Some examples of structure preservation

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Structure preserving algorithms attempt to preserve the integrity of inherent physical or geometric properties.

Contents

- Experiments with the Euler and Implicit Euler methods

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- Symplectic property

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- Experiments with the Euler and Implicit Euler methods
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- Symplectic Runge–Kutta methods

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- Experiments with some symplectic methods
- Symplectic Runge–Kutta methods
- A symplectic general linear method
- Preservation of quadratic invariants
- Conclusions

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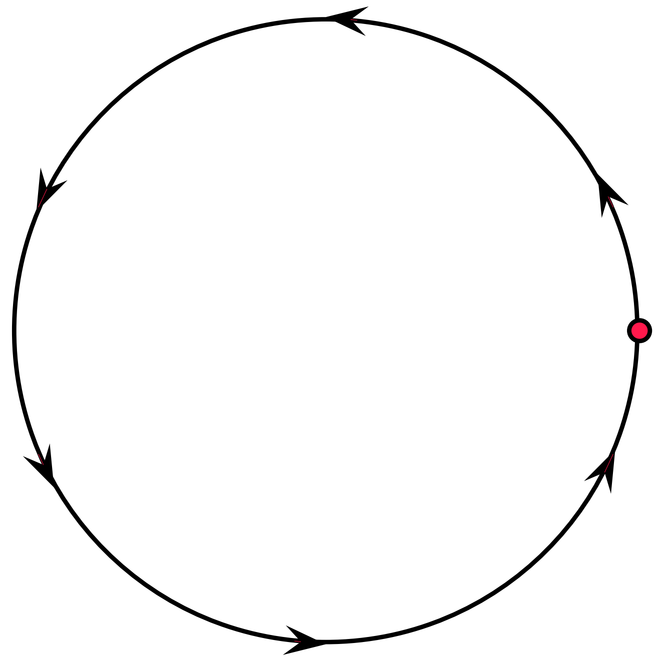

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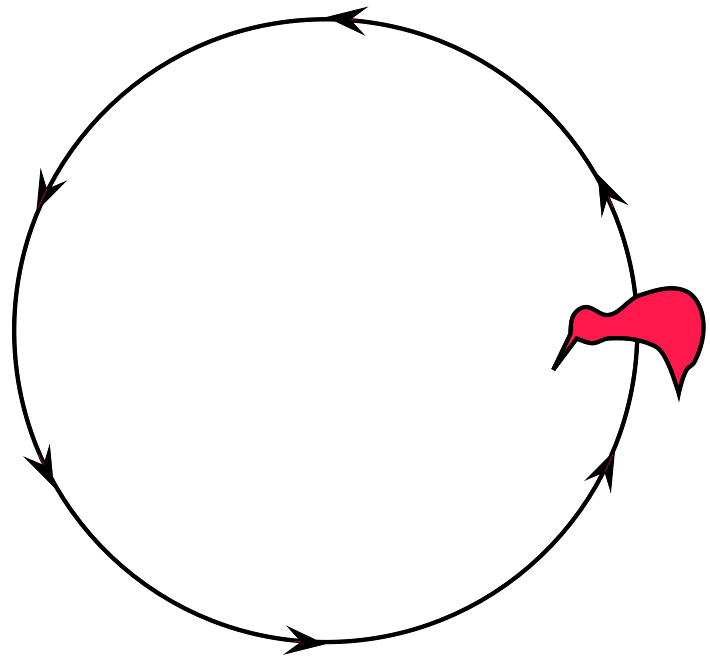

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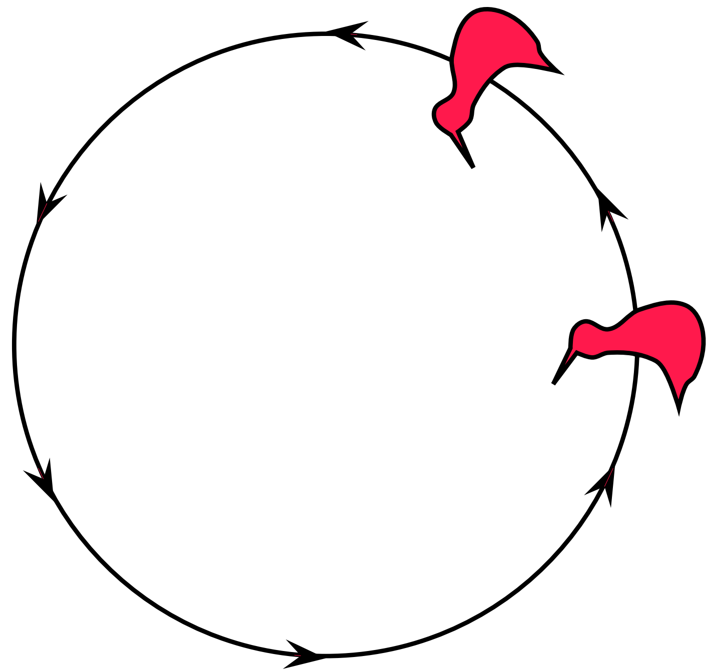

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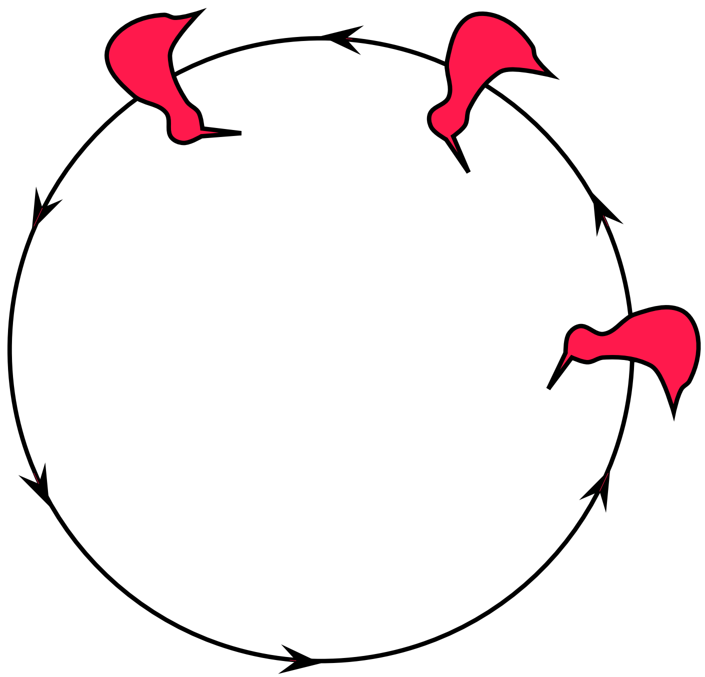

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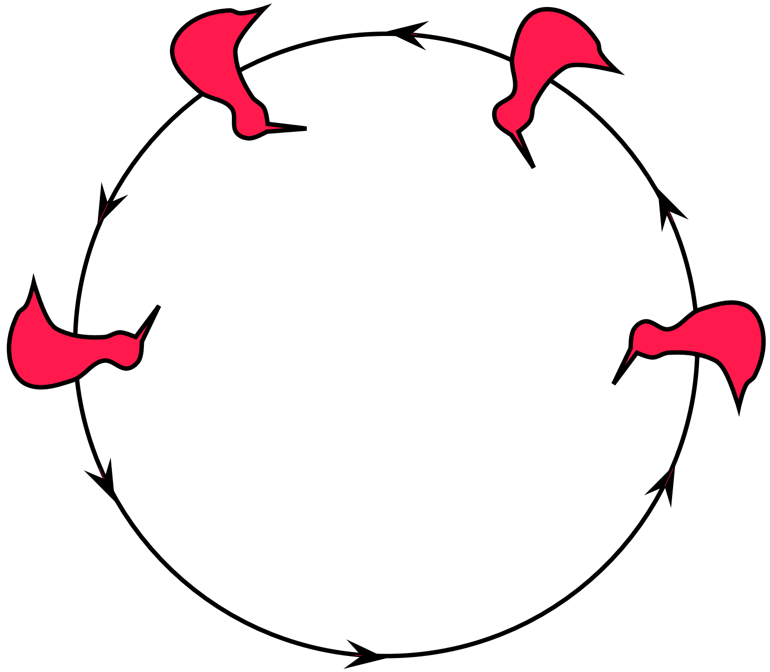

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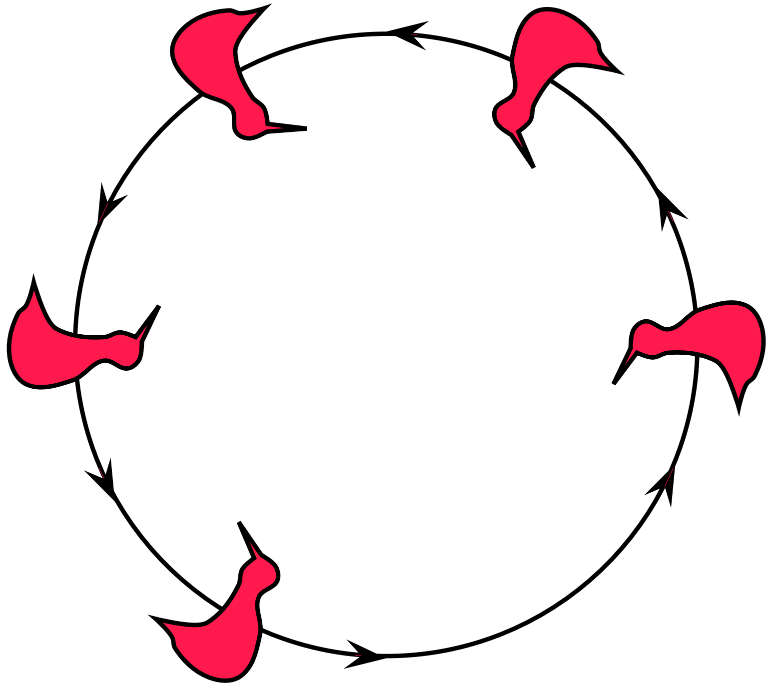

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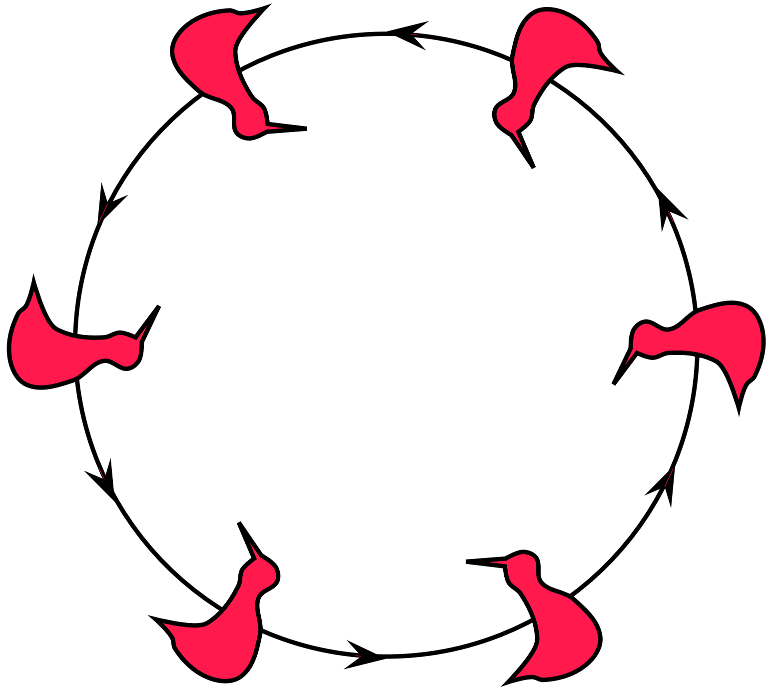

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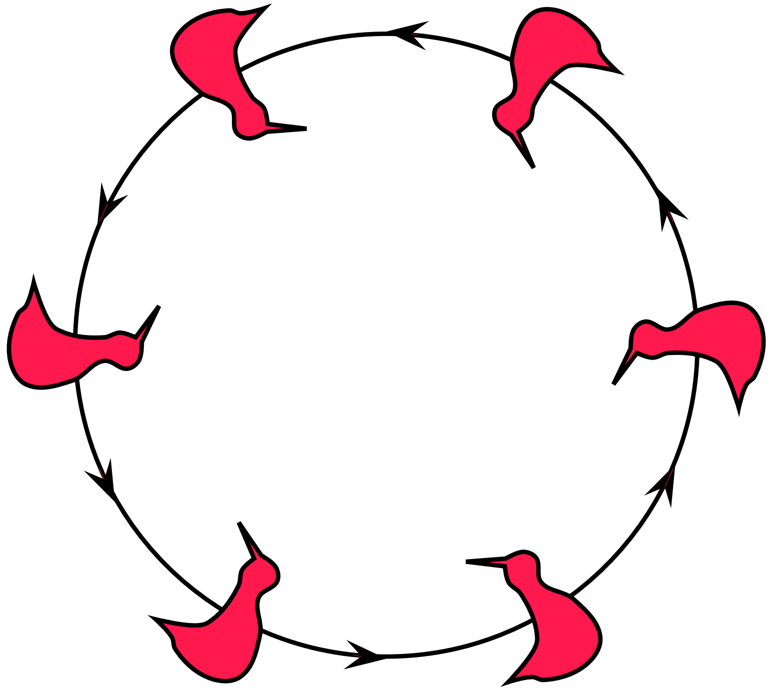

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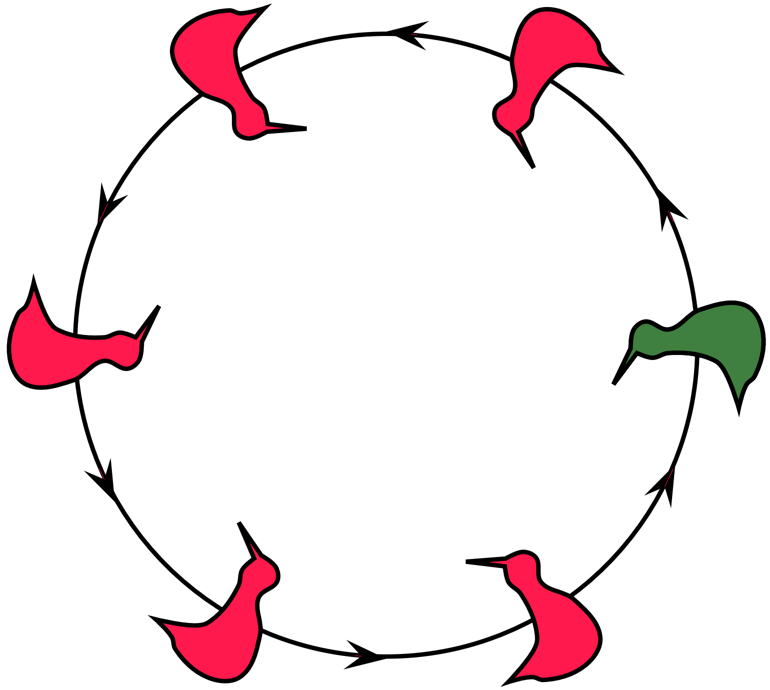

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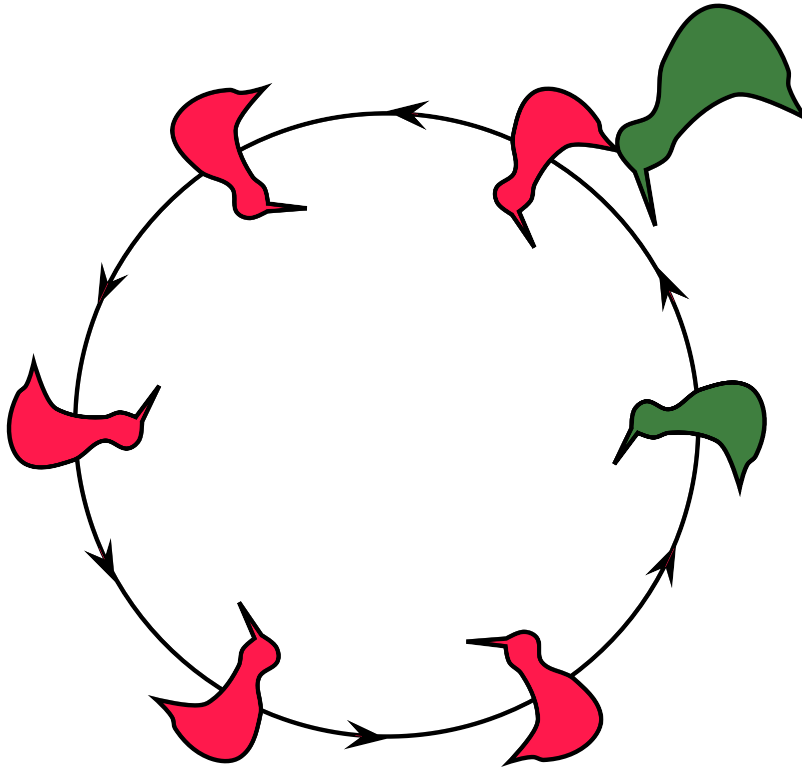

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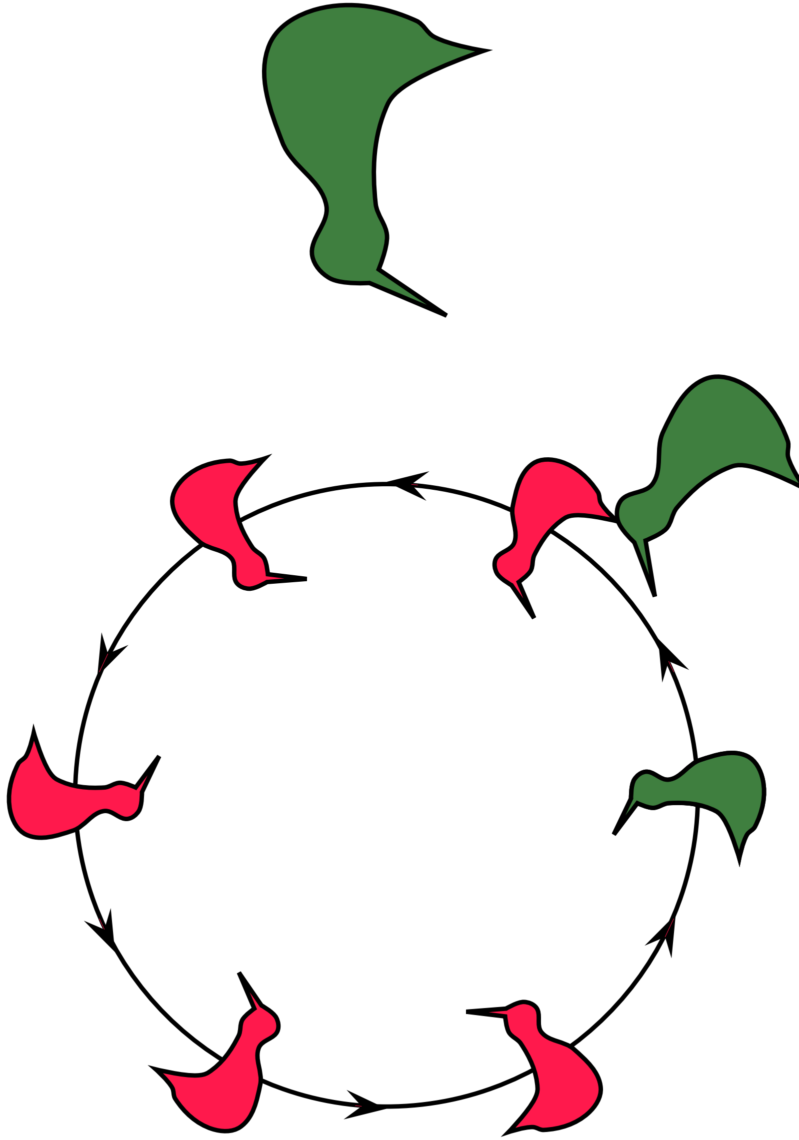

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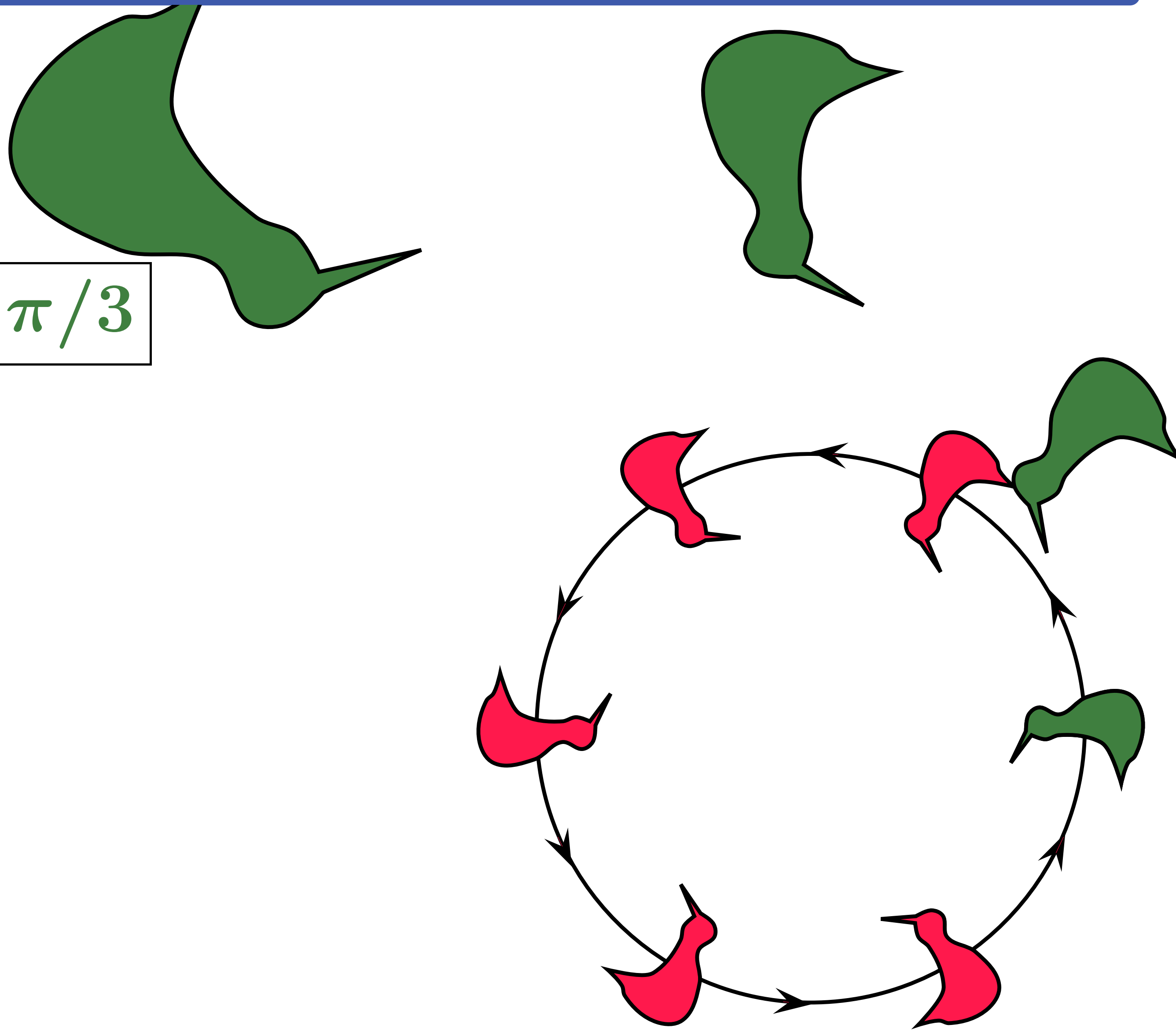

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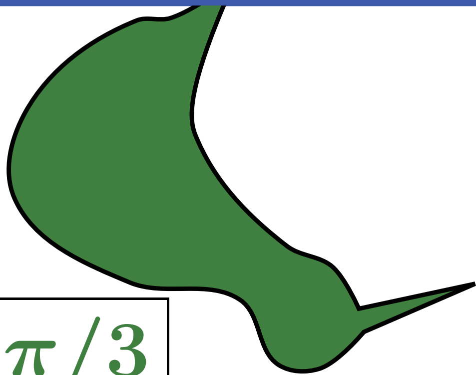

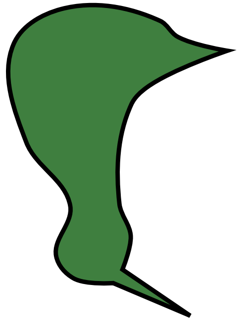

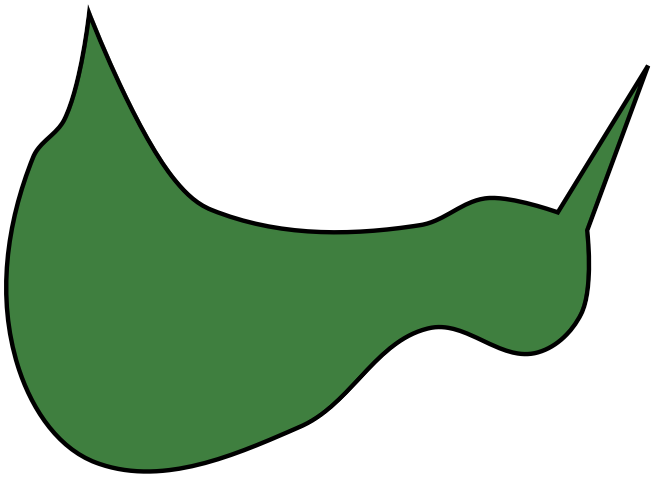

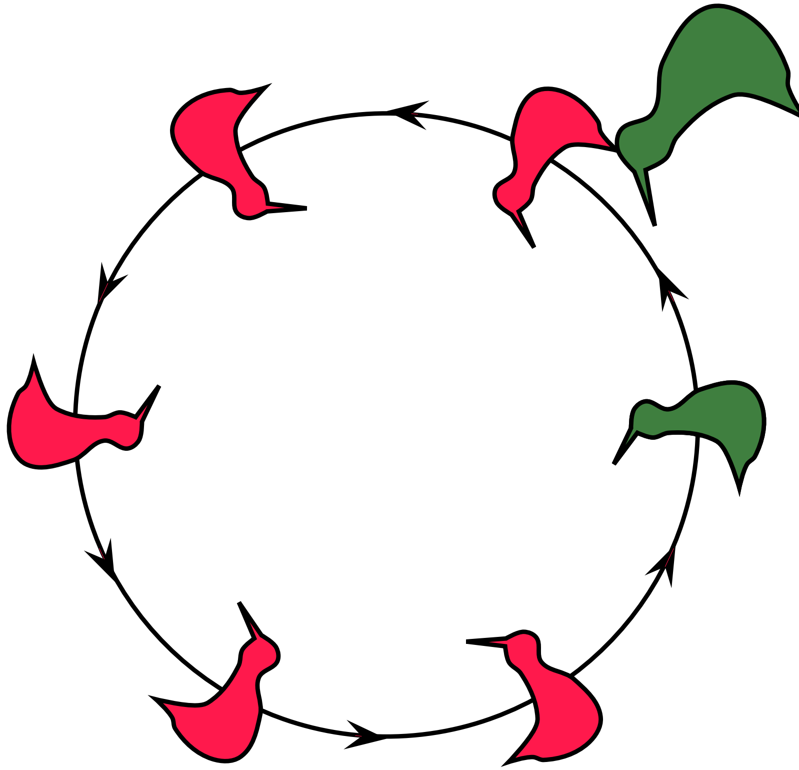

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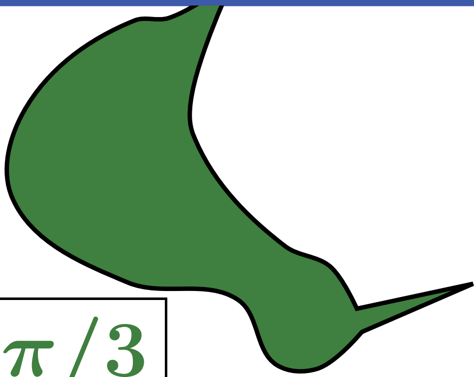

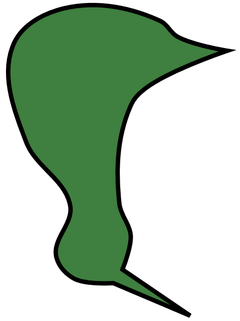

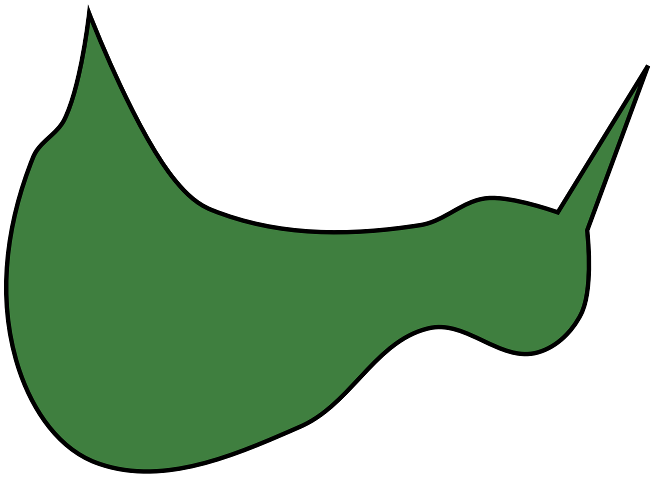

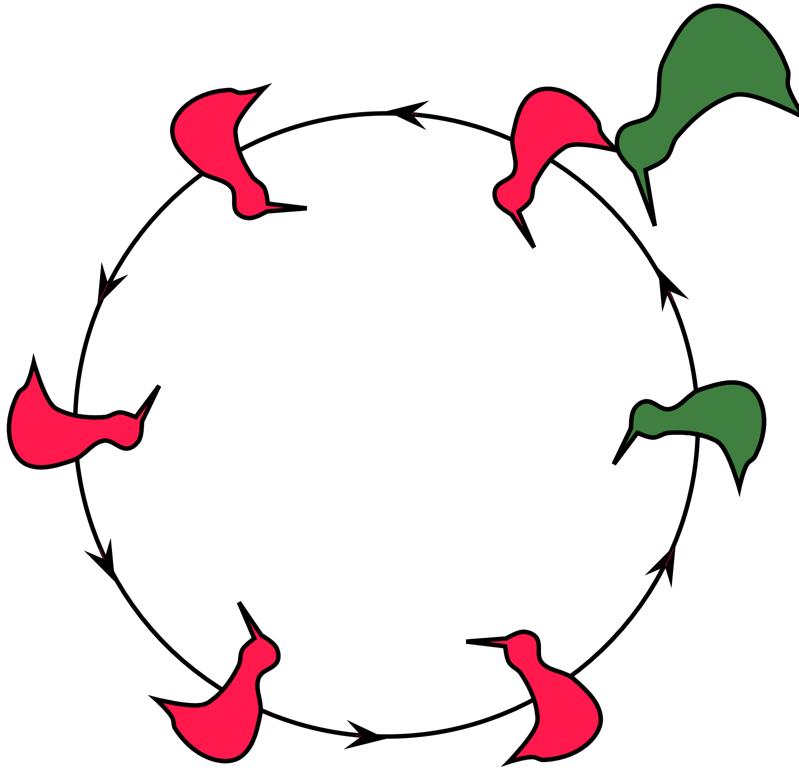

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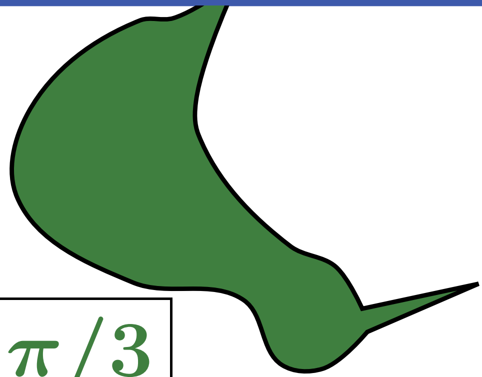

