

# **The Discrete Variational Method and Its Application**

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# Contents

1. Introduction
2. The discrete variational method
3. Numerical experiments for  
nonlinear partial differential equation
4. Conclusion

# **1. Introduction**

# Purpose

We consider

- **one general procedure that preserve energy properties(energy conservation , energy dissipation, mass conservation etc)**
- **nonlinear PDE with variable coefficients which is arised from population gene model.**

# **Numerical scheme that preserve energy properties**

Advantage

Physical reasonable numerical solutions

Robust numerical scheme

## **Ordinary differential equation**

Greenspan, Hairer, Itoh, Maeda, Marsden, McLachlan,  
Munthe-Kaas, Owren, Quispel, Sanz-Serna, Yoshida etc

## **Partial differential equation**

FDS · · · Fei, Li, Vu-Quoc, Vazquez etc

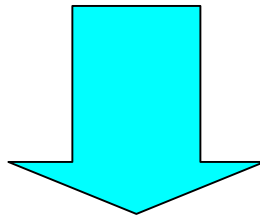
FEM · · · Du, French, Nikolaidis etc

Multi symplectic method · · · Bridge, Hong, Reich etc

## **2. The discrete variational method**

**What is**

**“ The discrete variational method” ?**

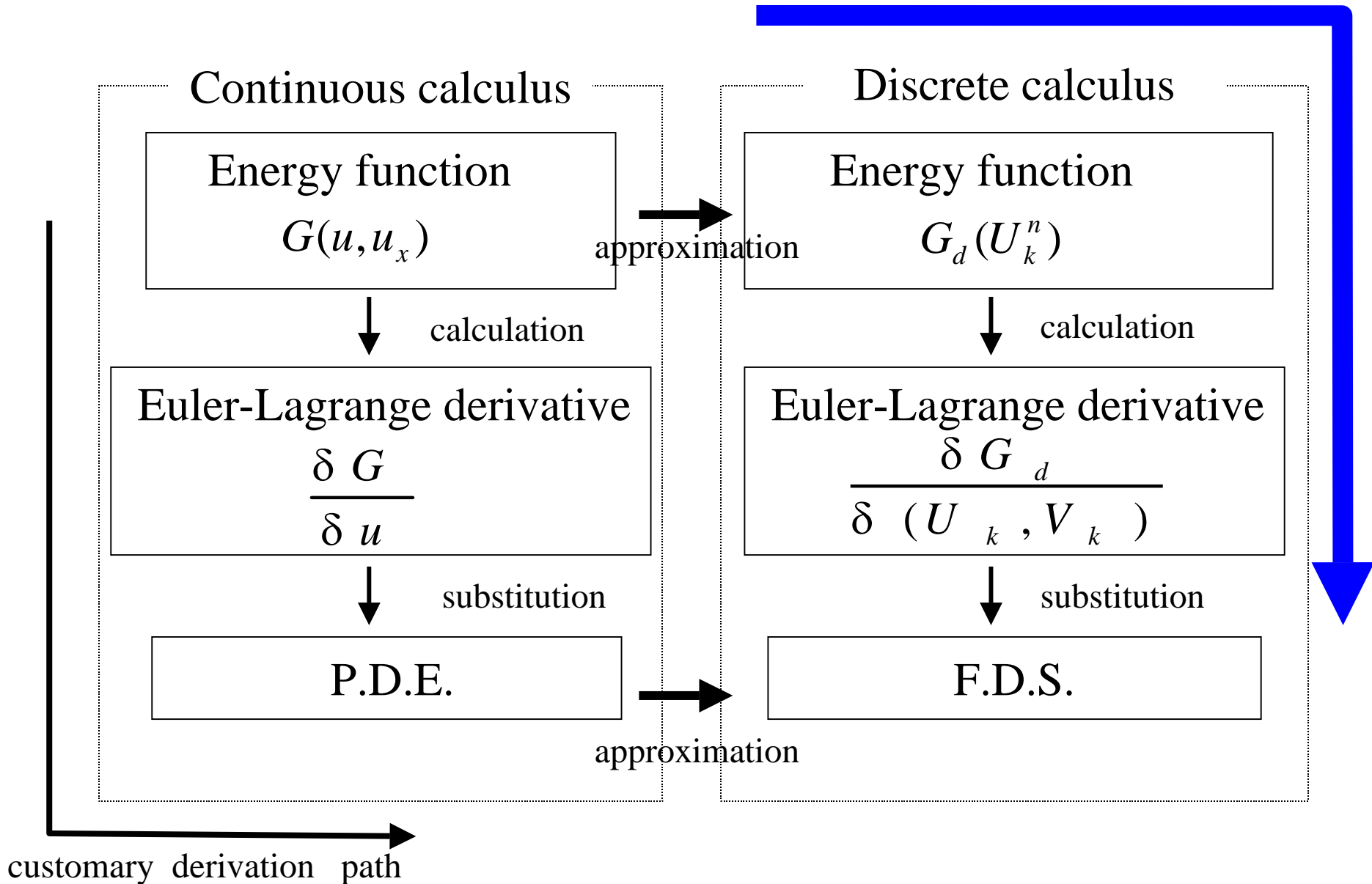


**One general procedure of designing**

**FDS for PDE**

**that preserve energy properties**

## 2.1 Concept of the discrete variational method

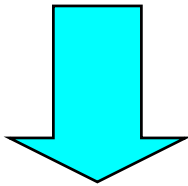


D. Furihata (Osaka University, Japan)

- Finite difference schemes for  $\frac{\partial u}{\partial t} = \left(\frac{\partial}{\partial x}\right)^\alpha \frac{\delta G}{\delta u}$  that inherit energy conservation or dissipation property, J.Comput.Phys.**156**(1999), 181-205.

- Finite difference schemes for nonlinear wave equation that inherit energy conservation property, J.Comput.Appl.Math. 134(2001),37-57.

$$\frac{\partial u}{\partial t} = \left( \frac{\partial}{\partial x} \right)^\alpha \frac{\delta G}{\delta u}$$



$$\frac{d}{dt} \int G(u, u_x) dx = 0 : \alpha \text{ is odd}$$

(eg KdV eq etc)

$$(-1)^{\frac{\alpha}{2}+1} \frac{d}{dt} \int G(u, u_x) dx \leq 0 : \alpha \text{ is even}$$

(eg Cahn-Hilliard eq, linear heat eq etc)

T. Matsuo (Nagoya University, Japan)

- Complex valued problem (e.g. NLS eq etc)
- Pseudo spectral method

## 2.2 Calculus of variation

### 1st step

$$J[u] \stackrel{\text{def}}{=} \int_a^b G(u, u_x) dx : \text{total energy}$$

where

$$G(u, u_x) : \text{energy function}$$

### 2nd step

$$J[u + \delta u] - J[u] \cong \int_a^b \frac{\delta G}{\delta u} \delta u dx + \left[ \frac{\partial G}{\partial u_x} \delta u \right]_a^b.$$



Integration by parts

### 3rd step

$$\frac{\partial u}{\partial t} = \frac{\partial^\alpha}{\partial x^\alpha} \left( \frac{\delta G}{\delta u} \right).$$

## 2.3 Calculus of discrete variation

### 1st step

$$J_d[U_k] = \sum_{k=0}^N G_d(U_k) \Delta x.$$

where

$G_d(U_k)$ : discrete energy function

### 2nd step

$$J_d[U_k] - J_d[V_k] = \sum_{k=0}^N \frac{\delta G_d}{\delta (U_k, V_k)} (U_k - V_k) \Delta x + \left[ \frac{\partial G_d}{\partial \delta (U_k, V_k)} \right]_0^N$$



Summation by parts

### 3rd step

$$\frac{U_k^{n+1} - U_k^n}{\Delta t} = \delta_k^{(\alpha)} \frac{\delta G_d}{\delta (U_k^{n+1}, U_k^n)}.$$

# Notations

$$\Delta x = \frac{b-a}{N} : \text{space mesh size}$$

$$\Delta t : \text{time mesh size}$$

$$U_k^n \cong u(a + k\Delta x, n\Delta t) : \text{numerical solution}$$

$$\sum_{k=0}^N U_k \Delta x = \left( \frac{1}{2} U_0 + \sum_{k=1}^{N-1} U_k + \frac{1}{2} U_N \right) \Delta x : \text{trapezoidal rule}$$

$$\delta_k^+ U_k = \frac{U_{k+1} - U_k}{\Delta x} : \text{Euler difference operator}$$

$$\delta_k^- U_k = \frac{U_k - U_{k-1}}{\Delta x} : \text{backward difference operator}$$

$$\delta_k^{(1)} U_k = \frac{U_{k+1} - U_{k-1}}{2\Delta x} : \text{1st central difference operator}$$


$$\delta_k^{(2)} U_k = \frac{U_{k+1} - 2U_k + U_{k-1}}{(\Delta x)^2} : \text{2nd central difference operator}$$

### 3. Numerical experiments for nonlinear partial differential equation

# 3.1 Target Equation

$$(1) \begin{cases} \frac{\partial u}{\partial t} = -\frac{\delta G}{\delta u} \text{ where} \\ \frac{\delta G}{\delta u} = -d \frac{\partial^2 u}{\partial x^2} - u(u - a(x))(1 - u), \text{ in } \Omega = [a, b], t > 0, \\ \frac{\partial u}{\partial x}(a, t) = \frac{\partial u}{\partial x}(b, t) = 0, \text{ : Neumann condition} \\ u(x, 0) = u_0(x) \geq 0, \text{ : Initial condition.} \end{cases}$$

$d(> 0)$  : diffusion coefficient,

$a(x) \in C^0(\Omega)$ ,  **amount of contamination**

$G(u, u_x) = \frac{1}{2} d \left( \frac{\partial u}{\partial x} \right)^2 + \frac{a(x)}{2} u^2 - \frac{1 - a(x)}{3} u^3 + \frac{1}{4} u^4$  : energy function,

$\frac{\delta G}{\delta u} \stackrel{def}{=} \frac{\partial G}{\partial u} - \frac{\partial}{\partial x} \frac{\partial G}{\partial u_x}$  : Euler – Lagrange derivative.

