12. The equation $\partial\phi/\partial t - \alpha\partial^2\phi/\partial x^2 = 0$ is to be solved in the domain $0 \le x \le 1$, $t > 0$ with boundary conditions $\phi(0,t) = 0$, $\phi(1,t) = \phi_R$ and the initial condition $\phi(x,0) = 0$. Show via the separation of variables technique, that the solution is

$$\phi = \phi_R x + \sum_{k=1}^{\infty} \frac{2\phi_R(-1)^k \exp\left(-k^2\pi^2\alpha t\right)\sin(k\pi x)}{k\pi}.$$

Solution:

Determine the solution of

$$\frac{\partial\phi}{\partial t} - \frac{\partial^2\phi}{\partial x^2} = 0 \tag{1}$$

in $0 \le x \le 1$, $t > 0$ with $\phi(0,t) = 0$, $\phi(1,t) = \phi_R$ and $\phi(x,0) = 0$.

Separation of variables: $\phi(x,t) = X(x)T(t)$ yields

$$\frac{1}{T}\frac{dT(t)}{dt} - \frac{1}{X}\frac{d^2X(x)}{dx^2} = 0$$

Assume: $(1/T)dT/dt = -c^2$ such that $\frac{d^2X(x)}{dx^2} + c^2X = 0$

i) $c = 0$: $T = const$ and from $d^2X/dx^2 = 0$ we obtain $X(x) = ax + b$. Thus

$$\phi_0 = XT = ax + b$$

solves (1). With $a = \phi_R$ and $b = 0$, $\phi_0 = \phi_R x$ satisfies the boundary conditions.

ii) $c \neq 0$: $X(x) = d\sin(cx) + e\cos(cx)$ and $T(t) = \exp(-c^2t)$ such that

$$\phi_c = \exp(-c^2t)\,(d\sin(cx) + e\cos(cx))$$

is a solution of (1).

Boundary condition at $x = 0$: $\phi_c(0,t) = e\exp\left(-c^2t\right) = 0 \;\; => \;\; e = 0$

Boundary condition at $x = 1$:

$\phi_c(1,t) + \phi_0(1,t) = d\exp\left(-c^2t\right)\sin(cx) + \phi_R = \phi_R \;\; => \;\; c = k\pi$

Thus we can write the solution as:

$$\phi(x,t) = \phi_R x + \sum_{k=1}^{\infty} d_k \exp(-k^2\pi^2\alpha t)\sin(k\pi x) \tag{2}$$

Note the term with $k = 0$ corresponds to a constant which was already eliminated from ϕ_0 and the sum over $k = -1 \,..\, -\infty$ can be neglected because the terms are proportional to the corresponding terms with positive k values (linear dependent). (2) satisfies the boundary conditions.

Initial conditions:

$$\phi(x,0) = \phi_R x + \sum_{k=1}^{\infty} d_k \sin(k\pi x) = 0 \tag{3}$$

To determine the d_k we multiply (3) with $\sin(l\pi x)$ and integrate from 0 to 1. Here we assume $l > 0$ (the case $l < 0$ is easily shown to yield the same result). The first term in (3) yields:

$$\begin{aligned}
\phi_R \int_0^1 x \sin(l\pi x) dx &= -\frac{\phi_R}{l\pi} \left[x\cos(l\pi x)\right]_0^1 + \frac{\phi_R}{l\pi} \int_0^1 \cos(l\pi x) dx \\
&= -\frac{\phi_R}{l\pi} \cos(l\pi) + \frac{\phi_R}{(l\pi)^2} \left[\sin(l\pi x)\right]_0^1 \\
&= -\frac{\phi_R}{l\pi} (-1)^l
\end{aligned}$$

