An Introduction to Numerical Continuation Methods

with Applications

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Persistence of Solutions

- Newton's method for solving a nonlinear equation [B83][1]

$$\mathbf{G}(\mathbf{u}) \;=\; \mathbf{0}\ , \qquad \mathbf{G}(\cdot)\ ,\ \mathbf{u}\ \in\ \mathbb{R}^n\ ,$$

  may not converge if the "initial guess" is not close to a solution.

- However, one can put a homotopy parameter in the equation.

- Actually, most equations already have parameters.

- We will discuss persistence of solutions to such equations.

[1] See Page 83^+ of the Background Notes on Elementary Numerical Methods.

The Implicit Function Theorem

Let $\mathbf{G} : \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}^n$ satisfy

(**i**) $\mathbf{G}(\mathbf{u}_0, \lambda_0) = \mathbf{0}$, $\mathbf{u}_0 \in \mathbb{R}^n$, $\lambda_0 \in \mathbb{R}$.

(**ii**) $\mathbf{G}_\mathbf{u}(\mathbf{u}_0, \lambda_0)$ is nonsingular (*i.e.*, $\mathbf{u}_0$ is an isolated solution) ,

(**iii**) $\mathbf{G}$ and $\mathbf{G}_\mathbf{u}$ are smooth near $\mathbf{u}_0$.

Then there exists a unique, smooth solution family $\mathbf{u}(\lambda)$ such that

- $\mathbf{G}(\mathbf{u}(\lambda), \lambda) = \mathbf{0}$, for all λ near λ_0 ,
- $\mathbf{u}(\lambda_0) = \mathbf{u}_0$.

NOTE : The IFT also holds in more general spaces $\cdots$

EXAMPLE : **A Simple Homotopy** .

(`Course demo` : `Simple-Homotopy`[2])

Let

$$g(u,\lambda) \quad = \quad (u^2-1)\;(u^2-4) \quad + \quad \lambda\; u^2\; e^{\frac{1}{10}u} \; .$$

When $\lambda = 0$ the equation

$$g(u,0) \quad = \quad 0 \; ,$$

has four solutions , namely,

$$u \quad = \quad \pm\, 1 \; , \qquad \text{and} \qquad u \quad = \quad \pm\, 2 \; .$$

We have

$$g_u(u,\lambda)\Big|_{\lambda=0} \quad \equiv \quad \frac{d}{du}(u,\lambda)\Big|_{\lambda=0} \quad = \quad 4u^3 - 10u \; .$$

[2] http://users.encs.concordia.ca/ doedel/

Since

$$g_u(u,0) \;=\; 4u^3 - 10u \;,$$

we have

$$g_u(-1,0) \;=\; 6 \;, \qquad\qquad g_u(\;1,0) \;=\; -6 \;,$$

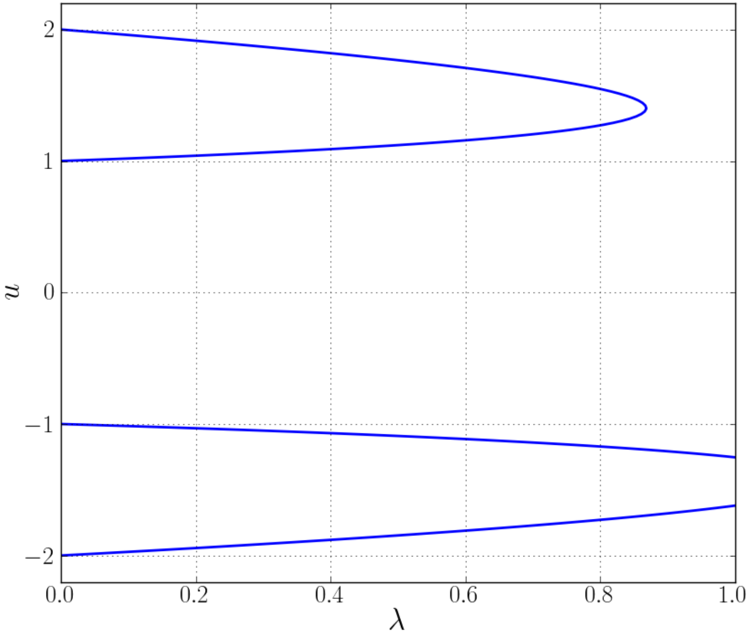
$$g_u(-2,0) \;=\; -12 \;, \qquad\qquad g_u(\;2,0) \;=\; 12 \;,$$

which are all nonzero .

Thus each of the four solutions when $\lambda = 0$ is isolated .

Hence each of these solutions persists as λ becomes nonzero,

(at least for "small" values of $|\,\lambda\,|$ $\cdots$).



Solution families of $g(u, \lambda) = 0$. Note the fold .

NOTE :

- Each of the four solutions at $\lambda = 0$ is isolated .

- Thus each of these solutions persists as λ becomes nonzero.

- Only two of the four homotopies reach $\lambda = 1$.

- The other two homotopies meet at a fold .

- IFT condition (**ii**) is not satisfied at the fold. (Why not?)

In the equation

$$\mathbf{G}(\mathbf{u},\lambda) \ = \ \mathbf{0} \ , \qquad \mathbf{u} \ , \ \mathbf{G}(\cdot,\cdot) \in \mathbb{R}^n \ , \quad \lambda \in \mathbb{R} \ ,$$

let

$$\mathbf{x} \ \equiv \ \begin{pmatrix} \mathbf{u} \\ \lambda \end{pmatrix} \ .$$

Then the equation can be written

$$\mathbf{G}(\mathbf{x}) \ = \ \mathbf{0} \ , \qquad \mathbf{G} \ : \ \mathbb{R}^{n+1} \ \longrightarrow \ \mathbb{R}^n \ .$$

DEFINITION :

A solution $\mathbf{x}_0$ of $\mathbf{G}(\mathbf{x}) \ = \ \mathbf{0}$ is regular if the matrix

$$\mathbf{G}^0_{\mathbf{x}} \ \equiv \ \mathbf{G}_{\mathbf{x}}(\mathbf{x}_0) \ , \qquad \text{(with } n \text{ rows and } n+1 \text{ columns)}$$

has maximal rank , *i.e.*, if

$$\text{Rank}(\mathbf{G}^0_{\mathbf{x}}) \ = \ n \ .$$

In the parameter formulation ,

$$\mathbf{G}(\mathbf{u}, \lambda) \;=\; \mathbf{0} \; ,$$

we have

$$\text{Rank}(\mathbf{G}_{\mathbf{x}}^0) \;=\; \text{Rank}(\mathbf{G}_{\mathbf{u}}^0 \mid \mathbf{G}_{\lambda}^0) \;=\; n \quad \Longleftrightarrow \quad \begin{cases} (\mathbf{i}) \quad \mathbf{G}_{\mathbf{u}}^0 \text{ is nonsingular,} \\ \\ \text{or} \\ \\ (\mathbf{ii}) \quad \begin{cases} \dim \mathcal{N}(\mathbf{G}_{\mathbf{u}}^0) \;=\; 1 \; , \\ \text{and} \\ \mathbf{G}_{\lambda}^0 \not\in \mathcal{R}(\mathbf{G}_{\mathbf{u}}^0) \; . \end{cases} \end{cases}$$

Here $\quad \mathcal{N}(\mathbf{G}_{\mathbf{u}}^0)$ denotes the null space of $\mathbf{G}_{\mathbf{u}}^0$,

and

$\mathcal{R}(\mathbf{G}_{\mathbf{u}}^0)$ denotes the range of $\mathbf{G}_{\mathbf{u}}^0$,

i.e., $\mathcal{R}(\mathbf{G}_{\mathbf{u}}^0)$ is the linear space spanned by the n columns of $\mathbf{G}_{\mathbf{u}}^0$.

COROLLARY (to the IFT) : Let

$$\mathbf{x}_0 \equiv (\mathbf{u}_0 , \lambda_0)$$

be a regular solution of

$$\mathbf{G}(\mathbf{x}) = \mathbf{0} .$$

Then, near $\mathbf{x}_0$, there exists a unique one-dimensional solution family

$$\mathbf{x}(s) \quad \text{with} \quad \mathbf{x}(0) = \mathbf{x}_0 .$$

PROOF : Since $\text{Rank}(\mathbf{G}_\mathbf{x}^0) = \text{Rank}(\mathbf{G}_\mathbf{u}^0 \mid \mathbf{G}_\lambda^0) = n$, we have that

(**i**) either $\mathbf{G}_\mathbf{u}^0$ is nonsingular and by the IFT we have

$$\mathbf{u} = \mathbf{u}(\lambda) \quad \text{near} \quad \mathbf{x}_0 ,$$

(**ii**) or else we can interchange colums in the Jacobian $\mathbf{G}_\mathbf{x}^0$ to see that the solution can locally be parametrized by one of the components of $\mathbf{u}$.

Thus a (locally) unique solution family passes through $\mathbf{x}_0$. **QED !**

NOTE :

- Such a solution family is sometimes called a solution branch .

- Case (**i**) is where the IFT applies directly .

- Case (**ii**) is that of a simple fold .

- Thus even near a simple fold there is a unique solution family .

- However, near such a fold, the family cannot be parametrized by λ.

More Examples of IFT Application

- We give examples where the IFT shows that a given solution persists (at least locally) when a problem parameter is changed.

- We also consider cases where the conditions of the IFT are not satisfied.

EXAMPLE : **The $A \to B \to C$ Reaction** .

(`Course demo` : `Chemical-Reactions/ABC-Reaction/Stationary`)

$$u_1' = -u_1 + D(1-u_1)e^{u_3} ,$$

$$u_2' = -u_2 + D(1-u_1)e^{u_3} - D\sigma u_2 e^{u_3} ,$$

$$u_3' = -u_3 - \beta u_3 + DB(1-u_1)e^{u_3} + DB\alpha\sigma u_2 e^{u_3} ,$$

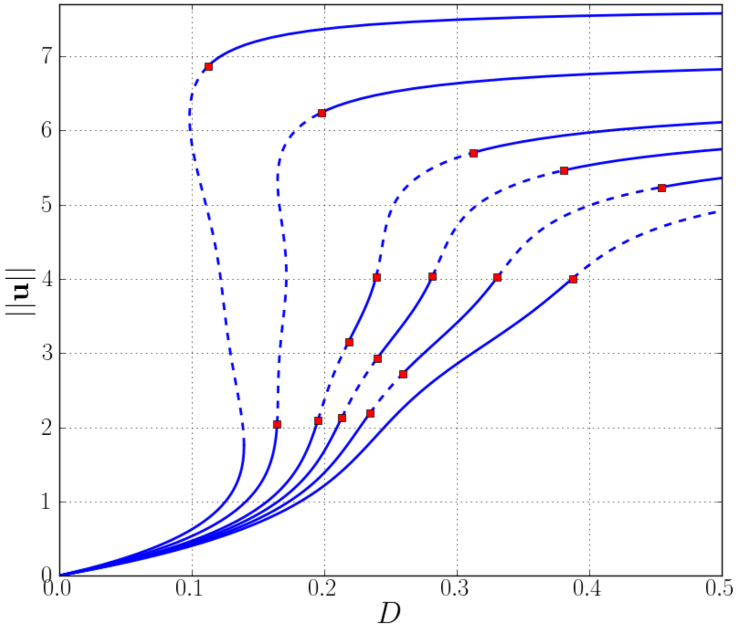
where

$1-u_1$ is the concentration of A , u_2 is the concentration of B ,

u_3 is the temperature, $\alpha = 1$, $\sigma = 0.04$, $B = 8$,

D is the Damkohler number , $\beta > 0$ is the heat transfer coefficient .

NOTE : The zero stationary solution at $D = 0$ persists (locally), because the Jacobian is nonsingular there, having eigenvalues -1, -1, and $-(1+\beta)$.



Families of stationary solutions of the $A \to B \to C$ reaction.

(From left to right : $\beta = 1.1$, 1.3 , 1.5 , 1.6 , 1.7 , 1.8 .)

NOTE :

In the preceding bifurcation diagram:

- $\| \mathbf{u} \| \quad = \quad \sqrt{u_1^2 + u_2^2 + u_3^2}$.
- Solid/dashed curves denote stable/unstable solutions.
- The red squares are Hopf bifurcations .

From the basic theory of ODEs:

- $\mathbf{u}_0$ is a stationary solution of $\mathbf{u}'(t) = \mathbf{f}(\mathbf{u}(t))$ if $\mathbf{f}(\mathbf{u}_0) = \mathbf{0}$.
- $\mathbf{u}_0$ is stable if all eigenvalues of $\mathbf{f}_{\mathbf{u}}(\mathbf{u}_0)$ are in the negative half-plane.
- $\mathbf{u}_0$ is unstable if one or more eigenvalues are in the positive half-plane.
- At a fold there is zero eigenvalue.
- At a Hopf bifurcation there is a pair of purely imaginary eigenvalues.

EXAMPLE (of IFT application) : **The Gelfand-Bratu Problem** .

(`Course demo : Gelfand-Bratu/Original`)

The boundary value problem

$$\begin{cases} u''(x) \ + \ \lambda \ e^{u(x)} & = \quad 0 \ , \quad \forall x \in [0,1] \ , \\ u(0) \ = \ u(1) & = \quad 0 \ , \end{cases}$$

defines the stationary states of a solid fuel ignition model.

If $\lambda = 0$ then $u(x) \equiv 0$ is a solution.

This problem can be thought of as an operator equation $\mathbf{G}(\mathbf{u};\lambda) = 0$.

We can use (a generalized) IFT to prove that there is a solution family

$$\mathbf{u} \ = \ \mathbf{u}(\lambda) \ , \qquad \text{for} \ \ |\lambda| \ \ \text{small} \ .$$

The linearization of $\mathbf{G}(\mathbf{u};\lambda)$ acting on $\mathbf{v}$, *i.e.*, $\mathbf{G}_{\mathbf{u}}(\mathbf{u};\lambda)\mathbf{v}$, leads to the homogeneous equation

$$\begin{aligned} v''(x) \ + \ \lambda\, e^{u(x)} v \quad &= \quad 0 \ , \\ v(0) \ = \ v(1) \quad &= \quad 0 \ , \end{aligned}$$

which for the solution $u(x) \equiv 0$ at $\lambda = 0$ becomes

$$\begin{aligned} v''(x) \ &= \ 0 \ , \\ v(0) \ = \ v(1) \ &= \ 0 \ . \end{aligned}$$

Since this equation only has the zero solution $v(x) \equiv 0$, the IFT applies.

Thus (locally) a unique solution family passes through $u(x) \equiv 0$, $\lambda = 0$.

In `Course demo` : `Gelfand-Bratu/Original` the BVP is implemented

as a first order system :

$$u_1'(t) \;=\; u_2(t) \; ,$$

$$u_2'(t) \;=\; -\lambda \; e^{u_1(t)} \; ,$$

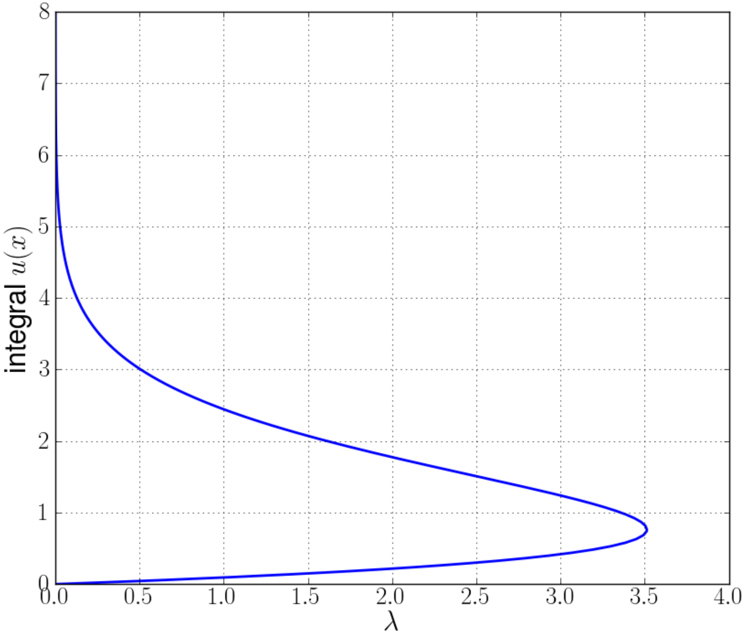
with boundary conditions

$$u_1(0) \;=\; 0 \; ,$$

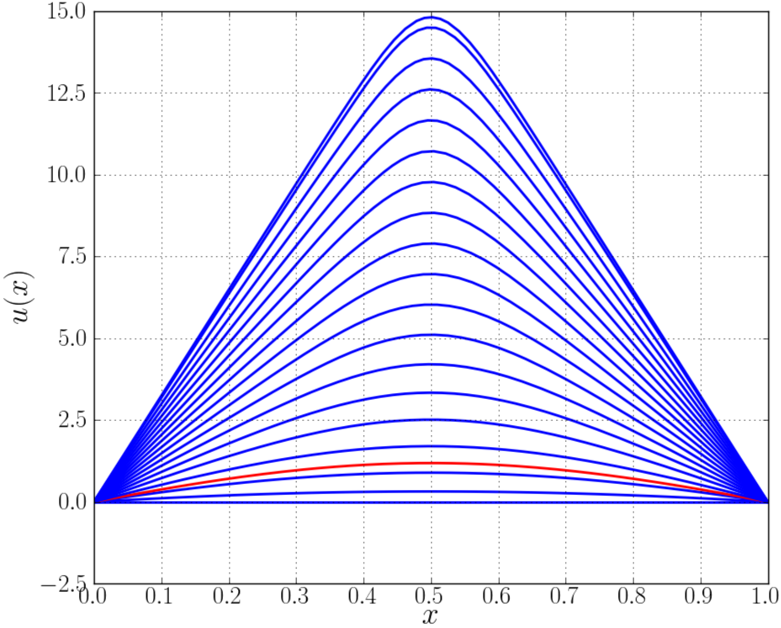
$$u_1(1) \;=\; 0 \; .$$

A convenient solution measure in the bifurcation diagram is the value of

$$\int_0^1 u_1(x) \; dx \; .$$



Bifurcation diagram of the Gelfand-Bratu equation.



Some solutions of the Gelfand-Bratu equation.
(The solution at the fold is colored red).

EXAMPLE : **A Boundary Value Problem with Bifurcations** .

(`Course demo` : `Basic-BVP/Nonlinear-Eigenvalue`)

$$u'' + \hat{\lambda}\, u(1 - u) = 0 ,$$

$$u(0) = u(1) = 0 ,$$

has $u(x) \equiv 0$ as a solution for all $\hat{\lambda}$.

QUESTION : Are there more solutions ?

Again, this problem corresponds to an operator equation $\mathbf{G}(\mathbf{u};\hat{\lambda}) = 0$.

Its linearization acting on $\mathbf{v}$ leads to the equation $\mathbf{G}_u(\mathbf{u};\hat{\lambda})\mathbf{v} = 0$, *i.e.*,

$$v'' + \hat{\lambda}\,(1 - 2u)v = 0 ,$$

$$v(0) = v(1) = 0 .$$

In particular, the linearization about the zero solution family $u \equiv 0$ is

$$v'' + \hat{\lambda}\, v = 0 \,,$$

$$v(0) = v(1) = 0 \,,$$

which for most values of $\hat{\lambda}$ only has the zero solution $v(x) \equiv 0$.

However, when

$$\hat{\lambda} = \hat{\lambda}_k \equiv k^2\pi^2 \,,$$

then there are nonzero solutions , namely,

$$v(x) = \sin(k\pi x) \,,$$

Thus the IFT does not apply at $\hat{\lambda}_k = k^2\pi^2$.

(We will see that these solutions are bifurcation points .)

In the implementation we write the BVP as a first order system .

We also use a scaled version of λ.

The equations are then

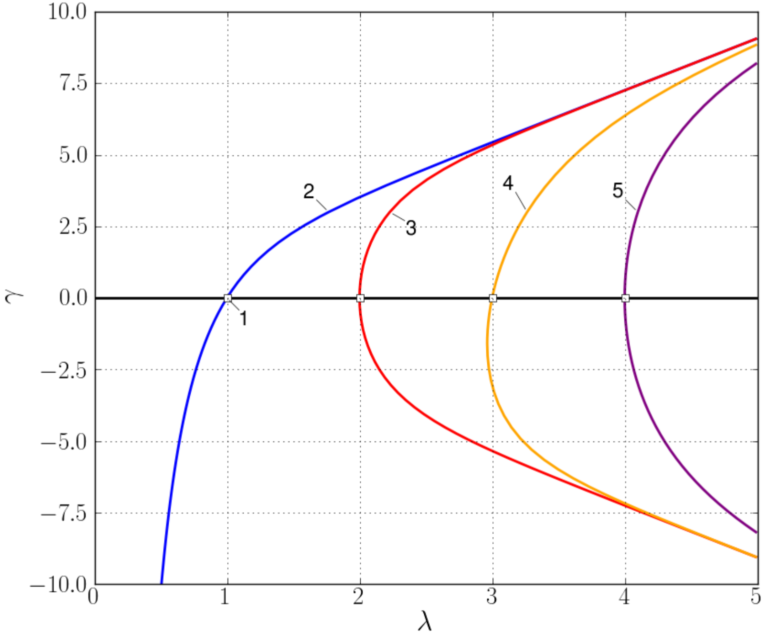
$$u_1' = u_2 ,$$

$$u_2' = \lambda^2\pi^2 \, u_1 \, (1 - u_1) ,$$

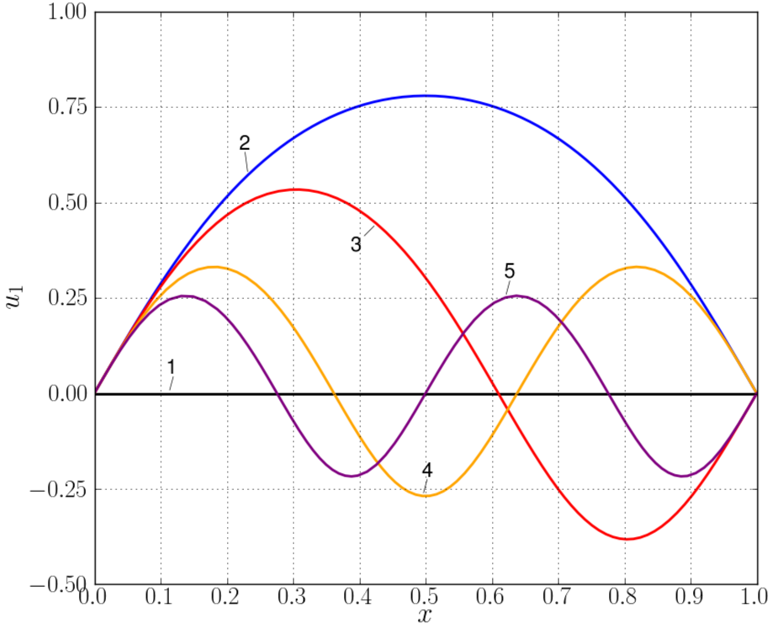
with $\hat{\lambda} = \lambda^2\pi^2$.

A convenient solution measure in the bifurcation diagram is

$$\gamma \equiv u_2(0) = u_1'(0) .$$



Solution families to the nonlinear eigenvalue problem.



Some solutions to the nonlinear eigenvalue problem.

Hopf Bifurcation

THEOREM : Suppose that along a stationary solution family $(\mathbf{u}(\lambda), \lambda)$, of

$$\mathbf{u}' = \mathbf{f}(\mathbf{u}, \lambda) ,$$

a complex conjugate pair of eigenvalues

$$\alpha(\lambda) \pm i\,\beta(\lambda) ,$$

of $f_{\mathbf{u}}(\mathbf{u}(\lambda), \lambda)$ crosses the imaginary axis transversally , *i.e.*, for some λ_0 ,

$$\alpha(\lambda_0) = 0 , \qquad \beta(\lambda_0) \neq 0 , \quad \text{and} \quad \dot{\alpha}(\lambda_0) \neq 0 .$$

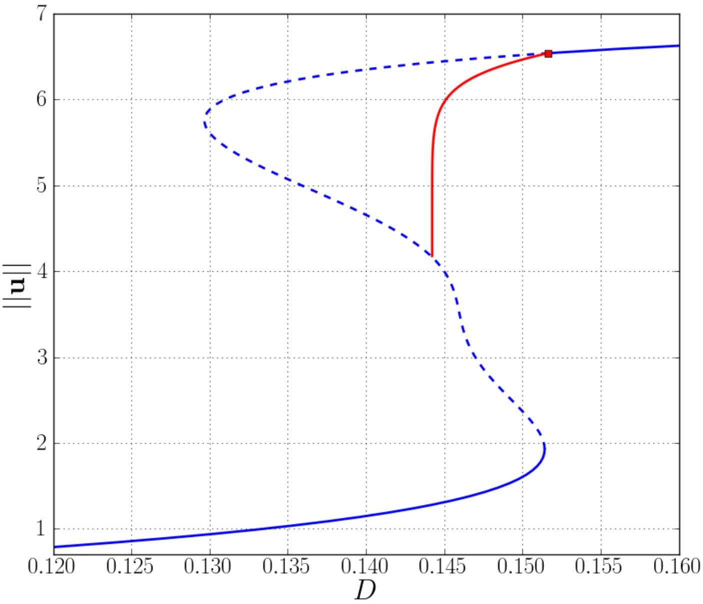
Also assume that there are no other eigenvalues on the imaginary axis .

