CS601: Software Development for Scientific Computing

Autumn 2021

Week3: Structured Grids (Contd..), Intermediate C++

Last Week..

- Program Development Environment – Demo
- 'C' subset of C++ and reference variables in C++
- Discretization and issues
  - scalability, approximation, and errors (discretization error and solution error), error estimates
  - mesh of cells/elements, cell shapes and sizes
- Structured Grids
  - 'Regularity' of cell connectivity (e.g. neighbors are similar kind of cells)
  - Case study – problem statement, representation (e.g. 2D arrays)

Review of Solution to Exercise: Product of Vectors

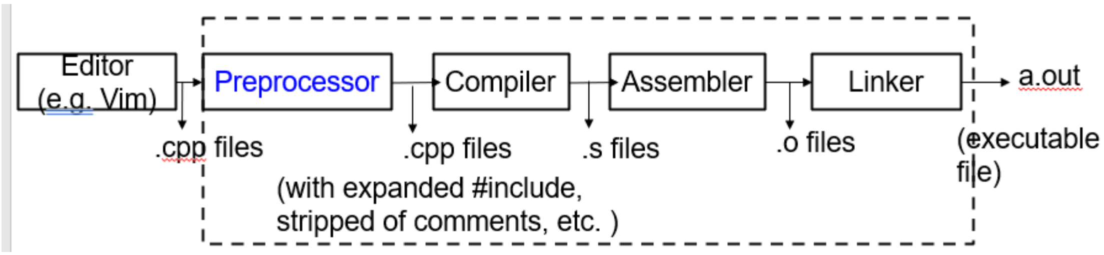
- Input sanity check using `istringstream`
- Good programming style: separation of the interface from implementation
  - Streams
  - Passing arrays to functions
  - Pragmas and preprocessor directives
  - Namespaces
- In the sample code, we have so many versions!

Demo

- streams, passing arrays to functions, namespaces, preprocessor directives.
  – Usage and Implementation (refer to week3_codesamples)

Detour - Conditional Compilation

- Set of 6 preprocessor directives and an operator.
  - #if
  - #ifdef
  - #ifndef
  - #elif
  - #else
  - #endif
- Operator ‘defined’



#if

```
#if <constant-expression>
cout<<"CS601";
#endif
```

//This line is compiled only if <constant-expression> evaluates to a value > 0 while preprocessing

```
#define COMP 0
#if COMP
cout<<"CS601"
#endif
```

No compiler error

```
#define COMP 2
#if COMP
cout<<"CS601"
#endif
```

Compiler throws error about missing semicolon

#ifdef

```
#ifdef identifier
cout<<“CS601”;
#endif
```

//This line is compiled only if identifier is defined before the previous line is seen while preprocessing.

`identifier` does not require a value to be set. Even if set, does not care about 0 or > 0.

```
#define COMP
#ifdef COMP
cout<<“CS601”
#endif
```

```
#define COMP 0
#ifdef COMP
cout<<“CS601”
#endif
```

```
#define COMP 2
#ifdef COMP
cout<<“CS601”
#endif
```

All three snippets throw compiler error about missing semicolon

#else and #elif

```
1. #ifdef identifier1
2. cout<<“Summer”
3. #elif identifier2
4. cout<<“Fall”;
5. #else
6. cout<<“Spring”;
7. #endif
```

//preprocessor checks if identifier1 is defined. if so, line 2 is compiled. If not, checks if identifier2 is defined. If identifier2 is defined, line 4 is compiled. Otherwise, line 6 is compiled.

`defined` operator

Example:

```
#if defined(COMP)
cout<<“Spring”;
#endif
```

//same as if #ifdef COMP

```
#if defined(COMP1) || defined(COMP2)
cout<<“Spring”;
#endif
```

//if either `COMP1` or `COMP2` is defined, the `printf` statement is compiled. As with `#ifdef`, `COMP1` or `COMP2` values are irrelevant.

Mathematical Model of the Grid

- Partial Differential Equations (PDEs):
  - Navier-Stokes equations to model water, blood flow, weather forecast, aerodynamics etc.
  - Elasticity (Lame-Navier equations)
  - Nutrient transport in blood flow
  - Heat conduction (Laplace / Poisson equation): *how heat conducts/diffuses through a material given the temperature at boundaries?*
  - Mechanics: *how does a mass reach from point p1 to point p2 in shortest time under gravitational forces?*

Notation and Terminology

- $\frac{\partial u}{\partial x} = \partial_x u$
- $\frac{\partial^2 u}{\partial x \partial y} = \partial_{xy} u$
- $\frac{\partial u}{\partial t} = \partial_t u$, t usually denotes time.
- Laplace operator $(\mathbf{L})$: of a two-times continuously differentiable scalar-valued function $u\colon \mathbb{R}^n \to \mathbb{R}$

