Computational Hydraulics

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Numerical Solution of Partial Differential Equations

Module 8

6 lectures

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Introduction

- In applied mathematics, partial differential equation is a subject of great significance
- These type of equations generally involves two or more independent variables that determine the behavior of the dependent variable.
- The partial differential equations are the representative equations in the fields of heat flow, fluid flow, electrical potential distribution, electrostatics, diffusion of matter etc.

Classification of PDEs

- Many physical phenomenon are a function of more than one independent variable and must be represented by a partial – differential equation, usually of second or higher order.

- We can write any second order equation (in two independent variable) as:

$$A\frac{\partial^2 u}{\partial x^2} + B\frac{\partial^2 u}{\partial x \partial y} + C\frac{\partial^2 u}{\partial y^2} + D\left(x, y, u, \frac{\partial u}{\partial x}, \frac{\partial u}{\partial y}\right) = 0$$

Classification of PDEs cont…

- The above partial differential equation can be classified depending on the value of $B^2 - 4AC$,

  Elliptic, if $B^2 - 4AC<0$;

  parabolic, if $B^2 - 4AC=0$;

  hyperbolic, if $B^2 - 4AC>0$.

- If *A,B,C* are functions of x,y,and/or u,the equation may change from one classification to another at various points in the domain

- For Laplace's and Poisson's equation, $B=0$, $A=C=1$, so these are always elliptic PDEs

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0$$

Classification of PDEs cont…

- 1D advective-dispersive transport process is represented through parabolic equation, where *B=0, C=0*, so $B^2 - 4AC=0$

$$D_l \frac{\partial^2 C}{\partial x^2} - \left(\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} \right) = 0$$

- 1D wave equation is represented through hyperbolic equation, where *B=0, A=1* and *C=-Tg/w*, so $B^2 - 4AC>0$

$$\frac{\partial^2 y}{\partial t^2} - \frac{Tg}{w} \frac{\partial^2 y}{\partial x^2} = 0$$

FD Approximation of PDEs

- One method of solution is to replace the derivatives by difference quotients
- Difference equation is written for each node of the mesh
- Solving these equations gives values of the function at each node of the grid network
- Let $h=\Delta x=$ spacing of grid work in x-direction
- Assume $f(x)$ has continuous fourth derivative w.r.t x and y.

FD Approximation of PDEs

- When f is a function of both x and y, we get the 2nd partial derivative w.r.t x, $\partial^2 u/ \partial x^2$, by holding y constant and evaluating the function at three points where x equals x_n, x_n+h and x_n-h. the partial derivative $\partial^2 u/ \partial y^2$ is similarly computed, holding x constant.
- To solve the Laplace equation on a region in the x-y plane, subdivide the region with equi-spaced lines parallel to x-y axes

FD Approximation of PDEs

- To solve Laplace equation on a *xy* plane, consider a region near (x_i, y_i), we approximate

$$\nabla^2 u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0$$

- Replacing the derivatives by difference quotients that approximate the derivatives at the point (x_i, y_i), we get

$$\begin{aligned}\nabla^2 u(x_i, y_i) &= \frac{u(x_{i+1}, y_i) - 2u(x_i, y_i) + u(x_{i-1}, y_i)}{(\Delta x)^2} \\ &+ \frac{u(x_i, y_{i+1}) - 2u(x_i, y_i) + u(x_i, y_{i-1})}{(\Delta y)^2} \\ &= 0\end{aligned}$$

FD Approximation of PDEs

- It is convenient to use double subscript on u to indicate the x- and y- values:

$$\nabla^2 u_{i,j} = \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{(\Delta x)^2} + \frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{(\Delta y)^2} = 0.$$

- For the sake of simplification, it is usual to take $\Delta x = \Delta y = h$

$$\nabla^2 u_{i,j} = \frac{1}{h^2}\left[u_{i+1,j} + u_{i-1,j} + u_{i,j+1} + u_{i,j-1} - 4u_{i,j}\right] = 0.$$

- We can notice that five points are involved in the above relation, known as five point star formula

FD Approximation of PDEs

- Linear combination of u's is represented symbolically as below

$$\nabla^2 u_{i,j} = \frac{1}{h^2}\begin{Bmatrix} & 1 & \\ 1 & -4 & 1 \\ & 1 & \end{Bmatrix} u_{i,j} = 0.$$

