Sept. 18 2009 _

Lecture 5: Introduction to Mathematica IV

Graphics

Graphics are an important part of exploring mathematics and conveying its results. An informative plot or graphic that conveys a complex idea succinctly and naturally to an educated observer is a work of creative art. Indeed, art is sometimes defined as "an elevated means of communication," or "the means to inspire an observation, heretofore unnoticed, in another." Graphics are art; they are necessary. And, I think they are fun.

For graphics, we are limited to two and three dimensions, but, with the added possibility of animation, sound, and perhaps other sensory input in advanced environments, it is possible to usefully visualize more than three dimensions. Mathematics is not limited to a small number of dimensions; so, a challenge —or perhaps an opportunity—exists to use artfulness to convey higher dimensional ideas graphically.

The introduction to basic graphics starts with two-dimensional plots.

Simple Plots

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Here are some examples of simple x-y plots and how to decorate them. We start with very simple examples and add a little more at each step to show how a plot can be developed incrementally. We leave all the steps in as cut-and-paste examples.

```
Plot[Sin[x] / x, {x, -5 Pi, 5 Pi}]
Options[Plot]
Plot[Sin[x] / x, {x, -5 Pi, 5 Pi},
  PlotStyle → {Red, Thick}]
Plot[Sin[x] / x, {x, -5 Pi, 5 Pi},
  PlotRange → {-0.25, 1.25},
PlotStyle → {Red, Thick},
  AxesLabel \rightarrow \left\{ "x", "\frac{\sin(x)}{m}" \right\}
Plot[Sin[x] /x, {x, -5 Pi, 5 Pi},
  PlotRange → {-0.25, 1.25}, PlotStyle → {Red, Thick},
  \mathtt{AxesLabel} \rightarrow \left\{ \texttt{"x", "} \frac{\mathtt{Sin (x)}}{} \texttt{"} \right\}, \ \mathtt{BaseStyle} \rightarrow
    {Large, FontFamily → "Helvetica", Italic}
Plot[Sin[x] / x, {x, -5 Pi, 5 Pi},
 PlotRange → {-0.25, 1.25}, PlotStyle → {Red, Thick},
  \mathtt{AxesLabel} \rightarrow \left\{ \texttt{"x", "} \frac{\mathtt{Sin (x)}}{} \texttt{"} \right\}, \ \mathtt{BaseStyle} \rightarrow
   {Large, FontFamily → "Helvetica", Italic},
  TicksStyle → {{Medium, Blue},
     {Medium, RGBColor[0.5, 0.2, 0]}}
```

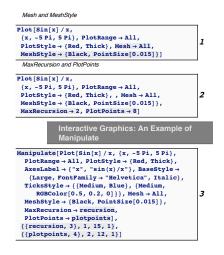
- 1: This is the simplest version of Plot: all it requires is an expression depending on a variable and a range over which to plot that variable.

 MATHEMATICA® has algorithms to select the region which is most likely to be of interest.
- 2: Tweaking the appearance of a plot will usually involve changing one of Plot's options.
- 3: Here we change PlotRange and PlotStyle explicitly. PlotStyle takes a list of graphics directives, and the type of PlotStyle directives will generally depend on what is being plotted (i.e., lines, points, surfaces).
- 4: The AxesLabel option is used here. The BasicMathInput-palette is useful to typesetting mathematical expressions.
- 5: The option BaseStyle can be used to specify the basic size, font, font-shape, etc for the entire plot.
- **6:** As a last example, we use a list of two styles for TickStyle to specify both x- and y-axis ticking characteristics.

Plotting Precision and an Example of Interaction

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Even for continuous functions, a graphical representation is a discrete object. The level of precision is associated with the *mesh*—which is the set where numerical evaluations are performed. More mesh points generally results in a smoother representation, but at the cost of longer computation and memory.



- 1: The option Mesh→All shows the points where Plot made numerical evaluations. Note that the points are not equally spaced, but are adapted to the plot (in this case, to the curvature). MeshStyle permits specification of how the mesh is visualized.
- 2: A simple way to control the mesh is with PlotPoints (which specifies how many points to sample initially) and MaxRecursion (which specifies how many times to try to optimize the adaptation of the points on the curve).
- 3: This is a simple example of using Manipulate to change PlotPoints and MaxRecursion interactively. Here, both of the options point to variables (recursion and plotpoints) that can be adjusted via a graphical interface.

