Scientific Computing for CS Students

Walter Gander
ETH Zürich
Switzerland
gander@inf.ethz.ch
http://www.inf.ethz.ch/personal/gander/

Abstract: At ETH Zürich we have redesigned our former courses on numerical analysis for the education of our compter science students. We make use of computer algebra for derivation of algorithms and for some proofs. Furthermore we try to explain the fundamentals, on which packages like the PDE Toolbox of MATLAB are built.

Curriculum at ETH for CS students

2 mandatory courses à 3h lecture + 2h exercises per week (2nd year)

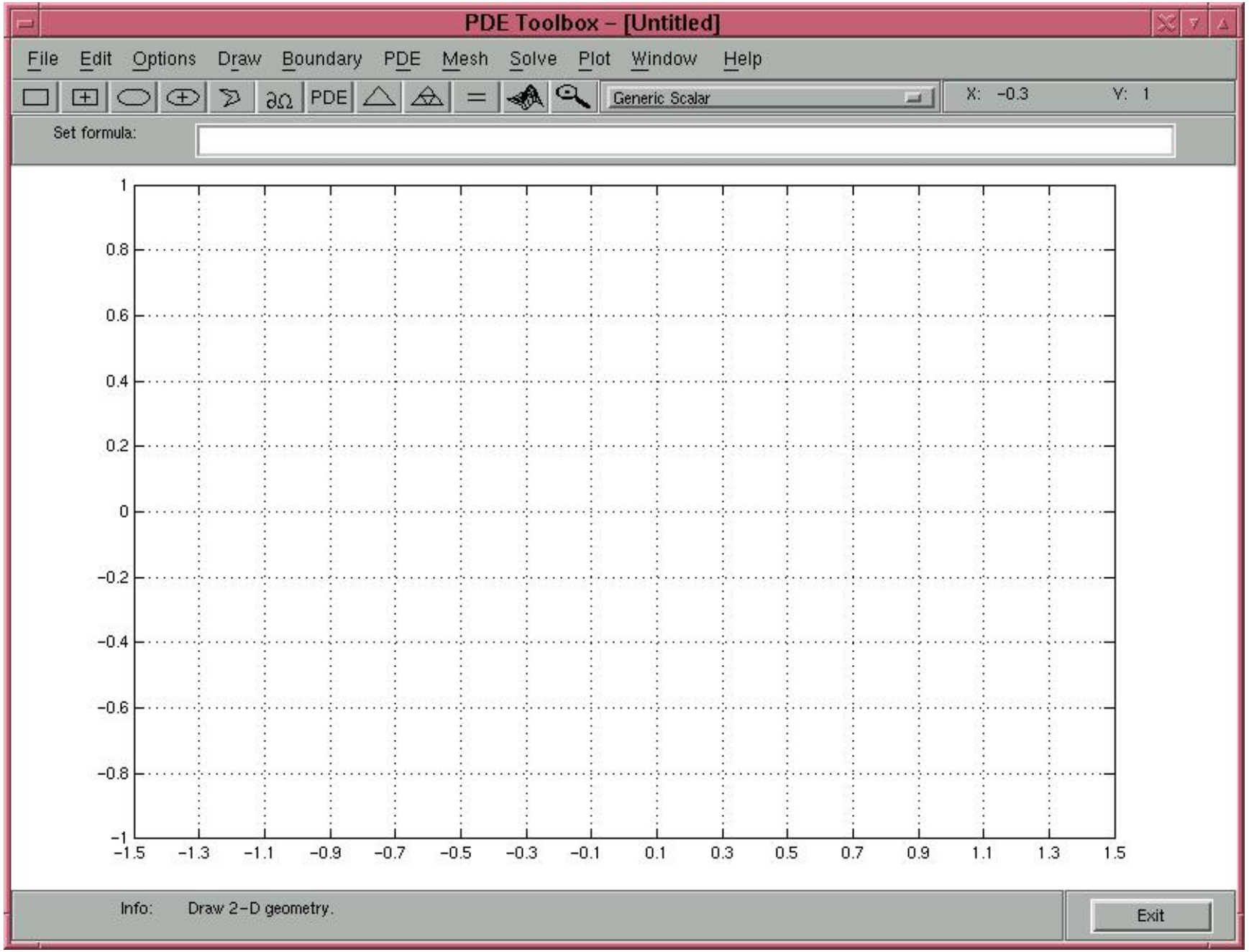
1. Numerical and Symbolic Computation (WS)
(arithmetic, exact computing, lin. and nonlinear eq., automatic differentiation, system of eq., least squares, interpolation/extrapolation)

2. Scientific Computation (SS)
(quadrature, ODE, BVP, calculus of variation, finite elements)

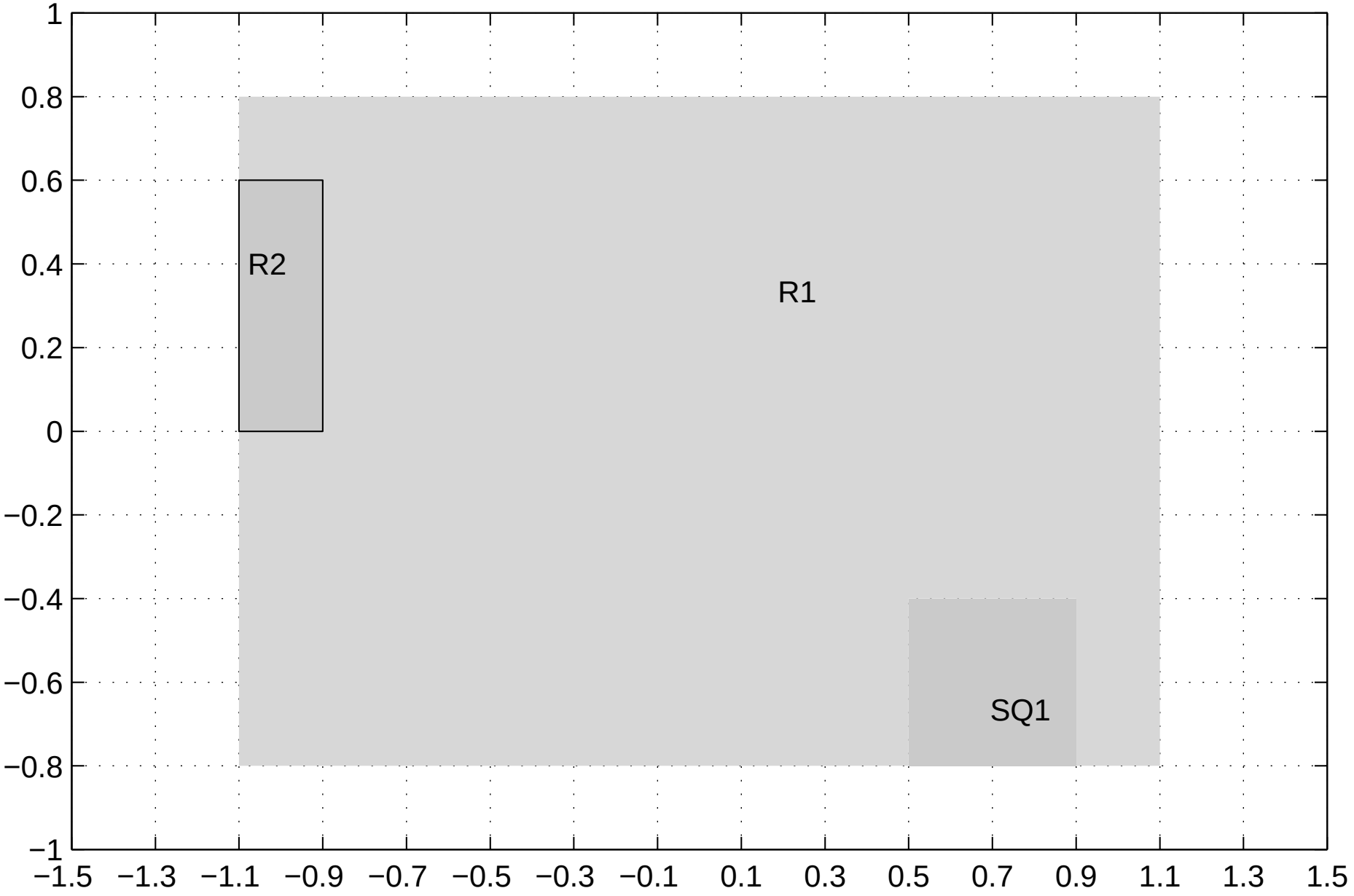
Goals:

- understand and implement algorithms
- explain software (Maple, Matlab)

