# Symplectic Integration of Hamiltonian Systems

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# Outline

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- Introduction of Background
- Pendulum Problem

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- Lagrange’s and Hamilton’s Equations
- Symplectic Transformations
- Examples of Symplectic Integrators

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- Lotka-Volteraa Problem
- Numerical results and conclusions

# Introduction of Background

- Introduction of Background

**They throw geometry out the door, and it comes back through the window.** **—————— —— H.G.Forder, Auckland 1973**

General ordinary differential equations (non-stiff and stiff)

solved

Runge–Kutta methods or linear multistep methods

- However

- astronomy
- molecular dynamics
- mechanics
- theoretical physics
- numerical analysis
- applied and pure mathematics

Need develop

- Numerical methods which preserve geometric properties of the flow.

- Introduction of Background

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- Hamiltonian systems form the most important class of ordinary differential equations.
- Some famous problems of Hamiltonian systems in physics:

1. Kepler Problem
2. Outer Solar system
3. Highly Oscillatory Problem

- The flow of Hamiltonian systems is symplectic.

Here,

- We study Symplectic integrators which preserve geometric properties of Hamiltonian systems' flow.

# The Pendulum Problem

- The Pendulum Problem

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- **The Pendulum as a Hamiltonian System**
- Hamiltonian problem

$$\dot{p} = -H_q(p,q) \qquad \dot{q} = H_p(p,q)$$

- where
- the *Hamiltonian H*($p_1$ , . . . ,$p_d$ , $q_1$ , . . .$q_d$ ) represents the total energy;
- $q_i$ are the position coordinates;
- $p_i$ the momenta for *i* = 1, . . . , *d*, with *d* the number of degrees of freedom;
- $H_p$ and $H_q$ are the vectors of partial derivatives.

- the solution curves of

$$H(p(t), q(t)) = Const$$

- i.e., the Hamiltonian is an invariant or a *first integral*.

- The Pendulum Problem

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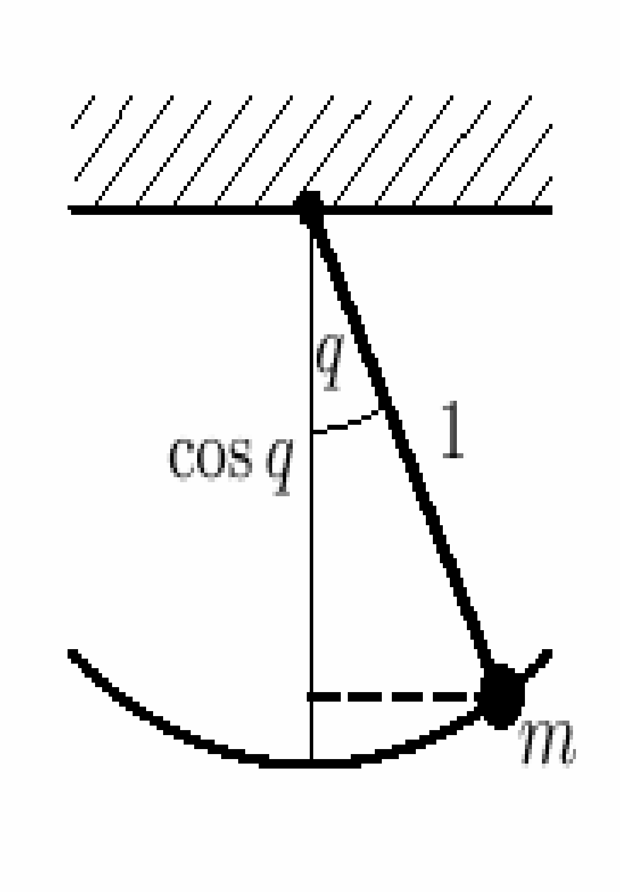
- **Pendulum.**

- The mathematical pendulum (mass *m* = 1, massless rod of length = 1, gravitational acceleration *g* = 1) is a system with one degree of freedom having the Hamiltonian

$$H(p,q) = \frac{1}{2}p^2 - \cos q$$

- So that the equations of motion become

$$\dot{p} = -sinq \qquad \dot{q} = p$$



- The Pendulum Problem

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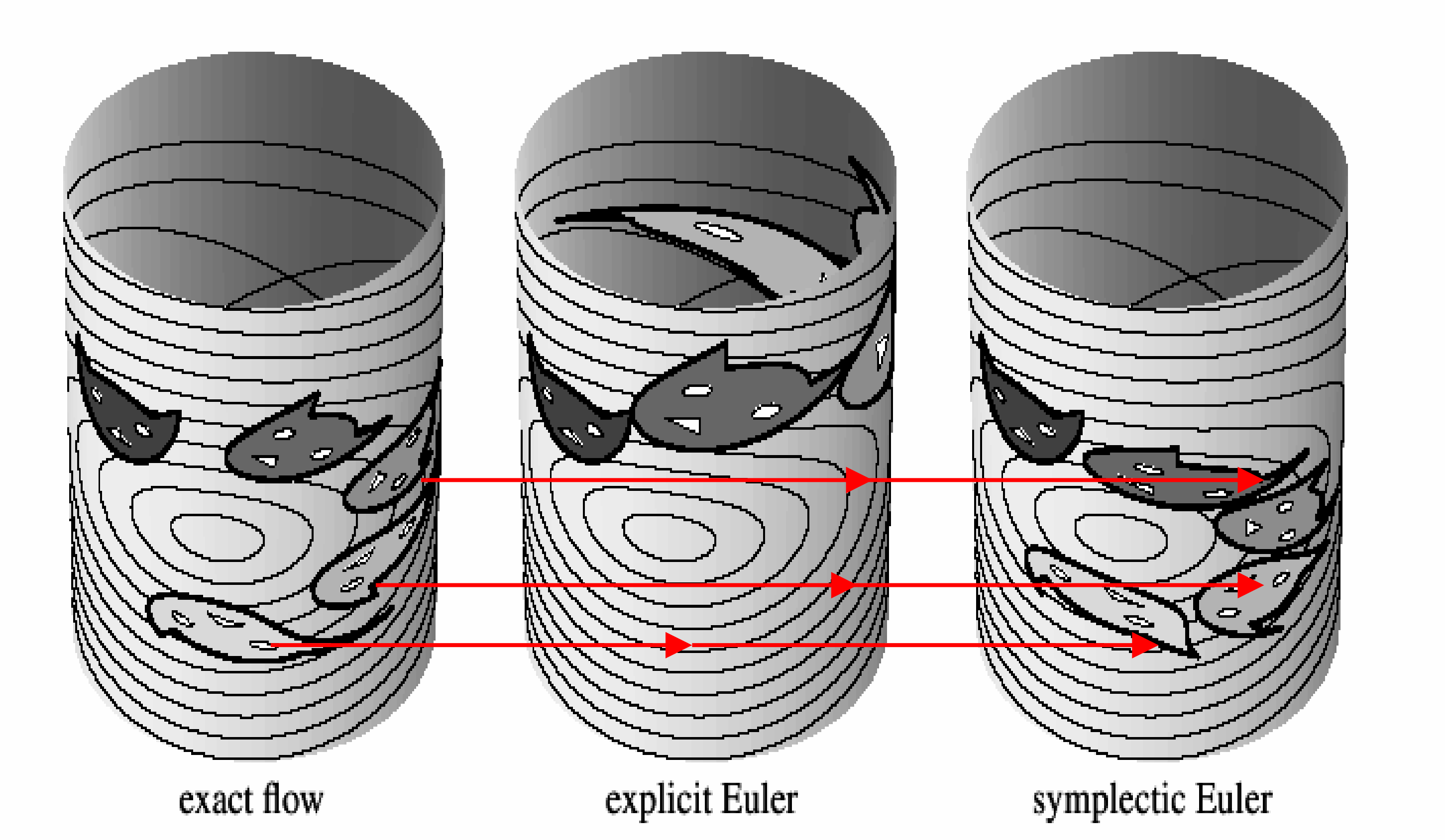
- **Area Preservation.**



