Simulation in Computer Graphics

Partial Differential Equations

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Motivation

- various dynamic effects and physical processes are described by partial differential equations (PDEs)
  - e.g., wave propagation, advection, diffusion

- we consider PDEs that describe the time rate of change of a quantity at fixed positions
Motivation

- this is a short overview of a large research field in mathematics and physics applied to the fields of animation and computer graphics

- goals:
  - you know what a PDE is
  - you know PDEs for specific effects
  - you know how to solve these PDEs with finite differences
Outline

- introduction
  - 1D advection
- mathematical background
  - definition
  - types
  - boundary conditions
  - numerical solution methods
- examples
  - advection
  - diffusion
  - wave equation
Advection

- simulation of temperate evolution
- consider temperature $T$ at position $x$ and time $t$
- start with known temperatures at time 0: $T(x, 0)$
- consider some wind speed $v$
- how to compute $T(x, t)$ at arbitrary position $x$ and time $t$
Advection Equation in 1D

- consider temperature change within a small time step $\Delta t$ at a fixed position $x_i$

- temperature is only advected
- no additional effects

\[
\frac{\Delta T}{v \Delta t} \approx \frac{\partial T(x,t)}{\partial x} \quad \Delta t \rightarrow 0
\]

\[
\frac{T(x_i, t+\Delta t)-T(x_i, t)}{\Delta t} = \frac{-\Delta T}{\Delta t} \approx \frac{\partial T(x,t)}{\partial t}
\]

\[
\frac{\partial T(x,t)}{\partial t} = -v \frac{\partial T(x,t)}{\partial x}
\]

$T$ depends on two variables (space and time)
$\partial / \partial t$ denotes the time derivative
$\partial / \partial x$ denotes the space derivative
Analytical Solution

- define an initial condition $T(x, 0)$
  - temperature distribution at all positions $x$ at time 0
- $T(x_i, t)$ at a position $x_i$ and time $t$ is obtained by shifting the temperature distribution at time 0 by the distance $vt$

$$T(x_i, t) = T(x_i - vt, 0)$$
Numerical Solution with Finite Differences

Discretization

- consider / sample the function $T(x, t)$ at discrete positions with distance $h$ and discrete times with time step $\Delta t$

$$x_i+1 - x_i = h$$
$$t_{j+1} - t_j = \Delta t$$

- approximate the partial derivatives with finite differences

$$\frac{\partial T(x, t)}{\partial t} \approx \frac{T(x_{i+1}, t_j) - T(x_i, t_j)}{\Delta t}$$
$$\frac{\partial T(x, t)}{\partial x} \approx \frac{T(x_{i+1}, t_j) - T(x_i, t_j)}{h}$$
Numerical Solution with Finite Differences

Approximate Computation of $T$

- \[
\frac{\partial T(x,t)}{\partial t} = -\nu \frac{\partial T(x,t)}{\partial x} \rightarrow \frac{T(x_i,t_{j+1})-T(x_i,t_j)}{\Delta t} = -\nu \frac{T(x_{i+1},t_j)-T(x_i,t_j)}{h}
\]

- can be solved for $T(x_i,t_{j+1})$
  \[
  T(x_i,t_{j+1}) = T(x_i,t_j) - \Delta t \cdot \nu \frac{T(x_{i+1},t_j)-T(x_i,t_j)}{h}
  \]

- from the initial condition, temperature $T(x_i,t_0)$ is known at all sample positions $x_i$ at some time $t_0$

- i.e., for all positions $x_i$, we can compute
  \[
  T(x_i,t_1) = T(x_i,t_0) - \Delta t \cdot \nu \frac{T(x_{i+1},t_0)-T(x_i,t_0)}{h}
  \]

- if we have computed $T(x_i,t_1)$ for all positions $x_i$, we can compute
  \[
  T(x_i,t_2) = T(x_i,t_1) - \Delta t \cdot \nu \frac{T(x_{i+1},t_1)-T(x_i,t_1)}{h}
  \]

