Presentación de proyecto con acceso a PRACE:

Artif cial photosynthesis

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Identify a challenge problem

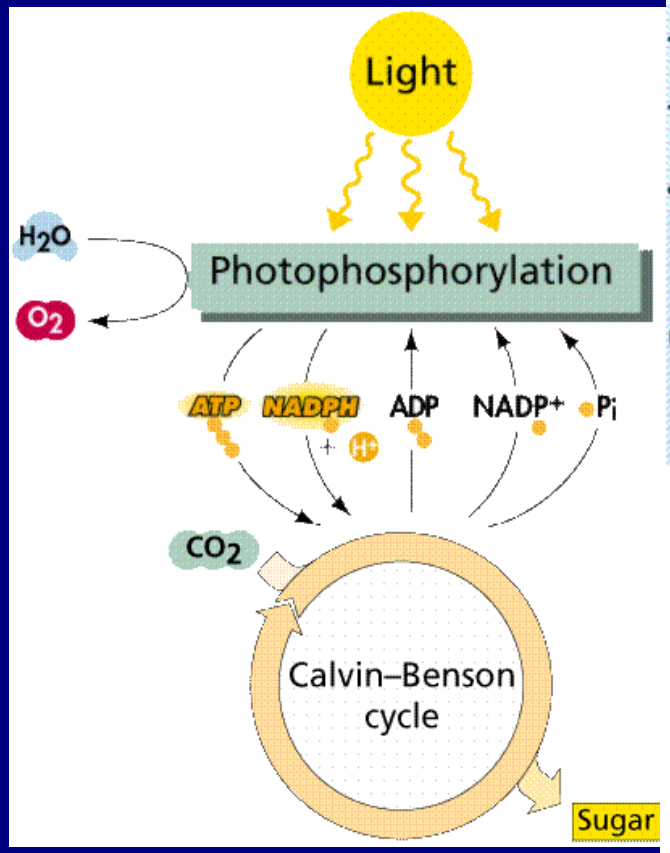
Identify/select the code; tests

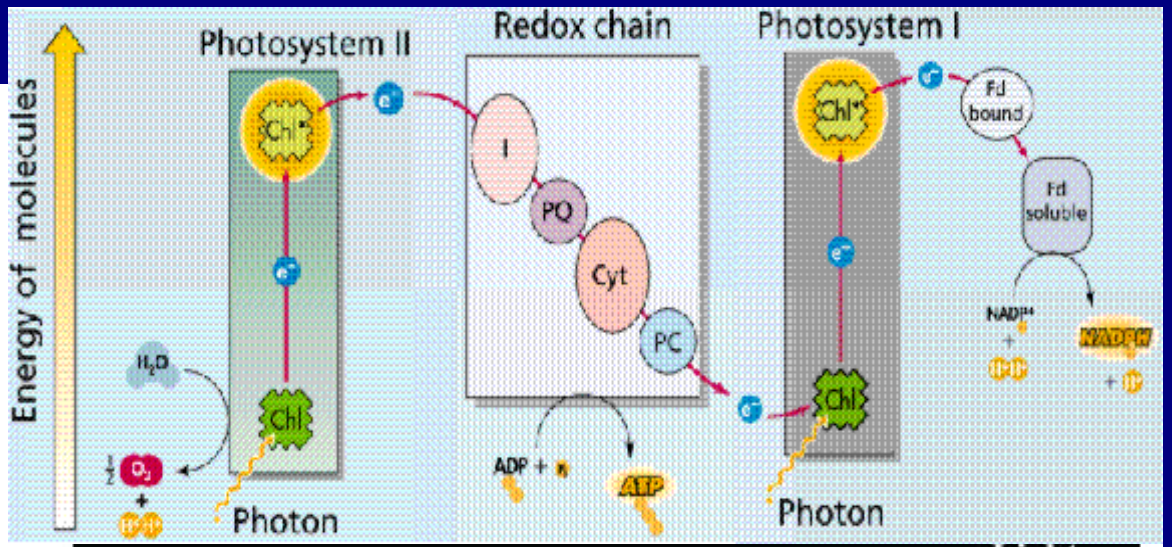
Adapt the code: massive paralell

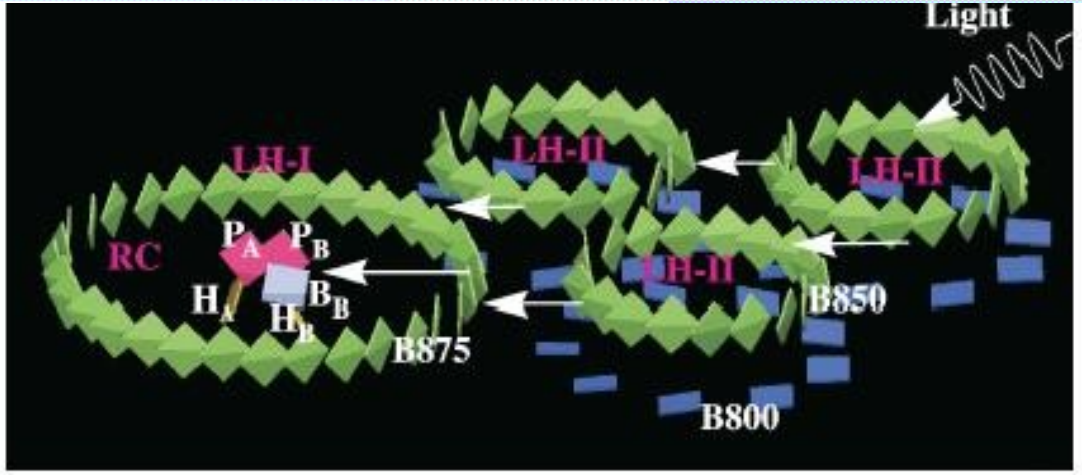
Detailed estimation of the needs: why PRACE?

Prepare the proposal

Photosynthesis. Process by which the plants cells use solar energy to produce ATP. The conversion of sunlight energy into usable chemical energy. Our atmosphere is oxidant thanks to this process.