Multiple Curves, Filling, and Excluding Points

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Here, simple examples of plotting several curves at the same time, of filling between curves, or between curves and the axis, and of telling plot to ignore certain points, are demonstrated.

```
\begin{split} & \textbf{Plot}[\textbf{Sin}[\textbf{x}] \, / \, \textbf{x}, \, \left(\textbf{x}, -5 \, \textbf{Pi}, \, 5 \, \textbf{Pi}\right), \\ & \textbf{PlotRange} \rightarrow \left\{-0.25, \, 1.25\right\}, \\ & \textbf{PlotStyle} \rightarrow \left\{\text{Red}, \, \textbf{Thick}\right\}, \\ & \textbf{TicksStyle} \rightarrow \left\{\left(\text{Medium}, \, \textbf{Blue}\right), \, \left(\text{Medium}, \, \textbf{RGSColor}[0.5, \, 0.2, \, 0]\right)\right\}, \\ & \left\{\text{Medium}, \, \textbf{RGBColor}[0.5, \, 0.2, \, 0]\right\}\right\}, \end{split}
   Filling → Automatic]
    Combining several curves
Plot[\{\sin[x] / x, \tan[x] / x\},
\{x, -5 \text{ Pi}, 5 \text{ Pi}\}, \text{ BaseStyle} \rightarrow \{\text{Thick}\}]
Plot[\{\sin[x] / x, \tan[x] / x\},

\{x, -5 \text{ Pi}, 5 \text{ Pi}\}, PlotStyle \rightarrow \{\{\text{Red}, \text{Thick}\}\},

\{\text{Hue}[0.3, 1, .5], \text{Thickness}[0.005]\}\}
    Removing points with Exclusions
Plot[Tan[x] / x, {x, -5 Pi, 5 Pi},
   BaseStyle → {Thick, Medium},
Exclusions → {-Pi/2, Pi/2}]
Plot[Tan[x] / x, {x, -5 Pi, 5 Pi},

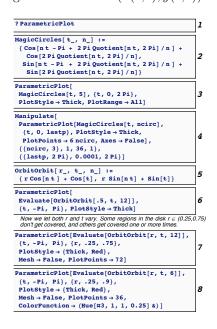
BaseStyle → {Thick, Medium}, Exclusions →
     Table[p, {p, -9 Pi/2, 9 Pi/2, Pi}]]
    Multiple curves with exclusions
Plot[{Sin[x]/x, Tan[x]/x}, {x, -5 Pi, 5 Pi},
    PlotStyle → {{Red, Thick}, {Hue[0.3, 1, .5],
Thickness[0.005]}}, Exclusions →
     Table[p, {p, -9 Pi/2, 9 Pi/2, Pi}]]
    Filling between curves
Plot[{Sin[x]/x, Tan[x]/x},
  {x, -5 Pi, 5 Pi}, PlotStyle → {{Red, Thick}, 
{Hue[0.3, 1, .5], Thickness[0.005]}},
PlotRange → {-0.25, 1.25}, Exclusions →
  Table[p, {p, -9 Pi/2, 9 Pi/2, Pi/2}],
Filling \rightarrow {2 \rightarrow {{1}, {RGBColor[1, 0, 0, 0.2],
                RGBColor[0, 0, 1, 0.2]}}}]
```

- 1: Simple filling to the x-axis can be produced with Filling \rightarrow Automatic.
- 2: When Plot gets a list of expressions as its first argument, it will superimpose the curves obtained from each. The curves' colors are chosen automatically, but can be specified. (n.b., if you find that the colors are not changing as you'd expect, try calling Evaluate on the list.) In this example, a vertical line appears for the $\tan(x)/x$ function where the values change as $\pm\infty$. To change the appearance of each curve, a list containing a style-directive list for each curve is used for the PlotStyle option. The first style, {Red,Thick}, uses simple directives for basic, easy-to-remember, control; the second style uses higher precision control with Hue and Thickness.
- **3:** The singularities in the function produce vertical lines in the above plots. To remove these features, the option Exclusions can get a list of points where the curve should be sliced and not evaluated.
- 4: Here, we use Table to produce a list of all the singularities in $\tan(x)/x$. This list is passed via Exclusions.
- 7: This is a more complex example of filling: here we ask for the filling to take place between the second curve and the first—and to use different filling styles when the first curve lies above or below the second curve.

Plotting Two Dimensional Parametric Curves and Mapped Regions

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Here are simple examples of using ParametricPlot to plot functions for curves in the form (x(t), y(t)) and regions in the form (x(s,t), y(s,t)).

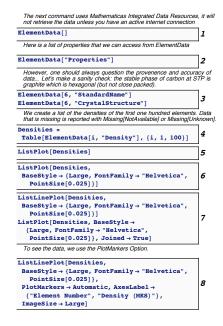


- 2: A function, MagicCircles[t,n], is defined to produce some interesting parametric plots. It returns data in the form $\{x(t),y(t)\}$ where $t \in (0,2\pi)$. The second argument, n, is a parameter which will determine how many circles get drawn.
- **3:** ParametricPlot is used with the PlotStyle option set for thick curves, and PlotRange set to All.
- 4: Here, we make ParametricPlot the first argument to Manipulate so that the number of circles can be varied (note, that we force n to iterate over integers). The trajectory of the curve can be visualized here by interactively changing the upper bound of t with lastp.
- 5: We cook up another function, OrbitOrbit[r,t,n], to demonstrate filling a region. Data is returned in the form $\{x(r,t),y(r,t)\}$, and n is a parameter.
- **6:** If r is fixed, ParametricPlot produces a curve as before.
- 7: Letting both r and t vary, produces a two-dimensional region—one might think of the region as the set of all the curves for different r.
- 8: This is a slightly advanced example where we use a *pure function* for the ColorFunction option. I'm including this example because I think it's pretty.

