# Implicit Spatial Discretization for Advection-Diffusion-Reaction Equation

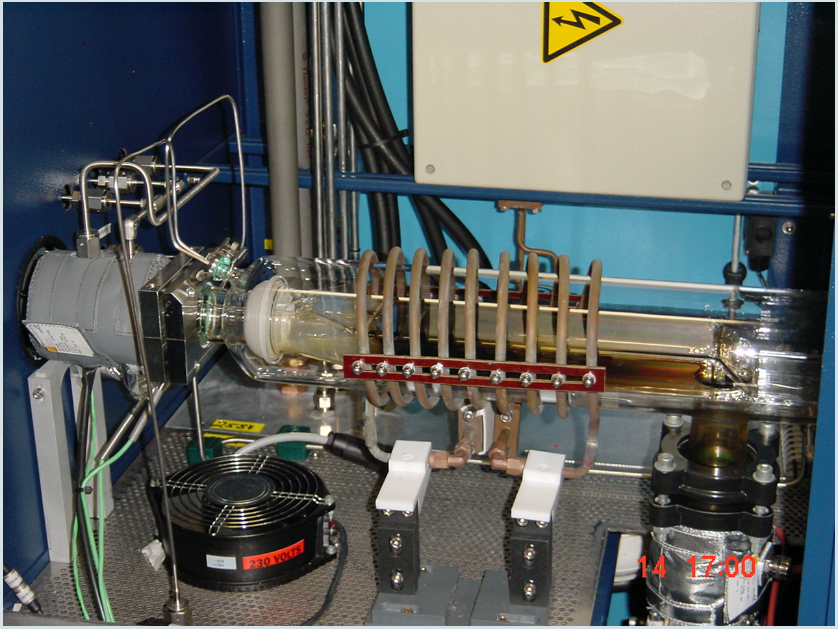
Kundan Kumar

10-Dec-2008

# Introduction

## Applications of Advection-Diffusion Reaction Equations

### Chemical Vapor Deposition



# Introduction

Setting:

- Advection-Diffusion-Reaction Equation
- $$\phi_t + u\phi_x = \epsilon\phi_{xx} + s(x,t),$$
- Advection Velocity : u
- Diffusion Coefficient : $\epsilon$
- Source term : $s(x,t)$

$$s(x,t) = b^2\epsilon\cos(b(x-ut)).$$

# Introduction

Setting:

- Exact Solution:

$$\phi = \cos(b(x - ut)) + \exp(-a^2 \epsilon t) \cos(a(x - ut)).$$

- Dirichlet Boundary Conditions.
- Initial Condition, $\phi(x, t)$ at $t = 0$.

# Contents

# 1. Discretization

$$\phi_t + u\phi_x = \epsilon\phi_{xx} + s(x,t)$$

Discretization:

$$\begin{aligned}\sum_{k=-1}^{1}\beta_k w'_{j+k}(t) &= h^{-2}\sum_{k=-1}^{1}\alpha_k w_{j+k}(t)\\ &+ \sum_{k=-1}^{1}\beta_k g_{j+k}(t)\end{aligned}$$

$$w_j(t) \approx \phi(x_j,t); \quad g_j(t) = s(x_j,t); \quad \sum_{k=-1}^{1}\beta_k = 1.$$

# Discretization

Vector Notation:

$$\begin{aligned} Bw'(t) &= Aw(t) + Bg(t), \\ A &= (a_{ij}) = (h^{-2}\alpha_{j-i}) \\ B &= (b_{ij}) = (\beta_{j-i}). \end{aligned}$$

Define:

$$\xi_k = (-1)^k \alpha_{-1} + \alpha_1, \quad \eta_k = (-1)^k \beta_{-1} + \beta_1.$$

## 1.1. Order Condition

Let $\phi_h$ be the restriction of the exact solution $\phi$ to the grid.
Spatial truncation error:

$$\sigma_h(t) = B\phi_h'(t) - A\phi_h(t) - Bg(t).$$

Truncation error in a point $(x_j, t)$ equals:

$$\sigma_{h,j}(t) = h^{-2}(C_0\phi + hC_1\phi_x + h^2C_2\phi_{xx} + h^3C_3\phi_{xxx} + \ldots)|_{(x_j,t)}$$

