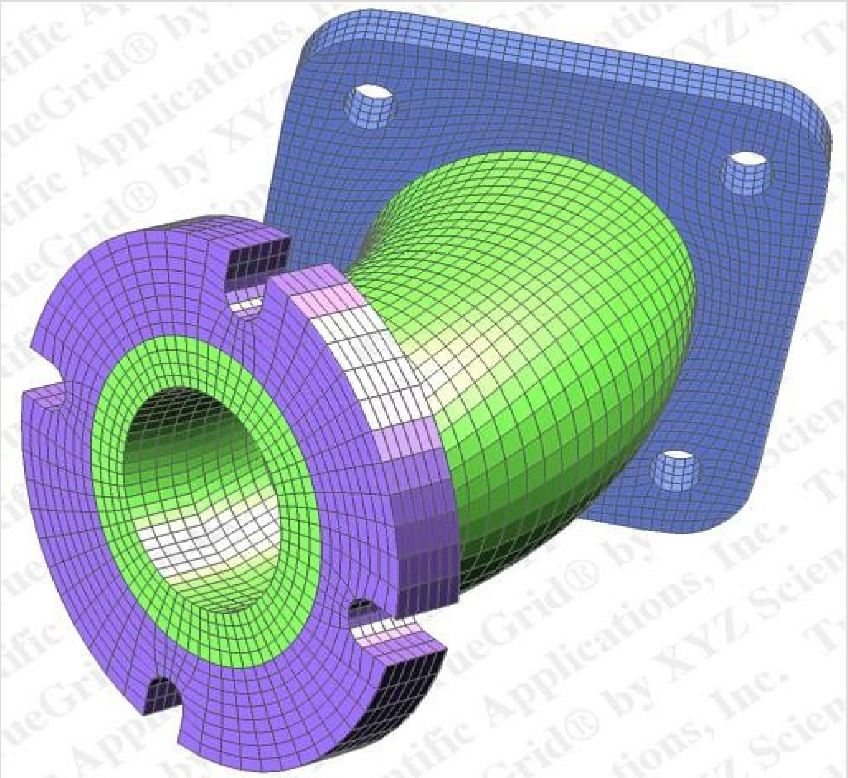
Nonstandard Finite Difference Methods for Numerical ODE/PDE

Sergey Voronin

Numerical Solution of ODEs and PDEs

Finite Difference Methods
Collocation Methods
Spectral Methods
Finite Element Methods



Review of Finite Differences

Grid Discretization

Replacement of Derivatives by their discrete approximations

Derivative approximations come from Taylor's expansion theorem

Why Use Finite Differences?

Relatively easy to implement on the computer.

Low space requirements. Even for schemes that cannot be expressed explicitly, iterative methods may be used to solve systems of equations produced by FD eliminating the need to store and manipulate large matrices.

May be adapted to more complex grids by using variable spacing.

Approximation Formulas (1)

$$\left(x_{i+1} = x_i + h \quad ; \quad t_{j+1} = t_j + k \right)$$

$$h = \Delta x \quad ; \quad k = \Delta t$$

$$u\left(x_{i+1}, t_j\right) = u\left(x_i, t_j\right) + h \frac{\partial u}{\partial x}\left(x_i, t_j\right) + \Theta\left(h^2\right)$$

$$\frac{\partial u}{\partial x}\left(x_i, t_j\right) = \frac{u\left(x_{i+1}, t_j\right) - u\left(x_i, t_j\right)}{h} + \Theta\left(h\right)$$

Approximation Formulas (2)

$$u\left(x_i+\frac{h}{2},t_j\right)=u(x_i,t_j)+\frac{h}{2}\frac{\partial u}{\partial x}(x_i,t_j)+\frac{h^2}{8}\frac{\partial^2 u}{\partial x^2}(x_i,t_j)+\Theta(h^3)$$

$$u\left(x_i-\frac{h}{2},t_j\right)=u(x_i,t_j)-\frac{h}{2}\frac{\partial u}{\partial x}(x_i,t_j)+\frac{h^2}{8}\frac{\partial^2 u}{\partial x^2}(x_i,t_j)+\Theta(h^3)$$

Subtract to get:

$$\frac{\partial u}{\partial x}(x_i,t_j)=\frac{u\left(x_i+\frac{h}{2},t_j\right)-u\left(x_i-\frac{h}{2},t_j\right)}{h}+\Theta(h^2)$$

Approximation Formulas (3)

$$u(x_{i+1}, t_j) = u(x_i, t_j) + h\frac{\partial u}{\partial x}(x_i, t_j) + \frac{h^2}{2}\frac{\partial u}{\partial x}(x_i, t_j) + \Theta(h^3)$$

$$u(x_{i-1}, t_j) = u(x_i, t_j) - h\frac{\partial u}{\partial x}(x_i, t_j) + \frac{h^2}{2}\frac{\partial u}{\partial x}(x_i, t_j) - \Theta(h^3)$$

Subtract to get:

$$\frac{\partial u}{\partial x}(x_i, t_j) = \frac{u(x_{i+1}, t_j) - u(x_{i-1}, t_j)}{2h} + \Theta(h^2)$$

Approximation Formulas (4)

$$u(x_{i+1}, t_j) = u(x_i, t_j) + h\frac{\partial u}{\partial x}(x_i, t_j) + \frac{h^2}{2}\frac{\partial^2 u}{\partial x^2}(x_i, t_j) + \frac{h^3}{6}\frac{\partial^3 u}{\partial x^3}(x_i, t_j) + \Theta(h^4)$$

$$u(x_{i-1}, t_j) = u(x_i, t_j) - h\frac{\partial u}{\partial x}(x_i, t_j) + \frac{h^2}{2}\frac{\partial^2 u}{\partial x^2}(x_i, t_j) - \frac{h^3}{6}\frac{\partial^3 u}{\partial x^3}(x_i, t_j) + \Theta(h^4)$$

Add to get:

$$\frac{\partial^2 u}{\partial x^2}(x_i, t_j) = \frac{u(x_{i+1}, t_j) - 2u(x_i, t_j) + u(x_{i-1}, t_j)}{h^2} + \Theta(h^2)$$

ODEs

Example: The Decay Equation

$$\frac{d}{dt}u(t) = -\lambda u(t) \quad ; \quad u(t_0) = u_0$$

In this case, the exact solution is known:

$$\frac{du(t)}{u(t)} = -\lambda\, dt \Rightarrow \int_{t_0}^{t} \frac{du(t)}{u(t)} = \int_{t_0}^{t} -\lambda\, dt \Rightarrow \ln\left[\frac{u(t)}{u(t_0)}\right] = -\lambda(t - t_0)$$

