

Computation in the Classroom: Open Source Physics Resources

Anne J. Cox, Professor of Physics
Eckerd College, St Petersburg, FL

I am delighted to have this opportunity to talk with you about integrating computation in the classroom. The Gordon Research Conference brought together researchers (practitioners) in computational physics and physics education with the goal of getting more computation into the classroom. I will briefly discuss why this is important, examine some of the barriers to this, and demonstrate some of the ways the Open Source Physics project has tried to address these barriers.

Why Computation in Classroom?

- Analytical skills

•Model building develops analytical skills and helps students understand concepts more deeply. Often when my students say the “program isn’t working” or “I don’t know if my program is working right or not” it is because they don’t understand the physics. They haven’t thought about what they expect (if they program a $-k*x^3$ force for example– what do they expect? Why?); At the intro level, if they leave the initial velocity zero and initial position zero, then the spring won’t oscillate.

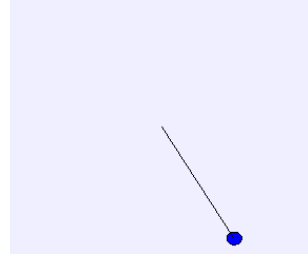
•More realistic problems– a less spherical cow? Computer allows you to solve problems that you don’t have the mathematical tools (or sophistication) to solve– this is why we use it in the first place– students need to see that

•Preparation: Computational physics is an area of research all its own: Theoretical, Experimental, Computational. This is what professional physicists do. We need our undergraduates to be equipped for graduate work.

•Fun– okay, not in the video game sense of fun, but maybe “fun” in that it is “satisfying” when you understand and even more so when you can make the simulation work.

Why Computation in Classroom?

