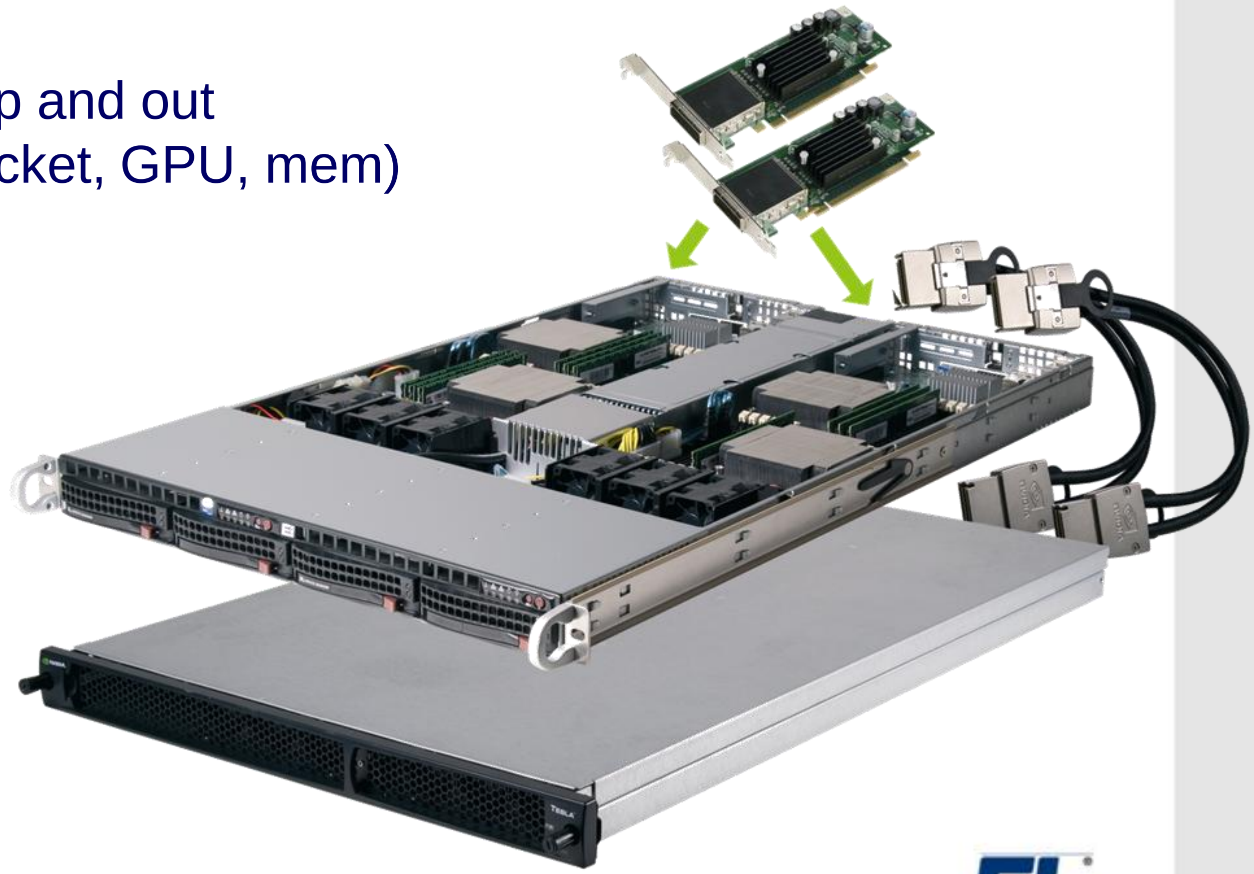
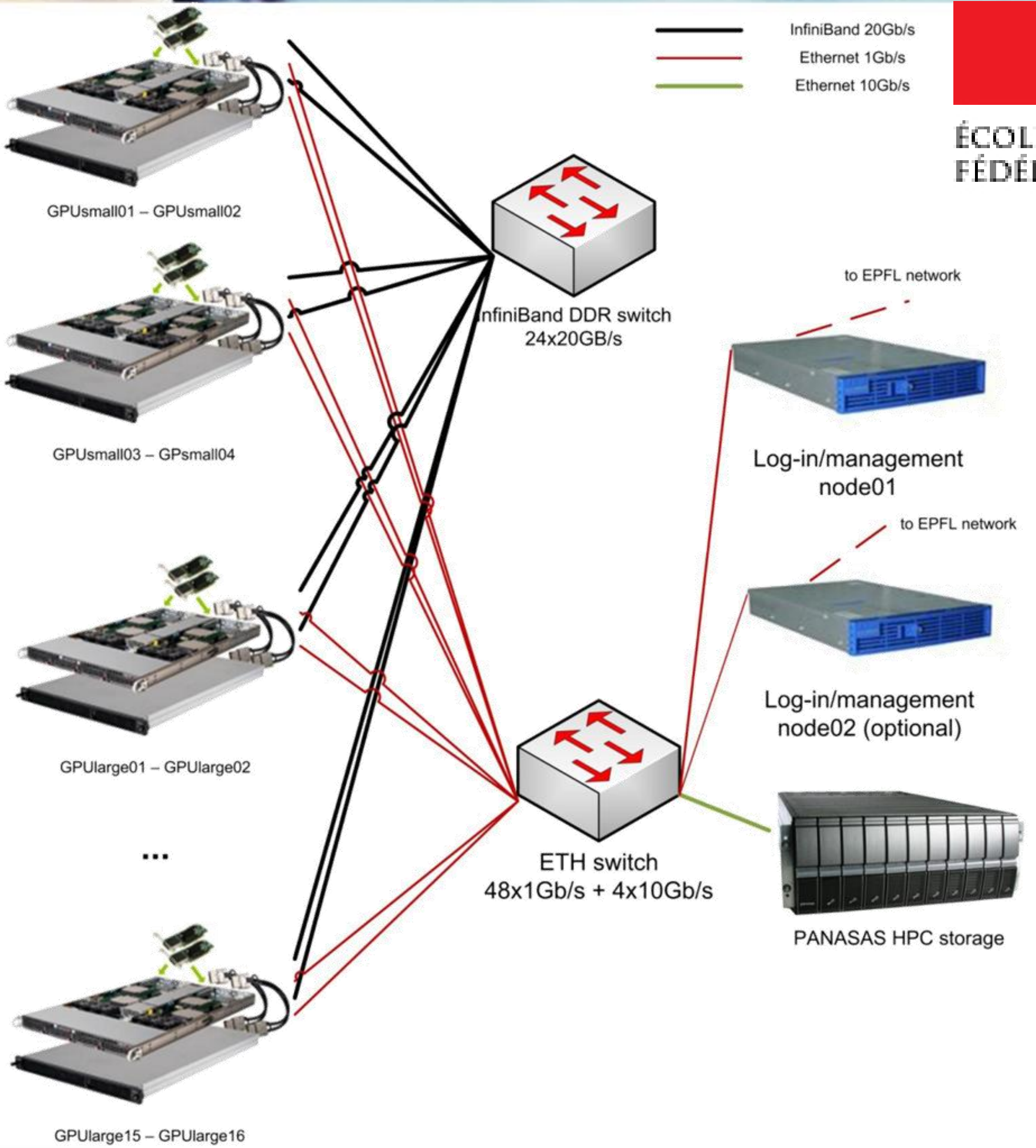
Building block:

