Partial Differential Equations

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Partial Derivative

- Derivative of a multi-variable function with respect to one variable, with the others fixed (making them constant)

- Ex.) $f(x,y) = x^2 + xy + y^2$

$$f_x \text{ or } f_{,x} \equiv \partial f/\partial x$$
$$f_{xx} \text{ or } f_{,xx} \equiv \partial^2 f/\partial x^2$$
$$\partial_x \equiv \partial/\partial x$$

$$\left.\frac{\partial f}{\partial x}\right|_{\substack{x=a\\y=b}} = \left.\frac{\partial}{\partial x}(x^2 + xy + y^2)\right|_{\substack{x=a\\y=b}}$$

$$= \left.\frac{d}{dx}(x^2 + xb + b^2)\right|_{x=a} = 2a + b$$

Partial Differential Equation

- Differential equation × multivariable function(s) × partial derivatives
- Variables in PDEs
  - Continuous variables
  - Two or more independent variables
    - State variables: functions of independent variables.

參考: Partial Differential Equation

- Examples
  - 1-D advection equation (or flow equation)
    - $cu_x + u_t = 0$
  - 1-D wave equation
    - $c^2u_{xx} - u_{tt} = 0$
  - 1-D diffusion equation (heat equation)
    - $u_t = Du_{xx}$
  - 2-D Poisson's equation
    - $u_{xx} + u_{yy} = f(x,y)$
  - 2-D Helmholtz equation
    - $u_{xx} + u_{yy} + k^2u = 0$

參考: Partial Differential Equation

- Examples
  - 1-D Klein-Gordon equation
    - $\psi_{tt} - \psi_{xx} + m^2\psi = 0$
  - 1-D incompressible Navier-Stokes equation
    - $u_t + u \cdot u_x - v^2 u_{xx} = -p_x/\rho$
  - Burgers' equation
    - $u_t + u \cdot u_x = v^2 u_{xx}$
  - Inviscid Burgers' equation
    - $u_t + u \cdot u_x = 0$
  - Black-Scholes equation
    - $V_t + \frac{1}{2}\sigma^2 s^2 V_{ss} + rsV_s - rV = 0$

參考: Laplace Operator (= Laplacian)

$$\Delta f = \nabla^2 f = \nabla \cdot \nabla f$$

$$\nabla = \frac{\partial}{\partial x}\hat{\boldsymbol{x}} + \frac{\partial}{\partial y}\hat{\boldsymbol{y}} + \frac{\partial}{\partial z}\hat{\boldsymbol{z}}$$

$$\Delta f = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2}.$$

$$\Delta f = \frac{1}{\rho}\frac{\partial}{\partial \rho}\left(\rho \frac{\partial f}{\partial \rho}\right) + \frac{1}{\rho^2}\frac{\partial^2 f}{\partial \varphi^2} + \frac{\partial^2 f}{\partial z^2}.$$

$$\Delta f = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial f}{\partial r}\right) + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta \frac{\partial f}{\partial \theta}\right) + \frac{1}{r^2 \sin^2\theta}\frac{\partial^2 f}{\partial \varphi^2}.$$

Types of 2nd order PDEs

- Elliptic equations
  - Poisson, Laplace (f = 0)

$$\Delta u = f(\vec{x})$$

- Parabolic equations
  - Heat, dispersion

$$\frac{\partial u}{\partial t} - \alpha \nabla^2 u = 0$$

- Hyperbolic equations
  - Advection(convection), wave

$$\frac{\partial^2 u}{\partial t^2} = c^2 \nabla^2 u$$

- Mixed type
  - Euler-Tricomi

$$\frac{\partial^2 u}{\partial x^2} = x \frac{\partial^2 u}{\partial y^2}$$

Types of 2nd order PDEs

- $Au_{xx} + 2Bu_{xy} + Cu_{yy} = F(u_x , u_y , u , ...)$
  - Elliptic equations if $AC - B^2 > 0$
    - $u_{xx} + u_{yy} = f(x,y)$
  - Parabolic equations if $AC - B^2 = 0$
    - $u_t = Du_{xx}$
  - Hyperbolic equations if $AC - B^2 < 0$
    - $c^2u_{xx} - u_{tt} = 0 \quad (\; = \; (c\,\partial_x + \partial_t)(c\,\partial_x - \partial_t)u \quad)$
    - $cu_x + u_t = 0$

Initial Conditions of PDEs

- Elliptic equations
  - Static. Steady-state solution. No initial condition is needed.

