Bob Eisenberg <bob.eisenberg@gmail.com>

Recrossings

Bob Eisenberg <beisenbe@rush.edu>
Reply-To: beisenbe@rush.edu
To: Chun Liu <liu@math.psu.edu>, Yoichiro Mori <ymori@umn.edu>
Cc: "Stuart A. Rice" <s-rice@uchicago.edu>, Bob Eisenberg <beisenbe@rush.edu>, Ardyth at Gmail <ardyth.eisenberg@gmail.com

Dear Chun and Yoichiro,

I have been corresponding with J. Ross Macdonald
who was the leader in impedance measurements in
electrochemistry for many decades about one thing
or another, and the following emerged, which I thought
might interest you both historically and logically (recrossings
and what needs to be done in ionic solutions).

Of course, this is all speculation, so there may be lots
of holes in it, for you and your generation to fill, I trust and
pray!!

As ever
Bob

PS I am sending a copy of this to Stuart Rice, hoping he
may be amused as well.

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---------- Forwarded message ----------
From: **Bob Eisenberg** <beisenbe@rush.edu>
Date: Sun, Sep 19, 2010 at 10:21 AM
Subject: Re: Ready for PNP-vi
To: "J. Ross Macdonald" <macd@email.unc.edu>
Cc: Bob Eisenberg <beisenbe@rush.edu>

I do not mention impedance measurements which were a wonderful larger scale task for me for some 20 years.

So to survive, I had to know a lot of different fields.

To other matters:

I have not read the epsilon algorithm paper and will try to do that today.

I look forward to reading the paper #207 which I have not read.

To treatments of finite size:

The issue about how to deal with finite size effects is very very sensitive as far as I am concerned, because it deals with issues of integrity, without which no theoretical treatment will succeed.

The fundamental issue must be a commitment to deal with a specific set of data sets, in the language and form that experimentalists in the field think important.

For ionic solutions, at this stage of our ignorance, the choice is very very easy. It is first and foremost the simplest properties of ionic solutions, called colligative properties in the ancient literature, that survives to this day, which are roughly speaking the free energy per mole of each ionic species. There are huge and accurate data sets on these and in my view theories and simulations must be tested first by their ability to deal with this data in a range of ionic solutions over many decades of concentration and in mixtures, including divalents and monovalents and worse.

The primitive model does reasonably well with this provided the dielectric constant of the solution (NOT of water) is used. This is true whether the primitive model is evaluated with MC or with (awful) approximate theories. We do not yet know how well a good mathematical theory (EnVarA) deals with the data because we have not yet computed the theory in three dimensions.

The problem with most of the electrostatics of proteins literature is that it consciously and deliberately avoids all issues in which linear Poisson Boltzmann is inadequate. (I use the words 'consciously and deliberately' because I have with my own eyes and ears heard such remarks from leaders in the field. Remember I knew about linear PB before they started their work in the 1980s so I grew up with them.) Almost all biology occurs in the regimes in which linear PB does not work (i.e., with divalents present, or at voltages larger than say 10 mV, or in mixtures). The motivations here have to do with money and career not science.

Other workers are now beginning to deal with finite size.
The problem with many treatments of finite size is that the authors do not deal with the realities of experiments. Indeed, Bazant is adamant and contemptuous in private conversation about all previous treatments of these problems, and does not agree that data needs to be fit. He is proud that he does not know statistical mechanics (he boasted of this repeatedly to me with many others present during my several visits with him a few years ago). I do not believe this approach can converge to a good result.

This is NOT to say that a simpler approach than EnVarA might not work. Too many negatives, let me say it positively.

simulations: the current flows would produce impossible effects).

The tragedy with Brownian motion theory is that it has ignored selfconsistency entirely (see attached) and so is irrelevant to diffusion in water, where (nearly) everything that dissolves has huge electric charge densities (even sucrose, although they add to zero when summed over the whole molecule).

I included this remark as a dig at Frauenfelder and Wolynes, not my favorite intellect, who have papers trying to determine the number of recrossings over the top of a barrier in 'Kramers' theory and use this to determine a transmission (fudge) factor to put in front of the exponential expression.

Zeev Schuss showed (attached) in an unpublished paper (that he has given me permission to circulate and have on my public FTP site) that the transmission factor (in the usual 1D version of Kramers' theory) is exactly and identically one half. He did not publish this because he found a Russian more or less pure math paper that proved the same thing in one incomprehensible paragraph in the 1920's. Only Zeev could understand the paragraph but he has stubborn integrity (which is one of the reasons I love him so much) and refused to publish it. Now I am trying to have him post it on the ArXiv but he is old and not well and not yet able to do it.

