Parallel Adaptive Discontinuous Galerkin Method for Chemical Transport Equations

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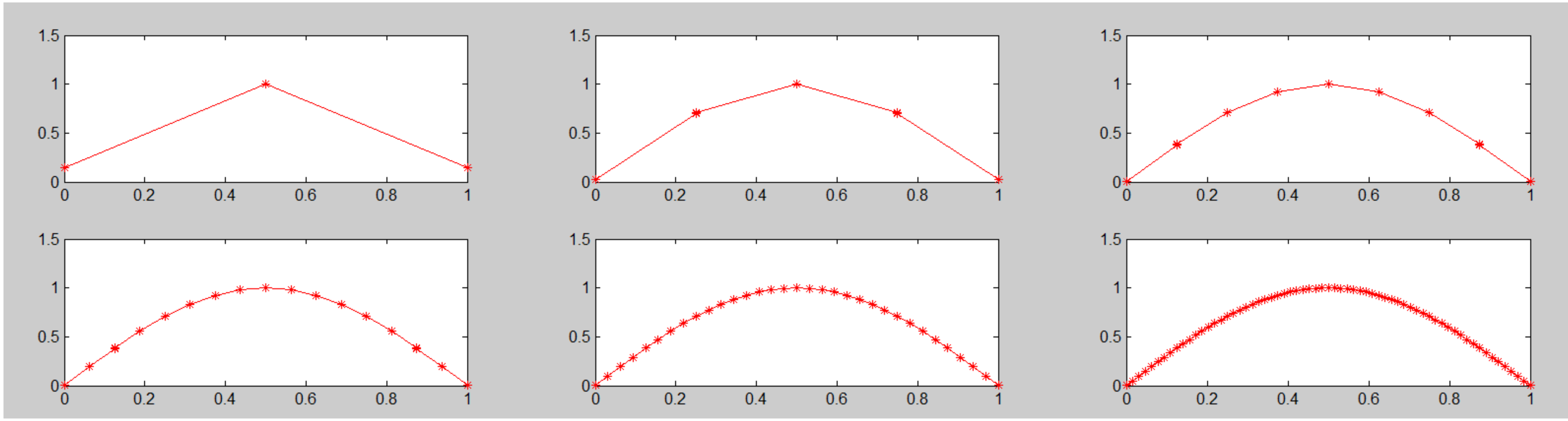
- Objective
  - Construct a 3D Parallel Adaptive computer code to solve a set of chemical transport equations
    - Using Discontinuous Galerkin Method (DG-FEM)

- Objective
- **Background**
- Current Progress
- Acknowledgements

Discontinuous Galerkin Method (DG-FEM)

- Discontinuous Galerkin Method (DG-FEM)
  - A class of Finite Element Method (FEM)
  - Finding approximate solutions to boundary value problems
  - Solving differential equations



Example: Solving Heat Equation (1D)

- 1D Poisson's Equation on domain $I=[a,b]$

$$
\begin{cases}
-u'' = f \\
u(a) = u(b) = 0
\end{cases}
$$

Example: Solving Heat Equation (1D)

- Multiply by an arbitrary function v

  (satisfying $v(a)=v(b)=0$)

$$-u'' v - f v = 0$$

- Integration (Strong-form)

$$-\int u'' v - \int f v = 0$$

Example: Solving Heat Equation (1D)

- Suppose v is continuous over I, integration by parts

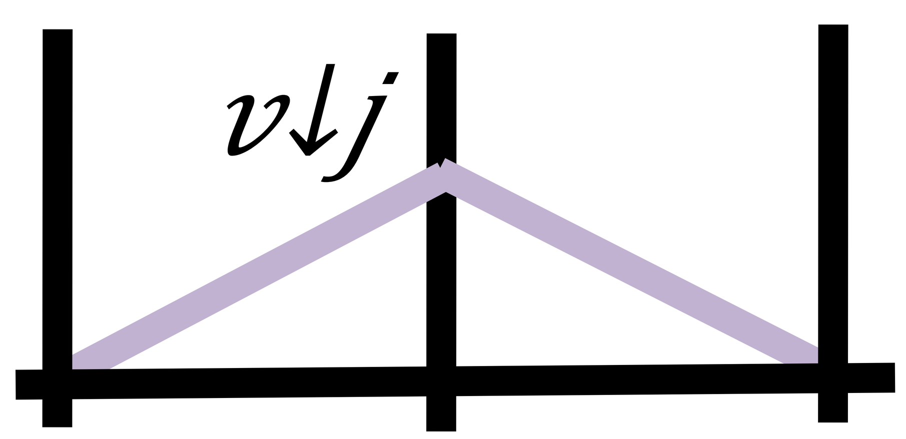
$$\int u' v' + [u' v]_I - \int f v = 0$$