- and so on ...
Numerical Solution with Finite Differences
Boundary Conditions

- at time $t_j$, the temperature is known at $n$ sample positions: $T(x_0, t_j), T(x_1, t_j), \ldots, T(x_{n-1}, t_j)$
- however, the computation of the temperature at $x_{n-1}$ requires the temperature at $x_n$
- setting boundary conditions / define missing values
  - e.g., periodic boundaries
  - $T(x_n, t_j) = T(0, t_j)$
  - temperature leaving/entering the right-hand side of the simulation domain, enters/leaves the left-hand side of the domain
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Definition

- a partial differential equation PDE describes the behavior of an unknown multivariable function $f$ using:
  - partial derivatives of $f$, e.g. $\frac{\partial f}{\partial t}$, $\frac{\partial f}{\partial x}$, $\frac{\partial^2 f}{\partial t^2}$, $\frac{\partial^2 f}{\partial x \partial t}$
  - the function $f$ and
  - the independent variables, e.g. $x, t$

- example: $\frac{\partial T(x,t)}{\partial t} = -\nu \frac{\partial T(x,t)}{\partial x}$

- notation $\frac{\partial T(x,t)}{\partial t} = T_t \quad \frac{\partial T(x,t)}{\partial x} = T_x \quad \frac{\partial^2 f}{\partial x \partial t} = f_{x,t}$

$T_t = -\nu T_x$

- ordinary differential equations are a special case for functions that depend on one variable
PDEs in Physics

- independent variables are
  - static problems: $x$ (1D), $x$, $y$ (2D), $x$, $y$, $z$ (3D)
  - dynamic problems: $x$, $t$ (1D+1), $x$, $y$, $t$ (2D+1), $x$, $y$, $z$, $t$ (3D+1)

- unknown functions are
  - scalars, e.g. temperature $T$, density $\rho$
  - vectors, e.g. displacement $\mathbf{u}$, velocity $\mathbf{v}$
PDE Classification

- order
  - given by the highest order of a partial derivative

- linearity
  - the function and its partial derivatives only occur linearly
  - coefficients may be functions of independent variables

- e.g. second-order linear PDE of function \( f(x, y) \) with two independent variables \( x, y \)
  - general form
    \[
    g_1(x, y) f_{xx} + g_2(x, y) f_{xy} + g_3(x, y) f_{yy} +
    g_4(x, y) f_x + g_5(x, y) f_y + g_6(x, y) f + g_7(x, y) = 0
    \]

- non-linear example
  \( f_{xx} \cdot f_{xy} = 0 \)
PDE Classification

- second-order PDEs
  \[ A(x,y)f_{xx} + B(x,y)f_{xy} + C(x,y)f_{yy} + \ldots + F(x,y,f,f_x,f_y) = 0 \]

- can be classified into
  - hyperbolic \( B^2 - A \cdot C > 0 \)
  - parabolic \( B^2 - A \cdot C = 0 \)
  - elliptic \( B^2 - A \cdot C < 0 \)

- classification
  - is geometrically motivated
  - is characterized by different mathematical and physical behavior
  - determines type of required boundary conditions
PDE Classification

- **hyperbolic**
  - time-dependent processes
  - reversible, not evolving to a steady state
  - undiminished propagation
  - e.g., wave motion

- **parabolic**
  - time-dependent processes
  - irreversible, evolving to a steady state
  - dissipative
  - e.g., heat diffusion

- **elliptic**
  - time-independent
  - already in a steady state
Boundary Conditions

- generally, many functions $f$ solve a PDE
- physical applications expect one solution
- $f$ is typically defined in a simulation domain $D$
- the physical solution is required to satisfy certain conditions on the boundary of $D$

