Introduction
- The irradiation of biological systems leads to the formation of radiolytic species such as H, OH, H₂, H₂O₂, eaq etc. [1]
- These species react with neighboring molecules, which result in damage in biological molecules such as DNA.
- Radiation chemistry is therefore very important to understand the radiobiological consequences of radiation [2].
- In this work, we discuss an approach based on the exact Green Functions for diffusion-influenced reactions which may be used to simulate radiation chemistry and eventually extended to study more complex systems, including DNA.

Green functions
- The exact Green functions for an isolated pair are known analytically [3-4]:

\[
\begin{align*}
\psi_{\text{free}}(t, r) &= \frac{1}{\pi} \int_0^\infty \frac{d\tau}{\tau^2} e^{-\tau^2} \frac{1}{\sqrt{\tau^2 + 1}} e^{-\frac{r^2}{4\tau^2}} \\
\psi_{\text{bound}}(t, r) &= \frac{1}{2} \int_0^\infty \frac{d\tau}{\tau^2} e^{-\tau^2} \frac{1}{\sqrt{\tau^2 + 1}} e^{-\frac{r^2}{4\tau^2}} \\
\psi_{\text{react}}(t, r) &= \frac{1}{4} \int_0^\infty \frac{d\tau}{\tau^2} e^{-\tau^2} \frac{1}{\sqrt{\tau^2 + 1}} e^{-\frac{r^2}{4\tau^2}} \\
\psi_{\text{products}}(t, r) &= \frac{1}{8} \int_0^\infty \frac{d\tau}{\tau^2} e^{-\tau^2} \frac{1}{\sqrt{\tau^2 + 1}} e^{-\frac{r^2}{4\tau^2}} 
\end{align*}
\]

- The coefficients \(a, \beta\) and \(\gamma\) are related to the reaction rate constants (\(k_0=4\pi RD\)):

\[
\begin{align*}
\alpha &= \frac{a + \beta}{2} + (\alpha + \beta) k_{1N} \\
\beta &= \frac{a + \beta}{2} - (\alpha + \beta) k_{1N} \\
\gamma &= \alpha - \beta
\end{align*}
\]


Chemical reactions and radiolytic yields
- The chemical reactions between radiolytic species with no electrostatic interaction (i.e. their charge product is 0) can be simulated by using the Green Functions described above.
- The radiation chemistry code can be used to simulate the time evolution of the radiolytic species (radiation chemistry) and radiochemical yields [5,6].

Assumptions of the model
- The pair of particles may react as follow [3]:

\[
A + B \rightarrow (AB)^{\text{products}}
\]

- Transitions from a state to another are defined:

<table>
<thead>
<tr>
<th>Initial state</th>
<th>State after one timestep</th>
</tr>
</thead>
<tbody>
<tr>
<td>Free (kₐ)</td>
<td>p(kₐ) (t₀) p(kₐ) (t₀) p(kₐ) (t₀)</td>
</tr>
<tr>
<td>Rev. bound (kₐ)</td>
<td>p(kₐ) (t₀) p(kₐ) (t₀) p(kₐ) (t₀)</td>
</tr>
<tr>
<td>Products (kₐ)</td>
<td>0 0 0</td>
</tr>
</tbody>
</table>

Sampling of the Green functions
- We have developed exact algorithms to sample the random variates \(r\) for \(p(r,t₀)\) and \(p(r,t|*)\) [4].
- The algorithm allow the simulation to be done in several timesteps (time discretization)

Radiation track structure and evolution in time

Conclusion
- This approach has been used successfully to simulate the time evolution of radiolytic species and to calculate radiochemical yields.
- The radiation track structure code RITRACKS [7] and the chemistry code will be of crucial importance in future models of DNA damage.

References