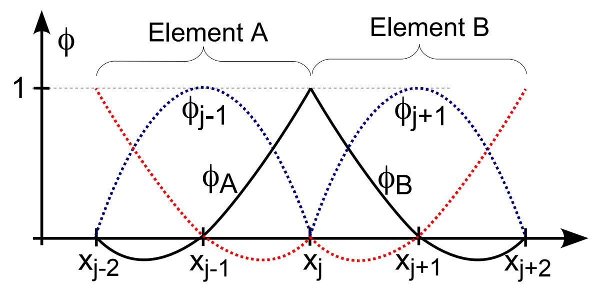
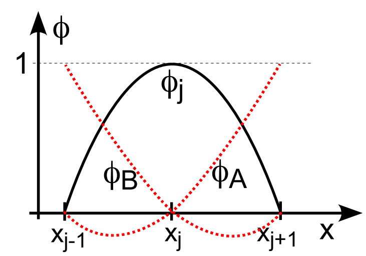
22. For the finite element method, second derivatives in a partial differential equation are determined by the terms $l_{ij} = \int \frac{\partial \phi_i}{\partial x}\frac{\partial \phi_j}{\partial x} dx$. Quadratic finite element base functions are given by $\phi_{A,B} = 0.5\xi(\xi \pm 1)$ on even nodes and for odd nodes they are $\phi_{odd} = (1-\xi^2)$. The transformation between x and ξ on even nodes is given by

$$\xi_A = 2\frac{x-0.5(x_{j-2}+x_j)}{x_j - x_{j-2}}$$
$$\xi_B = 2\frac{x-0.5(x_{j+2}+x_j)}{x_{j+2} - x_j}$$

Compute the second derivative coefficients l_{ij} for even and for odd nodes. (Note: You don't have to compute all nonzero coefficients if you make use of symmetry properties.)



Sketch of the quadratic base function at an even node x_j.



Sketch of the quadratic base function at an odd node x_j.

The second derivative coefficients $l_{ij} = \int \frac{\partial \phi_i}{\partial x}\frac{\partial \phi_j}{\partial x} dx$ are non zero only in regions where finite elements overlap.

a) For even nodes the above figure implies nonzero coefficients for $l_{j,j-2}$ (overlap of $\phi_{j,A}$ and $\phi_{j-2,B}$), $l_{j,j-1}$ (overlap of $\phi_{j,A}$ and ϕ_{j-1}), $l_{j,j}$ (overlap of $\phi_{j,A}$ with $\phi_{j,A}$ and $\phi_{j,B}$ with $\phi_{j,B}$), $l_{j,j+1}$ (overlap of $\phi_{j,B}$ and ϕ_{j+1}), and for $l_{j,j+2}$ (overlap of $\phi_{j,B}$ and $\phi_{j+2,A}$).

b) For j odd (odd numbered nodes, in the above figure they correspond to the elements centered at $j-1$ or $j+1$) we have overlap (nonzero contributions) only with the direct neighbors and with the elements themselves, i.e., $l_{j,j-1}$, $l_{j,j}$, and $l_{j,j+1}$.

Starting indexing with 0 we can address elements j as even and $j-1$ or $j+1$ as odd nodes.

With the transformation to local coordinates we have in element A

$$\frac{d}{dx_A} = \frac{d\xi}{dx_A}\frac{d}{d\xi} = \frac{2}{\Delta x_j}\frac{d}{d\xi}$$
$$dx_A = \frac{dx_A}{d\xi}d\xi = \frac{\Delta x_j}{2}d\xi$$

and in element B

$$\frac{d}{dx_B} = \frac{d\xi}{dx_B}\frac{d}{d\xi} = \frac{2}{\Delta x_{j+2}}\frac{d}{d\xi}$$
$$dx_B = \frac{dx_B}{d\xi}d\xi = \frac{\Delta x_{j+2}}{2}d\xi$$

with $\Delta x_j = x_j - x_{j-2}$ and $\Delta x_{j+2} = x_{j+2} - x_j$ and $x_A = x$ in interval A and $x_B = x$ in interval B. For odd nodes we have the same transformation except that we consider $\Delta x_{j+1} = x_{j+1} - x_{j-1}$.