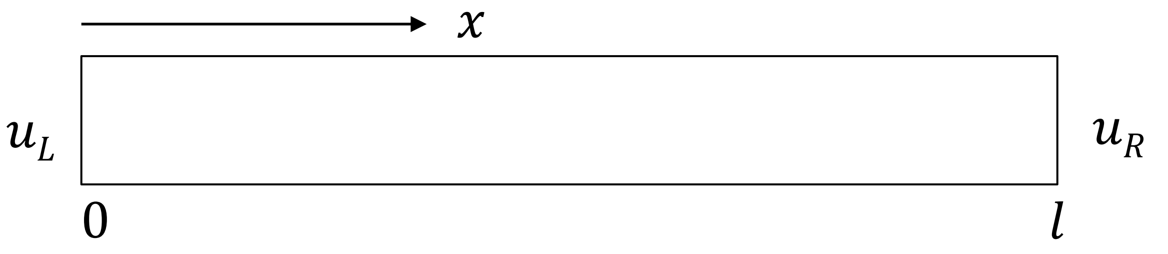
$$\Delta u \quad = \sum_{k=1}^{n} \partial_{kk} u$$

Important PDEs

- Three important types (*not a complete categorization by any means*):
  - Poisson problem: $-\Delta u = f$ (elliptic)
  - Heat equation: $\partial_t u - \Delta u = f$ (parabolic. Here, $\partial_t u = \frac{\partial u}{\partial t}$ = partial derivative w.r.t. time)
  - Wave equation: $\partial_t{}^2 u - \Delta u = f$ (Hyperbolic. Here, $\partial_t{}^2 u = \frac{\partial^2 u}{\partial t \partial t}$ = second-order partial derivative w.r.t. time)

Application: Heat Equation

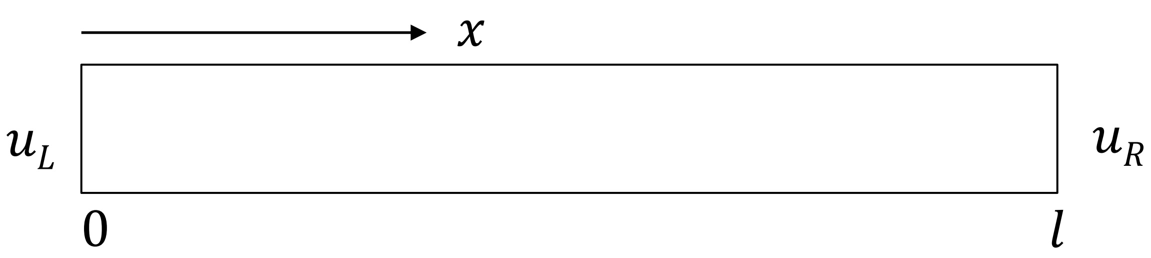
- Example: heat conduction through a rod



- $u = u(x, t)$ is the temperature of the metal bar at distance x from one end and at time t
- Goal: find u

Initial and Boundary Conditions

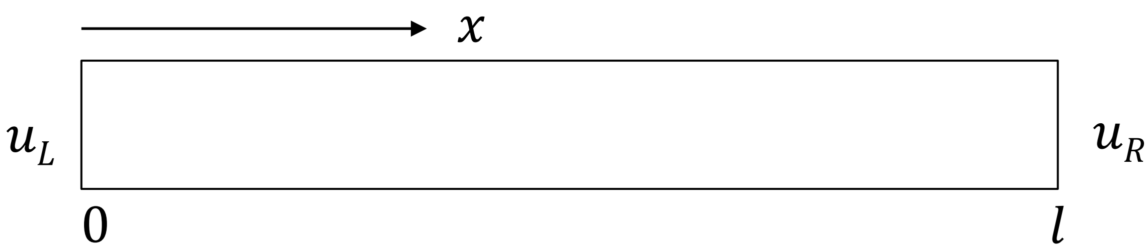
- Example: heat conduction through a rod



- Metal bar has length l and the ends are held at constant temperatures u_L at the left and u_R at the right
- Temperature distribution at the initial time is known $f(x)$, with $f(0) = u_L$ and $f(l) = u_R$

Equations

- Example: heat conduction through a rod



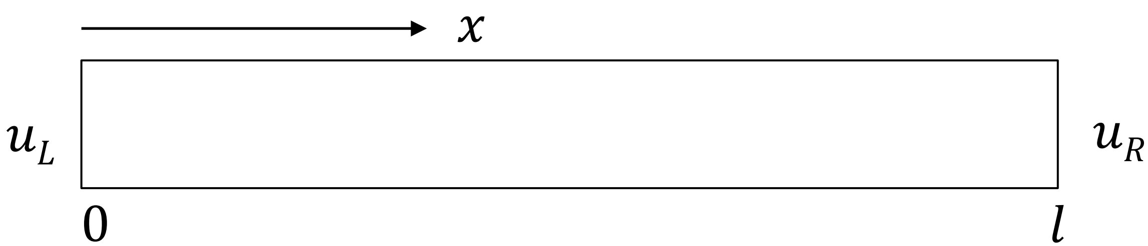
$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2} \qquad (0 < x < l, t > 0)$$

