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Bob Eisenberg <bob.eisenberg@gmail.com>

Continuum and Discrete Estimates of Stochastic Processes or Stochastic Elementary Events

Bob Eisenberg <beisenbe@rush.edu>   Thu, Jun 13, 2013 at 11:21 AM
Reply-To: beisenbe@rush.edu
To: Dezso Boda <dezsoboda@gmail.com>, Bob Eisenberg <beisenbe@rush.edu>
Cc: Jinn Liu 劉晉良 <jinnliu@mail.nhcue.edu.tw>

Dear Dezső

As usual, you hit the nail on the head.

BUT this is NOT NOT an unusual situation
in stochastics and probability theory.
(I have done a good deal of work on this
a long time ago and was trained by Zeev
Schuss who wrote the first textbook in
the field, and has the best textbook as
well

1.   Schuss, Z. 2009. Theory And Applications Of Stochastic Processes: An Analytical Approach New York:
Springer. 470 p.

2.   Schuss, Z. 1980. Theory and Applications of Stochastic Differential Equations. New York: John Wiley)

In probability theory or theory of stochastic processes, there is an underlying "set" (in quotes
because I am not a mathematician and do not use the exact mathematical meaning of the word set) of
trajectories or outcomes with a definite set of properties. That is to say, they have a definite distribution which is
always the same when measured accurately enough (i.e., with enough outcomes).

The physical properties produced by those trajectories or outcomes are however MEASURES
of the "set". They are NOT NOT the set itself.

Different methods use different measures and the choice of correct measure is always problematic. Measures
that have no bias (which has an exact meaning) are rarely the measures
which are most efficient (which does not have an exact meaning until a cost function is specified), or least
variance, etc etc

Metropolis Monte Carlo is ONE way to study the properties of the set.
Continuum partial differential equations describing densities is another.

The relation of these apples and oranges REQUIRES a theory of estimation.
This is a main result of the modern theory of probability and (separately) the
modern theory of stochastic processes.

That theory is not known for pde's (I know that because we tried to derive it.
For uncharged point particles, we succeeded beyond our wildest dreams

Eisenberg, R. S., M. M. Kłosek, and Z. Schuss. 1995. Diffusion as a chemical reaction: Stochastic trajectories

between fixed concentrations. J. Chem. Phys. 102:1767-1780.

For interacting particles, we did better than anyone else (I know of,
because we actually derived a NONequilibrium BBGKY hierarchy)

1.   Schuss, Z., B. Nadler, and R. S. Eisenberg. 2001. Derivation of Poisson and Nernst-Planck equations in a
bath and channel from a molecular model. Phys Rev E Stat Nonlin Soft Matter Phys 64:036116.

2.   Schuss, Z., B. Nadler, and R. S. Eisenberg. 2001. Derivation of PNP Equations in Bath and Channel from a
Molecular Model. Physical Review E 64:036116 036111-036114.

3.   Schuss, Z., B. Nadler, A. Singer, and R. Eisenberg. A PDE formulation of non-equilibrium statistical
mechanics for ionic permeation,. In: S. M. Bezrukov, editor; 2002; Washington, DC,. AIP.

I do not know whether either of these treatments survives coupling to Poisson, i.e., introducing charged particles
that satisfy electric field equations and boundary conditions.

For Monte Carlo, I am much less an expert, but I cannot yet find in the standard works

1.   Binder, K. 1995. The Monte Carlo Method in Condensed Matter Physics. New York: Springer.

2.   Gilks, W. R., S. Richardson, and D. J. Spiegelhalter. 1996. Markov Chain Monte Carlo in Practice. New
York: Chapman Hall/CRC. 486 p.

3.   Newman, M. E. J. and G. T. Barkema. 1999. Monte Carlo Methods in Statistical Physics. New York:
Oxford. 475 p.

4.   Landau, D. P. and K. Binder. 2000. A Guide to Monte Carlo Simulations in Statistical Physics. New York:
Cambridge University Press. 384 p.

5.   Christian, P. R. and G. Casella. 2004. Monte Carlo Statistical Methods

theorems that apply to spatially inhomogeneous systems within boundary conditions,
or to charged particles (with charge treated consistently with the field equations of
electricity and magnetism).

BUT Dezső knows MUCH more about this than I, and I will keep looking.

In both cases, I emphasize what is needed is a MATHEMATICAL theory of estimation.

If you doubt the need, just look up the literature of estimation of a Fourier Transform
by a discrete Fourier Transform (which includes binning problems, aliasing, picket fence
effects and so on) to see what complexity can arise (including car wheels that go backwards
in movies and TV).

