

**36. The DuFort-Frankel method** is given by

$$\frac{f_j^{n+1} - f_j^{n-1}}{2\Delta t} = \alpha L_{xx} f_j^n = \frac{\alpha}{\Delta x^2} (f_{j-1}^n - f_j^{n-1} - f_j^{n+1} + f_{j+1}^n)$$

**(a) Truncation error:**

Taylor expansion

$$f_i^{n+1} = \sum_{m=0}^{\infty} \frac{\Delta t^m}{m!} \left[ \frac{\partial^m f}{\partial t^m} \right]_i \quad (1)$$

Since we consider the diffusion equation we need to carry the Taylor expansion in time only up to half the order of the spatial derivative. Considering terms up to the 4th or 5th derivative in space it is sufficient to go up to the 2nd derivative in time. Note: for the corresponding expansion vor the convection or transport equation we need to carry the Taylor expansion in time as far as we carry the expansion in space.

**Term 1** in the equation:

$$\begin{aligned} \frac{f_j^{n+1} - f_j^{n-1}}{2\Delta t} &= \frac{1}{2\Delta t} \left\{ (1-1)f_j^n + (1+1)\Delta t \frac{\partial f}{\partial t} + (1-1)\frac{\Delta t^2}{2} \frac{\partial^2 f}{\partial t^2} + (1+1)\frac{\Delta t^3}{6} \frac{\partial^3 f}{\partial t^3} + \dots \right\} \\ &= \frac{\partial f}{\partial t} + \frac{\Delta t^2}{6} \frac{\partial^3 f}{\partial t^3} + O(\Delta t^4) \end{aligned}$$

**Term 2** in the equation (we separate the temporal and spatial variations on the right side):

$$\begin{aligned} \frac{f_j^{n+1} + f_j^{n-1}}{\Delta x^2} &= \frac{1}{\Delta x^2} \left\{ (1+1)f_j^n + (1-1)\Delta t \frac{\partial f}{\partial t} + (1+1)\frac{\Delta t^2}{2} \frac{\partial^2 f}{\partial t^2} + (1-1)\frac{\Delta t^3}{6} \frac{\partial^3 f}{\partial t^3} + \dots \right\} \\ &= \frac{1}{\Delta x^2} \left( 2f + \Delta t^2 \frac{\partial^2 f}{\partial t^2} + O(\Delta t^4) \right) \end{aligned}$$

**Term 3** also on the right side:

$$\begin{aligned} \frac{f_{j-1}^n + f_{j+1}^n}{\Delta x^2} &= \frac{1}{\Delta x^2} \left\{ (1+1)f_j^n + (1-1)\Delta x \frac{\partial f}{\partial x} + (1+1)\frac{\Delta x^2}{2} \frac{\partial^2 f}{\partial x^2} + (1-1)\frac{\Delta x^3}{6} \frac{\partial^3 f}{\partial x^3} \right. \\ &\quad \left. + (1+1)\frac{\Delta x^4}{24} \frac{\partial^4 f}{\partial x^4} + (1-1)\frac{\Delta x^5}{120} \frac{\partial^5 f}{\partial x^5} \right\} \\ &= \frac{1}{\Delta x^2} \left( 2f + \Delta x^2 \frac{\partial^2 f}{\partial x^2} + \frac{\Delta x^4}{12} \frac{\partial^4 f}{\partial x^4} \right) \end{aligned}$$

Combining the right side terms and using

$$\frac{\partial f}{\partial t} = \alpha \frac{\partial^2 f}{\partial x^2} \quad \text{and} \quad \frac{\partial^2 f}{\partial t^2} = \alpha^2 \frac{\partial^4 f}{\partial x^4}$$