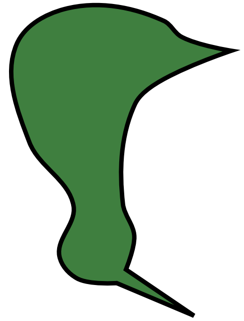

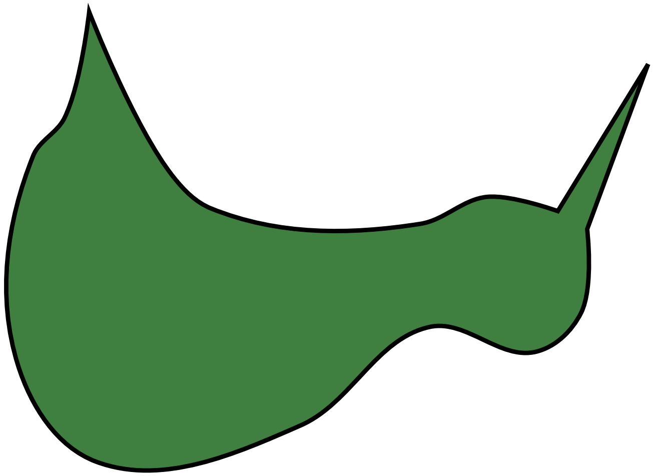

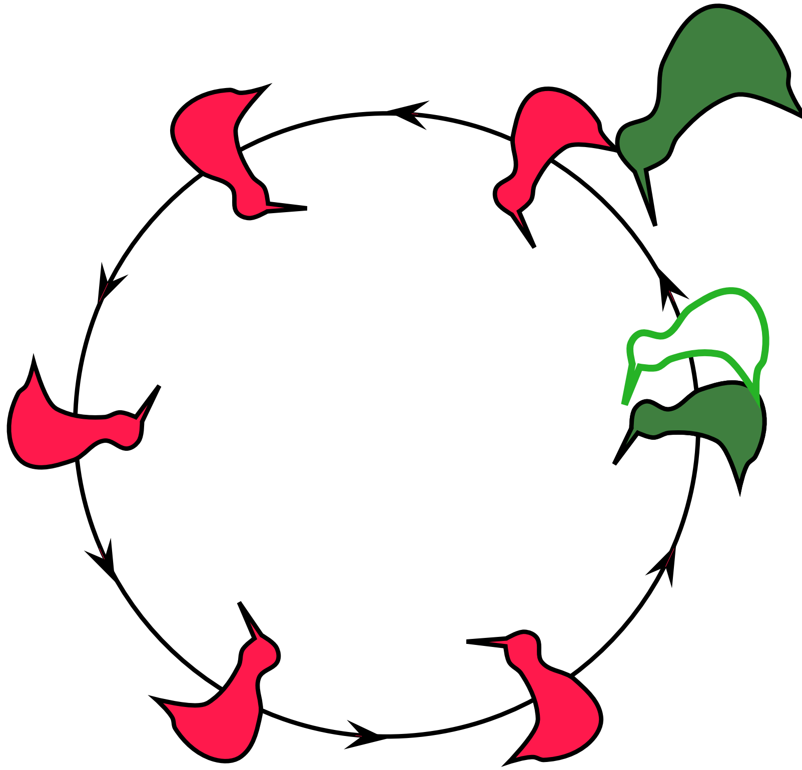

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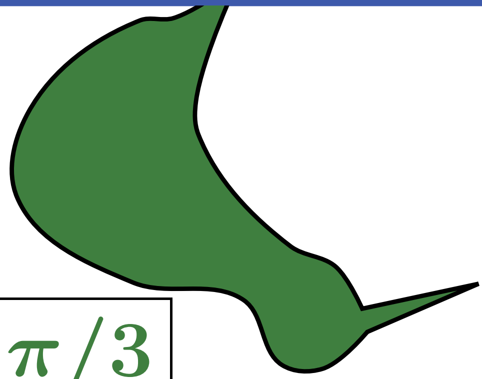

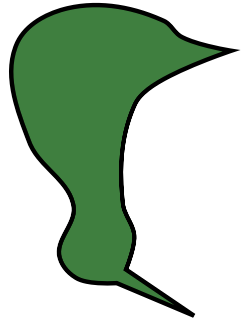

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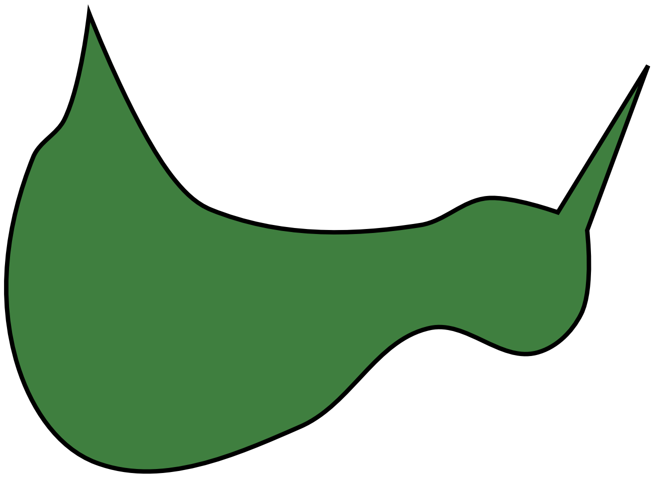

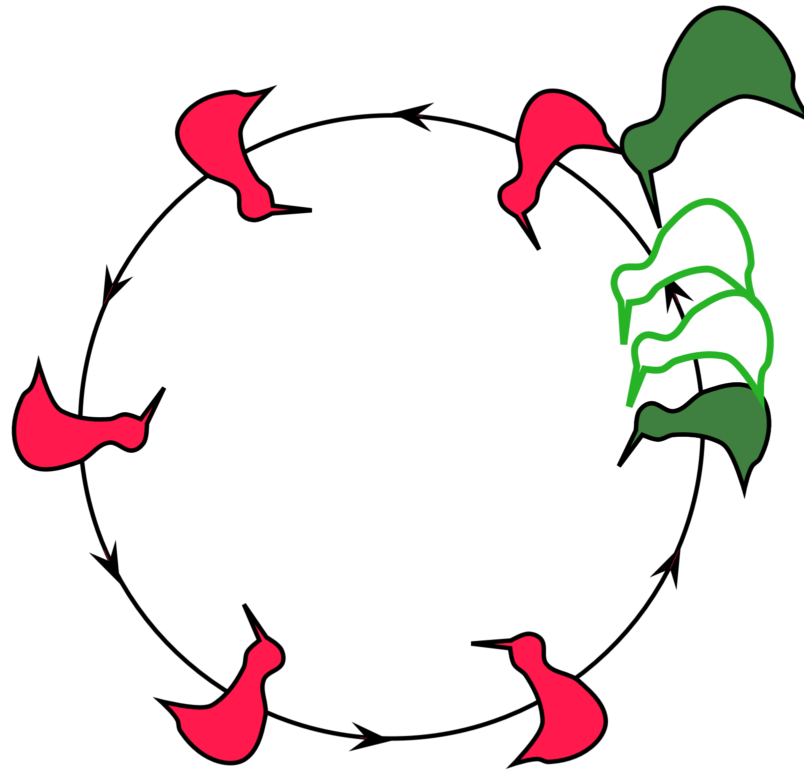

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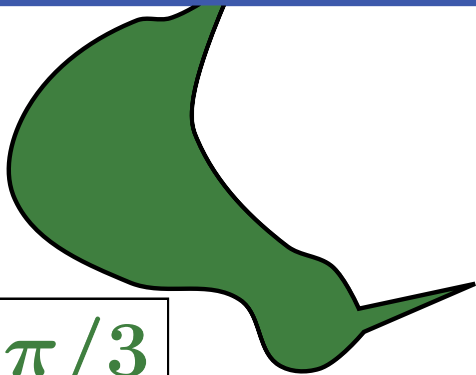

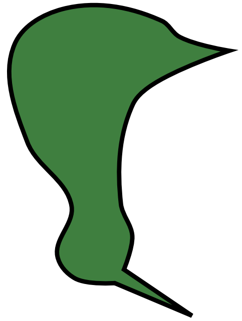

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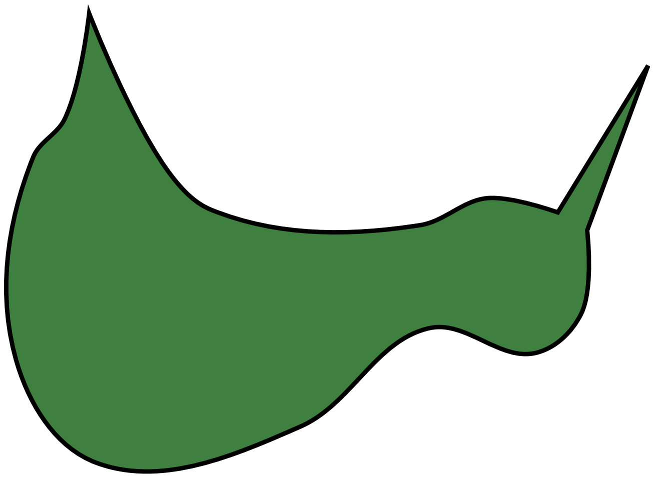

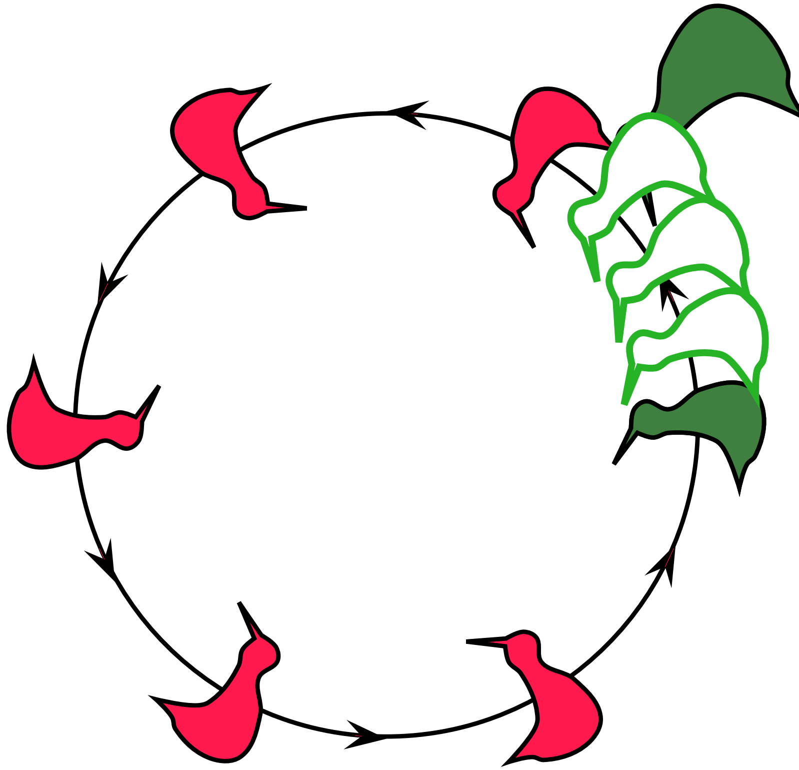

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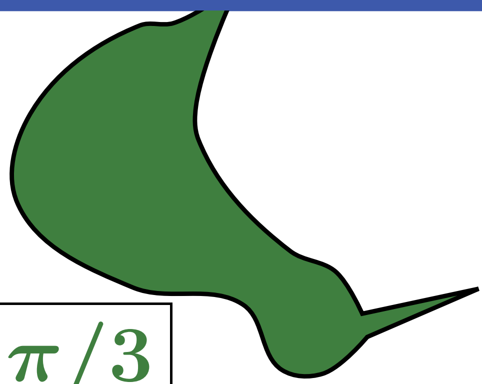

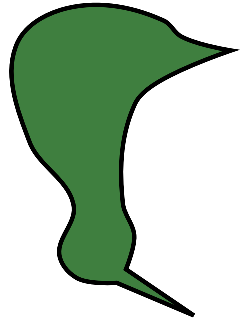

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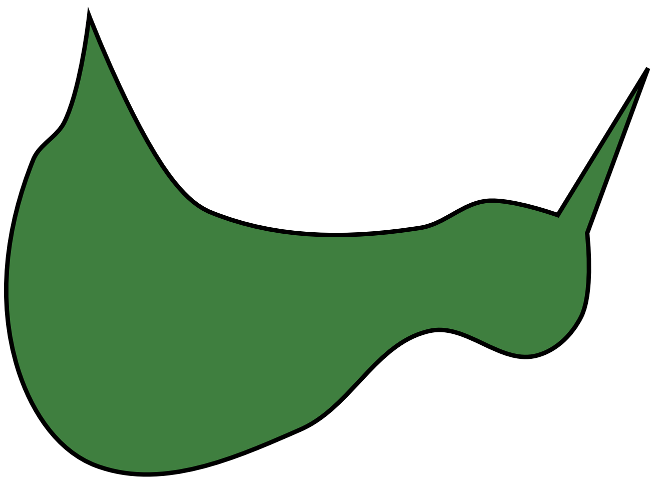

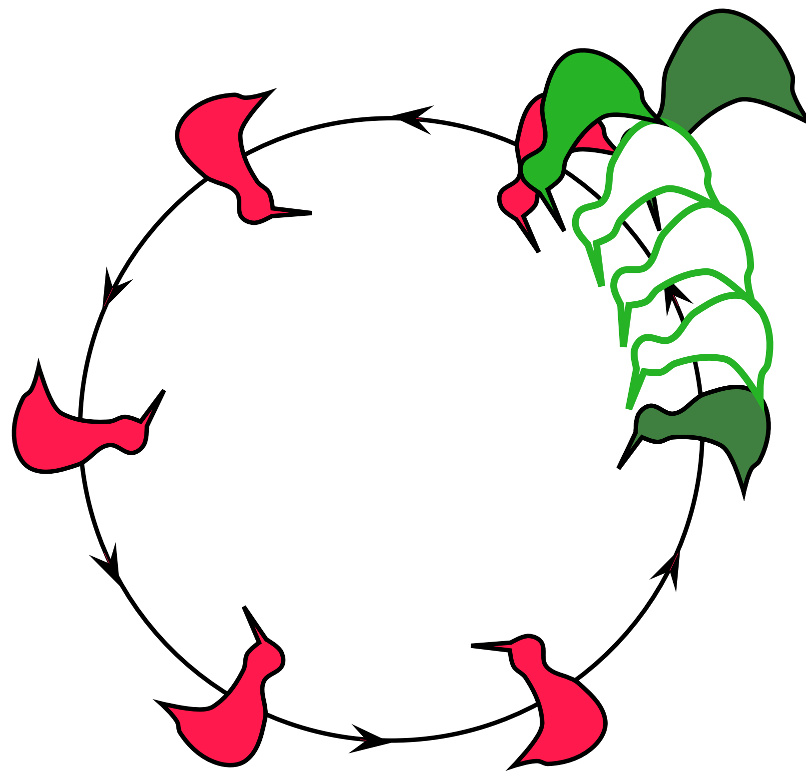

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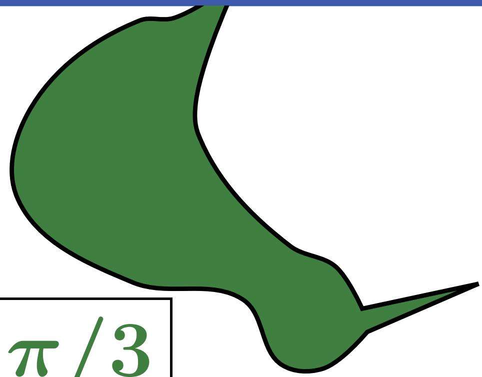

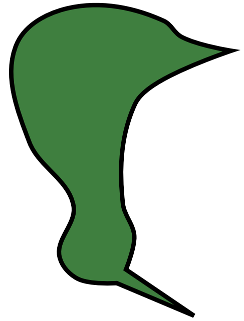

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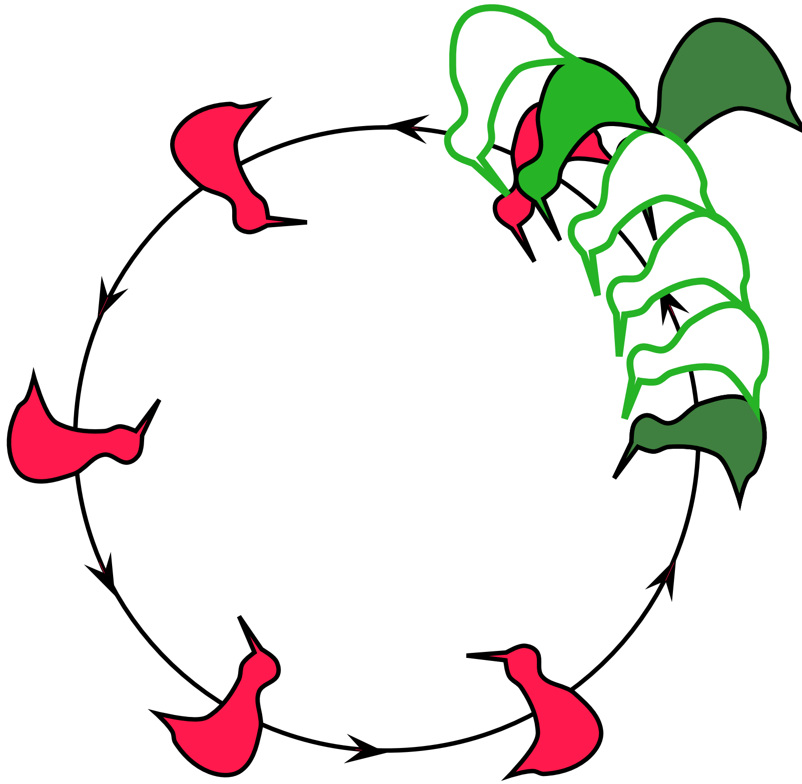

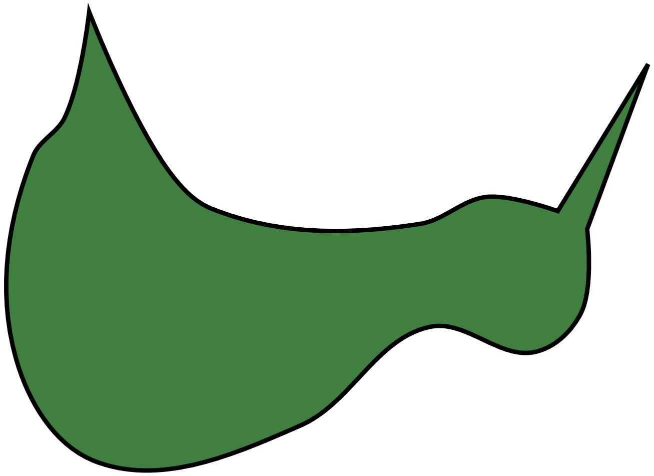

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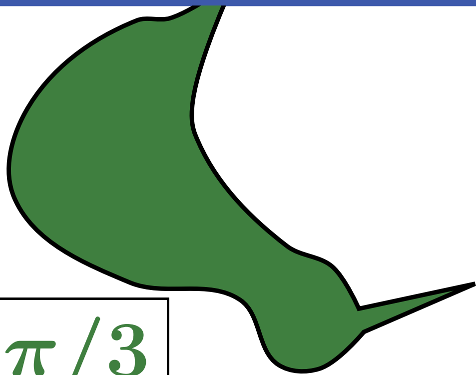

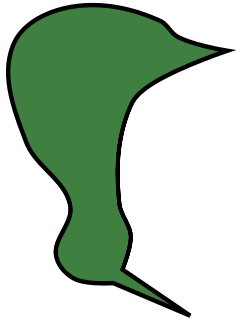

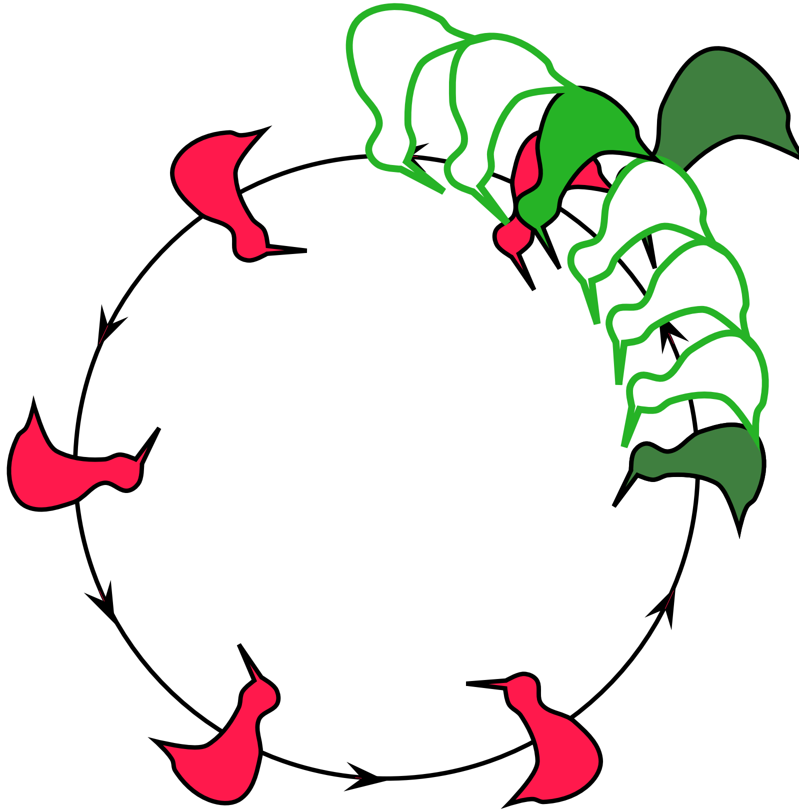

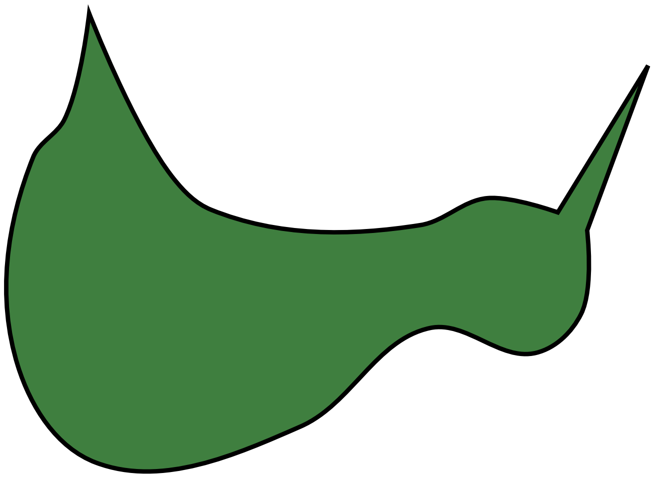

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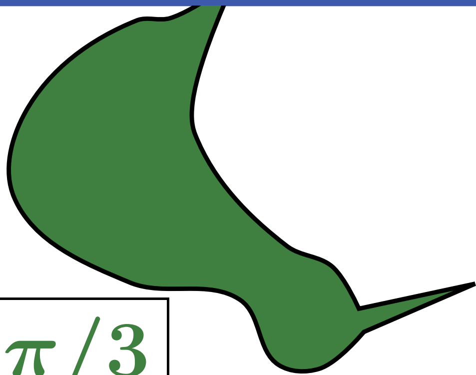

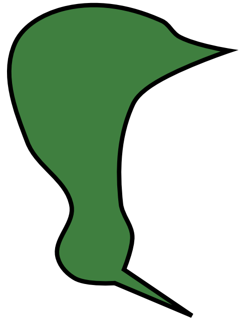

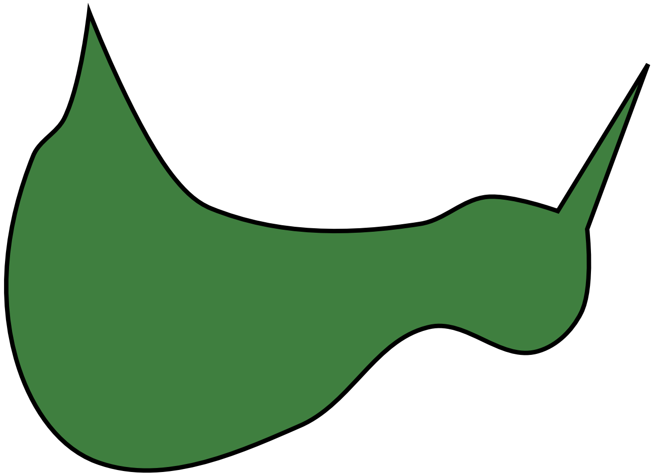

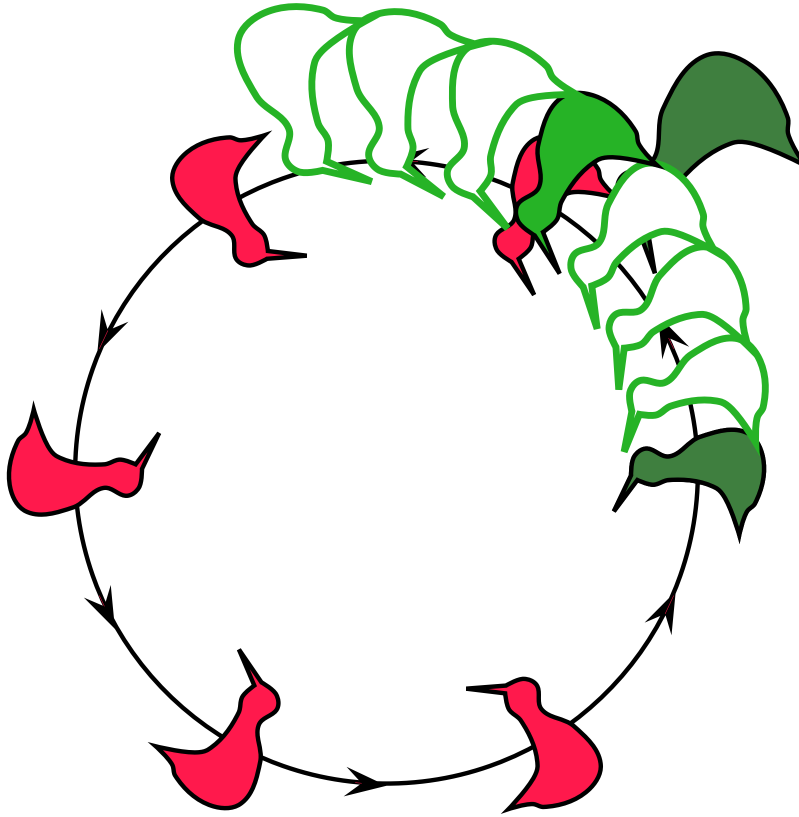

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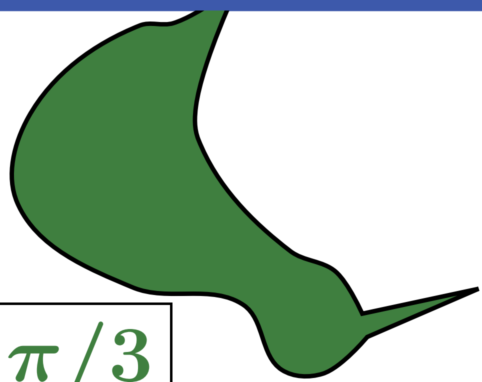

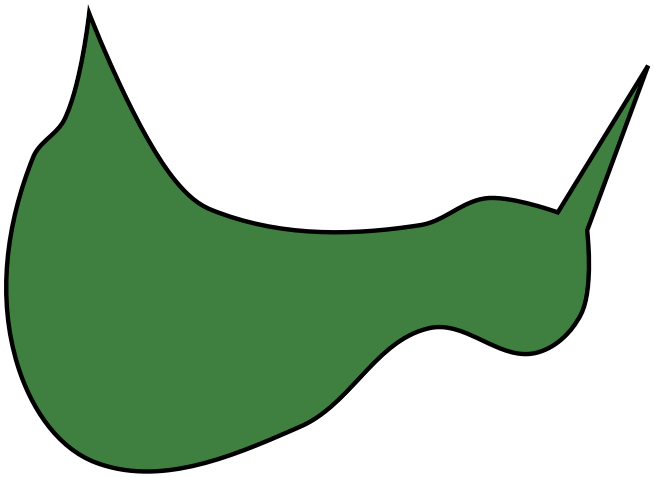

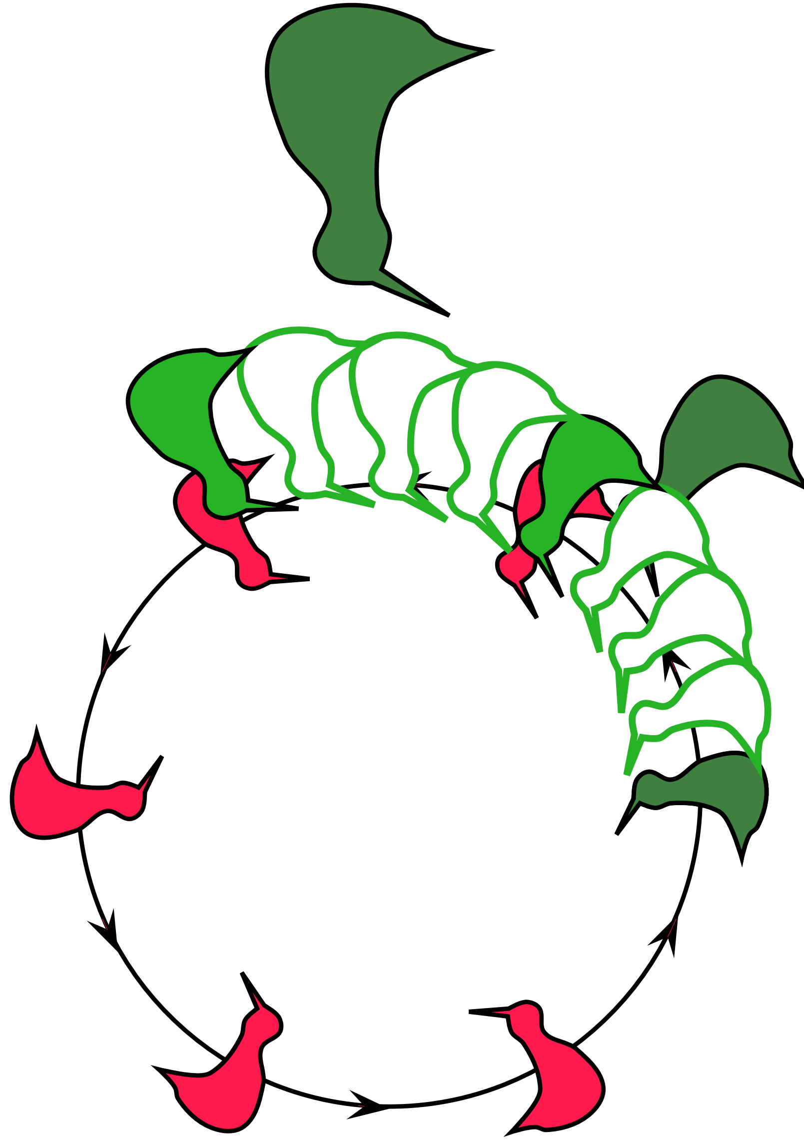

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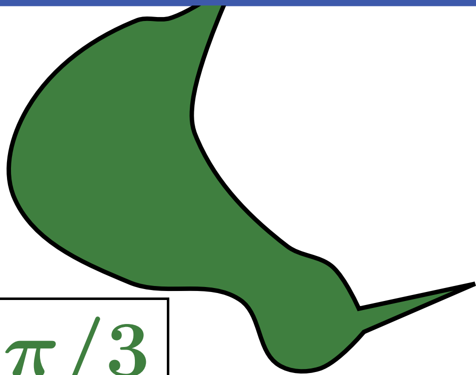