From Book ‘Geometric Numerical Integration’

# Lagrange’s and Hamilton’s Equations

- Lagrange's and Hamilton's Equations

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- derive the Hamilton's Equations from a mechanical problem.
- By theory from mechanics :

$$T = T(q, \dot{q})$$

- which represents the *kinetic energy*,where $q = (q_1, ..., q_d)^T$ as generalized coordinates.

$$U = U(q)$$

- representing the *potential energy*. Then, after denoting by

$$L = T - U$$

- the corresponding *Lagrangian*, the coordinates $q_1(t), ..., q_d(t)$ obey the differential equations

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}}\right) = \frac{\partial L}{\partial q}$$

- which constitute the *Lagrange equations* of the system.

- Lagrange’s and Hamilton’s Equations

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- Hamilton (1834) simplified the structure of Lagrange’s equations by
- introducing Poisson’s variables, the conjugate *momenta*

$$p_k = \frac{\partial L}{\partial \dot{q}_k}(q, \dot{q}) \qquad \text{for } k=1,\dots,d,$$

- considering the *Hamiltonian*

$$H := p^T \dot{q} - L(q, \dot{q})$$

- $H = H(p, q)$ obtained by expressing $\dot{q}$ as a function of $p$ and $q$
- for every $q$, a continuously differentiable bijection $\dot{q} \leftrightarrow p$. This map is called the *Legendre transform*.

## Lagrange’s and Hamilton’s Equations

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- **Theorem 1.** *Lagrange’s equations are equivalent to Hamilton’s equations*

$$\dot{p}_k = -\frac{\partial H}{\partial q_k}(p,q) \qquad \dot{q}_k = \frac{\partial H}{\partial p_k}(p,q) \qquad K=1,\ldots d$$

- *Proof.* The definitions conjugate momenta and Hamiltonian for the momenta *p* and for the Hamiltonian *H* imply that

$$\frac{\partial H}{\partial p} = \dot{q}^T + p^T \frac{\partial \dot{q}}{\partial p} - \frac{\partial L}{\partial \dot{q}} \frac{\partial \dot{q}}{\partial p} = \dot{q}^T$$

$$\frac{\partial H}{\partial q} = p^T \frac{\partial \dot{q}}{\partial q} - \frac{\partial L}{\partial q} - \frac{\partial L}{\partial \dot{q}} \frac{\partial \dot{q}}{\partial q} = -\frac{\partial L}{\partial q} = -\dot{p}$$

# Symplectic Transformations

- Symplectic Transformations

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- Properties of Hamiltonian systems

1. the Hamiltonian $H(p, q)$ is a *first integral* of the system

$$\dot{p}_k = -\frac{\partial H}{\partial q_k}(p,q) \qquad \dot{q}_k = \frac{\partial H}{\partial p_k}(p,q)$$

2. Its flow has a property called *symplecticity.*

- Symplectic Transformations

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- two-dimensional parallelograms lying in $R^{2d}$

$$\xi = \begin{pmatrix} \xi^p \\ \xi^q \end{pmatrix} \qquad \eta = \begin{pmatrix} \eta^p \\ \eta^q \end{pmatrix}$$

- In the (*p, q*) space ( $\xi_p, \xi_q, \eta_p, \eta_q$ are in $R^d$ ) as

$$P = \{ t\xi + s\eta \,|\, 0 \le t \le 1, 0 \le s \le 1 \}$$

- In the case *d* = 1, the *oriented area*

$$\text{or.area (P)} = \det \begin{pmatrix} \xi^p & \eta^p \\ \xi^q & \eta^q \end{pmatrix} = \xi^p \eta^q - \xi^q \eta^p$$

- In higher dimensions, we replace this by the *sum of the oriented areas of the projections of P onto the coordinate planes* ( $p_i, q_i$ ), i.e., by

$$\omega(\xi, \eta) := \sum_{i=1}^{d} \det \begin{pmatrix} \xi_i{}^p & \eta_i{}^p \\ \xi_i{}^q & \eta_i{}^q \end{pmatrix} = \sum_{i=1}^{d} (\xi_i^p \eta_i^q, \xi_i^q \eta_i^p)$$

- Symplectic Transformations

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- In matrix notation, this bilinear map acting on vectors of $R^{2d}$ has the form

$$\omega(\xi,\eta) = \xi^T J \eta \quad \text{with} \quad J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}$$

where *I* is the identity matrix of dimension *d*.