yields

$$\begin{aligned}
\frac{\alpha}{\Delta x^2} \left( f_{j-1}^n - f_j^{n-1} - f_j^{n+1} + f_{j+1}^n \right) &= \frac{\alpha}{\Delta x^2} \left[ 2f + \Delta x^2 \frac{\partial^2 f}{\partial x^2} + \frac{\Delta x^4}{12} \frac{\partial^4 f}{\partial x^4} - 2f - \Delta t^2 \frac{\partial^2 f}{\partial t^2} \right] \\
&= \alpha \left( \frac{\partial^2 f}{\partial x^2} + \frac{\Delta x^2}{12} \frac{\partial^4 f}{\partial x^4} - \alpha^2 \frac{\Delta t^2}{\Delta x^2} \frac{\partial^4 f}{\partial x^4} \right) \\
&= \alpha \frac{\partial^2 f}{\partial x^2} + \alpha \Delta x^2 \left( \frac{1}{12} - s^2 \right) \frac{\partial^4 f}{\partial x^4}
\end{aligned}$$

Compining all terms yields

$$\frac{\partial f}{\partial t} - \alpha \frac{\partial^2 f}{\partial x^2} - \alpha \Delta x^2 \left( \frac{1}{12} - s^2 \right) \frac{\partial^4 f}{\partial x^4} + \dots = 0$$

with the error

$$E = -\alpha \Delta x^2 \left( \frac{1}{12} - s^2 \right) \frac{\partial^4 f}{\partial x^4}$$

### (b) Amplification factor

Re-aranging terms in the algebraic equation (see problem 31) yields

$$f_j^{n+1} = \frac{2s}{1+2s} (f_{j-1}^n + f_{j+1}^n) + \frac{1-2s}{1+2s} f_j^n$$

Division by  $f_j^n$  with  $g = f_j^{n+1} / f_j^n$

$$g - \frac{2s}{1+2s} (\exp(ik\Delta x) + \exp(-ik\Delta x)) - \frac{1-2s}{1+2s} \frac{1}{g} = 0$$

or

$$g^2 - \frac{4s \cos k\Delta}{1+2s} g - \frac{1-2s}{1+2s} = 0$$

Solving this equation for  $g$ :

$$\begin{aligned}
g^2 - \frac{4s \cos k\Delta}{1+2s} g + \left( \frac{2s \cos k\Delta}{1+2s} \right)^2 &= \frac{1-2s}{1+2s} + \left( \frac{2s \cos k\Delta}{1+2s} \right)^2 \\
\left( g - \frac{2s \cos k\Delta}{1+2s} \right)^2 &= \frac{1}{(1+2s)^2} (1 - 4s^4 + 4s^2 \cos^2 k\Delta) \\
\text{and } g &= \frac{2s \cos k\Delta}{1+2s} \pm \frac{1}{1+2s} \sqrt{1 - 4s^2 \sin^2 k\Delta}
\end{aligned}$$

### c) Stability:

$\alpha$ ) First consider  $4s^2 \sin^2 k\Delta \leq 1$  such that the argument of the square root is positive. Assuming  $\cos k\Delta > 0$  we can consider just the “+” sign and consider

$$\frac{2s \cos k\Delta}{1+2s} + \frac{1}{1+2s} \sqrt{1 - 4s^2 \sin^2 k\Delta} \leq 1$$

=>

$$2s \cos k\Delta + \sqrt{1 - 4s^2 \sin^2 k\Delta} \leq 1 + 2s$$

This is obvious because  $\sqrt{1 - 4s^2 \sin^2 k\Delta} \leq 1$  and  $2s \cos k\Delta \leq 2s$ . Considering  $\cos k\Delta \leq 0$  and choosing “-” sign yields the requirement

$$-1 \leq \frac{2s \cos k\Delta}{1 + 2s} - \frac{1}{1 + 2s} \sqrt{1 - 4s^2 \sin^2 k\Delta}$$

i.e., the same condition as the one above.

$\beta$ ) Consider  $4s^2 \sin^2 k\Delta > 1$  renders the argument of the square root negative such that the square root is purely imaginary. Thus the requirement for stability is

$$|g|^2 = gg^* = \frac{(2s \cos k\Delta)^2 + 4s^2 \sin^2 k\Delta - 1}{(1 + 2s)^2} = \frac{4s^2 - 1}{4s^2 + 4s + 1} < 1$$

Thus the scheme is unconditionally stable.