$$u(t) = u_0 e^{-\lambda(t - t_0)}$$

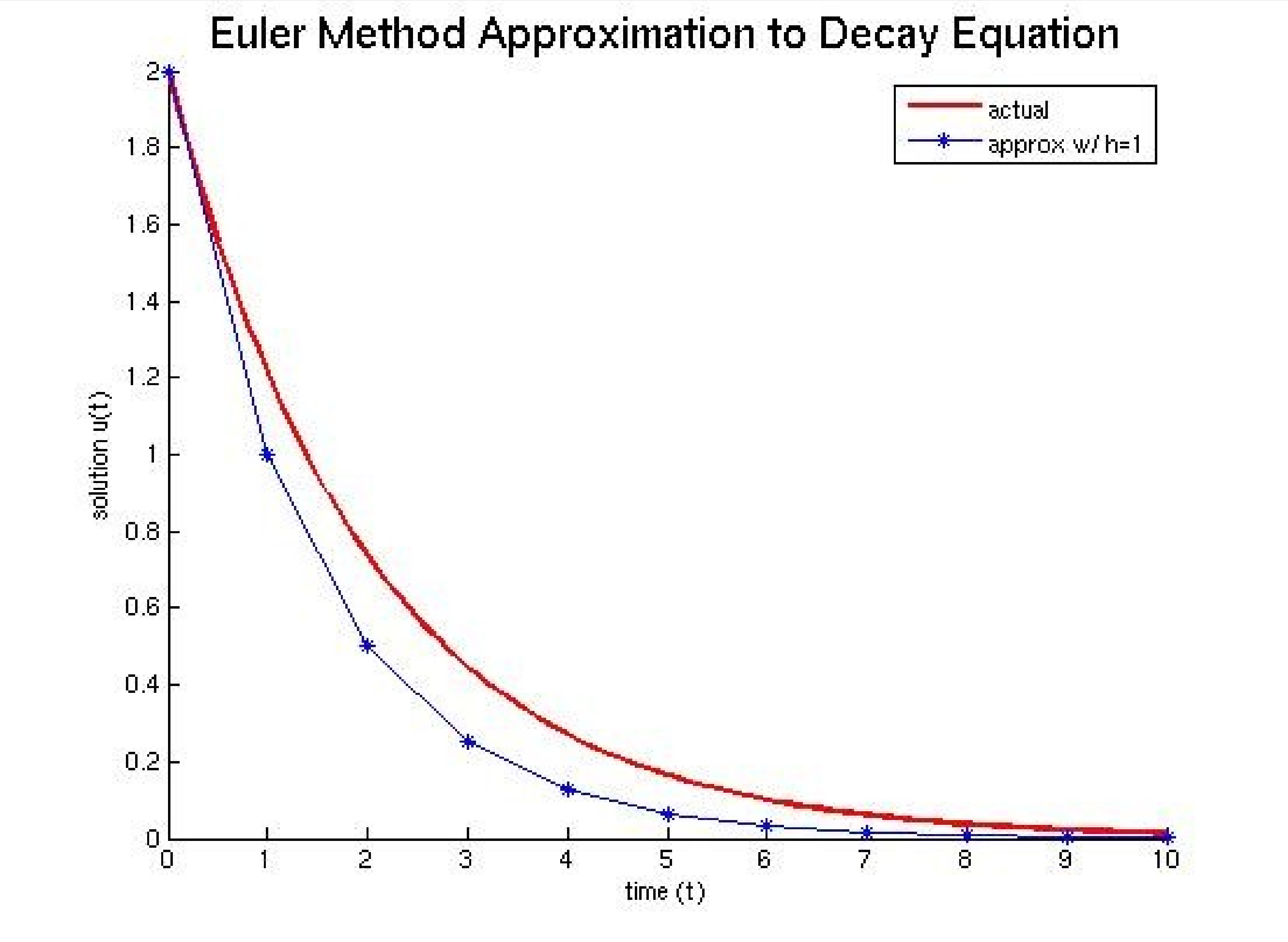
Application of FD

We apply the forward first order approximation for the time derivative to get the forward Euler scheme:

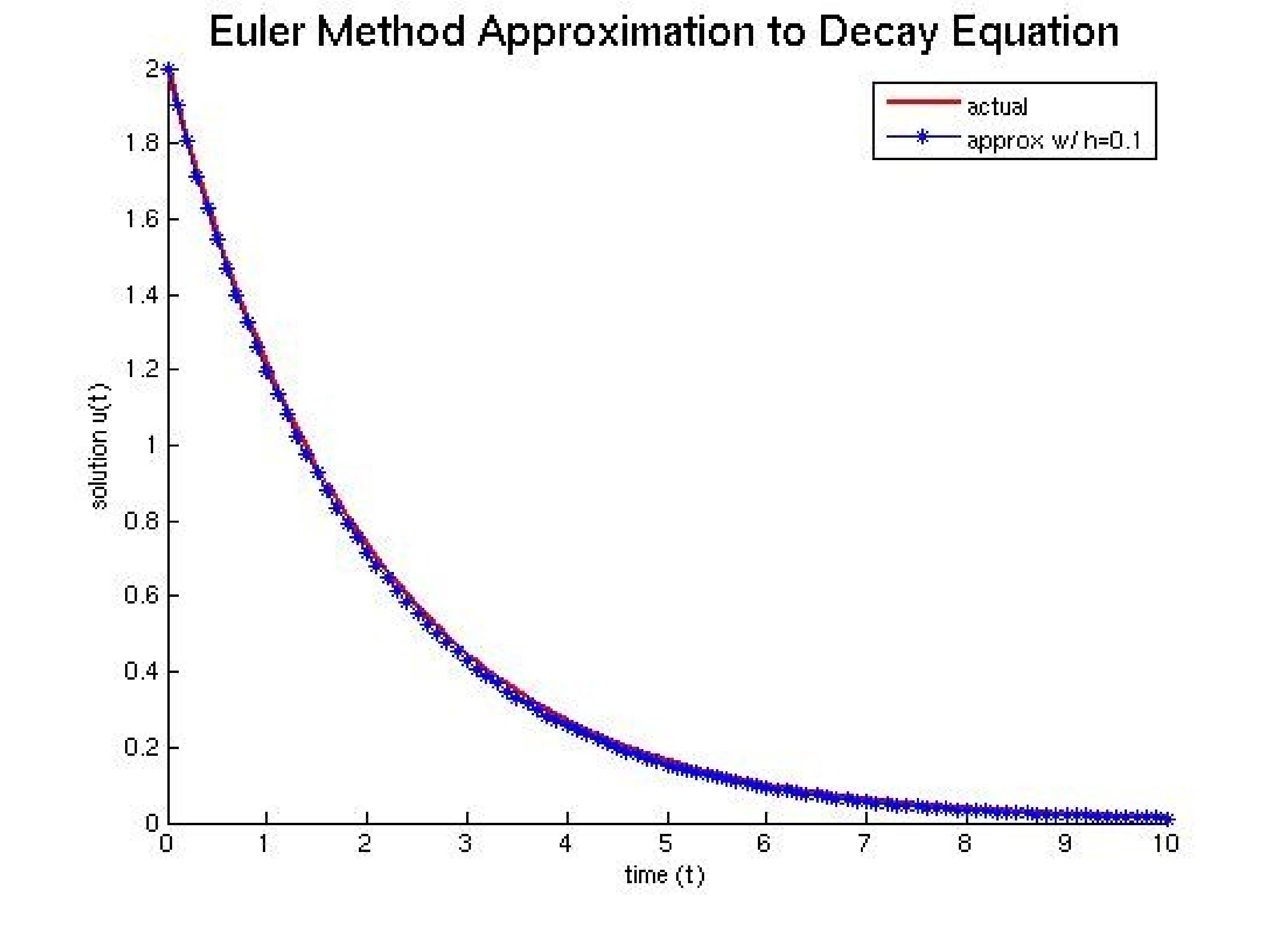
$$\frac{u_{k+1} - u_k}{h} = -\lambda u_k \Rightarrow u_{k+1} = (1 - \lambda h) u_k$$

Given u_0, we can march in time and determine u_k for all $k > 0$. For this example, let $u_0 = 2$ and $\lambda = 0.5$.

FD Approx Results (1)



FD Approx Results (2)



Can we do better?

We can decrease the error by decreasing the step size (h), but at a cost of computational increases.

We can use a faster converging method like Runge–Kutta, but sometimes, we cannot afford to cut the step size to get the accuracy that we need.

We can modify our scheme, by using a Nonstandard Finite Difference approach.

How do we apply NSFD?

First, we need to modify the FD derivative approximation:

$$\text{Original:} \quad \frac{\partial u}{\partial t} \Rightarrow \frac{u_{k+1} - u_k}{h}$$

$$\text{NSFD:} \quad \frac{\partial u}{\partial t} \Rightarrow \frac{u_{k+1} - \psi(h) u_k}{\phi(h)}$$

Rules for Constructing NSFD Schemes [Mickens]

1) “The orders of the discrete derivatives should be equal to the orders of the corresponding derivatives appearing in the differential equation.”

2) “Discrete Representations for derivatives must, in general, have non-trivial denominator functions.”

$\rightarrow \ \phi(h)$ not necessarily equal to h

Rules for Constructing NSFD Schemes (2) [Mickens]

3) “Non-linear terms should, in general, be replaced by non-local discrete approximations.”

$$u^2 \to u_{k+1} u_k \quad \text{or} \quad u^2 = 2u^2 - u^2 \to 2(u_k)^2 - u_{k+1} u_k$$

4) “Special conditions that hold for the solutions of the differential equations should also hold for the solutions of the finite difference scheme.”

A Look at the Original Scheme

$$\frac{u_{k+1} - u_k}{h} = -\lambda u_k \Leftrightarrow u_{k+1} = (1 - \lambda h) u_k$$

It violates rule 4. The solution to the decay equation monotonically decreases to zero if $u_0 \neq 0.$

But if λh is sufficiently large, this may not be the case.