- **Definition 2.1.** A linear mapping *A* : $R^{2d} \rightarrow R^{2d}$ is called *symplectic* if

$$A^T J A = J$$

Or, equivalently, if $\omega(A\xi, A\eta) = \omega(\xi,\eta)$ for all $\xi,\eta \in R^{2d}$

- Symplectic Transformations

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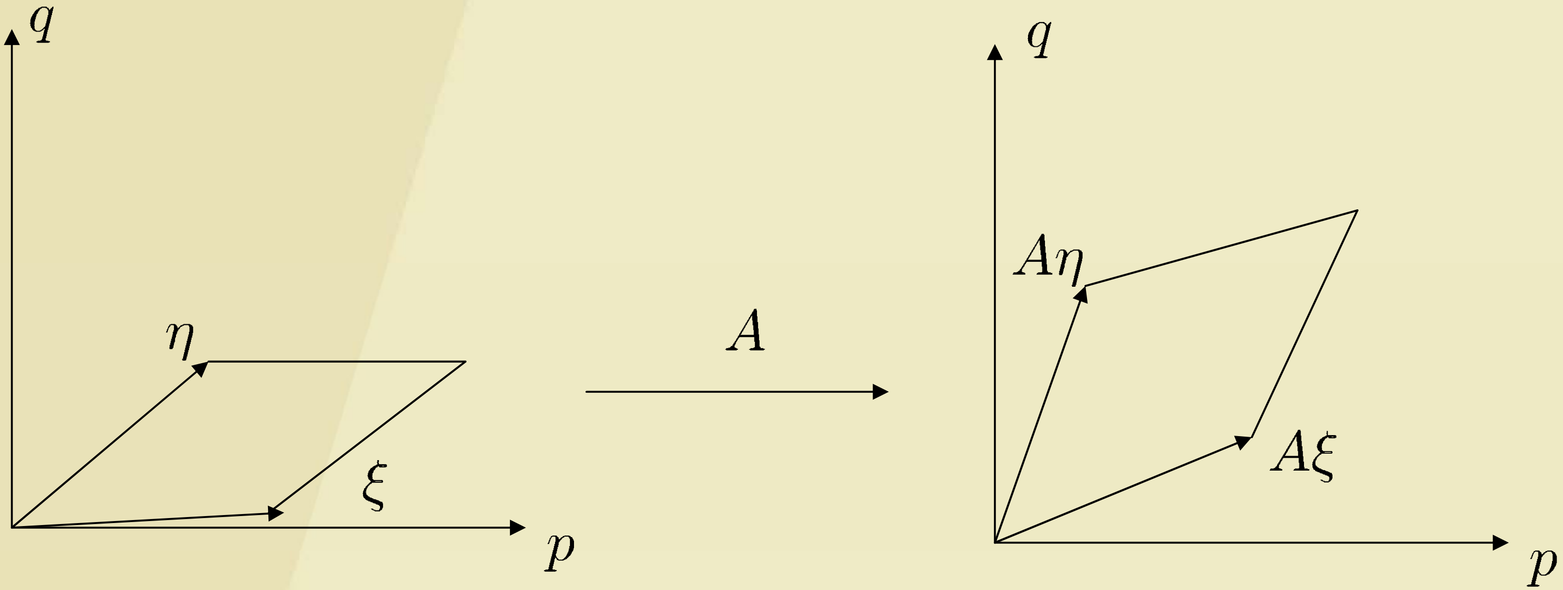

**Fig. 2.1.** Symplecticity (area preservation) of a linear mapping

- Symplectic Transformations

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- For nonlinear mappings

- **Definition 2.2.** A differentiable map $g : U \to R^{2d}$ (where $U \subset R^{2d}$ is an open set) is called *symplectic* if the Jacobian matrix $g(p, q)$ is everywhere symplectic,i.e.,if

$$g'(p,q)^T J g'(p,q) = J \quad \text{or} \quad \omega(g'(p,q)\xi, g'(p,q)\eta) = \omega(\xi,\eta)$$

- all symplectic mappings (also nonlinear ones) are *area preserving*.

## Symplectic Transformations

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- We use the notation $y = (p, q)$, and we write the Hamiltonian system in the form

$$\dot{y} = J^{-1}\nabla H(y)$$

Where J is the matrix we see before and $\nabla H(y) = H'(y)^T$.

- The flow $\varphi_t : U \rightarrow R^{2d}$ of a Hamiltonian system is the mapping that advances the

solution by time $t$, i.e., $\varphi_t\ (p_0, q_0) = (p(t, p_0, q_0), q(t, p_0, q_0))$

- where $(p(t, p_0, q_0), q(t, p_0, q_0))$ is the solution of the system corresponding to

initial values $p(0) = p_0$, $q(0) = q_0$ .

- Symplectic Transformations

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- **Theorem 2.3 (Poincar´e 1899).** *Let H (p, q) be a twice continuously differentiable function on U* $\subset R^{2d}$ *. Then, for each fixed t, the flow* $\varphi_t$ *is a symplectic transformation wherever it is defined.*

- Symplectic Transformations

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- *locally Hamiltonian*:

$$\dot{y} = f(y)$$

if for every $y_0 \in U$ there exists a neighbourhood where $f(y) = J^{-1}\nabla H(y)$ for some function *H*.

- **Theorem 2.4. (characteristic property for Hamiltonian systems)** *Let f : U $\rightarrow R^{2d}$ be continuously differentiable. Then, $\dot{y} = f(y)$ is locally Hamiltonian if and only if its flow $\varphi_t(y)$ is symplectic for all $y \in U$ and for all sufficiently small t.*

- **Lemma 2.5 (Integrability Lemma).** *Let $D \subset R^n$ be open and $f : D \rightarrow R^n$ be continuously differentiable, and assume that the Jacobian $f'(y)$ is symmetric for all $y \in D$. Then, for every $y_0 \in D$ there exists a neighbourhood and a function H(y) such that*

$$f(y) = \nabla H(y)$$

*on this neighbourhood*

# Examples of Symplectic Integrators

- Examples of Symplectic Integrators

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- In the following we show the symplecticity of various numerical methods when they are applied to the Hamiltonian system in the variables *y* = (*p, q*),

$$\dot{p} = -H_q(p,q)$$
$$\dot{q} = H_p(p,q)$$

Or equivalently $$\dot{y} = J^{-1}\nabla H(y)$$

- where $H_p$ and $H_q$ denote the column vectors of partial derivatives of the Hamiltonian *H*(*p, q*) with respect to *p* and *q*, respectively.