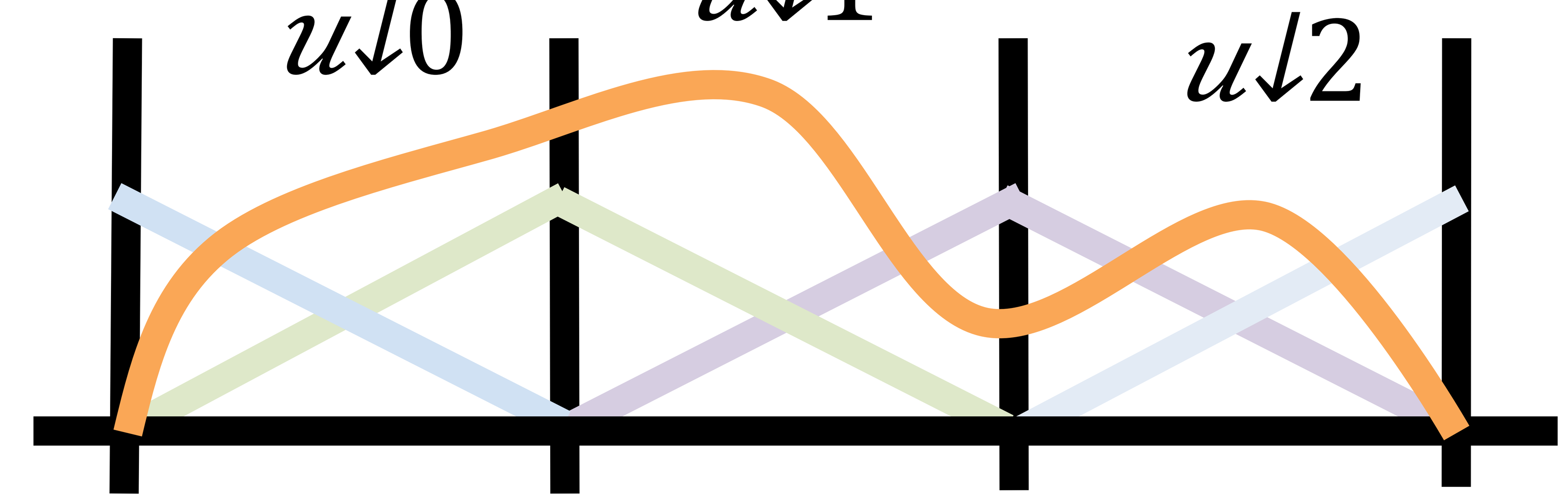
- Obtain Weak-form of *Finite Element Method*

$$\int u' v' - \int f v = 0$$

Example: Solving Heat Equation (1D)

- Choice of v: also serve as basis functions



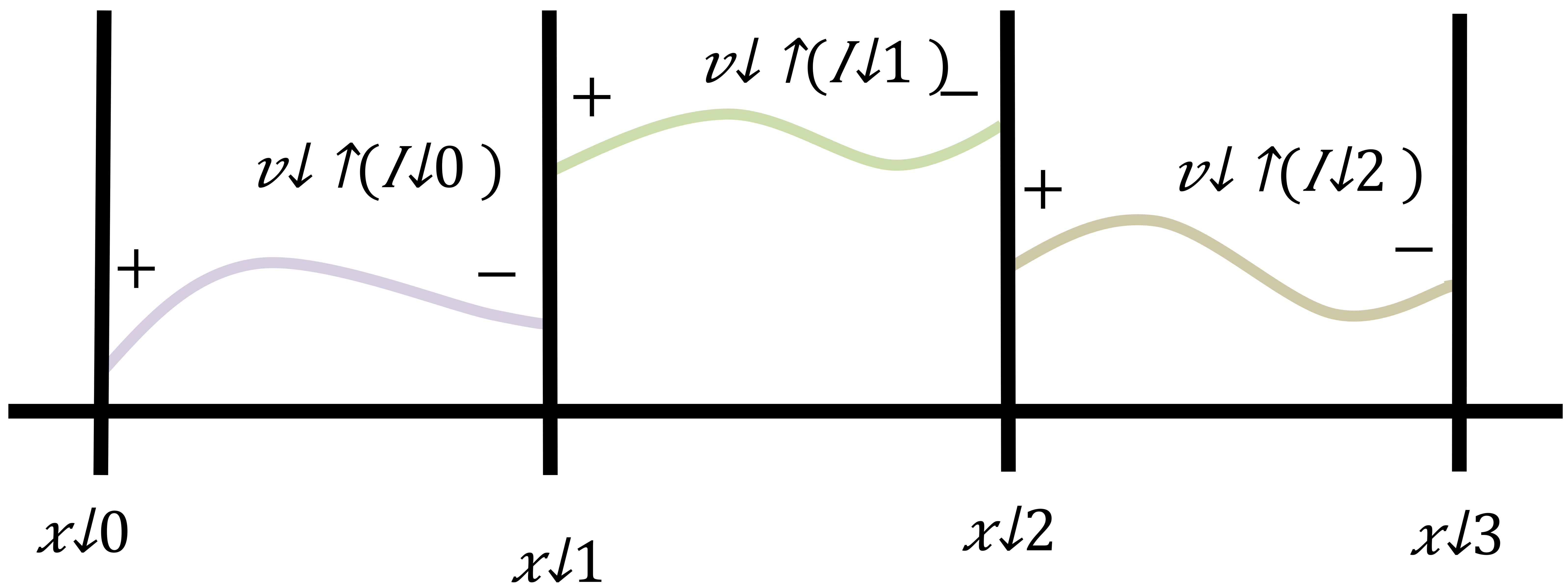


- Approximate $u_i = \sum_j u_j v_j$: linear combination of v_j

$$\begin{bmatrix} \int_I v_0' v_0' & \int_I v_1' v_0' & \int_I v_2' v_0' \\ \int_I v_0' v_1' & \int_I v_1' v_1' & \int_I v_2' v_1' \\ \int_I v_0' v_2' & \int_I v_1' v_2' & \int_I v_2' v_2' \end{bmatrix} \begin{bmatrix} u_0 \\ u_1 \\ u_2 \end{bmatrix} - \begin{bmatrix} \int_I f v_0 \\ \int_I f v_1 \\ \int_I f v_2 \end{bmatrix} = 0$$

