Water, water everywhere... How can we understand it?

An exploration of water using physical models and computer simulation

Chandler A. Becker, PhD
Material Measurement Laboratory
NIST

16 Mar. 2011

Arctichistorian01, wikimedia commons

Outline

- Goals/Introduction
- Water molecules
- Many water molecules + other stuff
- Too many water molecules
- Resources

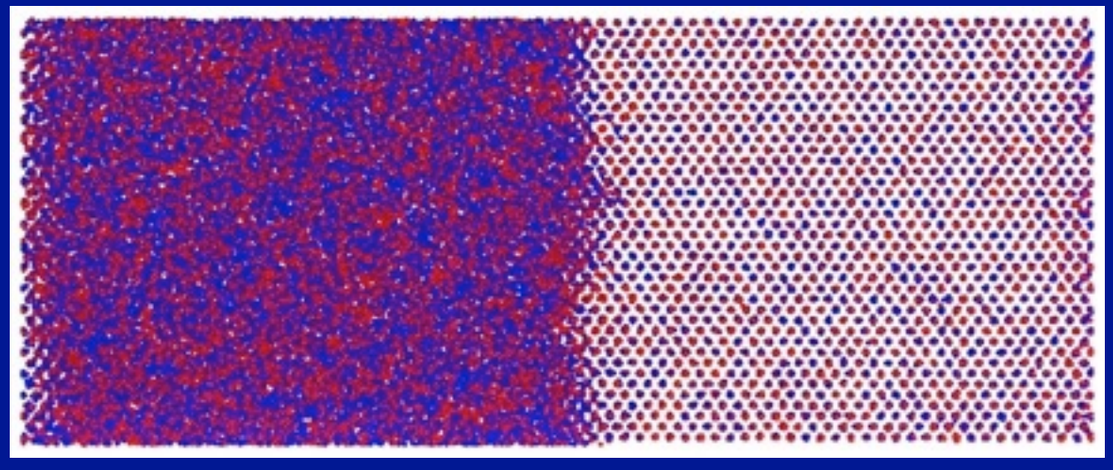
Bob Burkhardt, wikimedia commons

Goals

- Discuss water as something that hopefully fits into the middle-school curriculum
- Introduce materials science, and how computers can be used to complement experiments
- Examples of tools that can be used in the classroom or by advanced students

A bit of background about me...

- Materials Scientist @ NIST
- B.S. in physics, Ph.D. in materials science and engineering, worked as a programmer
- Adventure in Science organizer and mentor
- Interested in how materials behave and why, how they can be improved, and how we use(d) them
- For fun: Scottish fiddle, read mysteries and archaeology/history



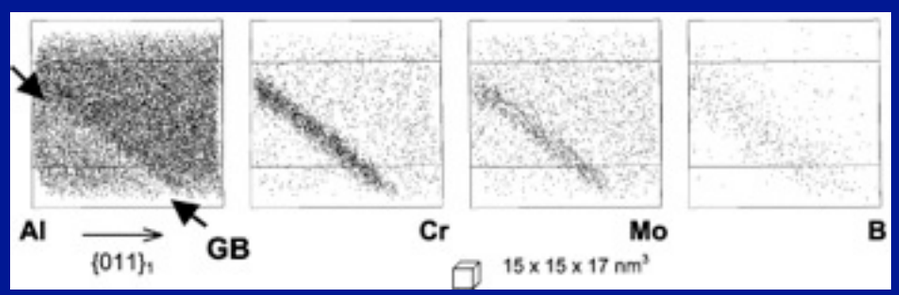
What is "Materials Science?"

- The study of stuff
- Stuff is everything around us -- biological, metallurgical, ceramic, polymer, molecular, ...
  - and all the combinations of these things
- Overlaps with physics, chemistry, biology, metallurgy, ceramics, engineering fields
- Different from traditional chemistry in the emphasis on solids, but the lines are very blurry
- Nice introduction: NOVA series "Making Stuff" on PBS (video.pbs.org)

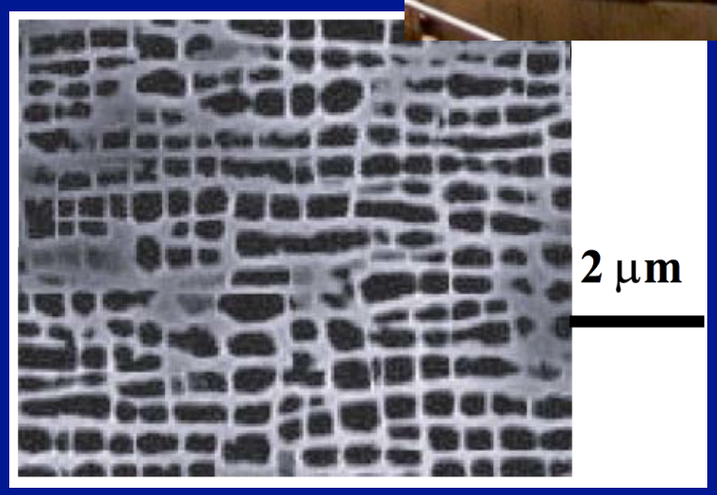
Application areas

- consumer products
  - electronics, plastics
- construction/infrastructure
  - concrete, steel
- transportation (e.g., jet engines)
- nanotechnology
- biomedical applications (e.g., hip replacements)

wikipedia.org



E. Cadel, et al., Acta Mat. (2002)



H.A. Calderon, et al., Microsc. Microanal. (2005)

Approaches used to study materials

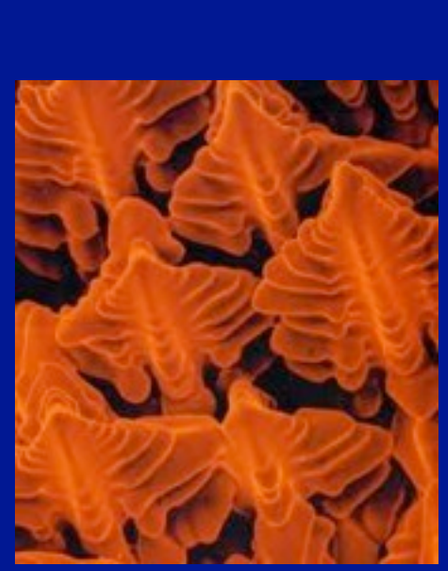
- Microscopy
- X-rays
- Chemical analysis
- Thermal behavior (melting, changes in density, latent heat)
- Stretching/bending/compressing/breaking them
- Mathematical models
- Any others?

Why computer simulations and models?

- Computer simulations and models can be used to complement and understand experiments
- They can be used to explore a wide range of variables without needing to do a separate experiment for each case
- We use them to test our understanding of physical processes. If the simulation does not agree with the experiment, we need to figure out why
- Practical applications: movies, video games, etc.
- More generally: companies rely increasingly on computers, and computer literacy is crucial for most careers

Metals and Water?

- "You study metals. What does that have to do with water?"
- Water and many metals share certain basic properties, so understanding one can provide insight into the other
- Example:
  - Dendrites

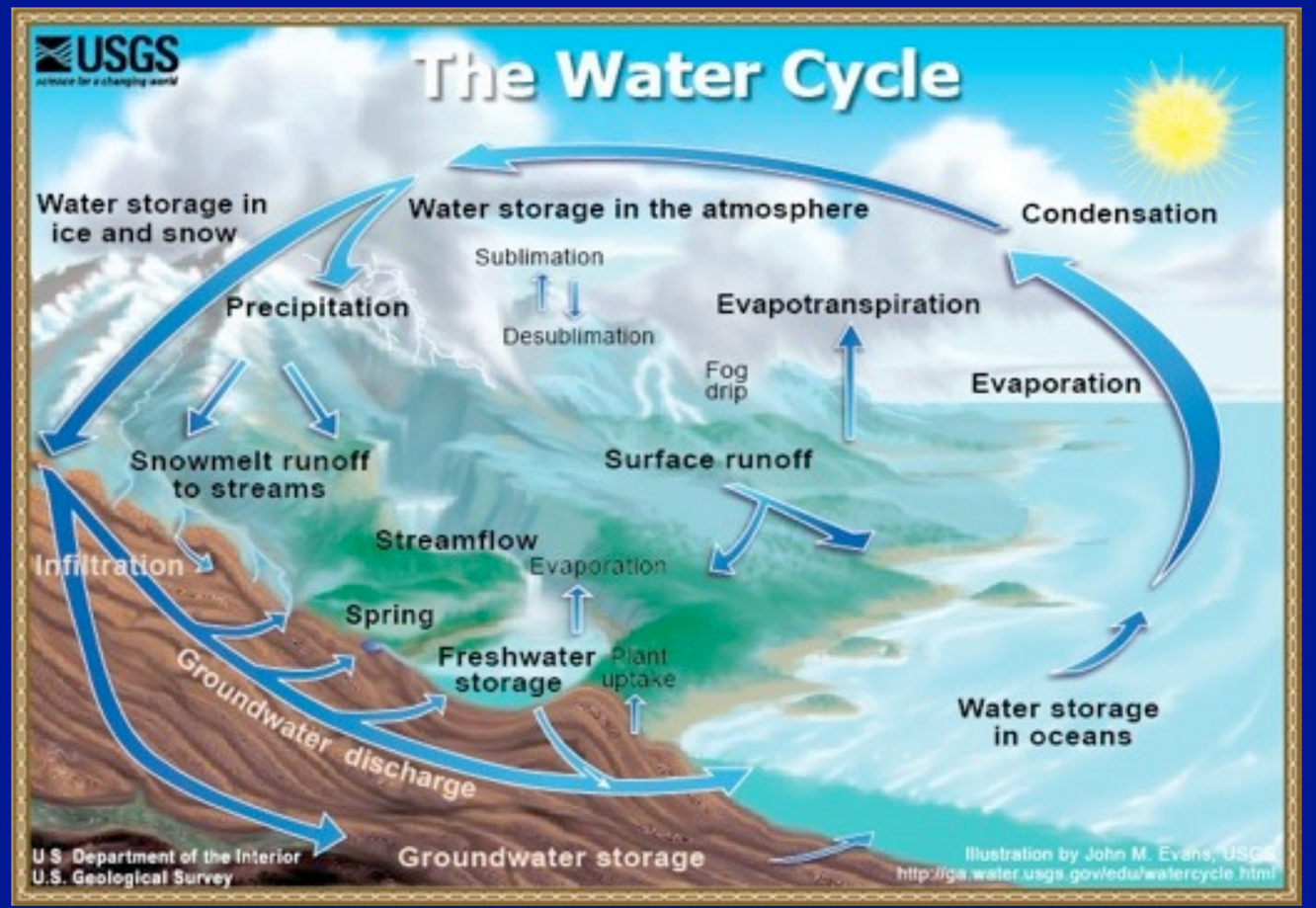


- However, many things are very different (crystal structure, chemical bonding, melting temperatures, strength, etc.), so they can't be treated exactly the same.