- plenty of MFLOPS
- DDR Infiniband
- easy to scale up and out
- upgradable (socket, GPU, mem)
- easy to isolate
- self contained
- modular
- rack-mount
- Linux
- CUDA



# System design:

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# A successful deployment

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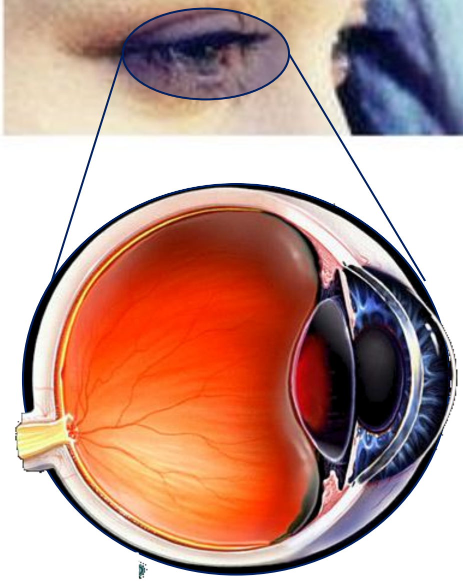
| System | Execution time (sec) | MFLUPS |
|---|---|---|
| 1xC870 GPU | 760 | 53 |
| 2xGT200 GPUs | 159 | 252 |
| 8xGT200 GPUs | 41.9 | 955 |

Timing of 10,000 iterations on an irregular domain with ~4,000,000 voxels on multi-GPU architectures. The performance is measured by using the de- facto standard unit for Lattice Boltzmann, that is Million of FLUid node lattice Updates per Second (MFLUPS).

A MFLUPS is equal, approximately, to 200 million floating point operations per second (MFLOPS).