Example: Solving Heat Equation (1D)

- Suppose v is discontinuous on x_j



- Integration by parts on each interval

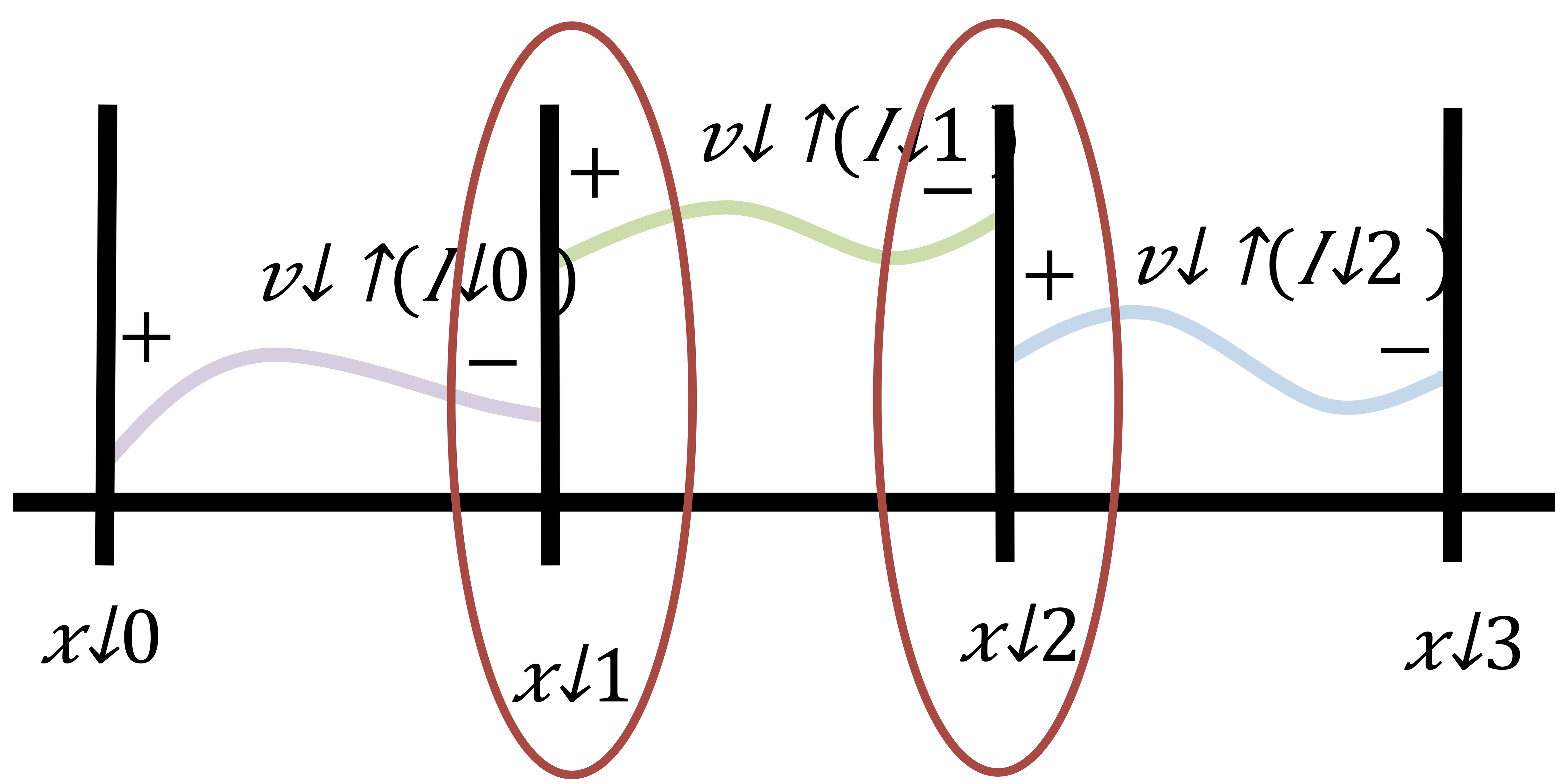
$$-\int u'' v = -\sum_j \int_{I_j} u'' v = \sum_j \left(\int_{I_j} u' v' \right) - \sum_j [u' v]_{x_j}^{x_{j+1}}$$

Example: Solving Heat Equation (1D)

