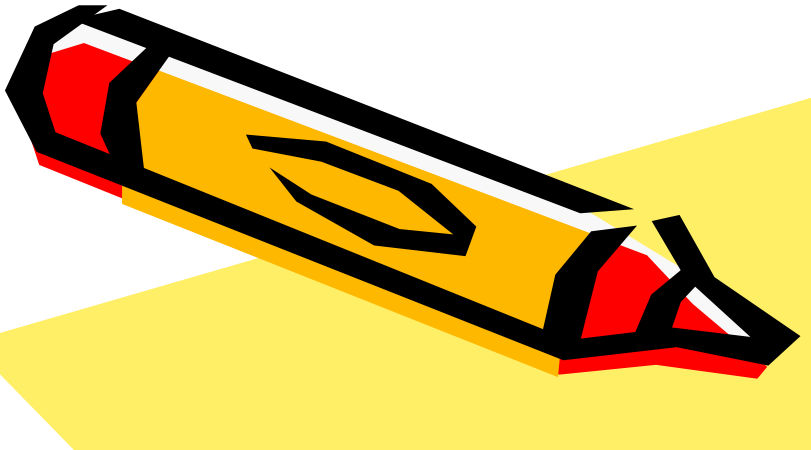


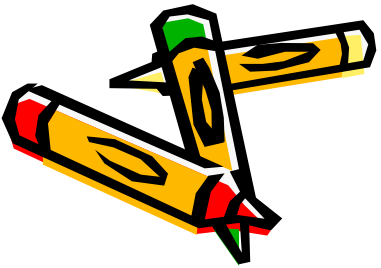
# Virtual Cell

邢锋

2010.11.19

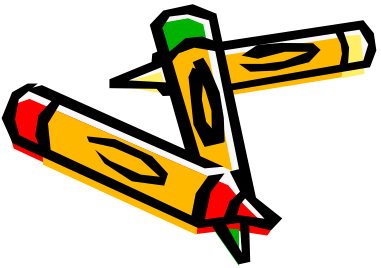
# 内容概览

虚拟细胞简介
软件产生背景及作者信息
软件下载地址及安装方法



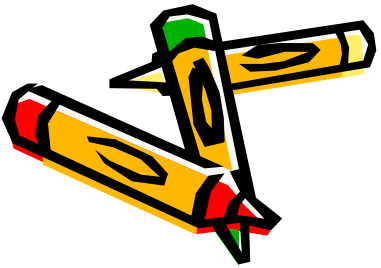
# 虚拟细胞简介

- 虚拟细胞即通过信息学和数学的原理，对细胞的结构和功能进行分析、整合和应用，模拟和再现细胞的生命现象，从而使生物学实验在人工环境里运行。
- 常用的软件：ECell，VCell，JSim
- 网站：http://www.ebi.ac.uk/biomodels-main/，http://www.e-cell.org/ecell/，http://www.nrcam.uchc.edu/，http://nsr.bioeng.washington.edu/jsim/



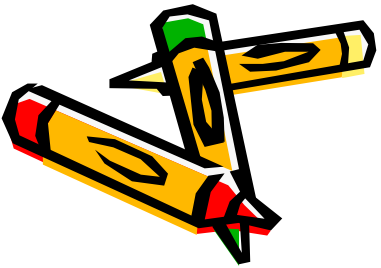
# 虚拟细胞发展

- 细胞生化和遗传机制的模拟：Mendes P；Meyers S
- 第一个虚拟细胞模型：原核细胞能量代谢模型（1997）
- 第二个：美国的真核细胞钙转运模型（1999）
- 美国的基于猪蛔虫精子游动细胞模型（2004）



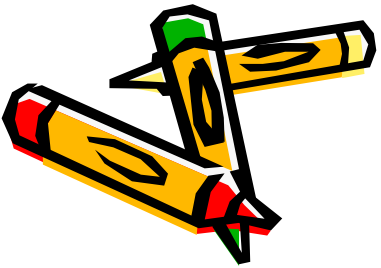
# 虚拟细胞研究意义

- 辅助科学实验
- 疾病诊断与防治
- 应用于教学及社会生活方面



# What is Virtual cell?

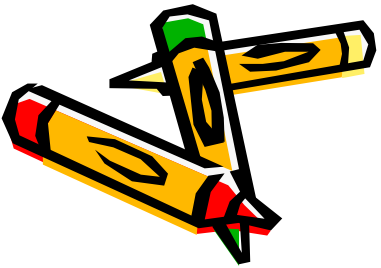
- The **Virtual cell (or Vcell)** is a software developed by **NRCAM**.
- This software platform has been designed to model cell biological processes.
- Vcell consists of a biological and mathematical framework. Scientists can create biological models from which the software will automatically generate mathematical code needed to run simulation.
- This software consists of **3 key components**, named **BioModel, Geometry** and **Math Model** documents, each of which is saved independently, althogh they do reference each other.
- Models can be reused, updated and published so they are available to the scientific community or they can be shared privately amongst collaborating groups.