NSFD Approach (1)

NSFD "algorithm" for scalar ODEs:

$$\frac{du}{dt} = f(u)$$

In this case, the derivative approximation is:

$$\frac{du}{dt} \to \frac{u_{k+1} - u_k}{\phi(h)}$$

$$\text{where } \phi(h) = \frac{1 - e^{-R^* h}}{R^*}$$

NSFD Approach (2)

R* is determined as follows:

$$\text{Find the fixed points of } \frac{du}{dt} \Rightarrow f(\bar{u}) = 0 \Rightarrow \{\bar{u}_1, \bar{u}_2, \ldots, \bar{u}_n\}$$

$$\text{Form the set } \{\mathrm{R}_i\} \text{ where } \mathrm{R}_i = \left.\frac{df}{du}\right|_{u=\bar{u}_i}$$

$$R^* = \max\{|\mathrm{R}_i|; i = 1, 2, \ldots, n\}$$

Application to Decay ODE (1)

$$\frac{du}{dt} = -\lambda u \Rightarrow f(\overline{u}) = -\lambda \overline{u} = 0 \Rightarrow \left\{ \overline{u}_i \right\} = \{0\}$$

$$R_1 = \left.\frac{df}{du}\right|_{u=\overline{u}_1} = \left.\frac{d}{du}[-\lambda u]\right|_{u=0} = -\lambda$$

$$R^* = \max\left\{ |-\lambda| \right\} = \lambda$$

$$\Rightarrow \phi(h) = \frac{1 - e^{-\lambda h}}{\lambda} \Rightarrow \frac{du}{dt} \to \frac{u_{k+1} - u_k}{\left(\dfrac{1 - e^{-\lambda h}}{\lambda} \right)}$$

Application to Decay ODE (2)

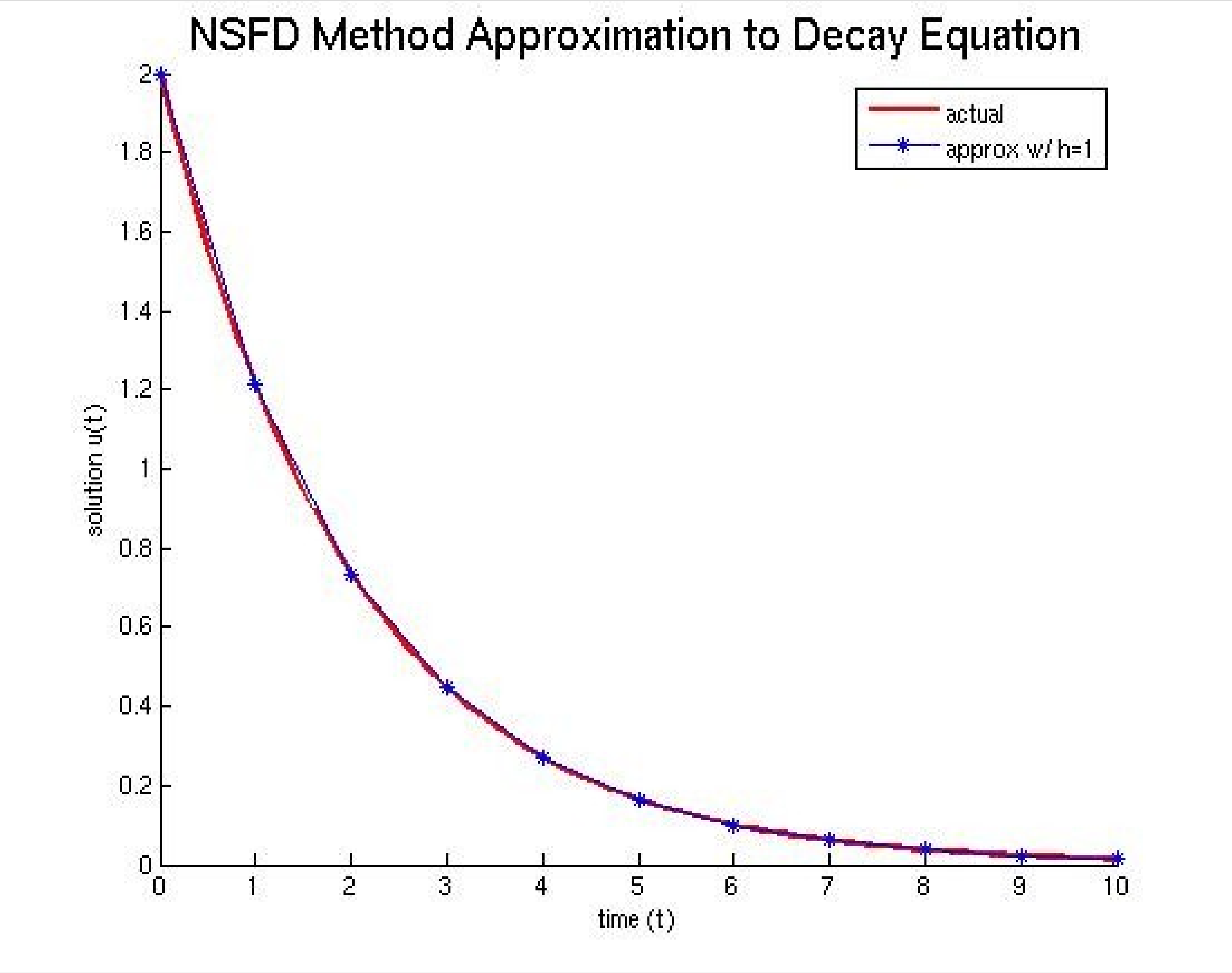
$$\frac{u_{k+1} - u_k}{\left(\frac{1 - e^{-\lambda h}}{\lambda}\right)} = -\lambda u_k \Rightarrow u_{k+1} = u_k - \left(\frac{1 - e^{-\lambda h}}{\lambda}\right)\lambda u_k$$

$$u_{k+1} = u_k - (1 - e^{-\lambda h})u_k \Rightarrow u_{k+1} = u_k - u_k + e^{-\lambda h}u_k$$

$$u_{k+1} = e^{-\lambda h}u_k \quad ; \quad u_0 \text{ given}$$

Compare with the exact solution: $u(t) = u_0 e^{-\lambda(t - t_0)}$

Application to Decay ODE (3)



Application to Logistical ODE (1)

$$\frac{du}{dt} = ru(1-u) = ru - ru^2 \quad ; \quad u(0) = u_0$$

$$\frac{du}{dt} \to \frac{u_{k+1} - u_k}{\phi(h)} \quad ; \quad u^2 \to u_{k+1} u_k$$

$$\phi(h) = \frac{1 - e^{-R^* h}}{R^*}$$

$$R^* = \max\{|R_i|; i = 1, 2, 3, \ldots, n\} \text{ where } R_i = \left.\frac{df}{du}\right|_{\bar{u} = \bar{u}_i}$$

Application to Logistical ODE (2)

$$f(\bar{u}) = r\bar{u}(1-\bar{u}) = 0 \Rightarrow \bar{u}_1 = 0, \ \bar{u}_2 = 1$$

$$R_1 = \left.\frac{df}{du}\right|_{u=\bar{u}_1} = (r - 2\bar{u}r)\Big|_{\bar{u}=0} = r - 0 = r$$

$$R_2 = \left.\frac{df}{du}\right|_{u=\bar{u}_2} = (r - 2\bar{u}r)\Big|_{\bar{u}=1} = r - 2r = -r$$

$$R^* = \max\{|r|, |-r|\} = r \Rightarrow \phi(h) = \frac{1-e^{-rh}}{r}$$

Application to Logistical ODE (3)

$$\frac{u_{k+1} - u_k}{\frac{1 - e^{-rh}}{r}} = r u_k - r u_{k+1} u_k$$

$$u_{k+1} - u_k = \frac{1 - e^{-rh}}{r} r u_k - \frac{1 - e^{-rh}}{r} r u_{k+1} u_k = A u_k - A u_{k+1} u_k$$

$$\text{where } A = 1 - e^{-rh}$$

$$u_{k+1}(1 + A u_k) = u_k (A + 1)$$

$$u_{k+1} = \frac{u_k (A + 1)}{(1 + A u_k)} \Rightarrow u_{k+1} = \frac{u_k \left(2 - e^{-rh}\right)}{1 + (1 - e^{-rh}) u_k}$$

Application to Logistical ODE (4)

NFSD Scheme for Logistic ODE:

$$u_{k+1} = \frac{u_k \left(2 - e^{-rh}\right)}{1 + \left(1 - e^{-rh}\right) u_k} \quad ; \quad u_0 \text{ given}$$

Let's compare this scheme to the classical fourth order Runge-Kutta scheme for different values of r and h.