Then there is a Hopf bifurcation, that is, a family of periodic solutions bifurcates from the stationary solution at $(\mathbf{u}_0, \lambda_0)$.

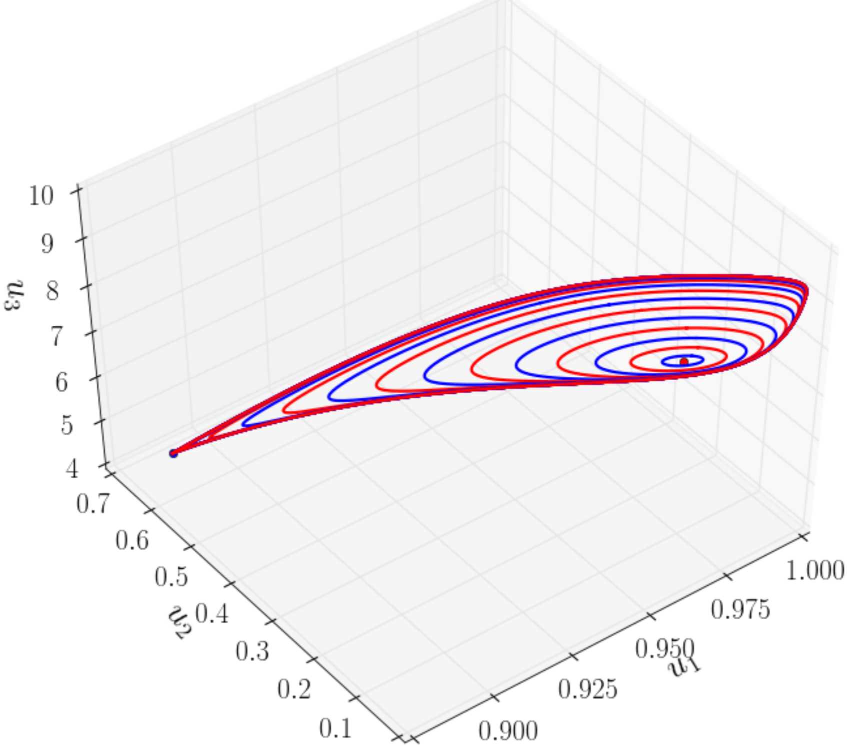
NOTE : The assumptions imply that $\mathbf{f}_{\mathbf{u}}^0$ is nonsingular, so that the stationary solution family is indeed (locally) a function of λ .

EXAMPLE : **The $A \to B \to C$ reaction** .

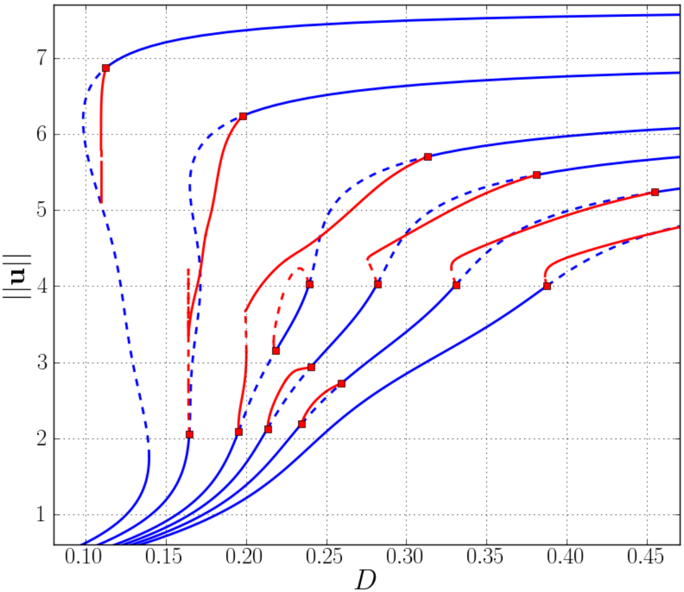
(`Course demo` : `Chemical-Reactions/ABC-Reaction/Homoclinic`)



A stationary (blue) and a periodic (red) family of the $A \to B \to C$ reaction for $\beta = 1.2$. The periodic orbits are stable and terminate in a homoclinic orbit .



The periodic family orbit family approaching a homoclinic orbit (black). The red dot is the Hopf point; the blue dot is the saddle point on the homoclinic.



Bifurcation diagram for $\beta = 1.1,\ 1.3,\ 1.5,\ 1.6,\ 1.7,\ 1.8$.

(For periodic solutions $\| \mathbf{u} \| = \frac{1}{T} \int_0^T \sqrt{u_1^2 + u_2^2 + u_3^2}\ dt$, where T is the period.)

EXAMPLE : **A Predator-Prey Model** .

(`Course demo` : `Predator-Prey/ODE/2D`)

$$\begin{cases} u_1' &= \quad 3u_1(1-u_1) - u_1u_2 \;-\; \lambda(1-e^{-5u_1}) \;, \\ u_2' &= \quad -u_2 \;+\; 3u_1u_2 \;. \end{cases}$$

Here u_1 may be thought of as "fish " and u_2 as "sharks ", while the term

$$\lambda\,(1-e^{-5u_1})\;,$$

represents "fishing", with "fishing-quota " λ .

When $\lambda = 0$ the stationary solutions are

$$\left.\begin{array}{rcl} 3u_1(1-u_1) - u_1u_2 & = & 0 \\ -u_2 \;+\; 3u_1u_2 & = & 0 \end{array}\right\} \Rightarrow \;(u_1,u_2) \;=\; (0,0)\;,\;(1,0)\;,\;(\frac{1}{3},2)\;.$$

The Jacobian matrix is

$$\mathbf{G}_{\mathbf{u}}(u_1, u_2 \ ; \ \lambda) \ = \ \begin{pmatrix} 3 - 6u_1 - u_2 - 5\lambda e^{-5u_1} & -u_1 \\ 3u_2 & -1 + 3u_1 \end{pmatrix}$$

so that

$$\mathbf{G}_{\mathbf{u}}(0, 0 \ ; \ 0) \ = \ \begin{pmatrix} 3 & 0 \\ 0 & -1 \end{pmatrix}; \quad \text{real eigenvalues } \ 3 \ , \ \text{-1} \quad \text{(unstable)}$$

$$\mathbf{G}_{\mathbf{u}}(1, 0 \ ; \ 0) \ = \ \begin{pmatrix} -3 & -1 \\ 0 & 2 \end{pmatrix}; \quad \text{real eigenvalues } \ \text{-3} \ , \ 2 \quad \text{(unstable)}$$

$$\mathbf{G}_{\mathbf{u}}(\frac{1}{3}, 2 \ ; \ 0) \ = \ \begin{pmatrix} -1 & -\frac{1}{3} \\ 6 & 0 \end{pmatrix}; \quad \text{complex eigenvalues } \ -\frac{1}{2} \pm \frac{1}{2}\sqrt{7}\ i \quad \text{(stable)}$$

All three Jacobians at $\lambda = 0$ are nonsingular .

Thus, by the IFT, all three stationary points persist for (small) $\lambda \neq 0$.

In this problem we can explicitly find all solutions:

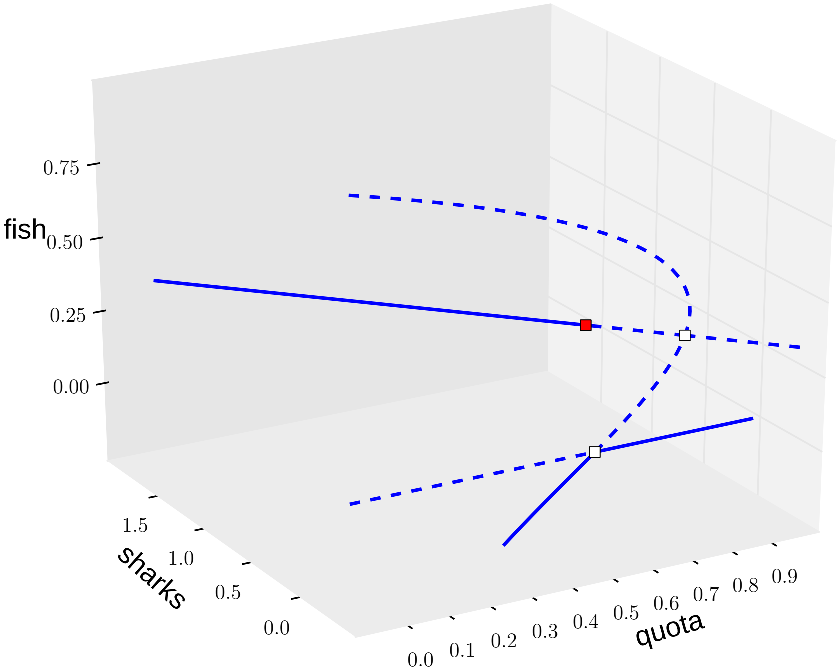
Family 1 :
$$(u_1, u_2) = (0 \, , \, 0)$$

Family 2 :
$$u_2 = 0 \, , \qquad \lambda = \frac{3u_1(1-u_1)}{1-e^{-5u_1}}$$

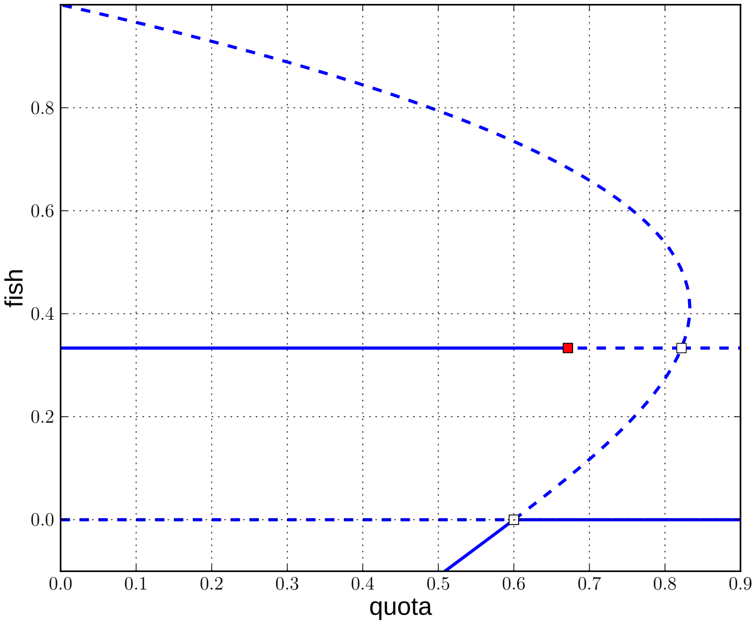
$$(\text{ Note that } \lim_{u_1 \longrightarrow 0} \lambda = \lim_{u_1 \longrightarrow 0} \frac{3(1-2u_1)}{5e^{-5u_1}} = \frac{3}{5} \,)$$

Family 3 :
$$u_1 = \frac{1}{3} \, , \qquad \frac{2}{3} - \frac{1}{3} u_2 - \lambda(1-e^{-5/3}) = 0 \Rightarrow u_2 = 2 - 3\lambda(1-e^{-5/3})$$

These solution families intersect at two bifurcation points , one of which is
$$(u_1, u_2, \lambda) = (0 \, , \, 0 \, , \, 3/5) \, .$$



Stationary solution families of the predator-prey model.
Solid/dashed curves denote stable/unstable solutions.
Note the bifurcations and Hopf bifurcation (red square).



Stationary solution families, showing fish versus quota.
Solid/dashed curves denote stable/unstable solutions.

Stability of Family 1 :

$$\mathbf{G}_{\mathbf{u}}(0,0\ ;\ \lambda)\ =\ \begin{pmatrix} 3-5\lambda & 0 \\ 0 & -1 \end{pmatrix};\quad \text{eigenvalues}\ \ 3-5\lambda,\ \ -1\ .$$

Hence the zero solution is :

$$\text{unstable if}\ \ \lambda < 3/5\ ,$$

and

$$\text{stable if}\ \ \lambda > 3/5\ .$$

Stability of Family 2 :

This family has no stable positive solutions.

- **Stability of Family 3** :

  At $\lambda_H \approx 0.67$ the complex eigenvalues cross the imaginary axis:

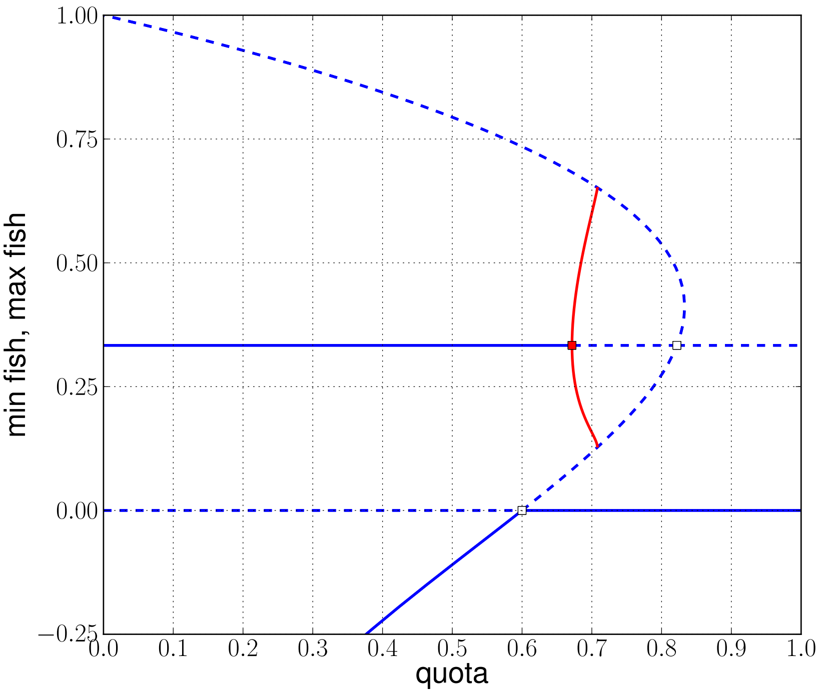
  - This crossing is a Hopf bifurcation ,

  - Beyond λ_H there are stable periodic solutions .

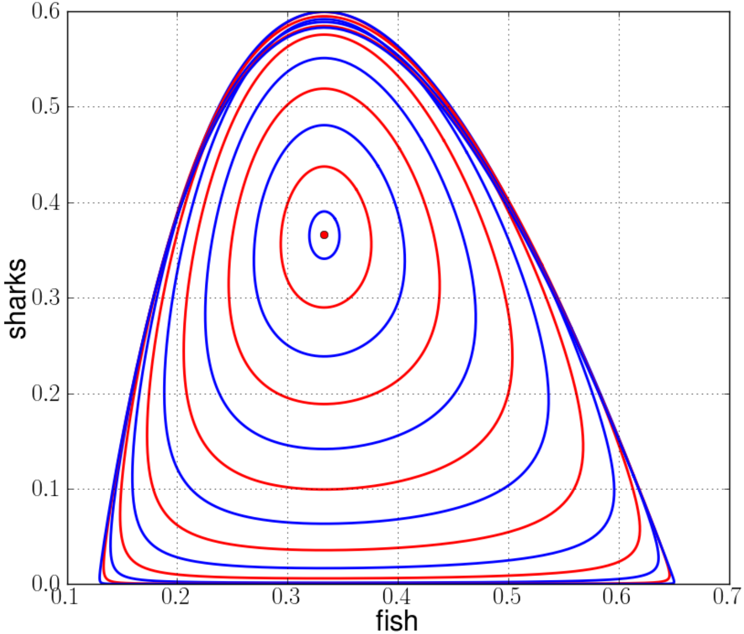
  - Their period T increases as λ increases.

  - The period becomes infinite at $\lambda = \lambda_\infty \approx 0.70$.

  - This final orbit is a heteroclinic cycle .



Stationary (blue) and periodic (red) solution families of the predator-prey model. (For the periodic solution family both the maximum and minimum are shown.)



Periodic solutions of the predator-prey model.
The largest orbits are close to a heteroclinic cycle.

The bifurcation diagram shows the solution behavior for (slowly) increasing λ :

- Family 3 is followed until $\lambda_H \approx 0.67$.

- Periodic solutions of increasing period until $\lambda = \lambda_\infty \approx 0.70$.

- Collapse to trivial solution (Family 1).

Continuation of Solutions

Parameter Continuation

Suppose we have a solution $(\mathbf{u}_0, \lambda_0)$ of

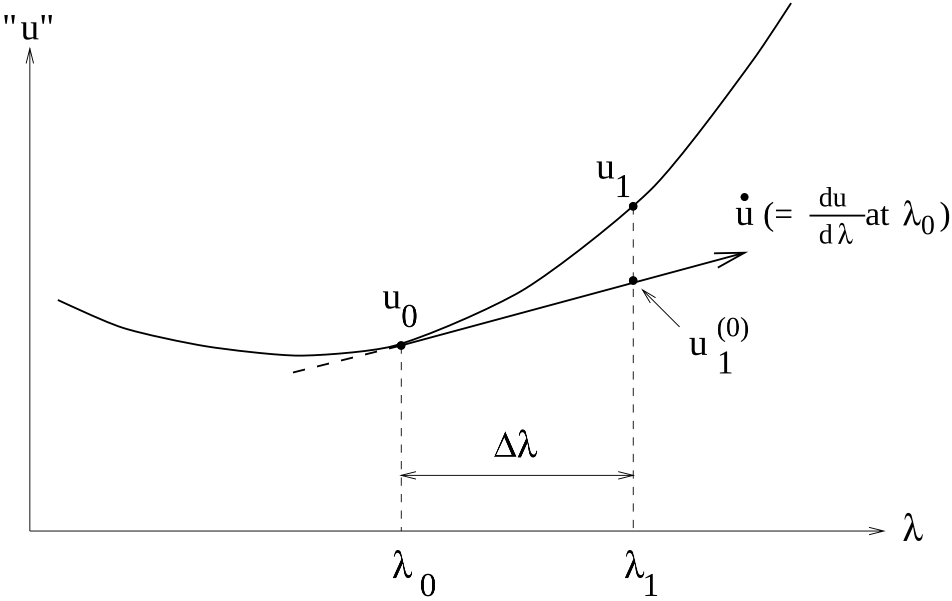
$$\mathbf{G}(\mathbf{u}, \lambda) = \mathbf{0} ,$$

as well as the derivative $\dot{\mathbf{u}}_0$.

Here

$$\dot{\mathbf{u}} \equiv \frac{d\mathbf{u}}{d\lambda} .$$

We want to compute the solution $\mathbf{u}_1$ at $\lambda_1 \equiv \lambda_0 + \Delta\lambda$.



Graphical interpretation of parameter-continuation.

To solve the equation

$$\mathbf{G}(\mathbf{u}_1 \ , \ \lambda_1) \ = \ \mathbf{0} \ ,$$

for $\mathbf{u}_1$ (with $\lambda = \lambda_1$ fixed) we use Newton's method

$$\left.\begin{array}{rcl} \mathbf{G}_{\mathbf{u}}(\mathbf{u}_1^{(\nu)}, \lambda_1) \ \Delta \mathbf{u}_1^{(\nu)} & = & - \ \mathbf{G}(\mathbf{u}_1^{(\nu)}, \lambda_1) \ , \\ \mathbf{u}_1^{(\nu+1)} & = & \mathbf{u}_1^{(\nu)} \ + \ \Delta \mathbf{u}_1^{(\nu)} \ . \end{array}\right. \qquad \nu \ = \ 0, 1, 2, \cdots \ .$$

As initial approximation use

$$\mathbf{u}_1^{(0)} \ = \ \mathbf{u}_0 \ + \ \Delta\lambda \ \dot{\mathbf{u}}_0 \ .$$

If

$$\mathbf{G}_{\mathbf{u}}(\mathbf{u}_1, \lambda_1) \quad \text{is nonsingular} \ ,$$

and $\Delta\lambda$ sufficiently small then this iteration will converge [B55].

After convergence, the new derivative $\dot{\mathbf{u}}_1$ is computed by solving

$$\mathbf{G}_{\mathbf{u}}(\mathbf{u}_1, \lambda_1)\ \dot{\mathbf{u}}_1 \ = \ -\,\mathbf{G}_\lambda(\mathbf{u}_1, \lambda_1)\ .$$

This equation is obtained by differentiating

$$\mathbf{G}(\mathbf{u}(\lambda), \lambda) \ = \ \mathbf{0}\ ,$$

with respect to λ at $\lambda \ = \ \lambda_1$.

Repeat the procedure to find $\mathbf{u}_2$, $\mathbf{u}_3$, $\cdots$.

NOTE :

- $\dot{\mathbf{u}}_1$ can be computed without another LU-factorization of $\mathbf{G}_{\mathbf{u}}(\mathbf{u}_1, \lambda_1)$.

- Thus the extra work to compute $\dot{\mathbf{u}}_1$ is negligible .

EXAMPLE : **The Gelfand-Bratu Problem** .

$$u''(x) \ + \ \lambda \, e^{u(x)} \ = \ 0 \quad \text{for} \quad x \in [0,1] \ , \qquad u(0) \ = \ 0 \ , \qquad u(1) \ = \ 0 \ .$$

We know that if $\lambda = 0$ then $u(x) \equiv 0$ is an isolated solution .

Discretize by introducing a mesh ,

$$0 \ = \ x_0 \ < \ x_1 \ < \ \cdots \ < \ x_N \ = \ 1 \ ,$$

$$x_j \ - \ x_{j-1} \ = \ h \ , \quad (1 \leq j \leq N) \ , \qquad h \ = \ 1/N \ .$$

The discrete equations are :

$$\frac{u_{j+1} \ - \ 2u_j \ + \ u_{j-1}}{h^2} \ + \ \lambda \, e^{u_j} \ = \ 0 \ , \qquad j = 1, \cdots, N-1 \ ,$$

with $u_0 \ = \ u_N \ = \ 0$.

Let

$$\mathbf{u} \equiv \begin{pmatrix} u_1 \\ u_2 \\ \cdot \\ u_{N-1} \end{pmatrix} .$$

Then we can write the discrete equations as

$$\mathbf{G}(\mathbf{u} , \lambda) = \mathbf{0} ,$$

where

$$\mathbf{G} : \mathbb{R}^{N-1} \times \mathbb{R} \rightarrow \mathbb{R}^{N-1} .$$

Parameter-continuation :

Suppose we have λ_0 , $\mathbf{u}_0$, and $\dot{\mathbf{u}}_0$. Set $\lambda_1 = \lambda_0 + \Delta\lambda$.

Newton's method :

$$\mathbf{G}_{\mathbf{u}}(\mathbf{u}_1^{(\nu)}, \lambda_1)\ \Delta\mathbf{u}_1^{(\nu)} = -\,\mathbf{G}(\mathbf{u}_1^{(\nu)}, \lambda_1)\ ,$$

$$\mathbf{u}_1^{(\nu+1)} = \mathbf{u}_1^{(\nu)} + \Delta\mathbf{u}_1^{(\nu)}\ ,$$

for $\nu = 0, 1, 2, \cdots$, with

$$\mathbf{u}_1^{(0)} = \mathbf{u}_0 + \Delta\lambda\ \dot{\mathbf{u}}_0\ .$$

After convergence compute $\dot{\mathbf{u}}_1$ from

$$\mathbf{G}_{\mathbf{u}}(\mathbf{u}_1, \lambda_1)\ \dot{\mathbf{u}}_1 = -\,\mathbf{G}_{\lambda}(\mathbf{u}_1, \lambda_1)\ .$$

Repeat the procedure to find $\mathbf{u}_2$, $\mathbf{u}_3$, $\cdots$.

