

RMACC High Performance Computing Symposium

Computational Thinking Links to Materials

Steven I. Gordon (sgordon@osc.edu)

August 11, 2014

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
Traffic Model Example	https://www.osc.edu/sites/osc.edu/files/staff_files/sgordon/trafficmodel.pdf
MATLAB Models Online	https://compsci.osc.edu/
Algebraic Thinking with Excel	http://shodor.org/talks/ncsi/excel/SimplePopulation.xls
Dynamic Variation with Excel	http://shodor.org/talks/ncsi/excel/Snake2.xls
Iteration and Diffusion with Excel	http://shodor.org/talks/ncsi/excel/SaltDiffusion.xls
Population dynamics with Vensim	http://shodor.org/talks/ncsi/vensim/BunnyComparison.mdl
Disease SIR Model with Vensim	http://shodor.org/talks/ncsi/vensim/AdvancedSIR.mdl
Malaria Model with Vensim	http://shodor.org/talks/ncsi/vensim/MalariaEpidModel.mdl



Falling objects with Vensim	http://shodor.org/talks/ncsi/vensim/FallingRockWithDrag.mdl
Pharmokinetics with Vensim	http://shodor.org/talks/ncsi/vensim/Pharma.mdl
Simple Sick Model with AgentSheets	http://shodor.org/talks/ncsi/agentsheets/SimpleSick.zip
Forest Fire with AgentSheets	http://shodor.org/talks/ncsi/agentsheets/AccessFire.zip
Precipitates from Solution with AgentSheets	http://shodor.org/talks/ncsi/agentsheets/precipitate.zip

Java Applets

Description	Link
Function Flyer for math education	http://www.shodor.org/interactivate/activities/MultiFunctionDataFly/
Histogram	http://www.shodor.org/interactivate/activities/Histogram/
Molecular model of ideal gas	http://www.phy.ntnu.edu.tw/ntnugava/index.php?topic=25
Predator prey	http://www.shodor.org/interactivate/activities/RabbitsAndWolves/
Spread of disease	http://shodor.org/talks/ncsi/agentsheets/SimplesickApplet/index.html
Forest fire	http://shodor.org/talks/ncsi/agentsheets/AccessFireApplet/index.html
Precipitation from solution	http://shodor.org/talks/ncsi/agentsheets/PrecipitateApplet/index.html

Links to XSEDE Resources

Description	Link
-------------	------



XSEDE User Portal	https://www.xsede.org/
Science Gateways	https://www.xsede.org/gateways-listing
Campus Champions	https://www.xsede.org/web/guest/campus-champions
Course training calendar	https://www.xsede.org/web/xup/course-calendar
Online courses	https://www.xsede.org/web/xup/online-training
Getting started (accounts and services)	https://www.xsede.org/using-xsede

Resources for Computational Modeling

Description	Link
National Science Digital Library (NSDL)	http://www.nsdl.org
Biology Workbench	http://mycyberbench.ncsa.illinois.edu/
GridChem	http://www.gridchem.org
Computational Science Education Reference Desk – National Science Digital Library – models with exercises and reviews	http://www.shodor.org/refdesk
HPC University – workshops and pointers to materials	http://hpcuniversity.org/
Computational modules on a variety of topics	http://www.capital.edu/cs-computational-science/
Shared science instructional modules and models	http://phet.colorado.edu/
Computational physics materials	http://www.ucomp.org/
Computational Science and Engineering Online – various chemistry, combustion, and nano-science java tools	http://cse-online.net/
Computational biology for biology educators	http://www.computationalscience.org/cbbe



Computational chemistry for chemistry educators	http://www.computationalscience.org/ccce
Agent based models for economics	http://www2.econ.iastate.edu/tesfatsi/ace.htm
Systems Dynamics Society Proceedings 2013	http://www.systemdynamics.org/conferences/2013/proceed/
MATLAB demos in engineering design	http://gershwin.ens.fr/vdaniel/Doc-Locale/Cours-Mirrored/Methodes-Maths/white/cappl/s0/mlabcappl/mlabcappl.html
Tools, lesson plans, and datasets relating to biological modeling	http://bioquest.org
NASA Aeronautics Models	http://www.grc.nasa.gov/WWW/k-12/aerores.htm
Engineering applets from Virginia Tech	http://www.engapplets.vt.edu/
Large number of physics and mathematics applets	http://www.falstad.com/mathphysics.html
Virtual Physics Laboratory	http://www.phy.ntnu.edu.tw/ntnujava/
Earthquake engineering resources	http://nees.org/education/for-teachers/collegiate-teachers

Digital Humanities and Social Science Resources

Description	Link
ICHASS - University of Illinois	http://www.ichass.illinois.edu/Home/Home.html
Digital Humanities Now	http://digitalhumanitiesnow.org/tag/resource/
Journal of Digital Humanities	http://journalofdigitalhumanities.org/
Alliance of Digital Humanities Organizations	http://adho.org/
dH Commons	http://dhcommons.org/
Association for Computers and the Humanities	http://ach.org/
Digital Social Research	http://www.digitalsocialresearch.net/wordpress/
Humanities and Social Sciences	http://www.hastac.org/



Collaboratory	
Online Guide for Newcomers to Agent Modeling	http://www2.econ.iastate.edu/tesfatsi/abmread.htm
Repast Open Source Agent Modeling	http://repast.sourceforge.net/
Brookings National Agent Based Model	http://www.brookings.edu/about/centers/dynamics/us-abm
Model Library with Advanced Vensim Models	http://models.metasd.com/
Simulation for the Social Scientist	http://cress.soc.surrey.ac.uk/s4ss/links.html
Repast Application Papers	http://repast.sourceforge.net/papers.php
Simulation of Historic Settlement Patterns	http://escholarship.org/uc/item/2zd1t887
Village Ecodynamics Project	http://village.anth.wsu.edu/about

Curriculum Resources

Competencies for an Undergraduate Curriculum

Minor Program in Computational Science Competency/Topic Overview

As part of the creation of an interdisciplinary undergraduate minor program in computational science put into place at a number of Ohio institutions, we formulated a set of competencies to serve as guidance in the creation of courses and course materials in computational science. The competency-based approach allows institutions to design their curriculum in a flexible way by integrating portions of the computational science materials into existing courses, by creating new courses focused on computational science, or doing a combination of the two.

The competencies were created by the participating faculty and then reviewed by a business advisory committee that offered some advice on topic emphasis and breadth. Since that time, a number of courses and instructional modules have been put into place and tested in a variety of instructional formats. In addition, there have been significant changes in computing technology with the advent of multi-core and many-core computational resources. The competencies below reflect the competencies based on these experiences.

Area 1: Simulation and Modeling [+]

Area 2: Programming and Algorithms [+]

Area 3: Differential Equations and Discrete Dynamical Systems [+]

Area 4: Numerical Methods [+]

Area 5: Optimization [+]

Area 6: Parallel Programming [+]

Area 7: Scientific Visualization [+]



Source: <http://hpcuniversity.org/educators/undergradCompetencies/>

Sources of Educational Materials

See <https://www.osc.edu/~sgordon/workshop/materials> - facsimile attached

XSEDE Resources

Getting started guide	https://www.xsede.org/using-xsede
Gateway listing	https://www.xsede.org/gateways-listing
Course calendar	https://www.xsede.org/web/xup/course-calendar
Online training	https://www.xsede.org/web/xup/online-training
User forums	https://www.xsede.org/web/xup/forums
Software search	https://www.xsede.org/web/xup/software

