

# **Calibrating Simulations Proceedings**

*Meeting at Rush University Medical Center*

*Jan 9-10, 2007*

*Sponsored by Army Research Office*

*David Stepp*

*and*

*Argonne National Laboratory, MCS Division*

*Bob Eisenberg (Senior Scientist)*

# Agenda

Monday Jan 8

## *Arrival*

*Dinner* in 'Hyatt at University Village', 625 South Ashland (at Harrison)  
Chicago, 60607. Telephone: (312) 243-7200

Tuesday Jan 9

7:30 *Breakfast and Registration* at Hyatt

8:45 *Greetings* from Dave Stepp, ARO, and Bob Eisenberg, Rush/Argonne

## Calibrations in Computational Electronics

9:00 *History* Dave Ferry

10:00 Coffee

## Calibrations in Physics of Fluids

10:30 *History* Doug Henderson

11:00 *Monte Carlo Simulations* Dezso Boda

11:30 *Density Functional Theory* Roland Roth

12:00 Goals and Organization of Meeting  
Dave Stepp

12:30 *Lunch*

## Calibrations in Molecular Dynamics

2:00 *History and Force Fields* Monte Pettitt

2:45 *Electrostatics of Ions in Solutions and Proteins* Benoit Roux

3:30 *Electrostatics, a different way* Tony Maggs, collaborator Joerg Rottler

4:15 *Organization of Wednesday Subgroups* Bob Eisenberg

6:00 *Reception*

6:30 *Dinner* at Phoenix Restaurant, Chinatown

*After Dinner* 10 minute Talks: *Why Calibrate?* Dave Ferry, Dave Stepp  
and other volunteers

# **Calibrating Simulations**

Wednesday Jan 9

7:30 *Breakfast at Hyatt*

## **8:30-10:15 Workgroups**

*Workgroup on Standards for Homogeneous Systems, leader Dezso Boda,*

Possible questions:

Standards for computations of electrostatics?

Standards for computations of free energy

*Workgroup on Standards for Inhomogeneous Systems, leader Roland Roth*

Possible questions:

Standards for computations of electrostatics?

Standards for computations of free energy

*Workgroup on Standards for Electrostatics of Channels, leader Marco Saraniti*

Possible questions:

Standards for equilibrium calculation (e.g., equilibrium potential)

Standards for nonequilibrium calculations (e.g., current/voltage curve)

## **Coffee 10:15-10:45**

11:30 *Reports from Workgroups, Discussion*

12:30 *Lunch*

2:00 *Workgroup Write-ups*

## **Coffee 3:30-4:00**

4:00 *Next Steps and Goodbye*

Dave Stepp

**Participants Calibrating Simulations Conference : January 9 & 10, 2007**

<b>Participant, Title &amp; Email</b>	<b>Affiliation &amp; Address</b>
1) Dezso Boda, Ph.D. Assistant Professor <a href="mailto:dboda@rush.edu">dboda@rush.edu</a>	Rush University Medical Center Dept. of Molecular Biophysics and Physiology 1750 W. Harrison Street Chicago, Illinois 60612 Voice: (312) 942-6751 Fax: (312) 942-8711
2) Robert Eisenberg, Ph.D. Professor <a href="mailto:beisenbe@rush.edu">beisenbe@rush.edu</a>	Rush University Medical Center Dept. of Molecular Biophysics and Physiology 1750 W. Harrison Street Chicago, Illinois 60612 Voice: (312) 942-6467 Fax: (312) 942-8711
3) Professor David Ferry Regents Professor of Electrical Engineering <a href="mailto:ferry@asu.edu">ferry@asu.edu</a>	Arizona State University Dept. of Electrical Engineering P.O. Box 875706 Tempe, Arizona 85287-5706 Voice: (480) 965-2570
4) Dirk Gillespie, Ph.D. Assistant Professor <a href="mailto:Dirk_Gillespie@rush.edu">Dirk_Gillespie@rush.edu</a>	Rush University Medical Center Dept. of Molecular Biophysics and Physiology 1750 W. Harrison Street Chicago, Illinois 60612 Voice: (312) 942-3089 Fax: (312) 942-8711
5) Douglas Henderson, Ph.D. Professor <a href="mailto:doug@chem.byu.edu">doug@chem.byu.edu</a>	Brigham Young University Department of Chemistry and Biochemistry Provo, Utah 84602 Voice: (801) 422-5934 Fax: (801) 422-0153
6) Dmitry Karpeev, Ph.D. <a href="mailto:karpeev@mcs.anl.gov">karpeev@mcs.anl.gov</a>	Argonne National Laboratory Mathematics and Computer Science Division Building 221, C228 9700 S. Cass Avenue Argonne, Illinois 60439 Voice: (630) 252-1870 Fax: (630) 252-5986

Subtotal Page 1:

<b>Participant, Title &amp; Email</b>	<b>Affiliation &amp; Address</b>
7) Matt Knepley, Ph.D.	Argonne National Laboratory Mathematics and Computer Science Division

[knepley@mcs.anl.gov](mailto:knepley@mcs.anl.gov)

Building 221, C228  
9700 S. Cass Avenue  
Argonne, Illinois 60439  
Voice: (630) 252-1870 Fax: (630) 252-5986

8) Anthony Maggs, Ph.D.