Simple Plots of Data

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One of Mathematica® 's integrated data resources, ElementData, is used to demonstrate plotting of discrete data.



- 1: ElementData will download physical data for the elements via an internet connection. This command won't work if you do not have an active connection. However, similar data remain in the now obsolete ChemicalElements package.
- 2: This produces a list of properties that are available. One should always suspect data sources! The stable form of carbon and graphite, is hexagonal but not close-packed.
- **3:** For example, this is how to access properties for carbon.
- 4: Table is used with ElementData to produce a list, Densities, of the first 100 elements for subsequent use. Missing data are indicated with the function Missing.
- 5: Simply using ListPlot produces an indexed scatter plot.
- **6:** Like Plot, we can use options in ListPlot and ListLinePlot to change the appearance of the graphic.
- 7: A set of line segments are drawn (approximating a curve) in ListLinePlot—which is equivalent to using ListPlot with the option PlotJoined set to True.
- 8: Using the PlotMarkers option, both the data and the line segments are visualized.

Getting More out of Displayed Data: Screen Interaction

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Putting too much information on a single data graphic can make it difficult to understand. Using pop-up windows with the mouse can be a nice way to improve graphical information flow. Here, we show how this can be done using Tooltip. In these examples, where the extra information appears can be altered by replacing Tooltip with StatusArea, Annotation, or PopupWindow.

```
Example with Toolip to make graphics interactive—put your mouse over a point and you get a pop-up with more information

ListLinePlot[Tooltip[Densities],

BaseStyle + {Large, FontFamily + "Helvetica",
    PointSize[0.025]},
    PlotMarkers + Automatic, AxesLabel +
    {"Element Number", "Density (MKS)"},
    ImageSize + Large!

This is a slightly more complicated example of Toolip. We create a data structure with (X(J)(W)) = (density(f), bulkmodulus(f)) and then tell Tooltip to pop-up the element's symbol when the mouse is over it.

ListPlot[
Table[Tooltip[{ElementData[i, "Density"],
    ElementData[i, "BulkModulus"]},
    ElementData[i, "BulkModulus"]},
    ElementData[i, "Abbreviation"],
    LabelStyle + (Large)], (i, 1, 100)],
    BaseStyle + (Large)], FontFamily - "Helvetica",
    PointSize[0.025]), PlotMarkers + Automatic,
    AxesLabel + {"Density", "Bulk Modulus"},
    IndgeSize + Full]
```

- 1: This is a simple example of Tooltip: wrapping the first argument to ListPlot or ListLinePlot inside Tooltip will show the value of each data point when the mouse is over it.
- 2: I like this example which uses <code>Tooltip[{xi,yi},labeli]</code> to produce an interesting way to pick material properties. Suppose we were interested in finding materials that are very stiff (large bulk modulus) but not very heavy (low density)—plotting modulus versus density will identify "interesting" elements in the northwest region of the plot. Using <code>Tooltip</code> with <code>ElementData[i,'Abbreviation'']</code> allows us to explore element properties without cluttering up the plot. I use <code>LabelStyle</code> as an option for <code>Tooltip</code> and <code>ImageSize</code> as an option for <code>ListPlot</code> to make things readable on the display.

Graphical Data Exploration, continued

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We use BarChart and PieChart in the BarCharts and PieCharts packages to explore the relative abundances of different crystal structures among the elements. A three-dimensional histogram of elements selected by their melting points and densities is produced with Histogram3D from the Histograms package.

```
Here we do a small exercise to get a graphical representation of which 
Crystal Structures the elements form, and represent the frequency of 
each type. First we create a list of known elemental crystal structures for 
the list 100 elements.
CrystalStructures = Table[ElementData[
     i, "CrystalStructure"], {i, 100}]
UniqueStructures = Tally[Cases[
CrystalStructures, Except[Missing[_]]]]
MatrixForm[UniqueStructures]
  Here is a bar chart showing the frequency of crystal structu
BarChart[Transpose[UniqueStructures][[2]],
 BarLabels ->
   Transpose[UniqueStructures][[1]]
 \label{eq:baseStyle} \begin{split} & \texttt{BaseStyle} \rightarrow \{\texttt{Large, FontFamily} \rightarrow \texttt{"Helvetica"} \} \,, \\ & \texttt{BarOrientation} \rightarrow \texttt{Horizontal, ImageSize} \rightarrow \texttt{Full}] \end{split}
Needs["PieCharts`"]
PieChart[Transpose[UniqueStructures][[2]],
 Transpose[UniqueStructures][[1]],
BassStyle → (Large, FontFamily → "Helvetica"),
ImageSize → Full]
  As a last example, we produce a 3D histogram. The height of each bar corresponds to the number of elements in a range of melting points and
   range of dens
Needs["Histograms`"]
histdata = DeleteCases[Table[
     HistogramCategories → {16, 24} ]
```

