

```
> restart;
with(PDEtools):
with(plots):
with(LinearAlgebra):
Digits := 14;
```

Nonlinear PDEs

The purpose of this worksheet is to discuss the solution of nonlinear PDEs using finite difference methods. For concreteness, we will concentrate on a diffusion equation with a potential:

$$\frac{\partial}{\partial t} u(t, x) = d \frac{\partial^2}{\partial x^2} u(t, x) + V(u(t, x)).$$

Here, d is the diffusion constant and V is a given (presumably nonlinear) function of $u(t, x)$. We take t as a time variable, hence this is an initial value problem. We'll take Dirichlet boundary conditions

$$u(t, -L) = u(t, L) = 0,$$

where L is a constant to be specified.

Stencils

Here is our PDE:

```
> pde := diff(u(t,x),t)=d*diff(u(t,x),x,x)+V(u(t,x));
```

$$pde := \frac{\partial}{\partial t} u(t, x) = d \left(\frac{\partial^2}{\partial x^2} u(t, x) \right) + V(u(t, x))$$

(1.1)

We will make use of the **GenerateStencil** procedure defined elsewhere:

```
> GenerateStencil := proc(F,N,{orientation:=center,stepsize:=h,showorder:=true,showerror:=false})
    local vars, f, ii, Degree, stencil, Error, unknowns, Indets, ans, Phi, r, n, phi;

    Phi := convert(F,D);
    vars := op(Phi);
    n := PDEtools[difforder](Phi);
    f := op(1,op(0,Phi));
```

```

if (nops([vars])<>1) then:
  r := op(1,op(0,op(0,Phi)));
else:
  r := 1;
fi:
phi := f(vars);
if (orientation=center) then:
  if (type(N,odd)) then:
    ii := [seq(i,i=-(N-1)/2..(N-1)/2)];
  else:
    ii := [seq(i,i=-(N-1)..(N-1),2)];
  fi;
elif (orientation=left) then:
  ii := [seq(i,i=-N+1..0)];
elif (orientation=right) then:
  ii := [seq(i,i=0..N-1)];
fi;
stencil := add(a[ii[i]]*subsop(r=op(r,phi)+ii[i]*stepsize,phi),i=1..N);
Error := D[r$N](f)(vars) - stencil;
Error := convert(series(Error,stepsize,N),polynom);
unknowns := {seq(a[ii[i]],i=1..N)};
Indets := indets(Error) minus {vars} minus unknowns minus {stepsize};
Error := collect(Error,Indets,'distributed');
ans := solve({coeffs(Error,Indets)},unknowns);
if (ans=NULL) then:
  print(`Failure: try increasing the number of points in the stencil`);
  return NULL;
fi:
stencil := subs(ans,stencil);
Error := convert(series(`leadterm`(D[r$N](f)(vars) - stencil),stepsize,N+20),polynom);
Degree := degree(Error,stepsize);
if (showorder) then:
  print(cat(`This stencil is of order `,Degree));
fi:
if (showerror) then:
  print(cat(`This leading order term in the error is `,Error));
fi:
convert(D[r$N](f)(vars) = stencil,diff);

end proc:
> forward_time := GenerateStencil(diff(u(t,x),t),2,orientation=right,stepsize=s);

```

```
backward_time := GenerateStencil(diff(u(t,x),t),2,orientation=left,stepsize=s);
centered_time := GenerateStencil(diff(u(t,x),x,x),3,orientation=center,stepsize=h);
```

This stencil is of order 1

$$\text{forward_time} := \frac{\partial}{\partial t} u(t,x) = -\frac{u(t,x)}{s} + \frac{u(t+s,x)}{s}$$

This stencil is of order 1

$$\text{backward_time} := \frac{\partial}{\partial t} u(t,x) = -\frac{u(t-s,x)}{s} + \frac{u(t,x)}{s}$$

This stencil is of order 2

$$\text{centered_time} := \frac{\partial^2}{\partial x^2} u(t,x) = \frac{u(t,x-h)}{h^2} - \frac{2u(t,x)}{h^2} + \frac{u(t,x+h)}{h^2} \quad (1.2)$$

```
> Label[1] := `FTCS`;
stencil[1] := subs(forward_time,centered_time,pde);
```

$$\text{stencil}_1 := -\frac{u(t,x)}{s} + \frac{u(t+s,x)}{s} = d \left(\frac{u(t,x-h)}{h^2} - \frac{2u(t,x)}{h^2} + \frac{u(t,x+h)}{h^2} \right) + V(u(t,x)) \quad (1.3)$$

```
> BTCS := subs(backward_time,centered_time,t=t+s,pde);
```

$$\text{BTCS} := -\frac{u(t,x)}{s} + \frac{u(t+s,x)}{s} = d \left(\frac{u(t+s,x-h)}{h^2} - \frac{2u(t+s,x)}{h^2} + \frac{u(t+s,x+h)}{h^2} \right) + V(u(t+s,x)) \quad (1.4)$$

```
> Label[2] := `CN`;
stencil[2] := (stencil[1]+BTCS)/2;
```

$$\begin{aligned} \text{stencil}_2 := & -\frac{u(t,x)}{s} + \frac{u(t+s,x)}{s} = \frac{1}{2} d \left(\frac{u(t,x-h)}{h^2} - \frac{2u(t,x)}{h^2} + \frac{u(t,x+h)}{h^2} \right) + \frac{1}{2} V(u(t,x)) \\ & + \frac{1}{2} d \left(\frac{u(t+s,x-h)}{h^2} - \frac{2u(t+s,x)}{h^2} + \frac{u(t+s,x+h)}{h^2} \right) + \frac{1}{2} V(u(t+s,x)) \end{aligned} \quad (1.5)$$