## Theorem(Energy Dissipation)

Let  $u$  be a solution of (1). Then the total energy

$$J[u] = \int_a^b G(u, u_x) dx$$

is dissipation with respect to  $t$

$$\frac{d}{dt} J[u] = \frac{d}{dt} \int_a^b G(u, u_x) dx \leq 0.$$

**Question Steady stable solution of (1) ?**

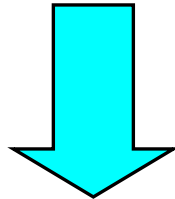
Does solution of (1) have multiplicity ?

Where is the transition layer ?

## 3.2 Proposed Scheme and Its Discrete Energy Property

Discretization of energy function

$$G(u, u_x) = \frac{1}{2} d \left( \frac{\partial u}{\partial x} \right)^2 + \frac{a(x)}{2} u^2 - \frac{1-a(x)}{3} u^3 + \frac{1}{4} u^4$$



$$G_d(U_k^n) = \frac{d}{2} \frac{(\delta_k^+ U_k^n)^2 + (\delta_k^- U_k^n)^2}{2} + \frac{a_k}{2} (U_k^n)^2 - \frac{1-a_k}{3} a_k (U_k^n)^3 + \frac{1}{4} (U_k^n)^4$$

where

$$a_k \cong a(x)$$

## 3.2 Proposed Scheme and Its Discrete Energy Property

$$(2) \left\{ \begin{array}{l} \frac{U_k^{n+1} - U_k^n}{\Delta t} = -\frac{\delta G_d}{\delta(U_k^{n+1}, U_k^n)} \text{ where} \\ \frac{\delta G_d}{\delta(U_k^{n+1}, U_k^n)} = -\frac{d}{2} \delta_k^{(2)} (U_k^{n+1} + U_k^n) + \frac{a_k}{2} (U_k^{n+1} + U_k^n) \\ -\frac{1-a_k}{3} \left\{ (U_k^{n+1})^2 + U_k^{n+1} U_k^n + (U_k^n)^2 \right\} \\ + \frac{1}{4} \left\{ (U_k^{n+1})^3 + (U_k^{n+1})^2 U_k^n + U_k^{n+1} (U_k^n)^2 + (U_k^n)^3 \right\}, k = 0, \dots, N, \\ U_{-1}^n = U_1^n = 0, U_{N+1}^n = U_{N-1}^n = 0, n = 0, 1, 2, \dots, \\ U_k^0 \geq 0, k = 0, \dots, N. \end{array} \right.$$

## **Theorem**(Discrete Energy Dissipation)

Let  $U_k^n$  be a solution of (2). Then the discrete total energy

$$J_d[U_k] = \sum_{k=0}^N G_d(U_k) \Delta x$$

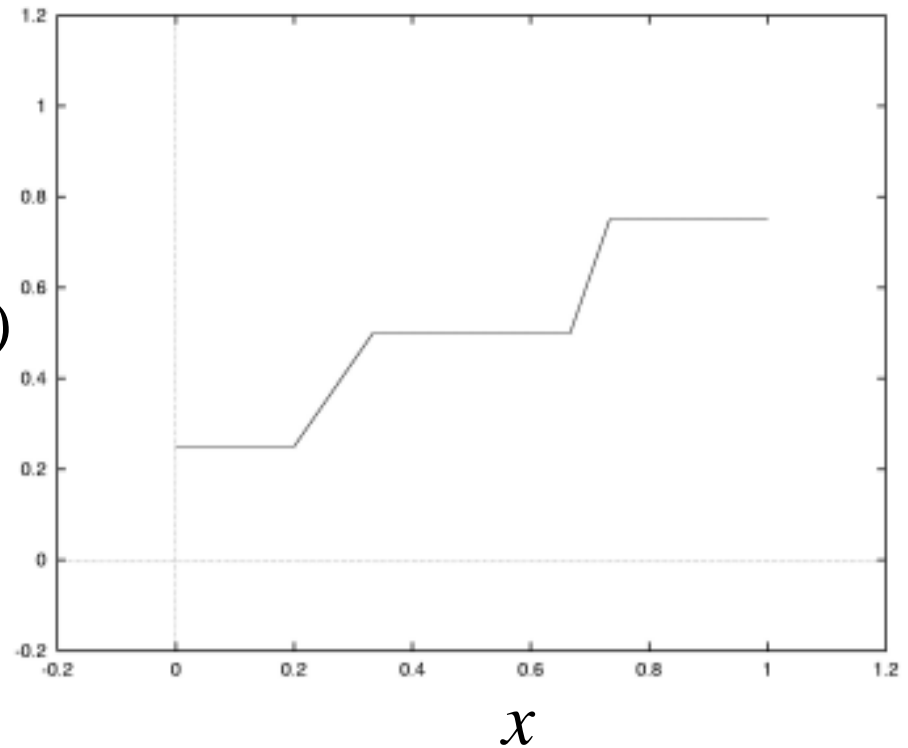
is dissipation with respect to  $n$ ,

$$\frac{1}{\Delta t} \left\{ J_d[U_k^{n+1}] - J_d[U_k^n] \right\} \leq 0.$$

# 3.3 Numerical experiments

variable coefficients

$$a(x) = \begin{cases} \frac{1}{4}, & 0 \leq x \leq \frac{30}{150}, \\ \frac{5}{18}x + \frac{7}{36}, & \frac{30}{150} \leq x \leq \frac{50}{150}, \\ \frac{1}{2}, & \frac{50}{150} \leq x \leq \frac{100}{150}, \\ \frac{15}{4}x - 2, & \frac{100}{150} \leq x \leq \frac{110}{150}, \\ \frac{3}{4}, & \frac{110}{150} \leq x \leq 1. \end{cases} \quad a(x)$$



# Numerical experiment

(Comparison of central difference scheme)

$$\Omega = [0,1]$$

$$\Delta x = \frac{1}{75} : \textit{space mesh size}$$

$$\Delta t = \frac{1}{100} : \textit{time mesh size}$$

$$d = 0.01 : \textit{diffusion coefficient}$$

$$u(x,0) = \begin{cases} 0.4, & 0 \leq x \leq \frac{20}{75}, \\ 0, & \frac{20}{75} < x \leq 1. \end{cases}$$

## Explicit scheme

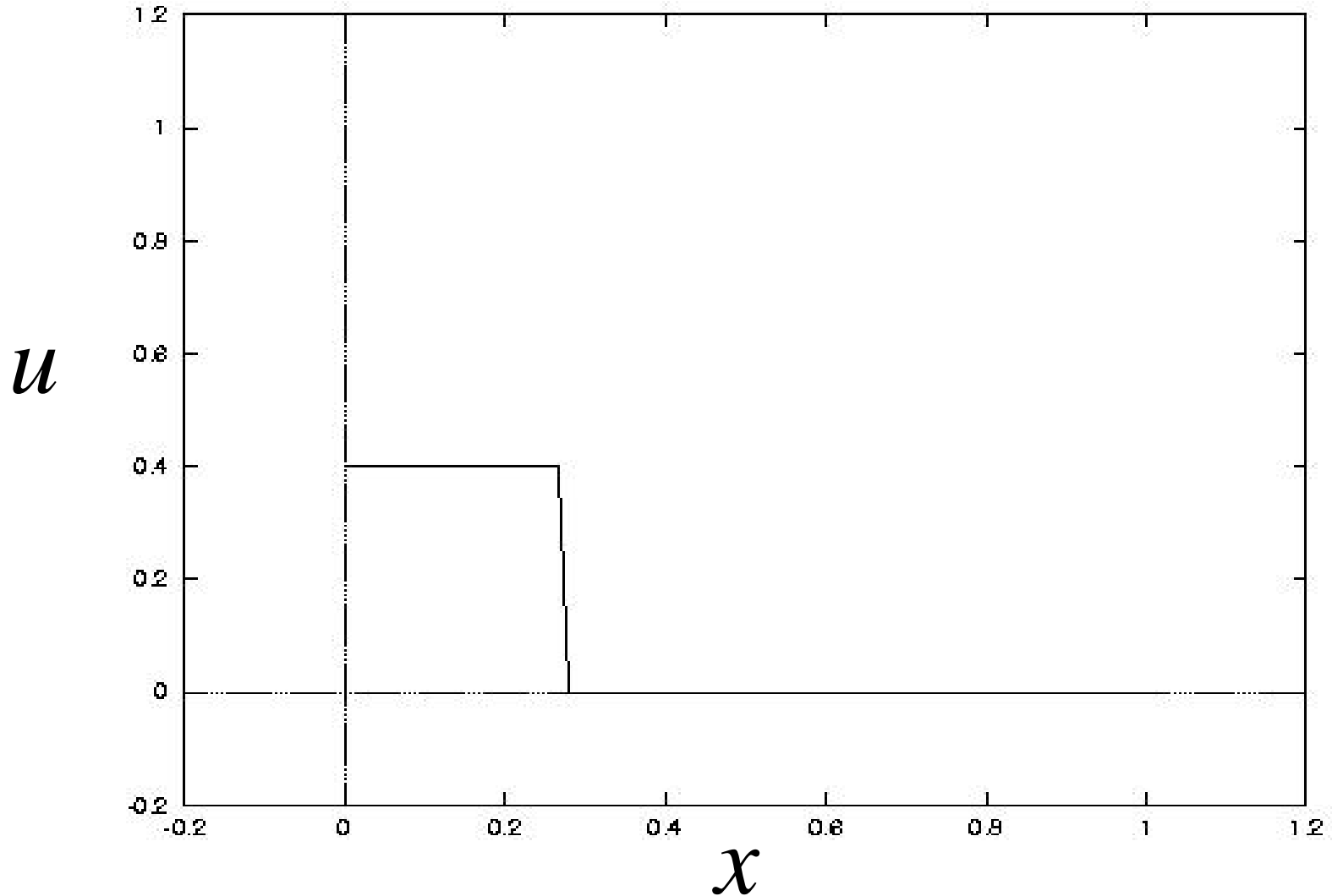
$$(3) \begin{cases} \frac{U_k^{n+1} - U_k^n}{\Delta t} = d \frac{U_{k+1}^n - 2U_k^n + U_{k-1}^n}{(\Delta x)^2} + U_k^n (U_k^n - a_k) (1 - U_k^n), & k=0, \dots, N, \\ U_{-1}^n = U_1^n = 0, \\ U_{N+1}^n = U_{N-1}^n = 0, \\ U_k^0 \geq 0, & k=0, \dots, N. \end{cases}$$