- Examples of Symplectic Integrators

**They throw geometry out the door, and it comes back through the window. ——————— —— H.G.Forder, Auckland 1973**

- **Definition 3.1.** A numerical one-step method is called *symplectic* if the one-step map

$$y_1 = \phi_h(y_0)$$

is symplectic whenever the method is applied to a smooth Hamiltonian system.

- **Theorem 3.1 (de Vogelaere 1956).** *The so-called symplectic Euler methods*

$$\begin{aligned} p_{n+1} &= p_n - hH_q(p_{n+1}, q_n) \\ q_{n+1} &= q_n + hH_p(p_{n+1}, q_n) \end{aligned} \quad \text{or} \quad \begin{aligned} p_{n+1} &= p_n - hH_q(p_n, q_{n+1}) \\ q_{n+1} &= q_n + hH_p(p_n, q_{n+1}) \end{aligned}$$

*are symplectic methods of order* 1.

- Examples of Symplectic Integrators

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- *Proof.*
- We consider only the method to the left. Differentiation with respect to ($p_n$, $q_n$) yields

$$\begin{pmatrix} 1+hH_{qp}^T & 0 \\ -hH_{pp} & I \end{pmatrix} \left( \frac{\partial(p_{n+1}, q_{n+1})}{\partial(p_n, q_n)} \right) = \begin{pmatrix} I & -hH_{qq} \\ 0 & I+hH_{qp} \end{pmatrix}$$

where the matrices $H_{pq}$ ,$H_{pp}$ , . . . of partial derivatives are all evaluated at ( $p_{n+1}$ ,$q_n$ ). This relation allows us to compute $\frac{\partial(p_{n+1}, q_{n+1})}{\partial(p_n, q_n)}$ and to check in a straightforward way the symplecticity condition

$$\left( \frac{\partial(p_{n+1}, q_{n+1})}{\partial(p_n, q_n)} \right)^T J \left( \frac{\partial(p_{n+1}, q_{n+1})}{\partial(p_n, q_n)} \right) = J$$

- Examples of Symplectic Integrators

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- **Theorem 3.2.** *The implicit midpoint rule*

$$y_{n+1} = y_n + hJ^{-1}\nabla H((y_{n+1}+y_n)/2)$$

*is a symplectic method of order 2.*

- *Proof.*
- Differentiation yields

$$(I - \frac{h}{2}J^{-1}\nabla^2 H)(\frac{\partial y_{n+1}}{\partial y_n}) = (I + \frac{h}{2}J^{-1}\nabla^2 H)$$

- Again it is straightforward to verify that $(\frac{\partial y_{n+1}}{\partial y_n})^T J(\frac{\partial y_{n+1}}{\partial y_n}) = J$ . Due to its symmetry,

the midpoint rule is known to be of order 2

# Numerical experiments

- Numerical experiments

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- **The Lotka–Volterra Mode**
- We start with an equation from mathematical biology which models the growth of animal species.
- Assumptions:

*1.* $u(t)$ is to represent the number of individuals of a certain species at time $t$

2. Its evolution is $du/dt = u \cdot a$, where $a$ is the reproduction rate.

*3.* $u(t)$ denotes the number of predators and $v(t)$ denotes the number of prey.

The we have *Lotka–Volterra model :*

$$\dot{u} = u(v-2)$$

$$\dot{v} = v(1-u)$$

- where the dots on $u$ and $v$ stand for differentiation with respect to time. (We have chosen the constants 2 and 1 arbitrarily.)

- Numerical experiments

**They throw geometry out the door, and it comes back through the window. ——— H.G.Forder, Auckland 1973**

$$\dot{y} = f(y)$$

- Every *y* represents a point in the *phase space*, *y* = (*u*, *v*) is in the phase plane .
- The vector-valued function *f*(*y*) represents a *vector field*

- **Flow of the System.**
- A fundamental concept is the *flow* over time *t*. denoted by $\varphi_t$, is thus defined by

$$\varphi_t(y_0) = y(t) \quad \text{if} \quad y(0) = y_0$$

- Numerical experiments

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- **Invariants.**
- If we divide the two equations by each other, we obtain a single equation between the variables *u* and *v*. After separation of variables we get

$$0 = \frac{1-u}{u}\dot{u} - \frac{v-2}{v}\dot{v} = \frac{d}{dt}I(u,v)$$

Where

$$I(u,v) = Inu - u + 2Inv - v$$

- so that *I*(*u*(*t*), *v*(*t*)) = *Const* for all *t*.
- We call the function *I* an *invariant* of the system.
- Every solution of model thus lies on a level curve of I.
- Some of these curves are drawn in the pictures of Fig. 4.1.

- Numerical experiments

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- three stages:

- U: prey
- V: predator

1. the prey population increases.
2. the predator population increases by feeding on the prey.
3. the predator population diminishes due to lack of food