Forward-time centered-space solution

```
> FTCS_stencil := expand(isolate(stencil[1],u(t+s,x)));
```

$$\text{FTCS_stencil} := u(t+s,x) = \frac{s d u(t,x-h)}{h^2} - \frac{2 s d u(t,x)}{h^2} + \frac{s d u(t,x+h)}{h^2} + s V(u(t,x)) + u(t,x) \quad (2.1)$$

```
> Subs := u(t,x-h)=u1,u(t,x)=u2,u(t,x+h)=u3;
```

```
Phi := unapply(subs(Subs,rhs(FTCS_stencil)),u1,u2,u3,h,s,d);
Subs := u(t,x-h) = u1, u(t,x) = u2, u(t,x+h) = u3
```

$$\Phi := (u1, u2, u3, h, s, d) \rightarrow \frac{s \, d \, u1}{h^2} - \frac{2 \, s \, d \, u2}{h^2} + \frac{s \, d \, u3}{h^2} + s \, V(u2) + u2 \quad (2.2)$$

```
> FTCS := proc(tau,L,N,M,d,f) local s, h, XX, X, T, PlotOptions, Title, u_past, u_future, p,
i, j:
```

```
# We first determine the time and space steps
```

```
X := j -> L*(-1 + j*2/(M+1));
T := i -> tau*i/N;
s := evalf(T(1)-T(0));
h := evalf(X(1)-X(0));
```

```
# We define an Array containing the x-coordinates of the spatial lattice
```

```
XX := Array(0..M+1,[seq(X(j),j=0..M+1)],datatype=float):
```

```
# The scheme will be based on two Arrays u_past and u_future:
```

```
# u_past corresponds to the field values on a given time step
# u_future corresponds to the field values at the next time step
# To begin, we fix u_past from the initial data.
```

```
u_past := Array(0..M+1,[seq(f(XX[j]),j=0..M+1)],datatype=float):
```

```
# Our goal will be a movie whose frames are plots of u at each time step
```

```
# The frames of our movie will be generated by a separate procedure that follows this one
```

```
p[0] := Frame[1](XX,u_past,s,h,T(0));
```

```
# Now we start the main calculation loop
```

```
# i will run over timesteps while j runs over spacesteps
```

```
for i from 1 to N do:
```

```
    # We initialize the u_future array and fix its values
    # at either end based on the boundary conditions
```

```

u_future := Array(0..M+1,datatype=float):
u_future[0] := 0:
u_future[M+1] := 0:

# The rest of the values of u_future are obtained by using the Phi procedure
# Notice the arguments of Phi are the values of u_past

for j from 1 to M do:
    u_future[j] := Phi(u_past[j-1],u_past[j],u_past[j+1],h,s,d):
od:

# Now, we get ready for the next time step by making u_future into the new u_past

ArrayTools[Copy](u_future,u_past):

# Finally, another frame of our movie is generated:

p[i] := Frame[1](XX,u_past,s,h,T(i));

od:

# After the loop is over, we have N plots p[i] that are the pictures of u at each time slice
# The display command assembles these into a movie, which is the output of the procedure

display(convert(p,list),insequence=true):

end proc:

Frame[1] := proc(xdata,ydata,s,h,T) local Title, PlotOptions:

    Title := typeset(`timestep = `,evalf[2](s),`, spacestep = `,evalf[2](h),`, `t=
evalf[2](T));
    PlotOptions := axes=boxed, labels=[x,u(t,x)], legend=["numerical solution (FTCS)
"], color=red;
    plot(Matrix([[xdata],[ydata]])^T,title=Title,PlotOptions);

end proc:
> V := u -> 1-u^2;
tau := 1;
N := 400;

```

```

M := 20;
L := 1;
d := 1;
s := evalf(2*L/(M+1));
h := evalf(tau/N);
f := x -> exp(-(4*x)^2);
movie[1] := FTCS(tau,L,N,M,d,f):
pds := pdsolve(pde, [u(t,-L)=0,u(t,+L)=0,u(0,x)=f(x)], numeric, timestep=s, spacestep=h):
movie[2] := pds:-animate(t=0..tau, frames=N+1, axes=boxed, legend=["pdsolve/numeric"], color=
blue):