$f(x, 0) = f_0(x)$

initial condition

$f(x_1, t) = f_1(t)$

Dirichlet condition

$f_x(x_2, t) = f_2(t)$

Neumann condition
Numerical Solution - Overview

Governing Equations IC / BC

Discretization

System of Algebraic Equations

Equation (Matrix) Solver

Approx. Solution

Continuous form

Finite Difference
Finite Volume
Finite Element
Spectral
Boundary Element

Discrete Nodal Values
e.g., CG
Discretization

- time derivatives
  - finite differences
- spatial derivatives
  - finite differences FDM, finite elements FEM, finite volumes FVM
- example
  - 1D advection
  - continuous form
  - discretizing the time derivative with FD
  - discretizing the spatial derivative with FD
  - algebraic equation

\[
\frac{\partial T(x,t)}{\partial t} = -u \frac{\partial T(x,t)}{\partial x}
\]

\[
\frac{\partial T(x,t)}{\partial t} \approx \frac{T(x_{i+1},t_j) - T(x_{i},t_j)}{\Delta t}
\]

\[
\frac{T(x_{i},t_{j+1}) - T(x_{i},t_{j})}{\Delta t} = -u \frac{T(x_{i+1},t_j) - T(x_{i},t_j)}{h}
\]
2D Sampling

- function $f$ is reconstructed at fixed sample positions at fixed time points
- simplest case: sampling of $f$ on a regular grid
  - e.g., 2D+1 dimensions
  - $f[i, j, t] = f(x_i, y_j, t_t) = f(x_0 + i \cdot h, y_0 + j \cdot h, t_0 + t \cdot \Delta t)$
  - $i \in (0, \ldots, n - 1), j \in (0, \ldots, m - 1), t \in (0, 1, 2, \ldots)$
  - grid spacing $h$ and time step $\Delta t$
2D Finite Difference Approximations

- **time derivative**
  \[ f_t[i, j, t] = \frac{f[i, j, t+1] - f[i, j, t]}{\Delta t} + O(\Delta t) \]
  time marching

- **spatial derivatives**
  \[ f_x[i, j, t] = \frac{f[i+1, j, t] - f[i, j, t]}{h} + O(h) \]
  forward scheme

  \[ f_x[i, j, t] = \frac{f[i, j, t] - f[i-1, j, t]}{h} + O(h) \]
  backward scheme

  \[ f_x[i, j, t] = \frac{f[i+1, j, t] - f[i-1, j, t]}{2h} + O(h^2) \]
  central scheme

- if information moves from left to right, backward is upwind, otherwise forward is upwind
- upwind is typically preferred
2D Finite Difference Approximations

- higher-order derivatives, e.g.
  - \[ f_{xx}[i, j, t] = \frac{f_x[i, j, t] - f_x[i-1, j, t]}{h} = \frac{f[i+1, j, t] - 2f[i, j, t] + f[i-1, j, t]}{h^2} + O(h^2) \]

- higher-order approximations, e.g.
  - \[ f_x[i, j, t] = \frac{f[i-2, j, t] - 8f[i-1, j, t] + 8f[i+1, j, t] - f[i+2, j, t]}{12h} + O(h^4) \]
  - \[ f_{xx}[i, j, t] = \frac{-f[i-2, j, t] + 16f[i-1, j, t] - 30f[i, j, t] + 16f[i+1, j, t] - f[i+2, j, t]}{12h^2} + O(h^4) \]
Explicit Solution Schemes - 1D Advection

- advection equation \( \frac{\partial f(x,t)}{\partial t} = -v \frac{\partial f(x,t)}{\partial x} \)

- upwind \((v > 0)\)
  \[
  \frac{f[i,t+1] - f[i,t]}{\Delta t} + v \frac{f[i,t] - f[i-1,t]}{h} = 0
  \]
  discretization

   \[
   f[i, t + 1] = f[i, t] - v \frac{\Delta t}{h} (f[i, t] - f[i - 1, t])
   \]
  solver (solution scheme)

- simple stability rule
  - information must not travel more than one grid cell per time step
    - \(v \Delta t < h \rightarrow \Delta t < \frac{h}{v}\)
    - \(v \Delta t < h \rightarrow \frac{v \Delta t}{h} = \sigma < 1\) CFL number
    - time step should be sufficiently small to result in \(\sigma < 1\)
Explicit Solution Schemes - 1D Advection