The second term in (3) yields:

$$\begin{aligned}
\sum_{k=1}^{\infty} d_k \int_0^1 \sin(l\pi x) \sin(k\pi x) dx &= \sum_{k=1}^{\infty} d_k \int_0^1 \frac{1}{2} \left[\cos\left((k-l)\,\pi x\right) - \cos\left((k+l)\,\pi x\right)\right] dx \\
&= \sum_{k=1}^{\infty} \frac{d_k}{2} \delta_{kl} \\
&= \frac{d_l}{2}
\end{aligned}$$

the combination yields

$$d_l = 2\frac{\phi_R}{l\pi}(-1)^l$$

such that the solution to (1) with the given boundary and initial conditions becomes

$$\phi = \phi_R x + \sum_{k=1}^{\infty} \frac{2\phi_R (-1)^k \exp(-k^2\pi^2\alpha t) \sin(k\pi x)}{k\pi}$$

Note that the linear term $\phi_R x$ is straightforward because it represents the time asymptotic (steady state) solution of constant heat conduction between the values of $\phi = 0$ and $\phi = \phi_R$. This solution is also similar to the one for the sim1 code.

13. Accuracy:

A three-level explicit discretization of $\frac{\partial T}{\partial t} - \alpha \frac{\partial^2 T}{\partial x^2} = 0$ can be written as

$$\frac{0.5T_j^{n-1} - 2T_j^n + 1.5T_j^{n+1}}{\Delta t} - \alpha \left[\frac{(1+d)(T_{j-1} - 2T_j + T_{j+1})^n}{\Delta x^2} - \frac{d(T_{j-1} - 2T_j + T_{j+1})^{n-1}}{\Delta x^2} \right] = 0$$

(a) Expand each term as a Taylor series to determine the truncation error of the complete equation for arbitrary values of d.

(b) Use the general technique to choose d as a function of $s = \alpha \Delta t / \Delta x^2$ so that the scheme is fourth-order accurate in Δx.

Hint: Terms involving $\partial T / \partial t$ (or higher derivatives of t) can be expressed as x derivatives by making use of $\partial T / \partial t = \alpha \partial^2 T / \partial x^2$. Terms with Δt in the expansion can be written as $\Delta t = s \Delta x^2 / \alpha$ since the time integration parameter is usually s.

Solution:

(a) Truncation error:

First term:

$$\begin{aligned}
Term_1 &= \frac{1}{\Delta t}\left[\frac{1}{2}T_j^{n-1} - 2T_j^n + \frac{3}{2}T_j^{n+1}\right] \\
&= \frac{1}{\Delta t}\left[\left(\frac{1}{2} - 2 + \frac{3}{2}\right)T_j^n + \left(-\frac{1}{2} + \frac{3}{2}\right)\Delta t \frac{\partial T_j^n}{\partial t} + \right. \\
&\quad \left. + \left(\frac{1}{2} + \frac{3}{2}\right)\frac{\Delta t^2}{2}\frac{\partial^2 T_j^n}{\partial t^2} + \left(-\frac{1}{2} + \frac{3}{2}\right)\frac{\Delta t^3}{6}\frac{\partial^3 T_j^n}{\partial t^3} + \ldots\right] \\
&= \frac{\partial T_j^n}{\partial t} + \Delta t \frac{\partial^2 T_j^n}{\partial t^2} + \frac{1}{6}\Delta t^2 \frac{\partial^3 T_j^n}{\partial t^3} + \ldots \\
&= \frac{\partial T_j^n}{\partial t} + \alpha^2 \Delta t \frac{\partial^4 T_j^n}{\partial x^4} + \frac{\alpha^3}{6}\Delta t^2 \frac{\partial^6 T_j^n}{\partial x^6} + ..
\end{aligned}$$

Where the last line is obtained from $\partial T / \partial t = \alpha \partial T^2 / \partial x^2$

