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Computational Thinking

ACSC Curriculum Workshop

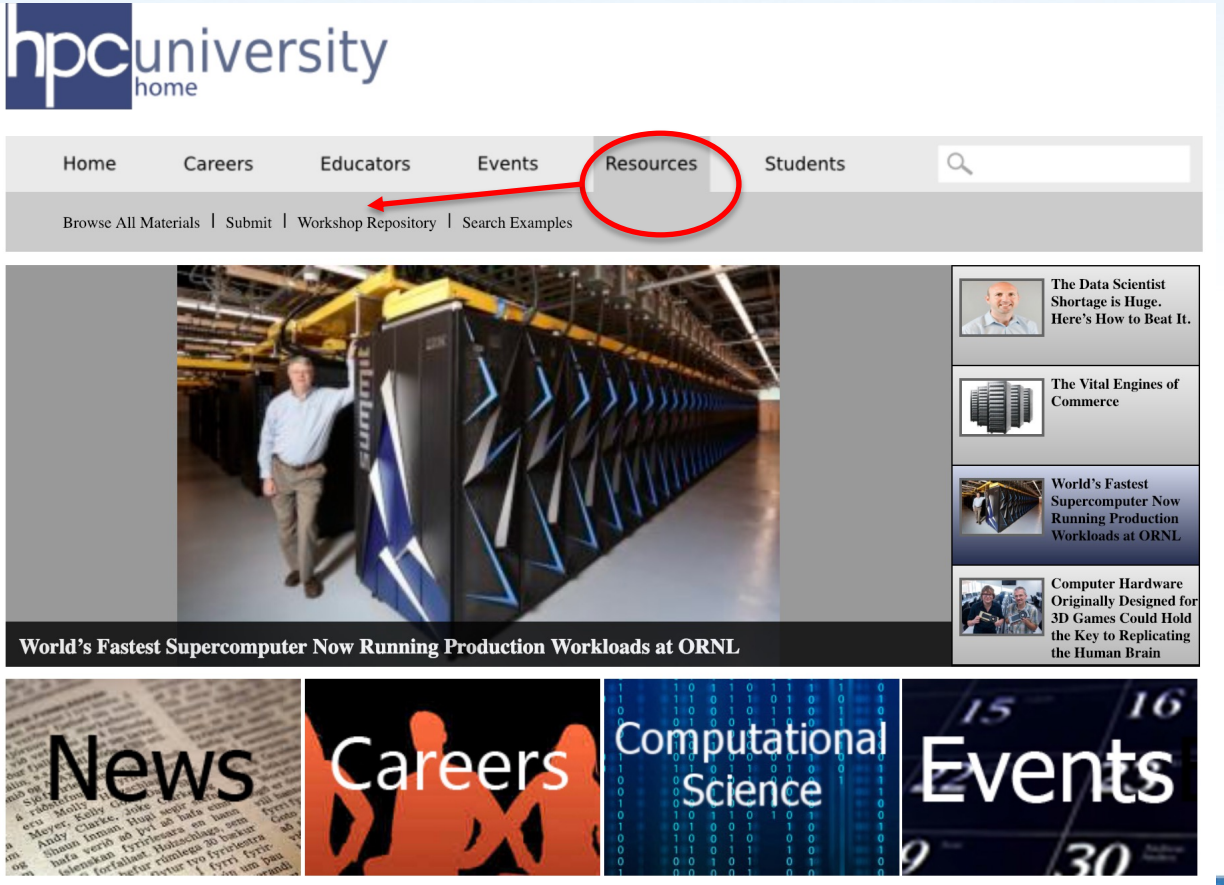
Kate Cahill (kcahill@osc.edu)

XSEDE

Extreme Science and Engineering Discovery Environment

Step 1: Get the presentation slides

http://hpcuniversity.org/trainingMaterials/254/



HPCUniversity.org

- Repository of materials
  - Workshop slides
  - Links to videos
  - Exercises
- Events calendar – conferences, deadlines
- Fellowships, Internships & Job Postings

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 to 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 computational & data science competencies:

http://hpcuniversity.org/educators/competencies/

Goals for this Session

- 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

Scale of Analysis

- For education depending on the size of the data or simulation – laptops OK
- Laptops will not work with larger datasets
- Large scale will require supercomputer access

Social Network Analysis

- Social media allows the connection of billions of people across the globe
- Social network analysis examines and analyzes 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?

Large Scale Example

- Six Degrees of Francis Bacon
  - Analysis of 16th – 17th Century social networks
  - Visualization tool built with JSON

http://www.sixdegreesoffrancisbacon.com/?ids=10003747&min_confidence=60&type=network

Analysis Tools

- NodeXL
  - Addon to Microsoft Excel
    - Social Media Research Foundation https://www.smrfoundation.org/
- Network package for R
- NetworkX package for python
- Other tools:
  - http://professorkhan.com/network-analysis-tools-for-data-visualization/

Step 2: Reference Materials

- https://www.osc.edu/~kcahill/XSEDE_Workshop_materials

- **Get data sets**

Presentation on formal programs in computational science
http://www.osc.edu/~sgordon/workshops/Comp_science_overview.pdf

Example Datasets

Description	Link
Package of datasets in zip file format	https://www.osc.edu/sites/osc.edu/files/staff_files/sgordon/workshop_data_0.zip

Starting with Simple Models and Tools

- Can use simple models to illustrate modeling principles and definitions
- Models of change in space and/or time:

HAVE = HAD + CHANGE

- Which phenomena employ this basic concept?

