

Numerical Methods for Physics

(401-1662-10 L)

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(C) Seminar für Angewandte Mathematik, ETH Zürich

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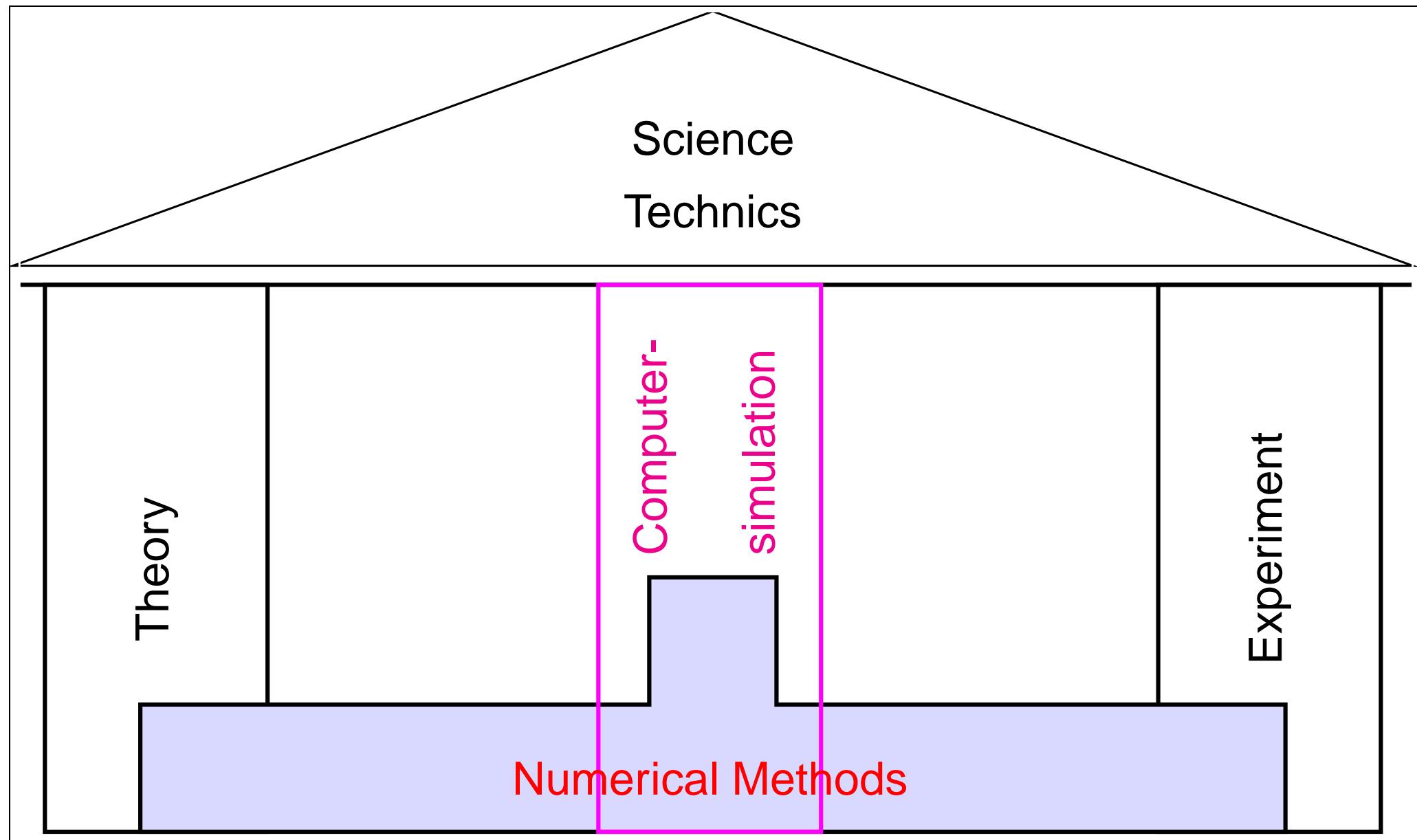
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0.1 About this course



