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Numerical Solutions of Partial Differential Equations and Introductory Finite Difference and Finite Element Methods

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Outline

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Need for Numerical Methods for PDE's

- Most of the PDEs are non-linear
- Most of them do not have analytical solutions
- Difficult to find analytical solution in most cases due to its complexity
- Even if the analytical solution can be found, computing it takes more time than that needed for numerical solution
- Computers are able to solve only discrete problems

Discretization Methods

- Finite Difference Method (FDM)
- Finite Element Method (FEM)
- Finite Volume Method (FVM)
- Spectral Method
- Lattice Gas Cellular Automata (LGCA)

Classification of PDEs

First order PDEs - Hyperbolic

$$\mathbf{Au_{xx} + Bu_{xy} + Cu_{yy} + Du_x + Eu_y + Fu = G(x,y)}$$

Second order PDEs are classified as

- Hyperbolic $B^2 - 4*A*C > 0$
- Parabolic $B^2 - 4*A*C = 0$
- Elliptical $B^2 - 4*A*C < 0$

- Classification useful
  - To identify solution methods applicable for the particular equation type

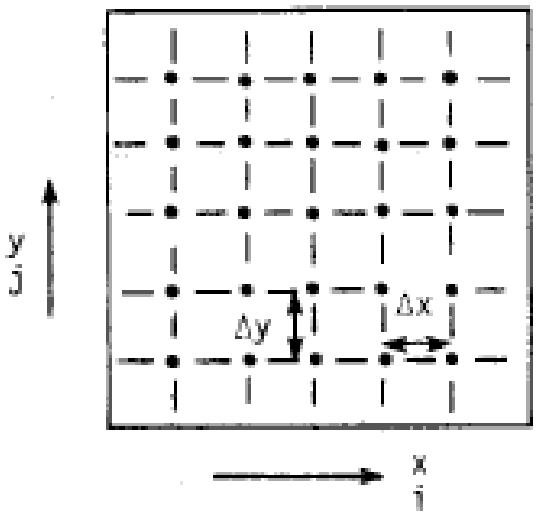
Classification of PDEs

- PDEs – Linear, Non-linear, Quasi-linear, Semi-linear, Homogenous, Non-homogenous
- Well-posed PDE
- Equilibrium and marching problems

Finite Difference Approximations

- Derivatives in a PDE is replaced by finite difference approximations
- Results in large algebraic system of equations instead of differential equation.
- Replace continuous problem domain by finite difference mesh or grid
- u(x,y) replaced by $u(i\Delta x, j\Delta y)$
- $u_{i,j}$ = u(x,y) $u_{i+1,j+1}$ = u(x+h,y+k)
- Methods of obtaining Finite Difference Equations – Taylor Series Expansion, Polynomial Fitting, Integral Method, Control Volume Approach

Finite Difference Approximations



Taylor Expansion of $u(x_0 + x, y_0)$ about $u(x_0, y_0)$

$$u(x_0+x, y_0) = u(x_0, y_0) + \frac{\partial u}{\partial x}\Delta x + \frac{\partial^2 u}{\partial x^2}\frac{(\Delta x)^2}{2!} + .. + \frac{\partial^n u}{\partial x^n}\frac{(\Delta x)^n}{n!}$$

Taylor Expansion of $u(x_0 - x, y_0)$ about $u(x_0, y_0)$

$$u(x_0 - x, y_0) = u(x_0, y_0) - \frac{\partial u}{\partial x}\Delta x + \frac{\partial^2 u}{\partial x^2}\frac{(\Delta x)^2}{2!} - .. + (-1)^n\frac{\partial^n u}{\partial x^n}\frac{(\Delta x)^n}{n!}$$

