PHYSICS 210

OVERVIEW OF FINITE DIFFERENCE APPROXIMATION

Discretization

- In numerical analysis one can often approximately solve continuum systems—typically differential equations—through a process known as discretization

- In the continuum case, and, for specificity, assuming that the unknown function depends on a single independent variable, t (time), the unknown will typically be defined on some interval $0 \le t \le t_{\text{max}}$ of the real number line and will thus constitute an infinite number of values

- In the discrete case, the unknown function will typically be defined only at a finite number of times t^n, $n = 1, 2, \ldots, n_t$ and will thus comprise a finite number of values

Discretization (continued)

- **1st FUNDAMENTAL PURPOSE OF DISCRETIZATION**
  - Reduce infinite number of “degrees of freedom” to finite number
- **WHY?**
  - Computational resources are finite
- **2nd FUNDAMENTAL PURPOSE OF DISCRETIZATION**
  - Replace differential equations with algebraic equations
- **WHY?**
  - Can solve algebraic equations (linear or non-linear) computationally

Finite Difference Approximation

- Finite difference approximation (**FDA**) is one specific approach to the discretization of continuum systems such as differential equations

- We choose to focus on it here for several reasons
  - Accessibility (requires a minimum of mathematical background)
  - Generality (can be applied to virtually any system of differential equations)
  - Simplicity (relatively easy to apply in many cases)
  - Sufficiency (for many problems, produces results of acceptable accuracy with reasonable computational cost)

- Other important approaches that we will not discuss
  - **Finite element approximation**
  - **Spectral approximation**

Finite Difference Approximation (continued)

- **BASIC IDEA**
  - Derivatives are replaced with algebraic "difference quotients", very similar in spirit to algebraic expressions that are encountered in the standard definition of a derivative in calculus

$$\frac{df(x)}{dx} \equiv f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

  - In the above

$$\frac{f(x+h) - f(x)}{h}$$

is a finite difference approximation of $f'(x)$

Key Steps in Solution of Differential System Using FDA

1. Formulate **precise** and **complete** mathematical description of the problem to solve, including
   - Specification of independent variables (coordinates)
     - $t,\ x,\ (t,x),\ (t,x,y),\ \ldots$
   - Specification of solution domain in terms of these independent variables
     - $0 \le t \le t_{\max},\ [0 \le x \le 1, 0 \le t \le t_{\max}],\ \ldots$
   - Specification of dependent variables and their type (e.g. scalar or vector, real or complex …)
     - $u(t),\ f(x),\ \psi(t,x),\ u(x,y),\ \vec{r}_i(t),\ \ldots$
   - Specification of differential equations governing dependent variables (for time dependent problems, will often call these the equations of motion)
   - Specification of sufficient initial and/or boundary conditions to ensure that the problem has a unique solution.