α is thermal diffusivity

(a constant if the material is homogeneous and isotropic.
copper = 1.14 $cm^2\,s^{-1}$, aluminium = 0.86 $cm^2\,s^{-1}$)

Equations

- Example: heat conduction through a rod



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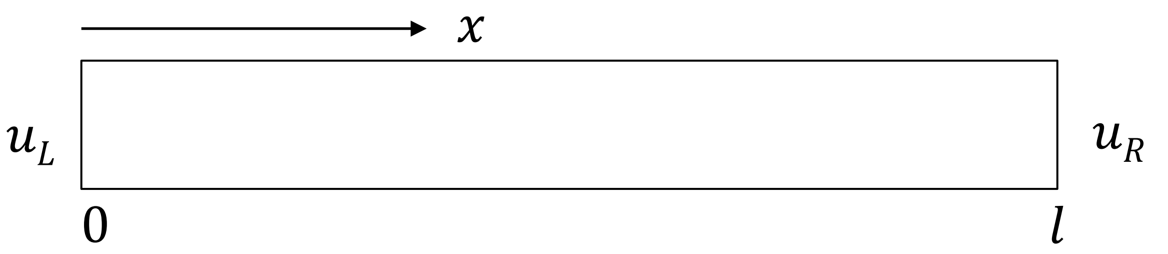
- *Exercise: what kind of a PDE is this? (Poisson/Heat/Wave?)*

Equations

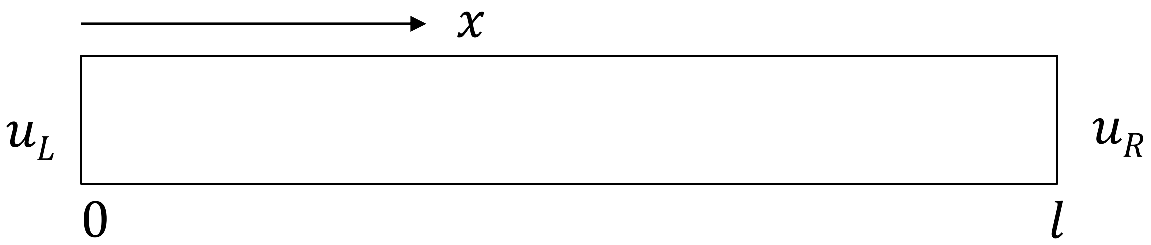
- Example: heat conduction through a rod



$\partial_t u = \alpha \Delta u$ as per the notation mentioned earlier

Equations

- Example: heat conduction through a rod



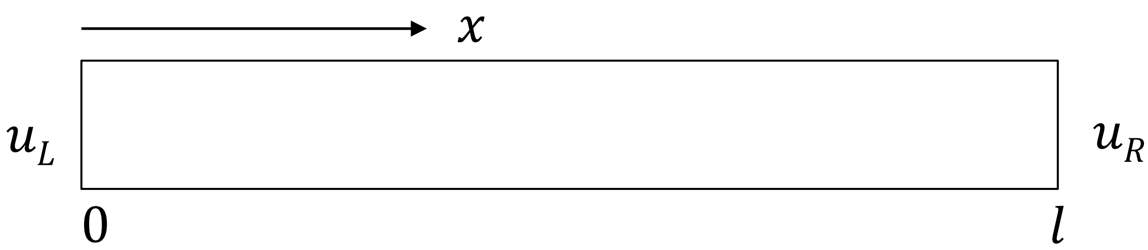
$$\partial_t u = \alpha \Delta u$$

Can also be written as:

$$\partial_t u - \alpha \Delta u = 0$$

Equations

- Example: heat conduction through a rod



$$\partial_t u - \alpha \Delta u = 0 \ ,$$

Based on initial and boundary conditions:

$$u(0, t) = u_L \ ,$$
$$u(l, t) = u_R \ ,$$
$$u(x, 0) \ = \ f(x)$$

Equations

- Summarizing:
  1. $\partial_t u - \alpha \Delta u = 0, 0<x<l, t>0$
  2. $u(0,t) = u_L, t > 0$
  3. $u(l,t) = u_R\,, t > 0$
  4. $u(x,0) = \ f(x), 0 < x < l$

- Solution:

$$u(x,t) \quad = \sum_{m=1}^{\infty} B_m e^{-m^2 \alpha \pi^2 t/l^2} \sin(\frac{m\pi x}{l}) \quad ,$$

where, $B_m = 2/l \int_0^l f(s) \sin\left(\frac{m\pi s}{l}\right) ds$

Equations

- Summarizing:
  1. $\partial_t u - \alpha \Delta u = 0, 0<x<l, t>0$
  2. $u(0,t) = u_L, t > 0$
  3. $u(l,t) = u_R, t > 0$
  4. *But we are interested in a numerical solution*