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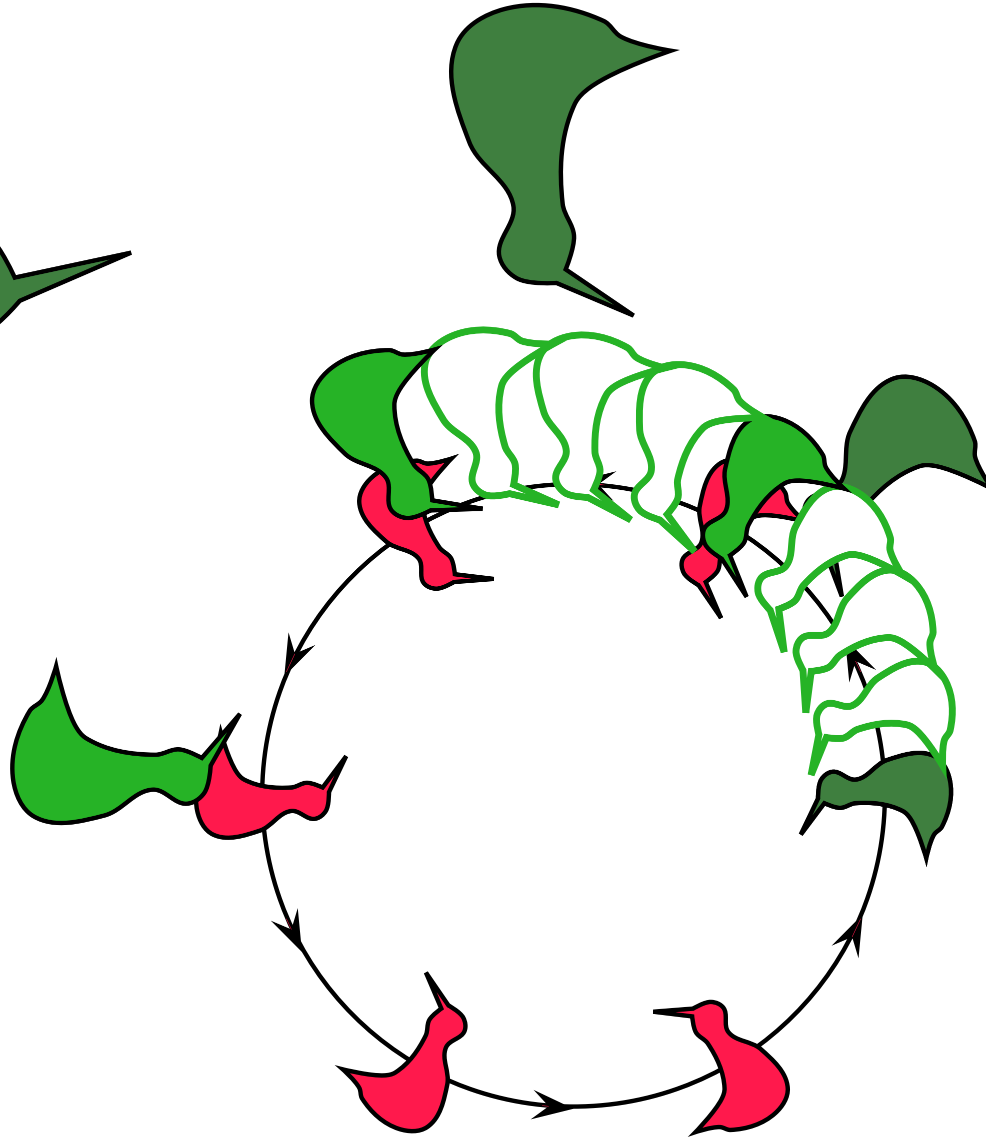

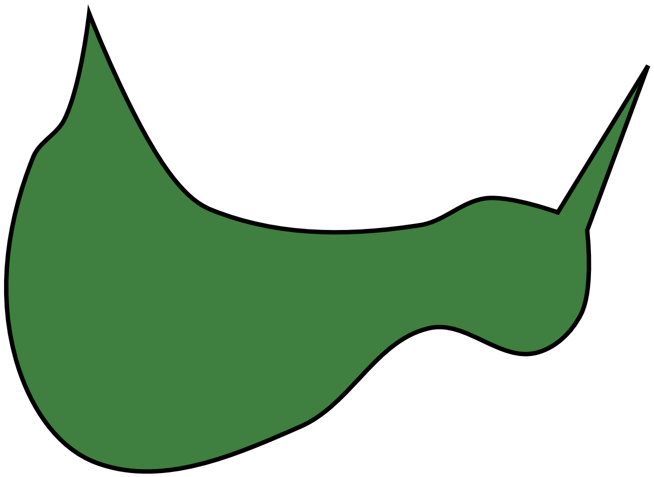

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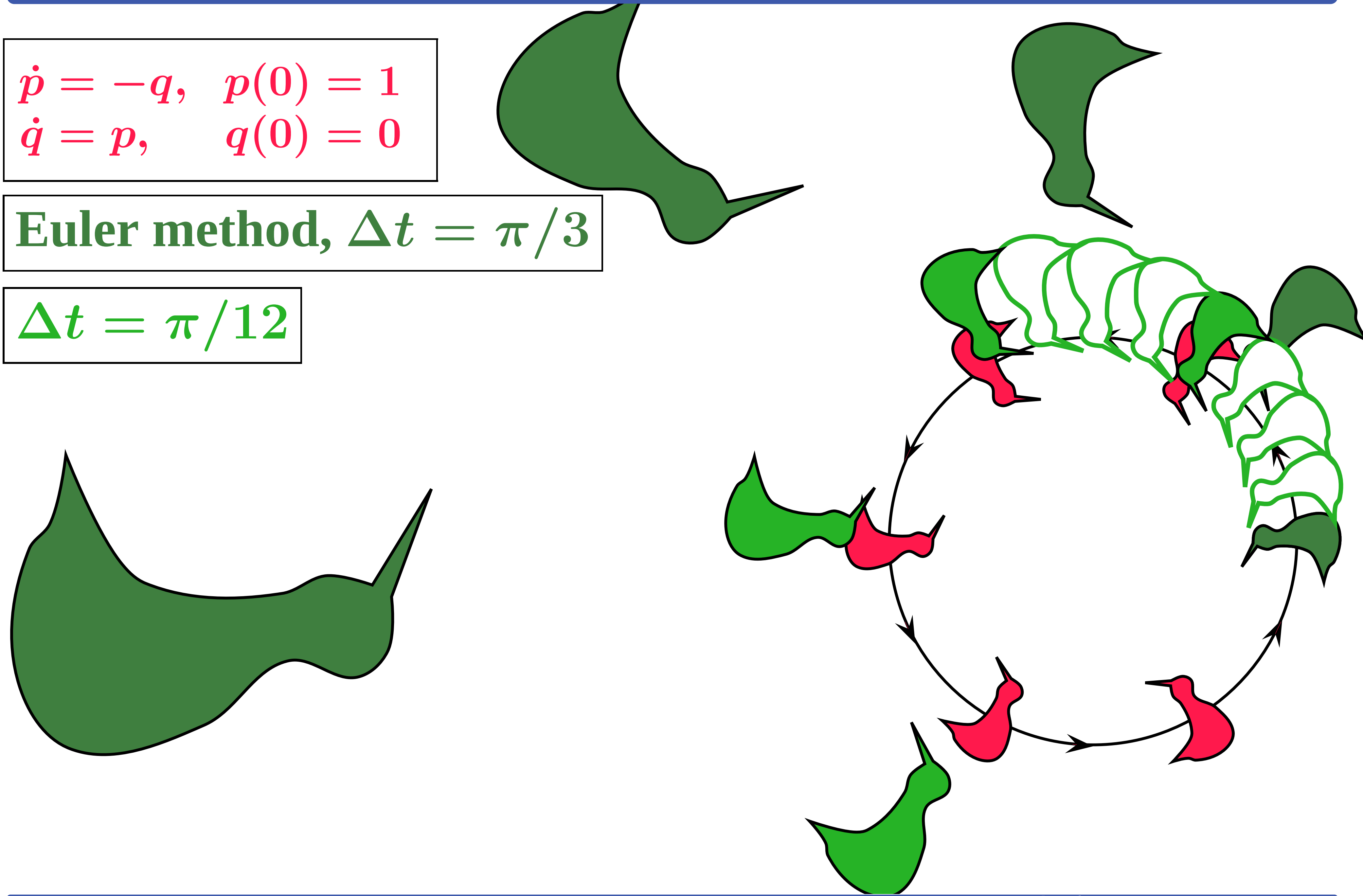

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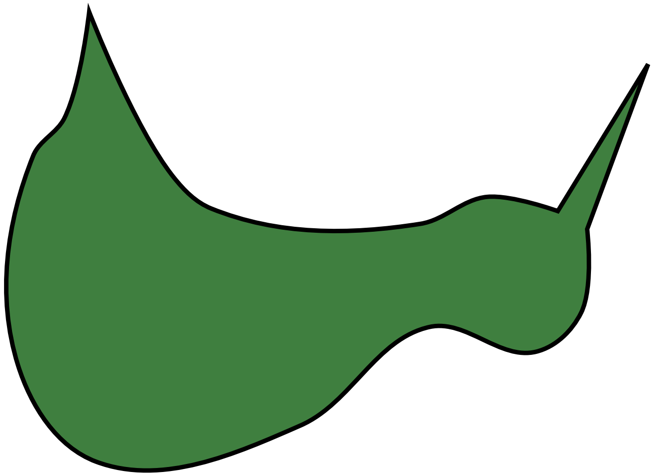

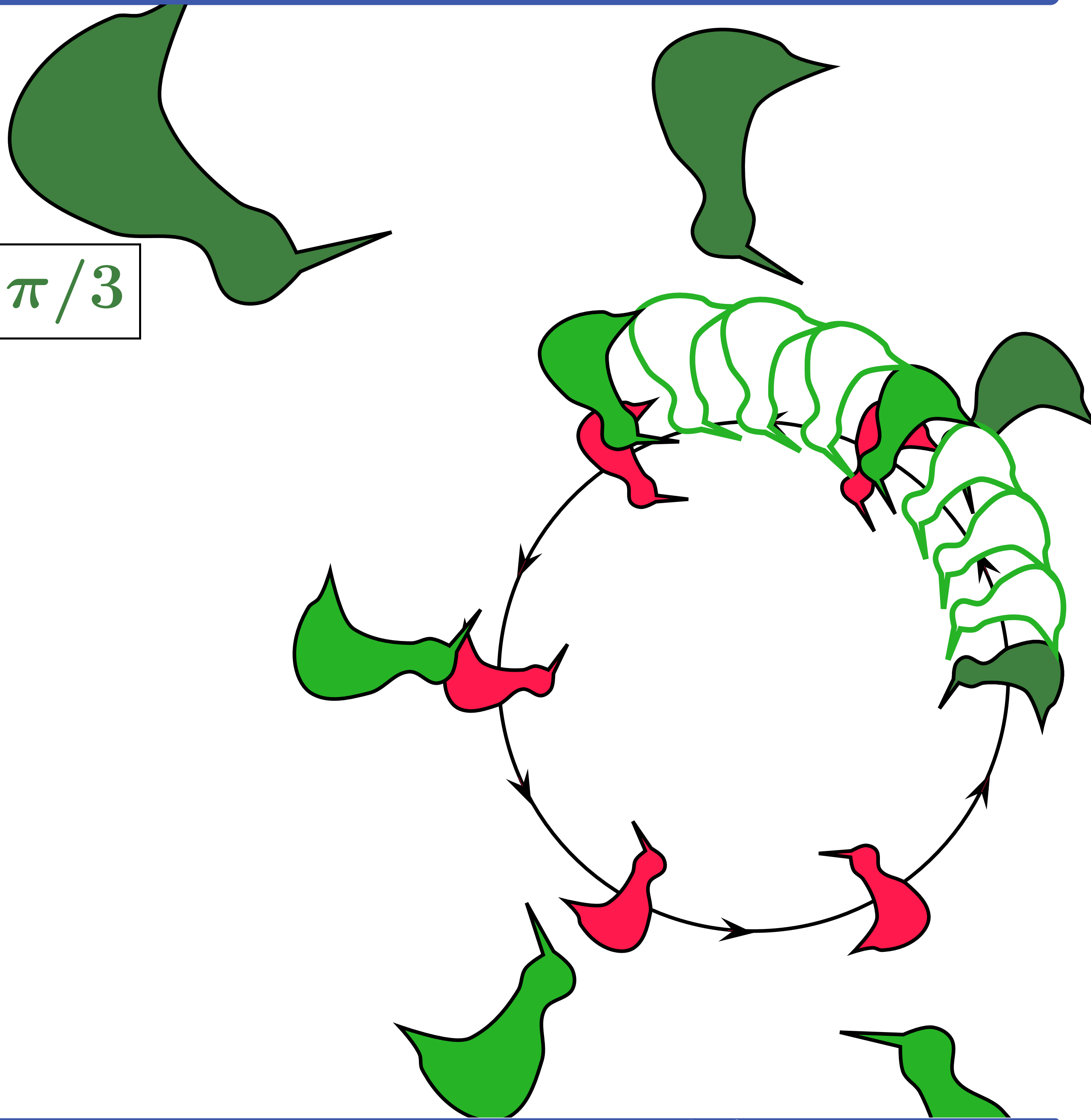

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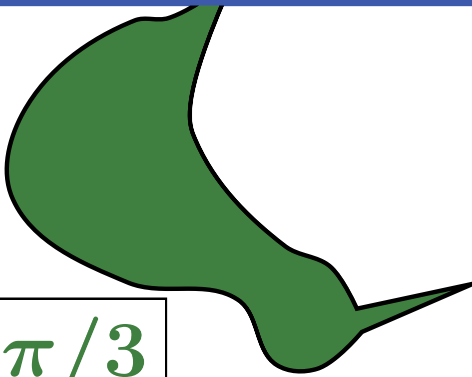

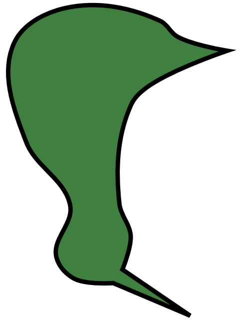

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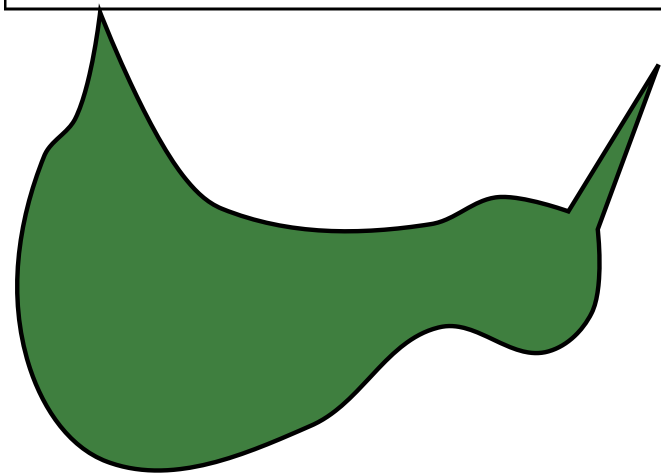

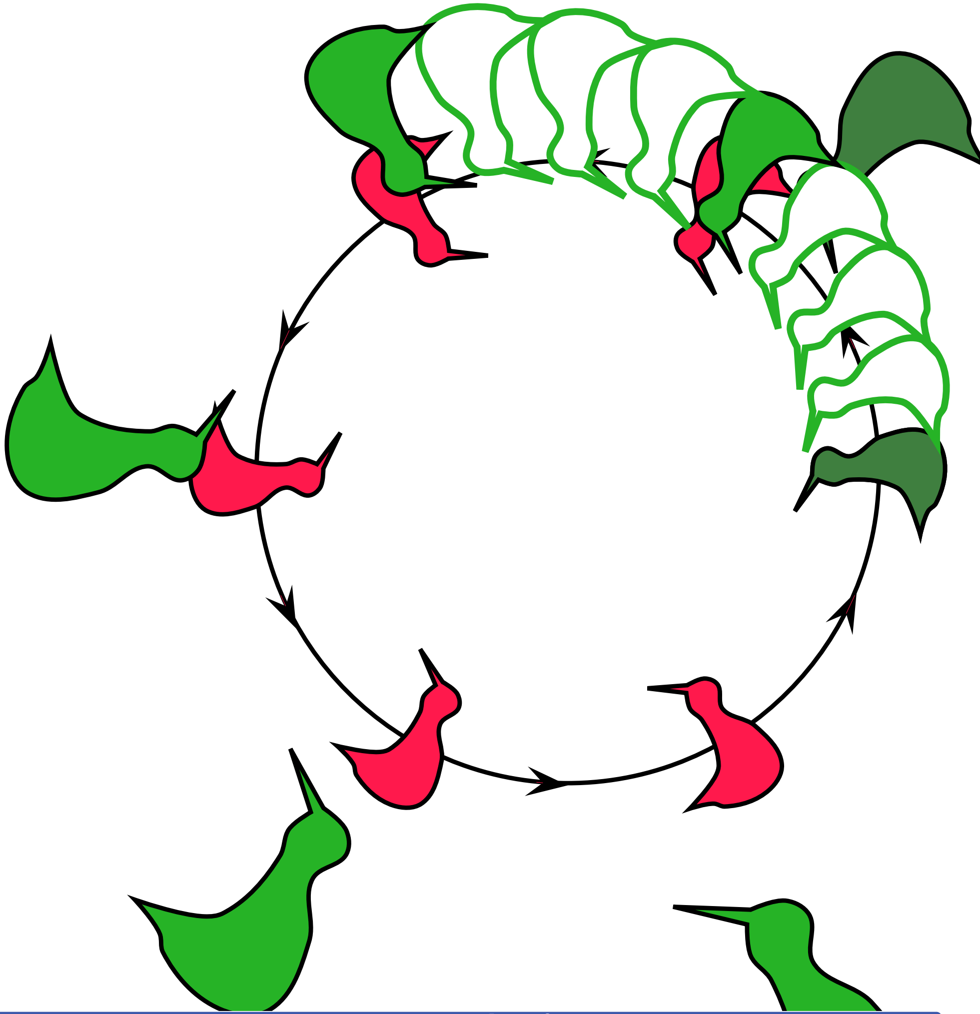

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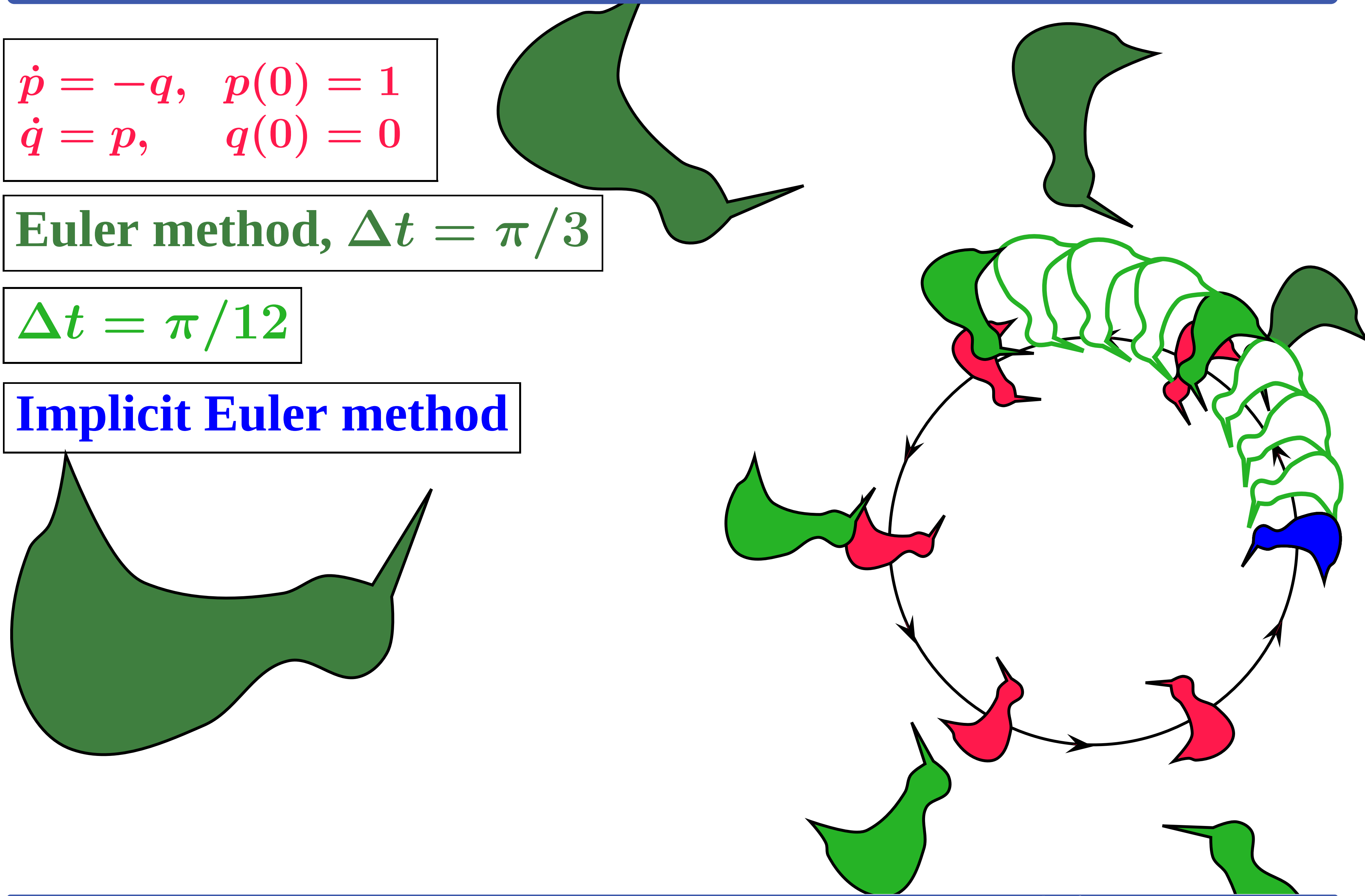

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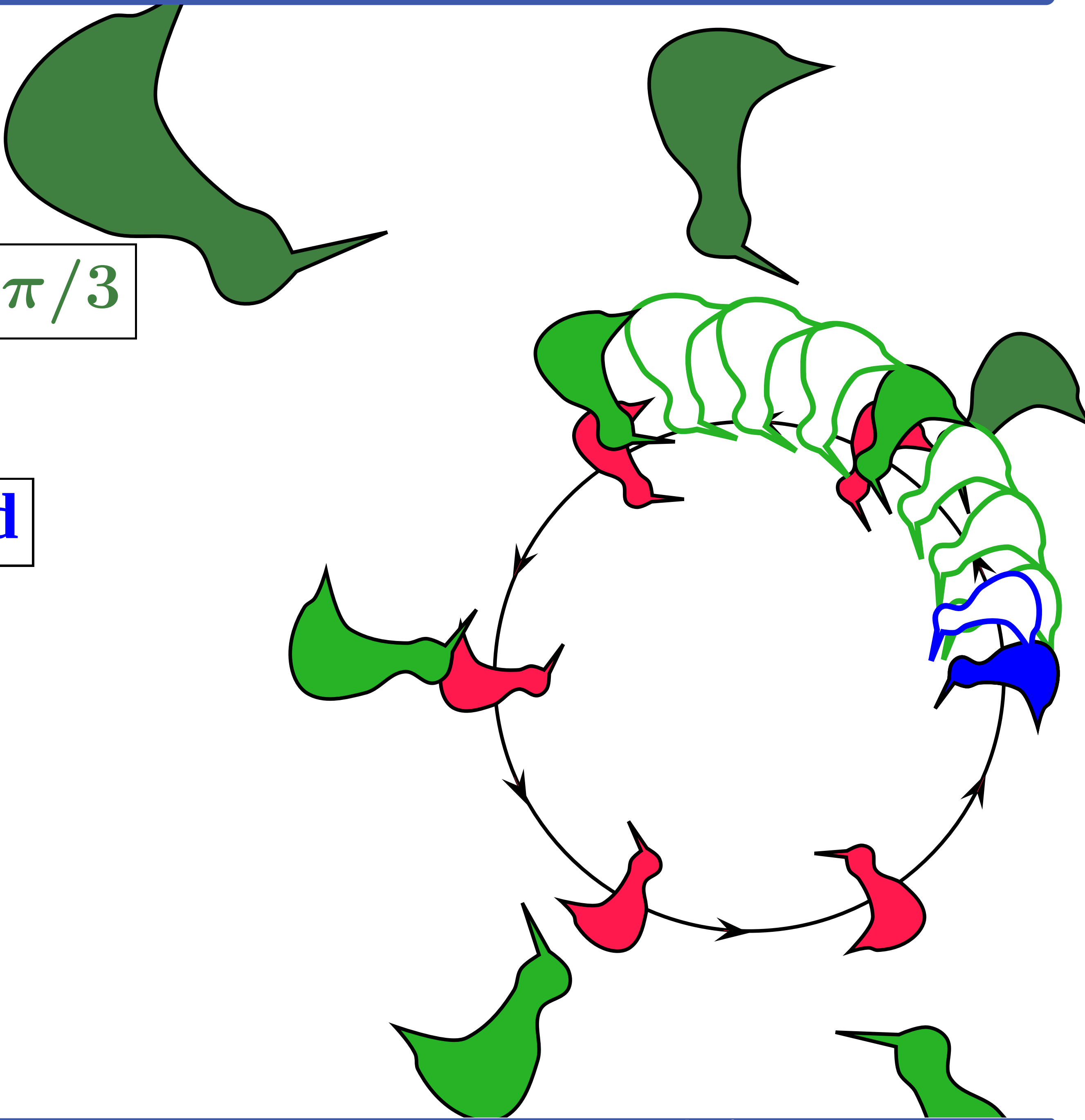

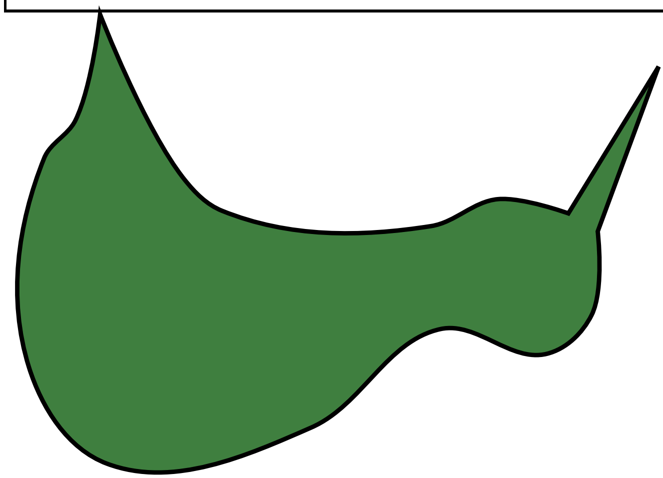

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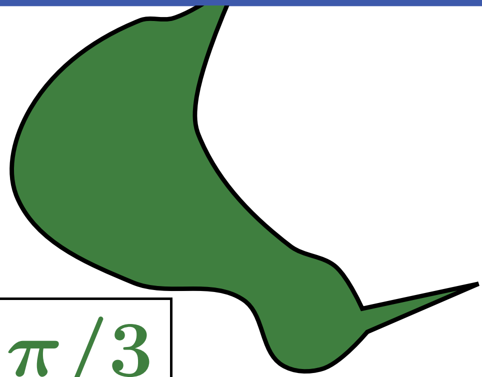

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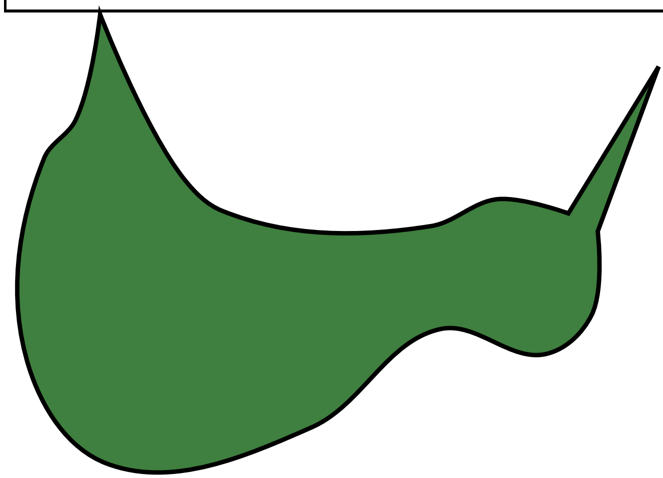