(a) Even nodes:

i) Element $l_{j,j-2}$:

$$
\begin{aligned}
l_{j,j-2} &= -\int_0^1 \frac{\partial \phi_j}{\partial x}\frac{\partial \phi_{j-2}}{\partial x}dx = -\int_{-1}^1 \frac{\partial \phi_A}{\partial \xi}\frac{\partial \phi_B}{\partial \xi}\left(\frac{d\xi}{dx_A}\right)^2 \frac{dx_A}{d\xi}d\xi \\
&= -\frac{2}{\Delta x_j}\int_{-1}^1 \left(\xi+\frac{1}{2}\right)\left(\xi-\frac{1}{2}\right)d\xi = -\frac{2}{\Delta x_j}\left[\frac{\xi^3}{3}-\frac{\xi}{4}\right]_{-1}^1 = -\frac{1}{3\Delta x_j}
\end{aligned}
$$

Element $l_{j,j-1}$:

$$
\begin{aligned}
l_{j,j-1} &= -\int_0^1 \frac{\partial \phi_j}{\partial x}\frac{\partial \phi_{j-1}}{\partial x}dx = -\frac{2}{\Delta x_j}\int_{-1}^1 \left(\xi+\frac{1}{2}\right)(-2\xi)\,d\xi \\
&= \frac{4}{\Delta x_j}\int_{-1}^1 \left(\xi^2-\frac{\xi}{2}\right)d\xi = \frac{4}{\Delta x_j}\left[\frac{\xi^3}{3}-\frac{\xi^2}{4}\right]_{-1}^1 = \frac{8}{3\Delta x_j}
\end{aligned}
$$

Element $l_{j,j}$:

$$
\begin{aligned}
l_{j,j} &= -\int_0^1 \left[\left(\frac{\partial \phi_A}{\partial x}\right)^2+\left(\frac{\partial \phi_B}{\partial x}\right)^2\right]dx = -\frac{2}{\Delta x_j}\int_{-1}^1 \left(\frac{\partial \phi_A}{\partial \xi}\right)^2 d\xi - \frac{2}{\Delta x_{j+2}}\int_{-1}^1 \left(\frac{\partial \phi_B}{\partial \xi}\right)^2 d\xi \\
&= -\frac{2}{\Delta x_j}\int_{-1}^1 \left(\xi+\frac{1}{2}\right)^2 d\xi - \frac{2}{\Delta x_{j+2}}\int_{-1}^1 \left(\xi-\frac{1}{2}\right)^2 d\xi \\
&= -\frac{2}{\Delta x_j}\int_{-1}^1 \left(\xi^2+\xi+\frac{1}{4}\right)d\xi - \frac{2}{\Delta x_{j+2}}\int_{-1}^1 \left(\xi^2-\xi+\frac{1}{4}\right)d\xi \\
&= -\frac{2}{\Delta x_j}\left[\frac{\xi^3}{3}+\frac{\xi}{4}\right]_{-1}^1 - \frac{2}{\Delta x_{j+2}}\left[\frac{\xi^3}{3}+\frac{\xi}{4}\right]_{-1}^1 = -\frac{7}{3\Delta x_j}-\frac{7}{3\Delta x_{j+2}}
\end{aligned}
$$

Symmetry implies that the coefficients $l_{j,j+1}$ and $l_{j,j+2}$ are the same as $l_{j,j-1}$ and $l_{j,j-2}$ except that Δx_j needs to be replaced by Δx_{j+2}, ie., such that for even nodes the 5 nonzero coefficients are

$$
\begin{aligned}
l_{j,j-2} = -\frac{1}{3\Delta x_j} \quad &, \quad l_{j,j+2} = -\frac{1}{3\Delta x_{j+2}} \\
l_{j,j-1} = \frac{8}{3\Delta x_j} \quad &, \quad l_{j,j+1} = \frac{8}{3\Delta x_{j+2}} \\
l_{j,j} = -\frac{7}{3\Delta x_j} - \frac{7}{3\Delta x_{j+2}}
\end{aligned}
$$