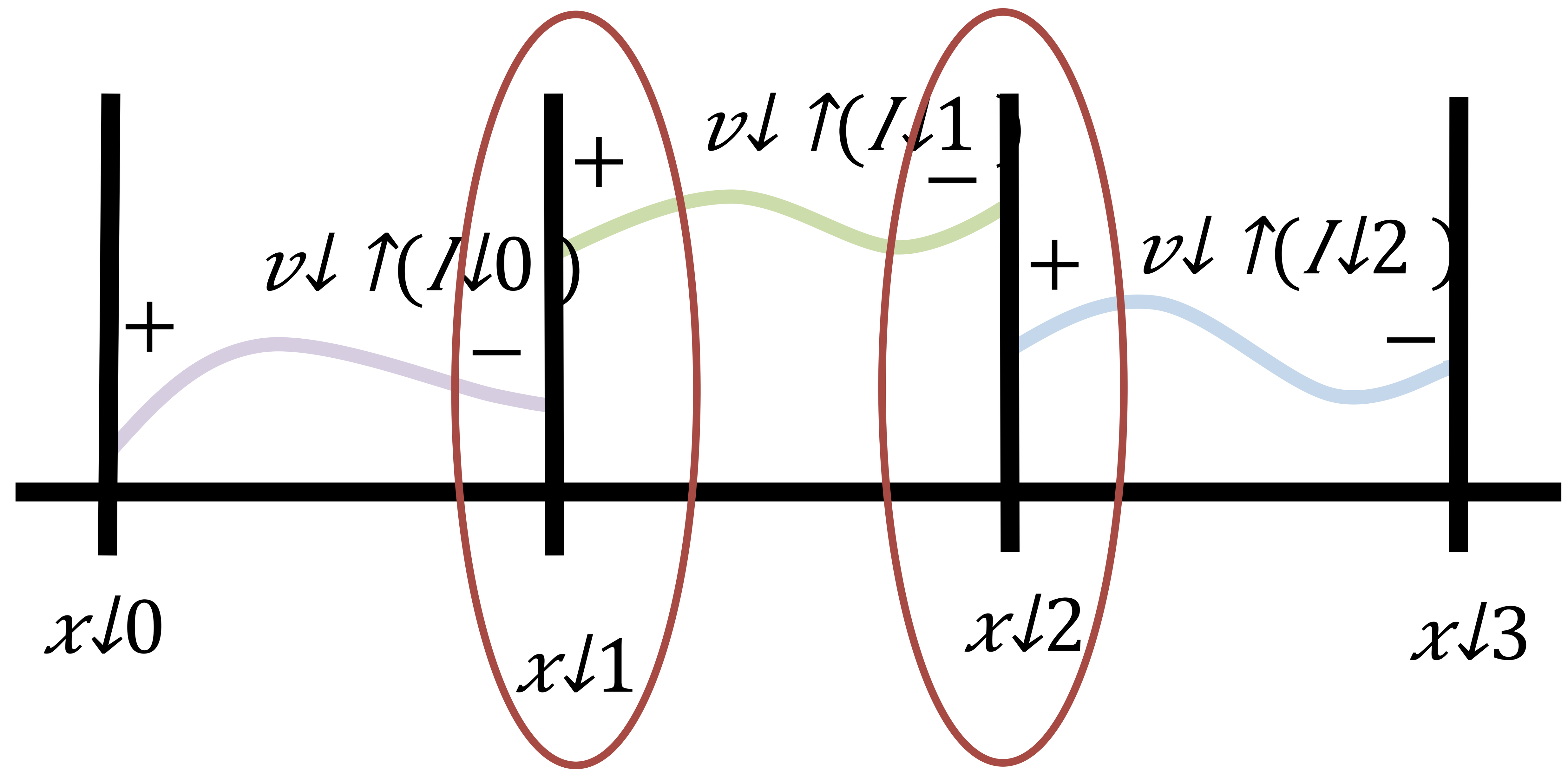
↑▒ [u′↑ v′]↓x↓j ↑x↓j+1 ↓↑ =∑j↑▒ u↑′ (x↓j↑+)v(x↓j↑+)−u↑′ (x↓j+1↑
(x↓j+1↑−)↓

▇= u↑′ (x↓0↑+)v(x↓0↑+)−u↑′ (x↓1↑−)v(x↓1↑−) + u↑′ (x↓1↑
+)v(x↓1↑+)−u↑′ (x↓2↑−)v(x↓2↑−) + u↑′ (x↓2↑
+)v(x↓2↑+)−u↑′ (x↓3↑−)v(x↓3↑−) ↓

=u↑′ (x↓0↑+)v(x↓0↑+)+∑**interiorj**↑▒ (**u↑′ (x↓j↑+)v(x↓j↑+)−u↑′ (x↓j↑−)v(x↓j↑**
−)↓)− u↑′ (x↓3↑−)v(x↓3↑−)



