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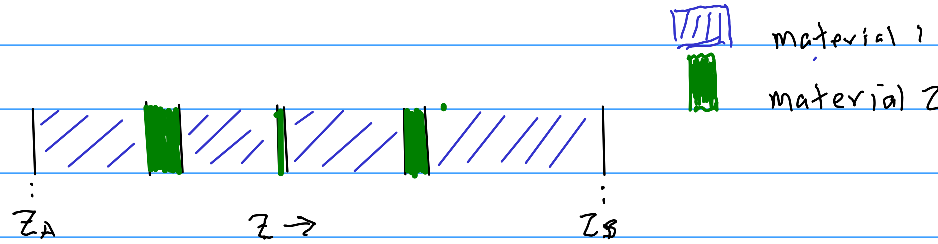
Fields institute mini-course : Lecture #3.

Numerical methods for the 1D Schroedinger - Poisson equation

Equations



$\kappa(z)$ = dielectric factor - piecewise constant, constant over each layer

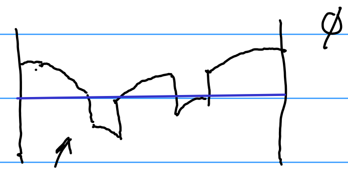
The potential $\phi(z) = \tilde{\phi}(z) + \phi_D(z) + \phi_B(z)$ where

$\phi_B(z)$ = "bandshift" - piecewise constant, constant over each layer

$$\frac{d}{dz}\kappa(z)\frac{d}{dz}\phi_D = -\rho_D(z) \qquad \phi_D(z_A) = g_A \qquad \phi_D(z_B) = g_B$$

$$\frac{d}{dz}\kappa(z)\frac{d}{dz}\tilde{\phi} = -\rho_e(z) \qquad \tilde{\phi}(z_A) = 0 \qquad \tilde{\phi}(z_B) = 0$$

Sample ϕ plot :



discontinuities due to ϕ_B

$$\rho_e(z) = 2\sum_{\lambda_j < E_f} \psi_j^*(z)\psi_j(z)\, W(\lambda_j, E_f) \qquad \left\{ (E_f - \lambda_j)\frac{m_r(z)}{2\pi\hbar^2} \right.$$

where

$$\left[\frac{\hbar^2}{2}\left[\frac{d}{dz}\left(\frac{1}{m_e(z)}\frac{d}{dz}\right) + \left[\tilde{\phi}(z) + \phi_D(z) + \phi_B(z)\right]\right]\right]\psi_j = \lambda_j\psi_j$$

$m_e(z)$ = effective mass - piecewise constant, constant over each layer

First computational task.

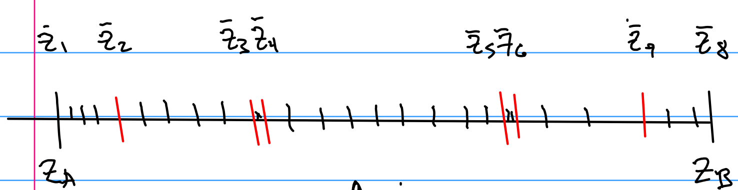
Solve problems of the form

$$\frac{d}{dz}\left(a(z) \frac{du}{dz} \right) = f(z) \qquad u(z_A) = g_A \qquad u(z_B) = g_B \qquad a(z) \text{ piecewise constant.}$$

General approach: set up a linear system of equations whose solution gives values that approximate the exact solution values.

Derive the discrete equations using a simple, but very useful technique "finite volume discretization".

Grid: Semi-uniform, a collection of M uniform grids, one for each material layer with N_j panels the jth layer.

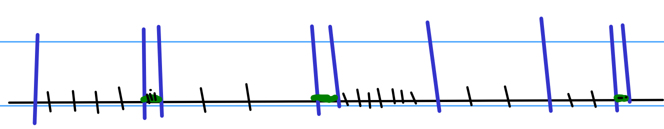


$\bar{z}_j$ = jth layer boundary location

N_j 'panels' $\quad h_j = \text{mesh width} = \dfrac{\bar{z}_{j+1} - \bar{z}_j}{N_j}$

Why a semi-uniform grid?