Here

$$\mathbf{G_u}(\ \mathbf{u}\ ,\ \lambda\ )\ =\ \begin{pmatrix} -\frac{2}{h^2}\ +\ \lambda e^{u_1} & \frac{1}{h^2} & & & \\ \frac{1}{h^2} & -\frac{2}{h^2}\ +\ \lambda e^{u_2} & \frac{1}{h^2} & & \\ & \cdot & \cdot & \cdot & \\ & & \cdot & \cdot & \cdot \\ & & & \frac{1}{h^2} & -\frac{2}{h^2}\ +\ \lambda e^{u_{N-1}} \end{pmatrix}\ .$$

Thus we must solve a tridiagonal system for each Newton iteration.

NOTE :

- The solution family has a fold where parameter-continuation fails !
- A better continuation method is "pseudo-arclength continuation ".
- There are also better discretizations, namely collocation , as used in `AUTO` .

Pseudo-Arclength Continuation

This method allows continuation of a solution family past a fold .

It was introduced by H. B. Keller (1925-2008) in 1977.

Suppose we have a solution $(\mathbf{u}_0, \lambda_0)$ of

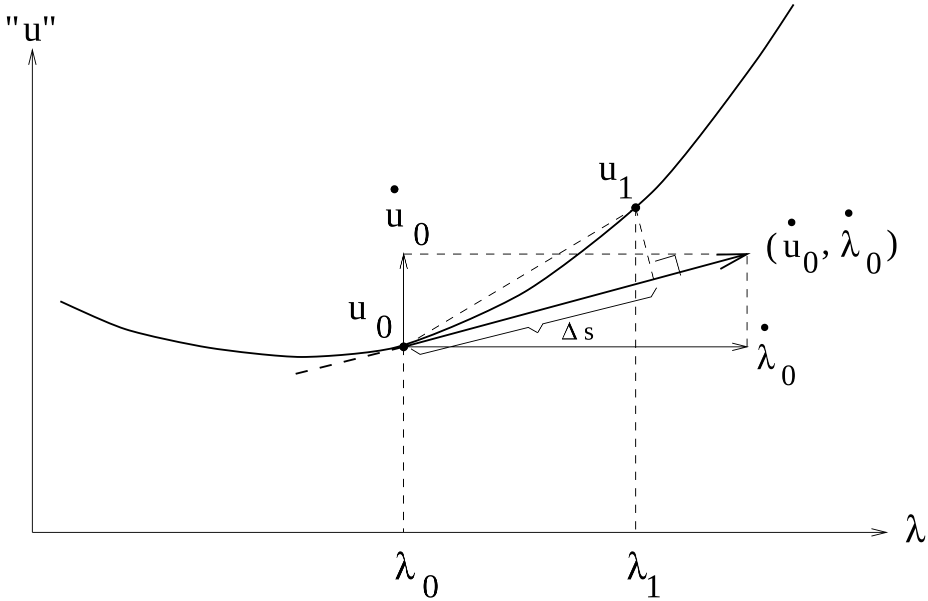
$$\mathbf{G}(\ \mathbf{u}\ ,\ \lambda\ )\ =\ \mathbf{0}\ ,$$

as well as the normalized direction vector $(\dot{\mathbf{u}}_0, \dot{\lambda}_0)$ of the solution family.

Pseudo-arclength continuation consists of solving these equations for $(\mathbf{u}_1, \lambda_1)$:

$$\mathbf{G}(\mathbf{u}_1, \lambda_1)\ =\ \mathbf{0}\ ,$$

$$\langle\ \mathbf{u}_1\ -\ \mathbf{u}_0\ ,\ \dot{\mathbf{u}}_0\ \rangle\ +\ (\lambda_1\ -\ \lambda_0)\ \dot{\lambda}_0\ -\ \Delta s\ =\ 0\ .$$



Graphical interpretation of pseudo-arclength continuation.

Solve the equations

$$\mathbf{G}(\mathbf{u}_1, \lambda_1) \;=\; \mathbf{0} \;,$$

$$\langle\ \mathbf{u}_1 \;-\; \mathbf{u}_0\ ,\ \dot{\mathbf{u}}_0\ \rangle \;+\; (\lambda_1 \;-\; \lambda_0)\ \dot{\lambda}_0 \;-\; \Delta s \;=\; 0\ .$$

for $(\mathbf{u}_1, \lambda_1)$ by Newton's method :

$$\begin{pmatrix} (\mathbf{G}^1_{\mathbf{u}})^{(\nu)} & (\mathbf{G}^1_{\lambda})^{(\nu)} \\ \\ \dot{\mathbf{u}}_0^* & \dot{\lambda}_0 \end{pmatrix} \begin{pmatrix} \Delta \mathbf{u}_1^{(\nu)} \\ \Delta \lambda_1^{(\nu)} \end{pmatrix} = - \begin{pmatrix} \mathbf{G}(\mathbf{u}_1^{(\nu)}, \lambda_1^{(\nu)}) \\ \\ \langle\ \mathbf{u}_1^{(\nu)} - \mathbf{u}_0\ ,\ \dot{\mathbf{u}}_0\ \rangle + (\lambda_1^{(\nu)} - \lambda_0)\dot{\lambda}_0 - \Delta s \end{pmatrix} .$$

Compute the next direction vector by solving

$$\begin{pmatrix} \mathbf{G}^1_{\mathbf{u}} & \mathbf{G}^1_{\lambda} \\ \\ \dot{\mathbf{u}}_0^* & \dot{\lambda}_0 \end{pmatrix} \begin{pmatrix} \dot{\mathbf{u}}_1 \\ \dot{\lambda}_1 \end{pmatrix} = \begin{pmatrix} \mathbf{0} \\ \\ 1 \end{pmatrix} \;,$$

and normalize it.

NOTE :

- We can compute $(\dot{\mathbf{u}}_1, \dot{\lambda}_1)$ with only one extra backsubstitution .

- The orientation of the family is preserved if Δs is sufficiently small.

- Rescale the direction vector so that indeed $\| \dot{\mathbf{u}}_1 \|^2 + \dot{\lambda}_1^2 = 1$.

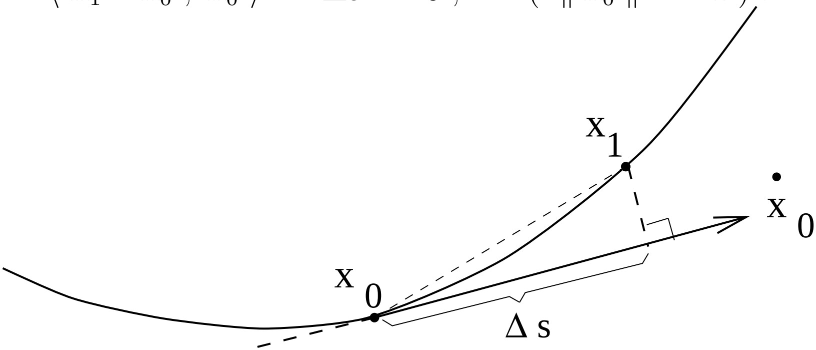
FACT : The Jacobian is nonsingular at a regular solution.

PROOF : Let $\mathbf{x} \equiv \begin{pmatrix} \mathbf{u} \\ \lambda \end{pmatrix} \in \mathbb{R}^{n+1}$.

Then pseudo-arclength continuation can be simply written as

$$\mathbf{G}(\mathbf{x}_1) \ = \ 0 \ ,$$

$$\langle \ \mathbf{x}_1 - \mathbf{x}_0 \ , \ \dot{\mathbf{x}}_0 \ \rangle \ - \ \Delta s \ = \ 0 \ , \qquad (\ \| \ \dot{\mathbf{x}}_0 \ \| \ = \ 1 \ ) \ .$$



Pseudo-arclength continuation.

The pseudo-arclength equations are

$$\mathbf{G}(\mathbf{x}_1) \;=\; 0 \;,$$

$$\langle\; \mathbf{x}_1 - \mathbf{x}_0 \;,\; \dot{\mathbf{x}}_0 \;\rangle \;-\; \Delta s \;=\; 0 \;, \qquad (\; \|\, \dot{\mathbf{x}}_0 \,\| \;=\; 1 \;) \;.$$

The Jacobian matrix in Newton's method at $\Delta s \;=\; 0$ is

$$\begin{pmatrix} \mathbf{G}_{\mathbf{x}}^0 \\ \dot{\mathbf{x}}_0^* \end{pmatrix} \;.$$

At a regular solution $\mathcal{N}(\mathbf{G}_{\mathbf{x}}^0) \;=\; \mathrm{Span}\{\dot{\mathbf{x}}_0\}$.

We must show that $\begin{pmatrix} \mathbf{G}_{\mathbf{x}}^0 \\ \dot{\mathbf{x}}_0^* \end{pmatrix}$ is nonsingular at a regular solution.

If on the contrary $\begin{pmatrix} \mathbf{G}_{\mathbf{x}}^{0} \\ \dot{\mathbf{x}}_0^{*} \end{pmatrix}$ is singular then for some vector $\mathbf{z} \neq \mathbf{0}$ we have :

$$\mathbf{G}_{\mathbf{x}}^{0}\, \mathbf{z} \;=\; \mathbf{0} \,,$$

$$\langle\, \dot{\mathbf{x}}_0 \,,\, \mathbf{z} \,\rangle \;=\; 0 \,,$$

Since by assumption $\mathcal{N}(\mathbf{G}_{\mathbf{x}}^{0}) = \text{Span}\{\dot{\mathbf{x}}_0\}$, we have

$$\mathbf{z} \;=\; c\, \dot{\mathbf{x}}_0 \,, \qquad \text{for some constant } c \,.$$

But then

$$0 \;=\; \langle\, \dot{\mathbf{x}}_0 \,,\, \mathbf{z} \,\rangle \;=\; c\, \langle\, \dot{\mathbf{x}}_0 \,,\, \dot{\mathbf{x}}_0 \,\rangle \;=\; c\; \|\, \dot{\mathbf{x}}_0 \,\|^2 \;=\; c \,,$$

so that $\mathbf{z} = \mathbf{0}$, which is a contradiction . **QED !**

EXAMPLE : **The Gelfand-Bratu Problem** .

Use pseudo-arclength continuation for the discretized Gelfand-Bratu problem.

Then the matrix

$$\begin{pmatrix} \mathbf{G_x} \\ \dot{\mathbf{x}}^* \end{pmatrix} = \begin{pmatrix} \mathbf{G_u} & \mathbf{G}_\lambda \\ \dot{\mathbf{u}}^* & \dot{\lambda} \end{pmatrix} ,$$

in Newton's method is a bordered tridiagonal matrix :

$$\begin{pmatrix}
\star & \star & & & & & & & \star \\
\star & \star & \star & & & & & & \star \\
 & \star & \star & \star & & & & & \star \\
 & & \star & \star & \star & & & & \star \\
 & & & \star & \star & \star & & & \star \\
 & & & & \star & \star & \star & & \star \\
 & & & & & \star & \star & \star & \star \\
 & & & & & & \star & \star & \star \\
\star & \star & \star & \star & \star & \star & \star & \star & \star
\end{pmatrix} .$$

which can be decomposed very efficiently .

Following Folds and Hopf Bifurcations

- At a fold the the behavior of a system can change drastically.

- How does the fold location change when a second parameter varies ?

- Thus we want the compute a locus of folds in 2 parameters.

- We also want to compute loci of Hopf bifurcations in 2 parameters.

Following Folds

Treat both parameters λ and μ as unknowns , and compute a solution family

$$\mathbf{X}(s) \equiv (\mathbf{u}(s) , \boldsymbol{\phi}(s) , \lambda(s) , \mu(s)) ,$$

to

$$\mathbf{F}(\mathbf{X}) \equiv \begin{cases} \mathbf{G}(\mathbf{u},\lambda,\mu) = \mathbf{0} , \\ \mathbf{G}_{\mathbf{u}}(u,\lambda,\mu)\ \boldsymbol{\phi} = \mathbf{0} , \\ \langle \boldsymbol{\phi} , \boldsymbol{\phi}_0 \rangle - 1 = 0 , \end{cases}$$

and the added continuation equation

$$\langle \mathbf{u}-\mathbf{u}_0 , \dot{\mathbf{u}}_0 \rangle + \langle \boldsymbol{\phi}-\boldsymbol{\phi}_0 , \dot{\boldsymbol{\phi}}_0 \rangle + (\lambda-\lambda_0)\dot{\lambda}_0 + (\mu-\mu_0)\dot{\mu}_0 - \Delta s = 0 .$$

As before,

$$(\dot{\mathbf{u}}_0 , \dot{\boldsymbol{\phi}}_0 , \dot{\lambda}_0 , \dot{\mu}_0) ,$$

is the direction of the family at the current solution point

$$(\mathbf{u}_0 , \boldsymbol{\phi}_0 , \lambda_0 , \mu_0) .$$

EXAMPLE : **The $A \to B \to C$ Reaction** .

(Course demo : Chemical-Reactions/ABC-Reaction/Folds-SS)

The equations are

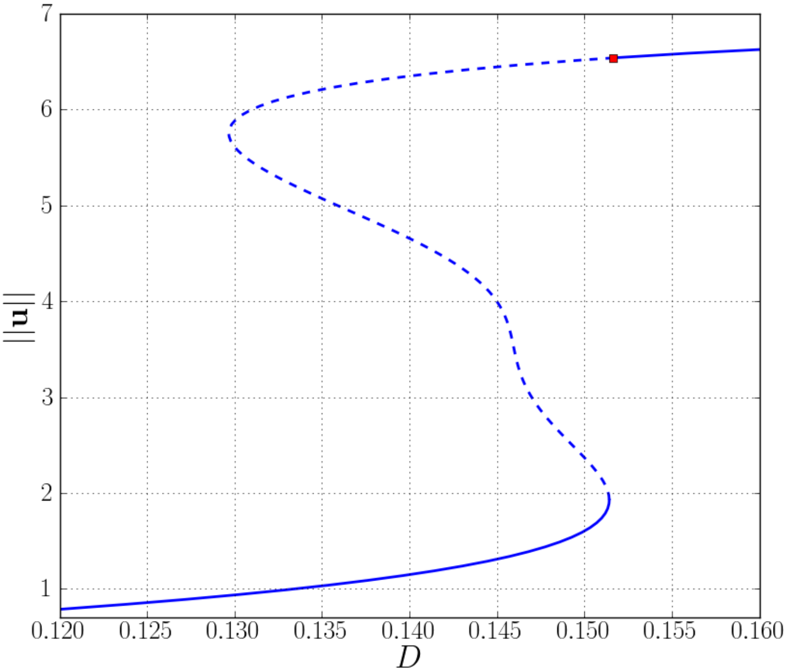
$$\begin{aligned} u_1' &= -u_1 + D(1-u_1)e^{u_3} , \\ u_2' &= -u_2 + D(1-u_1)e^{u_3} - D\sigma u_2 e^{u_3} , \\ u_3' &= -u_3 - \beta u_3 + DB(1-u_1)e^{u_3} + DB\alpha\sigma u_2 e^{u_3} , \end{aligned}$$

where

$1-u_1$ is the concentration of A , u_2 is the concentration of B ,

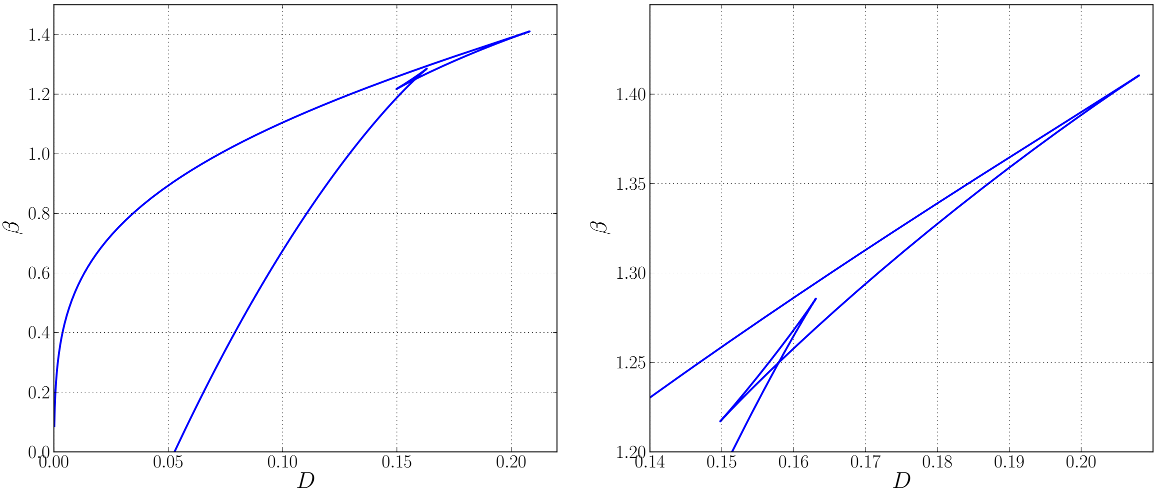
u_3 is the temperature , $\alpha = 1$, $\sigma = 0.04$, $B = 8$,

D is the Damkohler number , β is the heat transfer coefficient .



A stationary solution family for $\beta = 1.20$.

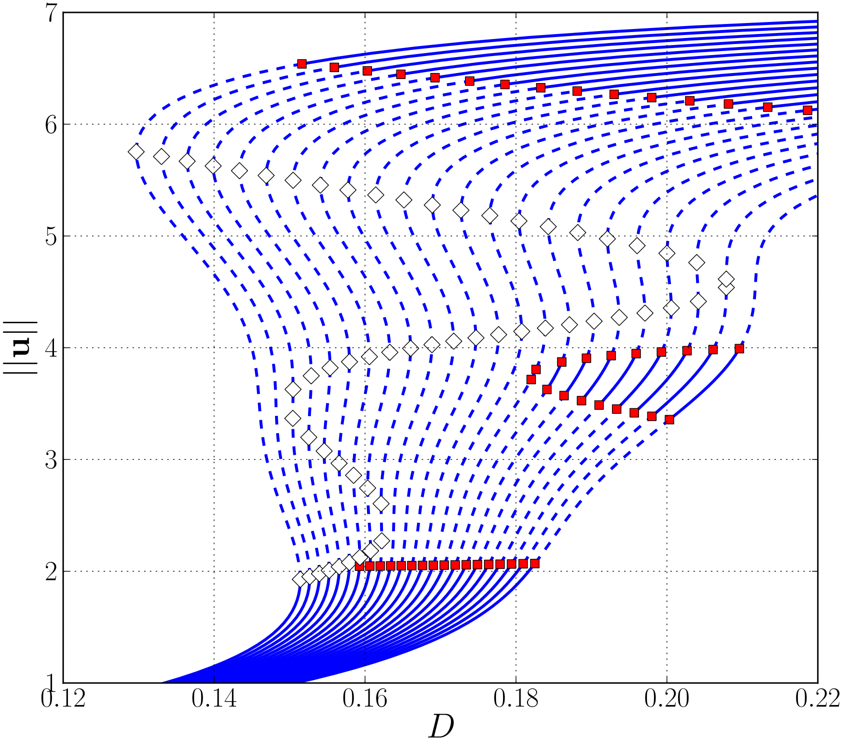
Note the two folds and the Hopf bifurcation .



A locus of folds (with blow-up) for the $A \to B \to C$ reaction.

Notice the two cusp singularities along the 2-parameter locus.

(There is a swallowtail singularity in nearby 3-parameter space.)



Stationary solution families for $\beta = 1.20,\ 1.21,\ \cdots\ ,\ 1.42.$
(Open diamonds mark folds, solid red squares mark Hopf points.)

Following Hopf Bifurcations

The extended system is

$$\mathbf{F}(\mathbf{u},\boldsymbol{\phi},\beta,\lambda;\mu) \;\equiv\; \begin{cases} \mathbf{f}(\mathbf{u},\lambda,\mu) \;=\; \mathbf{0}\ , \\[2ex] \mathbf{f}_{\mathbf{u}}(\mathbf{u},\lambda,\mu)\ \boldsymbol{\phi} \;-\; i\,\beta\,\boldsymbol{\phi} \;=\; \mathbf{0}\ , \\[2ex] \langle\ \boldsymbol{\phi}\ ,\ \boldsymbol{\phi}_0\ \rangle \;-\; 1 \;=\; 0\ , \end{cases}$$

where

$$\mathbf{F} \quad : \quad \mathbb{R}^n \times \mathbb{C}^n \times \mathbb{R}^2 \times \mathbb{R} \quad \rightarrow \quad \mathbb{R}^n \times \mathbb{C}^n \times \mathbb{C}\ ,$$

and to which we want to compute a solution family

$$(\ \mathbf{u}\ ,\ \boldsymbol{\phi}\ ,\ \beta\ ,\ \lambda\ ,\ \mu\ )\ ,$$

with

$$\mathbf{u} \in \mathbb{R}^n, \qquad \boldsymbol{\phi} \in \mathbb{C}^n, \qquad \beta,\ \lambda,\ \mu\ \in \mathbb{R}\ .$$

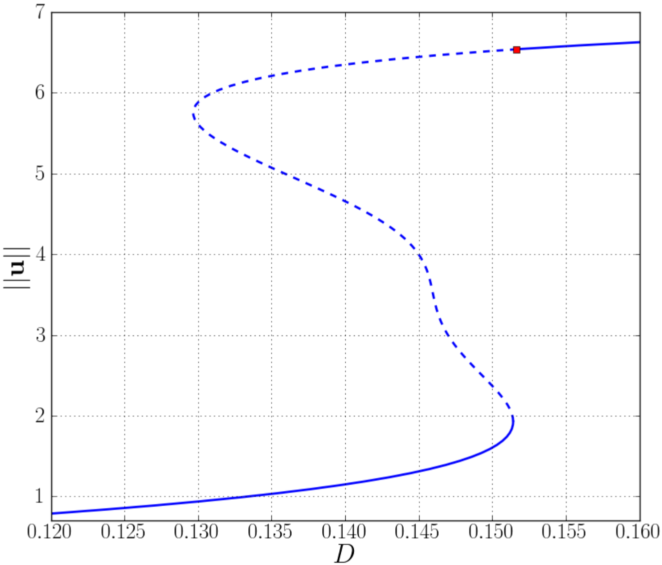
Above $\boldsymbol{\phi}_0$ belongs to a "reference solution "

$$(\ \mathbf{u}_0\ ,\ \boldsymbol{\phi}_0\ ,\ \beta_0\ ,\ \lambda_0\ ,\ \mu_0\ )\ ,$$

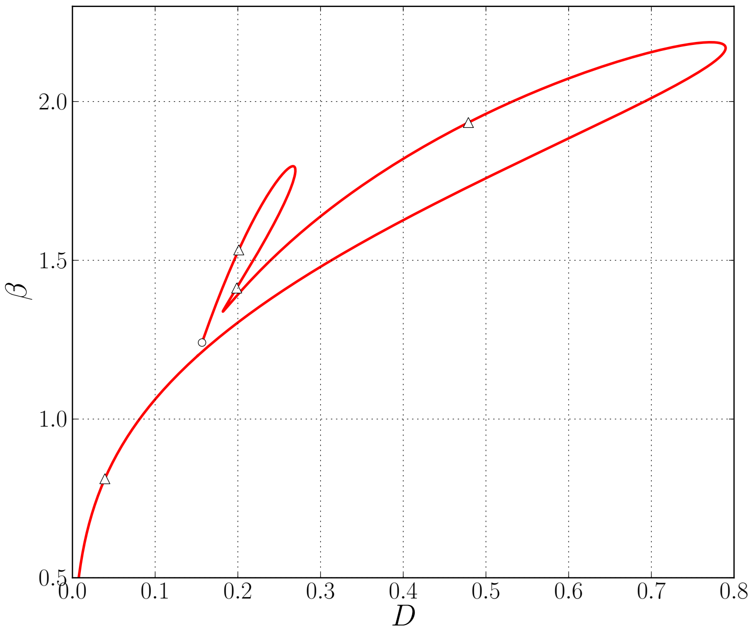
which normally is the latest computed solution along a family.

EXAMPLE : **The $A \to B \to C$ Reaction** .