- 1: CrystalStructures will be a list of the crystal structures of the most stable solid phase. (I am not sure what is meant by most stable—this is ambiguous, but that is what it says in the documentation)
- 2: UniqueStructures will be a list of pairs—each item will be comprised of a crystal structure and how many times it appears. We use Cases to remove missing data by using a pattern, and then use Tally to create the data structure.
- 3: Because BarChart needs data of the form {y1, y2, ...}, we need to manipulate the data. To get the data, Transpose will put the abundances into the second row, which is also the list we need. We use the first row of the transpose for the BarLabels option. The plot is easier to read if horizontal, so we use the BarOrientation option.
- 4: Here we simply replace the barchart with PieChart.
- 5: As a final example, we create a histogram of elements with similar densities and melting points. We use a pattern with an "or" in Cases to remove missing data with DeleteCases, because we cannot plot data where either the density or the melting point is missing.

Three-Dimensional Graphics

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Here we show examples of three-dimensional graphics, although it would be better to say, 3D graphics projected onto a 2D screen.

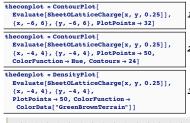
```
EPot[x_, y_, z_, xo_, yo_] :=
   \sqrt{(x-xo)^2 + (y-yo)^2 + z^2}
SheetOLatticeCharge[x_, y_,
  Sum[EPot[x, y, z, xo, yo], 
{xo, -5, 5}, {yo, -5, 5}]
   SheetOLatticeCharge represents the electric field produced by an 11 by 11 array of point charges arranged on the x-y plane at z = 0. The following command evaluates and plots the field variation in the plane z = 0.25:
Plot3D[
  Evaluate[SheetOLatticeCharge[x, y, 0.25]],
  \{x, -6, 6\}, \{y, -6, 6\}
  Note below how theplot is set to contain the output of the Plot3D command—it is now a symbol assigned to a graphics object. The number of plotpoints is increased so that we can resolve all the bumps. This will take a while to compute on most machines.
theplot = Plot3D[
   Evaluate[SheetOLatticeCharge[x, y, 0.25]], \{x, -6, 6\}, \{y, -6, 6\}, PlotPoints \rightarrow 60]
   This demonstrates the use of RegionFunction plot option which is
   function. Here, only the region inside a cylinder with radius 9 (x^2 + y^2
  92) is plotted.
Plot3D[
 Evaluate[SheetOLatticeCharge[x, y, 0.25]], \{x, -9, 9\}, \{y, -9, 9\}, PlotPoints \rightarrow 60, RegionFunction <math>\rightarrow (\sharp 1^2 + \sharp 2^2 \le 81 \&)]
   This demonstrates the use of the ColorFunction plot option which is pure function. Here we use one of Mathematica ColorData functions.
  Evaluate[SheetOLatticeCharge[x, y, 0.25]],
  {x, -9, 9}, {y, -9, 9}, PlotPoints
    egionFunction \rightarrow (#1^2 + #2^2 \leq 81 &),
    (ColorData["TemperatureMap"][#3] &)]
```

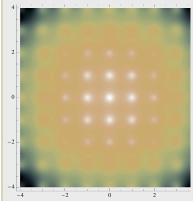
- 1: This is the electrostatic potential as a function of (x, y, z) due to a single positive charge located at $(x_o, y_o, z = 0)$ (i.e., anywhere on the z = 0 plane).
- 2: By summing over a square lattice of unit charges, this function (SheetOLatticeCharge) computes the electrostatic potential over a 11×11 square-lattice of point-charges centered on the z-plane as a function of x, y, and z.
- 3: Plot3D plots data of the form f(x,y) (f is the height above a point (x,y)). Therefore, we must fix one of the coordinates; here we visualize the electrostatic potential at a fixed height (z=0.25). Note that the bounds for both the "horizontal" and "into-screen" coordinates need to be specified.
 - You can rotate the graphics by dragging the mouse over the surface, translate by dragging with the shift-key held down, and zoom with the alt-key held down.
- 4: With sufficiently many PlotPoints, the structure of the potential at a fixed distance z=0.25 is made apparent. The finer details are not resolved at lower resolutions, but using 60 points in each direction may be overkill and this will be slow on older computers and may not fit on machines with little memory.
- 5: RegionFunction is new as of MATHEMATICA® 6. This is an advanced examples, but it demonstrates how one can plot over non-rectangular domains.
- **6:** As a last example, the use of the new ColorData functions for the ColorFunction option is demonstrated.

Colors and Contours: Three-Dimensional Graphics in Two Dimensions

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Three dimensions can also be visualized by drawing level sets (as in a topographical map) or by drawing colors (as in a relief map). The data burden is usually much smaller than a 3D graphics object, is sometimes easier to interpret, and is certainly easier to publish.