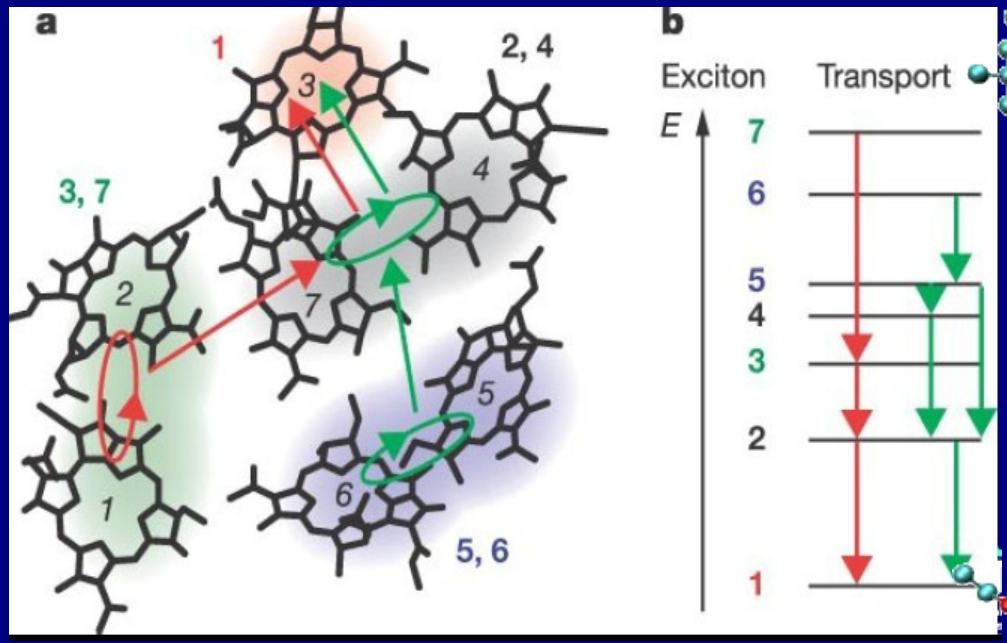


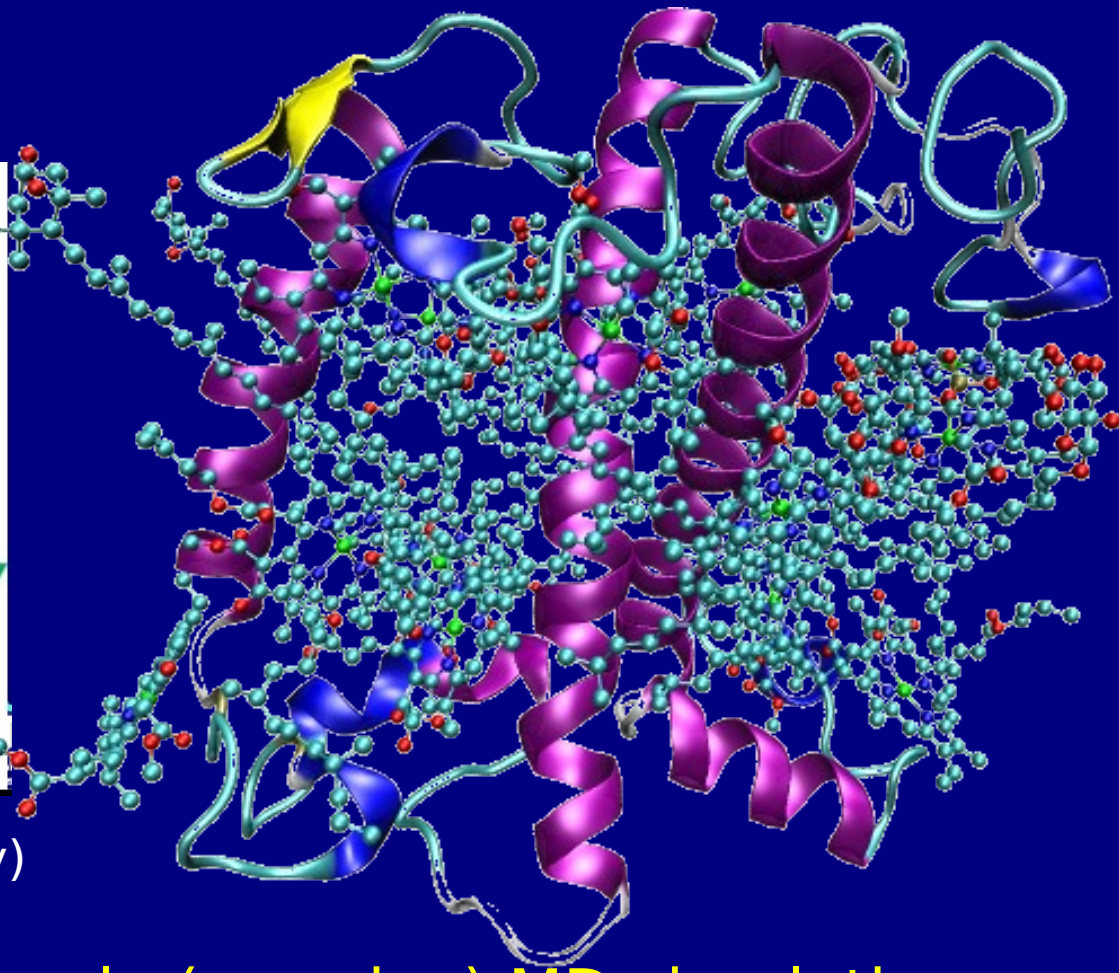


Chlorophylls are used to create a series of redox potentials that will give energy and e- to yield chemical energy