- Solution:

$$u(x,t) \quad = \sum_{m=1}^{\infty} B_m e^{-m^2 \alpha \pi^2 t / l^2} \sin\left(\frac{m\pi x}{l}\right) \quad ,$$

where, $B_m = 2/l \int_0^l f(s) \sin\left(\frac{m\pi s}{l}\right) ds$

Approximating Partial Derivatives

- Suppose $y = f(x)$
  - Forward difference approximation to the first-order derivative of f w.r.t. x is:

$$\frac{df}{dx} \approx \frac{\left(f(x+\delta x)-f(x)\right)}{\delta x}$$

  - Central difference approximation to the first-order derivative of f w.r.t. x is:

$$\frac{df}{dx} \approx \frac{\left(f(x+\delta x)-f(x-\delta x)\right)}{2\delta x}$$

  - Central difference approximation to the second-order derivative of f w.r.t. x is:

$$\frac{d^2 f}{dx^2} \approx \frac{\left(f(x+\delta x)-2f(x)+f(x-\delta x)\right)}{(\delta x)^2}$$

Approximating Partial Derivatives

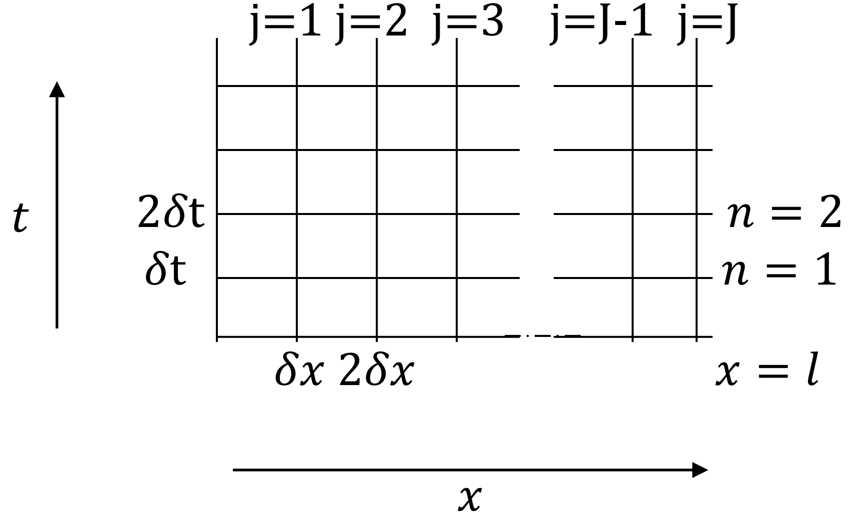
- In example heat application $f = u = u(x, t)$ and $\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2}$
  - First, approximating $\frac{\partial u}{\partial t}$:

    $\frac{\partial u}{\partial t} \approx \frac{(u(x,t+\delta t)-u(x,t))}{\delta t}$, where δt is a small increment in time
  - Next, approximating $\frac{\partial^2 u}{\partial x^2}$:

    $\frac{\partial^2 u}{\partial x^2} \approx \frac{(u(x+\delta x,t)-2u(x,t)+u(x-\delta x,t))}{(\delta x)^2}$, where δx is a small increment in space (along the length of the rod)

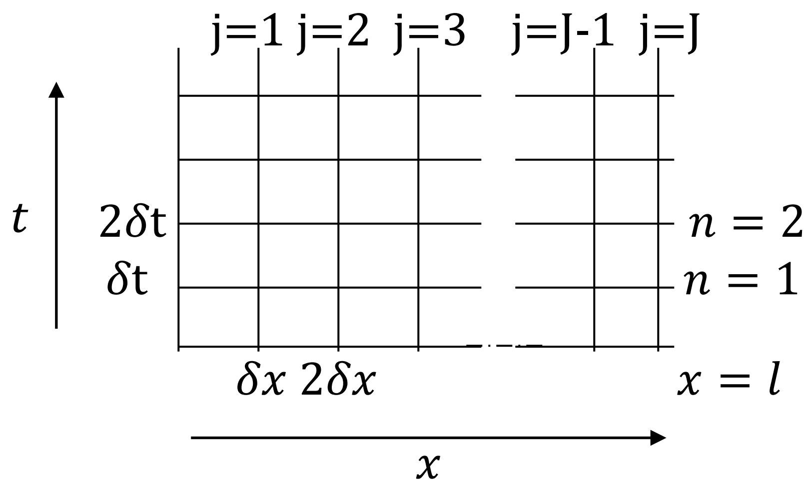
Approximating Partial Derivatives

- Divide length l into J equal divisions: $\delta x = l/J$ (space step)
- Choose an appropriate δt (time step)



Approximating Partial Derivatives

- Find sequence of numbers which approximate u at a sequence of (x, t) points (i.e. at the intersection of horizontal and vertical lines below)



- Approximate the exact solution $u(j \times \delta x, n \times \delta t)$ using the approximation for partial derivatives mentioned earlier

