Quaternions for Regularizing Celestial Mechanics – the Right Way

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Abstract

Quaternions, introduced by W. R. Hamilton (1844) as a generalization of complex numbers, lead to a remarkably simple representation of the regularization of the spatial case of binary collisions in celestial mechanics. The transformation suggested by Kustaanheimo and Stiefel (KS) in 1964 may be handled in complete formal agreement with the planar case regularized by Levi-Civita (1920) by means of a conformal squaring.

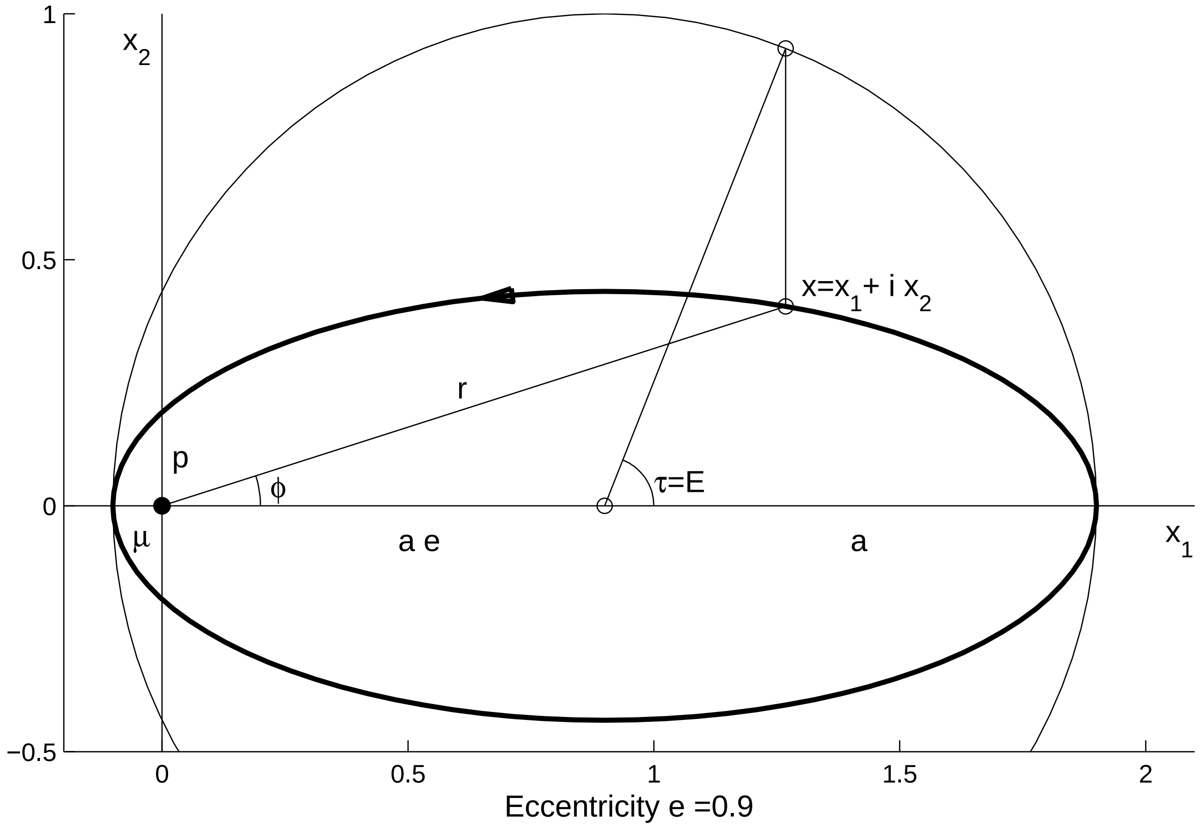
Outline

1. Kepler motion
2. Levi-Civita regularization
3. Kustaanheimo-Stiefel (KS) regularization
4. Quaternions
5. KS regularization with quaternions
6. The perturbed Kepler motion
7. Regularizing the restricted 3-body problem
8. Appendix: MATLAB code for animated Kepler motions