Typical Differential Equations In This Course

- Particle dynamics: Equations of motion from, e.g., Newton's second law

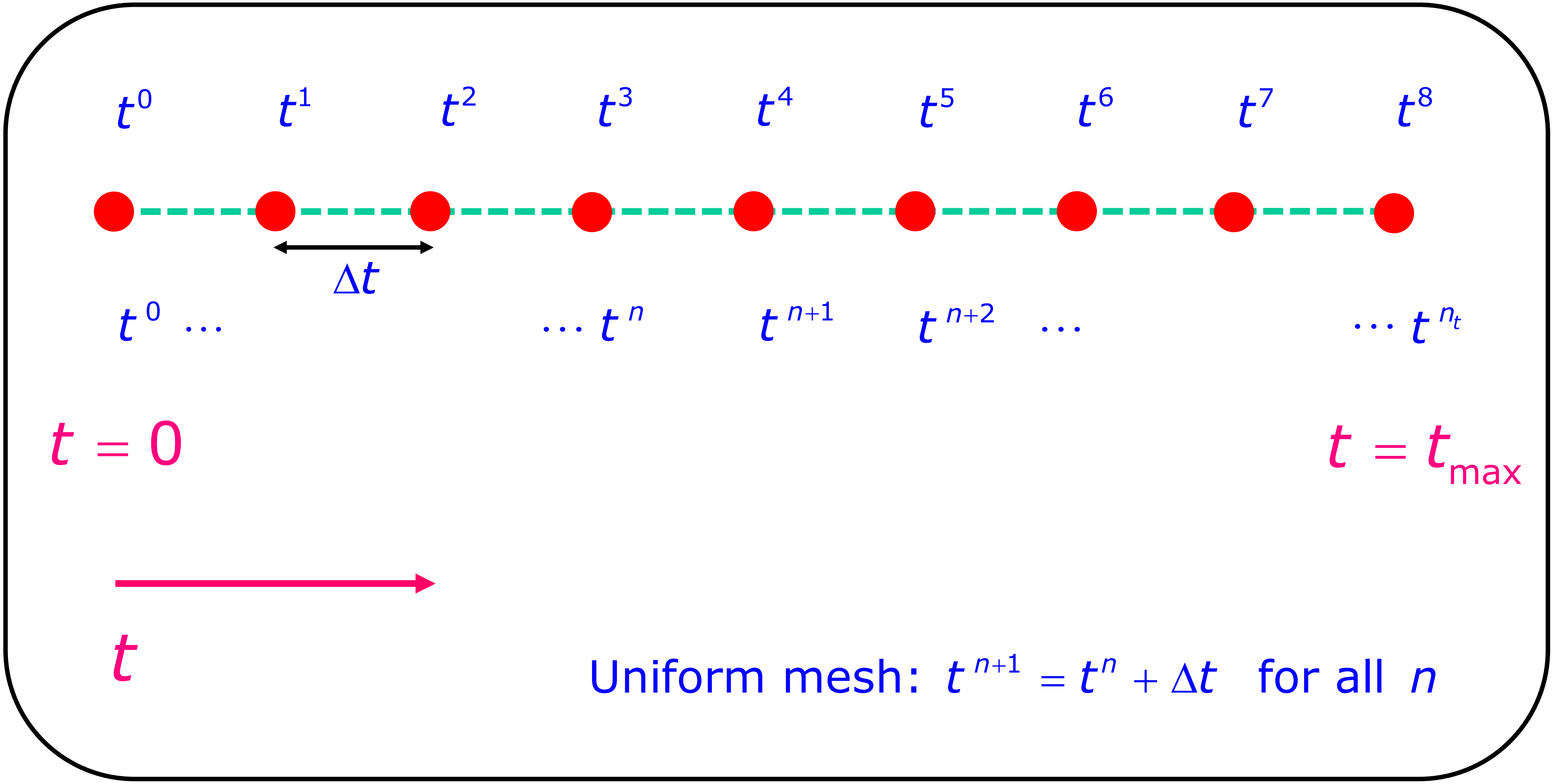
- Example: Single particle

Particle position: $x(t)$

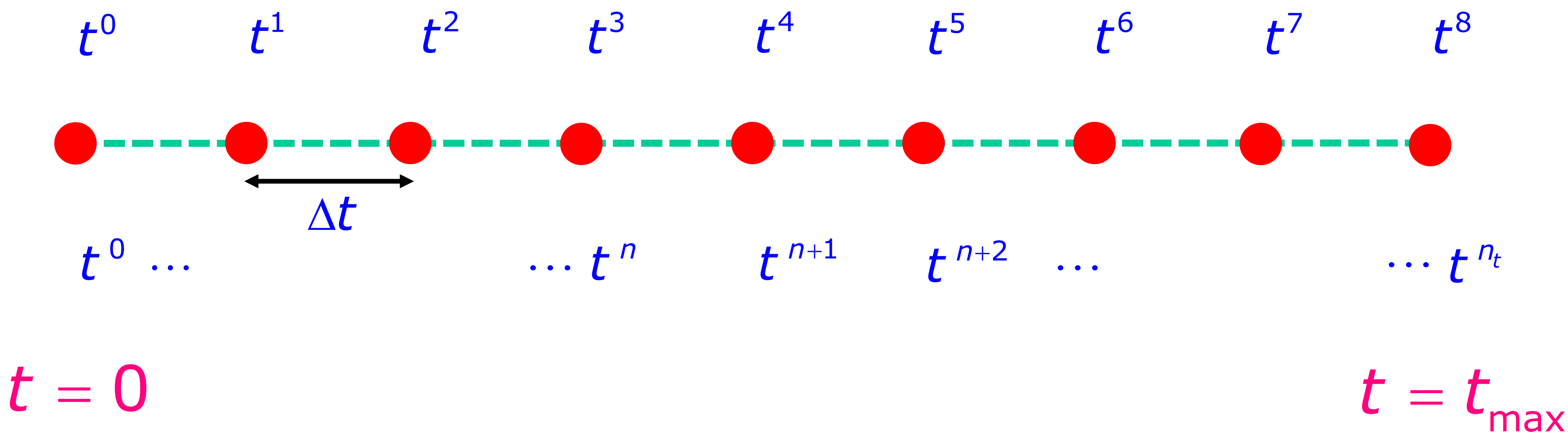
$$m\,a(t) = m\frac{d^2x(t)}{dt^2} = F_{\text{applied}}(t)$$