# 产生背景及发展

(1)1997年12月，James Schaff，Boris Slepchenko，Loew等人在“A General Computational Framework for Modeling Cellular Structure and Function”中提到了“Virtual Cell”的概念，并用Virtual Cell模拟了IP3对钙离子的调控作用，这是第一个用Virtual Cell做的虚拟细胞模型

(2)1999年James等人发表第一个公开的虚拟细胞模型，2000与2001年各有两个公开模型发表，后面发表的模型越来越多，现在已有数十个公开模型发表

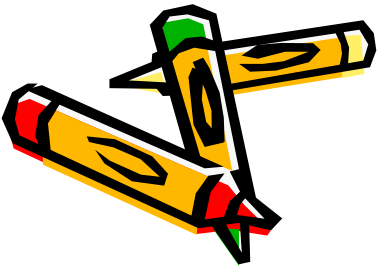


# Virtual Cell现状

- 它作为 NRCAM 在 NIH 中接受 NNCR 的资助
- Virtual Cell团队的名字为*CCAM*，坐落在康涅狄格健康研究中心大学
- 团队拥有一系列先进的显微成像设备

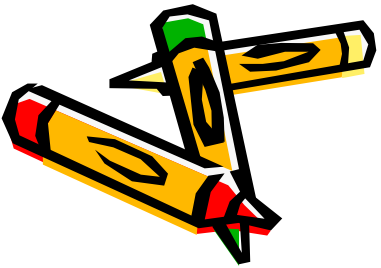
# 网站的相关介绍

- http://www.nrcam.uchc.edu/index.html
- 七个模块：Home，Run VCell Software，Technical Documents，Software Architecture，Publications，Calendar，CCAM



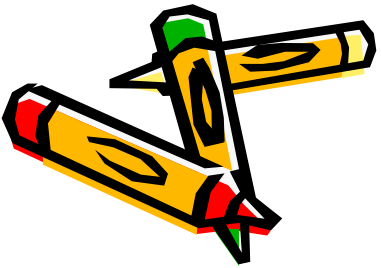
# 作者信息

- Director：Les Loew
  Email:les@volt.uchc.edu
- Lead Developer：Jim Schaff
- Mathematician：Boris Splepchenko
- Database Administrator：Frank Morgan
- Systems Administrator：Ion Moraru



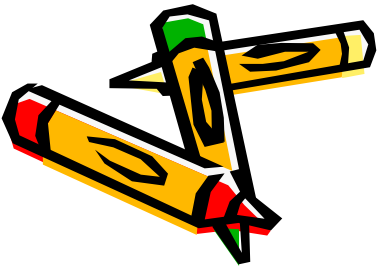
# 软件下载与安装

- 软件运行需要java Runtime Enviroment (JRE1.5 or later)，in Technical Documents
- 注册，使用Virtual Cell必须进行注册
- 安装JRE后，在Run VCell Software中点击Run VCell 4.7或Run VCell 4.8 Beta可以下载并直接运行，输入用户名之后即可运行

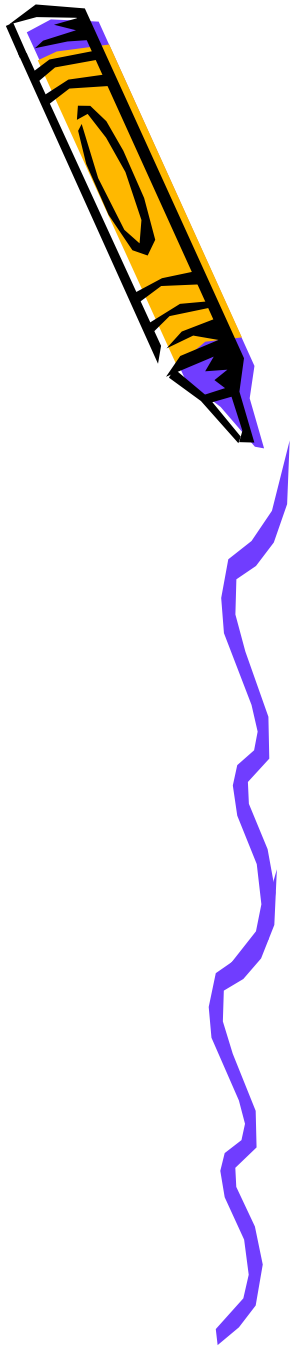


# 文件格式

- 输入输出格式支持XML，level1和level2的SBML，VCML；其中level1的SBML不支持随机模拟过程
- 另外支持Matlab中的m文件的输入和输出，m文件只支持确定性模拟过程，不支持随机模拟过程