Why is water important?

- Crucial for most life
  - Drinking supplies
- Cooling for manufacturing, combustion, etc.
- Medium for many reactions (industrial, medical, etc., applications)

Eyone, Wikimedia Commons



What are properties of water?

- Solid water (ice) floats. Usually.
  - What consequences does that have for ecosystems?

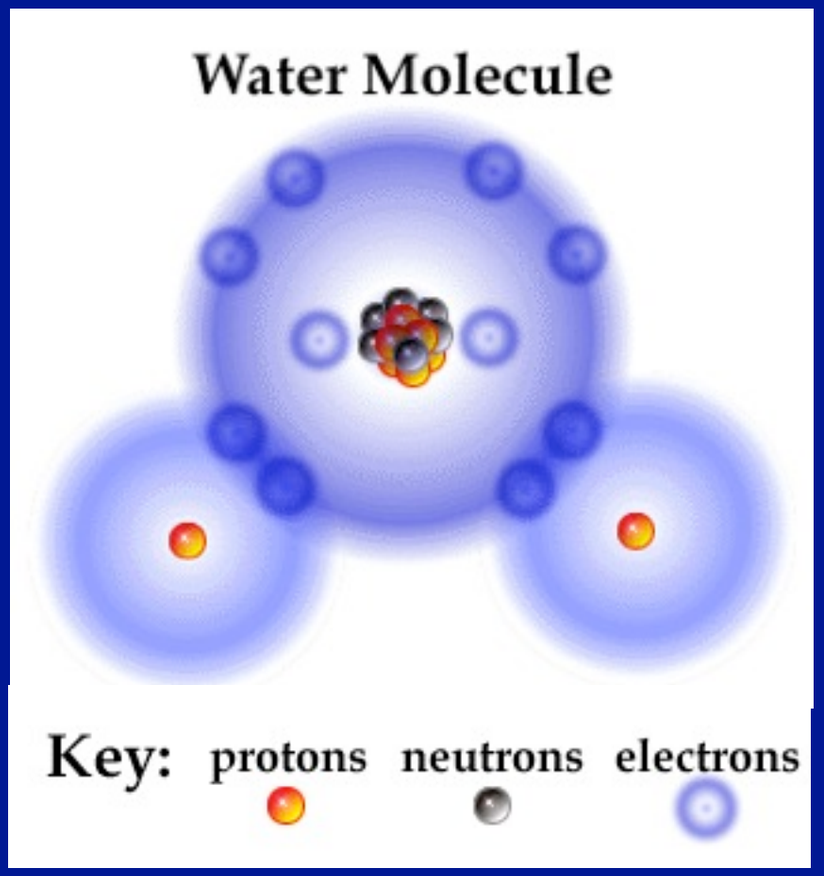
Wikimedia Commons

- liquid from 32 F (0 C) to 212 (100 C) if pure and at sea level
- Polar molecule
- "Universal solvent"

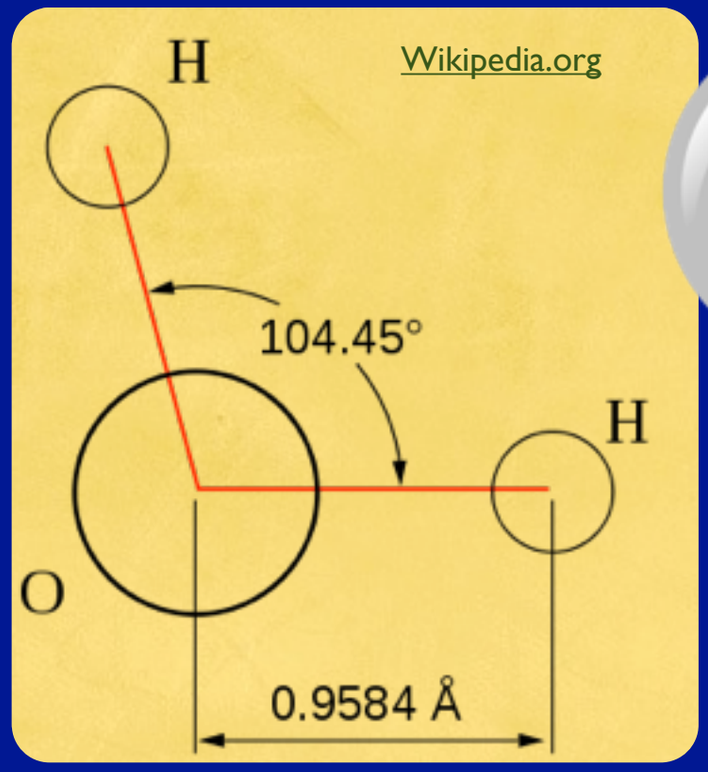
EnDumEn, Wikimedia Commons

Water is weird.

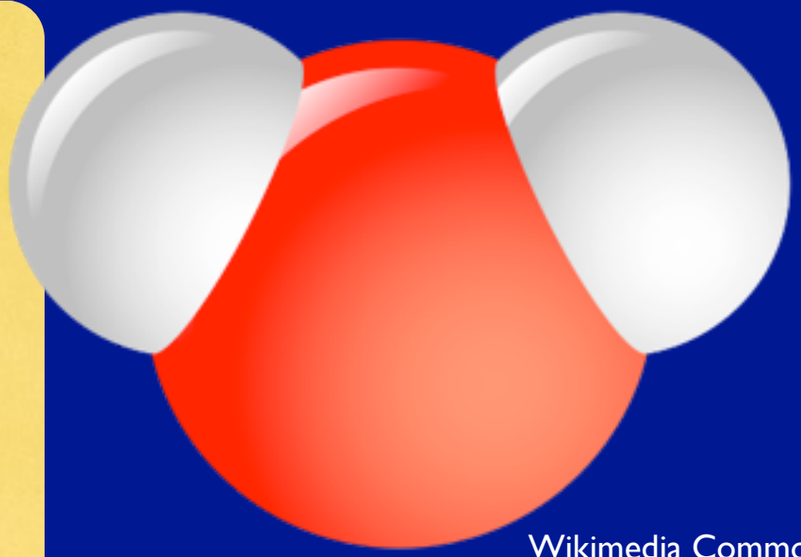
Molecules of H_2O



http://www.brooklyn.cuny.edu/bc/ahp/SDgraphics/PSgraphics/SD.PS.LG.Water.html

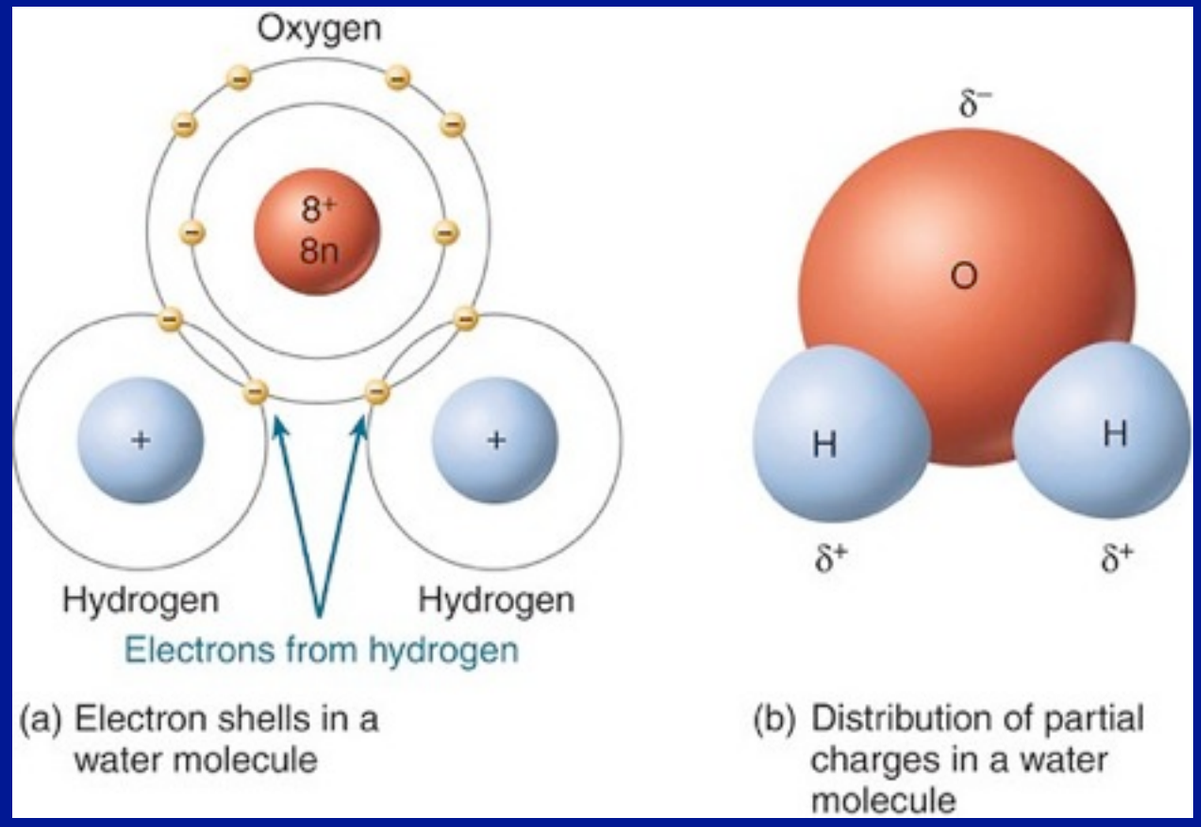


Wikipedia.org



Wikimedia Commons

craziestgadgets.com



NASA

Water Kit

- Build your own water molecules with the kit from 3-D Molecular Designs
- 12 water molecules (24 white H + 12 red O), 1 Na (blue), 1 Cl (green)
- http://www.3dmoleculardesigns.com
- Basic lesson plans:
  - http://www.3dmoleculardesigns.com/Water_Kit_Basic_Lesson_Plans.pdf
- Additional Resources:
  - http://www.3dmoleculardesigns.com/resources.php#water

WebMO Demo Server

http://www.webmo.net/demo/index

Google

- WebMO Home Page
- Features
- Pro Features
- Enterprise Features
- Compare Features
- System Requirements
- Screen Shots
- Working Demo
- Support
- Support Forum
- Testimonials
- Revision History
- Mailing List
- Curriculum Examples
- Workshops
- License Info
- Pricing
- Buy WebMO Pro/Ent
- Obtain Free License
- Download

Recent news

WebMO 10.1 is now available for free download!