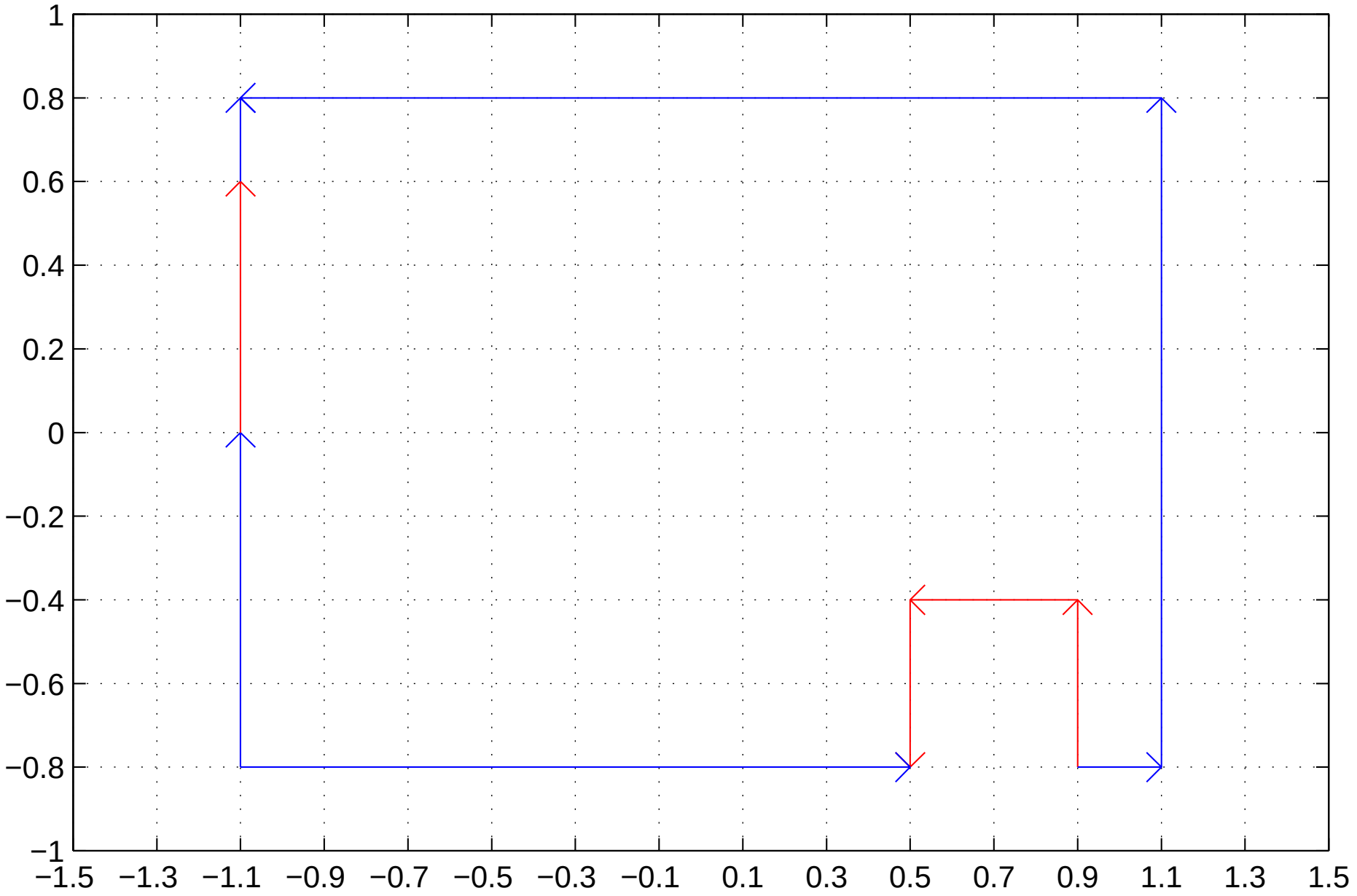
Matlab PDE-Toolbox



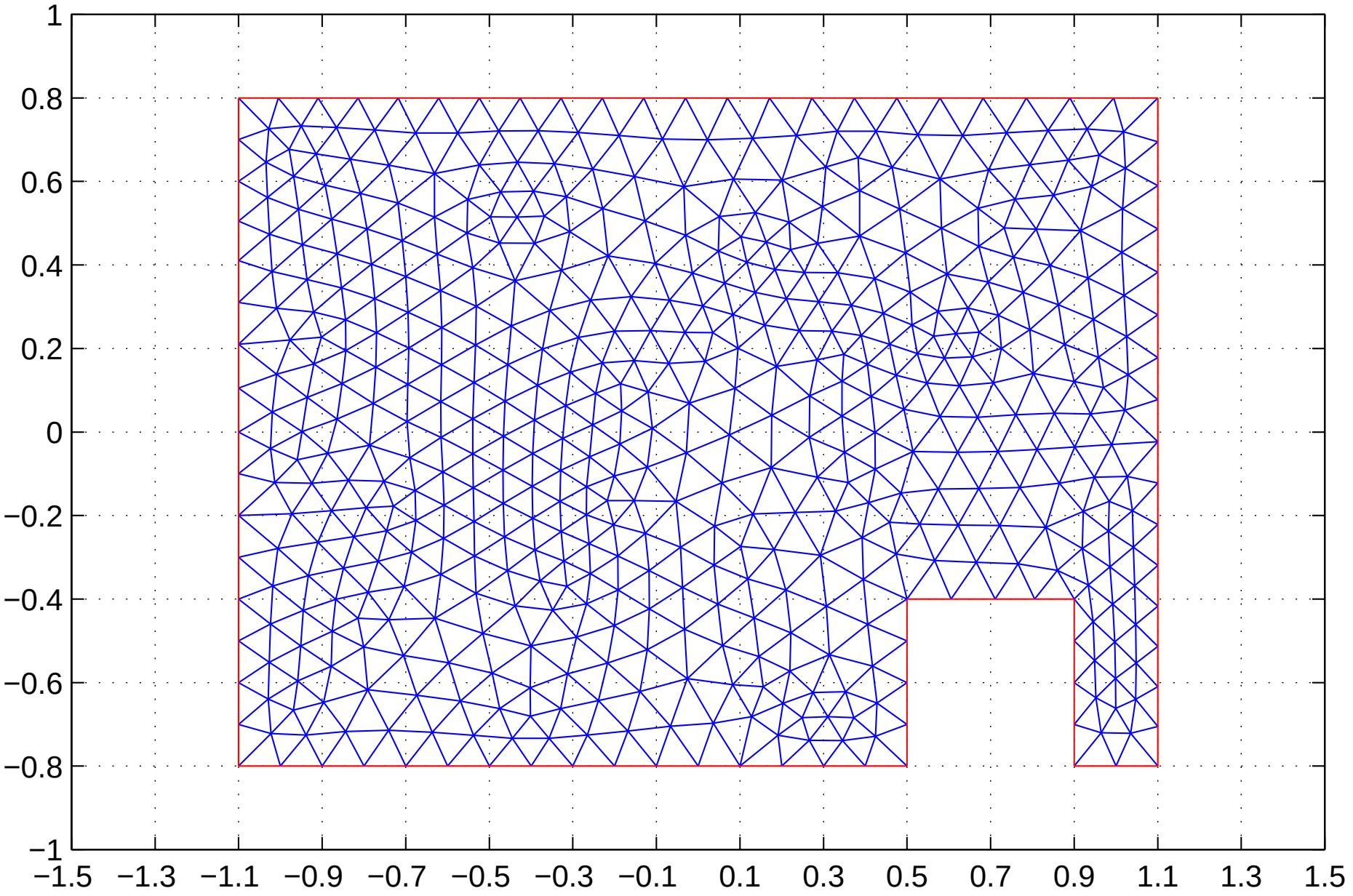
Define Domain



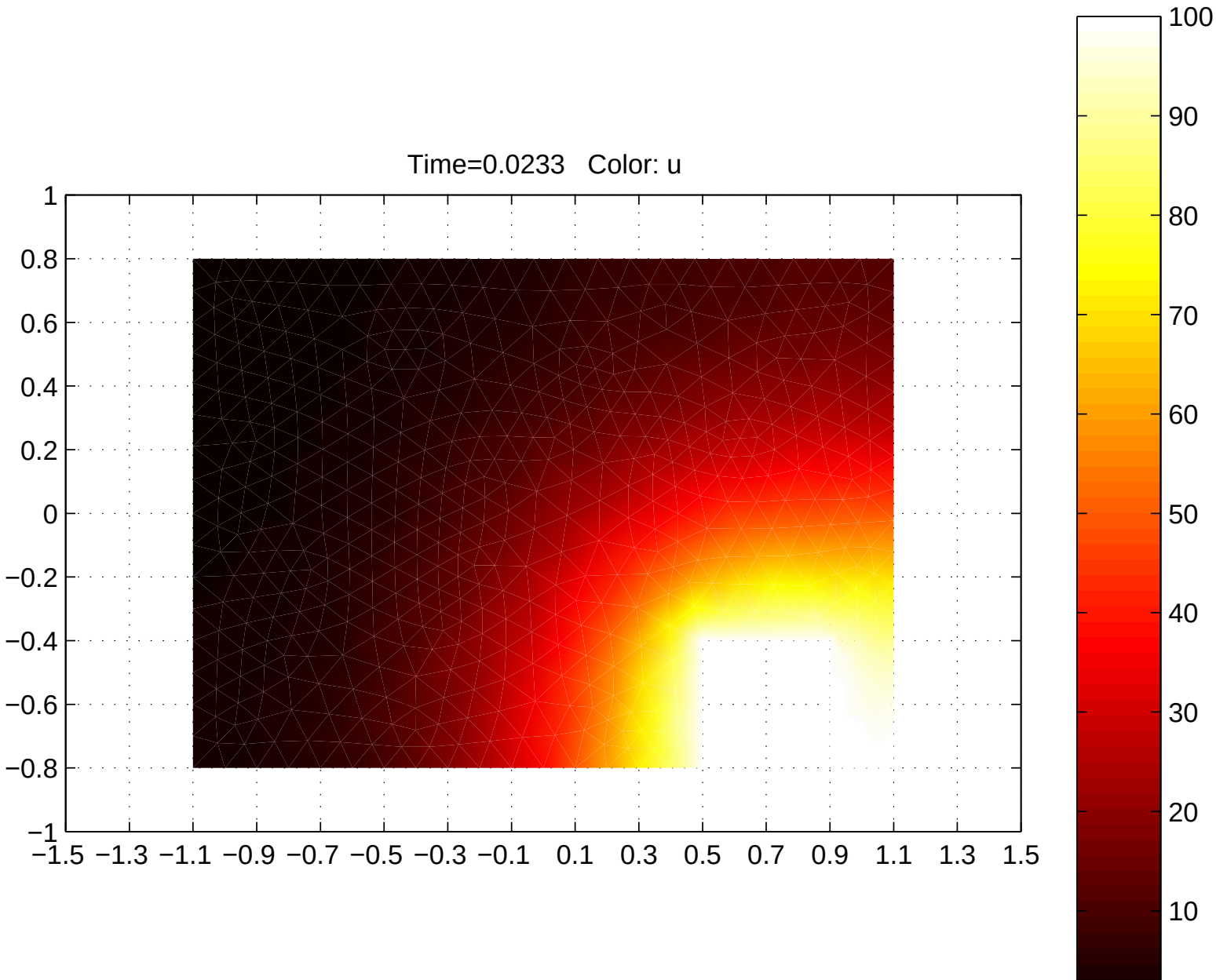
Define Boundary Conditions



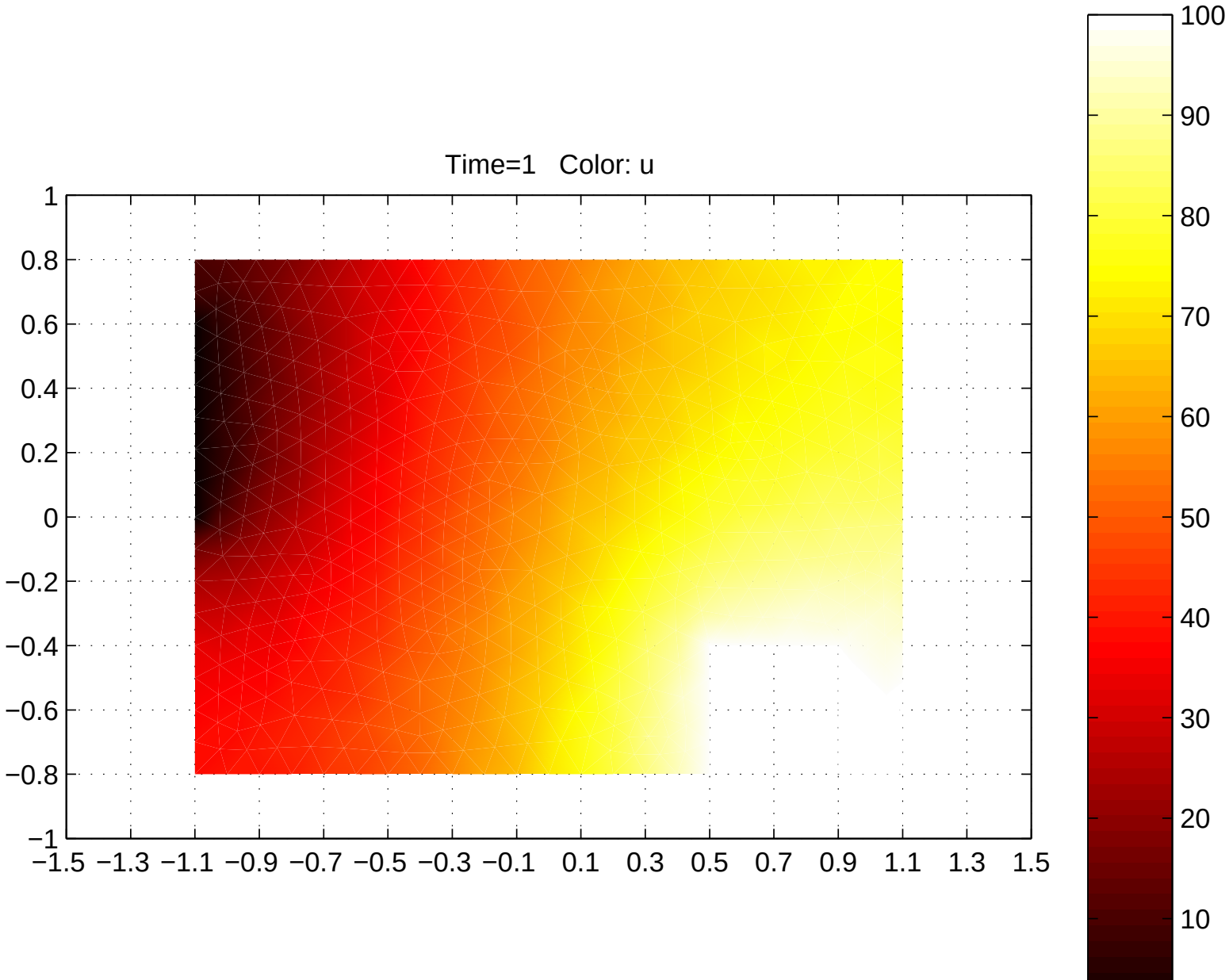
Create Mesh


1
0.8
0.6
0.4
0.2
0
−0.2
−0.4
−0.6
−0.8
−1
−1.5 −1.3 −1.1 −0.9 −0.7 −0.5 −0.3 −0.1 0.1 0.3 0.5 0.7 0.9 1.1 1.3 1.5

Solve


Time=0.0233 Color: u
1
0.8
0.6
0.4
0.2
0
−0.2
−0.4
−0.6
−0.8
−1
−1.5 −1.3 −1.1 −0.9 −0.7 −0.5 −0.3 −0.1 0.1 0.3 0.5 0.7 0.9 1.1 1.3 1.5
100
90
80
70
60
50
40
30
20
10

Asymptotic Solution



From Hairer-Wanner: Analysis by History:

> M. Cauchy annonce, que, pour se conformer au voeu du Conseil, il ne s'attachera plus à donner, comme il a fait jusqu'à présent, des demonstrations parfaitement rigoureuses.
>
> Conseil d'instruction de l'Ecole Polytechnique Paris, 24 nov. 1825
>
> (Mr. Cauchy announces that he will comply to the wish of the council and that he will not anymore, as he did till today, give perfectly rigorous proofs.)

