Maple

Lecture 13

Lecture course: Computational methods in Meso-Bio-Nano Science

by Dr.phil.nat.Dr.rer.pol. Matthias Hanauske

GOETHE UNIVERSITÄT FRANKFURT AM MAIN

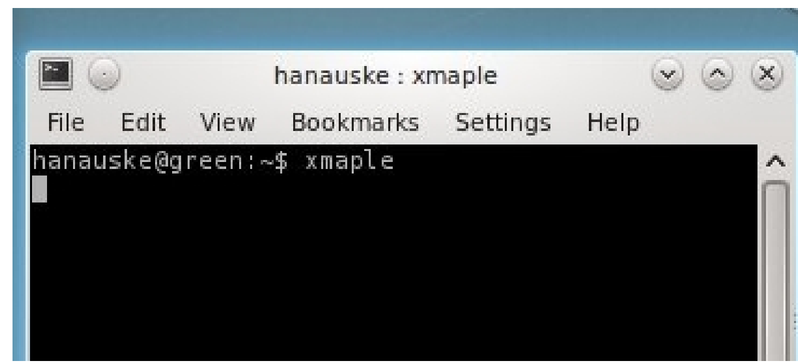
Contents

1. Getting started
2. Symbolic calculations
3. Numerical calculations
4. Visualization of data
5. Programming tools
6. Advanced examples

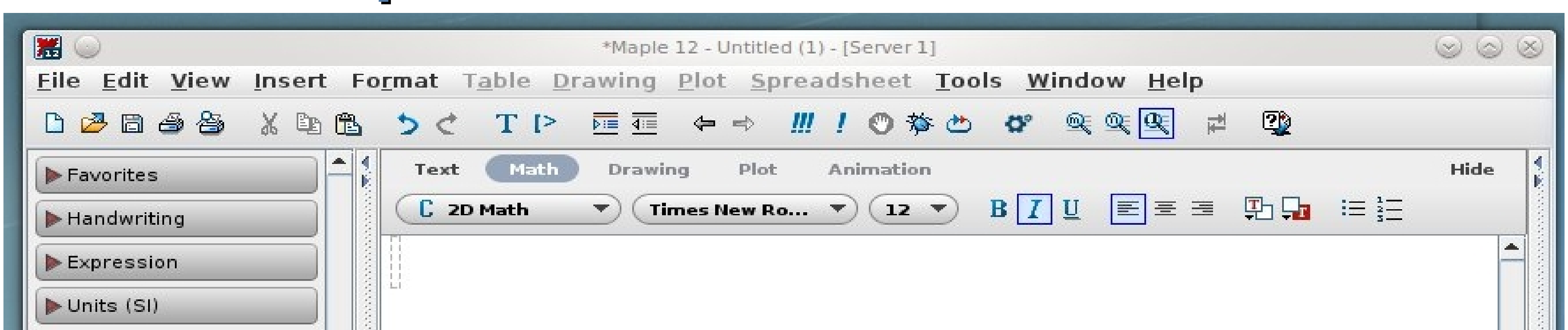
Getting started

Maple (Maplesoft) is a **computer algebra system**, first developed in 1980 by the Symbolic Computation Group at the **University of Waterloo** in **Waterloo, Ontario, Canada**. The first version (Maple 1.0) was released in 1982 and the current version (Maple 15) has been released in 2011.

To run Maple on a terminal at FIAS, please type “xmaple” in a Linux-shell and enter ‘return’.