- Parabolic or Hyperbolic equations
  - Initial-boundary-value problems (IBVPs)
  - Initial condition is defined as a function of space variables.

Boundary Conditions of PDEs

- Periodic boundary condition
  - If period = L,
    - $u(x+L) = u(x)$
- B. C. for elliptic or parabolic PDEs
  - Dirichlet B. C.
    - u(boundary) = value
  - Neumann B. C.
    - ∂u(boundary)$/\partial x$ = value
    - 2-D or 3-D: derivative normal to the boundary
  - Robin B. C.
    - Linear combination of Dirichlet & Neumann BCs.

Boundary Conditions of PDEs

- B. C. for hyperbolic PDEs
  - Cauchy B. C.
    - Both the function and derivative
    - For the 2nd order PDE with single initial condition
      - Dirichlet or Neumann BCs are applicable, but the solution is not unique.
  - If there are double initial conditions for every position, the solution is unique even with Dirichlet or Neumann BCs.
    - Cauchy problem: the 2nd order PDE with initial state distribution $u(t=0)$ and initial change rate distribution $\partial_t u(t=0)$

參考: Usual Modeling with PDEs

1. Selection of state variables from a phenomenological observation
2. Modeling of the interaction between the inner system (the main model) and the outer environment
3. Finding the equilibrium, conservation, and/or balance equations
4. Constitutive or material modeling (equivalent to approximation of the interaction among individuals in microscopic modeling)
5. Deriving a set of equations describing the evolution of the state variable(s) in time and space

參考: Usual Modeling with PDEs

- Constitutive Relation
  - A relation between two physical quantities
  - Types of constitutive relations
    1) Definitions or physical laws
    2) Phenomenological or empirical
    3) Derived from first-principles or microscopic model calculations

❖ Systems may be composed by different interconnected systems. One needs different models for each sub-system and compatibility conditions (as I. C. and/or B. C.) between contiguous systems.

Dismantling a PDE into ODEs

- Methods to solve a PDE by transforming it into a system of ODEs or ODE + PDE.
  - Method of characteristics (for hyperbolic equations)
  - Separation of variables
  - Method of lines

參考: Method of Characteristics

- Characteristic: a curve of singularities characterizing a hyperbolic equation
  - Ex.) simple case – advection equation
    - $cu_x + u_t = 0$ (c: constant)

Since c is the advection velocity,

$dx/dt = c \;\rightarrow\; x = ct + x_0 \;\rightarrow\; x_0 = x - ct$

$du/dt = (\partial u/\partial x)(dx/dt) + (\partial u/\partial t) = cu_x + u_t = 0$

$\rightarrow u = \mathrm{f}(x_0)$

$\therefore\; u = \mathrm{f}(x - ct)$: general solution

Separation of Variables

- Ex.) $$\frac{\partial^2 u}{\partial t^2} = \Delta u$$ (2-D)

Let $u = \mathrm{T}(t)\mathrm{V}(x,y)$

Then,

$$\frac{\frac{d^2}{dt^2}\mathrm{T}(t)}{\mathrm{T}(t)} = \frac{\nabla^2 \mathrm{V}(x,y)}{\mathrm{V}(x,y)} = -\lambda$$

✓ $\lambda \geq 0$ for steady state solutions

Separation of Variables

$$\frac{\frac{d^2}{dt^2}\mathrm{T}(t)}{\mathrm{T}(t)} = -\lambda$$

- $\lambda>0$: Let $\lambda=k^2$

  $\mathrm{T}(t) = A\cos(kt) + B\sin(kt)$

- $\lambda<0$: Let $\lambda=-\kappa^2$

  $\mathrm{T}(t) = A\exp(-\kappa t) + B\exp(\kappa t)$

Separation of Variables

- Separation of space variables depends on the system's symmetry
  - Cuboid → Cartesian coordinates
    - $V(x, y, z) = X(x)\,Y(y)\,Z(z)$
  - Cylinder → cylindrical coordinates
    - $V(r, \theta, z) = R(r)\,\Theta(\theta)\,Z(z)$
  - Sphere → spherical coordinates
    - $V(r, \theta, \varphi) = R(r)\,\Theta(\theta)\,\Phi(\varphi)$
  - Irregular shape: Go numerical!