- Will need FDA for second time derivative of *x(t)*

Example Finite Difference Mesh/Grid



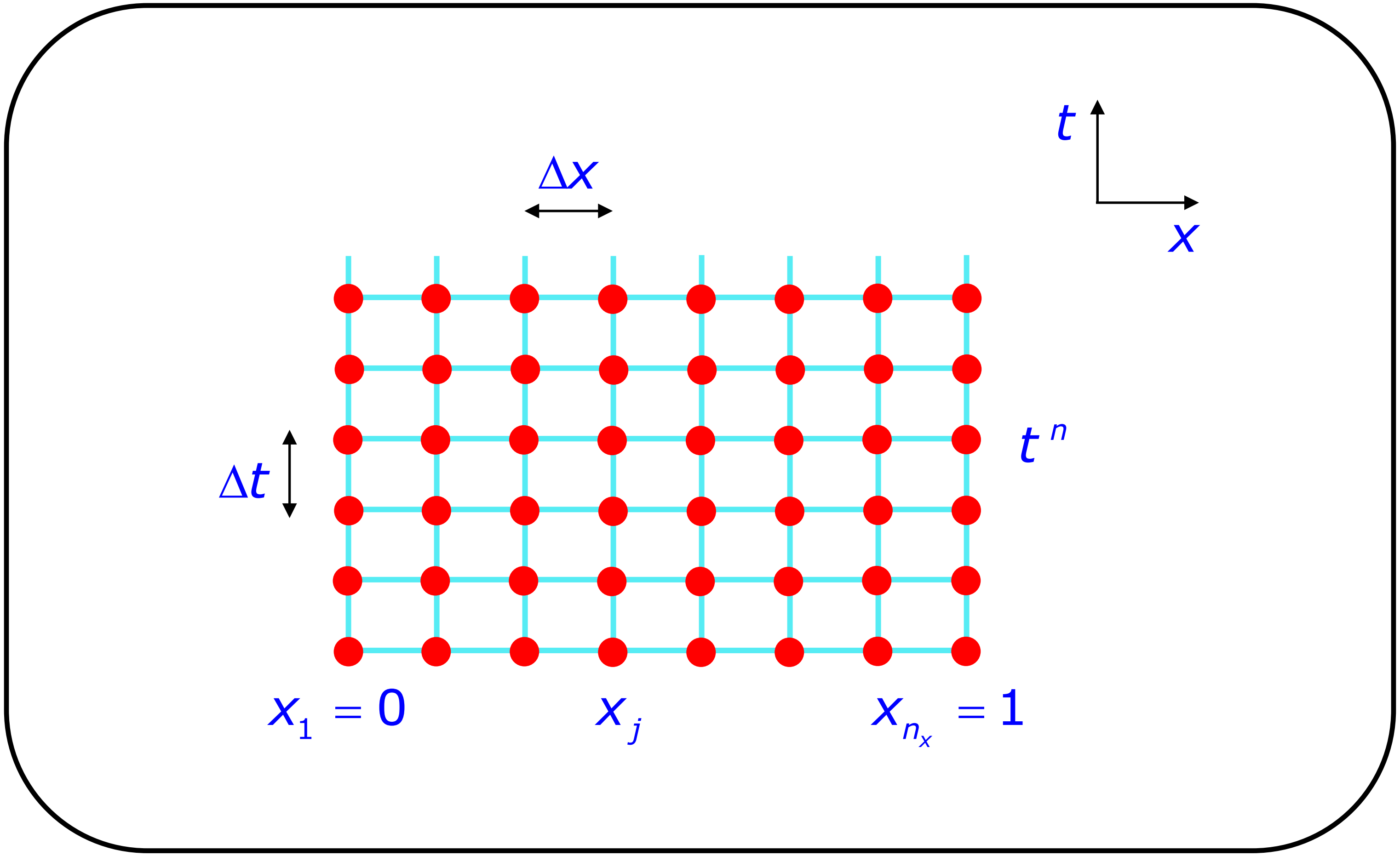
Example Finite Difference Mesh/Grid



Discrete particle position: $x^n \equiv x(t^n)$

Discrete equations of motion determine: $x^n \to x^{n+1} \to x^{n+2} \to \cdots$

Schematic Finite Difference Mesh (Space & Time)



Key Steps in Solution of Differential System Using FDA

2. Discretization: Step 1

   – Define finite difference **grid** (**mesh**, **lattice**) that replaces continuum solution domain with **finite** set of grid points at which discrete solution is to be computed

   – Mesh will be characterized be a set of spacings between adjacent points in each of the coordinate directions; in this course will typically assume that these are constants (so meshes will be called **uniform**)

   – Mesh spacings constitute fundamental parameters that control accuracy of particular FDA

   – Working assumption is that in the limit that the spacings tend to 0, the finite difference solution will **converge** to the continuum solution

Key Steps in Solution of Differential System Using FDA

3. Discretization: Step 2

   – Replace all derivatives—including any involved in the initial or boundary conditions—with finite difference approximations
   – This process yields a set of algebraic equations (linear or non-linear) for the discrete unknowns

4. Solution of algebraic equations

   – The solution of the algebraic equations is then accomplished computationally
   – Depending on the nature of the differential equations as well as the FDA used the sophistication/complexity of the algorithms required to do this efficiently can vary widely

Key Steps in Solution of Differential System Using FDA

5. Convergence testing / error analysis

   – Extremely important part of solution process (difficult to overemphasize importance)

   – Basic idea is to repeat calculations using same basic problem parameters, initial data, boundary conditions etc., but with varying mesh sizes (grid spacings)

   – Investigation of behaviour of finite difference solution as a function of mesh size allows us to estimate (and ultimately control) the accuracy of the solution, and to establish that the solution **is** converging to the desired continuum limit