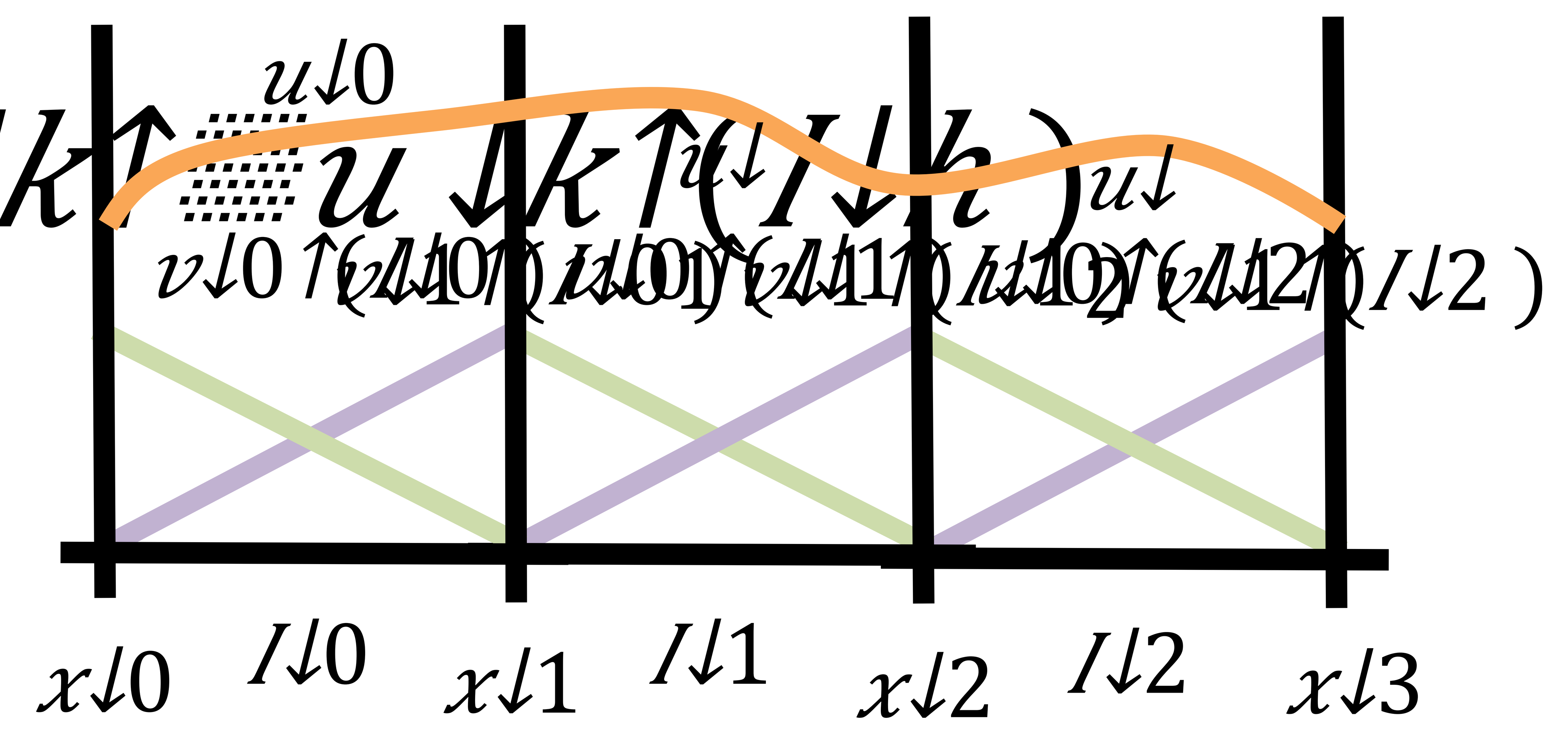
Example: Solving Heat Equation (1D)

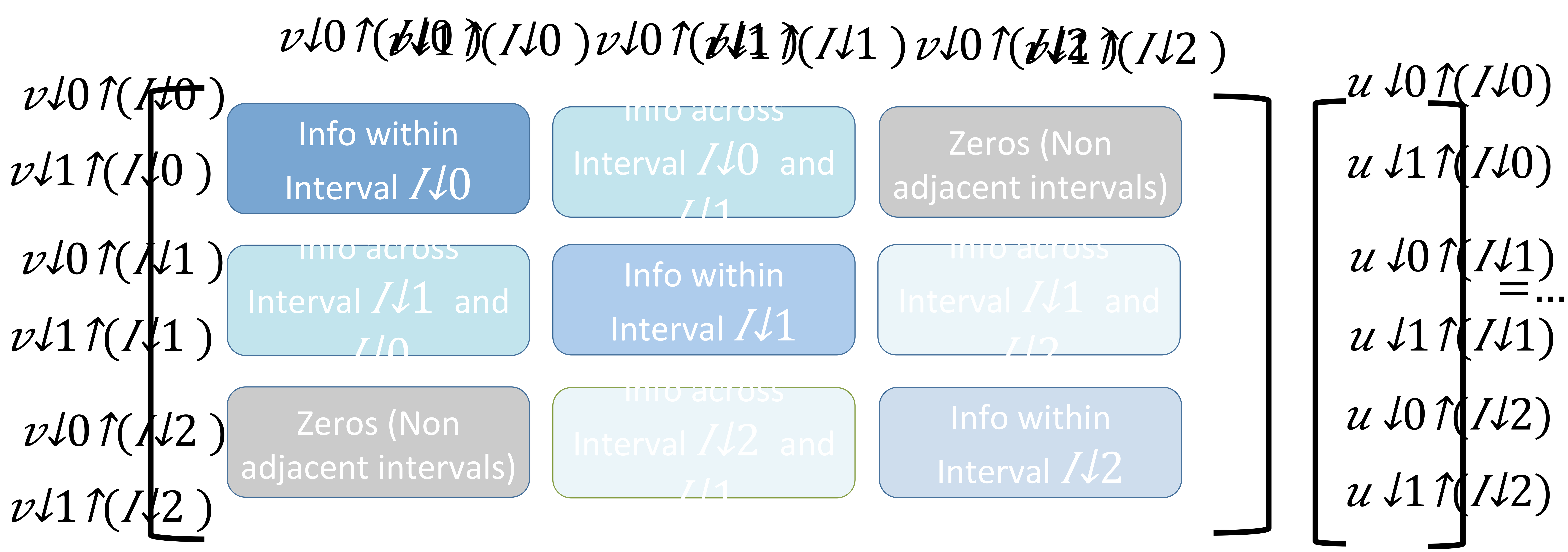


- Non-zero jumps at interior nodes
- Transfer intervals information between intervals
- Discontinuous Galerkin Methods

Example: Solving Heat Equation (1D)

- Approximate $u_h^{(I_h)} = \sum_k u_k^{(I_h)} v_k^{(I_h)}$
- Matrix formulation
  - In terms of blocks