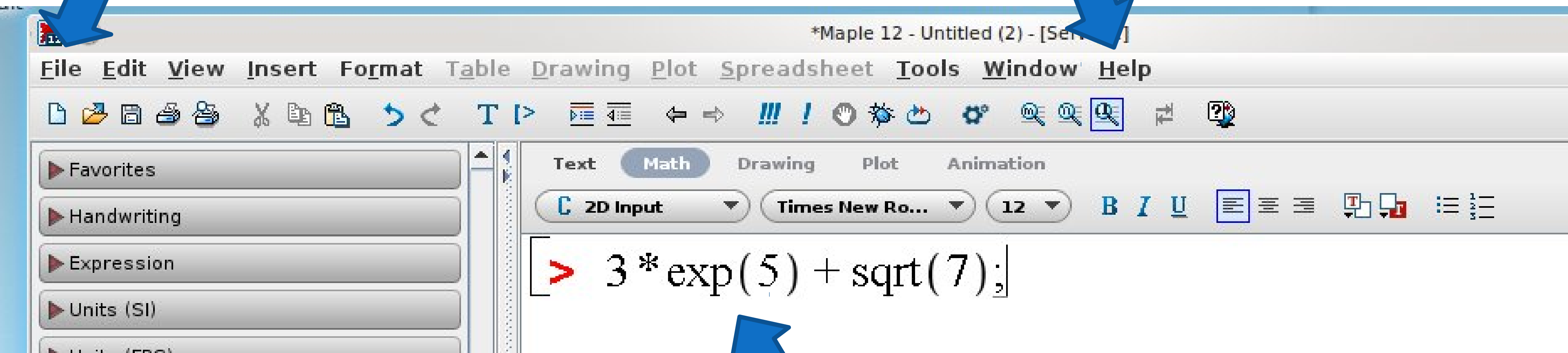
Maple 12



Getting started

By clicking at "File", you can create new 'Maple-Worksheeds' or load existing 'Worksheeds'

By clicking at "Help", you can learn about the different maple contents



To evaluate or execute something in Maple, you simply type the expression (as a Maple input) into the worksheet. Please use after each expression a semicolon ';' and press "enter".

Getting started

The first section of the “Maple Tutorium Worksheed” is displayed on the right. You can download it from the following **internetlink**

The red expressions are the Maple inputs written by the user, whereas the blue equations and numbers are the Maple outputs.

> **Maple Tutorium**

Getting started

```
> 3*exp(5)+sqrt(7);
```

$$3\,e^{5}+\sqrt{7} \qquad (1.1)$$

```
> evalf(3*exp(5)+sqrt(7));
```

$$447.8852286 \qquad (1.2)$$

```
> Digits := 20:
  evalf(3*exp(5)+sqrt(7));
```

$$447.88522861879440085 \qquad (1.3)$$

exp(5), sqrt(7) : Euler's number to the power of 5, root of 7

evalf(...) : Evaluates an expression

Digits:=20: : Defines the number of digits of any following output to 20

Symbolic calculations

Symbolic Calculations

```
> restart:
```

- Definition of Variables and Functions
- Simplification of expressions
- Symbolic differentiation and integration
- Solving algebraic equations
- Solving ordinary differential equations

restart:

All of the predefined variables, functions, … are erased

Symbolic calculations

Definition of Variables and Functions

```
> A:=3;
```

$$A := 3 \quad (2.1.1)$$

```
> A+2;
```

$$5 \quad (2.1.2)$$

```
> f:=(x)->sqrt(x);
```

$$f := \mathrm{sqrt} \quad (2.1.3)$$

```
> f(4);
```

$$2 \quad (2.1.4)$$

```
> g:=(x,y)->sin(x)+cos(y);
```

$$g := (x, y) \rightarrow \sin(x) + \cos(y) \quad (2.1.5)$$

```
> g(Pi/2,0);
```

$$2 \quad (2.1.6)$$

Symbolic calculations

Simplification of expressions

```
> Exp1:=f(x)*(x^(5/2)+x^(3/2));
```

$$Exp1 := \sqrt{x}\left(x^{5/2} + x^{3/2}\right) \quad (2.2.1)$$

```
> expand(Exp1);
```

$$x^3 + x^2 \quad (2.2.2)$$

```
> Exp2:=sin(x)^2+cos(x)^2;
```

$$Exp2 := \sin(x)^2 + \cos(x)^2 \quad (2.2.3)$$

```
> simplify(Exp2);
```

$$1 \quad (2.2.4)$$

expand(...) : Expands an expression

simplify(...) : Simplifies an expression

Symbolic calculations

Symbolic differentiation and integration

```
> diff(f(x),x);
```

$$\frac{1}{2}\frac{1}{\sqrt{x}} \quad (2.3.1)$$

```
> int(f(x),x);
```

$$\frac{2}{3}x^{3/2} \quad (2.3.2)$$

```
> int(f(x),x=0..5);
```

$$\frac{10}{3}\sqrt{5} \quad (2.3.3)$$

```
> diff(g(x,y),x);
```

$$\cos(x) \quad (2.3.4)$$

```
> int(int(g(x,y),x=0..Pi),y=0..Pi);
```

$$2\pi \quad (2.3.5)$$

```
> Int(Int(g(x,y),x=0..Pi),y=0..Pi)=
int(int(g(x,y),x=0..Pi),y=0..Pi);
```