Finite Difference Approximations

$$\left(\frac{\partial u}{\partial x}\right)_{x_o,y_o} = \frac{u(x_0 + x\ , y_0) - u(x_0, y_0)}{\Delta x} - \left(\frac{\partial^2 u}{\partial x^2}\right)_{x_o,y_o} \frac{\Delta x}{2!} - \ldots$$

$$\left(\frac{\partial u}{\partial x}\right)_{i,j} = \frac{u_{i+1,j} - u_{i,j}}{\Delta x} + O(\Delta x)$$

forward difference

$$\left(\frac{\partial u}{\partial x}\right)_{i,j} = \frac{u_{i,j} - u_{i-1,j}}{\Delta x} + O(\Delta x)$$

backward difference

$$\left(\frac{\partial u}{\partial x}\right)_{i,j} = \frac{u_{i+1,j} - u_{i-1,j}}{2\Delta x} + O(\Delta x)^2$$

central difference

$$\left(\frac{\partial^2 u}{\partial x^2}\right)_{i,j} = \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{(\Delta x)^2} + O(\Delta x)^2$$

second order difference

Boundary Conditions

- **Dirichlet BC** : The value of the function is specified

$$f \text{ is specified on the boundary}$$

- **Neumann BC** : The value of the derivative normal to the boundary is specified

$$\frac{\partial f}{\partial n} \text{ is specified on the boundary}$$

- **Mixed (Robin) BC** : Combination of the function and its normal derivative is specified

$$af + b\frac{\partial f}{\partial n} \text{ is specified on the boundary}$$

Truncation Error

Partial differential equation

$$\frac{\partial T}{\partial t} - \alpha \frac{\partial^2 T}{\partial x^2} = 0 = \underbrace{\frac{T_i^{n+1} - T_i^n}{\Delta t} - \frac{\alpha(T_{i+1}^n - 2T_i^n + T_{i-1}^n)}{(\Delta x)^2}}_{\text{Difference equation}} + \underbrace{\left[-\left(\frac{\partial^2 T}{\partial t^2}\right)_i^n \frac{\Delta t}{2} + \alpha \left(\frac{\partial^4 T}{\partial x^4}\right)_i^n \frac{(\Delta x)^2}{12} + \cdots \right]}_{\text{Truncation error}}$$

- Truncation error (residual) is the difference between the actual PDE and the difference equation, TE=PDE-FDE
- For the particular difference equation we say it is first order accurate in time and second order accurate in space, represented by $O(\Delta t) + O(\Delta x)^2, [O\Delta t, (\Delta x)^2]$
- Higher the order of truncation error, greater the accuracy of the solution obtained

Consistency, Stability, Convergence

- A finite difference equation is *consistent* with a PDE if the truncation error vanishes as the size of the grid spacing goes to zero independently
- In the previous scheme, T.E goes to zero by refining the spatial and temporal discretization
- However a scheme in which T.E is $O(\Delta t/\Delta x)$

  would not be formally consistent unless the mesh were refined in a manner such that $(\Delta t/\Delta x) \rightarrow 0$
- DuFort-Frankel scheme of heat equation

$$\frac{u_j^{n+1} - u_j^{n-1}}{2\,\Delta t} = \frac{\alpha}{(\Delta x)^2}\left(u_{j+1}^n - u_j^{n+1} - u_j^{n-1} + u_{j-1}^n\right)$$

$$+ \frac{\alpha}{12}\frac{\partial^4 u}{\partial x^4}\Big)_{n,j}(\Delta x)^2 - \alpha\frac{\partial^2 u}{\partial t^2}\Big)_{n,j}\left(\frac{\Delta t}{\Delta x}\right)^2 - \frac{1}{6}\frac{\partial^3 u}{\partial t^3}\Big)_{n,j}(\Delta t)^2$$

- Consistency implies FDE approximates PDE

Consistency, Stability, Convergence

- Consistency is necessary but not sufficient condition for convergence
- Constraint on mesh width and time-step, determined by stability
- Stability is in the strict sense applicable only to marching problems
- A finite difference scheme is said to be *stable* if errors from any source (round off + T.E) are not permitted to grow (i.e bounded) in the sequence of numerical procedure as calculation proceeds from first marching step to next
- Stability of a FDE is determined by von Neumann analysis, Discrete Perturbation Method

Consistency, Stability, Convergence

- A FDE method is *convergent* if the solution of the FDE approaches the exact solution of the PDE as the mesh is refined
- Lax-Richtmyer Equivalence Theorem

  Given a properly posed initial value problem and a finite-difference approximation to it that satisfies the consistency condition, stability is the necessary and sufficient condition for convergence
- Since conditions of consistency and stability are easily verifiable, using this theorem, any finite difference scheme can be checked for convergence