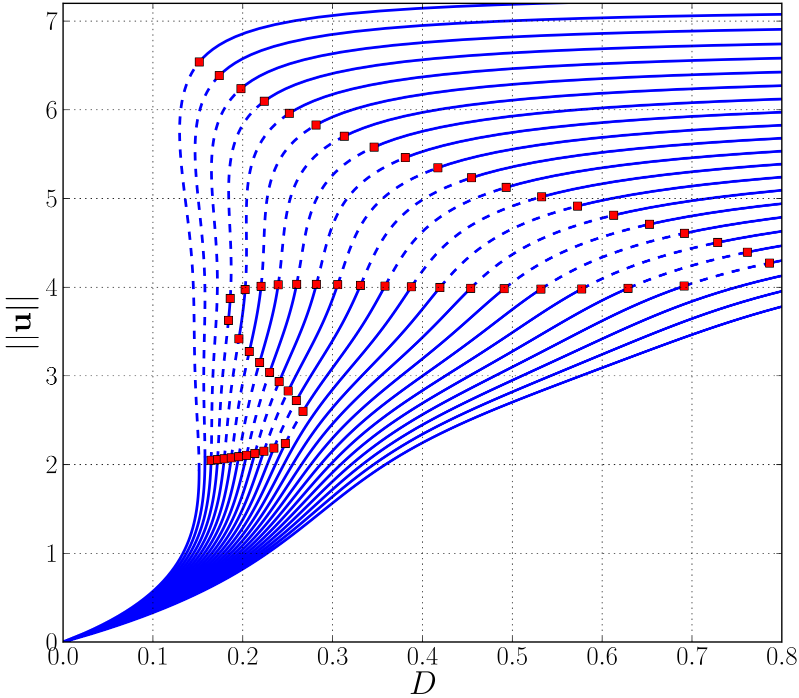
(Course demo : `Chemical-Reactions/ABC-Reaction/Hopf`)



The stationary family with Hopf bifurcation for $\beta = 1.20$.



The locus of Hopf bifurcations for the $A \longrightarrow B \longrightarrow C$ reaction.



Stationary solution families for $\beta = 1.20,\ 1.20,\ 1.25,\ 1.30,\ \cdots\ ,\ 2.30,$ with Hopf bifurcations (the red squares).

Boundary Value Problems

Consider the first order system of ordinary differential equations

$$\mathbf{u}'(t) \;-\; \mathbf{f}(\;\mathbf{u}(t)\;,\;\mu\;,\;\lambda\;)\;=\;\mathbf{0}\;, \qquad t \in [0,1]\;,$$

where

$$\mathbf{u}(\cdot)\;,\;\mathbf{f}(\cdot) \in \mathbb{R}^n\;, \qquad \lambda \in \mathbb{R}, \qquad \mu \in \mathbb{R}^{n_\mu}\;,$$

subject to boundary conditions

$$\mathbf{b}(\;\mathbf{u}(0)\;,\;\mathbf{u}(1)\;,\;\mu\;,\;\lambda\;)\;=\;\mathbf{0}\;, \qquad \mathbf{b}(\cdot) \in \mathbb{R}^{n_b}\;,$$

and integral constraints

$$\int_0^1 \mathbf{q}(\;\mathbf{u}(s)\;,\;\mu\;,\;\lambda\;)\;ds\;=\;\mathbf{0}\;, \qquad \mathbf{q}(\cdot) \in \mathbb{R}^{n_q}\;.$$

This boundary value problem (BVP) is of the form

$$\mathbf{F}(\ \mathbf{X}\ ) \quad = \quad \mathbf{0}\ ,$$

where

$$\mathbf{X} \quad = \quad (\ \mathbf{u}\ ,\ \mu\ ,\ \lambda\ )\ ,$$

to which we add the continuation equation

$$\langle\ \mathbf{X} - \mathbf{X}_0\ ,\ \dot{\mathbf{X}}_0\ \rangle\ -\ \Delta s \quad = \quad 0\ ,$$

where $\mathbf{X}_0$ represents the latest solution computed along the family.

In detail , the continuation equation is

$$\int_0^1 \langle\ \mathbf{u}(t) - \mathbf{u}_0(t)\ ,\ \dot{\mathbf{u}}_0(t)\ \rangle\ dt \ +\ \langle\ \mu - \mu_0\ ,\ \dot{\mu}_0\ \rangle$$
$$+\ (\lambda - \lambda_0)\dot{\lambda}_0 \ -\ \Delta s \ = 0\ .$$

NOTE :

- In the context of continuation we solve this BVP for $(\mathbf{u}(\cdot)\ ,\ \lambda\ ,\ \mu)$.

- In order for problem to be formally well-posed we must have

$$n_\mu \quad = \quad n_b + n_q - n \quad \geq \quad 0 \ .$$

- A simple case is

$$n_q = 0 \ , \qquad n_b = n \ , \qquad \text{for which} \quad n_\mu = 0 \ .$$

Discretization: Orthogonal Collocation

Introduce a mesh

$$\{ \, 0 \; = \; t_0 \; < \; t_1 \; < \; \cdots \; < \; t_N \; = \; 1 \, \} \, ,$$

where

$$h_j \; \equiv \; t_j \; - \; t_{j-1} \; , \qquad (1 \leq j \leq N) \; ,$$

Define the space of (vector) piecewise polynomials $\mathbb{P}_h^m$ as

$$\mathbb{P}_h^m \;\; \equiv \;\; \{ \; \mathbf{p}_h \in C[0,1] \; : \; \mathbf{p}_h \Big|_{[t_{j-1},t_j]} \in \mathbb{P}^m \; \} \; ,$$

where $\mathbb{P}^m$ is the space of (vector) polynomials of degree $\leq \; m$.

The collocation method consists of finding

$$\mathbf{p}_h \in \mathbb{P}_h^m \ , \qquad \mu \in \mathbb{R}^{n_\mu} \ ,$$

such that the following collocation equations are satisfied :

$$\mathbf{p}_h'(z_{j,i}) \ = \ \mathbf{f}(\ \mathbf{p}_h(z_{j,i})\ ,\ \mu,\ \lambda\ )\ , \qquad j = 1, \cdots, N\ , \quad i = 1, \cdots, m\ ,$$

and such that

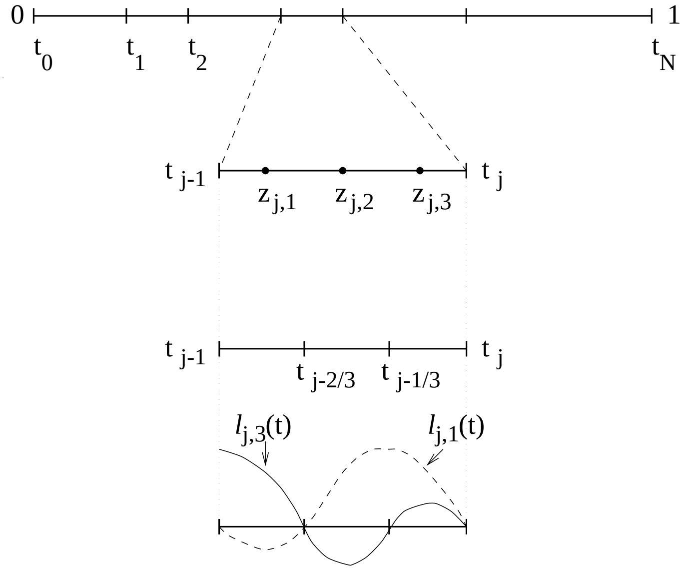
$$\mathbf{p}_h \ \text{ satisfies the } \ \text{boundary and integral conditions}\ .$$

The collocation points $z_{j,i}$ in each subinterval

$$[\ t_{j-1}\ ,\ t_j\ ]\ ,$$

are the (scaled) roots of the mth-degree orthogonal polynomial (Gauss points[3]).

[3] See Pages 261, 287 of the Background Notes on Elementary Numerical Methods.



The mesh $\{0 = t_0 < t_1 < \cdots < t_N \; = \; 1\}$, with collocation points and extended-mesh points shown for $m = 3$.

Also shown are two of the four local Lagrange basis polynomials .

Since each local polynomial is determined by

$$(m+1)\ n\ ,$$

coefficients, the total number of unknowns (considering λ as fixed) is

$$(m+1)\ n\ N\ +\ n_\mu\ .$$

This is matched by the total number of equations :

collocation : $m\ n\ N$,

continuity : $(N-1)\ n$,

constraints : $n_b\ +\ n_q\quad (\ =\ n\ +\ n_\mu\ )$.

Assume that the solution $\mathbf{u}(t)$ of the BVP is sufficiently smooth.

Then the order of accuracy of the orthogonal collocation method is m , *i.e.*,

$$\| \mathbf{p}_h - \mathbf{u} \|_\infty = \mathcal{O}(h^m) \ .$$

At the main meshpoints t_j we have superconvergence :

$$max_j \mid \mathbf{p}_h(t_j) - \mathbf{u}(t_j) \mid = \mathcal{O}(h^{2m}) \ .$$

The scalar variables λ and μ are also superconvergent .

Implementation

For each subinterval $[\ t_{j-1}\ ,\ t_j\ ]$, introduce the Lagrange basis polynomials

$$\{\ \ell_{j,i}(t)\ \}\ , \qquad j = 1, \cdots, N\ , \quad i = 0, 1, \cdots, m\ ,$$

defined by

$$\ell_{j,i}(t) \ = \ \prod_{k=0,k\neq i}^{m} \frac{t - t_{j-\frac{k}{m}}}{t_{j-\frac{i}{m}} \ - \ t_{j-\frac{k}{m}}}\ ,$$

where

$$t_{j-\frac{i}{m}} \ \equiv \ t_j \ - \ \frac{i}{m}\, h_j\ .$$

The local polynomials can then be written

$$\mathbf{p}_j(t) \ = \ \sum_{i=0}^{m} \ell_{j,i}(t)\ \mathbf{u}_{j-\frac{i}{m}}\ .$$

With the above choice of basis

$$\mathbf{u}_j \ \sim \ \mathbf{u}(t_j) \qquad \text{and} \qquad \mathbf{u}_{j-\frac{i}{m}} \ \sim \ \mathbf{u}(t_{j-\frac{i}{m}})\ ,$$

where $\mathbf{u}(t)$ is the solution of the continuous problem.

The collocation equations are

$$\mathbf{p}_j'(z_{j,i}) \ = \ \mathbf{f}(\ \mathbf{p}_j(z_{j,i})\ ,\ \mu\ ,\ \lambda\ )\ , \qquad i = 1, \cdots, m, \quad j = 1, \cdots, N\ .$$

The boundary conditions are

$$b_i(\ \mathbf{u}_0\ ,\ \mathbf{u}_N\ ,\ \mu\ ,\ \lambda\ )\ =\ 0\ , \qquad i = 1, \cdots, n_b\ .$$

The integral constraints can be discretized as

$$\sum_{j=1}^{N} \sum_{i=0}^{m} \omega_{j,i}\ q_k(\ \mathbf{u}_{j-\frac{i}{m}}\ ,\ \mu\ ,\ \lambda)\ =\ 0\ , \qquad k = 1, \cdots, n_q\ ,$$

where the $\omega_{j,i}$ are the Lagrange quadrature weights .

The continuation equation is

$$\int_0^1 \langle \mathbf{u}(t) - \mathbf{u}_0(t) , \dot{\mathbf{u}}_0(t) \rangle \, dt + \langle \mu - \mu_0 , \dot{\mu}_0 \rangle + (\lambda - \lambda_0) \dot{\lambda}_0 - \Delta s = 0 ,$$

where

$$(\mathbf{u}_0 , \mu_0 , \lambda_0) ,$$

is the previous solution along the solution family, and

$$(\dot{\mathbf{u}}_0 , \dot{\mu}_0 , \dot{\lambda}_0) ,$$

is the normalized direction of the family at the previous solution .

The discretized continuation equation is of the form

$$\sum_{j=1}^{N} \sum_{i=0}^{m} \omega_{j,i} \langle \mathbf{u}_{j-\frac{i}{m}} - (\mathbf{u}_0)_{j-\frac{i}{m}} , (\dot{\mathbf{u}}_0)_{j-\frac{i}{m}} \rangle$$

$$+ \langle \mu - \mu_0 , \dot{\mu}_0 \rangle + (\lambda - \lambda_0) \dot{\lambda}_0 - \Delta s = 0 .$$

Numerical Linear Algebra

The complete discretization consists of

$$m\,n\,N \;+\; n_b \;+\; n_q \;+\; 1\,,$$

nonlinear equations , with unknowns

$$\{\mathbf{u}_{j-\frac{i}{m}}\} \in \mathbb{R}^{mnN+n}\,, \qquad \mu \in \mathbb{R}^{n_\mu}\,, \qquad \lambda \in \mathbb{R}\,.$$

These equations are solved by a Newton-Chord iteration .

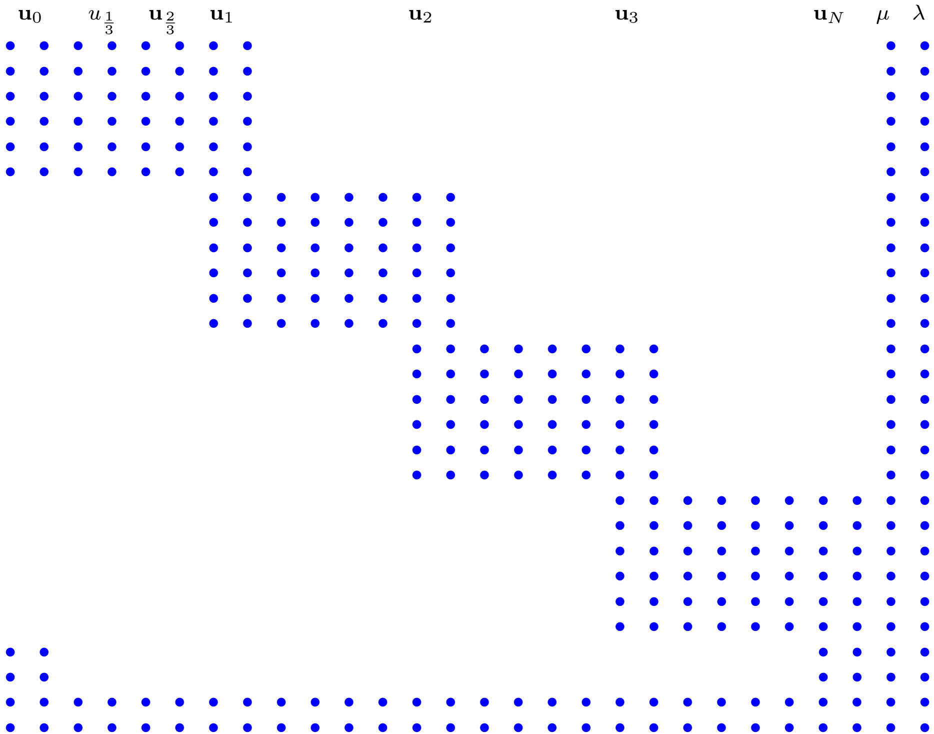
We illustrate the numerical linear algebra for the case

$$n = 2 \text{ ODEs} \quad , \quad N = 4 \text{ mesh intervals} \quad , \quad m = 3 \text{ collocation points} ,$$

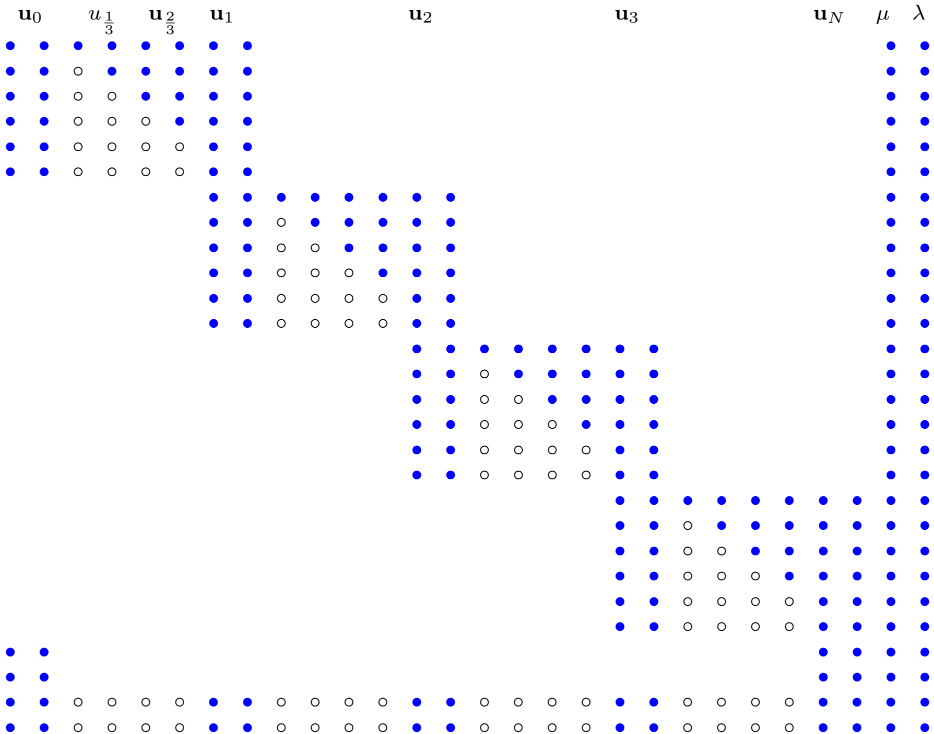
$$n_b = 2 \text{ boundary conditions} \quad , \quad n_q = 1 \text{ integral constraint} ,$$

and the continuation equation.

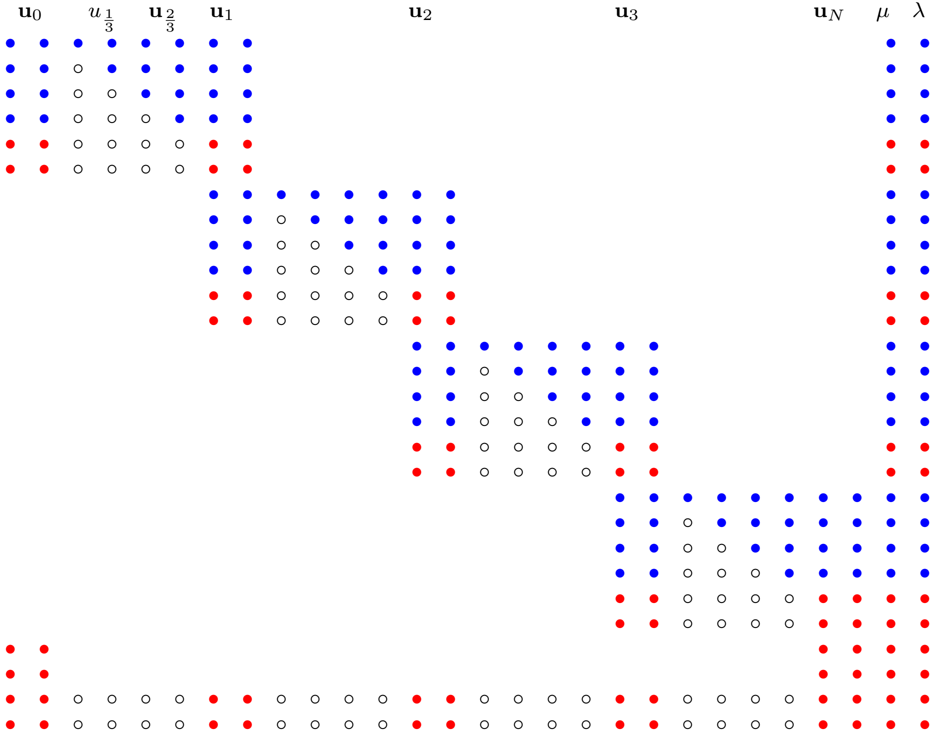
- The operations are also done on the right hand side , which is not shown.
- Entries marked "∘" have been eliminated by Gauss elimination.
- Entries marked "·" denote fill-in due to pivoting .
- Most of the operations can be done in parallel .



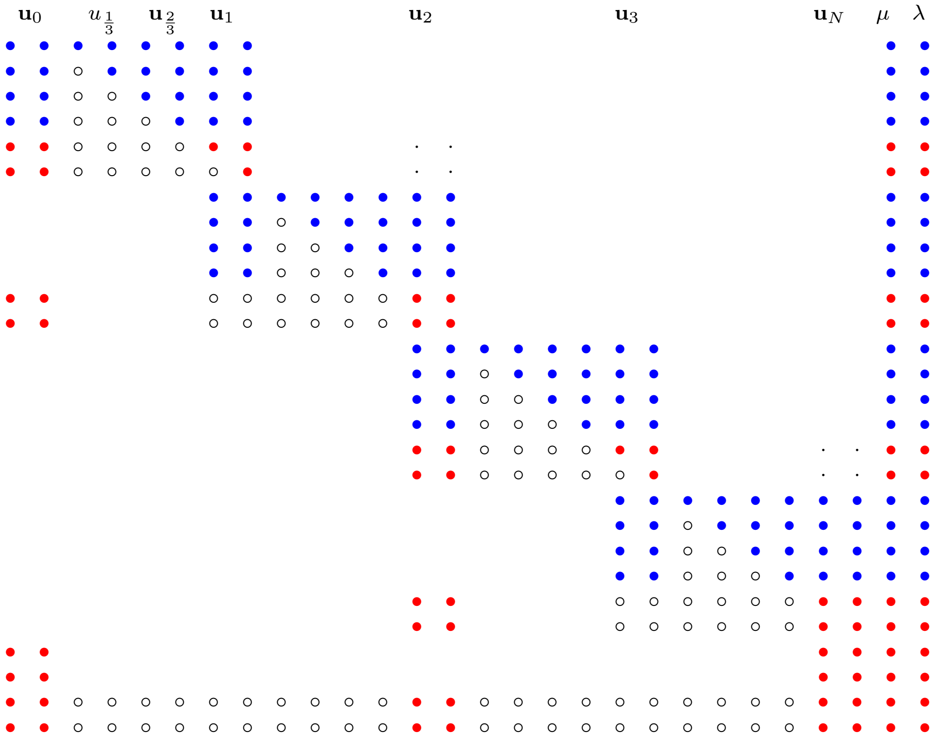
The structure of the Jacobian .



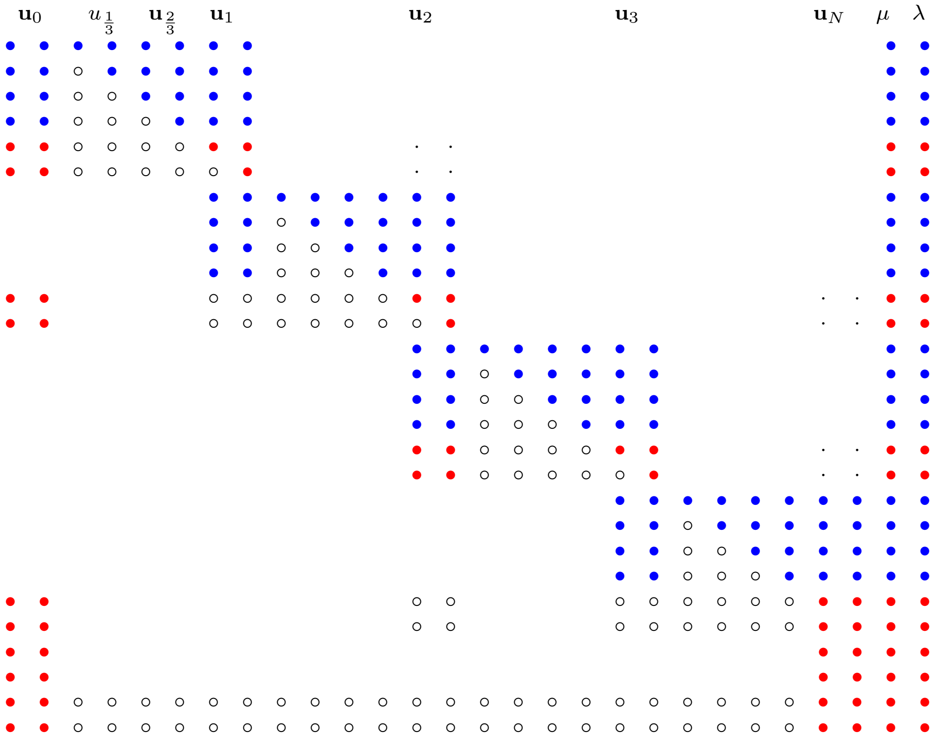
The system after condensation of parameters, which can be done in parallel .