- **downwind** ($v < 0$)
  \[
  \frac{f[i, t+1] - f[i, t]}{\Delta t} + v \frac{f[i+1, t] - f[i, t]}{h} = 0
  \]
  \[
  f[i, t + 1] = f[i, t] - v \frac{\Delta t}{h} (f[i + 1, t] - f[i, t])
  \]

- **centered, FTCS** (forward time centered space)
  \[
  \frac{f[i, t+1] - f[i, t]}{\Delta t} + v \frac{f[i+1, t] - f[i-1, t]}{2h} = 0
  \]
  \[
  f[i, t + 1] = f[i, t] - v \frac{\Delta t}{2h} (f[i + 1, t] - f[i - 1, t])
  \]

- **Leap-frog**
  \[
  \frac{f[i, t+1] - f[i, t-1]}{2\Delta t} + v \frac{f[i+1, t] - f[i-1, t]}{2h} = 0
  \]
  \[
  f[i, t + 1] = f[i, t - 1] - v \frac{\Delta t}{h} (f[i + 1, t] - f[i - 1, t])
  \]
Explicit Solution Schemes - 1D Advection

- **Lax-Wendroff**
  
  $$f[i, t + 1] =$$
  
  $$f[i, t] - v \frac{\Delta t}{2h} (f[i + 1, t] - f[i - 1, t]) + \frac{1}{2} \left( v \frac{\Delta t}{h} \right)^2 (f[i + 1, t] - 2f[i, t] + f[i - 1, t])$$

- **Beam-Warming** ($v > 0$)
  
  $$f[i, t + 1] =$$
  
  $$f[i, t] - v \frac{\Delta t}{2h} (3f[i, t] - 4f[i - 1, t] + f[i - 2, t]) + \frac{1}{2} \left( v \frac{\Delta t}{h} \right)^2 (f[i, t] - 2f[i - 1, t] + f[i - 2, t])$$

- **Lax-Friedrich**
  
  $$f[i, t + 1] =$$
  
  $$\frac{1}{2} (f[i + 1, t] - f[i - 1, t]) - v \frac{\Delta t}{2h} (f[i + 1, t] - f[i - 1, t])$$
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Advection in 2D and 3D

- 1D advection $f_t = -v f_x$
- generally, the velocity is a vector $\mathbf{v}$ with direction $\mathbf{n}_v$ and length $v$
- spatial derivative of $f$ in direction $\mathbf{n}_v$
  \[
  \frac{\partial f}{\partial \mathbf{n}_v} = \mathbf{n}_v \cdot \nabla f \quad \nabla f = \begin{pmatrix} f_x \\ f_y \end{pmatrix} \quad \nabla f = \begin{pmatrix} f_x \\ f_y \\ f_z \end{pmatrix}
  \]
- therefore, $f_t = -v (\mathbf{n}_v \cdot \nabla f) = -\mathbf{v} \cdot \nabla f$
2D Finite Difference Solution Scheme

- advection equation
  \[ f_t + \mathbf{v} \cdot \nabla f = f_t + v_x \cdot f_x + v_y \cdot f_y = 0 \]

- discretization
  \[ \frac{f[i,j,t+1] - f[i,j,t]}{\Delta t} + v_x \frac{f[i,j,t] - f[i-1,j,t]}{h} + v_y \frac{f[i,j,t] - f[i,j-1,t]}{h} = 0 \]

- solution scheme
  \[ f[i,j,t + 1] = f[i,j,t] - \Delta t \left( v_x \frac{f[i,j,t] - f[i-1,j,t]}{h} + v_y \frac{f[i,j,t] - f[i,j-1,t]}{h} \right) \]

- variant
  - velocity can vary with the location
  - PDE still first order and linear
  - \[ f_t + \mathbf{v}(x,y) \cdot \nabla f = 0 \]
**Diffusion in 1D**

