Step-by-step simulation of radiation of radiation chemistry using Green Functions for diffusion-influenced reactions

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Introduction

- The irradiation of biological systems leads to the formation of radiolytic species such as H, OH, H$_2$, H$_2$O, e$_{aq}$, 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]:

\[
\phi(x,t|x_0,t_0) = \frac{1}{\sqrt{2\pi\tau}} \exp\left(-\frac{(x-x_0)^2}{4\tau}\right)
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- The coefficients $\alpha, \beta$ and $\gamma$ are related to the reaction rate constants ($k_0=4\pi RD$):

\[
\alpha = \beta = \gamma = (1/\sqrt{\pi}) k_0 R
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- The chemical reactions are 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].

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.
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Assumptions of the model

- The pair of particle may react as follow [3]:

\[
A + B \rightarrow (AB) \rightarrow AB
\]

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\]

- Transitions from a state to another are defined:

<table>
<thead>
<tr>
<th>State after one timestep</th>
<th>Free (x)</th>
<th>Rev bound (*)</th>
<th>Products(**)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial state</td>
<td></td>
<td></td>
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</tr>
</tbody>
</table>

- The material balance condition is:

\[k_i p(t, r | *) = k_{ip}(t, r | r)\]

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- The boundary condition is:

\[Q(t | *) = \frac{4}{3} \pi r^2 p(t, r | *) dr\]

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Sampling of the Green functions

- We have developed exact algorithms to sample the random variables $r$ for $p(r, t | r_0)$ and $p(r, t | *)$ [4].
- The algorithm allow the simulation to be done in several timesteps (time discretization)

\[\text{Sampling algorithm}\]

<table>
<thead>
<tr>
<th>( \gamma )</th>
<th>( \alpha )</th>
<th>( \beta )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Max</td>
<td>Min</td>
<td>Median</td>
</tr>
</tbody>
</table>

Radiation track structure and evolution in time

- The Green Functions can be used to build a radiation chemistry code [4], by using average positions generated by sampling the inter-particle distance at each timestep

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References