Continuous Simulation with Ordinary Differential Equations

Seminar - Modeling and Simulation

Julian Busch
9busch@informatik.uni-hamburg.de

University of Hamburg
Department of Informatics
Scientific Computing

December 3, 2012

Outline

Introduction

- Changes in quantities can accurately be described with derivatives and be related to other quantities via equations
- Differential equations are a natural way to describe dynamically changing systems
- They arise in many different contexts such as
  - Physics & astronomy (celestial mechanics)
  - Geology (weather modeling)
  - Chemistry (reaction rates)
  - Biology, social sciences, economics, ...
- We will focus on the numerical simulation of systems modeled with Ordinary differential equations

Continuous Simulation

Recap:

- **Continuous System:** input, output and state variables are defined over a range of time
- **Discrete Systems:** input, output and state variables are defined for $t_0, t_1, t_2, \ldots$
- **Lumped Models:** only one independent variable (time)
- **Distributed Model:** more than one independent variable

Continuous Simulation

- Ordinary Differential Equations model Continuous and Lumped Systems
- Simulating a system means to solve its mathematical model and predict its behavior in different situations
- Many important differential equations cannot be solved exactly
  - Numerical methods are employed
  - The model is discretized

Example

Falling Ball:

- A ball is falling from a height of 100 m.
- When does it reach the ground?
- Assumption: only gravitational force is acting
- Model:

$$v'(t) = -9.8$$

$$x'(t) = v(t)$$

Initial conditions: $x(0) = 100,\ v(0) = 0$

Example

- Solution:

$$x(t) = 100 - 0.5(9.8)t^2$$

$$v(t) = -9.8t$$

- System can be simulated: vertical position and speed of the ball is given for any time t
- The ball reaches the ground at $t = 4.5175\ s$ with a velocity $v = -44.2719\ m/s$

Ordinary Differential Equations

Definition

An ordinary differential equation (ODE) is an equation containing a function of one independent variable and its derivatives.

- Ordinary: no partial derivatives
- Examples:

$$y'(t) = y(t),$$

$$x''(t) = \frac{F(t, x(t))}{m} \quad \text{(Newton's Second Law)}$$

Ordinary Differential Equations

- General form:

$$F\left(t, y, y', \ldots, y^{(n-1)}\right) = y^{(n)}$$

  where $y = y(t)$ and $y^{(n)}$ denotes the nth derivative of y
- t is called *independent variable* or *time variable*
- n is the *order* of the equation
- A *system* of coupled differential equations is specified, if y is a vector of functions and F is a vector valued function

Order Reduction

- Most solvers expect first order equations
- Higher order equations can be reduced to an equivalent first order system by introducing new functions for the derivatives:

$$\begin{pmatrix} y_1' \\ y_2' \\ \vdots \\ y_{n-1}' \\ y_n' \end{pmatrix} = \begin{pmatrix} y_2 \\ y_3 \\ \vdots \\ y_n \\ F(t, y_1, \ldots, y_n) \end{pmatrix}$$

Classifications

- Some classes of ODEs have special properties
- **Autonomous:** F does not depend on t, also named Time-invariant system
- **Linear:** F can be written as a linear combination of the derivatives of y

$$y^{(n)} = \sum_{i=0}^{n-1} a_i(t) y^{(i)} + r(t)$$

  - **Homogeneous:** $r(t) = 0$
  - **Inhomogeneous:** $r(t) \neq 0$
  - Determining stability of solutions is relatively easy

Solutions

- A solution is a function u that is n times differentiable and satisfies
$$F\left(t, u, u', \ldots, u^{(n-1)}\right) = u^{(n)}$$
- It can be defined on all of $\mathbb{R}$ (*global solution*) or only on a maximal time interval (*maximal solution*)
- Equations without additional conditions have a *general solution* that contains a number of independent constants
  - ODE describes the slope of a solution, not the actual values

Solutions

- The constants can be set to specific values to fulfill additional conditions, yielding a *particular solution*
- **Initial value problem:** specifies a particular solution by a given initial value $y(t_0) = y_0$
- **Boundary value problem:** conditions for more than one point are given, typically specified for the endpoints of some time-interval
- We will focus on Initial value problems

Exact Solutions

- Some but not all ODEs have solutions that can be written in exact and closed form
- Several techniques for solving exist, for example
  - Direct integration
  - Separation of variables
  - Laplace transform
  - Specialized methods for classes of equations