Focus

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- ▷ on **algorithms** (principles, scope, and limitations)
- ▷ on **implementation** (efficiency, stability)
- ▷ on **numerical experiments** (design and interpretation)

no emphasis on

- theory and proofs (unless essential for understanding of algorithms)
- hardware-related issues (e.g. parallelization, vectorization, memory access)

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Goals

- Knowledge of the fundamental algorithms in numerical mathematics
- Ability to choose the appropriate numerical method for concrete problems
- Ability to interpret numerical results
- Ability to implement numerical algorithms efficiently

Indispensable:

Learning by doing (→ exercises)

- ▷ active attendance of the lecture
- ▷ active participation to the exercises class
- ▷ at least **5 hours of additional work per week** (reading the lecture, answering the questions in the “Essential skills”-section, performing the numerical experiments from the slides and from the homework)

The final exam will take place at computer and will reside on **practical implementations**, based on the questions in the “Essential skills”-section of each chapter.

Reading instructions

This course materials are neither a textbook nor lecture notes.
They are meant to be supplemented by explanations given in class.

Some pieces of advice:

- these lecture slides are not designed to be self-contained, but to supplement explanations in class.
- this document is not meant for mere reading, but for working with,
- turn pages all the time and follow the numerous cross-references,
- study the relevant section of the course material when doing homework problems.

What to expect

The course is difficult and demanding (*ie.* ETH level)

- Do **not** expect to understand everything in class. The average student will
 - understand about one third of the material when attending the lectures,
 - understand another third when making a *serious effort* to solve the homework problems,
 - hopefully understand the remaining third when studying for the examination after the end of the course.

Perseverance will be rewarded!

Books

Parts of the following textbooks may be used as supplementary reading for this course. References to relevant sections will be provided in the course material.

- M. HANKE-BOURGEOIS, *Grundlagen der Numerischen Mathematik und des Wissenschaftlichen Rechnens*, Mathematische Leitfäden, B.G. Teubner, Stuttgart, 2002.
- P. DEUFLHARD AND A. HOHMANN, *Numerische Mathematik. Eine algorithmisch orientierte Einführung*, DeGruyter, Berlin, 1 ed., 1991.

- J. Stör and R. Bulirsch, *Einführung in die Numerische Mathematik*, 1976. English version, *Intro. to Numerical Mathematics*, Springer Verlag, 1980. Latest edition is 2002.
- Quarteroni, Sacco and Saleri, *Numerische Mathematik 1 + 2*, Springer Verlag 2002

Essential prerequisite for this course is a solid knowledge in basic calculus and linear algebra. Familiarity with the topics covered in the textbook [?] is taken for granted.

0.2 Appetizer

Example 0.2.1 (Euler method for pendulum equation).

Hamiltonian form of equations of motion for pendulum

$$\text{angular velocity } p := \dot{\alpha} \Rightarrow \frac{d}{dt} \begin{pmatrix} \alpha \\ p \end{pmatrix} = \begin{pmatrix} p \\ -\frac{g}{l} \sin \alpha \end{pmatrix}, \quad g = 9.8, l = 1. \quad (0.2.1)$$

- numerical solution with explicit/implicit Euler method (5.2.1)/(5.2.4),
- constant time-step $h = T/N$, end time $T = 5$ fixed, $N \in \{50, 100, 200\}$,

- initial value: $\alpha(0) = \pi/4$, $p(0) = 0$.