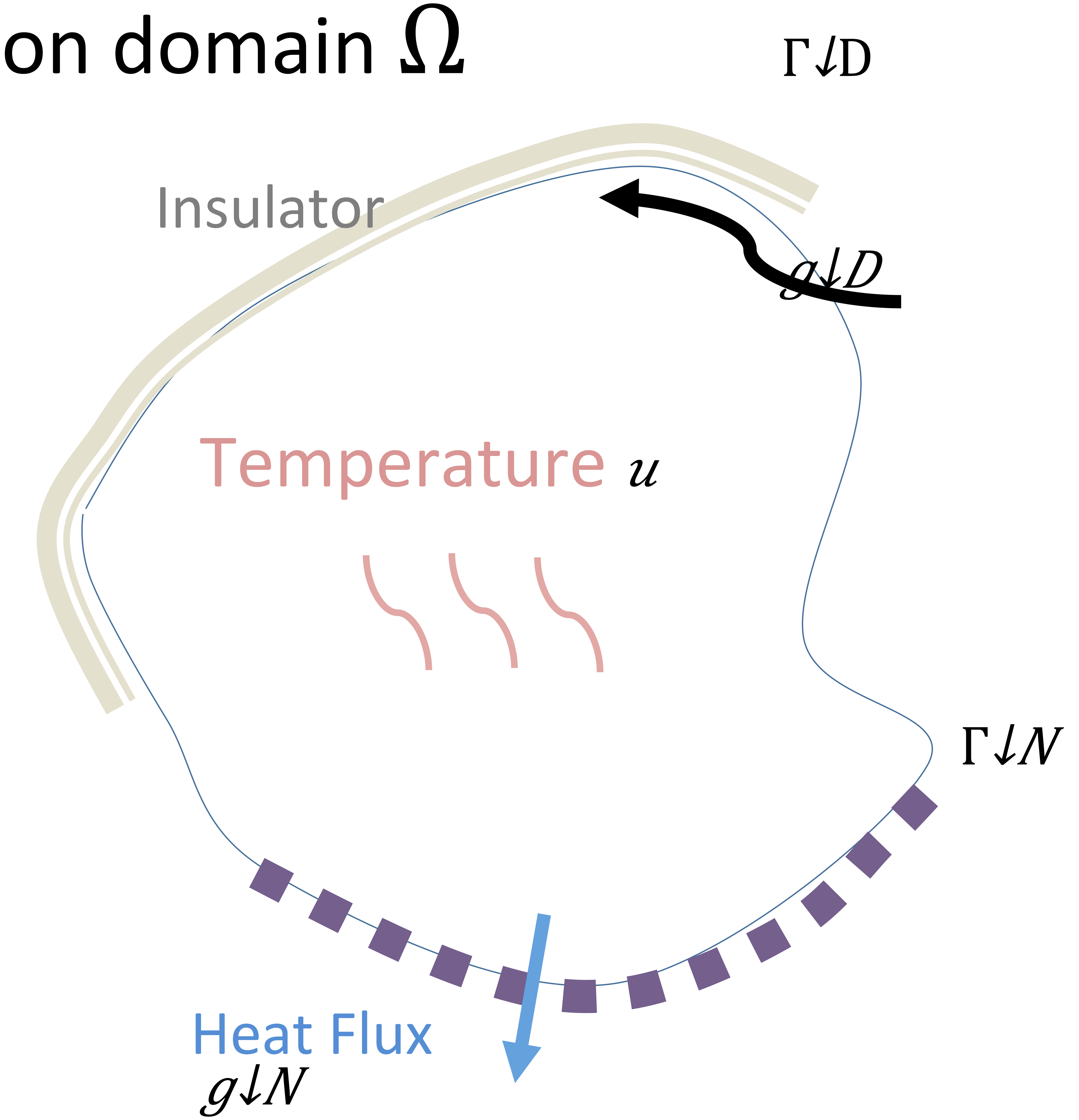




Example: Solving Heat Equation (1D)