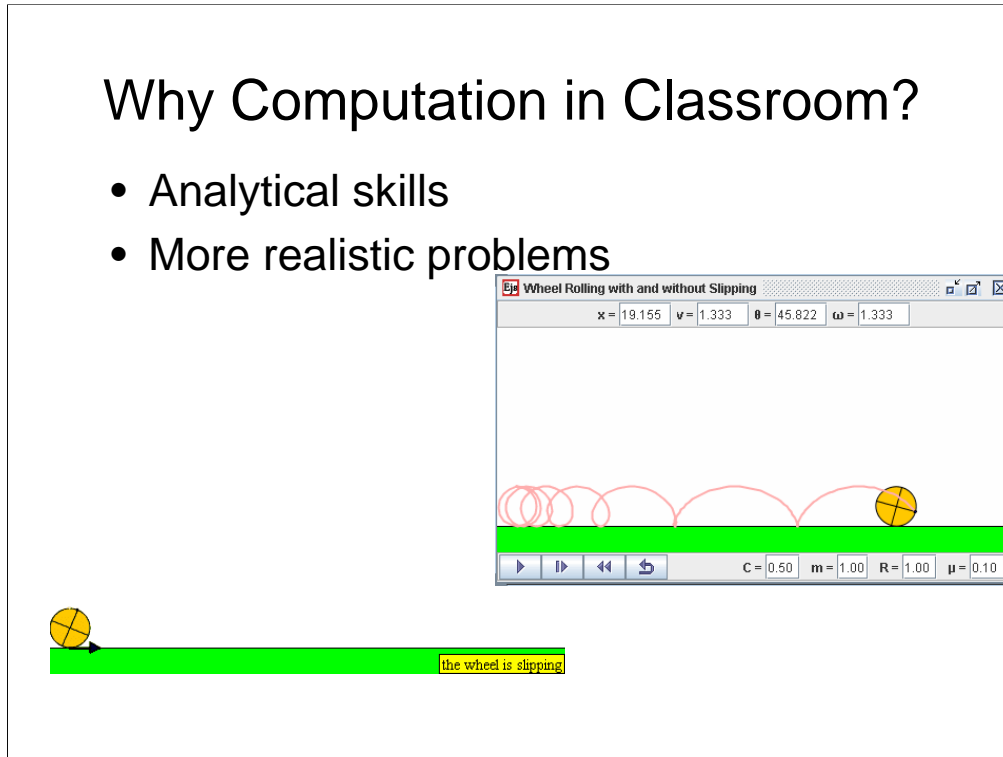
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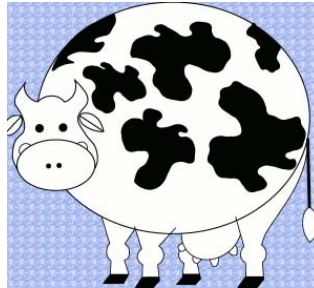
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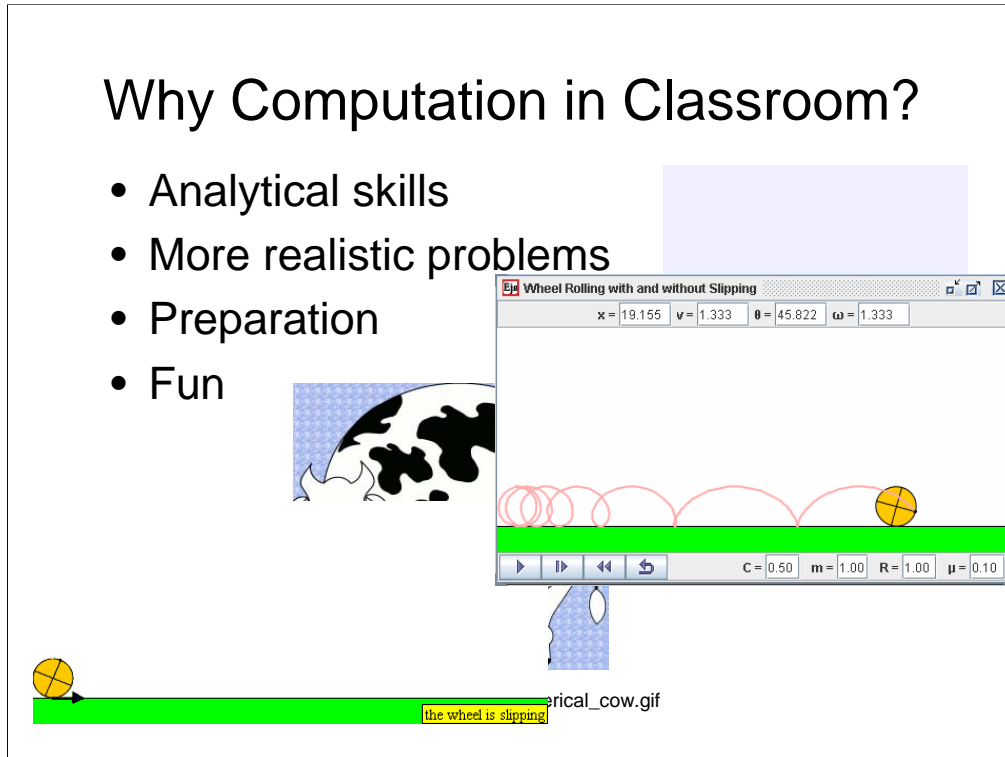


http://en.wikipedia.org/wiki/File:Spherical_cow.gif

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Barriers

- Finding materials
- Pedagogy
- Source availability
- High overhead

- Lots of material out there
- Animations and simulations without associated teaching materials
- Simulation without code: it is a simulation or an animation?
- Spend time teaching computational physics in class.