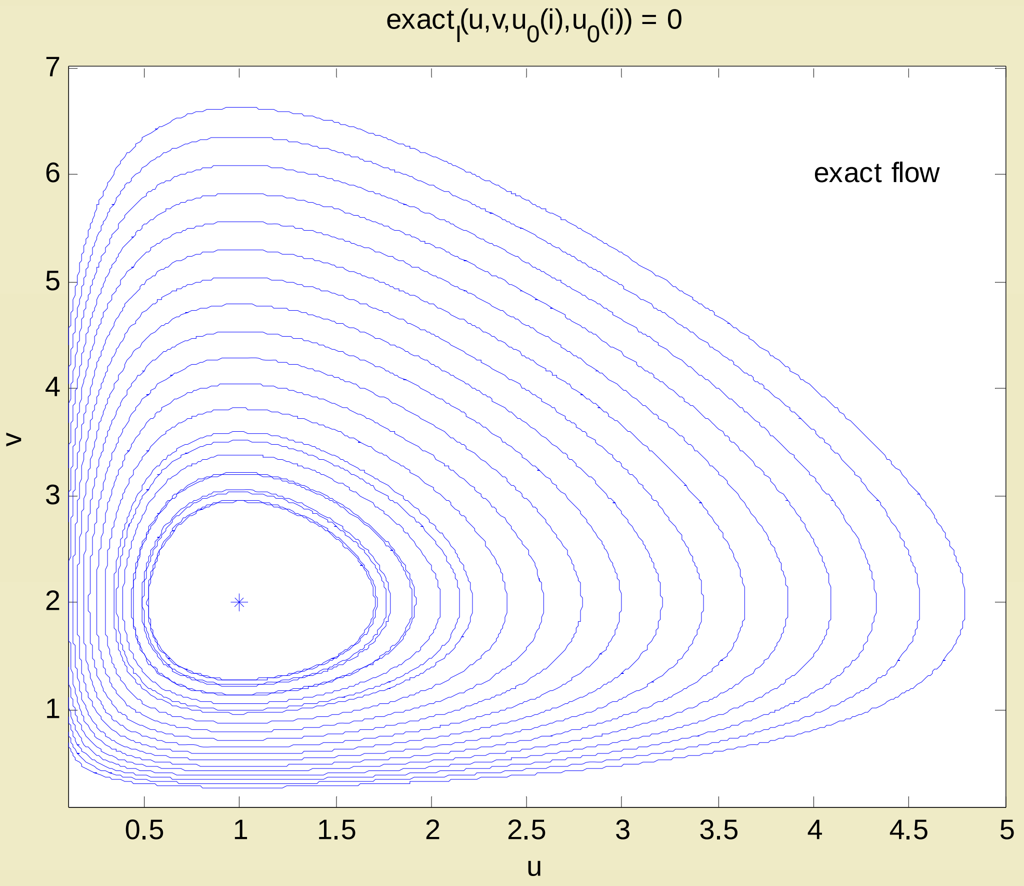

**Fig. 4.1.** exact flow

- Numerical results and conclusions

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- **Explicit Euler Method.**
- The simplest of all numerical methods for the system $\dot{y} = f(y)$ is the method formulated by Euler (1768),

$$y_{n+1} = y_n + hf(y_n)$$

- constant step size *h*
- given initial value *y*(0) = $y_0$.
- *Discrete or numerical flow*

$$\phi_h : y_n \longrightarrow y_{n+1}$$

- Numerical results and conclusions

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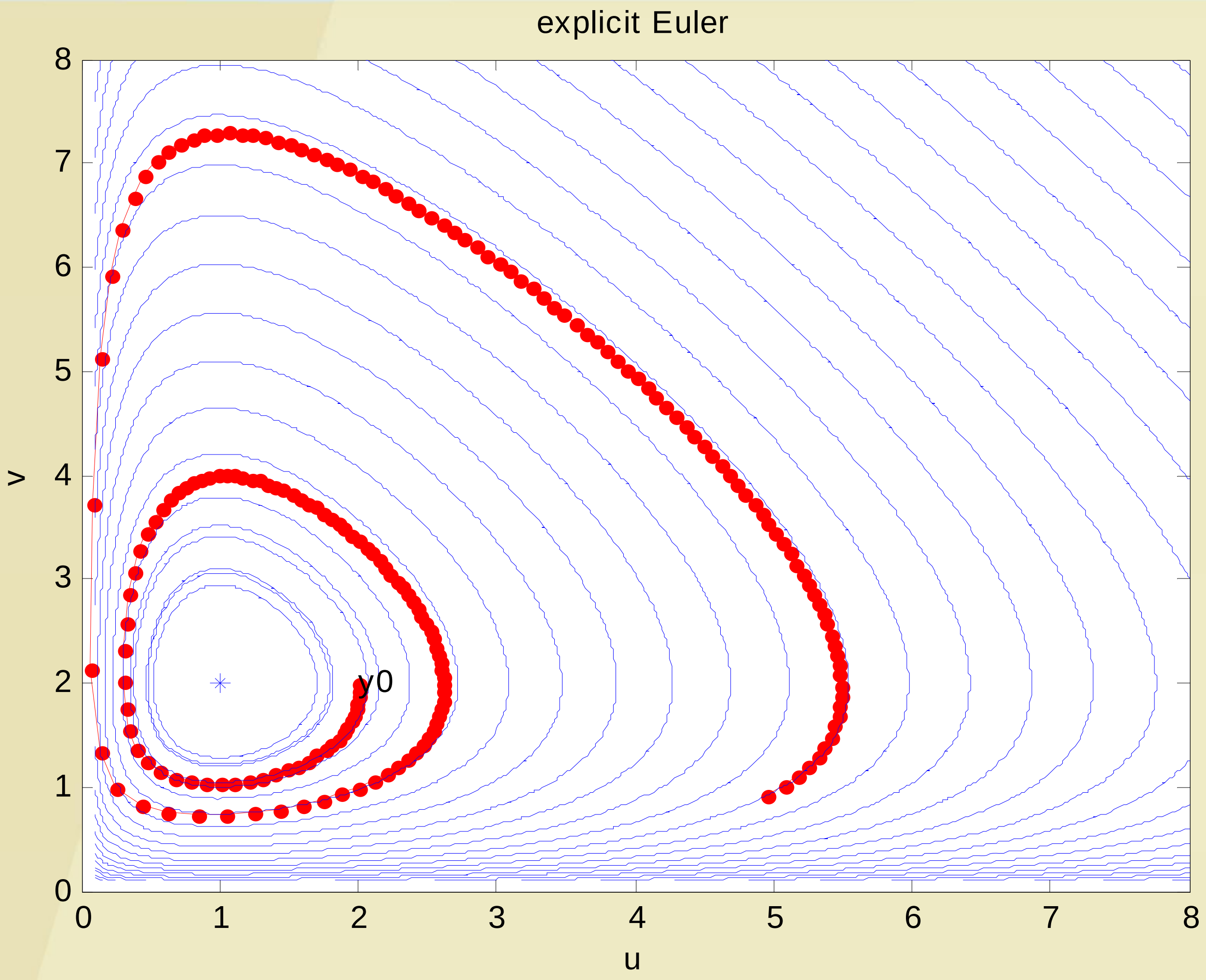

- **Implicit Euler Method.**
- The *implicit Euler method*

$$y_{n+1} = y_n + hf(y_{n+1})$$

- is known for its all-damping stability properties. In contrast to the last one, the approximation $y_{n+1}$ is defined implicitly and the implementation requires the numerical solution of a nonlinear system of equations.