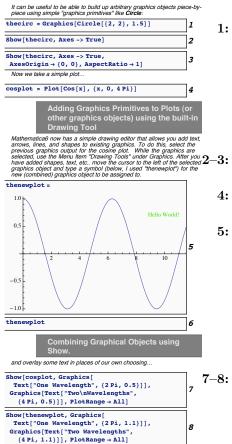


- 1: We reproduce the 3D graphics object for the sheet of electric charges using ContourPlot. Here, the number of contours are picked arbitrarily, but PlotPoints has to be increased to resolve details of the function. Moving the mouse over one of the contours will give a pop-up window for the value along that contour.
- 2: In the representation above, we might conclude that a positive charge (such as a hole) confined to z=0.25 could not be "trapped" because no minima are obvious. Increasing the number of contours with the Contours option improves the resolution so that local minima can be observed. Here we pass Hue to the ColorFunction option; however, I don't find this satisfactory because both the largest and the smallest values are red. In other words, the color scaling runs completely around the outside of a color wheel and ends up where it started.
 - Unless options are sent requesting otherwise, the values of the plot will be scaled so that the maximum and minimum values are 1 and 0. Thus, two plots would look the same whether the differences are very small or very large. This feature is controlled by ColorFunctionScaling.
- 3: Here, instead of a single color decorating the region between two neighboring contours, a color is plotted directly indicating the "height" of the function. ColorData is used with GreenBrownTerrain so that the high potentials look like snow-covered peaks and lower potentials look like green river-deltas.

Graphics Primitives, Drawing on Graphics, and Combining Graphical Objects

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Here, examples of placing *Graphics Primitives* into a *Graphics Object* are demonstrated by direct means: by a drawing tool, and by sequential combination.



1: A Circle is a graphics primitive, and making a primitive an argument to Graphics returns a "Graphics Object." When a graphics object is output, graphics appear. The graphical output can be suppressed by a trailing semicolon. In this case, thecirc is assigned to the graphics object and it is displayed. If a trailing semicolon appears (e.g., a unit circle thecirc = Graphics[Circle[]];), then the assignment is made to thecirc, but no graphics are sent to the display.

Additional options can be added to a graphics object with Show. The result is a new graphics object.

- 4: Here we create a graphics object and assign it to the symbol cosplot by simply using Plot.
- 5: If the mouse is clicked on the display of the graphics object, then it can be edited just like input. Clicking to the left of the object allows you to type a symbol for assignment to the graphics object. Shown here is the result of assigning a graphic to thenewplot. If the graphic is selected, then a *Drawing Tools Widget* can be pulled up under the Graphics menu item. With the widget, other primitives such as text, lines, arrows, and shapes can be combined. When the expression is evaluated, the combined graphics will be assigned to thenewplot.

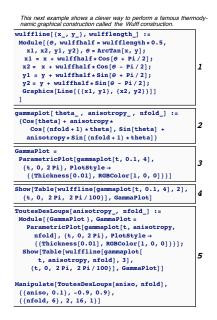
: Here, Show is used to add text via a graphics primitive to the original plot and to the new combined graphics object.

A Worked Example: The Two-Dimensional Wulff Construction

Download notebooks, pdf(color), pdf(bw), or html from http://pruffle.mit.edu/3.016-2009.

The Wulff construction is a famous thermodynamic construction that predicts the equilibrium enclosing-surface of an anisotropic isolated body. The anisotropic surface tension, $\gamma(\hat{n})$, is the amount of work (per unit area) required to produce a planar surface with outward normal \hat{n} . The construction proceeds by drawing a bisecting plane at each point of the polar plot $\gamma(\hat{n})\hat{n}$. The interior of all bisectors is the resulting Wulff shape.

A working example of the Wulff construction for a $\gamma(\theta)$ in two dimensions is produced here.



- 1: This function takes a point $\{x,y\}$ as an argument and then returns a graphics object of a line of specified length. The line is the perpendicular bisector required by the Wulff construction.
- 2: This is an example $\gamma(\hat{n})$ with the surface tension being smaller in the $\langle 11 \rangle$ -directions (if the anisotropy parameter is positive).
- 3: A particular instance of a γ -plot is assigned to GammaPlot.
- 4: Table is used to produce a list of graphics objects by calling wulf-fline function at one hundred points on the γ -plot. The equilibrium shape is the interior of all the curves and the γ -plot from which it derives is superimposed by collecting all the graphics together with Show.
- 5: All the above steps are collected together and bundled into a Module to produce a single visualization function, *ToutesDesLoups*. The function depends on the prior definition of gammaplot[t, \alpha, n].
- **6:** Here, *ToutesDesLoups* is used as the argument to Manipulate to visualize the effect of changing the anisotropy factor and the n-fold axis.