### 37. Implementation of the DuFort-Frankel and the Hopscotch (1D) schemes in program sim1:

First derive the algebraic equations needed for the DuFort-Frankel and the Hopscotch scheme and explain what changes you need to apply to sim1.f for the implementation. Carry out the implementation. Test the schemes first for a set of standard parameters used for the FTCS scheme with a grid number of 21 points and compare the result to the FTCS. Then use increasingly larger time steps for the new schemes and report your observations. Pay attention to the fact that the time steps should be chosen such that the final time is in fact the same as for the FTCS scheme.

DuFort-Frankel - Algebraic equation:

$$\frac{f_j^{n+1} - f_j^{n-1}}{2\Delta t} = \alpha L_{xx} f_j^n = \frac{\alpha}{\Delta x^2} (f_{j-1}^n - f_j^{n-1} - f_j^{n+1} + f_{j+1}^n)$$

multiplication with  $2\Delta t$  and definition  $s = \alpha\Delta t/\Delta x^2$  yields

$$f_j^{n+1} - f_j^{n-1} = 2s (f_{j-1}^n - f_j^{n-1} - f_j^{n+1} + f_{j+1}^n)$$

$$\Rightarrow (1 + 2s) f_j^{n+1} = (1 - 2s) f_j^{n-1} + 2s (f_{j-1}^n + f_{j+1}^n) \text{ or}$$

$$f_j^{n+1} = \frac{1 - 2s}{1 + 2s} f_j^{n-1} + \frac{2s}{1 + 2s} (f_{j-1}^n + f_{j+1}^n)$$

and the Hopscotch (1D) schemes in program sim1:

Hopscotch: 1st stage

$$\frac{\Delta f_j^{n+1}}{\Delta t} = \alpha L_{xx} f_j^n \quad j + n = \text{even}$$

Equation to solve:

$$f_j^{n+1} = (1 - 2s) f_j^n + s (f_{j-1}^n + f_{j+1}^n)$$

2nd stage:

$$\frac{\Delta f_j^{n+1}}{\Delta t} = \alpha L_{xx} f_j^{n+1}, \quad j + n = \text{odd}$$

Equation to solve:

$$f_j^{n+1} = \frac{1}{1 + 2s} f_j^n + \frac{s}{1 + 2s} (f_{j-1}^{n+1} + f_{j+1}^{n+1})$$

#### (a) Implementation of the two schemes:

The two schemes are implemented using the code modified for the two level scheme. The new program is called *sim1mul.f* and associated changes are in the data file *sim1m.dat* and the include file *sim1min*.

Changes are:

Introduction of the subroutines:

Subroutine *intduff* (DuFort-Frankel)

```

subroutine intduff
include 'sim1min'
integer i real s0,s1
s0 = (1.-2.*s)/(1.+2.*s)
s1 = 2.*s/(1.+2.*s)
do 10 i = 1,nx
10 foold(i) = fold(i)
do 20 i = 1,nx
20 fold(i) = f(i)
do 30 i = 2,nx-1
30 f(i) = s0*foold(i) + s1*( fold(i+1)+fold(i-1) )
return
end

```

Subroutines inthop1, inhop2 (2stages of the hopscotch)

```

subroutine inthop1
include 'sim1min'
integer i
real s0
s0 = 1.0-2.*s
do 20 i = 2+mod(nt,2),nx-1,2
20 f(i) = s0*f(i) + s*( f(i+1)+f(i-1) )
return
end
subroutine inthop2
include 'sim1min'
integer i real s0,s1
s0 = 1./(1.0+2.*s)
s1 = s/(1.0+2.*s)
do 20 i = 2+mod((nt+1),2),nx-1,2
20 f(i) = s0*f(i) + s1*( f(i+1)+f(i-1) )
return
end

```

In addition an new variable meth is introduced to select and kept track of the method used in the scheme. meth is added to sim1m.dat and sim1min and also written to the binary output file to print the method when a plot is generated by sim1.pro (with corresponding small changes). The main program of sim1mul.f is mainly modified as follows (instead of calling just the FTCS or the two-level schemes):

```

if (meth.eq.2 .or. meth.eq.4) then
nt = nt+1
time = time + dt
call intftcs
call bdcon
if (mod(nt,nout) .eq. 0) call out

