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Computational Thinking

South Carolina State University Regional Workshop

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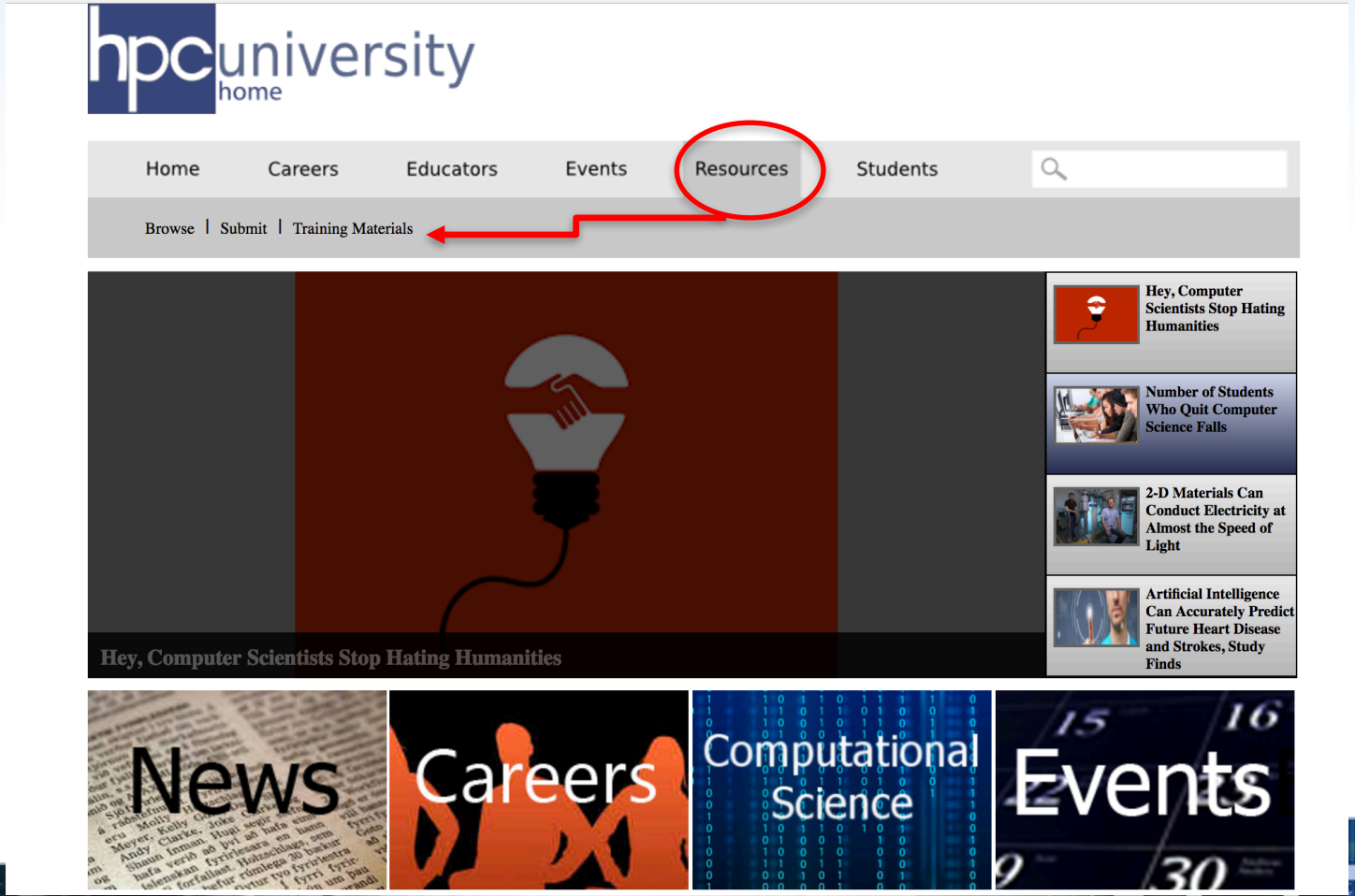
XSEDE

Extreme Science and Engineering Discovery Environment

NSF

Step 1: Get the presentation slides

http://hpcuniversity.org/trainingMaterials/241/



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 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

Step 2: Reference Materials

- https://www.osc.edu/~kcahill
  - Choose Computational Thinking Workshop Materials

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/

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?
- Example – go to datasets folder
- Open SimplePopulation.xls

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

Another simple model

- I am the average of my neighbors
- Representation of a space by a matrix of values representing location and adjacency
  - 2D or 3D
- What is modeled in this way?

More Excel tricks

- Open saltdiffusion.xlsx
  - Note the matrix of numbers
  - Each cell is calculated as the average of its neighbors
  - In D5 insert 50 or = B5
  - Note the change of color
  - Now use the F9 key to incrementally calculate the results
- Turned calculation to manual
- Added formatting to cells based on value

Built Models You Can Use in Classroom

- Go to workshop website referred to earlier
- Scroll down the list to Java Applets
  - Choose histogram
  - Ability to examine the impact of categorization on the description of a distribution
- Now scroll to Resources for Computational Modeling
  - 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 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

Some Sketch Tools

Auxiliary Variable (constant)

Box Variable (Level)

Arrow (connects cause and effect)

Rate

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

- AgentSheets
- 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?

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

Story behind this model

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

Second Example

- Go back and to rpanoff models list
- Select Flat_fire
- Note there are trees with three states
- Story behind this model

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?
  - Clck 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

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

HPCUniversity.org

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

Collaborative Online Courses

Applications of Parallel Computing will be offered in Spring 2018 https://cvw.cac.cornell.edu/apc/default

Prepared lectures, quizzes, and exercises online

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

Use XSEDE education allocations

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Questions and Discussion

Please complete a short on-line survey about this module at http://bit.ly/xsedesurvey . We value your feedback, and will use your feedback to help improve our training offerings.


Our reach will forever
exceed our grasp, but,
in stretching our horizon,
we forever improve our world.
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