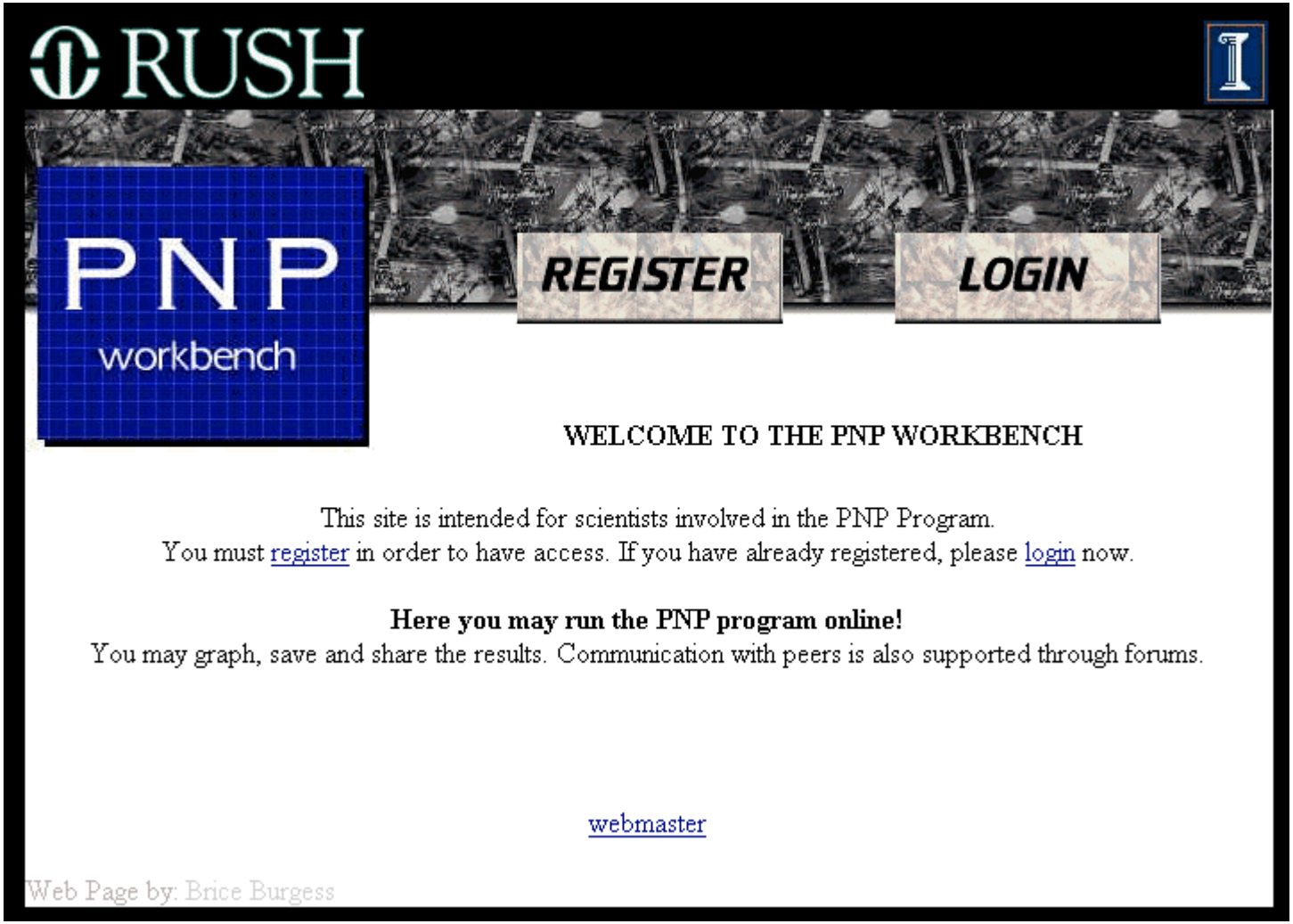
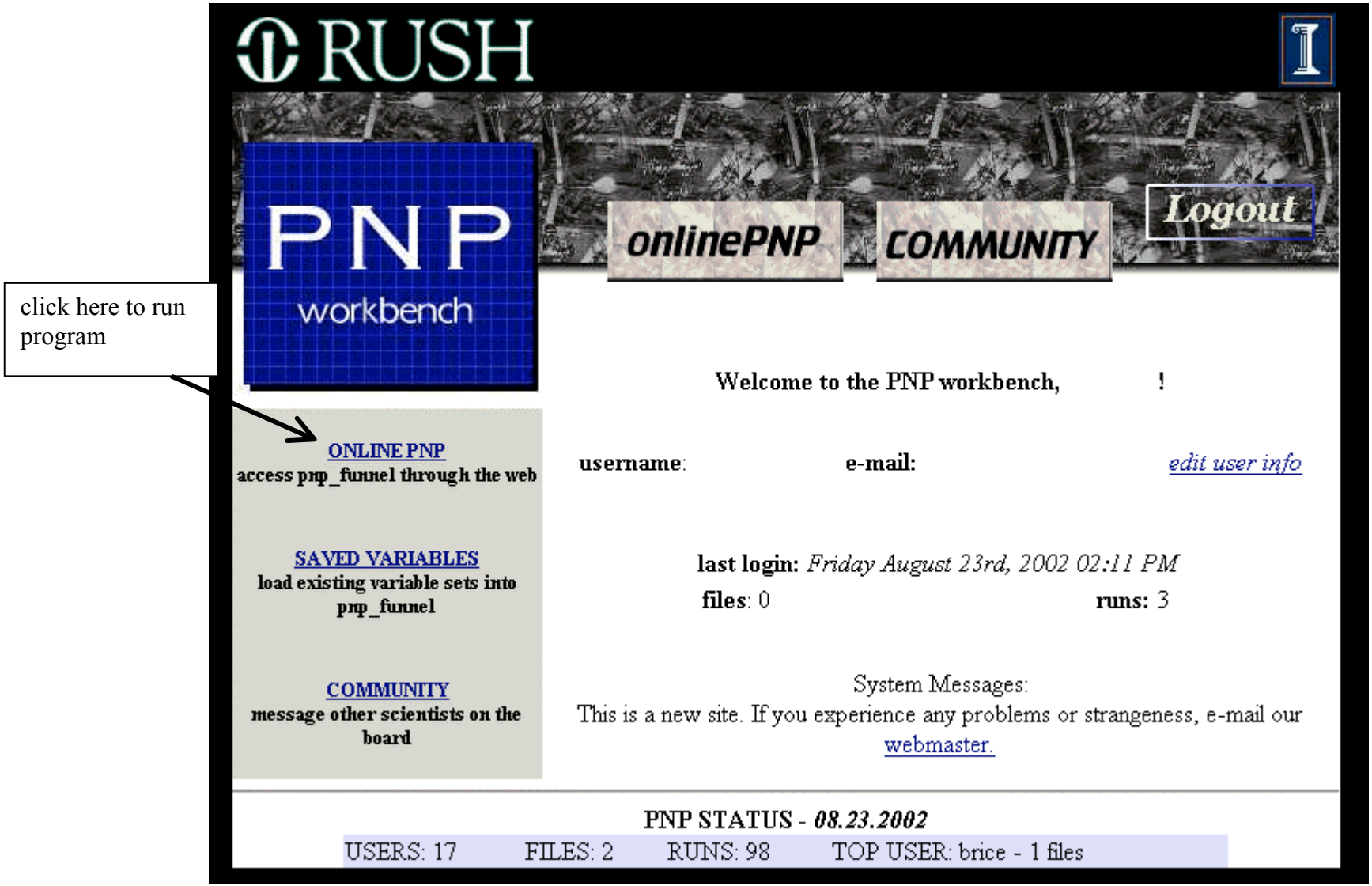
2002 Summer School on Computational Material Science