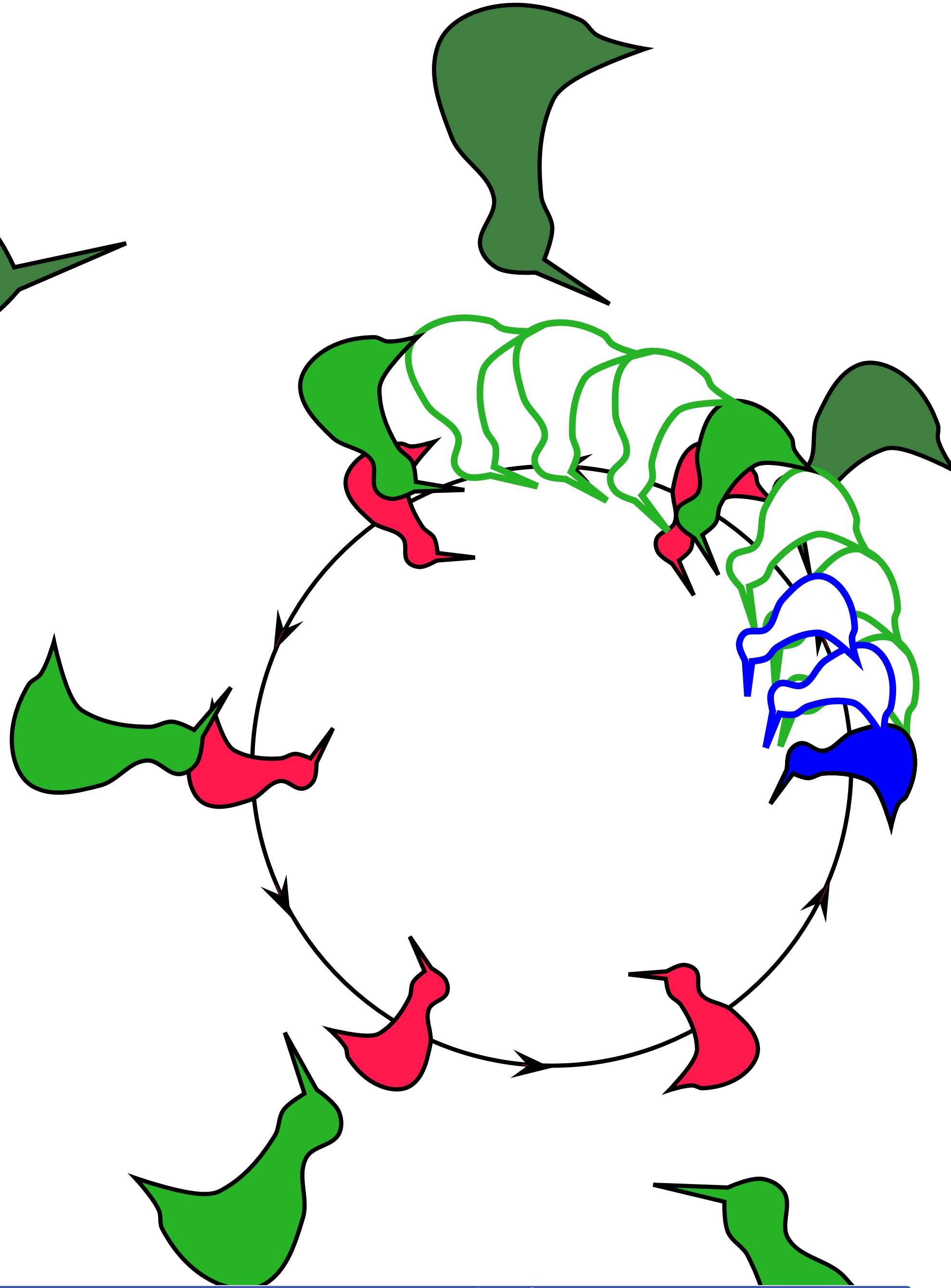

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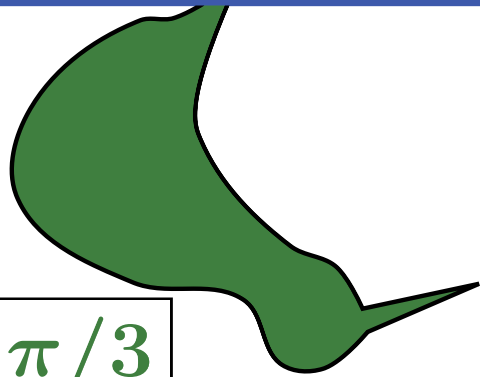

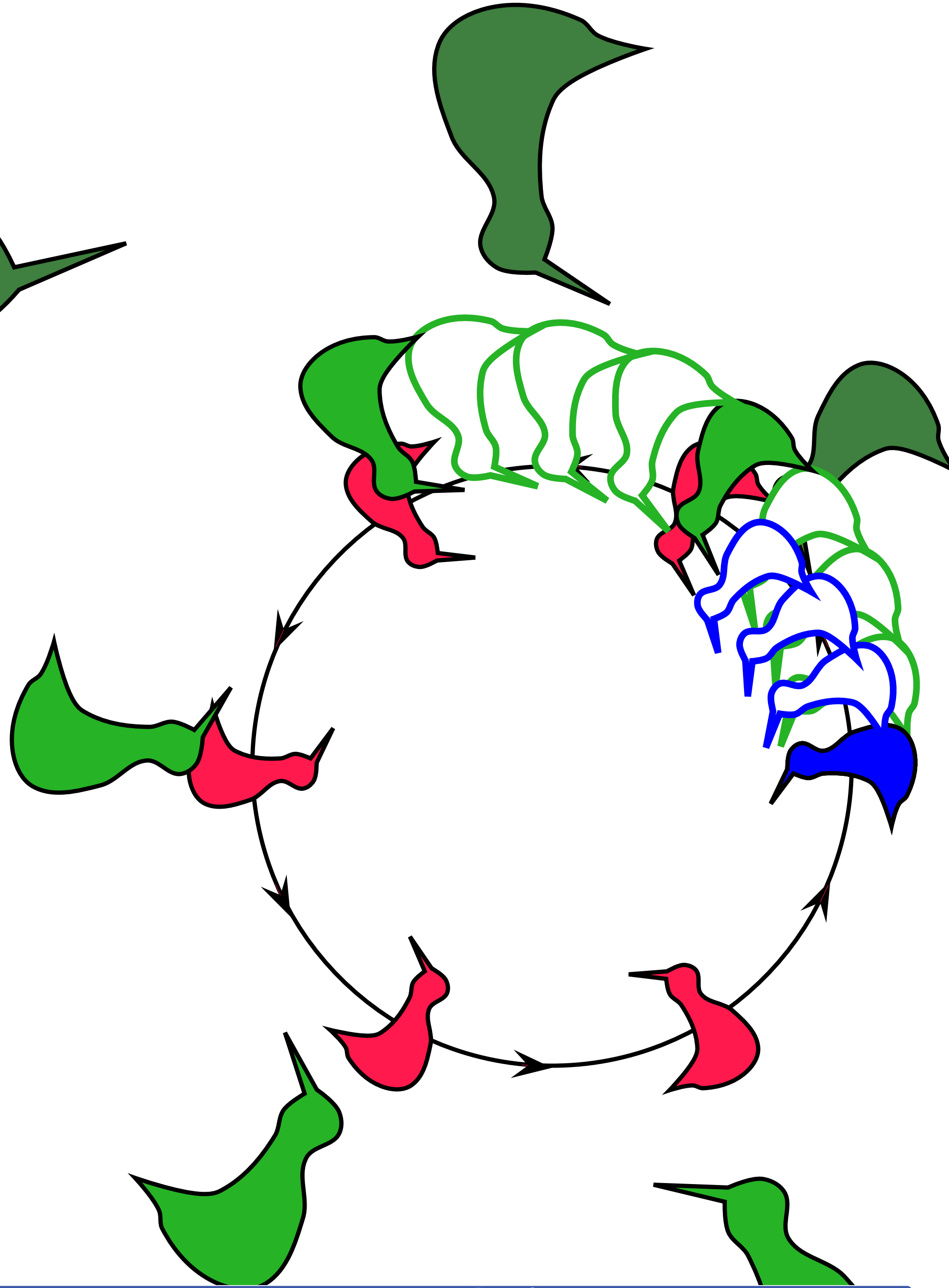

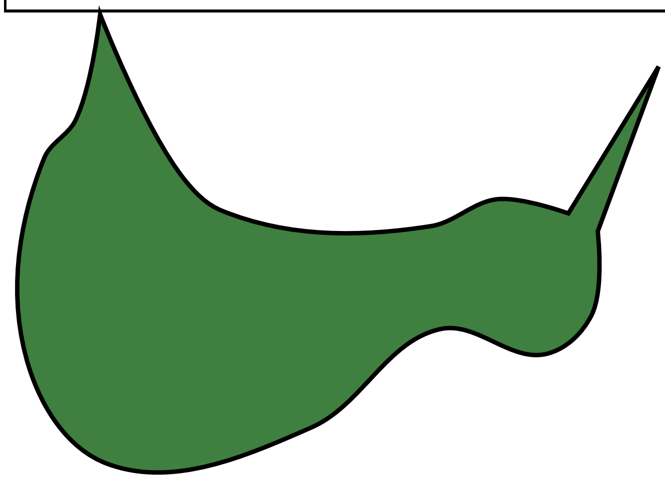

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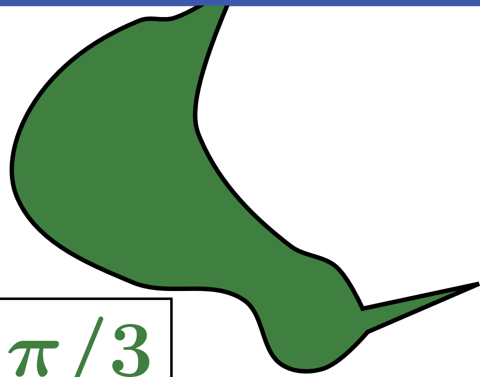

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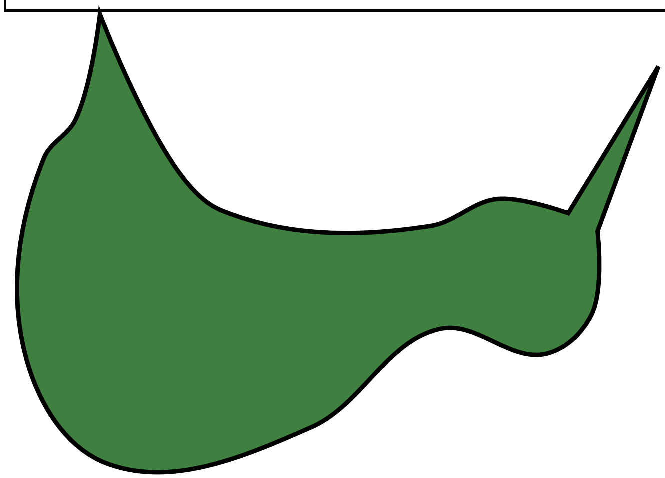

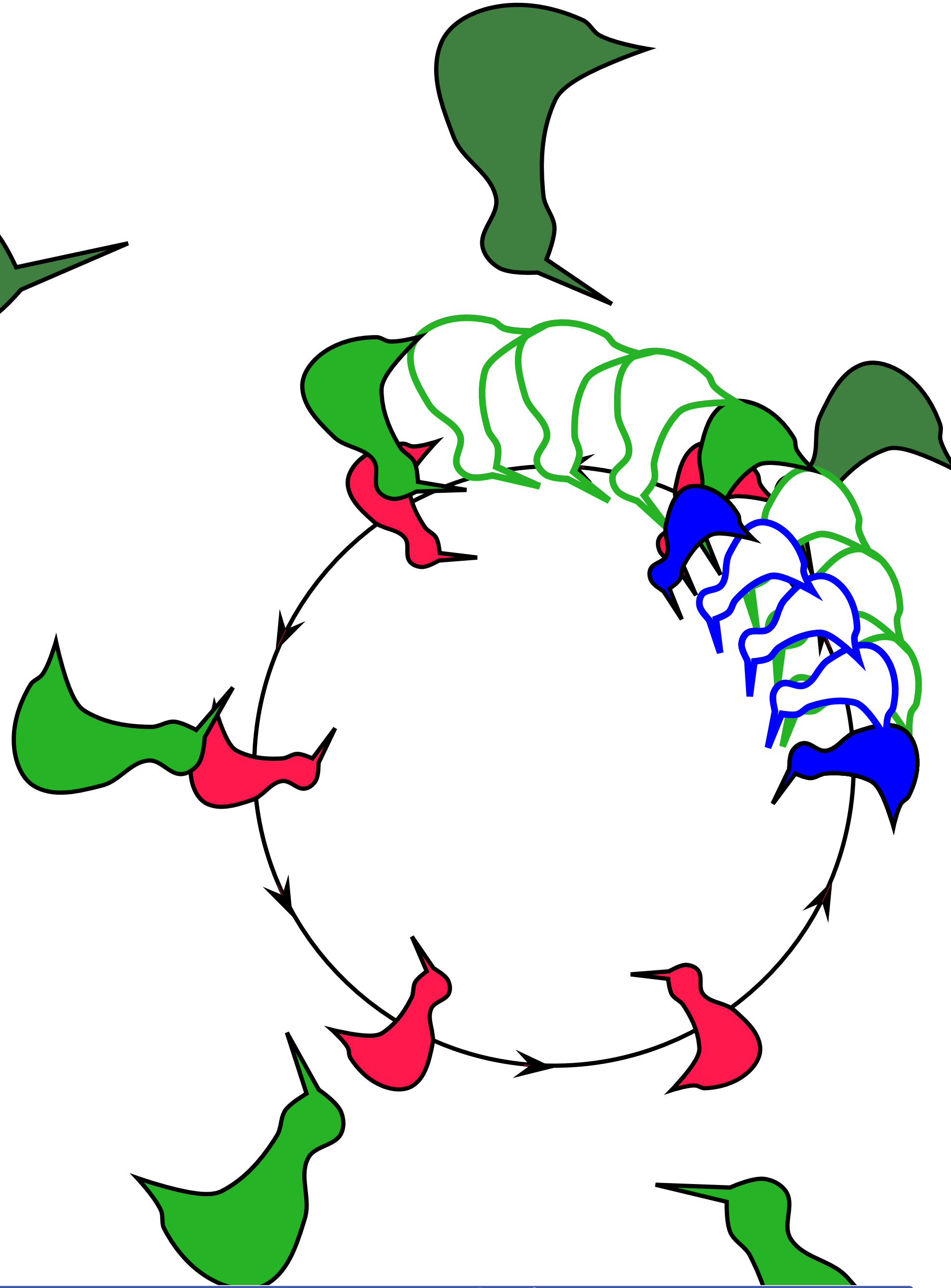

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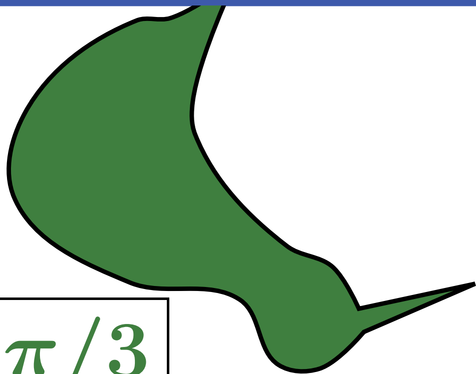

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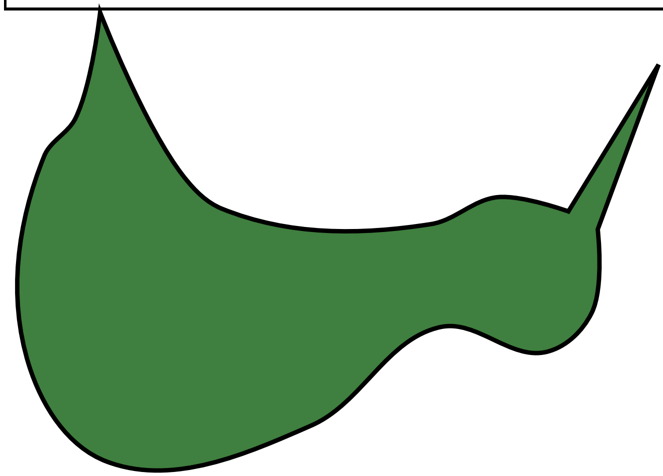

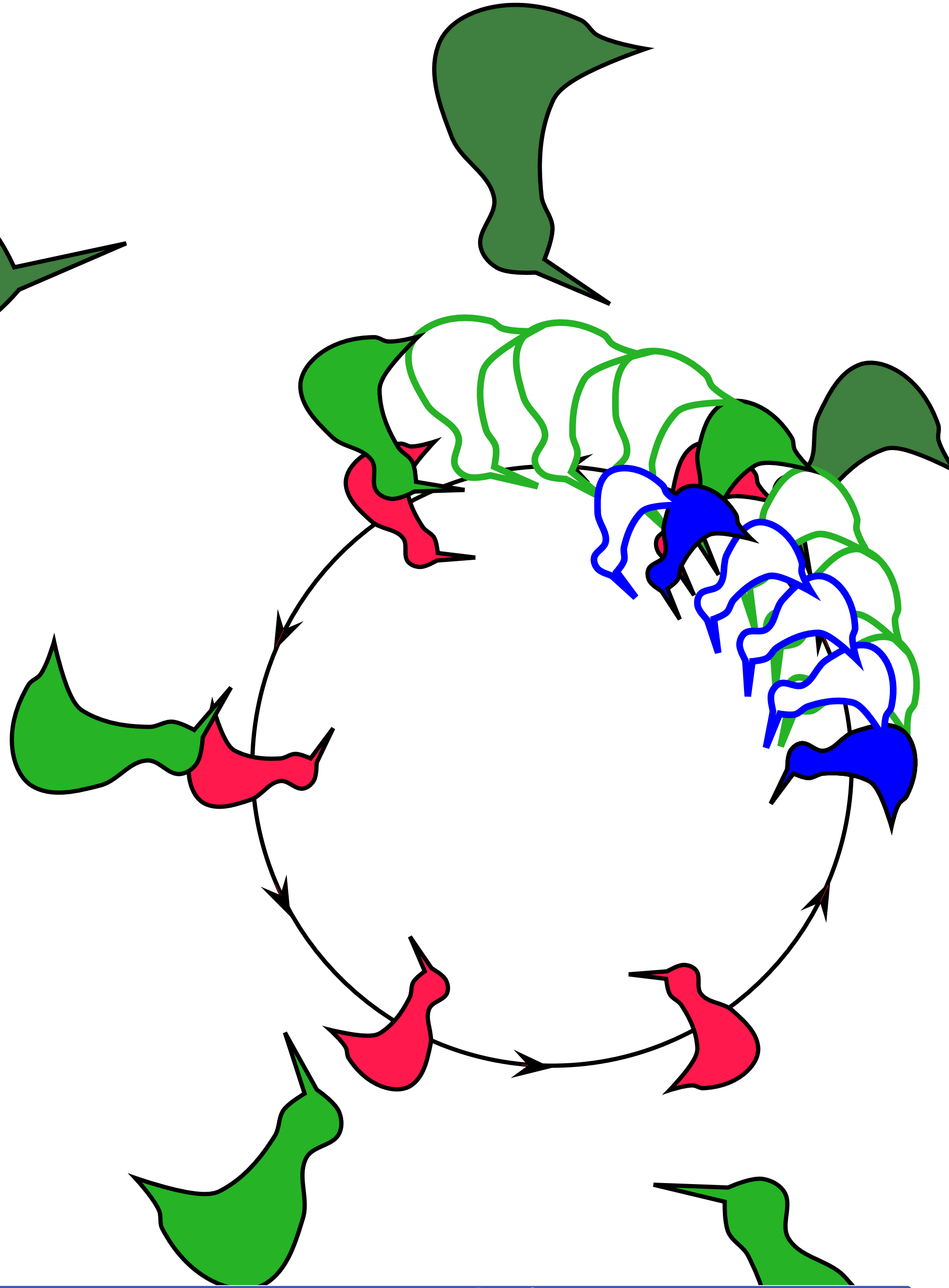

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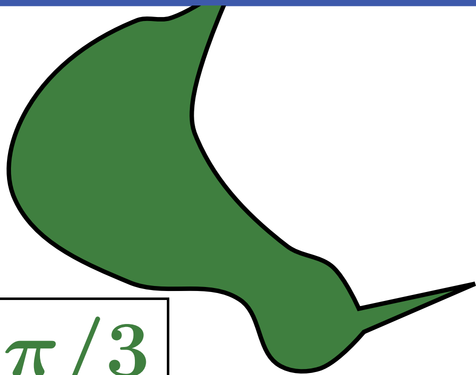

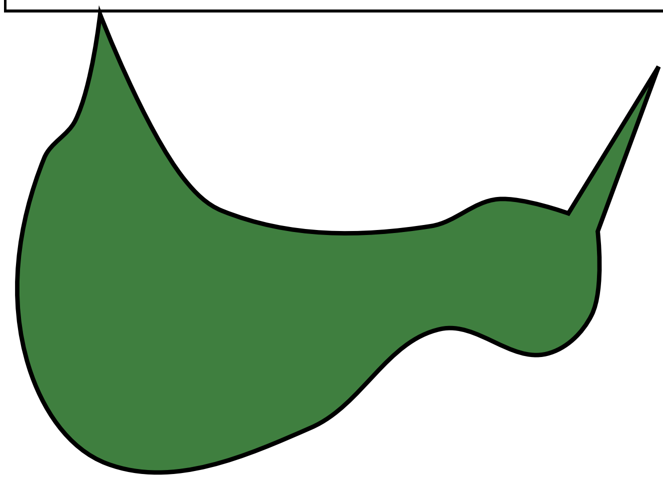

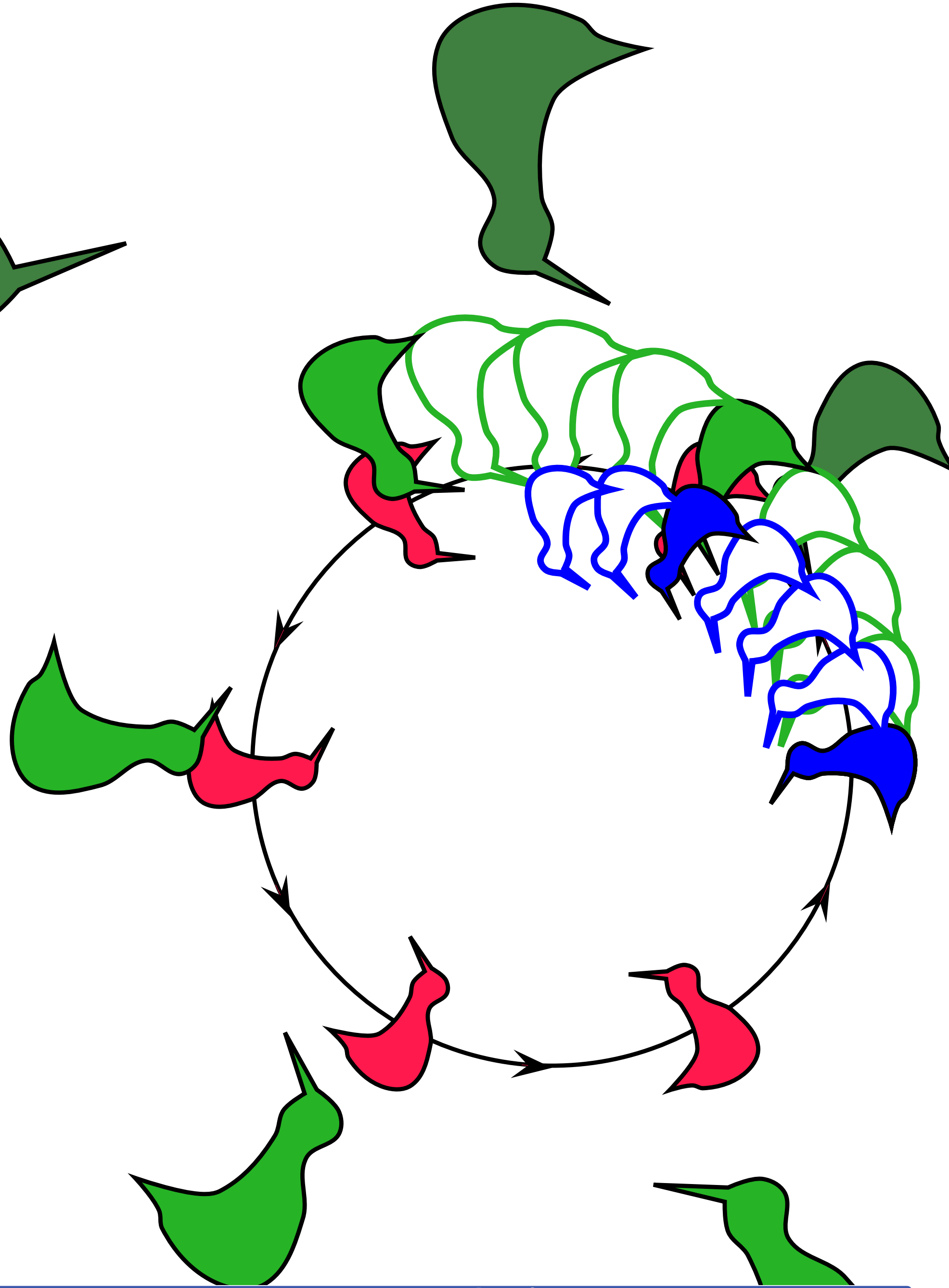

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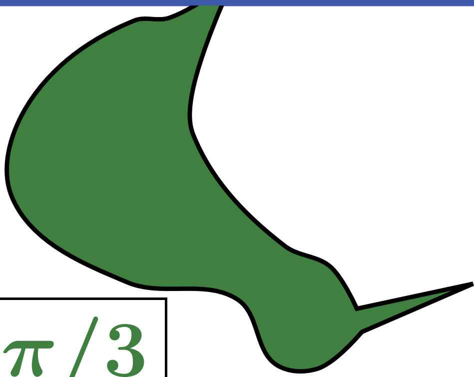

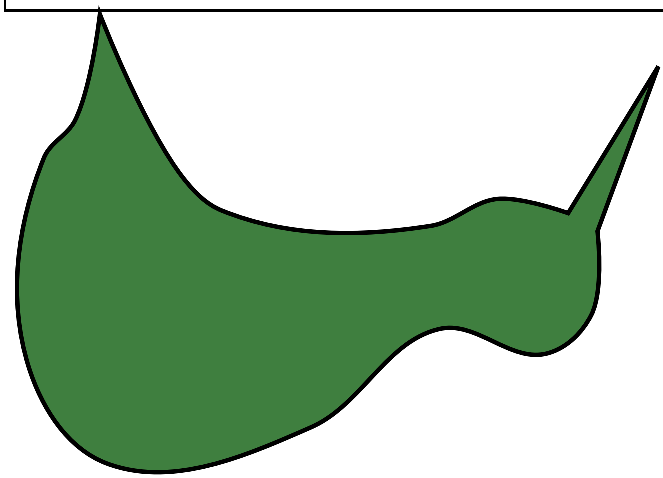

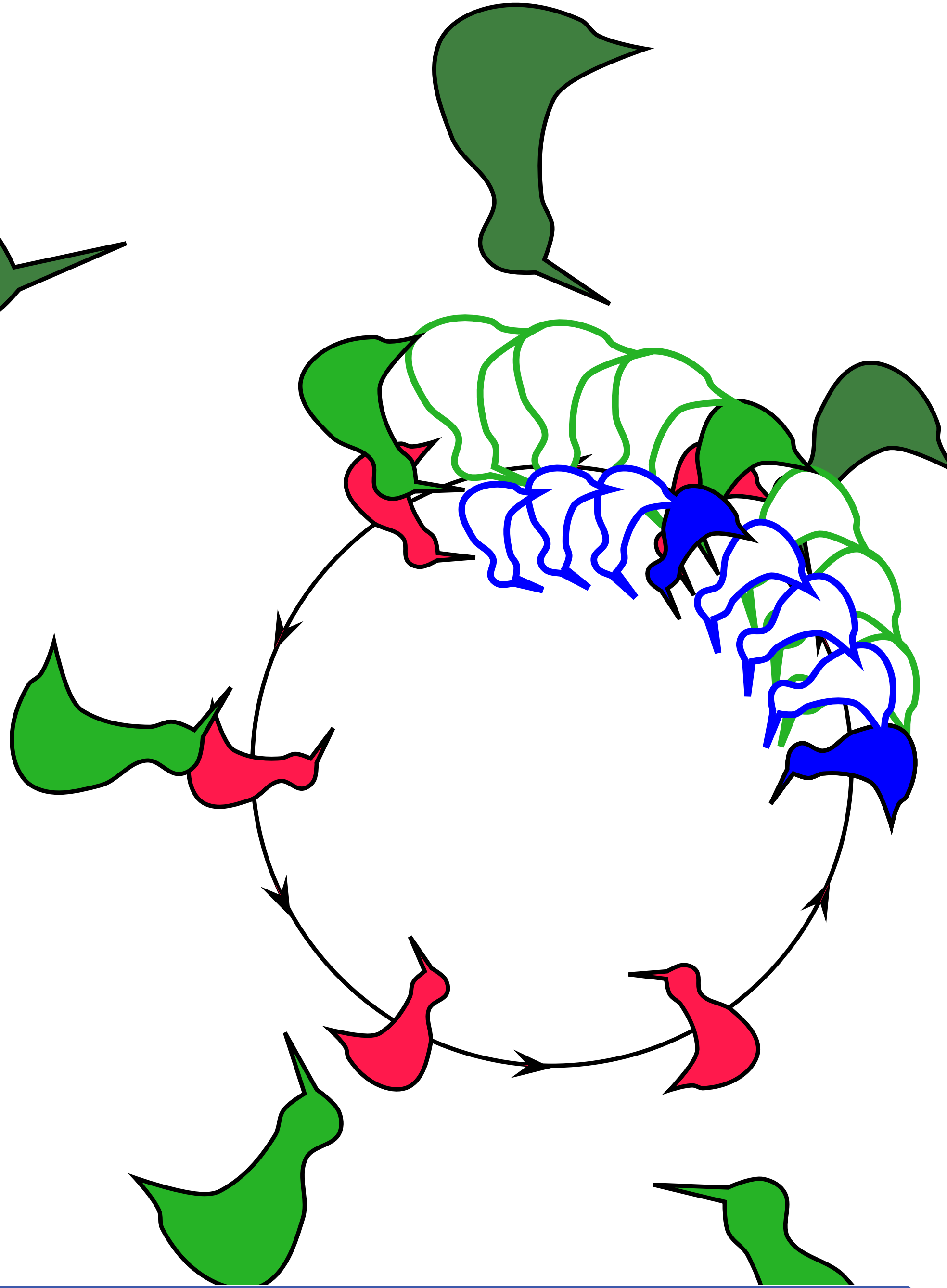

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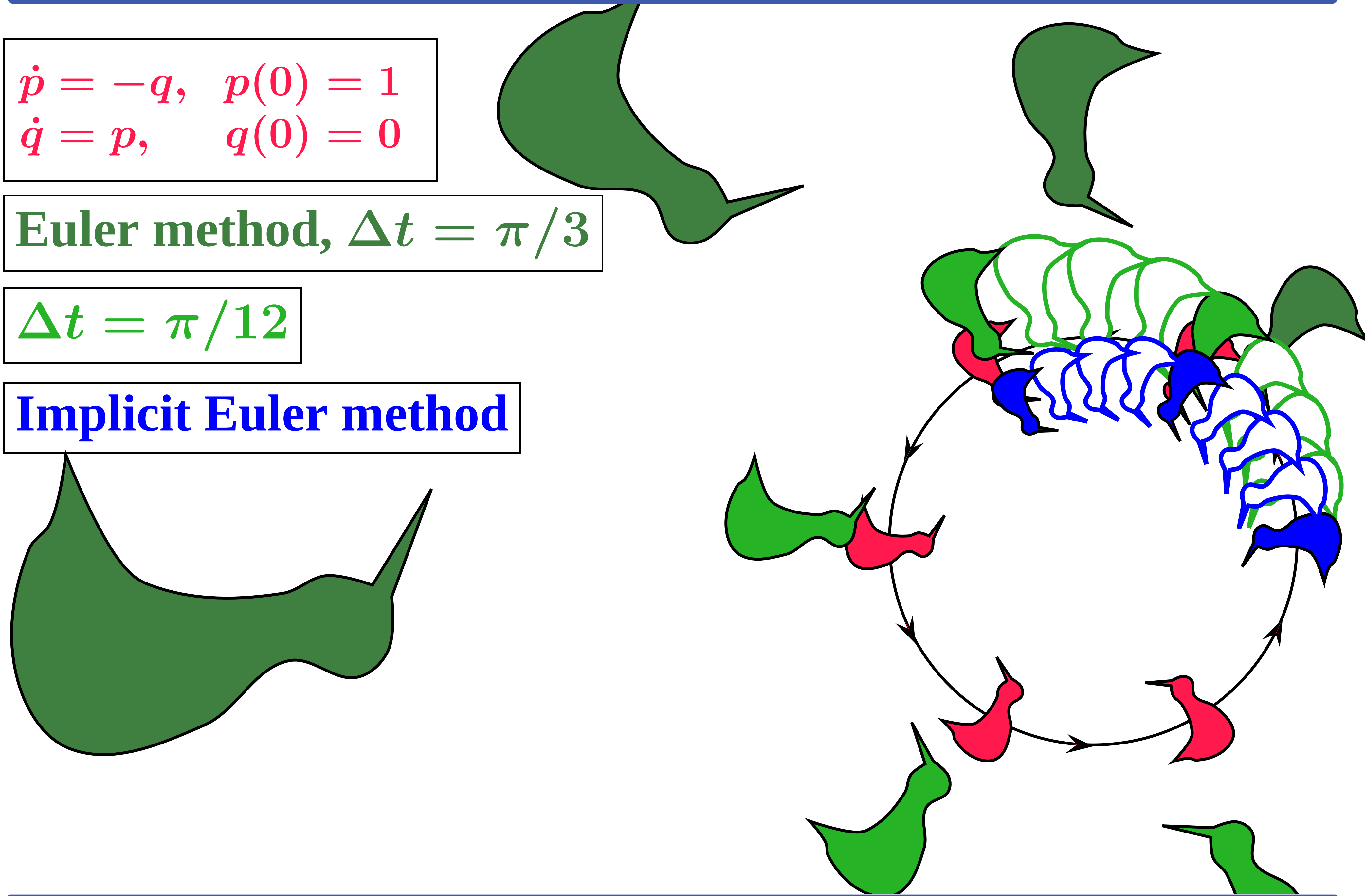