```

$$V := u \rightarrow 1 - u^2$$

$$\tau := 1$$

$$N := 400$$

$$M := 20$$

$$L := 1$$

$$d := 1$$

$$s := 0.095238095238095$$

$$h := 0.0025000000000000$$

$$f := x \rightarrow e^{-16x^2}$$

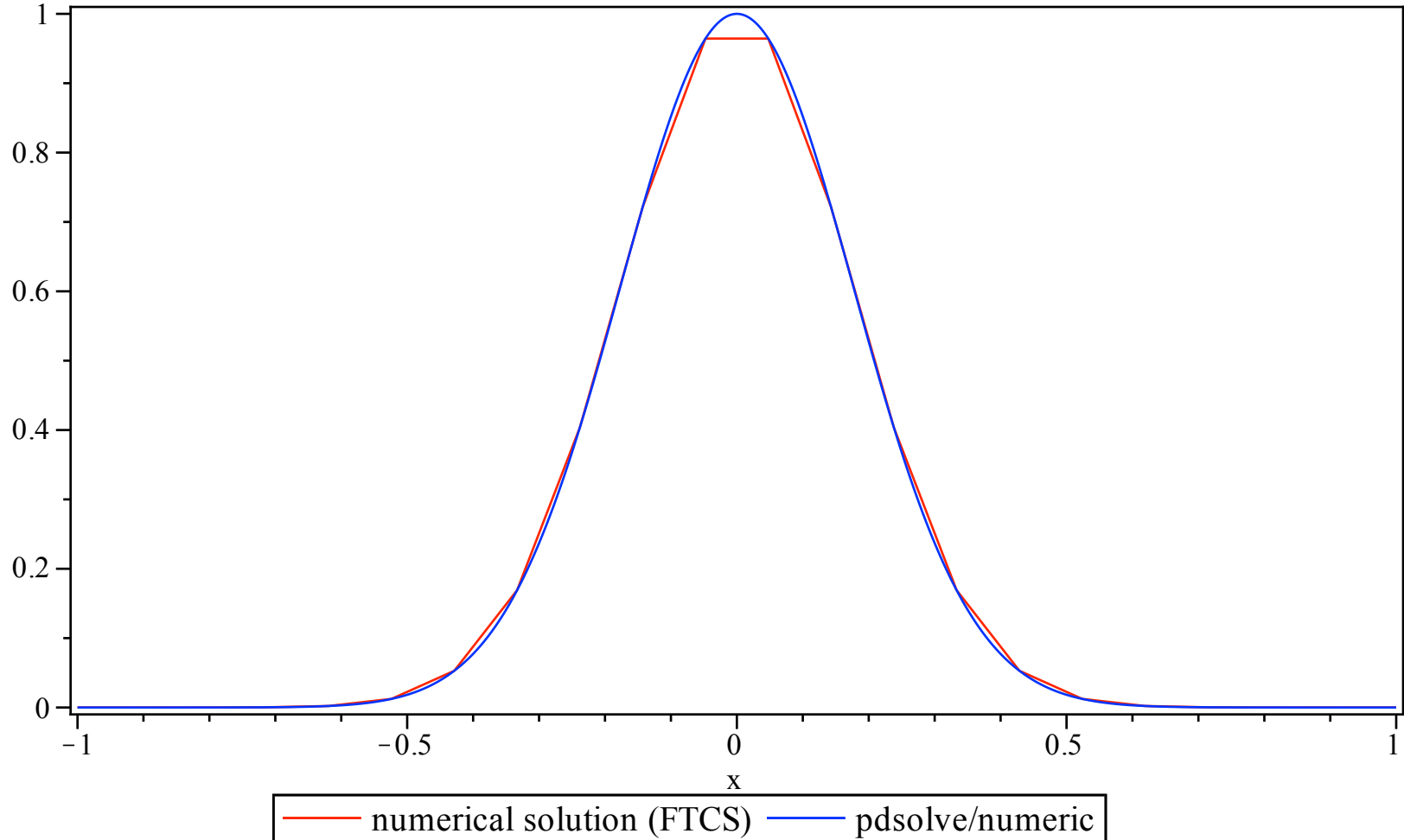
(2.3)

```

> display([movie[1],movie[2]]);

```

timestep = 0.0025, spacestep = 0.095, t = 0.



▼ Review of Newton's method to solve nonlinear algebraic equations

▼ Solving one equation for one unknown

```
> eq1 := F(x) = 0;
```

$$eq1 := F(x) = 0$$

(3.1.1)

```
> eq2 := x = x[guess] + delta;
```

$$eq2 := x = x_{guess} + \delta \quad (3.1.2)$$

```
> eq3 := subs(eq2,eq1);
```

$$eq3 := F(x_{guess} + \delta) = 0 \quad (3.1.3)$$

```
> eq4 := series(lhs(eq3),delta,2)=0;
```

$$eq4 := F(x_{guess}) + D(F)(x_{guess})\delta + O(\delta^2) = 0 \quad (3.1.4)$$

```
> eq5 := isolate(convert(eq4,polynomial),delta);
```

$$eq5 := \delta = -\frac{F(x_{guess})}{D(F)(x_{guess})} \quad (3.1.5)$$

```
> eq6 := x[`new guess`] = x[guess] + delta;
```

$$eq6 := x_{new\ guess} = x_{guess} + \delta \quad (3.1.6)$$

```
> eq7 := subs(eq5,eq6);
```

$$eq7 := x_{new\ guess} = x_{guess} - \frac{F(x_{guess})}{D(F)(x_{guess})} \quad (3.1.7)$$

```
> x_new := unapply(rhs(eq7),x[guess]);
```

$$x_{new} := y1 \rightarrow y1 - \frac{F(y1)}{D(F)(y1)} \quad (3.1.8)$$

```
> Newton[scalar] := proc(F,x0,eps)
  local maxsteps, CONTINUE, x, i:
  maxsteps := 20:
  CONTINUE := true:
  x[0] := evalf(x0):
  for i from 1 to maxsteps while (CONTINUE) do:
    x[i] := evalf(x_new(x[i-1])):
    if (abs(x[i]-x[i-1])<eps) then CONTINUE := false fi:
  od;
  Matrix([seq([x[j],F(x[j])],j=0..i-1)],datatype=float);
end proc;
```

```
> F := x -> sin(x)-x/2;
Newton[scalar](F,4,1e-10);
```

$$F := x \rightarrow \sin(x) - \frac{1}{2}x$$

4.	-2.75680249530790
1.61035171915210	0.194041927889040
1.96999160043930	-0.0636217292795800
1.89840009052060	-0.00238393487773000
1.89549913294010	-0.000003985297930000000
1.89549426704770	-1.124000000000000 10 ⁻¹¹
1.89549426703400	-2.000000000000000 10 ⁻¹⁴

(3.1.9)