Finding materials

Lennard-Jones Potential Simulation

- Google, wiki
- Digital library: NSDL and ComPADRE

The screenshot shows a search results page from ComPADRE. The search string is "lennard-jones potential simulation". The results are displayed in a table with columns for "Compadre Portal Results" and "Partner Results". The first result is "1. Lennard-Jones Potential Model [Computer Program]". The description of this result states: "The EJS Lennard-Jones Potential model shows the dynamics of a particle of mass m within this potential. You can drag particle to change its position and you can drag the energy-line to change its total energy. The Lennard-Jones potential function is a reasonably accurate model ...". To the right of the text is a small graph showing a potential energy curve with a red dot representing a particle's position and energy. Below the graph is a "Control Menu" with buttons for "Details", "Post a comment", and "Control Menu". The URL for the document is <http://www.compadre.org/portal/document/ServeFile.cfm?ID=8306&Doc...>. The page also includes a Google logo, a search bar, and navigation links like "Web", "Scholar", and "Books".

Google 145,000 hits (on 3/4/09 at 3 EST): in first 10 you get the wiki entry, several pdfs (to articles in journals you need to subscribe to), a book and two webpages with links to sims

ComPADRE: 9 hits– all programs

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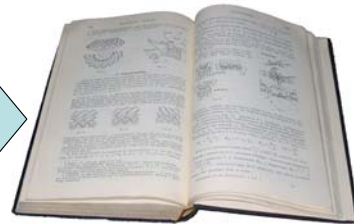
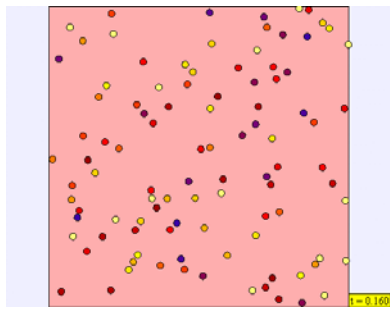
Pedagogy

- Curriculum
- PER

- directed interaction students don't just "play" with sims on their own (if given "play" time, will Txt, etc)
- Inspired by best practices and informed by PER
- STP Project chapter 1 starts explicit connection between Simulation Curriculum AND algorithm.

Connections

- Curriculum
- PER



<http://en.wikipedia.org/wiki/File:Dubbel2.jpg>

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1.4 Some Simple Simulations

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CHAPTER 1. FROM MICROSCOPIC TO MACROSCOPIC BEHAVIOR

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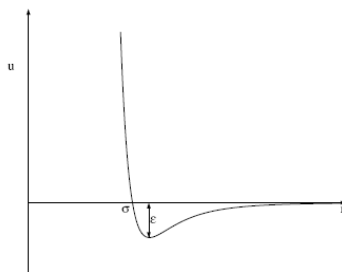


Figure 1.4. Plot of the Lennard-Jones potential $u(r)$ versus the distance between two particles.

