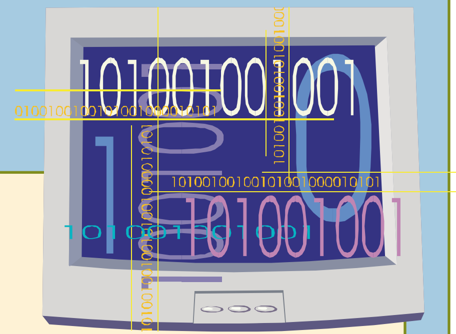
Math Matters

Apply It.



The math behind...
In silico cell models

Technical terms used:
In silico (means “performed in computer”), mathematical model, cell physiology, fluid dynamics, chemical kinetics, transport phenomena, and optimization

Uses and applications:
Cell models can be used: (1) to explore possible pathways for cell pharmacological and genetic manipulation; (2) to predict possible cell responses to a given perturbation; and (3) for education purposes in Cell Biology and Physiology. Moreover, the beauty of cell mathematical models relies on the ease with which they can be altered. That is, a cell model with two opposite assumptions can be formulated, resulting in simulations for multiple scenarios that try to answer the what ifs of the studied cell.

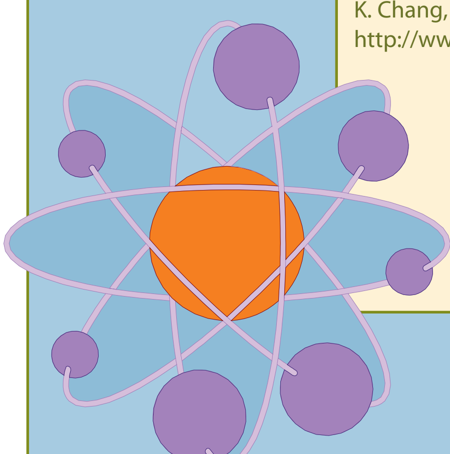
How it works:
First, one has to formulate the cell mathematical model. The model is composed of individual modules (e.g., a model for each transport protein expressed in the studied cell). It includes the kinetics and/or thermodynamics that describe the time- and space-dependent solute movement and solute-solute interactions throughout and around these cells. It is formulated from the molecular to the cellular level, and it can be extended to the tissue level. Second, one has to obtain the model parameters. These parameters are obtained by minimizing the distance between model and in situ, in vitro, or in vivo data reported in the literature. In addition, one could optimize the cell as a function of a desired output. Finally, one uses the model to perform the cell simulations under the desired setting.

Interesting fact:
The 2013 Nobel Prize in Chemistry was granted to three scientists for their in silico simulations to study complex reactions and design new drugs. In this regard, Professor Sven Lidin, Chairman of the 2013 Nobel Committee for Chemistry, said in a press release “Computer simulations have become as informative as the experiments. You still have to do the experiment. But the predictions that theory makes are becoming so much more powerful these days that we can perhaps save ninety percent of the experimenting and concentrate on the ten percent where we know that the most important results will lie.”

References:

M.H. Fogler, Principles and Models of Biological Transport (Springer, New York, ed. 2, 2008).

K. Chang, Without Test Tubes, 3 Win Nobel in Chemistry” (The New York Times, October 7, 2013; http://www.nytimes.com/2013/10/10/science/three-researchers-win-nobel-prize-in-chemistry.html?_r=0).



Submitted by Mónica Nadal-Quirós, University of Puerto Rico, San Juan, Math Matters, Apply it! Contest, February 2015

Society for Industrial and Applied Mathematics
www.siam.org
www.siam.org/careers/matters.php