(b) Odd nodes: The coefficients $l_{j,j-1}$ and $l_{j,j+1}$ involve the same integrals as those for even nodes at $(j,j-1)$ and $(j,j+1)$ except that we deal with the interval $\Delta x_{j+1} = x_{j+1}-x_{j-1}$.The coefficient at (j,j) is given by

$$
\begin{aligned}
l_{j,j} &= -\int_0^1 \left(\frac{\partial \phi_j}{\partial x}\right)^2 dx = -\int_{-1}^1 (-2\xi)^2\left(\frac{d\xi}{dx}\right)^2 \frac{dx}{d\xi}d\xi \\
&= -\frac{8}{\Delta x_{j+1}}\int_{-1}^1 \xi^2 d\xi = \frac{8}{\Delta x_j}\left[\frac{\xi^3}{3}\right]_{-1}^1 = -\frac{16}{3\Delta x_{j+1}}
\end{aligned}
$$

In summary the 3 nonzero coefficients for odd nodes are

$$
\begin{aligned}
l_{j,j-1} &= \frac{8}{3\Delta x_{j+1}} \quad , \quad l_{j,j+1} = \frac{8}{3\Delta x_{j+1}} \\
l_{j,j} &= -\frac{16}{3\Delta x_{j+1}}
\end{aligned}
$$

The following was not required for this homework!

1. Note: For a uniform grid $\Delta x_{j+2} = \Delta x_{j+1} = \Delta x_j = 2\Delta x$ because Δx_j spans 2 grid spacings.

2. Note: In order interpret the coeffecients in terms of a 2nd derivative operator on has to normalize these by the weight from the mass operator. On even notes this weight is

$$
w_{j,even} = -\frac{\Delta x_j}{30} + \frac{\Delta x_j}{15} + 2\frac{\Delta x_j + \Delta x_{j+2}}{15} + \frac{\Delta x_{j+2}}{15} - \frac{\Delta x_{j+2}}{30} = \frac{1}{6}\left(\Delta x_j + \Delta x_{j+2}\right)
$$

On odd notes this weight is

$$
w_{j,odd} = \frac{\Delta x_{j+1}}{15} + 8\frac{\Delta x_{j+1}}{15} + \frac{\Delta x_{j+1}}{15} = \frac{2}{3}\Delta x_{j+1}
$$

with the weighted 2nd derivative operators

$$
\begin{aligned}
L_{xx}^{even} &= \frac{2}{\Delta x_j + \Delta x_{j+2}}\left(-\frac{1}{\Delta x_j}, \frac{8}{\Delta x_j}, -\frac{7\left(\Delta x_j + \Delta x_{j+2}\right)}{\Delta x_j \Delta x_{j+2}}, \frac{8}{\Delta x_{j+2}}, -\frac{1}{\Delta x_{j+2}}\right) \\
L_{xx}^{odd} &= \frac{4}{\Delta x_{j+1}^2}(1, -2, 1)
\end{aligned}
$$

and the weighted mass operators

$$
\begin{aligned}
M^{even} &= \frac{1}{5\left(\Delta x_j + \Delta x_{j+2}\right)}\left(-\Delta x_j, 2\Delta x_j, 4\left(\Delta x_j + \Delta x_{j+2}\right), 2\Delta x_{j+2}, -\Delta x_{j+2}\right) \\
M^{odd} &= \frac{1}{10}(1, -8, 1)
\end{aligned}
$$

3. Finally for a uniform grid with $\Delta x_{j+2} = \Delta x_{j+1} = \Delta x_j = 2\Delta x$ these operators are

$$
\begin{aligned}
L_{xx}^{even} &= \frac{1}{\Delta x^2}\left(-\frac{1}{4}, 2, -\frac{7}{2}, 2, -\frac{1}{4}\right) \\
L_{xx}^{odd} &= \frac{1}{\Delta x^2}(1, -2, 1) \\
M^{even} &= \frac{1}{10}(-1, 2, 4, 2, -1) \\
M^{odd} &= \frac{1}{10}(1, -8, 1)
\end{aligned}
$$

