

Nano-Scale Device Simulations Using PROPHET Lab. Exercise I

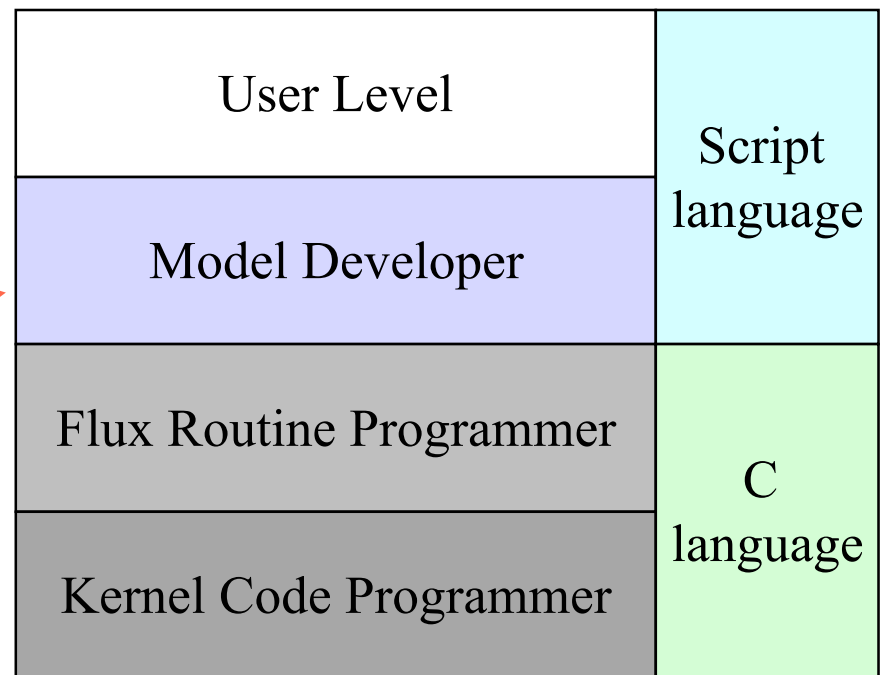
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PROPHET Roadmap

- Lect. #1: basics
 - **Problem set**
 - **Description in Breeze Lab #1**
 - **Access through nanoHUB**
- Lect. #2: PDE def.
- Advanced topics
 - Nano-bio devices
 - Nano-wire devices
 - Organic semiconductor nano-devices
 - <http://www.nanohub.org>

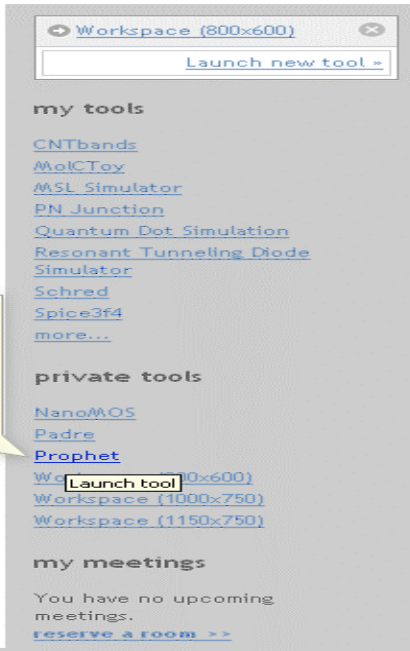


Ex. 0: Log On

- Register @ www.nanohub.org and login
- Launch PROPHET

Tool:
Prophet

Summary:
Framework for solving systems of partial differential equations (PDEs) in time and 1, 2, or 3 space dimensions



Workspace (800x600)