Separation of Variables

- Because the time variable part is usually easily separated, the method of variable separation can be used with other methods.
  - Time part: ODE (often analytically solvable)
  - Space part: a numerical method

Superposition Principle

- If f and g are solutions of a homogeneous PDE,

  $u = af + bg$ is also a solution. (a,b: constants)

  – A PDE is a homogeneous PDE if $u = 0$ is its solution. Otherwise, it is an inhomogeneous PDE.

- If h is a solution of an inhomogeneous PDE,

  $u = af + bg + h$ is also a solution.

❖ This principle is used for separation of variables before initial conditions are applied.

Method of Lines

1. Discretizing space (usually by finite difference methods)
2. PDE → ODEs on a grid: an ODE for each grid point → system of ODEs
   - Method of lines can be used to construct or analyze a numerical method by leaving the time variable continuous.
3. Solve the system of ODEs by an ODE solver

Method of Lines

- Example: Bioreactor model

J. Chem. Technol. Biotechnol. **74**, 78 (1999); Automatica **28**, 873 (1992)

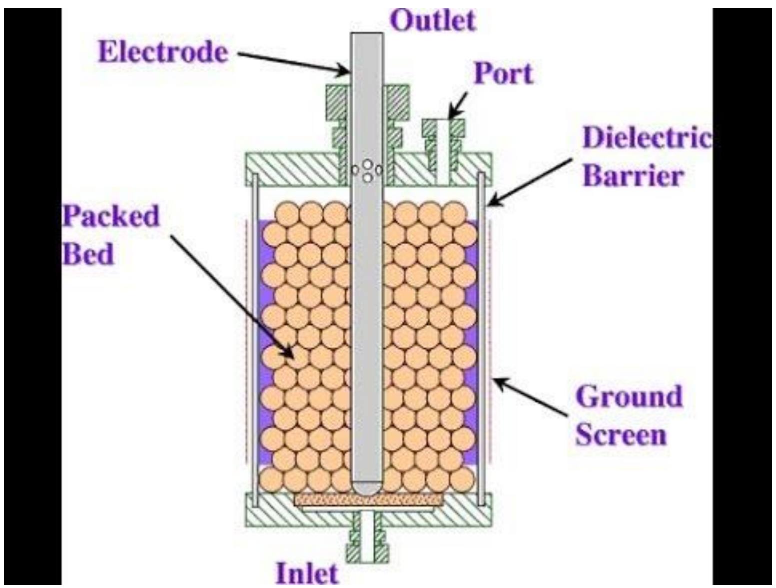


Figure from quora.com

- A fixed bed bioreactor
- Two reactions
  1. Growth:
     substrate + biomass
     → entrapped on a bed
  2. Death of micro-organisms
- State variables
  - X: biomass concentration
  - S: substrate concentration

Method of Lines

- Example: Bioreactor model

J. Chem. Technol. Biotechnol. **74**, 78 (1999); Automatica **28**, 873 (1992)

$$\partial X/\partial t = \mu(X, S)X - k_{\mathrm{d}} X$$

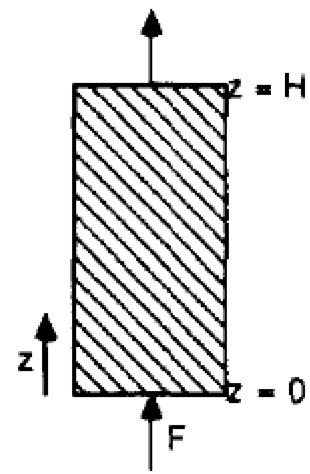
$$\partial S/\partial t = -(F/A)\partial S/\partial z - k_{\mathrm{Y}}\, \mu(X, S)X$$

$$dX_i/\mathrm{d}t = \mu(X_i, S_i)X_i - k_{\mathrm{d}} X_i$$

$$\mathrm{d}S_i/\mathrm{d}t = -(F/A)(S_i - S_{i-1})/\Delta z - k_{\mathrm{Y}}\, \mu(X_i, S_i)X_i$$

$$S_i = S(z_i, t), \quad X_i = X(z_i, t), \quad z_i = i\Delta z,$$

$$S_0 = S_{\mathrm{in}}$$



F : flow
A : area of cross-section

Numerical Methods for PDEs

– Traditional space discretization

- Finite Difference Method (FDM)
  - Numerical differentiation on a uniform mesh
- Finite Element Method (FEM)
  - Sub-domain division → Element equation over each sub-domain → Connecting solutions
- Finite Volume Method (FVM)
  - PDEs are recast in a conservative form by using the divergence theorem and are solved over discrete volumes. (Application in fluid dynamics)