# Creating Biomodel



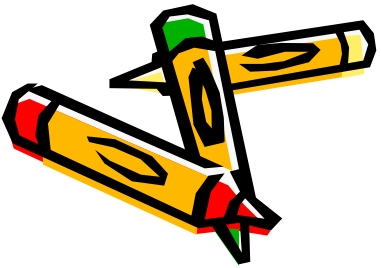
Defining compartments

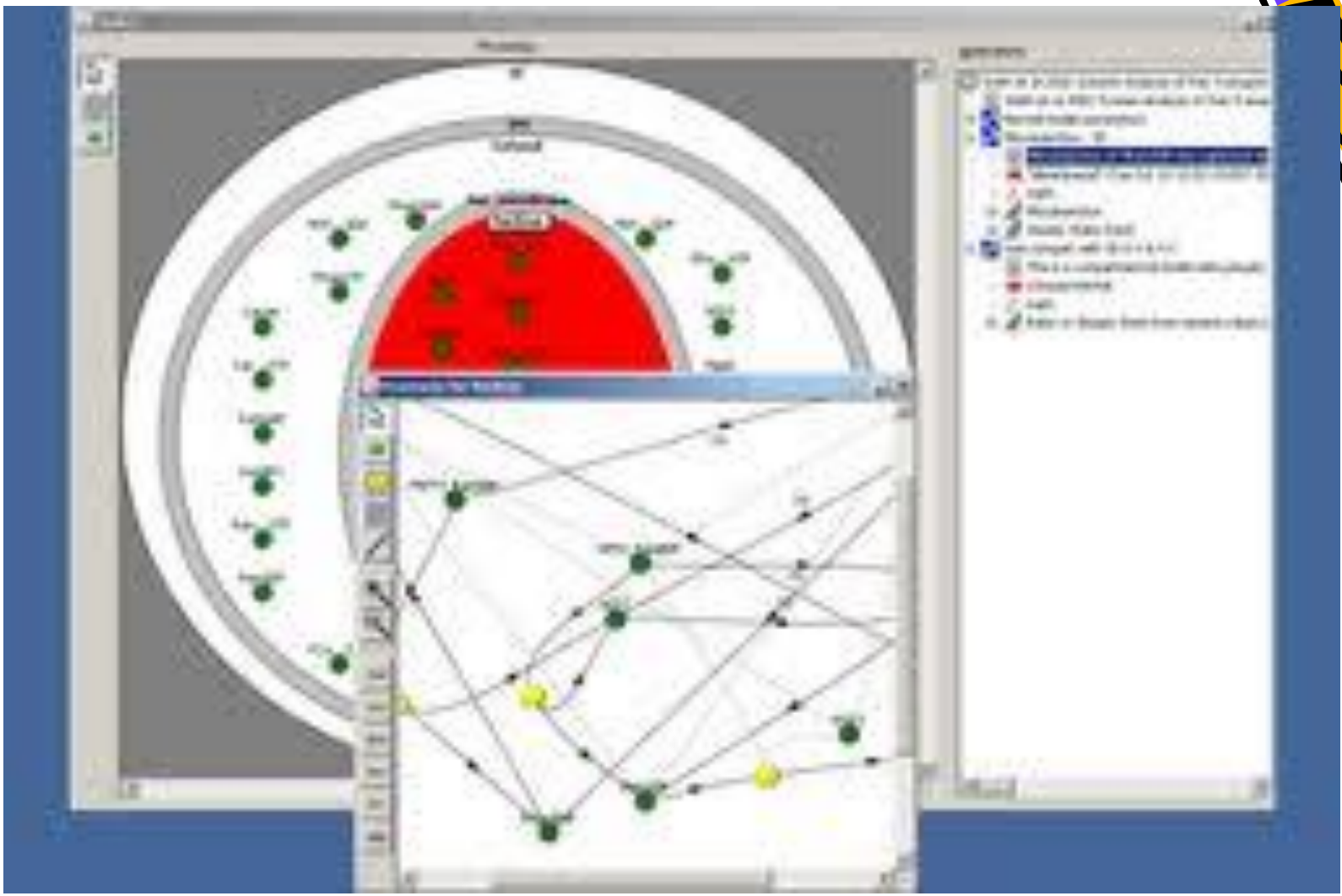
↓

Creating Species

↓

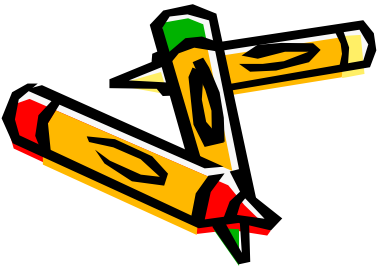
Defining Reactions





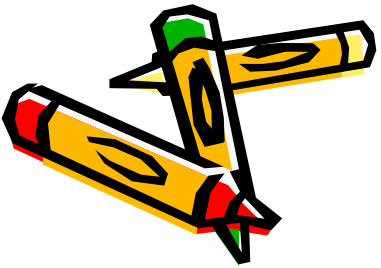
# Creating Application

- Structure Mapping between Model and Geometry.
- Define Initial condition of the system.
- Reaction Mapping.
- We can view the software generated math code describing our model and equations used in simulations.
- Simulation results.



# How to View Virtual Cell Published Models

- Login to the Virtual Cell.
- Go to File>Open>BioModel>Shared Models
- In the 'BioModel Database' pane, find the name of the VC User published model account you are looking for; expand that User's set of public models (see screenshot).
- Double click the model you are interested in viewing.
- If you wish to modify the model or run new simulations, you may copy it into your VC Workspace under your own User account.



# 谢谢