```

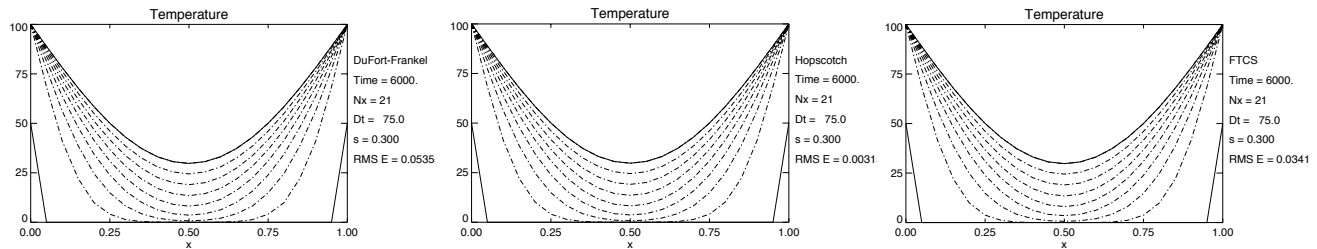
```

endif
do while( (nt .lt. ntmax) .and.
+       (time .lt.(tmax-0.001*dt)) )
  nt = nt+1
  time = time + dt
  write(*,*) 'time', time
  if (meth.eq.1) call intftcs
  if (meth.eq.2) call intduff
  if (meth.eq.4) call int2l
  if (meth.eq.3) then
    call inthop1
    call bdcon
    call inthop2
  endif
  call bdcon
  if (mod(nt,nout) .eq. 0)
    call out
  end do

```

**(b) Test of schemes and comparison with FTCS:**

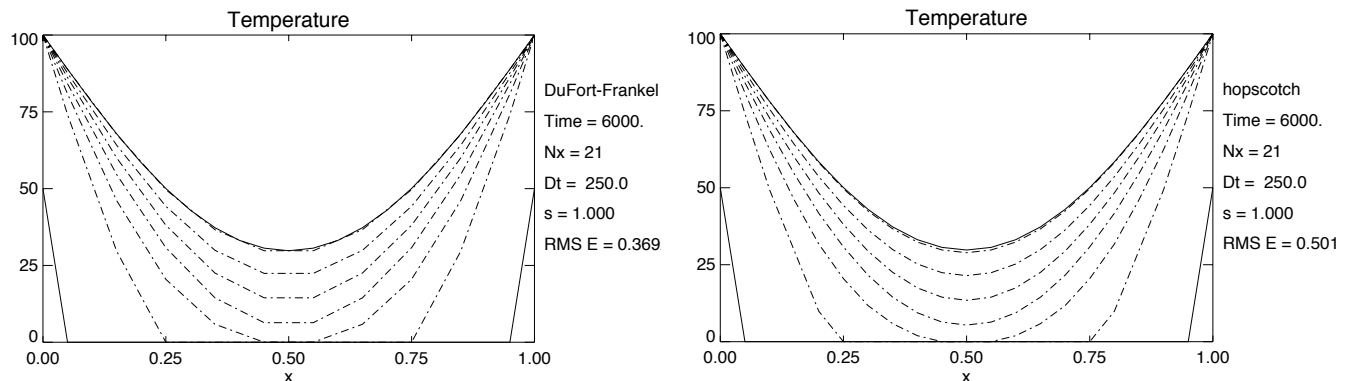
The following plots show DuFort-Frankel, Hopscotch, and FTCS results for  $s = 0.3$ .