Simple Models with Excel

- Open datasets folder
- Open simplepopulation.xlsx
  - Principle – HAVE=HAD+Change
- 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
- http://www.shodor.org/talks-new/

Built Models You Can Use in Classroom

- http://www.shodor.org/interactivate/
- Select Activities - Statistics
  - Choose histogram
  - Ability to examine the impact of categorization on the description of a distribution
- Resources for Computational Modeling
  - https://phet.colorado.edu/
  - Find Shared science instructional modules - PHET

Explore Other Relevant Examples

- Look at sites relevant to your discipline
  - Computational physics
  - Computational chemistry
  - More Shodor examples
  - Engineering
  - Economics
  - And so on

Systems Modeling

- Effective method for analyzing behavior across disciplines
- Simple interactions can lead to complex outcomes
- A way to understand behavior through structure
- Focus on interconnectedness of system elements

Reference: *Thinking in Systems* by Donella H. Meadows

Systems Model Tools

- There are several systems modeling packages that can provide similar learning experiences
- iThink; Berkeley Madonna; Stella
- Vensim
  - Free education version
  - Graphical user interface to modeling
- Open bunnycomparison.mdl

Reviewing a Simple Model with Vensim

- Several simple models of a rabbit population
- 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 **bunnies 1**
  - 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 **birf rate 1**
  - Click in the box and then 2 inches to the right – name it **death rate**
- Note that the diagram represents adding to the population with births and decreasing the population with deaths

More to Add

- Auxiliary variable
  - birth rate 0.5
  - Death rate 0.02
- Connect the components with the arrow tool
  - Birf rate to bunnification
  - Death rate to bunnification
  - Bunnies 1 to bunnification
- 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
    - bunnies 1 * birf rate 1 – (bunnies 1 * death rate)

More Model

- Constants
  - Bunnies 1 = Initial value 2
  - Death rate = 0.02
  - Birf rate 1 = 0.5

More Vensim Examples

- Other examples
  - Advanced SIR
  - Pharma model
- Can save runs under different names
- Compare runs on the same graph
- Interactively change parameters to find a target

Explore Other Built Models

- http://www.shodor.org/talks-new/vensim/

- Vensim model building tutorial video:

http://vensim.com/building-a-simple-vensim-model/

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

- AgentCubes
- Netlogo
- StarLogo
- Repast (with a supercomputer version)
- Swarm

Agent Models Tell A Story

- Should describe the behaviors before model building
- Example of simple disease model
  - Agents: People
  - People are either healthy or sick
  - For a contagious disease, what is the story of the interaction of healthy and sick people?

Story behind model

- Agents with two states
- If they “meet” there is some probability that a healthy person will become sick
- Examine the program syntax

Moving to Supercomputer Scale

- Once students understand the basic principles of a particular type of model – can scale models to run on supercomputers
- Use community codes or science gateways
- Approach the problems in a similar way
  - Make multiple runs to understand system behavior
  - Pose problems that change a finite set of model parameters to answer specific questions

Collaborative Online Courses

Applications of Parallel Computing will be offered in Spring 2022

Prepared lectures, quizzes, and exercises online

Collaborating faculty at local institutions create a local course number and supervise their students

Use XSEDE education allocations

Reference Materials Reminder

- https://www.osc.edu/~kcahill
  - Choose Computational Thinking Workshop Materials
  - This presentation is here:
    - http://hpcuniversity.org/trainingMaterials/254/
- Introduction to Computational Thinking Across the Curriculum
  - 2 day workshops this month!
    - ~~June 15-16: Modeling with Spreadsheets and Web resources~~
    - June 22-23: Systems Modeling
    - June 29-30: Agent-based Modeling
    - Register on the XSEDE Portal

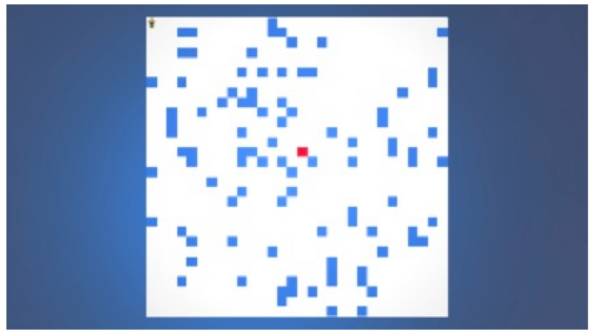

Our reach will forever
exceed our grasp, but,
in stretching our horizon,
we forever improve our world.
XSEDE
Extreme Science and Engineering
Discovery Environment

Mostly hidden Excel Capabilities

- Slider bar
  - Access via Developer menu
  - File/options/customize ribbon
  - Choose All tabs – move Developer and turn it on
- Insert Scroll Bar
- Associate its value with a cell D11
- Value of 50
- Value of D8 is D11/100
- **Close this spreadsheet**

Defining Agent Behavior

- Login to www.agentcubesonline.com
  - Username shodor0
  - Password: sh0d0r1f1c
- Click on AgentCubes logo at top
- Type rpanoff in the search box at bottom
- Choose CLASS_SIR on the bottom



CLASS_SIR
By ncsi-shodor