- This approximation has error of order *O(h²)*,provided u is sufficiently smooth enough
- We can also derive nine point formula for Laplace's equation by similar methods to get

$$\nabla^2 u_{i,j} = \frac{1}{6h^2}\begin{Bmatrix} 1 & 4 & 1 \\ 4 & -20 & 4 \\ 1 & 4 & 1 \end{Bmatrix} u_{i,j} = 0.$$

- In this case of approximation the error is of order $O(h^6)$, provided u is sufficiently smooth enough

Methods of solution

- approximation through FD at a set of grid points (x_i,y_i), a set of simultaneous linear equations results which needs to be solved by ***Iterative methods***

Liebmann's Method

- Rearrange the FD form of Laplace's equation to give a diagonally dominant system
- This system is then solved by Jacobi or Guass-Seidel iterative method
- The major drawback of this method is the slow convergence which is acute when there are a large system of points, because then each iteration is lengthy and more iterations are required to meet a given tolerance.

SOR method of solution

S.O.R method – Accelerating Convergence

- Relaxation method of Southwell, is a way of attaining faster convergence in the iterative method.
- Relaxation is not adapted to computer solution of sets of equations
- Based on Southwell's technique, the use of an overrelaxation factor can give significantly faster convergence
- Since we handle each equation in a standard and repetitive order, this method is called ***successive overrelaxation*** (S.O.R)

SOR method of solution cont…

- Applying SOR method to Laplace's equation as given below:

$$\nabla^2 u_{i,j} = \frac{1}{h^2}\begin{Bmatrix} & 1 & \\ 1 & -4 & 1 \\ & 1 & \end{Bmatrix} u_{i,j} = 0.$$

- The above equation leads to

$$u_{ij}^{(k+1)} = \frac{u_{i+1,j}^{(k)} + u_{i-1,j}^{(k+1)} + u_{i,j+1}^{(k)} + u_{i,j-1}^{(k+1)}}{4}$$

- We now both add and subtract $u_{ij}^{(k)}$ on the right hand side, getting

$$u_{ij}^{(k+1)} = u_{ij}^{(k)} + \left[\frac{u_{i+1,j}^{(k)} + u_{i-1,j}^{(k+1)} + u_{i,j+1}^{(k)} + u_{i,j-1}^{(k+1)} - 4u_{ij}^{(k)}}{4}\right]$$

SOR method of solution cont…

- The numerator term will be zero when final values, after convergence, are used, term in bracket called"residual", which is "relaxed" to zero
- We can consider the bracketed term in the equation to be an adjustment to the old value $u_{ij}^{(k)}$, to give the new and improved value $u_{ij}^{(k+1)}$
- If instead of adding the bracketed term, we add a larger value (thus "overrelaxing"), we get a faster convergence.
- We modify the above equation by including an overrelaxation factor ω to get the new iterating relation.

SOR method of solution cont…

- The new iterating relation after overrelaxation ω is as:

$$u_{ij}^{(k+1)} = u_{ij}^{(k)} + \omega\left[\frac{u_{i+1,j}^{(k)} + u_{i-1,j}^{(k+1)} + u_{i,j+1}^{(k)} + u_{i,j-1}^{(k+1)} - 4u_{ij}^{(k)}}{4}\right]$$

- Maximum acceleration is obtained for some optimum value of ω which will always lie in between 1.0 to 2.0 for Laplace's equation

ADI method of solution

- Coefficient matrix is sparse matrix, when an elliptical PDE is solved by FD method
- Especially in the 3D case, the number of nonzero coefficients is a small fraction of the total, this is called sparseness
- The relative sparseness increases as the number of equations increases
- Iterative methods are preferred for sparse matrix, until they have a tridiagonal structure

ADI method of solution

- Mere elimination does not preserve the sparseness until the matrix itself is tridiagonal
- Frequently the coefficient matrix has a band structure
- There is a special regularity for the nonzero elements
- The elimination does not introduce nonzero terms outside of the limits defined by the original bands

ADI method of solution

- Zeros in the gaps between the parallel lines are not preserved, though, so the tightest possible bandedness is preferred
- Sometimes it is possible to order the points so that a pentadiagonal matrix results
- The best of the band structure is tridiagonal, with corresponding economy of storage and speed of solution.