Numerical Methods for PDEs

– Others

- Lattice Boltzmann Method
  - Transforming PDEs to integral equations. Matrix-free.
- Boundary Element Method
  - FEM on boundaries.
- Spectral Element Method
- Differential Quadrature Method

Simple FDM

- Example methods of applying finite differences directly
  - Euler method
    - Time derivative → Forward or Backward 2-point
  - Five-point stencil
    - 2D space Laplacian → Central 3-point
  - Leapfrog method
    - Time derivative → Central 3-point
    - Space derivative → Central 3-point

FDM for 1-D Parabolic PDE

- Forward Euler method

$$\frac{\partial u}{\partial t} \to \frac{u(\vec{x}, t+\delta) - u(\vec{x}, t)}{\delta}$$

  - δ: time interval (Δt)

Ex.) $\partial_t u = \triangle u \;\rightarrow\; u(\vec{x}, t + \delta) = u(\vec{x}, t) + \delta \triangle_h u(\vec{x}, t)$

  - h: space interval (Δx)

  - This method is explicit.
  - However, parabolic PDEs are often too stiff to apply this method.

FDM for 1-D Parabolic PDE

- Forward Euler method
  - 1-D diffusion equation

$$u_t = Du_{xx}$$ (uniform grids)

- Let $U_i^k = u(x_i, t_k)$ where $x_i = ih + x_0$, $t_k = k\delta + t_0$

$$u_t \to \frac{U_i^{k+1} - U_i^k}{\delta}$$

$$u_{xx} \to \frac{U_{i+1}^k - 2U_i^k + U_{i-1}^k}{h^2}$$

$$u_t = Du_{xx} \to \frac{U_i^{k+1} - U_i^k}{\delta} = D\frac{U_{i+1}^k - 2U_i^k + U_{i-1}^k}{h^2}$$

- Let $\gamma = D\delta/h^2$, then

$$U_i^{k+1} = \gamma U_{i+1}^k + (1 - 2\gamma)U_i^k + \gamma U_{i-1}^k$$

FDM for 1-D Parabolic PDE

- Forward Euler method
  - 1-D diffusion equation

$$u_t = D u_{xx}$$

    - Let the domain = $[0, L]$
    - Dirichlet boundary conditions

$$u(0) = c \;\rightarrow U_0^k = c$$
$$u(L) = c \;\rightarrow U_N^k = c$$

    - Neumann boundary conditions
      1) Forward FD or Backward FD
      2) Ghost boundary points

FDM for 1-D Parabolic PDE

- Forward Euler method
  - Discrete maximum principle

$$\max_i \left|U_i^{k+1}\right| \leq \max_i \left|U_i^k\right| \quad \text{for every } k$$

→ (sufficient) Stability condition for 1-D diffusion eq.

$$\gamma \leq \frac{1}{2} \rightarrow 2D\delta \leq h^2$$

  - Algorithm for 1-D diffusion equation
    1. Setting parameters
    2. Setting the initial condition & time-invariant Dirichlet BCs.
    3. Loop: applying $U_i^{k+1} = \gamma U_{i+1}^k + (1 - 2\gamma)U_i^k + \gamma U_{i-1}^k$ with Neumann & time-variant BCs.

Do It Yourself

- Make your code to solve

$$u_t = 4u_{xx} + 1, \qquad 0 < x < 1, t > 0$$

  – Initial condition: $u(x,0) = 0, 0 < x < 1$
  – Boundary conditions: $u(t,0) = u(t,1) = 0, t \geq 0$

with the forward Euler method.

– Wen Shen 11.5-2

❖The main formula is a little bit changed.

- Check out the results every time step.
  – [option]: numbers, graphs, animation

Five-point Stencil (2D)

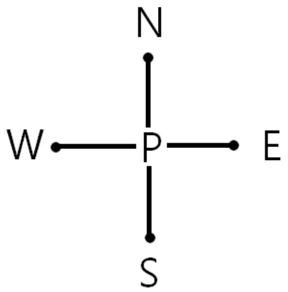
- 5-point discrete Laplacian (2D)

  $\triangle u = u_{xx} + u_{yy}$

  – Let $U_{i,j} = u(x_i, y_j)$ where $x_i = ih$, $y_j = jh$

  $u_{xx,\,h} = (U_{i-1,j} - 2U_{i,j} + U_{i+1,j})/h^2$

  $u_{yy,\,h} = (U_{i,j-1} - 2U_{i,j} + U_{i,j+1})/h^2$



$$\triangle_h u = u_{xx,\,h} + u_{yy,\,h}$$
$$= (U_{i-1,j} + U_{i+1,j} + U_{i,j-1} + U_{i,j+1} - 4U_{i,j})/h^2$$