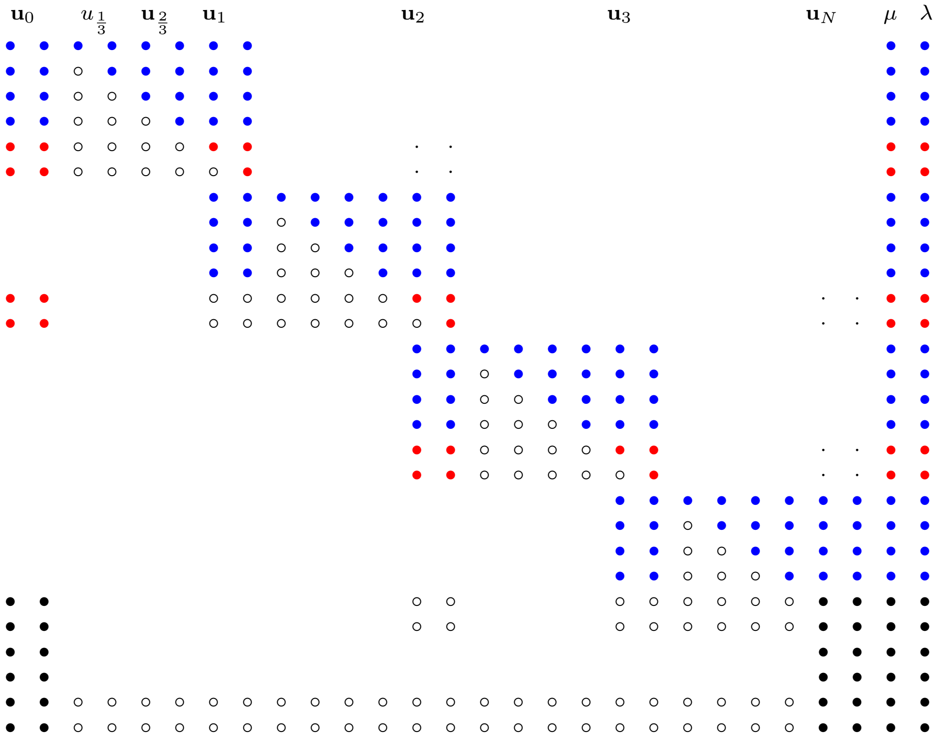
The preceding matrix, showing the decoupled • subsystem .



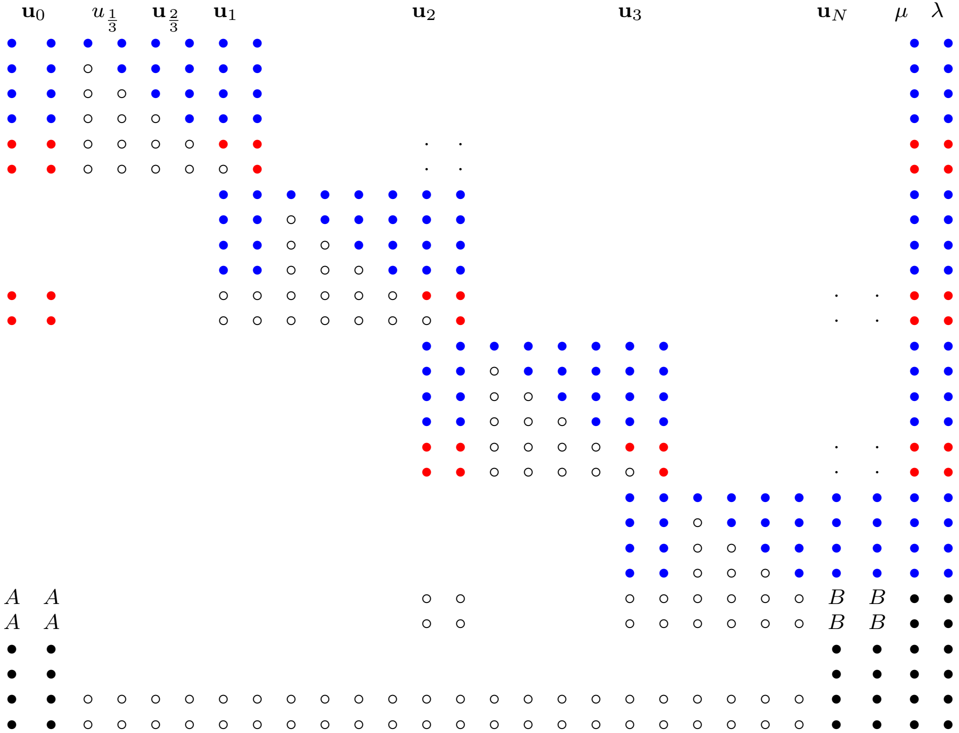
Stage 1 of the nested dissection to solve the decoupled ● subsystem.



Stage 2 of the nested dissection to solve the decoupled • subsystem.



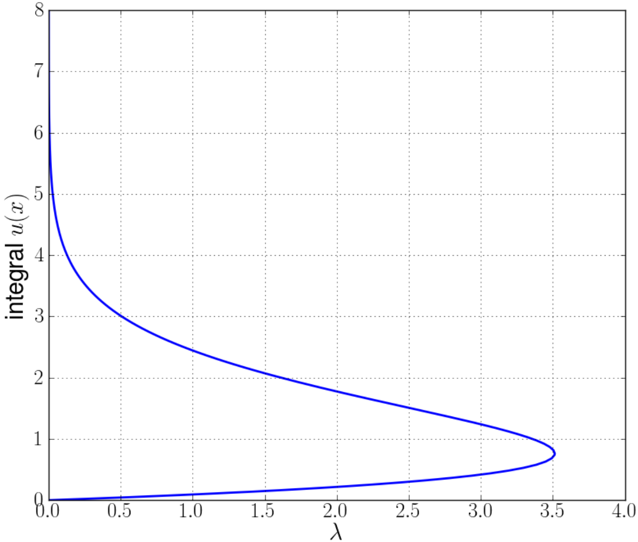
The preceding matrix showing the final decoupled ● subsystem .



The approximate Floquet multipliers are the eigenvalues of $\mathbf{M} \equiv -\mathbf{B}^{-1}\mathbf{A}$.

Accuracy Test

The Table shows the location of the fold in the Gelfand-Bratu problem, for 4 Gauss collocation points per mesh interval, and N mesh intervals .



N	Fold location
2	3.5137897550
4	3.5138308601
8	3.5138307211
16	3.5138307191
32	3.5138307191

Periodic Solutions

- Periodic solutions can be computed efficiently using a BVP approach.

- This method also determines the period very accurately.

- Moreover, the technique can compute unstable periodic orbits.

Consider

$$\mathbf{u}'(t) \;=\; \mathbf{f}(\;\mathbf{u}(t)\;,\;\lambda\;)\;, \qquad \mathbf{u}(\cdot)\;,\;\mathbf{f}(\cdot)\in\mathbb{R}^n\;, \qquad \lambda\in\mathbb{R}\;.$$

Fix the interval of periodicity by the transformation

$$t \;\rightarrow\; \frac{t}{T}\;.$$

Then the equation becomes

$$\boxed{\mathbf{u}'(t) \;=\; T\;\mathbf{f}(\;\mathbf{u}(t)\;,\;\lambda\;)}\;, \qquad \mathbf{u}(\cdot)\;,\;\mathbf{f}(\cdot)\in\mathbb{R}^n\;, \qquad T\;,\;\lambda\in\mathbb{R}\;.$$

and we seek solutions of period 1 , *i.e.*,

$$\boxed{\mathbf{u}(0) \;=\; \mathbf{u}(1)}\;.$$

Note that the period T is one of the unknowns .

The above equations do not uniquely specify $\mathbf{u}$ and T :

Assume that we have computed

$$(\ \mathbf{u}_{k-1}(\cdot) \ , \ T_{k-1} \ , \ \lambda_{k-1} \ ) \ ,$$

and we want to compute the next solution

$$(\ \mathbf{u}_{k}(\cdot) \ , \ T_{k} \ , \ \lambda_{k} \ ) \ .$$

Then $\mathbf{u}_k(t)$ can be translated freely in time :

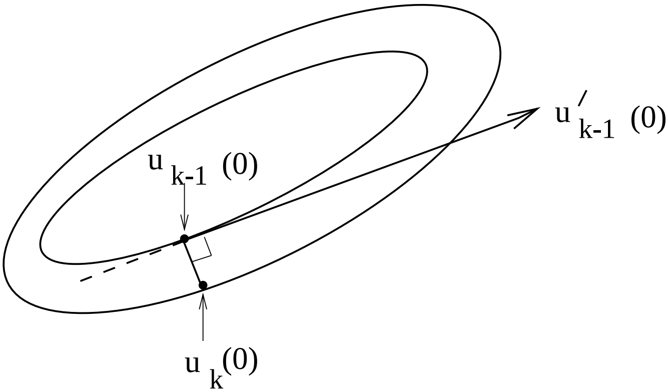
If $\mathbf{u}_k(t)$ is a periodic solution, then so is $\mathbf{u}_k(t + \sigma)$, for any σ .

Thus, a phase condition is needed.

An example is the Poincaré phase condition

$$\langle \mathbf{u}_k(0) - \mathbf{u}_{k-1}(0) , \mathbf{u}'_{k-1}(0) \rangle = 0 .$$

(But we will derive a numerically more suitable integral phase condition .)



Graphical interpretation of the Poincaré phase condition.

An Integral Phase Condition

If $\tilde{\mathbf{u}}_k(t)$ is a solution then so is

$$\tilde{\mathbf{u}}_k(t+\sigma) \ ,$$

for any σ .

We want the solution that minimizes

$$D(\sigma) \ \equiv \ \int_0^1 \| \ \tilde{\mathbf{u}}_k(t+\sigma) \ - \ \mathbf{u}_{k-1}(t) \ \|_2^2 \ dt \ .$$

The optimal solution

$$\tilde{\mathbf{u}}_k(t+\hat{\sigma}) \ ,$$

must satisfy the necessary condition

$$D'(\hat{\sigma}) \ = \ 0 \ .$$

Differentiation gives the necessary condition

$$\int_0^1 \langle\ \tilde{\mathbf{u}}_k(t+\hat{\sigma})\ -\ \mathbf{u}_{k-1}(t)\ ,\ \tilde{\mathbf{u}}_k'(t+\hat{\sigma}\ \rangle\ dt\ =\ 0\ .$$

Writing

$$\mathbf{u}_k(t)\ \equiv\ \tilde{\mathbf{u}}_k(t+\hat{\sigma})\ ,$$

gives

$$\int_0^1 \langle\ \mathbf{u}_k(t)\ -\ \mathbf{u}_{k-1}(t)\ ,\ \mathbf{u}_k'(t)\ \rangle\ dt\ =\ 0\ .$$

Integration by parts, using periodicity, gives

$$\boxed{\int_0^1\ \langle\ \mathbf{u}_k(t)\ ,\ \mathbf{u}_{k-1}'(t)\ \rangle\ dt\ =\ 0\ .}$$

This is the integral phase condition.

Continuation of Periodic Solutions

- Pseudo-arclength continuation is used to follow periodic solutions .

- It allows computation past folds along a family of periodic solutions.

- It also allows calculation of a "vertical family" of periodic solutions.

For periodic solutions the continuation equation is

$$\int_0^1 \langle \mathbf{u}_k(t) - \mathbf{u}_{k-1}(t) \ , \ \dot{\mathbf{u}}_{k-1}(t) \ \rangle \ dt \ + \ (T_k - T_{k-1})\dot{T}_{k-1} \ + \ (\lambda_k - \lambda_{k-1})\dot{\lambda}_{k-1} = \Delta s \ .$$

SUMMARY :

We have the following equations for periodic solutions :

$$\mathbf{u}_k'(t) \ = \ T\ \mathbf{f}(\ \mathbf{u}_k(t)\ ,\ \lambda_k\ )\ ,$$

$$\mathbf{u}_k(0) \ = \ \mathbf{u}_k(1)\ ,$$

$$\int_0^1 \langle\ \mathbf{u}_k(t)\ ,\ \mathbf{u}_{k-1}^{'}(t)\ \rangle\ dt \ = \ 0\ ,$$

with continuation equation

$$\int_0^1 \langle\ \mathbf{u}_k(t) - \mathbf{u}_{k-1}(t)\ ,\ \dot{\mathbf{u}}_{k-1}(t)\ \rangle\ dt\ +\ (T_k - T_{k-1})\dot{T}_{k-1}\ +\ (\lambda_k - \lambda_{k-1})\dot{\lambda}_{k-1} = \Delta s\ ,$$

where

$$\mathbf{u}(\cdot)\ ,\ \mathbf{f}(\cdot)\ \in\ \mathbb{R}^n\ , \qquad \lambda\ , T\ \in\ \mathbb{R}\ .$$

Stability of Periodic Solutions

In our continuation context, a periodic solution of period T satisfies

$$\mathbf{u}'(t) \;=\; T\,\mathbf{f}(\,\mathbf{u}(t))\;, \qquad \text{for } t \in [0,1]\;,$$

$$\mathbf{u}(0) \;=\; \mathbf{u}(1)\;,$$

(for given value of the continuation parameter λ).

A small perturbation in the initial condition

$$\mathbf{u}(0) \;+\; \epsilon\,\mathbf{v}(0)\;, \qquad \epsilon \text{ small}\;\;,$$

leads to the linearized equation

$$\mathbf{v}'(t) \;=\; T\,\mathbf{f}_{\mathbf{u}}(\,\mathbf{u}(t)\,)\,\mathbf{v}(t)\;, \qquad \text{for } t \in [0,1]\;,$$

which induces a linear map

$$\mathbf{v}(0) \;\rightarrow\; \mathbf{v}(1)\;,$$

represented by

$$\mathbf{v}(1) \;=\; \mathbf{M}\,\mathbf{v}(0)\;.$$

$$\mathbf{v}(1) \;=\; \mathbf{M}\ \mathbf{v}(0)$$

The eigenvalues of $\mathbf{M}$ are the Floquet multipliers that determine stability.

$\mathbf{M}$ always has a multiplier $\mu = 1$, since differentiating

$$\mathbf{u}'(t) \;=\; T\ \mathbf{f}(\ \mathbf{u}(t))\ ,$$

gives

$$\mathbf{v}'(t) \;=\; T\ \mathbf{f}_{\mathbf{u}}(\ \mathbf{u}(t)\ )\ \mathbf{v}(t)\ ,$$

where

$$\mathbf{v}(t) \;=\; \mathbf{u}'(t)\ , \quad \text{with} \quad \mathbf{v}(0) \;=\; \mathbf{v}(1)\ .$$

$$\mathbf{v}(1) \;=\; \mathbf{M}\;\mathbf{v}(0)$$

- If $\mathbf{M}$ has a Floquet multiplier μ with $|\,\mu\,| \;>\; 1$ then $\mathbf{u}(t)$ is unstable .

- If all multipliers (other than $\mu = 1$) satisfy $|\,\mu\,| \;<\; 1$ then $\mathbf{u}(t)$ is stable .

- At folds and branch points there are two multipliers $\mu = 1$.

- At a period-doubling bifurcation there is a real multiplier $\mu = -1$.

- At a torus bifurcation there is a complex pair on the unit circle.

EXAMPLE : **The Lorenz Equations** .

(`Course demo` : `Lorenz`)

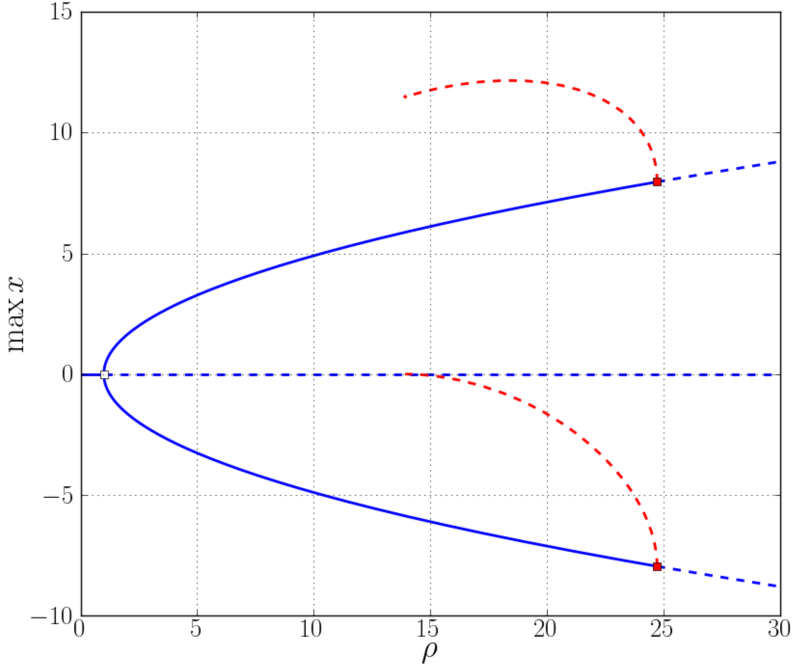
These equations were introduced in 1963 by Edward Lorenz (1917-2008)

as a simple model of atmospheric convection :

$$
\begin{aligned}
x' &= \sigma\ (y - x)\ , \\
y' &= \rho\ x\ -\ y\ -\ x\ z\ , \\
z' &= x\ y\ -\ \beta\ z\ ,
\end{aligned}
$$

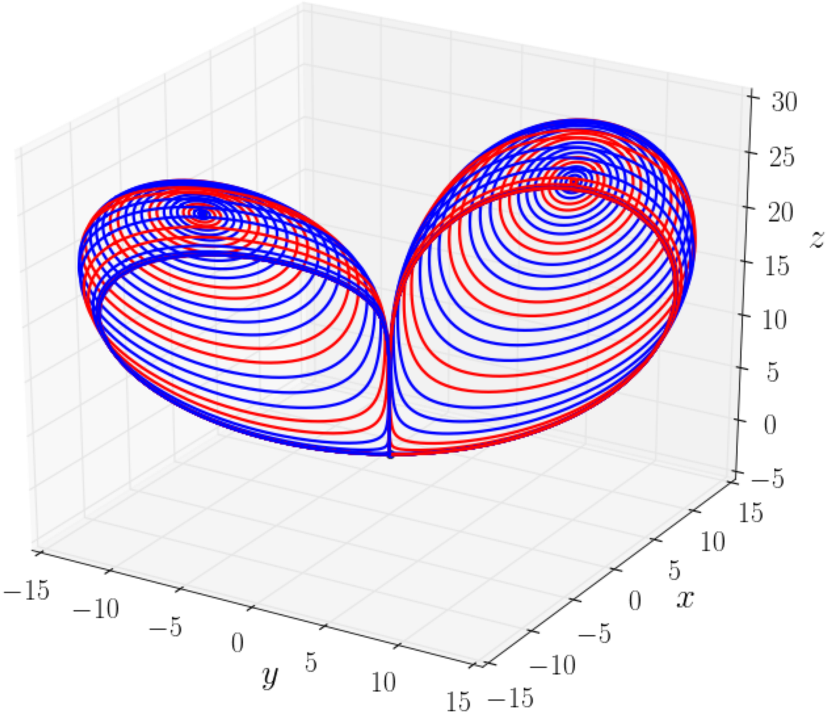
where (often)

$$\sigma = 10 \quad , \quad \beta = 8/3 \quad , \quad \rho = 28\ .$$



Bifurcation diagram of the Lorenz equations for $\sigma = 10$ and $\beta = 8/3$.

Course demo : Lorenz/Basic



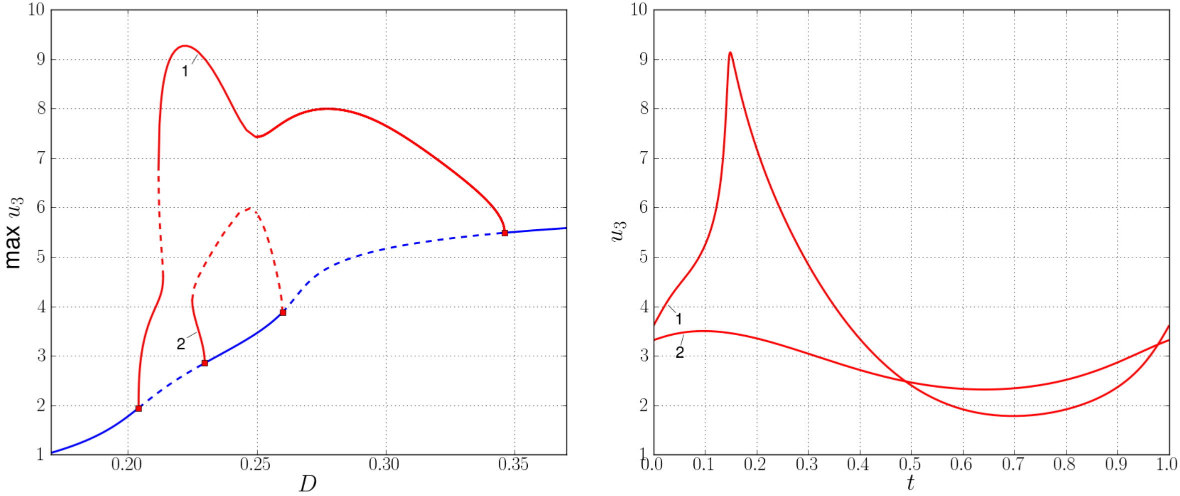
Unstable periodic orbits of the Lorenz equations.

In the Lorenz Equations :

- The zero stationary solution is unstable for $\rho > 1$.
- Two nonzero stationary families bifurcate at $\rho = 1$.
- The nonzero stationary solutions are unstable for $\rho > \rho_H$.
- At $\rho_H \approx 24.7$ there are Hopf bifurcations .
- Unstable periodic solution families emanate from the Hopf bifurcations.
- These families end in homoclinic orbits (infinite period) at $\rho \approx 13.9$.
- At $\rho = 28$ (and a range of other values) there is the Lorenz attractor .

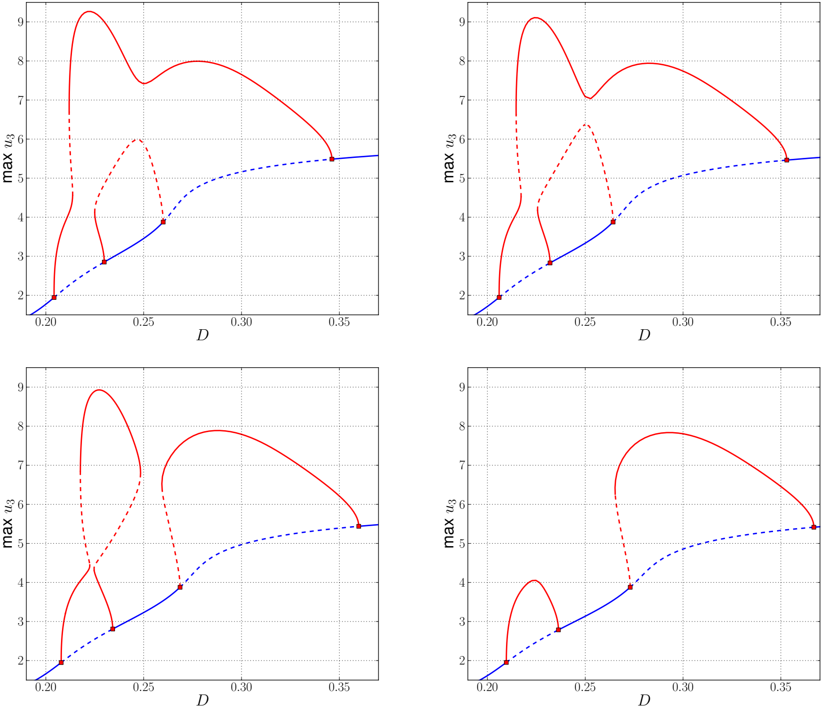
EXAMPLE : **The $A \to B \to C$ Reaction** .

(`Course demo` : `Chemical-Reactions/ABC-Reaction/Periodic`)



Stationary and periodic solution families of the $A \to B \to C$ reaction: $\beta = 1.55$.

Note the coexistence of stable solutions, for example, solutions 1 and 2 .



Top left: $\beta = 1.55$, right: $\beta = 1.56$, Bottom left: $\beta = 1.57$, right: $\beta = 1.58$.

(**QUESTION** : Is something missing somewhere ?)

Following Folds for Periodic Solutions

Recall that periodic orbits families can be computed using the equations

$$\mathbf{u}'(t) \; - \; T \, \mathbf{f}(\, \mathbf{u}(t) \, , \, \lambda \,) \; = \; \mathbf{0} \, ,$$

$$\mathbf{u}(0) \; - \; \mathbf{u}(1) \; = \; \mathbf{0} \, ,$$

$$\int_0^1 \langle \, \mathbf{u}(t) \, , \; \mathbf{u}_0'(t) \, \rangle \, dt \; = \; 0 \, ,$$

where $\mathbf{u}_0$ is a reference orbit , typically the latest computed orbit.

The above boundary value problem is of the form

$$\mathbf{F}(\, \mathbf{X} \, , \, \lambda \,) \; = \; \mathbf{0} \, ,$$

where

$$\mathbf{X} \; = \; (\, \mathbf{u} \, , \, T \,) \, .$$

At a fold with respect to λ we have

$$\mathbf{F}_{\mathbf{X}}(\ \mathbf{X}\ ,\ \lambda\ )\ \mathbf{\Phi}\ \ =\ \ \mathbf{0}\ ,$$

$$\langle\ \mathbf{\Phi}\ ,\ \mathbf{\Phi}\ \rangle\ \ =\ \ 1\ ,$$

where

$$\mathbf{X}\ \ =\ \ (\ \mathbf{u}\ ,\ T\ )\qquad ,\qquad \mathbf{\Phi}\ \ =\ \ (\ \mathbf{v}\ ,\ S\ )\ ,$$

i.e., the linearized equations about $\mathbf{X}$ have a nonzero solution $\mathbf{\Phi}$.