$$\int_0^{\pi}\int_0^{\pi}(\sin(x)+\cos(y))\,dx\,dy = 2\pi \quad (2.3.6)$$

diff(...), int(...) : Differentiates, integrates a function

Diff(...), Int(...) : Just displays the differentiation, integration (does not evaluate it)

Symbolic calculations

solve(...) : Solves an equation or a system of equations

Solving algebraic equations

```
> Eq1:=x^2-3*x+1=0;
```

$$Eq1 := x^2 - 3\,x + 1 = 0$$

```
> solve(Eq1,x);
```

$$\frac{3}{2} + \frac{1}{2}\sqrt{5},\ \frac{3}{2} - \frac{1}{2}\sqrt{5}$$

```
> evalf(solve(Eq1,x));
```

$$2.618033988,\ 0.381966012$$

dsolve(...) : Solves a differential equation or a system of differential equations (with or without specific initial conditions)

Solving ordinary differential equations

```
> DGL1:=diff(x(t),t)=3*x(t);
```

$$DGL1 := \frac{d}{dt}\,x(t) = 3\,x(t)$$

```
> dsolve(DGL1,x(t));
```

$$x(t) = \_C1\,e^{3\,t}$$

```
> dsolve({DGL1,x(0)=10},x(t));
```

$$x(t) = 10\,e^{3\,t}$$

Numerical calculations

Numerical Calculations

```
> restart:
```

- Limit finding
- Minimum (maximum) of lists
- Interpolation
- Numerical integration
- Solving ordinary differential equations

Numerical calculations

Limit finding

```
> Limit(sin(x)/x,x=0)=limit(sin(x)/x,x=0);
```

$$\lim_{x \to 0} \frac{\sin(x)}{x} = 1$$

Minimum (maximum) of lists

```
> List:={2,32,13,7};
```

$$\{2, 7, 13, 32\}$$

```
> min(List);
```

$$2$$

```
> max(List);
```

$$32$$

limit(...) : **Numerical calculation of the limit of a function**

{... , ... , ...} : **Unordered list of numbers or variables**

min(...), max(...) : **Minimum or maximum of a list of numbers**

Numerical calculations

Interpolation

```
> with(Statistics):
> Xvalues:=[0,1,2,3,4];
```

$$[0, 1, 2, 3, 4]$$

```
> Yvalues:=[0.2,0.98,4.1,8.8,17];
```

$$[0.2, 0.98, 4.1, 8.8, 17]$$

```
> Fit(a+b*x^2, Xvalues, Yvalues, x);
```

$$-0.0633103448275848246 + 1.04655172413793096\, x^2$$

Numerical integration

```
> int(1/exp(x*ln(x)), x=1..infinity);
```

$$\int_1^{\infty} \frac{1}{e^{x \ln(x)}}\, dx$$

```
> evalf(int(1/exp(x*ln(x)), x=1..infinity));
```

$$0.7041699604$$

with(Statistics): : Loads the extra Maple package “Statistics”