# Into the eye



Eye

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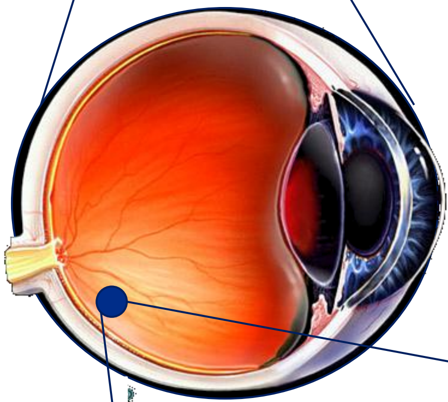
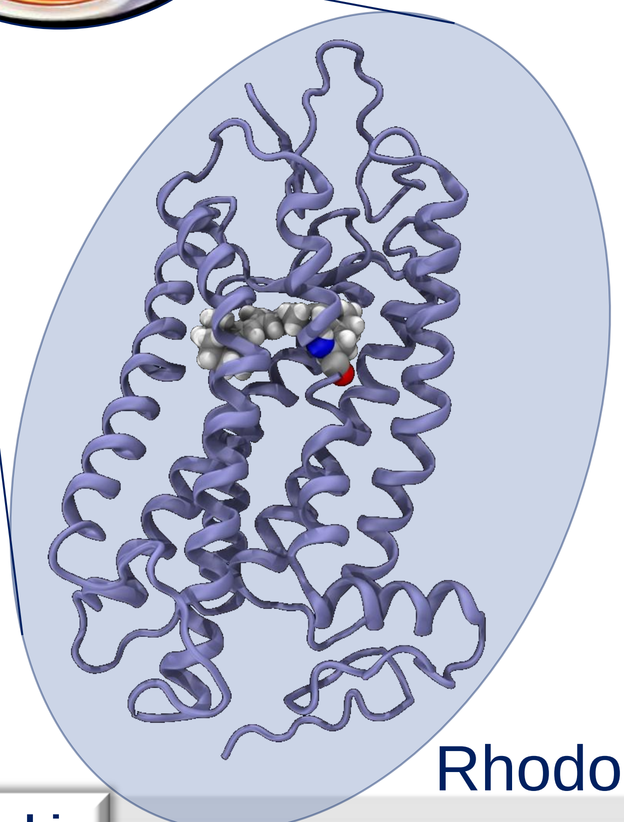
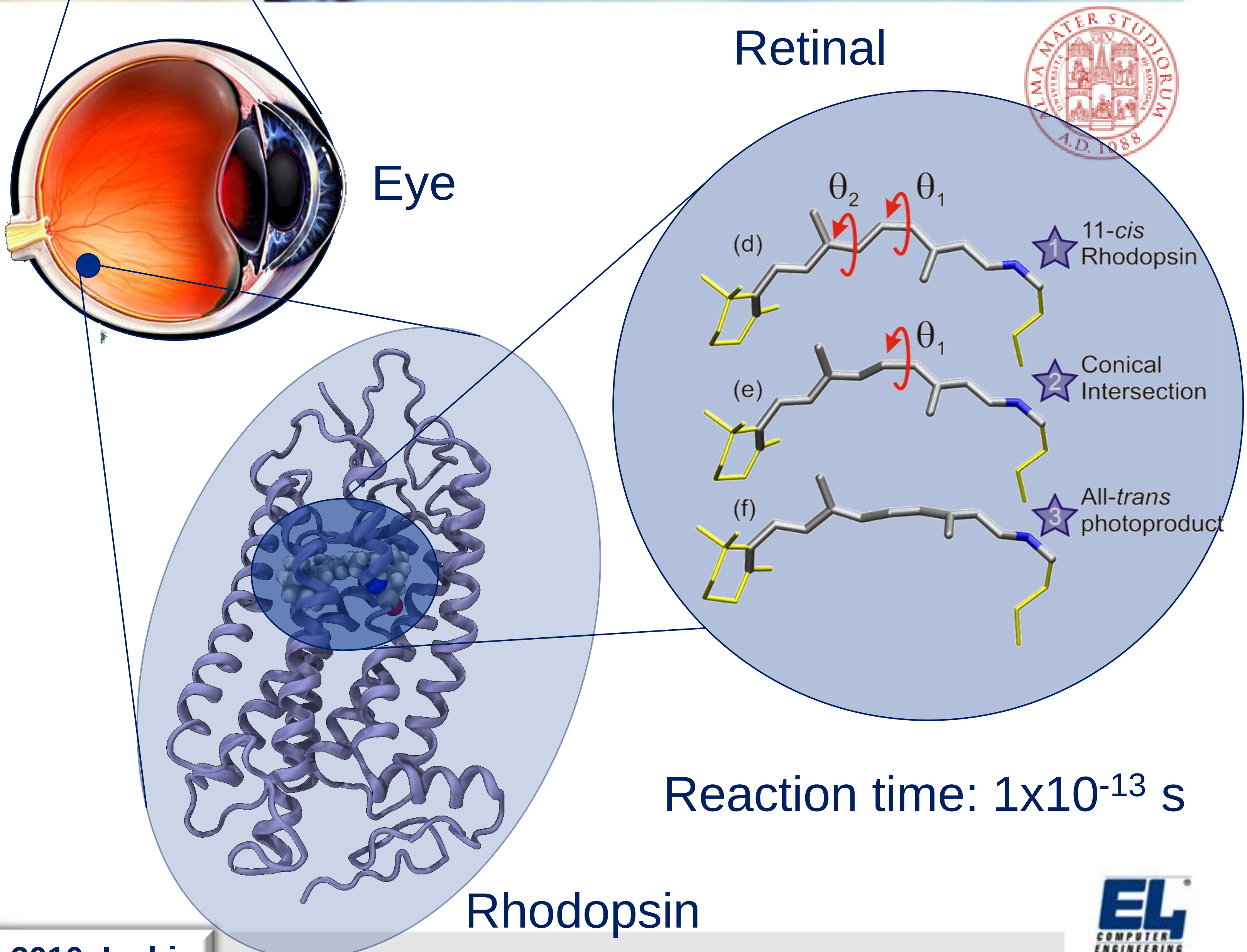