WebMO 10.1 Pro and Enterprise have a variety of additional features and is available for purchase.

WebMO can now be installed on Windows, Mac, and Unix servers!

January 25, 2011

WebMO Demo Server

The WebMO Demo Server is now up and running! Log in as follows:

Username: **guest**
Password: **guest**

Job Time Limit: Because the WebMO Demo Server is a shared resource, jobs are limited to one minute (60 seconds) of CPU time!

Java Requirements for WebMO

WebMO requires a web browser to support Java 2, LiveConnect, and Cascading Style Sheet technology.

- **Windows 9X/ME/NT/2000/XP/Vista:** WebMO works with Internet Explorer, Firefox, and other browsers. Sun's Java engine version 1.4 or higher is required.
- **Mac OS X:** WebMO works with Safari, Firefox, and other browsers on OS X 10.3 and higher. Java 1.4.2 or higher is required (available from Apple as a System Update). Some browser versions require a plug-in to enable LiveConnect (available from SourceForge.net). Instructions for pre-10.3 are linked below.
- **Unix/Linux:** WebMO works with Firefox and other browsers. Sun's java engine and a plug-in are required.

See WebMO supported web browsers for details and Java installation instructions.

Tutorial

Useful tutorial

WebMO Login

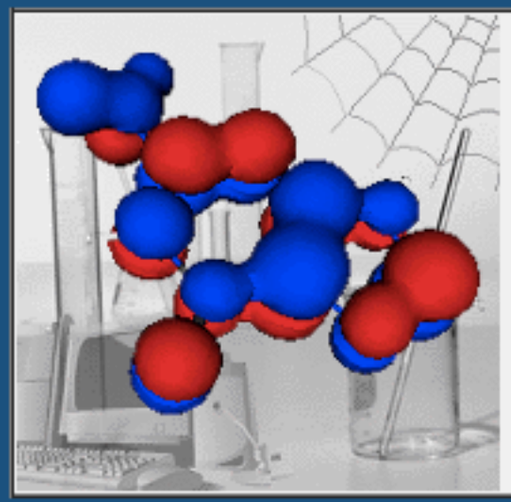
http://buchner.chem.hope.edu/~webmodemo/cgi-bin/webmo/login.cgi

Google

WebMO Login

Version: 10.1.002e
Computational Chemistry on the WWW

Username: guest
Password: guest



Username

Password

Login

WebMO

Wednesday, March 16, 2011

WebMO Job Manager

http://buchner.chem.hope.edu/~webmodemo/cgi-bin/webmo/jobmgr.cgi

Google

WebMO Job Manager

Status

guest
webmo
1:00
unlimited
0 jobs

Folders

Inbox
SCF_DFT_CMPR...
Trash

Manage folders
Empty trash

Search

Displayed jobs
Search

New Job | Refresh | Download | Move To | Delete | Utilities | Logout

	Number	Name	Description	Date	Status	Time	Actions
			Show all	Show all	Show all	Show all	
☐	74236	C3H6O	Geometry Optimization - Mopac	1/25/2011 16:40	Complete	0.1 sec	
☐	74235	C3H6OC3H6O	Geometry Optimization - Mopac	1/25/2011 16:38	Complete	0.1 sec	
☐	74234	C3H6O	Vibrational Frequencies - Mopac	1/25/2011 16:36	Complete	0.0 sec	
☐	74233	C3H6O	Vibrational Frequencies - Mopac	1/25/2011 16:26	Complete	0.0 sec	
☐	74232	C3H8O	Vibrational Frequencies - Mopac	1/25/2011 16:18	Complete	0.0 sec	
☐	74231	C2H6O	Vibrational Frequencies - Mopac	1/25/2011 16:15	Complete	0.0 sec	
☐	74230	C2H6O	Vibrational Frequencies - Mopac	1/25/2011 16:14	Complete	0.0 sec	
☐	74229	C2H6O	Molecular Energy - Mopac	1/25/2011 16:14	Complete	0.0 sec	
☐	74228	C2H6O	Vibrational Frequencies - Mopac	1/25/2011 16:10	Complete	0.0 sec	
☐	74227	C2H6O	Vibrational Frequencies - Mopac	1/25/2011 16:06	Complete	0.0 sec	
☐	74226	CH4O	Vibrational Frequencies - Mopac	1/25/2011 15:58	Complete	0.0 sec	
☐	74225	CH4O	Vibrational Frequencies - Mopac	1/25/2011 15:54	Complete	0.0 sec	
☐	74224	CH4	Vibrational Frequencies - Mopac	1/25/2011 15:48	Complete	0.0 sec	
☐	74223	CH4	Vibrational Frequencies - Mopac	1/25/2011 15:45	Complete	0.1 sec	
☐	74222	H2O	Vibrational Frequencies - Mopac	1/25/2011 15:41	Complete	0.0 sec	
☐	74221	CO2	Vibrational Frequencies - Mopac	1/25/2011 15:31	Complete	0.0 sec	

To make a water molecule in WebMO

- Choose "New Job"
- Under "Build", select "O"
- Click somewhere in the middle. A red oxygen atom will appear.
- Under "Clean-Up", select "Comprehensive -- idealized". Hydrogens (white) will be added at the correct angle.
- Click on the right arrow in the bottom right corner to continue.

(Lost? There is a tutorial on www.webmo.net/demo/index)

Build Molecule

http://buchner.chem.hope.edu/~webmodemo/cgi-bin/webmo/build_molecule.cgi

Google

Build Molecule

Status

guest
webmo
1:00
unlimited
0 jobs

Progress

- Job manager
- **Build molecule**

Build a new molecule using the WebMO editor, or import an existing molecule from a file. Additionally, you can export the molecule to a variety of file formats.

- Choose engine
- Job options
- Submit job

Editor help

File Edit Tools View Build Adjust Clean-Up Help

Build Mode - O (click = add atom; drag = add bond; click & drag = add atom & bond; letter = change atom)

Import Molecule Export Molecule

Choose Computational Engine

http://buchner.chem.hope.edu/~webmodemo/cgi-bin/webmo/build_molecule.cgi

Google

Choose Computational Engine

Status

guest
webmo
1:00
unlimited
0 jobs

Progress

- Job manager
- Build molecule
- **Choose engine**

Choose the desired computational engine from those installed.

- Job options
- Submit job

Help

Engine	Description
Gamess	Ab initio and semi-empirical calculations
Gaussian	Ab initio and semi-empirical calculations
Molpro	Ab initio calculations
Mopac	Semi-empirical calculations
NWChem	Ab initio calculations
PQS	Ab initio, semi-empirical, and mechanics
PSI	Ab initio calculations
QChem	Ab initio calculations
Tinker	Molecular mechanics calculations
Select Server	buchner.chem.hope.edu

Tradeoffs: the most accurate calculations are generally the most expensive (time, resources). The question is often, "what is the minimum accuracy I need to answer my question?"

Ab initio = you tell it which atom types to use, and it will treat the electrons (charge) realistically. It is the most accurate, but it is also expensive, limiting the number of atoms in a calculation.

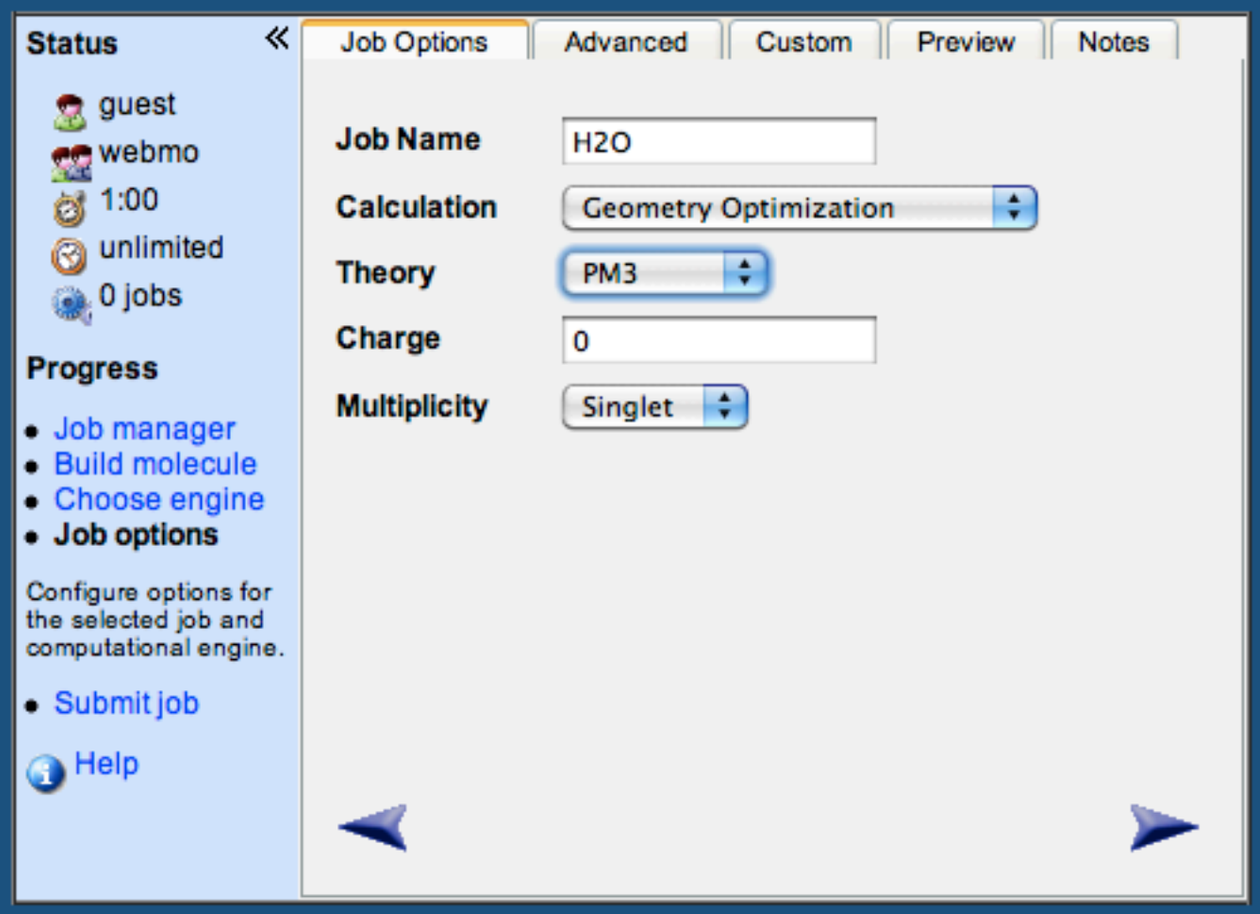
Semi-empirical = an approximation that still treats individual atoms/molecules but is less accurate than "ab initio." It is faster. This allows calculations with larger numbers of molecules.

