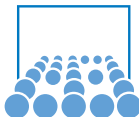


Scientific Computing I

Module 4: Numerical Methods for ODE

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Part I: Basic Numerical Methods

Motivation: Direction Fields

Euler's Method

Discretized Model vs. Discrete Model

Implicit Euler

Analysis of Numerical Schemes for ODE

Local Discretisation Error

Global Discretisation Error

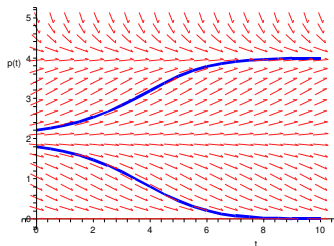
Order of Consistency/Convergence

Motivation: Direction Fields

- given: initial value problem:

$$\dot{y}(t) = f(t, y(t)), \quad y(t_0) = y_0$$

- easily computable: direction field



- idea: “follow the arrows”

“Following the Arrows”

- direction field illustrates slope for given time t_n and value y_n :

$$\dot{y}_n = f(t_n, y_n)$$

- “follow arrows” = make a small step in the given direction:

$$y_{n+1} := y_n + \tau \dot{y}_n = y_n + \tau f(t_n, y_n)$$

- motivates numerical scheme:

$$\begin{aligned} y_0 &:= y_0 \\ y_{n+1} &:= y_n + \tau f(t_n, y_n) \quad \text{for } n = 0, 1, 2, \dots \end{aligned}$$

Euler's Method

- numerical scheme is called **Euler's method**:

$$y_{n+1} := y_n + \tau f(t_n, y_n)$$

- results from **finite difference** approximation:

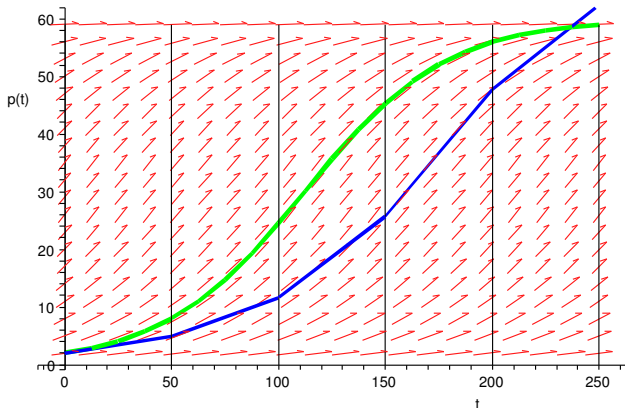
$$\frac{y_{n+1} - y_n}{\tau} \approx \dot{y}_n = f(t_n, y_n)$$

(difference quotient instead of derivative)

- or from truncation of Taylor expansion:

$$y(t_{n+1}) = y(t_n) + \tau \dot{y}(t_n) + \mathcal{O}(\tau^2)$$

Euler's Method and Direction Fields



use direction at the **beginning** of the timestep

Euler's Method – 1D examples

- model of Malthus, $\dot{p}(t) = \alpha p(t)$:

$$p_{n+1} := p_n + \tau \alpha p_n$$

- Logistic Growth, $\dot{p}(t) = \alpha (1 - p(t)/\beta) p(t)$:

$$p_{n+1} := p_n + \tau \alpha \left(1 - \frac{p_n}{\beta}\right) p_n$$

- Logistic growth with threshold:

$$p_{n+1} := p_n + \tau \alpha \left(1 - \frac{p_n}{\beta}\right) \left(1 - \frac{p_n}{\delta}\right) p_n$$

Euler's Method in 2D

- Euler's method is easily extended to systems of ODE \rightarrow use vector notation:

$$\mathbf{y}_{n+1} := \mathbf{y}_n + \tau f(t_n, \mathbf{y}_n)$$

- example: nonlinear extinction model

$$\dot{p}(t) = \left(\frac{71}{8} - \frac{23}{12}p(t) - \frac{25}{12}q(t) \right) p(t)$$

$$\dot{q}(t) = \left(\frac{73}{8} - \frac{25}{12}p(t) - \frac{23}{12}q(t) \right) q(t)$$

