AN INTRODUCTION TO COMPACT FINITE DIFFERENCES

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Numerical methods for partial differential equations

There are many methods which may be called upon to solve systems of partial differential equations. Examples include:

- Finite difference methods
- Finite volume methods
- Finite element methods
- Spectral/Galerkin methods
- Lattice Boltzmann methods
- Smoothed particle hydrodynamics
- Radial basis functions

Finite difference methods — a simple case

- The central idea is that differential equations are replaced by difference equations.

- For example, if we wish to solve
$$\frac{du}{dx} = -au$$
on the set of discrete points, x_0, x_1, $x_2 \cdots$, where there is a constant steplength, h, then at $x = x_n$ we may replace du/dx by the forward difference,
$$\frac{du}{dx}(x_n) \simeq \frac{u_{n+1} - u_n}{h},$$
where u_n is the numerical approximation to the exact value, $u(x_n)$.

- The right hand side may also be interpreted as the slope of the tangent to $u(x)$ at $x = x_n$. Hence we obtain,
$$\frac{u_{n+1} - u_n}{h} = -au_n \qquad \Longrightarrow \qquad u_{n+1} = (1 - ah)u_n,$$
a difference equation!

Finite difference methods — Taylor's series

- The finite difference approximation to a derivative is usually derived by using a Taylor's series expansion. If we focus on $x = x_n$, then we have,

$$u(x_{n+1}) = u(x_n + h) = u(x_n) + hu'_n + \tfrac{1}{2}h^2u''_n + \tfrac{1}{6}h^3u'''_n + \tfrac{1}{24}h^4u''''_n + O(h^5) \quad (1)$$
$$u(x_{n-1}) = u(x_n - h) = u(x_n) - hu'_n + \tfrac{1}{2}h^2u''_n - \tfrac{1}{6}h^3u'''_n + \tfrac{1}{24}h^4u''''_n + O(h^5) \quad (2)$$

- If we add together Eqs. (1) and (2), then

$$u(x_{n+1}) + u(x_{n-1}) = 2u(x_n) + h^2u''_n + \tfrac{1}{12}h^4u''''_n + O(h^6).$$

  Upon rearrangement we find that,

$$u''_n = \frac{u_{n-1} - 2u_n + u_{n+1}}{h^2} - \tfrac{1}{12}h^2u''''_n + O(h^4).$$

- Upon neglecting the error terms in red, we have the finite difference approximation,

$$u''_n \simeq \frac{u_{n-1} - 2u_n + u_{n+1}}{h^2}.$$

  The error associated with this approximation is of $O(h^2)$, a 2nd order method.

Finite difference methods — Taylor's series

- Recapping the Taylor's series:

$$u(x_{n+1}) = u(x_n + h) = u(x_n) + hu_n' + \tfrac{1}{2}h^2u_n'' + \tfrac{1}{6}h^3u_n''' + \tfrac{1}{24}h^4u_n'''' + O(h^5) \quad (1)$$

$$u(x_{n-1}) = u(x_n - h) = u(x_n) - hu_n' + \tfrac{1}{2}h^2u_n'' - \tfrac{1}{6}h^3u_n''' + \tfrac{1}{24}h^4u_n'''' + O(h^5) \quad (2)$$

- If we subtract Eq. (2) from Eq. (1), then

$$u(x_{n+1}) - u(x_{n-1}) = 2hu_n' + \tfrac{1}{3}h^3u_n''' + O(h^5).$$

Upon rearrangement we find that,

$$u_n' = \frac{u_{n+1} - u_{n-1}}{2h} - \tfrac{1}{6}h^2u_n''' + O(h^4).$$

- Upon neglecting the error terms in red, we have the finite difference approximation,

$$u_n' \simeq \frac{u_{n+1} - u_{n-1}}{2h}.$$

The error associated with this approximation is again of $O(h^2)$, a 2nd order method.

Finite difference methods — notations and representations

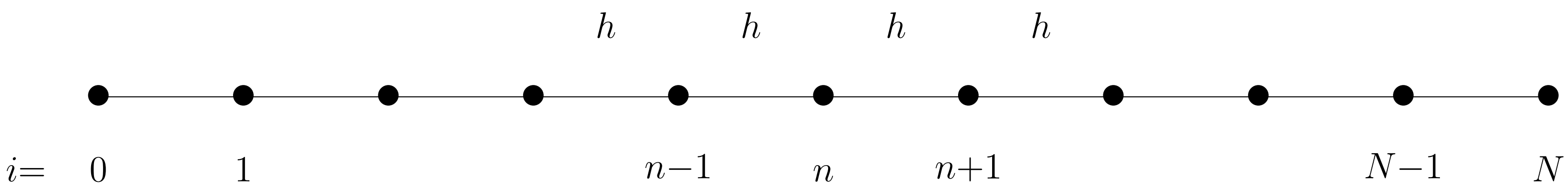
In many contexts the following notation is used:

$$u_n' \simeq \frac{u_{n+1} - u_{n-1}}{2h} \equiv \delta_x\, u_n$$

and

$$u_n'' \simeq \frac{u_{n-1} - 2u_n + u_{n+1}}{h^2} \equiv \delta_x^2\, u_n.$$

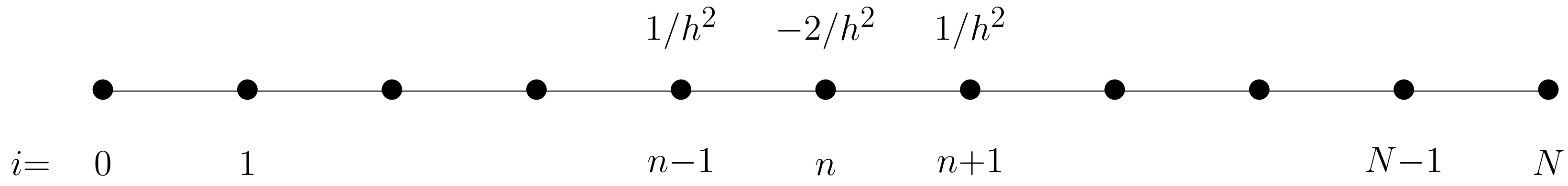
If the following grid is visualized,



then...

Finite difference methods — notations and representations

$u_n'' = (u_{n-1} - 2u_n + u_{n+1})/h^2$ may be represented using the coefficients:



or in finite difference stencil or finite difference molecule form,

$$u_n'' = \left(\frac{1}{h^2} \quad -\frac{2}{h^2} \quad \frac{1}{h^2}\right) u_n,$$

or

$$u_n'' = \tfrac{1}{h^2}(1, \ -2, \ 1)u_n.$$

Similarly,

$$u_n' = \tfrac{1}{2h}(-1, \ 0, \ 1)u_n.$$

Finite difference methods — example of a second order method

- Let us solve $u'' - 4u = -4x^2$ numerically, subject to $u(0) = u(1) = 0$.

- The analytical solution is

$$u = x^2 + \tfrac{1}{2} - \tfrac{1}{2}\cosh 2x + \frac{\tfrac{1}{2}\cosh 2 - \tfrac{3}{2}}{\sinh 2}\sinh 2x.$$

- The finite difference approximation is

$$\tfrac{1}{h^2}(1,\ -2,\ 1)u_n - 4u_n = -4x_n^2$$

at $x = x_n$, the general point. It is valid for $n = 1, \cdots, N-1$, and we use $u_0 = u_N = 0$.

- For $N = 5$ and where $h = \frac{1}{5}$, the assembled set of difference equations is

$$\begin{pmatrix} -2-4h^2 & 1 & 0 & 0 \\ 1 & -2-4h^2 & 1 & 0 \\ 0 & 1 & -2-4h^2 & 1 \\ 0 & 0 & 1 & -2-4h^2 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{pmatrix} = h^2 \begin{pmatrix} -4x_1^2 \\ -4x_2^2 \\ -4x_3^2 \\ -4x_4^2 \end{pmatrix}.$$

Finite difference methods — example of a second order method

Table of results.

N	$u_{N/2}$	error	error$/h^2$
10	0.101 126 67	0.000 819 05	0.081 905 30
20	0.101 740 30	0.000 205 43	0.082 170 24
40	0.101 894 33	0.000 051 40	0.082 236 83
80	0.101 932 87	0.000 012 85	0.082 253 50
160	0.101 942 51	0.000 003 21	0.082 257 67
∞	0.101 945 73	0	

We see the typical behaviour for a second order accurate method where the error, which is roughly proportial to h^2, reduces by a factor of 4 when h is halved.

Finite difference methods — higher orders of accuracy

- Second order accurate methods are typical when solving PDEs, but we are used to better schemes for ODEs such as the fourth and sixth order Runge-Kutta methods. Can we do better than second order with finite differences?

- We may, but with larger stencils. The following schemes

				$-\frac{1}{12}h^2$	$\frac{4}{3}h^2$	$-\frac{5}{2}h^2$	$\frac{4}{3}h^2$	$-\frac{1}{12}h^2$			
	●	●	●	●	●	●	●	●	●	●	●
$i=$	0	1			$n-1$	n	$n+1$			$N-1$	N

			$\frac{1}{90}h^2$	$-\frac{1}{3}20h^2$	$\frac{3}{2}h^2$	$-\frac{49}{18}h^2$	$\frac{3}{2}h^2$	$-\frac{3}{20}h^2$	$\frac{1}{90}h^2$		
	●	●	●	●	●	●	●	●	●	●	●
$i=$	0	1			$n-1$	n	$n+1$			$N-1$	N

have 4th and 6th order accuracies, respectively, but involve five and seven points.

- Near boundaries even more points are needed to maintain the accuracy.

Compact differences for an ODE

We shall solve $u'' + bu = f(x)$.

- The finite difference approximation for the second derivative was shown to be:

$$u''_n = \frac{u_{n-1} - 2u_n + u_{n+1}}{h^2} - \tfrac{1}{12}h^2 u''''_n + O(h^4). \tag{1}$$

- We may now achieve an $O(h^4)$ approximation if we can model the u'''' term which is in the first error term on the right hand side.

- We may find an expression for u'''' by differentiating the original equations twice:

$$u'''' = f'' - bu'',$$

where it is assumed here that b is a constant, for the sake of simplicity.

- Hence Eq. (1) becomes,

$$u''_n = \frac{u_{n-1} - 2u_n + u_{n+1}}{h^2} - \tfrac{1}{12}h^2 \Big(f'' - bu''\Big) + O(h^4).$$

Compact differences for an ODE

- We had:

$$u_n'' = \frac{u_{n-1} - 2u_n + u_{n+1}}{h^2} - \tfrac{1}{12}h^2\Big(f'' - bu''\Big) + O(h^4), \tag{2}$$

  and therefore the original ODE becomes,

$$u_n'' + bu_n - f = \frac{u_{n-1} - 2u_n + u_{n+1}}{h^2} + bu_n - \tfrac{1}{12}h^2\Big(f'' - bu''\Big) + O(h^4),$$

  and we may develop this in two different ways.

- First way: Use the usual three-point stencil for u''. Eventually this leads to

$$\left[\frac{1}{h^2} + \frac{b}{12},\ \ -\frac{2}{h^2} + \frac{10b}{12},\ \ \frac{1}{h^2} + \frac{b}{12}\right] u_n = \left[\frac{1}{12},\ \ \frac{10}{12},\ \ \frac{1}{12}\right] f_n.$$

- Second way: Find u'' from Eq. (2) and substitute that into the orginal equation:

$$\left[\frac{1}{h^2},\ \ -\frac{2}{h^2},\ \ \frac{1}{h^2}\right] u_n + b\left(1 - \frac{bh^2}{12}\right) u_n = \left[\frac{1}{12},\ \ -\frac{2}{12},\ \ \frac{1}{12}\right] f_n + \left(1 - \frac{bh^2}{12}\right) f_n.$$

- Slightly different forms are available for the right hand sides if $f(x)$ is given analytically.

Finite difference methods — example of a fourth order method

N	$u_{N/2}$	error	error$/h^2$
10	0.10112667	0.00081905	0.08190530
20	0.10174030	0.00020543	0.08217024
40	0.10189433	0.00005140	0.08223683
80	0.10193287	0.00001285	0.08225350
160	0.10194251	0.00000321	0.08225767
∞	0.101 945 73	0	

Second order method

N	$u_{N/2}$	error	error$/h^4$
10	0.10194737	-0.00000164	-0.01642592
20	0.10194583	-0.00000010	-0.01644530
40	0.10194573	-0.00000001	-0.01645018
80	0.10194573	0.00000000	-0.01645140

First way

N	$u_{N/2}$	error	error$/h^4$
10	0.10194464	0.00000109	0.01090290
20	0.10194566	0.00000007	0.01095157
40	0.10194572	0.00000000	0.01096380
80	0.10194573	0.00000000	0.01096671

Second way

We see the typical behaviour for a fourth order accurate method where the error, which is roughly proportial to h^4, reduces by a factor of 16 when h is halved.

A fourth order method for a more general ODE

- We shall develop a fourth order method for the ODE,

$$u'' + au' + bu = f(x).$$

- Application of the Taylor's series developed earlier leads to.

$$\delta_x^2 u_n + a\delta_x u_n + bu_n - \frac{h^2}{12}u_n'''' - \frac{ah^2}{6}u_n''' = f_n.$$

- Differentiation of the ODE yields

$$u''' = f' - au'' - bu'$$

and

$$u'''' = f'' - au''' - bu''.$$

- Substitution into the red terms eventually gives,

$$\left[1 + \left(\frac{a^2+b}{12}\right)h^2\right]\delta_x^2 u_n + a\left[1 + \frac{b}{12}h^2\right]\delta_x u_n + b_n u_n = f_n + \frac{ah^2}{12}\delta_x f_n + \frac{h^2}{12}\delta_x^2 f_n.$$

A fourth order method for a more general ODE

We shall solve

$$u'' + 4u' + 3u = -16e^{-5x}$$

subject to $u(0) = 0$ and $u(1) = e^1 + e^{-3} - 2e^{-5}$. The analytical solution is

$$u = e^{-x} + e^{-3x} - 2e^{-5x}.$$

Table of results.

N	$u_{N/2}$	error	error$/h^4$
10	0.66544157	0.00004925	0.49250582
20	0.66548778	0.00000304	0.48715954
40	0.66549063	0.00000019	0.48582812
80	0.66549081	0.00000001	0.48549544

Once more we see the typical behaviour for a fourth order accurate method.

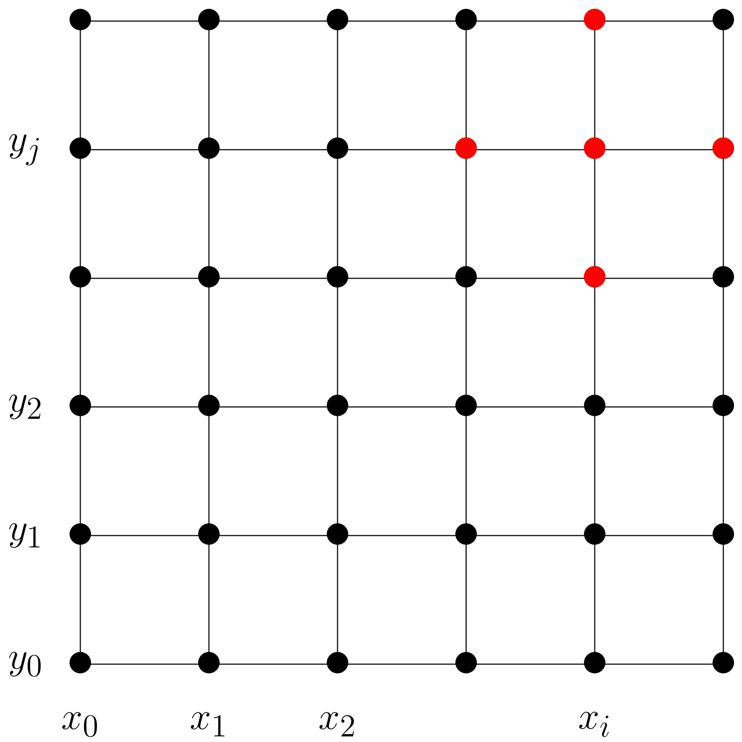
Some general comments about solving ODEs with 4th order compact methods

- Unlike second order methods, fourth order compact methods are tailored to the equation which is being solved.
- When programmed correctly they will exhibit the error-reducing properties which are associated with an $O(h^4)$ method. Slight errors of programming or analysis will manifest themselves as second order methods.
- These methods may also be applied to systems with other types of boundary condition, such Neumann or Robin conditions.
- They can also be applied to nonlinear equations.
- It is possible to take this theory still further and produce 6th order accurate solvers but still retaining the three-point compact stencil.

- What happens with PDEs? We shall consider Poisson's equations.

Compact differences for the 2D Poisson's equation

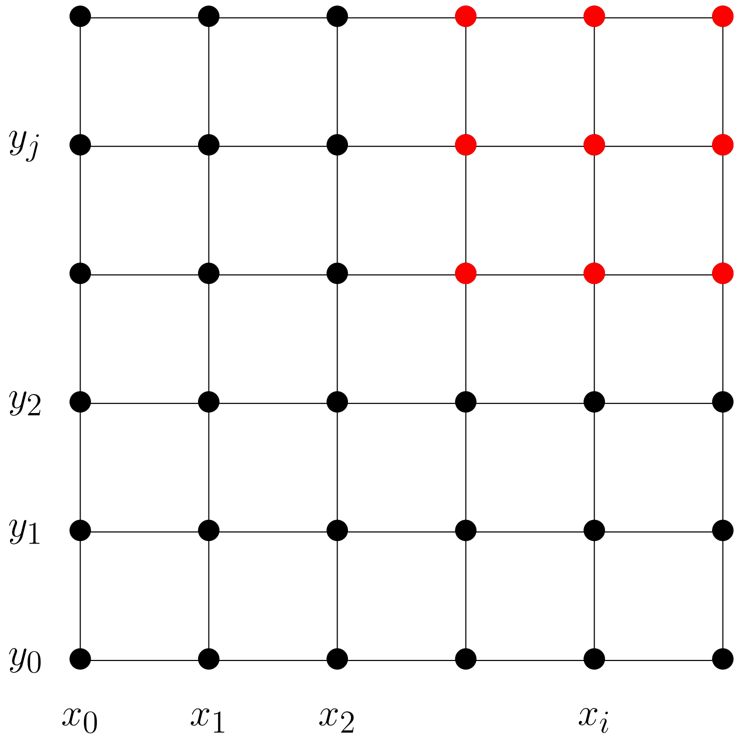
For simplicity we shall consider a square grid steplengths of magnitude, h, in both the x and y directions.



The red nodes represent the classical finite difference stencil which is used to solve Poisson's equation in 2D.

Compact differences for the 2D Poisson's equation

Our aim will be determine a nine-point stencil:



Compact differences for the 2D Poisson's equation

Poisson's equation is

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = f(x, y) \qquad \text{or} \qquad u_{xx} + u_{yy} = f.$$

Using Taylor's series as before we obtain,

$$u_{xx} = \frac{1}{h^2}\Big(1,\ -2,\ 1\Big)u_{ij} - \frac{h^2}{12}u_{xxxx} + O(h^4),$$

$$u_{yy} = \frac{1}{h^2}\begin{pmatrix} 1 \\ -2 \\ 1 \end{pmatrix} u_{ij} - \frac{h^2}{12}u_{yyyy} + O(h^4).$$

The order $O(h^2)$ errors may be accounted for by using the appropriate derivatives of the Poisson's equation. Hence

$$u_{xxxx} = f_{xx} - u_{xxyy}, \qquad u_{yyyy} = f_{yy} - u_{xxyy}.$$

Compact differences for the 2D Poisson's equation

Therefore we obtain,

$$u_{xx} + u_{yy} - f = \frac{1}{h^2}\begin{pmatrix} 0 & 1 & 0 \\ 1 & -4 & 1 \\ 0 & 1 & 0 \end{pmatrix} u_{i,j} - f_{i,j} - \frac{h^2}{12}\Big(f_{xx} + f_{yy} - 2u_{xxyy}\Big) + O(h^4).$$

The mixed fourth partial derivative has a compact stencil:

$$u_{xxyy} = \frac{1}{h^4}\begin{pmatrix} 1 & -2 & 1 \\ -2 & 4 & -2 \\ 1 & -2 & 1 \end{pmatrix} u_{i,j} + O(h^2).$$

After some manipulations we eventually obtain the following compact difference equation,

$$\frac{1}{6h^2}\begin{pmatrix} 1 & 4 & 1 \\ 4 & -20 & 4 \\ 1 & 4 & 1 \end{pmatrix} u_{i,j} = \frac{1}{12}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 8 & 1 \\ 0 & 1 & 0 \end{pmatrix} f_{i,j}.$$

Compact differences for the 2D Poisson's equation

$$\frac{1}{6h^2}\begin{pmatrix} 1 & 4 & 1 \\ 4 & -20 & 4 \\ 1 & 4 & 1 \end{pmatrix} u_{i,j} = \frac{1}{12}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 8 & 1 \\ 0 & 1 & 0 \end{pmatrix} f_{i,j}.$$

The finite difference formula on the left hand side is a well-known fourth-order accurate nine-point formula which may be used when f = constant, but an analysis of this stencil by itself using Taylor's series will imply that it only has second order accuracy.

The present analysis guarantees fourth order accuracy because we have accounted for the inhomogeneous term, $f(x, y)$, in our derivation.

Comparison between the 2nd order, standard 4th order and compact 4th order methods

2nd order

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

4th order

$$\frac{1}{h^2}\begin{pmatrix} 0 & 0 & -1/12 & 0 & 0 \\ 0 & 0 & 4/3 & 0 & 0 \\ -1/12 & 4/3 & -5 & 4/3 & -1/12 \\ 0 & 0 & 4/3 & 0 & 0 \\ 0 & 0 & -1/12 & 0 & 0 \end{pmatrix} u_{i,j} = f_{i,j}.$$

Compact 4th order

$$\frac{1}{6h^2}\begin{pmatrix} 1 & 4 & 1 \\ 4 & -20 & 4 \\ 1 & 4 & 1 \end{pmatrix} u_{i,j} = \frac{1}{12}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 8 & 1 \\ 0 & 1 & 0 \end{pmatrix} f_{i,j}.$$

The application of compact differences to Poisson's equation

We shall solve

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

in the unit square, $0 \le x \le 1$ and $0 \le y \le 1$.

The boundary conditions are that $u = 0$ on all four boundaries.

The value of u at the centre is computed to be $u(\frac{1}{2}, \frac{1}{2}) = 2.385891352$ (9DPs).

The application of compact differences to Poisson's equation

N	$u_{N/2,N/2}$	error	error$/h^2$
10	2.316727002892	0.069164349348	6.9164
20	2.368308146803	0.017583205436	7.0333
40	2.381476871123	0.004414481117	7.0632
80	2.384786557124	0.001104795116	7.0707
160	2.385615079383	0.000276272857	7.0726
320	2.385822278850	0.000069073390	7.0731

Second order method

N	$u_{N/2,N/2}$	error	error$/h^4$
10	2.386695367753	-0.000804015514	-8.040155137405
20	2.385941851193	-0.000050498953	-8.079832482579
40	2.385894511633	-0.000003159394	-8.088047424053
80	2.385891549040	-0.000000196800	-8.060930122156

Fourth order compact method

For this example compact differences with $N = 20$ gives a more accurate solution than second order differences with $N = 320$.

Conclusions and comments

- For second order methods it is generally the case that each derivative is simply replaced by its finite difference stencil, but for compact fourth order methods the appropriate scheme depends on the form of the equation being solved.

- The derivation of the compact 4th order scheme takes much longer than for a 2nd order scheme, as does the programming, but there is a substantial gain in accuracy and speed of computation.

- The general methodology may still be applied to nonlinear equations.

- It may also be applied in 3D.

- It is not restricted to Dirichlet boundary conditions.

- This methodology can be applied at an interface between two media with continuity of flux conditions.

- The multigrid method may be applied to accelerate iterative convergence.