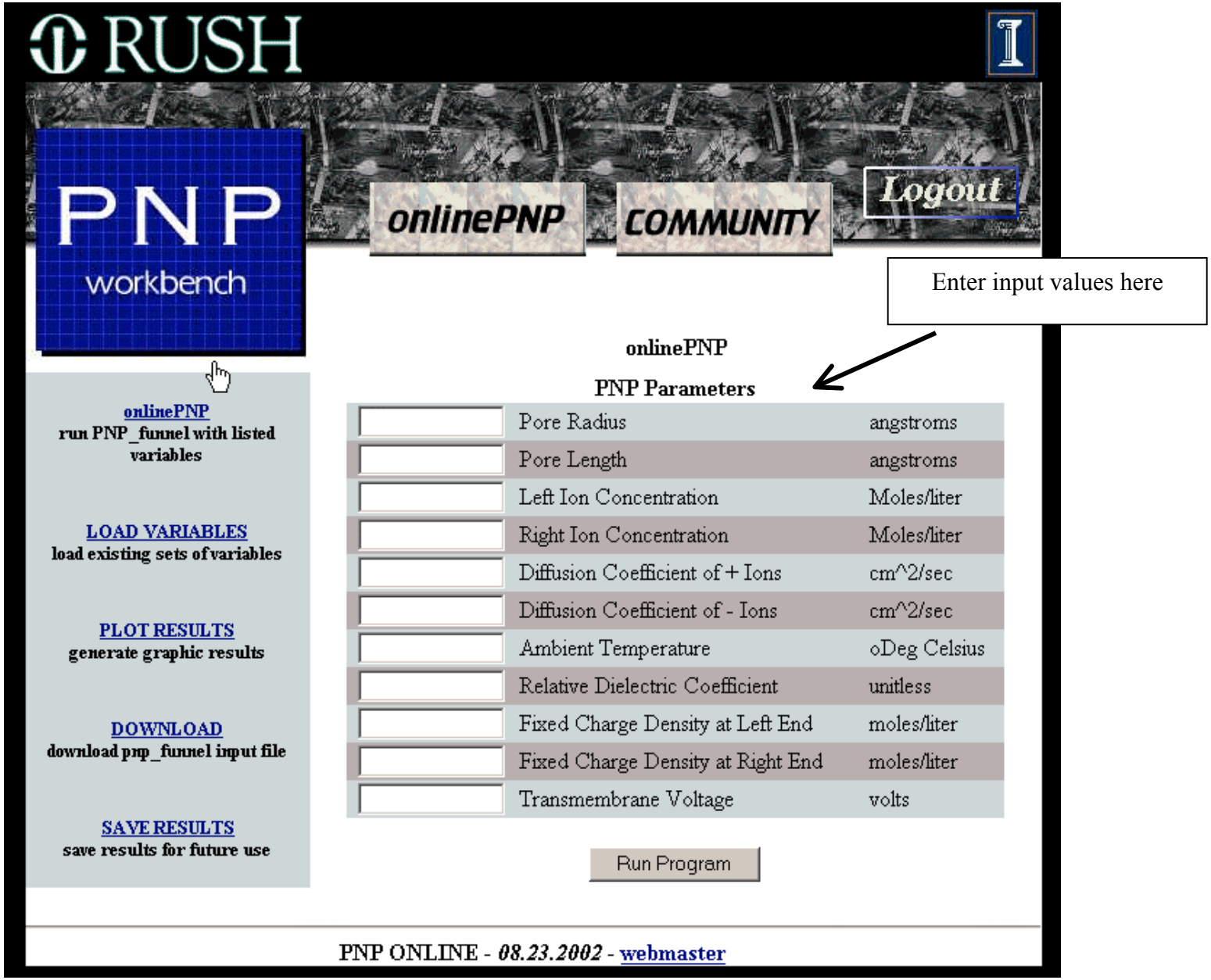
Lab exercises on transport in ionic channels – Trudy A. van der Straaten