Approximating Partial Derivatives

$$\frac{\partial u}{\partial t} \approx \frac{\big(u(x, t + \delta t) - u(x, t)\big)}{\delta t}$$

$$= \frac{(u_j^{n+1} - u_j^n)}{\delta t}$$

where u_j^{n+1} denotes taking j steps along x direction and $n + 1$ steps along t direction

Similarly, $\frac{\partial^2 u}{\partial x^2} \approx \frac{\big(u(x+\delta x,t) - 2u(x,t) + u(x-\delta x,t)\big)}{(\delta x)^2}$

$$= \frac{(u_{j+1}^n - 2\, u_j^n + u_{j-1}^n)}{(\delta x)^2}$$

Approximating Partial Derivatives

Plugging into $\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2}$:

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

This is also called as difference equation because you are computing difference between successive values of a function involving discrete variables.

Approximating Partial Derivatives

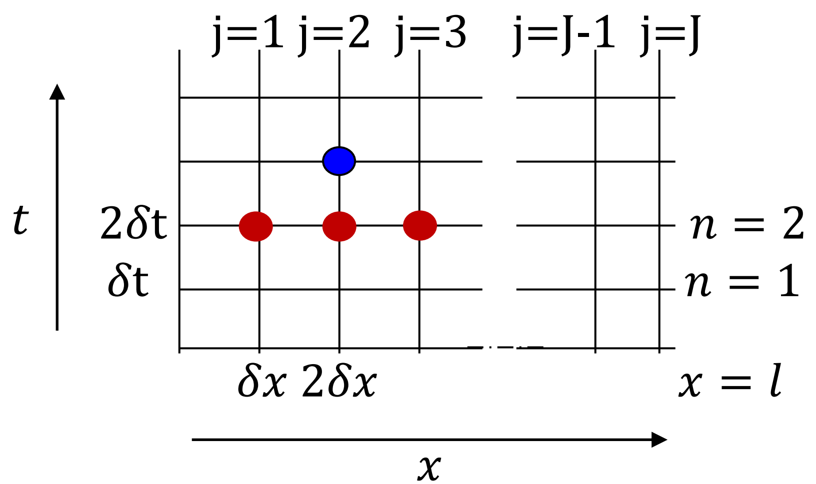
Simplifying:

$$u_j^{n+1} = u_j^n + r(u_{j+1}^n - 2\, u_j^n + u_{j-1}^n)$$
$$= ru_{j-1}^n + (1\ - 2r)u_j^n + ru_{j+1}^n,$$
$$where\ r = \alpha \frac{\delta t}{(\delta x)^2}$$

Approximating Partial Derivatives

visualizing,

$$u_j^{n+1} = ru_{j-1}^n + (1 - 2r)u_j^n + ru_{j+1}^n$$



To compute the value of function at blue dot, you need 3 values indicated by the red dots – 3-point stencil

Approximating Partial Derivatives

- Initial and boundary conditions tell us that:
  $u(0,t) = u_L$,
  $u(l,t) = u_R$,
  $u(x,0) = f(x)$

- $u_0^0, u_1^0\, u_2^0, \ldots.\, u_J^0$ are known (at time t=0, the temperature at all points along the distance is known as indicated by $f(x) = f_j$).
- u_0^1 is $u_{L,}\, u_J^1$ is u_R
- Now compute points on the grid from left-to-right:

Approximating Partial Derivatives

- Now compute points on the grid from left-to-right:

$$u_1^1 = u_1^0 + r(u_0^0 - 2u_1^0 + u_2^0)$$
$$u_2^1 = u_2^0 + r(u_1^0 - 2u_2^0 + u_3^0)$$

.

.

$$u_{J-1}^1 = u_{J-1}^0 + r\left(u_{J-2}^0 - 2u_{J-1}^0 + u_J^0\right)$$

- This constitutes the computation done in the first time step.
- Now do the second time step computation…and so on..

Numerical Methods for Solving PDEs

- Finite Difference Methods
- Finite Volume Methods
- Finite Element Methods
- Boundary Elements Methods
- Isogeometric Analysis
- Spectral Methods

Programming Assignment 1: heads-up

- *Steady-state* heat equation for a metal plate with boundaries at constant temperature

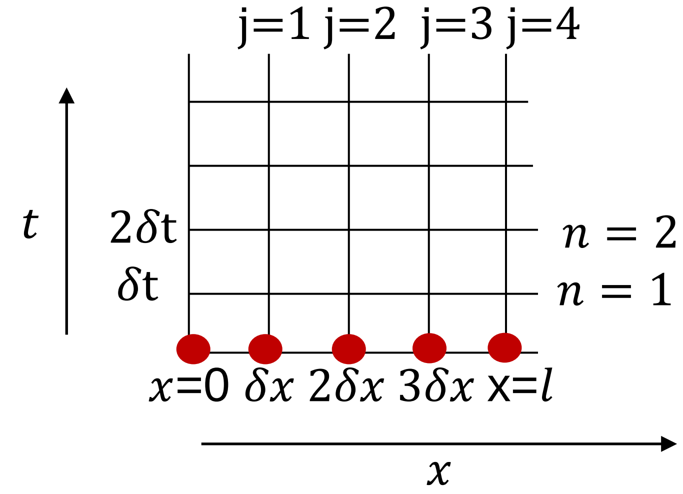
Explicit Difference Method: Stability

- Given: $l = 1,$
  $u(0, t) = u_L = 0,$
  $u(l, t) = u_R = 0,$
  $u(x, 0) = f(x) = x(l - x)$
  $\alpha = 1,$
- Choose: $\delta x = 0.25, \delta t = 0.075$
- Solve.

