PDESOL Application Examples[1]

ADVECTION EQUATION (11 sec)

First-order convective (hyperbolic) PDE. Shows the propagation of a finite discontinuity (step change) along x. Advantage of upwind approximations for the convective term is illustrated.

$$\frac{\partial U}{\partial t} = -v\frac{\partial U}{\partial x}$$

$$U(x,0) = 0$$
$$U(0,t) = 1$$

```
U_x = dxu(U,v)
U_t = -v*U_x
```

```
U@t0 = 0
U@xL = 1
```

ONE-DIMENSIONAL BURGERS' EQUATION (75 sec)

A standard test problem for PDE numerical methods, with known analytical solutions. The equation is of the hyperbolic-parabolic type. For small values of μ, the Burgers' equation is strongly hyperbolic, and the solutions can exhibit steep moving fronts which are difficult to resolve numerically. This example presents solutions for a case of Burgers' equation with front sharpening as time progresses (μ= 0.003).

$$\frac{\partial u}{\partial t} = -u\frac{\partial u}{\partial x} + \mu\frac{\partial^2 u}{\partial x^2}$$

$$a = 0.05(x - 0.5 + 4.95t)/\mu$$
$$b = 0.25(x - 0.5 + 0.75t)/\mu$$
$$c = 0.5(x - 0.375)/\mu$$
$$\Phi = \frac{0.1e^{-a} + 0.5e^{-b} + e^{-c}}{e^{-a} + e^{-b} + e^{-c}}$$

$$u(x,0) = \frac{0.1e^{-a(x,0)} + 0.5e^{-b(x,0)} + e^{-c}}{e^{-a(x,0)} + e^{-b(x,0)} + e^{-c}}$$
$$u(0,t) = \Phi(0,t)$$
$$u(l,t) = \Phi(l,t)$$

```
u_x = dxu5b(u,1)
u_xx = dxx(u,DD)
u_t = - u*u_x +
        vis*u_xx
```

```
u@t0=(0.1*exp(-a0)+0.5*exp(-b0)+exp(-c))/
     (exp(-a0)+exp(-b0)+exp(-c))

u@xL = phi@xL
u@xU = phi@xU
```

KORTEWEG-DE VRIES EQUATION (264 sec)

Classical nonlinear PDE which balances front sharpening and dispersion to produce solitons, i.e. traveling waves that do no change shape or speed. A special third-order derivative routine is used to evaluate the dispersion term without the need for boundary conditions, as long as the computed solitons do not closely approach the finite boundaries that are used in place of the infinite boundaries.

$$\frac{\partial U}{\partial t} = -6U\frac{\partial U}{\partial x} - \frac{\partial^3 U}{\partial x^3}$$

$$U(x,0) = \frac{0.5}{\left(\cosh(0.5x)\right)^2}$$

```
U_x = dx(U)
U_xxx = dxxx7c(U)
U_t =  - 6*U*U_x - U_xxx
```

```
U@t0 = 0.5/(cosh(0.5*x))^2
```

KORTEWEG-DE VRIES EQUATION WITH TWO-PULSE INITIAL CONDITION (386 sec)

Same as above, with two-pulse initial condition of different amplitudes and speeds. As the solution progresses, the faster pulse catches up and merges with the slower pulse. The two original pulses eventually reappear, and continue to travel in their original shape.

$$\frac{\partial U}{\partial t} + 6U\frac{\partial U}{\partial x} + \frac{\partial^3 U}{\partial x^3} = 0$$

$$U(x,0) = \frac{0.5x2}{\left(\cosh(0.5\sqrt{2}(x+15)\right)^2} + \frac{0.5x0.5}{\left(\cosh(0.5\sqrt{0.5}(x-15)\right)^2}$$

```
U_x = dx(U)
U_xxx = dxxx7c(U)
U_t = - 6*U*U_x - U_xxx
```

```
U@t0 =
 0.5*2/(cosh(0.5*sqrt(2)*(x+15)))^2 +
 0.5*0.5/(cosh(0.5*sqrt(0.5)*(x-15)))^2
```

CUBIC SCHRÖDINGER EQUATION (395 sec)

The Cubic Shrödinger Equation (CSE) governs the movement of solitons traveling with constant velocity and amplitude (without changing shape). When separated into real and imaginary parts, the CSE gives two coupled PDEs. The equations require a fine grid in space in order to resolve the sharp spatial variations of the solitons; 401 points are used in the example (802 equations).