Round off error

- D = exact solution of difference equation
- N = numerical solution from a computer with finite accuracy

$$\text{Round-off error} = \epsilon = N - D$$
$$N = D + \epsilon$$

$$\frac{T_i^{n+1} - T_i^n}{\Delta t} = \frac{\alpha}{2(\Delta x)^2}(T_{i+1}^n - 2T_i^n + T_{i-1}^n)$$

- Substituting,

$$\frac{D_i^{n+1} + \epsilon_i^{n+1} - D_i^n - \epsilon_i^n}{\alpha\,\Delta t} = \frac{D_{i+1}^n + \epsilon_{i+1}^n - 2D_i^n - 2\epsilon_i^n + D_{i-1}^n + \epsilon_{i-1}^n}{(\Delta x)^2}$$

- Since D must satisfy difference equation, same is true for round off error

$$\frac{\epsilon_i^{n+1} - \epsilon_i^n}{\alpha\,\Delta t} = \frac{\epsilon_{i+1}^n - 2\epsilon_i^n + \epsilon_{i-1}^n}{(\Delta x)^2}$$

von Neumann Analysis

- **For stability, error should be bounded**
- **Error variation can be represented as where k_m is wave number**

$$\left| \frac{\epsilon_i^{n+1}}{\epsilon_i^n} \right| \leq 1$$

$$e(x,t) = \sum_m b_m(t) e^{ik_m x}$$

$$k_m = \frac{2\pi}{\lambda} \text{ or } k_m = \frac{2\pi m}{L}$$

$$\lambda_{min} = 2L/N \qquad k_m = \frac{2\pi}{2L/N} = \frac{2\pi}{L}\frac{N}{2}$$

$$m = N/2$$

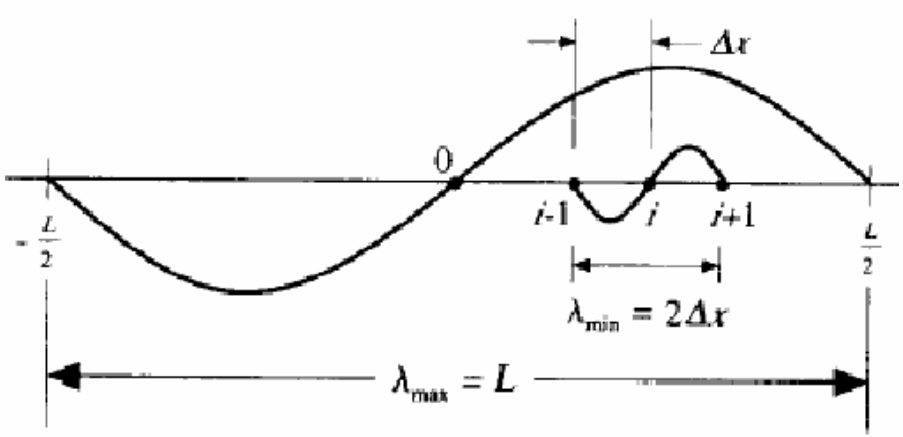


Illustration of max and min wavelengths for Fourier components in round off error

von Neumann Analysis

- Since the difference equation is linear and the behavior of each term is same as that of the series, we consider single term
- Since we seek solution of the form $z^n e^{ik_m x}$

$$z = e^{a\,\Delta t} \qquad z^n = e^{an\,\Delta t} = e^{at}$$

$$\epsilon_m(x, t) = e^{at} e^{ik_m x}$$

- Substituting error term in FDE and satisfying the following condition leads to constraint on time-step and mesh width for stable difference scheme

$$\left| \frac{\epsilon_i^{n+1}}{\epsilon_i^n} \right| = |e^{a\,\Delta t}| \leq 1$$

