Computational Science Skills

- Computational science provides skills needed in the present and future workforce
  - Understanding of modeling techniques that are used in research and business
  - Data management skills
  - Analytical skills
  - Teamwork skills
  - Communications skills
- Inquiry-based education approach engages students in learning
Acquiring the Appropriate Skills

• Begin with basic modeling skills
  – What is a model?
    • Models of physical systems
    • Models of social systems
  – How do you create a model?
    • Understanding cause and effect
    • Representing the relationships in mathematical terms
  – How do you implement the model on the computer
  – How do you know if the model is “right”
Steps Toward Competency

• Investigate how models have been used to gain insights about complex systems
  – Observe and manipulate built models on personal computers
• Use modeling tools to add new components to existing models
• Build new models of interesting systems
• Use the model to explore the system
• Present results in writing and orally
Progression of Technical Skills

• Using modeling tools on a personal computer
• Learning programming skills
• Advancing applied math skills
• Applying skills to the student’s academic major
  – Starting with simple models on personal computers
  – Expanding to large-scale applications on supercomputers
Integrating Materials into the Curriculum

• Model competencies

• http://hpcuniversity.org/educators/competencies/
Goals for the Sessions

• Demonstrate the pedagogy for computational science education

• Progression of possible activities
  – Using complete models to demonstrate principles
  – Running models to gain insights into system behavior
  – Modifying models to relax assumptions
  – Building new models
What We Will Cover

- Introduce materials and models that can be incorporated for classroom use
- Introduce simple tools that can be used to build and demonstrate modeling techniques
- Provide a list of resources you can explore in detail later
Reference Materials

- [https://www.osc.edu/~sgordon](https://www.osc.edu/~sgordon)
  - Choose Workshop Materials
  - Then Links to other materials
Simple Models with Excel

• Open datasets folder
• Open simplepopulation.xlsx
  – Principle – HAVE = HAD + Change
• Open SystemDynamics.xlsx
  – Principle – adding limits to the system
• Open saltdiffusion.xlsx
  – Principle – “I am the average of my neighbors”
More Examples

• Examples from several of the tools we will be using in this workshop along with lesson plans

Systems Models

• There are several systems modeling packages that can provide similar learning experiences
• Vensim
  – Free education version
  – Graphical users interface to modeling
• Open bunnycomparison.mdl
Social Network Analysis

• Social media allows the connection of billions of people across the globe

• Social network analysis examines and analyzed those connections
  – Email exchanges
  – Blog posts
  – Twitter
  – Wikis, etc.
Analyzing Social Media

• Behavior patterns on many issues
  – Who are the key leaders?
  – What are the key questions?
  – How does the discussion change over time?
  – Are there significant subgroups?
  – What are the strengths of the relationships?
Analysis Tools

• NodeXL
  – Addin to Microsoft Excel
  – Companion book with many examples
    • “Analyzing Social Media Networks with NodeXL”
      Hansen, Schneiderman, and Smith

• Extensions to the R Statistical Package
• NetworkX library for python and Sage
• Netminer
Scale of Analysis

• For instruction – PC tools ok
• PCs will not work for very large datasets
• Need tools ported to supercomputers
• SDSC Boot Camp on graph analytics
  – http://www.sdsc.edu/services/data_science/graph_analytics.html
NodeXL Overview

• Open NodeXL Template
• NodeXL Menu
  – Import from several social media sites
  – Tools to create and manipulate a graph
  – Uses other Excel features to allow for further data analysis
• Simple example for today to demonstrate some features
Senate Voting 2007

- Dataset showing US Senate voting records and degree of agreement on voting
- Open senateraw.xls
Building a Simple Model with Vensim

• Let’s now build a simple model of a rabbit population

• From the Start Menu, choose Vensim
  – Choose File New from the menu, 30 for final timestep, 0.125 as the increment, Year for time units

• We are going to add items to the sketch that represent different components of the a simple population model
Some Sketch Tools

- Auxiliary Variable (constant)
- Box Variable (Level)
- Arrow (connects cause and effect)
- Rate
Add to Your Sketch

• Box variable – label as Rabbit Population
  – Click on the tool, drag it to the open area and drop it

• Rate variable
  – Click on tool; click 2 inches to the left of Rabbit Population then click inside of the Box; name it Births
  – Click in the box and then 2 inches to the right – name it deaths

• Note that the diagram represents adding to the population with births and decreasing the population with deaths
More to Add

• Auxiliary variable
  – birth rate (under births)
  – Average lifetime (under deaths)

• Connect the components with the arrow tool
  – Birth rate to births
  – Average lifetime to deaths
  – Population to births
  – Population to deaths

• Make pull on the circle in the last two to get a curved arrow – just for aesthetics

• Save it
The Sketch and the Model

• The logic of the model is in the sketch
  – What does it show?
  – What is left out?