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.

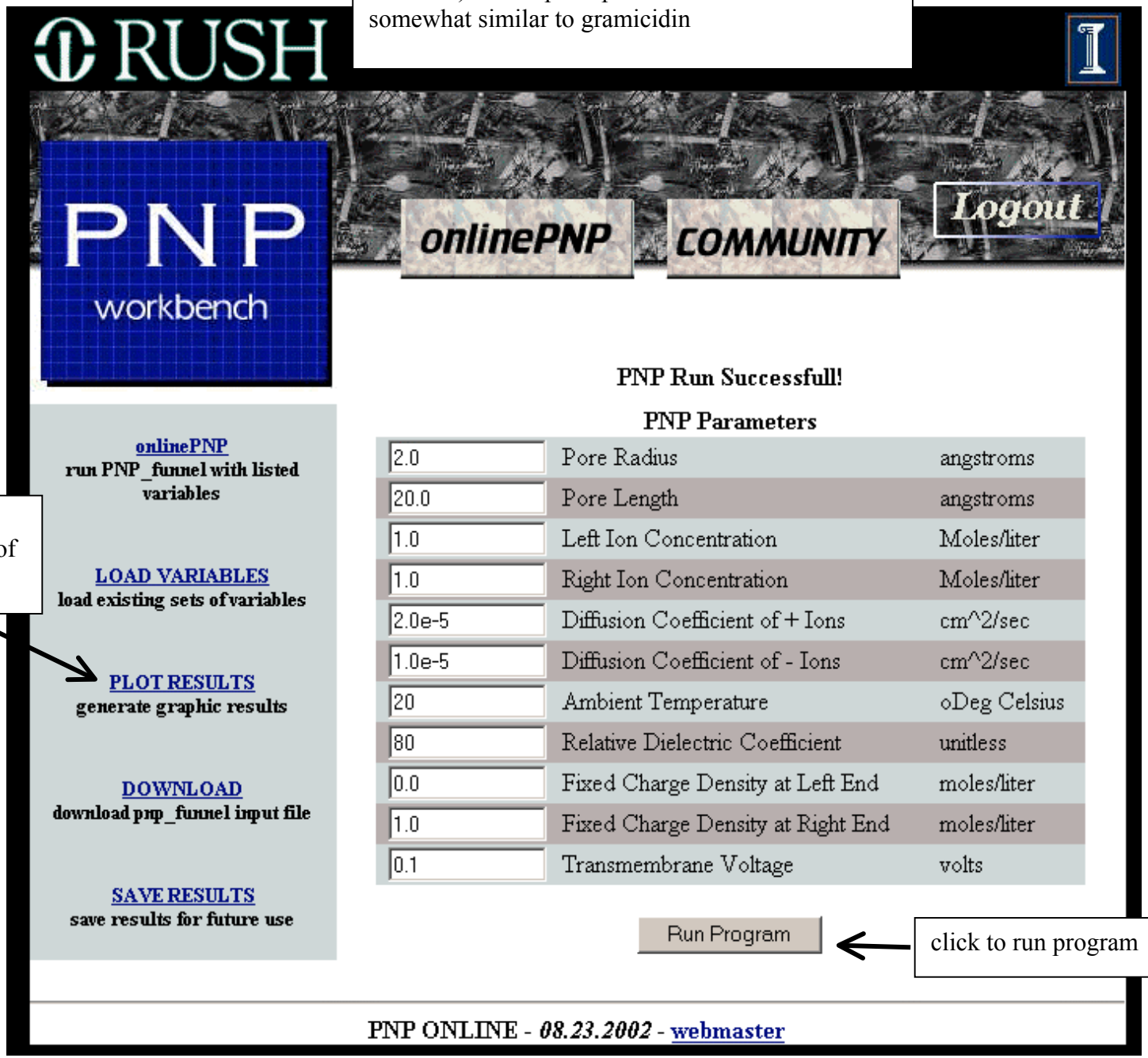


After login, the user will reach the following page




RUSH
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
Pore Radius angstroms
Pore Length angstroms
Left Ion Concentration Moles/liter
Right Ion Concentration Moles/liter
Diffusion Coefficient of + Ions cm^2/sec
Diffusion Coefficient of - Ions cm^2/sec
Ambient Temperature oDeg Celsius
Relative Dielectric Coefficient unitless
Fixed Charge Density at Left End moles/liter
Fixed Charge Density at Right End moles/liter
Transmembrane Voltage volts
Run Program
PNP ONLINE - 08.23.2002 - webmaster