About KC Cole. I had many (i.e., about 10) conversations with him and have all his reprints from days when I was a student at Woods Hole (1960-1962). He stoked my interests in impedance measurements.

Hope I have answered all your questions!
I have to do some legal work for my wife and then will look to your papers (if football does not paralyze me entirely).

As ever
Bob

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with separate physical mechanisms (coming from separate
physical structures) to control amplitude and 'duty factor'
(what channel people call open probability).

The amplitude is responsible for the selectivity between
different ions.

The gating (duty factor) is basically responsible for the sensitivity
to specific inputs (which are different for each of the thousands
of types of channels. Some channels respond to voltage, some
to temperature, some to specific chemicals etc).

The total current through the membrane (which determines the
macroscopic function) is the 'sum' of the responses of many
channels (thousand to billions sometimes) each opening and closing.

The attached long review hopes to explain this clearly.
Let me know how I fail and I will explain better.

You chose the right two papers for citation.

I hope I have answered everything

As ever
Bob

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On Wed, Sep 15, 2010 at 10:20 AM, J. Ross Macdonald <macd@email.unc.edu> wrote:

> Dear Bob:
>
> Perhaps we are still having trouble with emails. Please find below my last message to you of 8/24. I hope you got it, b
>
> I have suggested that you might be a reviewer of my PNP MS submitted to JPCondens Matter. No reviewer reports sc
>
> I sent copies of your forthcoming impressive JCP paper to two of my correspondents, both of whom found it to be of r
>
> Best wishes,

from orthogonality of problems we have
worked on, to the necessity of adherence
to Poisson.

Attached is the JCP paper that was accepted
in final form a few weeks before I knew of your
PNP work. I will send the literature reference when
it is out in the next week or two.

I also attach two older PNP papers you might want
to cite as entries of your readers into PNP in the
biological (nonlinear) context.

As ever
Bob

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On Mon, Aug 23, 2010 at 2:45 PM, J. Ross Macdonald <macd@email.unc.edu> wrote:

See interline inputs below.
R

On 8/23/2010 12:43 PM, Bob Eisenberg wrote:

> Dear Ross
>
> I have had a chance to read the PNPContinuum paper
> and find it fascinating.

Thank you. I am glad you found it interesting. It has a lot of stuff in it, at least some of which is novel. I
me know.

> After our JCP paper appears, I will post the JCP paper
> on the ArXiv and add a page or two giving your paper(s)
> as references. Please send me the correct literature
> reference for your paper.

I look forward to reading the JCP paper. Please keep me informed as to when and how.

Your work and mine has been somewhat orthogonal. Had I known of it, I would have mentioned it in the
in proof. Please send me reference citations of two or three of your papers that would be appropriate

My work has been mostly involved with linear response, although a couple of numerical papers by Fran
situations (e.g. #'s126,131). I have dealt mostly with simpler situations than you have done, and I am h
accomplish.

> b) My former student and present (independent) colleague Dirk Gillespie has
> done the nonequilibrium problem in this domain and has spectacularly
> good fits to large amounts of data. I include a few of his papers. There
> are many more.
>
> If they are confusing, let me know and I will try to translate and explain.
>
> c) I think the generation recombination mechanism should be included
> in a few specific channel models. Let me know if you or your younger
> colleagues would like to do something on that.

Possibly. Maybe my Italian colleague, Giovanni Barbero, would like to try this.

Best wishes,

Ross

> As ever
> Bob
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>
> On Sat, Aug 21, 2010 at 9:27 AM, J. Ross Macdonald <macd@email.unc.edu> wrote:
> > Dear Bob:
> >
> > See Interlined material below.
> >
> > I agree with you comments on our different IS approaches. I do not claim to have done anyth
> > although I have reviewed a few manuscripts in the area.

current work. If so, what are your plans?

What should I read about your work on PNP?
I certainly want to cite it properly.

Thank you for your willingness to do this. Some of my relevant PNP papers are #'s 11 (the fir
between plane parallel electrodes), 92, 100, 122, 124, and 183. But most of this is cited and
who repeated my work unknowingly, in my pending PNP MS. I attach it and invite your comme
but changes can be made in the next go around if appropriate.

So here is some more reading for you!

R

As ever
Bob

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