$$\frac{\partial v}{\partial t} = -\frac{\partial^2 w}{\partial x^2} - \left(v^2 + w^2\right)w$$
$$\frac{\partial w}{\partial t} = \frac{\partial^2 v}{\partial x^2} + \left(v^2 + w^2\right)v$$
$$|u| = |v + iw| = \sqrt{v^2 + w^2}$$

$$v(x,0) = \sqrt{2}\cos(x/2)/\cosh(x)$$
$$w(x,0) = \sqrt{2}\cos(x/2)/\cosh(x)$$
$$v(0,t) = w(0,t) = 0$$
$$v(l,t) = w(l,t) = 0$$

```
V_xx = dxx(V,DD)
W_xx = dxx(W,DD)

V_t = -W_xx - (V^2+W^2)*W
W_t =  V_xx + (V^2+W^2)*V

NORM = sqrt(V^2+W^2)
```

```
V@t0 = sqrt(2)*cos(0.5*x)/cosh(x)
W@t0 = sqrt(2)*sin(0.5*x)/cosh(x)

V@xL = 0  ;   W@xL = 0
V@xU = 0  ;   W@xU = 0
```

RIVER POLLUTION MODEL WITH POINT SOURCE (3 sec)

Hyperbolic-parabolic or convective-diffusion equation. The equation models pollutant concentrations in a river and includes a spatial point source p(x,t), turned on during a finite time interval over the course of the solution. Note the special outflow boundary condition and the use of the step function to specify the point source.

$$\frac{\partial U}{\partial t} = D\frac{\partial^2 U}{\partial x^2} - v\frac{\partial U}{\partial x} - rU + p(x,t)$$

$p(x,t)=0$ for $0 \le x < l/2$
$p(l/2,t)=100$ for $0 \le t \le 10$
$p(l/2,t)=0$ for $t > 10$
$p(x,t)=0$ for $l/2 < x \le l$

$$U(x,0) = 0$$
$$U(0,t) = 0$$
$$\frac{\partial U}{\partial t}(l,t) = -v\frac{\partial U}{\partial x}(l,t)$$

```
Ux = dxu5b(U,1)
Uxx = dxx(U,DD)
U_t = D*Uxx-v*Ux-
      r*U + pp
```

```
p = 100*(step(t) -
         step(t-10))
pp = p*(step(x-249.95) -
        step(x-250.05))
```

```
U@t0 = 0
U@xL = 0
U_t@xU = -v*Ux@xU
```

[1] Note the similarity between mathematical statements and PDESOL statements. Operators for spatial derivatives are explained in the Help file. Numbers in parenthesis are the run-times obtained on a Pentium 90 machine.

FOURIER SECOND LAW IN CYLINDRICAL COORDINATES (28 sec)

Parabolic PDE governing diffusion in cylindrical geometry. The example shows how the "divide by zero" at r = 0 can be avoided in PDESOL by using the operator “>“.

$$\frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial r^2} + \frac{1}{r}\frac{\partial T}{\partial r}$$

$T(x,0) = 0$

$\frac{\partial T}{\partial r}(0,t) = 0$

$T(l,t) = 25$

```
T_r = dx(T)
T_rr = dx(T_r)
T_t = T_rr + (1/(x>0.001))*T_r
T_t@xL = 2*T_rr@x
```

```
T@t0 = 0
T_r@xL = 0
T@xU = 25
```

ONE-DIMENSIONAL WAVE EQUATION (4 sec)

Second order hyperbolic PDEs, i.e. PDEs which are second-order in time, can be integrated by expressing them as systems of two first-order PDEs. The one-dimensional wave equation is used to illustrate this procedure.

$$\frac{\partial^2 U}{\partial t^2} - \frac{\partial^2 U}{\partial x^2} = 0$$

$U(x,0) = \sin(\pi x)$

$\frac{\partial U}{\partial t}(x,0) = 0$

$U(0,t) = U(1,t) = 0$

```
U1_x = dx(U1)
U1_xx = dx(U1x)
U1_t = U2
U2_t = U1_xx
```

```
U1@t0 = sin(pi*x)
U2@t0 = 0
U1@xL = 0
U1@xU = 0
```

FOUR-PASS SHELL AND TUBE HEAT EXCHANGER (6 sec)

Mixed PDE/ODE system with stirred tank ODE boundary conditions to simulate mixing in the headers.