1. Kepler Motion

$$\ddot{x} + \mu \frac{x}{|x|^3} = 0\,, \quad x = \binom{x_1}{x_2} \in \mathbb{R}^2 \quad \text{or} \quad x = x_1 + i\,x_2 \in \mathbb{C}$$

$$\dot{(\,)} = \frac{d}{dt}(\,), \quad t = \text{time}, \quad \mu = \text{gravitational parameter}$$



Explicit solution, Kepler formulas

$a =$ major semi-axis $\quad r =$ radial distance $\quad p =$ semi latus rectum

$e =$ eccentricity $\quad \varphi =$ polar angle $\quad E =$ eccentric anomaly

$$\left.\begin{array}{rcl} x_1 & = & a\,(e + \cos E) \\ x_2 & = & a\sqrt{1-e^2} \cdot \sin E \end{array}\right\} \Longrightarrow \quad r = |x| = a\,(1 + e\,\cos E)$$

$$t = \sqrt{\frac{a^3}{\mu}} \cdot (E + e\,\sin E)\,, \qquad \frac{dt}{dE} = \sqrt{\frac{a}{\mu}} \cdot r$$

Further explicit formulas

Orbit in polar coordinates

$$\begin{aligned} r &= \frac{p}{1 - e\,\cos(\varphi)}\,, \quad p = a\,(1-e^2) \\ \tan(\tfrac{\varphi}{2}) &= \sqrt{\frac{1-e}{1+e}}\,\tan(\tfrac{E}{2}) \end{aligned}$$

Conservation of energy: $\frac{1}{2}|\dot{x}|^2 - \frac{\mu}{r} = -h\,, \quad h = \frac{\mu}{2\,a}$

Conservation of angular momentum: $|x \times \dot{x}| = \sqrt{\mu\,p}$

2. Levi-Civita regularization

Conformal squaring: $\boxed{x \;=\; u^2 \in \mathbb{C}}$

$$
\begin{aligned}
x &= x_1 + i\,x_2 = a\,\left(e + \cos E + i\,\sqrt{1-e^2}\,\sin E\right) \quad \Longleftarrow \\
u &= \sqrt{a\,(1+e)}\,\cos(\frac{E}{2}) + i\,\sqrt{a\,(1-e)}\,\sin(\frac{E}{2})
\end{aligned}
$$

Regularization procedure

Step 1. Time transformation: $dt = c^{-1}\,r\,d\tau, \quad c > 0$

Case 1: $c = 1$, $\tau =$ fictitious time, Sundman transformation

Case 2: $c = \sqrt{2\,h}$, $\tau = E =$ eccentric anomaly

Step 2. Conformal squaring: $x \;=\; u^2 \in \mathbb{C}$

Step 3. Use the energy integral for eliminating u'

The formal regularization procedure, $c = 1$

$$\ddot{x} + \mu \frac{x}{r^3} = 0\,, \qquad \frac{1}{2}\,|\dot{x}|^2 - \frac{\mu}{r} = -h\,, \quad r = |x|$$

Step 1:

$$\tfrac{d}{dt} = r^{-1}\,\tfrac{d}{d\tau}\,, \qquad \tfrac{d^2}{dt^2} = r^{-2}\,\tfrac{d^2}{d\tau^2} - r'\,r^{-3}\,\tfrac{d}{d\tau}\,, \qquad (\;)' = \tfrac{d}{d\tau}(\;)$$

$$\Longrightarrow\; r\,x'' - r'\,x' + \mu\,x = 0\,, \qquad \frac{1}{2}\,r^{-2}\,|x'|^2 - \frac{\mu}{r} = -h$$

Step 2: $x = u^2,\; x' = 2uu',\; x'' = 2(uu'' + u'^2),\; r = u\bar{u},\; r' = u'\bar{u} + u\bar{u}'$

$$\Longrightarrow\; r\cdot 2uu'' + \underbrace{r\cdot 2u'^2 - u'\bar{u}\cdot 2uu'}_{0} - u\bar{u}'\cdot 2uu' + \mu u^2 = 0$$

Energy equation $\Longrightarrow\; \frac{1}{2} r^{-2}\cdot 4uu'\bar{u}\bar{u}' - \frac{\mu}{r} = -h$ or $2\,u'\,\bar{u}' = \mu - r\,h$