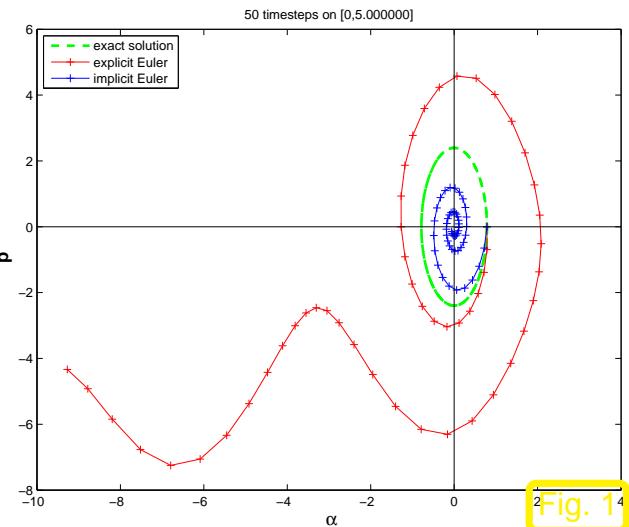


Fig. 1

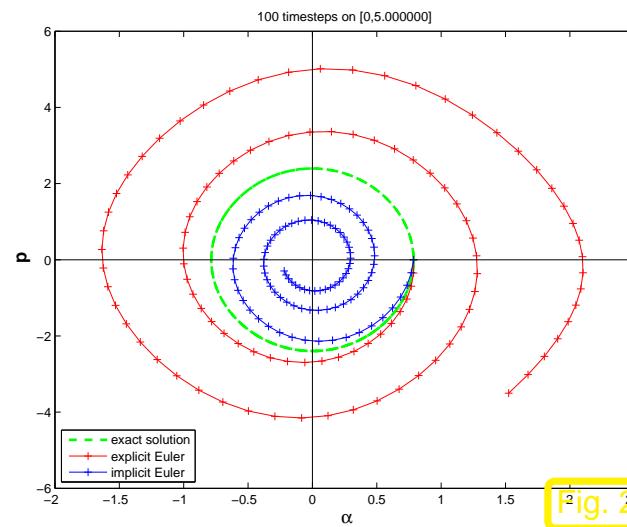


Fig. 2

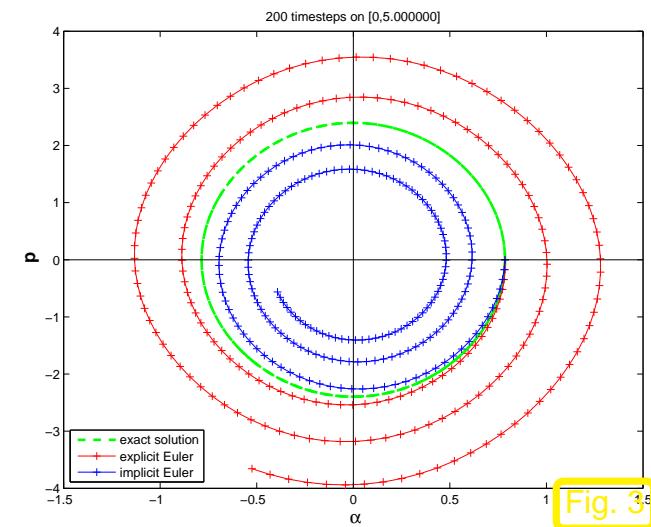
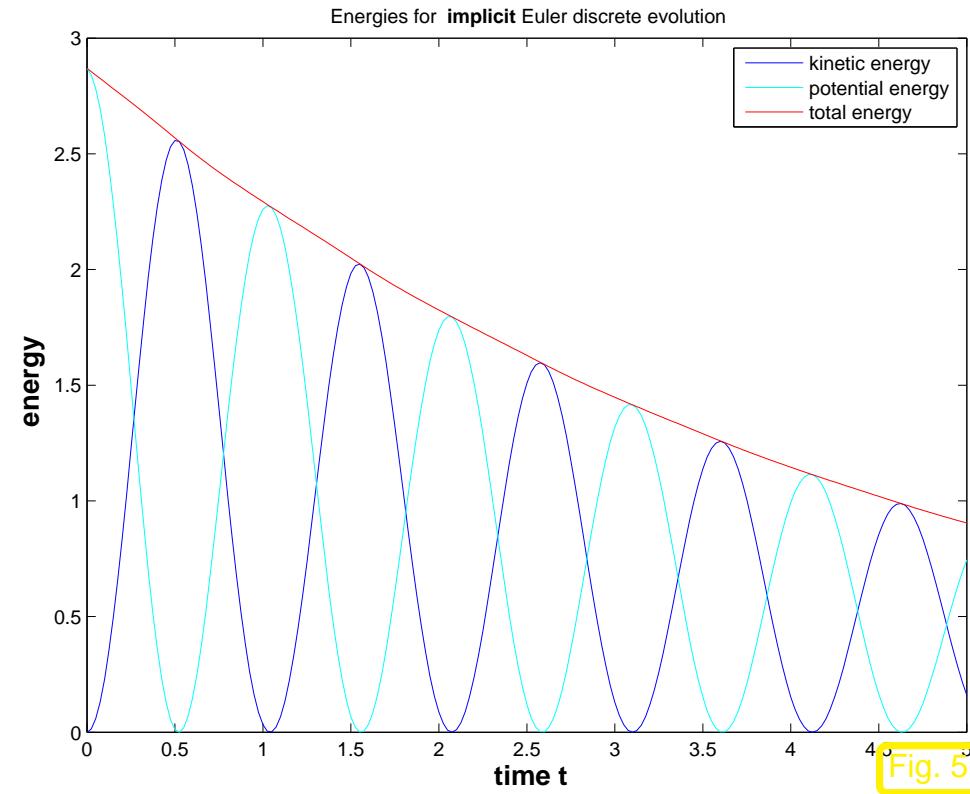
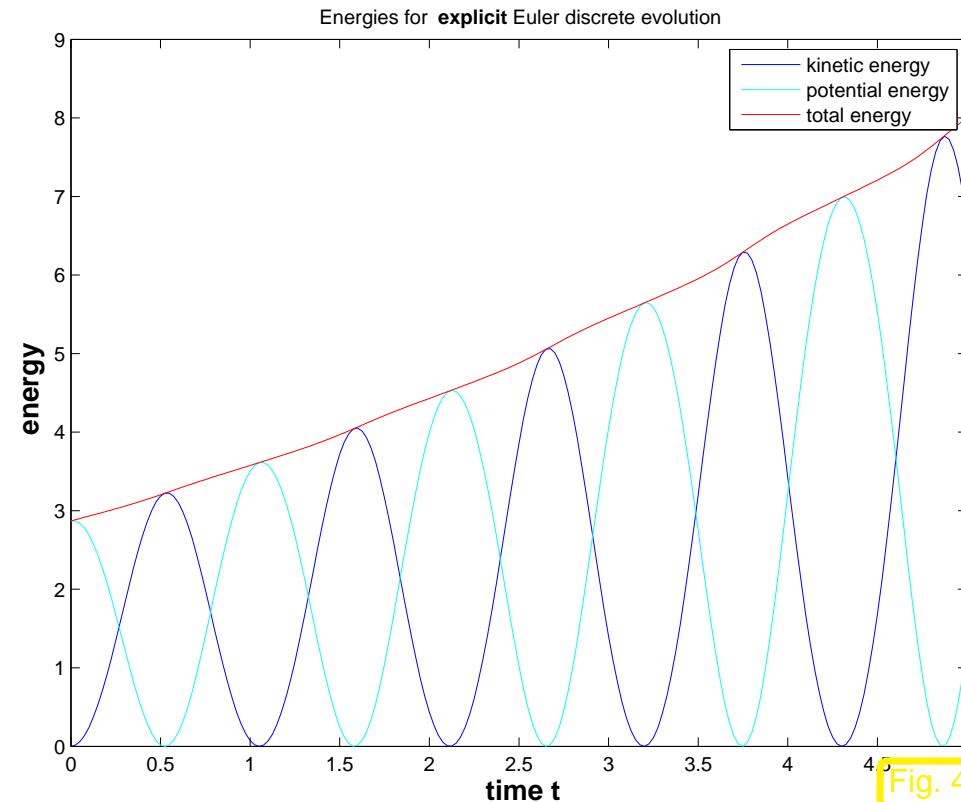


Fig. 3

Behavior of the computed energy: kinetic energy : $E_{\text{kin}}(t) = \frac{1}{2}p(t)^2$
 potential energy : $E_{\text{pot}}(t) = -\frac{g}{l} \cos \alpha(t)$



- ☞ explicit Euler: increase of total energy
- ☞ implicit Euler: decrease of total energy ("numerical friction")