Eye



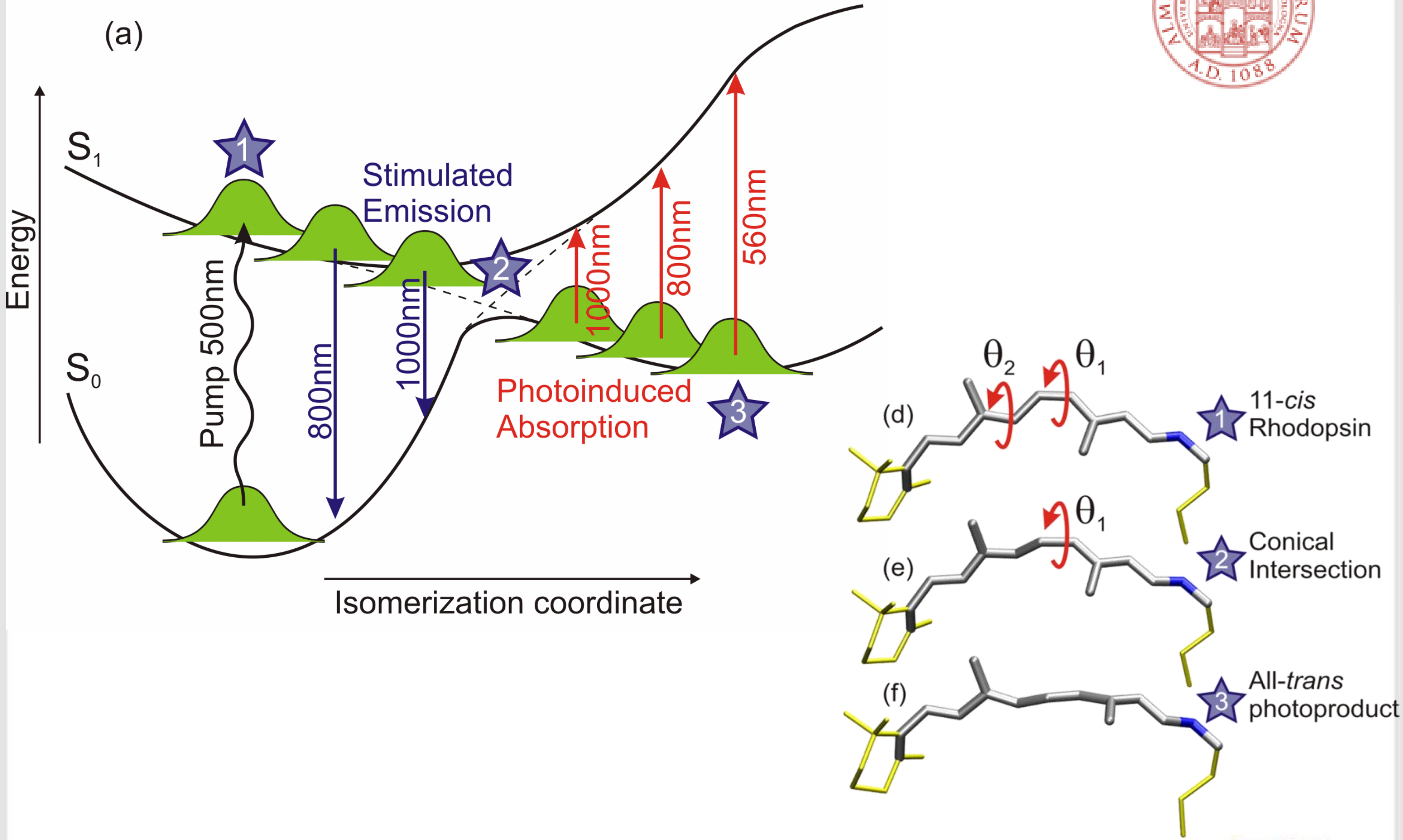
Rhodopsin

# Into the eye

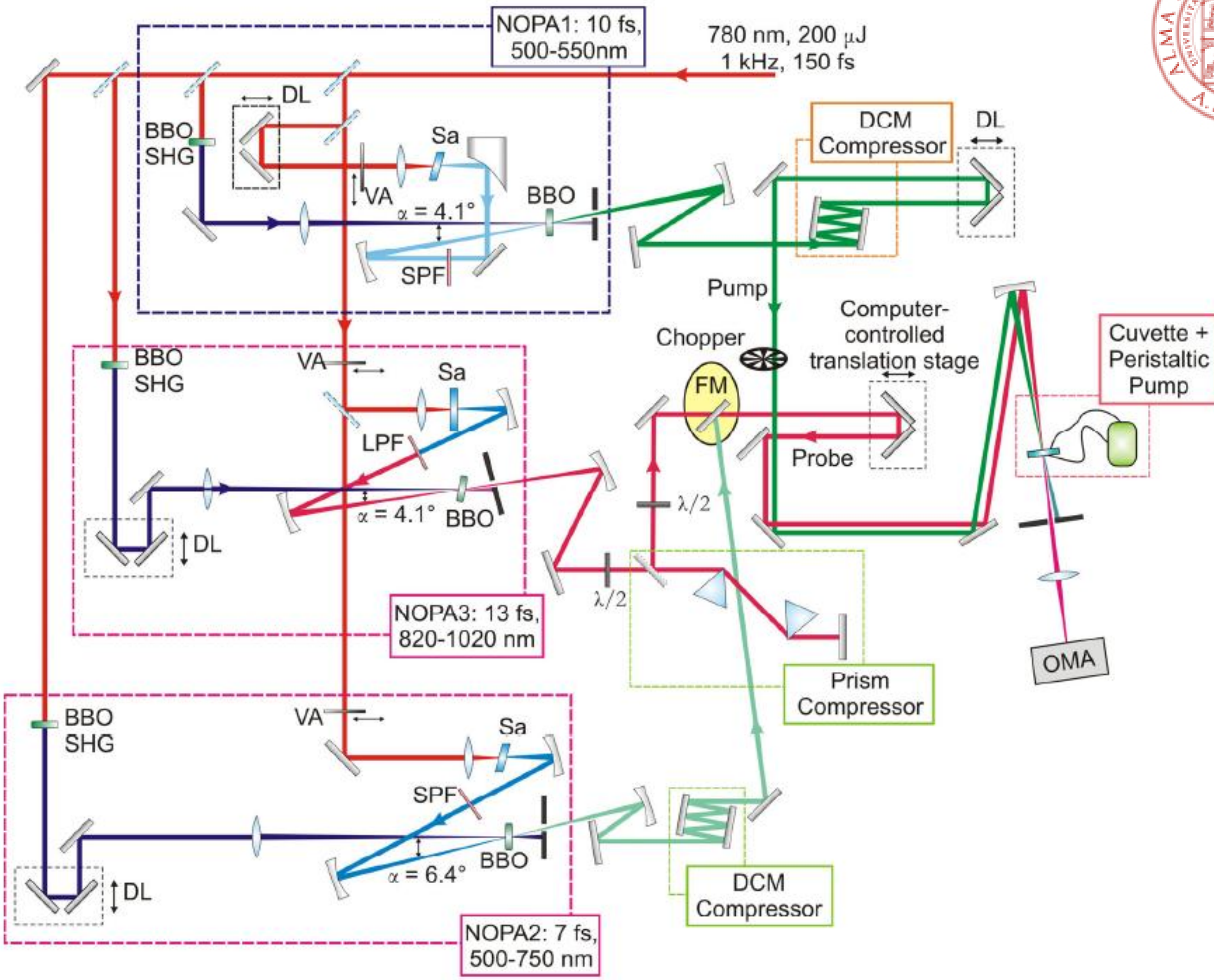



Reaction time: $1x10^{-13}$ s

# Pump & probe


(a)
Energy
$S_1$
$S_0$
Pump 500nm
800nm
1000nm
Stimulated Emission
Photoinduced Absorption
1000nm
800nm
560nm
1
2
3
Isomerization coordinate
(d)
(e)
(f)
$\theta_2$
$\theta_1$
$\theta_1$
1 11-*cis* Rhodopsin
2 Conical Intersection
3 All-*trans* photoproduct

# Experimental setup



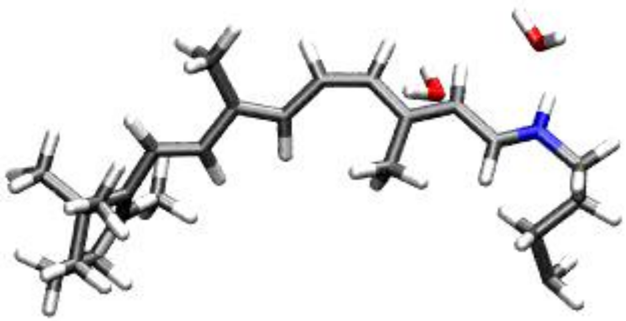
# Theoretical setup

• QM: Retinal chromophore, CASSCF(12,12) / 6-31G*
• MM: Rhodopsin protein, fixed at crystal structure values, Amber
movable waters 2a/2b, lysin296

