Nano-Scale Device Simulations Using PROPHET Lab. Exercise II

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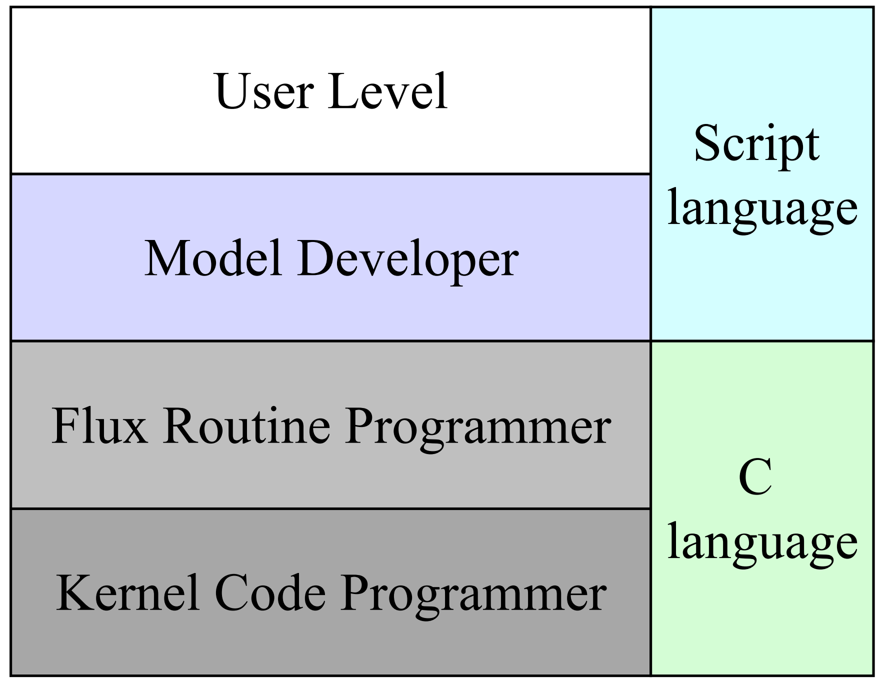
PROPHET Roadmap

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



Ex. 3(a): Modified Diffusion Eq.

Run the two given scripts “diffusion1.pf” and “diffusion2.pf” which solve for the two diffusion equations, respectively:

$$\partial n(\vec{r},t)/\partial t - D\nabla \cdot \nabla n(\vec{r},t) = 0$$

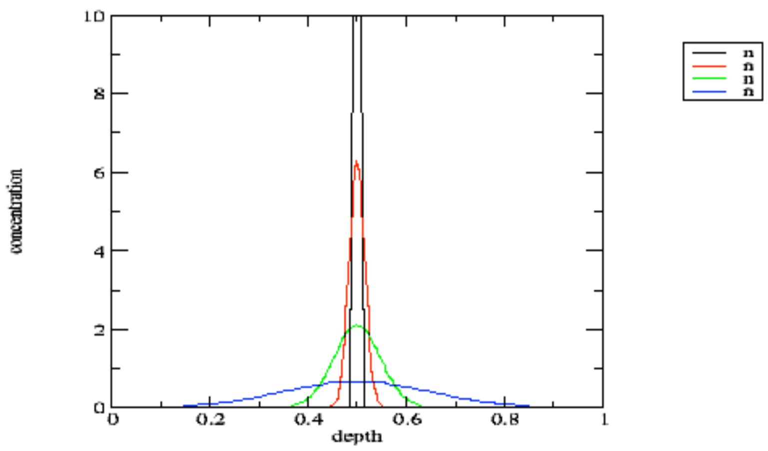
$$\partial n(\vec{r},t)/\partial t - D\nabla \cdot \nabla \sqrt{n(\vec{r},t)} = 0$$

and examine the difference in SYSTEM definitions and the simulated results. Change the diffusion coefficient Dix to see its impact on output.

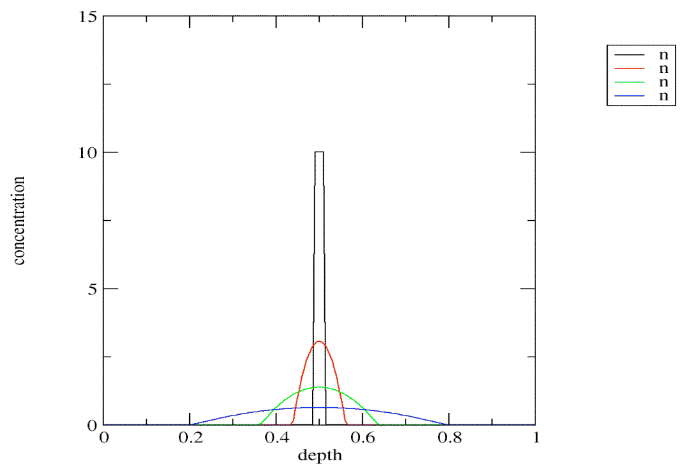
Ex. 3(b): Modified Diffusion Eq.