- Euler's method:

$$p_{n+1} = p_n + \tau \left(\frac{71}{8} - \frac{23}{12}p_n - \frac{25}{12}q_n \right) p_n$$

$$q_{n+1} = q_n + \tau \left(\frac{73}{8} - \frac{25}{12}p_n - \frac{23}{12}q_n \right) q_n$$

Discretized Model vs. Discrete Model

- example: model of Malthus/radioactive decay ($\dot{p} = -\alpha p$):

$$p_{n+1} := p_n - \tau\alpha p_n, \quad \alpha > 0$$

- compare to discrete model:

$$p_{n+1} := p_n - \delta p_n, \quad \delta > 0$$

with decay rate δ (“percentage”)

- obvious restriction in the discrete model: $\delta < 1$
- obvious restriction for τ in the discretized model?

$$\tau\alpha < 1 \Rightarrow \tau < \alpha^{-1}$$

- not that simple in non-linear models or systems of ODE!

Implicit Euler

- Euler's method ("explicit Euler"):

$$y_{n+1} := y_n + \tau f(t_n, y_n)$$

- implicit Euler:

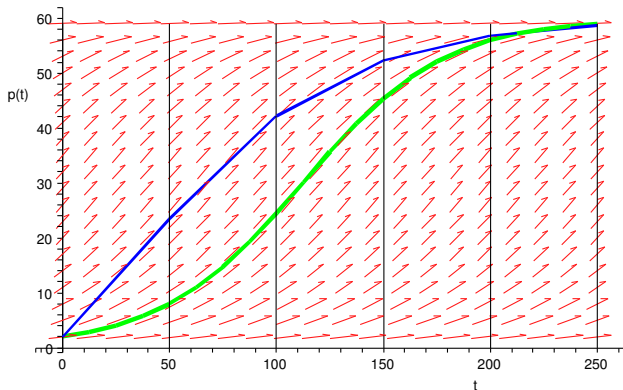
$$y_{n+1} := y_n + \tau f(t_{n+1}, y_{n+1})$$

- results from **finite difference** approximation:

$$\frac{y_{n+1} - y_n}{\tau} \approx \dot{y}_{n+1} = f(t_{n+1}, y_{n+1})$$

- explicit formula for y_{n+1} not immediately available
- to do: solve equation for y_{n+1}

Implicit Euler and Direction Fields



use direction at **end** of the timestep

Implicit Euler – Examples

- example: Model of Malthus/radioactive decay

$$p_{n+1} := p_n - \tau\alpha p_{n+1} \Rightarrow p_{n+1} = \frac{1}{1 + \tau\alpha} p_n$$

- correct (discrete) model?

$\alpha > 0$: then $0 < (1 + \tau\alpha)^{-1} < 1$ for any τ

$\alpha < 0$: then $\tau < -\alpha^{-1}$ required!

- in physics $\alpha > 0$ is more frequent!
(damped systems, friction, ...)
- implicit schemes preferred when explicit schemes require very small τ

Implicit Euler – 2D Example

- example: arms race

$$p_{n+1} = p_n + \tau (b_1 + a_{11}p_{n+1} + a_{12}q_{n+1})$$

$$q_{n+1} = q_n + \tau (b_2 + a_{21}p_{n+1} + a_{22}q_{n+1})$$

- solve linear system of equations:

$$(1 - \tau a_{11})p_{n+1} - \tau a_{12}q_{n+1} = p_n + \tau b_1$$

$$-\tau a_{21}p_{n+1} + (1 - \tau a_{22})q_{n+1} = q_n + \tau b_2$$

(for each time step $n \rightarrow n + 1$)

- in vector notation: $(I - \tau A)\mathbf{y}_{n+1} = \mathbf{y}_n + \tau \mathbf{b}$

Local Discretisation Error

- local influence of using differences instead of derivatives
- example: Euler's method

$$l(\tau) = \max_{[a,b]} \left\{ \left\| \frac{y(t+\tau) - y(t)}{\tau} - f(t, y(t)) \right\| \right\} = \frac{\tau}{2} \|\ddot{y}_n\| + O(\tau^2)$$

