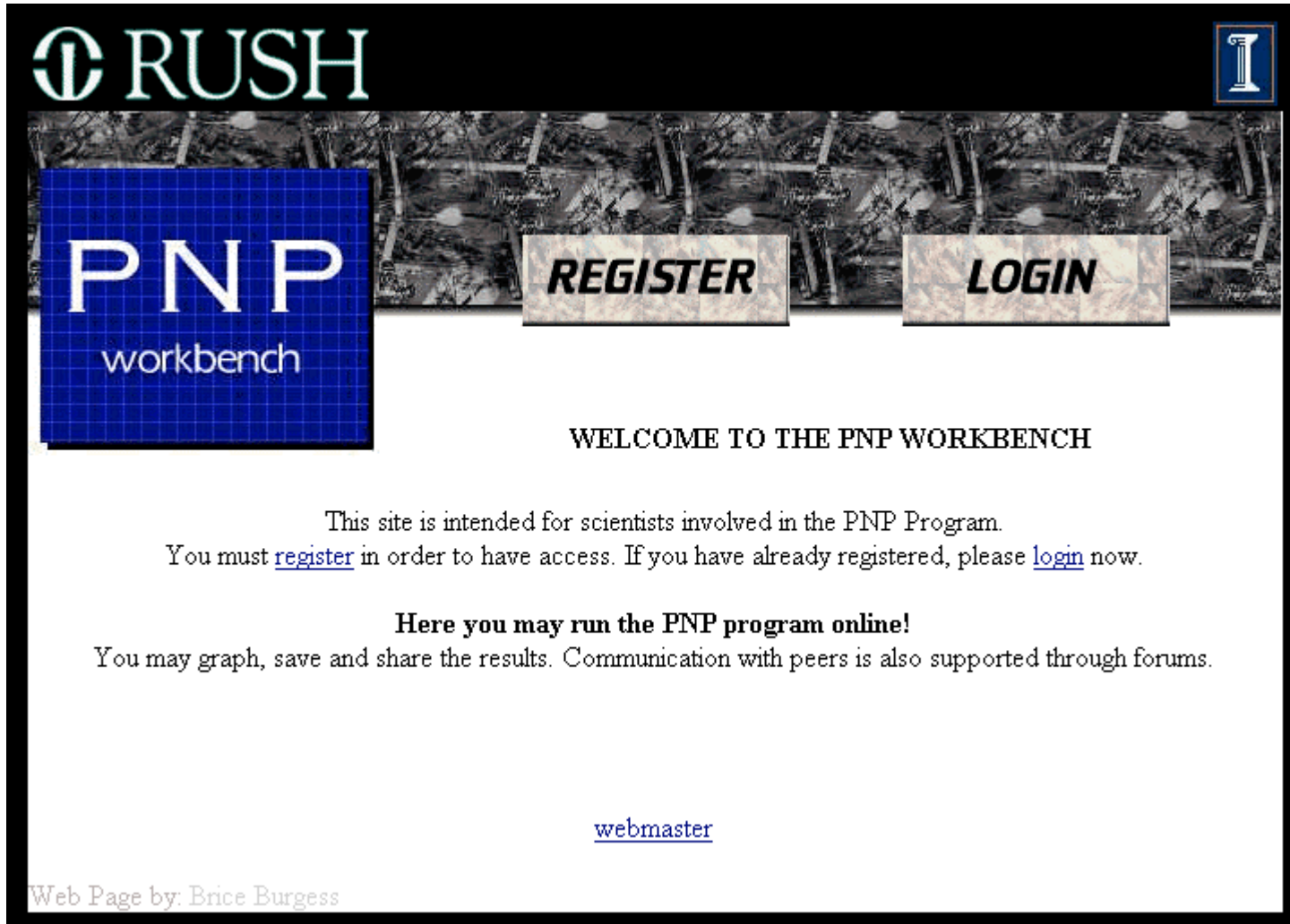


2002 Summer School on Computational Material Science

Lab exercises on transport in ionic channels – Trudy A. van der Straaten

A simple 1-D Poisson-Nernst-Plank (drift-diffusion) solver is available on-line at the site <http://lipidraft.ncsa.uiuc.edu/~pnp>. New users should register first, to gain access to the environment.



The screenshot shows the homepage of the PNP Workbench. At the top left, there is a logo with a stylized 'P' and 'N' inside a circle, followed by the word 'RUSH' in a large, green, serif font. In the top right corner, there is a small blue square icon with a white column. Below the header, there is a horizontal banner with a background image of a forest. On the left side of the banner is a blue square with a white grid pattern containing the text 'PNP workbench' in white. In the center of the banner are two buttons: 'REGISTER' and 'LOGIN', both in a bold, black, sans-serif font. Below the banner, the text 'WELCOME TO THE PNP WORKBENCH' is centered. Further down, there is a paragraph of text: 'This site is intended for scientists involved in the PNP Program. You must [register](#) in order to have access. If you have already registered, please [login](#) now.' Below this is another paragraph: 'Here you may run the PNP program online! You may graph, save and share the results. Communication with peers is also supported through forums.' At the bottom center, there is a link for '[webmaster](#)'. In the bottom left corner, there is a small text credit: 'Web Page by: Brice Burgess'.

After login, the user will reach the following page

**RUSH**

**PNP**  
workbench

[onlinePNP](#) [COMMUNITY](#) [Logout](#)

click here to run program

[ONLINE PNP](#)  
access `pnp_funnel` through the web

[SAVED VARIABLES](#)  
load existing variable sets into  
`pnp_funnel`

[COMMUNITY](#)  
message other scientists on the  
board

Welcome to the PNP workbench, !

username: e-mail: [edit user info](#)

last login: *Friday August 23rd, 2002 02:11 PM*  
files: 0 runs: 3

System Messages:  
This is a new site. If you experience any problems or strangeness, e-mail our [webmaster](#).