- Numerical results and conclusions

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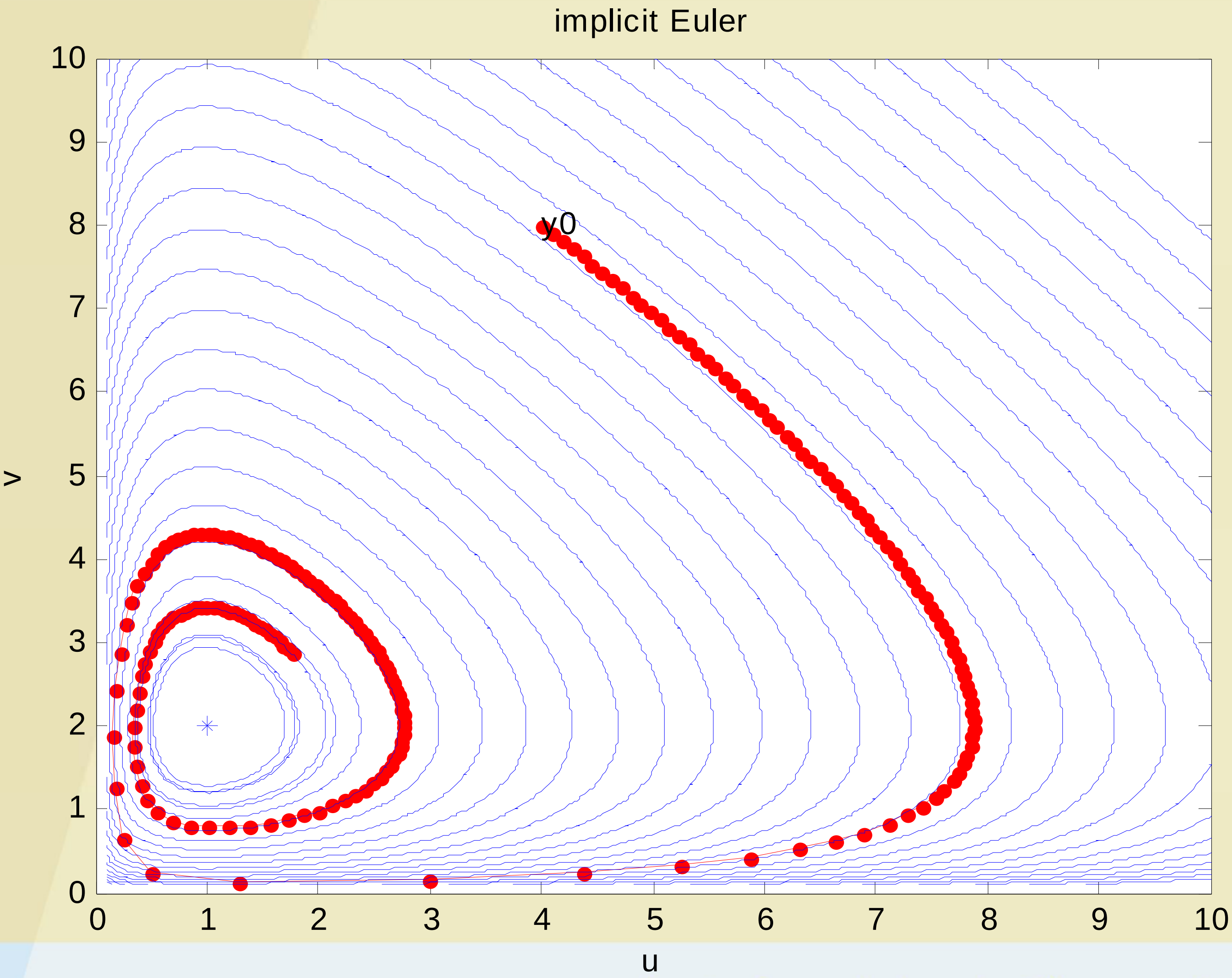

- **Implicit Midpoint Rule.**
- Taking the mean of $y_n$ and $y_{n+1}$ in the argument of *f*, we get the *implicit midpoint rule*

$$y_{n+1} = y_n + hf\left(\frac{y_{n+1} + y_n}{2}\right)$$

- It is a *symmetric* method, which means that the formula is left unaltered after exchanging $y_n \leftrightarrow y_{n+1}$ and *h* ↔−*h*