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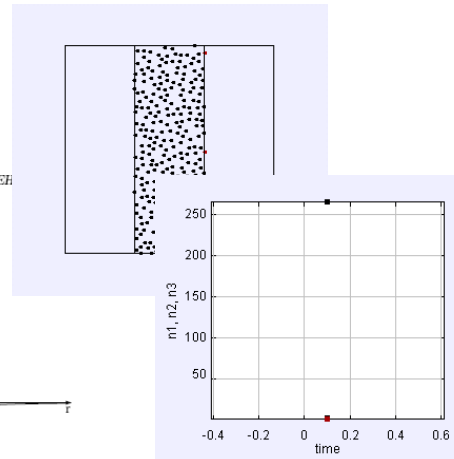
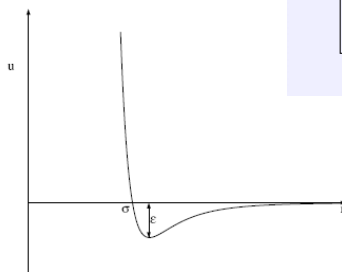
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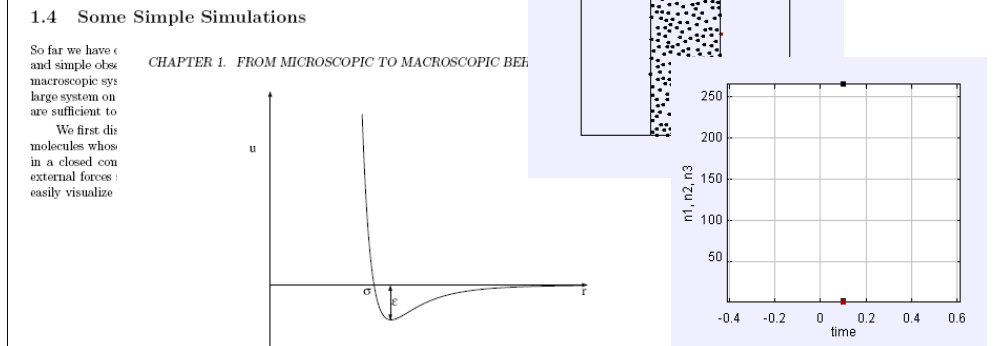
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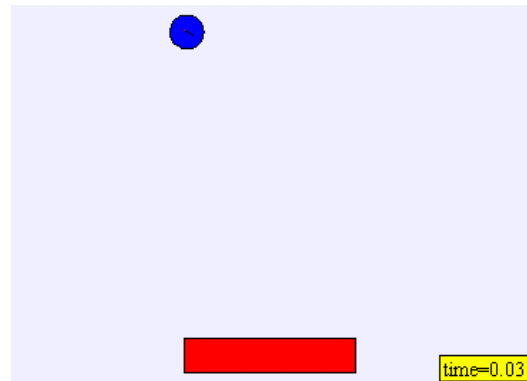
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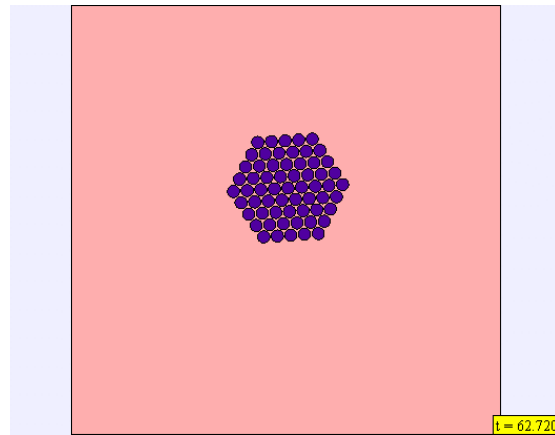
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- Eclipse workspace available for OSP materials.

Animation? Simulation?



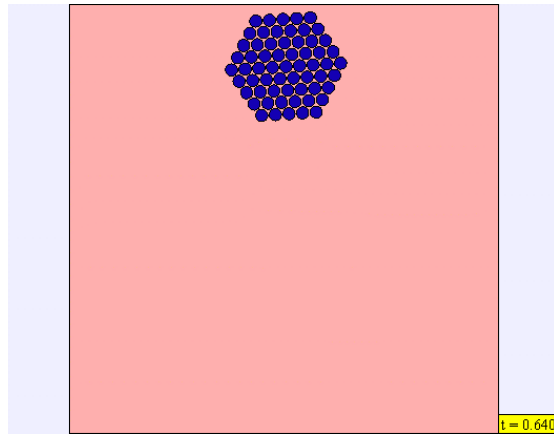
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- Animation? Simulation?
- Open Source Physics (OSP) Project



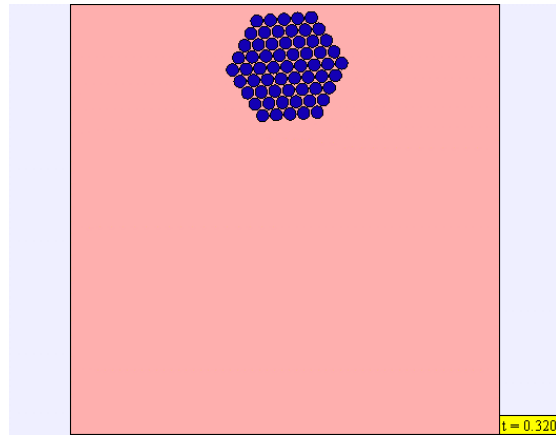
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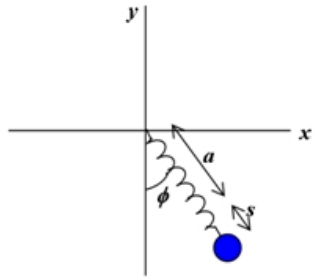
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Easy High Overheads (Ejs)