## Discrete energy function

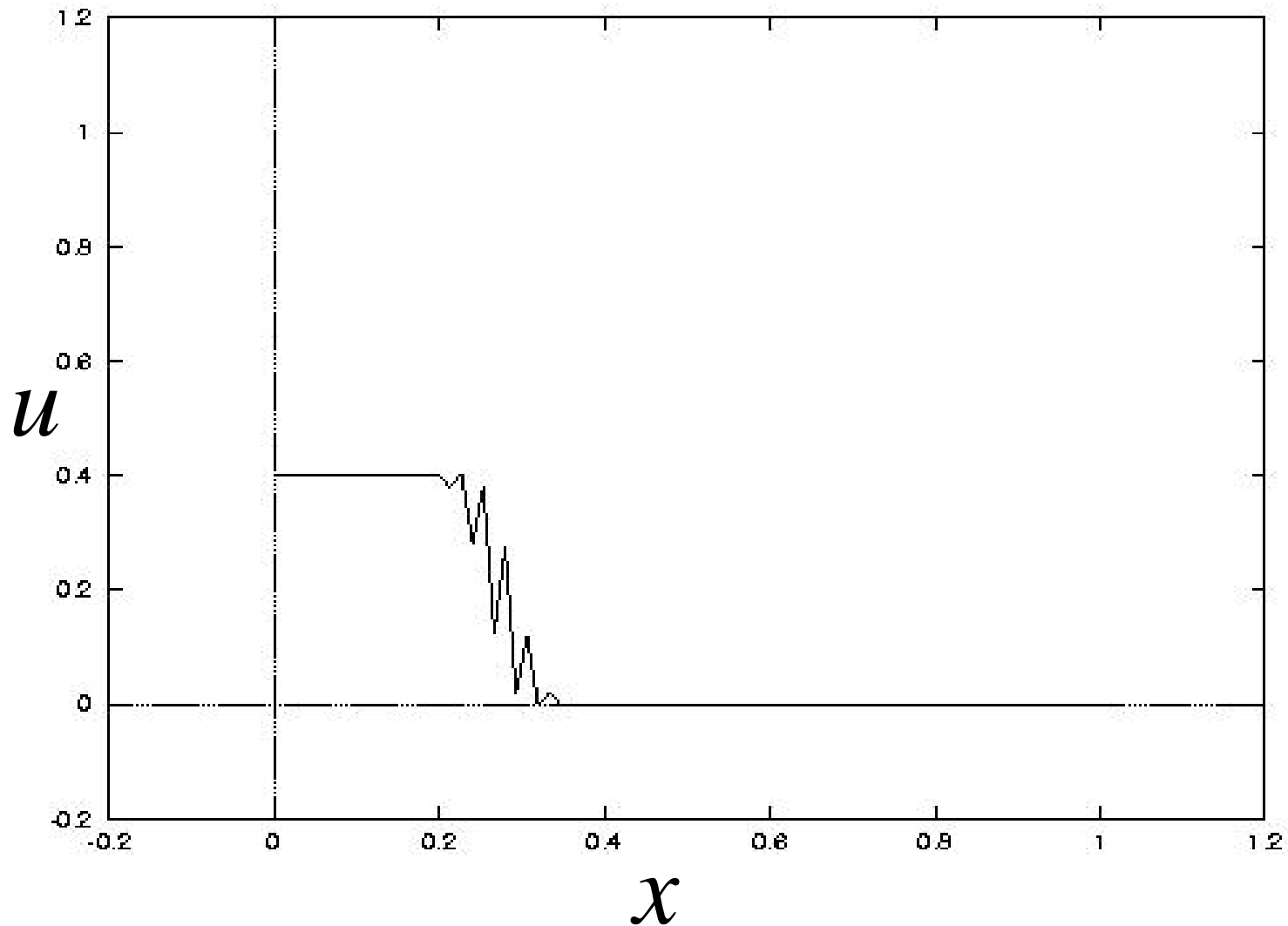
$$G_d(U_k^n) = -\frac{d}{2} (\delta_k^{(1)} U_k^n)^2 + \frac{a_k}{2} (U_k^n)^2 - \frac{1-a_k}{3} a_k (U_k^n)^3 + \frac{1}{4} (U_k^n)^4$$

# Numerical experiment of explicit scheme

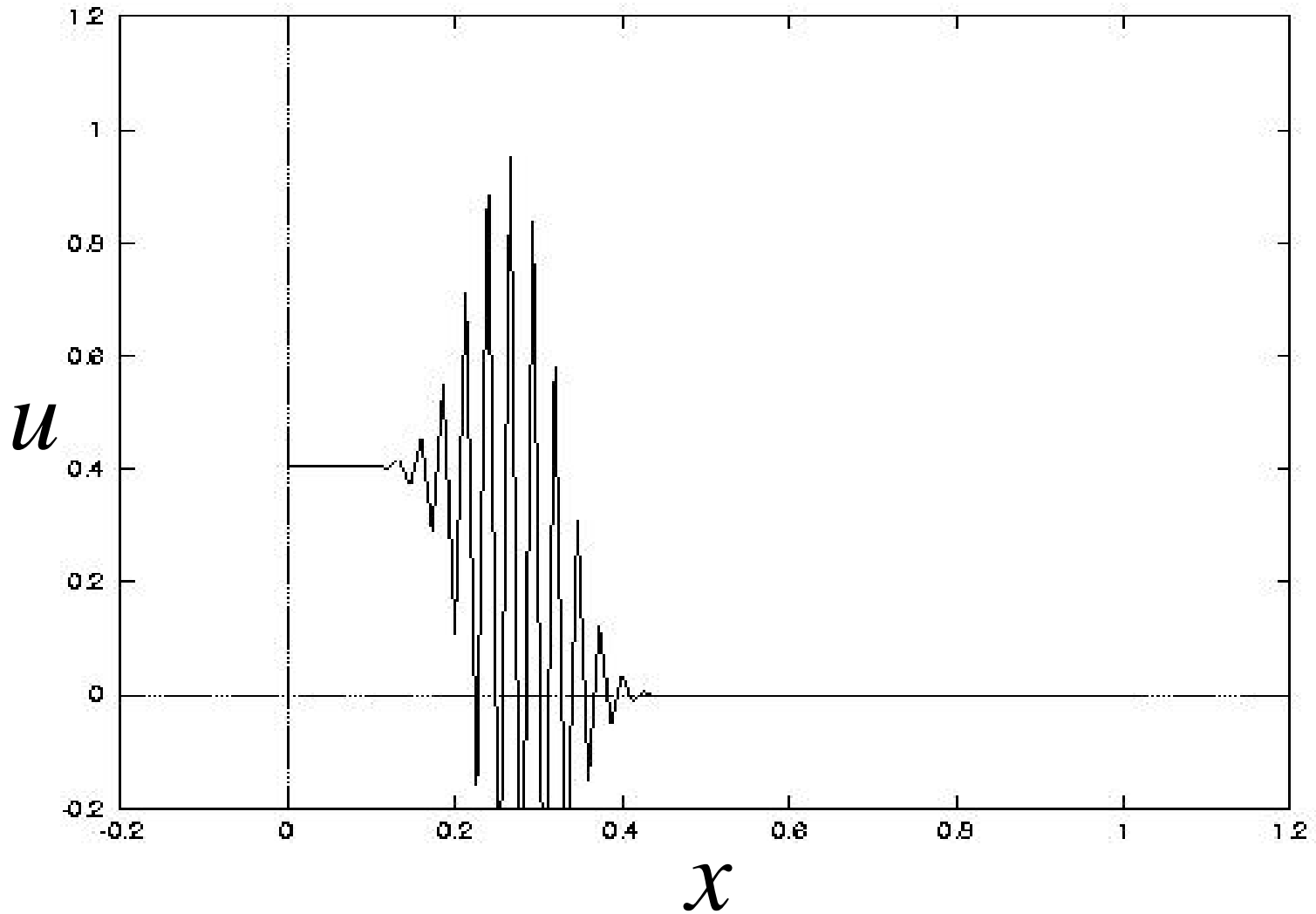
Initial value (time step  $n=0$ )



