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Bob Eisenberg <bob.eisenberg@gmail.com>

Re: Estimators and Continuum Theories have much in common

Xiantao Li <xli@math.psu.edu> Wed, Feb 4, 2015 at 1:19 PM
Reply-To: xli@math.psu.edu
To: bob.eisenberg@gmail.com, Chun Liu <liu@math.psu.edu>, Andrew Belmonte <alb18@psu.edu>, "Bob Eisenberg beisenbe@rush" <beisenbe@rush.edu>

Dear Bob,
If my understanding is correct, you need a procedure to map molecular trajectories to quantities that are measured and analyzed in experiments. Examples include number density, current, momentum fluxes, stress, temperature etc.

If this is the case, I think the question has two parts, the first of which is the correct mathematical formula for the corresponding quantities, and the second one is how to take the average, especially when the system is out-of-equilibrium. This is something that I have worked on before and I have several papers to address these issues. In many cases, the formulas can be identified from fundamental conservation laws. The functional form depends on the interatomic potentials. For the second part, the averaging procedure has to be consistent with either the Heisenberg or Schrodinger's view. Some of these issues have been (or will be) illustrated in my blog site:
https://sites.psu.edu/moleculardynamics/about/

For the accuracy of the molecular trajectories, the mathematical term for the divergence is instability in the Lyapunov sense. For example, a nonlinear pendulum, when perturbed, may oscillate with a different frequency, and therefore, eventually becomes off phase. For systems near a thermodynamic equilibrium, however, it is sufficient to maintain the accuracy within the correlation time, typically a few pico seconds. So long time accuracy is irrelevant. For nonlinear processes, this is not understood.

Meanwhile, I will clear my schedule for the workshop to make sure we have enough time to discuss.

Xiantao

On Wednesday2/4/15 7:00 AM, Bob Eisenberg wrote:

> Dear Xiantao
>
> I know how busy family life can be.
> I look forward to more time together
> in March.
>
> YOU better than anyone else can
> solve the puzzle of making MD satisfy
> the laws of electricity.
>
> Note a problem we have not discussed
> but that is quite relevant to the conference.
>
> Let's assume for the minute that MD produced
> perfect trajectories lasting long enough to
> deal with macroscopic phenomena

How do you deal with that number of numbers
i.e., that number of trajectories?

How do you compare them with experiments which
almost never measure trajectories directly?

ANSWER You need an estimator in the
EXACT meaning of that word in probability
and statistics (there is a large and important
theory of estimation in statistics and probability
and in the theory of stochastic processes).
**Crafting the estimator will have almost the
same problems as crafting a continuum
theory, in my view.**

**"Crafting" is an unusual English/American
word but an important one in this context.
It implies a mixture of math, science,
and art/intuition**

**As ever
Bob**

As ever
Bob

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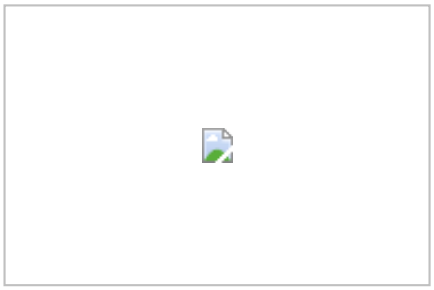
New hospital tower at Rush



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On Tue, Feb 3, 2015 at 4:04 PM, xiantao li <xli@math.psu.edu> wrote:

> Dear Bob,
> My apologies! I got so busy at home these days and I did not get a chance to talk to you. I hope that you had a nice trip back to Chicago.
> I also hope that during the workshop in March, we can get together and discuss the ideas that we presented in the proposal, and see how to proceed with the approach. I believe that the approach is consistent with the energetic variations, and it is also consistent with the molecular dynamics models.
>
> Xiantao
>
> On 2/2/15 11:16 AM, Bob Eisenberg wrote:
>
> > you won't miss anything new!
> >
> > stay warm and dry
> >
> > as ever
> > Bob
> >
> > ~~~~~~~~~~~~~~~~~~
> > Return Address for email: beisenbe@rush.edu or bob.eisenberg@gmail.com
> >
> > Bob aka RS Eisenberg
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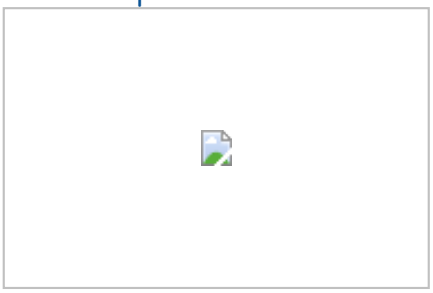

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On Mon, Feb 2, 2015 at 11:11 AM, xiantao li <xli@math.psu.edu> wrote:

> Dear Bob and Chun,
>
> I have to stay home this morning due to the school closure, and unfortunately, I will miss the lunch seminar. But I will come to the colloquium this afternoon. See you then.
>
> Xiantao