Explicit Approach

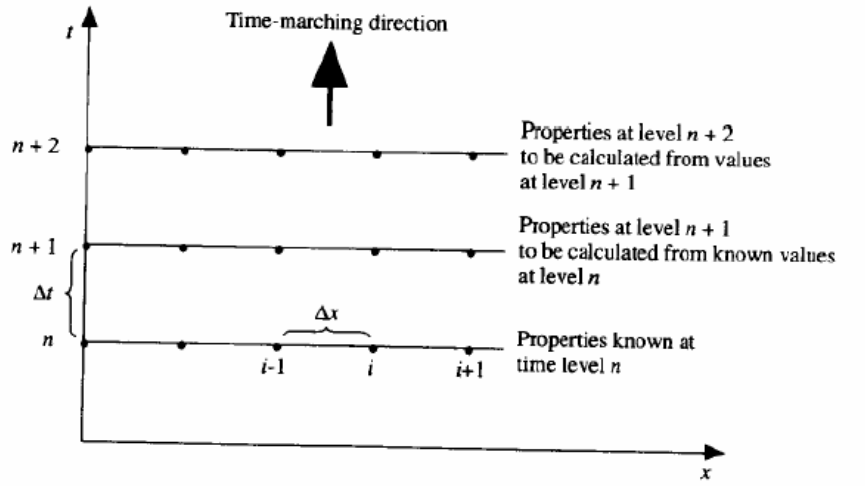
- Explicit approach is one in which each difference equation contains only one unknown and therefore can be solved explicitly for this unknown in a straightforward manner.
- Consider one dimensional heat equation

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2}$$

$$\frac{T_i^{n+1} - T_i^n}{\Delta t} = \alpha \frac{(T_{i+1}^n - 2T_i^n + T_{i-1}^n)}{(\Delta x)^2}$$

$$T_i^{n+1} = T_i^n + \alpha \frac{\Delta t}{(\Delta x)^2} (T_{i+1}^n - 2T_i^n + T_{i-1}^n)$$

Explicit Approach



- Easy to set up
- Constraint on mesh width, time-step
- Less computer time

Implicit Approach

- An implicit approach is one in which the unknowns must be obtained by means of simultaneous solutions of difference equations applied at all grid points arrayed at a given time level.
- Crank-Nicolson finite difference for 1D heat conduction

$$\frac{T_i^{n+1} - T_i^n}{\Delta t} = \alpha \frac{1/2(T_{i+1}^{n+1} + T_{i+1}^n) + 1/2(-2T_i^{n+1} - 2T_i^n) + 1/2(T_{i-1}^{n+1} + T_{i-1}^n)}{(\Delta x)^2}$$

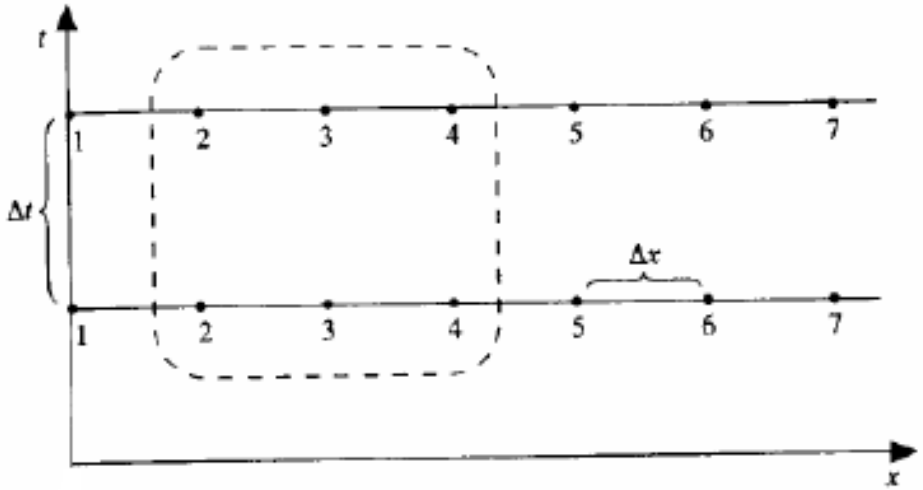
$$AT_{i-1}^{n+1} - BT_i^{n+1} + AT_{i+1}^{n+1} = K_i$$

$$A = \frac{\alpha \Delta t}{2(\Delta x)^2} \quad B = 1 + \frac{\alpha \Delta t}{2(\Delta x)^2} \quad K_i = -T_i^n - \frac{\alpha \Delta t}{2(\Delta x)^2}(T_{i+1}^n - 2T_i^n + T_{i-1}^n)$$