• Now must enter the equations
  – Click on the equations tool (second from right)
  – Unidentified items turn black

• Click on Births
  – Fill in by clicking on the variables and operators
    • Births*Rabbit Population
    • Units – type in rabbits/year
More Model

• Rabbit Population
  – Births – deaths (unit rabbits)
  – Initial value 1000

• Rest
  – Average lifetime = 8 (years)
  – Birth rate = 0.125 (fraction/year)
  – Deaths = rabbit population/average lifetime

• Check the model
  – Model Check Model
  – Model Check Units
Run the Model

• Create the label for the run – equilibrium
• Hit enter or click on the first runner
• To see outcomes
  – Click on a variable then a tool on the side
  – Try it with the graph for Rabbit Population
  – Why did it come out as a constant?
• Change the model
  – Title to Exponential Growth
  – Click on SyntheSim (second runner)
  – Drag birth rate to 0.2
  – Click stop
  – Look at graph
Adding Visualization Tools

- Click on View and choose New
- Insert custom graph
  - Control panel
  - Choose graph
  - Add Name and Title
  - X Axis – (Sel) Time
  - Variable (Sel) Rabbit population
- Drag I/O Object to Pallet
- Output custom graph – choose Rabbit population
Add Slider Bars

• I/O Object
  – Input slider
  – Make one for average lifetime

• Run model interactively

• Can use slider bar and see the impacts
Explore Other Built Models

- http://www.shodor.org/talks-new/vensim/
Not So Secret Agent

• What is an agent?
  – An autonomous entity that acts according to a set of rules or constraints
  – Multiple agents are involved in complex systems, each acting in a particular way
  – Agents that “meet” then interact to produce another set of outcomes
  – The resulting outcomes are often different than one would expect due to the complexity of the interactions
  – Most agent-based models introduce the idea of randomness in the interaction rules – i.e. Monte Carlo simulations
Some Modeling Conveniences

• Agents can act both in space and in time
  – Explicit spatial movement is often important to accurately represent some phenomena
  – More difficult to do with other approaches
  – More realistic representations of spatial phenomena are possible
Some Examples

• Spatially explicit models of the spread of disease
• Growth of urban areas
• Supply chain optimization
• Human cell and immune system models
• Biochemical processes
• Consumer behavior and economics models
Tools

- AgentSheets
- Netlogo
- StarLogo
- Repast (with a supercomputer version)
- Swarm
Let’s Demonstrate

• Open AgentSheets
  – File Open Project
  – Work your way to the Datasets Folder
  – Open Forest Fire

• Opens several windows
  – Worksheet – graphical representation of the space being modeled and the agents in that space
  – Simulation properties – default settings for important variables
  – Gallery – Agents used in this simulation
Running the Model

• Click on the finger in the pallet on the Worksheet window then a tree and Run
  – Observe the behavior – what is the result?
  – Click Stop then Reset
  – Now change the burnprob on Simulation Properties to 5.0
  – How do the results compare?
Agents and Behavior

• Agents can have several states
  – E.G. Tree – green, on fire, burnt over
  – Each state has an editable depiction

• Right click on the tree or click the tree and use the Gallery – Edit Behavior
  – Simple graphical programming environment
  – Click on red border for top component then Explain
  – Notice the other changes of state which produce a change in the agent Tree
Changing the Model

• Let’s suppose that the forest we are working in is most prone to major fires when there are strong winds from a particular direction – E.G. California Santa Anna winds

• How would we change the agent behavior to reflect this idea?
Modifying an Existing Model

• Open Access Fire
  – Same as current model
  – Let’s add some directional information by changing the behavior of the tree
  – Right click on the tree – Edit Behavior
  – Change the reaction of the tree to only seeing trees from the West.
  – Change the burnprob name to burnprobw
  – Edit the simulation properties to change burnpro to burnprobw and set an initial value
  – Try it out and check the logic
Building a New Model

- Frog and the Princess
Reference Materials

• https://www.osc.edu/~sgordon
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Our reach will forever exceed our grasp, but, in stretching our horizon, we forever improve our world.