23. Modification of Fivol

Extend the program FIVOL to solve the equation

$$\frac{\partial \phi}{\partial x} + \frac{\partial \phi}{\partial y} - \alpha \left(\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} \right) = S$$

The linear terms can be included in a similar way as discussed for the finite volume method and first order derivatives. The source term S can be treated in the same way as the term $\partial q / \partial t$ which has been discussed for the first order derivatives. Test the program for the case $S = (\cos(2\theta) - \sin(2\theta)) / r^2$ by obtaining solutions for the same boundary conditions and parameter values as in homework 21 except for r_X which should be chosen as $r_X = 1.0$. Compare the solutions with the exact solution $\phi = (\sin\theta)/r$.

We can rewrite the equation as

$$\frac{1}{\alpha} \left(S - \frac{\partial \phi}{\partial x} - \frac{\partial \phi}{\partial y} \right) + \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = 0$$

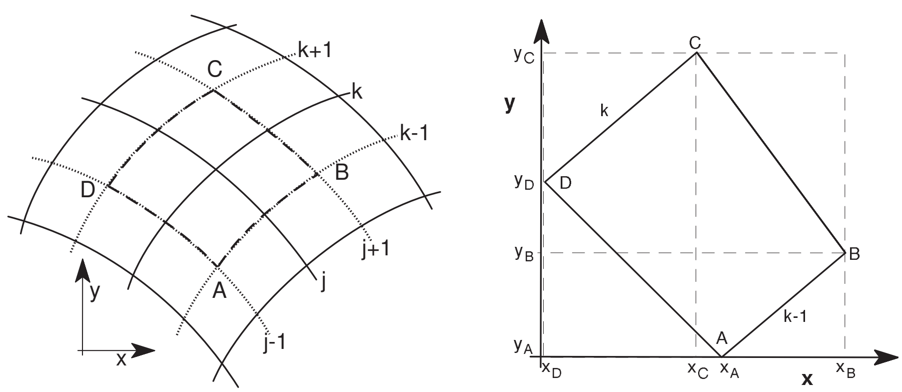
where the terms of the second derivative are already computed in the program FIVOL (see the derivation from class) such that we only need to add the additional term

$$\frac{1}{\alpha} \left(S - \frac{\partial \phi}{\partial x} - \frac{\partial \phi}{\partial y} \right)$$

which is done following exactly the procedure outlined in class. First the residual method requires to evaluate

$$T = \int_{\overline{ABCD}} \left[S - \frac{\partial \phi}{\partial x} - \frac{\partial \phi}{\partial y} \right] dxdy$$

over the area of $\overline{ABCD}$.



With $\mathbf{H} = (\phi, \phi)$ such that $\partial \phi / \partial x + \partial \phi / \partial y = \nabla \cdot \mathbf{H}$ this term becomes

$$T = \int_{\overline{ABCD}} S dV - \oint_{\partial ABCD} \mathbf{H} \cdot \mathbf{n} ds$$

In Cartesian coordinates the surface element vector $d\mathbf{s} = (dx, dy)$ such that the normal vector $\mathbf{n}ds = (dy, -dx)$ and $\mathbf{H} \cdot \mathbf{n}ds = \phi dy - \phi dx$. Thus

$$T = A_r S_{jk} - \sum_{ABCD} (\phi \Delta y - \phi \Delta x)$$

with A_r =area of $\overline{ABCD}$. Using the notations $\Delta y_{AB} = y_B - y_A$, $\Delta x_{AB} = x_B - x_A$, and the averages $\phi_{AB} = 0.5\left(\phi_{j,k-1} + \phi_{j,k}\right)$, and applying these to all sections of $\overline{ABCD}$ we obtain

$$\begin{aligned} T &= A_r S_{jk} - 0.5\left(\phi_{j,k-1} + \phi_{j,k}\right)(\Delta y_{AB} - \Delta x_{AB}) - 0.5\left(\phi_{j+1,k} + \phi_{j,k}\right)(\Delta y_{BC} - \Delta x_{BC}) \\ &\quad - 0.5\left(\phi_{j,k+1} + \phi_{j,k}\right)(\Delta y_{CD} - \Delta x_{CD}) - 0.5\left(\phi_{j-1,k} + \phi_{j,k}\right)(\Delta y_{DA} - \Delta x_{DA}) \end{aligned}$$