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- memory hook: insert exact solution $y(t)$ into

$$\frac{y_{n+1} - y_n}{\tau} - \dot{y}_n$$

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$$\frac{y_{n+1} - y_n}{\tau} - \dot{y}_n$$

A numerical scheme is called **consistent**, if

$$l(\tau) \rightarrow 0 \quad \text{for } \tau \rightarrow 0$$

Global Discretisation Error

- compare numerical solution with exact solution
- example: Euler's method

$$e(\tau) = \max_{k=0, \dots, k_{max}} \{ \|y_k - y(t_k)\| \}$$

$y(t)$ exact solution;

y_k solution of the discretized equations (depends on τ)

A numerical scheme is called **convergent**, if

$$e(\tau) \rightarrow 0 \quad \text{for } \tau \rightarrow 0$$

Global Discretisation Error – Explicit Euler

$$\begin{aligned}
 \mathbf{e}_{n+1} &= \mathbf{y}_{n+1} - \mathbf{y}(t_{n+1}), \\
 \mathbf{y}_{n+1} &= \mathbf{y}_n + \tau \mathbf{f}(t_n, \mathbf{y}_n), \\
 \mathbf{y}(t_{n+1}) &= \mathbf{y}(t_n) + \tau \mathbf{f}(t_n, \mathbf{y}(t_n)) + \tau^2 \frac{\ddot{\mathbf{y}}(t_n)}{2} + O(\tau^3), \\
 \Rightarrow |\mathbf{e}_{n+1}| &\stackrel{\cdot}{\leq} |\mathbf{e}_n| + \tau M |\mathbf{e}_n| + N\tau^2 \\
 &= (1 + M\tau) |\mathbf{e}_n| + N\tau^2 \\
 &\leq (1 + \tau M)^2 |\mathbf{e}_{n-1}| + (1 + \tau M) N\tau^2 + N\tau^2 \\
 &\leq \dots \leq e^{(n+1) \cdot \tau M} \underbrace{|\mathbf{e}_0|}_{=0} + N\tau^2 \frac{e^{(n+1) \cdot \tau M} - 1}{\tau M} \\
 &= N\tau \frac{e^{(n+1) \cdot \tau M} - 1}{M} = N\tau \frac{e^{(t_{n+1} - t_0)M} - 1}{M} = O(\tau).
 \end{aligned}$$

Order of Consistency/Convergence

A numerical scheme is called **consistent** of order p (p -th order consistent), if

$$I(\tau) = \mathcal{O}(\tau^p)$$

A numerical scheme is called **convergent** of order p (p -th order convergent), if

$$e(\tau) = \mathcal{O}(\tau^p)$$

We have shown that the explicit Euler method is consistent and convergent of order 1.

For more complicated ODE or numerical schemes
→ see lecture(s) in Numerical Programming

Part II: Advanced Numerical Methods

Runge-Kutta-Methods

2nd-order Runge-Kutta

4th-order Runge-Kutta

Multistep Methods

Adams-Bashforth

Adams-Moulton

Explicit Midpoint Rule

Problems for Numerical Methods for ODE

Ill-Conditioned Problems

Stability

Stiff Equations

Summary

Runge-Kutta-Methods

- 1st idea: use additional evaluations of f :

$$y_{n+1} = y_n + \tau \sum_{i=1}^p \beta_i f(t_n^i, y_n^i) \text{ with } t_n^i \in [t_n; t_{n+1}]$$

open questions: Where to obtain $y_n^i, i = 1, \dots, p$? How to choose $\beta_i, i = 1, \dots, p$?

- 2nd idea: numerical approximations for missing values of y :

$$y_n^i := y_n + \tau \sum_{j=1}^p \alpha_{i,j} f(t_n^j, y_n^j)$$

explicit Runge-Kutta: $\alpha_{i,j} = 0$ if $j \geq i$.