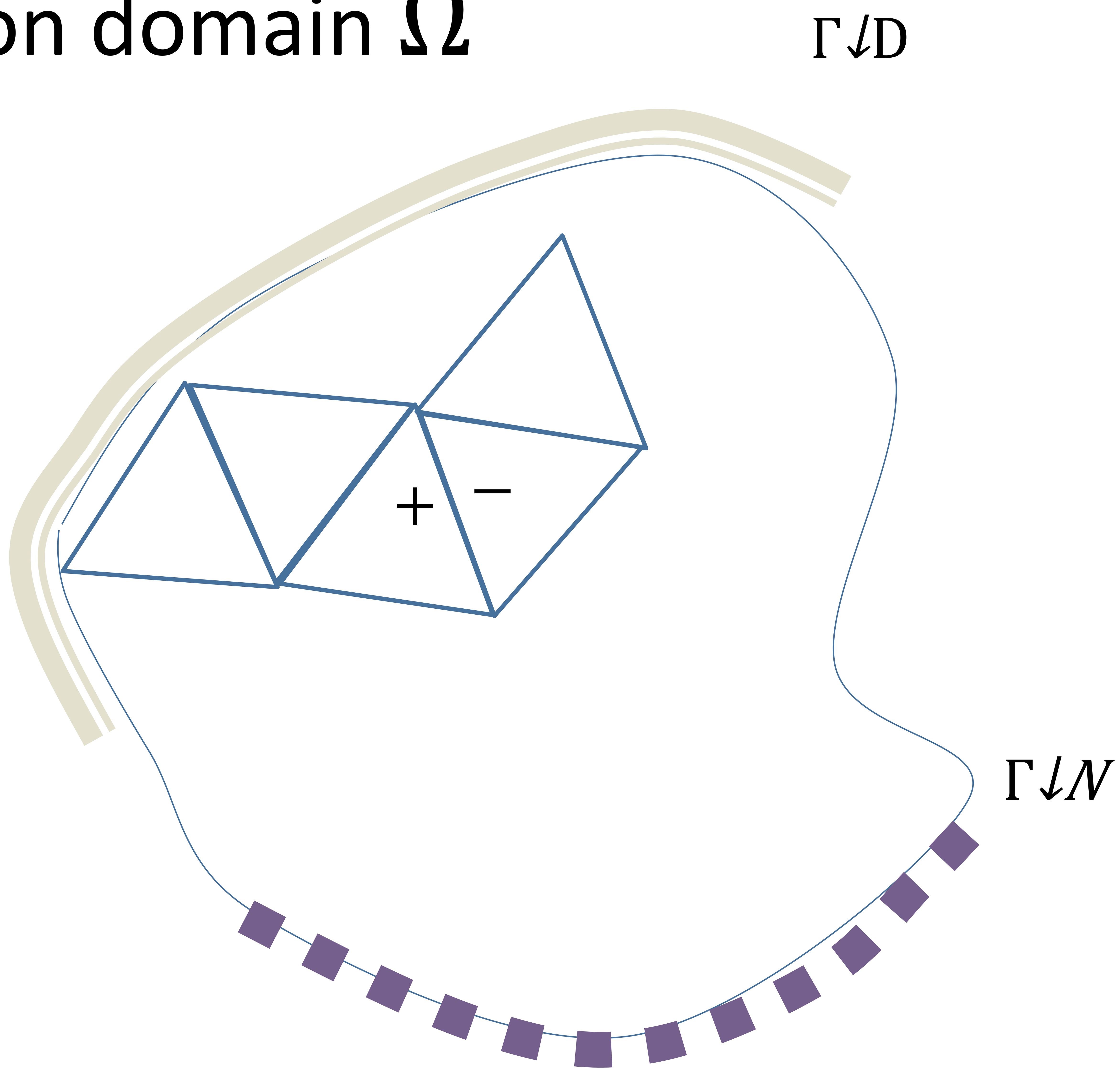
- 2D Poisson's Equation on domain Ω

$$
\begin{cases}
-\Delta u = f \\
u = g_D \text{ on } \Gamma_D \\
\partial u/\partial n = g_N \text{ on } \Gamma_N
\end{cases}
$$



Example: Solving Heat Equation (1D)

- 2D Poisson's Equation on domain Ω
- Partition the domain into triangles
- DG-FEM: Jumps across edges



Why DG-FEM over FEM

- Cons:
  - Large number of degrees of freedom
- Pros:
  - Increase of accuracy
  - Sparse matrix
  - Facilitation of parallelization
    - Information within or across local matrix blocks