Configure Mopac Job Options

http://buchner.chem.hope.edu/~webmodemo/cgi-bin/webmo/choose_engine.cgi

Google

Configure Mopac Job Options



Other calculation options include:

- Molecular Energy
- Vibrational Frequencies
- Thermochemistry
- Molecular Orbitals

There are also lots of options under the tabs.

WebMO Job Manager

http://buchner.chem.hope.edu/~webmodemo/cgi-bin/webmo/jobmgr.cgi

Google

WebMO Job Manager

When the status says "Complete", click the "Name" (H2O)

Status

guest
webmo
1:00
unlimited
0 jobs

Folders

Inbox
SCF_DFT_CMPR...
Trash

Manage folders
Empty trash

Search

Displayed jobs
Search

New Job | Refresh | Download | Move To | Delete | Utilities | Logout

Number	Name	Description	Date	Status	Time	Actions
74242	H2O	Geometry Optimization - Mopac	1/25/2011 16:55	Running	0.0 sec	
74241	C2H6O	Vibrational Frequencies - Mopac	1/25/2011 16:53	Complete	0.1 sec	
74240	C2H6O	Geometry Optimization - Mopac	1/25/2011 16:51	Complete	0.1 sec	
74239	C2H6O	Vibrational Frequencies - Mopac	1/25/2011 16:47	Complete	0.1 sec	
74238	C2H6O	Geometry Optimization - Mopac	1/25/2011 16:46	Complete	0.7 sec	
74237	C3H6O	Vibrational Frequencies - Mopac	1/25/2011 16:42	Complete	0.1 sec	
74236	C3H6O	Geometry Optimization - Mopac	1/25/2011 16:40	Complete	0.1 sec	
74235	C3H6OC3H6O	Geometry Optimization - Mopac	1/25/2011 16:38	Complete	0.1 sec	
74234	C3H6O	Vibrational Frequencies - Mopac	1/25/2011 16:36	Complete	0.0 sec	
74233	C3H6O	Vibrational Frequencies - Mopac	1/25/2011 16:26	Complete	0.0 sec	
74232	C3H8O	Vibrational Frequencies - Mopac	1/25/2011 16:18	Complete	0.0 sec	
74231	C2H6O	Vibrational Frequencies - Mopac	1/25/2011 16:15	Complete	0.0 sec	
74230	C2H6O	Vibrational Frequencies - Mopac	1/25/2011 16:14	Complete	0.0 sec	
74229	C2H6O	Molecular Energy - Mopac	1/25/2011 16:14	Complete	0.0 sec	
74228	C2H6O	Vibrational Frequencies - Mopac	1/25/2011 16:10	Complete	0.0 sec	
74227	C2H6O	Vibrational Frequencies - Mopac	1/25/2011 16:06	Complete	0.0 sec	

View Job 74242: H2O, Geometry Optimization - Mopac

Status

guest
webmo
1:00
unlimited
0 jobs

Summary

- H2O
- Job # 74242
- 1/25/2011
- 0.0 sec

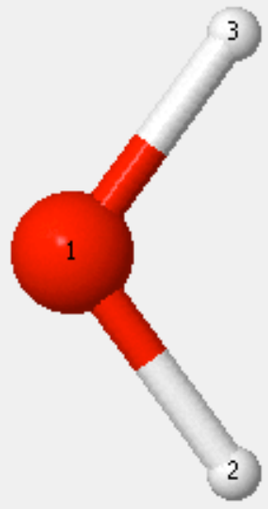
Actions

Job Manager
Raw output
All files
Print
Help

Notes

Molecule Viewer | Data Viewer

File Edit View Help



View Mode – Rotate (drag = rotate XY; alt-drag = rotate Z)

Reset Viewer | New Job Using This Geometry | Export Molecule

Calculated Quantities

Quantity	Value
Geometry Sequence	

Step	Energy
0	-42.17675
1	-48.02339
2	-52.96029
3	-53.36703
4	-53.42500
5	-53.43282
6	-53.43283

Animation speed: 5

Loop: None

Route	
Symmetry	C2v
PM3 Heat of Formation	-53.43283 kcal/mol
Dipole Moment	1.739 Debye

Partial Charges

Atom	Symbol	Charge
1	O	-0.358562
2	H	0.179281
3	H	0.179281

Bond Order

Atom	Symbol	1 O	2 H	3 H
1	O	1.935716		
2	H	0.967858	0.967858	
3	H	0.967858	0.000000	0.967858

Server	buchner.chem.hope.edu (0)
CPU time	0.01 sec

http://buchner.chem.hope.edu/~webmodemo/cgi-bin/webmo/jobmgr.cgi

Google

View Job 74242: H2O, Geometry Optimization - Mopac

Status

- guest
- webmo
- 1:00
- unlimited
- 0 jobs

Summary

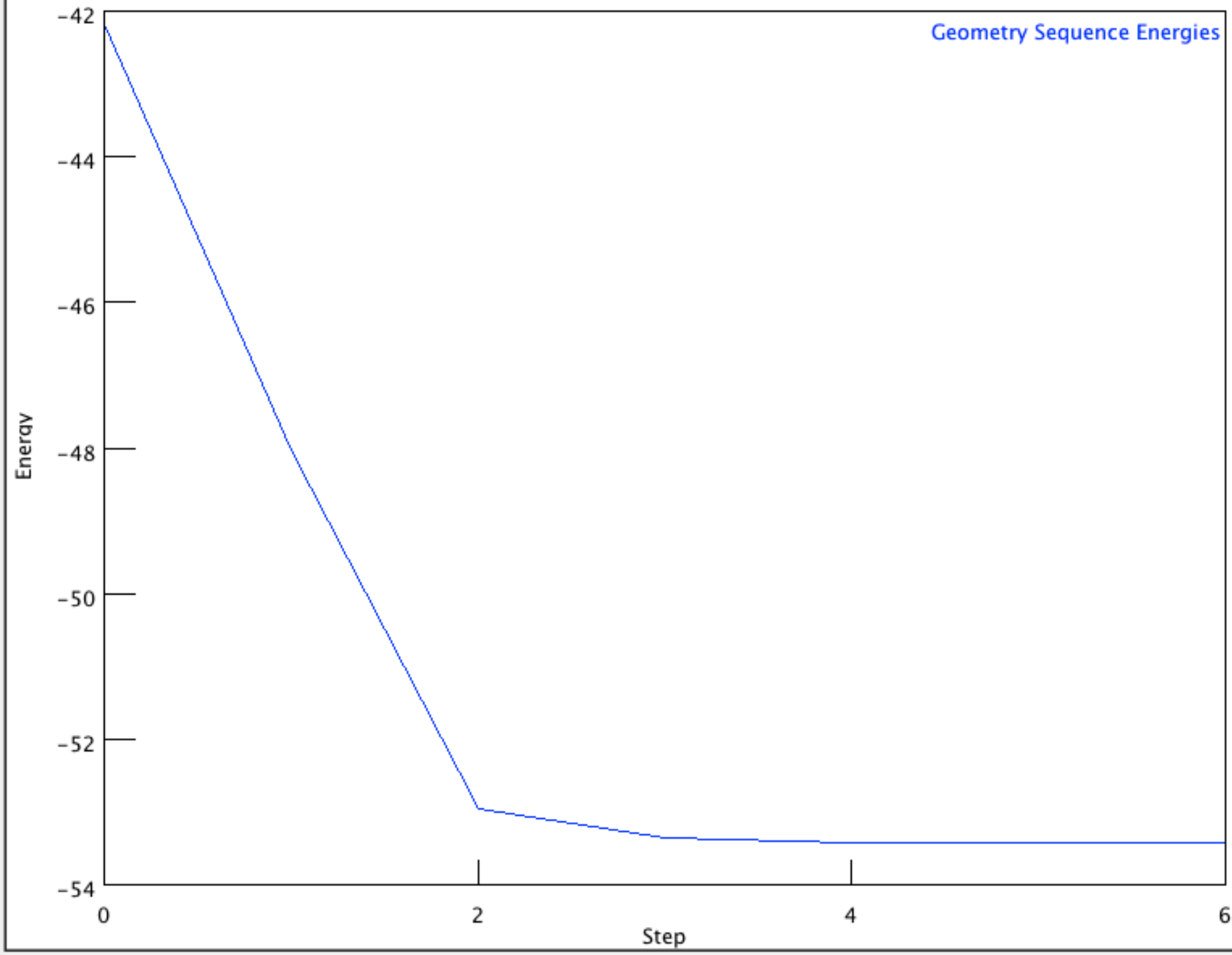
- H2O
- Job # 74242
- 1/25/2011
- 0.0 sec

Actions

- Job Manager
- Raw output
- All files
- Print
- Help

Notes

Molecule Viewer | Data Viewer



Reset Viewer | New Job Using This Geometry | Export Molecule

http://buchner.chem.hope.edu/~webmodemo/cgi-bin/webmo/jobmgr.cgi

Google

View Job 74242: H2O, Geometry Optimization - Mopac

Status

- guest
- webmo
- 1:00
- unlimited
- 0 jobs

Summary

- H2O
- Job # 74242
- 1/25/2011
- 0.0 sec

Actions

- Job Manager
- Raw output
- All files
- Print
- Help

Notes

Molecule Viewer | Data Viewer

File Edit View Help

View Mode – Rotate (drag = rotate XY; alt-drag = rotate Z)

Reset Viewer | New Job Using This Geometry | Export Molecule

http://buchner.chem.hope.edu/~webmodemo/cgi-bin/webmo/jobmgr.cgi

Google

guest
webmo
1:00
unlimited
0 jobs

Summary

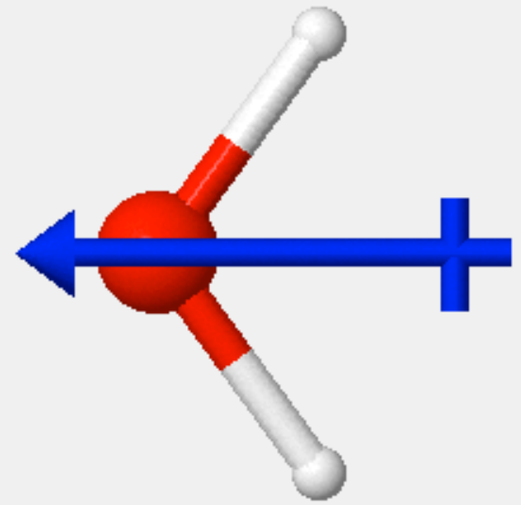
- H2O
- Job # 74242
- 1/25/2011
- 0.0 sec