Towards the color of plants:

e.g. Spinach



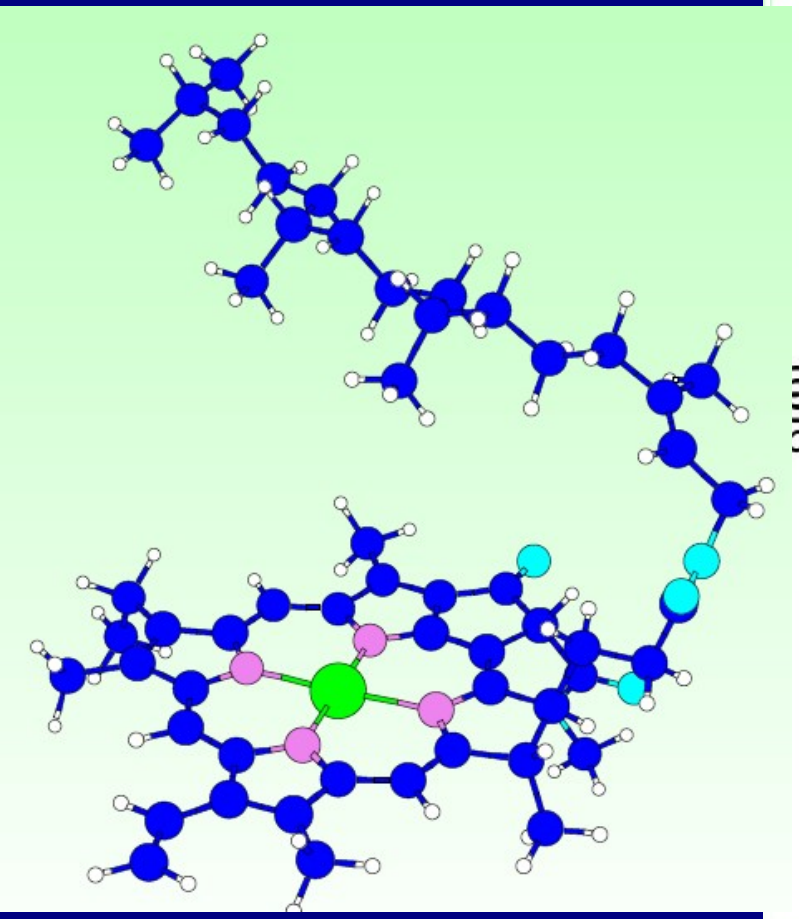