- 3rd idea: choose β_i and $\alpha_{i,j}$ such that order of consistency is maximal (use quadrature rules)

Runge-Kutta-Methods of 2nd Order

- example: 2nd-order Runge-Kutta (“method of Heun”)

$$\begin{aligned}y_n^I &= y_n, \\y_n^{II} &= y_n + \tau f(t_n, y_n^I), \\y_{n+1} &= y_n + \tau \frac{1}{2} (f(t_n, y_n^I) + f(t_{n+1}, y_n^{II})).\end{aligned}$$

- interpretation of the steps:

- $y_n^{II} = y_n + \tau f(t_n, y_n^I)$

→ Euler step to obtain estimate y_n^{II} for solution at time t_{n+1}

- $y_{n+1} = y_n + \tau \frac{1}{2} (f(t_n, y_n^I) + f(t_{n+1}, y_n^{II}))$

→ Euler step using an averaged direction

(averages directions obtained from t_n, y_n^I and t_{n+1}, y_n^{II})

- exercise: draw these steps into direction field!

Runge-Kutta-Methods of 2nd Order (2)

- further example: “modified Euler” (also 2nd order)

$$\begin{aligned}y_n^I &= y_n, \\y_n^{II} &= y_n + \frac{\tau}{2} f(t_n, y_n^I), \\y_{n+1} &= y_n + \tau f\left(t_n + \frac{\tau}{2}, y_n^{II}\right)\end{aligned}$$

- interpretation of the steps:

1. $y_n^{II} = y_n + \frac{\tau}{2} f(t_n, y_n^I)$

→ Euler step with step size $\tau/2$

to obtain estimate y_n^{II} for solution at time $t_{n+\frac{1}{2}}$

2. $y_{n+1} = y_n + \tau f\left(t_n + \frac{\tau}{2}, y_n^{II}\right)$

→ Euler step using direction obtained from $t_{n+\frac{1}{2}}, y_n^{II}$

- exercise: draw these steps into direction field!

Runge-Kutta-Method of 4th order

classical 4th-order Runge-Kutta:

- intermediate steps:

$$t_n^I = t_n, \quad y_n^I = y_n, \quad (1)$$

$$t_n^{II} = t_n + \frac{\tau}{2}, \quad y_n^{II} = y_n + \frac{\tau}{2} f(t_n^I, y_n^I), \quad (2)$$

$$t_n^{III} = t_n + \frac{\tau}{2}, \quad y_n^{III} = y_n + \frac{\tau}{2} f(t_n^{II}, y_n^{II}), \quad (3)$$

$$t_n^{IV} = t_{n+1}, \quad y_n^{IV} = y_n + \tau f(t_n^{III}, y_n^{III}). \quad (4)$$

- explicit scheme:

$$y_{n+1} = y_n + \frac{\tau}{6} \left(f(t_n^I, y_n^I) + 2f(t_n^{II}, y_n^{II}) + 2f(t_n^{III}, y_n^{III}) + f(t_n^{IV}, y_n^{IV}) \right)$$

- How would you translate this method into efficient pseudo-code?
Remember that unnecessary evaluations of f can be very costly!

Pseudo-Code Runge-Kutta-Method of 4th order

```
f[1] = f(t,y[n]);  
dt2 = dt/2;  
t2 = t + dt2;  
f[2] = f(t2, y[n] + dt2*f[1]);  
f[3] = f(t2, y[n] + dt2*f[2]);  
t = t + dt;  
f[4] = f(t, y[n] + dt*f[3]);  
y[n+1] = y[n] + dt * (f[1] + 2*f[2] + 2*f[3] + f[4]);
```

Note: each $f[. . .]$ will be a vector (1D array) for systems of ODE

Multistep Methods

- 1st idea: use previous steps for computation:

$$y_{n+s} = g(y_n, y_{n+1}, \dots, y_{n+s-1})$$

Multistep Methods

- 1st idea: use previous steps for computation:

$$y_{n+s} = g(y_n, y_{n+1}, \dots, y_{n+s-1})$$

- 2nd idea: use integral form of ODE

$$\begin{aligned} \dot{y}(t) &= f(t, y(t)) \\ \int_{t_{n+s-1}}^{t_{n+s}} \dot{y}(\theta) d\theta &= \int_{t_{n+s-1}}^{t_{n+s}} f(\theta, y(\theta)) d\theta \\ y(t_{n+s}) - y(t_{n+s-1}) &= \int_{t_{n+s-1}}^{t_{n+s}} f(\theta, y(\theta)) d\theta =? \end{aligned}$$

