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Bob Eisenberg <bob.eisenberg@gmail.com>

Re: Thanks for the delightful lunch!

Bob Eisenberg <beisenbe@rush.edu> Fri, Jan 11, 2013 at 8:01 AM
Reply-To: beisenbe@rush.edu
To: John Prausnitz <prausnit@cchem.berkeley.edu>, Chun Liu <liu@math.psu.edu>, Craig Evans <evans@math.berkeley.edu>, Rich J Saykally <saykally@berkeley.edu>, Bob Eisenberg <beisenbe@rush.edu>, Allen Tzyy-Leng Horng 2 <tlhorng123@gmail.com>, Tai-Chia Lin 林太家 <tclin@math.ntu.edu.tw>, YunKyong Hyon <hyon70@gmail.com>, Yoichiro Mori <ymori@umn.edu>, Stephen Harris <harris.steveharris@gmail.com>

Dear John

Thanks for the email and kind comments.

I certainly was vague about how to implement the transformation from reductionist to gestalt.....because I only know how to do it in one case!

The attached paper shows how we implemented the gestalt approach for the primitive model (note that we did it twice, once with a LJ model of ions and another with the Rosenfeld DFT model. The details of the latter are in the appendices). The Eisenberg Hyon Liu paper has full details and is meant to be tutorial. The Horng paper is a simplification that is much easier to compute. But the idea is the same.

We also showed how to work through an idealized electrodiffusion model (no finite size in this case) so we could deal with water flow and cell volume effects in biological tissues (Mori paper).

The advantages of the (energetic) variational approach EnVarA are

1) It automatically deals with boundary conditions and thus with flows that arise from spatially nonuniform boundary conditions.

2) thus EnVarA automatically deals with devices (that have inputs and outputs and power supplies, all at different locations and thus requiring spatially nonuniform boundary conditions)

3) EnVarA allows combinations of different 'fields' as in the Mori paper where we derive (we arrogantly think for the first time) fully consistent descriptions of water flow, cell and tissue volume, and electrodiffusion.

4) Added components (i.e., additional ions) are added in consistently with minimal adjustable parameters. This fact can be a little hard to see in our papers since the additional components are indicated by subscripts BUT the additional components can have profound effects and interactions. The side chains of proteins are handled as additional components in this way and they determine a large part of the special behavior of calcium and sodium channels. (I spare you the papers giving the evidence that we can in fact deal with both realistically.) The Horng paper shows this most

explicitly.

5) Because the electric field is handled by Poisson with boundary conditions, no issues of approximation or convergence arise in the primitive model (beyond those of numerical analysis, which are nontrivial, of course, hence the Horng and other papers I am not sending you.)

6) From a more general point of view, the EnVarA approach allows treatment of very complex problems. I include a paper by Chun Liu showing such an example, and a paper or two by Doi showing his approach to liquid crystals which is similar.

7) I do NOT know how to embed classical chemical reactions
in this energetic variational approach, HOWEVER, once the
free energy and dissipation of the chemical reaction is specified
by equations, the inclusion is straightforward, albeit hard work.

8) The central idea is that the chemical tradition uses the thermodynamic
limit throughout its theories. Scientists see the world through the spectacles
of their theories, to quote a book I am reading, and so boundary conditions
and electric fields are very difficult to include in the chemical tradition.
The electric field REQUIRES boundary conditions if it is to be specified
by Poisson or Maxwell the way physicists do. Saying "at infinity" is vague
and not sufficient to actually allow solution of the equations. These difficulties
appear in classical chemistry as problems in convergence of Coulomb's law
integrated over infinite domains. The problems can NOT be waved away.
In fact it is the existence of those problems that forced Poisson etc to
use partial differential equations to describe the electric field.

Please let me know if this is of any help.
It is my responsibility to make clear what we think we have done here.
I can do that ONLY when you (all) tell me where I have failed.
I will then try again!!

I hope to have many opportunities to work through these ideas
together,

As ever
Bob

PS This work depends entirely on the foundations built by
Chun Liu and involves very hard work by many collaborators.
I am sending them copies of this email, so they can participate
in this conversation if they (and you!) wish. Craig Evans and
Rich Saykally at Berkeley and Steve Harris (LBL) have had
many discussions with me on these subjects so I am copying
them as well. I hope you do not mind.

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On Thu, Jan 10, 2013 at 5:51 PM, John Prausnitz <prausnit@cchem.berkeley.edu> wrote:

Dear Bob,

Thank you for your splendid company at lunch today. I learned much. While I do not (as yet) understand all of the details of your integrated method to describe phenomena, I like the general tone: Away with reductionism! Don't neglect context!

We can call your work Gestalt Physical Chemistry.

With best wishes,

Sincerely,

John

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Bob Eisenberg wrote, On 1/10/2013 3:35 PM:

> Dear John
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> Thank you for the delightful lunch, conversation,
> most useful reprints about polarization!
>
> I hope we have a chance to have many more
>
> As ever
> Bob
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6 attachments

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