Actions

Job Manager
Raw output
All files
Print
Help

Notes

File Edit View Help



View Mode – Rotate (drag = rotate XY; alt-drag = rotate Z)

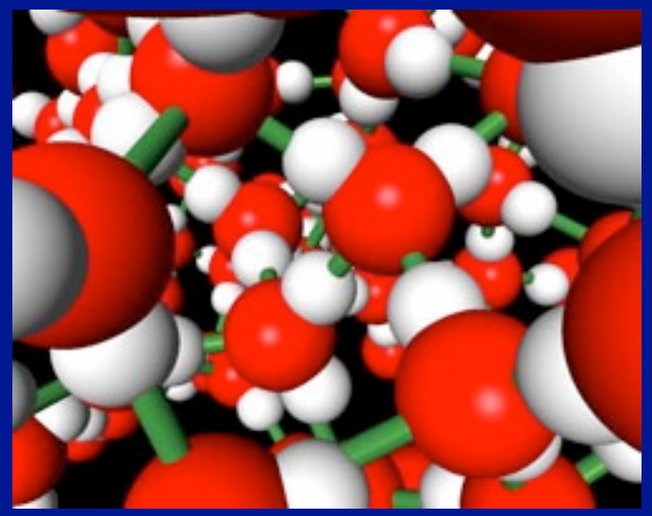
Reset Viewer | New Job Using This Geometry | Export Molecule

Calculated Quantities

Quantity	Value

Many H_20 molecules + other stuff

- Molecular simulation can be used to look at groups of water molecules and their interactions with other ions/ molecules.



F.W. Starr/Wesleyan Univ.

Formation of water shells around ions

http://mw2.concord.org/public/student/solution/watershell.html

Google

Formation of Water Shells Around Ions

Charge on the purple ion

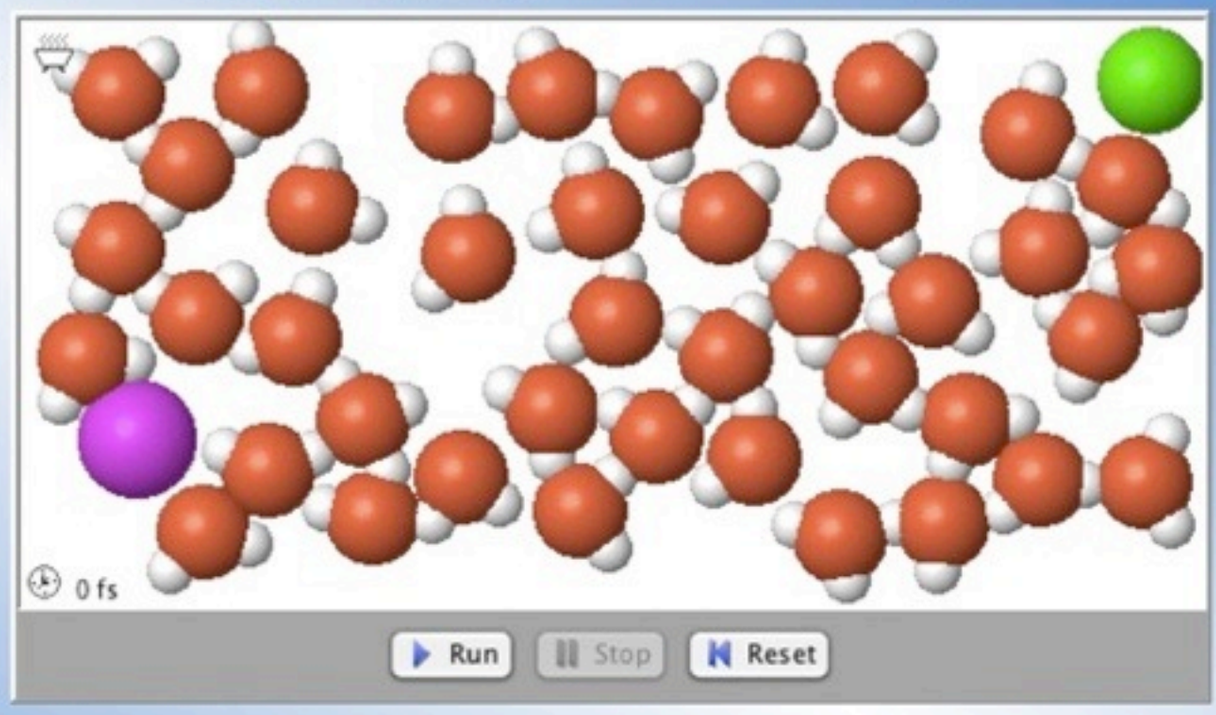
-5e 0e 5e

Charge on the green ion

-5e 0e 5e

Show Hydrogen Bonds Show Charges Cool Heat Spacefilling

Water is a great solvent, but all substances that water can dissolve must be either polar or ionic (either positively or negatively charged). The polar water molecules attract charged particles and push out non-charged particles. Water is attracted to itself, to other polar molecules, ionic substances, and to polar substances.



In solution, water molecules form a "shell" around ions. This model illustrates how ions solvated by water molecules move. Note, however, **this 2D model does not depict the real shell structure, which in reality is 3D**.

Molecular Workbench
http://mw.concord.org

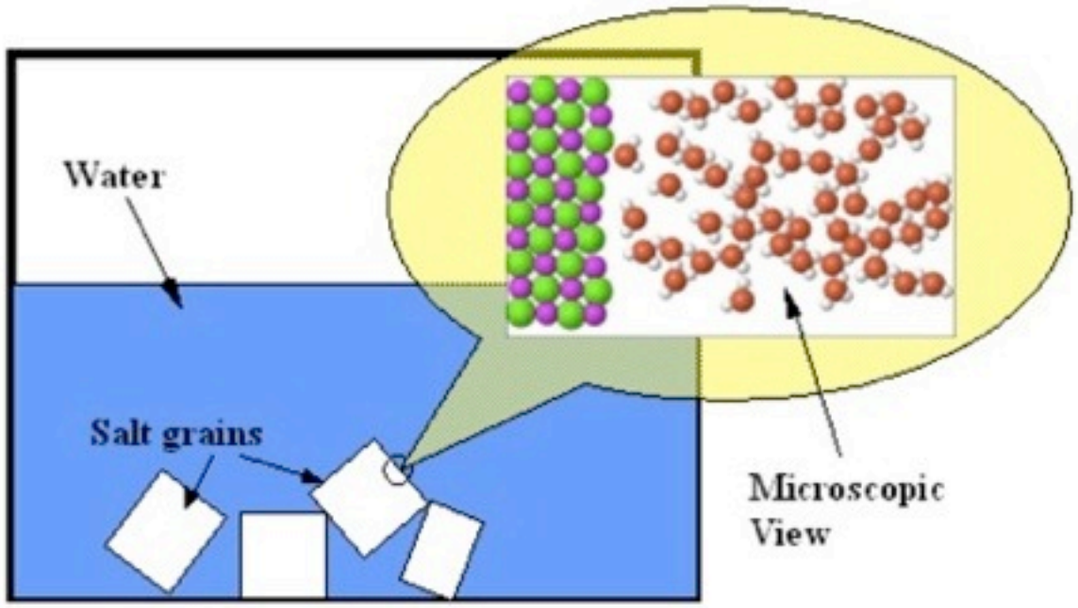
Dissolving Salt in Water

http://mw2.concord.org/public/student/solution/dissolve.html

Google

Dissolving Salt in Water

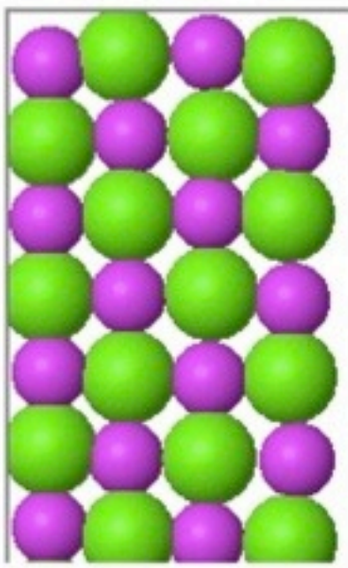
Key concept: solubility. The simulation demonstrates that dissolution occurs because the electrostatic interactions between water and salt ions compete with the electrostatic interactions among the salt ions themselves and therefore cause the structure of ionic crystal to fall apart.



Run the model first. You should see that the salt crystal does not change shape. Then use the following button to add water to the salt crystal:

Add water

Use the following button to return to the starting salt crystal:

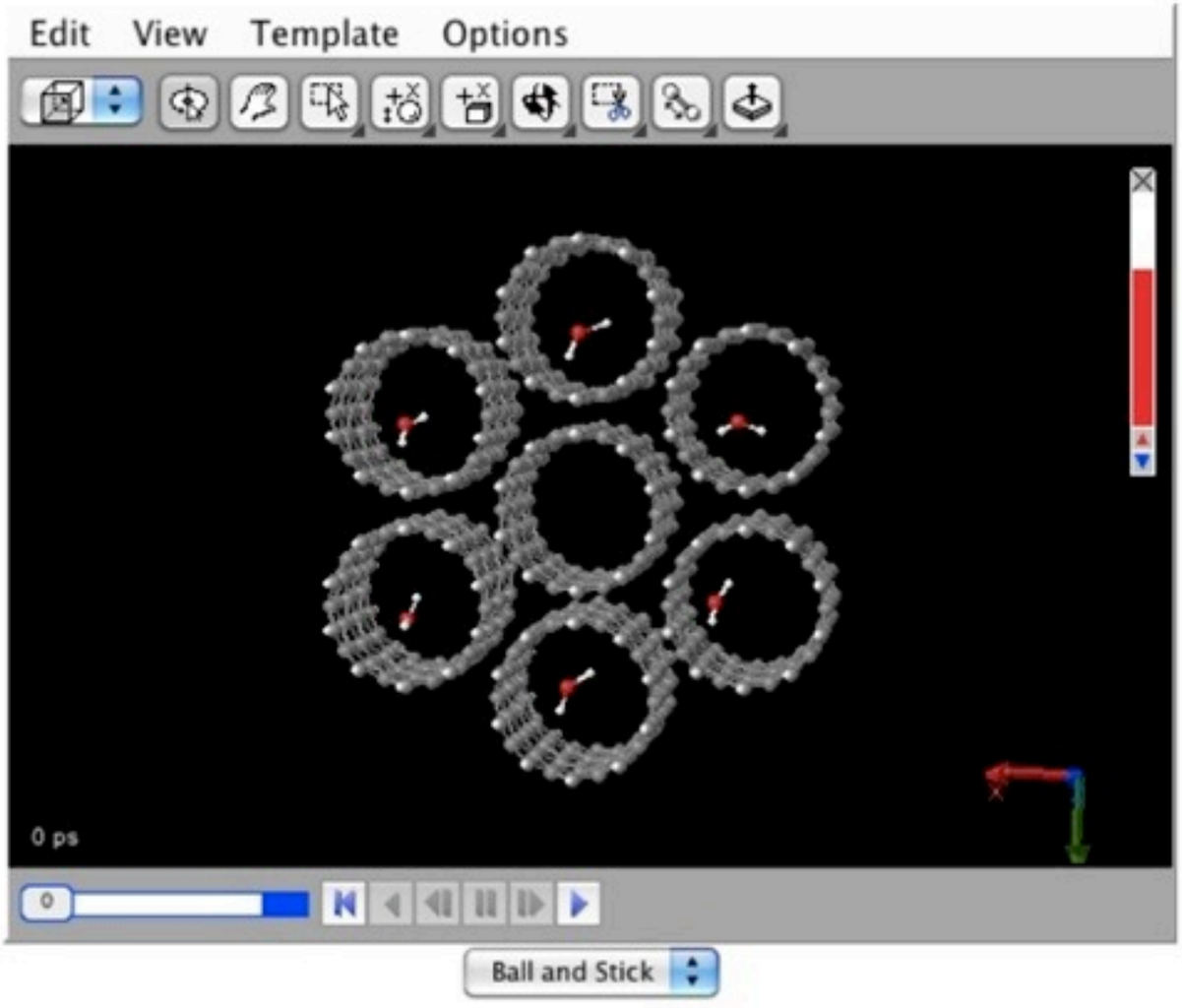


A race of water molecules through a cluster of carbon nanotubes

http://mw2.concord.org/public/student/nano/waterrace.html

Google

A race of water molecules through a cluster of carbon nanotubes



Note about this model: This model has 998 atoms, just 2 atoms under the current limit we set (1000). It has 1342 radial bonds, 2386 angular bonds and 910 torsional bonds. If we had taken into account of the calculations for all the atoms and bonds, it would have been so slow that it will probably take a few hours to simulation 100 picoseconds. To simplify the simulation, we fix the seven nanotubes all together and let only the water molecules move. We think this is a good approximation, because nanotubes must be rigid in real world applications so that they can remain stable.

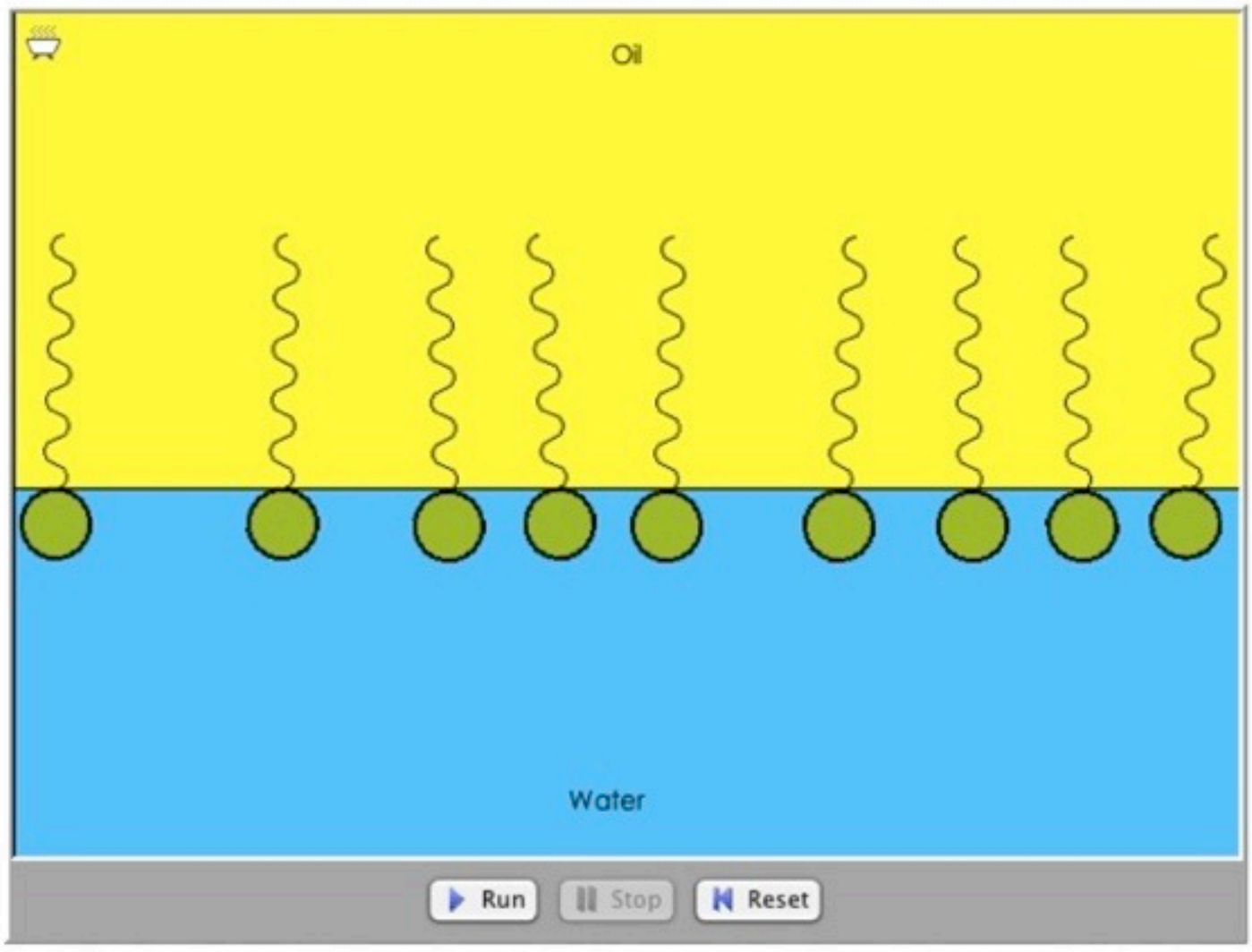
Although the nanotubes are fixed, their interactions with the water molecules are still calculated. Therefore, such a simplification can be thought of as water molecules moving in the static force fields formed by the carbon atoms of the nanotubes.

Lipid molecules form a monolayer at an oil-water interface

http://mw2.concord.org/public/student/biomodels/monolayer.html

Google

Lipid molecules form a monolayer at an oil-water interface



Use the "Flip" button to switch the environment and observe how lipid molecules respond to the change.
You may also try dragging the molecules away from the interface line and see how they reform a monolayer.
Note: You have to stop the simulation in order to drag the molecules.

Flip | Take a snapshot

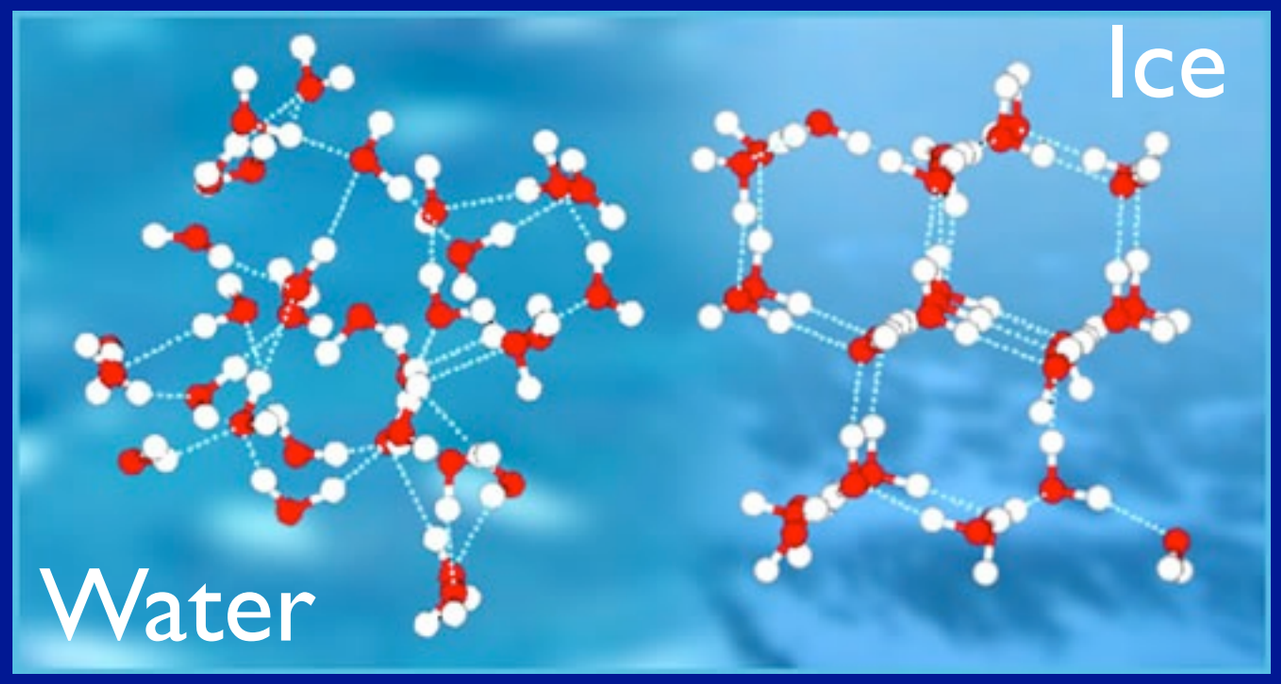
Molecular Workbench
http://mw.concord.org

Snowflakes

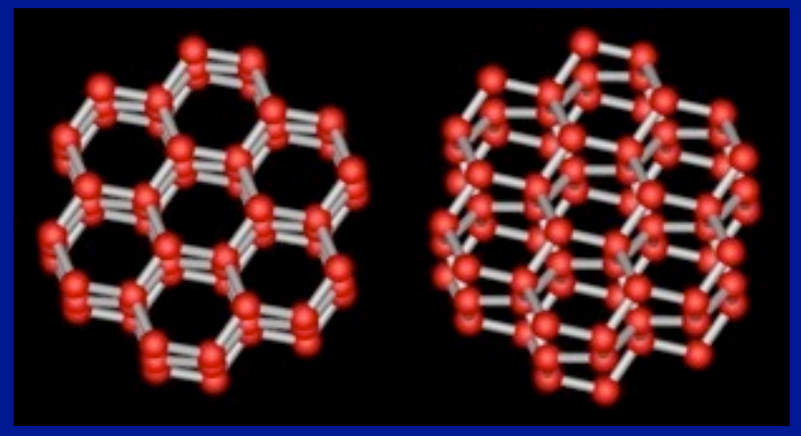
- We are fascinated by snowflakes
  - are no two really alike?
- But, it is not well understood exactly how they form or what controls their shapes
- Applications: understanding effects of pollution, antifreeze (ice cream, cellular damage)
- Great website: snowcrystals.com

What happens to make a snowflake?