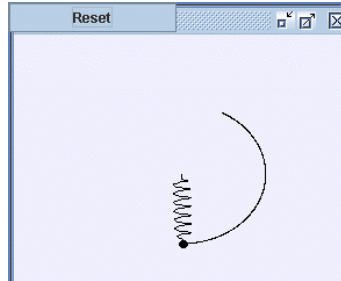
By Francisco Esquembre
Built on OSP code library



Lowers the programming overhead
Feedback from programming

Easy Java Simulations (Ejs)

By Francisco Esquembre
Built on OSP code library



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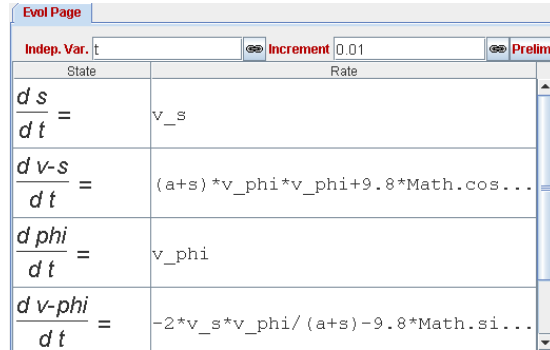
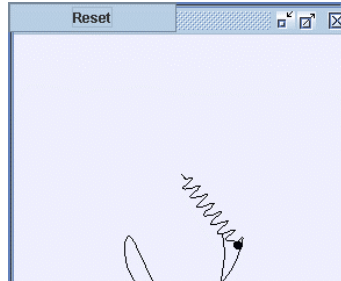
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State	Rate
$\frac{d s}{d t} =$	v_s
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$\frac{d \phi}{d t} =$	v_phi
$\frac{d v-\phi}{d t} =$	0

Lowers the programming overhead
Feedback from programming

Easy Java Simulations (Ejs)

By Francisco Esquembre
Built on OSP code library



State	Rate
$\frac{d s}{d t}$	v_s
$\frac{d v_s}{d t}$	$(a+s)*v_{\phi}+9.8*\text{Math.cos}...$
$\frac{d \phi}{d t}$	v_{ϕ}
$\frac{d v_{\phi}}{d t}$	$-2*v_s*v_{\phi}/(a+s)-9.8*\text{Math.si}...$

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ComPADRE details

- OSP Collection
- Topical
 - STP
 - Quantum Exchange
 - Others coming soon
- uComp- coming soon





- SIMULATIONS
- EJS
- MODELING
- CURRICULUM
- PROGRAMMING
- TOOLS
- BROWSE MATERIALS
- RELATED SITES
- DISCUSSION
- ABOUT OSP

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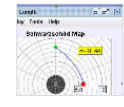
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resource (2)

Subjects	Levels	Resource Types
Astronomy Fundamentals	- Upper Undergraduate Lower Undergraduate	- Simulation Curriculum support

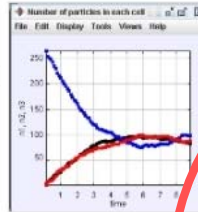
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Computer Program Detail Page

[STP MD Approach To Equilibrium Three Partitions Program](#)

written by Harvey Gould, Jan Tobochnik, Wolfgang Christian, and Anne Cox

The MDApproachToEquilibriumThreePartitions program simulates a system of particles in two dimensions interacting via the Lennard-Jones potential. The program shows the particles in the box as a function of time once the partitions dividing the box into three sections are removed.