The formal regularization procedure, continued

Step 3: Elimination of u' from the last two equations and division by ru:

$$\boxed{2\,u'' + h\,u = 0\,, \quad u \in \mathbb{C}}$$

- A harmonic oscillator in 2 dimensions, frequency $\omega = \sqrt{h/2}$
- All Kepler formulas may be conveniently derived from the above ODE and the transformation rules
- Initial conditions from a complex square root, e.g.

$$u = \sqrt{x} = \frac{x + |x|}{\sqrt{2\,(|x| + \mathrm{Re}\,x)}}$$

3. The Kustaanheimo-Stiefel (KS) regularization

$$\ddot{x} + \mu \frac{x}{r^3} = 0 , \qquad \frac{1}{2} |\dot{x}|^2 - \frac{\mu}{r} = -h , \quad r = |x| , \quad x \in \mathbb{R}^3$$

Step 2: The KS transformation (Hopf map)

$$u = (u_0, u_1, u_2, u_3)^T \in \mathbb{R}^4 \mapsto x = (x_0, x_1, x_2)^T \in \mathbb{R}^3$$

$$\begin{aligned} x_0 &= u_0^2 - u_1^2 - u_2^2 + u_3^2 \\ x_1 &= 2\,(u_0\,u_1 - u_2\,u_3) \\ x_2 &= 2\,(u_0\,u_2 + u_1\,u_3) \end{aligned}$$

with the bilinear differential relation

$$u_3\,du_0 - u_2\,du_1 + u_1\,du_2 - u_0\,du_3 = 0$$

A few references

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4. Quaternions

W. R. Hamilton (1844): On quaternions, or a new system of imaginaries in algebra. Philos. Mag. **25**, 489-495.

Three independent imaginary units, i, j, k, satisfying

$$i^2 = j^2 = k^2 = -1$$

$$i\,j = -j\,i = k, \quad j\,k = -k\,j = i, \quad k\,i = -i\,k = j\,.$$

The object $u = u_0 + i\,u_1 + j\,u_2 + k\,u_3$ with $u_l \in \mathbb{R}$ is called a quaternion, $u \in \mathbb{U}$. The above multiplication rules and vector space addition define the quaternion algebra:

- Multiplication is non-commutative in general, but $u\,c = c\,u \;\forall\; c \in \mathbb{R}$
- Multiplication is associative, $(u\,v)\,w = u\,(v\,w)$

Miscellaneous definitions and properties

Conjugation: $\bar{u} = u_0 - i\, u_1 - j\, u_2 - k\, u_3$

$\bar{\bar{u}} = u$

Real quaternion: A quaternion $u \in \mathbb{U}$ is real, $u \in \mathbb{R}$,

if and only if $u = \bar{u}$

Modulus $|u|$: $u\, \bar{u} = \bar{u}\, u = |u|^2 = \sum_{l=0}^{3} u_l^2$

u commutes with $\bar{u}$

Conjugation of a product: $\overline{u\, v} = \bar{v}\, \bar{u}$

5. KS regularization with quaternions

a) Preliminaries

Let $u = u_0 + i\,u_1 + j\,u_2 + k\,u_3$

Definition: $\boxed{u^\star = u_0 + i\,u_1 + j\,u_2 - k\,u_3}$ "star conjugation"

We have: $u^\star = k^{-1}\,\bar{u}\,k = -k\,\bar{u}\,k$

Properties: $(u^\star)^\star = u$

$|u^\star|^2 = |u|^2$

$(u\,v)^\star = v^\star\,u^\star$

KS regularization, continued

b) The KS transformation

Consider the map $\boxed{x = u\,u^\star}$ with $u \in \mathbb{U}$

Due to $x^\star = (u^\star)^\star\, u^\star = x$ we identically have $x_3 = 0$; therefore the quaternion $x = x_0 + i\,x_1 + j\,x_2$ may be associated with a vector $\in \mathbb{R}^3$.

In components:

$$\begin{aligned} x_0 &= u_0^2 - u_1^2 - u_2^2 + u_3^2 \\ x_1 &= 2\,(u_0\,u_1 - u_2\,u_3) \\ x_2 &= 2\,(u_0\,u_2 + u_1\,u_3) \end{aligned}$$

The KS transformation or Hopf map (p. 10) !