Application to Logistical ODE (5)

Runge-Kutta scheme for $\dfrac{du}{dt} = f(u) = ru(1-u)$:

$$u_{k+1} = u_k + \frac{h}{6}(k_1 + 2k_2 + 2k_3 + k_4) \quad ; \quad u_0 \text{ given, where:}$$

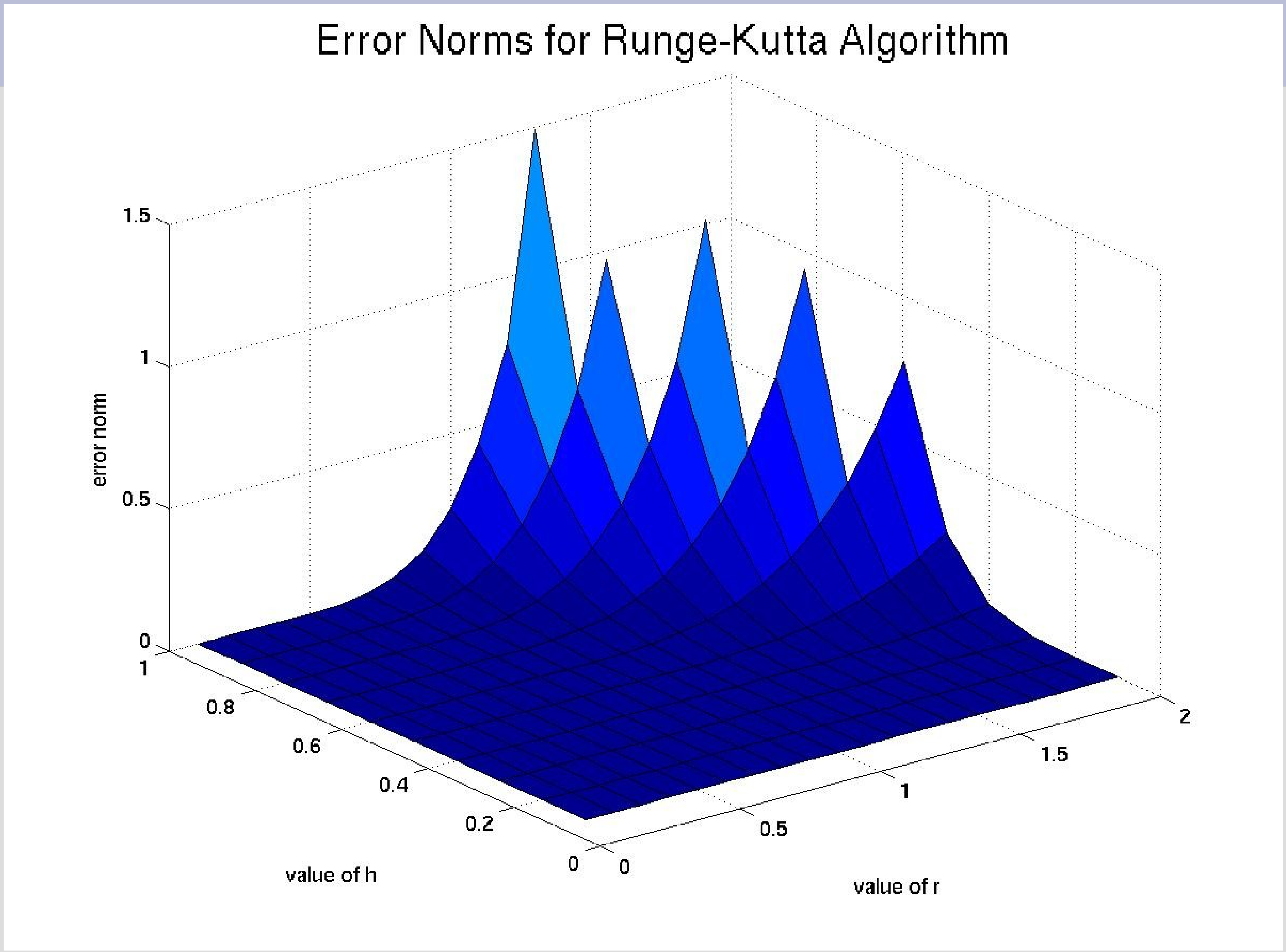
$$k_1 = f(u_k)$$

$$k_2 = f\left(u_k + \frac{h}{2}k_1\right)$$

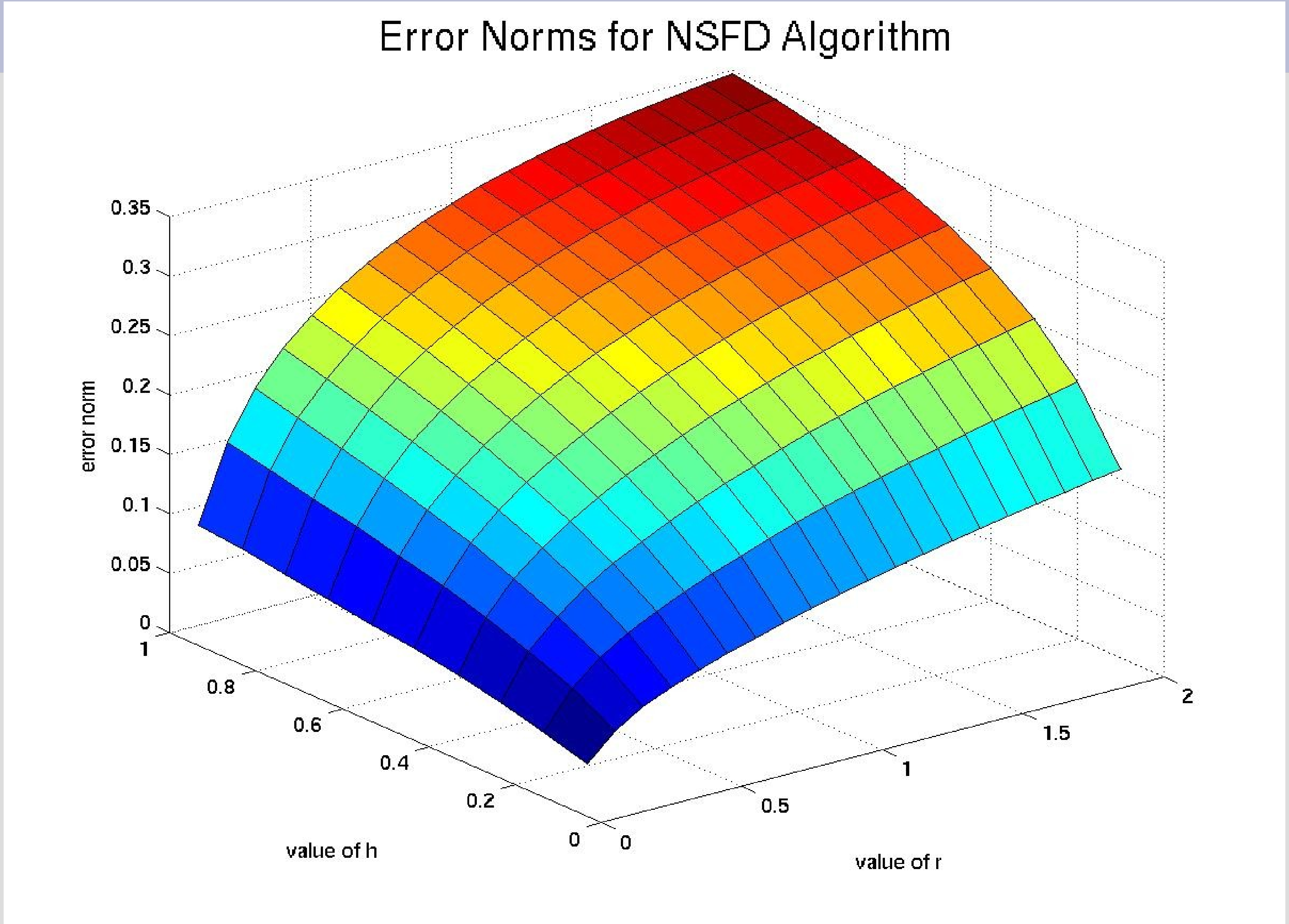
$$k_3 = f\left(u_k + \frac{h}{2}k_2\right)$$

$$k_4 = f(u_k + hk_3)$$

Application to Logistical ODE (6)



Application to Logistical ODE (7)



NSFD and PDE

Sample Problem – 1D Wave Equation

$$\frac{\partial^2 u(x,t)}{\partial t^2} - v^2(x)\frac{\partial^2 u(x,t)}{\partial x^2} = 0 \quad ; \quad 0 < x < L; \quad 0 < t < T$$

with boundary conditions:

$$u(0,t) = u(L,t) = 0, \quad t > 0$$

and initial conditions:

$$u(x,0) = f(x) \text{ and } u_t(x,0) = g(x), \quad 0 \leq x \leq L$$

Standard Finite Differences (1)

$$\frac{\partial^2 u}{\partial t^2}(x_i, t_j) = \frac{u(x_i, t_{j+1}) - 2u(x_i, t_j) + u(x_i, t_{j-1})}{(\Delta t)^2} + \Theta\left((\Delta t)^2\right)$$

$$\frac{\partial^2 u}{\partial x^2}(x_i, t_j) = \frac{u(x_{i+1}, t_j) - 2u(x_i, t_j) + u(x_{i-1}, t_j)}{h^2} + \Theta(h^2)$$

$$\frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{(\Delta t)^2} - \frac{v_{i+1}^2 u_{i+1,j} - v_i^2 2u_{i,j} + v_{i-1}^2 u_{i-1,j}}{h^2} = 0$$

In this case, we can proceed to write an explicit scheme for $u_{i,j+1}$.