Launch new tool >

my tools

- [CNTbands](#)
- [MolCToy](#)
- [MSL Simulator](#)
- [PN Junction](#)
- [Quantum Dot Simulation](#)
- [Resonant Tunneling Diode Simulator](#)
- [Schred](#)
- [Spice3f4](#)
- [more...](#)

private tools

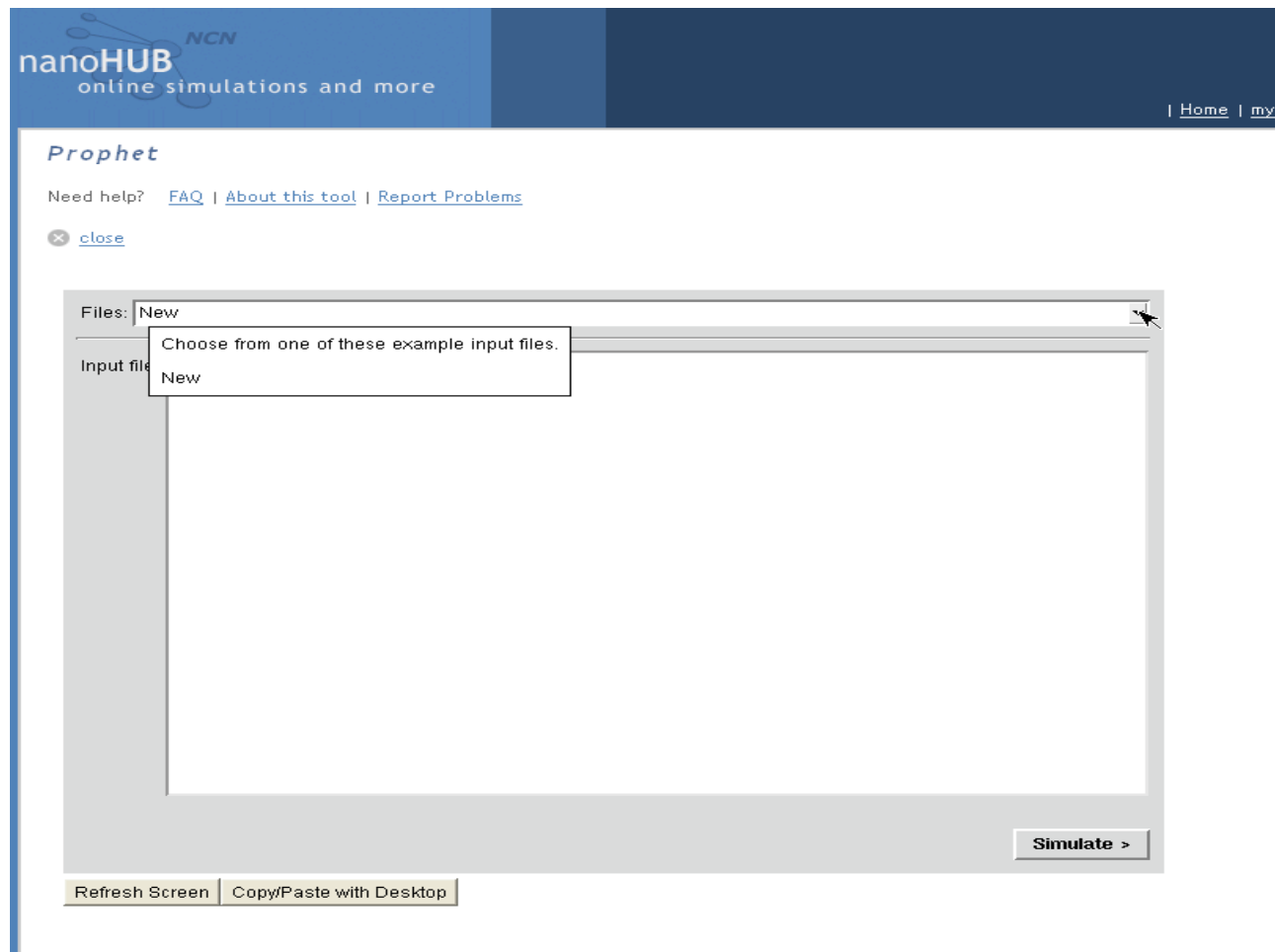
- [NanoMOS](#)
- [Padre](#)
- [Prophet](#)
- [Workspace \(800x600\)](#)
- [Workspace \(1000x750\)](#)
- [Workspace \(1150x750\)](#)

my meetings

You have no upcoming meetings.