**Order Condition**: The discretization has order $q$ if:

$$\sigma_h = O(h^q),$$

translates to:

$$C_k = O(h^{q+2-k}), \quad k = 0, 1, \cdots, q+2.$$

## Order Condition

Error coefficients:

$$C_0 = -\xi_0, \quad C_1 = -\xi_1 - uh\eta_0,$$

$$C_k = \frac{-1}{k!}(\xi_k + kuh\eta_{k-1} - k(k-1)\epsilon\eta_{k-2}); \quad k \geq 2.$$

where,

$$\xi_k = (-1)^k \alpha_{-1} + \alpha_1, \quad \eta_k = (-1)^k \beta_{-1} + \beta_1.$$

Use the order condition to determine $\alpha_j$ and $\beta_j$.

# 2. Examples

**Explicit Central Difference**

$$w_j' = \frac{u}{2h}(w_{j-1} - w_{j+1}) + \frac{\epsilon}{h^2}(w_{j-1} - 2w_j + w_{j+1}) + g_j,$$

**Implicit Central Difference**

$$\begin{aligned}\frac{1}{6}(w_{j-1}' + 4w_j' + w_{j+1}') &= \frac{u}{2h}(w_{j-1} - w_{j+1}) \\ &+ \frac{\epsilon}{h^2}(w_{j-1} - 2w_j + w_{j+1}) + \frac{1}{6}(g_{j-1} + 4g_j + g_{j+1})\end{aligned}$$

# Examples

Define:

$$\mu = uh/\epsilon \qquad \text{(Peclet Number)}.$$

**Explicit Adaptive Upwinding**

$$w_j' = \frac{u}{2h}(w_{j-1} - w_{j+1}) + \frac{\epsilon + 0.5uh\kappa}{h^2}(w_{j-1} - 2w_j + w_{j+1}) + g_j,$$

Where $\kappa$ is defined as:

$$\kappa = \max(0, 1 - 2/\mu).$$

# Examples

**Implicit Adaptive Upwinding**

$$
\begin{aligned}
\frac{1}{2}\kappa w'_{j-1} + (1-\frac{1}{2}\kappa)w'_j &= \frac{u}{2h}(w_{j-1}-w_{j+1}) \\
&+ \frac{\epsilon + 0.5uh\kappa}{h^2}(w_{j-1}-2w_j+w_{j+1}) \\
&+ \frac{1}{2}\kappa g_{j-1} + (1-\frac{1}{2}\kappa)g_j .
\end{aligned}
$$

# Examples

Peclet Number $\mu$:

$$\mu = uh/\epsilon.$$

**Explicit Exponential Fitting**

$$w_j' = \sum_{k=-1}^{1} \alpha_k w_{j+k} + g_j,$$

$$\alpha_{-1} = uh\frac{\exp(\mu)}{\exp(\mu)-1}, \alpha_1 = uh\frac{1}{\exp(\mu)-1}, \alpha_0 = -(\alpha_1 + \alpha_{-1}).$$

## Implicit Exponential Fitting

$$\beta_{-1} w'_{j-1} + \beta_0 w'_j + \beta_1 w'_{j+1} = \sum_{k=-1}^{1} \alpha_k w_{j+k} + \beta_{-1} g_{j-1} + \beta_0 g_j + \beta_1 g_{j+1}.$$

where

$$\beta_{-1} = \frac{1}{2}\left(\frac{\exp(\mu)}{\exp(\mu)-1} - \frac{1}{\mu}\right),$$

$$\beta_0 = \frac{1}{2},$$

$$\beta_1 = \frac{1}{2}\left(\frac{1}{\mu} - \frac{1}{\exp(\mu)-1}\right).$$

# Examples

Compact Schemes:

$$
\begin{aligned}
\alpha_{-1} &= \epsilon + \frac{1}{2}uh - uh(\beta_1 - \beta_{-1}), \\
\alpha_1 &= \epsilon - \frac{1}{2}uh - uh(\beta_1 - \beta_{-1}), \\
\alpha_0 &= -(\alpha_{-1} + \alpha_1), \\
\beta_{-1} &= \frac{1}{\gamma}(6 + 3\mu - \mu^2), \\
\beta_0 &= \frac{1}{\gamma}(60 - 4\mu^2), \\
\beta_1 &= \frac{1}{\gamma}(6 - 3\mu - \mu^2)
\end{aligned}
$$