Standard Finite Differences (2)

$$u_{i,j+1} = 2(1 - s_i)u_{i,j} + s_{i+1}u_{i+1,j} + s_{i-1}u_{i-1,j} - u_{i,j-1}$$

where $s_i = (v(ih))^2 \dfrac{(\Delta t)^2}{h^2}$ and CFL: $\Delta t \leq \dfrac{h}{\|v\|_\infty}$

with initial conditions:

$\rightarrow u_{i,0} = f(ih)$

since, $u_{i,1} - u_{i,-1} = 2g(ih)\Delta t$

$$\rightarrow u_{i,1} = f(ih) + g(ih)\Delta t + \frac{1}{2}\left[s_{i+1} f\left((i+1)h\right) - 2s_i f\left(ih\right) + s_{i-1} f\left((i-1)h\right)\right]$$

and boundary conditions:

$u_{0,j} = u_{n,j}$

NSFD and the Wave PDE (1)

$$\frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{(\Delta t)^2} - \frac{v_{i+1}^2 u_{i+1,j} - v_i^2 2u_{i,j} + v_{i-1}^2 u_{i-1,j}}{h^2} = 0$$

$$\Leftrightarrow \left[\frac{\overline{d}_t^2}{(\Delta t)^2} - v^2(x)\frac{\overline{d}_x^2}{h^2}\right]\overline{u}(x,t) = 0$$

where $\overline{u}(x,t) \to u(x,t)$ as $h \to 0$ and $\Delta t \to 0$

In the above expression, $\overline{u}(x,t)$ is an approximation to the actual solution $u(x,t)$. One NSFD approach is to make the scheme exact with respect to a particular solution of the wave equation.

NSFD and the Wave PDE (2)

We know a particular exact solution:

$$u_0(x,t) = e^{i(kx - wt)}$$

which represents a wave travelling in the $+x$ direction with frequency $f = 2\pi w$ and wavelength λ, where:

$$w = \frac{2\pi}{f} \text{ and } k = \frac{2\pi}{\lambda}; \text{ also, since } \lambda f = v \Rightarrow v = \frac{w}{k}$$

$$\Rightarrow \left[\frac{\overline{d}_t^2}{(\Delta t)^2} - v^2(x) \frac{\overline{d}_x^2}{h^2} \right] u_0(x,t) = \varepsilon \neq 0$$

NSFD and the Wave PDE (3)

We want to make the scheme exact with respect to a particular solution:

$$\Rightarrow \left[\frac{\overline{d}_t^{\,2}}{(\Delta t)^2} - v^2(x) \frac{\overline{d}_x^{\,2}}{h^2} \right] e^{i(kx-wt)} = 0$$

$$\overline{d}_x^{\,2} \left[e^{i(kx-wt)} \right] = e^{i[k(x+h)-wt]} + e^{i[k(x-h)-wt]} - 2e^{i(kx-wt)}$$

$$= e^{i[(kx-wt)+kh]} + e^{i[(kx-wt)-kh]} - 2e^{i(kx-wt)}$$

$$= e^{i(kx-wt)} \left(e^{ikh} + e^{-ikh} \right) - 2e^{i(kx-wt)} = 2e^{i(kx-wt)} \left[\cos(kh) - 1 \right]$$

NSFD and the Wave PDE (4)

$$\Rightarrow \overline{d}_x^{\,2}\left[e^{i(kx-wt)}\right] = 2e^{i(kx-wt)}\left[\cos(kh)-1\right] = 2u_0(x,t)\left[\cos(kh)-1\right]$$

Via a similar derivation:

$$\overline{d}_t^{\,2}\left[e^{i(kx-wt)}\right] = 2e^{i(kx-wt)}\left[\cos(w\Delta t)-1\right] = 2u_0(x,t)\left[\cos(w\Delta t)-1\right]$$

Recall that we want: $\left[\frac{\overline{d}_t^{\,2}}{(\Delta t)^2} - v^2(x)\frac{\overline{d}_x^{\,2}}{h^2}\right]u_0(x,t) = 0 \Rightarrow \left[\overline{d}_t^{\,2} - v^2(x)\frac{(\Delta t)^2}{h^2}\overline{d}_x^{\,2}\right]u_0(x,t) = 0$

We substitute the above results and solve for the combined operator:

$$p^2(x) = v^2(x)\frac{\overline{d}_x^{\,2}}{h^2}$$

NSFD and the Wave PDE (5)

$$\Rightarrow \; 2u_0(x,t)\left[\cos(w\Delta t)-1\right]-v^2(x)\frac{(\Delta t)^2}{h^2}2u_0(x,t)\left[\cos\left(k(x)h\right)-1\right]=0$$

$$\Rightarrow \; p^2(x)=v^2(x)\frac{(\Delta t)^2}{h^2}=\frac{\cos(w\Delta t)-1}{\cos\left(k(x)h\right)-1}=\frac{\sin^2\left(\frac{w\Delta t}{2}\right)}{\sin^2\left(\frac{k(x)h}{2}\right)}$$

$$\Rightarrow \; \left[\bar{d}_t^{\,2}-p^2(x)\bar{d}_x^{\,2}\right]u_0(x,t)=0$$

In other words, with the above substitution for the $p^2(x)$ operator, the scheme is exact with respect to a particular solution of the PDE.

NSFD and the Wave PDE (6)

We can now derive the NSFD scheme:

$$\left[\bar{d}_t^{\,2} - p^2(x)\bar{d}_x^{\,2}\right]\bar{u}(x,t) = 0 \quad \text{where} \quad p^2(x) = \frac{\sin^2\left(\frac{w\Delta t}{2}\right)}{\sin^2\left(\frac{k(x)h}{2}\right)}$$

Upon expanding, we may rewrite the above as:

$$\bar{u}(x,t+\Delta t) = 2\bar{u}(x,t) - \bar{u}(x,t-\Delta t) + p^2\bar{d}_x^{\,2}\bar{u}(x,t)$$

$$\Rightarrow \bar{u}(x,t+\Delta t) = 2\bar{u}(x,t) - \bar{u}(x,t-\Delta t) + p^2(x+h)\bar{u}(x+h,t) + p^2(x-h)\bar{u}(x-h,t)$$

NSFD Scheme for the Wave PDE

$$u_{i,j+1} = 2\left(1 - p_i^2\right)u_{i,j} + p_{i+1}^2 u_{i+1,j} + p_{i-1}^2 u_{i-1,j} - u_{i,j-1}$$

$$\text{where } p_i^2 = \frac{\sin^2\left(\frac{w\,\Delta t}{2}\right)}{\sin^2\left(\frac{k_i h}{2}\right)} \text{ and } k_i = k(ih) = \frac{w}{v(ih)} \text{ and CFL: } \Delta t \le \frac{h}{\|v\|_\infty}$$

with initial conditions:

$$u_{i,0} = f_i$$

$$u_{i,1} = f_i + g_i \Delta t + \frac{1}{2}\left[p_{i+1}^2 f_{i+1} - 2p_i^2 f_i + p_{i-1}^2 f_{i-1}\right]$$

and boundary conditions:

$$u_{0,j} = u_{n,j} = 0$$

Comparing NSFD and Std FD

$$\frac{\partial^2 u(x,t)}{\partial t^2} - v^2(x)\frac{\partial^2 u(x,t)}{\partial x^2} = 0 \quad ; \quad 0 < x < L ; \quad 0 < t < T$$