- phase transition when liquid freezes into solid
- seed with crystal growth as water droplets attach
- different faces have different energy (generally, systems want to minimize the energy)
- What are the effects of temperature? solute? freezing rate? other variables?



Lawrence Berkeley Laboratory

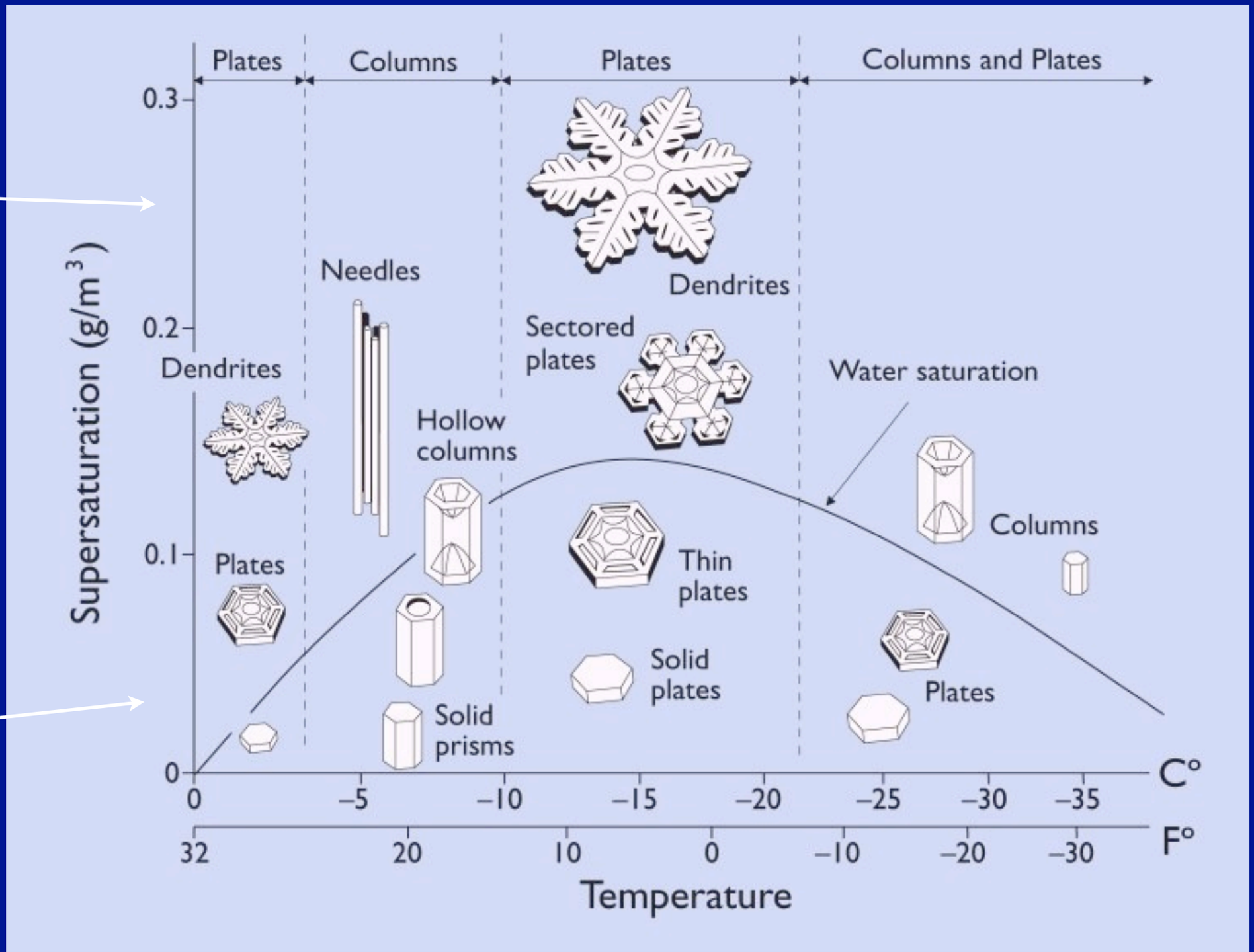


www.its.caltech.edu

Snowflake morphologies

Wetter →

Drier →



www.its.caltech.edu/~atomic/snowcrystals/primer/morphologydiagram.jpg

Snowflakes

Experiment (photo)

Kenneth G. Libbrecht, Caltech

Computer simulation

David Griffeaths, U. Wisc.; Antoine Clappier

David Griffeaths, U. Wisc, http://psoup.math.wisc.edu/Snowfakes

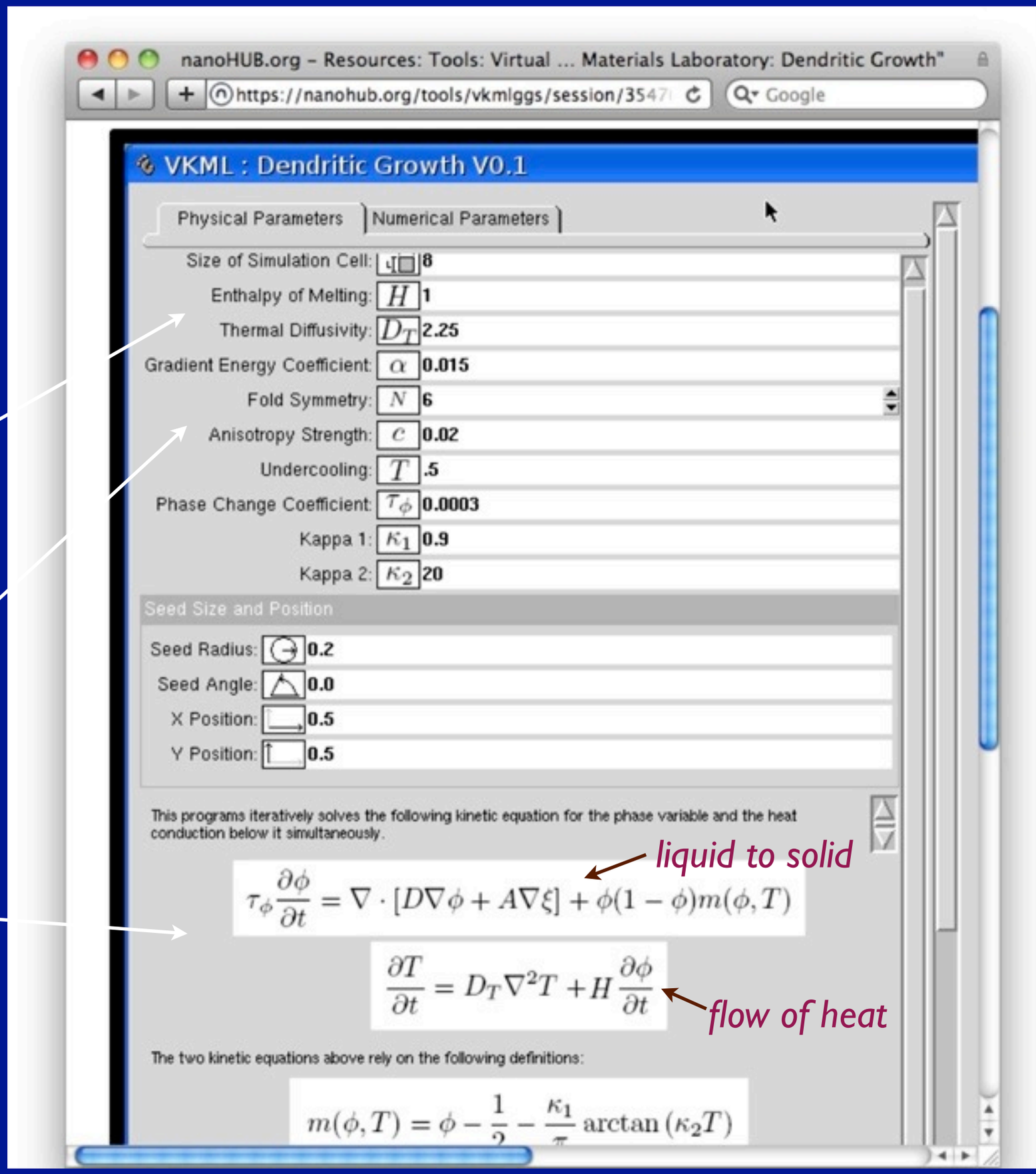
We can model many of the processes:

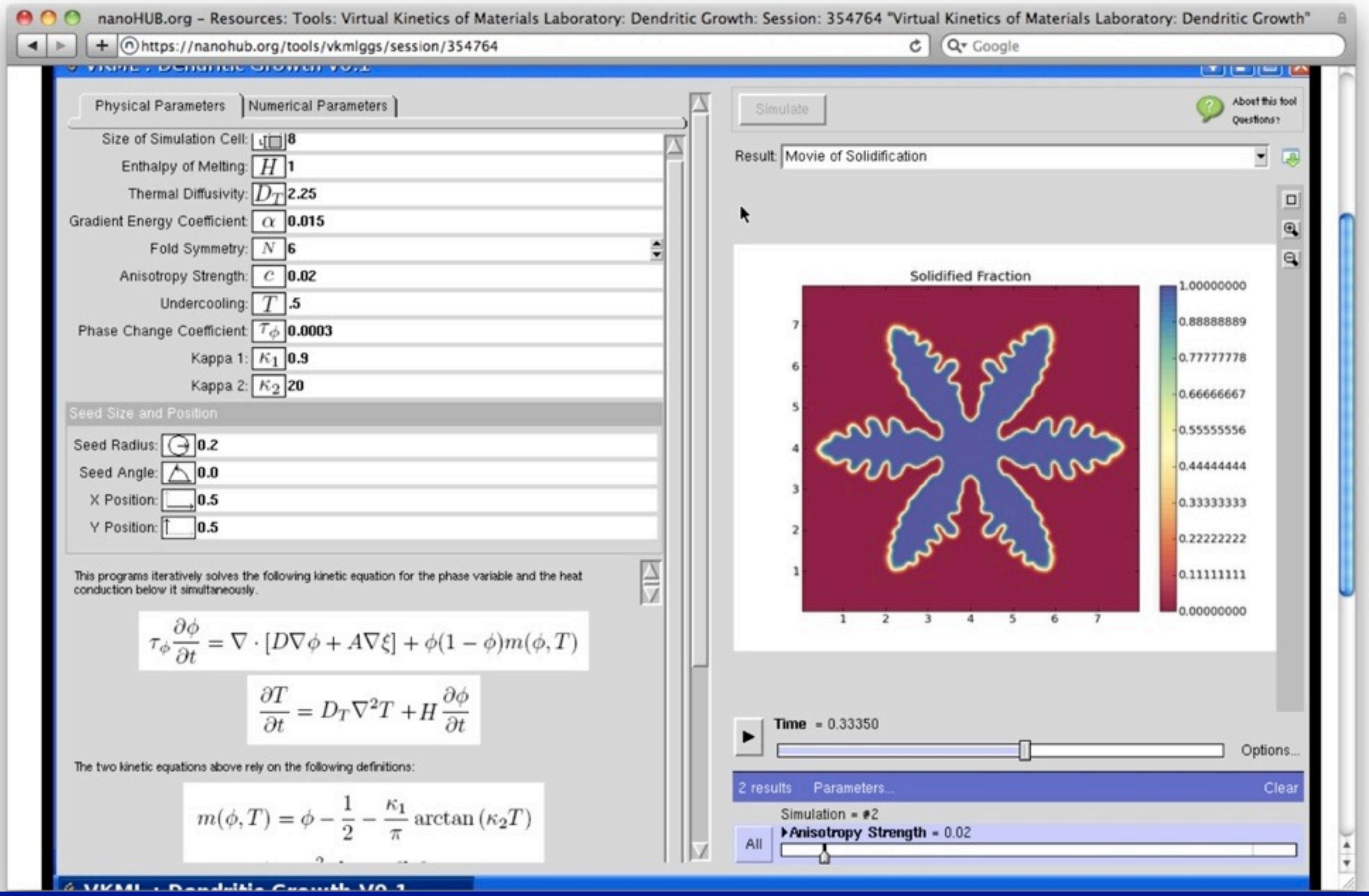
Virtual Kinetics of Materials Laboratory: Dendritic Growth
https://nanohub.org/tools/vkmlggs

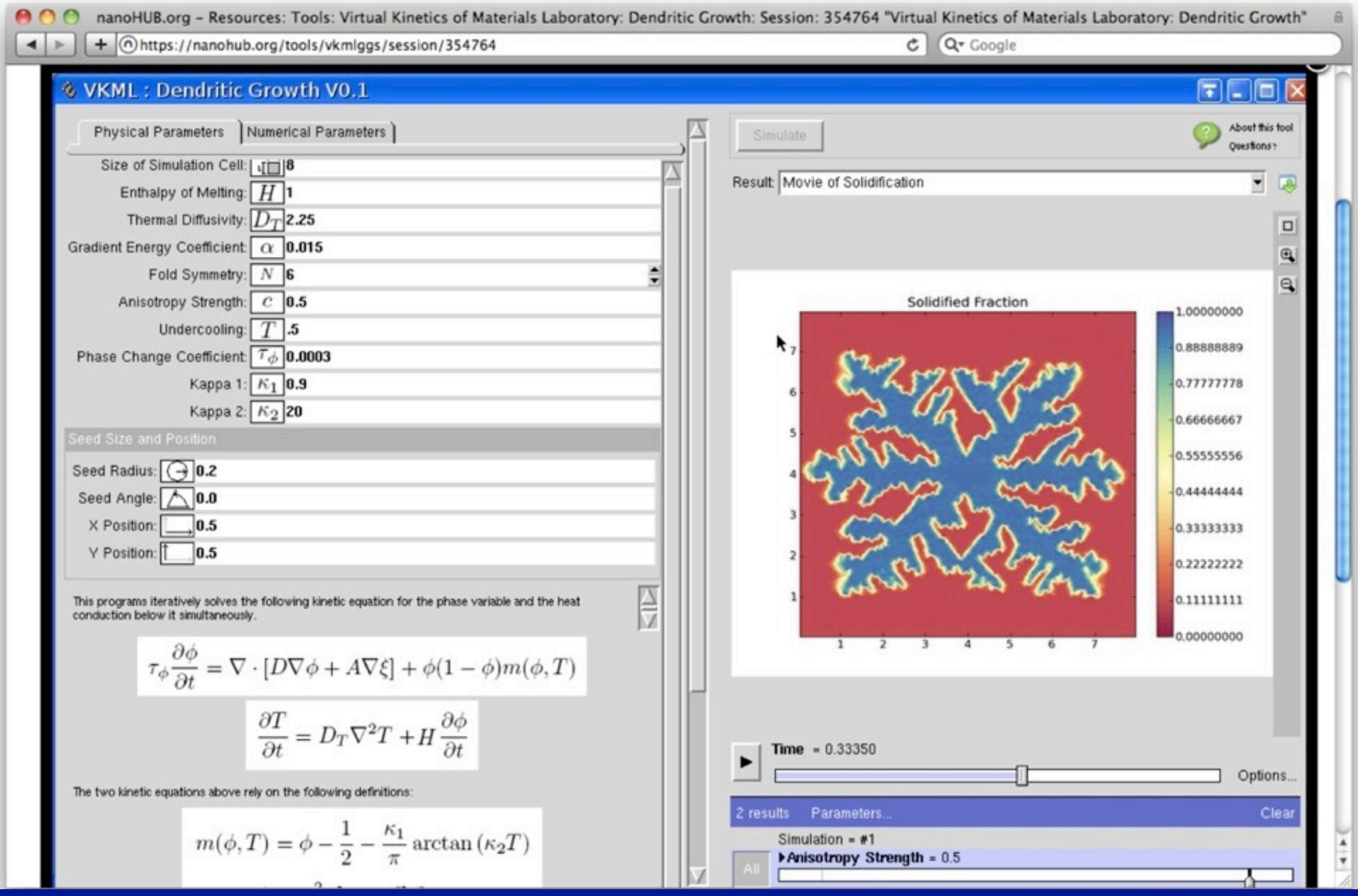
Mouse over each parameter name to see a description

See what happens when you change:
Enthalpy of Melting
Fold symmetry
Anisotropy Strength

These equations describe how the dendrite grows.
Don't worry about the details.
They are an example of the kinds of problem that is hard for humans to solve, but for which computers are great.




nanoHUB.org - Resources: Tools: Virtual Kinetics of Materials Laboratory: Dendritic Growth: Session: 354764 "Virtual Kinetics of Materials Laboratory: Dendritic Growth"
https://nanohub.org/tools/vkmlggs/session/354764
Google
Physical Parameters
Numerical Parameters
Size of Simulation Cell: 8
Enthalpy of Melting: H 1
Thermal Diffusivity: D_T 2.25
Gradient Energy Coefficient: α 0.015
Fold Symmetry: N 6
Anisotropy Strength: ε 0.02
Undercooling: T .5
Phase Change Coefficient: τ_φ 0.0003
Kappa 1: κ_1 0.9
Kappa 2: κ_2 20
Seed Size and Position
Seed Radius: 0.2
Seed Angle: 0.0
X Position: 0.5
Y Position: 0.5
This programs iteratively solves the following kinetic equation for the phase variable and the heat conduction below it simultaneously.
$$\tau_\phi \frac{\partial \phi}{\partial t} = \nabla \cdot [D\nabla\phi + A\nabla\xi] + \phi(1-\phi)m(\phi,T)$$
$$\frac{\partial T}{\partial t} = D_T \nabla^2 T + H\frac{\partial \phi}{\partial t}$$
The two kinetic equations above rely on the following definitions:
$$m(\phi,T) = \phi - \frac{1}{2} - \frac{\kappa_1}{\pi}\arctan(\kappa_2 T)$$
Simulate
About this tool
Questions?
Result: Movie of Solidification
Solidified Fraction
1.00000000
0.88888889
0.77777778
0.66666667
0.55555556
0.44444444
0.33333333
0.22222222
0.11111111
0.00000000
Time = 0.33350
Options...
2 results
Parameters...
Clear
Simulation = #2
All
Anisotropy Strength = 0.02


nanoHUB.org – Resources: Tools: Virtual Kinetics of Materials Laboratory: Dendritic Growth: Session: 354764 "Virtual Kinetics of Materials Laboratory: Dendritic Growth"
https://nanohub.org/tools/vkmlggs/session/354764
Google
VKML : Dendritic Growth V0.1
Physical Parameters
Numerical Parameters
Size of Simulation Cell: 8
Enthalpy of Melting: H 1
Thermal Diffusivity: D_T 2.25
Gradient Energy Coefficient: α 0.015
Fold Symmetry: N 6
Anisotropy Strength: ε 0.5
Undercooling: T .5
Phase Change Coefficient: τ_ϕ 0.0003
Kappa 1: κ_1 0.9
Kappa 2: κ_2 20
Seed Size and Position
Seed Radius: 0.2
Seed Angle: 0.0
X Position: 0.5
Y Position: 0.5
This programs iteratively solves the following kinetic equation for the phase variable and the heat conduction below it simultaneously.
$$\tau_\phi \frac{\partial \phi}{\partial t} = \nabla \cdot [D\nabla\phi + A\nabla\xi] + \phi(1-\phi)m(\phi,T)$$
$$\frac{\partial T}{\partial t} = D_T \nabla^2 T + H\frac{\partial \phi}{\partial t}$$
The two kinetic equations above rely on the following definitions:
$$m(\phi,T) = \phi - \frac{1}{2} - \frac{\kappa_1}{\pi}\arctan(\kappa_2 T)$$
Simulate
About this tool
Questions?
Result: Movie of Solidification
Solidified Fraction
1.00000000
0.88888889
0.77777778
0.66666667
0.55555556
0.44444444
0.33333333
0.22222222
0.11111111
0.00000000
Time = 0.33350
Options...
2 results
Parameters...
Clear
Simulation = #1
All
Anisotropy Strength = 0.5

Additional resources

- Model kits:
  - http://3dmoleculardesigns.com
- Snowflakes:
  - snowcrystals.com
  - http://psoup.math.wisc.edu/3dMovies/3dMovies.htm
- Lots of great simulation tools:
  - http://mw.concord.org/modeler/showcase/index.html

Contact Information

- Chandler A. Becker, Ph.D.
- Materials Research Engineer

  Material Measurement Laboratory

  National Institute of Standards and Technology

  Gaithersburg, MD 20899
- Tel: 301-975-5344
- Email: chandler.becker@nist.gov

- Feel free to contact me with questions