Numerical Computing

Topics: finite arithmetic, interval arithmetic, floating-point numbers, rounding errors, stability, well and ill-conditioned problems

Example: notion of convergence

Cauchy: $\{x_n\}$ convergent $\iff \|x_n - x_m\| < \varepsilon, \quad \forall n, m > N$

"epsilonic" for mathematicians

finite machine: no limit computations possible,

need approximation, i.e. termination criteria

limit computations in a computer algebra system (PhD D. Gruntz, 1996)

Thesis: good algorithms work thanks to rounding errors

Square root (Heron): $x_1 = a, \quad x_{i+1} = \frac{1}{2}\left(x_i + \frac{a}{x_i}\right)$

termination criterion?

check successive iterates: $|x_{i+1} - x_i| < \varepsilon$ often wrong

check residual: $a - x_n^2 \approx 0$ better, but also often wrong

P. Rechenberg, G. Pomberger: Informatik-Handbuch, 1997:

```
SquareRoot (↓ a ↓ eps↑ x):
begin
   x := a/10;
   while |a − x^2| >eps∗a do
         x := (x + a/x)/2
   end
end SquareRoot
```

Use Monotonicity

For Newton's iteration: $\sqrt{a} < x_{n+1} < x_n, \forall n$ (if $x_0 > \sqrt{a}$)

finite arithmetic: necessarily some $x_{n+1} \geq x_n$

$xa = (1 + a)/2;$
$xn = (xa + a/xa)/2;$
while $xn < xa,$
  $xa = xn$
  $xn = (xa + a/xa)/2;$
end

- elegant (no bells and whistles)
- machine-independent (works on any computer)
- no "epsilonic"
- does not work in theory
- makes use of finite arithmetic

Bisection

$f(x)$ continuous, $f(a) < 0$, $f(b) > 0 \Rightarrow \exists s$, $a \leq s \leq b$ s.t. $f(s) = 0$

Usual algorithm:

```
while b-a> eps
   x = (a+b)/2;
   if f(x) <0, a=x; else b=x; end
end
```

Better termination criterion:

```
x = (a+b)/2;
while (a<x) & (x<b)
   if f(x) <0, a=x; else b=x; end
   x = (a+b)/2;
end
```

Does not work in exact arithmetic!

Symbolic/Analytic versus Numerical Computation

$y'' = x^2 y + x + 1 - \frac{1}{x}$

```
> dsolve(diff(y(x),x$2) = x^2 *y(x) + x+1-10*x,y(x));
```

$$y(x) =$$
$$-1/8\,x^{3/2}\left(-4\,BesselI(1/4,1/2\,x^2)\pi^2\,csgn(x)hypergeom([1/4],[3/2,3/4],1/16\,x^4)\right.$$
$$+2\,BesselI(1/4,1/2\,x^2)\pi\sqrt{2}\left(\Gamma(3/4)\right)^2 x\;hypergeom([1/2],[3/2,\tfrac{11}{8}],1/16\,x^4)$$
$$+9\,BesselI(1/4,1/2\,x^2)\pi^{3/2}\sqrt{2}\left(\Gamma(3/4)\right)^2 x\;BesselK(3/4,1/2\,x^2)$$
$$StruveL(1/4,1/2\,x^2)+4\,x\left(\Gamma(3/4)\right)^2 BesselK(1/4,1/2\,x^2)$$
$$hypergeom([1/2],[3/2,5/4],1/16\,x^4)+$$
$$9\,x\left(\Gamma(3/4)\right)^2 BesselK(1/4,1/2\,x^2)\sqrt{2}\pi^{3/2}$$
$$\left.BesselI(-3/4,1/2\,x^2)StruveL(1/4,1/2\,x^2)\right)\pi^{-1}\left(\Gamma(3/4)\right)^{-1}+$$
$$\_C1\,\sqrt{x}BesselI(1/4,1/2\,x^2)+\_C2\,\sqrt{x}BesselK(1/4,1/2\,x^2)$$

Topics from symbolic computation

1. Polynomial arithmetic: e.g. Karatsuba algorithm for multiplication: $O(n^{1.585})$ instead of $O(n^2)$

2. Euclidian algorithm

for computing inverse elements in number fields, e.g. in $Q(\sqrt{2})$.
Factorization of polynomials.

3. Deriving of formulas with Maple[a], e.g.:

   - order of convergence for Newton's method for multiple roots.
   - proof that the order of convergence for the secant method is $(1+\sqrt{5})/2$

4. Automatic differentiation, e.g. for the "billiard problem"

[a] W. Gander and D. Gruntz Derivation of Numerical Methods using Computer Algebra, SIAM Review, Vol 41, Number 3, 1999.

Convergence of the Secant Method

$f(x)$, $f(s) = 0$ simple zero

$$x_{k+1} = F(x_k, x_{k-1}) = x_k - \frac{f(x_k)\,(x_k - x_{k-1})}{f(x_k) - f(x_{k-1})}$$

```
F := (u,v) -> u - f(u)*(u-v)/(f(u)-f(v));
x[k+1] = F(x[k],x[k-1]);
f(s) := 0:
e2 = normal(readlib(mtaylor)(F(s+e1,s+e0) - s, [e0,e1], 4));
```

$$e2 = \frac{1}{2}\,\frac{e0\,(\mathrm{D}^{(2)})(f)(s)\,e1}{\mathrm{D}(f)(s)}$$

```
%/e1/e0;
simplify(subs(e2=K*e1^p, e1=K*e0^p, %/K^p),assume=positive);
```

$$e0^{(p^2-p-1)} = \frac{1}{2}\,\frac{K^{-p}\,(\mathrm{D}^{(2)})(f)(s)}{\mathrm{D}(f)(s)}$$

```
solve(ln(lhs(%)), p);
```

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

convergence factor $p = (1+\sqrt{5})/2 = 1.618033989$

Derivation of Simpson's Rule

```
f := x-> a0 + a1*x + a2*x^2;
solve( {f(a)=y0, f(a+h)=y1, f(a+2*h)=y2},{a0,a1,a2});
assign(%);
i := int(f(x), x=a..a+2*h);
simplify(%);
```

$$\left\{a0 = 1/2\,\frac{3\,ay0\,h+a^2y0-2\,a^2y1+a^2y2-4\,ay1\,h+ay2\,h+2\,y0\,h^2}{h^2},\right.$$
$$a1 = -1/2\,\frac{3\,y0\,h+2\,ay0-4\,ay1+2\,ay2-4\,y1\,h+y2\,h}{h^2},\ a2 = 1/2\,\left.\frac{y0-2\,y1+y2}{h^2}\right\}$$
$$i := \frac{3\,ay0\,h+a^2y0-2\,a^2y1+a^2y2-4\,ay1\,h+ay2\,h+2\,y0\,h^2}{h}$$
$$-\frac{(3\,y0\,h+2\,ay0-4\,ay1+2\,ay2-4\,y1\,h+y2\,h)\left((a+2\,h)^2-a^2\right)}{4h^2}+\frac{(y0-2\,y1+y2)\left((a+2\,h)^3-a^3\right)}{6h^2}$$

$$1/3\,h\,(y0+4\,y1+y2)$$

Newton-Cotes Integration

```
f := interp([0,1,2], [y1, y2, y3],z);
Q := int(f,z=0..2)/2;
```

$$1/6\,y3 + 2/3\,y2 + 1/6\,y1$$

Derivation of the Integration Formula for quad8 in Matlab 5

```
f:=interp([0,1,2,3,4,5,6,7,8], [y1,y2,y3,y4,y5,y6,y7,y8,y9],z):
Q := int(f,z=0..8);
```

$$\frac{3956}{14175}\,y1 + \frac{23552}{14175}\,y2 - \frac{3712}{14175}\,y3 + \frac{41984}{14175}\,y4 - \frac{3632}{2835}\,y5$$
$$+\frac{41984}{14175}\,y6 - \frac{3712}{14175}\,y7 + \frac{23552}{14175}\,y8 + \frac{3956}{14175}\,y9$$

More elegant

```
> closedcotes := n -> factor(int(interp([seq(i*h, i=0..n)],
                    [seq(f(i*h), i=0..n)], z),z=0..n*h)):
```

```
> simpson := closedcotes(2);
```

$$\frac{h}{3}\left(f(0)+4\,f(h)+f(2\,h)\right)=\frac{b-a}{6}\left(f(0)+4\,f(h)+f(2\,h)\right)$$

```
> milne := closedcotes(4);
```

$$\frac{2}{45}\,h\left(7\,f(0)+32\,f(h)+12\,f(2\,h)+32\,f(3\,h)+7\,f(4\,h)\right)$$

Discretization Error

```
> for i from 1 by 1 to 4 do
> rule := closedcotes(i);
> err := taylor(rule - int(f(x), x= 0..i*h), h=0,i+4);
> od;
```

We obtain for the following first terms of the Taylor series:

i	rule	error
1	Trapezoidal	$\frac{1}{12}\, f''(0)\, h^3$
2	Simpson	$\frac{1}{90}\, f^{(4)}(0)\, h^5$
3	$\frac{3}{8}$-Rule	$\frac{3}{80}\, f^{(4)}(0)\, h^5$
4	Milne	$\frac{8}{945}\, f^{(6)}(0)\, h^7$