Explicit Difference Method: Stability

- Initialize u_j^0 values from initial and boundary conditions i.e. *get time-step 0 values*

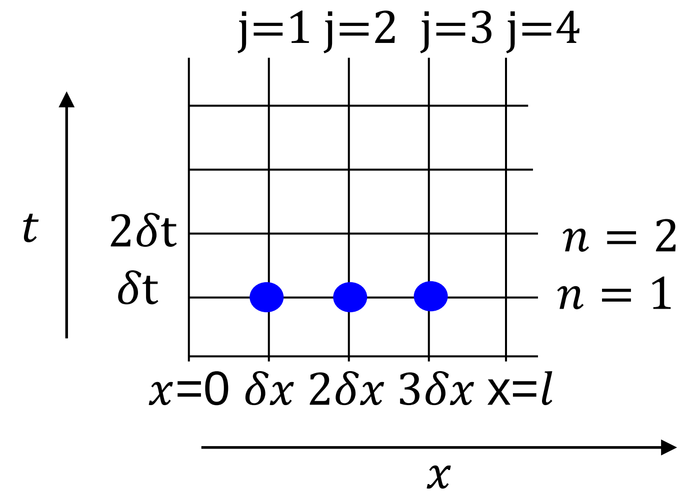
$u_0^0 = 0$
$u_1^0 = f(\delta x) = \delta x(l - \delta x) = .1875$
$u_2^0 = f(2\delta x) = 2\delta x(l - 2\delta x) = .25$
$u_3^0 = f(3\delta x) = 3\delta x(l - 3\delta x) = .1875$
$u_4^0 = 0$



Explicit Difference Method: Stability

- Compute time-step 1 values

$$u_j^{n+1} = ru_{j-1}^n + (1 - 2r)u_j^n + ru_{j+1}^n$$

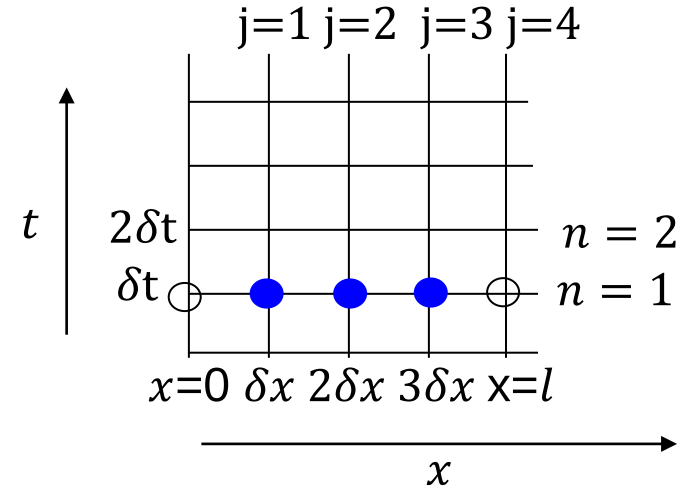


Explicit Difference Method: Stability

- Compute time-step 1 values

$$u_j^{n+1} = ru_{j-1}^n + (1 - 2r)u_j^n + ru_{j+1}^n$$

What about values of $u(x,t)$ at ○ ?



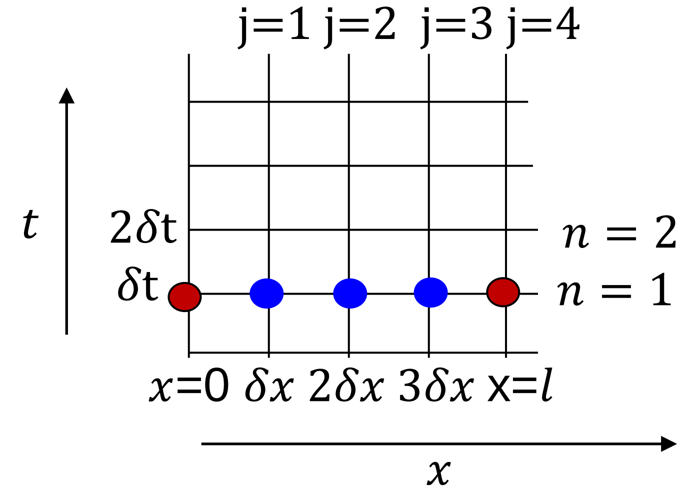
Explicit Difference Method: Stability

- Compute time-step 1 values

$$u_j^{n+1} = ru_{j-1}^n + (1 - 2r)u_j^n + ru_{j+1}^n$$

What about values of $u(x,t)$ at ○ ?