Modulus: $|x| = \sqrt{x\,\bar{x}} = \sqrt{u\,(u^\star\,\bar{u^\star})\,\bar{u}} = \sqrt{|u^\star|^2\,|u|^2} = |u|^2$

KS regularization, continued

c) Fibration instead of inverse map

Find all u with $u\,u^\star = x = x_0 + i\,x_1 + j\,x_2$

First step: Particular solution v with $v = v^\star = v_0 + i\,v_1 + j\,v_2$,
in analogy to p. 9 for the complex case,

$$v = \frac{x + |x|}{\sqrt{2\,(|x| + x_0)}}\,.$$

Second step: All solutions u of $u\,u^\star = x$ are given by

$$u = v\,e^{k\,\varphi} = v\,(\cos\varphi + k\,\sin\varphi)\,, \quad \varphi \in \mathbb{R}$$

Proof (sketch): $\quad u\,u^\star = v\,e^{k\,\varphi}\,e^{-k\,\varphi}\,v^\star = v\,v^\star = x$ $\square$

KS regularization, continued

d) Differentiation

We have

$$dx = du\ u^\star + u\ du^\star\ .$$

The bilinear relation of KS (p. 10),

$$2\,(u_3\,du_0 - u_2\,du_1 + u_1\,du_2 - u_0\,du_3) = 0\,,$$

may be written as the commutator relation

$$u\ du^\star - du\ u^\star = 0\ ;$$

therefore

$$\boxed{dx = 2\ u\ du^\star = 2\ du\ u^\star}$$

Remark: With the above bilinear relation the tangential map of $u \mapsto u\,u^\star$ behaves like a tangential map in a commutative algebra.

KS regularization, continued

e) The formal regularization procedure (cf. p. 8)

Step 1 yields, as on p. 8: $r\,x'' - r'\,x' + \mu\,x = 0$ (*)

Energy relation, as on p. 8:

$$\frac{1}{2}\,r^{-2}\cdot 4\,u\,(u^{\star\prime}\,\bar{u}^{\star\prime})\,\bar{u} - \frac{\mu}{r} = -h \qquad \Longrightarrow \qquad 2\,|u'|^2 = \mu - r\,h$$

Step 2: Differentiation yields

$$\begin{aligned} x &= u\,u^\star & \qquad r &= u\,\bar{u} \\ x' &= 2\,u\,u^{\star\prime} & \qquad r' &= u'\,\bar{u} + u\,\bar{u}' \\ x'' &= 2\,u\,u^{\star\prime\prime} + 2\,u'\,u^{\star\prime} \end{aligned}$$

The non-commutative computations

Substitution into (*) yields

$$(u\,\bar u)\,(2\,u\,u^{\star\prime\prime} \;+\; \underbrace{2\,u\,'u^{\star\prime}) - (u'\,\bar u}_{\substack{2(u\bar u)u'u^{\star\prime} - 2u'(\bar u u)u^{\star\prime} \\ =0}} \;+\; u\,\bar u')\,2\,\underbrace{u\,u^{\star\prime}}_{u'\,u^\star} + \mu\;u\,u^\star \;=\; 0$$

Together with the energy relation, after left-multiplication by $r^{-1}\,u^{-1}$ and star-conjugation:

$$\boxed{2\,u'' + h\,u = 0\,, \quad u \in \mathbb{U}}$$

in perfect formal agreement with the planar case, p. 9.

6. The perturbed Kepler problem

$$\ddot{x} + \mu \frac{x}{|x|^3} = \varepsilon f(x,t)\,,$$

where $x \in \mathbb{R}^3$ is the position vector, $f : \mathbb{R}^3 \times \mathbb{R} \mapsto \mathbb{R}^3$ is a perturbing function, and ε is a small parameter. Alternatively, the symbols $x, f \in \mathbb{U}$ will be considered as quaternions with a vanishing k-component.