In detail :

$$\mathbf{v}'(t)\ -\ T\ \mathbf{f}_{\mathbf{u}}(\ \mathbf{u}(t)\ ,\ \lambda\ )\ \mathbf{v}\ -\ S\ \mathbf{f}(\ \mathbf{u}(t)\ ,\ \lambda\ )\ \ =\ \ \mathbf{0}\ ,$$

$$\mathbf{v}(0)\ -\ \mathbf{v}(1)\ \ =\ \ \mathbf{0}\ ,$$

$$\int_0^1\ \langle\ \mathbf{v}(t)\ ,\ \mathbf{u}_0'(t)\ \rangle\ dt\ \ =\ \ 0\ ,$$

$$\int_0^1\ \langle\ \mathbf{v}(t)\ ,\ \mathbf{v}(t)\ \rangle\ dt\ \ +\ \ S^2\ \ =\ \ 1\ .$$

The complete extended system to follow a fold is

$$\mathbf{F}(\ \mathbf{X}\ ,\ \lambda\ ,\ \mu\ )\ =\ \mathbf{0}\ ,$$

$$\mathbf{F_X}(\ \mathbf{X}\ ,\ \lambda\ ,\ \mu\ )\ \mathbf{\Phi}\ =\ \mathbf{0}\ ,$$

$$\langle\ \mathbf{\Phi}\ ,\ \mathbf{\Phi}\ \rangle\ -\ 1\ =\ 0\ ,$$

with two free problem parameters λ and μ .

To the above we add the continuation equation

$$\langle\ \mathbf{X}-\mathbf{X}_0\ ,\ \dot{\mathbf{X}}_0\ \rangle\ +\ \langle\ \mathbf{\Phi}-\mathbf{\Phi}_0\ ,\ \dot{\mathbf{\Phi}}_0\ \rangle\ +\ (\lambda-\lambda_0)\ \dot{\lambda}_0\ +\ (\mu-\mu_0)\ \dot{\mu}_0\ -\ \Delta s\ =\ 0\ .$$

In detail :
$$\mathbf{u}'(t) \; - \; T \, \mathbf{f}(\, \mathbf{u}(t) \, , \, \lambda \, , \, \mu \,) \; = \; \mathbf{0} \, ,$$
$$\mathbf{u}(0) \; - \; \mathbf{u}(1) \; = \; \mathbf{0} \, ,$$
$$\int_0^1 \langle \, \mathbf{u}(t) \, , \, \mathbf{u}_0'(t) \, \rangle \, dt \; = \; 0 \, ,$$

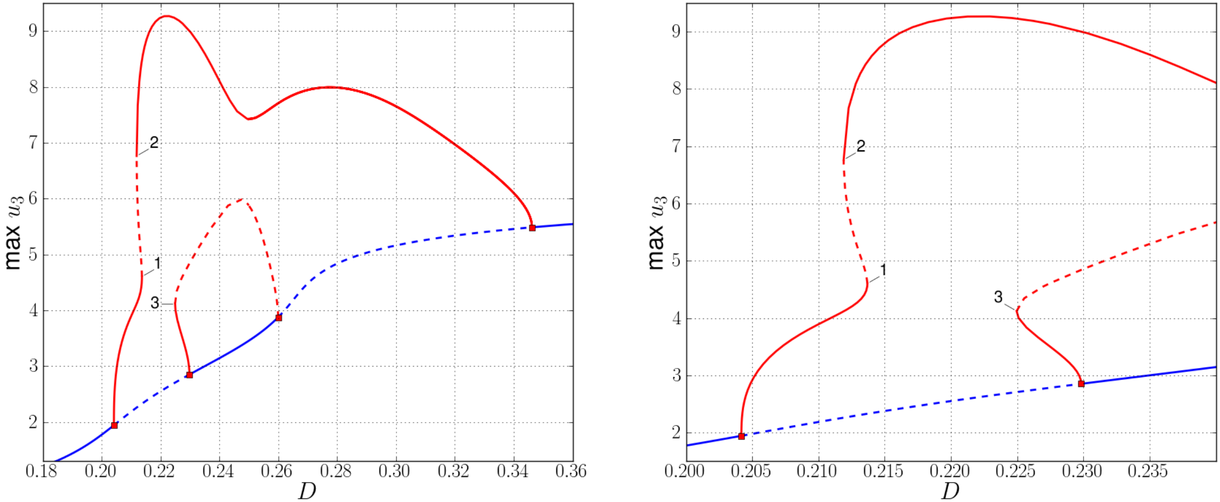
$$\mathbf{v}'(t) \; - \; T \, \mathbf{f}_{\mathbf{u}}(\, \mathbf{u}(t) \, , \, \lambda \, , \, \mu \,) \, \mathbf{v} \; - \; S \, \mathbf{f}(\, \mathbf{u}(t) \, , \, \lambda \, , \, \mu \,) \; = \; \mathbf{0} \, ,$$
$$\mathbf{v}(0) \; - \; \mathbf{v}(1) \; = \; \mathbf{0} \, ,$$
$$\int_0^1 \langle \, \mathbf{v}(t) \, , \, \mathbf{u}_0'(t) \, \rangle \, dt \; = \; 0 \, ,$$

with normalization
$$\int_0^1 \langle \, \mathbf{v}(t) \, , \, \mathbf{v}(t) \, \rangle \, dt \; + \; S^2 \; - \; 1 \; = \; 0 \, ,$$

and continuation equation
$$\int_0^1 \langle \, \mathbf{u}(t) - \mathbf{u}_0(t) \, , \, \dot{\mathbf{u}}_0(t) \, \rangle \, dt \; + \; \int_0^1 \langle \, \mathbf{v}(t) - \mathbf{v}_0(t) \, , \, \dot{\mathbf{v}}_0(t) \, \rangle \, dt \; +$$
$$+ \; (T_0 - T)\dot{T}_0 \; + \; (S_0 - S)\dot{S}_0 \; + \; (\lambda - \lambda_0)\dot{\lambda}_0 \; + \; (\mu - \mu_0)\dot{\mu}_0 \; - \; \Delta s \; = \; 0 \, .$$

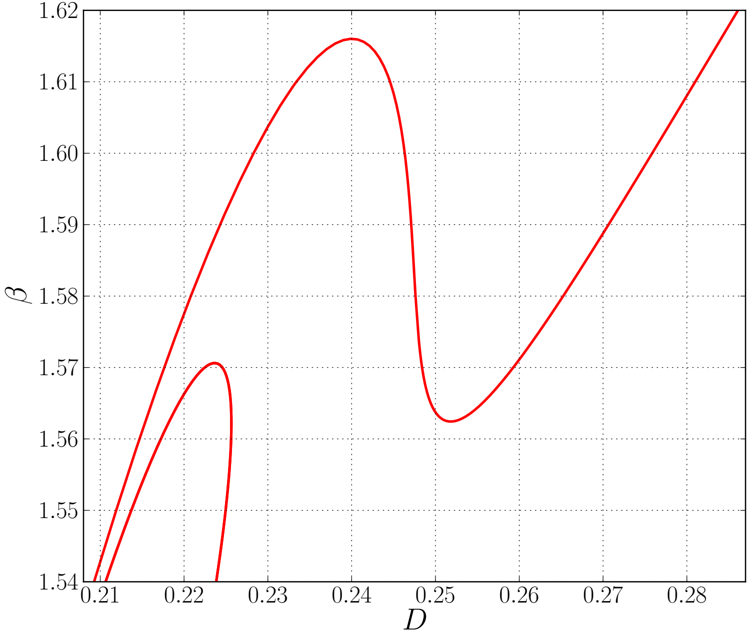
EXAMPLE : **The $A \to B \to C$ Reaction** .

(`Course demo` : `Chemical-Reactions/ABC-Reaction/Folds-PS`)

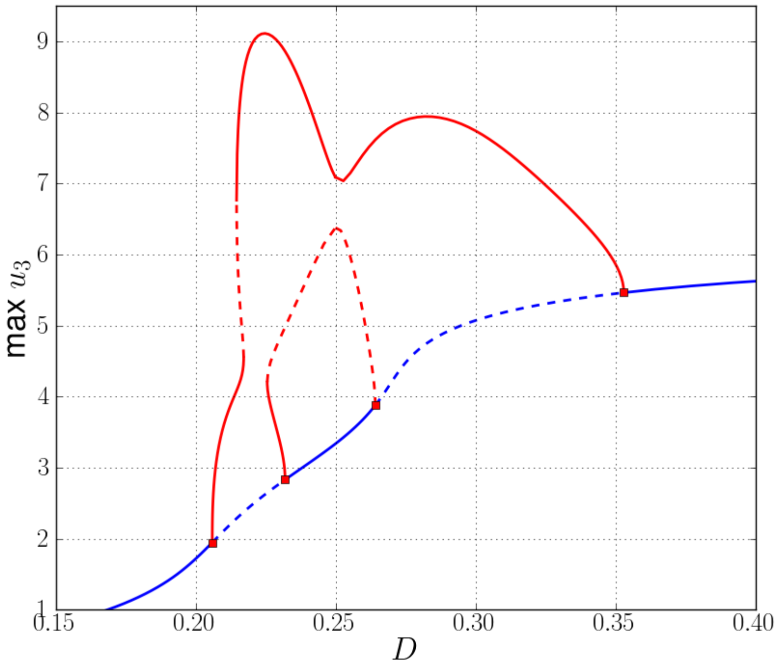


Stationary and periodic solution families of the $A \to B \to C$ reaction .

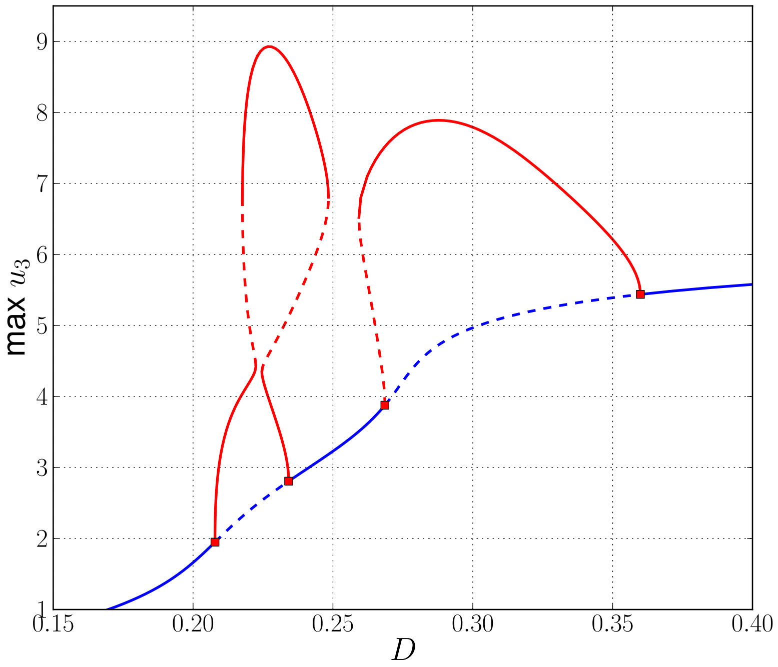
(with blow-up) for $\beta = 1.55$. Note the three folds , labeled 1, 2, 3 .



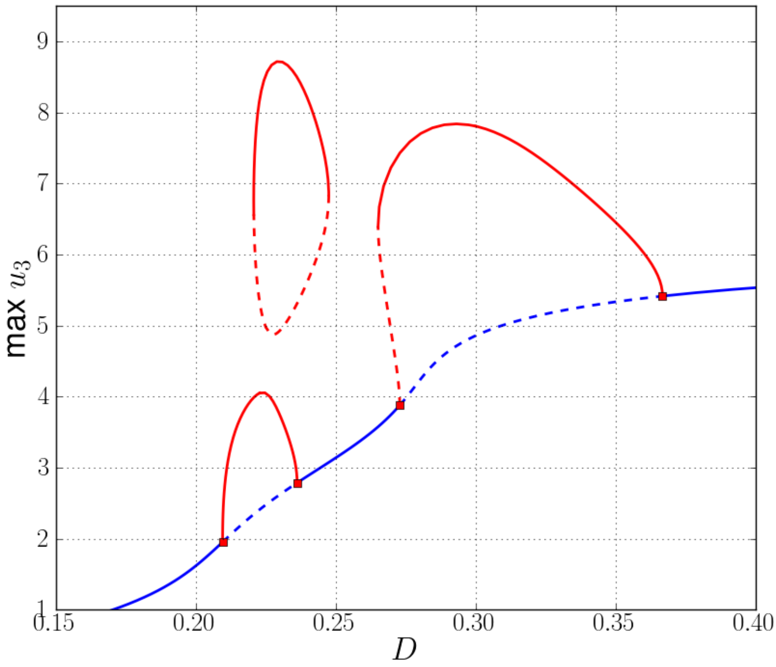
Loci of folds along periodic solution families for the $A \to B \to C$ reaction.



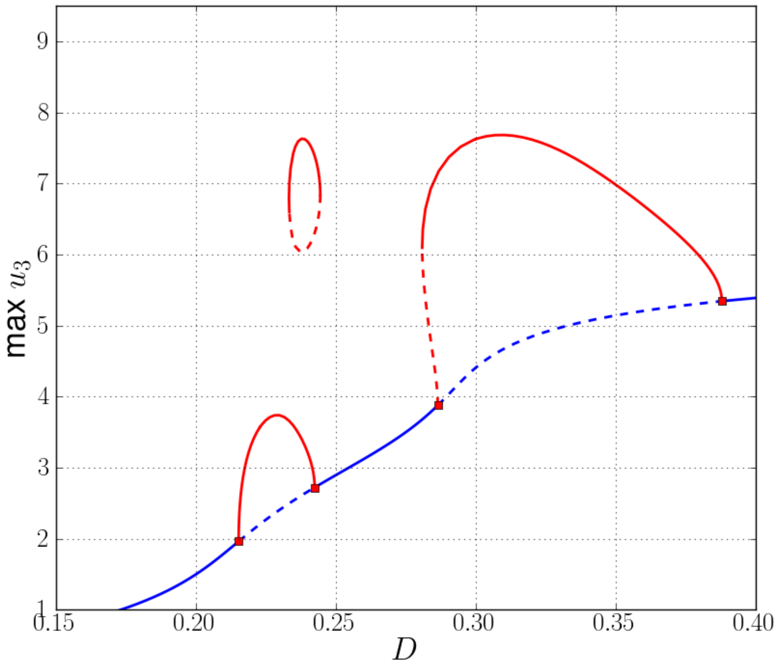
Stationary and periodic solution families of the $A \rightarrow B \rightarrow C$ reaction: $\beta = 1.56$.



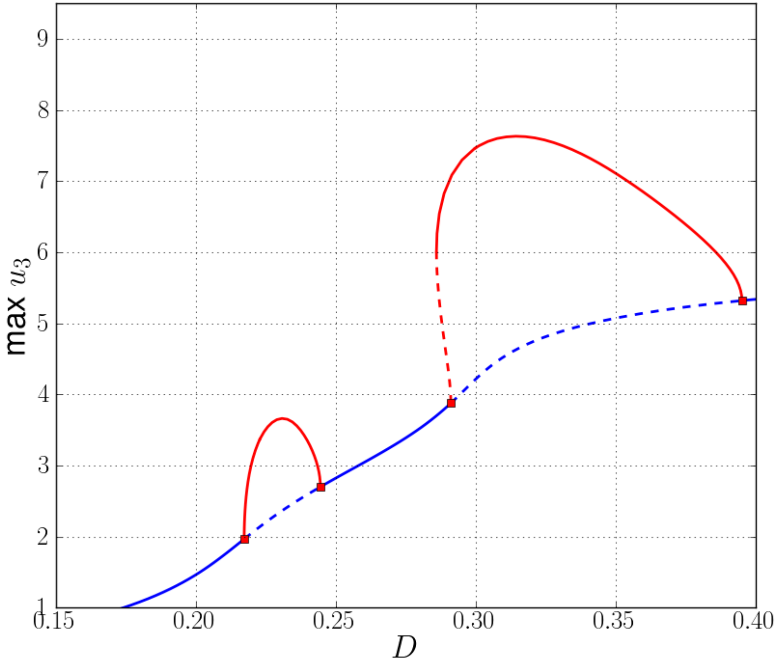
Stationary and periodic solution families of the $A \rightarrow B \rightarrow C$ reaction: $\beta = 1.57$.



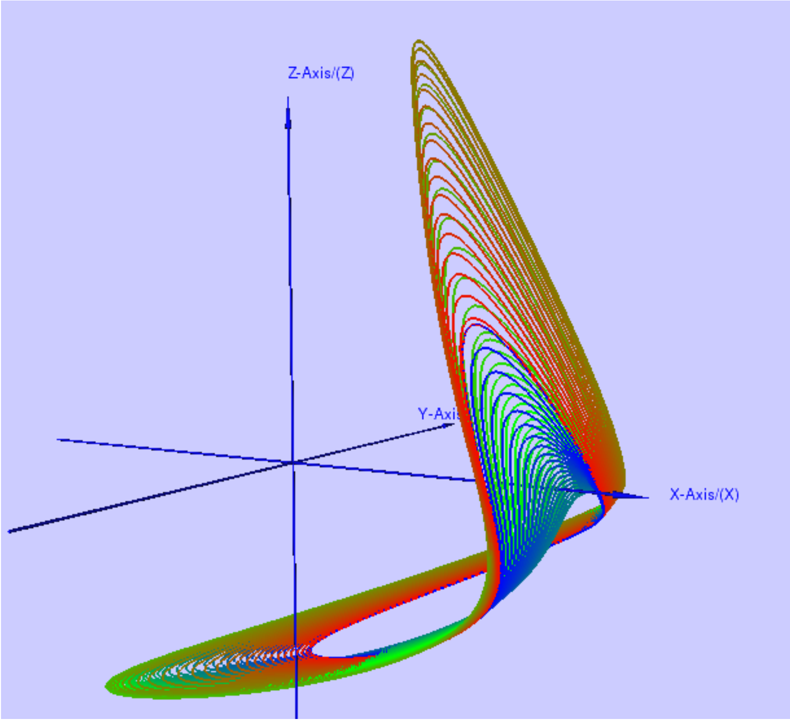
Stationary and periodic solution families of the $A \rightarrow B \rightarrow C$ reaction: $\beta = 1.58$.



Stationary and periodic solution families of the $A \to B \to C$ reaction: $\beta = 1.61$.



Stationary and periodic solution families of the $A \to B \to C$ reaction: $\beta = 1.62$.



Periodic solutions along the isola for $\beta = 1.58$.
(Stable solutions are blue, unstable solutions are red.)

Following Period-doubling Bifurcations

Let $(\ \mathbf{u}(t)\ ,\ T\ )$ be a periodic solution , *i.e.*, a solution of

$$\mathbf{u}'(t)\ -\ T\,\mathbf{f}(\ \mathbf{u}(t)\ ,\ \lambda\ )\ =\ \mathbf{0}\ ,$$

$$\mathbf{u}(0)\ -\ \mathbf{u}(1)\ =\ \mathbf{0}\ ,$$

$$\int_0^1 \langle\ \mathbf{u}(t)\ ,\ \mathbf{u}_0'(t)\ \rangle\ dt\ =\ 0\ ,$$

where $\mathbf{u}_0$ is a reference orbit .

A necessary condition for a period-doubling bifurcation is that the following linearized system have a nonzero solution $\mathbf{v}(t)$:

$$\mathbf{v}'(t)\ -\ T\,\mathbf{f}_{\mathbf{u}}(\ \mathbf{u}(t)\ ,\ \lambda\ )\ \mathbf{v}(t)\ =\ \mathbf{0}\ ,$$

$$\mathbf{v}(\mathbf{0})\ +\ \mathbf{v}(\mathbf{1})\ =\ \mathbf{0}\ ,$$

$$\int_0^1 \langle\ \mathbf{v}(t)\ ,\ \mathbf{v}(t)\ \rangle\ dt\ =\ 1\ .$$

The complete extended system to follow a period-doubling bifurcation is

$$\mathbf{u}'(t) \; - \; T\,\mathbf{f}(\;\mathbf{u}(t)\;,\;\lambda\;,\;\mu\;) \;=\; \mathbf{0}\;,$$

$$\mathbf{u}(0) \; - \; \mathbf{u}(1) \;=\; \mathbf{0}\;,$$

$$\int_0^1 \langle\; \mathbf{u}(t)\;,\;\mathbf{u}_0'(t)\;\rangle\; dt \;=\; 0\;,$$

$$\mathbf{v}'(t) \; - \; T\,\mathbf{f}_{\mathbf{u}}(\;\mathbf{u}(t)\;,\;\lambda\;)\;\mathbf{v}(t) \;=\; \mathbf{0}\;,$$

$$\mathbf{v}(\mathbf{0}) \; + \; \mathbf{v}(\mathbf{1}) \;=\; \mathbf{0}\;,$$

$$\int_0^1 \langle\; \mathbf{v}(t)\;,\;\mathbf{v}(t)\;\rangle\; dt \;-\; 1 \;=\; 0\;,$$

and continuation equation

$$\int_0^1 \langle\; \mathbf{u}(t) - \mathbf{u}_0(t)\;,\;\dot{\mathbf{u}}_0(t)\;\rangle\; dt \;+\; \int_0^1 \langle\; \mathbf{v}(t) - \mathbf{v}_0(t)\;,\;\dot{\mathbf{v}}_0(t)\;\rangle\; dt \;+$$

$$+\;(T_0 - T)\dot{T}_0 \;+\; (\lambda - \lambda_0)\dot{\lambda}_0 \;+\; (\mu - \mu_0)\dot{\mu}_0 \;-\; \Delta s \;=\; 0\;.$$

EXAMPLE : **Period-Doubling Bifurcations in the Lorenz Equations** .

(`Course demo` : `Lorenz/Period-Doubling`)

- The Lorenz equations also have period-doubling bifurcations .

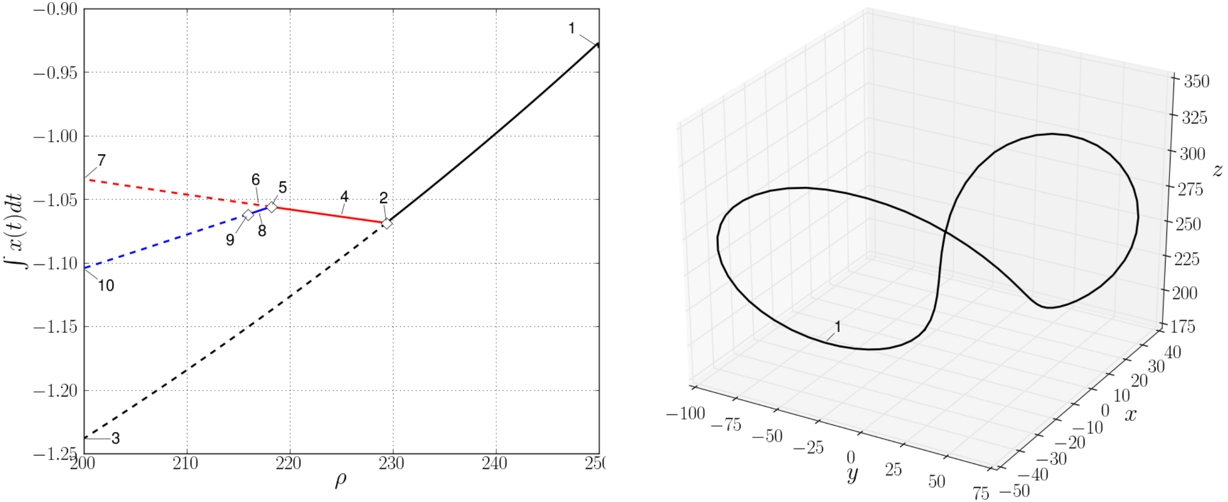
- In fact, there is a period-doubling cascade for large ρ .

- We start from numerical data .

- (Such data may be from simulation , *i.e.*, initial value integration .)

- We also want to compute loci of period-doubling bifurcations .