• Geometry optimization

• Numerical frequency calculation

• Generate initial conditions by thermal sampling of Retinal ground state vibrational modes at 300 K, C-H and N-H stretching modes not sampled



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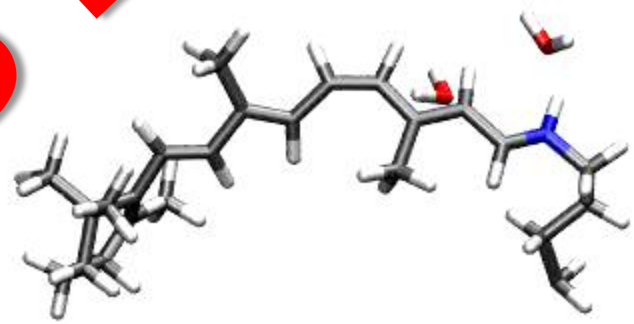

# Timing

**Expectation time:**
**25 days for each of the 200 calculations:**
**120000 h**

**With 7 jobs per node we have extrapolated :**
**500000 h**

**We need to optimize: a single job takes**
**3 months**

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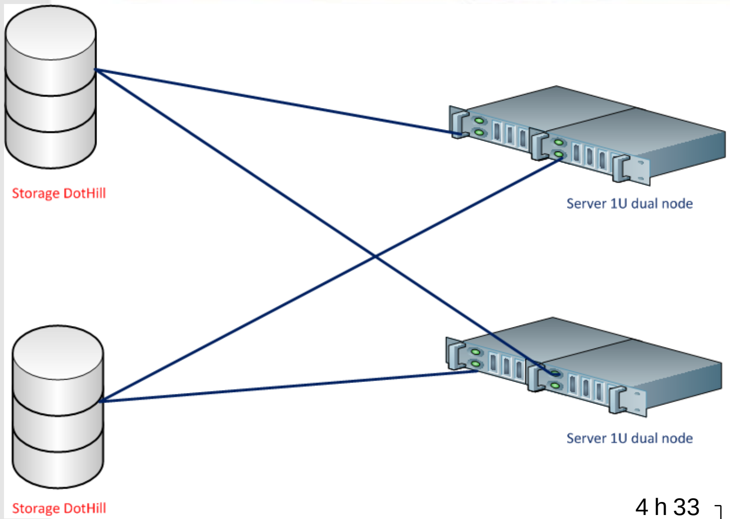
**Bottleneck disks :**
**Transfer rate or access time?**