Second term (symmetry => all odd orders in the Taylor expansion vanish and even order are just multiplied with 2 because of T_{j-1} and T_{j+1} !). Expansion is at time level n:

$$\begin{aligned}
Term_2 &= \frac{1}{\Delta x^2}\left[T_{j-1} - 2T_j + T_{j+1}\right]^n \\
&= \frac{1}{\Delta x^2}\left[(1 - 2 + 1)T_j + 2\frac{\Delta x^2}{2}\frac{\partial^2 T_j}{\partial x^2} + 2\frac{\Delta x^4}{24}\frac{\partial^4 T_j}{\partial x^4} + 2\frac{\Delta x^6}{720}\frac{\partial^6 T_j}{\partial x^6} + \ldots\right]^n \\
&= \frac{\partial^2 T_j^n}{\partial x^2} + \frac{\Delta x^2}{12}\frac{\partial^4 T_j^n}{\partial x^4} + \frac{\Delta x^4}{360}\frac{\partial^6 T_j^n}{\partial x^6} + \ldots
\end{aligned}$$

Third term: this is identical to the second term with the only difference that it is for time level $n-1$ such that we need Taylor expansion in time of the expansion of $Term_2$:

$$
\begin{aligned}
Term_3 &= Term_2^{n-1} \\
&= \frac{\partial^2}{\partial x^2}\left(T_j^n - \Delta t\frac{\partial T_j^n}{\partial t} + \frac{\Delta t^2}{2}\frac{\partial^2 T_j^n}{\partial t^2} - ..\right) \\
&\quad + \frac{\Delta x^2}{12}\frac{\partial^4}{\partial x^4}\left(T_j^n - \Delta t\frac{\partial T_j^n}{\partial t} + ..\right) + \frac{\Delta x^4}{360}\frac{\partial^6}{\partial x^6}\left(T_j^n - ..\right) \\
&= \frac{\partial^2 T_j^n}{\partial x^2} + \left(-\alpha\Delta t + \frac{\Delta x^2}{12}\right)\frac{\partial^4 T_j^n}{\partial x^4} + \left(\alpha^2\frac{\Delta t^2}{2} - \alpha\Delta t\frac{\Delta x^2}{12} + \frac{\Delta x^4}{360}\right)\frac{\partial^6 T_j^n}{\partial x^6}
\end{aligned}
$$

Substituting $\alpha\Delta t = s\Delta x^2$ to eliminate the Δt terms yields for the three terms

$$
\begin{aligned}
Term_1 &= \frac{\partial T_j^n}{\partial t} + \alpha s\Delta x^2\frac{\partial^4 T_j^n}{\partial x^4} + \frac{\alpha}{6}s^2\Delta x^4\frac{\partial^6 T_j^n}{\partial x^6} + .. \\
-\alpha(1+d)\,Term_2 &= -\alpha(1+d)\left(\frac{\partial^2 T_j^n}{\partial x^2} + \frac{\Delta x^2}{12}\frac{\partial^4 T_j^n}{\partial x^4} + \frac{\Delta x^4}{360}\frac{\partial^6 T_j^n}{\partial x^6} + ...\right) \\
\alpha d\,Term_3 &= \alpha d\left(\frac{\partial^2 T_j^n}{\partial x^2} + \left(-s + \frac{1}{12}\right)\Delta x^2\frac{\partial^4 T_j^n}{\partial x^4} + \left(\frac{s^2}{2} - \frac{s}{12} + \frac{1}{360}\right)\Delta x^4\frac{\partial^6 T_j^n}{\partial x^6}\right)
\end{aligned}
$$

Taking the sum and collecting all terms and their coefficients gives:

$$
\begin{aligned}
\frac{\partial T_j^n}{\partial t} - \alpha\frac{\partial^2 T_j^n}{\partial x^2} \qquad & +\alpha\left(s - \tfrac{1+d}{12} + d\left(-s + \tfrac{1}{12}\right)\right)\Delta x^2\tfrac{\partial^4 T_j^n}{\partial x^4} \\
& +\alpha\left(\tfrac{s^2}{6} - \tfrac{1+d}{360} + d\left(\tfrac{s^2}{2} - \tfrac{s}{12} + \tfrac{1}{360}\right)\right)\Delta x^4\tfrac{\partial^6 T_j^n}{\partial x^6} \quad = 0
\end{aligned}
$$