time step  $n=50$

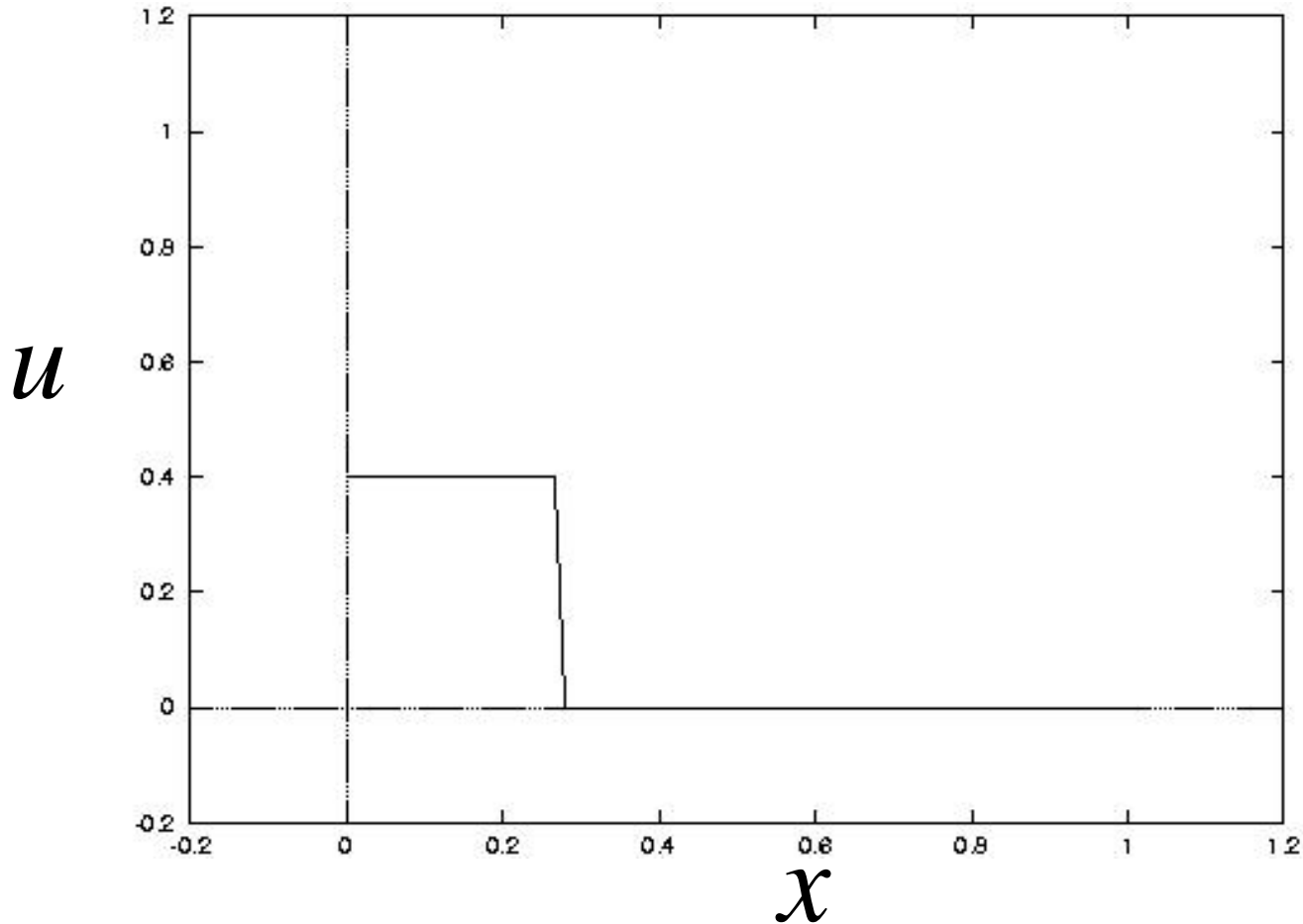


time step  $n=160$

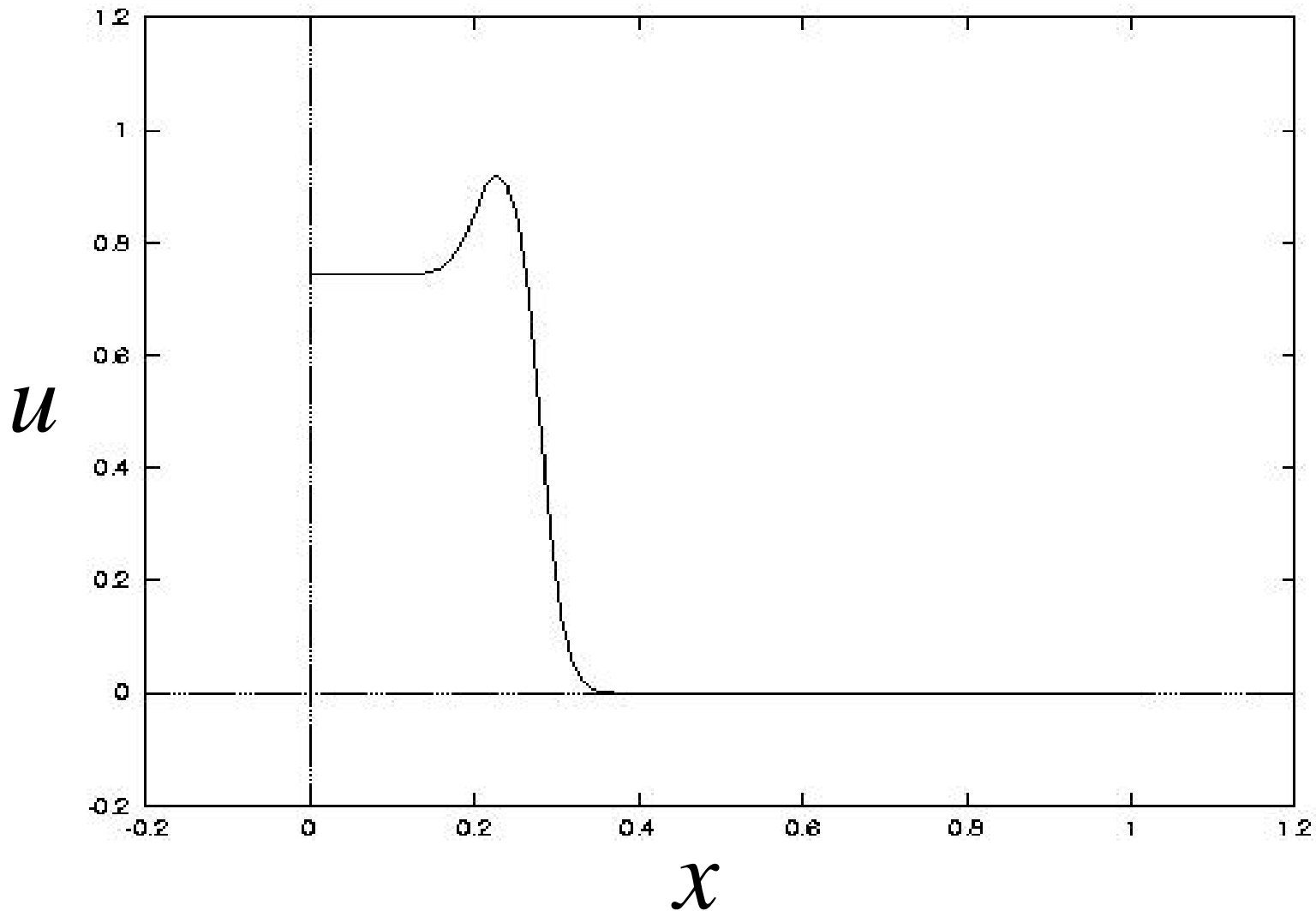


# Numerical experiment proposed scheme

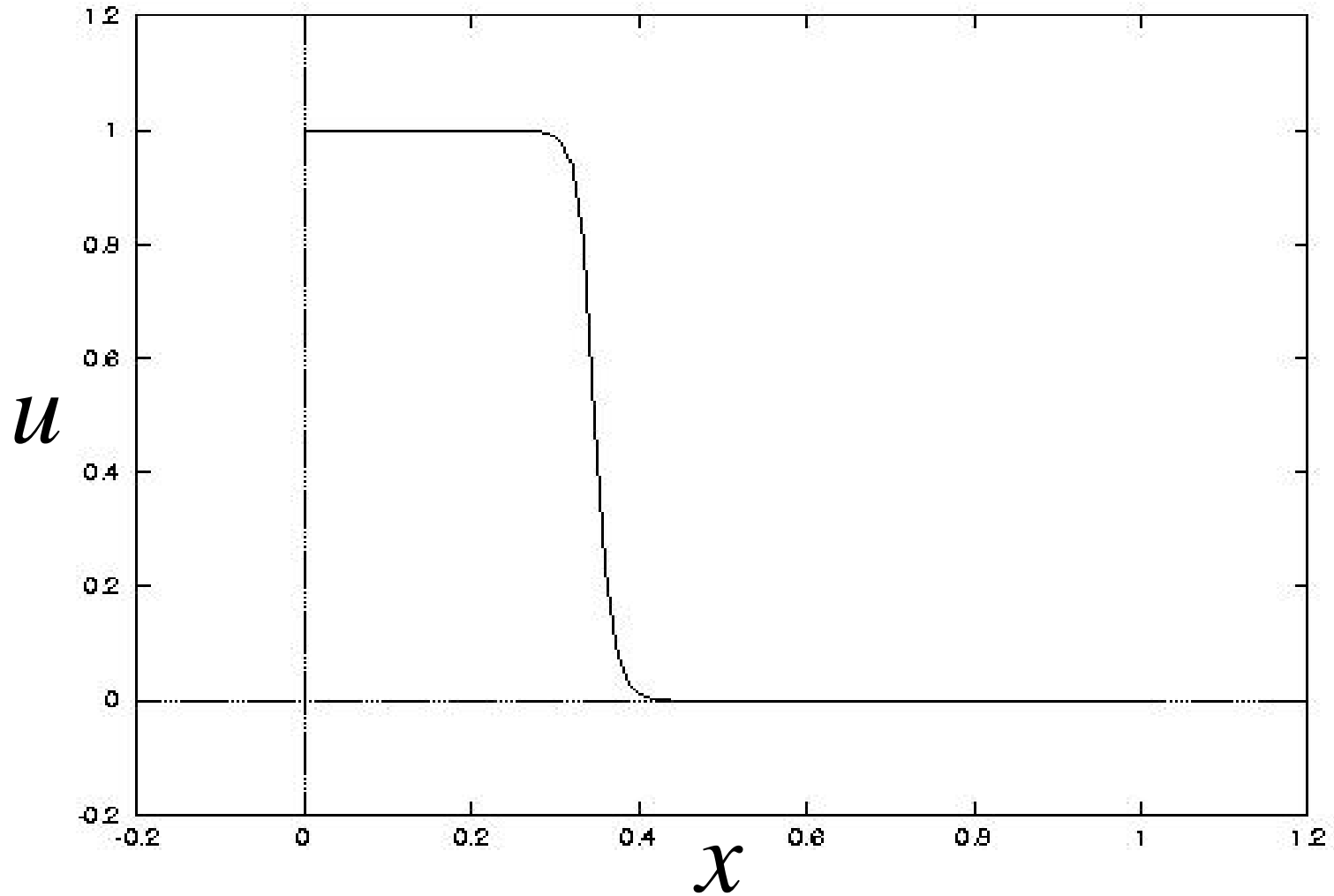
Initial value (time step  $n=0$ )