Implicit Approach

- Can be solved using

Thomas Algorithm



- Complicated to set up
- Larger computer time
- No constraint on time step

Weak/Variational Formulation

- A variational method is one in which approximate solutions of the form $u_N = \sum_{j=1}^{N} c_j \phi_j + \phi_0$ are sought, where c_j are determined using an integral statement and ϕ_j. are approximate functions

  The difference $A(u_N) - f$ is called residual of the approximation $R \equiv A(u_N) - f = A\left(\sum_{j=1}^{N} c_j \phi_j + \phi_0\right) - f \neq 0$

- The weighted-integral form of the differential equation is given below
- Parameters c_j are determined by requiring residual to vanish in the weighted-integral sense

$$\int_{\Omega} w\, R(x, y, c_j)\, dx\, dy = 0 \quad (i = 1, 2, \ldots, N)$$

Weak/Variational Formulation

- A weak form is a weighted-integral statement of differential equation, in which differentiation is distributed among weight function and dependent variable and includes natural boundary conditions of the problem
- Sole purpose of weighted integral statement is to obtain N linearly independent algebraic relations between the coefficients c_j
- Weighted integral statement requires ϕ_j to be as many times differentiable as in the differential equation
- However, weak form requires less stringent condition on dependent variable and natural boundary condition is included in the form, hence approximate solution has to satisfy only essential conditions of the problem
- Weak form can developed if the equations are second-order or higher, even if they are non-linear

Weak/Variational Formulation

Method to obtain weak formulation of differential equation:

1) Obtain the weighted-integral statement of the differential equation
2) Distribute the differentiation between approximate solution and weight function using integration by parts and use boundary terms to identify the form of primary and secondary variables
3) Modify boundary terms by restricting the weight function to satisfy the homogenous form of the specified essential boundary conditions of the problem

Resulting equation is called weak/variational form of the differential equation

Weak / Variational Formulation

- Consider an example

$$-\frac{d}{dx}\left[a(x)\frac{du}{dx}\right] = q(x) \quad \text{for } 0 < x < L$$

$$u(0) = u_0, \qquad \left(a\frac{du}{dx}\right)\Big|_{x=L} = Q_0$$

$$u \approx U_N = \sum_{j=1}^{N} c_j \phi_j(x) + \phi_0(x)$$

$$0 = \int_0^L w\left[-\frac{d}{dx}\left(a\frac{du}{dx}\right) - q\right] dx \longrightarrow \langle 1 \rangle$$

$$0 = \int_0^L \left\{w\left[-\frac{d}{dx}\left(a\frac{du}{dx}\right)\right] - wq\right\} dx$$

$$= \int_0^L \left(\frac{dw}{dx}a\frac{du}{dx} - wq\right) dx - \left[wa\frac{du}{dx}\right]_0^L \longrightarrow \langle 2 \rangle$$

$w(0) = 0$, because $u(0) = u_0$

$$\left(a\frac{du}{dx}\right)\Big|_{x=L} = Q_0$$

$$0 = \int_0^L \left(a\frac{dw}{dx}\frac{du}{dx} - wq\right) dx - w(L)Q_0 \longrightarrow \langle 3 \rangle$$

Weak/Variational formulation

$$B(w, u) = \int_0^L a \frac{dw}{dx} \frac{du}{dx} dx, \qquad l(w) = \int_0^L wq\, dx + w(L)Q_0$$

$$B(w, u) = l(w)$$

where B(w,v) and l(w) are called functionals

Variational problem now corresponds to finding u for all sufficiently differentiable w which satisfies the homogenous form of the specific essential conditions of the problem

$$u - u^* + w$$

w can be viewed as variation of the actual solution

$$w = \delta u$$

u is the variational solution

Since u^* and u satisfy essential boundary conditions, it follows that w must satisfy homogenous form of the essential boundary conditions

Rayleigh-Ritz Method

- In this method, coefficients c_j are determined using the weak form of the differential equation and the weight functions are restricted to approximate functions

$$u_N = \sum_{j=1}^{N} c_j \phi_j + \phi_0 \qquad w = \phi_i \ (i = 1, 2, \ldots, N)$$