Fit(...) : Fits a model function to data

evalf(int(...)) : Numerical calculation of an integral

Numerical calculations

Solving ordinary differential equations

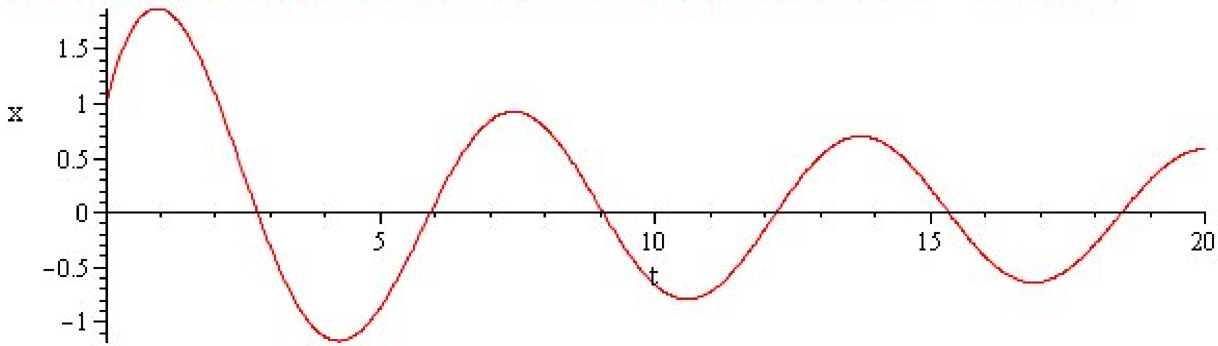
```
> DGL2:=(t+1)^2*(diff(x(t),t,t))+(t+1)*(diff(x(t),t))+((t+1)^2
  -0.25)*x(t) = 0;
```

$$(t+1)^2 \left(\frac{d}{dt}\left(\frac{d}{dt}x(t)\right)\right) + (t+1)\left(\frac{d}{dt}x(t)\right) + \left((t+1)^2 - 0.25\right)x(t) = 0 \qquad (3.5.1)$$

```
> Ergebnis:=dsolve({DGL2, x(0) = 1, (D(x))(0) = 2}, type=
  numeric,output=listprocedure);
```

$$\left[t = \mathbf{proc}\,(t)\ \ldots\ \mathbf{end\ proc},\ x(t) = \mathbf{proc}\,(t)\ \ldots\ \mathbf{end\ proc},\ \frac{d}{dt}x(t) = \mathbf{proc}\,(t)\ \ldots\ \mathbf{end\ proc}\right] \qquad (3.5.2)$$

```
> with(plots):
> odeplot(Ergebnis,[t,x(t)],0..20,numpoints=1000);
```



dsolve(...,type=numeric) : Numerical calculation of a differential equation

odeplot(...) : Plots solution curves obtained from dsolve(...)

Visualization of data

Visualisation of Data

```
> restart:
```

- 2D plots
- Contour plots
- 3D surface plots
- Spacecurves
- Animations

Visualization of data

Visualisation of Data

```
> restart:
```

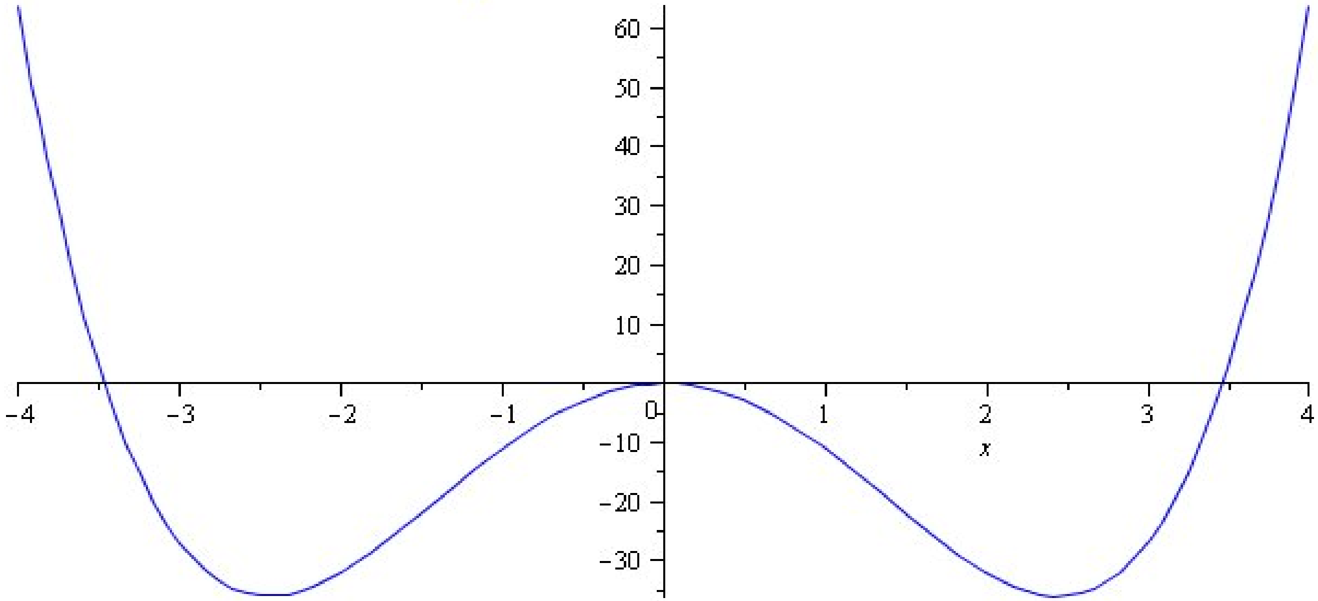
- 2D plots
- Contour plots
- 3D surface plots
- Spacecurves
- Animations