**PNP STATUS - 08.23.2002**

USERS: 17 FILES: 2 RUNS: 98 TOP USER: brice - 1 files

## PNP workbench

*onlinePNP*

*COMMUNITY*

*Logout*

Enter input values here

[onlinePNP](#)  
run PNP\_funnel with listed variables

[LOAD VARIABLES](#)  
load existing sets of variables

[PLOT RESULTS](#)  
generate graphic results

[DOWNLOAD](#)  
download pnp\_funnel input file

[SAVE RESULTS](#)  
save results for future use

### onlinePNP PNP Parameters

<input type="text"/>	Pore Radius	angstroms
<input type="text"/>	Pore Length	angstroms
<input type="text"/>	Left Ion Concentration	Moles/liter
<input type="text"/>	Right Ion Concentration	Moles/liter
<input type="text"/>	Diffusion Coefficient of + Ions	cm <sup>2</sup> /sec
<input type="text"/>	Diffusion Coefficient of - Ions	cm <sup>2</sup> /sec
<input type="text"/>	Ambient Temperature	oDeg Celsius
<input type="text"/>	Relative Dielectric Coefficient	unitless
<input type="text"/>	Fixed Charge Density at Left End	moles/liter
<input type="text"/>	Fixed Charge Density at Right End	moles/liter
<input type="text"/>	Transmembrane Voltage	volts

Run Program

CASE A) A sample input set for a channel somewhat similar to gramicidin



**onlinePNP**

**COMMUNITY**

**Logout**

**PNP Run Successful!**

**PNP Parameters**

<input type="text" value="2.0"/>	Pore Radius	angstroms
<input type="text" value="20.0"/>	Pore Length	angstroms
<input type="text" value="1.0"/>	Left Ion Concentration	Moles/liter
<input type="text" value="1.0"/>	Right Ion Concentration	Moles/liter
<input type="text" value="2.0e-5"/>	Diffusion Coefficient of + Ions	cm <sup>2</sup> /sec
<input type="text" value="1.0e-5"/>	Diffusion Coefficient of - Ions	cm <sup>2</sup> /sec
<input type="text" value="20"/>	Ambient Temperature	oDeg Celsius
<input type="text" value="80"/>	Relative Dielectric Coefficient	unitless
<input type="text" value="0.0"/>	Fixed Charge Density at Left End	moles/liter
<input type="text" value="1.0"/>	Fixed Charge Density at Right End	moles/liter
<input type="text" value="0.1"/>	Transmembrane Voltage	volts

Click here to generate plots of results on-line

[onlinePNP](#)  
run PNP\_funnel with listed variables

[LOAD VARIABLES](#)  
load existing sets of variables

[PLOT RESULTS](#)  
generate graphic results

[DOWNLOAD](#)  
download pnp\_funnel input file

[SAVE RESULTS](#)  
save results for future use

Run Program

click to run program

Data entered in the interface above:

CASE A) Pore radius = 2.0 Å  
Pore Length = 20.0 Å  
Left ion concentration = 1 Moles/liter  
Right ion concentration = 10 Moles/liter  
Diffusion Coefficient of + ions = 2.0E-5 cm<sup>2</sup>/s  
Diffusion Coefficient of - ions = 1.0E-5 cm<sup>2</sup>/s  
Ambient temperature = 20° C  
Relative Dielectric coefficient = 80  
Fixed charge density at left end = 0.0 Mole/liter  
Fixed charge density at right end = 1.0 Mole/liter  
Transmembrane voltage (bias) = 0.1 V

Try other cases with the following changes:

CASE B) Left ion concentration = 1 Moles/liter  
Right ion concentration = 10 Moles/liter  
Transmembrane voltage (bias) = 0.1 V

CASE C) Left ion concentration = 1 Moles/liter  
Right ion concentration = 10 Moles/liter  
Transmembrane voltage (bias) = 0.0 V

CASE D) Left ion concentration = 1 Moles/liter  
Right ion concentration = 10 Moles/liter  
Transmembrane voltage (bias) = - 0.2 V

Other sample input files are available at the site.





# PNP

workbench

*onlinePNP*

*COMMUNITY*

*Logout*

[onlinePNP](#)  
run PNP\_funnel with listed variables

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[PLOT RESULTS](#)  
generate graphic results

[DOWNLOAD](#)  
download pnp\_funnel input file

[SAVE RESULTS](#)  
save results for future use

## PNP Variables Loaded

### PNP Parameters

<input type="text" value="4.0"/>	Pore Radius	angstroms
<input type="text" value="30.0"/>	Pore Length	angstroms
<input type="text" value="96.1e-3"/>	Left Ion Concentration	Moles/liter
<input type="text" value="641.0e-3"/>	Right Ion Concentration	Moles/liter
<input type="text" value="2.892363e-07"/>	Diffusion Coefficient of + Ions	cm <sup>2</sup> /sec
<input type="text" value="1.795128e-06"/>	Diffusion Coefficient of - Ions	cm <sup>2</sup> /sec
<input type="text" value="28.85"/>	Ambient Temperature	oDeg Celsius
<input type="text" value="80.0"/>	Relative Dielectric Coefficient	unitless
<input type="text" value="+1.0"/>	Fixed Charge Density at Left End	moles/liter
<input type="text" value="-6.0"/>	Fixed Charge Density at Right End	moles/liter
<input type="text" value="-0.2"/>	Transmembrane Voltage	volts

Run Program