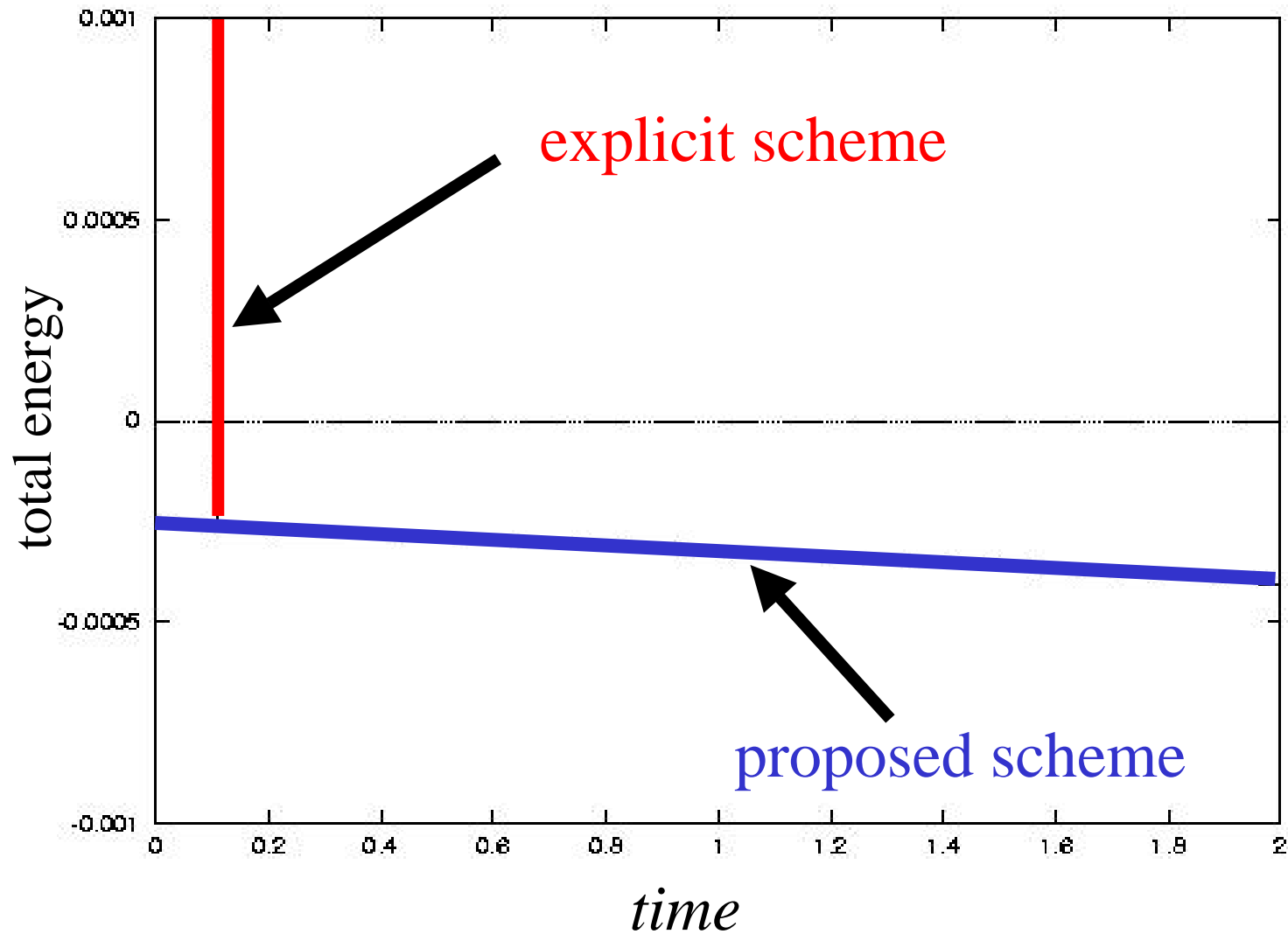
time step  $n=50$



time step  $n=200$



# Time evolution of discrete total energy



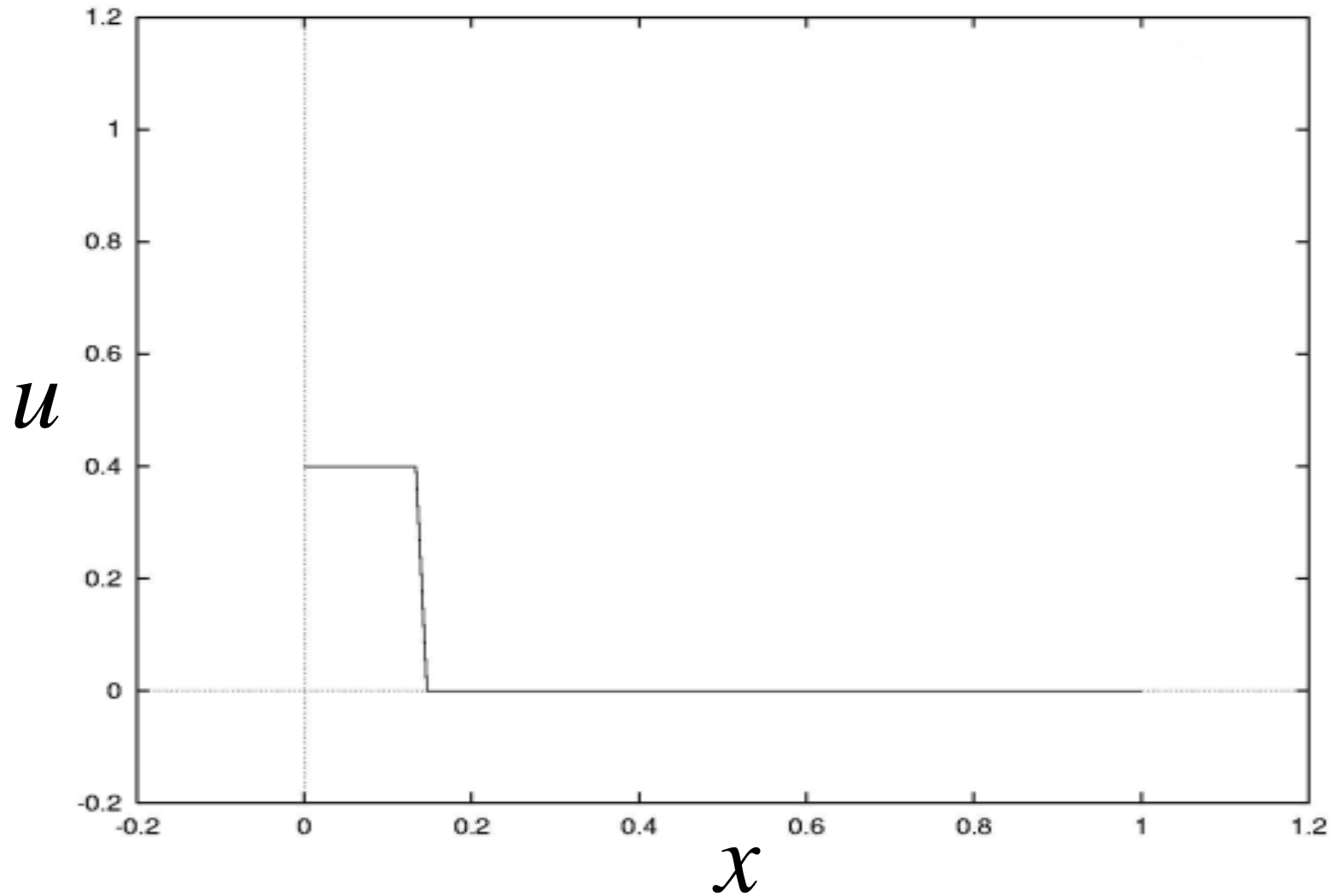
# Numerical experiments

Initial conditions are

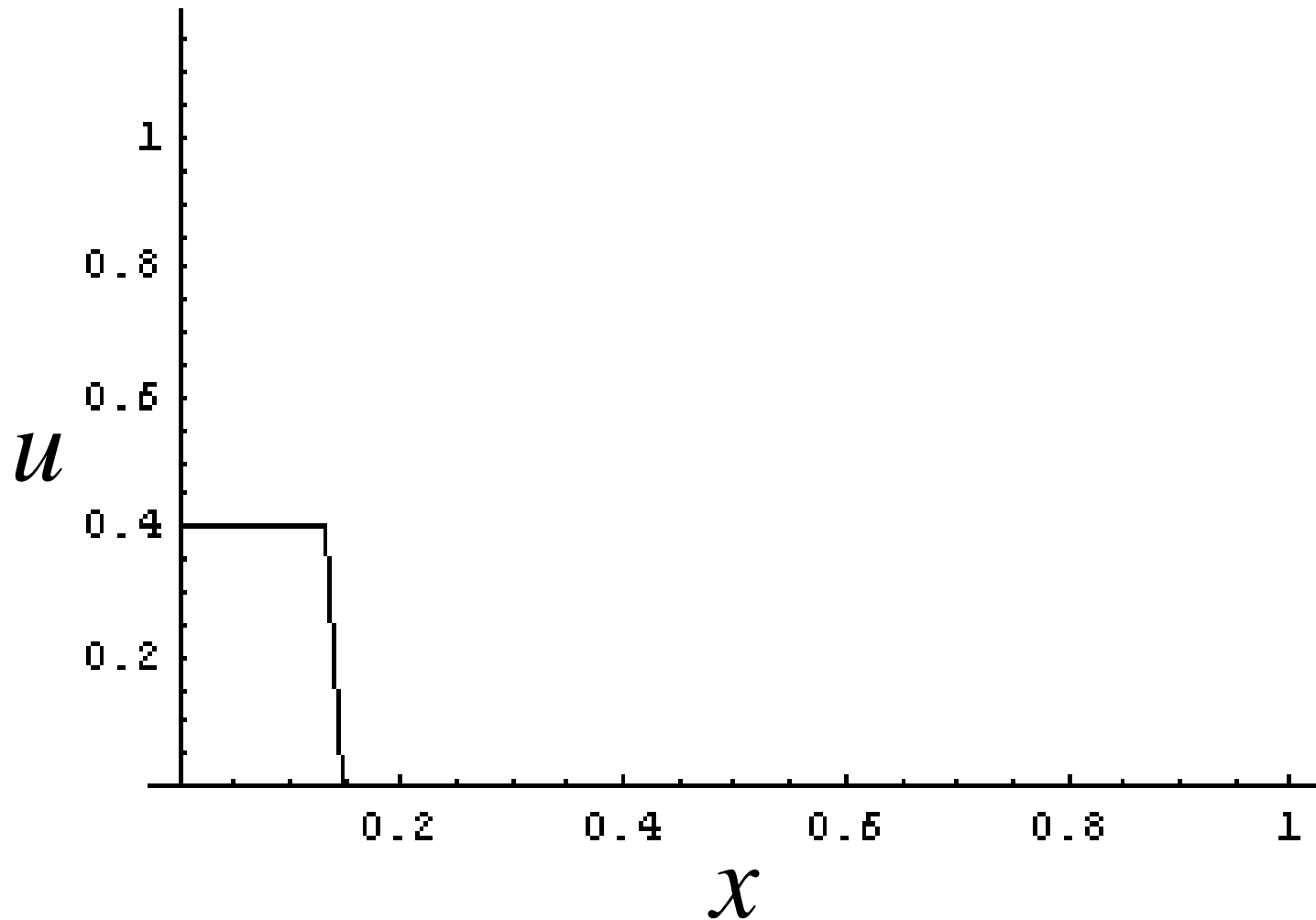
1. 
$$u(x,0) = \begin{cases} 0.4, & 0 \leq x \leq \frac{10}{75}, \\ 0, & \frac{10}{75} < x \leq 1. \end{cases}$$

2. 