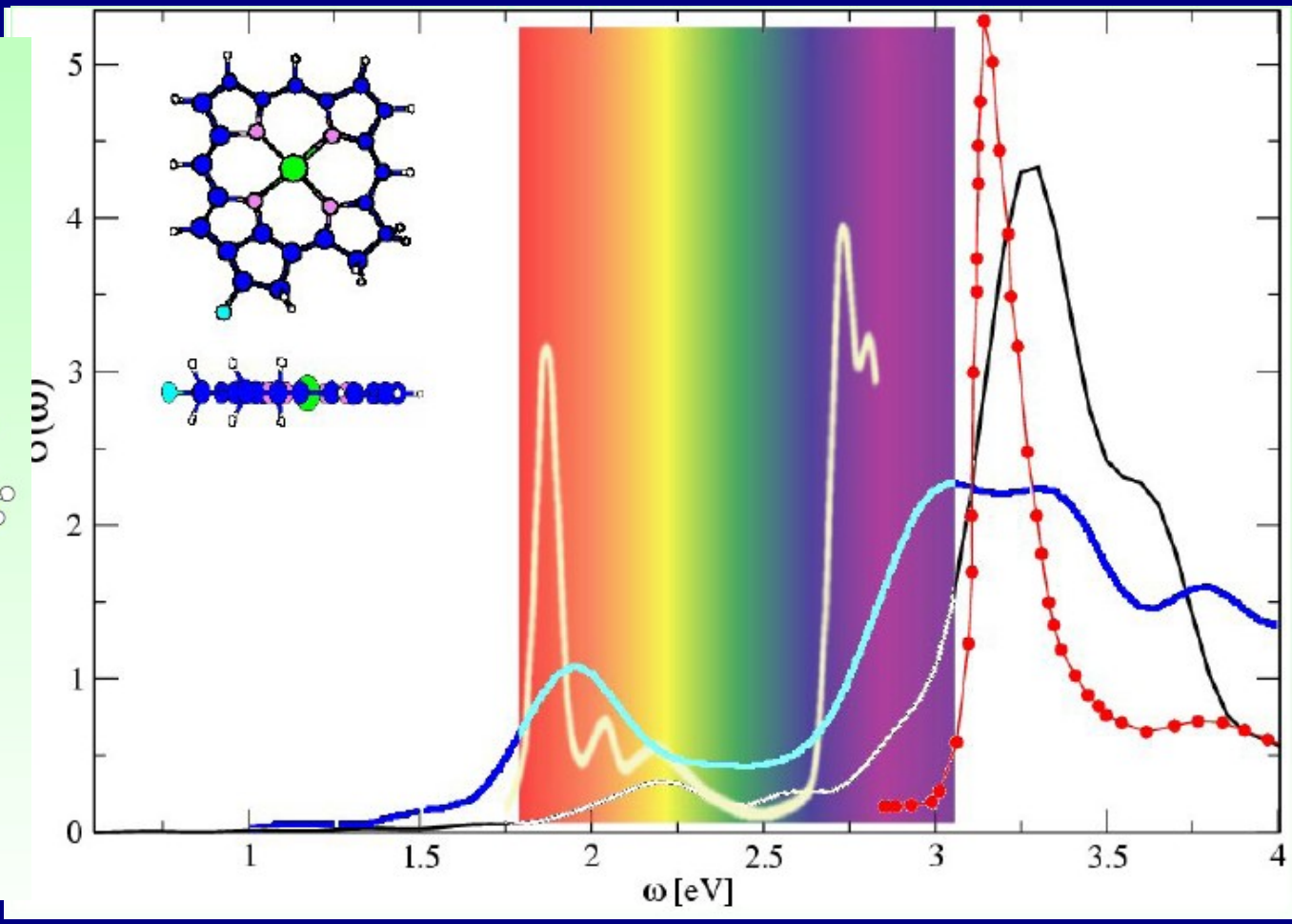
Fleming et al Nature (2005),.... (Berkeley)