$$u(0,t) = u(L,t) = 0, \quad t > 0$$

$$u(x,0) = f(x) \text{ and } u_t(x,0) = g(x), \quad 0 \le x \le L$$

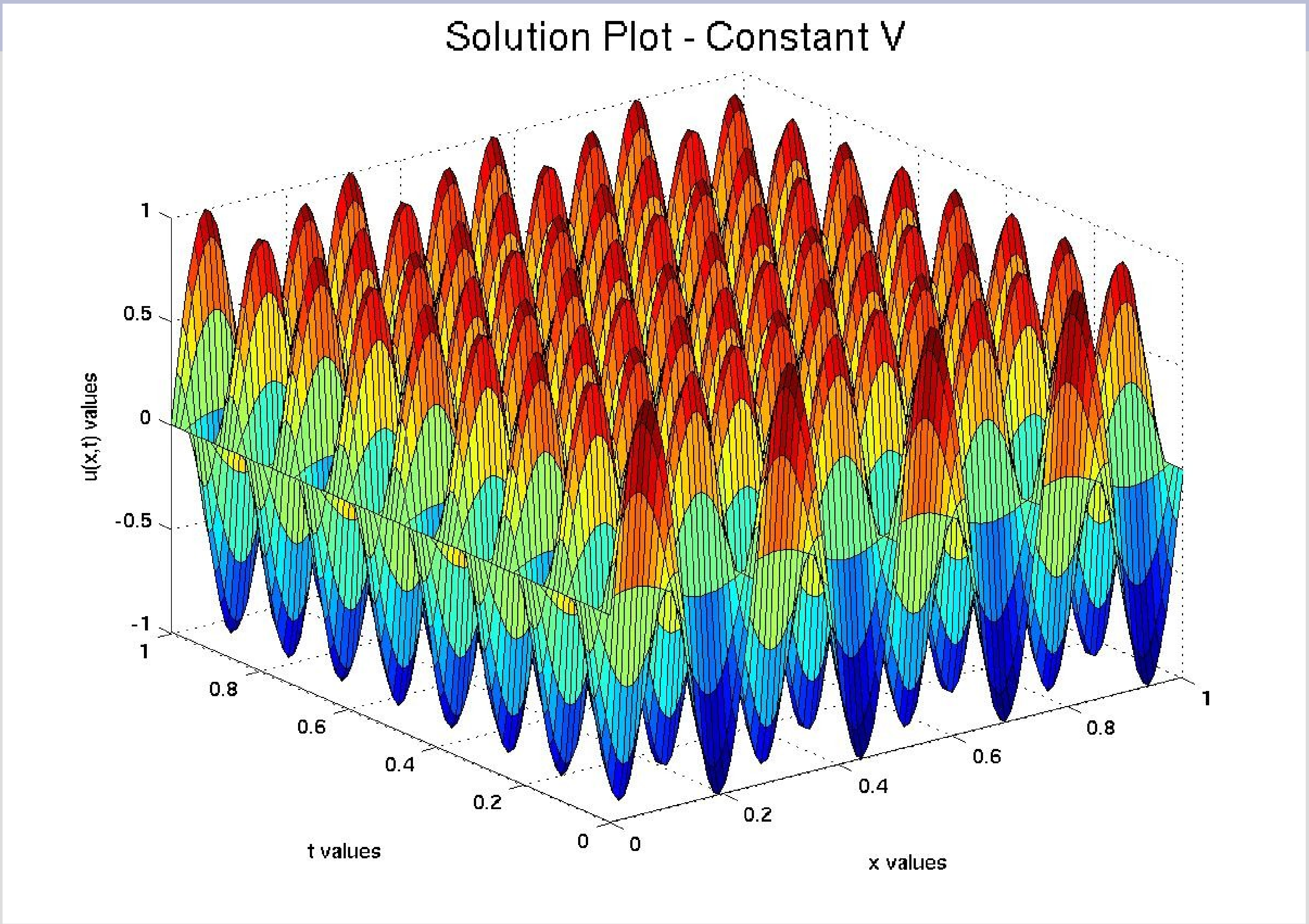
$$L = 1 \quad ; \quad T = 1 \quad ; \quad h = \frac{0.1}{64} \quad ; \quad k = \frac{0.02}{64}$$

$$f(x) = \sin(w\pi x) \quad ; \quad g(x) = 0$$

1. Constant v case: $v = 2$

2. Variable v case: $v(x) = 1 + x^2$

Constant V Solution



Constant V Errors

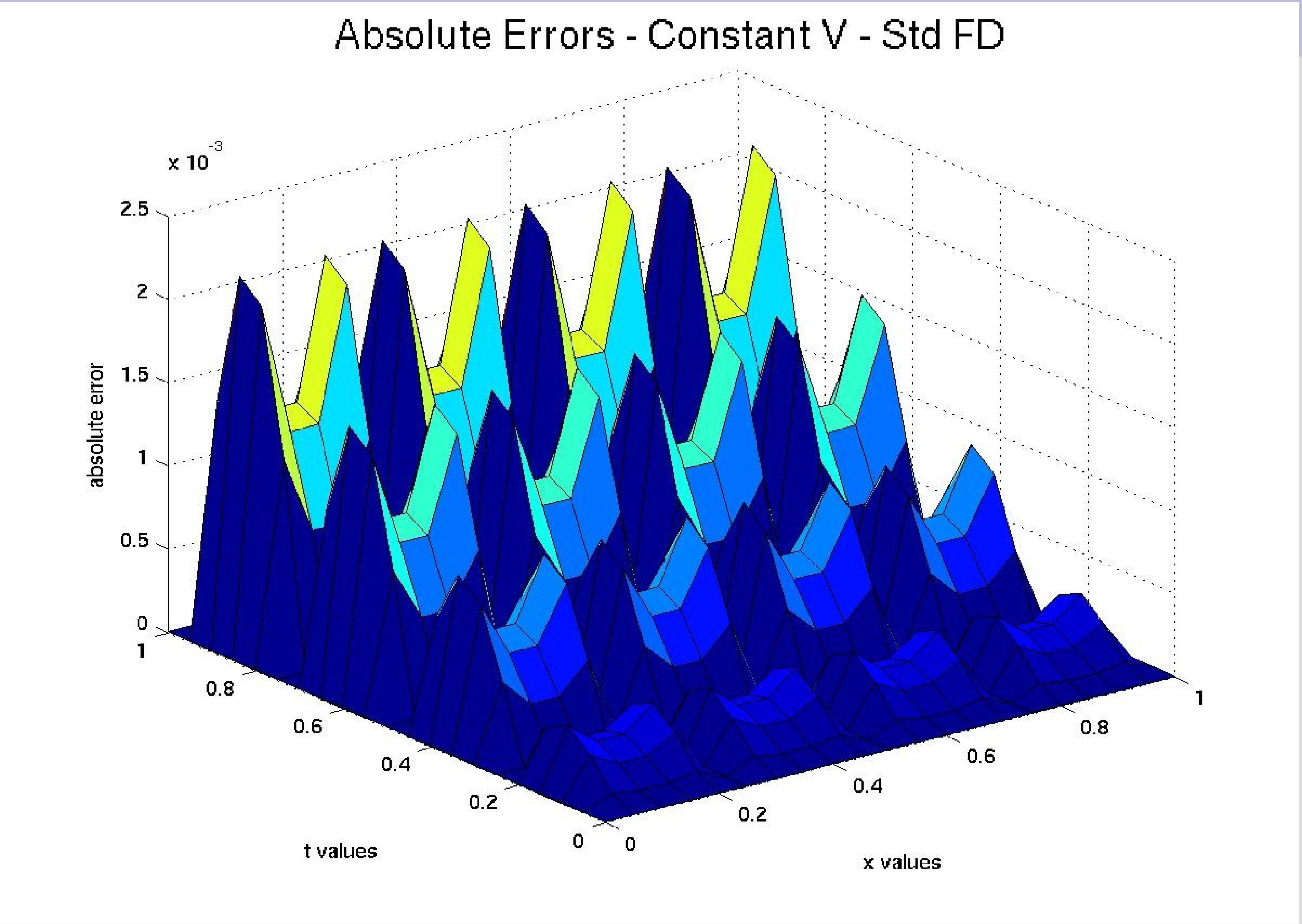
Standard Algorithm Errors:

h = 0.1	k = 0.02	max absolute error = 1.53884
h = 0.025	k = 0.005	max absolute error = 0.554372
h = 0.00625	k = 0.00125	max absolute error = 0.0351087
h = 0.0015625	k = 0.0003125	max absolute error = 0.00220772