Graphical Animation: Using Time as a Dimension in Visualization

Animations can be very effective tools to illustrate time-dependent phenomena in scientific presentations. Animations are sequences of multiple images—called frames—that are written to the screen interatively at a constant rate: if one second of real time is represented by N frames, then a real-time animation would display a new image every 1/N seconds.

There are two important practical considerations for computer animation:

frame size An image is a an array of pixels, each of which is represented as a color. The amount of

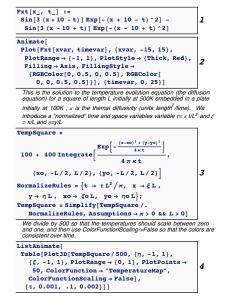
memory each color requires depends on the current image depth, but this number is typically 2-5 bytes. Typical video frames contain 1024×768 pixel images which corresponds to about 2.5 MBytes/image and shown at 30 frames per second corresponding to about 4.5 GBytes/minute. Storage and editing of video is probably done at higher spatial and temporal resolution. Each frame must be read from a source—such as a hard disk—and transferred to the graphical memory (VRAM) before the screen can be redrawn with a new image. Therefore, along with storage space the rate of memory transfer becomes a practical issue when constructing an animation.

animation rate Humans are fairly good at extrapolating action between sequential images. It depends on the difference between sequential images, but animation rates below about 10 frames per second begin to appear jerky. Older Disney-type cartoons were typically displayed at about 15 frames per second, video is displayed at 30 frames per second. Animation rates above about 75 frames per second yield no additional perceptable "smoothness." The upper bound on computer displays is typically 60 hertz.

Animation

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Animations are a nice way to visualize an extra dimension, like time. An animation is composed of a sequence of displayed graphics (frames) that are displayed iteratively. Animations are fairly easy to create—and can be great fun.

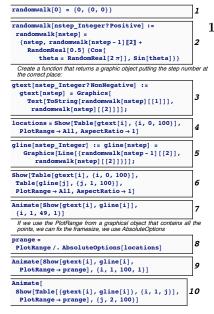


- 1: We will create a simple animation by cooking up a function f(x,t) and then plotting it for a range of x and for a sequence of t's.
- **2:** This plot would be the frame associated with t = 0.
- 3: Using Plot as the argument to Animate produces the animation. Note, xvar 'belongs' to Plot while timevar belongs to Animate. Can you imagine what the animation would look like if we animated over x and plotted over t? No? Try it!
- We will produce a three-dimensional animation of how the temperature would change in a flat plate, if at time t=0 there is a square at a different temperature than the rest of the plate. The governing partial differential equation is $\partial T/\partial t = \kappa \nabla^2 T$ and for initial conditions T(x, y, t = 0) = 500 when -L/2 < x, y < L/2 and T = 100otherwise, the closed form solution can be expressed as an integral. To make a plot, we must send a function that can be evaluated numerically. To do this, we must non-dimensionalize variables (also known, as dimensional scaling or normalizing variables). This is done by dividing variables having physical units (such as x), with a characteristic quantity in the model that has the same physical units (here, we will use the model's length L to produce a dimensionless variable $\xi = x/L$) NormalizeRules is a set of rules that can be applied to our physical problem. After the normalization rules are applied, the properly scaled solution should be a non-dimensional temperature-quantity as a function of non-dimensional space- and time-quantities.
- finally, we will use Plot3D inside ListAnimate. Plot3D's argument is scaled by dividing by the maximum temperature, so that all temperature-like quantities scale between zero and one. We turn off ColorFunctionScaling so that the 'meaning' of each color remains constant in the animation. ListAnimate takes a list of frames that are produced via Table.

An Example of Animating a Random Walk

Download notebooks, pdf(color), pdf(bw), or html from http://pruffle.mit.edu/3.016-2009.

A random walk process is an important concept in diffusion and other statistical phenomena. Functions to simulate a random walk in two dimensions are constructed and then visualized with animations.



- 1–2: This is a recursive function that simulates a random walk process. Each step in the random walk is recorded as a list structure, { {iteration number}, { x , y }}, and assigned to randomwalk [iteration number]. For each step (or iteration), a number between 0 and 1/2 is selected (for the magnitude of the displacement), and an angle between 0 and 2π is selected (for the direction), with each of these numbers being selected randomly from a uniform distribution (using RandomReal). The function includes an assignment, so all previous values are stored in memory.
 - **3:** The function *gtext* calls *randomwalk* to create a text graphics-object located at the position corresponding to nstep.
 - 4: This shows the history of a random walk after 50 iterations by combining the graphics objects created by *gtext*. The resulting graphics object gets assigned, because we will use some information contained in it later.
 - 5: To improve the physical interpretation of the previous graphic, it would be an aid to the eye if the individual jumps were indicated. To do this, the function *gline* calls *randomwalk* to create a line graphics-object connecting the position corresponding to nstep to its previous position.
 - 7: Thus, we could animate by combining the line and the text with Show and using that as the argument to Animate. However, this result will be unsatisfactory because the "length scale" of each frame will not be consistent.
 - 8: To solve this problem, we find the bounds of a graphics object (locations) that contains all the points, and then query its PlotRange using AbsoluteOptions and this is assigned to a symbol prange.
 - 9: The animation is consistent now, but could still use some improvement.
- 10: Here, we animate the graphics object that also contains the history of prior jumps. This is not a terribly efficient way to do this because we recreate the early steps many times over, but it works for our purposes.