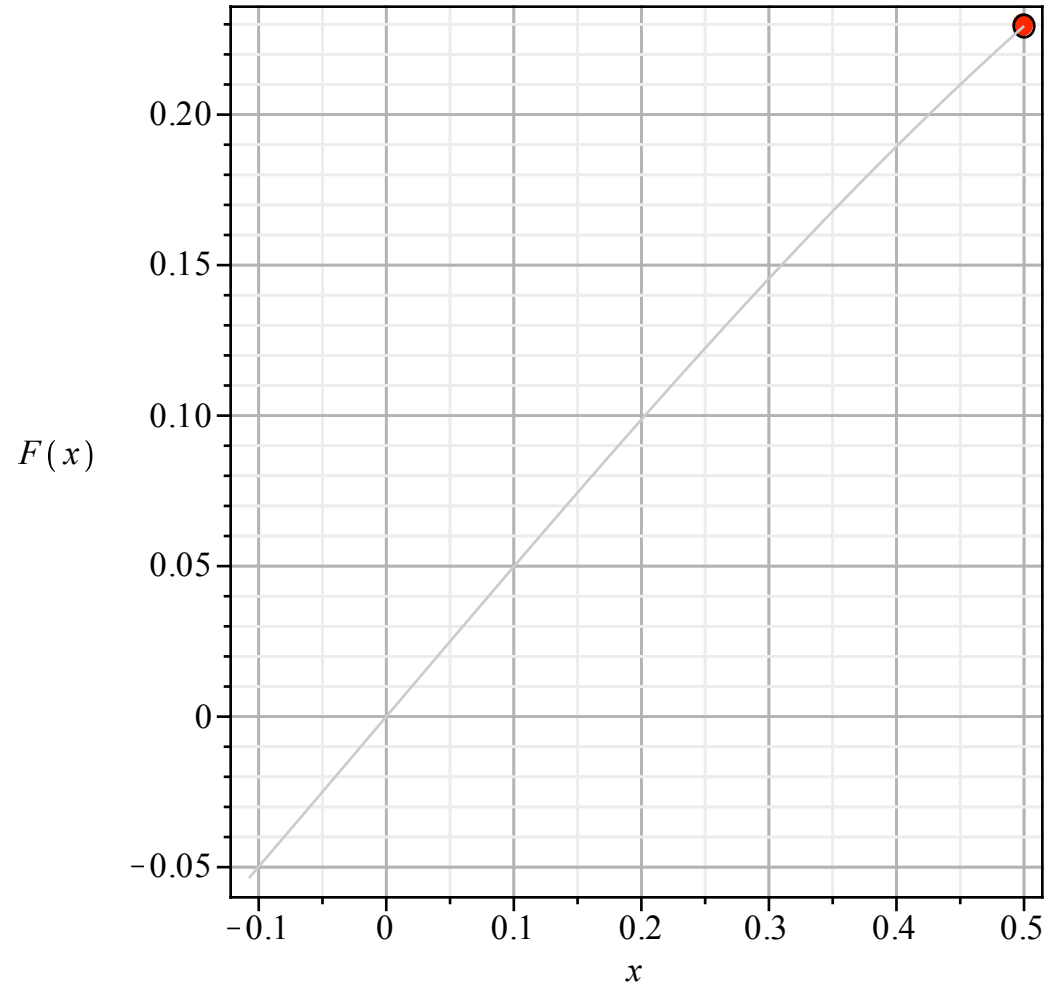
```

> Newton[movie] := proc(F,x0,eps)
  local data, i, r, ngon, q, p:
  data[0] := Newton[scalar](F,x0,eps):
  for i from 1 to 2 do:
    data[i] := Column(data[0],i):
    r[i] := (max(data[i])-min(data[i]))/75:
  od;
  ngon := (n,x,y,rx,ry,phi,Color) -> polygonplot([seq([x+rx*cos(2*Pi*i/n+phi),
    y+ry*sin(2*Pi*i/n+phi)], i = 1 .. n)],color=Color):
  q := plot(F(x),x=min(data[1])..max(data[1]),color=grey,axes=boxed,gridlines=true,
labels=[x,'F(x)']):
  for i from 1 to Dimension(data[0])[1] do:
    p[i] := display(ListTools[Reverse]([q,seq(ngon(20,data[0][j,1],data[0][j,2],r
[1],r[2],0,yellow),j=1..i-1),
      ngon(20,data[0][i,1],data[0][i,2],r[1],r[2],0,red))],title=[typeset
(`Iteration`,i,`:`,
      x[i]=evalf[4](data[0][i,1]))]);
    od:
  display(convert(p,list),insequence=true);
end proc:
> F := x -> sin(x)-x/2;
Newton[movie](F,0.5,1e-6);
Newton[movie](F,4.0,1e-6);
Newton[movie](F,1.0,1e-6);

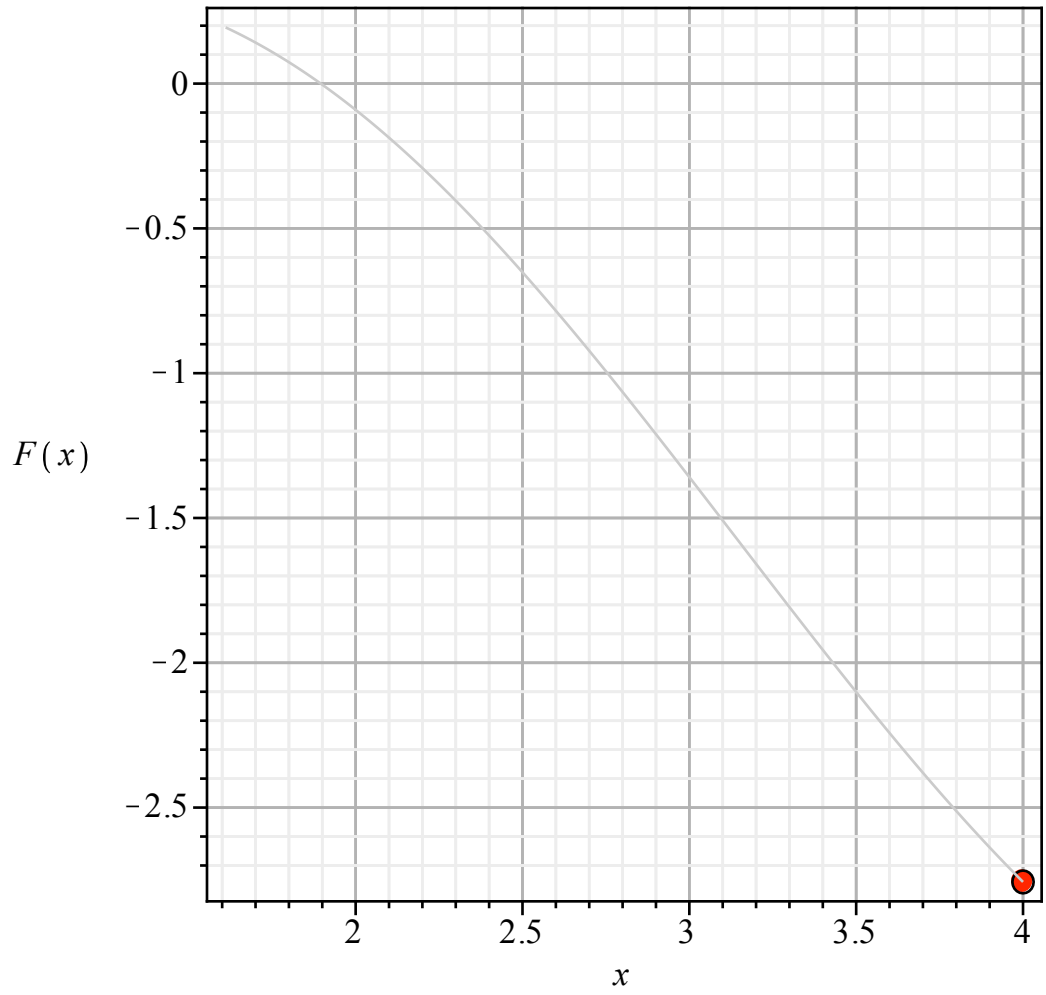
```