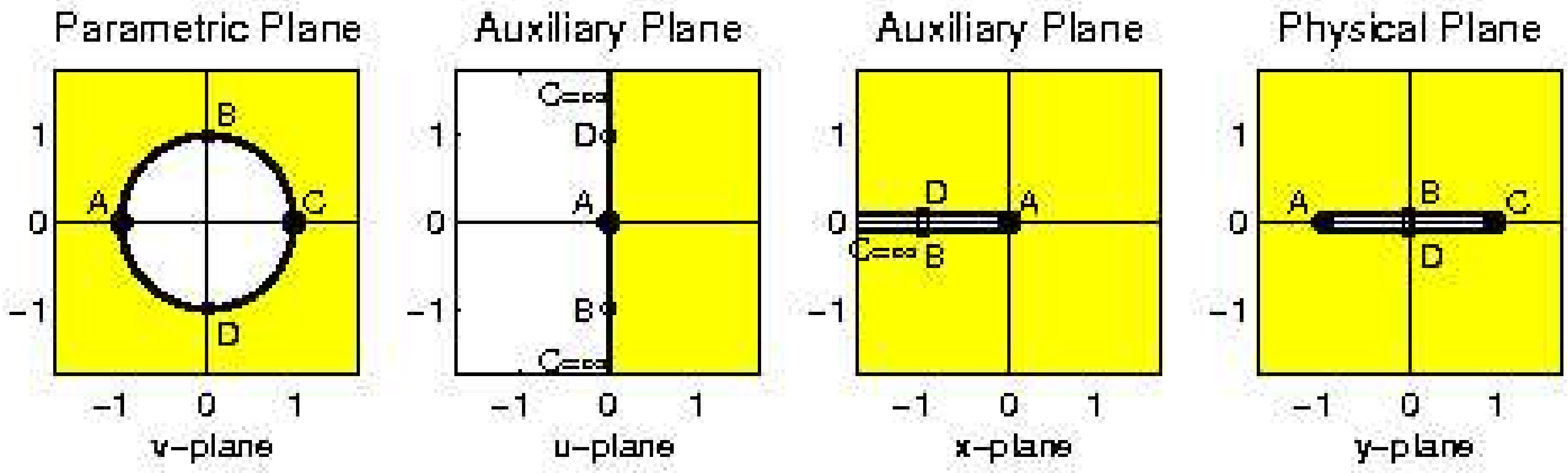
Equivalent regularized system:

$$\begin{aligned} 2\,u'' + h\,u &= \varepsilon\, r\, f(x,t)\,\bar{u}^\star\,, & r &= |u|^2 \\ t' &= r\,, & x &= u\,u^\star \\ h' &= -\langle x', \varepsilon f(x,t)\rangle & \text{or} \quad h &= r^{-1}\,(\mu - 2\,|u'|^2) \end{aligned}$$

7. Regularizing the restricted 3-body problem

- Motion of a massless particle under the gravitational force of two heavy primaries moving on circular orbits
- Use a rotating coordinate system, traditionally centered at the center of mass, such that the primaries are fixed at the complex positions $-\mu$ and $1-\mu$, respectively $(0 < \mu < 1)$
- We discuss the simultaneous regularization of both types of collisions. G. D. Birkhoff (1915): time transformation (Step 1): $dt = r_1\, r_2\, d\tau$, where $r_1,\ r_2$ are the distances of the particle from the primaries
- Coordinate transformation in 2 dimensions (Step 2): A sequence of conformal mappings $v \in \mathbb{C} \mapsto u \mapsto x \mapsto y$, where for simplicity we choose $y \in \mathbb{C}$ as a normalized physical coordinate with the primaries located at $y = -1$ and $y = 1$

The Joukowsky-Birkhoff transformation



$$v \mapsto u = \frac{v+1}{v-1} \qquad u \mapsto x = u^2 \qquad x \mapsto y = \frac{x+1}{x-1}$$

Composition of the three mappings

Two dimensions:

$$y = \frac{\left(\frac{v+1}{v-1}\right)^2 + 1}{\left(\frac{v+1}{v-1}\right)^2 - 1} \qquad \text{or} \qquad y = \frac{1}{2}\left(v + \frac{1}{v}\right)$$

Three dimensions: $v, u, x, y \in \mathbb{U}, \quad x = x^\star, \; y = y^\star$

$$v \mapsto u = 1 + 2\,(v-1)^{-1}, \quad u \mapsto x = u\,u^\star, \quad x \mapsto y = 1 + 2\,(x-1)^{-1}$$