$$\frac{\partial T_1}{\partial t} = -v\frac{\partial T_1}{\partial x} + \frac{UA_h}{A\rho C_p}(T_5 - T_1)$$

$$\frac{\partial T_2}{\partial t} = v\frac{\partial T_2}{\partial x} + \frac{UA_h}{A\rho C_p}(T_6 - T_2)$$

$$\frac{\partial T_3}{\partial t} = -v\frac{\partial T_3}{\partial x} + \frac{UA_h}{A\rho C_p}(T_7 - T_3)$$

$$\frac{\partial T_4}{\partial t} = v\frac{\partial T_4}{\partial x} + \frac{UA_h}{A\rho C_p}(T_8 - T_4)$$

$$\frac{\partial T_5}{\partial t} = \frac{UA_h}{A_m\rho_m C_{pm}}(T_1 - T_5) + \frac{U_0 A_{h0}}{A_m\rho_m C_{pm}}(T_9 - T_5)$$

$$\frac{\partial T_6}{\partial t} = \frac{UA_h}{A_m\rho_m C_{pm}}(T_2 - T_6) + \frac{U_0 A_{h0}}{A_m\rho_m C_{pm}}(T_9 - T_6)$$

$$\frac{\partial T_7}{\partial t} = \frac{UA_h}{A_m\rho_m C_{pm}}(T_3 - T_7) + \frac{U_0 A_{h0}}{A_m\rho_m C_{pm}}(T_9 - T_7)$$

$$\frac{\partial T_8}{\partial t} = \frac{UA_h}{A_m\rho_m C_{pm}}(T_4 - T_8) + \frac{U_0 A_{h0}}{A_m\rho_m C_{pm}}(T_9 - T_8)$$

$$\frac{\partial T_9}{\partial t} = -v_s\frac{\partial T_9}{\partial x} + \frac{U_0 A_{h0}}{A_s\rho_s C_{ps}}((T_5 - T_9) + (T_6 - T_9) + (T_7 - T_9) + (T_8 - T_9))$$

$$V_1\frac{dT_0(t)}{dt} = Q(T_4(0,t) - T_0(t))$$

$T_1(x,0) = T_2(x,0) = T_3(x,0) =$
$T_4(x,0) = T_5(x,0) = T_6(x,0) =$
$T_7(x,0) = T_8(x,0) = T_9(x,0) = 0$

$T_0(0) = 0$

$T_9(0,t) = TSI$

$V_1\frac{dT_1(0,t)}{dt} = Q(T_i - T_1(0,t))$

$V_2\frac{dT_2(l,t)}{dt} = Q(T_1(l,t) - T_2(l,t))$

$V_2\frac{dT_3(0,t)}{dt} = Q(T_2(0,t) - T_3(0,t))$

$V_2\frac{dT_4(l,t)}{dt} = Q(T_3(l,t) - T_4(l,t))$

```
T1_x =  dxu(T1,1)
T1_t = -C1*T1_x + C3*(T5-T1)

T2_x =  dxu(T2,-1)
T2_t = C1*T2_x + C3*(T6-T2)

T3_x =  dxu(T3,1)
T3_t = -C1*T3_x + C3*(T7-T3)

T4_x =  dxu(T4,-1)
T4_t = C1*T4_x + C3*(T8-T4)

T5_t = C4*(T1-T5) + C5*(T9-T5)
T6_t = C4*(T2-T6) + C5*(T9-T6)
T7_t = C4*(T3-T7) + C5*(T9-T7)
T8_t = C4*(T4-T8) + C5*(T9-T8)

T9_x =  dxu(T9,1)
T9_t = -C2*T9_x - 4*C6*T9 +
        C6*(T5+T6+T7+T8)

T0_t = B1*(T4@xL-T0)
```

```
T1@t0 = 0.
T2@t0 = 0.
T3@t0 = 0.
T4@t0 = 0.
T5@t0 = 0.
T6@t0 = 0.
T7@t0 = 0.
T8@t0 = 0.
T9@t0 = 0.

T0@t0 = 0.

T9@xL = TSI
T1_t@xL = B1*(TI-T1@xL)
T2_t@xU = B2*(T1@xU-T2@xU)
T3_t@xL = B2*(T2@xL-T3@xL)
T4_t@xU = B2*(T3@xU-T4@xU)
```

BLACK AND SCHOLES EQUATION (0.2 sec)

The Black and Scholes equation governs the price of any derivative security dependent on a non-dividend-paying stock. This example is for an american put option.

$$\frac{\partial f}{\partial t} = rf - rf\frac{\partial f}{\partial x} - \frac{1}{2}\sigma^2 x^2\frac{\partial^2 f}{\partial x^2}$$

$f(x,t) = MAX(50 - x, f)$

$f(x,0) = MAX(50 - x, 0)$

$f(0,t) = 50$

$f(l,t) = 0$

```
f_x=dx(f)
f_xx=dxx(f,DD)
f_t = -(r*f - r*f*f_x -
        0.5*sigsq*x^2*f_xx)
```

```
f = (50-x) > f
f@t0=(50-x)>0
f@xL=50
f@xU=0
```

PACKED HUMIDIFICATION COLUMN (1 sec)

PDE system with an ODE equation to simulate a PI controller plus many intermediate variables.

