NSFD Schemes: A Methodology for Constructing Structure Preserving Discretizations for Differential Equations

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AMS Special Session: "Highly Accurate and Structure-Preserving Numerical Methods for Nonlinear PDE's"

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Purpose of Special Session

Discuss possible resolutions of the fact that standard methods (such as Runge-Kutta, linear multi-step procedures, etc.) do not generally allow the incorporation of *a priori* given structural features of the differential equations into the discretizations of the differential equations.

Dynamic Consistency $\longrightarrow$ Qualitative Properties

- Positivity
- Conservation laws/symmetries
- Monotonicity
- Boundedness
- And so on...

Definition of "Dynamic Consistency"

Consider two "systems," S and S'. Let S have the property P. If S' also has the property P, then S' is said to be dynamic consistent with S, with respect to property P.

Comment

The two systems, S and S', do not have to be of the same "type." For example, S might be an isolated subsystem of the physical universe, while S' could be a data set gotten from probing S. Or, S could be a differential equation, while S' is a particular discretization of it.

Goals of the Presentation

- Discuss, in general terms, the full modeling process
- Indicate the non-uniqueness of this process (at every step)
- Show, within the context of structure-preserving algorithms/geometric integration, that the nonstandard finite difference (NSFD) methodology (Mickens, 1989) is a particularly powerful technique to discretize differential equations

Mickens, Ronald E. "Exact solutions to a finitedifference model of a nonlinear reaction-advection equation: Implications for numerical analysis." Numerical Methods for Partial Differential Equations 5.4 (1989): 313-325.

Two Issues

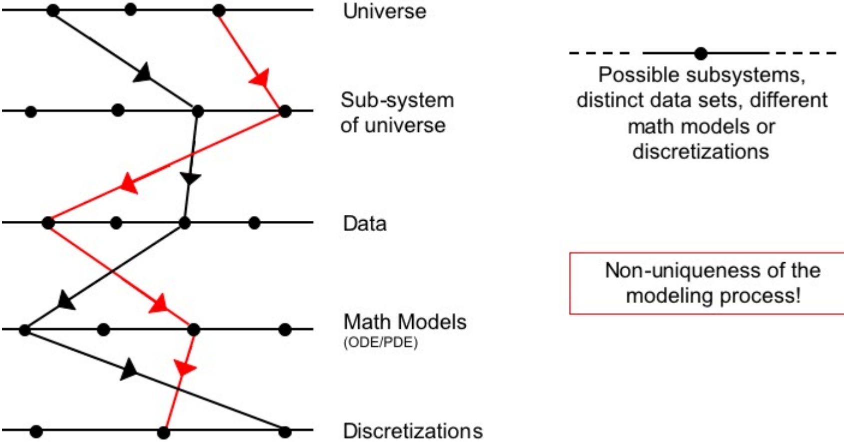
- No fully realistic differential equation model of physical phenomena can be solved and expressed exactly in terms of a "finite" combination of "elementary functions"
- Hence, the need exists for some form of discretization which can be used to calculate numerical approximations to the solutions of the differential equations.

Comment

The modeling of physical differential equations are never exact.

Example: The heat/diffusion partial differential equation

Multi-Paths to Discretizations



Non-uniqueness of the modeling process!

NSFD Methodology – Preliminaries

- Subequations
- Exact finite difference schemes
- Two examples of exact schemes
- Lessons learned, generalization to construct an NSFD scheme methodology

Sub-Equations

Consider, for example, the differential equation

$$M_1 + M_2 + M_3 = M_4$$

where M_i is a linear or nonlinear function of the dependent variables and/or their derivatives, and/or the independent variables.

Some subequations are:

$$\begin{aligned} M_1 + M_2 &= 0 \\ M_1 &= M_4 \\ M_2 + M_3 &= M_4 \\ M_1 + M_2 + M_3 &= 0 \end{aligned}$$

and so on . . .

Examples of Subequations

$$u_t + auu_x = Du_{xx} + \lambda_1 u - \lambda_2 u^2$$

Burgers-Fisher PDE

$$u_t + auu_x = 0$$

$$u_t = \lambda_1 u - \lambda_2 u^2$$

$$Du_{xx} + \lambda_1 u = 0$$

$$auu_x = Du_{xx}$$

Exact Finite Difference Schemes (for ODEs)

$$\frac{dx(t)}{dt} = f(x,p), \quad x(t_0) = x_0, \quad p = \text{parameters: } p_1, p_2, \dots, p_m$$

- Solution: $x(t) = \sum(x_0, t_0, t, p)$
- Note: $x(t_0) = \sum(x_0, t_0, t_0, p) = x_0$

Define

$$t \to t_k = kh, \quad h = \Delta t; \quad k \in \mathbb{Z}$$

$$x(t) \to x(t_k) = x_k$$

The exact finite difference scheme is

$$x_{k+1} = \sum(x_k, t_k, t_{k+1}, p)$$

where the number of parameters is $m+1 : (p, h)$.

- Note: $x(t_k) = x_k$, where $h > 0$ is defined

Example A: Linear Decay ODE

$$\frac{dx(t)}{dt} = -\lambda x(t), \quad x(t_0) = x_0 > 0$$

Solution:

$$x(t) = x_0 e^{-\lambda(t-t_0)}, \quad t > t_0$$

Exact Scheme:

$$x_{k+1} = x_k e^{-\lambda h}$$

which can be rewritten to the form

$$\frac{x_{k+1} - x_k}{\phi(\lambda, h)} = -\lambda x_k$$

where the denominator function $\phi(\lambda, h) = \frac{1-e^{-\lambda h}}{\lambda}$.