FDM for 1-D Hyperbolic PDE

- Simple advection equation

$$\partial_x u + \partial_t u = 0$$

- Backward central (or BTCS)
  - Let $U_i^k = u(x_i, t_k)$ where $x_i = ih$, $t_k = k\delta$
  - Time: backward difference
    - $\partial_{t,\delta} U_i^k = (U_i^{\,k} - U_i^{\,k-1})/\delta$
  - Space: central difference
    - $\partial_{x,h} U_i^k = (U_{i+1}^{\,k} - U_{i-1}^{\,k})/(2h)$

$\rightarrow u_i^{\,k+1} - u_i^{\,k} + \gamma(u_{i+1}^{\,k+1} - u_{i-1}^{\,k+1}) = 0$

where $\gamma = \delta/(2h)$

FDM for 1-D Hyperbolic PDE

- Backward central (or BTCS)

$$\gamma u_{i+1}{}^{k+1} + u_i{}^{k+1} - \gamma u_{i-1}{}^{k+1} = u_i{}^{k}$$

  – Matrix-vector form: $\mathbf{M}\mathbf{u}^{k+1} = \mathbf{u}^{k}$

    - In case of Dirichlet B. C., 0 at the ends,

$$\mathbf{M} = \begin{pmatrix} 1 & \gamma & 0 & 0 & \cdots & 0 \\ -\gamma & 1 & \gamma & 0 & \cdots & 0 \\ 0 & -\gamma & 1 & \gamma & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & -\gamma & 1 & \gamma & 0 \\ 0 & \cdots & 0 & -\gamma & 1 & \gamma \\ 0 & \cdots & 0 & 0 & -\gamma & 1 \end{pmatrix}$$

FDM for 1-D Hyperbolic PDE

- Backward central (or BTCS)

$$\gamma u_{i+1}{}^{k+1} + u_i{}^{k+1} - \gamma u_{i\text{-}1}{}^{k+1} = u_i{}^{k}$$

  - Algorithm
    1. Setting parameters
    2. Setting $\mathbf{u}^0$ & time-invariant Dirichlet BCs.
    3. If BCs have no variation in time, set $\mathbf{M}$ under Neumann BCs before the main loop → find $\mathbf{M}^{-1}$
    4. Loop: solving $\mathbf{M}\mathbf{u}^{k+1} = \mathbf{u}^k$ with time-variant BCs.
       - ❖ The different form of the PDE can change $\mathbf{M}$.
  - Stability
    - Unconditionally stable because $\|\mathbf{M}\| > 1$

FDM for 1-D Hyperbolic PDE

- Simple advection equation

$$\partial_x u + \partial_t u = 0$$

- Leapfrog method
  - Let $U_i^k = u(x_i, t_k)$ where $x_i = ih, t_k = k\delta$
  - Time: central difference
    - $\partial_{t,\delta} U_i^k = (U_i^{k+1} - U_i^{k-1})/(2\delta)$
  - Space: central difference
    - $\partial_{x,h} U_i^k = (U_{i+1}^k - U_{i-1}^k)/(2h)$

  → $U_i^{k+1} = U_i^{k-1} - \gamma(U_{i+1}^k - U_{i-1}^k)$

where $\gamma = \delta/h$

FDM for 1-D Hyperbolic PDE

- Leapfrog method
  - Stability condition: $\gamma \leq 1$
  - Algorithm
    1. Setting parameters
    2. Setting the initial condition & time-invariant Dirichlet BCs.
    3. Beginning with the Euler method
    4. Loop: applying $U_i^{k+1} = U_i^{k-1} - \gamma(U_{i+1}^{k} - U_{i-1}^{k})$ with Neumann & time-variant Dirichlet BCs.