- Numerical results and conclusions

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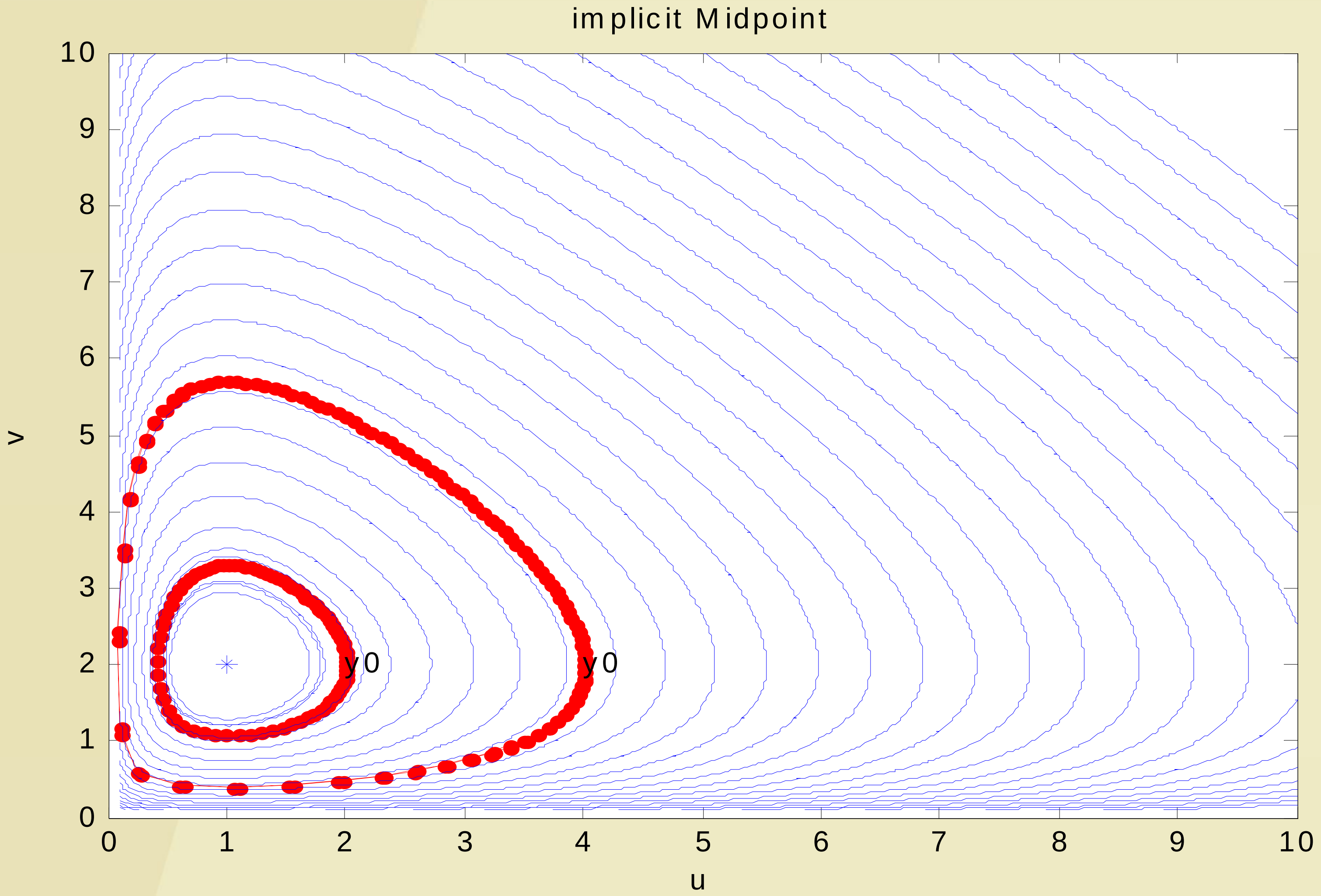

- **Symplectic Euler Methods.**
- For *partitioned* systems

$$\dot{u} = a(u,v)$$
$$\dot{v} = b(u,v)$$

- we consider also *partitioned* Euler methods

$$u_{n+1} = u_n + ha(u_n, v_{n+1}) \qquad\qquad u_{n+1} = u_n + ha(u_{n+1}, v_n)$$

or

$$u_{n+1} = u_n + hb(u_n, v_{n+1}) \qquad\qquad u_{n+1} = u_n + hb(u_{n+1}, v_n)$$

- which treat one variable by the implicit and the other variable by the explicit Euler method.

- Numerical results and conclusions

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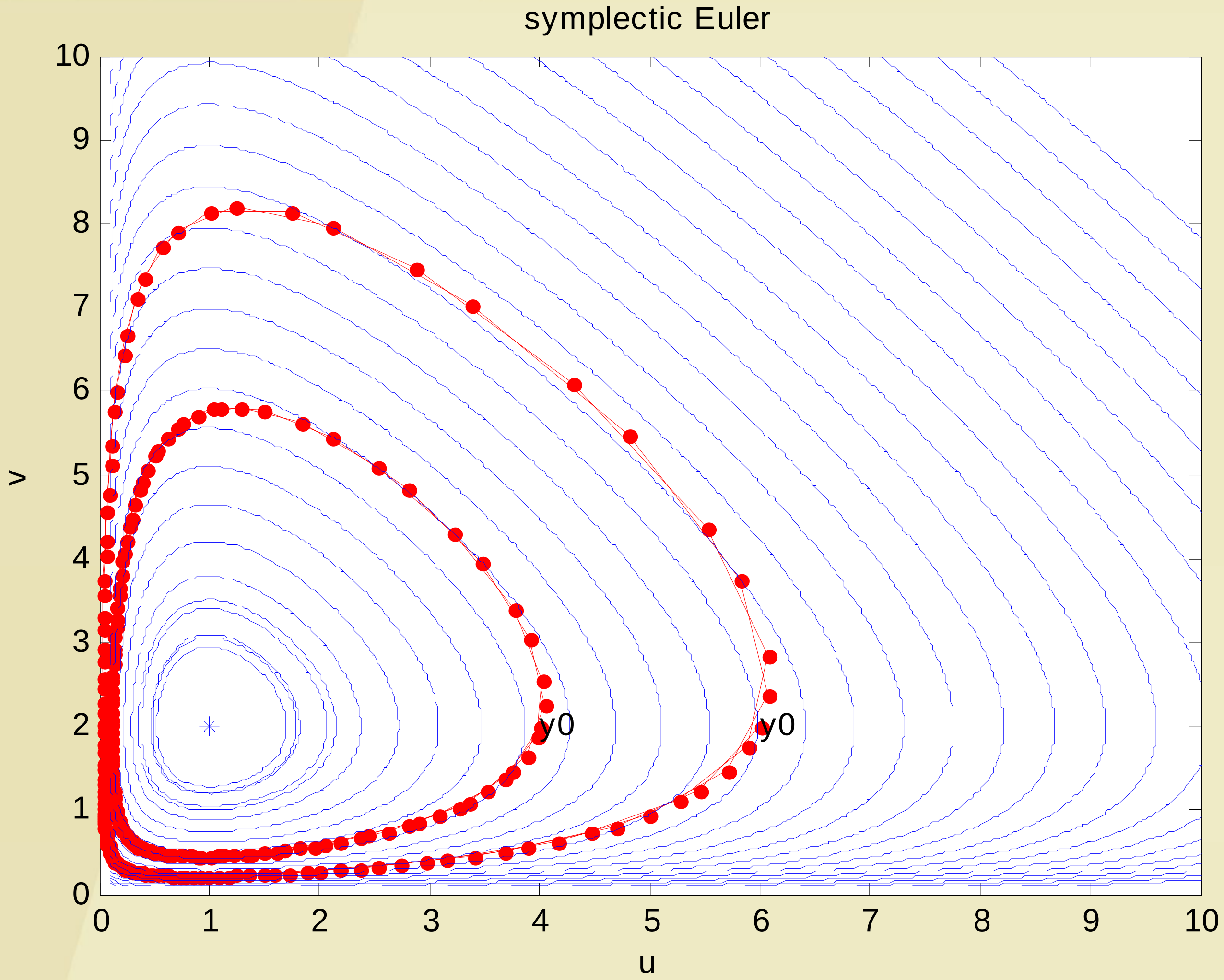