Worked Example (part A): Visualizing the Spinodal and Common Tangent Construction

Download notebooks, pdf(color), pdf(bw), or html from http://pruffle.mit.edu/3.016-2009.

The spinodal and common tangent construction is a fundamental thermodynamic concept used for the creation of an alloy phase diagram from molar-free energies. This construction appears repeatedly in studies of materials. An example of visualizing this construction as a function of temperature will be worked out in detail for the case of a single curve and a binary alloy.

First, we will work out all the steps in detail that are used to build up a single visualization, and then we will collect it all together in a reusable function.

```
A prototype molar free energy of mixing using the same xlogx function for
the ideal entropy of mixing terms. The temperature term is a scaled
energy (RT), and it is assumed that enthalpies have been scaled so that
the temperatures of interest (if there are any) are between T=0 and T=10.
  x\log x[1] = x\log x[0.0] = x\log x[1.0] = 0;
 Here is the shape of our prototype free energy at T=3/2
p1 = Plot[Gmolar[x, 3/2]
    \{x, 0, 1\}, PlotStyle \rightarrow Thick]
  We will need the bounds of the above graphics object:
{{graphxmin, graphxmax},
 {graphymin, graphymax}} =
PlotRange /. AbsoluteOptions[p1, PlotRange]
  First let's determine where the spinodal region (by finding where the second derivative with respect to composition is negative
ddg = D[Gmolar[x, 3/2], {x, 2}]
   Then, use RegionPlot to illustrate the range over which spinodal decomposition is spontaneous
p2 = RegionPlot[ddg < 0,
    {x, graphxmin, graphxmax},
{T, graphymin, graphymax},
PlotStyle→RGBColor[0, 1, .5, 0.1]]
   Show them both together to identify the spinodal region
Show[p1, p2]
                                                                                         6
```

- 1: We cook up a prototypical molar free-energy as a function of molar composition, X, and temperature T. The $x \log x$ terms are calculated with a handy function, $x \log x$, which will handle the zeroes without numerical difficulty at $0 \log[0]$.
- 2: The molar free-energy is plotted at a particular temperature (T = 1.5) and assigned to a symbol, pl.
- 3: We will need the bounds of the plot to create other graphical objects. We grab the bounds with AbsoluteOptions and assign them to variables using a handy assignment construction {a,b} = List.
- **4:** The spinodal region is the easiest to visualize—it is the region where the second derivative of the molar free-energy is negative. The second derivative is assigned to ddg.
- 5: RegionPlot evaluates its first argument over a square region and fills where the argument is true. It is exactly what we need in order to visualize the spinodal region. We use the bounds that we calculated from the free energy curve as the bounds for RegionPlot.
- **6:** Showing both plots together, we visualize the spinodal region.

Worked Example (part B): Visualizing the Spinodal and Common Tangent Construction

Download notebooks, pdf(color), pdf(bw), or html from http://pruffle.mit.edu/3.016-2009.

The common tangent is any finite line segment that touches the molar free-energy at two points which have the same derivative. For phase diagrams, we are interested only in lower common tangents (i.e., lines that touch the molar free-energy, but always lie below all values). One can picture the common tangent by imagining that an elastic string is stretched along a molar free-energy curve; the common tangents are where the string pulls away from the the curves.

The common tangent is related to the *convex hull* that appears in computational geometry.

```
We can use the ConvexHull to find the common tangent lines; this function is in the Computational Geometry Package.
<< ComputationalGeometry
                                                                                                            1
   First we compute a list of values along the molar free energy curve, then compute those that lie outside the common tangent(s) (i.e., the convex hull). Because the points are given in order, we might as well sort them on the way back out. Note, the convex hull program gives the indices of the vertices that are on the hull.
npoints = 100:
gvals = Table[{x, Gmolar[x, 3/2]},
     {x, 0, 1, 1/N[npoints - 1]}];
    We only want the lower convex hull; therefore we add some "fictive" points to the beginning and the end of the data. The the fictive points add a rectangle to the top of the curve that should be part of the computed convex hull.
gmax = Max[Transpose[gvals][[2]]];
 PrependTo[gvals, {0, 10 * Abs[gmax]}];
AppendTo[gvals, {1, 10 * Abs[gmax]}];
    After we compute this hull, we shift the hull by one and take off its first 
and last element. We strip the first and last element from the discrete 
values of free energy as well.
chul1 = Sort[ConvexHull[gvals]];
 chull = Drop[Drop[chull - 1, 1],
gvals = Drop[Drop[gvals, 1], -1]
   The common tangent(s) correspond to gaps in the vertex list of the common tangent. We will use Split to find the set of continous sequences
convexparts = Split[chull, (#2 - #1 < 2) &]
     {{1, 2, 3, 4, 5, 6}, {95, 96, 97, 98, 99, 100}}
```

 To calculate convex hulls, the ComputationalGeometry package is needed.