Analytical solution may be inexact

$$y'' + 5y' + 4y = 1 - e^x, \quad y(0) = y'(0) = 0$$

```
de := diff(y(x),x$2)+5*diff(y(x),x)+4*y(x) = 1-exp(x);
dsolve({de, y(0)=0, D(y)(0)=0}, y(x));
```

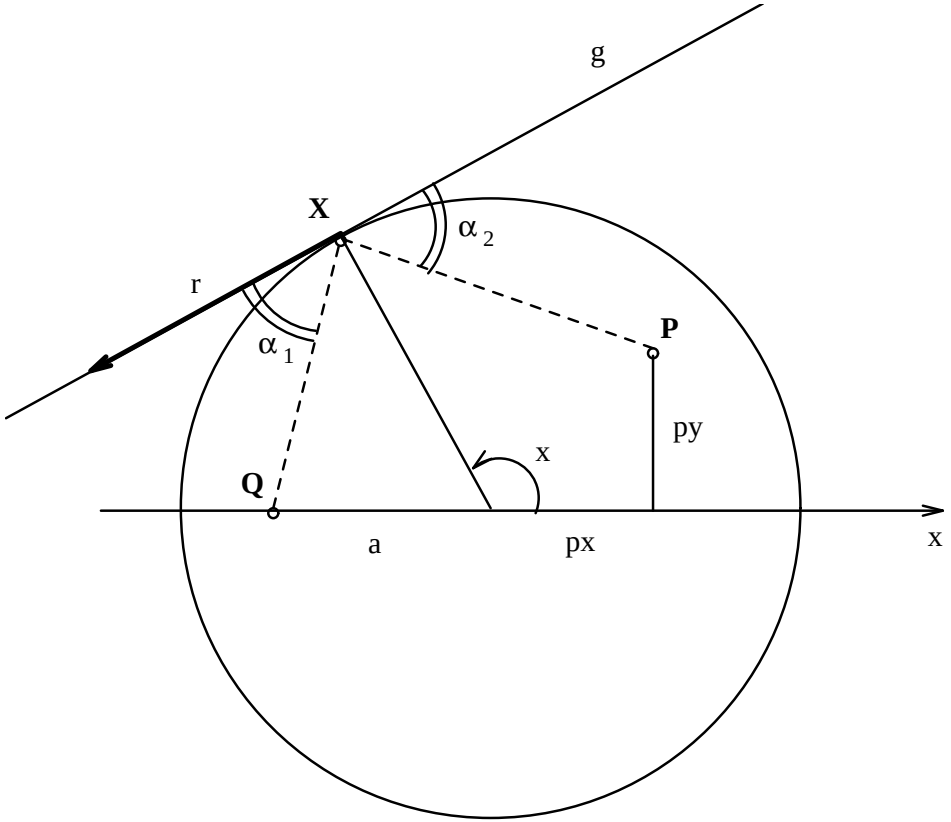
$$y(x) = \frac{e^x}{20}\left(5\,e^{-x} - 2\right) + \frac{1}{60}\,e^{-4\,x} - \frac{e^{-x}}{6}$$

```
f:= unapply(rhs(%),x);
for x from 0 by 0.001 to 0.01 do  print(evalf(f(x))) od;
```

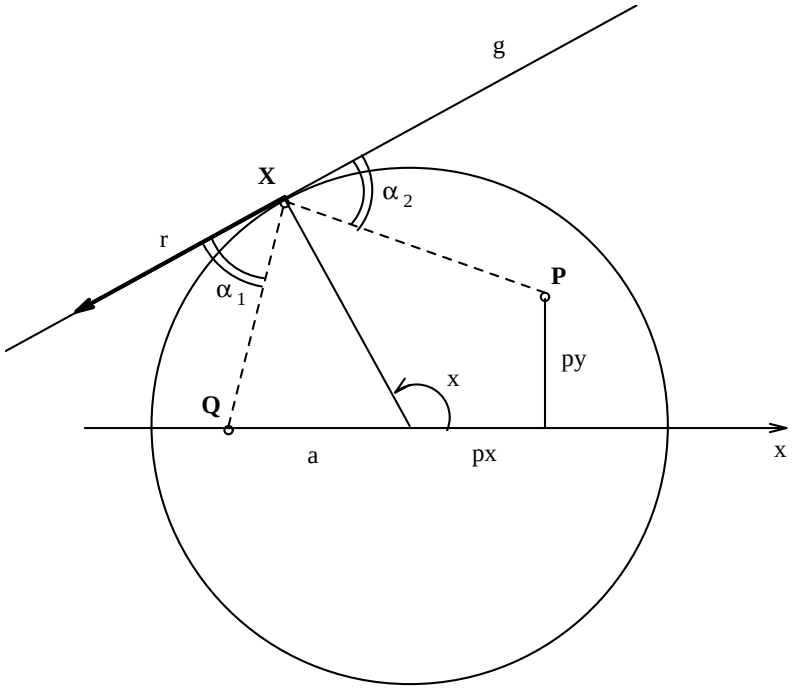
	MAPLE exact	MAPLE (series)	Runge Kutta $h = 10^{-3}$
x	y	y	y
1.0E-03	-.1498500750E-9	-.1665001417E-9	-1.6649995450E-10
2.0E-03	-.1347302699E-8	-.1330671200E-8	-1.3306708206E-09
3.0E-03	-.4436670003E-8	-.4486534425E-8	-4.4865337977E-09
4.0E-03	-.1055768469E-7	-.1062414507E-7	-1.0624143938E-08
5.0E-03	-.2064650894E-7	-.2072960938E-7	-2.0729606977E-08
6.0E-03	-.3578464671E-7	-.3578510160E-7	-3.5785096100E-08
7.0E-03	-.5675134695E-7	-.5676888099E-7	-5.6768868635E-08
8.0E-03	-.8457072070E-7	-.8465530880E-7	-8.4655282685E-08
9.0E-03	-.1204114060E-6	-.1204148653E-6	-1.2041481369E-07
1.0E-02	-.1649918048E-6	-.1650141667E-6	-1.6501407093E-07

cancellation in analytical expression!

Circular Billiard Problem



W. Gander and D. Gruntz, *The Billard Problem*, Int. J. Math. Educ. Sci. Technol., 1992, Vol. 23, No. 6, 825-830



Equation for X

- Rotational symmetry
- Unit circle $\Rightarrow \mathbf{X} = \begin{pmatrix} \cos x \\ \sin x \end{pmatrix} \Rightarrow \mathbf{r} = \begin{pmatrix} -\sin x \\ \cos x \end{pmatrix}$
- $\alpha_1 = \alpha_2 \iff (\mathbf{e}_{XQ} + \mathbf{e}_{XP})^T \mathbf{r} = 0.$

Computer algebra system Maple

```
xp1 := px-cos(x);
xp2 := py-sin(x);
xq1 := a-cos(x);
xq2 := -sin(x);

lp := sqrt((xp1)**2 + (xp2)**2);
ep1 := xp1/lp; ep2 := xp2/lp;

lq := sqrt((xq1)**2 + (xq2)**2);
eq1 := xq1/lq; eq2 := xq2/lq;

f := (ep1+eq1)*sin(x) - (ep2+eq2)*cos(x);
```

Result of Maple Computation (red: Parameters)

$$f(x) := \left(\frac{px - \cos x}{\sqrt{(px - \cos x)^2 + (py - \sin x)^2}} + \frac{a - \cos x}{\sqrt{(a - \cos x)^2 + \sin x^2}} \right) \sin x$$

$$- \left(\frac{py - \sin x}{\sqrt{(px - \cos x)^2 + (py - \sin x)^2}} - \frac{\sin x}{\sqrt{(a - \cos x)^2 + \sin x^2}} \right) \cos x = 0$$

For the solution with Newton's method we need the derivative

```
> D(f);
```

$$f'(x) =$$

$$\left(\frac{\sin(x)}{\sqrt{(px-\cos(x))^2+(py-\sin(x))^2}} - 1/2\,\frac{(px-\cos(x))(2\,(px-\cos(x))\sin(x)-2\,(py-\sin(x))\cos(x))}{\left((px-\cos(x))^2+(py-\sin(x))^2\right)^{3/2}} + \right.$$

$$\left. \frac{\sin(x)}{\sqrt{(a-\cos(x))^2+(\sin(x))^2}} - 1/2\,\frac{(a-\cos(x))(2\,(a-\cos(x))\sin(x)+2\,\sin(x)\cos(x))}{\left((a-\cos(x))^2+(\sin(x))^2\right)^{3/2}} \right) \sin(x) +$$

$$\left(\frac{px-\cos(x)}{\sqrt{(px-\cos(x))^2+(py-\sin(x))^2}} + \frac{a-\cos(x)}{\sqrt{(a-\cos(x))^2+(\sin(x))^2}} \right) \cos(x)$$