and $\gamma$ is a scaling factor given by:

$$\gamma = 72 - 6\mu^2.$$

# 3. Stability

Requirement:

$$||\exp(tB^{-1}A)|| \leq C, \quad \text{for all} \ \ t > 0.$$

We can write:

$$A = V\,\text{diag}(a_k)V^{-1}, \quad B = V\,\text{diag}(b_k)V^{-1},$$

with $a_k, b_k$ eigenvalues of $A$, $B$ respectively. Define global error $e(t)$:

$$e(t) = \phi_h(t) - w(t), \quad \hat{e}(t) = V^{-1}e(t)$$

Discretization error $\sigma_h(t)$:

$$\sigma_h(t) = B\phi_h'(t) - A\phi_h(t) - Bg(t), \quad \hat{\sigma}_h(t) = V^{-1}\sigma_h(t).$$

# Stability

The error equation then reads:

$$b_k \frac{d}{dt}\hat{e}(t) = a_k \hat{e}(t) + \hat{\sigma}_h(t).$$

Stability if:

$$Re(a_k/b_k) \leq 0 \quad \text{and} \quad |a_k| + |b_k| > 0.$$

**Result**: For the three point scheme considered with $C_0 = C_1 = 0, C_2 = O(h)$, and assume that:

$$h^{-2}|\alpha_0| + |\beta_0 - \frac{1}{2}| > 0,$$

then the stability condition holds iff:

$$2ah(\beta_1 - \beta_{-1}) \geq \alpha_0, \quad \text{and} \quad \alpha_0(1 - 2\beta_0) \geq 0.$$

# 4. Time Integration Aspect

Ode system:

$$Bw'(t) = Aw + Bg(t).$$

Define:

$$F(t, w) = Aw(t) + Bg(t).$$

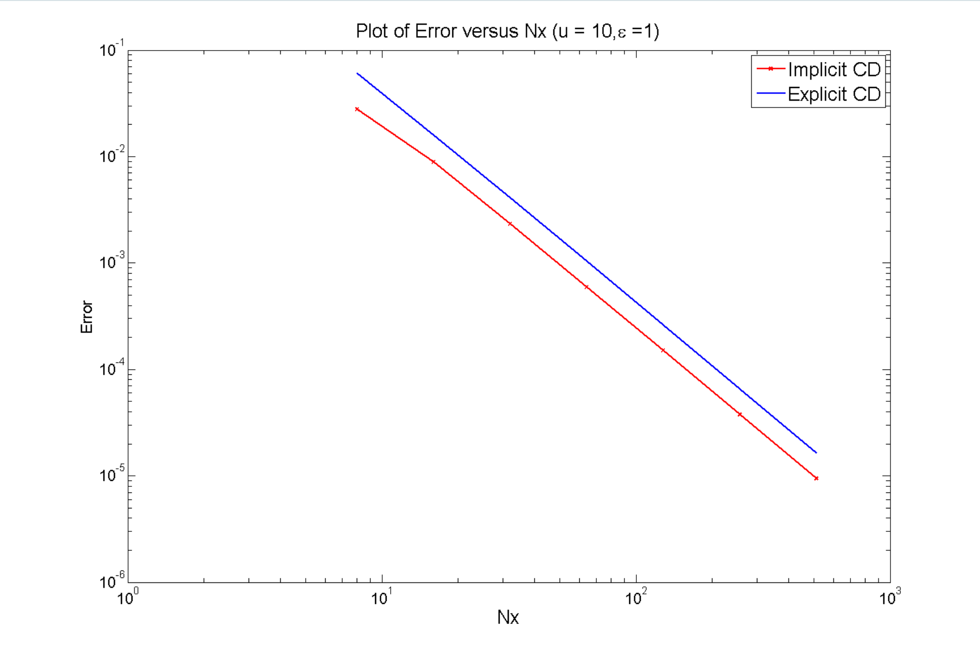
- We use the $\theta$ method (with $\theta = 0.5$:

$$Bw_{n+1} = Bw_n + 0.5\tau F(t_n, w_n) + 0.5\tau F(t_{n+1}, w_{n+1}).$$

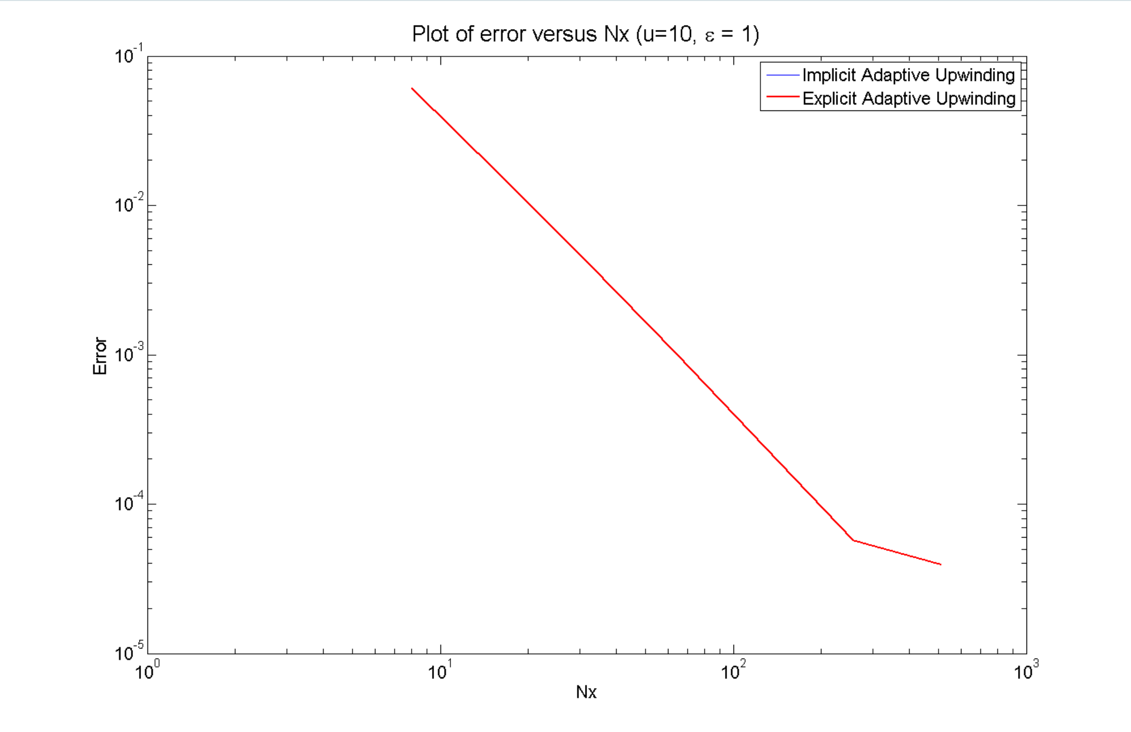
- With Explicit method, there is some amount of 'implicitness'!.
- Stability conditions in general become more stringent in case of implicit discretization method.
- For an implicit A-stable ODE method for time stepping, little difference between the two methods.

