The riojascience@home project is oriented to the study of chemical reactions theoretically. So, theories as quantum and classical mechanics are applied to study how reactions are produced.
As there are no few chemical reactions, the efforts of the project are focused on two kinds of processes: gas phase and enzymatic reactions.

1. Gas Phase Reactions:

The study of gas phase reactions are interesting in different classes of environments such as atmospheric and space chemistry or the study of combustion processes. Very often these reactions are elementary, meaning that they occur in a single reactive step, and quite simple where no more than two species are involved. This simple scenario lets to apply high-level theories to describe the reactive process or even to **develop** new theoretical tools to obtain a better accuracy with the reality.

The triqct program implemented on the riojascience@home project simulates the dynamics of gas phase reactions. It solves the Hamilton equations (you can also see Hamiltonian mechanics) from reactants to products for a certain initial condition of the reactants (collision or internal energy, approaching way, angular momentum), the simulation (equations solving) is performed along the time (related to an integration step) until the products are formed (or not). This is a trajectory.
To describe the real system it is necessary to simulate the trajectory in all of the possible (the more the better, at least) initial conditions, so thousand or million or trajectories are necessary to be calculated.

The simplest, and maybe the most important, property is the reaction probability that is calculated dividing the trajectories that lead to products by the total trajectories simulated, but trough these simulations much more information about the studied reaction can be extracted.

The regular way to operate is to try to reproduce experimental measurements by the simulations. If the obtained agreement is good, the theoretical information is supposed to be a good way to explain the measurements and we can get more information that cannot be obtained even in experiments.

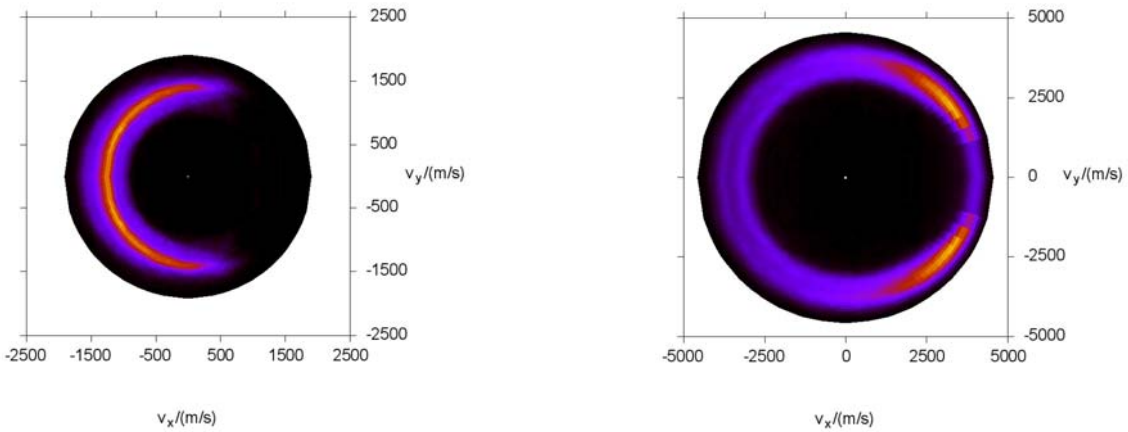
1.1 An example: simulating crossed-beam experiments with Triqct.

For example, a class of experiment that can be simulated by this program (or others related) is crossed-beam experiment. If the experiment is designed to study A + B → AB reaction a molecular beam of molecules of A is crossed with other beam of molecules of B in a vacuum chamber. Then the product AB is analyzed using different techniques such as time-of-flight spectrometers (TOF) or CCD cameras. Very interesting information about the dynamics of the reaction (how it is produced) can be extracted from these experiments and this information can be completed and explained by means of theoretical simulations.

1.1.1 The O + CH_4 reaction and velocity-flux maps.

An example of these studies performed using riojascience@home is the study of the stereo-dynamics of the reaction O + CH_4 → OH + CH_3. This reaction is a primary step in the combustion process of the hydrocarbon and because is the simplest reaction of the oxygen atom with hydrocarbons lets a strong interaction between experiments and simulations giving us information about the reaction at an atomic level.

Two experimental groups have measured (among other things) the center-of-mass velocity-flux maps of the products at different collision energies (see references [1]and [2]). Form the triqct calculations performed on the riojascience@home platform we analyzed the velocity-flux maps of the OH fragment reproducing the experimental behavior.



