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Bob Eisenberg <bob.eisenberg@gmail.com>

Re: Request for CI account (fwd)

Bob Eisenberg <beisenbe@rush.edu>   **Tue, Mar 8, 2011 at 8:00 AM**
Reply-To: beisenbe@rush.edu
To: Jim Fonseca <jefonseca@gmail.com>
Cc: Gary Leaf <leaf@mcs.anl.gov>, Ardyth at Gmail
<ardyth.eisenberg@gmail.com>, Bob Eisenberg <bob.eisenberg@gmail.com>

Dear Jim

Your insights are fabulous.

THIS SPECIAL RESULT MUST NOT BE LOST.
We need to write it up as a degenerative case of
what can happen at least for the arXiv and an Argonne
Report.

This is EXACTLY because of what Jim said

a) the effect of induced charge is to change the NATURE of
the channel.

b) the effect occurs even when induced charge is that of a perfect
dielectric, without lags or nonlinearity. Imagine what could happen
if the polarization charge lagged or lagged with different time courses
in different locations, or was nonlinear.

c) induced charge has been said by eveyone studying gating current
to control conductance. Now they believe there is a special machine.
A real paper saying "Polarization Charge can control Selectivity" would
be very interesting and even revolutionary!!

GREAT FIND.

As ever

Bob

PS Ardyth, could you share this with Jim if it arrives while he is on his way to our place.??
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Return Address for email: beisenbe@rush.edu

Bob aka RS Eisenberg

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On Mon, Mar 7, 2011 at 3:21 PM, Jim Fonseca <jefonseca@gmail.com> wrote:

> Dear Gary,
> I emailed LCRC about the hour request.
>
> Also, congratulations, you have made a Chloride selective Sodium channel. I wonder what the referees will think of that! The calciums, as well as chlorides, are accumulating (up to a couple dozen Molar) just outside the channel, like sprinkles on the top and bottom of the protein 'donut', if you will. I think it's actually mimicking a plasma. The chloride

concentration in the channel ranges from 1 M to 100 M. There is no Na or Ca, however there is a little bit of K! I've seen simulations like this blow up before. I think it just means the model does not hold when such strong (induced boundary) charges involved.

On the other hand, it's very interesting to think that (any kind of?) selectivity may be achieved by controlling the region's dielectric constant--or perhaps that selectivity is only an artifact of the continuum solvent model. Bob-is this somewhat similar to what you have said about possible harmonic charge movements and their effect on selectivity?

Thanks,
Jim

On Mon, Mar 7, 2011 at 2:11 PM, Gary Leaf <leaf@mcs.anl.gov> wrote:
> Jim: Shashi submitted the account request. In two days we will hear from them.
>
> Regarding the fusion account, Shashi suggests we ask for an additional 240K core hours this week. The justification is that the jobs use anywhere from 15 - 90 wallclock time on 24 processors. An 'average'/typical run is about 50 hours. Since this request is web based, would you again make the request?
> Also we should not forget that Rolf is also on this account.
>
> I am processing the rest of the Studies.
> In particular, the Na/Ka/Ca
> %)pwd
> /fusion/gpfs/project/dynamics/ION-TRANSPORT/SODIUMCHANNEL/ PHYSIODIVLNT_IIIKaCa
> (fusion-63%)
>
> This has NaCl=120mM; KCl=2mM; CaCl2 = 3mM.
> PR = 3.0 3.5 4.0
> E_chan = 40 20 10 04 (For PR=3.0, we have 80 as well.)
> The results are unusual in that at E_chan = 10 & 04, we get a Large # of Ca (like 69) and the occup results are very suspect

with STDs on the same order as the occupancy. This Na/Ka/Ca
case

may have to be examined in detail.
You an find the ferror_new summarys in the file Survey_Fix* in the
above directory.

GKL

---------- Forwarded message ----------
Date: Mon, 7 Mar 2011 13:35:42 -0600 (CST)
From: Shashi Aithal <aithal@mcs.anl.gov>
To: leaf@mcs.anl.gov
Subject: Request for CI account

The following information was submitted for approval.
Your account should be created 2 business days after your sponsor,
Daniel S. Katz, has approved the request.
Once your account has been approved and created, you will need to
call the CI Help Desk at 773-834-4102, to receive your intial password.

You will be required to answer your secret question to complete the
process.

First Name: Gary
Last Name: Leaf
Email: leaf@mcs.anl.gov
Username: leaf
Sponsor: Daniel S. Katz
Daytime Phone Number: 630-252-7241
Secret Question: Name of my first dog
Default Shell: /bin/bash

Resources:
Workstation: Yes
HNL Workstation: No
Default Email: leaf@ci.uchicago.edu
Teraport Cluster: No
Gridlab Cluster: No

BIRN: No
townsend: No

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