# 5. Numerical Computations

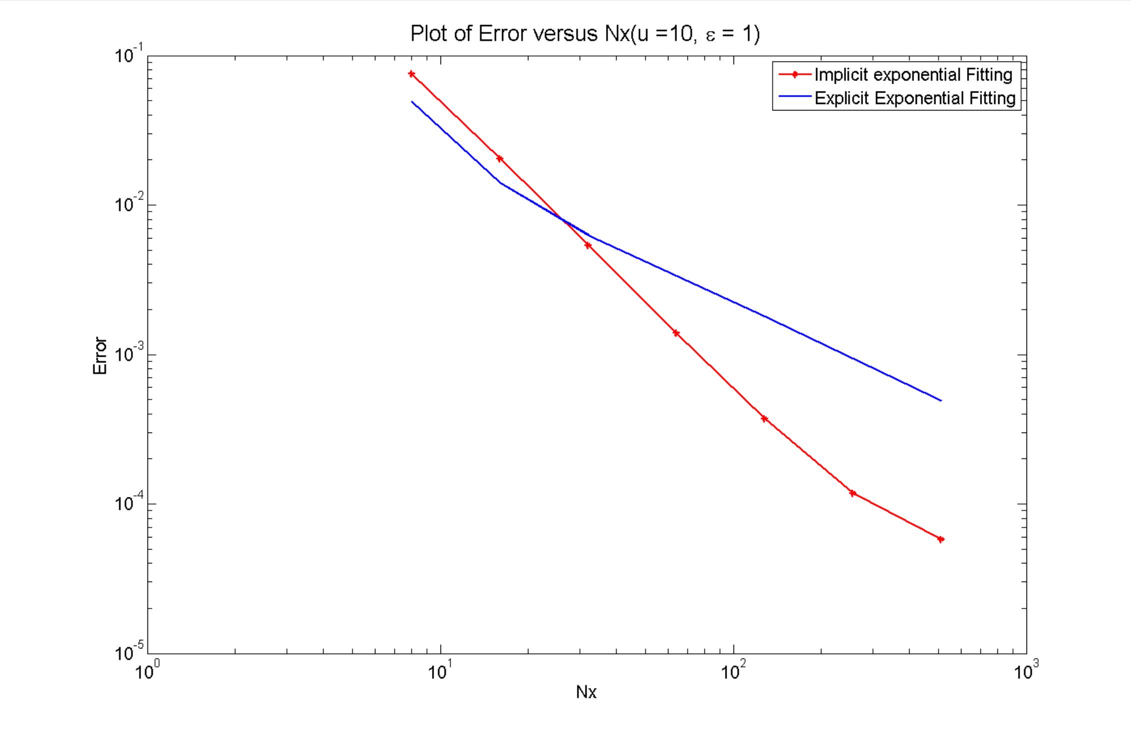
## Error for Implicit vs Explicit Central Difference



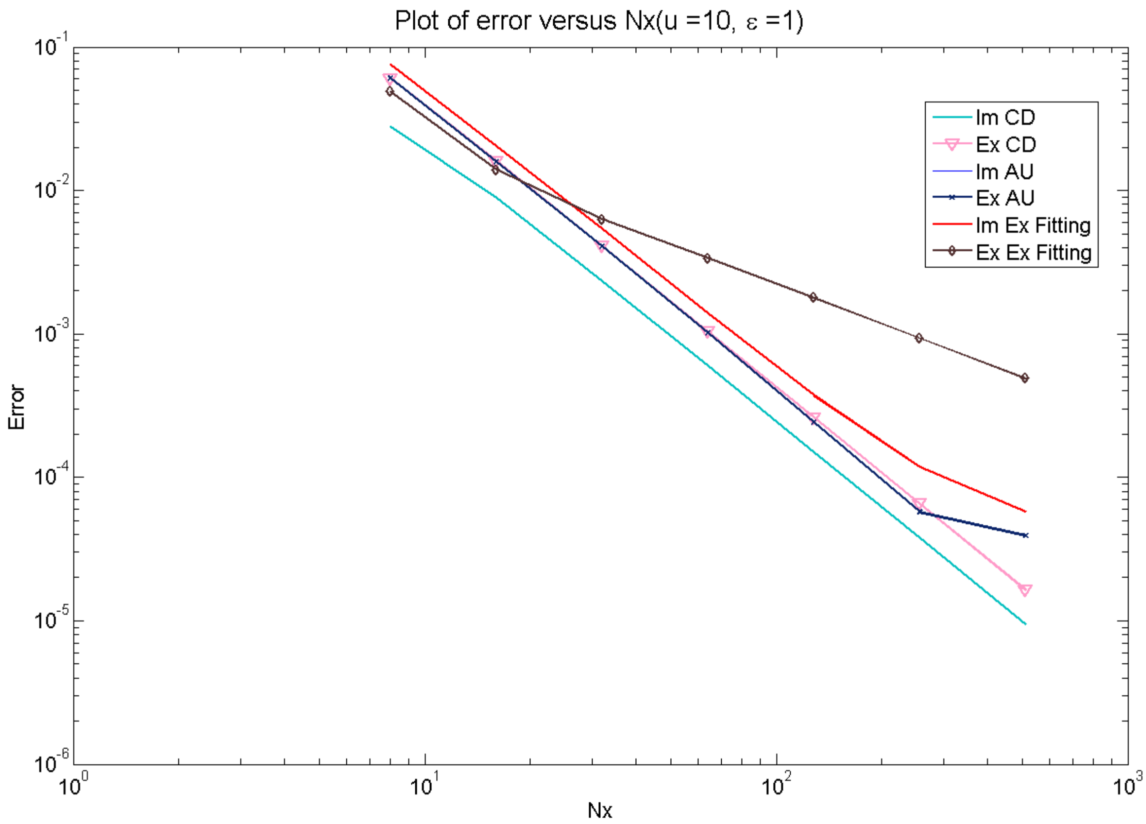
# Implicit vs Explicit Adaptive Upwinding