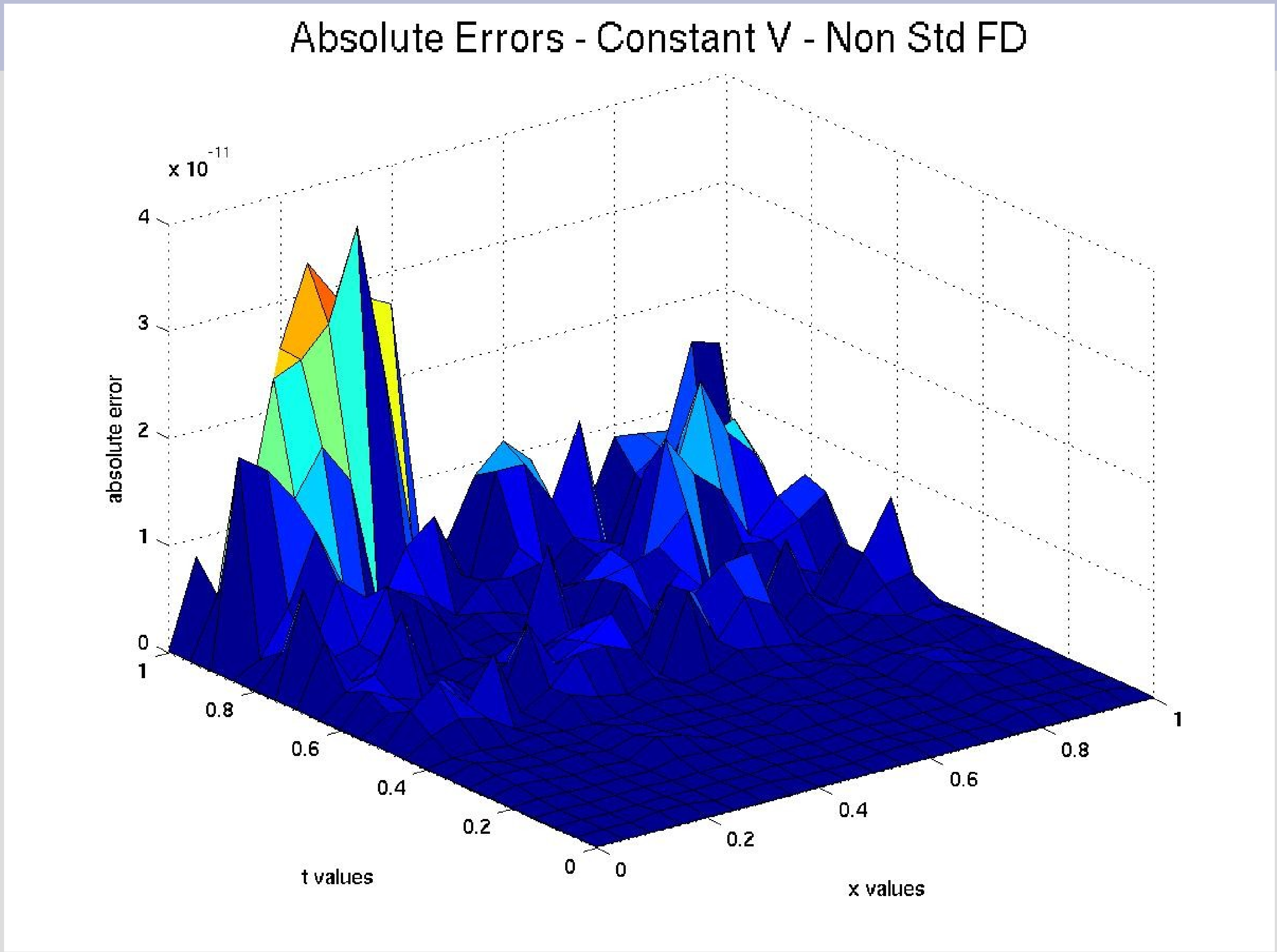
Non-Standard Algorithm Errors:

h = 0.1	k = 0.02	max absolute error = 5.88418e-15
h = 0.025	k = 0.005	max absolute error = 1.21569e-14
h = 0.00625	k = 0.00125	max absolute error = 1.08599e-11
h = 0.0015625	k = 0.0003125	max absolute error = 3.64967e-11