Multistep and Numerical Quadrature

- 3rd idea: use numerical method for integration
→ interpolate f using a polynomial p :

$$y(t_{n+s}) - y(t_{n+s-1}) = \int_{t_{n+s-1}}^{t_{n+s}} f(\theta, y(\theta)) d\theta \approx \int_{t_{n+s-1}}^{t_{n+s}} p(\theta) d\theta$$

where

$$p(t_{n+j}) = f(t_{n+j}, y(t_{n+j})) \quad \text{for } j = 0, \dots, s-1.$$

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where

$$p(t_{n+j}) = f(t_{n+j}, y(t_{n+j})) \quad \text{for } j = 0, \dots, s-1.$$

- compute integral and obtain quadrature rule:

$$y_{n+s} = y_{n+s-1} + \tau \sum_{j=0}^{s-1} \beta_j f(t_{n+j}, y(t_{n+j}))$$

Adams-Bashforth

- $s = 1 \Rightarrow$ use y_n only to compute y_{n+1} (Euler's method):

$$p(t) = f(t_n, y_n), \quad y_{n+1} = y_n + \tau f(t_n, y_n)$$

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$$p(t) = f(t_n, y_n), \quad y_{n+1} = y_n + \tau f(t_n, y_n)$$

- $s = 2 \Rightarrow$ use y_n and y_{n+1} to compute y_{n+2} :

$$p(t) = \frac{t_{n+1} - t}{\tau} f(t_n, y_n) + \frac{t - t_n}{\tau} f(t_{n+1}, y_{n+1}),$$
$$y_{n+2} = y_{n+1} + \frac{\tau}{2} (3f(t_{n+1}, y_{n+1}) - f(t_n, y_n))$$

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- usually consistent of s -th order
- modified at start (no previous values available)

Adams-Moulton

- use idea of Adams-Bashforth, but:
include value y_{n+s} in polynomial $p \Rightarrow$ **implicit scheme**

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- first order: implicit Euler

$$p(t) = f(t_{n+1}, y_{n+1}), \quad y_{n+1} = y_n + \tau f(t_{n+1}, y_{n+1})$$

- second order: Crank-Nicolson method (trapezoidal rule)

$$y_{n+1} = y_n + \frac{\tau}{2} (f(t_n, y_n) + f(t_{n+1}, y_{n+1}))$$

Adams-Moulton

- use idea of Adams-Bashforth, but:
include value y_{n+s} in polynomial $p \Rightarrow$ **implicit scheme**
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$$p(t) = f(t_{n+1}, y_{n+1}), \quad y_{n+1} = y_n + \tau f(t_{n+1}, y_{n+1})$$

- second order: Crank-Nicolson method (trapezoidal rule)

$$y_{n+1} = y_n + \frac{\tau}{2} (f(t_n, y_n) + f(t_{n+1}, y_{n+1}))$$

- how to obtain y_{n+s} ?
 - solve (nonlinear) equation \Rightarrow difficult!
 - easier and more common: *predictor-corrector* approach

Explicit Midpoint Rule

- formally a multi-step scheme: $y_{n+2} = g(y_n, y_{n+1})$
- derive from symmetric difference quotient:

$$\begin{aligned}\dot{y}(t) &= f(t, y(t)) \\ \frac{y(t + \tau) - y(t - \tau)}{2\tau} &= f(t, y(t))\end{aligned}$$

- leads to the following time-stepping scheme:

$$y_{n+2} = y_n + 2\tau f(t_{n+1}, y_{n+1})$$

- 2nd-order accurate with low computational effort, but tends to be instable (see below)

Problems for Numerical Methods for ODE

Short overview on possible problems:

- **Ill-Conditioned Problems:**
small changes in the input \Rightarrow big changes in the exact solution of the ODE

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big errors in the numerical solution compared to the exact solution (for arbitrarily small time steps although the method is consistent)

Problems for Numerical Methods for ODE

Short overview on possible problems:

- **Ill-Conditioned Problems:**
small changes in the input \Rightarrow big changes in the exact solution of the ODE
- **Instability:**
big errors in the numerical solution compared to the exact solution (for arbitrarily small time steps although the method is consistent)
- **Stiffness:**
small time steps for explicit single-step methods required for non-oscillatory behaviour of the approximate solution (although the exact solution is smooth)

III-Conditioned Problems

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- small changes in input entail completely different results
- numerical treatment of such problems is always difficult!
- discriminate:
 - only at critical points?
 - everywhere?
- possible risks:
 - non-precise input
 - round-off errors,...
- question: what are you interested in?
 - really the solution for specific initial condition?
 - statistical info on the solution?
 - general behaviour (patterns)?

Stability: Example explLMM2

Example:

$$\dot{y}(t) = y(t), \quad y(0) = 1$$

- exact solution: $y(t) = (e^t)$
- well-conditioned: $y_\varepsilon(0) = 1 + \varepsilon \Rightarrow y_\varepsilon(t) - y(t) = \varepsilon e^t$

Stability: Example explLMM2

Example:

$$\dot{y}(t) = y(t), \quad y(0) = 1$$

- exact solution: $y(t) = (e^t)$
- well-conditioned: $y_\varepsilon(0) = 1 + \varepsilon \Rightarrow y_\varepsilon(t) - y(t) = \varepsilon e^t$
- use following explicit multistep scheme ($s = 2$):

$$y_{n+2} = -4y_{n+1} + 5y_n + \tau \cdot [4 \cdot f(t_{n+1}, y_{n+1}) + 2 \cdot f(t_n, y_n)]$$

- leads to numerical scheme:

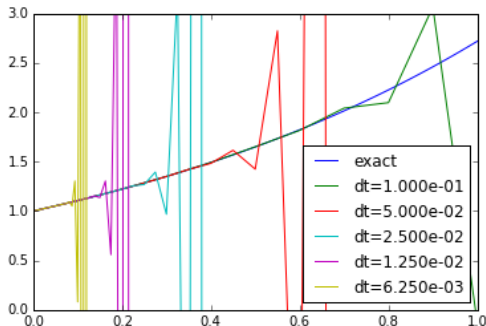
$$y_{n+2} = -4y_{n+1} + 5y_n + \tau \cdot [4y_{n+1}] + 2y_n]$$

- consistency of the method: order 3

Stability: Example explLMM2 (2)

Observation:

for start with exact initial values: $y_0 = y(0)$ and $y_1 = y(\tau)$



⇒ multistep method explLMM2 is 3rd-order consistent, but does not converge here: instable behaviour

Stability

- reason: difference equation generates spurious solutions
- analysis: roots μ_j of characteristic polynomial ?all $|\mu_j| < 1$?

Stability of ODE schemes:

- single step methods: always stable
- multistep methods: additional stability conditions
- in general:
consistency + zero-stability = convergence

Stability: Example Explicit Midpoint Rule

Example ODE (Dahlquist):

$$\dot{y}(t) = -10y(t), \quad y(0) = 1$$

- exact solution: $y(t) = (e^{-10t})$

Stability: Example Explicit Midpoint Rule

Example ODE (Dahlquist):

$$\dot{y}(t) = -10y(t), \quad y(0) = 1$$

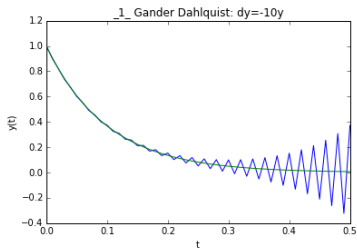
- exact solution: $y(t) = (e^{-10t})$
- use explicit midpoint rule ($s = 2$):

$$y_{n+2} = y_n + 2\tau f(t_{n+1}, y_{n+1})$$

- starting steps: $y_0 = y(0) = 1, \quad y_1 = y(\tau) = e^{-10\tau}$
- method is zero-stable