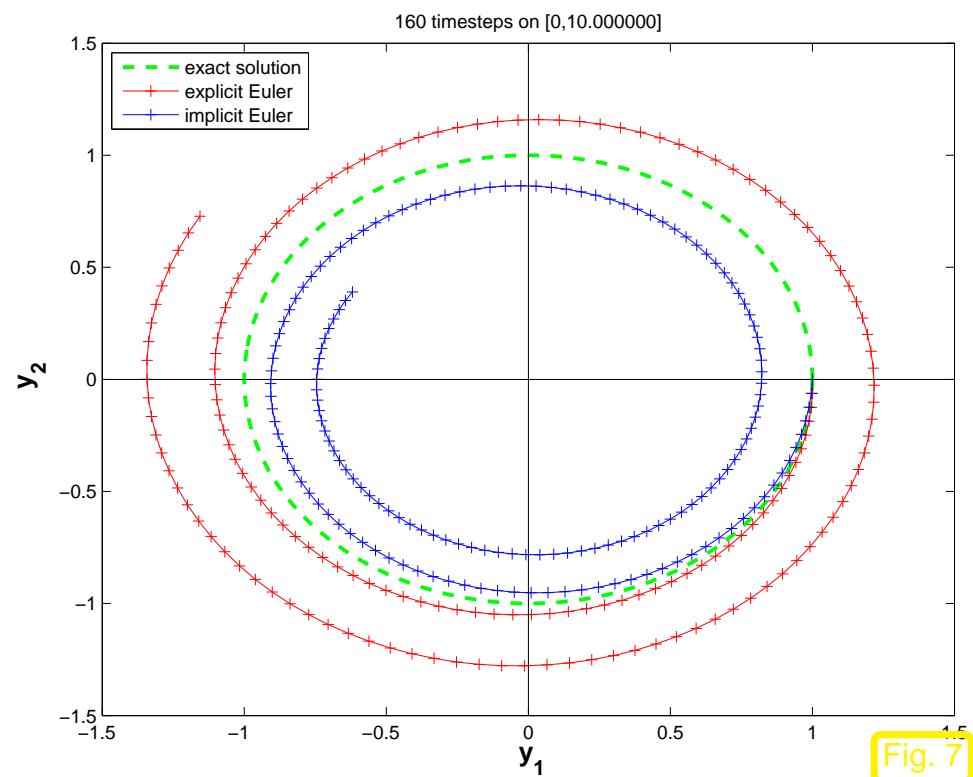
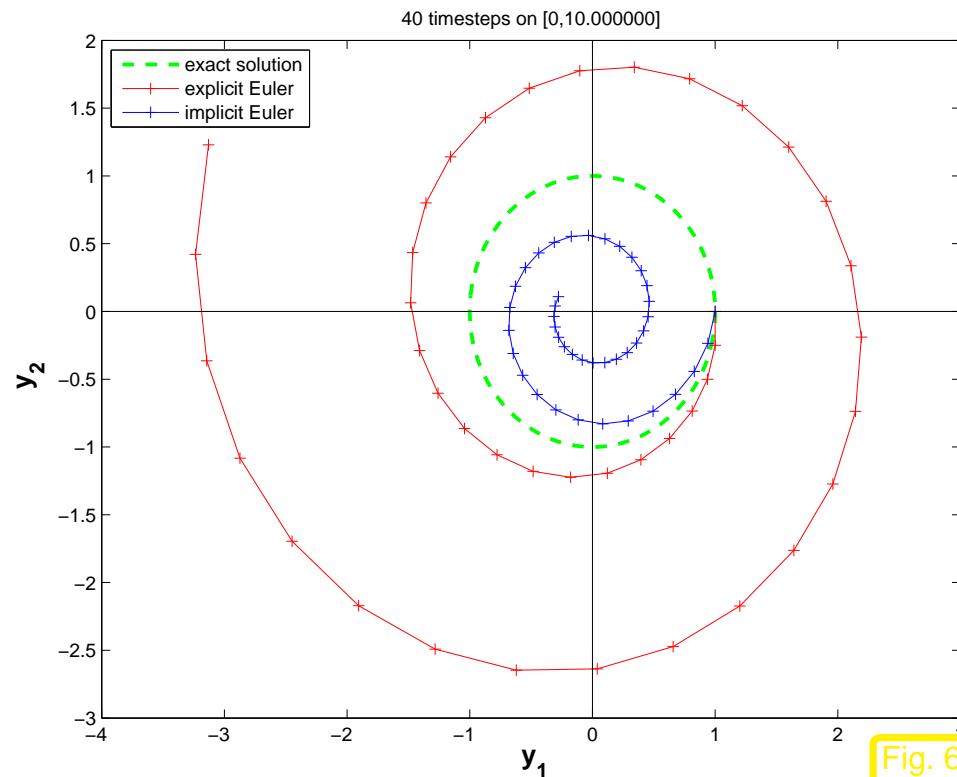
Example 0.2.2 (Euler method for long-time evolution).