Some problems consist of a mixture of very thin layers and very thick layers; we don't want a small mesh width in the thin layers to dictate the mesh widths in all the other layers.

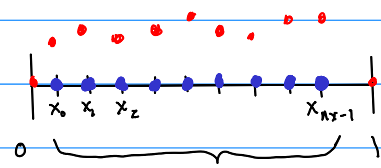


Background: Finite Volume Discretization.

Single uniform grid

(1D) $\frac{\partial}{\partial x}\left(a(x)\frac{\partial u}{\partial x}\right) = f(x) \quad x \in [0,1] \quad u(0) = u(1) = 0 \quad (*)$

$u_i \doteq u(x_i)$



M panels

$hx = \frac{1}{M}$

$nx = M-1$ interior points.

Seek approximate values $u_i \approx u(x_i)$

at interior grid points x_i.

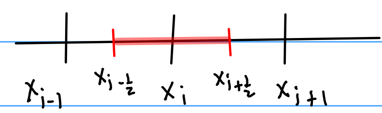
$x_i = (i+1)\,hx \quad i = 0,1,2,\cdots nx-1$ and $hx = \frac{1}{M}$.

Obtain an equation for each u_i by requiring

an integral approximation to $(*)$ hold in a finite volume

$[x_{i-1/2}, x_{i+1/2}] \qquad \left(x_{i+1/2} = x_i + \frac{hx}{2} \quad x_{i-1/2} = x_i - \frac{hx}{2} \right)$

$$\frac{d}{dx}\left(a(x)\frac{du}{dx}\right) = f(x) \Rightarrow \int_{x_{i-1/2}}^{x_{i+1/2}} \frac{d}{dx}\left(a(s)\frac{du}{\partial x}\right) ds = \int_{x_{i-1/2}}^{x_{i+1/2}} f(s)\,ds.$$



$$\Rightarrow \quad a(x)\frac{du}{dx}\Big|_{x_{i-1/2}}^{x_{i+1/2}} = \int_{x_{i-1/2}}^{x_{i+1/2}} f(s)\,ds.$$

Obtain equations by approximating this exact relation, with $\frac{du}{\partial x}\Big|_{x_{i+1/2}} \doteq \frac{u_{i+1}-u_i}{hx}$, $\frac{du}{\partial x}\Big|_{x_{i-1/2}} \doteq \frac{u_i - u_{i-1}}{hx}$ and the midpoint rule for the integral of f.

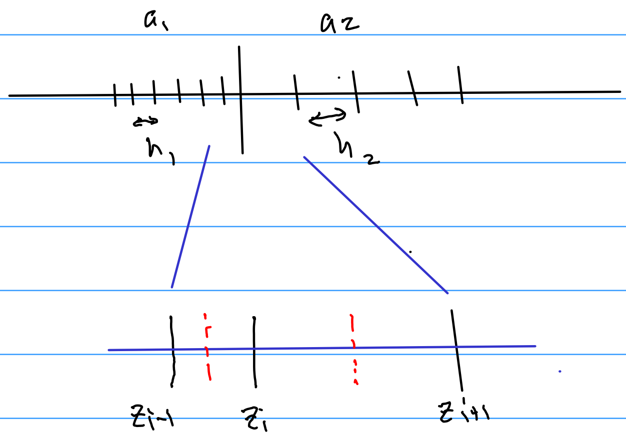
$$\approx \quad \boxed{a_{i+1/2}\frac{[u_{i+1}-u_i]}{hx} - a_{i-1/2}\frac{[u_i - u_{i-1}]}{hx} = f_i\, hx}$$

u_0, u_{nx} given

$$\begin{bmatrix} -(a_{1/2}+a_{3/2}) & a_{3/2} & & & \\ a_{3/2} & (a_{3/2}+a_{5/2}) & a_{5/2} & & \\ & a_{5/2} & \ddots & \ddots & \\ & & \ddots & \ddots & \ddots \\ & & & \ddots & \ddots \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ \\ u_{nx-1} \end{bmatrix} = (hx) \begin{bmatrix} f_1 \\ f_2 \\ \vdots \\ \\ f_{nx-1} \end{bmatrix} + \begin{bmatrix} -(a_{\frac{1}{2}}u_0)/hx \\ \\ \\ \\ -(a_{nx-1/2}u_{nx})/hx \end{bmatrix}$$

"Symmetric tridiagonal"

What changes have to be made when one is using a semi-uniform mesh?
The only change has to do with the creation of the equations at points that are layer boundaries. :



$$\int_{z_{i-1/2}}^{z_{i+1/2}} \frac{d}{dz}\, a(z) \frac{d}{dz} \quad dz = \int_{z_{i-1/2}}^{z_{i+1/2}} f(z)\, dz$$

$$\Rightarrow \quad a_2 \frac{du}{dz}\bigg|_{z_{i+1/2}} - a_1 \frac{du}{dz}\bigg|_{z_{i-1/2}} = \int_{z_{i-1/2}}^{z_{i+1/2}} f(z)\, dz.$$

$$a_2 \left(\frac{u_{i+1} - u_i}{h_2} \right) - a_1 \left(\frac{u_i - u_{i-1}}{h_1} \right) \cong f(z_i) \left(\frac{h_a}{2} + \frac{h_b}{2} \right)$$

This leads to a system of equations that is symmetric tri-diagonal, which, when one includes the modification of the right hand side that is due to the boundary conditions, has the form

$$\begin{bmatrix} \ddots & \ddots & & 0 \\ \ddots & \ddots & \ddots & \\ & \ddots & \ddots & \ddots \\ 0 & & \ddots & \ddots \end{bmatrix} \vec{u} = D\vec{f} - \vec{f}_{bdry} \qquad D = \begin{bmatrix} h_1 & & & & & \\ & h_1 & & & & \\ & & \ddots & & & \\ & & & (h_1+h_2)/2 & & \\ & & & & h_2 & \\ & & & & & \ddots \\ & & & & & & (h_2+h_3)/2 \\ & & & & & & & \ddots \end{bmatrix}$$

due to the change in mesh sizes

So, solution procedure for

$$\frac{d}{dz} k(z) \frac{\partial}{\partial z} \phi = \rho \qquad \phi(z_a) = g_a \quad \phi(z_b) = g_b$$

(1) Construct matrices associated with the discrete approximation obtained using finite volume based discretizations.

Grid specification $\rightsquigarrow L$ (tri-diagonal matrix)

$+$ $\rightsquigarrow D$ (diagonal matrix of mesh weights).

$k(z)$

Boundary value forcing term.

(2) Given ρ, form $\rho^* = D\rho - \begin{bmatrix} \frac{k_1 \phi(z_A)}{h_1} \\ 0 \\ 0 \\ 0 \\ \frac{k_m \phi(z_B)}{h_m} \end{bmatrix}$

(3) Solve $L\vec{\phi} = \rho^*$ to obtain $\phi_i \simeq \phi(z_i)$.

Note: L is symmetric tri-diagonal so using a standard tri-diagonal solver, $L\vec{\phi} = \rho^*$ can be obtained in $O(n)$ operations where $n =$ dimension of L.

(calls the solver for you.)

In Matlab or Octave, use phi = L \ ρStar

or, you can write your own tri-diagonal solver (a typical exercise given in numerical analysis classes)

Generally, when creating discrete approximations to self-adjoint operators one strives to obtain symmetric matrices. Why? Symmetric matrices have properties that facilitate the construction of efficient solution procedures.