ADI method of solution cont…

- A method for the steady state heat equation, called the alternating-direction-implicit (A.D.I) method, results in tridiagonal matrices and is of growing popularity.
- A.D.I is particularly useful in 3D problems, but the method is more easily explained in two dimensions.
- When we use A.D.I in 2D, we write Laplace's equation as

$$\nabla^2 u = \frac{u_L - 2u_0 + u_R}{(\Delta x)^2} + \frac{u_A - 2u_0 + u_B}{(\Delta y)^2} = 0$$

Where the subscripts L,R,A, and B indicate nodes left, right, above, and below the central node 0. If $\Delta x = \Delta y$, we can rearrange to the iterative form

ADI method of solution

- Iterative form is as:

$$u_L^{(k+1)} - 2u_0^{(k+1)} + u_R^{(k+1)} = -u_A^{(k)} + 2u_0^{(k)} - u_B^{(k)}$$

- Using above equation, we proceed through the nodes by rows, solving a set of equations (tri-diagonal) that consider the values at nodes above and below as fixed quantities that are put into the RHS of the equations

- After the row-wise traverse, we then do a similar set of computations but traverse the nodes column-wise:

$$u_A^{(k+2)} - 2u_0^{(k+2)} + u_B^{(k+2)} = -u_L^{(k+1)} + 2u_0^{(k+1)} - u_R^{(k+1)}$$

ADI method of solution

- This removes the bias that would be present if we use only the row-wise traverse
- The name ADI comes from the fact that we alternate the direction after each traverse
- It is implicit, because we do not get u_0 values directly but only through solving a set of equations
- As in other iterative methods, we can accelerate convergence. We introduce an acceleration factor, ρ, by rewriting equations

$$u_0^{(k+1)} = u_0^{(k)} + \rho\left(u_A^{(k)} - 2u_0^{(k)} + u_B^{(k)}\right) + \rho\left(u_L^{(k+1)} - 2u_0^{(k+1)} + u_R^{(k+1)}\right)$$

$$u_0^{(k+2)} = u_0^{(k+1)} + \rho\left(u_L^{(k+1)} - 2u_0^{(k+1)} + u_R^{(k+1)}\right) + \rho\left(u_A^{(k+2)} - 2u_0^{(k+2)} + u_B^{(k+2)}\right).$$

ADI method of solution

- Rearranging further to give the tri-diagonal systems, we get

$$-u_L^{(k+1)} + \left(\frac{1}{\rho} + 2\right) u_0^{(k+1)} - u_R^{(k+1)} = u_A^{(k)} - \left(\frac{1}{\rho} - 2\right) u_0^{(k)} + u_B^{(k)}$$

$$-u_A^{(k+2)} + \left(\frac{1}{\rho} + 2\right) u_0^{(k+2)} - u_B^{(k+2)} = u_L^{(k+1)} - \left(\frac{1}{\rho} - 2\right) u_0^{(k+1)} + u_R^{(k+1)}.$$

CGHS method

- The conjugate Gradient (CG) method was originally proposed by Hestens and Stiefel (1952).
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- The gradient method solves N x N nonsingular system of simultaneous linear equations by iteration process. There are various forms of conjugate gradient method
- The finite difference approximation of the ground water flow governing equation at all the I.J nodes in a rectangular flow region (J rows and I columns) will lead to a set of I.J linear equations and as many unknowns,

CGHS method

- The I.J equations can be written in the matrix notations as

$$\overline{A}\,\overline{H} = \overline{Y}$$

- Where A = banded coefficient matrix,
- H= the column vector of unknowns
- Y= column vector of known quantities
- Giving an initial guess H_i for the solution vector H, we can write as follow

$$H_{i+1} = H_i + d_i$$

CGHS method

- Where d_i is a direction vector, H_i is the approximation to the solution vector H at the i th iterative step.
- A CG method chooses d_i such that at each iteration the B norm of the error vector is minimized, which is defined as

$$\|e_{i+1}\|_{\overline{B}} = < \overline{B} e_{i+1}, e_{i+1} >^{0.5}$$

- where

$$\overline{e}_{i+1} = \overline{H} - \overline{H}_{i+1} = \overline{e}_i - \overline{d}_i$$

CGHS method

- In which e_{i+1} is the error at the (i+1)th iteration. In the above equation angle bracket denotes the Euclidean inner product, which is defined as

$$<x, y> = \sum_{i=1}^{n} x_i y_i$$

- In the previous equation B is a symmetric positive definite (spd) inner product matrix. In the case of symmetric positive definite matrix A, such as that arising from the finite difference approximation of the ground water flow equation, the usual choice for the inner product matrix is *B=A*