- density $\rho(x)$ describes the concentration of a substance in a tube with cross section $A$
- conduction law: the mass flow through an area $A$ (flux) is prop. to the neg. gradient of the density normal to $A$

\[
\frac{dm}{dtA} = \frac{d\rho(x)Adx}{dtA} = k\rho_x(x + dx) - k\rho_x(x)
\]

\[
\rho_t = k\frac{\rho_x(x + dx) - \rho_x(x)}{dx} = k\rho_{xx}
\]

\[
\rho_t = k\rho_{xx} \quad k - \text{conductivity}
\]
Diffusion in 2D and 3D

- equation
  \[ f_t = k \nabla^2 f = k \Delta f = k (f_{xx} + f_{yy}) \quad f_t = k (f_{xx} + f_{yy} + f_{zz}) \]
  - Laplace operator
  - 2D
  - 3D

- intuition for second spatial derivative
- constant gradient, i.e. \( f(x) = a + bx \), has no effect

 Flux, no change

 Flux, positive change
2D Finite Difference Solution Scheme

- diffusion equation
  \[ f_t - k (f_{xx} + f_{yy}) = 0 \]

- discretization
  \[
  \frac{f[i,j,t+1]-f[i,j,t]}{\Delta t} - k \left( \frac{f[i+1,j,t]-2f[i,j,t]+f[i-1,j,t]}{h^2} + \frac{f[i,j+1,t]-2f[i,j,t]+f[i,j-1,t]}{h^2} \right) = 0
  \]

- solution scheme
  \[
  f[i,j,t+1] = f[i,j,t] + \Delta t k \left( \frac{f[i+1,j,t]+f[i-1,j,t]+f[i,j+1,t]+f[i,j-1,t]-4f[i,j,t]}{h^2} \right)
  \]

- intuition
  - if the average value of the neighboring cells is larger than the cell value, the value increases and vice versa
Wave Equation in 1D

- function $u(x)$ is the displacement of the string normal to $x$
- assuming small displacement and constant stress $\sigma$
- force acting normal to cross section $A$ is $f = \sigma A$
- component in $u$-direction $f_u \approx \sigma A u_x$
- Newton’s Second Law for an infinitesimal segment

\[
(\rho A dx) u_{tt} = \sigma A u_x (x + dx) - \sigma A u_x (x)
\]

$\rho_{tt} = \sigma u_{xx}$
Wave Equation in 2D and 3D

- 1D wave equation \( f_{tt} = -c^2 f_{xx} \)  
  \( c \) – speed of wave propagation

- 2D: \( f_{tt} = c^2 \nabla^2 f = c^2 \Delta f = c^2 (f_{xx} + f_{yy}) \)

- 3D: \( f_{tt} = c^2 (f_{xx} + f_{yy} + f_{zz}) \)

- 2D finite difference solution scheme

\[
v[i, j, t + 1] = v[i, j, t] + \Delta t c^2 \frac{f[i+1,j,t]+f[i-1,j,t]+f[i,j+1,t]+f[i,j-1,t]-4f[i,j,t]}{h^2}
\]

\[
f[i, j, t + 1] = f[i, j, t] + \Delta t v[i, j, t + 1]
\]
Demo

- combination of wave equation, advection, and diffusion
  \[
  f_{tt} = c^2 \nabla^2 f \quad \text{wave equation}
  \]
  \[
  f_t = -v_{adv} \cdot \nabla f \quad \text{advection equation}
  \]
  \[
  f_t = k \nabla^2 f \quad \text{diffusion equation}
  \]

- update rule (spatial derivatives not discretized)
  \[
  v[i, j, t + 1] = v[i, j, t] + \Delta t c^2 \nabla^2 f[i, j, t]
  \]
  \[
  u[i, j, t + 1] = u[i, j, t] + \Delta t \left( v[i, j, t + 1] + k \nabla^2 f[i, j, t] - v_{adv} \cdot \nabla f[i, j, t] \right)
  \]
Literature