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



Click here to generate plots of results on-line

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^2/s
Diffusion Coefficient of – ions = 1.0E-5 cm^2/s
Ambient temperature = 20º 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

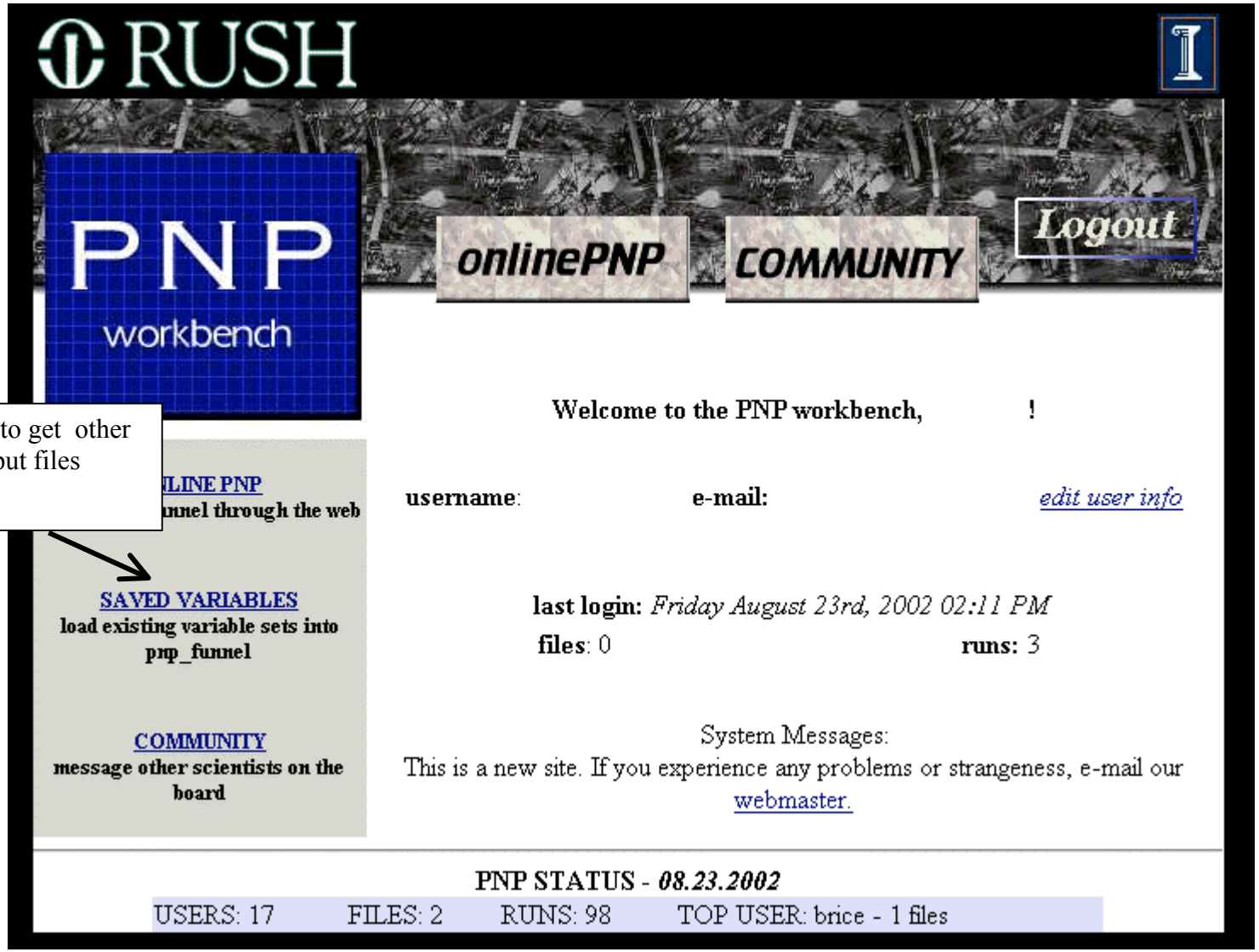
Try other cases with the following changes:

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.



click here to get other sample input files

Example of input file available on line