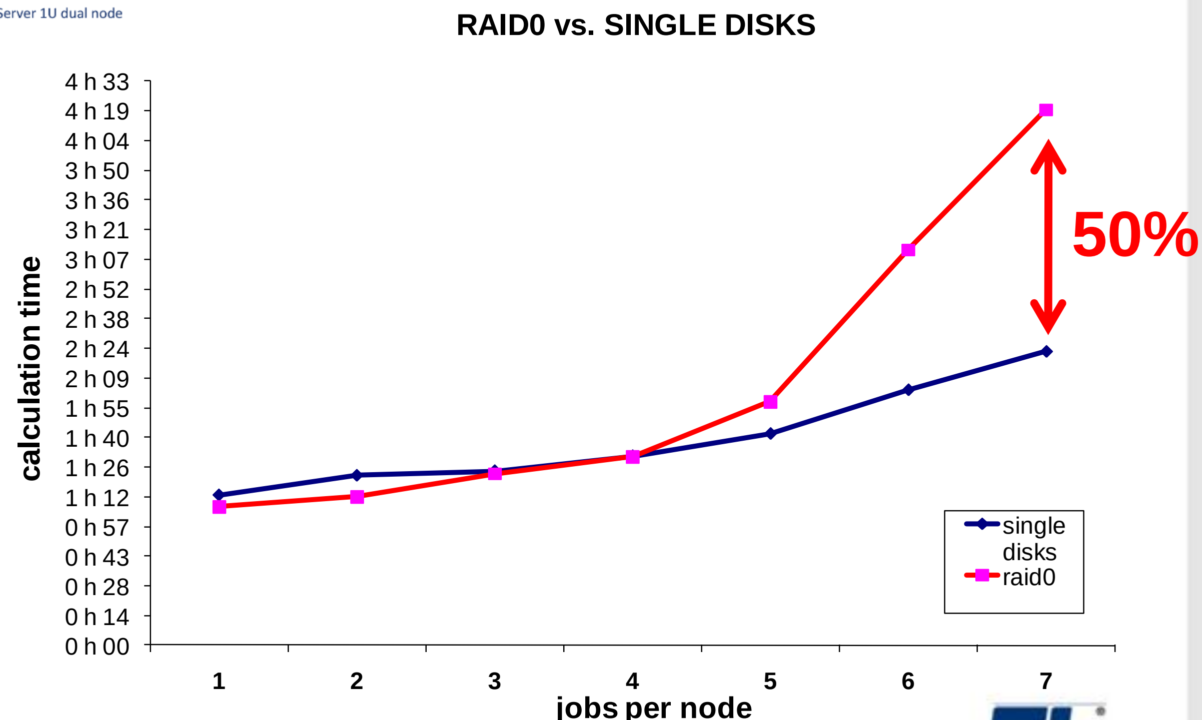
# Benchmarking



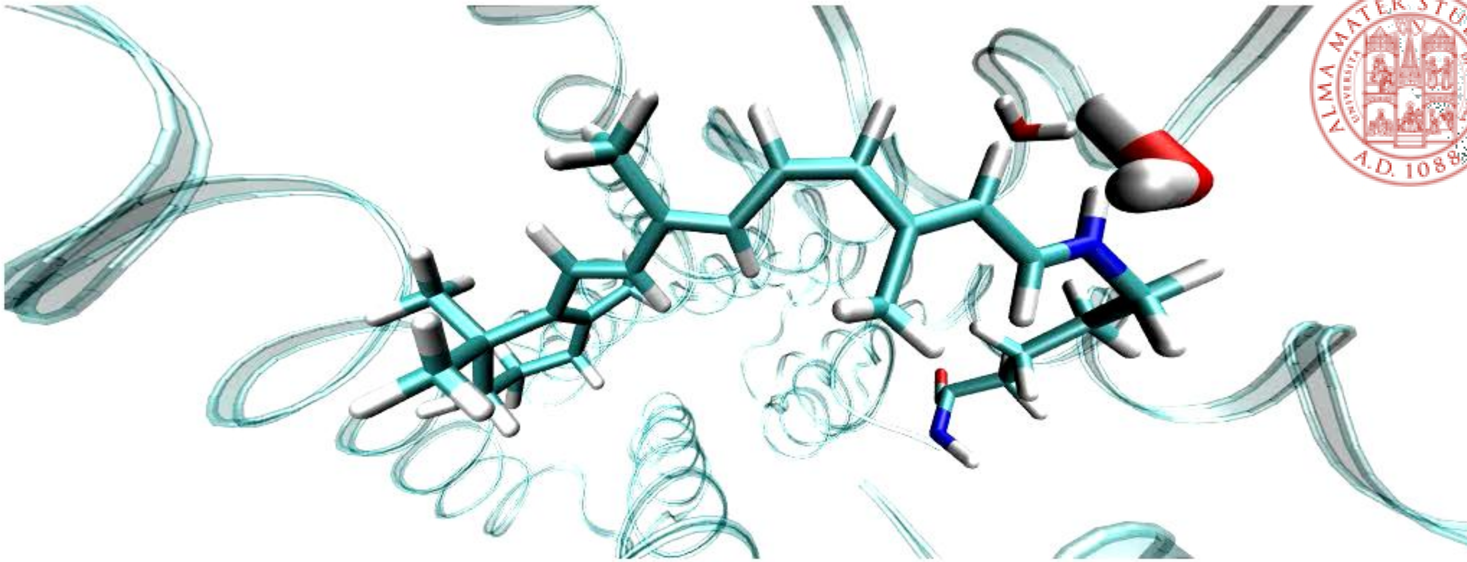

**2 dual node 1U**
**2 storage unit with 12 sas disks**

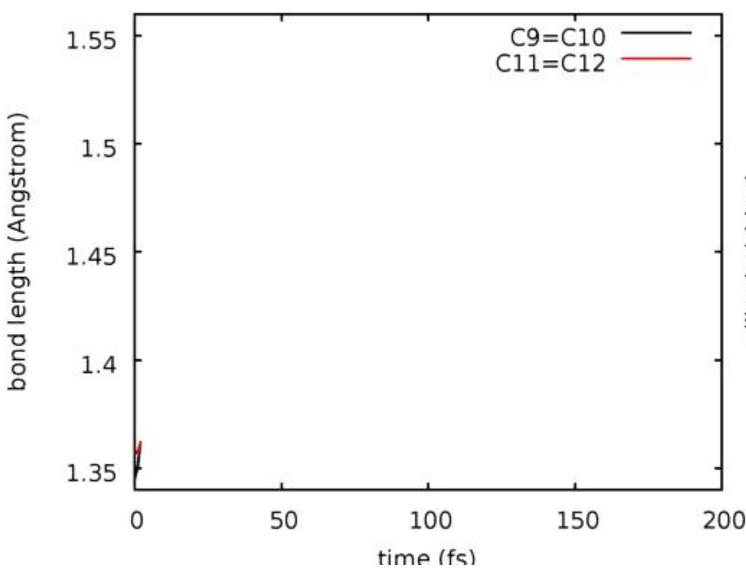
**Runs incresing the job per node**

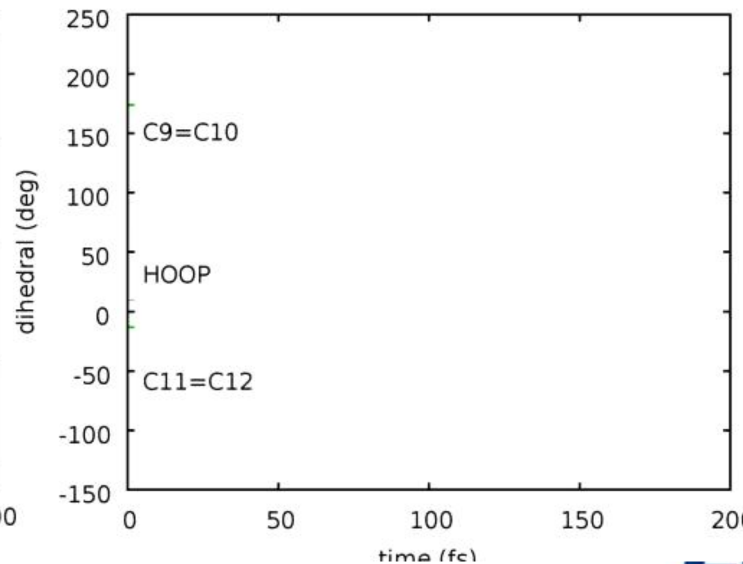