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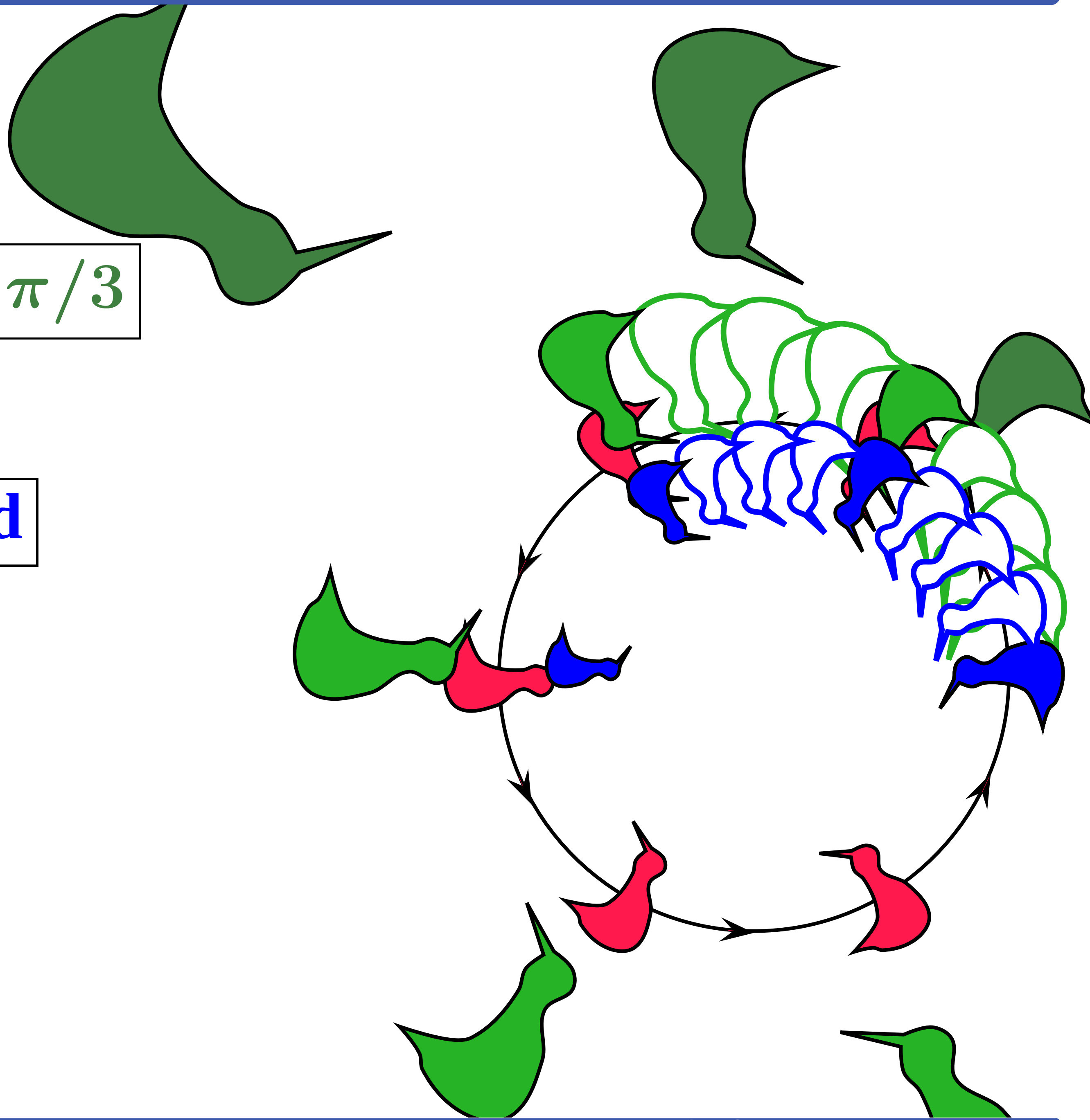

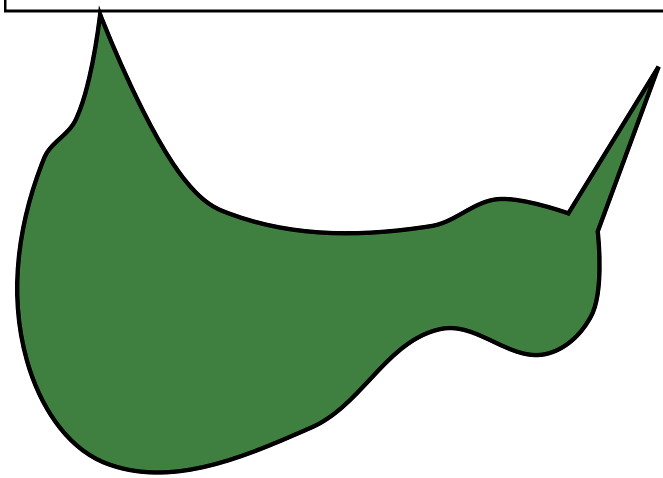

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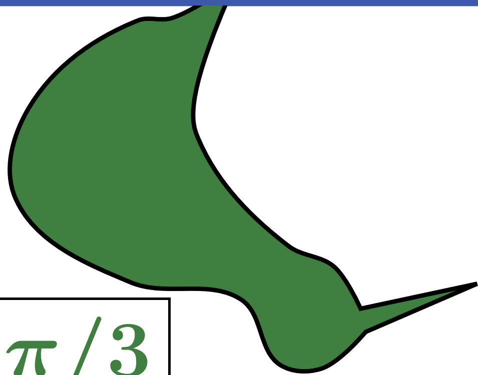

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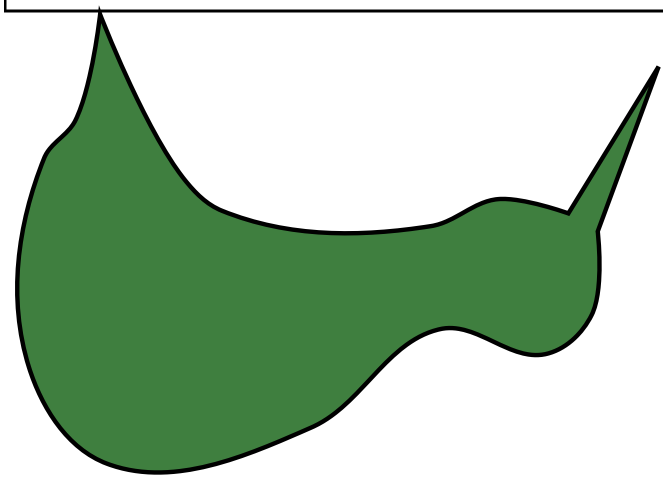

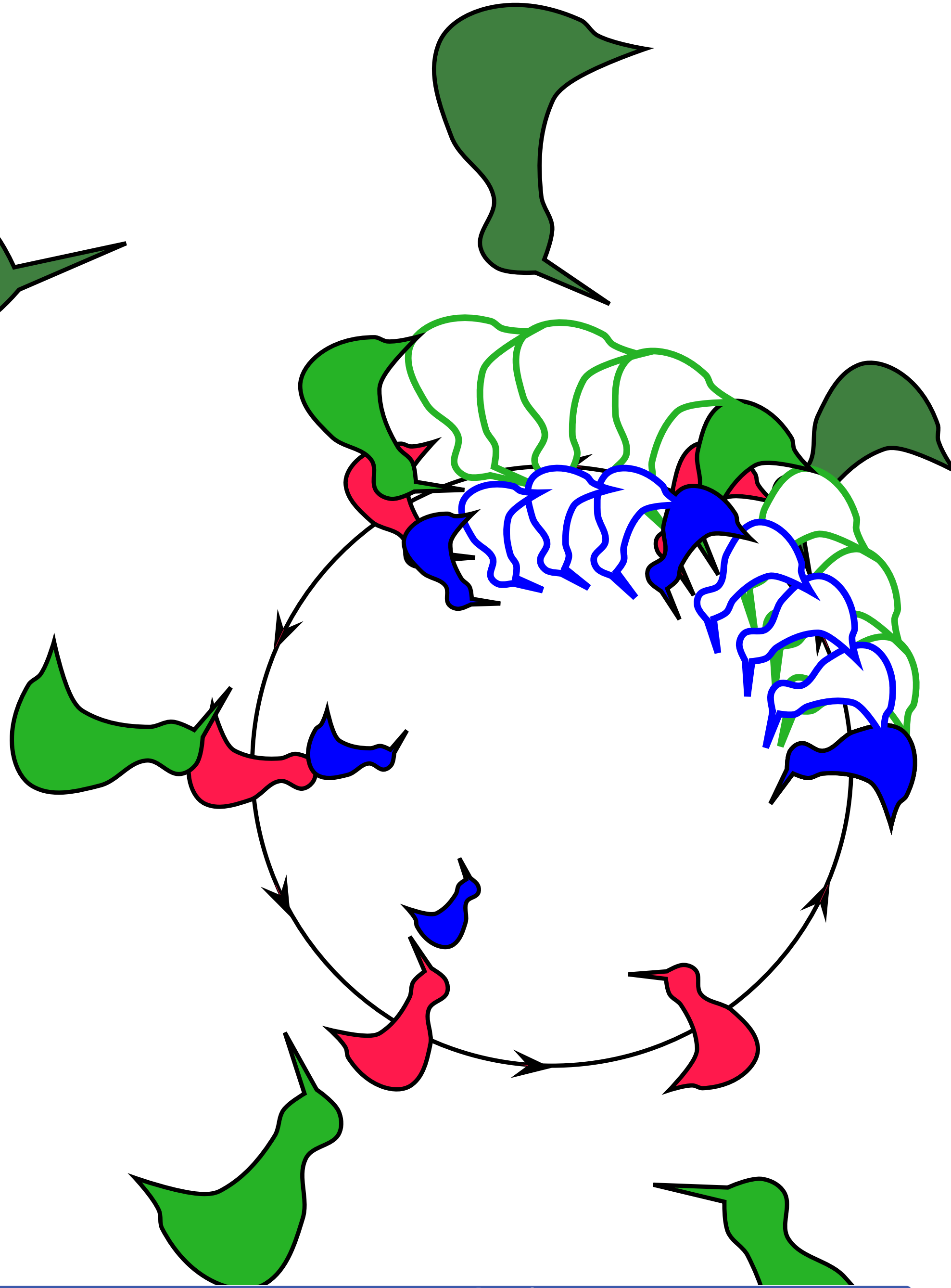

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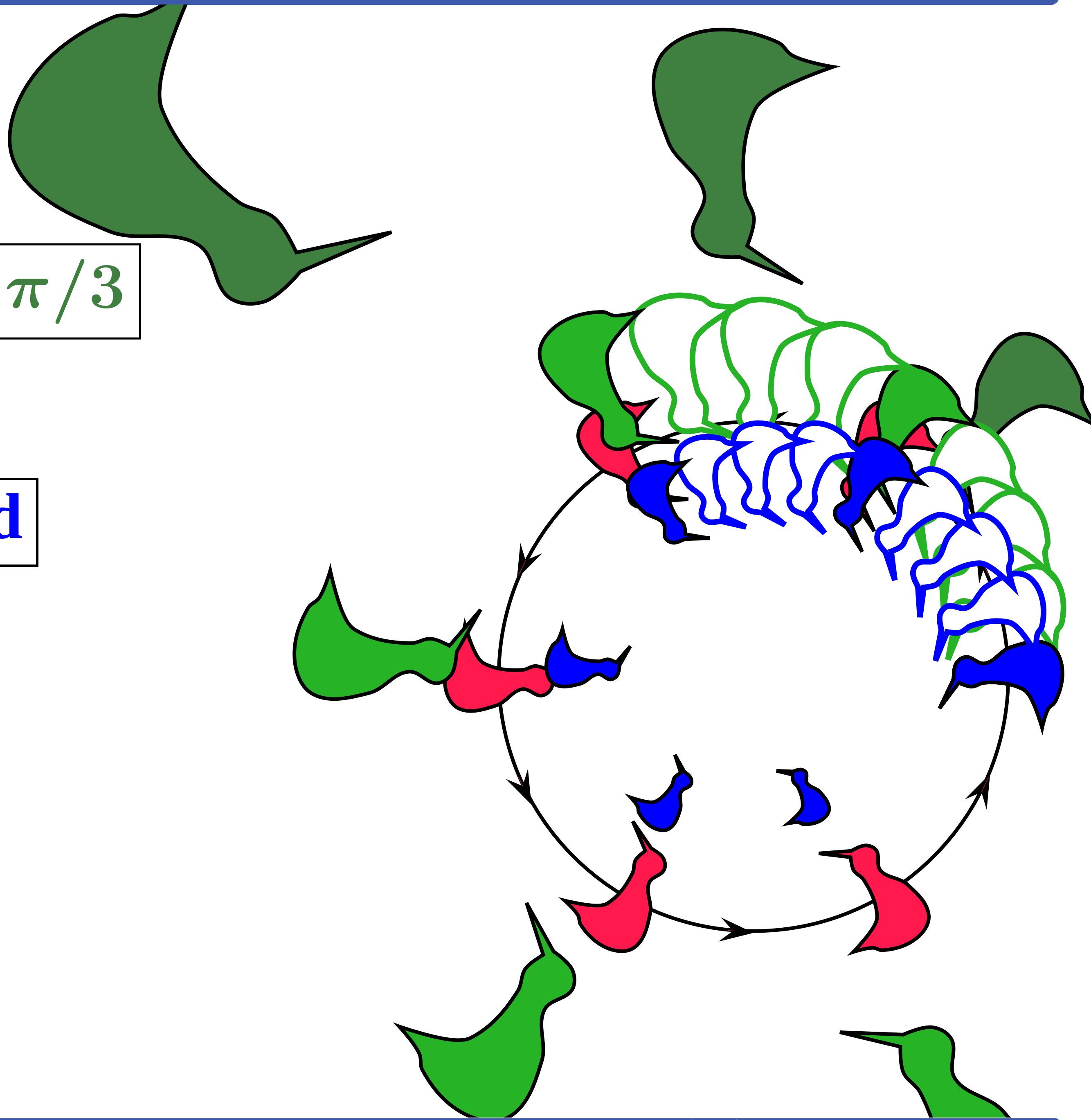

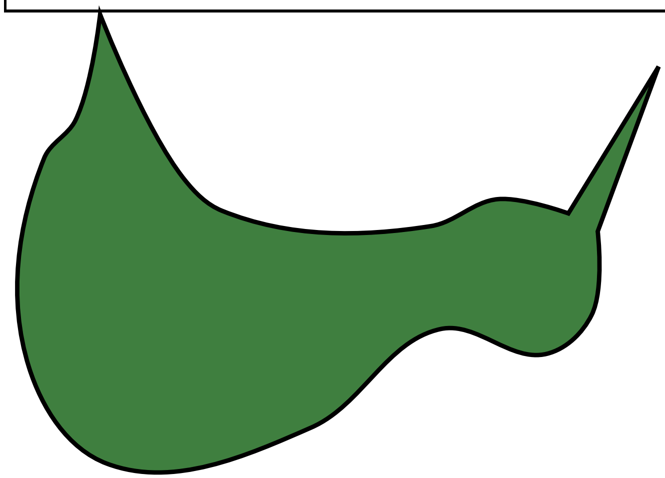

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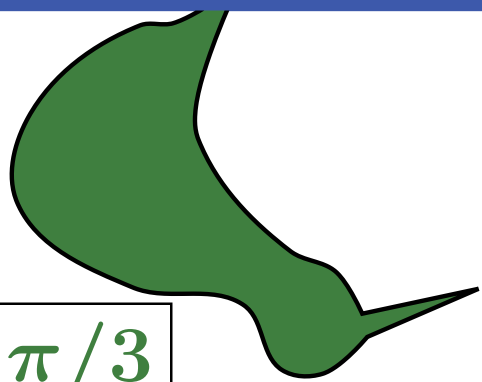

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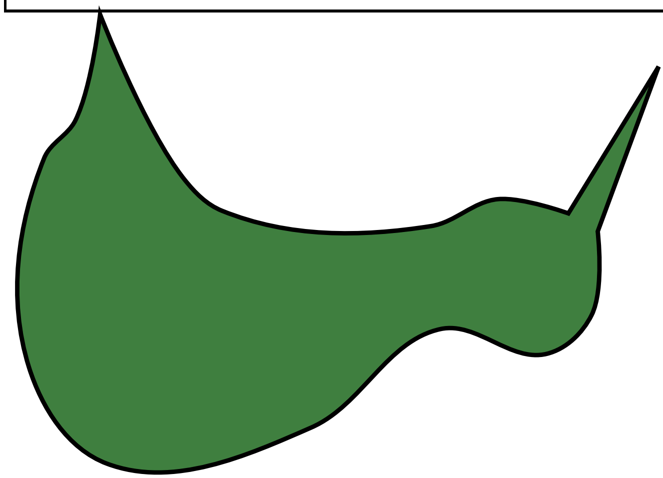

Hamiltonian problems

The differential equation in these computations is an example of a system of the form, based on a "Hamiltonian" $H(p, q)$:

$$\dot{p} = -\frac{\partial H}{\partial q}, \quad \dot{q} = \frac{\partial H}{\partial p}.$$

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One property of an equation of this form is that $H(p(t), q(t))$ is invariant, because

$$\dot{H} = \frac{\partial H}{\partial q}\dot{q} + \frac{\partial H}{\partial p}\dot{p} = \frac{\partial H}{\partial q}\frac{\partial H}{\partial p} - \frac{\partial H}{\partial p}\frac{\partial H}{\partial q} = 0.$$

Symplectic property

Another conservation property possessed by Hamiltonian problems is the “symplectic property”.

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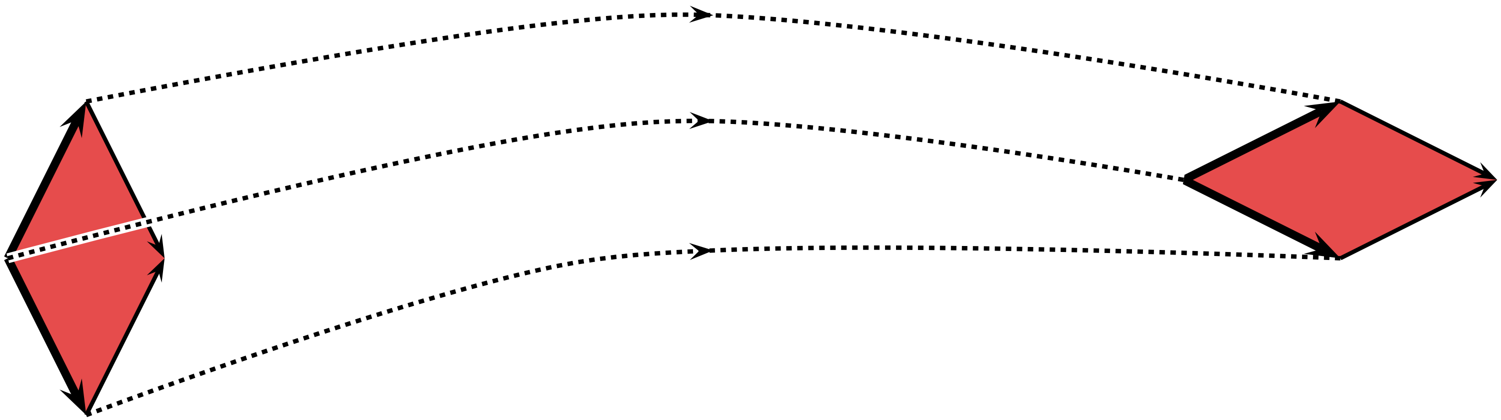
Consider two small vectors defining a parallelogram at time zero. At any later time t, the area of the corresponding parallelogram is unchanged.



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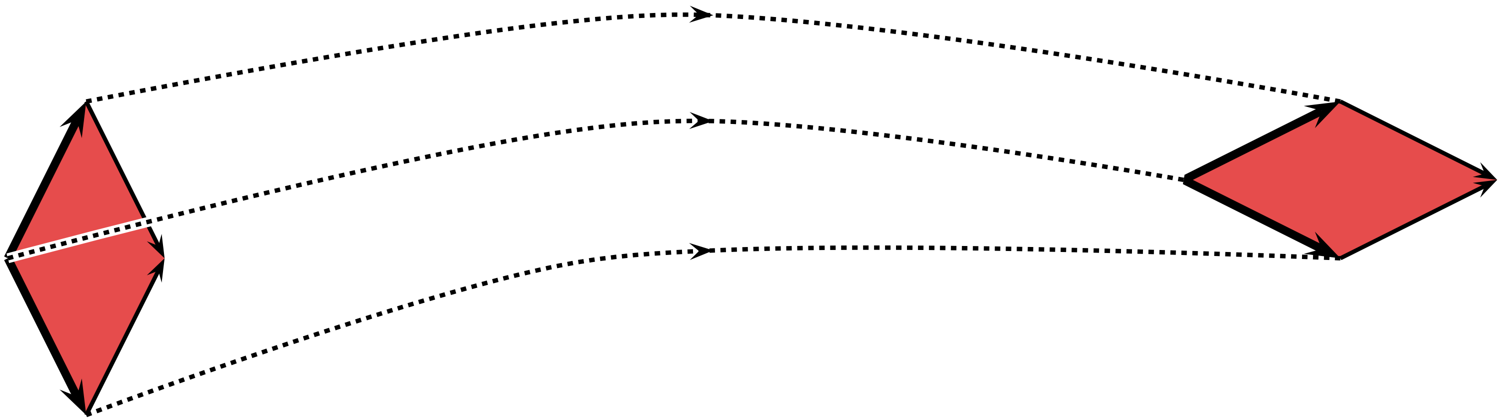

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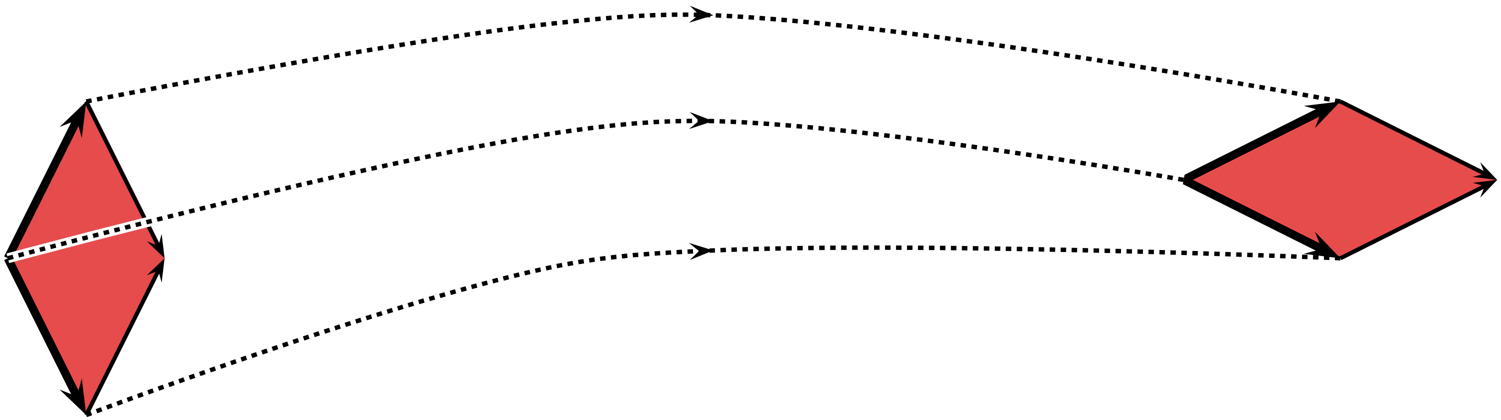

This means that the determinant of the 2×2 matrix formed from the two small vectors is conserved.

The reason for this hinges on a well-known fact.

Well-known fact 1 *Let X denote a matrix-valued function of t which satisfies the differential equation*

$$\dot{X}(t) = M(t)X(t),$$

and let $D(t) = \det(X(t))$.

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Proof. Let $\Xi(t)$ denote the adjoint matrix of $X(t)$ and write the columns of X as x_i and the rows of Ξ as ξ_i^T. We have

$$\begin{aligned}\dot{D} = \sum_{i=1}^{n} \xi_i^T \dot{x}_i &= \sum_{i=1}^{n} \xi_i^T M x_i \\ = \operatorname{tr}(\Xi M X) &= \operatorname{tr}(M X \Xi) \\ = \operatorname{tr}(M)D.\end{aligned}$$

Theorem 2 *Let* $X(t)$ *denote the matrix*

$$X(t) = \begin{bmatrix} dp_1(t) & dp_2(t) \\ dq_1(t) & dq_2(t) \end{bmatrix},$$

where $(p + dp_1, q + dq_1)$ *and* $(p + dp_2, q + dq_2)$ *are solutions to*

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Then $\det(X(t))$ *is constant.*

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Proof. Taking account of Well-Known Fact 1, we need only to prove that the trace of the Jacobian matrix is zero. The Jacobian matrix is

$$\begin{bmatrix} -\frac{\partial^2 H}{\partial p \partial q} & -\frac{\partial^2 H}{\partial q^2} \\ \frac{\partial^2 H}{\partial p^2} & \frac{\partial^2 H}{\partial q \partial p} \end{bmatrix},$$

which does indeed have zero trace.