[reserve a room >>](#)

PROPHET Web GUI



The screenshot shows the PROPHET Web GUI interface. At the top, there is a nanoHUB logo with the text "nanoHUB online simulations and more" and a navigation menu with links for "Home" and "my r". Below the header, the page title is "Prophet". There are links for "Need help? FAQ | About this tool | Report Problems" and a "close" button. The main content area features a "Files: New" section with a sub-section "Input files" containing a "New" button. A tooltip above the "New" button reads "Choose from one of these example input files." At the bottom right of the main area is a "Simulate >" button. At the bottom left, there are buttons for "Refresh Screen" and "Copy/Paste with Desktop".

Ex. 1(a): 1-D Poisson Eq.

Prophet

Need help? [FAQ](#) | [About this tool](#) | [Report Problems](#)

[close](#)

```
Files: poisson1d.pf
Input file: #filename: "poisson1d.pf"
#create dbase entry for sysvar u
dbase createlist name=library/physics/silicon/u
dbase prefix=library/physics/silicon/u
dbase create name=dirichlet.x0 rval=0.0
dbase create name=dirichlet.x1 rval=1.0
dbase create name=scale rval=1.0
dbase create name=Dix rval=1
dbase prefix=""

#define system poisson
system name=poisson
+ sysvars=u
+ term0=box_div_lapflux(u|u)@{silicon}
+ term1=nodal_copy(c|u)@{silicon}
+ term2=dirichlet.default_dirichlet(0|u)@{silicon/x0, silicon/x1}

#define simulation mesh and boundaries
grid xloc=0,1 xdel=0.005 dim=1
boundary xmin=0 xmax=0 name=x0
boundary xmin=1 xmax=1 name=x1

#define fixed charge
field set=c val=5
#initialize sysvar u
field set=u val=0

#solve and plot
```

[Simulate >](#)

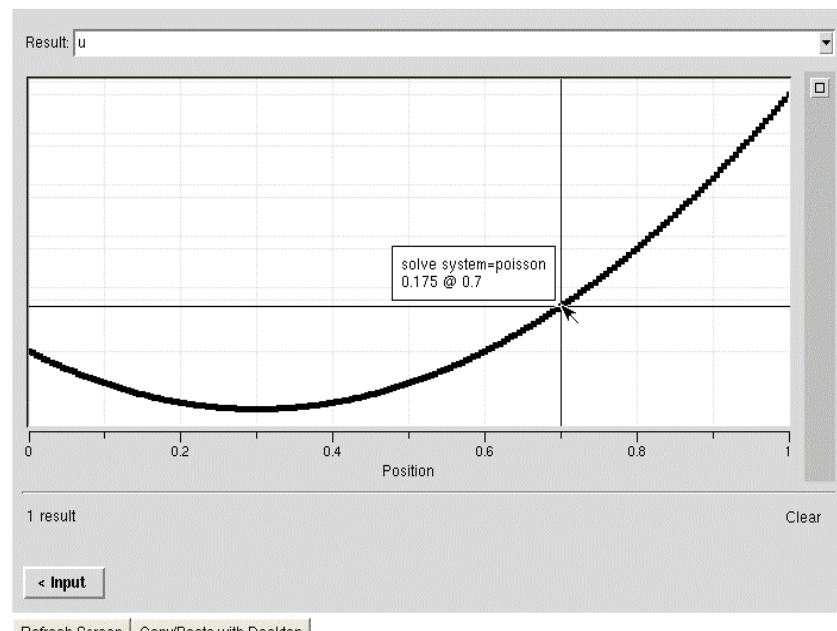
[Refresh Screen](#) | [Copy/Paste with Desktop](#)