Visualization of data

2D plots

```
> f:=(x)->x^4-12*x^2;
  plot(f(x),x=-4..4,color=blue);
```

$$f := x \rightarrow x^4 - 12\,x^2$$



plot(...,options) : Plots a function f(x)

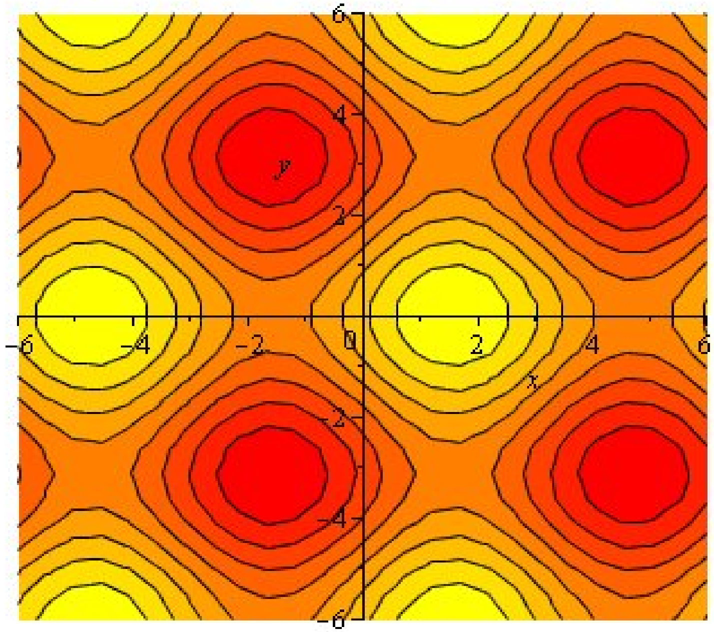
options : Various options are available (e.g. color, font, labels, linestyle, thickness, title, view, …), see help pages “plot, options”

Visualization of data

Contour plots

```
> with(plots):
  f:=(x,y)->sin(x)+cos(y);
  contourplot(f(x,y),x=-6..6,y=-6..6,filledregions = true);
```