Since the sum $\Delta y_{AB} + \Delta y_{BC} + \Delta y_{CD} + \Delta y_{DA} = 0$ (see Figure) and the same for Δx, the expression becomes

$$\begin{aligned} T &= A_r S_{jk} - 0.5\phi_{j,k-1}(\Delta y_{AB} - \Delta x_{AB}) - 0.5\phi_{j+1,k}(\Delta y_{BC} - \Delta x_{BC}) \\ &\quad - 0.5\phi_{j,k+1}(\Delta y_{CD} - \Delta x_{CD}) - 0.5\phi_{j-1,k}(\Delta y_{DA} - \Delta x_{DA}) \end{aligned}$$

The area (see Figure) is evaluated from

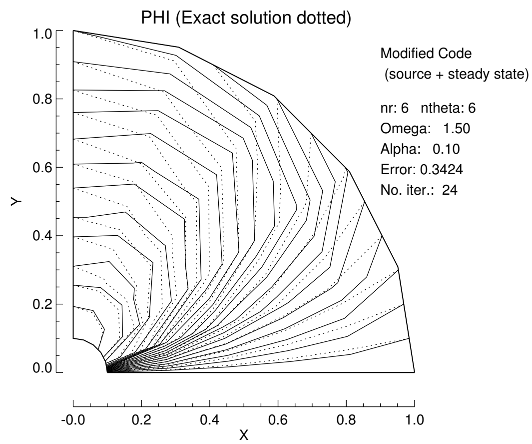
$$\begin{aligned} A_r &= (x_B - x_A)(y_C - y_A) - 0.5(x_B - x_A)(y_B - y_A) - 0.5(x_B - x_C)(y_C - y_B) \\ &\quad - 0.5(x_C - x_D)(y_C - y_D) - 0.5(x_A - x_D)(y_D - y_A) \\ &= 0.5\left(x_A(y_B - y_D) + x_B(y_C - y_A) + x_C(y_D - y_B) + x_D(y_A - y_C)\right) \\ &= 0.5\left((x_C - x_A)(y_D - y_B) + (x_D - x_B)(y_A - y_C)\right) \end{aligned}$$

In the program we need to introduce new arrays for A_r, S, the new parameter α, and it is convenient to introduce arrays for $\Delta y_{AB} - \Delta x_{AB}$, $\Delta y_{BC} - \Delta x_{BC}$, $\Delta y_{CD} - \Delta x_{CD}$, and $\Delta y_{DA} - \Delta x_{DA}$. We compute these arrays in the computation of the initial conditions and the matrix coefficients. We then need to add the term T/α to the residual. Finally one should remember to change the exact solution the subroutine startcon.

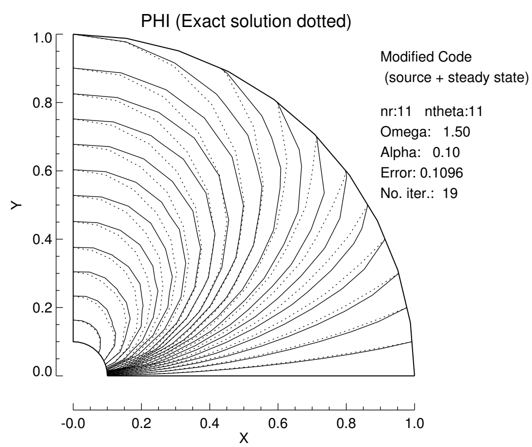
The file diffivol lists the changes of these modifications in detail (using the diff command in unix/linux).