Modify the script to build a PDE system for equation:

$$\partial n(\vec{r},t)/\partial t - D\nabla \cdot \nabla n(\vec{r},t)^2 = 0$$



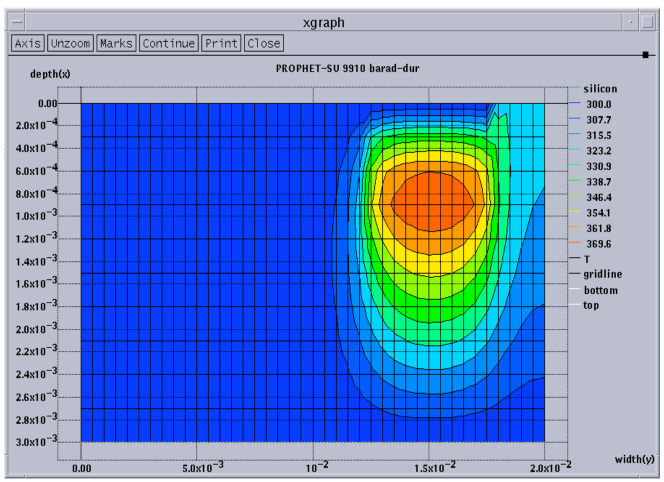
Normal diffusion process



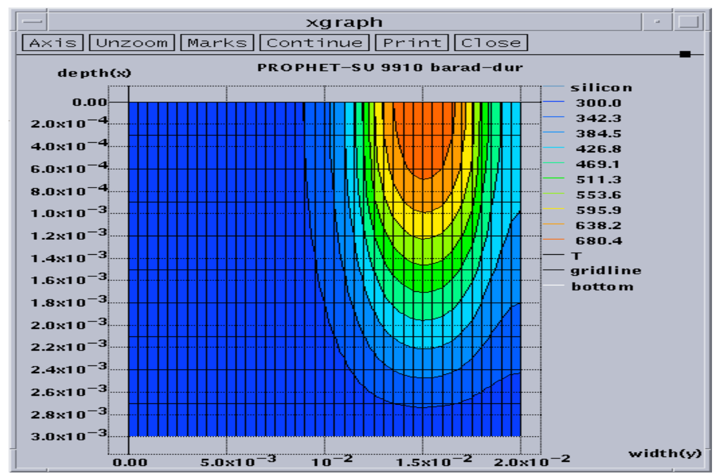
Modified diffusion process

Ex. 4: Thermal Diffusion with B.C.

When solving thermal transport equation, the thermal boundary conditions play an important role in determining the temperature distribution. In the given script “diffusion3.pf”, modify the 2D structure by removing the top thermal contact and examine the difference in temperature profile.



With top heat sink



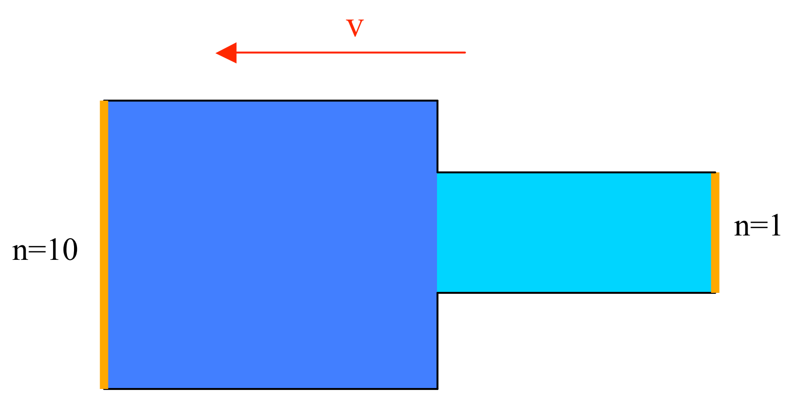
Without top heat sink

Ex. 5: Drift-Diffusion-Reaction

Consider a cell composed of a cell body to which is attached a tubular "process", e.g. the axon of a neuron. Suppose some substance n, e.g. a metabolite, is generated in the cell body and transport along the process under the combined drift-diffusion-reaction process. Modify the given script "iontransport1.pf" to simulate concentration profile at different reaction rate.

Equation: $$\partial n / \partial t = D\nabla^2 n - \vec{v} \cdot \nabla n - \alpha n$$

Cell structure:



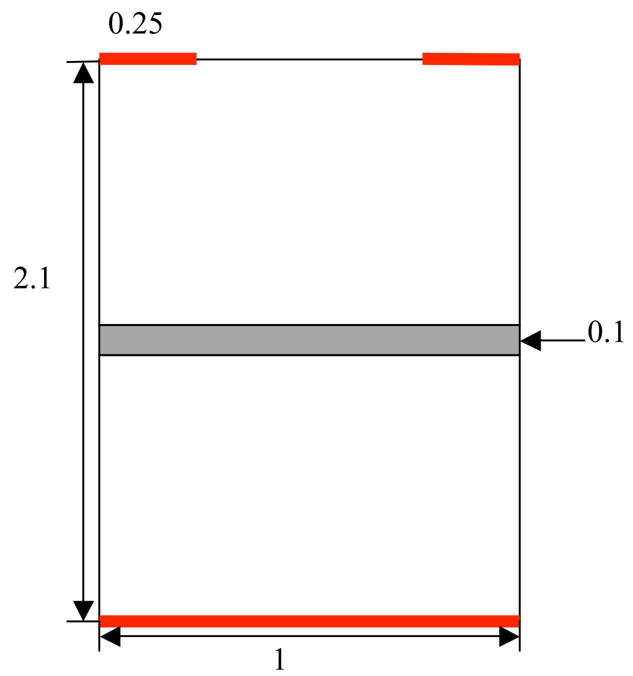
Ex. 6: optical & acoustic phonon system

Develop a new PROPHET system to solve the following heat transport PDEs:

$$\frac{\partial T_o}{\partial t} = P - \frac{T_o - T_a}{\tau}$$

$$\frac{\partial T_a}{\partial t} = \nabla \bullet \nabla T_a + \frac{T_o - T_a}{\tau}$$

where the two sysvars are optical phonon temperature and acoustic phonon temperature.



Simulated structure.

Ex. 6: Optical & Acoustic Phonon System

Hint: In this exercise, you are required to develop the entire script including the use of SYSTEM/DBASE/GRID/SOLVE commands for the coupled PDEs.

Expected acoustic phonon temperature profile: