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UNITED NATIONS EDUCATIONAL, SCIENTIFIC AND CULTURAL ORGANIZATION

INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS

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**WINTER COLLEGE ON "MULTILEVEL TECHNIQUES IN
COMPUTATIONAL PHYSICS"**

Physics and Computations with Multiple Scales of Lengths
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Multigrid Methods for Transport Models

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Multi Grid Methods
for
Transport Models

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Applications

- Satellite Electronics Shielding
- Radiation Effects on Electronics
- Solar Wind Models
- Nuclear Reactor Design
- Radiation Detector Design
- Radiation Effects on Materials

Linear Boltzmann Transport Equations

$N(\underline{x}, \vec{\Omega}, E, T)$ Density of Particles

\underline{x} position

$\vec{\Omega}$ direction

E energy

T time

$$\frac{\partial N}{\partial T} = -\vec{\Omega} \cdot \mathbf{v} \nabla N - \sigma_t \mathbf{v} N + S(\underline{x}, \vec{\Omega}, E, T)$$

S - sources

$\sigma_t dt =$ Collision Probability

Time Independent

$$\Psi = \mathbf{v} N \quad \text{flux}$$

$$\vec{\Omega} \cdot \nabla \Psi + \sigma_t \Psi = S(\underline{x}, \vec{\Omega}, E)$$

Sources

i) Scattering Source

Particles at position \underline{x} that scatter

from to

$E' \rightarrow E$

$\vec{\Omega}' \rightarrow \vec{\Omega}$

due to a collision

$$S_s = \int dE' \int d\vec{\Omega}' \sum_{i,s} (\underline{x}, \vec{\Omega}' \rightarrow \vec{\Omega}, E' \rightarrow E) \Psi(\underline{x}, \vec{\Omega}', E')$$

ii) Fission Source

$$S_f = \int dE' \int d\vec{\Omega}' \sum_{i,f} (\underline{x}, \vec{\Omega}' \rightarrow \vec{\Omega}, E' \rightarrow E) \Psi(\underline{x}, \vec{\Omega}', E')$$

iii) Other Sources

$$Q(\underline{x}, \vec{\Omega}, E)$$

Multi Group

Discrete Energies

$\Psi^{(k)}(x, \vec{\Omega})$ - Flux with energy $E^{(k)}$

$$\vec{\Omega} \cdot \nabla \Psi^k + \sigma_t \Psi^k = \sigma_s \int d\vec{\Omega}' \sum_s^k (x, \vec{\Omega}' \rightarrow \vec{\Omega}) \Psi^k(x, \vec{\Omega}') + Q$$

$$\sigma_a = \sigma_t - \sigma_s \quad \text{probability particle will}$$

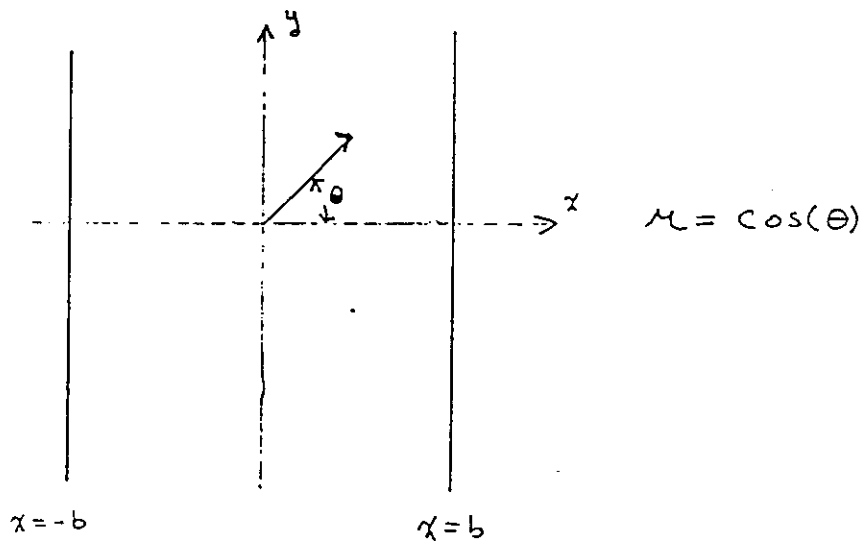
- be absorbed
- be scattered with energy other than $E^{(k)}$.

- Particles lost become source for other energy levels
- Without fission particles generally lose energy
- Sequentially solve for $E^{(k)}, E^{(k-1)}, \dots, E^{(1)}$

3-D Single Group

$$\vec{\Omega} \cdot \nabla \Psi + \sigma_t \Psi = \sigma_s \int d\vec{\Omega}' \Sigma_s(\vec{x}, \vec{\Omega}' \rightarrow \vec{\Omega}) \Psi(\vec{x}, \vec{\Omega}') + Q$$

Slab Geometry



Anisotropic

$$\mu \frac{\partial \Psi}{\partial x} + \sigma_t \Psi = \sigma_s \frac{1}{2} \int_{-1}^1 \Sigma_s(\vec{x}, \mu' \rightarrow \mu) \Psi(\vec{x}, \mu') d\mu' + Q$$

Isotropic

$$\mu \frac{\partial \Psi}{\partial x} + \sigma_t \Psi = \sigma_s \frac{1}{2} \int_{-1}^1 \Psi(\vec{x}, \mu') d\mu' + Q$$

Most Difficult

$$\sigma_s = \sigma_t$$

No Particles lost

$$\sigma_t b \gg 1$$

Slab optically dense

$$\frac{\mu}{\sigma_t} \frac{\partial \psi}{\partial x} + \psi = \frac{1}{2} \int_{-1}^1 \Sigma_s(x, \mu' \rightarrow \mu) \psi(x, \mu') d\mu' + \hat{Q}$$

$$-b \leq x \leq b \quad \psi(-b, \mu) = g_1(\mu) \quad \mu > 0$$

$$\psi(b, \mu) = g_2(\mu) \quad \mu < 0$$

Transformation: $x = bz$

$$\frac{\mu}{\sigma_t b} \frac{\partial \hat{\psi}}{\partial z} + \hat{\psi} = \frac{1}{2} \int_{-1}^1 \Sigma_s(z, \mu' \rightarrow \mu) \hat{\psi}(z, \mu') d\mu' + \hat{Q}$$

$$-1 \leq z \leq 1 \quad \hat{\psi}(-1, \mu) = g_1(\mu) \quad \mu > 0$$

$$\hat{\psi}(1, \mu) = g_2(\mu) \quad \mu < 0$$

Singularly Perturbed Problem

$$\hat{\psi} = \frac{1}{2} \int_{-1}^1 \Sigma'_s(z, \mu' \rightarrow \mu) \hat{\psi}(z, \mu') d\mu' + Q \quad (*)$$

Infinite Number of Solutions

Suppose

$$\xi(z, \mu) = \frac{1}{2} \int_{-1}^1 \Sigma'_s(z, \mu') \xi(z, \mu') d\mu'$$

Then for any $f(z)$

$$\underline{\xi(z, \mu) f(z)} = \frac{1}{2} \int_{-1}^1 \Sigma'_s(z, \mu') \underline{\xi(z, \mu') f(z)} d\mu'$$

and

$$\hat{\psi} + \xi(z, \mu) f(z)$$

satisfies (*).

- Lower frequency in space more nearly singular
- In many Applications the operator is nearly singular on all frequencies of interest

Motivation

- Many Important Applications depend upon efficient solution of Single Group Transport Model
- Single Group Problem is illconditioned in Optically Dense Media

Numerical Solution

- Problem Formulation
- Discrete Approximation
- Solution Algorithm
- Software Development

Discrete Approximation Angle

S_N Equations

$$\mu \frac{\partial \psi}{\partial x} + \sigma_s \psi = \sigma_s \frac{1}{2} \int_{-1}^1 \Sigma_s(x, \mu' \rightarrow \mu) \psi(x, \mu') d\mu' + Q$$

Let

$$K \cdot = \frac{1}{2} \int_{-1}^1 \Sigma_s(x, \mu' \rightarrow \mu) \cdot d\mu'$$

By construction

Eigenvectors of K are

Legendre Polynomials 1-D

Spherical Harmonics 2,3-D

S_N - Assume the variation in Angle of $\psi(x, \mu)$ can be expressed by the first N eigenvectors of K

1-D S_N Equations

Legendre Polynomials $\{P_\ell(\mu)\}_{\ell=0}^{N-1}$

Quadrature Points $\{\mu_1, \dots, \mu_N\}$

Weights $\{\omega_1, \dots, \omega_N\}$

Let

$$\Psi_m(x) = \Psi(x, \mu_m)$$

Moments:

$$\phi_\ell(x) = \frac{1}{2} \int_{-1}^1 \Psi(x, \mu) P_\ell(\mu) d\mu = \sum_{m=1}^N \Psi_m(x) P_\ell(\mu_m) \omega_m$$

By Assumption

$$\phi_\ell(x) = 0 \quad \ell \geq N$$

Inverse Transformation

$$\Psi_m(x) = \sum_{\ell=0}^{N-1} (2\ell+1) \phi_\ell(x) P_\ell(\mu_m)$$

1-D S_N Equations

$$\mu_m \frac{\partial}{\partial x} \Psi_m(\omega) + \sigma_t \Psi_m(x) = S_m(\omega) + Q_m \quad m=1, \dots, N$$

$$S_m = \sum_{\ell=0}^{N-1} (2\ell+1) \sigma_\ell \phi_\ell(\omega) \rho_\ell(\mu_m)$$

$$\phi_\ell(\omega) = \sum_{m=1}^N \Psi_m(x) \rho_\ell(\mu_m) \omega_m$$

Algebraically

$$\underline{\Psi}(x) = (\Psi_1(x), \dots, \Psi_N(x))^T$$

$$D \frac{\partial}{\partial x} \underline{\Psi} + \sigma_t \underline{\Psi} = \underline{T}^{-1} \underline{\Sigma} \underline{T} \underline{\Psi}(x) + \underline{Q}$$

$$D = \begin{pmatrix} \mu_1 & & \\ & \ddots & \\ & & \mu_N \end{pmatrix}$$

$$\underline{\Sigma} = \begin{pmatrix} \sigma_0 & & \\ & \ddots & \\ & & \sigma_{N-1} \end{pmatrix}$$

$$\sigma_t \geq \sigma_0$$

$$\left(\sigma_t = \sigma_0 \quad \text{Pure Scattering} \right)$$

1-D S_N Equations Isotropic

$$\sigma_a = 0 \quad \ell > 0$$

$$\sigma_0 = \sigma_t \quad \text{pure scattering}$$

$$\Sigma = \begin{pmatrix} \sigma_0 & & \\ & \ddots & \\ & & 0 \end{pmatrix}$$

$$T^{-1} \Sigma T = \sigma_0 \begin{pmatrix} | & & \\ \vdots & & \\ | & & \end{pmatrix} \begin{matrix} (\omega_1, \omega_2, \dots, \omega_N) \\ \vdots \\ \end{matrix}$$

$$= \sigma_0 \underline{\mathbf{1}} \underline{\omega}^T = R$$

$$D \frac{\partial^2}{\partial x^2} \underline{\psi} + \sigma_a \underline{\psi} = \sigma_a \underline{R} \underline{R} + Q$$

Solution Algorithm

- In Optically Dense Medium, Transport is Diffusive in Nature
- Diffusion Synthetic Acceleration (DSA)
 - Preconditions by Inverse of Diffusion Operator
 - Very successful for Isotropic Scattering
- Why Multigrid?
 - DSA Fails for Anisotropic Scattering and Inhomogeneous Material
 - Multigrid Excellent Technique for Diffusion-like Problems

Isotropic Scattering

- Multigrid in space

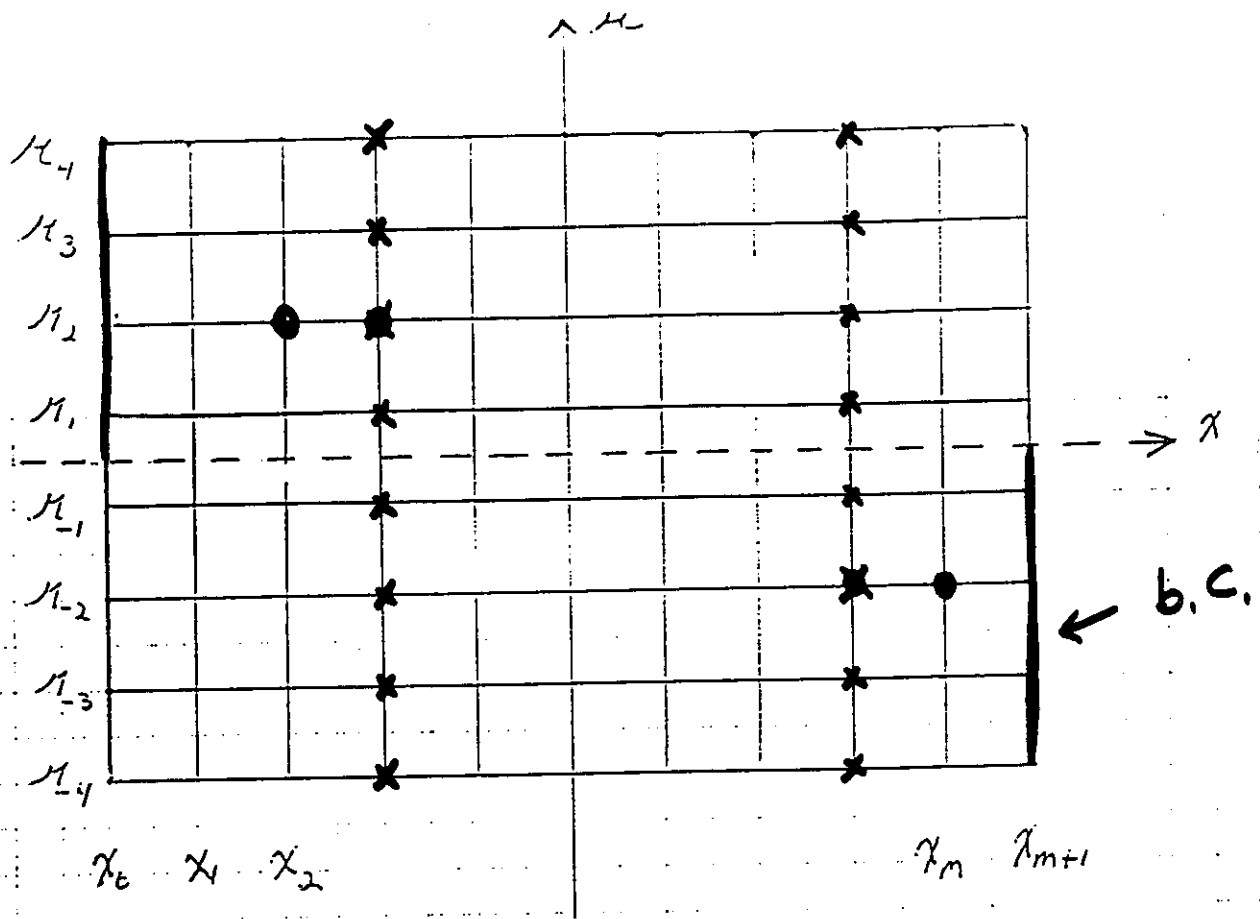
Anisotropic Scattering

- Multigrid in Angle
- S_2 Isotropic Problem on Coarse Grid

Multi Grid Depends upon

- Effective Smoothing
- Efficient Grid Transfer
- Inexpensive Solution on Coarsest Grid

Upwind Difference



$$\psi_{0,j} = g_{0j} \quad (j = 1, \dots, \frac{M}{2})$$

$$\epsilon \mu_j \frac{\psi_{ij} - \psi_{i-1,j}}{h} + \psi_{ij} = \sum_{k=-4}^4 w_k \psi_{ik} + g_{ij}$$

$$\epsilon \mu_j \frac{\psi_{i+1,j} - \psi_{ij}}{h} + \psi_{ij} = \sum_{k=-4}^4 w_k \psi_{ik} + g_{ij}$$

$$\psi_{m+1,j} = g_{2j} \quad (j = -1, \dots, -\frac{M}{2})$$

Write

$$\frac{\varepsilon}{h} D(\psi_{i,+} - \psi_{i-1,+}) + \psi_{i,+} = R(\psi_{i,+} + \psi_{i,-}) + \underline{e}_{i,+}$$

$$\frac{\varepsilon}{h} D(\psi_{i,-} - \psi_{i+1,-}) + \psi_{i,-} = R(\psi_{i,+} + \psi_{i,-}) + \underline{e}_{i,-}$$

where

$$\underline{\psi}_{i,+} = \begin{pmatrix} \psi_{i,1} \\ \vdots \\ \psi_{i,N} \end{pmatrix}$$

$$\underline{\psi}_{i,-} = \begin{pmatrix} \psi_{i,-1} \\ \vdots \\ \psi_{i,-N} \end{pmatrix}$$

$$D = \begin{pmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_N \end{pmatrix}$$

$$R = \underline{\underline{1}} \underline{\underline{\omega}}^T$$

$$\underline{\underline{1}} = (1, 1, \dots, 1)^T$$

$$\underline{\underline{\omega}} = (\omega_1, \omega_2, \dots, \omega_N)^T$$

$$(\underline{\underline{1}}^T \underline{\underline{\omega}} = \frac{1}{2})$$

x-line Relaxation (Transport Sweep)

$$\frac{\varepsilon}{h} D(\psi_{i,t}^{l+1} - \psi_{i-1,t}^{l+1}) + \psi_{i,t}^{l+1} = R(\psi_{i,t}^l + \psi_{i,-}^l) + \underline{g}_{i,t}$$

$$\frac{\varepsilon}{h} D(\psi_{i,-}^{l+1} - \psi_{i+1,-}^{l+1}) + \psi_{i,-}^{l+1} = R(\psi_{i,t}^l + \psi_{i,-}^l) + \underline{g}_{i,-}$$

For $\frac{\varepsilon}{h} \gg 1$ Effective Smoother

For $\frac{\varepsilon}{h} < 1$ Ineffective Smoother

For Some Problems

$$h = 10^{-3}$$

$$\varepsilon = 10^{-6}$$

$$\frac{\varepsilon}{h} = 10^{-3}$$

On Finest Grid!

n -line Relaxation

$$\frac{\epsilon}{h} D (\psi_{i,t}^{LH} - \psi_{i-1,t}^L) + \psi_{i,t}^{LH} = R (\psi_{i,t}^{LH} + \psi_{i,-}^{LH}) + \underline{b}_{i,t}$$

$$\frac{\epsilon}{h} D (\psi_{i,-}^{LH} - \psi_{i+1,-}^L) + \psi_{i,-}^{LH} = R (\psi_{i,t}^{LH} + \psi_{i,-}^{LH}) + \underline{b}_{i,-}$$

Rewrite as

$$\begin{bmatrix} I + \frac{\epsilon}{h} D - R & -R \\ -R & I + \frac{\epsilon}{h} D - R \end{bmatrix} \begin{pmatrix} \psi_{i,t}^{LH} \\ \psi_{i,-}^{LH} \end{pmatrix} = \begin{pmatrix} \frac{\epsilon}{h} D \psi_{i-1,t}^L + \underline{b}_{i,t} \\ \frac{\epsilon}{h} D \psi_{i+1,-}^L + \underline{b}_{i,-} \end{pmatrix}$$

• Blocks Easily Invertible

Diagonal plus Rank one

Sherman Morrison Formula

$$(\mathbf{I} - \underline{v} \underline{w}^T)^{-1} = (\mathbf{I} + \xi \underline{v} \underline{w}^T)$$

$$\xi = \frac{1}{1 - \underline{w}^T \underline{v}}$$

Multiply by: $(\mathbf{I} - \underline{v} \underline{w}^T)(\mathbf{I} + \xi \underline{v} \underline{w}^T) = \mathbf{I}$

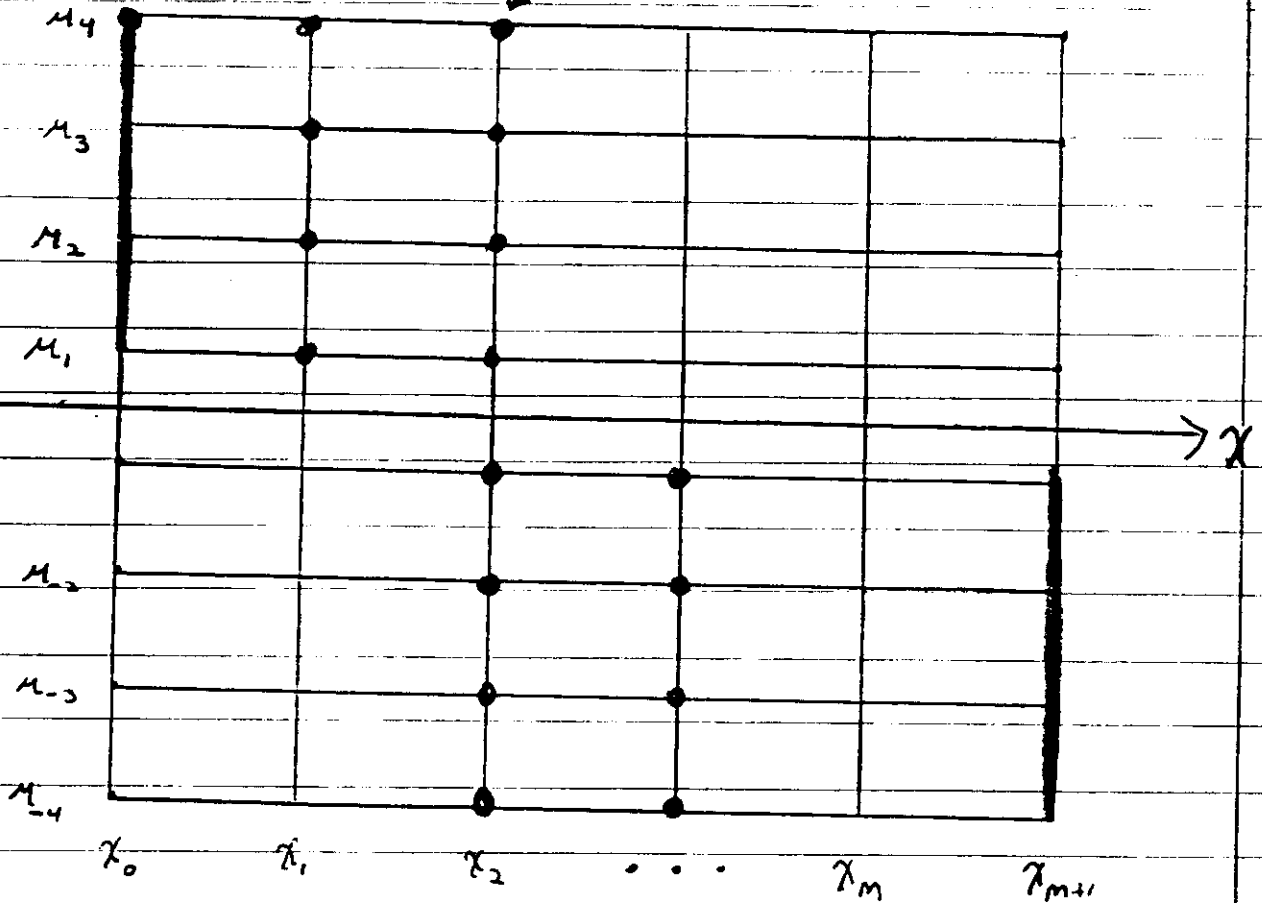
Solve for ξ .

General Formula

$$(\mathbf{A}_0 - \underline{v} \underline{w}^T)^{-1} = \mathbf{A}_0^{-1} + \xi \mathbf{A}_0^{-1} \underline{v} \underline{w}^T \mathbf{A}_0^{-1}$$

$$\xi = \frac{1}{1 - \underline{w}^T \mathbf{A}_0^{-1} \underline{v}}$$

Solve for



A-line Relaxation

Solve for \bullet $\psi(x_2, \mu_j)$

Using \bullet $\psi(x_3, \mu_j)$ $\mu_j < 0$
 $\psi(x_1, \mu_j)$ $\mu_j > 0$

Multi grid Algorithm

Linear Interpolation } upwind Diff.
Injection } on
Coarse Grid

Red/Black n -line Relaxation

Convergence Factor

2-Grid $r = O\left(\frac{\epsilon}{h}\right)$ (proof)

Multi grid (Numerical proof)

$V(1,0)$ cycle

$\frac{\epsilon}{h}$

r

.1

.136

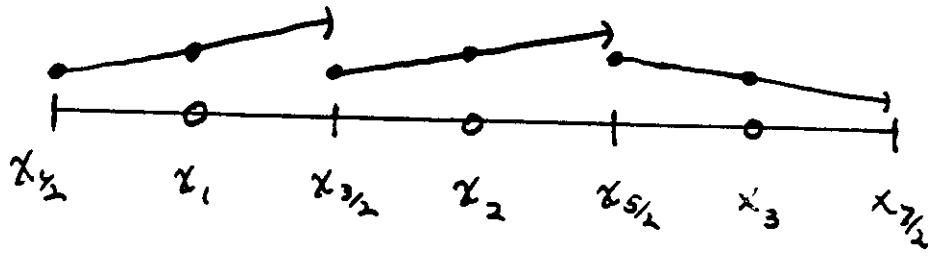
.01

.0136

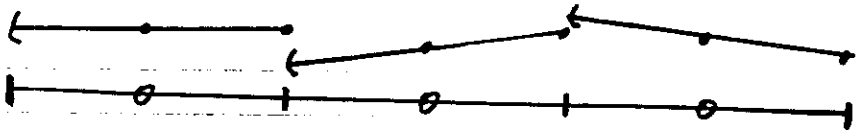
.001

.00140

Modified Linear Discontinuous Difference (MLD)



$\mu < 0$
←



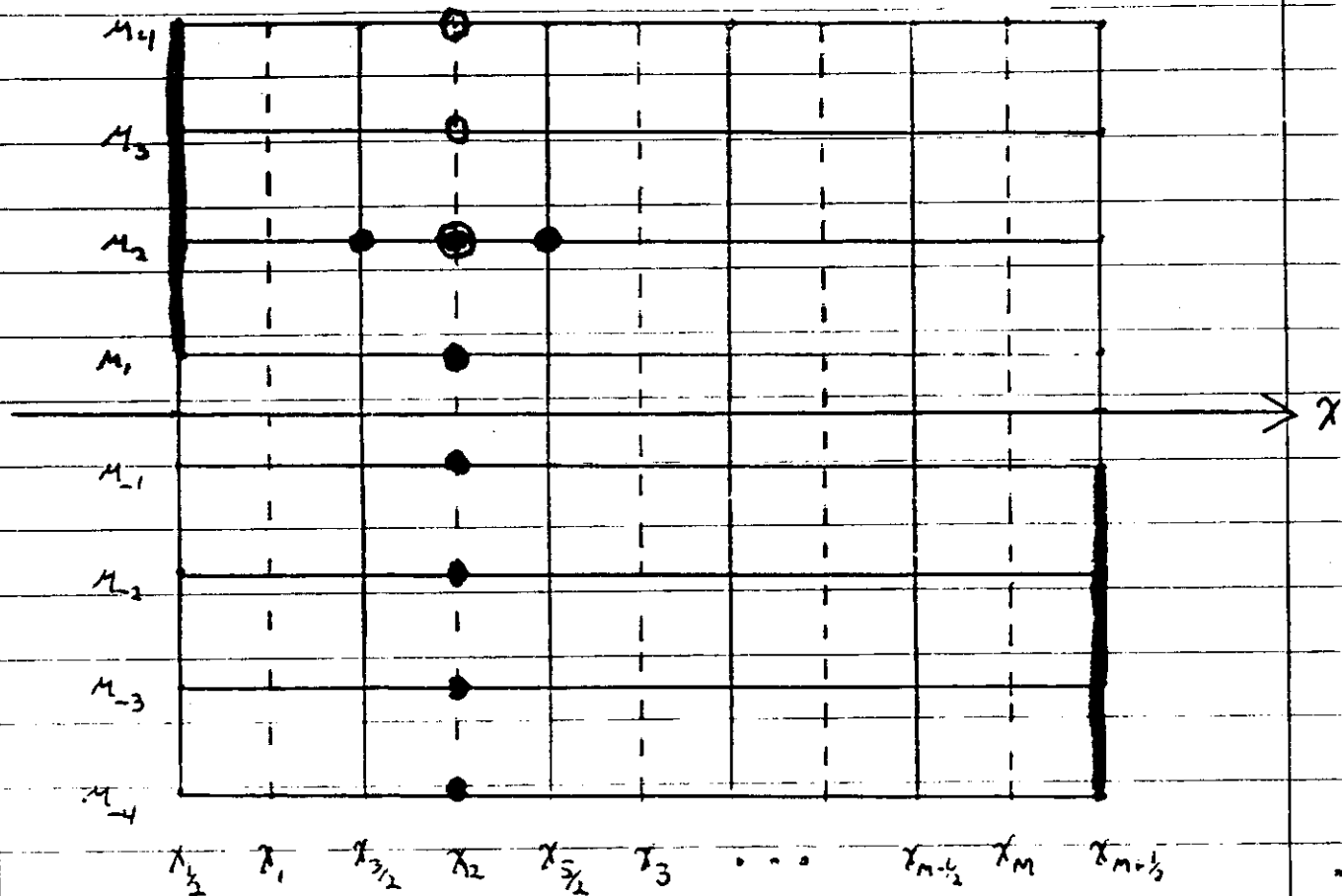
$\mu > 0$
→

	$I + \frac{2\varepsilon}{h}D$ $-R$	$-2R$	$-\frac{2\varepsilon}{h}D$	R	
$-\frac{\mu\varepsilon}{h}D$		$I - R$	$-R$		
		$-R$	$I - R$		$-\frac{\mu\varepsilon}{h}D$
	R	$-\frac{2\varepsilon}{h}D$	$-2R$	$I + \frac{2\varepsilon}{h}D$ $-R$	

$\psi_{1/2}^+$
 $\psi_{1/2}^-$
 ψ_1^+
 ψ_1^-
 $\psi_{3/2}^+$
 $\psi_{3/2}^-$

$$A \Psi = Q$$

Cell Center Equations



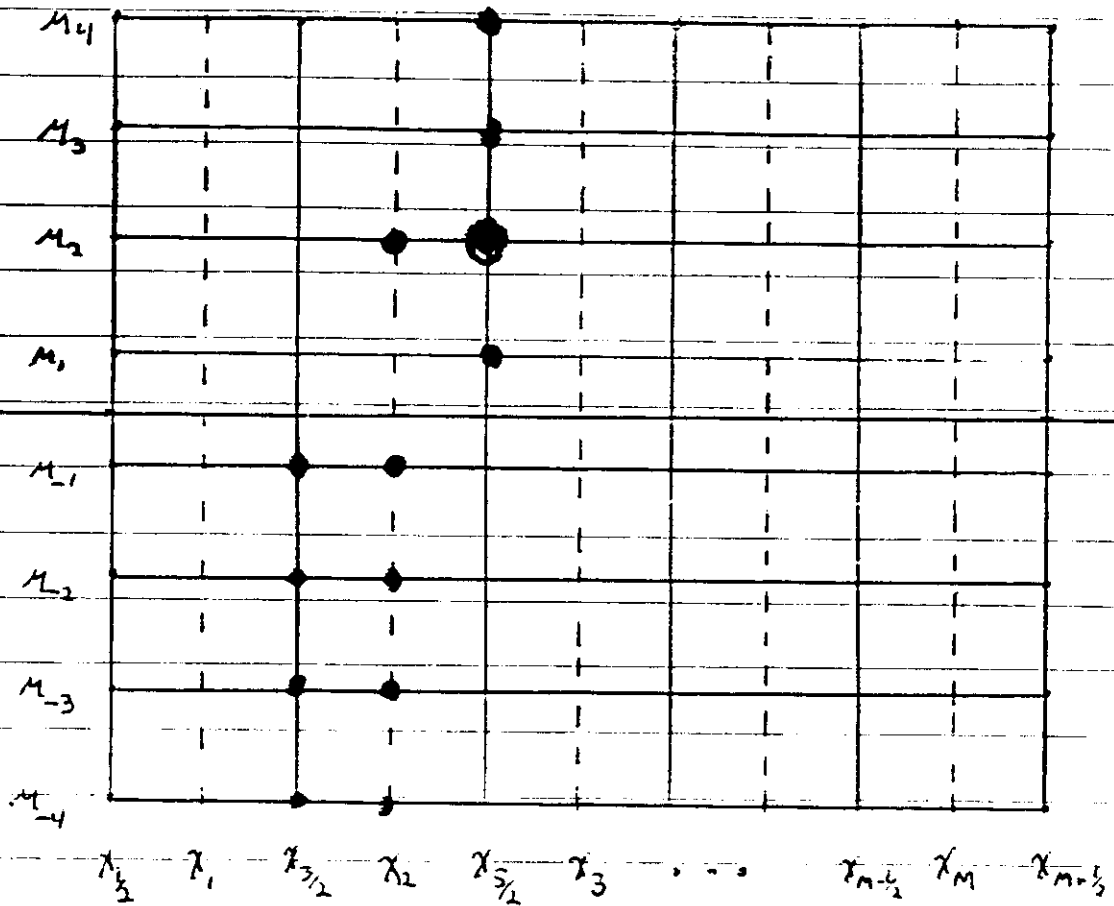
$\mu_j > 0$

$$|\mu_j| \varepsilon \frac{\psi_{i+\frac{1}{2},j} - \psi_{i-\frac{1}{2},j}}{h} + \psi_{i,j} = \sum_k w_k \psi_{ik} + \mathcal{G}_{ij}$$

$\mu_j < 0$

$$-|\mu_j| \varepsilon \frac{\psi_{i+\frac{1}{2},j} - \psi_{i-\frac{1}{2},j}}{h} + \psi_{i,j} = \sum_k w_k \psi_{ik} + \mathcal{G}_{ij}$$

Cell Edge Equations



$$\mu_j > 0$$

$$\mu_j \varepsilon \frac{\psi_{i+1/2, j} - \psi_{i, j}}{h/2} + \psi_{i+1/2, j} = \sum_{k>0} w_k \psi_{i+1/2, k}$$

$$+ \sum_{k<0} w_k (2\psi_{i, k} - \psi_{i-1/2, k}) + q_{i, j}$$

Why Modified Linear Discontinuous

More Accurate

Upwind $O(h)$

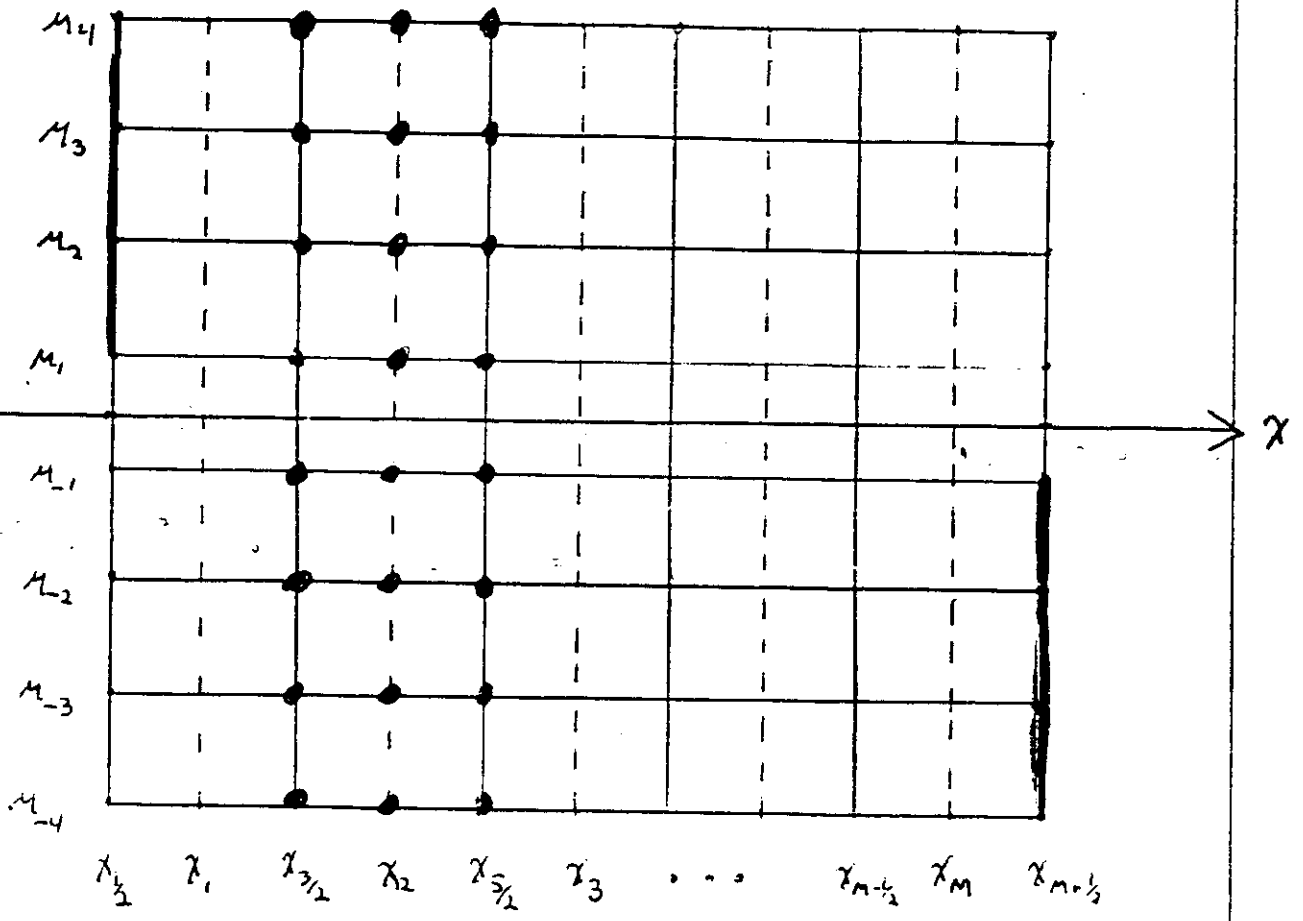
MLD $O(h^2)$

Diffusion Limit

MLD reproduces diffusion as $\frac{\epsilon}{h} \rightarrow 0$

Upwind does not

Block Equations



Given values at \bullet $\left(\begin{array}{l} \psi(x_{3/2}, M_j) \quad M_j = 0 \\ \psi(x_2, M_j) \quad M_j = 20 \end{array} \right)$

Solve simultaneously for values at \bullet

27-141 50 SHEETS
22-142 100 SHEETS
22-144 200 SHEETS

Modified Linear Discontinuous

Red/Black μ -line Relaxation

$$A_0 + R_0$$

R_0 rank 2

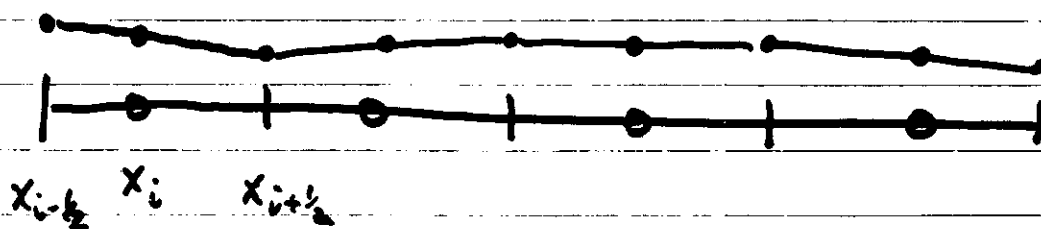
A_0^{-1} Easy

$$(A_0 + R_0)^{-1} = (A_0^{-1} + \sum A_0^{-1} R_0 A_0^{-1})$$

- Effective smoother for all values of $\frac{\epsilon}{h}$
- For $\frac{\epsilon}{h} \ll 1$ error becomes

Piecewise linear across cells

Independent of angle (μ)



$$e_i = \frac{e_{i-1/2} + e_{i+1/2}}{2} + O\left(\frac{\epsilon}{h}\right)$$

Coarse Grid Operator

For $\frac{\epsilon}{h} > 1$ use MLD

For $\frac{\epsilon}{h} < 1$ use Upwind

Grid

Operator

h

$\frac{\epsilon}{h}$

MLD

$2h$

$\frac{\epsilon}{2h}$

MLD

$4h$

$\frac{\epsilon}{4h}$

MLD

\vdots

$2^{p-1}h$

$\frac{\epsilon}{2^{p-1}h}$

MLD

$2^p h$

$\frac{\epsilon}{2^p h} < .1$

↓
UW

↓
UW

Switch

• If $\frac{\epsilon}{h} < .1$ on Finest Grid then

Switch to Upwind on first

Coarse Grid

Convergence Rates

$V(1,0)$ cycle

$\frac{E}{h}$ (Finest Grid)

r

40

.95

10

.97

2.6

.110

1.3

.116

.66

.114

.32

.097

.16

.096

.04

.045

.01

.069

.001

.077

.0001

.078

.00002

.080

Anisotropic Scattering

Multi Grid in Space (Jim Morel)

- S_N Equations
- LD Differencing
- 2 Block μ -line Relaxation
- Element interpolation/restriction

V-cycle rate .4 - .6

- independent of ϵ/h
- large material discontinuities

Problem

Expensive Inversion of Full Blocks

$$S_{16} \quad N = 16$$

Block 64 90,000 operations

MultiGrid IN Angle

S_N Equations

$$D \frac{\partial \underline{\psi}}{\partial x} + \sigma_t \underline{\psi} = T^{-1} \Sigma T \underline{\psi} + \underline{q}$$

$$D = \begin{pmatrix} \mu_1 & & \\ & \ddots & \\ & & \mu_n \end{pmatrix} \quad \Sigma = \begin{pmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_{n-1} \end{pmatrix} \quad \sigma_t \geq \sigma_0$$

Shifted x-line Sweep (Transport)

$$D \frac{\partial \underline{\psi}^{k+1}}{\partial x} + (\sigma_t - \alpha) \underline{\psi}^{k+1} = T^{-1} (\Sigma - \alpha I) T \underline{\psi}^k + \underline{q}$$

- Solve Transport Equation
- Stable for $(\sigma_t - \alpha) > 0$

Residual

$$r^{k+1} = T^{-1} (\Sigma - \alpha I) T (\underline{\psi}^{k+1} - \underline{\psi}^k)$$

Multi Grid in Angle

Moment Representation

$$\underline{r}^{k+1} = (\underline{\Sigma}^{-1} - \alpha \underline{I})(\underline{\phi}^{k+1} - \underline{\phi}^k)$$

Choose

$$\alpha = \frac{\sigma_{\frac{N+1}{2}} + \sigma_{N-1}}{2}$$

Smoothing Rate ($\sigma_+ = \sigma_0$)

$$\rho = \frac{\sigma_{\frac{N+1}{2}} - \sigma_{N-1}}{2\sigma_0 - (\sigma_{\frac{N+1}{2}} + \sigma_{N-1})}$$

On moments $\frac{N+1}{2} \dots N-1$

Multi Grid IN Angle

Coarse Grid Equations (Moment)

Interpolation $P = \begin{bmatrix} I_{N/2} \\ 0 \end{bmatrix}$

Restriction $Q = [I_{N/2}, 0]$

$$\underbrace{(QMP)}_{\tilde{M}} \frac{\partial}{\partial x} \phi + G_t I_{N/2} \phi = \underbrace{Q \Sigma P}_{\tilde{\Sigma}} \phi + P \tilde{f}$$

Moment equations associated
with a $S_{N/2}$ problem with
 $P \tilde{f}$ as a source term

Multi Grid In Angle

Coarse Grid Operator Flux Rep.

Quadrature points $\{\tilde{\mu}_1, \dots, \tilde{\mu}_{N/2}\}$
weights $\{\tilde{\omega}_1, \dots, \tilde{\omega}_{N/2}\}$

$$\tilde{\Psi}_m(x) = \sum_{l=0}^{N/2-1} (2l+1) \phi_l(x) P_l(\tilde{\mu}_m)$$

$$\phi_l(x) = \sum_{m=1}^{N/2} \tilde{\Psi}_m(x) P_l(\tilde{\mu}_m) \tilde{\omega}_m$$

$$\tilde{D} \frac{\partial \tilde{\Psi}}{\partial x} + \sigma_t \tilde{\Psi} = \tilde{T}^{-1} \tilde{\Sigma} \tilde{T} \tilde{\Psi} + \tilde{T}^{-1} P \tilde{\Gamma}$$

No simple relation between

Ψ and $\tilde{\Psi}$

Multi Grid in Angle

$$S_N \rightarrow S_{N/2} \rightarrow \rightarrow S_2$$

S_2 Moment Representation

$$\begin{pmatrix} 0 & 1 \\ \frac{1}{3} & 0 \end{pmatrix} \begin{pmatrix} \frac{\partial}{\partial x} \phi_0 \\ \frac{\partial}{\partial x} \phi_1 \end{pmatrix} + (\sigma_z - \alpha) \begin{pmatrix} \phi_0 \\ \phi_1 \end{pmatrix} = \begin{pmatrix} \sigma_0 - \alpha & 0 \\ 0 & \sigma_1 - \alpha \end{pmatrix} \begin{pmatrix} \phi_0 \\ \phi_1 \end{pmatrix} + \begin{pmatrix} \sigma_2 \\ \sigma_1 \end{pmatrix}$$

Choose $\alpha = \sigma_1$

Isotropic S_2 Equation

Multi Grid in Angle

Fokker Planck Scattering

Smoothing Rate ≤ 0.6

Coarsest Grid Isotropic S_2