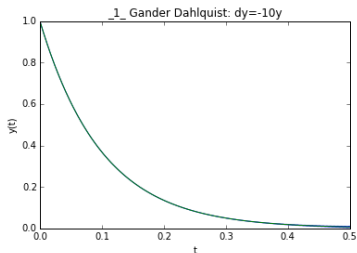
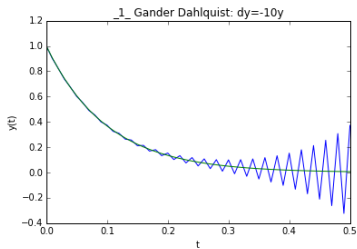
Stability: Example Explicit Midpoint Rule (2)

python demo: different $\tau = 0.01, 0.001 \Rightarrow$ Martini glass effect



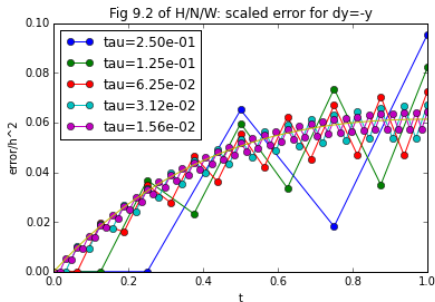
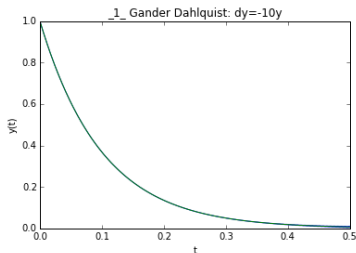
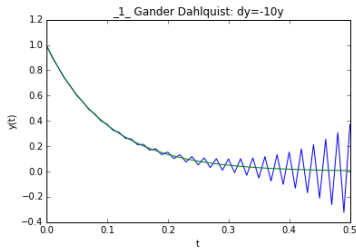
Stability: Example Explicit Midpoint Rule (2)

python demo: different $\tau = 0.01, 0.001 \Rightarrow$ Martini glass effect



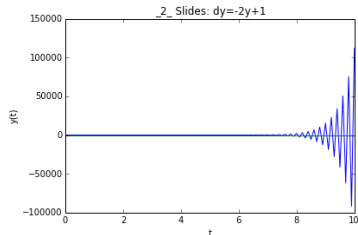
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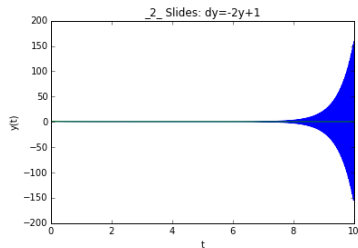
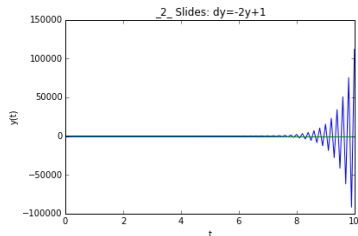
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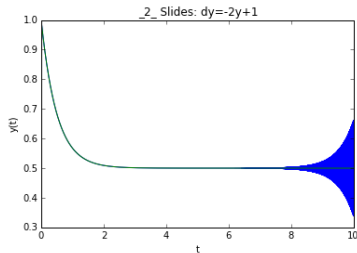
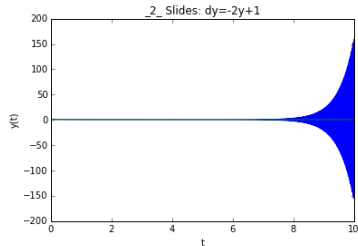
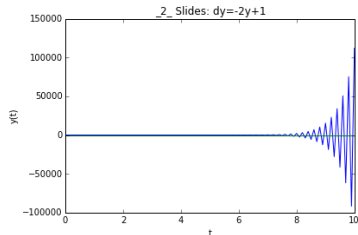
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- oscillations and divergence for $\delta t > 0.002$
- Why that? Consistency and stability are **asymptotic** terms!

Stiff Equations – Summary

Typical situation:

- one term in the ODE demands very small explicit time step
- but does not contribute much to the accuracy of the solution

Remedy: use implicit (or semi-implicit) methods

Summary

Runge-Kutta-methods:

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(Extrapolation methods:)

- for very long runtimes
- for very high accuracy