Further substituting $\alpha\Delta t = s\Delta x^2$gives a truncation error of:

$$
Error = \alpha\Delta x^2\left(s - \frac{1}{12} - ds\right)\frac{\partial^4 T_j^n}{\partial x^4} + \alpha\Delta x^4\left(\frac{s^2}{6} - \frac{1}{360} + d\left(\frac{s^2}{2} - \frac{s}{12}\right)\right)\frac{\partial^6 T_j^n}{\partial x^6} + ..
$$

(b) Fourth-order accuracy implies:

$$
d = 1 - \frac{1}{12s}
$$

such that the leading error term in (**??**) is zero and the leading order truncation error becomes

$$
\begin{aligned}
Error &= \alpha\Delta x^4\left(\frac{s^2}{6} - \frac{1}{360} + \frac{1}{2}\left(s - \frac{1}{12}\right)\left(s - \frac{1}{6}\right)\right)\frac{\partial^6 T_j^n}{\partial x^6} \\
&= \alpha\Delta x^4\left(\frac{2}{3}s^2 - \frac{1}{8}s + \frac{1}{240}\right)\frac{\partial^6 T_j^n}{\partial x^6}
\end{aligned}
$$

14. Simulation of the diffusion equation - SIM1:

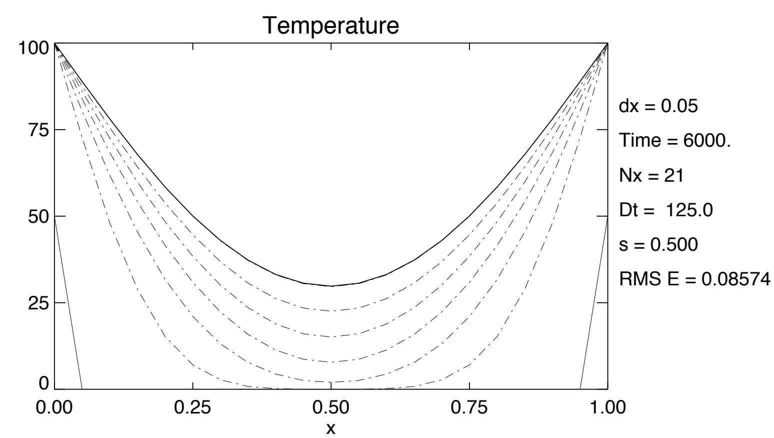
Try to understand the simulation code sim1. Run the code for different parameters by varying the time step through s, and Δx (by means of nx). Plot results for $\Delta x = 0.1$ and 0.05 (fixed α ans $s = 0.5$) with the provided IDL program (or another choice of a plotting routine but in a similar format as shown in class). To compare results change the output parameter for the different resolutions such that outputs are generated at the same physical time. Now change α to half the initial value. Generate again output at the same physical times (for $\Delta x = 0.05$). Understand and comment at which time levels output is generated depending on the altered parameters. If you change s to half its value (keeping α and Δx fixed) how do you need to change the output parameter to generate output at the same physical times? Finally run the program for $s = 1/6$ (again with output at the same physical times) How does the error change for different resolution and different values of s? What is the reason for the change in the error?