Example B: Logistic Equation

$$\frac{dx(t)}{dt} = \lambda_1 x(t) - \lambda_2 x(t)^2, \quad x(t_0) = x_0 > 0$$

Exact Scheme

$$\frac{x_{k+1} - x_k}{\phi(\lambda_1, h)} = \lambda_1 x_k - \lambda_2 x_{k+1} x_k$$

$$\phi(\lambda_1, h) = \frac{1 - e^{-\lambda_1 h}}{\lambda_1}$$

Nonstandard Finite Difference Methodology

- Formulated from constructions of hundreds of ODEs/PDEs whose exact solutions are *a priori* known

Results:

1) Derivative Discretizations

$$\frac{dx}{dt} \to \frac{x_{k+1} - x_k}{\phi(h,p)}$$

- $\phi(h,p)$ can be explicitly calculated in terms of the characteristic time-scales of the system.
- For ordinary differential equations, several "effective" techniques exist for determining explicit expressions for $\phi(h,p)$
- In general, we may use

$$\phi(h,p) = \frac{1 - e^{-rh}}{r}, \quad \frac{1}{r} = \text{smallest characteristic system time}$$

Nonstandard Finite Difference Methodology Continued

Results:

2) Non-local discretization of functions of the dependent variables

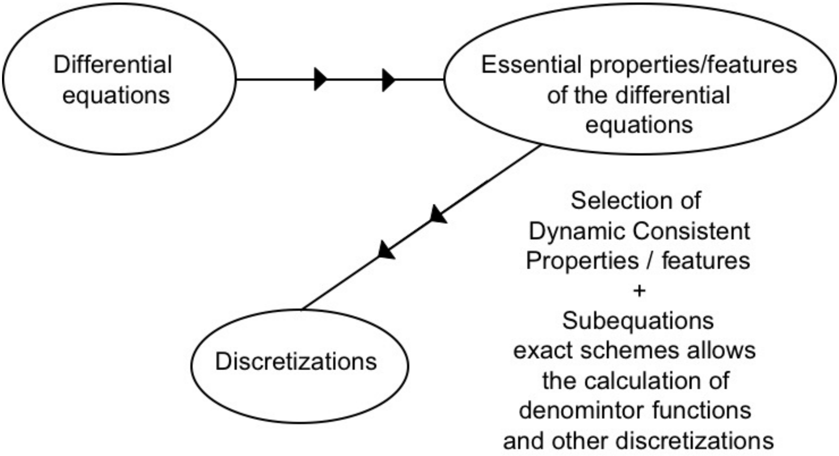
$$x^2 \rightarrow x_{k+1}x_k, \quad 2x_k^2 - x_{k+1x_k} \quad \text{(1st-order ODE)}$$

$$x^3 \rightarrow \left(\frac{x_{k+1} + x_{k-1}}{2}\right) x_k^2 \quad \text{(2nd-order ODE)}$$

$$x^2 \rightarrow \left(\frac{x_{k+1} + x_k + x_{k-1}}{3}\right) x_k \quad \text{(2nd-order ODE)}$$

$$x^{1/3} \rightarrow \frac{x_{k+1}}{x_k^{2/3}} \quad \text{(1st-order ODE)}$$

NSFD Procedure for Discretization



Application A: A Newton Mickens Law of Cooling

$$\frac{dx}{dt} = -\lambda_1 x - \lambda_2 x^p, \quad \lambda_1 > 0, \quad \lambda_2 \geq 0, \quad x(t_0) \neq 0$$

- Properties:
  1. Positivity
  2. Real solution
  3. Monotonic solutions
- $0 < p < 1, p = \frac{2m+1}{2N+1}, (N, m) : 0, 1, 2, \ldots ; 0 \leq m < N.$
- Useful subequation

$$\frac{dx}{dt} = -\lambda_1 x \quad \xrightarrow{\text{exact scheme}} \quad \frac{x_{k+1} - k_k}{\phi} = -\lambda_1 x_k$$

where $\phi = \frac{1-e^{-\lambda_1 h}}{\lambda_1}$

Application A: A Newton Mickens Law of Cooling

NSFD Scheme

$$\frac{x_{k+1} - x_k}{\phi} = -\lambda_1 x_k - \lambda_2 \frac{x_{k+1}}{(x_k)^{2/3}}$$

$$x_{k+1} = \left(\frac{x^{2/3}}{x^{2/3} + \lambda_2 \phi} \right) e^{-\lambda_1 h} x_k$$

Application B: Burgers-Fisher Equation

$$u_t + auu_x = Du_{xx} + \lambda_1 u - \lambda_2 u^2$$

(All parameters non-negative)

- Positivity and boundedness: $0 \leq u(x,t) \leq \frac{\lambda_1}{\lambda_2}$
- Sub-equations $u_t + auu_x = 0, Du_{xx} + \lambda_1 u = 0$
- NSFD scheme

$$\frac{u_m^{k+1} u_m^k}{\Delta t} + a u_m^{k+1} \left(\frac{u_m^k - u_{m-1}^k}{\Delta x} \right) = D \frac{u_{m+1}^k - 2u_m^k + u_{m-1}^k}{\left(\frac{4D}{\lambda_1}\right) \sin^2 \left[\left(\frac{\lambda_1}{D} \right) \left(\frac{\Delta x}{2} \right) \right]} + \lambda_1 u_m^k - \lambda_2 \bar{u}_m^k u_m^{k+1}$$

where $\bar{u}_m^k = \frac{u_{m+1}^k + u_m^k + u_{m-1}^k}{3}$

Summary ...

Future Problems...

Thanks!

Questions?