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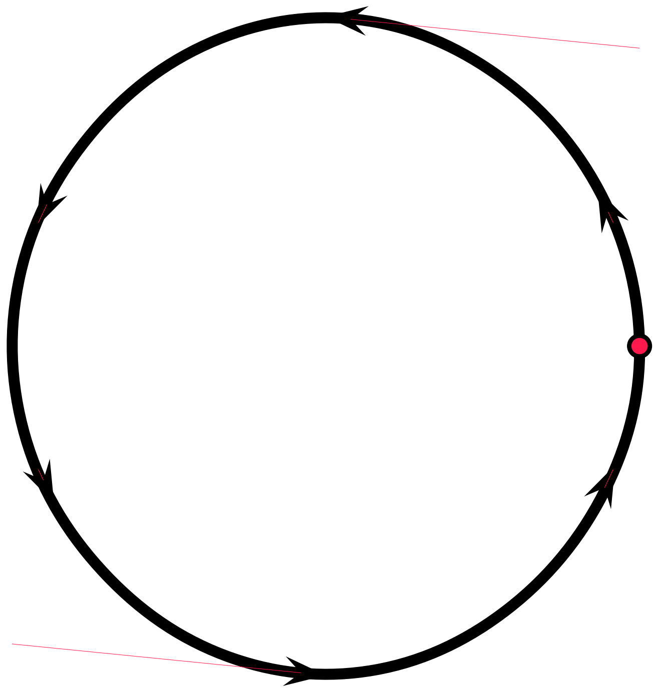

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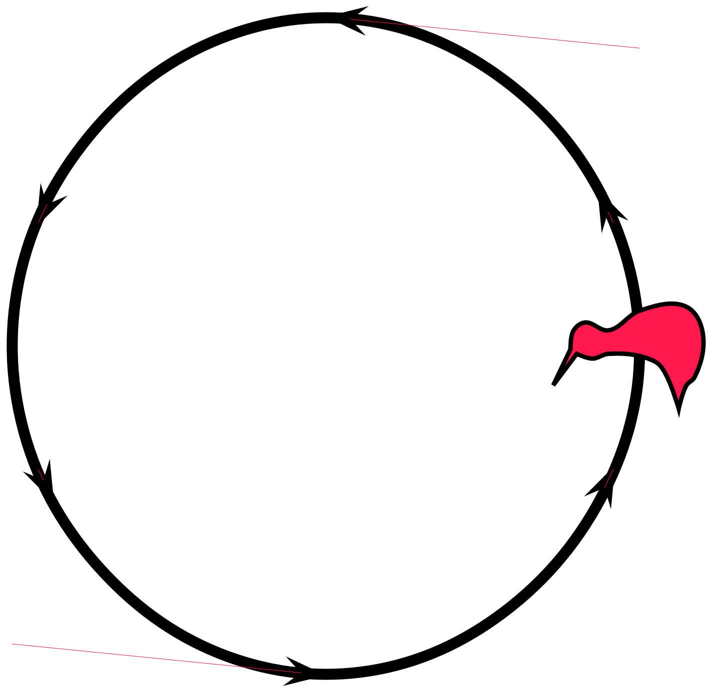

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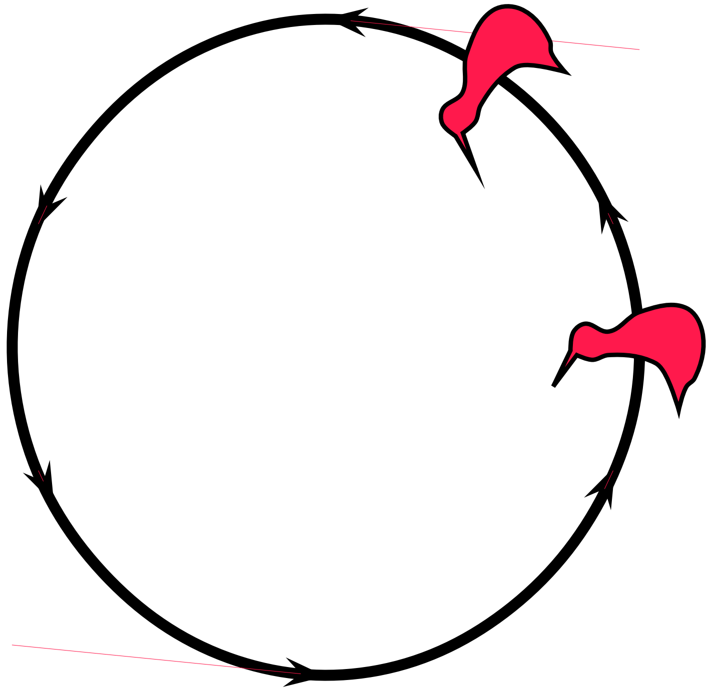

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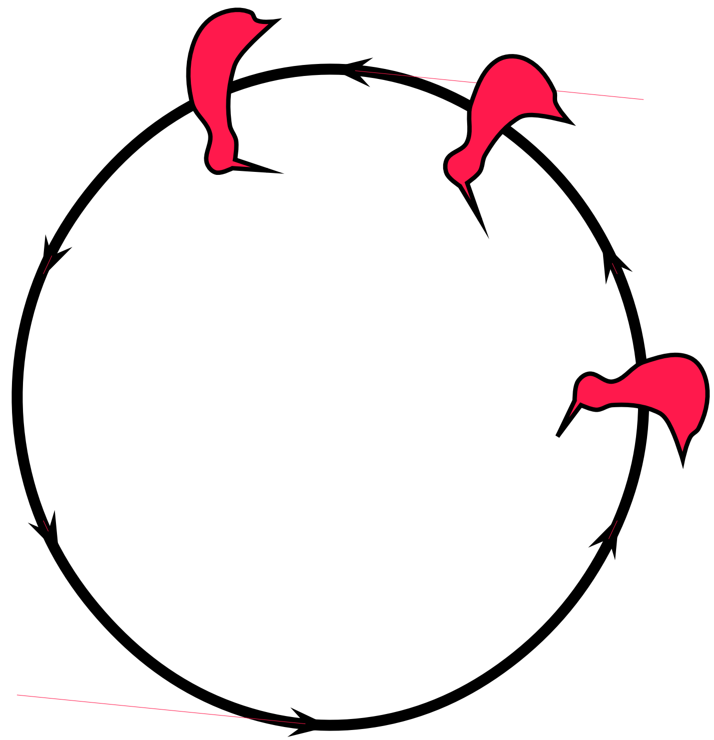

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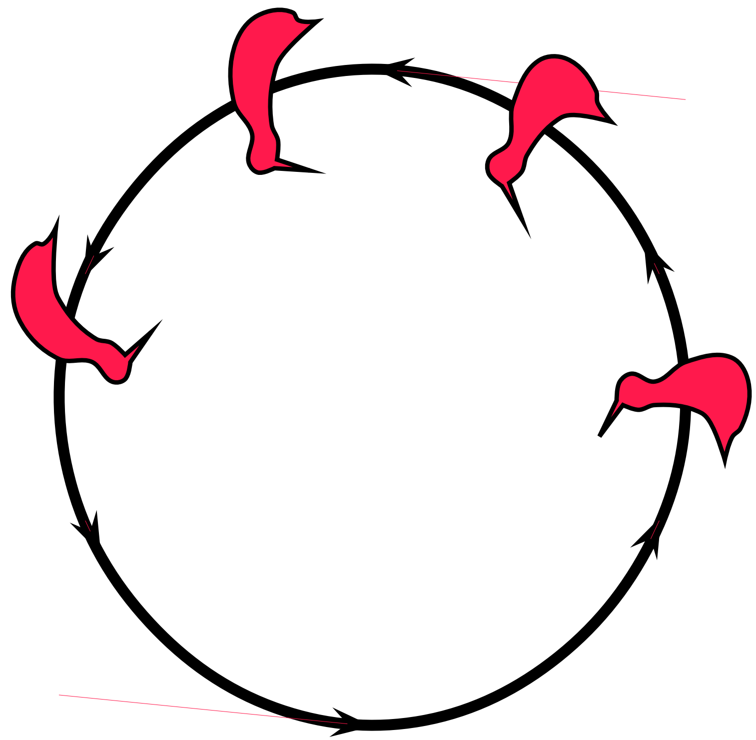

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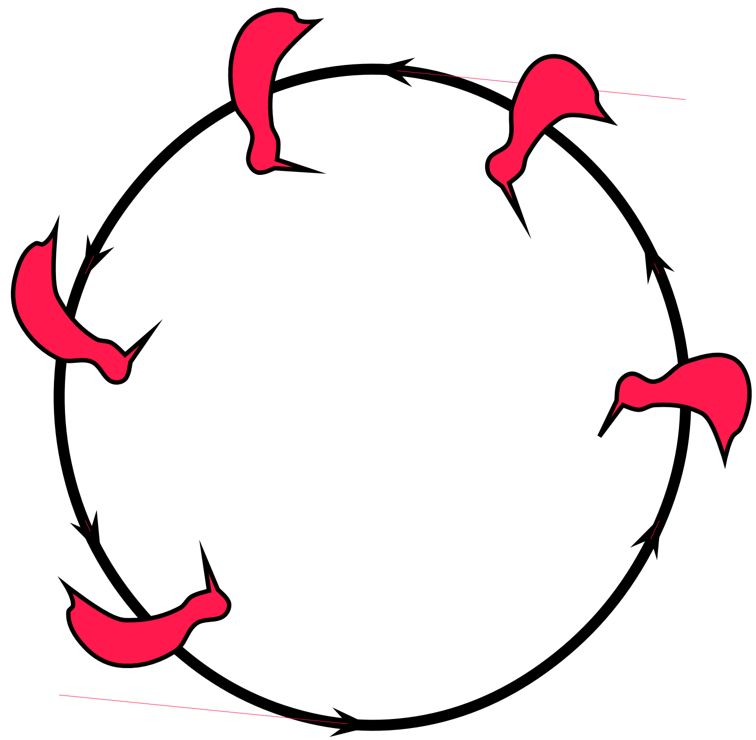

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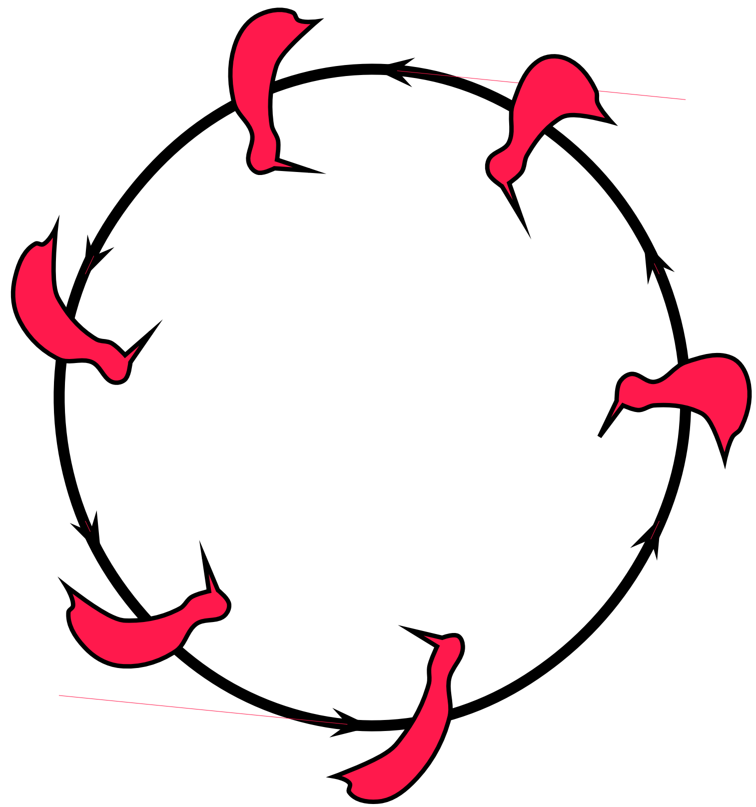

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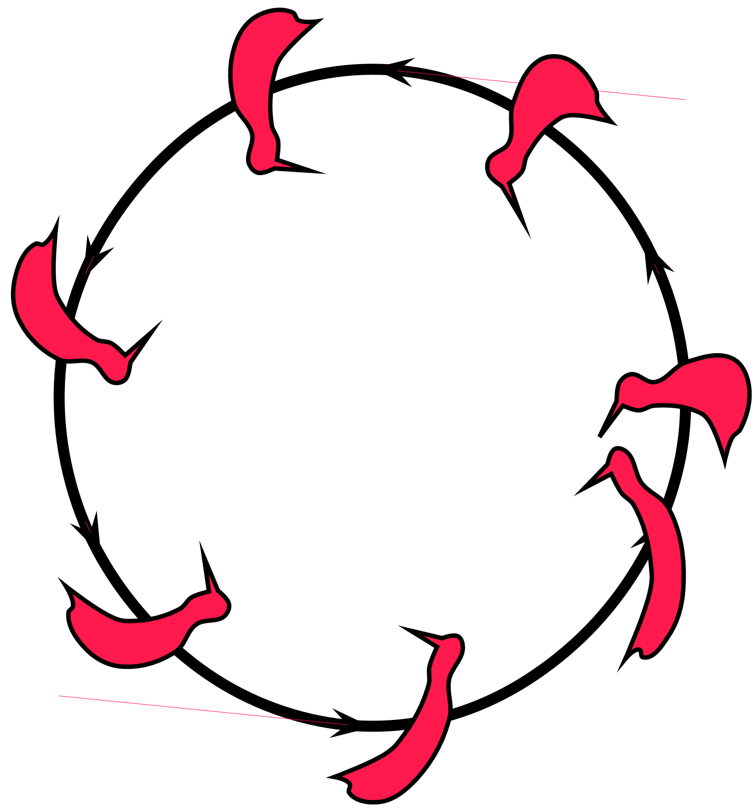

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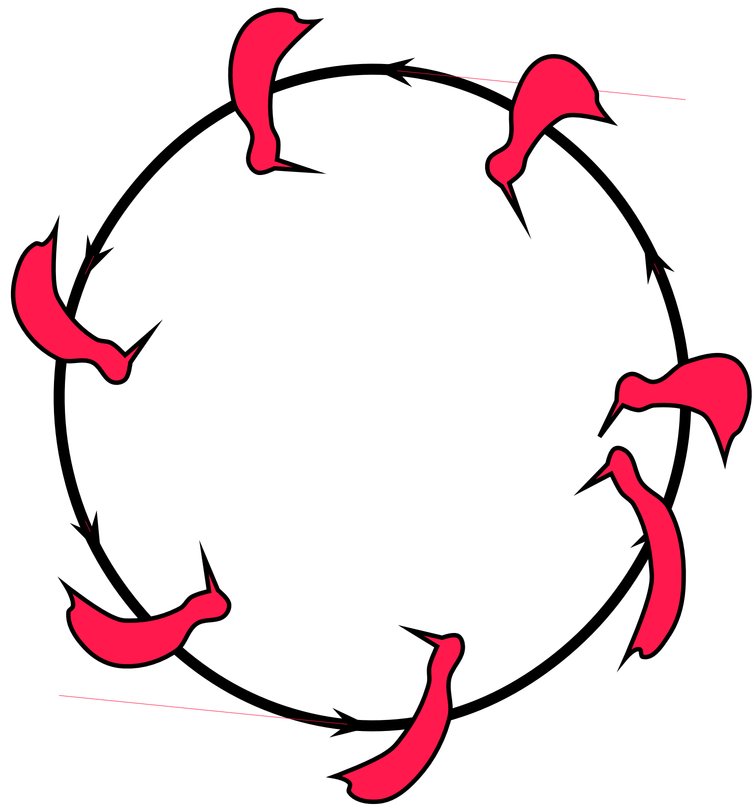
Gauss method

$$\begin{array}{c|cc} \frac{3-\sqrt{3}}{6} & \frac{3-2\sqrt{3}}{12} & \frac{1}{4} \\ \frac{3+\sqrt{3}}{6} & \frac{1}{4} & \frac{3+2\sqrt{3}}{12} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

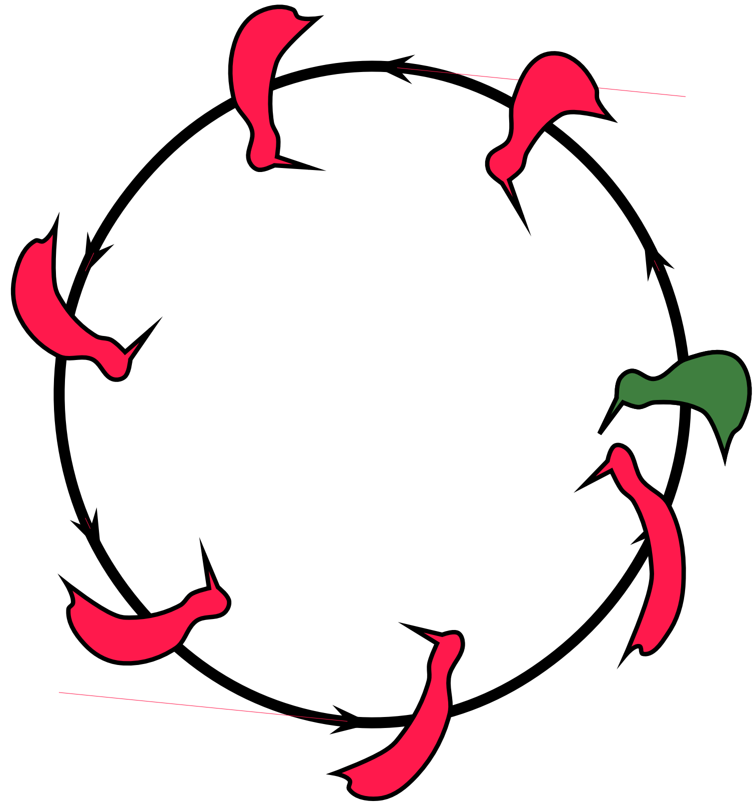


Experiments with some symplectic methods

$$\dot{p} = -\sin(q), \quad p(0) = 1$$
$$\dot{q} = p, \quad q(0) = 0$$

Gauss method

$\frac{3-\sqrt{3}}{6}$	$\frac{3-2\sqrt{3}}{12}$	$\frac{1}{4}$
$\frac{3+\sqrt{3}}{6}$	$\frac{1}{4}$	$\frac{3+2\sqrt{3}}{12}$
	$\frac{1}{2}$	$\frac{1}{2}$

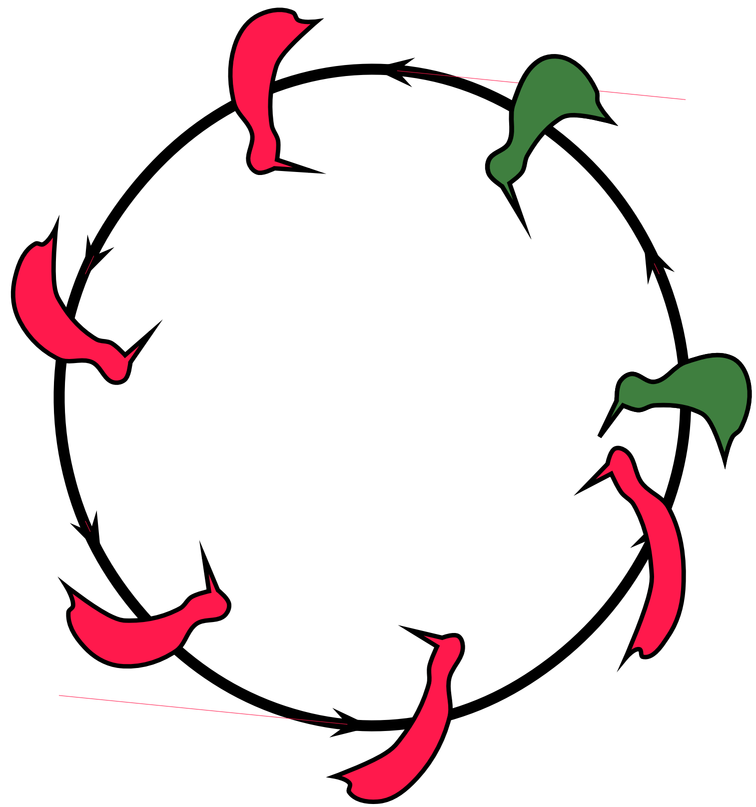


Experiments with some symplectic methods

$$\dot{p} = -\sin(q), \quad p(0) = 1$$
$$\dot{q} = p, \quad q(0) = 0$$

Gauss method

$$\begin{array}{c|cc} \frac{3-\sqrt{3}}{6} & \frac{3-2\sqrt{3}}{12} & \frac{1}{4} \\ \frac{3+\sqrt{3}}{6} & \frac{1}{4} & \frac{3+2\sqrt{3}}{12} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

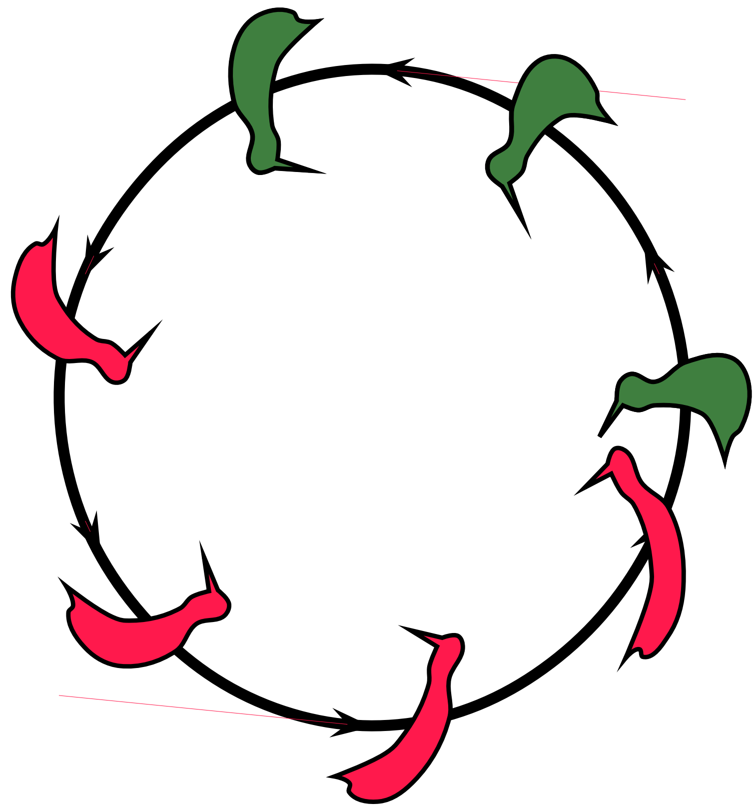


Experiments with some symplectic methods

$$\dot{p} = -\sin(q), \quad p(0) = 1$$
$$\dot{q} = p, \quad q(0) = 0$$

Gauss method

$$\begin{array}{c|cc} \frac{3-\sqrt{3}}{6} & \frac{3-2\sqrt{3}}{12} & \frac{1}{4} \\ \frac{3+\sqrt{3}}{6} & \frac{1}{4} & \frac{3+2\sqrt{3}}{12} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

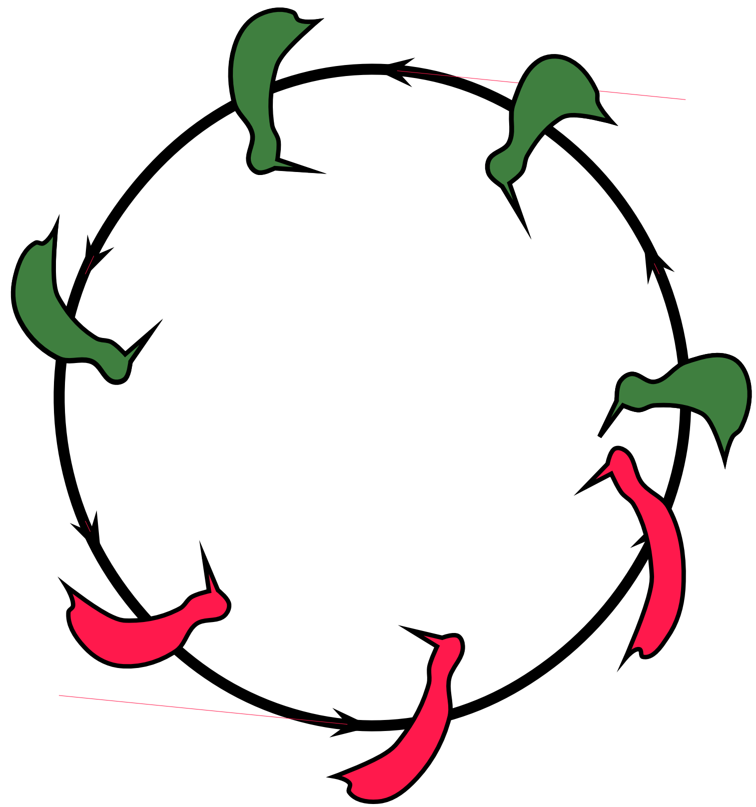


Experiments with some symplectic methods

$$\dot p = -\sin(q), \quad p(0) = 1$$
$$\dot q = p, \quad q(0) = 0$$

Gauss method

$\frac{3-\sqrt{3}}{6}$	$\frac{3-2\sqrt{3}}{12}$	$\frac{1}{4}$
$\frac{3+\sqrt{3}}{6}$	$\frac{1}{4}$	$\frac{3+2\sqrt{3}}{12}$
	$\frac{1}{2}$	$\frac{1}{2}$

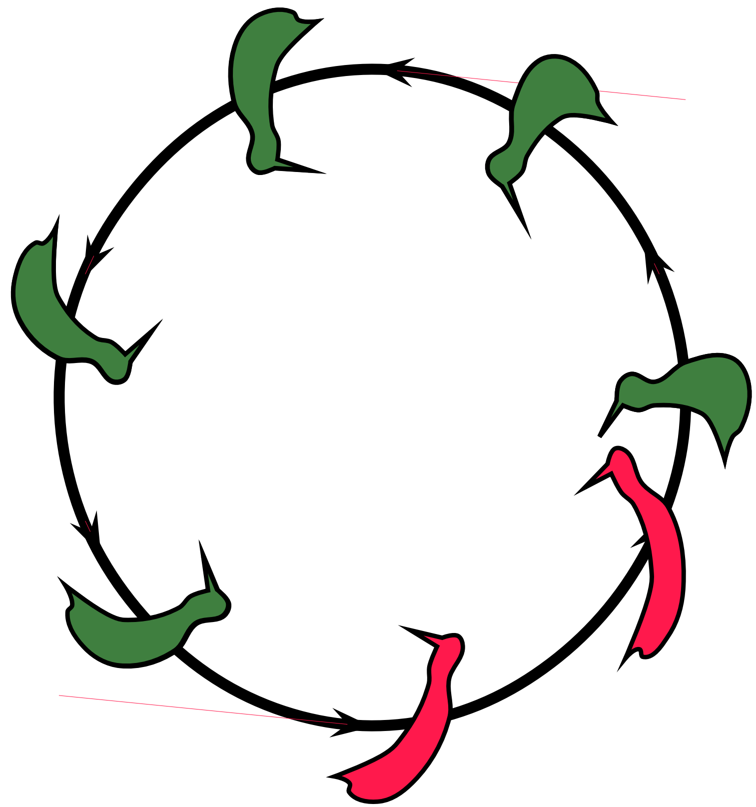


Experiments with some symplectic methods

$$\dot{p} = -\sin(q), \quad p(0) = 1$$
$$\dot{q} = p, \quad q(0) = 0$$

Gauss method

$$\begin{array}{c|cc} \frac{3-\sqrt{3}}{6} & \frac{3-2\sqrt{3}}{12} & \frac{1}{4} \\ \frac{3+\sqrt{3}}{6} & \frac{1}{4} & \frac{3+2\sqrt{3}}{12} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

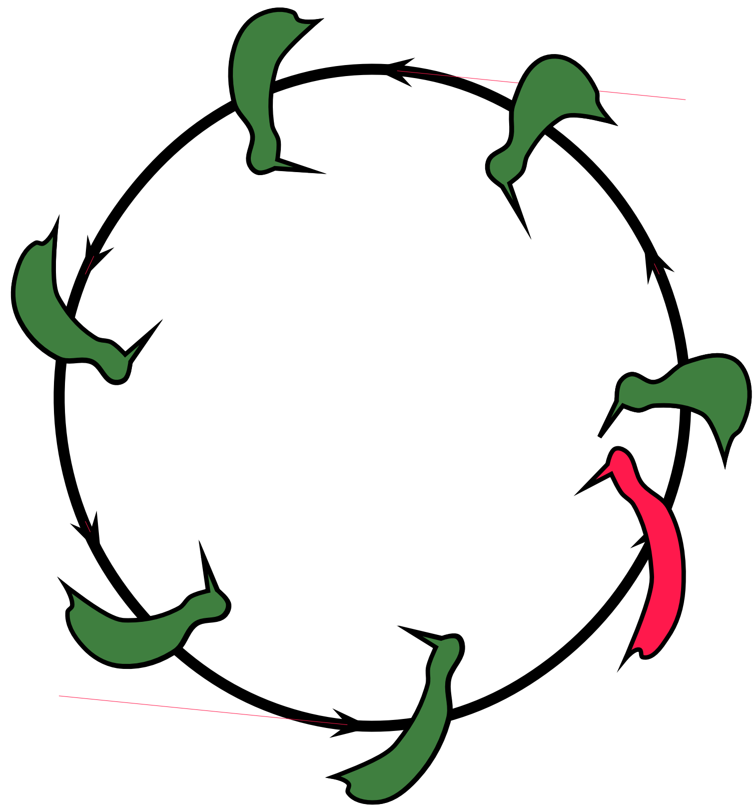


Experiments with some symplectic methods

$$\dot{p} = -\sin(q), \quad p(0) = 1$$
$$\dot{q} = p, \quad q(0) = 0$$

Gauss method

$$\begin{array}{c|cc} \frac{3-\sqrt{3}}{6} & \frac{3-2\sqrt{3}}{12} & \frac{1}{4} \\ \frac{3+\sqrt{3}}{6} & \frac{1}{4} & \frac{3+2\sqrt{3}}{12} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

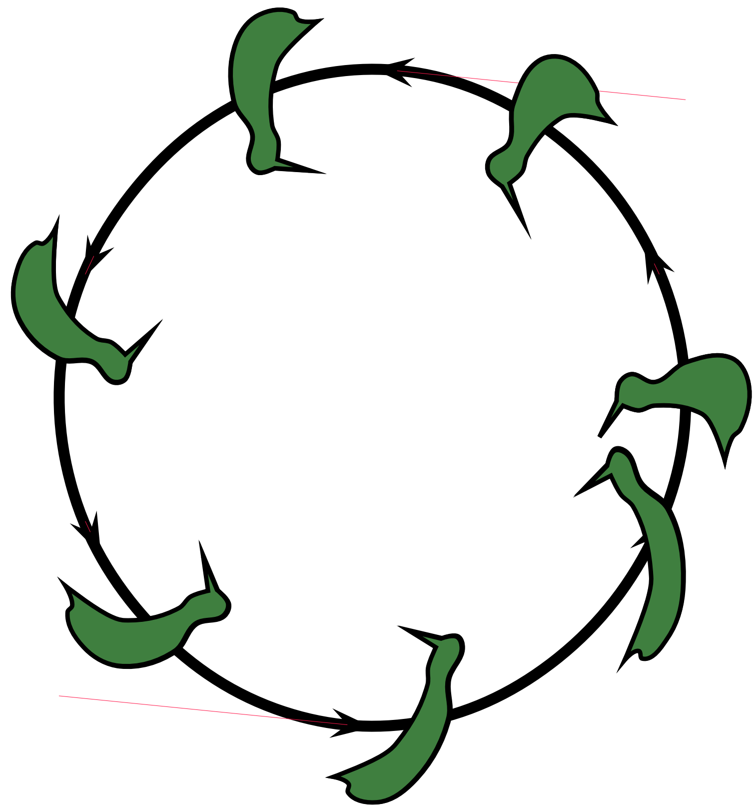


Experiments with some symplectic methods

$$\dot{p} = -\sin(q), \quad p(0) = 1$$
$$\dot{q} = p, \quad q(0) = 0$$

Gauss method

$\frac{3-\sqrt{3}}{6}$	$\frac{3-2\sqrt{3}}{12}$	$\frac{1}{4}$
$\frac{3+\sqrt{3}}{6}$	$\frac{1}{4}$	$\frac{3+2\sqrt{3}}{12}$
	$\frac{1}{2}$	$\frac{1}{2}$