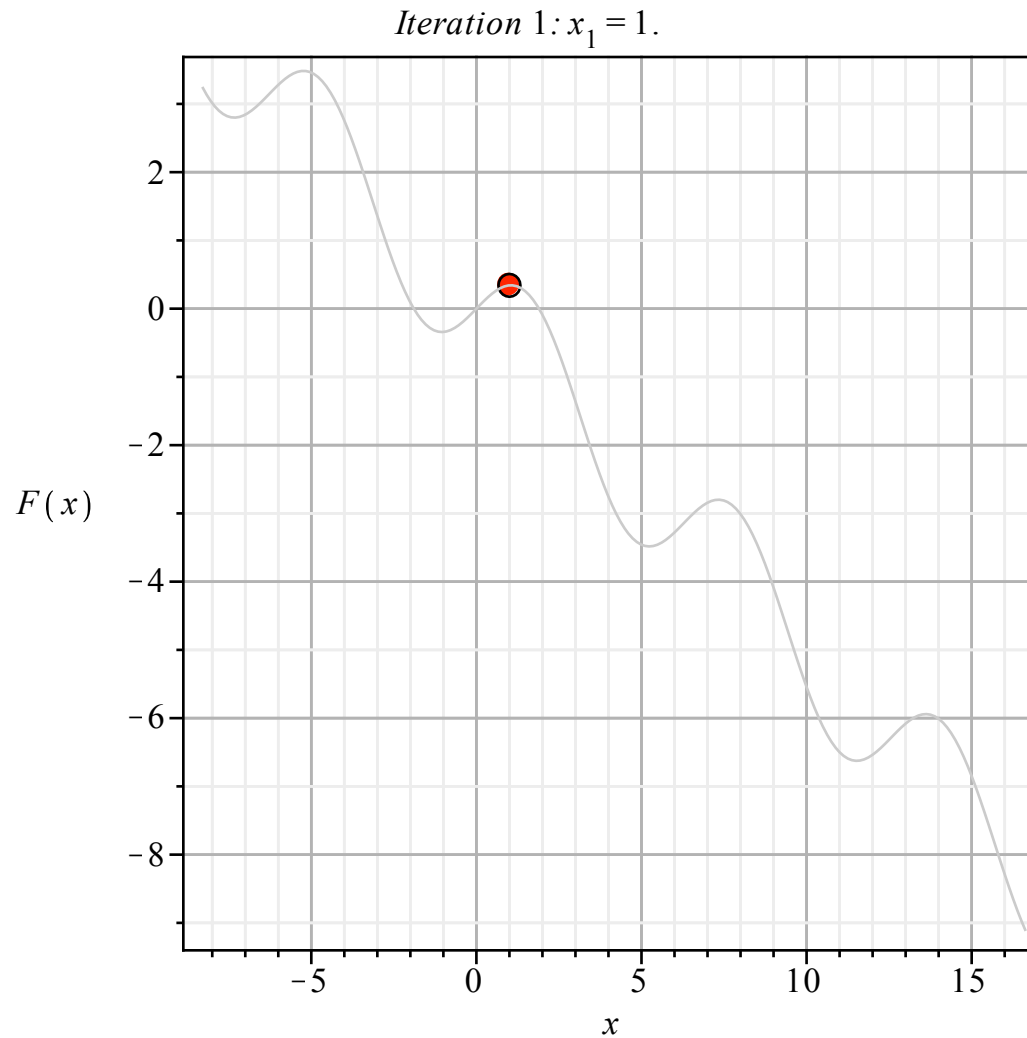
$$F := x \rightarrow \sin(x) - \frac{1}{2}x$$

Iteration 1: $x_1 = 0.5000$



Iteration 1: $x_1 = 4$.