Input script poisson1d.pf

Prophet

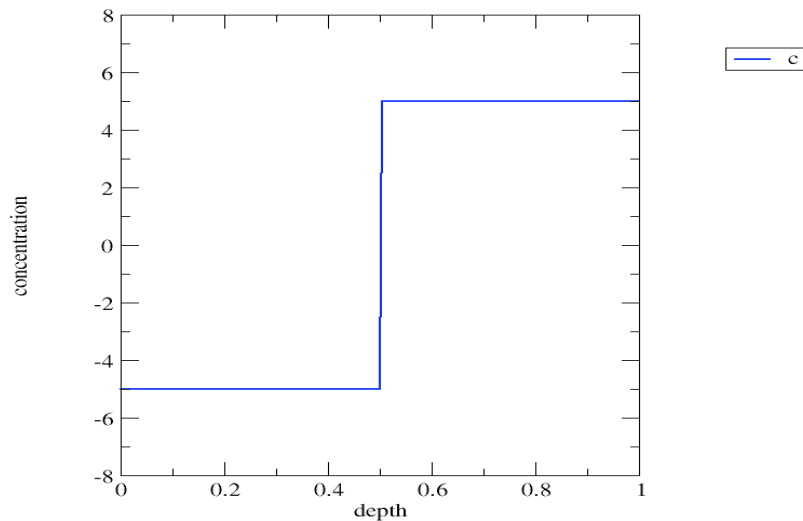
Need help? [FAQ](#) | [About this tool](#) | [Report Problems](#)

[close](#)

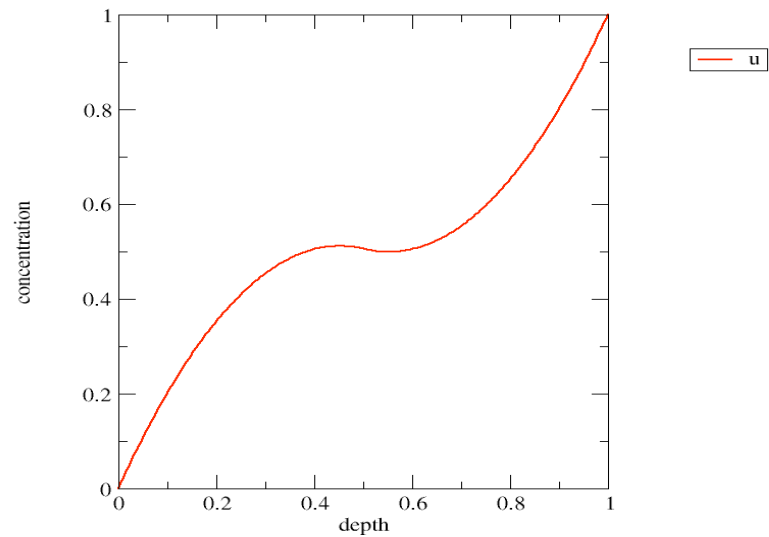


Output potential plot

Ex. 1(b): 1-D Poisson Eq.



Input: step-wise charge profile



Expected output: potential profile

Ex. 2(a): 2-D Poisson Eq.