MDApproachToEquilibriumThreePartitions is part of a suite of Open Source Physics programs that model aspects of Statistical and Thermal Physics (STP). The program is distributed as a ready-to-run (compiled) Java archive. Double-clicking the stpMDApproachToEquilibriumThreePartitions.jar file will run the program if Java is installed. Additional Open Source Physics programs for Statistical and Thermal Physics are available and can be found by searching ComPADRE for Open Source Physics, STP or Statistical and Thermal Physics.

Please note that this resource requires at least version 1.5 of Java.

<http://www.compadre.org/STP/document/ServeFile.cfm?ID=8159&DocID=8...>

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Related Materials

- References**
- [STP Textbook Chapter 1: From Classical to Statistical Mechanics](#)

- Is Part Of**
- [Statistical and Thermal Physics \(STP\) Application](#)

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Similar Materials

- [STP MD Approach To Equilibrium Two Partitions Program](#)

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Computer Program Detail Page

[Molecular Dynamics Demonstration Model](#)
written by Wolfgang Christian

The EJS Molecular Dynamics Demonstration model is constructed using the Lennard-Jones potential truncated at a distance of 3 molecular diameters. The motion of the molecules is governed by Newton's laws, approximated using the Verlet algorithm with the indicated Time step. For sufficiently small time steps dt, the system's total energy should be approximately conserved. Users can select various initial configurations using the drop down menu.

Ejs Molecular Dynamics Demonstration model was created using the Easy Java Simulations (Ejs) modeling tool. It is distributed as a ready-to-run (compiled) Java archive. Double clicking the js_stp_md_MolecularDynamicsDemo.jar file will run the program if Java is installed. Ejs is a part of the Open Source Physics Project and is designed to make it easier to access, modify, and generate computer models. Additional Ejs models for statistical mechanics are available. They can be found by searching ComPADRE for Open Source Physics, OSP, or Ejs.

Please note that this resource requires at least version 1.5 of Java.

<http://www.compadre.org/STP/1.6/ejs/serenice/mmt/0001&DocID=9...>

[View the source code document attached to this resource.](#)

- **Molecular Dynamics Demonstration Model source code**
 The source code zip archive contains an XML representation of the Molecular Dynamics Demo Model. [Unzip this archive in your Ejs workspace to compile and run](#)