$$u(x,0) = \begin{cases} 0.4, & 0 \leq x \leq \frac{70}{75}, \\ 0, & \frac{70}{75} < x \leq 1. \end{cases}$$

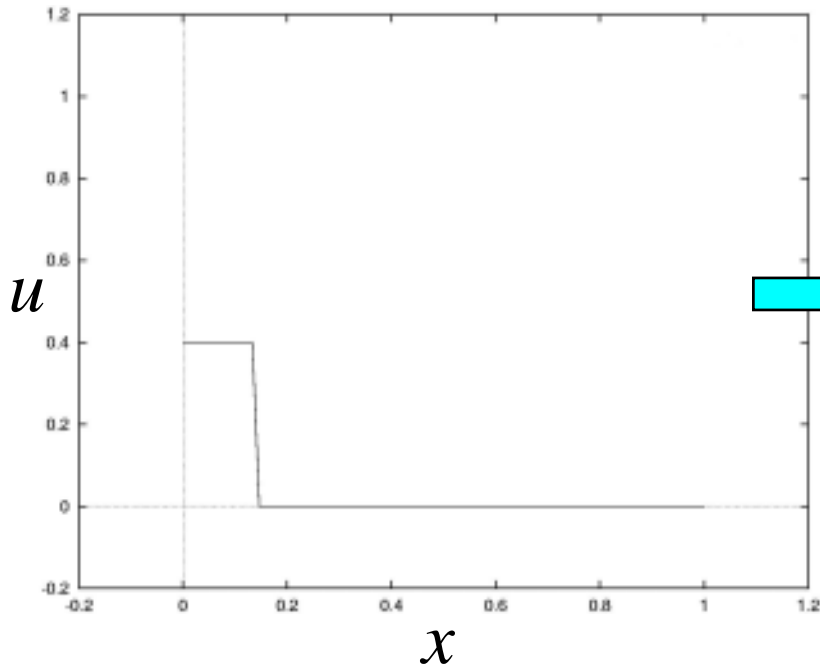
# Initial value 1



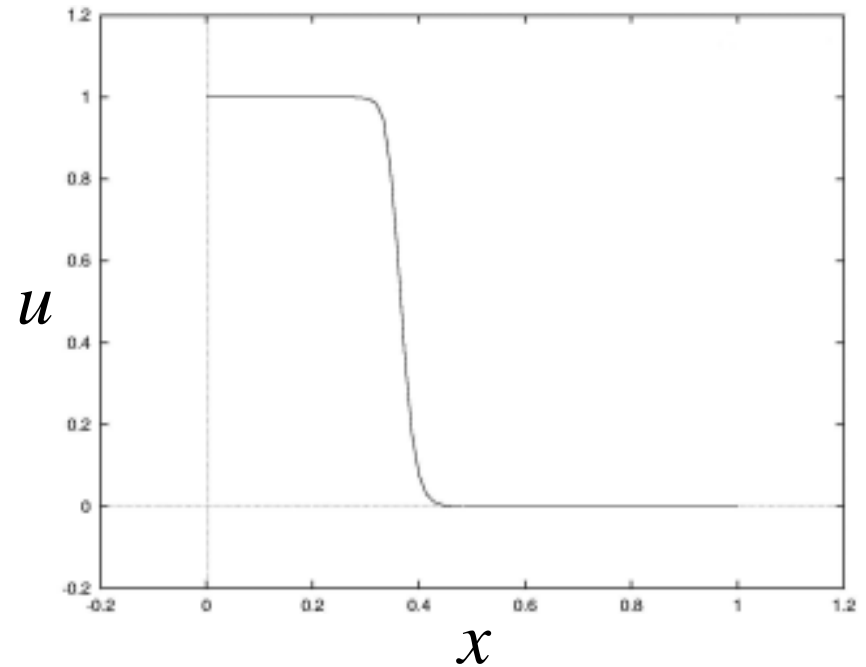
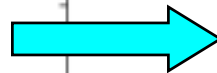
# Simulation of initial value 1



# Initial condition 1

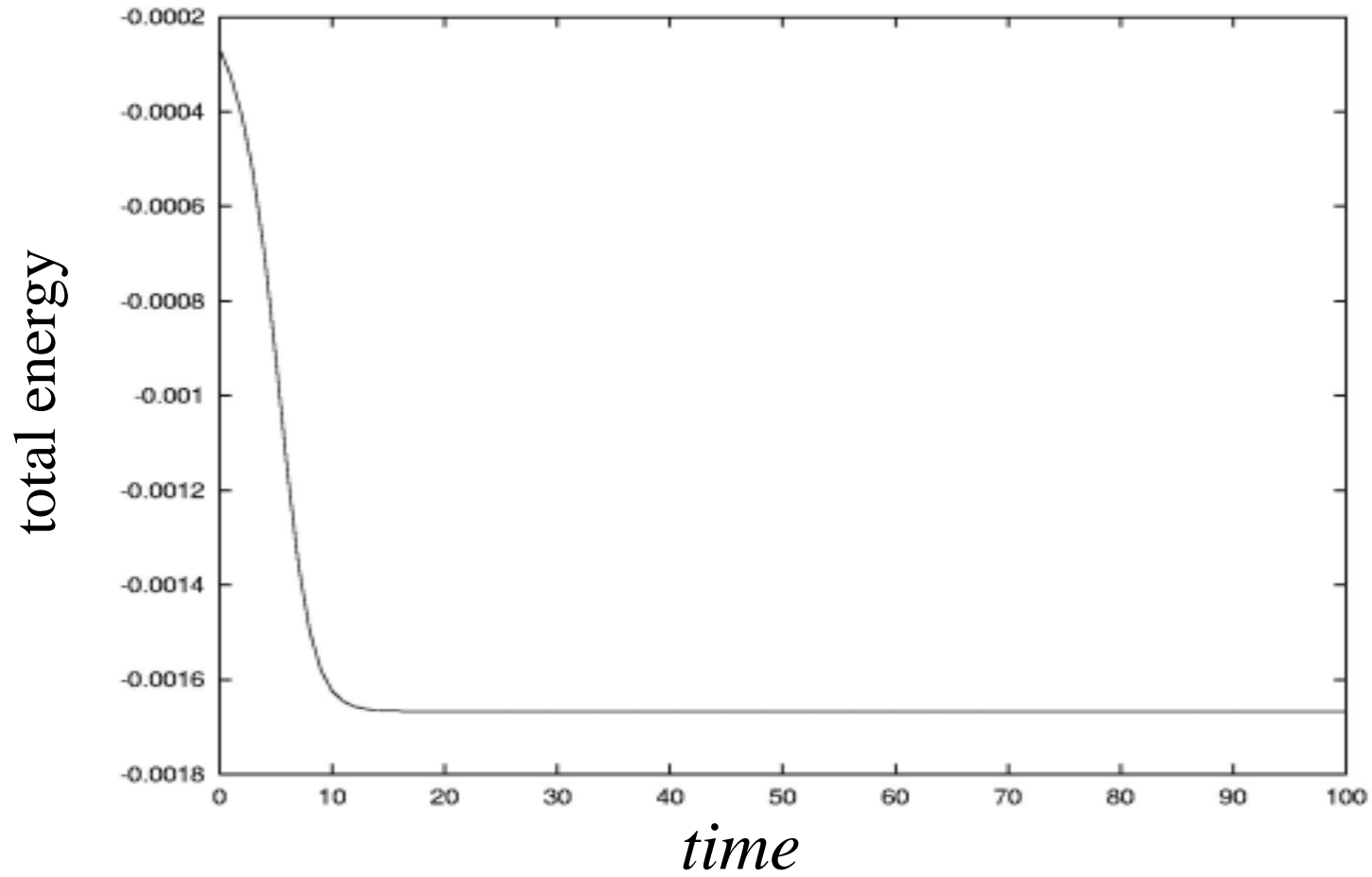


Initial value  
( $t=0$ , time step  $n=0$ )