Get it from boundary conditions



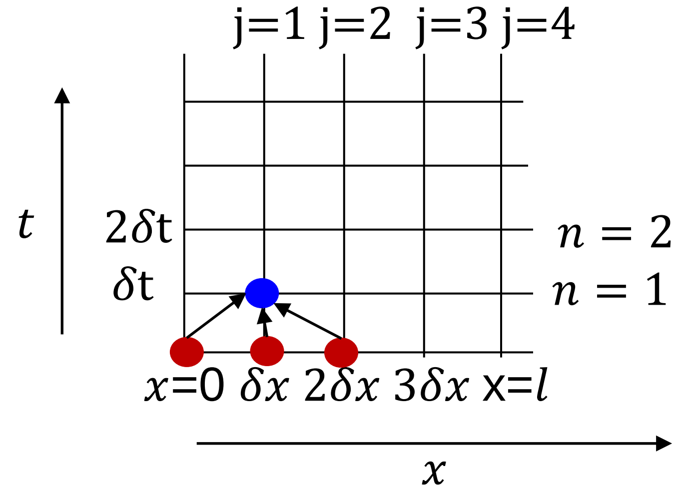
Explicit Difference Method: Stability

- Compute time-step 1 values

$$u_j^{n+1} = ru_{j-1}^n + (1 - 2r)u_j^n + ru_{j+1}^n$$

$r = \alpha\delta t/(\delta x)^2$ = 1.2

u_1^1 = $u_1^0 + r(u_0^0 - 2u_1^0 + u_2^0)$ = 0.03678



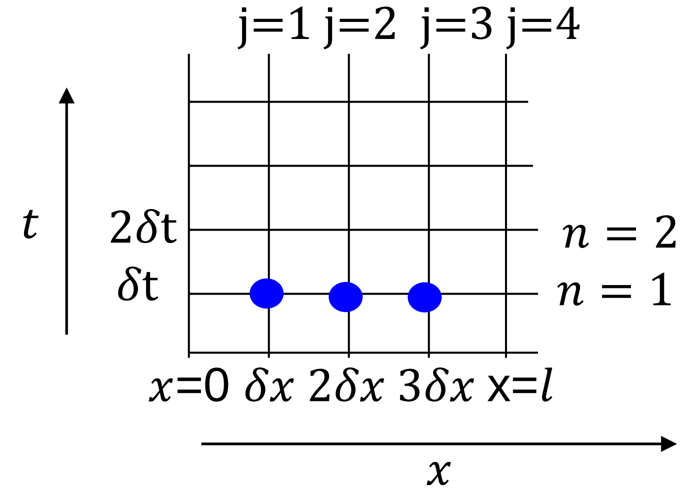
Explicit Difference Method: Stability

- Compute time-step 1 values

$u_j^{n+1} = ru_{j-1}^n + (1 - 2r)u_j^n + ru_{j+1}^n$

$r = \alpha\delta t/(\delta x)^2$ = 1.2

u_1^1 = $u_1^0 + r(u_0^0 - 2u_1^0 + u_2^0)$=0.03678
u_2^1 = $u_2^0 + r(u_1^0 - 2u_2^0 + u_3^0)$=0.1
u_3^1 = $u_3^0 + r(u_2^0 - 2u_3^0 + u_4^0)$=0.03678