Large scale (massive) MD simulations

J.L. Alonso, X. Andrade, P. Echenique, F. Falceto, D. Prada, AR PRL (2008)

Towards the color of plants: The real Chlorophyll molecule



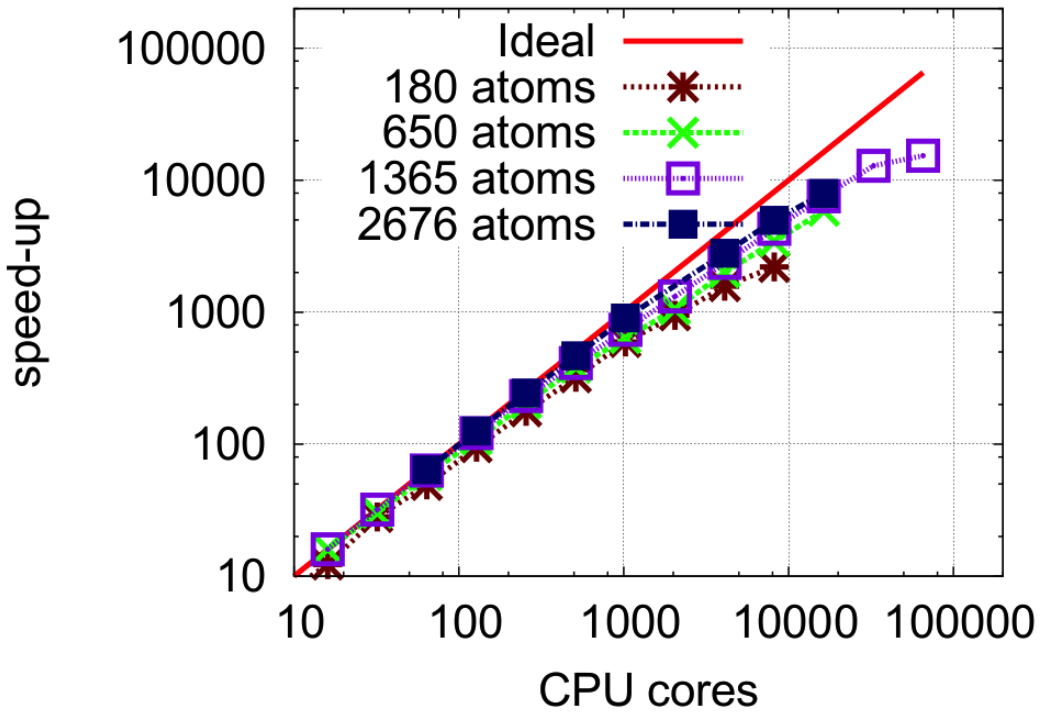


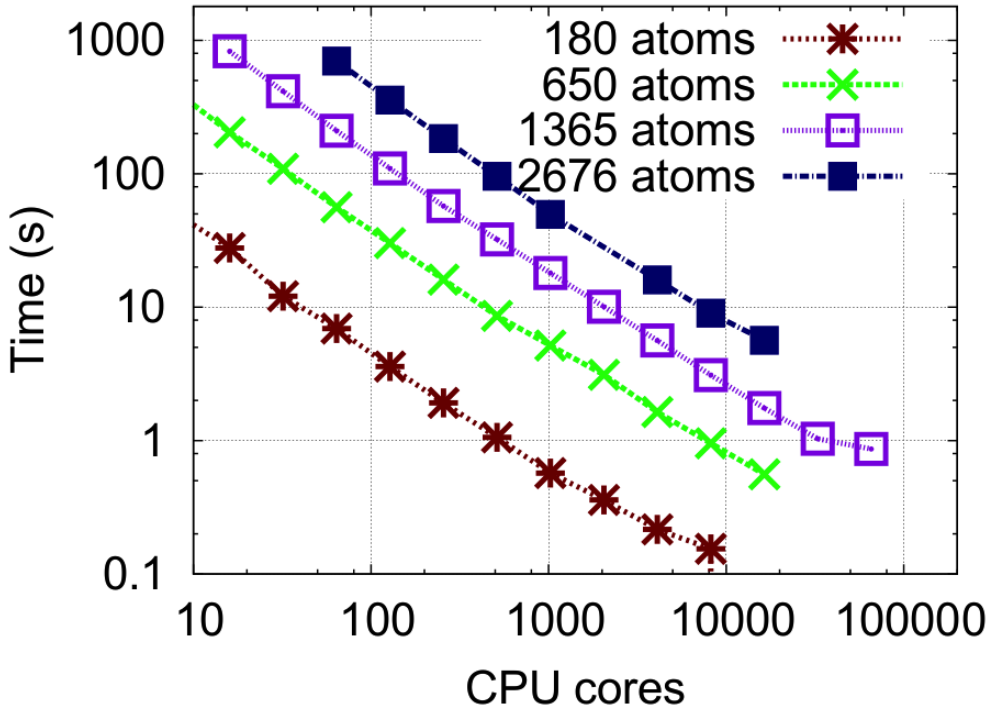
TDDFT: All observables are functionals of n(r,t) (Runge&Gross 1984)

Linear and non linear phenomena accessible

Octopus Code http://www.tddft.org

Time-Dependent Density Functional Theory, Lecture Notes in Physics, Springer Vols. 837, 706 (2012, 2006)





PRACE application form **7th PRACE Project Access Call**

Detailed Project Document

6. Justify the number of core hours requested. This should include information such as: run type, wall clock time per step, number of jobs per run type, the number of CPU cores and the total core hours per run type. This information should take the form of a table like the one shown below with example data. Explain how the core hours requested will be used (1 page).

Run type	# Runs	# Steps/Run	Walltime/Step	# CPU cores	Total core hours/Type Run
GS 5879	1	150	3.3 h	128	63,360
TD 5879	3	3,000	25 s	16,384	1,024,000
GS 9000	1	150	12 h	128	230,400
TD 9000	3	3,000	70 s	16,384	2,867,200
					4,184,960

At least, we have to run a GS for 5879 atoms system lasting 3 hours and 20 minutes per iterations and another GS calculation for the system of 9000 atoms lasting around 12 hours per iteration, with a total amount of 150 in both cases.

Respecting to the TD calculation; each TD iteration will need around 25 seconds in the case of 5879 atoms; and, 70 s with 9000 atoms. We will require at least 3000 iterations and 3 different executions per system.

Thank you!!!!

For more details see:
http://nano-bio.ehu.es
http://etsf.eu