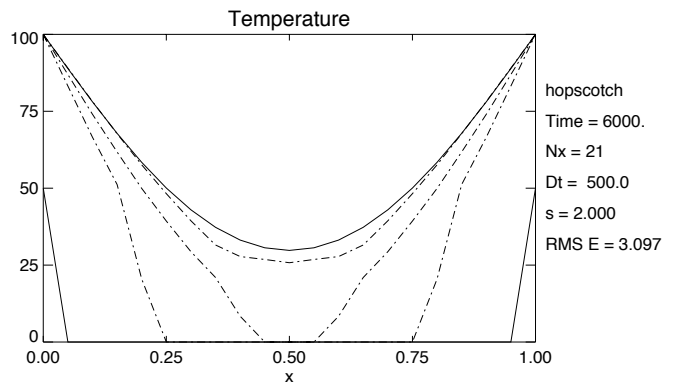
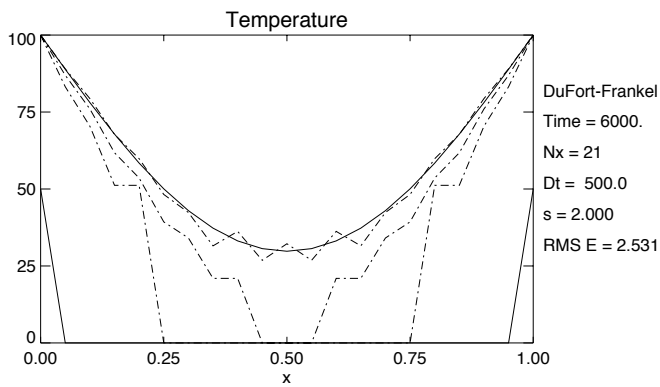
Note that differences are small since the rms error is small. Note that the Hopscotch scheme is remarkable better than the other two.

**(c) Selected results for increasing integration steps:**

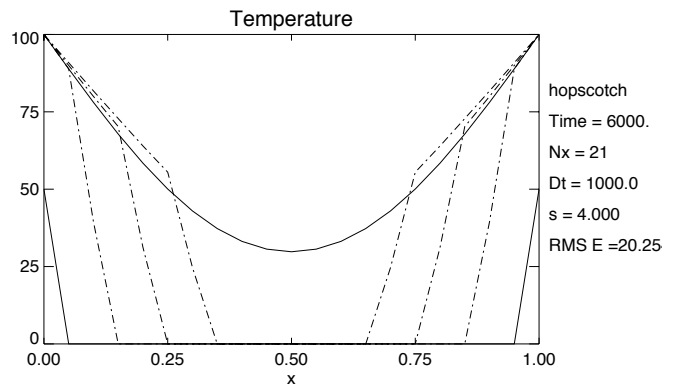
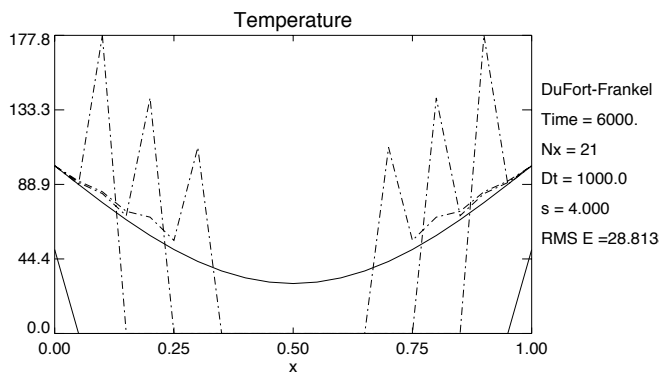
The next plots show results for the DuFort-Frankel, Hopscotch for  $s = 1.0$  (where the FTCS is already unstable)



$s = 2.0$ :