**Reduction of the Calculation time from 500000 h to 250000 h**



# Simulation results

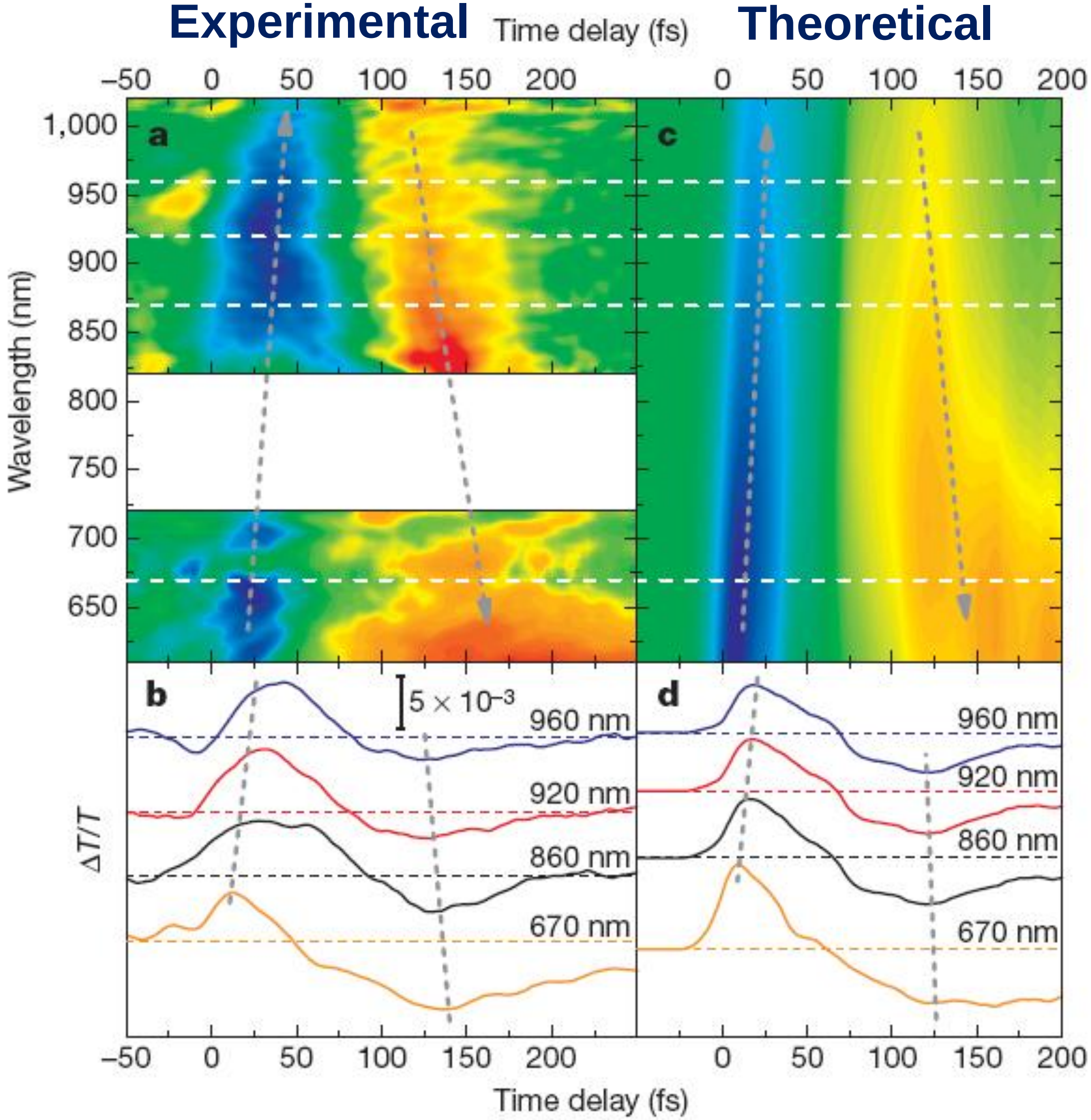




# Experiment vs calculations

**Experimental** **Theoretical**




**Starting from the crystal structure of the protein and the foundalmenal constants, we are able to reproduce the full behaviour of the system**