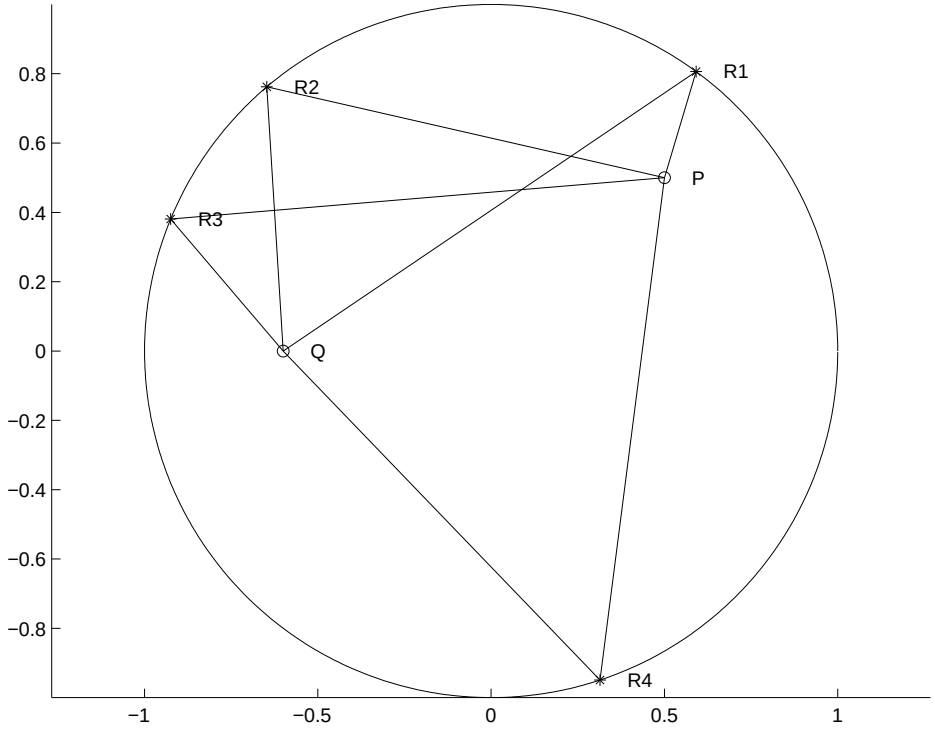
$$- \left(- \frac{\cos(x)}{\sqrt{(px-\cos(x))^2+(py-\sin(x))^2}} - 1/2\,\frac{(py-\sin(x))(2\,(px-\cos(x))\sin(x)-2\,(py-\sin(x))\cos(x))}{\left((px-\cos(x))^2+(py-\sin(x))^2\right)^{3/2}} - \right.$$

$$\left. \frac{\cos(x)}{\sqrt{(a-\cos(x))^2+(\sin(x))^2}} + 1/2\,\frac{\sin(x)(2\,(a-\cos(x))\sin(x)+2\,\sin(x)\cos(x))}{\left((a-\cos(x))^2+(\sin(x))^2\right)^{3/2}} \right) \cos(x) +$$

$$\left(\frac{py-\sin(x)}{\sqrt{(px-\cos(x))^2+(py-\sin(x))^2}} - \frac{\sin(x)}{\sqrt{(a-\cos(x))^2+(\sin(x))^2}} \right) \sin(x)$$

Better Solution by Automatic Differentiation

```
function [y ys] = ffs(x)
% computes the functions f and its derivative  fs for the
% billiard problem
global px py a
 cs = -sin(x);                                          c =  cos(x);
 ss = cos(x);                                           s = sin(x);
 xp1s =  -cs ; xp2s =  -ss;                             xp1 = px-c ;  xp2 = py-s;
 xq1s =   -cs ; xq2s = -ss;                             xq1 =  a-c ;  xq2 = -s;
 hs = (xp1*xp1s + xp2*xp2s)/sqrt(xp1^2 + xp2^2);        h = sqrt(xp1^2 + xp2^2);
 ep1s = (h*xp1s - xp1*hs)/h^2;                          ep1 = xp1/h;
 ep2s = (h*xp2s - xp2*hs)/h^2;                          ep2 = xp2/h;
 hs = (xq1*xq1s + xq2*xq2s)/sqrt(xq1^2 + xq2^2);        h = sqrt(xq1^2 + xq2^2);
 eq1s = (h*xq1s - xq1*hs)/h^2;                          eq1  = xq1/h;
 eq2s = (h*xq2s - xq2*hs)/h^2;                          eq2  = xq2/h;
 ys = (ep1s+eq1s)*s+(ep1+eq1)*ss-(ep2s+eq2s)*c-(ep2+eq2)*cs;
                                                        y = (ep1+eq1)*s - (ep2+eq2)*c;
```



Solutions for $P = (0.5, 0.5)$ **and** $Q = (-0.6, 0)$

Analytical Solution?

"Rationalizing" with $t = \tan(x/2)$ in $f(x) \Rightarrow \sin(x) = \frac{2t}{(1+t^2)}$,
$\cos(x) = \frac{1-t^2}{1+t^2}$

$$f(x) = g(t) = \frac{2\,t}{1+t^2}\left(\frac{px-\frac{1-t^2}{1+t^2}}{\sqrt{\left(px-\frac{1-t^2}{1+t^2}\right)^2+\left(py-\frac{2\,t}{1+t^2}\right)^2}}+\frac{a-\frac{1-t^2}{1+t^2}}{\sqrt{\left(a-\frac{1-t^2}{1+t^2}\right)^2+\frac{4\,t^2}{(1+t^2)^2}}}\right)$$

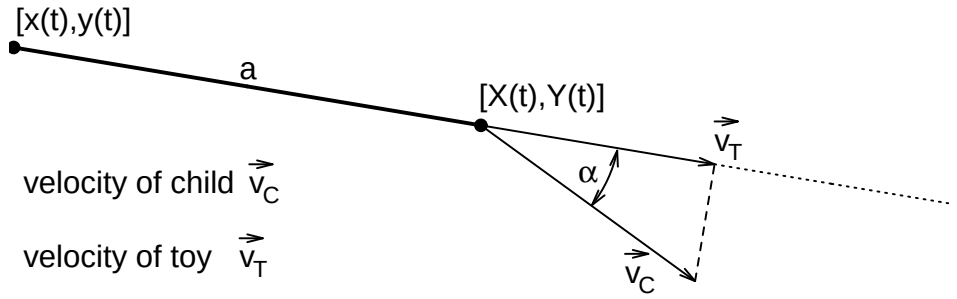
$$-\frac{1-t^2}{1+t^2}\left(\frac{py-\frac{2\,t}{1+t^2}}{\sqrt{\left(px-\frac{1-t^2}{1+t^2}\right)^2+\left(py-\frac{2\,t}{1+t^2}\right)^2}}-\frac{2\frac{t}{1+t^2}}{\sqrt{\left(a-\frac{1-t^2}{1+t^2}\right)^2+\frac{4\,t^2}{(1+t^2)^2}}}\right)=0$$

```
> sols := {solve(g = 0, t)};
```

$$RootOf\left((py\,a+py)\_Z^4+(4\,px\,a+2\,a+2\,px)\_Z^3-6\,\_Z^2 py\,a+(-4\,px\,a+2\,a+2\,px)\_Z-py+py\,a\right)$$

+ polynomial of degree 2 (squaring)

Toy/Child Problem



$$(X-x)^2+(Y-y)^2=a^2, \quad \begin{pmatrix} X-x \\ Y-y \end{pmatrix} = \lambda \begin{pmatrix} \dot{x} \\ \dot{y} \end{pmatrix} \quad \text{with} \quad \lambda > 0.$$

$$||\vec{v_T}|| = ||\vec{v_C}|| \cos(\alpha) = \vec{v_T} \cdot \vec{w}$$

```
function zs = f(t,z)
%
[X Xs Y Ys] = child(t);
v =[Xs; Ys];
w =[X-z(1); Y-z(2)];
w = w/norm(w);
zs = (v'*w)*w;
```