Initial value problem for , $D = \mathbb{R}^2$:

$$\dot{\mathbf{y}} = \begin{pmatrix} y_2 \\ -y_1 \end{pmatrix} , \quad \mathbf{y}(0) = \mathbf{y}_0 \quad \Rightarrow \quad \mathbf{y}(t) = \begin{pmatrix} \cos t & \sin t \\ -\sin t & \cos t \end{pmatrix} \mathbf{y}_0 .$$

Note that $I(\mathbf{y}) = \|\mathbf{y}\|$ is constant.

(movement with constant velocity on the circle)

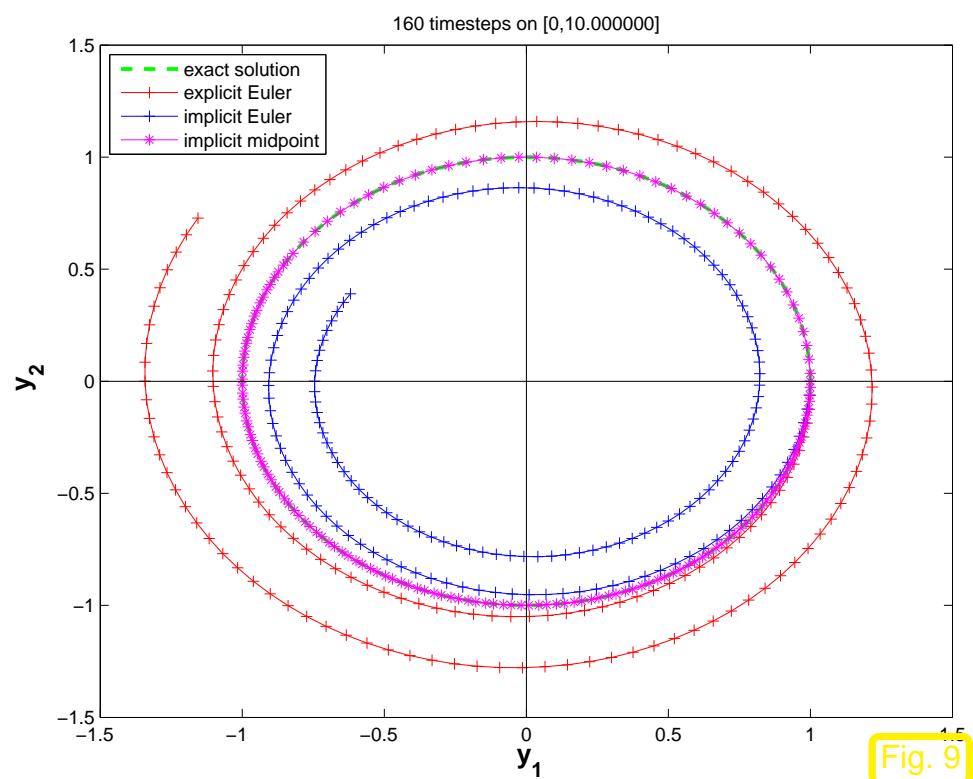
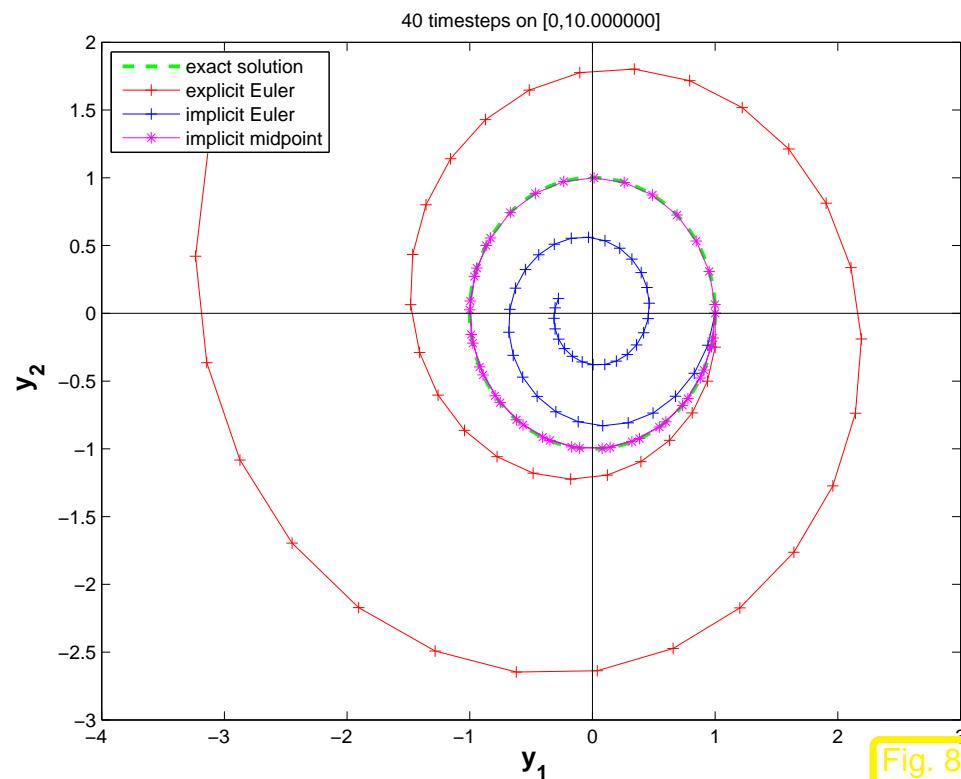