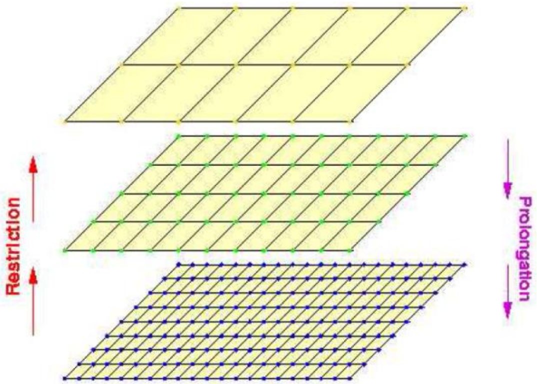
參考: Multi-Grid Technique

- Use of different scales of discretization
- Ex.) use of coarse and fine grids
  - Coarse grid: smooth function
  - Fine grid: highly oscillating function
  - A coarse grid can be used for correction of a fine-grid solution.

❖ This can be applied to any discretizing method (FDM, FEM, ……).

參考: Multi-Grid Technique

- Algorithm framework
  1. Smoothing: rough calculation on a fine grid
  2. Restriction: fine → coarse (error transfer)
  3. Calculation on the coarse grid
  4. Interpolation or prolongation: coarse → fine
  5. Further calculation on the fine grid



Picture from Borzì

Domain Decomposition Technique

- BVP on domain → BVPs on subdomains
  - In addition to boundary conditions, we need conditions at interfaces or in overlapping regions
- Usefulness
  1. Efficient parallel computing
  2. It is often useful to use different time steps or grids on different subdomains.
  - More often used for FEM than FDM

Domain Decomposition Technique

- Overlap conditions
    1. Domains overlap
    2. Domains do not overlap, but they are appended with buffer regions
    3. Without buffer regions, domains intersect only along an interface

Domain Decomposition Technique

- Simple example: FDM of 1-D heat eq.
  - $\partial_t u = \partial^2{}_x u$
  - $u(x\,, 0) = f(x)\,;\, u(0, t) = u(1, t) = 0$
  - Let $U_i^n \equiv u(x_i\,, t_n)$ where $x_i = ih$, $t_n = n\delta$
  - Assume each subdomain ranges from one interface point to the next interface point. Then,
    - $U_i^n = 0$ at boundary points
    - $\partial_{t,\,\delta} U_i^n = \partial^2{}_{x,\,h}\, U_i^{n\text{-}1}$ at interface points
    - $\partial_{t,\,\delta} U_i^n = \partial^2{}_{x,\,h}\, U_i^n$ at interior points

Ref.) C. N. Dawson *et al*., “A Finite Difference Domain Decomposition Algorithm for Numerical Solution of the Heat Equation”, Math. Comput. **57**, 63 (1991).

Domain Decomposition Technique

- Simple example: FDM of 1-D heat eq.
  - $U_i^n = 0$ at boundary points
  - $\partial_{t,\delta} U_i^n = \partial^2_{x,h} U_i^{n-1}$ at interface points
  - $\partial_{t,\delta} U_i^n = \partial^2_{x,h} U_i^n$ at interior points

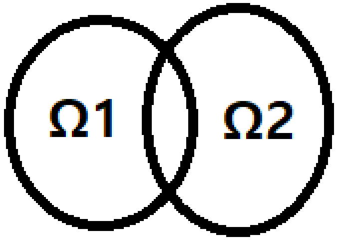
  where $\partial_{t,\delta} U_i^n = (U_i^n - U_i^{n-1})/\delta$,

  $$\partial^2_{x,h} U_i^n = (U_{i-1}^n - 2U_i^n + U_{i+1}^n)/h^2$$

  – Explicit for interface and implicit for interior
    - After computing the interface values, the interior values in each subdomain are computed.

Domain Decomposition Technique

- Overlapping domain cases
    - $\Omega = \Omega_1 \cup \Omega_2$



- Schwarz iteration
    - PDE → $\mathbf{Au} = \mathbf{b}$ form
    - Supposing $\mathbf{Au}_1^{k} = \mathbf{b}$ & $\mathbf{Au}_2^{k} = \mathbf{b}$,
    - Solve $\mathbf{Au}_1^{k+1} = \mathbf{b}$ & $\mathbf{Au}_2^{k+1} = \mathbf{b}$ under the B. C. $\mathbf{u}_1^{k+1} = \mathbf{u}_2^{k}$ on $\partial\Omega_1 \cap \Omega_2$ & $\mathbf{u}_2^{k+1} = \mathbf{u}_1^{k+1}$ on $\partial\Omega_2 \cap \Omega_1$
    - Convergence depends on boundary conditions and size of the overlapping region

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Investigation

- About the **Navier-Stokes** equation
- About the **Black-Scholes** equation
- About the **Euler-Tricomi** equation

❖ Not about numerical methods for these equations.