▼ Solving n equations for n unknowns

```
> Newton[vector] := proc(Sys,Vars,guess,eps)
  local N, vars, i, sys, linearization, linear_sys,
        A, b, X, CONTINUE, maxsteps, delta, Subs, d:
  N := nops(Sys):
  vars := convert(Vars,list):
```

```

for i from 1 to N do:
  if (type(Sys[i],equation)) then:
    sys[i] := (lhs-rhs)(Sys[i]):
  else:
    sys[i] := Sys[i]:
  fi;
od;
sys := convert(sys,list);
linearization := map(u->u+epsilon*d[u],vars);
linear_sys := map(u->subs(epsilon=1,convert(series(u,epsilon,2),polynom)),subs
(linearization,sys));
A,b := LinearAlgebra[GenerateMatrix](linear_sys,map(u->d[u],vars));
Subs := seq(vars[i]=q[i],i=1..N);
A := unapply(subs(Subs,A),q);
b := unapply(subs(Subs,b),q);
X[0] := evalf(Vector(guess));
maxsteps := 50:
CONTINUE := true:

for i from 1 to maxsteps while (CONTINUE) do:
  X[i] := LinearAlgebra[LinearSolve](evalf(A(X[i-1])),evalf(b(X[i-1]))) + X[i-1]:
  delta := X[i]-X[i-1]:
  delta := sqrt(delta^%T.delta)/N;
  if (delta<eps) then CONTINUE := false fi:
od;

if (CONTINUE) then:
  return `maximum number of iterations exceeded`;
else:
  return convert(X[i-1],list):
fi:

end proc:

```

> sys := [2*x+y^2-z-1,x-y^3+z^2,z^2-x^2];
vars := [x,y,z];
guess := [-4,2,-4];
Newton[vector](sys,vars,guess,1e-14);

$$\text{sys} := [2x + y^2 - z - 1, x - y^3 + z^2, z^2 - x^2]$$

$$\text{vars} := [x, y, z]$$

$$\text{guess} := [-4, 2, -4]$$

$$[-3.76230632494549, 2.18227091007178, -3.76230632494549] \quad (3.2.1)$$

```
> fsolve(sys);
```

$$\{x = -3.7623063249455, y = 2.1822709100718, z = -3.7623063249455\} \quad (3.2.2)$$

Crank-Nicholson solution

```
> v := 'v':
d := 'd':
s := 's':
h := 'h':
j := 'j':
```

```
> expand(stencil[2]/2/h^2);
```

$$-\frac{1}{2} \frac{u(t,x)}{h^2 s} + \frac{1}{2} \frac{u(t+s,x)}{h^2 s} = \frac{1}{4} \frac{du(t,x-h)}{h^4} - \frac{1}{2} \frac{du(t,x)}{h^4} + \frac{1}{4} \frac{du(t,x+h)}{h^4} + \frac{1}{4} \frac{V(u(t,x))}{h^2} \quad (4.1)$$

$$+ \frac{1}{4} \frac{du(t+s,x-h)}{h^4} - \frac{1}{2} \frac{du(t+s,x)}{h^4} + \frac{1}{4} \frac{du(t+s,x+h)}{h^4} + \frac{1}{4} \frac{V(u(t+s,x))}{h^2}$$

```
> Subs := seq(u(t+s,x+jj*h)=phi[j+jj],jj=-1..1),seq(u(t,x+jj*h)=psi[j+jj],jj=-1..1);
```

$$Subs := u(t+s,x-h) = \phi_{j-1}, u(t+s,x) = \phi_j, u(t+s,x+h) = \phi_{j+1}, u(t,x-h) = \psi_{j-1}, u(t,x) = \psi_j, u(t,x+h) = \psi_{j+1} \quad (4.2)$$

```
> stencil[2] := expand(isolate(subs(Subs,stencil[2]),phi));
```

$$stencil_2 := -2\phi_j h^2 + ds\phi_{j-1} - 2ds\phi_j + ds\phi_{j+1} + V(\phi_j)sh^2 = -2h^2\psi_j - s d\psi_{j-1} + 2s d\psi_j - s d\psi_{j+1} - s h^2 V(\psi_j) \quad (4.3)$$

```
> master_CN := unapply(stencil[2],phi,psi,d,s,h,j);
```

$$master_CN := (\phi, \psi, d, s, h, j) \rightarrow -2\phi_j h^2 + ds\phi_{j-1} - 2ds\phi_j + ds\phi_{j+1} + V(\phi_j)sh^2 = -2h^2\psi_j - s d\psi_{j-1} + 2s d\psi_j - s d\psi_{j+1} - s h^2 V(\psi_j) \quad (4.4)$$

```
> phi := 'phi':
```

```
psi := 'psi':
```

```
M := 5:
```

```
phi[0],psi[0],psi[M+1],phi[M+1] := 0,0,0,0;
```

```
Vector([seq(master_CN(phi,psi,d,s,h,j),j=1..M)]);
```