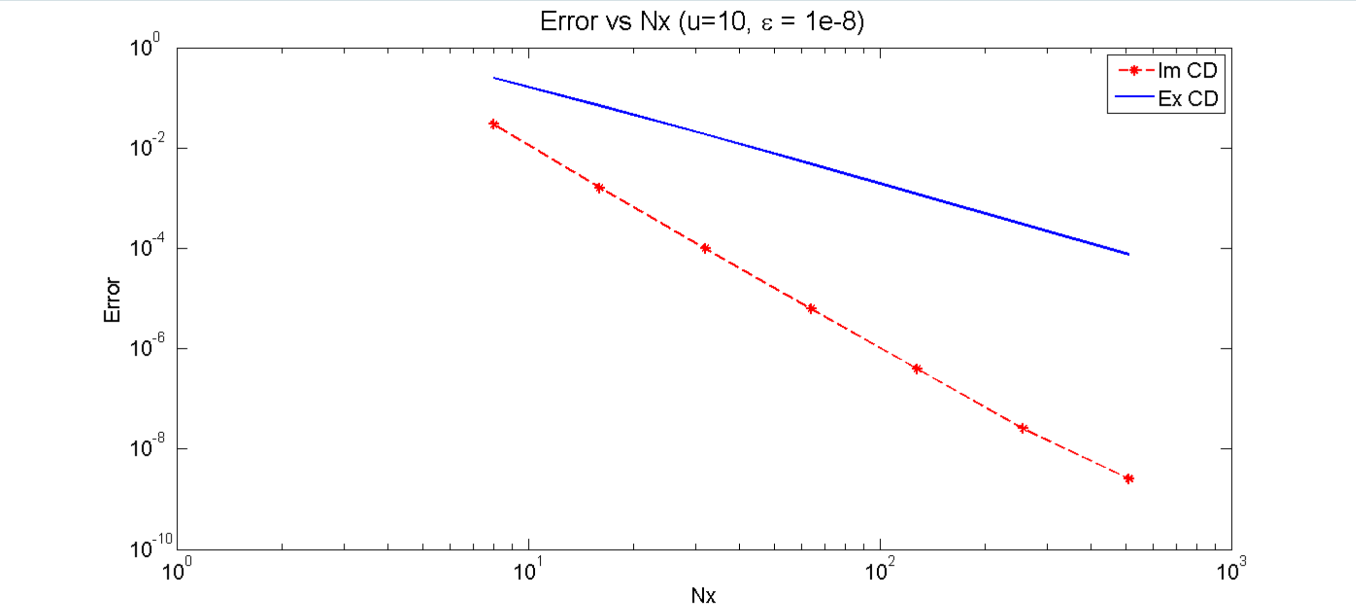
# Implicit vs Explicit Exponential Fitting