Solution:

Following are a few examples to show changes associated with program parameters of sim1.f. The time stepping is determined by the choice of the parameter s. with $s = \alpha\Delta t/\Delta x^2$, the time step associated with a particular s value is $\Delta t = s\Delta x^2/\alpha$. For $\alpha = 10^{-5}$ and $s = 0.5$ (default values) the time step is

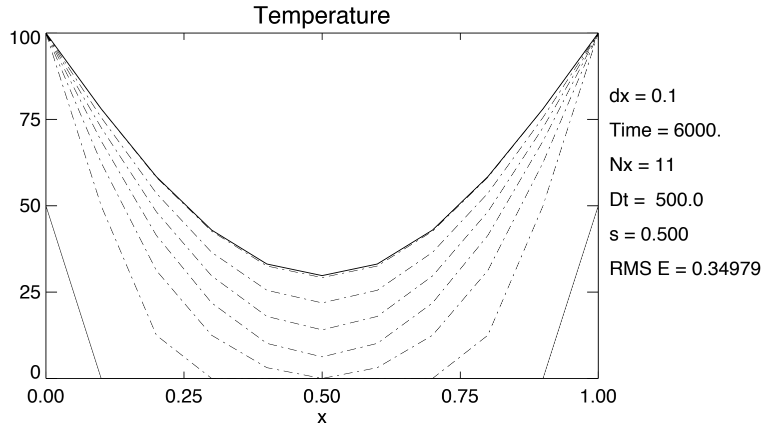
$$\Delta t = \begin{cases} 125 & for \quad \Delta x = 0.05 \\ 500 & for \quad \Delta x = 0.1 \end{cases}$$

A binary output of the data is generated every n_{out} integration steps. The default values (web version of the program) are $\Delta x = 0.05$ (from $N_x = 21$) and $n_{out} = 8$ resulting in ouputs at time intervals of 1000 time units. The corresponding result using these **default values** is plotted below (case 1):



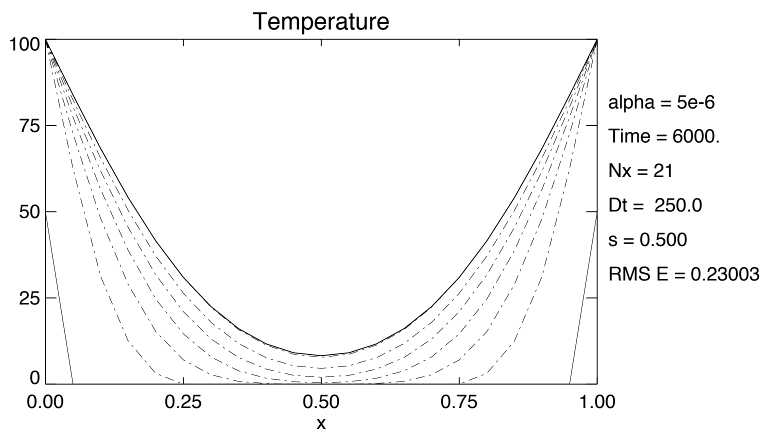
The plot represents the evolution of temperature in increments of 1000 time units. The solid line represents the analytic solution from class for comparison with the last numerical solution at time $t = 6000$.

Reducing the resolution to $\Delta x = 0.1$ yields $\Delta t = 500$ which requires $n_{out} = 2$ to generate output at the same physical time. The result is plotted below (case 2).



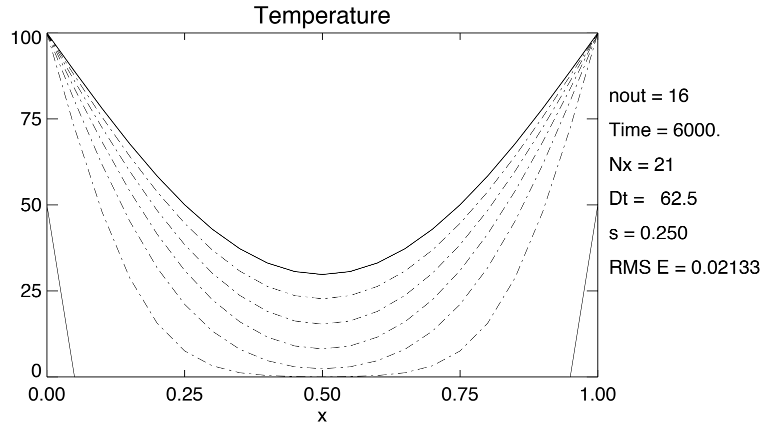
Clearly for half as many gridpoints the solution is not as smooth and the error is large enough that the numerical and analytical solutions are not overplotted at time $t = 6000$. However, only 12 integration steps in total were required to generate the solution.