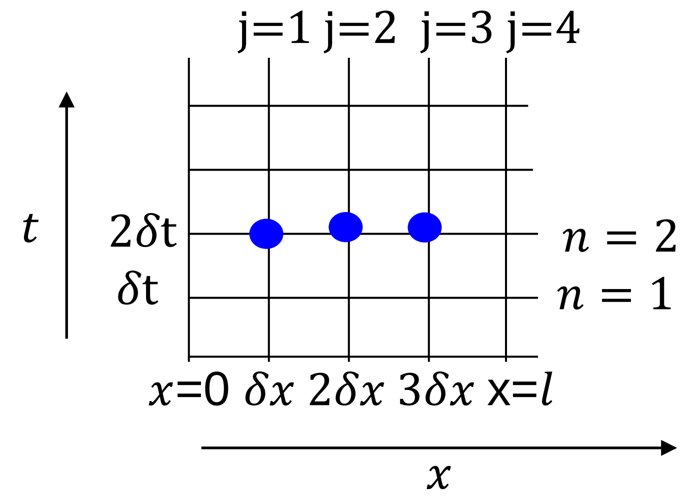


Explicit Difference Method: Stability

- Compute time-step 2 values

$$u_j^{n+1} = ru_{j-1}^n + (1 - 2r)u_j^n + ru_{j+1}^n$$

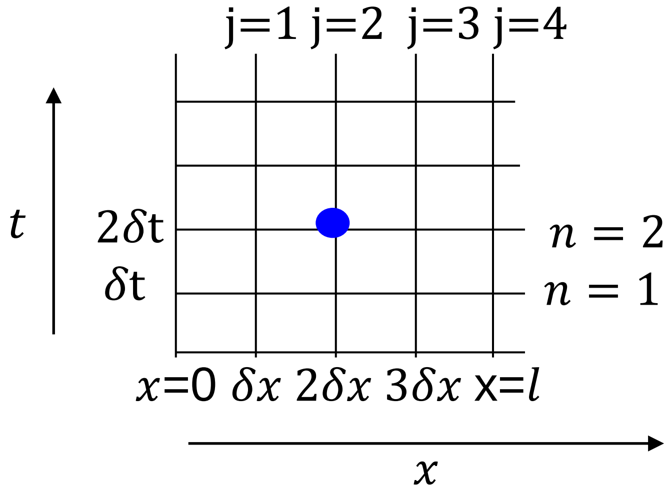
$u_1^2 = u_1^1 + r(u_0^1 - 2u_1^1 + u_2^1)$=0.06851
$u_2^2 = u_2^1 + r(u_1^1 - 2u_2^1 + u_3^1)$=**-0.05173**
$u_3^2 = u_3^1 + r(u_2^1 - 2u_3^1 + u_4^1)$=0.06851



Explicit Difference Method: Stability

- Temperature at $2\delta x$ after $2\delta t$ time units went into negative! (when the boundaries were held constant at 0)
  - Example of *instability*

$u_2^2 = u_2^1 + r(u_1^1 - 2u_2^1 + u_3^1) =$ **-0.05173**



The solution is stable (for heat diffusion problem) only if the approximations for $u(x,t)$ do not get bigger in magnitude with time

Explicit Difference Method: Stability

- The solution for heat diffusion problem is stable only if:

$$r \leq \frac{1}{2}$$

Therefore, choose your time step in such a way that:

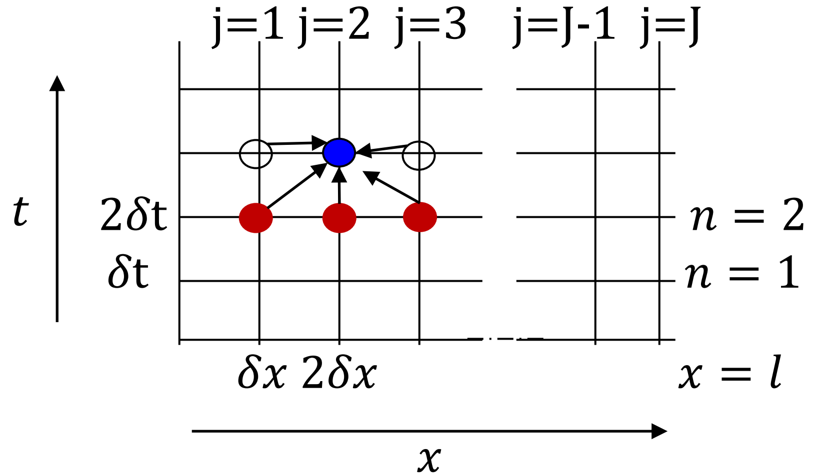
$$\delta t \leq \frac{\delta x^2}{2\alpha}$$

But this is a severe limitation!

Implicit Method: Stability

- Overcoming instability:

$$u_j^{n+1} = u_j^n + 1/2\, r(u_{j-1}^n - 2u_j^n + u_{j+1}^n + u_{j-1}^{n+1} - 2u_j^{n+1} + u_{j+1}^{n+1})$$



To compute the value of function at blue dot, you need 6 values indicated by the red dots (known) and 3 additional ones (unknown) above

Implicit Method: Stability

- Overcoming instability:

$$u_j^{n+1} = u_j^n + 1/2\, r(u_{j-1}^n - 2u_j^n + u_{j+1}^n + u_{j-1}^{n+1} - 2u_j^{n+1} + u_{j+1}^{n+1})$$

- Extra work involved to determine the values of unknowns in a time step
  - Solve a system of simultaneous equations. Is it worth it?

Definitions

- Consider a region of interest R in, say, xy plane. The following is a *boundary-value problem*:

  $$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = f(x, y) \qquad \text{(1)}$$

  where f is a given function in R and

  $$u = g,$$

  where the function g tells the value of function u at boundary of R
- if $f = 0$ everywhere, then Eqn. (1) is Laplace's Equation
- if $f \neq 0$ somewhere in R, then Eqn. (1) is Poisson's Equation

Suggested Reading

- *J.W. Thomas. Numerical Partial Differential Equations: Finite Difference Methods*

- *Parabolic PDEs:* *https://learn.lboro.ac.uk/archive/olmp/olmp_resources/pages/workbooks_1_50_jan2008/Workbook32/32_4_prblc_pde.pdf*