CGHS method

- A symmetric matrix A is said to be positive definite if $x^T Ax > 0$ whenever $x \neq 0$ where x is any column vector. So the resulting conjugate gradient method minimizes the A norm of the error vector (i.e. $\|e_{i+1}\|_{\overline{A}}$).
- The convergence of conjugate gradient method depend upon the distribution of eigenvalues of matrix A and to a lesser extend upon the condition number [k(A)] of the matrix. The condition number of a symmetric positive definite matrix is defined as

$$k(\overline{A}) = \lambda_{\max} / \lambda_{\min}$$

CGHS method

- Where λ_{max} and λ_{min} are the largest and smallest eigenvalues of A respectively. When k(A) is large, the matrix is said to be ill-conditioned, in this case conjugate gradient method may converge slowly.
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- The condition number may be reduced by multiplying the system by a pre-conditioning matrix K-1. Then the system of linear equation given by the equation… can be modified as

$$\overline{K}^{-1}\overline{A}\overline{H} = \overline{K}^{-1}\overline{Y}$$

CGHS method

- Different conjugate methods are classified depending upon the various choices of the pre-conditioning matrix.
- The choice of K matrix should be such that only few calculations and not much memory storage are required in each iteration to achieve this. With a proper choice of pre-conditioning matrix, the resulting preconditioned conjugate gradient method can be quite efficient.
- A general algorithm for the conjugate gradient method is given as follow:

CGHS method

- Initialize

$$\overline{H}_0 = Arbitrary - initial - guess$$

$$\overline{r}_0 = \overline{Y} - \overline{A}\,\overline{H}_0$$

$$\overline{s}_0 = \overline{K}^{-1}\overline{r}_0$$

$$\overline{p}_0 = \overline{s}_0$$

$$i = 0$$

- Do while till the stopping criteria is not satisfied

CGHS method

- Cont…

$$a_i = <\bar{s}_i, \bar{r}_i> / <\bar{A}\bar{p}_i, \bar{p}_i>$$

$$\bar{H}_{i+1} = \bar{H}_i + \bar{a}_i \bar{p}_i$$

$$\bar{r}_{i+1} = \bar{r}_i - a_i \bar{A}\bar{p}_i$$

$$\bar{s}_{i+1} = \bar{K}^{-1}\bar{r}_{i+1}$$

$$b_i = <\bar{s}_{i+1}, \bar{r}_{i+1}> / <s_i, r_i>$$

$$\bar{p}_{i+1} = \bar{s}_{i+1} + b_i \bar{p}_i$$

$$i = i + 1$$

End do

CGHS method

- Where r_0 is the initial residue vector, s_0 is a vector, p_0 is initial conjugate direction vector, r_{i+1},s_{i+1} and p_{i+1} are the corresponding vectors at (i+1)th iterative step, k-1 is the preconditioning matrix and A is the given coefficient matrix. This conjugate algorithm has following two theoretical properties:
- (a) the value $\{H_i\}i>0$ converges to the solution H within n iterations
- (b) the CG method minimizes $\|H_i - H\|$ for all the values of i

CGHS method

- There are three types of operations that are performed by the CG method: inner products, linear combination of vectors and matrix vector multiplications.
- The computational characteristics of these operations have an impact on the different conjugate gradient methods.

Assignments

1. The equation

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

is an elliptic equation. Solve it on the unit square, subject to u=0 on the boundaries. Approximate the first derivative by a central-difference approximation. Investigate the effect of size of Δx on the results, to determine at what size reducing it does not have further effect.

2. Write and run a program for poisson's equation. Use it to solve

$$\nabla^2 u = xy(x-2)(y-2)$$

On the region $0 \le x \le 2, 0 \le y \le 2,$ with u=0 on all boundaries except for y=0, where u=1.0.

Assignments

3. Repeat the exercise 2, using A.D.I method. Provide the Poisson equation as well as the boundary conditions as given in the exercise 2.

4. The system of equations given here (as an augmented matrix) can be speeded by applying over-relaxation. Make trials with varying values of the factor to find the optimum value. (In this case you will probably find this to be less than unity, meaning it is under-relaxed.)

$$\begin{bmatrix} 8 & 1 & -1 & | & 8 \\ 1 & -7 & 2 & | & -4 \\ 2 & 1 & 9 & | & 12 \end{bmatrix}$$