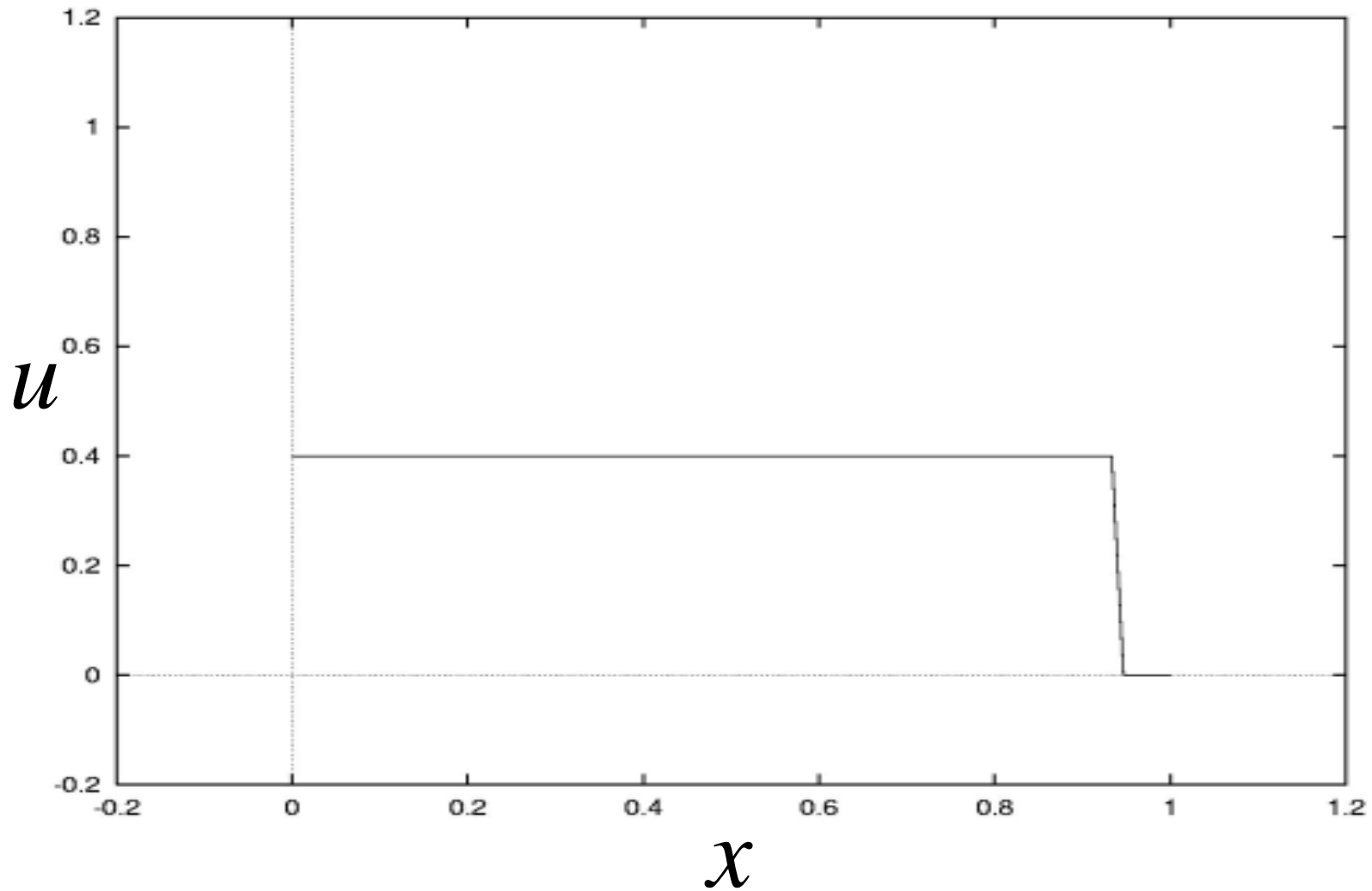


Stable Solution  
( $t=100$ , time step  $n=10000$ )

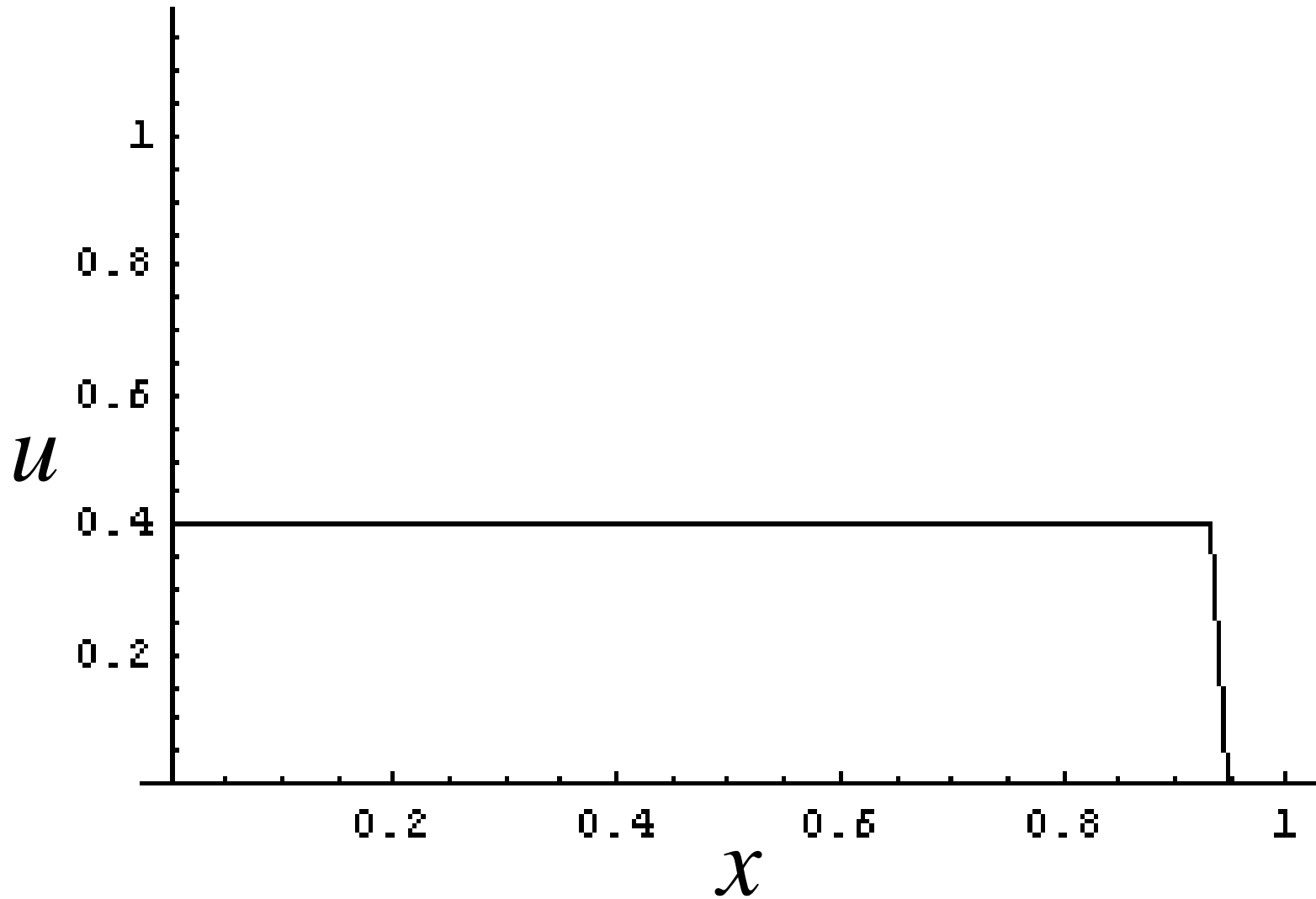
# Time evolution of discrete total energy