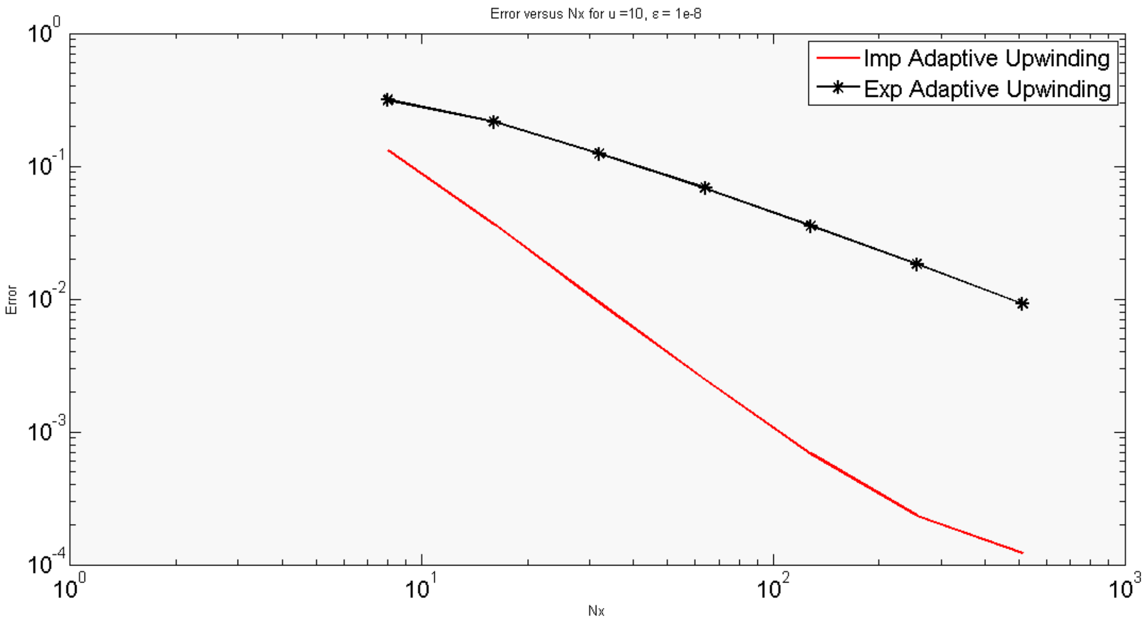
# Implicit vs Explicit



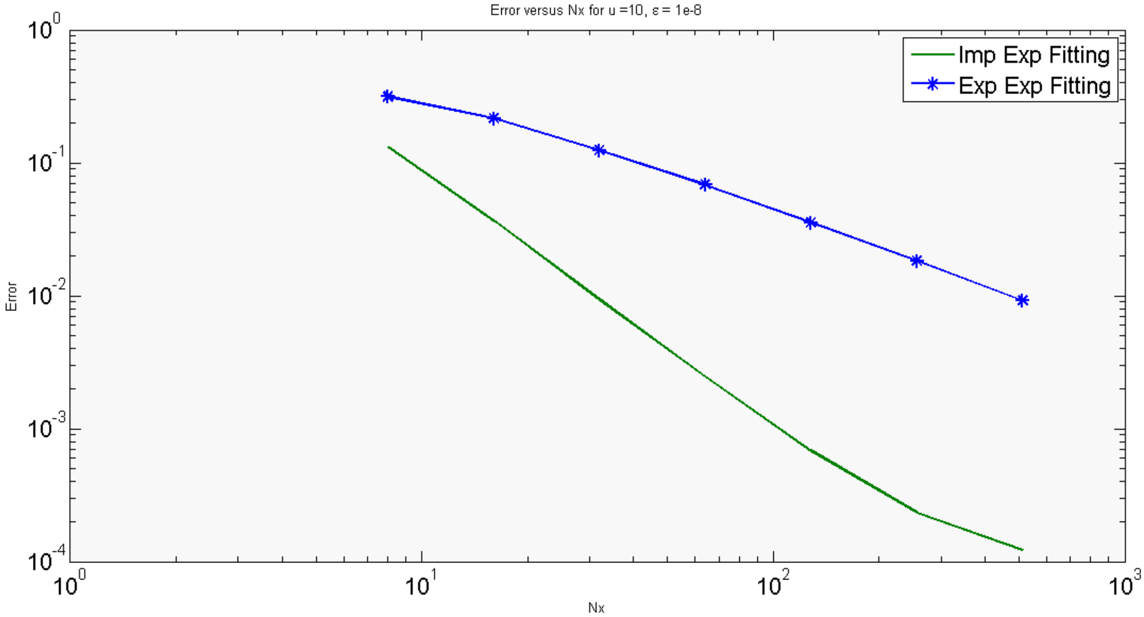
# Implicit vs Explicit Central Difference



# Implicit vs Explicit Adaptive Upwinding



# Implicit vs Explicit Exponential Fitting



# 6. Conclusion

When do we use Implicit Spatial Discretization?

- To achieve higher order without using wider stencils.
- To reduce the artificial oscillations in the numerical solution.
- Provides extra degrees of freedom for the numerical scheme.

Disadvantages

- Positivity may be lost.
- Stringent conditions for explicit time integration methods.