Prophet

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Files: poisson2d

```

Input file:
# poisson2d
#
#filename: "poisson2d.pf"
#create dbase entry for sysvar u
dbase createlist name=library/physics/silicon/u
dbase prefix=library/physics/silicon/u
dbase create name=dirichlet.contact0 rval=0.0
dbase create name=dirichlet.contact1 rval=1.0
dbase create name=scale rval=1.0
dbase create name=Dix rval=1
dbase prefix=""

#define system poisson
system name=poisson
+ sysvars=u
+ term0=box div lapflux(u|u)@(silicon)
+ term1=nodal.copy(c|u)@(silicon)
+ term2=dirichlet.default_dirichlet(0|u)@(silicon/contact0,silicon/contact1)

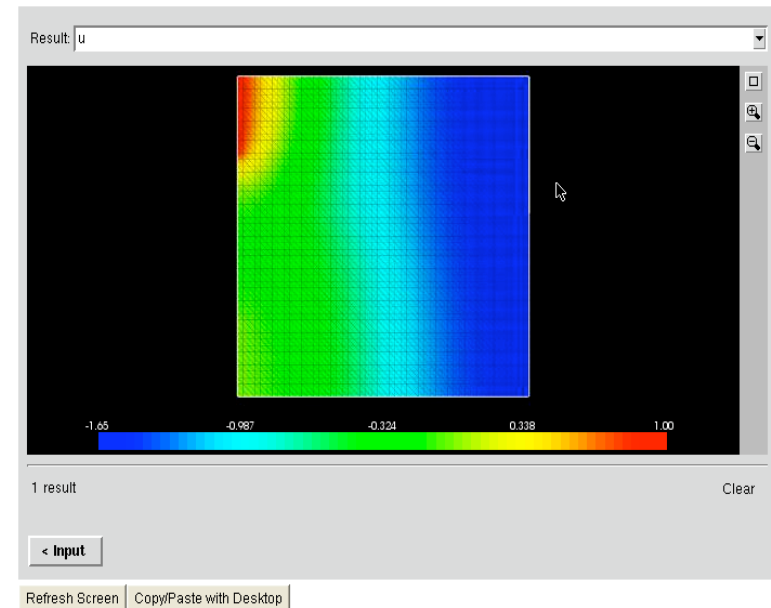
#define simulation mesh and boundaries
grid xloc=0,1 xdel=0.02 yloc=0,1 ydel=0.02 dim=2
boundary xmin=0 xmax=0 ymin=0 ymax=0.25 name=contact0
boundary xmin=0 xmax=0 ymin=0.75 ymax=1 name=contact1

#define fixed charge
field set=c1 val=5
field set=c2 val=-10 xrange=[0:0.5] yrange=[0:0.5]
    
```

Input script: poisson2d.pf

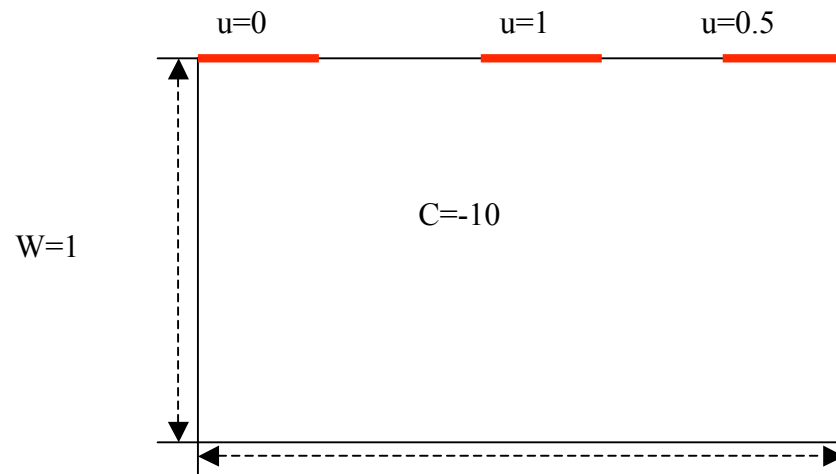
Prophet

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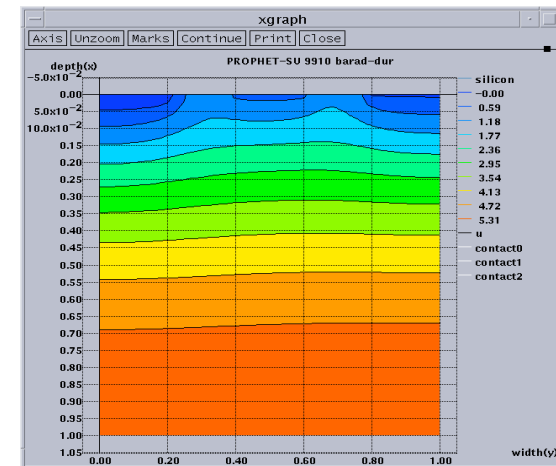


Output: 2d potential profile

Ex. 2(b): 2-D Poisson Eq.



- define structure and C profile using grid, boundary, and field commands
- specify Dirichlet boundary value using dbase
- minor change in system: add interface “silicon/contact2” at the end of term2



Expected 2D potential profile