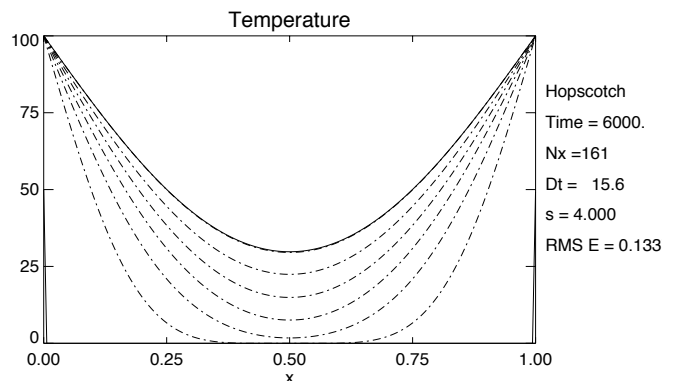
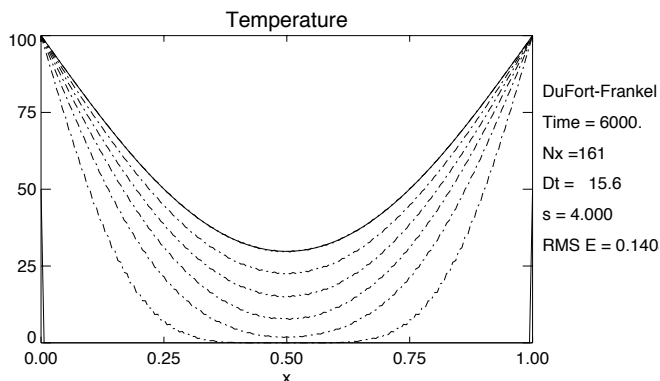


$s = 4.0$ :

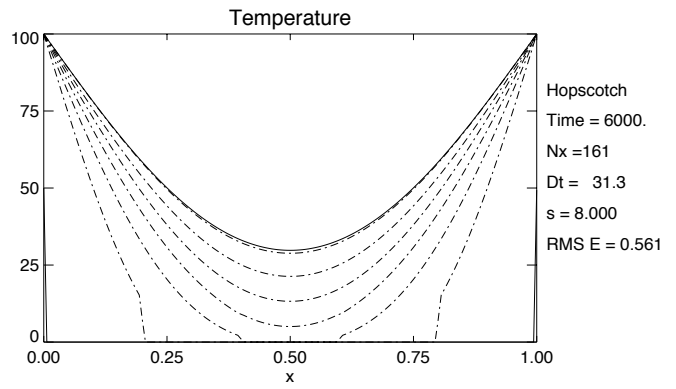
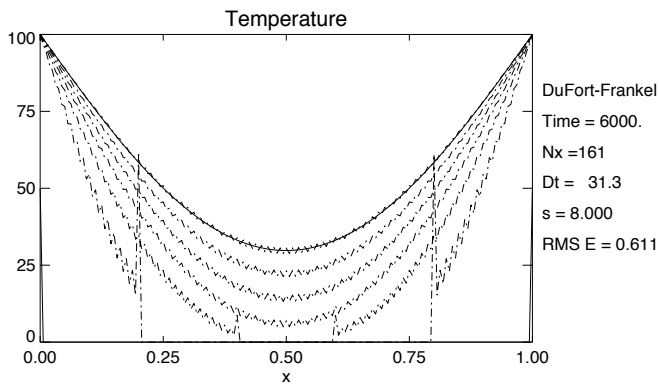


The results show that indeed both the DuFort-Frankel and the Hopscotch scheme are stable for all chosen values of  $s$ . However, the error increases although it is comparable between the two methods. Note that the choice  $s = 4.0$  yields  $\Delta t = 1000$  such that the result for  $n_x = 21$  used only 6 integration steps which is insufficient to propagate the diffusion across all grid points. While the DuFort-Frankel scheme tends to develop grid oscillations for large time steps the Hopscotch is smooth but tends to underestimate the actual solution. The lack of temporal resolution appears to imply that the results for  $s = 4$  is not really acceptable. However, the following plots show cases for  $s = 4$  and  $s = 8$  but on a 161 grid:

$s = 4.0, n_x = 161$ :



$s = 8.0, n_x = 161$ :



The result for  $s = 4.0$ ,  $n_x = 161$  shows that a larger choice of  $s$  is possible if the grid is sufficiently refined (thus lowering particularly the error associated with a large  $\Delta t$ ). This implies that the advantage of a larger  $s$  value becomes important for a sufficiently small grid spacing. This may be required in boundary layer problems, problems where the diffusion coefficient strongly varies, or equations where convection and diffusion are important.