[tony@turner.pct.espci.fr](mailto:tony@turner.pct.espci.fr)

Laboratoire de Physico-Chimie Theorique  
ESPCI  
10 Rue Vauquelin  
75005, Paris, France  
Voice: (331)40794732

9) Wolfgang Nonner, Ph.D.  
Professor

[wnonner@chroma.med.miami.edu](mailto:wnonner@chroma.med.miami.edu)

University of Miami  
Department of Physiology and Biophysics  
1600 N.W. 10th Avenue  
Room 6025B RMSB Bldg  
Miami, Florida 33136  
Voice: (305) 243-5536 Fax: (305) 243-5931

10) B. Montgomery Pettitt, Ph.D.  
Professor

[pettitt@uh.edu](mailto:pettitt@uh.edu)

University of Houston  
Department of Chemistry  
4800 Calhoun Road  
Houston, Texas 77004  
Voice: (713) 743-3263

11) Umberto Ravaioli, Ph.D.  
Professor

[ravaioli@uiuc.edu](mailto:ravaioli@uiuc.edu)

University of Illinois at Urbana-Champaign  
Beckman Institute Room 3255  
Dept. of Electrical and Computer Engineering  
405 N. Mathews Avenue  
Urbana, Illinois 61801  
Voice: (217) 244-5765

12) Roland Roth, Ph.D.

[Roland.Roth@mf.mpg.de](mailto:Roland.Roth@mf.mpg.de)

Max Planck Institut für Metallforschung  
Heisenbergstrasse 3  
Stuttgart, Germany D-70569  
Voice: (49) 711 6891907

:

**Participant, Title & Email**

**Affiliation & Address**

13) Joerg Rottler, Ph.D.

[jrotter@phas.ubc.ca](mailto:jrotter@phas.ubc.ca)

University of British Columbia  
Department of Physics and Astronomy  
6224 Agricultural Road  
Vancouver, BC V6T 1Z1, Canada  
Voice: (604) 822-3510

14) Benoit Roux, Ph.D.  
Professor

[roux@uchicago.edu](mailto:roux@uchicago.edu)

University of Chicago  
Inst of Molecular Pediatric Science  
Gordon Center for Integrative Science  
929 East 57th Street  
Chicago, Illinois 60637  
Voice: (773) 834-3557 Fax: (773) 834-3557

15) Marco Saraniti, Ph.D.  
Professor

[saraniti@iit.edu](mailto:saraniti@iit.edu)

Illinois Institute of Technology  
Dept. of Electrical and Computer Engineering  
Siegel Hall Suite 136  
3301 S. Dearborn Street  
Chicago, Illinois 60613793  
Voice: (312) 567-8813 Fax: (312) 567-8976

16) Gerhard Klimeck  
Professor

[gekco@purdue.edu](mailto:gekco@purdue.edu)

Purdue University  
School of Electrical & Computer Engineering  
465 Northwestern Avenue  
West Lafayette, IN 47907  
(765) 494-9212

Clemens Heitzinger

[clemensH@Purdue.edu](mailto:clemensH@Purdue.edu)

Purdue University  
School of Electrical and Computer Engineering  
465 Northwestern Avenue  
West LaFayette, IN 47907

18) David M. Stepp, Ph.D.

[david.m.stepp@us.army.mil](mailto:david.m.stepp@us.army.mil)

U.S. Army Research Office  
AMSRD-ARL-RO-EM  
Materials Science Division  
P.O.Box 12211  
Research Triangle, NC 27709-2211

## Specific Recommendations

- 1) Calibrations of electrostatics in bulk, channels, and proteins (i.e., homogeneous and inhomogeneous systems) for equilibrium depend on Gauss' law (1,2).
  - a. The charge (of all types, mobile, permanent and polarization) within **any** bounded domain must **at all times and under any conditions** equal the electric flux out of the domain. (Electric flux is the surface integral of the normal derivative of the electric field  $\oiint \mathbf{E} \cdot d\mathbf{S}$  ).
  - b. Gauss' law should be checked in the homogeneous bulk, in domains much larger than the periodic domain used in periodic boundary conditions (pbc). The same size domain should be checked if pbc are not used.
  - c. Gauss' law should be checked in the homogeneous bulk within the periodic domain used in periodic boundary conditions. The same size domain should be checked if pbc are not used.
  - d. Gauss law should be checked in an inhomogeneous system of bulk solution, membrane, bulk solution that does not contain a channel.
  - e. Gauss law should be checked in an inhomogeneous system of bulk solution, membrane, bulk solution that does contain a channel.
  - f. Gauss law should be checked in subdomains of the channel system, antechambers (i.e., access regions), selectivity filters, etc.
- 2) Calibrations of inhomogeneous nonequilibrium systems need also to check flow laws, namely Ohm's law and Fick's law. Macroscopic flows should follow these laws in the wide (but not complete) domains in which they are known to describe ionic solutions. The simulation will apply fixed voltages or concentrations gradients and compute flows. A range of voltages and concentrations would be checked.
- 3) Calibrations of inhomogeneous equilibrium systems need to check sum rules defining contact pressure, etc. in the domains listed above (1 a.-f.). The sum rules are define precisely in (3-6)

## References

1. Feynman, R. P., R. B. Leighton, and M. Sands. 1963. The Feynman: Lectures on Physics, Mainly Electromagnetism and Matter. New York: Addison-Wesley Publishing Co.
2. Jackson, J. D. 1975. Classical Electrodynamics. New York: Wiley. 848 p.
3. Henderson, D., L. Blum, and J. L. Lebowitz. 1979. An exact formula for the contact value of the density profile of a system of charged hard spheres near a charged wall. J. Electronal. Chem. 102:315-319.
4. Henderson, J. R. 1992. Statistical Mechanical Sum Rules. In Fundamentals of Inhomogeneous Fluids. D. Henderson, editor. Marcel Dekker. New York. 23-84.
5. Martin, P. A. 1988. Sum Rules in Charged Fluids. Reviews of Modern Physics 60:1076-1127.
6. Blum, L. and D. Henderson. 1992. Statistical Mechanics of Electrolyte at Interfaces. In Fundamentals of Inhomogeneous Fluids. D. Henderson, editor. Marcel Dekker. New York. 606.