- Numerical results and conclusions

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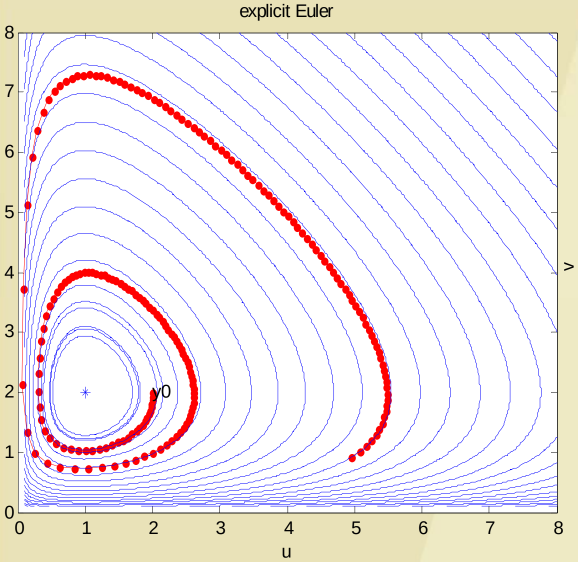
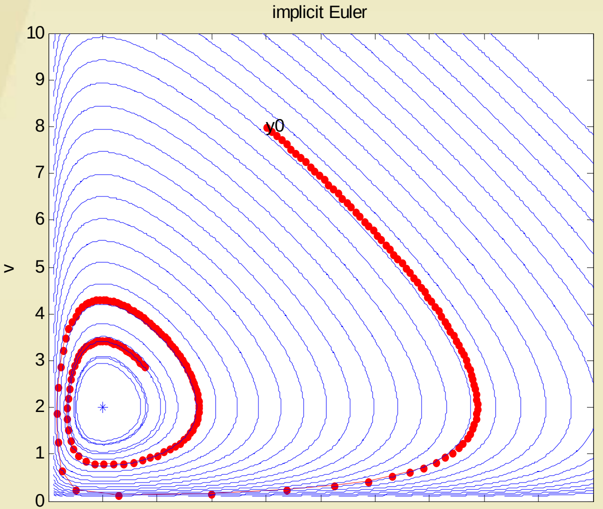
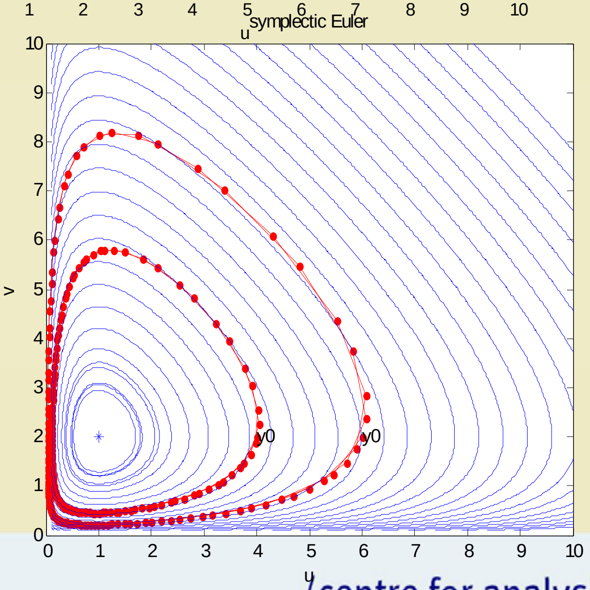
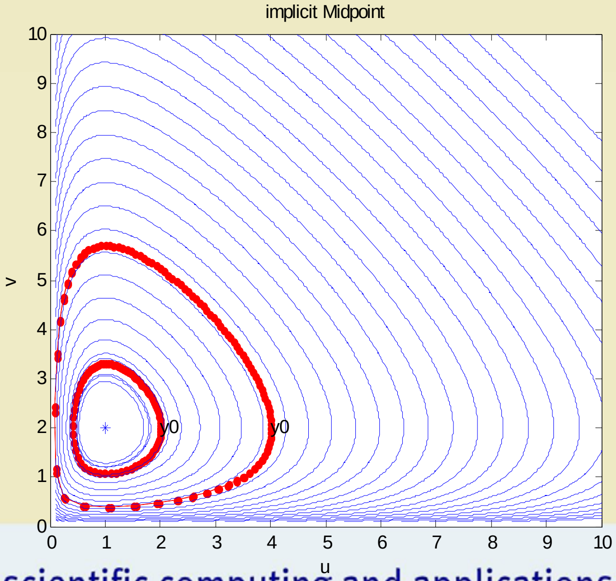




- step sizes $h = 0.12$
- explicit Euler method has initial values (2, 2)
- (4, 8) for the implicit Euler method

- (4,2) and (2,2) for implicit midpoint rule
- (4,2) and (6,2) for symplectic Euler method





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- **Numerical Results for the Lotka–Volterra Problem**

- the explicit and implicit Euler methods show wrong qualitative behaviour.

- Implicit Mdipoint Rule gives a numerical solution that lies apparently on a closed curve as does the exact solution.

- The symplectic Euler method (implicit in *u* and explicit in *v*), however, gives a numerical solution that lies apparently on a closed curve as does the exact solution.

# Thank you