$$\phi_0, \psi_0, \psi_6, \phi_6 := 0, 0, 0, 0$$

$$\begin{aligned}
 -2\phi_1 h^2 - 2ds\phi_1 + ds\phi_2 + V(\phi_1)sh^2 &= -2h^2\psi_1 + 2sd\psi_1 - sd\psi_2 - sh^2V(\psi_1) \\
 -2\phi_2 h^2 + ds\phi_1 - 2ds\phi_2 + ds\phi_3 + V(\phi_2)sh^2 &= -2h^2\psi_2 - sd\psi_1 + 2sd\psi_2 - sd\psi_3 - sh^2V(\psi_2) \\
 -2\phi_3 h^2 + ds\phi_2 - 2ds\phi_3 + ds\phi_4 + V(\phi_3)sh^2 &= -2h^2\psi_3 - sd\psi_2 + 2sd\psi_3 - sd\psi_4 - sh^2V(\psi_3) \\
 -2\phi_4 h^2 + ds\phi_3 - 2ds\phi_4 + ds\phi_5 + V(\phi_4)sh^2 &= -2h^2\psi_4 - sd\psi_3 + 2sd\psi_4 - sd\psi_5 - sh^2V(\psi_4) \\
 -2\phi_5 h^2 + ds\phi_4 - 2ds\phi_5 + V(\phi_5)sh^2 &= -2h^2\psi_5 - sd\psi_4 + 2sd\psi_5 - sh^2V(\psi_5)
 \end{aligned}$$

(4.5)

```

> CN := proc(tau,L,N,M,d,f)
  local X, T, s, h, XX, u_past, u_future, Title, PlotOptions, p, A, P,
    i, phi, psi, sys, vars, guess:

  # Defining the lattice parameters/functions as before:
  X := j -> L*(-1 + j*2/(M+1));
  T := i -> tau*i/N;
  s := evalf(T(1)-T(0));
  h := evalf(X(1)-X(0));

  # Set the initial data
  XX := Array(0..M+1, [seq(X(j), j=0..M+1)], datatype=float);
  psi := map(z->f(z), XX);
  # Plot the first frame
  p[0] := Frame[2](XX, psi, s, h, T(0));

  # Here is the main calculation loop (notice the LinearSolve command)
  for i from 1 to N do:
    phi := 'phi':
    phi[0], psi[0], psi[M+1], phi[M+1] := 0, 0, 0, 0;
    sys := [seq(master_CN(phi, psi, d, s, h, j), j=1..M)];
    vars := [seq(phi[j], j=1..M)];
    guess := [seq(psi[j], j=1..M)];
    phi := Newton[vector](sys, vars, guess, 1e-5);
    psi := Array(0..M+1, [0, op(phi), 0], datatype=float);
    p[i] := Frame[2](XX, psi, s, h, T(i));
  od:

  # Assemble the output movie

```

```
display(convert(p,list),insequence=true);
```

```
end proc;
```

```
# Here is the plotting subroutine
```

```
Frame[2] := proc(xdata,ydata,s,h,T) local Title, PlotOptions:
```

```
    Title := typeset(`timestep = `,evalf[2](s),`, spacestep = `,evalf[2](h),`, `, `t=evalf[2](T));
```

```
    PlotOptions := axes=boxed, labels=[x,u(t,x)], legend=["Crank-Nicholson"], color=magenta;
```

```
    plot(Matrix([[xdata],[ydata]])^%T,title=Title,PlotOptions);
```

```
end proc:
```

```
> V := u -> 5*u*(1-u);
```

```
tau := 5;
```

```
N := 400;
```

```
M := 100;
```

```
L := 5;
```

```
d := 1;
```

```
f := x -> exp(-(10*x)^2);
```

```
s := evalf(2*L/(M+1));
```

```
h := evalf(tau/N);
```

```
movie[1] := FTCS(tau,L,N,M,d,f);
```

```
movie[2] := CN(tau,L,N,M,d,f);
```

```
pds := pdsolve(pde,[u(t,-L)=0,u(t,+L)=0,u(0,x)=f(x)],numeric,timestep=s,spacestep=h):
```

```
movie[3] := pds:-animate(t=0..tau,frames=N+1,axes=boxed,legend=["pdsolve/numeric"],color=blue):
```