$$f := (x, y) \rightarrow \sin(x) + \cos(y)$$



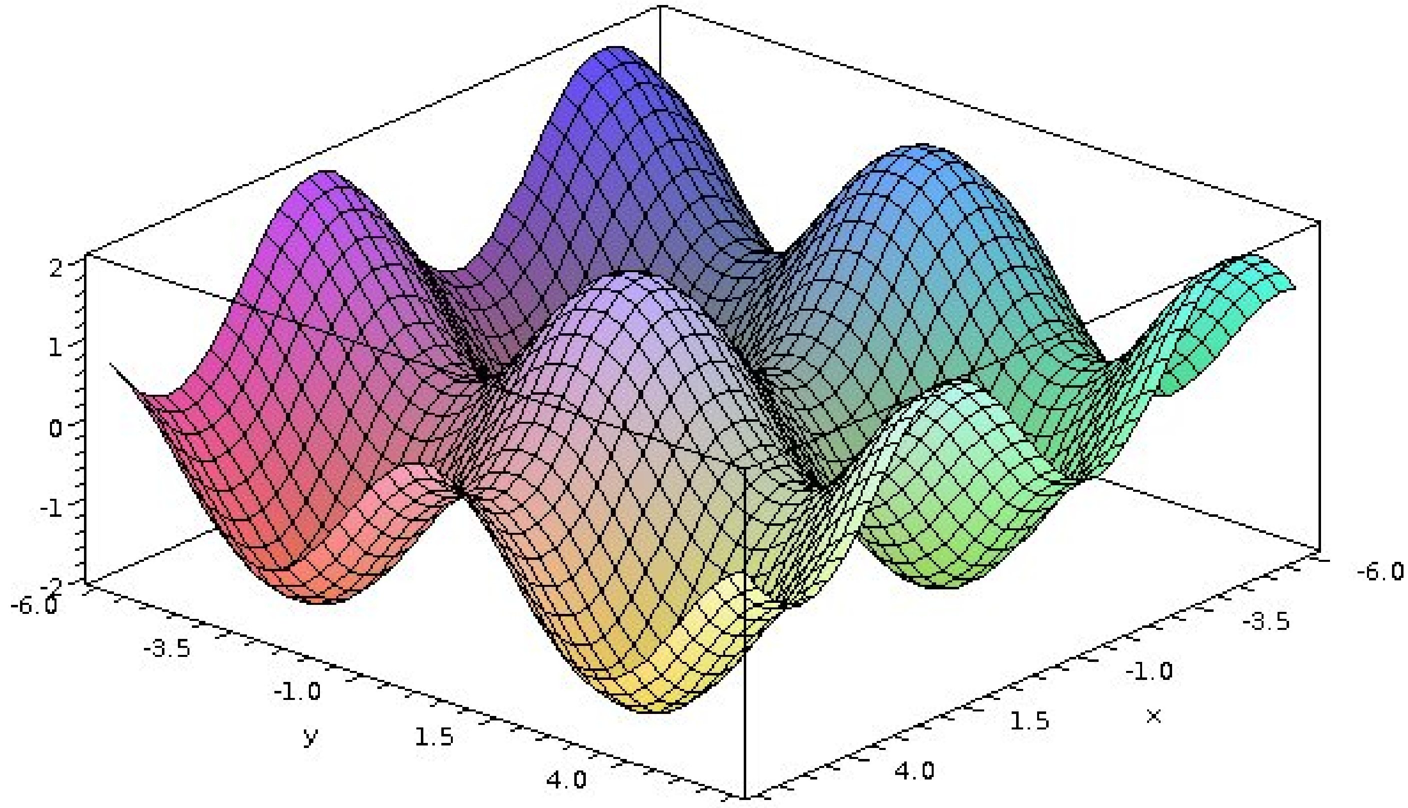
with(plots) : Loads Maple package for special plots

contourplot(...) : Displays a countourplot of a function f(x,y)

Visualization of data

3D surface plots

```
> plot3d(f(x,y),x=-6..6,y=-6..6,axes=boxed,numpoints=1500);
```

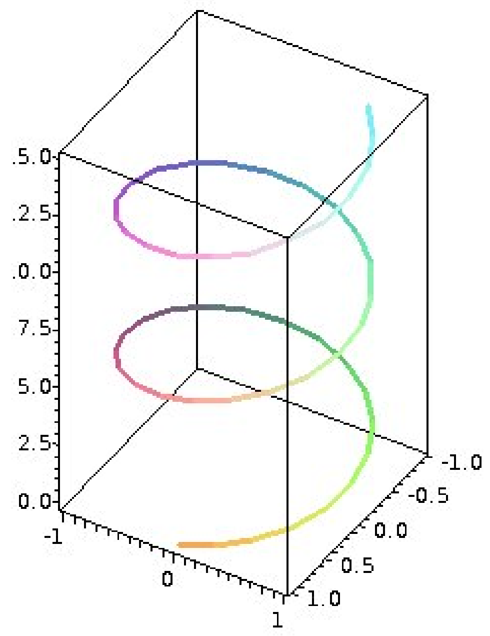


plot3d(...) : **Displays a surfaceplot of a function f(x,y)**

Visualization of data

Spacecurves

```
> spacecurve([cos(t), sin(t), t], t = 0 .. 15,axes=boxed,thickness=3);
```



spacecurve(...) : Displays a spacecurve [x(t),y(t),z(t)] in a three dimensional space