Experiments with some symplectic methods

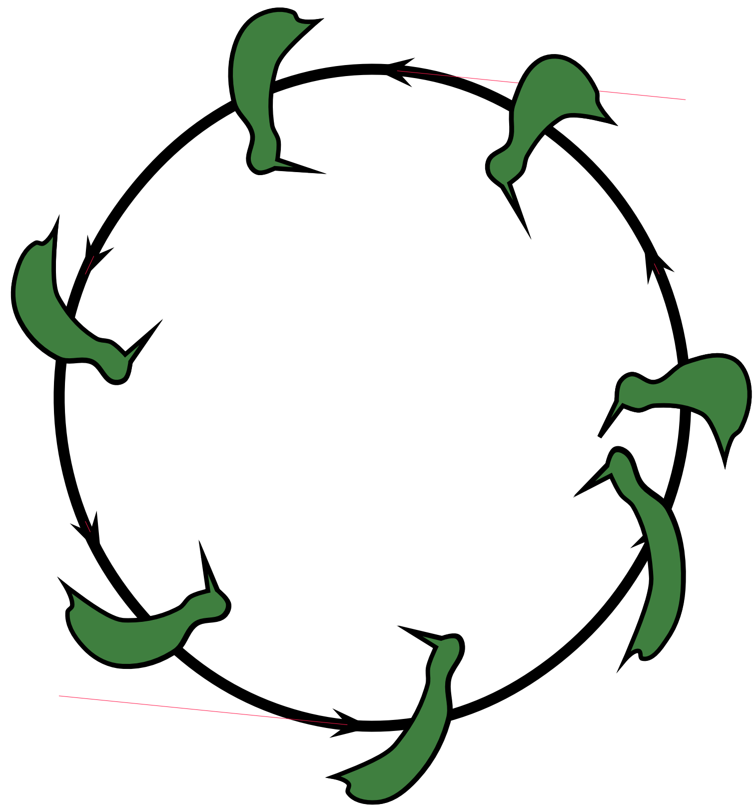
$$\dot{p} = -\sin(q), \quad p(0) = 1$$
$$\dot{q} = p, \quad q(0) = 0$$

Gauss method

$\frac{3-\sqrt{3}}{6}$	$\frac{3-2\sqrt{3}}{12}$	$\frac{1}{4}$
$\frac{3+\sqrt{3}}{6}$	$\frac{1}{4}$	$\frac{3+2\sqrt{3}}{12}$
	$\frac{1}{2}$	$\frac{1}{2}$

Mid-point rule

$\frac{1}{2}$	$\frac{1}{2}$
	1



Experiments with some symplectic methods

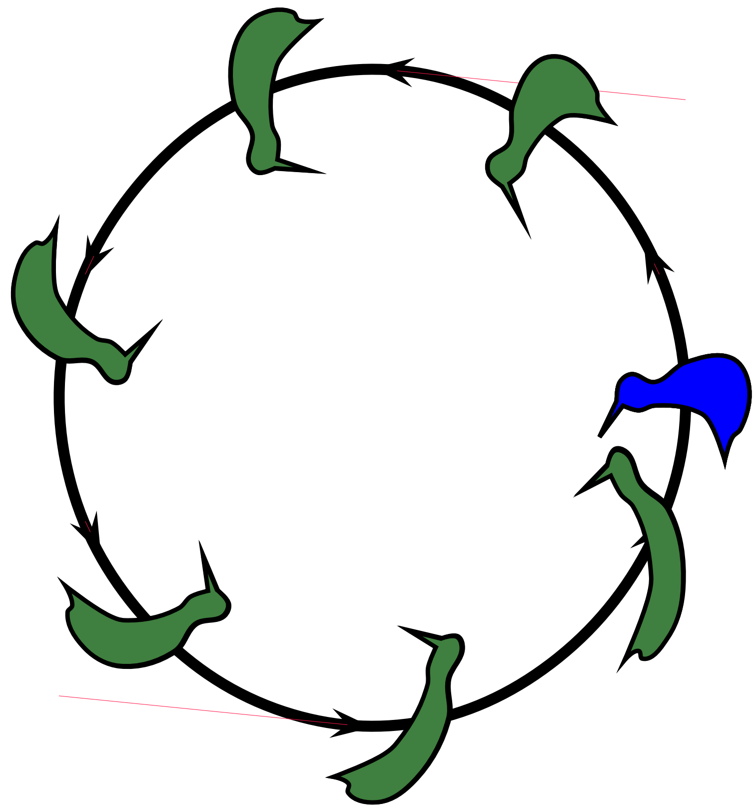
$$\dot{p} = -\sin(q), \quad p(0) = 1$$
$$\dot{q} = p, \quad q(0) = 0$$

Gauss method

$\frac{3-\sqrt{3}}{6}$	$\frac{3-2\sqrt{3}}{12}$	$\frac{1}{4}$
$\frac{3+\sqrt{3}}{6}$	$\frac{1}{4}$	$\frac{3+2\sqrt{3}}{12}$
	$\frac{1}{2}$	$\frac{1}{2}$

Mid-point rule

$\frac{1}{2}$	$\frac{1}{2}$
	1



Experiments with some symplectic methods

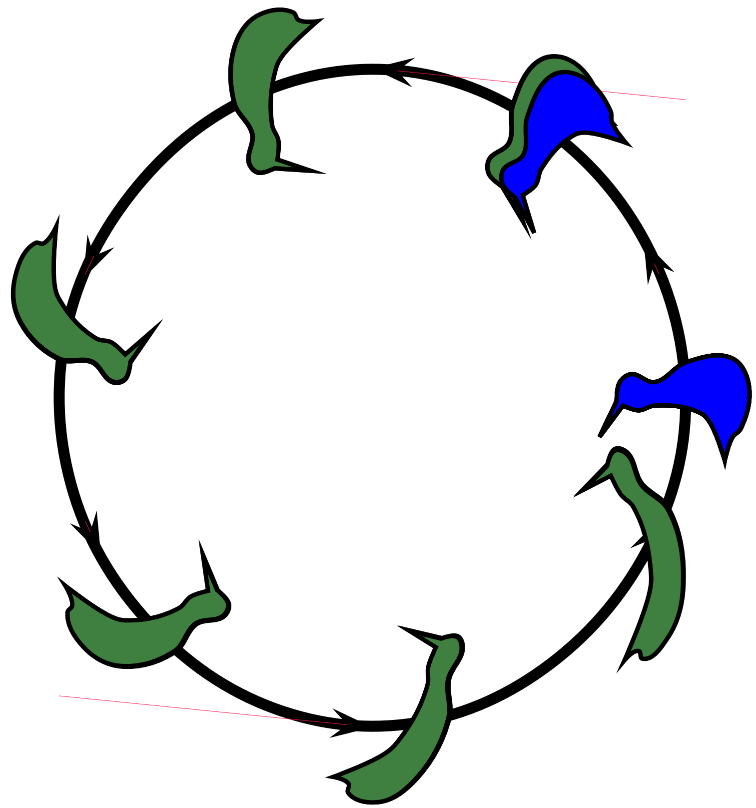
$$\dot{p} = -\sin(q), \quad p(0) = 1$$
$$\dot{q} = p, \quad q(0) = 0$$

Gauss method

$\frac{3-\sqrt{3}}{6}$	$\frac{3-2\sqrt{3}}{12}$	$\frac{1}{4}$
$\frac{3+\sqrt{3}}{6}$	$\frac{1}{4}$	$\frac{3+2\sqrt{3}}{12}$
	$\frac{1}{2}$	$\frac{1}{2}$

Mid-point rule

$\frac{1}{2}$	$\frac{1}{2}$
	1



Experiments with some symplectic methods

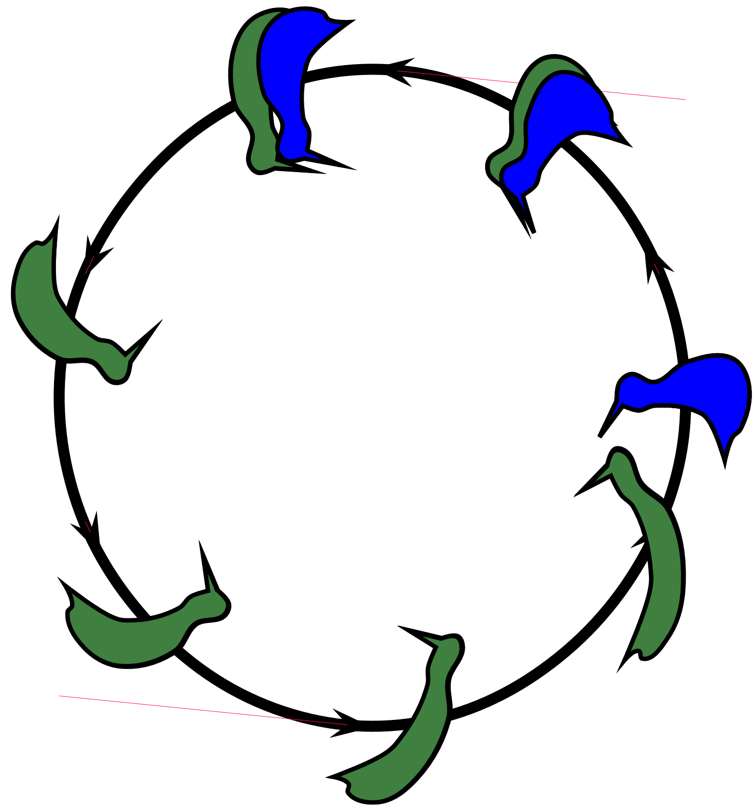
$$\dot{p} = -\sin(q), \quad p(0) = 1$$
$$\dot{q} = p, \quad q(0) = 0$$

Gauss method

$$\begin{array}{c|cc} \frac{3-\sqrt{3}}{6} & \frac{3-2\sqrt{3}}{12} & \frac{1}{4} \\ \frac{3+\sqrt{3}}{6} & \frac{1}{4} & \frac{3+2\sqrt{3}}{12} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

Mid-point rule

$$\begin{array}{c|c} \frac{1}{2} & \frac{1}{2} \\ \hline & 1 \end{array}$$



Experiments with some symplectic methods

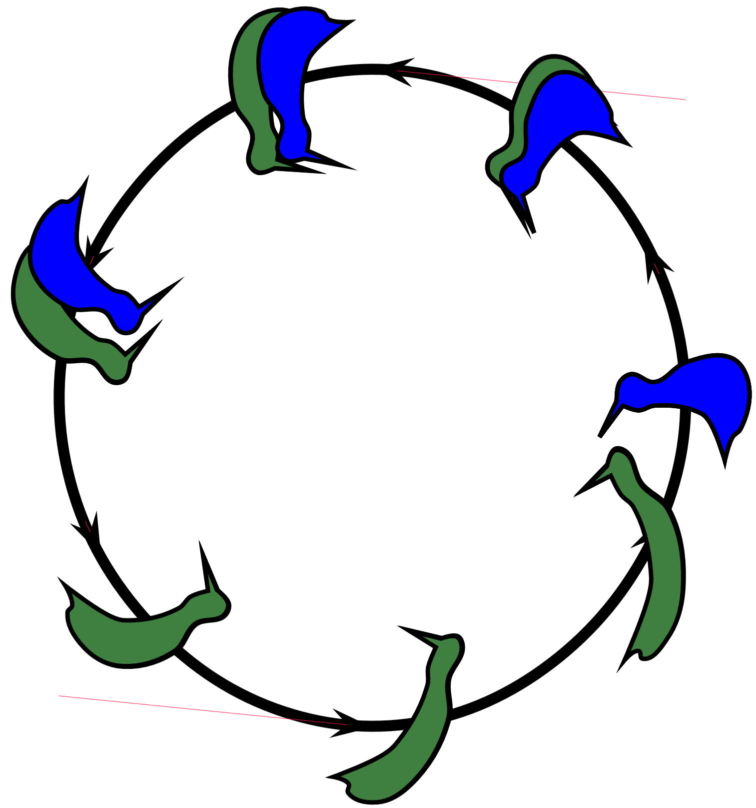
$$\dot{p} = -\sin(q), \quad p(0) = 1$$
$$\dot{q} = p, \quad q(0) = 0$$

Gauss method

$$\begin{array}{c|cc} \frac{3-\sqrt{3}}{6} & \frac{3-2\sqrt{3}}{12} & \frac{1}{4} \\ \frac{3+\sqrt{3}}{6} & \frac{1}{4} & \frac{3+2\sqrt{3}}{12} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

Mid-point rule

$$\begin{array}{c|c} \frac{1}{2} & \frac{1}{2} \\ \hline & 1 \end{array}$$



Experiments with some symplectic methods

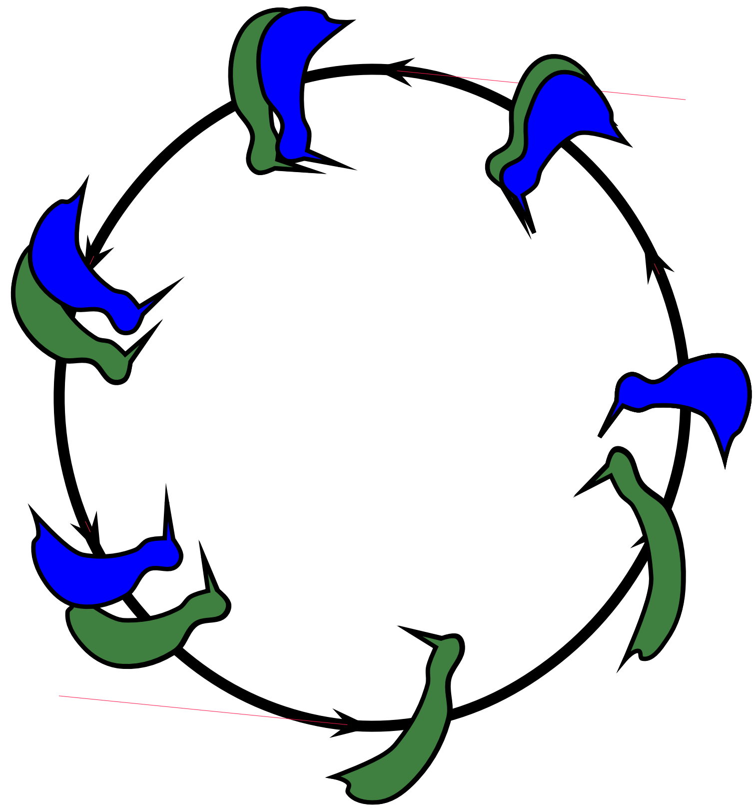
$$\dot{p} = -\sin(q), \quad p(0) = 1$$
$$\dot{q} = p, \quad q(0) = 0$$

Gauss method

$$\begin{array}{c|cc} \frac{3-\sqrt{3}}{6} & \frac{3-2\sqrt{3}}{12} & \frac{1}{4} \\ \frac{3+\sqrt{3}}{6} & \frac{1}{4} & \frac{3+2\sqrt{3}}{12} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

Mid-point rule

$$\begin{array}{c|c} \frac{1}{2} & \frac{1}{2} \\ \hline & 1 \end{array}$$



Experiments with some symplectic methods

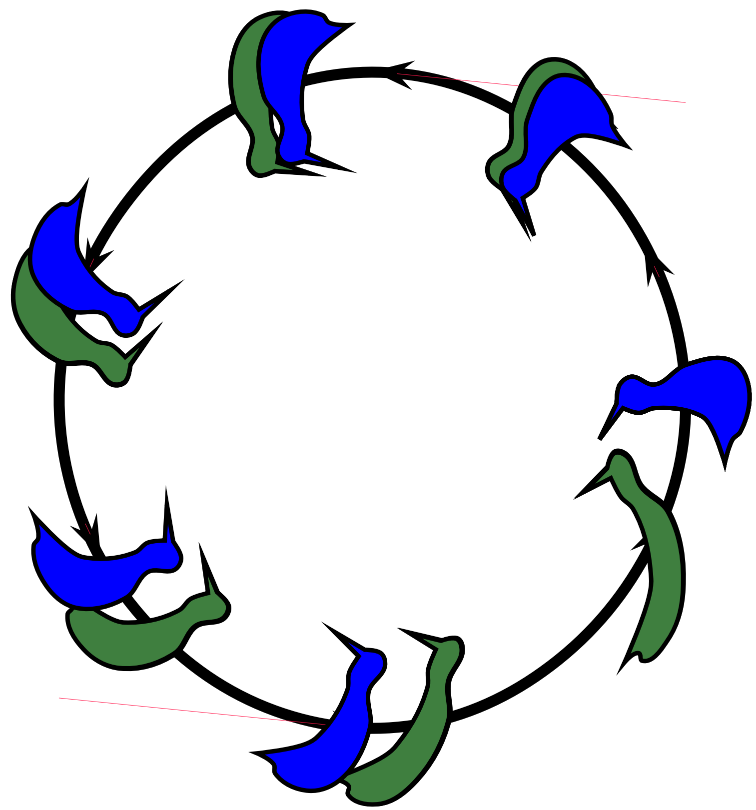
$$\dot{p} = -\sin(q), \quad p(0) = 1$$
$$\dot{q} = p, \quad q(0) = 0$$

Gauss method

$\frac{3-\sqrt{3}}{6}$	$\frac{3-2\sqrt{3}}{12}$	$\frac{1}{4}$
$\frac{3+\sqrt{3}}{6}$	$\frac{1}{4}$	$\frac{3+2\sqrt{3}}{12}$
	$\frac{1}{2}$	$\frac{1}{2}$

Mid-point rule

$\frac{1}{2}$	$\frac{1}{2}$
	1



Experiments with some symplectic methods

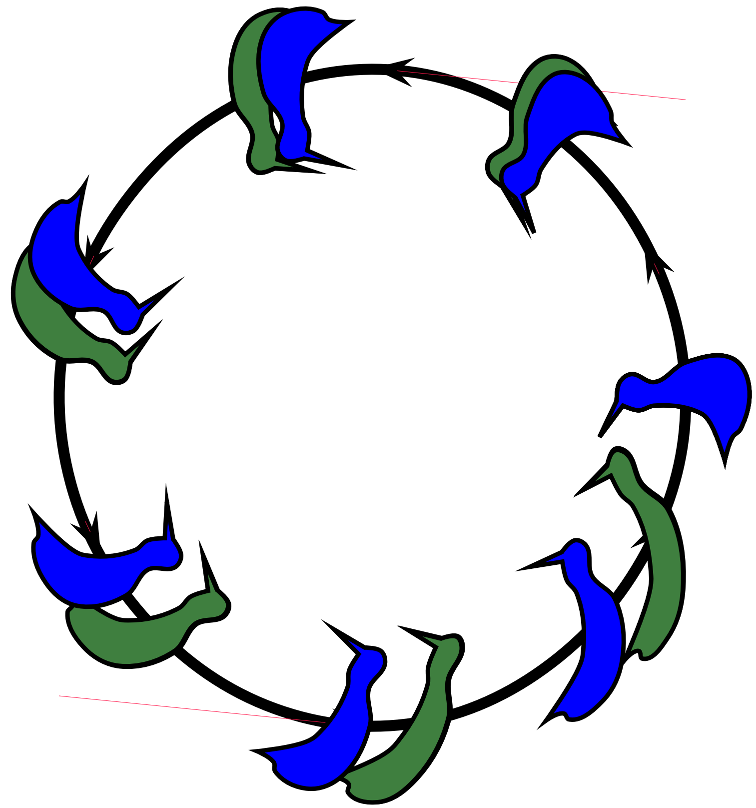
$$\dot{p} = -\sin(q), \quad p(0) = 1$$
$$\dot{q} = p, \quad q(0) = 0$$

Gauss method

$\frac{3-\sqrt{3}}{6}$	$\frac{3-2\sqrt{3}}{12}$	$\frac{1}{4}$
$\frac{3+\sqrt{3}}{6}$	$\frac{1}{4}$	$\frac{3+2\sqrt{3}}{12}$
	$\frac{1}{2}$	$\frac{1}{2}$

Mid-point rule

$\frac{1}{2}$	$\frac{1}{2}$
	1



Experiments with some symplectic methods

$$\begin{aligned} \dot p &= -\sin(q), & p(0) &= 1 \\ \dot q &= p, & q(0) &= 0 \end{aligned}$$

Gauss method

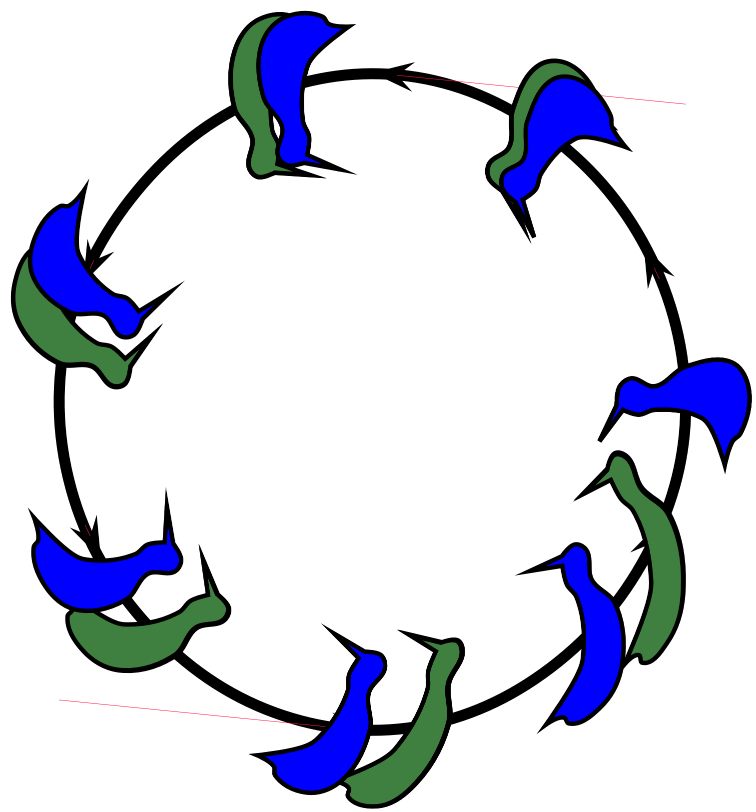
$$\begin{array}{c|cc} \frac{3-\sqrt{3}}{6} & \frac{3-2\sqrt{3}}{12} & \frac{1}{4} \\ \frac{3+\sqrt{3}}{6} & \frac{1}{4} & \frac{3+2\sqrt{3}}{12} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

Mid-point rule

$$\begin{array}{c|c} \frac{1}{2} & \frac{1}{2} \\ \hline & 1 \end{array}$$

General linear method

$$\left[\begin{array}{cc|cc} \frac{3+\sqrt{3}}{6} & 0 & 1 & \frac{-3-2\sqrt{3}}{3} \\ -\frac{\sqrt{3}}{3} & \frac{3+\sqrt{3}}{6} & 1 & \frac{3+2\sqrt{3}}{3} \\ \hline \frac{1}{2} & \frac{1}{2} & 1 & 0 \\ \frac{1}{2} & -\frac{1}{2} & 0 & -1 \end{array}\right]$$



Experiments with some symplectic methods

$$\dot p = -\sin(q),\quad p(0) = 1$$
$$\dot q = p,\quad q(0) = 0$$

Gauss method

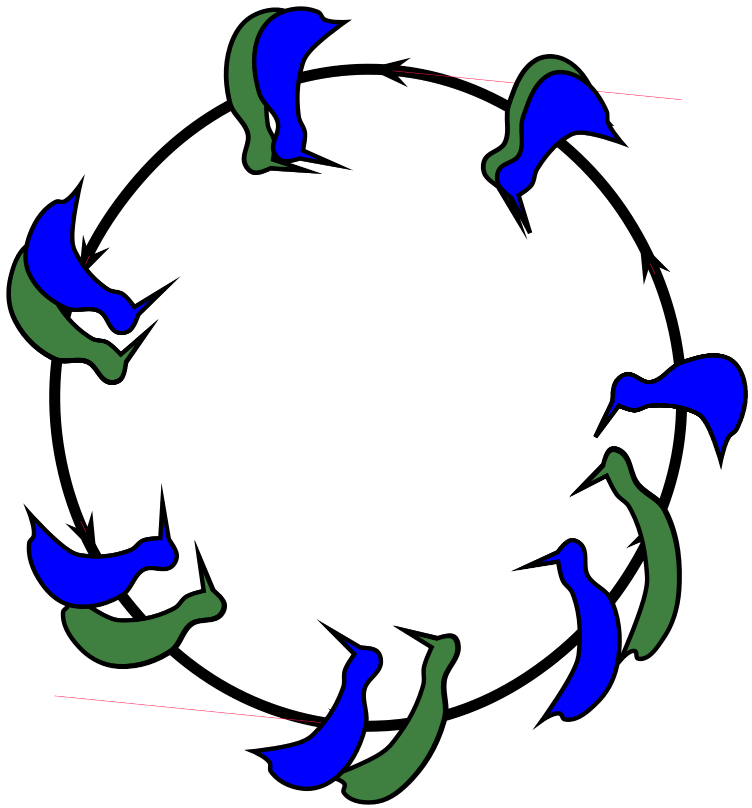
$$\begin{array}{c|cc} \frac{3-\sqrt3}{6} & \frac{3-2\sqrt3}{12} & \frac14 \\ \frac{3+\sqrt3}{6} & \frac14 & \frac{3+2\sqrt3}{12} \\ \hline & \frac12 & \frac12 \end{array}$$

Mid-point rule

$$\begin{array}{c|c} \frac12 & \frac12 \\ \hline & 1 \end{array}$$

General linear method

$$\left[\begin{array}{cc|cc} \frac{3+\sqrt3}{6} & 0 & 1 & \frac{-3-2\sqrt3}{3} \\ -\frac{\sqrt3}{3} & \frac{3+\sqrt3}{6} & 1 & \frac{3+2\sqrt3}{3} \\ \hline \frac12 & \frac12 & 1 & 0 \\ \frac12 & -\frac12 & 0 & -1 \end{array}\right]$$



This requires a starting method

Experiments with some symplectic methods

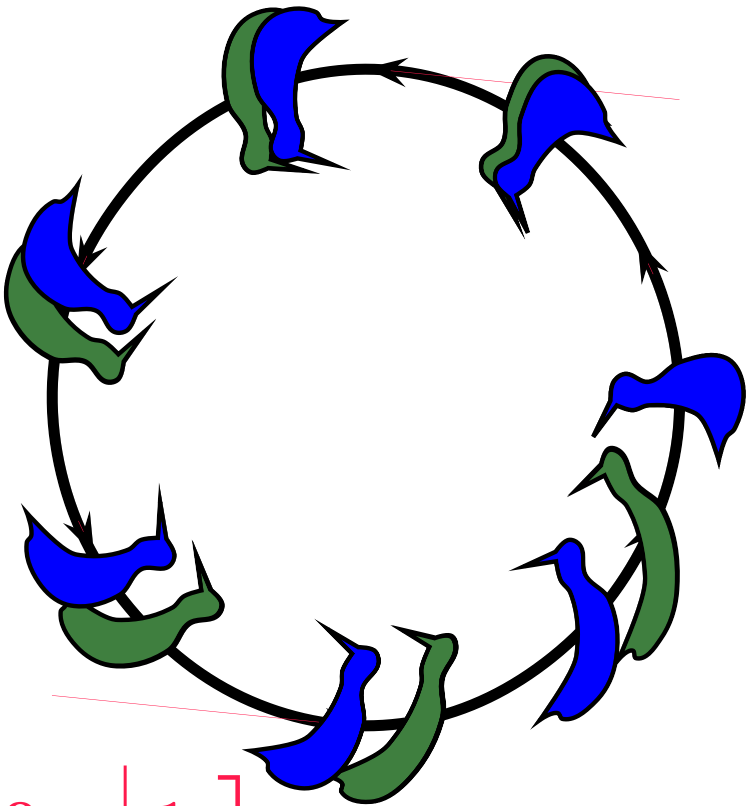
$$\dot{p} = -\sin(q), \quad p(0) = 1$$
$$\dot{q} = p, \quad q(0) = 0$$

Gauss method

$$\begin{array}{c|cc} \frac{3-\sqrt{3}}{6} & \frac{3-2\sqrt{3}}{12} & \frac{1}{4} \\ \frac{3+\sqrt{3}}{6} & \frac{1}{4} & \frac{3+2\sqrt{3}}{12} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

Mid-point rule

$$\begin{array}{c|c} \frac{1}{2} & \frac{1}{2} \\ \hline & 1 \end{array}$$



General linear method

$$\left[\begin{array}{cc|cc} \frac{3+\sqrt{3}}{6} & 0 & 1 & \frac{-3-2\sqrt{3}}{3} \\ -\frac{\sqrt{3}}{3} & \frac{3+\sqrt{3}}{6} & 1 & \frac{3+2\sqrt{3}}{3} \\ \hline \frac{1}{2} & \frac{1}{2} & 1 & 0 \\ \frac{1}{2} & -\frac{1}{2} & 0 & -1 \end{array}\right] \qquad \left[\begin{array}{cc|c} \frac{3+\sqrt{3}}{6} & 0 & 1 \\ -\frac{3+\sqrt{3}}{3} & \frac{3+\sqrt{3}}{6} & 1 \\ \hline 0 & 0 & 1 \\ \frac{\sqrt{3}-1}{8} & \frac{1-\sqrt{3}}{8} & 0 \end{array}\right]$$

Experiments with some symplectic methods

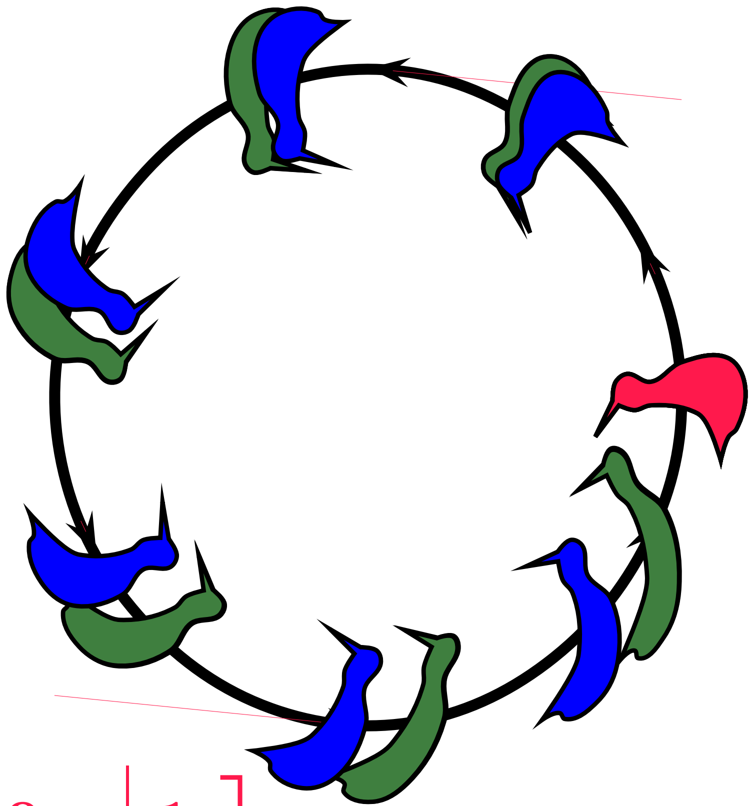
$$\dot{p} = -\sin(q), \quad p(0) = 1$$
$$\dot{q} = p, \quad q(0) = 0$$

Gauss method

$$\begin{array}{c|cc} \frac{3-\sqrt{3}}{6} & \frac{3-2\sqrt{3}}{12} & \frac{1}{4} \\ \frac{3+\sqrt{3}}{6} & \frac{1}{4} & \frac{3+2\sqrt{3}}{12} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