(Course demo : Lorenz/Period-Doubling)

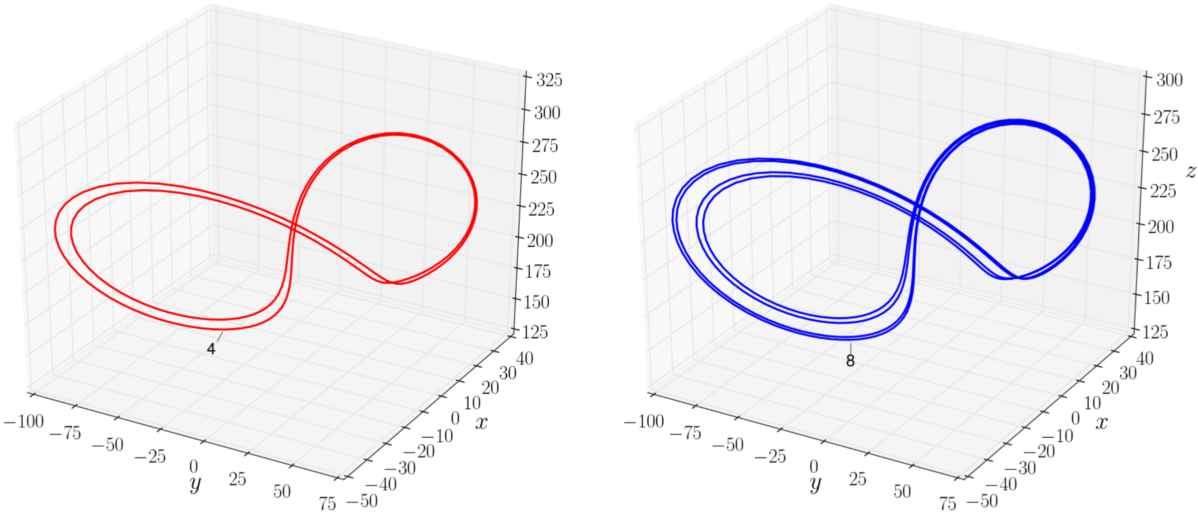


Left panel : Solution families of the Lorenz equations.

The open diamonds denote period-doubling bifurcations .

Right panel : Solution 1 was found by initial value integration .

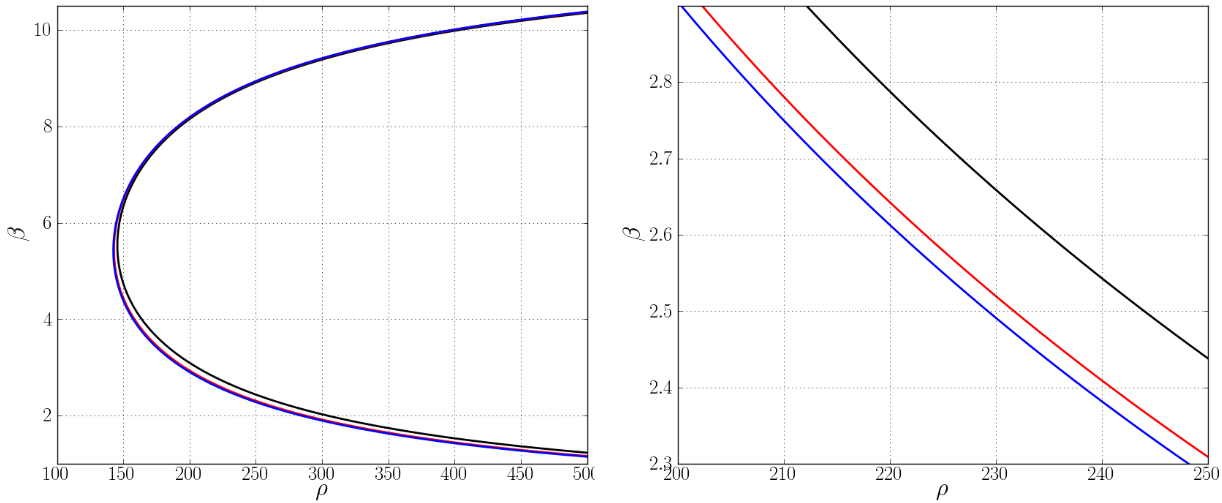
(Course demo : Lorenz/Period-Doubling)



Left panel : A primary period-doubled solution.

Right panel : A secondary period-doubled solution.

(Course demo : Lorenz/Period-Doubling)



Loci of period-doubling bifurcations for the Lorenz equations (with blow-up) .

Black: primary, Red: secondary, Blue: tertiary period-doublings .

Periodic Solutions of Conservative Systems

EXAMPLE : **A Model Conservative System** .

(`Course demo` : `Vertical-HB`)

$$u_1' = - u_2 ,$$

$$u_2' = u_1 (1 - u_1) .$$

PROBLEM :

- This system has a family of periodic solutions, but no parameter !

- The system has a constant of motion , namely the Hamiltonian

$$H(u_1, u_2) = -\frac{1}{2} u_1^2 - \frac{1}{2} u_2^2 + \frac{1}{3} u_1^3 .$$

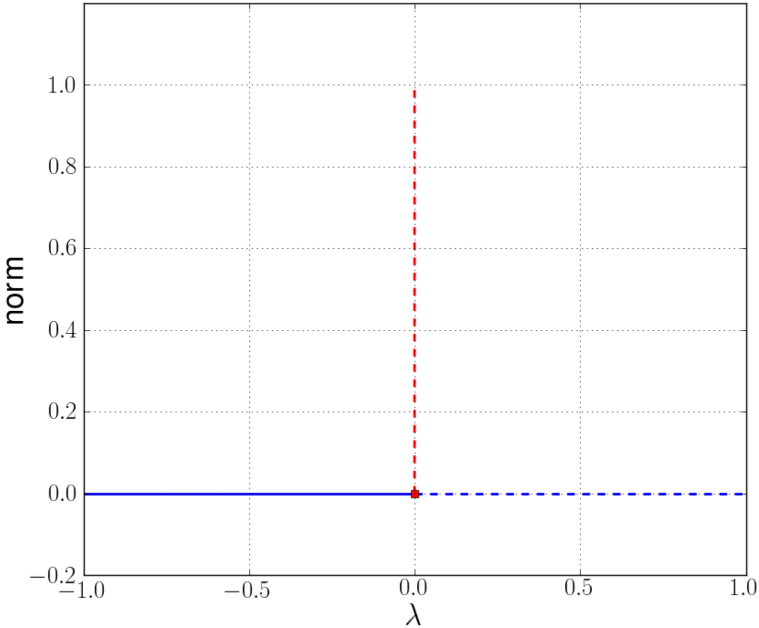
REMEDY :

Introduce an unfolding term with unfolding parameter λ :

$$u_1' = \lambda\, u_1 - u_2 \ ,$$

$$u_2' = u_1\,(1 - u_1) \ .$$

Then there is a vertical Hopf bifurcation from the trivial solution at $\lambda = 0$.



Bifurcation diagram of the vertical Hopf bifurcation problem.
(`Course demo` : `Vertical-HB`)

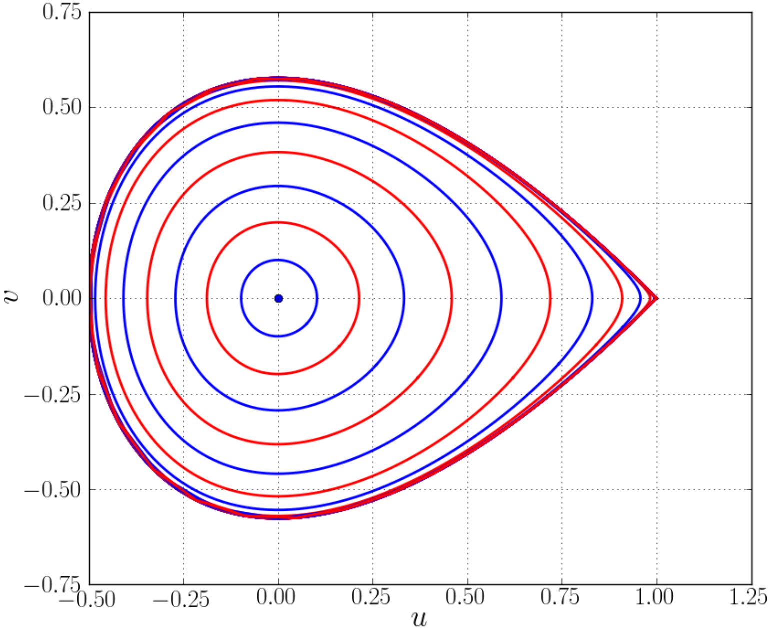
NOTE :

- The family of periodic solutions is vertical .

- The parameter λ is solved for in each continuation step.

- Upon solving, λ is found to be zero , up to numerical precision.

- One can use standard BVP continuation and bifurcation algorithms.



A phase plot of some periodic solutions.

EXAMPLE : **The Circular Restricted 3-Body Problem (CR3BP)** .

(`Course demo` : `Restricted-3Body/Earth-Moon/Orbits`)

$$x'' = 2y' + x - \frac{(1-\mu)(x+\mu)}{r_1^3} - \frac{\mu(x-1+\mu)}{r_2^3} ,$$

$$y'' = -2x' + y - \frac{(1-\mu)\, y}{r_1^3} - \frac{\mu\, y}{r_2^3} ,$$

$$z'' = -\frac{(1-\mu)\, z}{r_1^3} - \frac{\mu\, z}{r_2^3} ,$$

where

$$r_1 = \sqrt{(x + \mu)^2 + y^2 + z^2} , \qquad r_2 = \sqrt{(x-1+\mu)^2 + y^2 + z^2} .$$

and

(x, y, z) denotes the position of the zero-mass body .

NOTE : For the Earth-Moon system $\mu \approx 0.01215$.

The CR3BP has one integral of motion , namely, the "Jacobi-constant" :

$$J \; = \; \frac{x'^2 \; + \; y'^2 \; + \; z'^2}{2} \; - \; U(x, y, z) \; - \; \mu \, \frac{1 - \mu}{2} \; ,$$

where

$$U \; = \; \frac{1}{2}(x^2 + y^2) \; + \; \frac{1 - \mu}{r_1} \; + \; \frac{\mu}{r_2} \; ,$$

and

$$r_1 \; = \; \sqrt{(x + \mu)^2 \; + \; y^2 \; + \; z^2} \; , \qquad r_2 \; = \; \sqrt{(x - 1 + \mu)^2 \; + \; y^2 \; + \; z^2} \; .$$

Boundary value formulation :

$$\begin{aligned} x' &= T\ v_x \\ y' &= T\ v_y \\ z' &= T\ v_z \end{aligned}$$

$$\begin{aligned} v_x' &= T\ [\ 2v_y\ +\ x\ -\ (1-\mu)(x+\mu)r_1^{-3}\ -\ \mu(x-1+\mu)r_2^{-3}\ +\ \lambda\ v_x\ ] \\ v_y' &= T\ [\ -2v_x\ +\ y\ -\ (1-\mu)yr_1^{-3}\ -\ \mu yr_2^{-3}\ +\ \lambda\ v_y\ ] \\ v_z' &= T\ [\ -(1-\mu)zr_1^{-3}\ -\ \mu zr_2^{-3}\ +\ \lambda\ v_z\ ] \end{aligned}$$

with periodicity boundary conditions

$$x(1) = x(0)\ ,\quad y(1) = y(0)\ ,\quad z(1) = z(0)\ ,$$

$$v_x(1) = v_x(0)\ ,\quad v_y(1) = v_y(0)\ ,\quad v_z(1) = v_z(0)\ ,$$

$+$ phase constraint $+$ continuation equation .

Here T is the period of the orbit.

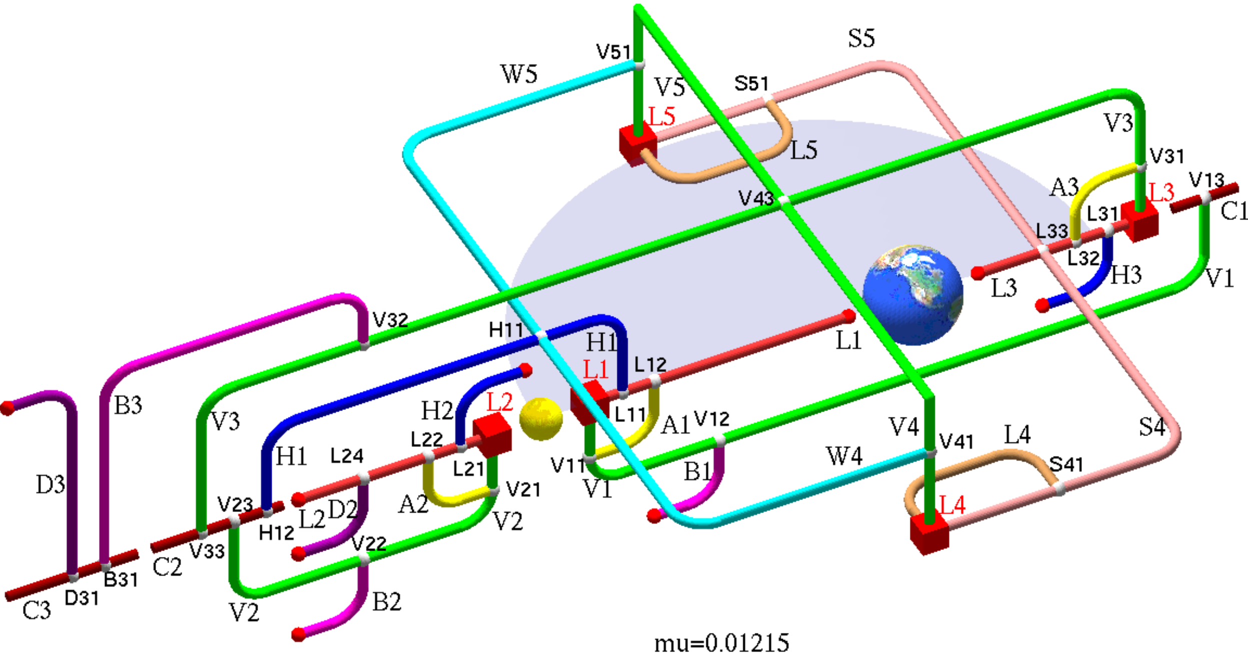
NOTE :

- One can use BVP continuation and bifurcation algorithms.

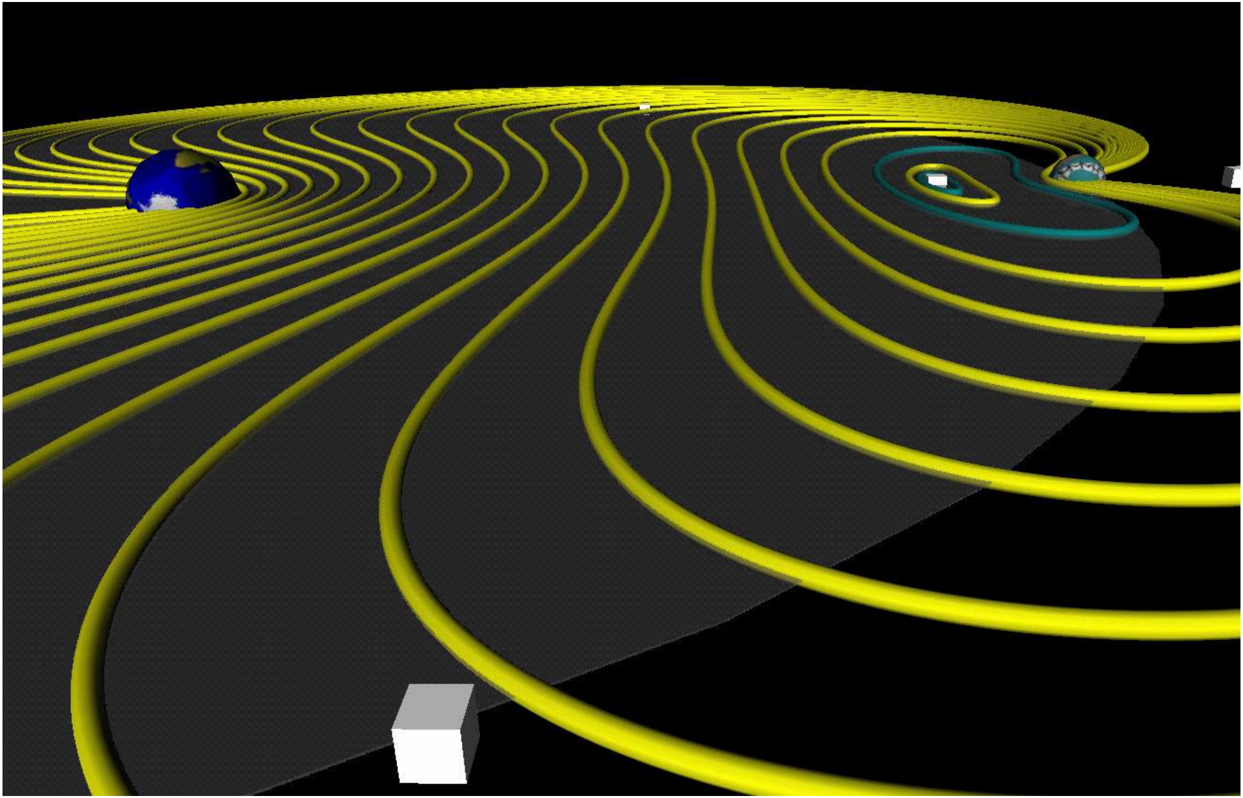
- The unfolding term $\lambda \, \nabla v$ regularizes the continuation.

- λ will be zero , once solved for.

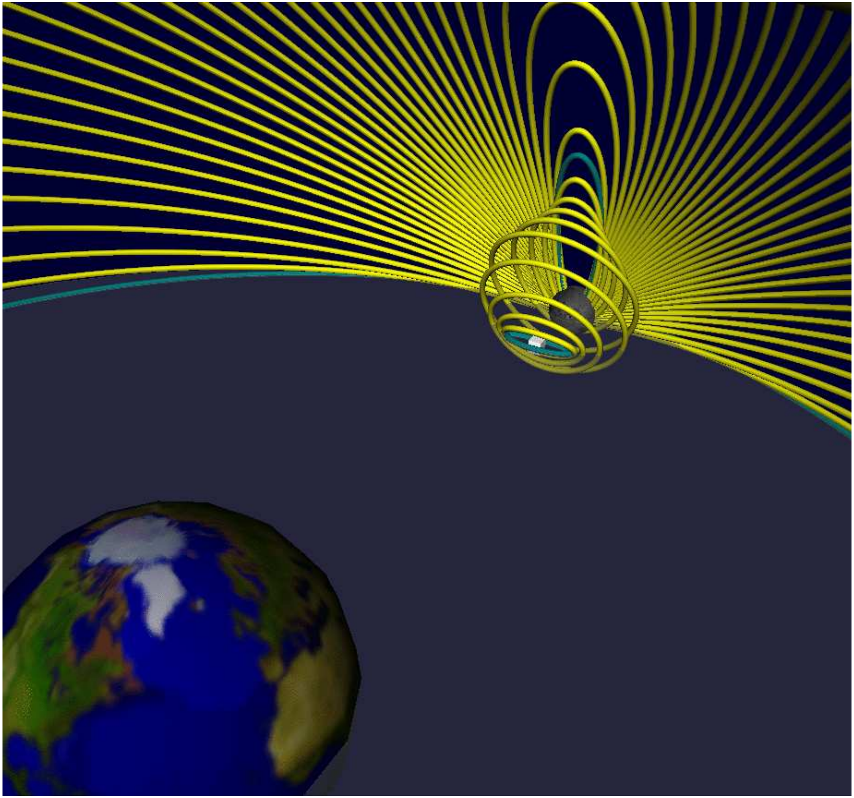
- Other unfolding terms are possible.



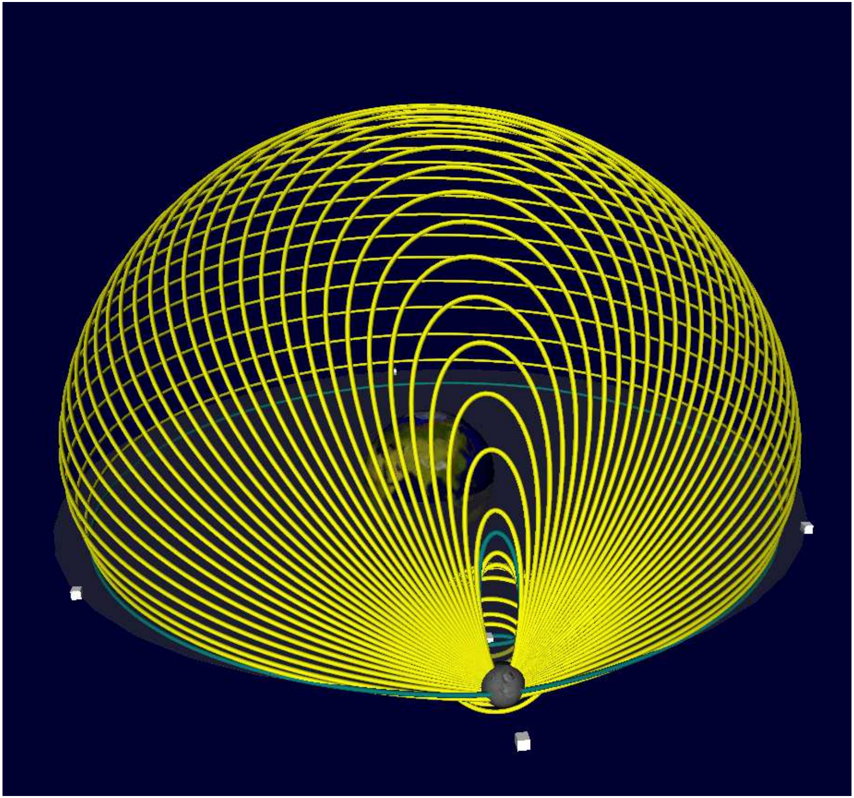
Schematic bifurcation diagram of periodic solution families of the Earth-Moon system .



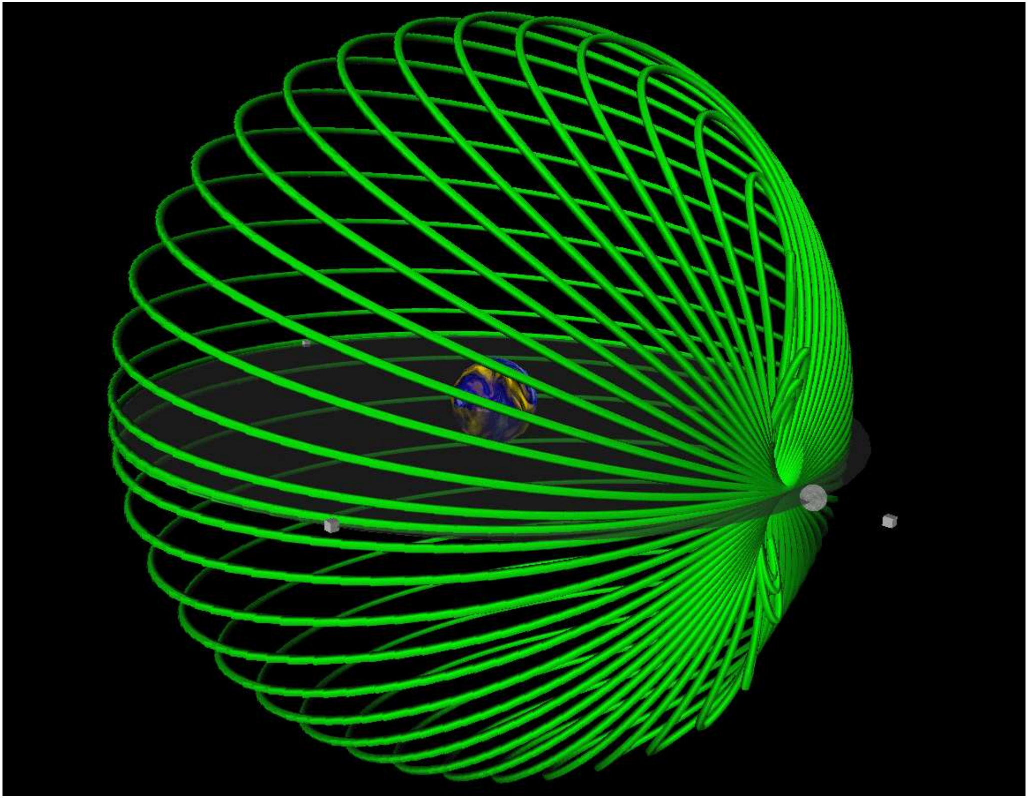
The planar Lyapunov family L1.