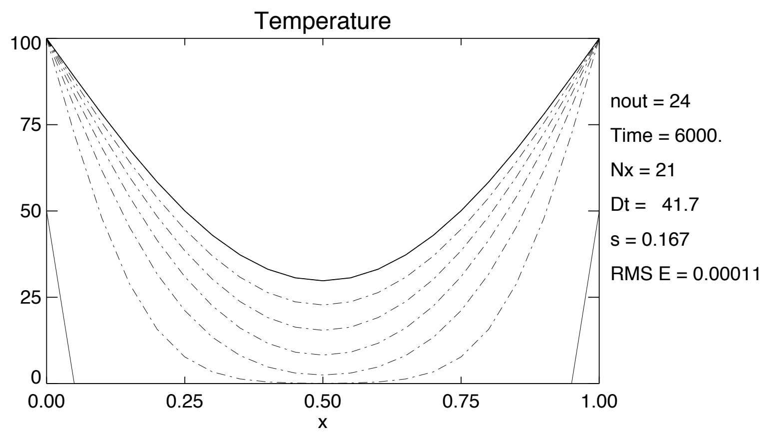
Changing the value of the diffusion coefficient to half its initial value implies $\alpha = 0.5 \cdot 10^{-5}$ and $\Delta t = 250$ for $s = 0.5$. This implies $n_{out} = 4$ to generate matching outputs. The result is plotted below (case 3):



As expected the smaller diffusion coefficient leads to slower diffusion. Since time scales inversly proportional to the diffusion coefficient the solution above corresponds to the default solution at time $t = 3000$.

Finally changing s to $s = 0.25$ (other parameters are default $\alpha = 10^{-5}$and $N_x = 21$) generates $\Delta t = 62.5$ and requires $n_{out} = 16$. Similarly using $1/6$ implies $\Delta t = 125/3$ and $n_{out} = 24$. Note that the last change of s should be applied directly in the program (which requires re-compilation) because it is more accurate to compute s as 1/6 than to provide it as a decimal number in the data input file sim1.dat. The results for $s = 0.25$ and $s = 1/6$ are presented in the plots below (cases 4 and 5).





The table below summarizes parameters and results for the cases above. Cases are numbered in the sequence of appearance.

Case	s	Δx	Δt	α	n_t	RMS
1	0.5	0.05	125	10^{-5}	48	0.086
2	0.5	0.1	500	10^{-5}	12	0.350
3	0.5	0.05	250	$0.5 \cdot 10^{-5}$	24	0.230
4	0.25	0.05	62.5	10^{-5}	96	0.0213
5	1/6	0.05	41.67	10^{-5}	144	0.00011

The parameter n_t is the total number of integration steps required to obtain the final result. In general more integration steps generate a more accurate result. More specifically, case 2 with half the resolution has an error of 4 times the default case consistent with the truncation error $\sim \Delta x^2$. The lower diffusion coefficient generate an error similar to the lower resolution. Here it is important to note that any error also satisfies the diffusion equation such that errors should decrease significantly with increasing time (or numerb of integration steps). The lowest error are generated by cases 4 and 5. For case 4 this is caused by a smaller coefficient in the leading error term due to the value of $s = 0.25$. The choice of $s = 1/6$ eliminates the 2nd order error in Δx altogether such that the leading error term is now Δx^4. Combined with a rather small coefficient , this reduces the error very significantly, however, at the expense of more operations since $n_t$is 3 times the number of the reference case.