Visualization of data

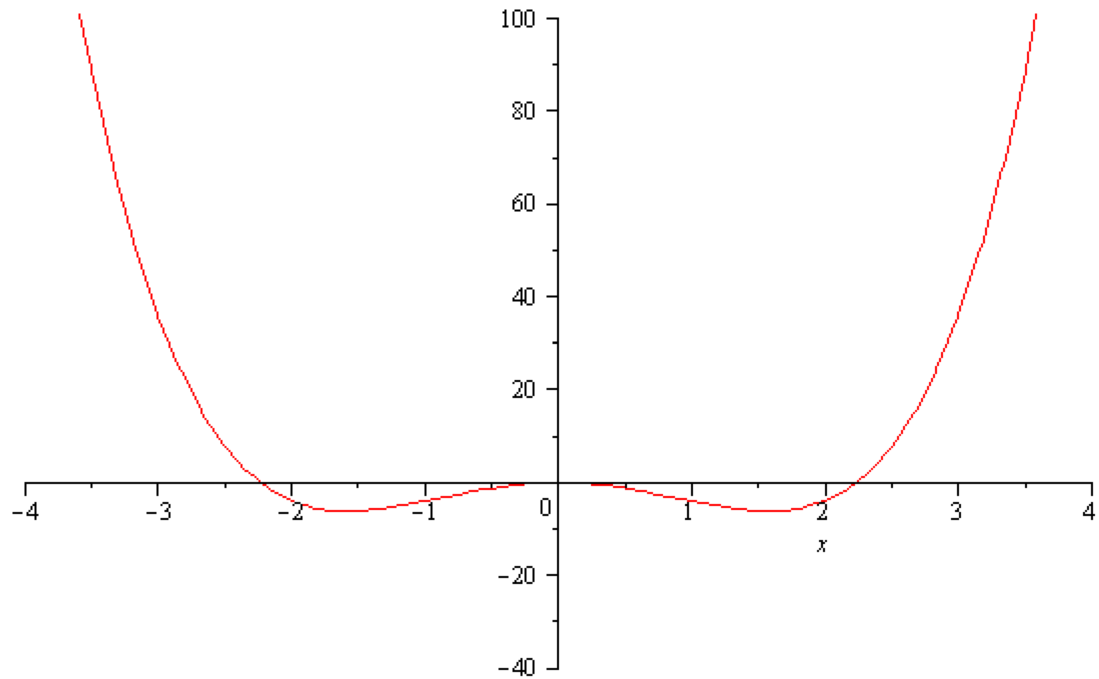
Animations

```
> f:=(x,a)->x^4-a*x^2;
  animate(f(x,a),x=-4..4,a=5..12,view=[-4..4,-40..100]);
```

$$f := (x, a) \rightarrow x^4 - a\,x^2$$

animate(...) :