SOOO
this is an elaborate way of saying I do not know how to compare these
apples and oranges in a rigorous way.

Indeed, I do not know how to compare the two images (i.e., estimates)
of the same oranges, if one is done discretely at variable resolution
and the other is done with continuous functions.

Lest Dezső think that discrete is definitely better, please remember that
the Maxwell equations involve ONLY continuous functions of charge and

these are the most general laws known, accurate to some 20 significant
figures from the (unobservable) diameter of an electron to astronomical
distances.

as ever
Bob

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Bob Eisenberg (or Robert S. Eisenberg). WebSite: http://www.phys.rush.edu/RSEisenberg/
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On Thu, Jun 13, 2013 at 10:43 AM, Dezso Boda <dezsoboda@gmail.com> wrote:
> Dear Jinn,
>
> I am sorry for misunderstanding. I am still confused.
>
> In this case we seem to plot two different profiles. How can you compare apple with orange?
>
> Dezső
>
> On Thu, Jun 13, 2013 at 9:19 AM, jinnliu <jinnliu@mail.nhcue.edu.tw> wrote:
>> Dear Dezső,
>>
>> Our conclusion on the disagreement between MC and PF profiles of oxygen ions is that
>> the Monte Carlo profile is not correct from the Poisson-Fermi viewpoint but is correct and feasible from the
>> Monte Carlo viewpoint and should be interpreted or used with care.
>>
>> Moreover, the definition and implementation of the concetration is very different between MC and PF. We
>> spend about 3 pages in our paper to explain this, in fear of any misinterpretation or misunderstanding about
>> our statements made in the paper.
>>
>> We did not use the word "unphysical" for the MC oxygen profile. In fact, we have shown that, even for the
>> delta functions, MC profiles are still physical and correct.
>>
>> What we really stress is that the MC profiles may not statisfy the saturation condition defined in our paper
>> (Eqs. (8) and (23)). And the saturation condition can only be used to verify PF profiles. The saturation
>> condition does not apply to MC profiles.
>>
>> We say and show that the Poisson-Boltzmann profile in Fig. 2 is "unphysical" (the proof statement is in the
>> last paragraph on P. 18).
>>
>> Please allow me to reiterate that we have shown that the MC oxygen profile in Fig. 2 is correct and feasible
>> (of course physical as well). But the MC profile cannot be used for PF calculations by finite difference
>> approximation.
>>
>>
>> Best,
>>
>> Jinn

-----Original message-----
From: Dezso Boda<dezsoboda@gmail.com>
To: beisenbe<beisenbe@rush.edu>
Cc: Jinn Liu 劉晉良<jinnliu@mail.nhcue.edu.tw>
Date: Thu, 13 Jun 2013 07:43:39 +0200
Subject: Re: Comments from Dezso
Dear Jinn,

I did not have time to read through the whole manuscript; I just read the parts where you explain why do you think that the ionic (oxygen) profiles plotted in our MC papers is unphysical.

I totally disagree. There is no any saturation condition for the one-particle density profile. It can by as high as you want. If oxygen ions tend to spend a lot of time at one position, concentration there will be high. It can be high. It is physical. It can even by infinite if an ion is fixed as in a crystal at 0 K.

The misunderstanding is probably coming from our different methods. You use a lattice method. You have an oxygen there or you do not have one. Implying an upper limit makes sense.

In MC, however, we have ions moving around. They can be anywhere. The definition for the density profile is what people use for local one-particle density. Take a small volume, dV, and measure how much oxygen-center you find in it on average, dN. The density is dN/dV. It is a well defined limiting value and not sensitive to the size of the volume element as soon as it is large enough. I checked.

So, I think your flat oxygen profile is an artifact of the theory you are using, while the MC profile is correct that any decent theory should be able to reproduce.

Best wishes,
Dezső

On Wed, Jun 12, 2013 at 7:07 PM, Bob Eisenberg <beisenbe@rush.edu> wrote:
> Dear Jinn and Dezso
>
> Dezso will be reading our paper and give us comments
> in the next week.
>
> He is concerned about depletion layers that go to zero
> (because that would produce no current) and the flat
> profile of the oxygens.
>
> I will let him speak for himself, however.
>
> Thank you Dezso in advance!!!
>
> As ever
> Bob
>
>
>
>
> Robert Eisenberg
> Bard Endowed Professor and Chair
> Department of Molecular Biophysics
> Rush University Medical Center
> =======================================

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--==Mailed via NHCUE Webmail==--