# The paper

Vol 000|00 Month 2010|doi:10.1038/nature09346 nature

LETTERS

## Conical intersection dynamics of the primary photoisomerization event in vision

Dario Polli[1], Piero Altoè[2], Oliver Weingart[3,4], Katelyn M. Spillane[5], Cristian Manzoni[1], Daniele Brida[1], Gaia Tomasello[2], Giorgio Orlandi[2], Philipp Kukura[6], Richard A. Mathies[5], Marco Garavelli[2] & Giulio Cerullo[1]

Ever since the conversion of the 11-*cis* retinal chromophore to its all-*trans* form in rhodopsin was identified as the primary photochemical event in vision[1], experimentalists and theoreticians have tried to unravel the molecular details of this process. The high quantum yield of 0.65 (ref. 2), the production of the primary ground-state rhodopsin photoproduct within a mere 200 fs (refs 3–7), and the storage of considerable energy in the first stable bathorhodopsin intermediate[8] all suggest an unusually fast and efficient photoactivated one-way reaction[9]. Rhodopsin's unique reactivity is generally attributed to a conical intersection between the potential energy surfaces of the ground and excited electronic states[10,11] and thereby enables the efficient and ultrafast conversion of photon energy into chemical energy[12–16]. But obtaining direct experimental evidence for the involvement of a conical intersection is challenging: the energy gap between the electronic states of the reacting molecule changes significantly over an ultrashort timescale, which calls for observational methods that combine high temporal resolution and a broad spectral observation window. Here we show that ultrafast optical spectroscopy with sub-20-fs time resolution and spectral coverage from the visible to the near-infrared allows us to follow rhodopsin isomerization. We track coherent wave-packet motion from the photoexcited Franck–Condon region to the photoproduct by monitoring the loss of reactant emission and the subsequent appearance of photoproduct absorption, and find excellent agreement between the experimental observations and molecular dynamics calculations that involve a true electronic states crossing. Taken together, these findings constitute the most compelling evidence to date for the existence and importance of conical intersections in visual photochemistry.

We initiated the photoisomerization reaction in the retinal chromophore of purified rhodopsin by 10-fs 500-nm pump pulses resonant with the ground-state absorption. The photoinduced dynamics were then probed by delayed ultra-broadband few-optical-cycle probe pulses, either in the visible wavelength region (500–720 nm) or in the near-infrared (NIR, 820–1,020 nm), generated by synchronized optical parametric amplifiers[17]. The temporal resolution was <20 fs over the entire monitored spectral range. Figure 1a presents a differential transmission ($\Delta T/T$) map as a function of probe wavelength and pump–probe time delay. Immediately following excitation from the ground state ($S_0$) to the first excited singlet state ($S_1$), we observed a positive $\Delta T/T$ signal (blue in the figure) with maximum intensity at ~650 nm, which is assigned to stimulated emission from the excited state due to the negligible ground-state absorption in this wavelength range. The stimulated emission signal rapidly shifts to the red while losing intensity and disappearing to wavelengths longer than 1,000 nm within ~75 fs. At this time, the $\Delta T/T$ signal changes sign and turns into a weak photoinduced absorption signal (red in the figure), which initially appears at 1,000 nm and then gradually shifts to the blue and increases in intensity. For delays longer than 200 fs, the photoinduced absorption signal stabilizes as a long-lived band peaking at 560 nm, indicating the formation of the all-*trans* photoproduct[3]. We emphasize that the use of a sub-15-fs NIR probe is the key to observing the transition between the excited and ground electronic states. Time traces at selected probe wavelengths are shown in Fig. 1b, highlighting the red shift of the stimulated emission signal and the subsequent blue shift of the photoinduced absorption.

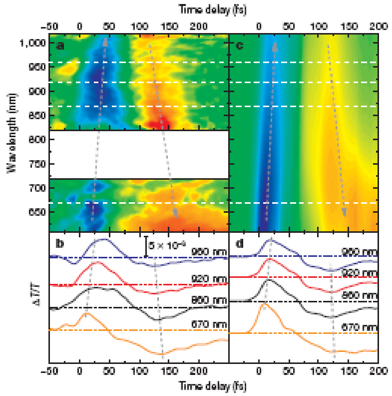



**Figure 1 | Wave-packet dynamics through the rhodopsin conical intersection.** **a**, **c**, Experimental (**a**) and simulated (**c**) differential transmission ($\Delta T/T$) map as a function of time delay and wavelength in the visible and NIR spectral regions. The white area in the experimental data around 750 nm corresponds to the 'blind region' of our set-up. Grey lines are guides to the eye, highlighting the shifts of the stimulated emission (blue) and photoinduced absorption (red/orange) signals in time. **b**, **d**, Experimental (**b**) and simulated (**d**) $\Delta T/T$ dynamics at selected probe wavelengths.

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Marco Costi
Cosimo Gianfreda

# Thank you

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