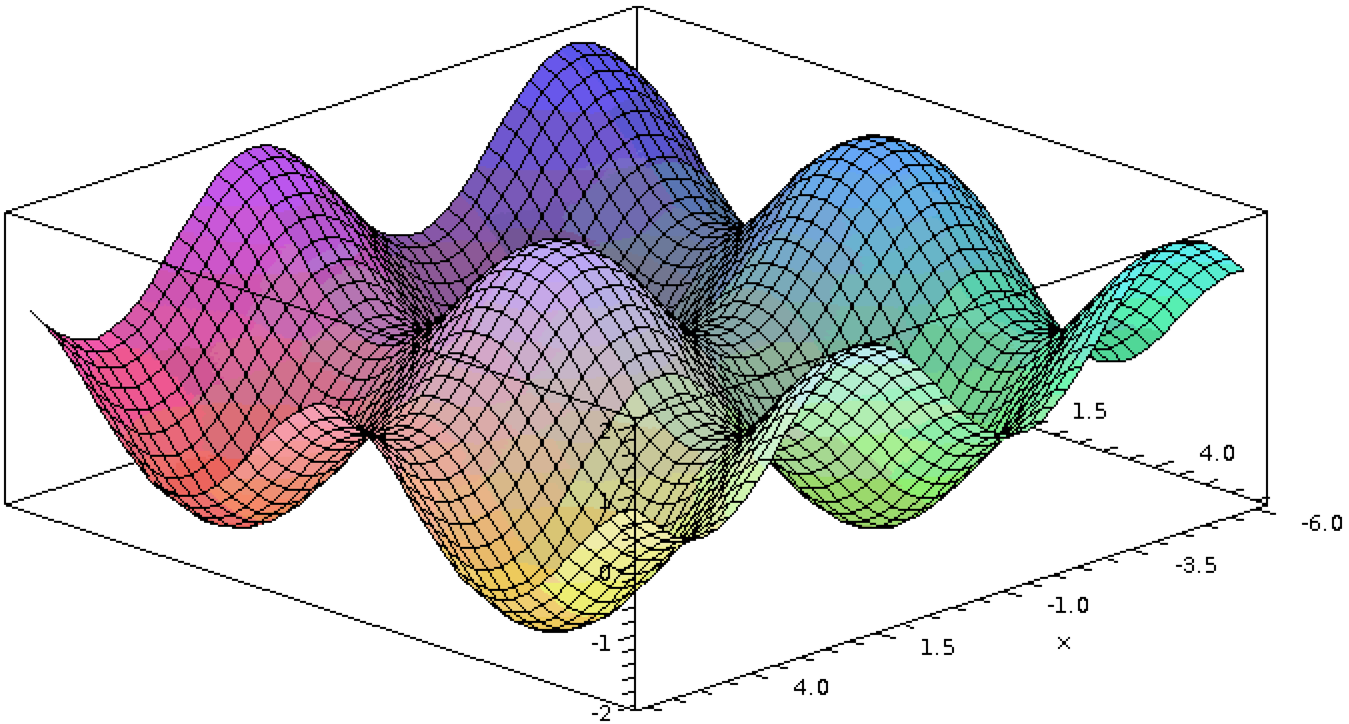
Animates a function f(x,a). It displays the function f(x,a) within a (x,y)-2D-plot, and the parameter “a” is used as the animation parameter within a given range.



Visualization of data

```
> f:=(x,y,t)->sin(x)+cos(t*y);
  animate3d(f(x,y,t),x=-6..6,y=-6..6,t=1..2,axes=boxed,numpoints=2000);
```

$$f := (x, y, t) \rightarrow \sin(x) + \cos(t\,y)$$



animate3d(...) : Animates a function f(x,y,t). It displays the function f(x,y,t) within a (x,y,z)-3D-plot, and the parameter "t" is used as the animation parameter within a given range.

Programming tools

Programming tools

```
>
```

Loops

```
> a:=1:
  for i from 1 by 1 to 10 do
  a:=a*i:
  od:
  a;
                                   3628800
> factorial(10);
                                   3628800
```

If procedures

```
> a:=12:
  b:=34:
  if b < a then
  print("a is greater than b") else print("a is not greater than b")
  end if:
                          "a is not greater than b"
```

A variety of different programming tools are available within Maple. Loops (e.g. for, while) and if-procedures can be used inside a Maple worksheed.

Advanced Examples

Further examples of mathematical physics

- The double pendulum within Hamilton's theory
- Lagrangian mechanics of various physical systems
- The Foucault's pendulum on the earth and on a neutron star
- Simulation of the transit of Venus on the 8. June 2004
- Replicator Dynamics of unsymetrical evolutionary games
- Evolutionary Quantum Game Theory with Maple

The examples are available at the following internet site
http://th.physik.uni-frankfurt.de/~hanauske/new/maple/

Maple Links

- **http://www.maplesoft.com/**
- **http://www.maplesoft.com/applications/**

Maple

Thank you for your attention

Lecture 13

Lecture course: Computational methods in Meso-Bio-Nano Science

GOETHE UNIVERSITÄT FRANKFURT AM MAIN