Jogger and Dog

- $\dot{x}^2 + \dot{y}^2 = w^2$ dog velocity
- velocity of dog parallel to difference vector

$$\begin{pmatrix}\dot{x}\\ \dot{y}\end{pmatrix} = \lambda \begin{pmatrix}X-x\\ Y-y\end{pmatrix} \quad \text{with } \lambda > 0$$

$$\Rightarrow w^2 = \dot{x}^2 + \dot{y}^2 = \lambda^2 \left|\left|\begin{pmatrix}X-x\\ Y-y\end{pmatrix}\right|\right|^2 \text{ and } \Rightarrow \lambda = \frac{w}{\left|\left|\begin{pmatrix}X-x\\ Y-y\end{pmatrix}\right|\right|} > 0$$

$$\begin{pmatrix}\dot{x}\\ \dot{y}\end{pmatrix} = \frac{w}{\left|\left|\begin{pmatrix}X-x\\ Y-y\end{pmatrix}\right|\right|} \begin{pmatrix}X-x\\ Y-y\end{pmatrix}$$

Demos: Toy/Child Problem

d0: child walking on straight line pushing toy

d1: child walking on circle, long rod

d2: child walking on circle, rod equal radius

d3: child walking on sin-curve

d4: jogger on ellipse, fast dog

d5: jogger on ellipse, slower dog

Gauss Quadrature $\int_{-1}^{1} f(x)\,dx \approx w_1 f(x_1) + w_2 f(x_2) + w_3 f(x_3)$

6 unknowns: $w_1, w_2, w_3, x_1, x_2, x_3$ demand exact values for monomes x^j:

$$w_1 x_1^j + w_2 x_2^j + w_3 x_3^j = \int_{-1}^{1} x^j\,dx, \quad j = 0, \ldots, 5$$

```
u1 := w1 +w2 +w3:   u2 := w1*x1  +w2*x2  +w3*x3:
u3 := w1*x1^2+w2*x2^2+w3*x3^2: u4 := w1*x1^3+w2*x2^3+w3*x3^3:
u5 := w1*x1^4+w2*x2^4+w3*x3^4: u6 := w1*x1^5+w2*x2^5+w3*x3^5:
solve({u1=2,u2=0,u3=2/3,u4=0,u5=2/5,u6=0}, {w1,w2,w3,x1,x2,x3});
```

$$\{x3 = RootOf(-3 + 5\_Z^2), x1 = 0, x2 = -RootOf(-3 + 5\_Z^2),$$
$$w2 = 5/9, w3 = 5/9, w1 = 8/9\}$$

```
fsolve({u1=2,u2=0,u3=2/3,u4=0,u5=2/5,u6=0}, {w1,w2,w3,x1,x2,x3});
```

$$\{x1 = -5.1250001 \times 10^{-24}, x2 = -0.7745966692 x3 = 0.7745966692,$$
$$w1 = 0.8888888888, w2 = 0.5555555556, w3 = 0.5555555556, \}$$

Gauss Quadratur and orth. Polynomes

Polynome-division:

$$P_{2n-1}(x) = H_{n-1}(x)Q_n(x) + R_{n-1}(x)$$

$$\int_{-1}^{1} P_{2n-1}\,dx = \int_{-1}^{1} H_{n-1}Q_n\,dx + \int_{-1}^{1} R_{n-1}\,dx$$

$$\sum_{i=1}^{n} w_i P_{2n-1}(x_i) = \sum_{i=1}^{n} w_i H_{n-1}(x_i)Q_n(x_i) + \sum_{i=1}^{n} w_i R_{n-1}(x_i)$$

$$\text{error:} = \int_{-1}^{1} H_{n-1}Q_n\,dx - \sum_{i=1}^{n} w_i H_{n-1}(x_i)Q_n(x_i) + \int_{-1}^{1} R_{n-1}\,dx - \sum_{i=1}^{n} w_i R_{n-1}(x_i)$$

1. Q_n O-Pol. on $(-1,1) \Rightarrow \int_{-1}^{1} H_{n-1}Q_n\,dx = 0$
2. x_i zero of $Q_n \Rightarrow \sum_{i=1}^{n} w_i H_{n-1}(x_i)Q_n(x_i) = 0$
3. w_i according to Newton-Cotes $\Rightarrow \int_{-1}^{1} R_{n-1}\,dx = \sum_{i=1}^{n} w_i R_{n-1}(x_i)$

```
with(orthopoly);
X := sort([fsolve(P(12,0,0,x)=0,x)]);
f := interp(X,[y1,y2,y3,y4,y5,y6,y7,y8,y9,y10,y11,y12],z):
Q:=  int(f,z=-1..1);
```

$$X := [-0.9815606342, -0.9041172564, -0.7699026742, -0.5873179543, -0.3678314990, -0.1252334085, 0.1252334085, 0.3678314990, 0.5873179543, 0.7699026742, 0.9041172564, 0.9815606342]$$

$$Q := +0.04717506586\, y1 + 0.1069394295\, y2 + 0.1600776434\, y3 + 0.2031689029\, y4 + 0.2334973032\, y5 + 0.2491475198\, y6 + 0.2491470907\, y7 + 0.2334921379\, y8 + 0.2031674530\, y9 + 0.1600783833\, y10 + 0.1069391353\, y11 + 0.04717532540\, y12$$

Unstable ! but `Digits := 30;`

$$
\begin{aligned}
Q = {} & 0.047175336386511827194615958213 1\, y1 + \\
& 0.106939325995318430960254714440\, y2 + \\
& 0.160078328543346226334652551494\, y3 + \\
& 0.203167426723065921749064450415\, y4 + \\
& 0.233492536538354808760849926553\, y5 + \\
& 0.249147045813402785000562439776\, y6 + \\
& 0.249147045813402785000562434283\, y7 + \\
& 0.233492536538354808760849896404\, y8 + \\
& 0.203167426723065921749064452856\, y9 + \\
& 0.160078328543346226334652528161\, y10 + \\
& 0.106939325995318430960254716884\, y11 + \\
& 0.047175336386511827194615961783 2\, y12
\end{aligned}
$$

Theory of Golub-Welsh

1. Three term recurrence relation $p_{i+1} = (x - \delta_{i+1})p_i - \gamma_{i+1}^2 p_{i-1} \iff$

$$\begin{pmatrix} xp_0 \\ xp_1 \\ \vdots \\ xp_{n-1} \end{pmatrix} = \begin{pmatrix} \delta_1 & 1 & & \\ \gamma_2^2 & \delta_2 & 1 & \\ & \ddots & \ddots & \ddots \\ & & \gamma_n^2 & \delta_n \end{pmatrix} \begin{pmatrix} p_0 \\ p_1 \\ \vdots \\ p_{n-1} \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ \vdots \\ p_n \end{pmatrix}$$

2. $\exists\ \tilde{T} \sim T$, with $\tilde{T}$ symmetric, $\tilde{T}U = U \begin{pmatrix} x_1 & & \\ & \ddots & \\ & & x_n \end{pmatrix}$

3. normalize $U^T U = I \Rightarrow w_i = u_{1i}^2 \int_a^b w(x)\, dx$

Variational problem: Ritz Ansatz

$$-\frac{d}{dx}(py') + qy = f$$

is Euler-Lagrange equation of $(\delta L = 0)$

$$L = \int_0^\pi (py'^2 + qy^2 - 2fy)\, dx$$

Ritz-Ansatz

$$y^h(x) = \sum_{j=1}^{N} c_j \varphi_j(x)$$

$$L^h = \mathbf{c}^T A\mathbf{c} + \mathbf{b}^T\mathbf{c} + \gamma$$

$$\delta L^h = 0 \iff 2A\mathbf{c} + \mathbf{b} = 0$$

$$\mathcal{D}(u(x)) = -u''(x) + 2u(x) = f(x), \quad u(0) = 0, u'(\pi) = 0$$

For $f(x) = \frac{17}{4}\sin(\frac{3}{2}\,x)$, solution : $u(x) = \sin(\frac{3}{2}\,x)$

```
DG := u -> -D(D(u)) + 2*u - f:  f  := x -> 17/4*sin(3/2*x):
dsolve({DG(u)(x)=0, u(0)=0, D(u)(Pi)=0}, u(x)): assign(%):
y := x -> c1*(x-x^2/(2*Pi)) + c2*x*exp(-x/Pi);
integrand := diff(y(x),x)^2+2*y(x)^2-2*f(x)*y(x);
```

$$y := x \mapsto c1\,\left(x - 1/2\,\frac{x^2}{\pi}\right) + c2\,xe^{-\frac{x}{\pi}}$$

$$\mathit{integrand} := \left(c1\,\left(1 - \frac{x}{\pi}\right) + c2\,e^{-\frac{x}{\pi}} - c2\,\frac{x}{\pi}e^{-\frac{x}{\pi}}\right)^2 +$$

$$2\,\left(c1\,\left(x - \frac{x^2}{2\pi}\right) + c2\,xe^{-\frac{x}{\pi}}\right)^2 - \frac{17}{2}\sin(\frac{3x}{2})\left(c1\,\left(x - \frac{x^2}{2\pi}\right) + c2\,xe^{-\frac{x}{\pi}}\right)$$