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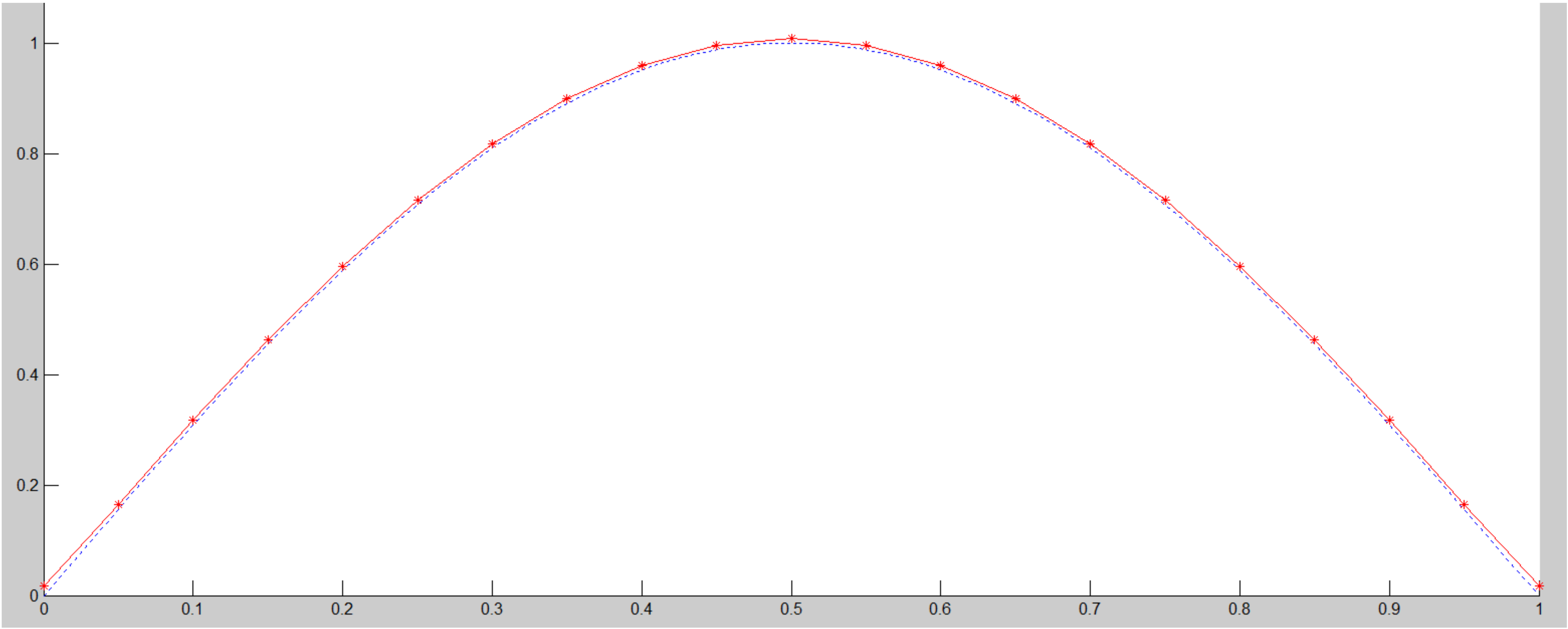
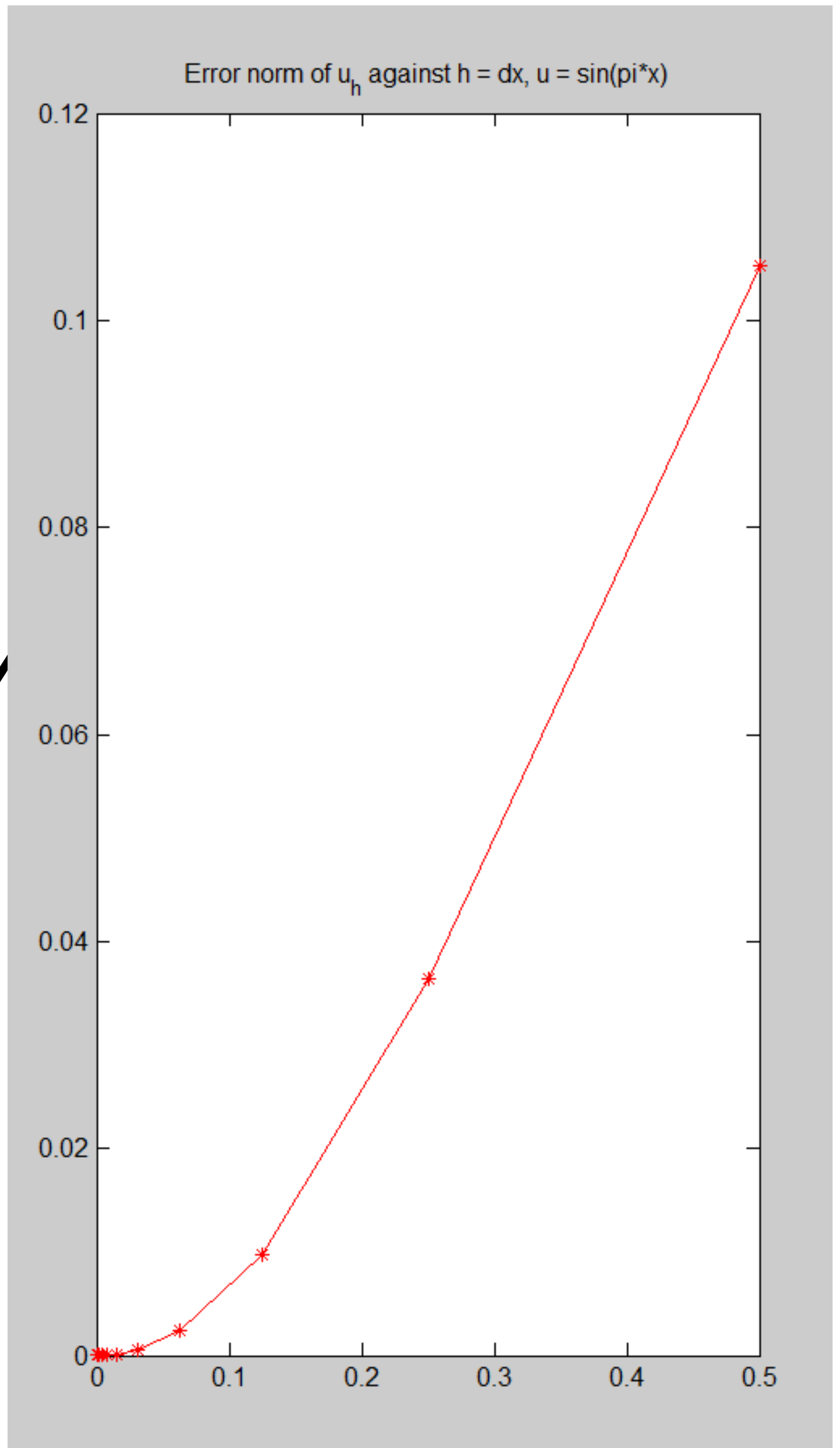
Current Progress

- Understand 1D DG serial code
  - Example: $f=\pi^2 \sin(\pi x)$, $u(0)=u(1)=0$
  - Basis functions $v_0 = 1-x$, $v_1 = x$
  - Number of intervals = 20



Current Progress

- Understand 1D DG serial code
    - Example: $f=\pi^2 \sin(\pi x)$, $u(0)=u(1)=0$
    - Basis functions $v_0 = 1-x$, $v_1 = x$
    - Number of intervals = 20
- Norm behaviors
    - $\left(\sum_{I} \int_{I} (u-u_h)^2 \, dx \right)^{1/}$



Current Progress

- Understand 1D DG serial code
- Extend the 1D serial code to parallel code
- Understand 2D DG serial code
- Extend *the 2D DG serial code to parallel code*
- Extend the 2D DG parallel code to *cover chemical transport equations (?)*
- Expand to 3D parallel code (?)
- Expand the code to be adaptive (?)

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