$$\frac{dei}{dt} = e$$
$$\frac{\partial y}{\partial t} = -p1\frac{\partial y}{\partial x} + P2(ys - y)$$
$$\frac{\partial tl}{\partial t} = P4\frac{\partial tl}{\partial x} - P5(tl - tg) - P6(ys - y)p7$$
$$\frac{\partial ev}{\partial t} = -p1\frac{\partial ep}{\partial x} + P3(tl - tg) + P2(ys - y)p7$$

$ei(x,0) = 0$

$y(x,0) = 0.01$

$tl(x,0) = 43.33$

$ev(x,0) = CVA\,tl(x,0) + y(x,0)(CVV\,tl(x,0) + DHVAP)$

$e = tl(l,t) - TLSET$

$xcon = XSS + KC(e + ei / TI)$

$0 < xcon < 1$

$v = CVDP\,xcon$

$p1 = \frac{v}{G\,S}$

$tg = (ev - y\,DHVAP) / (CVA + y\,CVV)$

$ep = CPA\,tg + y(CPV\,tg + DHVAP)$

$p = 10^{(7.96681 - 3002.4 / (378.4 + 1.8tl + 32))}$

$ys = p / (760 - p)$

$p7 = CVV\,tg + DHVAP$

$y(0,t) = 0.01$

$tl(l,t) = 43.33$

$tg(0,t) = 43.33$

$ep(0,t) = CPA\,tg(0,t) + y(0,t)(CPV\,tg(0,t) + DHVAP)$

$\frac{\partial ev}{\partial t}(0,t) = 0$

```
ei_t = e

y_x = dxu(y,1)
y_t = -p1*y_x+P2*(ys-y)

tl_x = dxu(tl,-1)
tl_t = P4*tl_x-P5*(tl-tg)-
       P6*(ys-y)*p7

ep_x = dxu(ep,1)
ev_t = -p1*ep_x+P3*(tl-tg)+
        P2*(ys-y)*p7
```

```
ei@t0 = 0
y@t0 = 0.01
tl@t0 = 43.33
ev@t0 = CVA*tl@t0 +
       y@t0*(CVV*tl@t0+DHVAP)

e = tl@xL - TLSET
xcon = XSS+KC*(e+(1/TI)*ei)
xcon = (xcon > 0.0) < 1.0
v = CVDP*xcon
p1 = v/(G*S)
tg = (ev-y*DHVAP)/(CVA+y*CVV)
ep = CPA*tg+y*(CPV*tg+DHVAP)
p = 10^(7.96681 -
3002.4/(378.4+1.8*tl+32))
ys = p/(760.0-p)
p7 = CVV*tg + DHVAP

y@xL = 0.01
tl@xU = 43.33
tg@xL = 43.33
ep@xL = CPA*tg@xL +
       y@xL*(CPV*tg@xL+DHVAP)

ev_t@xL = 0
```

PANCREATIC RESPONSE TO AN INFUSION OF GLUCOSE (0.4 sec)

Nonlinear ODE system with conditional RHS. Note the usage of the operator “>“ to specify the conditional RHS member and the operator “step” to specify a finite duration of a condition.

$$C_g\frac{dG}{dt} = Q + I_n - G_g IG - D_d G, \quad G < G_k$$
$$C_g\frac{dG}{dt} = Q + I_n - G_g IG - D_d G - M_u(G - G_k), \quad G \ge G_k$$
$$C_i\frac{dI}{dt} = -A_a I, \quad G < G_0$$
$$C_i\frac{dI}{dt} = -A_a I + B_b(G - G_0), \quad G \ge G_0$$

$I_n = Q_t, \quad 0 \le t < 0.5$

$I_n = 0, \quad 0.5 \le t \le 12$

$G(0) = 81.14$

$I(0) = 5.671$

```
G_t=(Q+IN-GG*I*G-DD*G-(MU*(G-GK)>0))/CG
I_t=(-AA*I+(BB*(G-G0)>0))/CI
```

```
IN = step(0.5-t)*QT
G@t0 = 81.14
I@t0 = 5.671
```

A VERY STIFF ODE PROBLEM (2 sec)

This example considers a second-order, linear ODE system, with a ratio of eigenvalues of 1000000 (L1 = -1000000, L2 = -1), illustrating the use of an explicit integrator (RKF45) and an implicit stiff integrator (LSODES) for the different time scales of the problem.

$$\frac{dy_1}{dt} = -ay_1 + by_2$$
$$\frac{dy2}{dt} = by_1 - ay_2$$

$a = 500000.5$

$b = 499999.5$

$y_1(0) = 0$

$y_2(0) = 2$

```
y1_t = -a*y1+b*y2
y2_t =  b*y1-a*y2
```

```
y1@t0 = 0
y2@t0 = 2
```