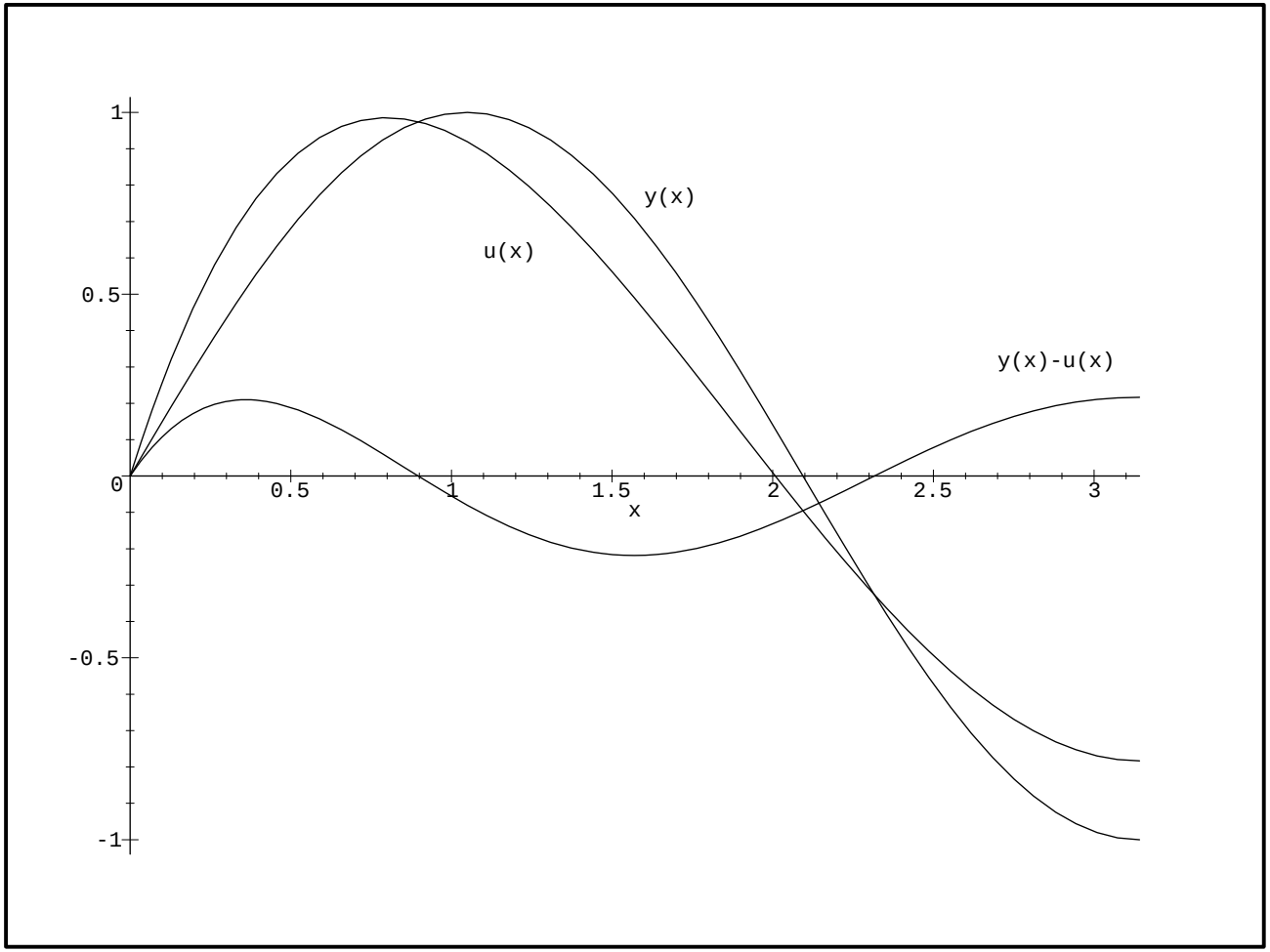
```
L := int(integrand,x=0..Pi): evalf(L);
```

$$L := -0.8016693423\,c1 - 1.582748542\,c2 + 14.51403010\,c2\,c1 + 9.315538006\,c1^2 + 5.691636323\,c2^2$$

```
v := linalg[grad](L, [c1,c2]):
solve({v[1],v[2]}, {c1,c2}):  evalf(%);
```

$$\{c2 = 12.52353174,\ c1 = -9.713086137\}$$

```
assign(%);
plot({y(x), u(x), y(x)-u(x)}, x=0..Pi, color=black);
```


1
0.5
0
-0.5
-1
0.5
1
1.5
2
2.5
3
x
y(x)
u(x)
y(x)-u(x)

Method of Galerkin

$$Dy = -\frac{d}{dx}(py') + qy = f, \qquad \text{Ritz-Ansatz:} \quad y^h(x) = \sum_{j=1}^{N} c_j \varphi_j(x)$$

Residual $\rho = Dy^h - f$

c_j such that residual is orthogonal to $\{\psi_j(x)\}, \quad i = 1, \ldots, N$

$$\Longleftrightarrow \int_0^\pi \rho\, \psi_j(x)\, dx = 0, \quad i = 1, \ldots, N$$

system of lin. eq. for c_j: $A\mathbf{c} = \mathbf{b}$

$$a_{ij} = \int_0^\pi \psi_i(x) D\varphi_j(x)\, dx, \quad b_i = \int_0^\pi f(x)\psi_i(x)\, dx$$

```
DG := u -> -D(D(u)) + 2*u - f:   f  := x -> 17/4*sin(3/2*x):
dsolve({DG(u)(x)=0, u(0)=0, D(u)(Pi)=0}, u(x)): assign(%):
psi1 := x -> sin(x):  psi2 := x -> cos(x):
y := x -> c1*(x-x^2/(2*Pi)) + c2*x*exp(-x/Pi);
eq := {int(DG(y)(t)*psi1(t), t=0..Pi), int(DG(y)(t)*psi2(t),t=0..Pi)}:
evalf(eq);  fsolve(eq, {c1,c2});
plot({y(x), u(x), y(x)-u(x)}, x=0..Pi, color=black);
```

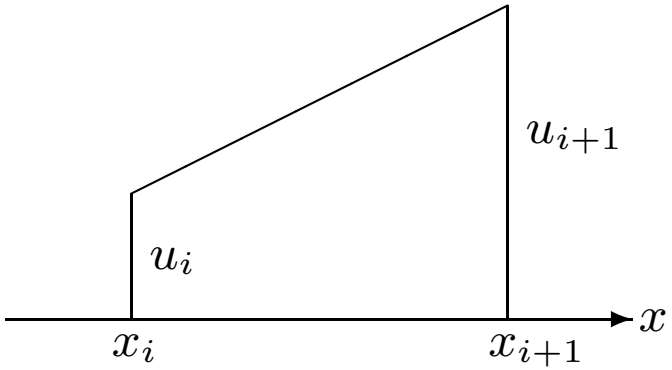
$$\{-1.038400155\,c2 - 5.100000003 - 2.000000001\,c1,$$
$$5.051451973\,c1 - 3.400000002 + 4.146353669\,c2\}$$

$$\{c2 = 10.68573206, c1 = -8.098032910\}$$

Finite element method

1. discretization (intervals, triangles)
2. elements $u_i^e(x) = \sum_{k=1}^{p} u_k N_k(x)$

knot variables u_i, form functions $N_k(x)$



$u_i^e(\xi) = u_i(1-\xi) + u_{i+1}\xi, \quad \xi = \frac{x-x_i}{x_{i+1}-x_i}$

3. Ritz-ansatz $u^h = \sum_{i=1}^{N} u_i^e N_i$

minimize functional or apply the method of Galerkin

Conclusions

- scientific computing makes use of powerful software for numerical and symbolic computing
- interesting and more realistic problems can be solved in class
- formulas used in numerical analysis and error estimates can be derived using a computer algebra system
- the students can concentrate more on learning principles instead of mechanically applying recipes

References

1. W. Gander and D. Gruntz
   The Billard Problem
   Int. J. Math. Educ. Sci. Technol., 1992, Vol. 23, No. 6, 825-830.

2. W. Gander and J. Hřebíček, ed.
   Solving Problems in Scientific Computing using Maple and Matlab
   Springer, third edition 1997.

3. W. Gander and D. Gruntz
   Derivation of Numerical Methods using Computer Algebra,
   SIAM Review, Vol 41, Number 3, 1999.

4. W. Gander and W. Gautschi
   Adaptive Quadrature - Revisited,
   BIT Vol. 40, No. 1, March 2000, pp. 84–101.