$$V := u \rightarrow 5u(1-u)$$

$$\tau := 5$$

$$N := 400$$

$$M := 100$$

$$L := 5$$

$$d := 1$$

$$f := x \rightarrow e^{-100x^2}$$

$$s := 0.099009900990099$$

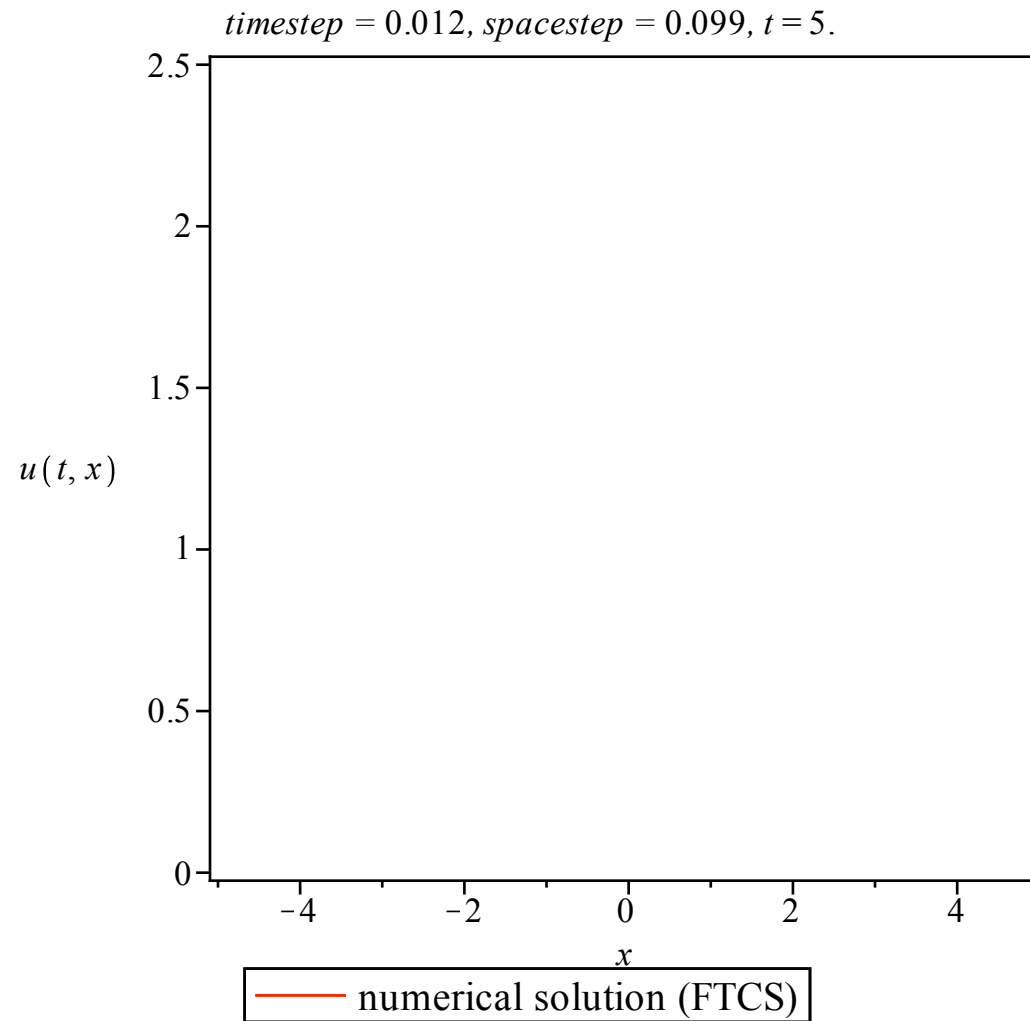

```
h := 0.0125000000000000
```

```
movie1 := PLOT(...)
```

```
movie2 := PLOT(...)
```

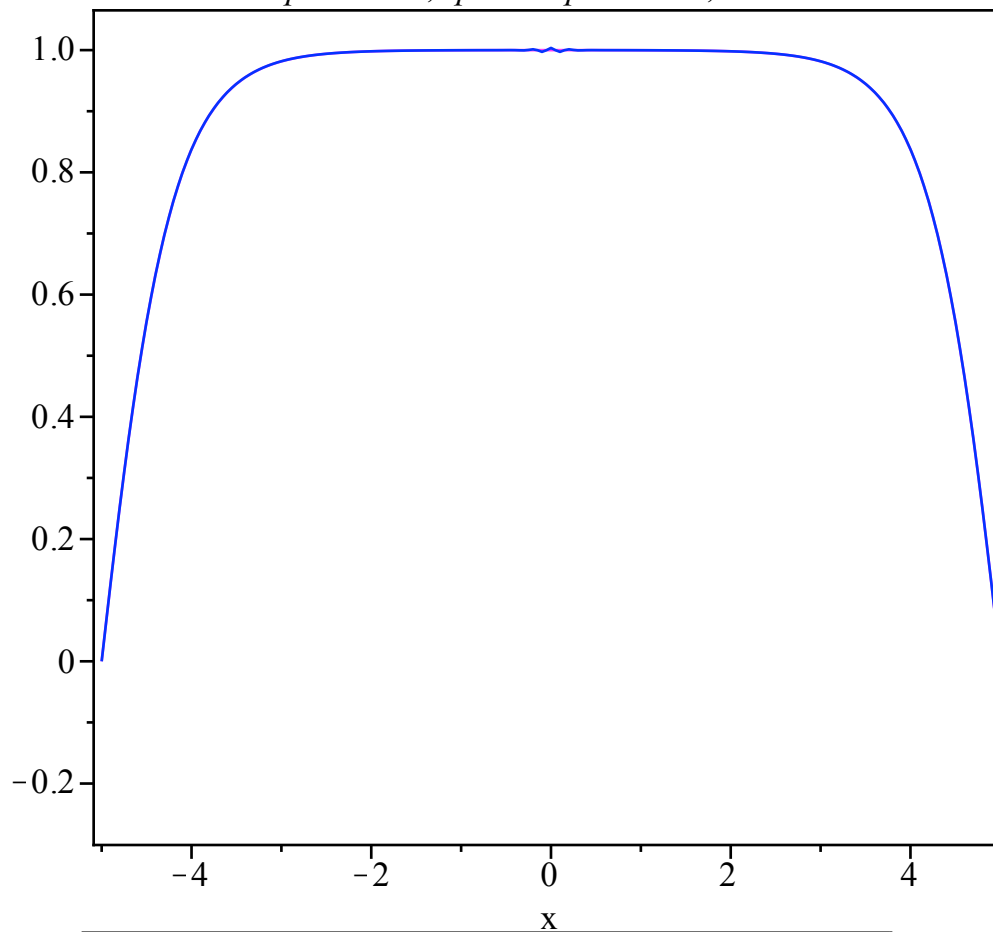
(4.6

```
> movie[1];
```



```
> display([movie[2], movie[3]]);
```

timestep = 0.050, spacestep = 0.099, t = 5.



— Crank-Nicholson — pdsolve/numeric