Example

- Consider the equation $y' = y$
- If $y \neq 0$ on its whole domain, we can write it as $\frac{y'}{y} = 1$ so that

$$\int \frac{y'}{y} dt = \int 1 dt = t + C$$

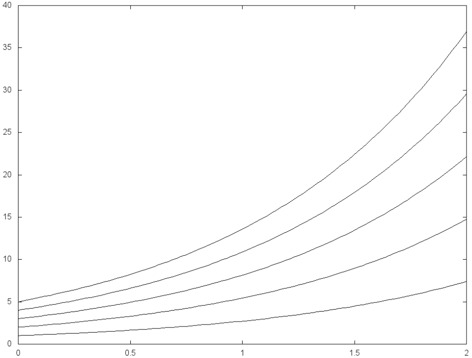
- Since an antiderivative of $\frac{y'}{y}$ is $ln|y|$, we get

$$ln|y| = t + C \quad \text{or} \quad y = \pm e^{C} \cdot e^{t}$$

- Solutions have the form $y = Ae^{t}$ $(A \neq 0)$
- $y = 0$ is a solution for $A = 0$

Example

- A given initial value $y(0) = y_0$ specifies the particular solution $y = y_0 e^t$



Initial Value Problems

- Given: the initial state y_0 of a system at time t_0 and an ODE that determines its evolution
- Want: a function $y(t)$ that describes the state of the system as a function of time
- Most numerical methods expect first order equations as an input:
$$y' = F(t, y), \qquad y(t_0) = y_0$$
- The IVP has a unique solution, provided F is sufficiently smooth (continuous in t and Lipschitz-continuous in y)

Numerical Methods

- Many important problems cannot be solved analytically
- Goal: predict future values of y by simulating the systems behavior
- Calculate a sequence of approximations $y_1, y_2, y_3, \ldots$ for y at consecutive points in time $t_0 + h, t_0 + 2h, t_0 + 3h, \ldots$
- h is called *step size*

Euler's Method

- Probably the most simple and popular method
- Trivial case of several more general techniques
- Consider the Taylor expansion of y around t_n:

$$y(t_n + h) = y(t_n) + hy'(t_n) + \frac{1}{2}h^2 y''(t_n) + O(h^3)$$

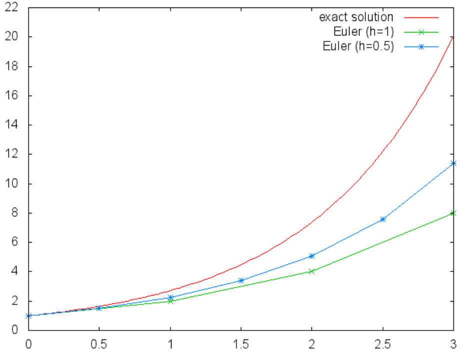
- Euler's method uses the first two terms as an approximation for $y(t_{n+1})$:

$$y_{n+1} = y_n + hF(t_n, y_n)$$

Euler's Method

Geometrical description:

- Start at initial value
- Take small steps along the tangent lines through the previous approximations



Stability of Solutions

- Roughly speaking, the *stability* for an ODE reflects the sensitivity of its solution to perturbations
- If the solutions are *stable*, they converge with time so that perturbations are damped out
- If the solutions are *unstable*, they diverge with time so that perturbations will grow
- When stepping from one approximation to the next, we land on a different solution from what we started from
- The stability of the solutions has an influence on whether the incurred error grows or decreases with time

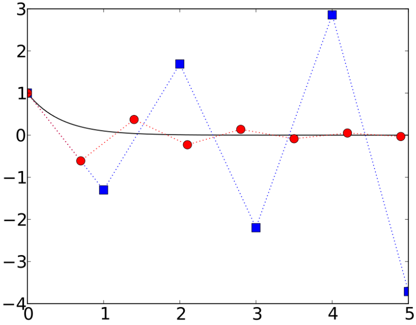
Stiffness

- ODEs for which stable solutions converge too rapidly are called *stiff*
- Some methods are inefficient for stiff equations
- Example: Euler's Method applied to the IVP

$$y' = -2.3y, \quad y(0) = 1$$

with step-sizes $h = 1$ and $h = 0.7$

Stiffness



- Numerical solution for $h = 1$ oscillates and grows without bound, stiffness forces very small step-sizes

image: `http://en.wikipedia.org/wiki/File:Instability_of_Euler%27s_method.svg`

Analysis

Numerical Analysis offers several concepts to evaluate the quality of numerical methods:

- **Global truncation error:** difference between computed and true solution passing through initial value:

$$e_n = y_n - y(t_n)$$

- **Local truncation error:** error made in one step of the method

$$l_n = y_n - u_{n-1}(t_n)$$

  where u_{k-1} is the solution passing through the previous approximation
- Want: small global error, but can only control local error

Analysis

- **Order:** method has order p, if

$$l_n = O(h^{p+1})$$

  (How much does the local error decrease with the step-size?)
- **Stability:** method is stable if it produces stable solutions, so that errors are not magnified
  - Stability depends on the stability of the ODE being solved, the method itself and the step-size
  - A method with low stability can produce high global errors despite a high order
  - Several different definitions exist

Analysis of Euler's Method

- Euler's Method has Order 1 (compare to Taylor series)
- It can produce unstable solutions (as seen before)
- Not effective for stiff equations

Backward Euler Method

- Use $F(t_{n+1}, y_{n+1})$ instead of $F(t_n, y_n)$:

$$y_{n+1} = y_n + hF(t_{n+1}, y_{n+1})$$

- Need to solve an algebraic equation
- Fixed-point iteration or Newton's method often used
- Starting guess for iteration can be obtained from explicit method or previous solution
- Same order as Euler's Method
- But: better stability and effective for stiff equations

Generalizations

- Exploit values available upon reaching t_n: $y_n, y_{n-1}, \ldots$ and $F(t_n, y_n), F(t_{n-1}, y_{n-1}), \ldots$
- **Explicit methods** use information at time t_n for the solution at time t_{n+1}
  - e.g. Euler Method
- **Implicit methods** use information at time t_{n+1}
  - Needs to evaluate F with argument y_{n+1} before its value is known
  - Generally more stable than comparable explicit methods
  - e.g. Backward Euler Method
- Important classes of methods: Backward Differentiation Formulas, Adams Methods, Runge-Kutta Methods

Trapezoidal Rule

- Implicit second order method
- Combines Euler & Backward Euler:

$$y_{n+1} = y_n + \frac{h}{2}\left(F(t_n, y_n) + F(t_{n+1}, y_{n+1})\right)$$

- Starting guess for y_{n+1} can be provided by an explicit method
- Correct it with the implicit formula, either repeatedly (fixed point iteration) or a fixed number of times
- The two methods are called a *predictor-corrector pair*

Heun's Method

- Heun's Method results from predicting with Euler's Method and correcting once with the Trapezoidal rule:

$$p_{n+1} = y_n + hF(t_n, y_n)$$

$$y_{n+1} = y_n + \frac{h}{2}\left(F(t_n, y_n) + F(t_{n+1}, p_{n+1})\right)$$

- Performing a single correction amounts to an explicit method
- Heun's method has order 2

Example: Euler vs. Trapezoidal rule

- Consider the IVP

$$y' = -15y, \quad y(0) = 1$$

with the exact solution $y(t) = e^{-15t}$

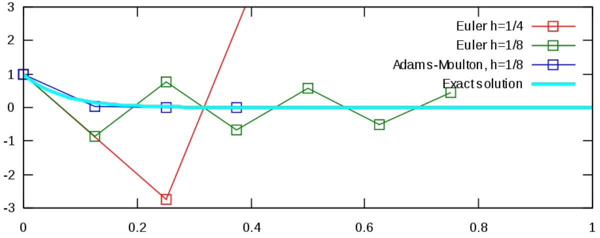


image: `http://en.wikipedia.org/wiki/File:StiffEquationNumericalSolvers.svg`

Adaptive step size

- It is appropriate to use a different size for each step to keep the local error below some tolerance level
- Sometimes the step-size can be increased to save computation time
- Sometimes it has to be reduced to ensure accuracy and stability
- The Runge-Kutta-Fehlberg method RK45 achieves this by producing 5th- and 4th-order estimates
  - The difference provides an estimate for the local error
  - The step-size is then adapted to the error estimate
  - `ode45` in matlab/octave

Application: N-body Simulation

The gravitational N-body problem:

- Predict the motion of N gravitationally interacting particles
- Applications range from systems of few bodies to solar systems and even systems of galactic and cosmological scale
- We will model our solar system, considering the Sun, the eight inner and outer planets and the dwarf-planet Pluto ($N = 10$)