Composition yields: $\boxed{y = 1 + (v^\star - 1)\,(v^\star + v)^{-1}\,(v-1)}$

Proof

$$(*) \qquad y = 1 + 2\left(u\,u^\star - 1\right)^{-1} \qquad \text{with} \qquad u = 1 + 2\,(v-1)^{-1}$$

Because of

$$\begin{aligned} u\,u^\star - 1 &= (u-1)\,(u^\star - 1) + u - 1 + u^\star - 1 \\ &= 4\,(v-1)^{-1}\,(v^\star - 1)^{-1} + 2\,(v-1)^{-1} + 2\,(v^\star - 1)^{-1} \end{aligned}$$

we write $(*)$ as

$$y = 1 + 2\,(v^\star - 1)\,\underbrace{(v^\star - 1)^{-1}\left(u\,u^\star - 1\right)^{-1}(v-1)^{-1}}_{D^{-1}}\,(v-1)\,.$$

$$\begin{aligned} \Longrightarrow\ D &= (v-1)\Big(4\,(v-1)^{-1}(v^\star - 1)^{-1} + 2(v-1)^{-1} + 2(v^\star - 1)^{-1}\Big)(v^\star - 1) \\ &= 4 + 2\,(v^\star - 1) + 2\,(v-1) = 2\,(v + v^\star)\,, \end{aligned}$$

whence the statement follows.

Conclusions

- The “language” of quaternions allows for a concise formalism for developing the Kustaanheimo-Stiefel theory of regularization of the perturbed spatial Kepler problem.

- The use of ”star-conjugation”,

$$u = u_0 + i\,u_1 + j\,u_2 + k\,u_3\,, \quad u^\star = u_0 + i\,u_1 + j\,u_2 - k\,u_3\,,$$

  yields a spatial regularization theory in perfect formal agreement with Levi-Civita’s planar regularization using complex numbers.

- Both collision types in the spatial restricted problem of three bodies may be regularized simultaneously by means of a generalization of the Joukowsky-Birkhoff mapping, elegantly representable in terms of quaternions.

8. Appendix: MATLAB code for animated Kepler motions

```
function ind = kepler(e,N,Nrev)        % Save as kepler.m
% e=eccentricity, N steps/revol.   Call: e.g., kepler(0.8,160,8)
% Nrev revol's of Kepler motion in phys.coord (Nrev/2 in reg.c.)
a=1; mu=1; b=a*sqrt(1-e^2);
a1=sqrt(a*(1+e)); b1=sqrt(a*(1-e)); n1=sqrt(a^3/mu);
N2=2*N; t=n1*[0:N2]'*4*pi/N2; E=t-e*sin(t); E0=1+0*E;
tol=sqrt(eps); ind=0; while any(abs(E-E0)>tol), ind=ind+1;
               E0=E; E=E-(E+e*sin(E)-t)./(1+e*cos(E)); end;
x = a*(e+cos(E)); y = b*sin(E);
u = a1*cos(E/2);  v = b1*sin(E/2);
X = x(1); Y = y(1); U = u(1); V = v(1);
clf; subplot(2,1,1); p = plot(x,y,'b',X,Y,'LineWidth',2);
axis equal; hold on; plot(0,0,'ko','LineWidth',6,'MarkerSize',6);
```

```
title(strcat('Kepler motion and Levi-Civita regularization, e = ',...
      num2str(e)),'FontSize',15);
xlabel('Physical system','FontSize',12);
subplot(2,1,2); q = plot(u,v,'c',U,V,'LineWidth',2);
axis equal; hold on; plot(0,0,'ko','LineWidth',6,'MarkerSize',6);
xlabel('Regularized system','FontSize',12);
set(p(2),'LineWidth',6,'Marker','o','MarkerSize',6,'Color','r');
set(q(2),'LineWidth',6,'Marker','o','MarkerSize',6,'Color','m');
for k=1:ceil(Nrev/2),
  for k=1:N2,
    set(p(2),'Xdata',x(k),'Ydata',y(k));
    set(q(2),'Xdata',u(k),'Ydata',v(k));
    pause(.0015);
  end
end  % Template by Peter Arbenz, Computational Science, ETH Zurich
```