☞ explicit Euler: numerical solution flies away

☞ implicit Euler: numerical solution falls off into the center

Can we avoid the energy drift ?

Example 0.2.3 (Implicit midpoint rule for circular motion).



Implicit midpoint rule: perfect conservation of length !



Example 0.2.4 (Implicit midpoint rule for pendulum).

Initial values and problem as in Bsp. 5.4.1

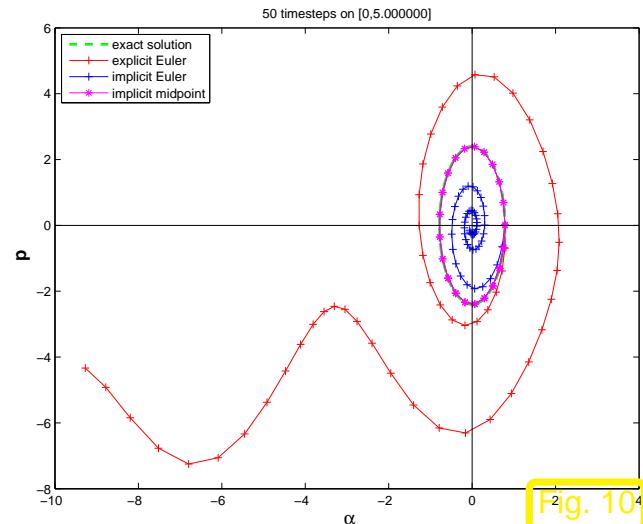


Fig. 10

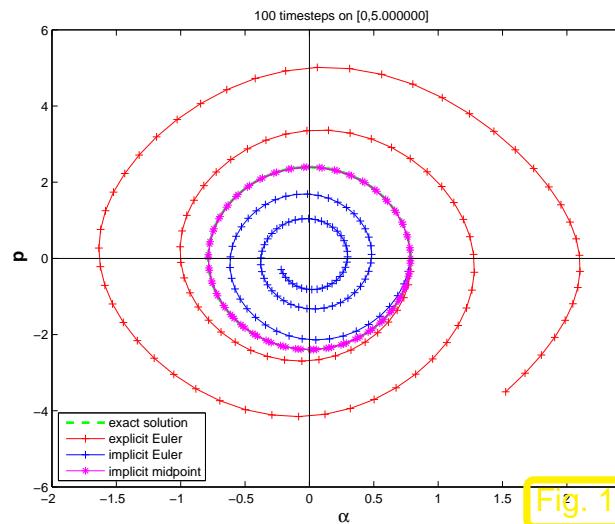


Fig. 11

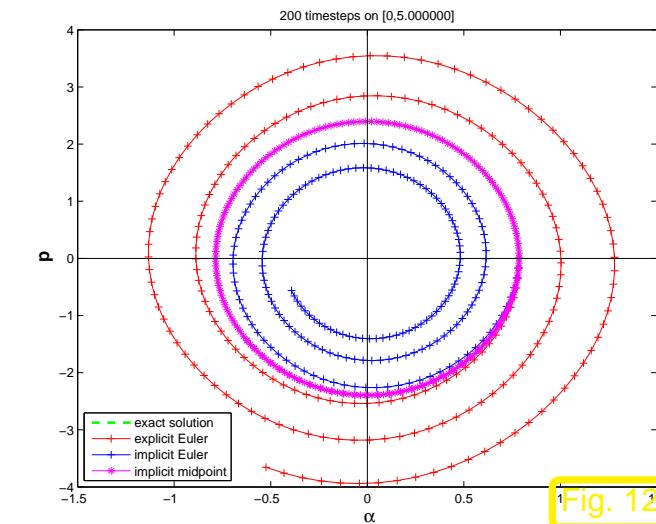


Fig. 12

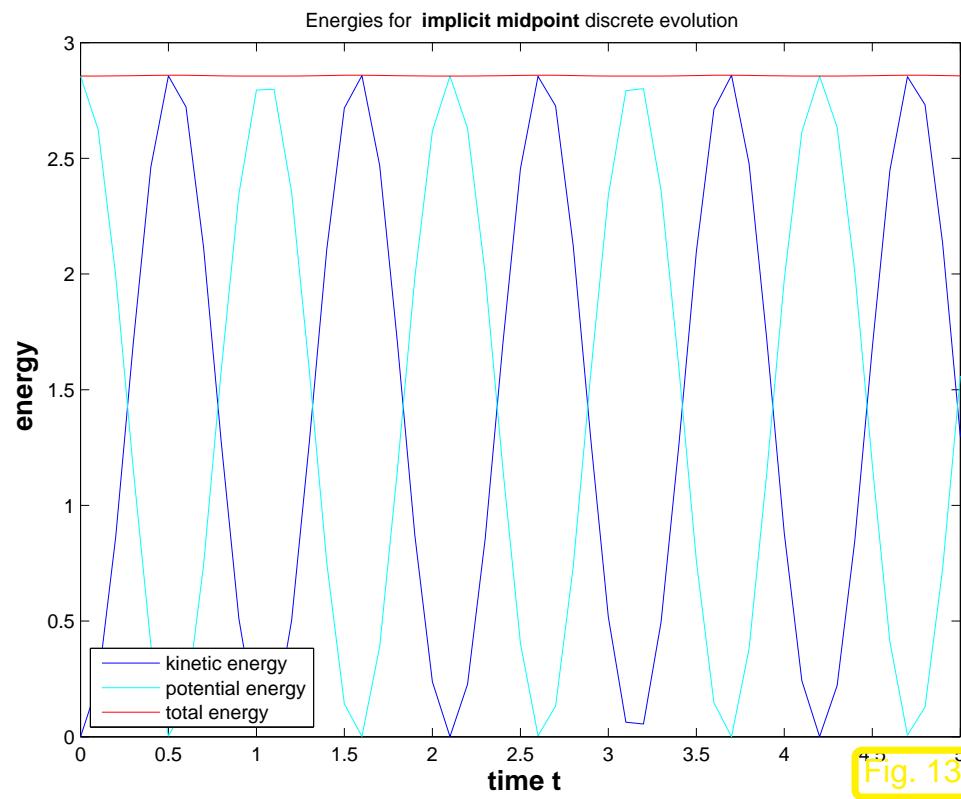


Fig. 13

◇ Behavior of the energy of the numerical solution computed with the midpoint rule (5.4.2), $N = 50$.
 No energy drift although large time step)



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