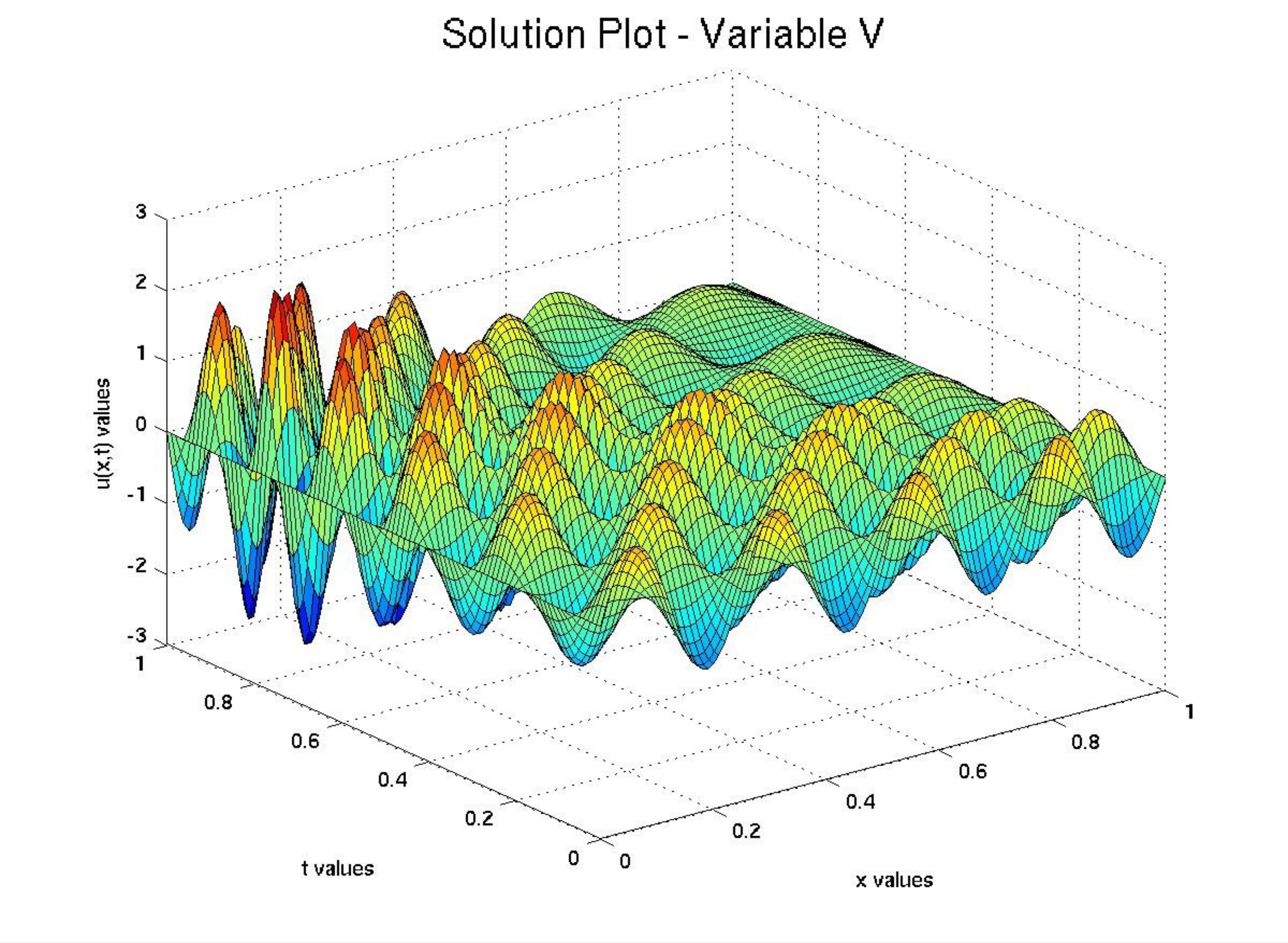
Constant V Error – Std FD



Constant V Error – NSFD



Variable V Solution



Variable V Errors

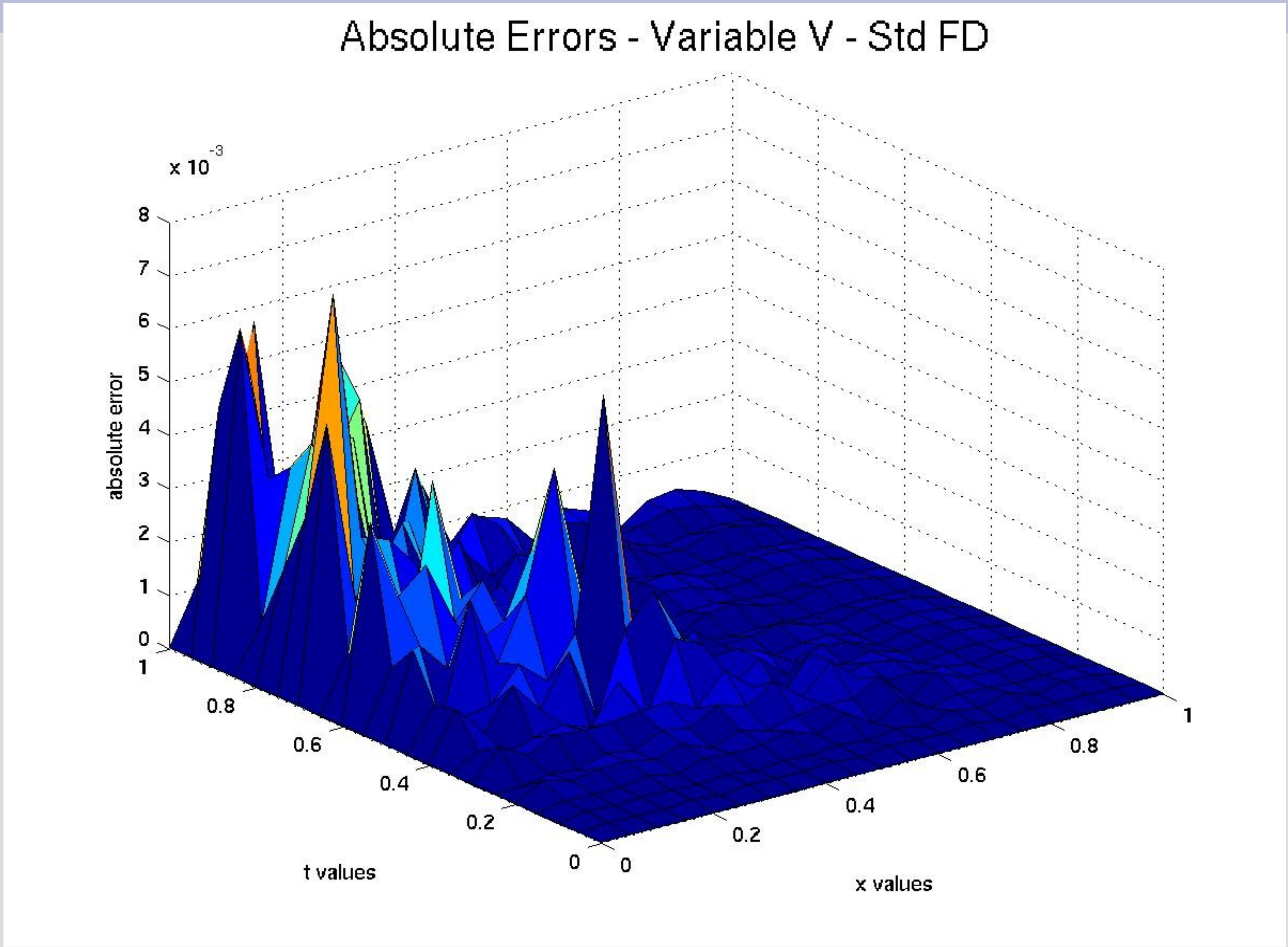
Standard Algorithm Errors:

h = 0.1	k = 0.02	max absolute error = 1.99215
h = 0.025	k = 0.005	max absolute error = 2.43195
h = 0.00625	k = 0.00125	max absolute error = 0.177339
h = 0.0015625	k = 0.0003125	max absolute error = 0.00728029

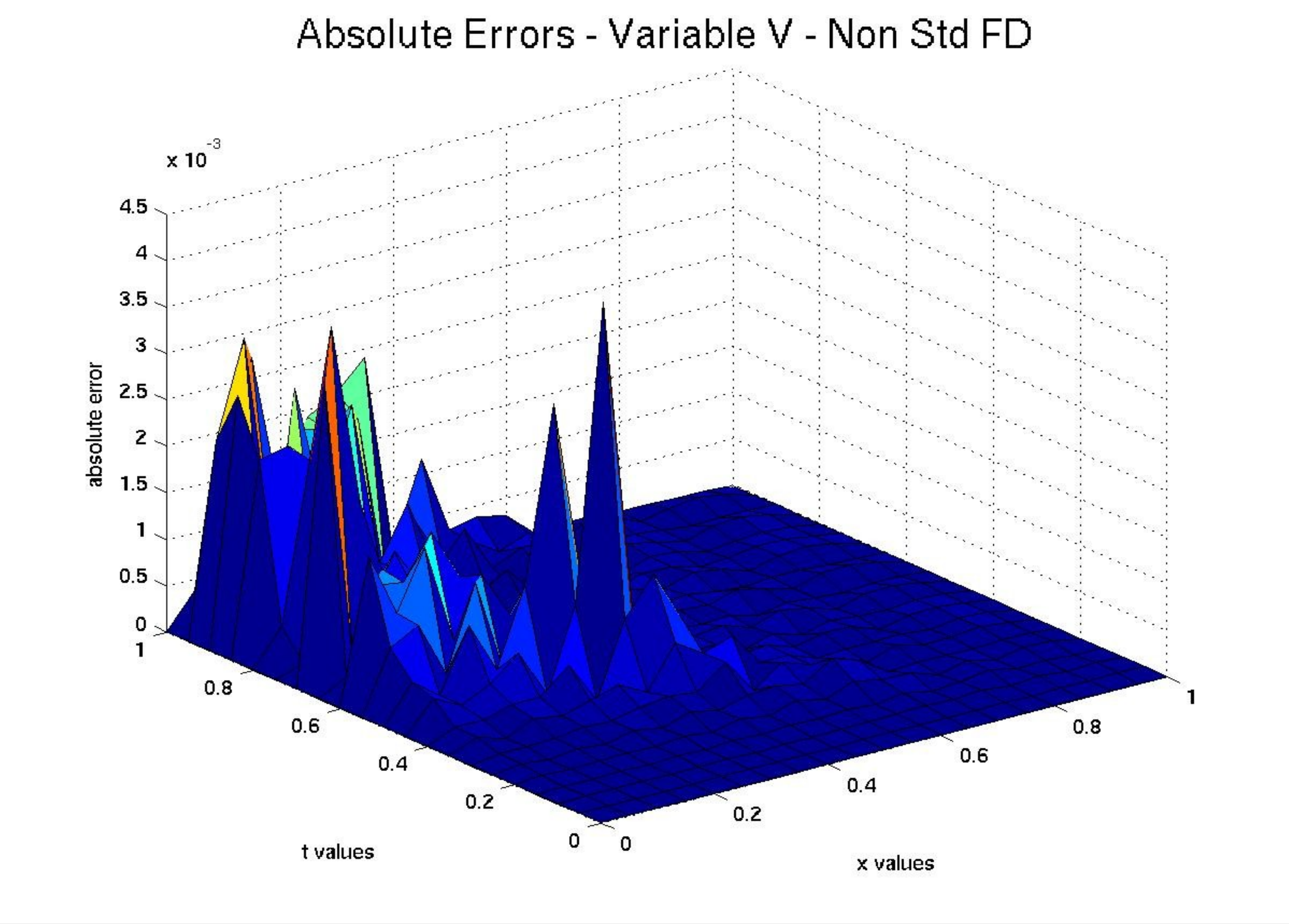
Non-Standard Algorithm Errors:

h = 0.1	k = 0.02	max absolute error = 2.007
h = 0.025	k = 0.005	max absolute error = 1.41017
h = 0.00625	k = 0.00125	max absolute error = 0.107026
h = 0.0015625	k = 0.0003125	max absolute error = 0.00414318

Variable V Error – Std FD



Variable V Error – NSFD



Summary and Conclusions (1)

The provided codes demonstrate that Non-Standard Finite Difference Methods can be effective in the numerical solution of some ODEs and PDEs.

In our Decay ODE test case, the NSFD algorithm resulted in an exact scheme. For the logistic ODE, we saw that the distribution of errors from the NSFD method was favorable even to a higher order Runge-Kutta method.

For our Wave Equation PDE test case, the NSFD algorithm is exact for the constant velocity case and produces less error than the standard FD algorithm in the variable velocity case.

Summary and Conclusions (2)

The NSFD method is in general, as easy to apply as the standard finite difference method. The computational costs of the method are similar to standard schemes.

NSFD is effective because it attempts to modify an existing FD scheme based on the properties of the individual equation, such as limiting properties and particular solutions.

NSFD is not a universal method. It is a growing collection of approaches to various differential equations.

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