Mid-point rule

$$\begin{array}{c|c} \frac{1}{2} & \frac{1}{2} \\ \hline & 1 \end{array}$$

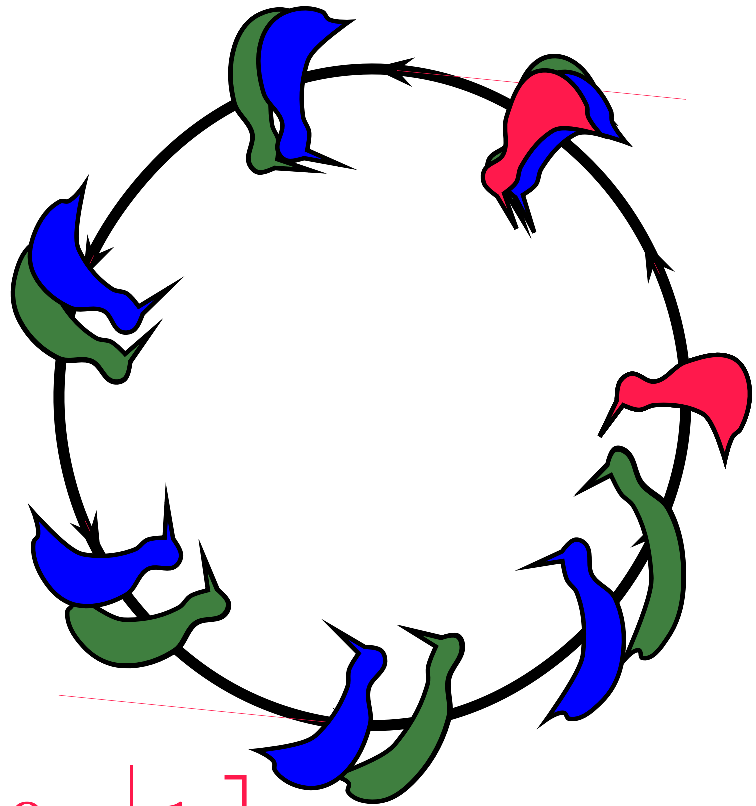


General linear method

$$\left[\begin{array}{cc|cc} \frac{3+\sqrt{3}}{6} & 0 & 1 & \frac{-3-2\sqrt{3}}{3} \\ -\frac{\sqrt{3}}{3} & \frac{3+\sqrt{3}}{6} & 1 & \frac{3+2\sqrt{3}}{3} \\ \hline \frac{1}{2} & \frac{1}{2} & 1 & 0 \\ \frac{1}{2} & -\frac{1}{2} & 0 & -1 \end{array}\right] \qquad \left[\begin{array}{cc|c} \frac{3+\sqrt{3}}{6} & 0 & 1 \\ -\frac{3+\sqrt{3}}{3} & \frac{3+\sqrt{3}}{6} & 1 \\ \hline 0 & 0 & 1 \\ \frac{\sqrt{3}-1}{8} & \frac{1-\sqrt{3}}{8} & 0 \end{array}\right]$$

Experiments with some symplectic methods

$$\dot p = -\sin(q), \quad p(0) = 1$$
$$\dot q = p, \quad q(0) = 0$$



Gauss method

$$\begin{array}{c|cc} \frac{3-\sqrt{3}}{6} & \frac{3-2\sqrt{3}}{12} & \frac{1}{4} \\ \frac{3+\sqrt{3}}{6} & \frac{1}{4} & \frac{3+2\sqrt{3}}{12} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

Mid-point rule

$$\begin{array}{c|c} \frac{1}{2} & \frac{1}{2} \\ \hline & 1 \end{array}$$

General linear method

$$\left[\begin{array}{cc|cc} \frac{3+\sqrt{3}}{6} & 0 & 1 & \frac{-3-2\sqrt{3}}{3} \\ -\frac{\sqrt{3}}{3} & \frac{3+\sqrt{3}}{6} & 1 & \frac{3+2\sqrt{3}}{3} \\ \hline \frac{1}{2} & \frac{1}{2} & 1 & 0 \\ \frac{1}{2} & -\frac{1}{2} & 0 & -1 \end{array}\right] \qquad \left[\begin{array}{cc|c} \frac{3+\sqrt{3}}{6} & 0 & 1 \\ -\frac{3+\sqrt{3}}{3} & \frac{3+\sqrt{3}}{6} & 1 \\ \hline 0 & 0 & 1 \\ \frac{\sqrt{3}-1}{8} & \frac{1-\sqrt{3}}{8} & 0 \end{array}\right]$$

Experiments with some symplectic methods

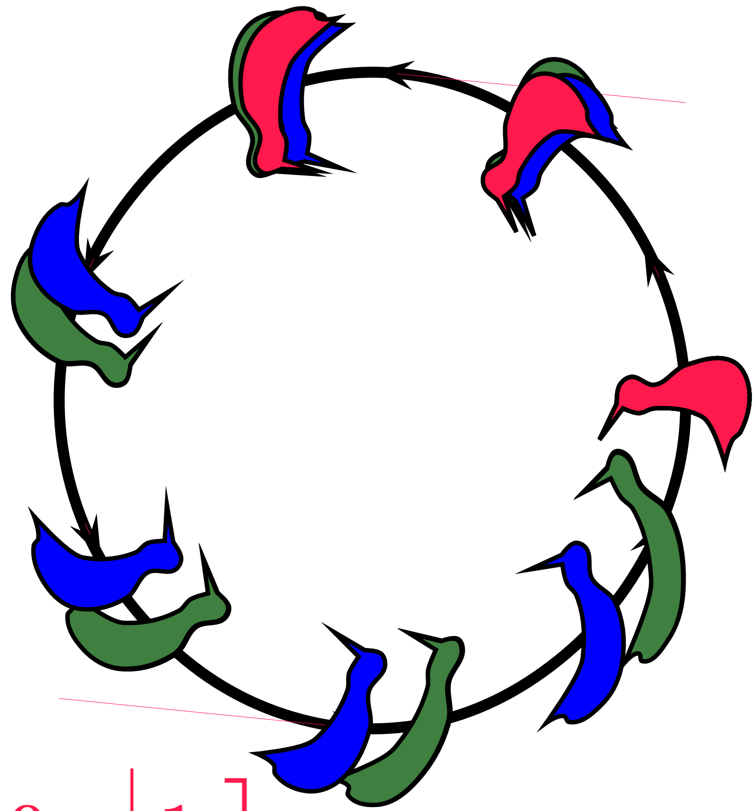
$$\begin{aligned} \dot{p} &= -\sin(q), & p(0) &= 1 \\ \dot{q} &= p, & q(0) &= 0 \end{aligned}$$

Gauss method

$$\begin{array}{c|cc} \frac{3-\sqrt{3}}{6} & \frac{3-2\sqrt{3}}{12} & \frac{1}{4} \\ \frac{3+\sqrt{3}}{6} & \frac{1}{4} & \frac{3+2\sqrt{3}}{12} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

Mid-point rule

$$\begin{array}{c|c} \frac{1}{2} & \frac{1}{2} \\ \hline & 1 \end{array}$$



General linear method

$$\left[\begin{array}{cc|cc} \frac{3+\sqrt{3}}{6} & 0 & 1 & \frac{-3-2\sqrt{3}}{3} \\ -\frac{\sqrt{3}}{3} & \frac{3+\sqrt{3}}{6} & 1 & \frac{3+2\sqrt{3}}{3} \\ \hline \frac{1}{2} & \frac{1}{2} & 1 & 0 \\ \frac{1}{2} & -\frac{1}{2} & 0 & -1 \end{array}\right] \qquad \left[\begin{array}{cc|c} \frac{3+\sqrt{3}}{6} & 0 & 1 \\ -\frac{3+\sqrt{3}}{3} & \frac{3+\sqrt{3}}{6} & 1 \\ \hline 0 & 0 & 1 \\ \frac{\sqrt{3}-1}{8} & \frac{1-\sqrt{3}}{8} & 0 \end{array}\right]$$

Experiments with some symplectic methods

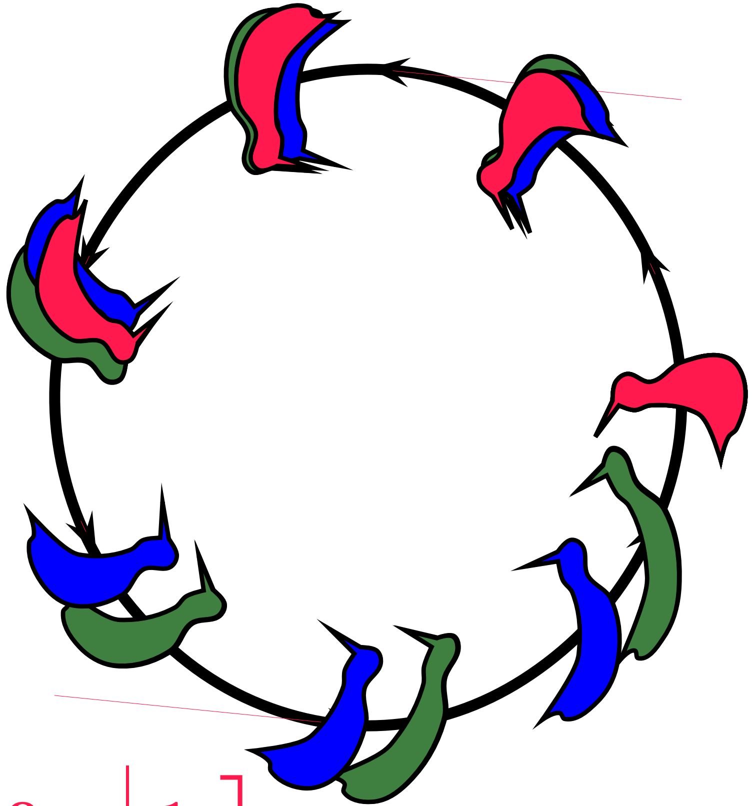
$$\begin{aligned} \dot{p} &= -\sin(q), & p(0) &= 1 \\ \dot{q} &= p, & q(0) &= 0 \end{aligned}$$

Gauss method

$$\begin{array}{c|cc} \frac{3-\sqrt{3}}{6} & \frac{3-2\sqrt{3}}{12} & \frac{1}{4} \\ \frac{3+\sqrt{3}}{6} & \frac{1}{4} & \frac{3+2\sqrt{3}}{12} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

Mid-point rule

$$\begin{array}{c|c} \frac{1}{2} & \frac{1}{2} \\ \hline & 1 \end{array}$$



General linear method

$$\left[\begin{array}{cc|cc} \frac{3+\sqrt{3}}{6} & 0 & 1 & \frac{-3-2\sqrt{3}}{3} \\ -\frac{\sqrt{3}}{3} & \frac{3+\sqrt{3}}{6} & 1 & \frac{3+2\sqrt{3}}{3} \\ \hline \frac{1}{2} & \frac{1}{2} & 1 & 0 \\ \frac{1}{2} & -\frac{1}{2} & 0 & -1 \end{array}\right] \qquad \left[\begin{array}{cc|c} \frac{3+\sqrt{3}}{6} & 0 & 1 \\ -\frac{3+\sqrt{3}}{3} & \frac{3+\sqrt{3}}{6} & 1 \\ \hline 0 & 0 & 1 \\ \frac{\sqrt{3}-1}{8} & \frac{1-\sqrt{3}}{8} & 0 \end{array}\right]$$

Experiments with some symplectic methods

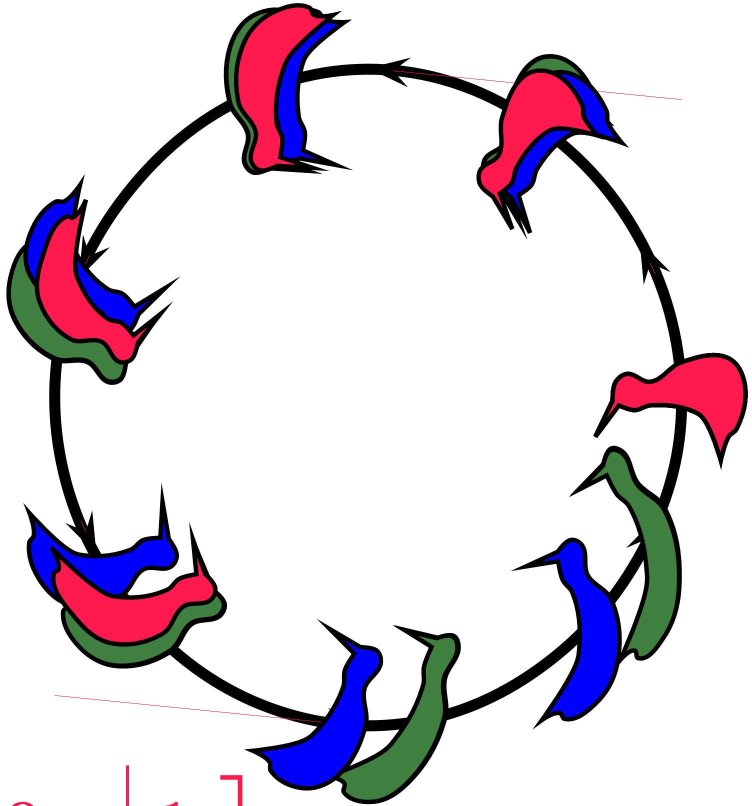
$$\begin{aligned} \dot p &= -\sin(q), & p(0) &= 1 \\ \dot q &= p, & q(0) &= 0 \end{aligned}$$

Gauss method

$$\begin{array}{c|cc} \frac{3-\sqrt{3}}{6} & \frac{3-2\sqrt{3}}{12} & \frac{1}{4} \\ \frac{3+\sqrt{3}}{6} & \frac{1}{4} & \frac{3+2\sqrt{3}}{12} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

Mid-point rule

$$\begin{array}{c|c} \frac{1}{2} & \frac{1}{2} \\ \hline & 1 \end{array}$$



General linear method

$$\left[\begin{array}{cc|cc} \frac{3+\sqrt{3}}{6} & 0 & 1 & \frac{-3-2\sqrt{3}}{3} \\ -\frac{\sqrt{3}}{3} & \frac{3+\sqrt{3}}{6} & 1 & \frac{3+2\sqrt{3}}{3} \\ \hline \frac{1}{2} & \frac{1}{2} & 1 & 0 \\ \frac{1}{2} & -\frac{1}{2} & 0 & -1 \end{array}\right] \qquad \left[\begin{array}{cc|c} \frac{3+\sqrt{3}}{6} & 0 & 1 \\ -\frac{3+\sqrt{3}}{3} & \frac{3+\sqrt{3}}{6} & 1 \\ \hline 0 & 0 & 1 \\ \frac{\sqrt{3}-1}{8} & \frac{1-\sqrt{3}}{8} & 0 \end{array}\right]$$

Experiments with some symplectic methods

$$\dot p = -\sin(q), \quad p(0) = 1$$
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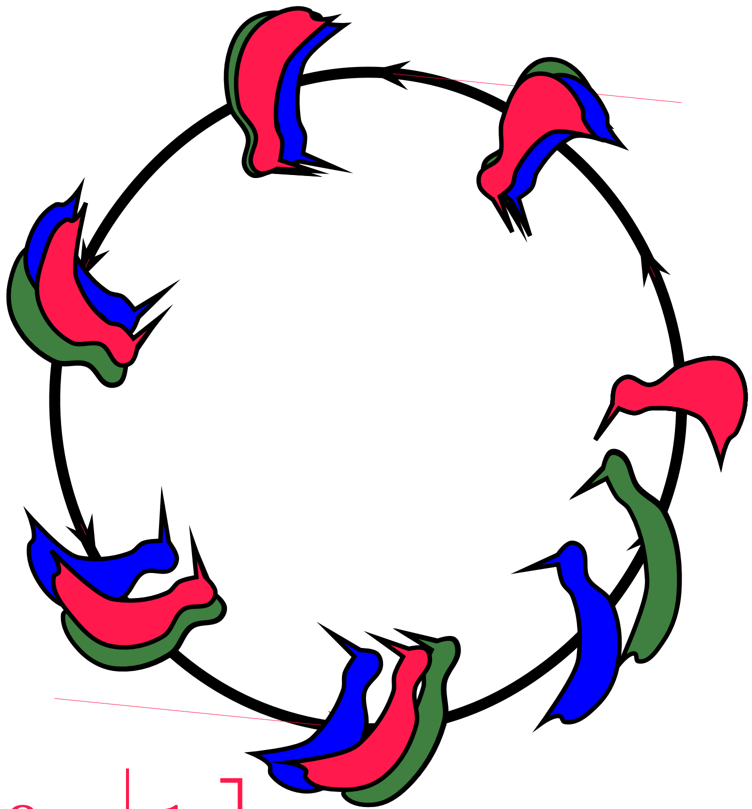

Gauss method

$$\begin{array}{c|cc} \frac{3-\sqrt{3}}{6} & \frac{3-2\sqrt{3}}{12} & \frac{1}{4} \\ \frac{3+\sqrt{3}}{6} & \frac{1}{4} & \frac{3+2\sqrt{3}}{12} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

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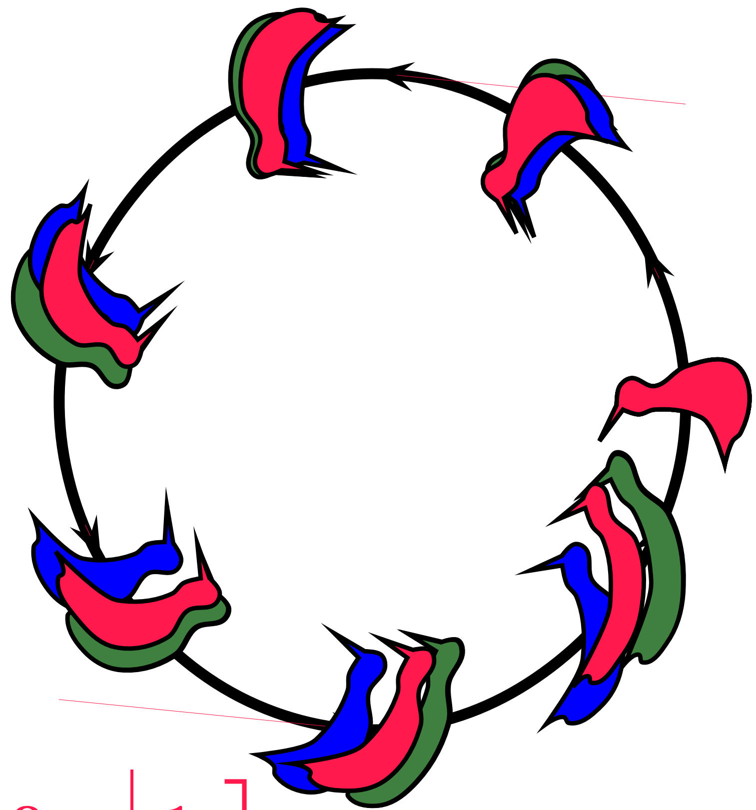

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In a step from t_{n-1} to $t_n = t_{n-1} + h$, Y_i approximates $y(t_{n-1} + hc_i)$ and $F_i \approx y'(t_{n-1} + hc_i)$ is computed from the differential equation $y'(t) = f(y(t))$.

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These quantities, together with the output approximation $y_n \approx y(t_n)$, are computed by

$$\begin{aligned} Y_i &= y_{n-1} + h \sum_{j=1}^{s} a_{ij} F_j, \qquad i = 1, 2, \ldots, s, \\ y_n &= y_{n-1} + h \sum_{i=1}^{s} b_i F_i. \end{aligned}$$

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Here is the coefficient tableau, in the form of a partitioned matrix, for this method:

$$\begin{bmatrix} A & U \\ B & V \end{bmatrix} = \left[\begin{array}{cc|cc} \frac{3+\sqrt{3}}{6} & 0 & 1 & \frac{-3-2\sqrt{3}}{3} \\ -\frac{\sqrt{3}}{3} & \frac{3+\sqrt{3}}{6} & 1 & \frac{3+2\sqrt{3}}{3} \\ \hline \frac{1}{2} & \frac{1}{2} & 1 & 0 \\ \frac{1}{2} & -\frac{1}{2} & 0 & -1 \end{array}\right]$$

For input $y_1^{[n-1]}$ and $y_2^{[n-1]}$ to step number n, the stages and the output values are computed by

$$
\begin{aligned}
Y_1 &= a_{11}hF_1 + a_{12}hF_2 + u_{11}y_1^{[n-1]} + u_{12}y_2^{[n-1]}\\
Y_2 &= a_{21}hF_1 + a_{22}hF_2 + u_{21}y_1^{[n-1]} + u_{22}y_2^{[n-1]}\\
y_1^{[n]} &= b_{11}hF_1 + b_{12}hF_2 + v_{11}y_1^{[n-1]} + v_{12}y_2^{[n-1]}\\
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\end{aligned}
$$

Substitute the coefficients from the matrices A, U, B, V:

$$
\begin{aligned}
Y_1 &= \tfrac{3+\sqrt{3}}{6}hF_1 + y_1^{[n-1]} - \tfrac{3+2\sqrt{3}}{3}y_2^{[n-1]}\\
Y_2 &= -\tfrac{\sqrt{3}}{3}hF_1 + \tfrac{3+\sqrt{3}}{6}hF_2 + y_1^{[n-1]} + \tfrac{3+2\sqrt{3}}{3}y_2^{[n-1]}\\
y_1^{[n]} &= \tfrac{1}{2}hF_1 + \tfrac{1}{2}hF_2 + y_1^{[n-1]}\\
y_2^{[n]} &= \tfrac{1}{2}hF_1 - \tfrac{1}{2}hF_2 - y_2^{[n-1]}
\end{aligned}
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Theorem 3 *The new general linear method has order 4.*

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Proof. Given an input approximation

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found by replacing x_0 by $x_1 = x_0 + h$ in (1) and expanding about x_0.

By Taylor expansions we find

$$Y_1 = y\left(x_0 + h\tfrac{3+\sqrt{3}}{6}\right) + \tfrac{9+5\sqrt{3}}{108} h^3 y^{(3)}(x_0) + O(h^4),$$

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Now consider the symplectic property of the new method.

For a general linear method to be symplectic, there would need to exist a diagonal matrix D and a symmetric matrix G, each of them positive definite, such that

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To actually use a method like this, there has to be a starting method to prepare for the very first step. This can be provided by the method

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Preservation of quadratic invariants

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but for a general linear method satisfying the symplectic property, we will be happy if

$$\sum_{i,j=1}^{r} g_{ij}\big((y_i^{[n]})^T M (y_j^{[n]})\big) = \sum_{i,j=1}^{r} g_{ij}\big((y_i^{[n-1]})^T M (y_j^{[n-1]})\big).$$

After a little manipulation, and using the conditions that

$$V^T G V = G,$$
$$B^T G V = DU,$$
$$B^T G B = DA + A^T D,$$

it is found that

$$\sum_{i,j=1}^{r} g_{ij} (y_i^{[n]})^T M (y_j^{[n]}) - \sum_{i,j=1}^{r} g_{ij} (y_i^{[n-1]})^T M (y_j^{[n-1]})$$
$$= 2h \sum_{i=1}^{s} d_i F_i^T M Y_i$$
$$= 0.$$

As an example of this result, consider the differential equation system due to Euler

$$\begin{aligned} A\dot{w}_1 &= (B - C)w_2 w_3, \\ B\dot{w}_2 &= (C - A)w_3 w_1, \\ C\dot{w}_3 &= (A - B)w_1 w_2, \end{aligned}$$

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This differential equation system has two quadratic invariants:

$$E = Aw_1^2 + Bw_2^2 + Cw_3^2,$$
$$F = A^2 w_1^2 + B^2 w_2^2 + C^2 w_3^2.$$

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For the case

$$[A, B, C] = [4, 3, 2], \qquad y_0 = [1, 1, 0]^T.$$

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and a stepsize $h = 0.1$, the method was applied for $n = 100,000$ steps.

It was found that E_n/E_0 and F_n/F_0 do not deviate very much from 1.

Let E_n and F_n denote the values of these "invariants" as computed from the results of n steps of a numerical method.

For the fourth order symplectic Runge–Kutta method we have considered, the values of these quantities do not change at all.

It is more interesting to see what happens in the case of the new symplectic general linear method.

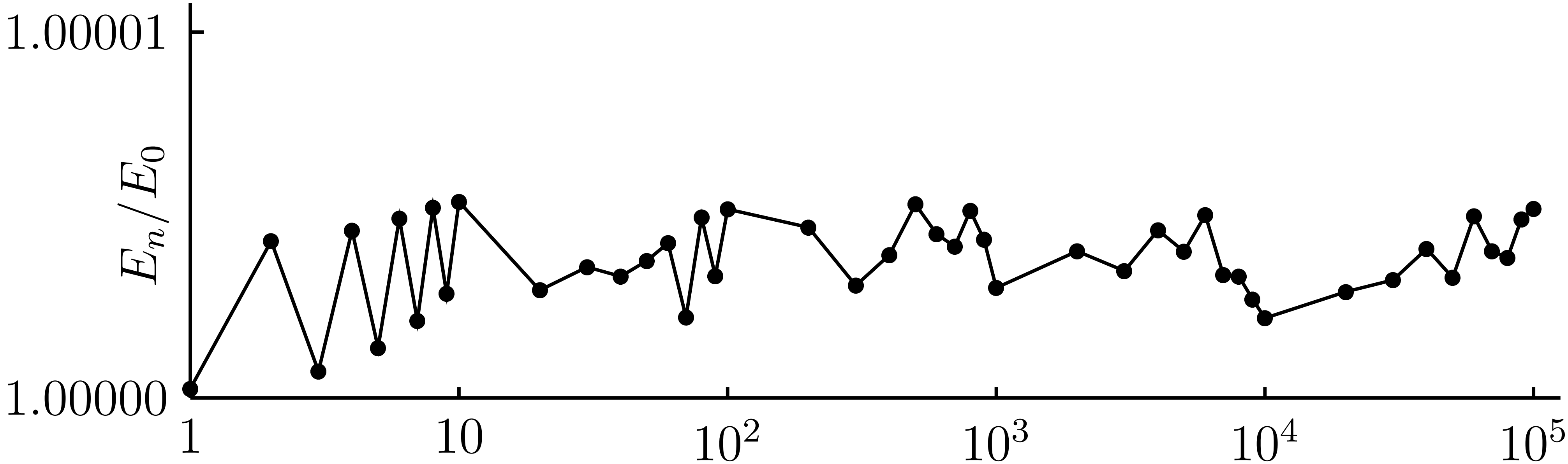
For the case

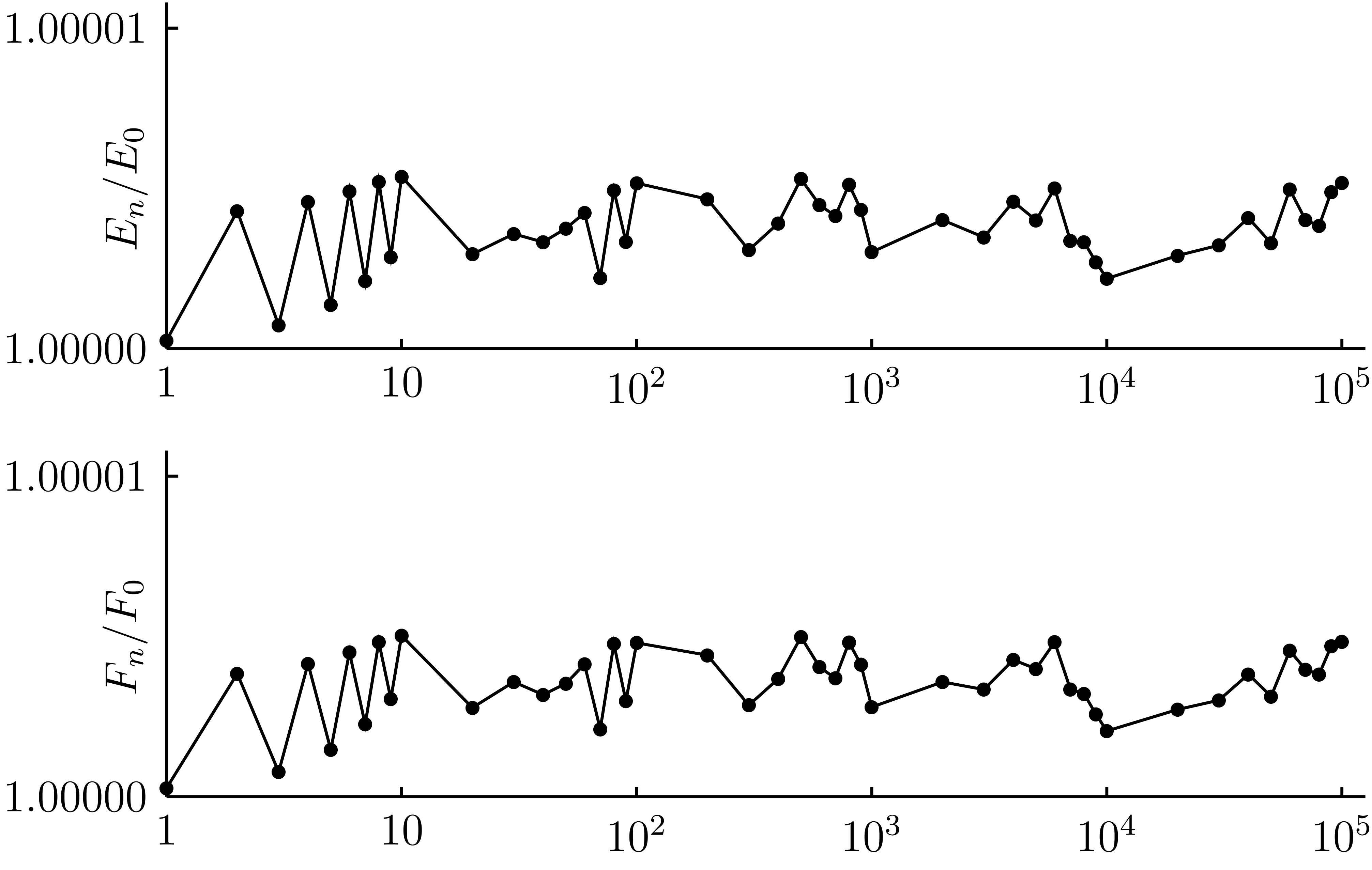
$$[A, B, C] = [4, 3, 2], \qquad y_0 = [1, 1, 0]^T.$$

and a stepsize $h = 0.1$, the method was applied for $n = 100,000$ steps.

It was found that E_n/E_0 and F_n/F_0 do not deviate very much from 1.

Results are shown on the next page.


1.00001
1.00000
E_n/E_0
1
10
10^2
10^3
10^4
10^5


1.00001
1.00000
E_n/E_0
1
10
10^2
10^3
10^4
10^5
1.00001
1.00000
F_n/F_0
1
10
10^2
10^3
10^4
10^5

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