If B is bilinear, then $B\left(\phi_i, \sum_{j=1}^{N} c_j \phi_j + \phi_0\right) = l(\phi_i) \quad (i = 1, 2, \ldots, N)$

$$\sum_{j=1}^{N} B(\phi_i, \phi_j) c_j = l(\phi_i) - B(\phi_i, \phi_0)$$

$$\sum_{j=1}^{N} B_{ij} c_j = F_i, \qquad B_{ij} = B(\phi_i, \phi_j), \qquad F_i = l(\phi_i) - B(\phi_i, \phi_0)$$

provides N linear algebraic equations to determine c_j and the approximate solution of the problem

Rayleigh-Ritz Method

Approximate functions should follow the following conditions:

1) ϕ_i should at least satisfy the homogenous form of the essential boundary conditions of the problem
2) They should be linearly independent
3) $\{\phi_i\}$ should be complete. For algebraic polynomials, the set should contain all terms of the lowest order admissible and up to the highest order desired

Rayleigh-Ritz method can be applied to all problems, including non-linear ones, which have weak forms

Method of Weighted Residual (MWR)

- The weighted residual method is a generalization of the Rayleigh-Ritz method, in that weight functions are chosen from independent set of functions and requires only weighted-integral form of the equation
- Since weighted-integral form is made use of, approximate solutions should satisfy both natural and essential boundary conditions of the problem
- Weight functions should be linearly independent
- Galerkin Method, Least Squares Method, Collocation Method

Method of Weighted Residual (MWR)

$$A(u) = f \quad in\ \Omega,$$

where A is a differential operator, acting on dependent variable u, f is a function of independent variables

$$u_N = \sum_{j=1}^{N} c_j \phi_j + \phi_0$$

- The difference $A(u_N) - f$ is called residual of the approximation

$$R \equiv A(u_N) - f = A\left(\sum_{j=1}^{N} c_j \phi_j + \phi_0\right) - f \neq 0$$

- Parameters c_j are determined by requiring residual to vanish in the weighted-integral sense

$$\int_{\Omega} \psi_i(x, y) R(x, y, c_j)\, dx\, dy = 0 \quad (i = 1, 2, \ldots, N)$$

Galerkin Method

- Weighted-integral method with choice of weight functions equal to approximation functions

$$\sum_{j=1}^{N} A_{ij} c_j = F_i$$

where

$$A_{ij} = \int_{\Omega} \phi_i A(\phi_j)\, dx\, dy, \qquad F_i = \int_{\Omega} \phi_i [f - A(\phi_0)]\, dx\, dy$$

- This is not the same as Rayleigh-Ritz method. This method uses weighted-integral method whereas latter uses variational form to determine undetermined coefficients c_j
- Approximation functions have to satisfy all the specified boundary conditions. This requirement will increase the order of the polynomial expressions used in this method

Finite Element Method

- A geometrically complex domain is represented by a collection of geometrically sub domains called finite elements
- Over each finite element, approximation functions (generally piecewise polynomials) are derived i.e., variational method applied to each element
- Algebraic relations among the undetermined coefficients (nodal values) are obtained by satisfying the governing differential equation in weighted-integral sense over each element
- Undetermined parameters represent approximate solutions at finite number of points called nodes
- Thus, finite element method is element-wise application of variational method
- The weighted-integral form are required to generate necessary and sufficient number of algebraic equations to determine the unknown coefficients in the approximate solution

Errors

- Errors in finite element method:

1) Domain approximation error
2) Approximation error
3) Computational error

Convergence: Finite element solution u_h is said to converge in the energy norm to true solution u if

$$\|u - u_h\|_m \leq ch^p \quad \text{for } p > 0$$

p–rate of convergence, h-characteristic length of element

p depends on order of derivative of u in weak form and order of polynomials used to approximate u

Hence, error can be reduced either by reducing the size of the elements or increasing the degree of approximation

Summary

- Finite Difference Methods are preferred when the domain is simple as they are easy to set up.
- Any finite difference scheme can be applied, provided it is consistent and satisfies the stability constraint (von Neumann analysis)
- Variational method also provides good approximation of the solution, however, there is no procedure for construction of approximation functions
- Finite Element Method is preferred if the problem domain is geometrically complex. It also overcomes the problem of variational method as the approximation functions can be determined even for complex domains

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Thank you