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- 2: ConvexHull operates on discrete data. Discrete data are created by evaluating *Gmolar* at npoints evenly-spaced mesh-points. We use Table and assign the discrete data list to gvals.
- 3: ConvexHull calculates the *entire hull* (i.e., the polygon that encloses all other points), and we are only interested in the lower hull. Thus, we add a rectangle to the top of the data which is guaranteed to be part of the hull, calculate the hull and discard the upper parts. Here we use PrependTo to add a point ten times higher than the maximum value on the left side of the region, and use AppendTo to add a corresponding point to the right side of the region. We have thus added a known rectangle that we will remove later.
- 4: ConvexHull returns a list of indices of points from the original data. Because the original data was created in an orderly left-to-right way, we can use Sort to put the data in a predictable form. Because there was an additional point added at the beginning of gvals, we will need to shift the indices down by one (by subtracting 1 from each index), and then we use Drop to remove the first and last elements of both chull and gvals.
- 5: Thinking about the indices on the convex hull, any ordered sequence of the sorted list must be part of original discrete data and also part of the convex hull. We are interested in connecting the last point of any isolated sequence to the first point of the next sequence. We can use Split to find the isolated sequences.

Worked Example (part C): Visualizing the Spinodal and Common Tangent Construction

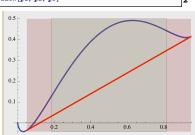
Download notebooks, pdf(color), pdf(bw), or html from http://pruffle.mit.edu/3.016-2009.

With the information contained in the convex hull data, graphical objects are created to represent the gaps in that data. The gaps coincide with the common tangents.

```
Now we create graphics objects for each of the two-phase regions (i.e., the gaps in the convex hull) and collect them all into a graphics list for subsequent display.

len = Length[convexparts];
graphicslist = {};
i = 1;
While[i + 1 ≤ len, leftpoint =
    gwals[[Last[convexparts[[i]]]];
    rightpoint = gwals[[
        First[convexparts[[i+1]]]];
    ctline = {Red, Thick,
        Line[{leftpoint, rightpoint}]};
    twophaseregion = {RGBColor[0.5, 0, 0, 0.2],
        Rectangle[{leftpoint[1]], graphymin},
        (rightpoint[[1]], graphymax]);
    AppendTo[graphicslist, ctline];
    AppendTo[graphicslist, twophaseregion];
    i++
    j
p3 = Graphics[graphicslist]

Show[p1, p2, p3]
```



- 1: We traverse the list convexparts and construct graphical objects corresponding to the regions of isolated sequences. Because it is possible that a curve may have any number of common tangents, we accumulate graphics primitives in a list as we encounter common tangents. A graphics object is created from the list of graphics primitives.
 - The number of isolated sequences is assigned to len and we start with an empty list graphicslist. Then, we loop over the list of length len. At each iteration in the loop, we identify the last vertex on the previous point of the convex hull sequence and the first part of the next sequence. We use those indices to extract the points on the curve that have been stored in gvals. With the two points, we create red lines for the common tangents—and with the extra graphical information about the original plot, draw a rectangle for the region.

Finally, a new graphics object (p3) is created.

2: Our final visualization is obtained by showing all three graphics objects together.

Worked Example (part D): Visualizing the Spinodal and Common Tangent Construction

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The previous three parts illustrate how one might actually go about developing a complex visualization: create simple working parts and then integrate them together into something more complex. (Don't get the impression that I didn't make any errors or silly conceptual mistakes as I created this example! It was very time consuming and, while it looks fairly straightforward in hindsight, it was a challenge to build.) However, once finished, it is useful to collect everything into a single function that can be reused.

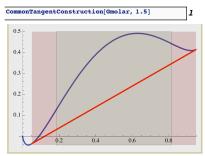
1: Here is the result, CommonTangentConstruction, which collects the previous three examples together and returns a single graphical object. CommonTangentConstruction takes two arguments for the molar free-energy function, Gm, and temperature T, and an optional third argument for the precision to calculate the hull. The optional argument is indicated by the :100 and will default to 100 if not passed to the function.

The first argument must be the name of a defined function of composition and temperature.

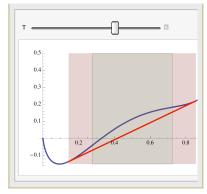
Worked Example (part E): Visualizing the Spinodal and Common Tangent Construction

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Examples of visualizing with CommonTangentConstruction are presented here.







- 1: This is the construction at T = 1.5.
- 2: Here we use the construction as an argument to Manipulate so that we can observe the effect of temperature on the spinodal and common tangent construction.