Model

- Combining Newton's Law of Universal Gravitation and the Second Law of Motion yields the following second order system:

$$a_i = \frac{\mathrm{d}^2 r_i}{\mathrm{d}t^2} = G \cdot \sum_{j \neq i} \frac{m_j (r_j - r_i)}{\|r_j - r_i\|^3} \qquad (i = 1, \ldots, N)$$

  (consisting of $3N$ equations, one per body and coordinate)
- Initial values for the positions r_i and velocities v_i can be obtained from `http://ssd.jpl.nasa.gov/?horizons`

Model

- Before the presented numerical methods can be applied, the system must be reduced to a first order system
- We do so by introducing the first derivative of position, the velocity, to get the following first order system:

$$\frac{\mathrm{d}r_i}{\mathrm{d}t} = v_i \qquad (i = 1, \ldots, N)$$
$$\frac{\mathrm{d}v_i}{\mathrm{d}t} = a_i = G \cdot \sum_{j \neq i} \frac{m_j(p_j - p_i)}{\|p_j - p_i\|^3} \qquad (i = 1, \ldots, N)$$

(consisting of now $6N$ equations)

Simulation

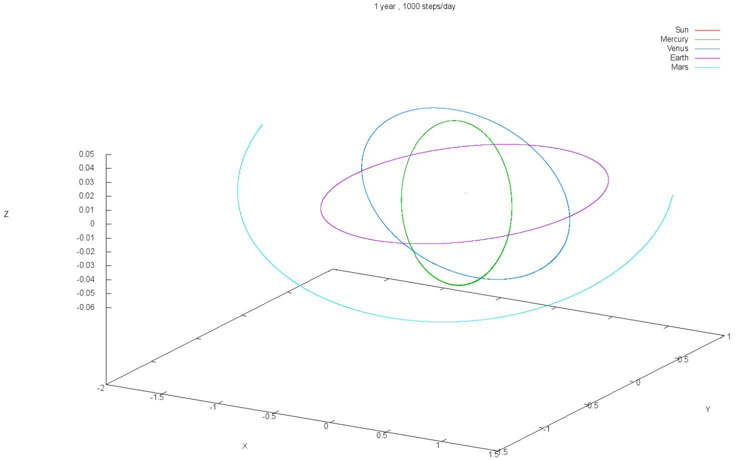
- For simplicity, we will use Euler's method to solve the equations
- Starting with the initial values, a series of approximations for the position and velocity of all bodies is calculated
- The values after a time-step of length h are given by

$$r_i(t_{n+1}) = r_i(t_n) + hv_i(t_n) \quad \text{and}$$

$$v_i(t_{n+1}) = v_i(t_n) + ha_i(t_n)$$

Simulation

- The obtained values can be used to plot the bodies' trajectories:



Conclusion

- Many different numerical methods for solving ODEs exist
- Higher order methods provide better accuracy but are more expensive
- When dealing with stiff ODEs, implicit methods should be employed (BDF, Adams-Moulton, ...)
- Most solvers use variable step-sizes
- The choice of an appropriate method for a given problem is crucial

References I

- Samir Al-Amer.
  Se207: Modeling and simulation.
  http://faculty.kfupm.edu.sa/SE/samirha/SE207_072/SE207_March2008.htm, 2008.
- John C. Butcher.
  Numerical Methods for Ordinary Differential Equations.
  John Wiley & Sons, 2008.
- Florin Diacu.
  The solution of the n-body problem.
  The Mathematical Intelligencer, 18, No. 3:66–70, 1996.

References II

Dimitry Gorinevsky.
Ee392m: Control engineering methods for industry.
http://www.stanford.edu/class/archive/ee/ee392m/ee392m.1034/Lecture2_Models.pdf, Winter Quarter 2002-2003.

Michael T. Heath.
Scientific computing: An introductory survey, chapter 9.
http://www.cse.uiuc.edu/heath/scicomp/notes/chap09.pdf, 2002.

Piet Hut and Michele Trenti.
N-body simulations (gravitational).
Scholarpedia, 3(5):3930, 2008.

References III

S. Thompson and L. F. Shampine.
Initial value problems.
Scholarpedia, 2(2):2861, 2007.

Wikipedia.
Numerical methods for ordinary differential equations — wikipedia, the free encyclopedia, 2012.
[Online; accessed 10-November-2012].

Wikipedia.
Ordinary differential equation — wikipedia, the free encyclopedia, 2012.
[Online; accessed 10-November-2012].