Simulation of experiment referenced at [1] (left; E_{col} = 14.7 kcal/mol) and at [2] (right; E_{col} = 64 kcal/mol

1 J. Zhang and K. Liu. Imaging the Reaction Dynamics of O(^{3}P) + CH_4 → OH + CH_3. Chem. Asian J. 2011. DOI: 10.1002/asia.201100414

2 J. Zhang et al. Crossed-Beams Studies of the Dynamics of the H-Atom Abstraction Reaction, O(^{3}P) + CH_4 → OH + CH_3 at Hyperthermal Collision Energies. J. Phys. Chem. A 2011. DOI: 10.1021/jp20137t

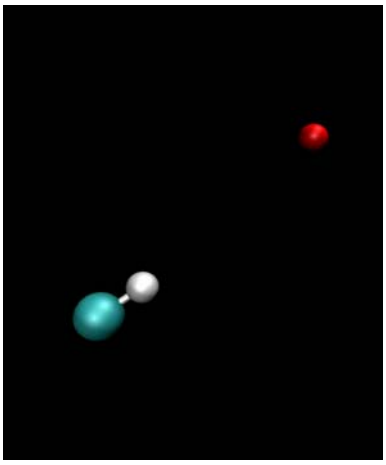
These diagrams represent the velocity components, relative to the system's center of masses, of the OH product once is produced in the reaction. They are the results of the simulations (performed at riojascience platform) of the referenced experiments where a beam of O atoms collides with other of CH_4. The difference between them is that in the first experiment (and simulation) the collision is produced at a relative translational energy i.e. collision energy of 14.7 kcal/mol whereas in the second experiment, this energy is much higher: 64 kcal/mol.

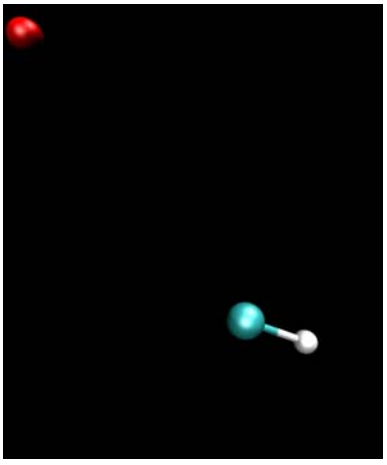
The interpretation of the first diagram is that the OH product is produced mainly backwards from the point that reaction is produced, thus, the maximum signal (red arc) is in the zone of negative v_x components. On the other hand in the second experiment the most intense peaks of the distribution are found at positive v_x values, meaning that an important part of the OH is produced forward when reaction occurs. The theoretical results are not perfect (don't forget it is classical dynamics!) but triqct simulations can reasonably reproduce these experimental evidences (sorry, we cannot show here the experimental results by published paper's copyright) so the theoretical information can explain the observed behavior too (or to raise a theory at least).

1.1.2 To rebound or to not-rebound that's the question.

For example, the known as microscopic mechanism (maybe nanoscopic mechanism would be better) can be analyzed by visualizing the time evolution of the atoms' movement along the simulated reactive trajectories. Obviously, thousand or million of trajectories cannot be visualized one by one, so a property to identify the representative mechanisms should be found first and then analyze the percentage of each, but an example of how the trajectories are is below.

From the triqct simulations two main mechanisms have been found for this reaction, thus the reactive simulated trajectories mainly occur through a rebound mechanism or a non-rebound mechanism.





Rebound (left) and non-rebound (right) trajectories. Note that CH_3 moiety is represented by a blue ball.

Thus, when the simulation is done at the lower collision energy a high percentage of trajectories occurs via the rebound trajectories, leading to a flux-map where the relative velocity is backwards as the OH product "rebounds" once is produced. Note that this rebound is produced in a wide range of angles because a semi-circle signal is obtained in the diagram.
When the collision energy augments this mechanism becomes less important (but is doesn't disappears) and the non-rebound one takes a main role thus, the OH peaks are observed in the forward part of the diagram. In conclusion, the existence of a rebound reaction mechanism and the change in its weight in the dynamical behavior of the reaction can explain the change in the experimentally measured velocity-flux maps.

This is only a little example of the information that can be extracted from the simulations, and the triqct program can be applied to the study of other reactions.

1.2. Triqct on riojascience@home

The riojascience@home project offers us an ideal platform to perform trajectory calculations because we can calculate million of trajectories in days giving us information with a so high quality in statistics that can only be obtained using huge regular computational clusters of hundreds of processors for weeks.
These kinds of calculations are basic Science; they are performed to make deeper the knowledge of how the simplest reactions occur, but the obtained information from these simulations can help to understand and simulate more complex systems, but it is hard, when the number of atoms to simulate increases, the simulations become harder. We are working on this; our intention is to implement new programs and algorithms on the platform that let the study, through trajectory calculations, of bigger systems.