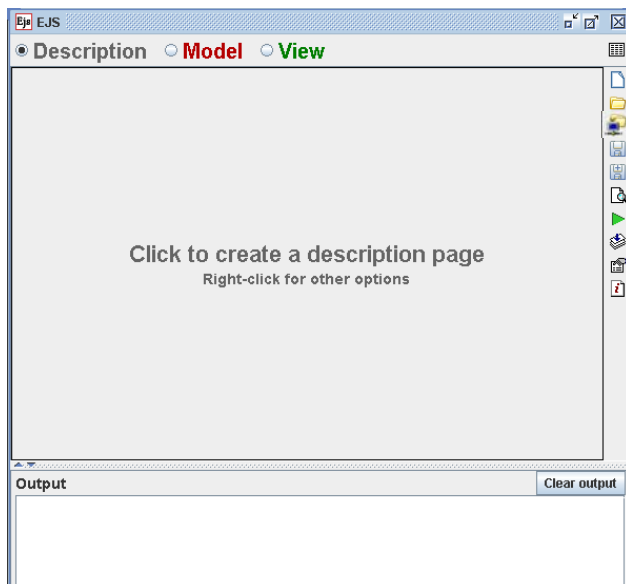
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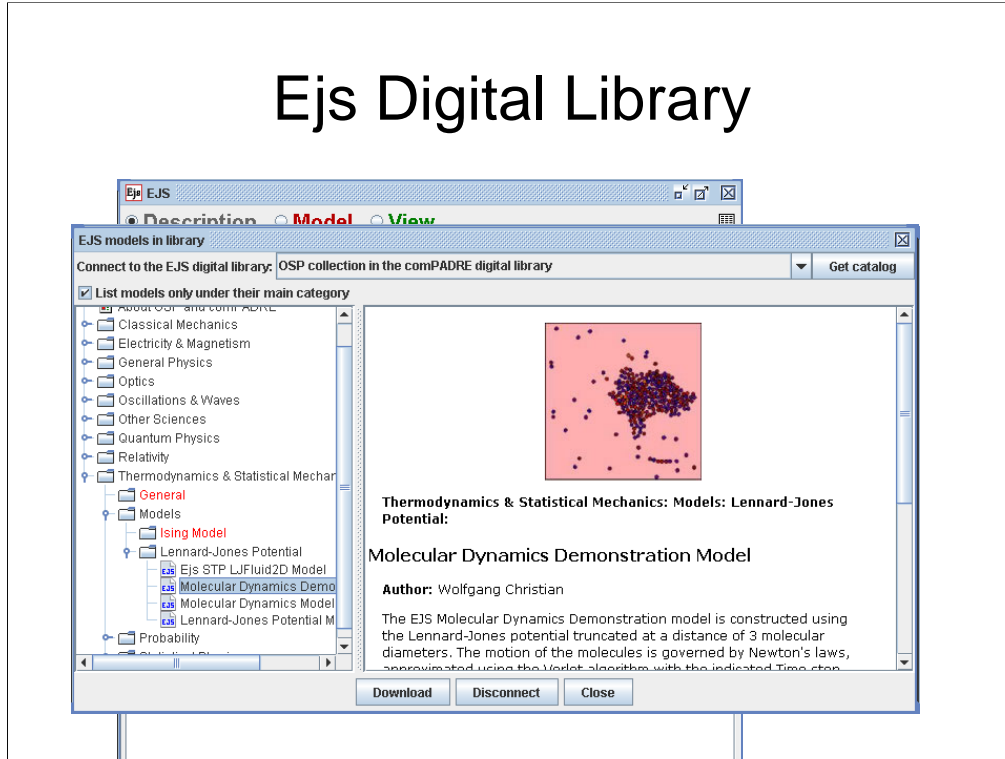
Similar Materials

- [Ejs STP LJFluid2D Model](#)
- [Ejs Hard Disk Gas Model](#)
- [Ejs Hard Sphere Gas Model](#)
- [More...](#)

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Ejs Digital Library



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Mouse over the boxes to the left to find collections designed for your needs.

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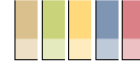
An **NSDL** Pathway

The comPADRE Pathway, a part of the National Science Digital Library, is a growing network of educational resource collections supporting teachers and students in Physics and Astronomy. As a user you may explore collections designed to meet your specific needs and help build the network by recommending resources, commenting on resources, and starting or joining discussions. To recommend a web resource, visit the [Suggest a Resource page](#) on the [Physical Sciences Resource Center](#).

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Filing Cabinet

Your filing cabinet allows you to store and organize resources into folders for later use. For details, please visit the [Filing Cabinet help](#).

Additionally, you may share selected folders with other comPADRE members, or browse other members' [shared folders](#).

Private Folders

[General Resources](#) (0)

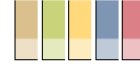
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	Statistical and Thermal Physics (3)
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	└─ Chapter 3: Concepts of Probability (14)
	└─ Chapter 4: The Methodology of Statistical Mechanics (8)
	└─ Chapter 5: Magnetic Systems (10)
	└─ Chapter 6: Noninteracting Particle Systems (6)
	└─ Chapter 7: Chemical Potential and Phase Equilibria (3)
	└─ Chapter 8: Classical Gases and Liquids (6)
	└─ Chapter 9: Critical Phenomena (2)
	Computation in the Classroom: APS March Mtg 09: A6.00004 (7)
	Cari Hall Folders Profile

Acknowledgements



Mario Belloni, Wolfgang Christian, Harvey Gould, Jan Tobochnik, Bill Junkin, Doug Brown



Lyle Barbarto, Bruce Mason, Matt Riggsbee



NSF DUE-0442581.

www.compadre.org/OSP