Running the modified code for the resolutions 6×6, 11×11, and 21×21 yields the following results with the analytic solution $\phi = (\sin\theta)/r$ dotted. They all use a value of $\alpha = 0.1$ such that the convection term dominates. The number of iteration for convergence is slightly larger than for the original code. Also the error is now about 2 to 3 times as large as for the original code but quite comparable to the error for the distorted domains (Problem 18).

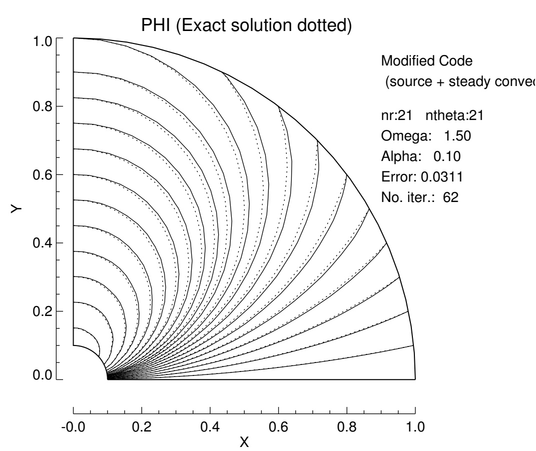
For the resolution 6×6:



For the resolution 11×11:



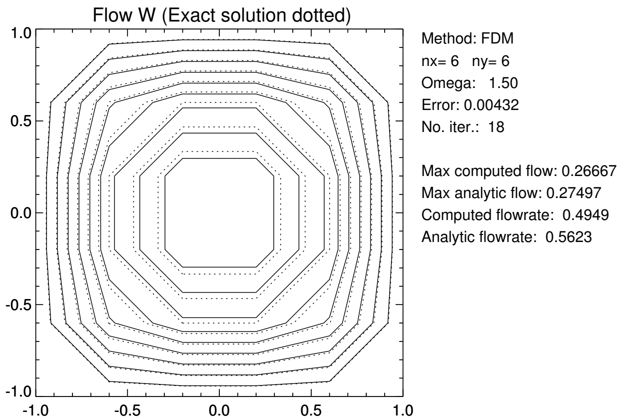
For the resolution 21×21:

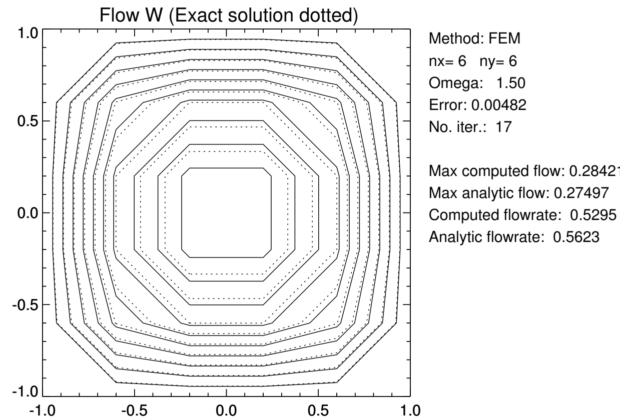


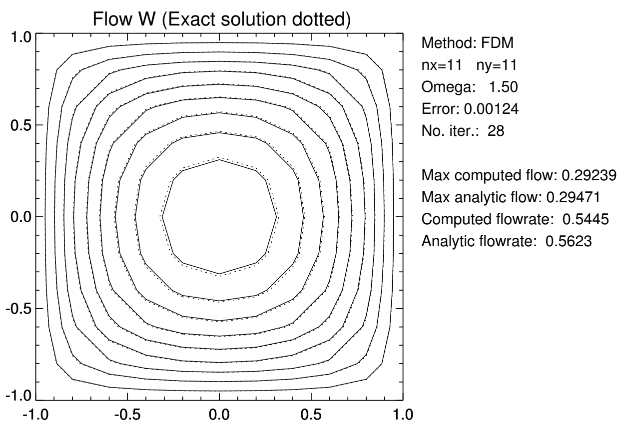
24. Program DUCT

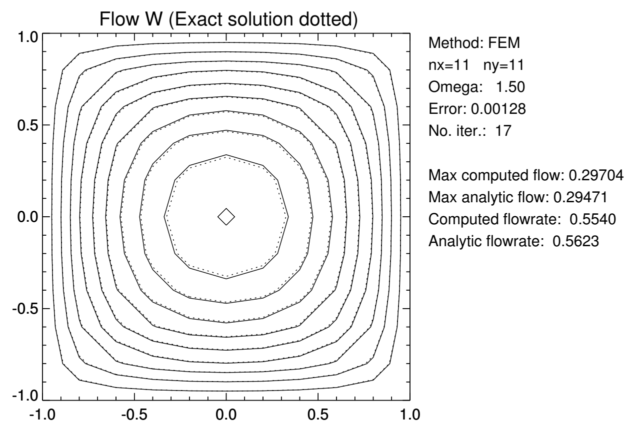
To become familiar with the program run the program DUCT for grid resolutions of 6×6, 11×11, and 21×21. determine the rms error for the finite differences and finite element methods (you can switch between them with a parameter). Tabulate and comment your results. Plot an example for the coarse and the fine grid spacing.

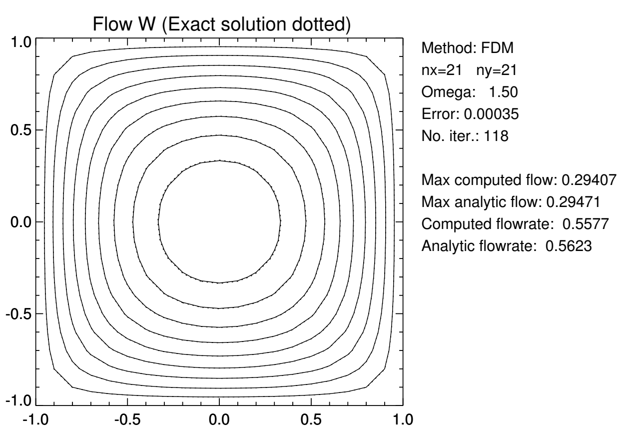
Finite difference (fdm): **Finite elements (FEM)**

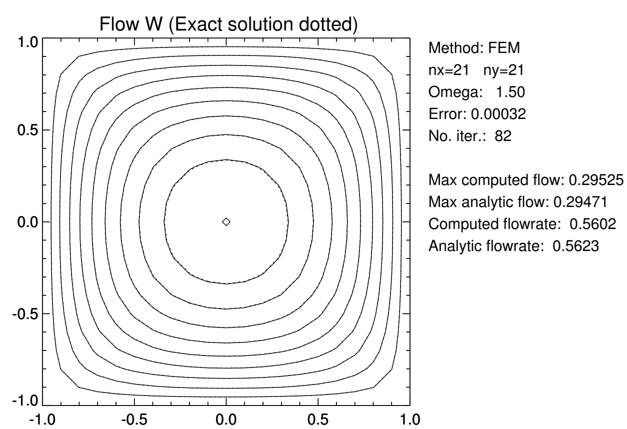












Comparison of the different runs:

method	resolution	rms error	Δ max flow	Δ flow rate
fdm	6×6	0.00432	-0.00830	-0.0674
fdm	11×11	0.00124	-0.00232	-0.0178
fdm	21×21	0.00035	-0.00064	-0.0046
fem	6×6	0.00482	0.00924	-0.0328
fem	11×11	0.00128	0.00233	-0.0083
fem	21×21	0.00032	0.00054	-0.0021

Summary: Finite difference and finite element methods provide quite similarly accurate results. In terms of rms error and maximum flow the results are very similar. The integral flow appears to be captured better by the finite element method. In both cases the errors decreases with Δx^2.

26. Select a class project. Try to formulate goals for the project and become familiar with the methodology. Provide a brief report (not more than three pages) on this progress with your project. Particularly list also any problems you may have encountered. This report as any future reports should demonstrate that you have indeed thought about the problem and made first progress (or not if documented by a corresponding discussion of the problems).