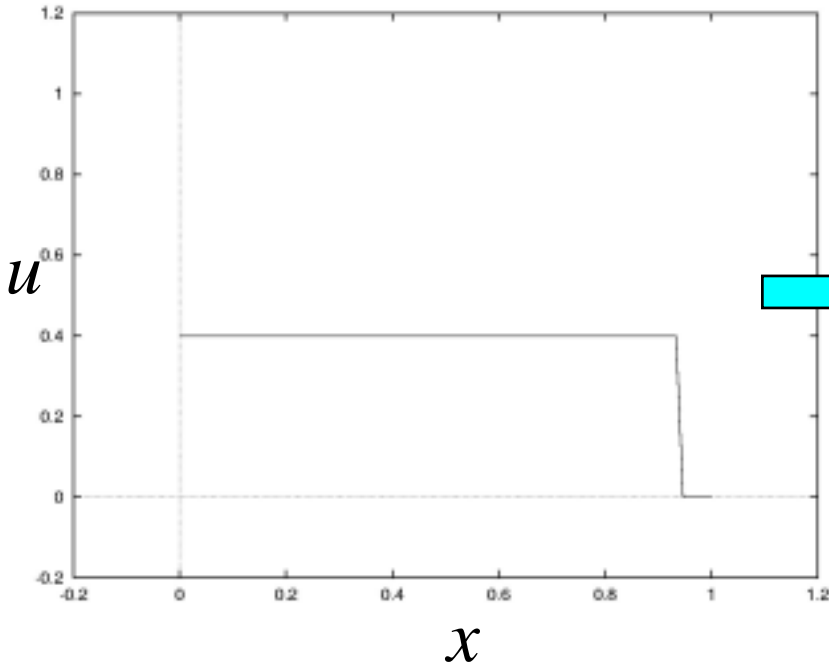
# Initial value 2



# Simulation of initial value 2

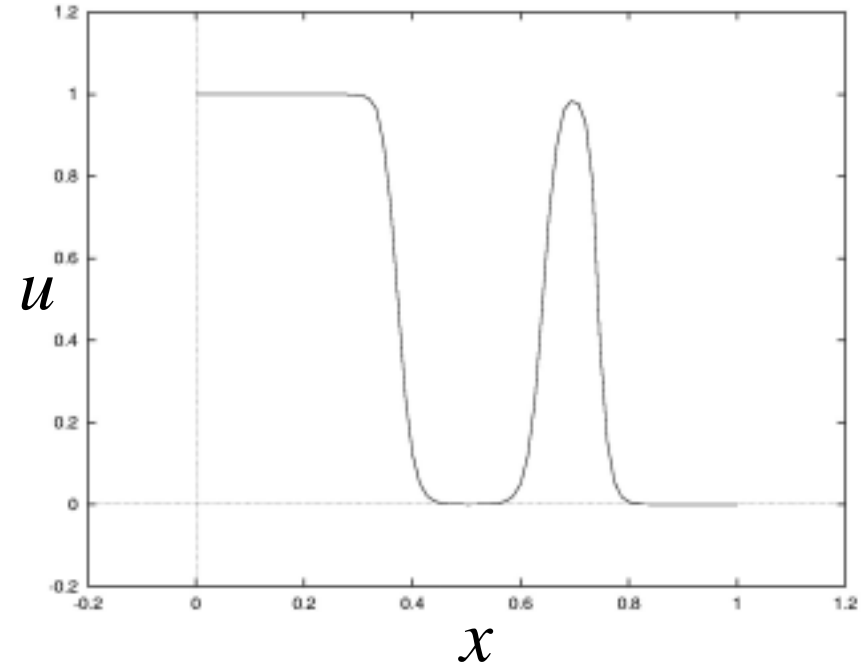


# Initial condition 2



Initial value

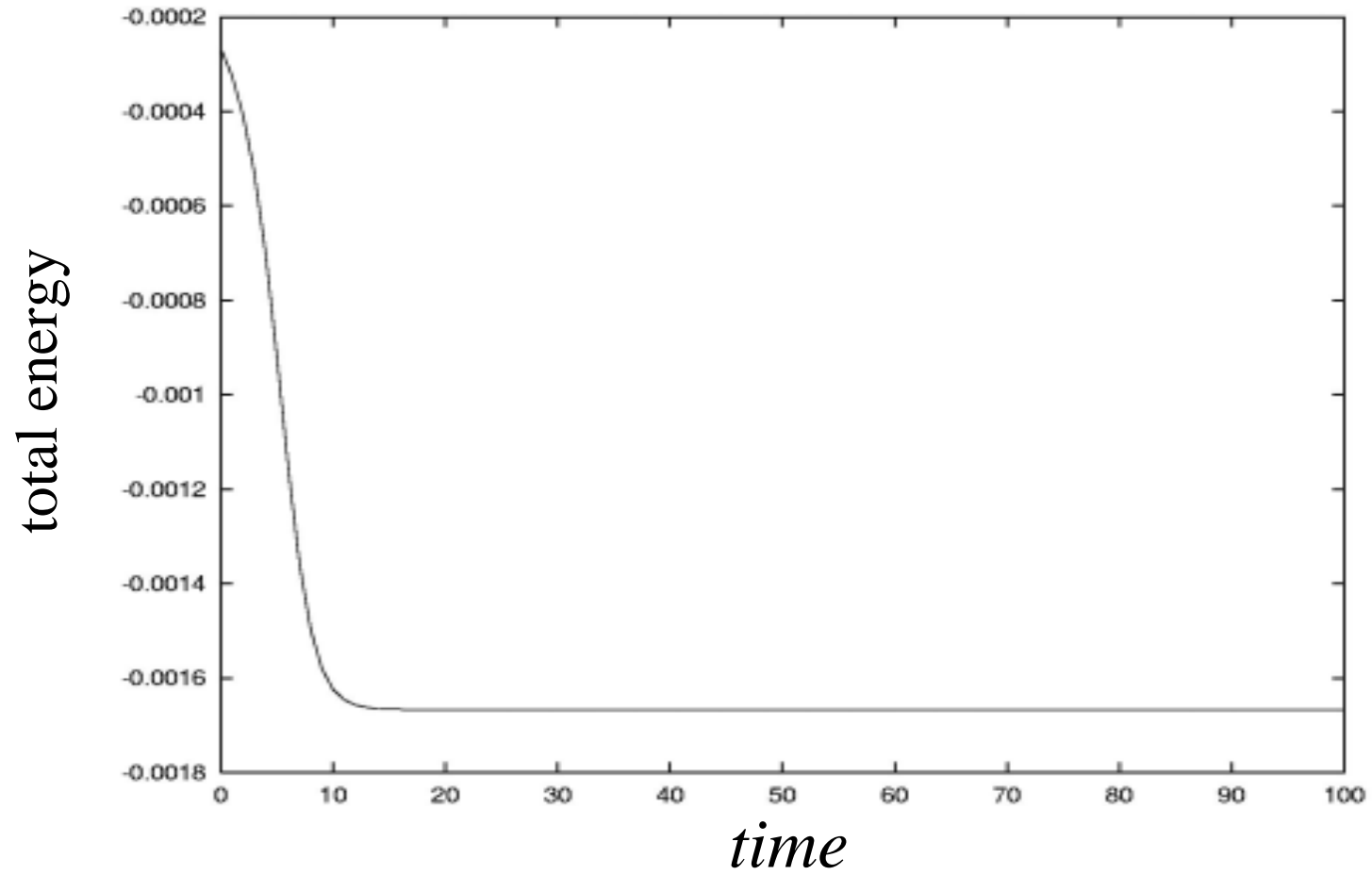
( $t=0$ , time step  $n=0$ )



Stable Solution

( $t=100$ , time step  $n=10000$ )

# Time evolution of discrete total energy

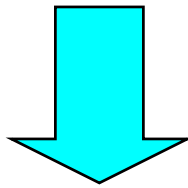


## 4. Conclusion

- Proposed scheme is
  - preserve energy dissipation property,
  - robust.
- We have the conjecture for target equation
  - the solution of (2) has multiplicity which depends on initial value.

# Appendix

$$\frac{\partial^2 u}{\partial t^2} = - \frac{\delta G}{\delta u}$$



$$\frac{d}{dt} \int G(u, u_x) dx = 0 : \alpha \text{ is odd}$$

(eg sine-Gordon eq, linear wave eq etc)

# The discrete Euler-Lagrange derivative

$$\frac{\delta G_d}{\delta (U_k, V_k)} \stackrel{def}{=} \sum_{l=1}^m \left( \frac{df_l}{d(U_k, V_k)} \frac{g_l^+(\delta_k^+ U_k) g_l^-(\delta_k^- U_k) + g_l^+(\delta_k^+ V_k) g_l^-(\delta_k^- V_k)}{2} - \delta_k^+ W_l^-(U_k, V_k) - \delta_k^- W_l^+(U_k, V_k) \right)$$

where

$$\delta_k^\pm W_l^\mp(U_k, V_k) = \left( \frac{f_l(U_k) + f_l(V_k)}{2} \right) \left( \frac{g_l^\mp(\delta_k^\mp U_k) + g_l^\mp(\delta_k^\mp V_k)}{2} \right) \frac{dg_l^\pm}{d(\delta_k^\pm U_k, \delta_k^\pm V_k)}$$

and

$$\frac{df}{d(a, b)} \stackrel{def}{=} \begin{cases} \frac{f(b) - f(a)}{b - a} & : a \neq b, \\ \frac{df}{da} & : a = b. \end{cases}$$

We apply the summation by parts formula to difference

$J_d[U_k] - J_d[V_k]$ , to obtain

$$J_d[U_k] - J_d[V_k] = \sum_{k=0}^N \frac{\delta G_d}{\delta(U_k, V_k)} (U_k - V_k) \Delta x + \left[ \frac{\partial G_d}{\partial \delta(U_k, V_k)} \right]_0^N$$

where

$$\frac{\delta G_d}{\delta \delta(U_k, V_k)} \stackrel{\text{def}}{=} \frac{1}{2} \sum_{l=1}^m \left( W_l^+(U_k, V_k) s_k^+(U_k - V_k) + W_l^-(U_k, V_k) s_k^-(U_k - V_k) \right. \\ \left. (s_k^+ W_l^-(U_k, V_k) + s_k^- W_l^+(U_k, V_k)) (U_k - V_k) \right).$$

Therefore we can regard  $J_d[U_k] - J_d[V_k]$  as a discrete analogue of  $J[u + \delta u] - J[u]$ .

## Summation by parts

$$\begin{aligned} & \sum_{k=0}^N \left[ \frac{(\delta_k^+ U_k)(\delta_k^+ V_k) + (\delta_k^- U_k)(\delta_k^- V_k)}{2} \right] \Delta x + \sum_{k=0}^N (\delta_k^{(2)} U_k) V_k \Delta x \\ &= \frac{1}{2} \left[ (\delta_k^{(2)} U_k) (s_k^{(1)} + 1) U_k + (s_k^{(1)} + 1) U_k (\delta_k^{(1)} V_k) \right]_0^N \end{aligned}$$

where

$$s_k^+ U_k = U_{k+1},$$

$$s_k^- U_k = U_{k-1},$$

$$s_k^{(1)} U_k = \frac{s_k^+ + s_k^-}{2} U_k.$$