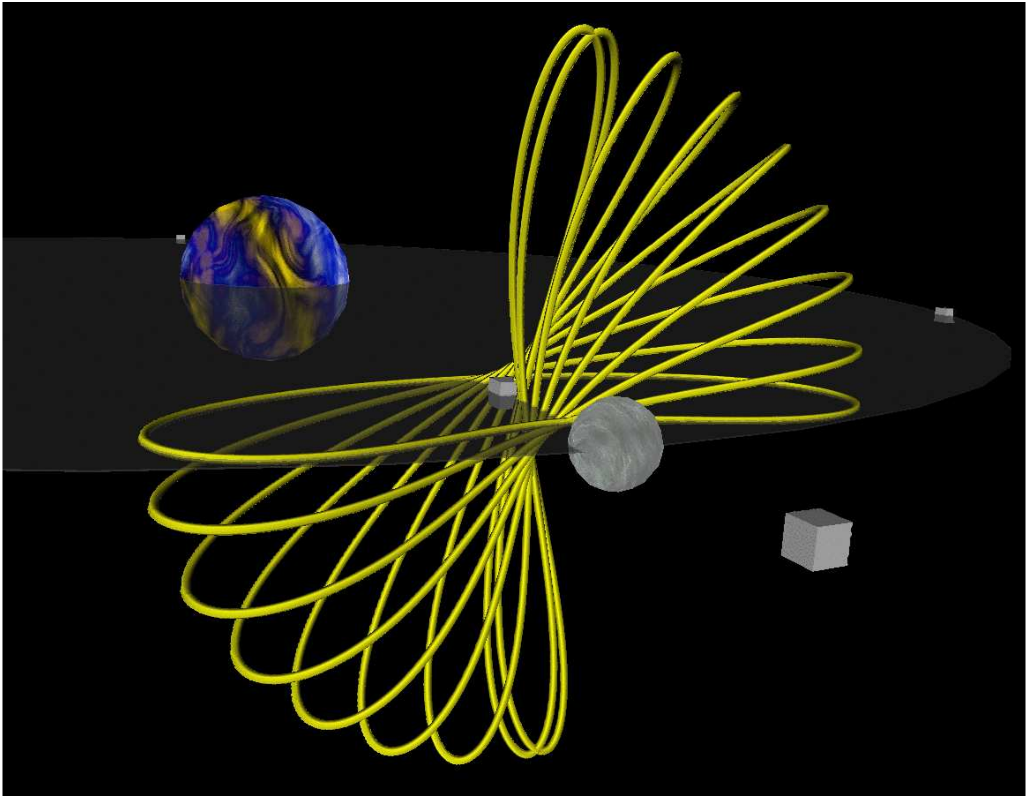
The Halo family H1.



The Halo family H1.



The Vertical family V1.



The Axial family A1.

Stable and Unstable Manifolds

EXAMPLE : **Phase-plane orbits: Fixed length** .

These can be computed by orbit continuation .

Model equations are

$$x' = \epsilon x - y^3 ,$$

$$y' = y + x^3 .$$

where $\epsilon > 0$ is small.

- There is only one equilibrium , namely, $(x, y) = (0, 0)$.
- This equilibrium has eigenvalues ϵ and 1 ; it is a source .

For the computations :

- The time variable t is scaled to $[0,1]$.

- The actual integration time T is then an explicit parameter :

$$x' = T\ (\ \epsilon x\ -\ y^3\ )\ ,$$

$$y' = T\ (\ y\ +\ x^3\ )\ .$$

These constraints are used :

- To put the initial point on a small circle around the origin :

$$
\begin{aligned}
x(0) - r\cos(2\pi\theta) &= 0 \ , \\
y(0) - r\sin(2\pi\theta) &= 0 \ .
\end{aligned}
$$

- To keep track of the end points :

$$
\begin{aligned}
x(1) - x_1 &= 0 \ , \\
y(1) - y_1 &= 0 \ .
\end{aligned}
$$

- To keep track of the length of the orbits

$$
\int_0^1 \sqrt{x'(t)^2 + y'(t)^2}\, dt - L = 0 \ .
$$

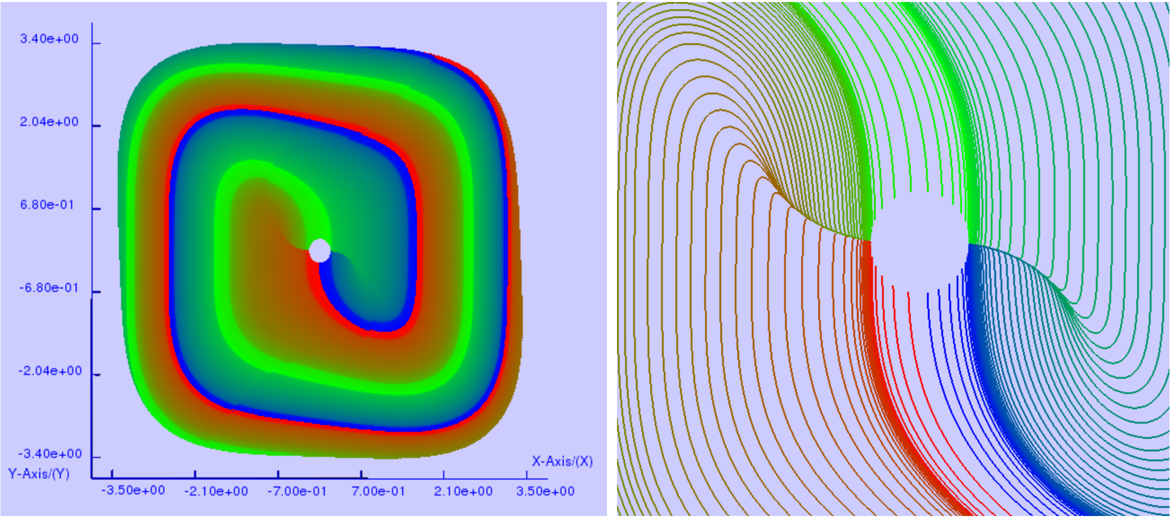
The computations are done in 3 stages :

- In the first run an orbit is grown by continuation :
  - The free parameters are T, L, x_1, y_1 .
  - The starting point is on the small circle of radius r.
  - The starting point is in the strongly unstable direction .
  - The value of ϵ is 0.5 in the first run.

- In the second run the value of ϵ is decreased to 0.01 :
  - The free parameters are ϵ, T, x_1, y_1 .

- In the third run the initial point is free to move around the circle :
  - The free parameters are θ, T, x_1, y_1 .

(Course demo : Basic-Manifolds/2D-ODE/Fixed-Length)



Unstable Manifolds in the Plane: Orbits of Fixed Length .
(The right-hand panel is a blow-up, and also shows fewer orbits.)

EXAMPLE : **Phase-plane orbits: Variable length** .

These can also be computed by orbit continuation .

Model equations are

$$\begin{aligned} x' &= \epsilon x - y^2 , \\ y' &= y + x^2 . \end{aligned}$$

- The origin $(x, y) = (0, 0)$ is an equilibrium .
- The origin has eigenvalues ϵ and 1 ; it is a source .
- Thus the origin has a 2-dimensional unstable manifold .
- We compute this stable manifold using continuation .
- (The equations are 2D; so we actually compute a phase portrait.)

For the computations :

- The time variable t is scaled to $[0,1]$.
- The actual integration time T is then an explicit parameter :

$$
\begin{aligned}
x' &= T(\epsilon x - y^2) \ , \\
y' &= T(y + x^2) \ .
\end{aligned}
$$

NOTE :

- There is also a nonzero equilibrium

$$
(x,y) \ = \ (\epsilon^{\frac{1}{3}}, -\epsilon^{\frac{2}{3}}) \ .
$$

- It is a saddle (1 positive, 1 negative eigenvalue).

These constraints are used :

- To put the initial point on a small circle at the origin :

$$x(0) - r\cos(2\pi\theta) = 0 \ ,$$
$$y(0) - r\sin(2\pi\theta) = 0 \ .$$

- To keep track of the end points :

$$x(1) - x_1 = 0 \ ,$$
$$y(1) - y_1 = 0 \ .$$

- To keep track of the length of the orbits we add an integral constraint :

$$\int_0^1 \sqrt{x'(t)^2 + y'(t)^2}\, dt - L = 0 \ .$$

- To allow the length L to contract :

$$(T_{\max} - T)(L_{\max} - L) - c = 0 \ .$$

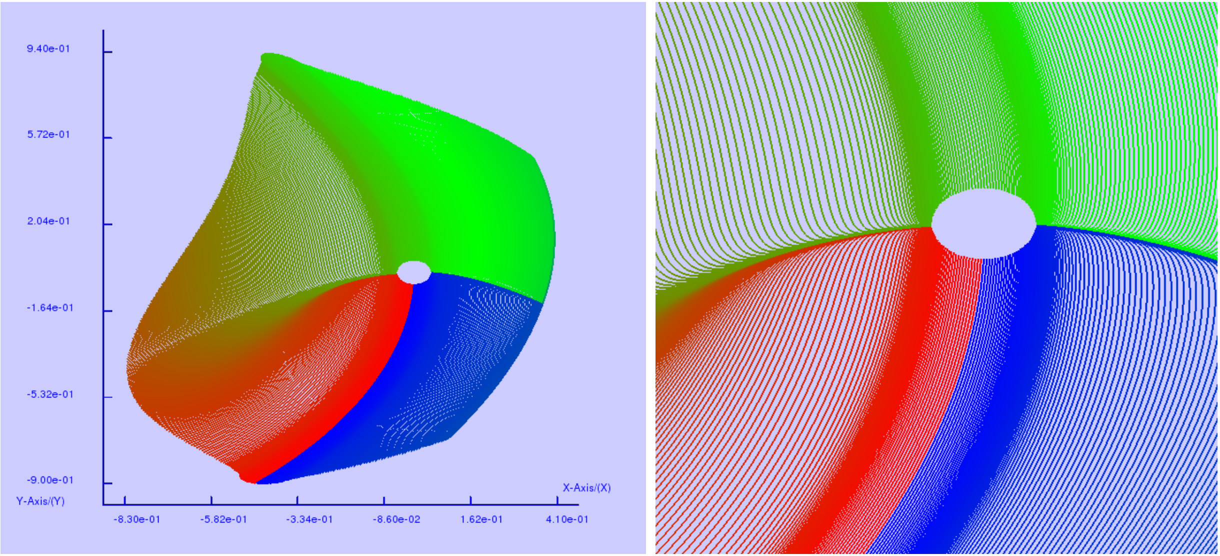
Again the computations are done in 3 stages :

- In the first run an orbit is grown by continuation :
  - The free parameters are T, L, x_1, y_1, c .
  - The starting point is on a small circle of radius r.
  - The starting point is in the strongly unstable direction .
  - In this first run $\epsilon = 0.5$.

- In the second run the value of ϵ is decreased to 0.05 :
  - The free parameters are ϵ, T, L, x_1, y_1 .

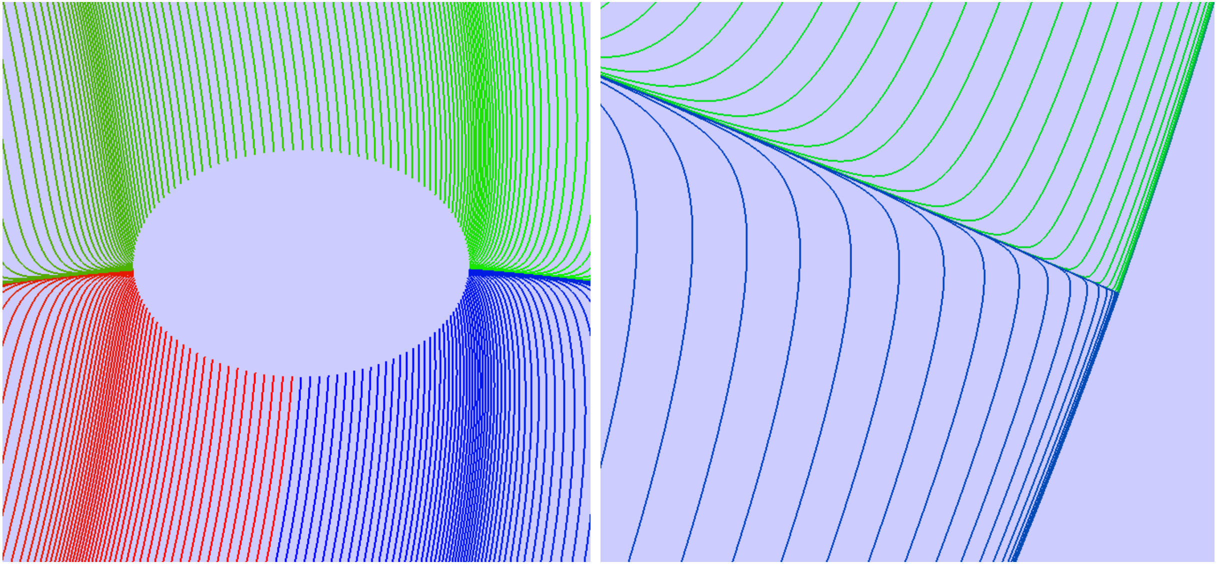
- In the third run the initial point is free to move around the circle :
  - The free parameters are θ, T, L, x_1, y_1 .

(Course demo : Basic-Manifolds/2D-ODE/Variable-Length)



Unstable Manifolds in the Plane: Orbits of Variable Length .

(Course demo : Basic-Manifolds/2D-ODE/Variable-Length)



Unstable Manifolds in the Plane: Orbits of Variable Length (Blow-up).

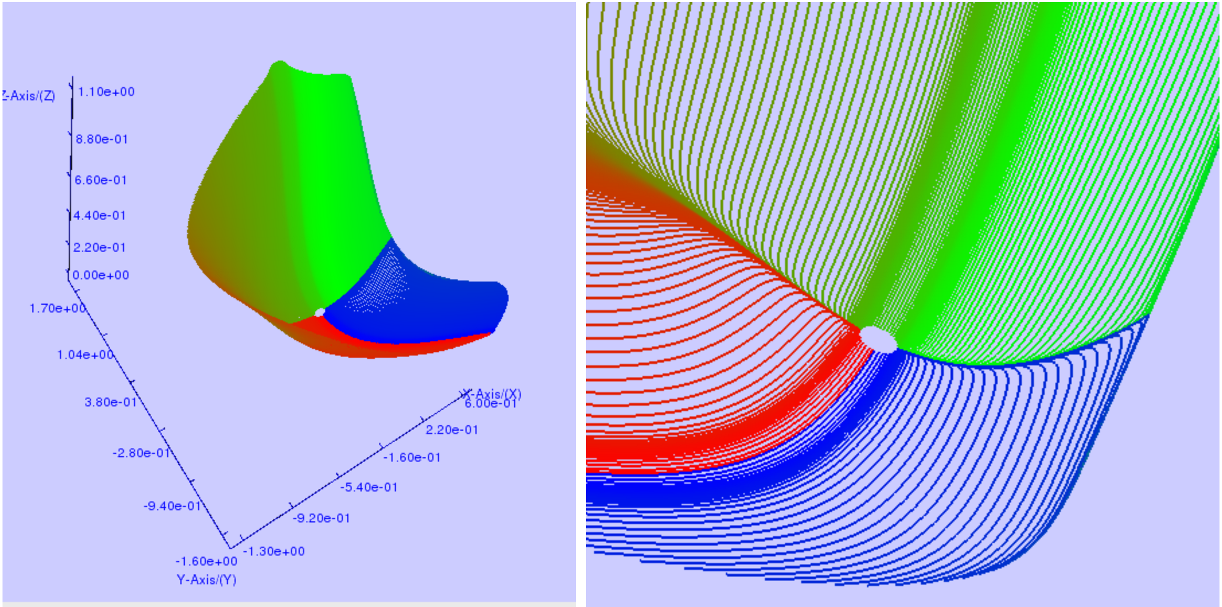
EXAMPLE : A 2D unstable manifold in $\mathbb{R}^3$.

This can also be computed by orbit continuation. The model equations are

$$\begin{aligned} x' &= \epsilon x - z^3 \ , \\ y' &= y - x^3 \ , \\ z' &= -z + x^2 + y^2 \ . \end{aligned}$$

- We take $\epsilon = 0.05$.
- The origin is a saddle with eigenvalues ϵ, 1, and -1.
- Thus the origin has a 2-dimensional unstable manifold .
- The initial point moves around a circle in the 2D unstable eigenspace .
- The equations are 3D; so we will compute a 2D manifold in $\mathbb{R}^3$.
- There is also a nonzero saddle , so we use retraction .
- The set-up is similar to the 2D phase-portrait example.

(Course demo : Basic-Manifolds/3D-ODE/Variable-Length)



Unstable Manifolds in $\mathbb{R}^3$: Orbits of Variable Length .

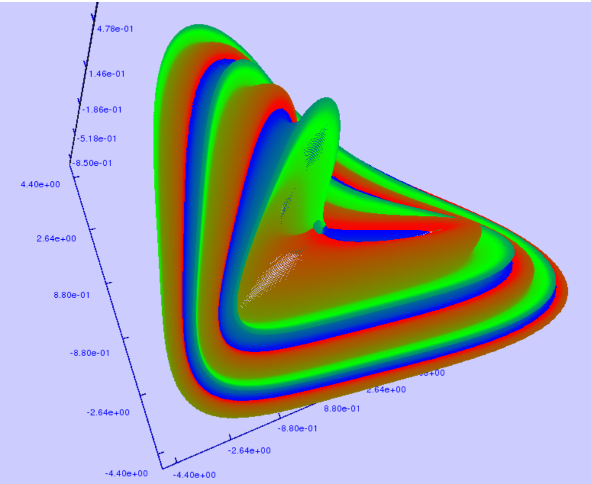
EXAMPLE : **Another 2D unstable manifold in $\mathbb{R}^3$** .

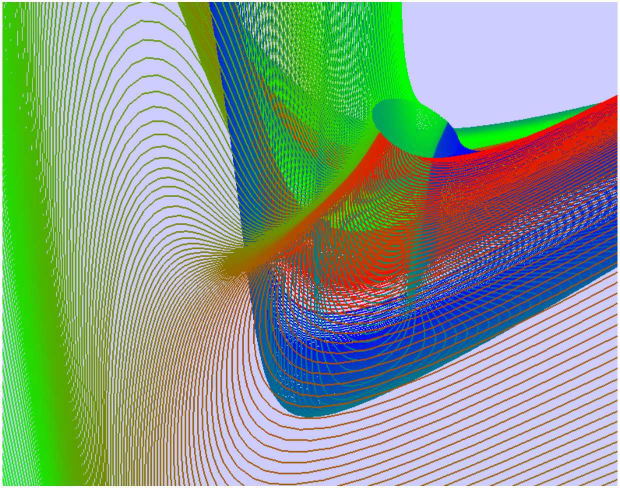
The model equations are

$$\begin{aligned} x' &= \epsilon x - y^3 + z^3 \ , \\ y' &= \ y + x^3 + z^3 \ , \\ z' &= -z - x^2 + y^2 \ . \end{aligned}$$

- We take $\epsilon = 0.05$.
- The origin is a saddle with eigenvalues ϵ, 1, and -1.
- Thus the origin has a 2-dimensional unstable manifold .
- The initial point moves around a circle in the 2D unstable eigenspace .
- The equations are 3D; so we will compute a 2D manifold in $\mathbb{R}^3$.
- No retraction is needed, so we choose to compute orbits of fixed length .
- The set-up is similar to the 2D phase-portrait example.

(Course demo : Basic-Manifolds/3D-ODE/Fixed-Length)





Unstable Manifolds in $\mathbb{R}^3$: Orbits of Fixed Length .

The Lorenz Manifold

- For $\rho > 1$ the origin is a saddle point .

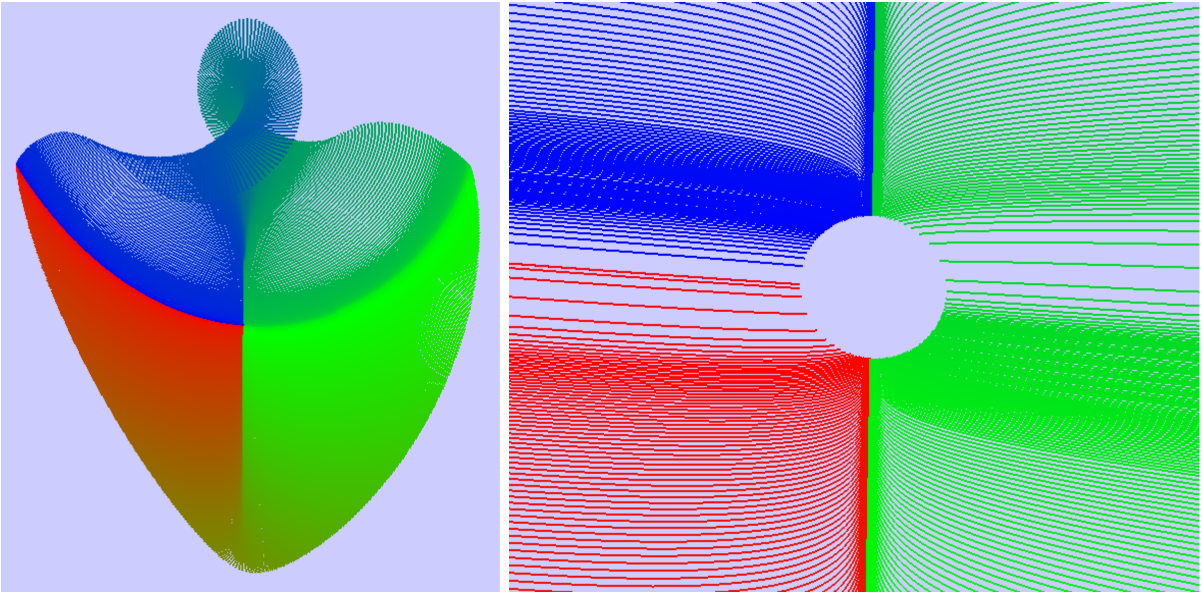
- The Jacobian has two negative and one positive eigenvalue .

- The two negative eigenvalues give rise to a 2D stable manifold .

- This manifold is known as as the Lorenz Manifold .

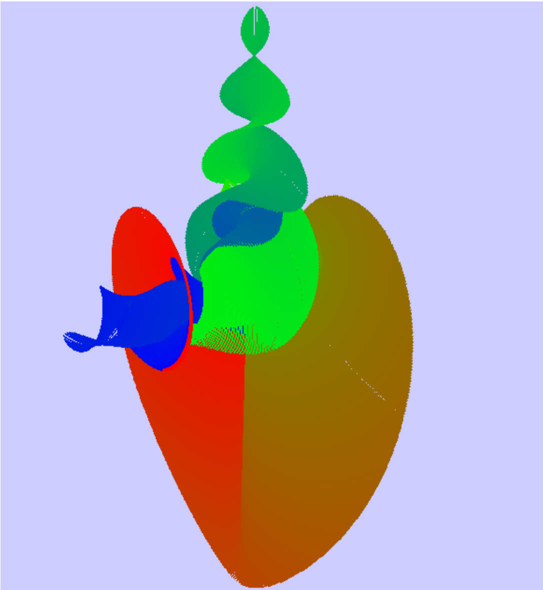
- The set-up is as for the earlier 3D model, using fixed length .

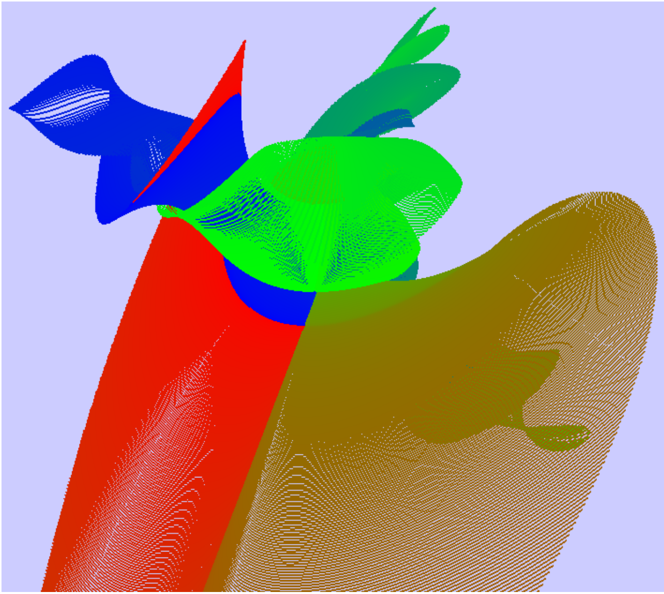
Course demo : Lorenz/Manifolds/Origin/Fixed-Length



Part of the Lorenz Manifold (with blow-up). Orbits have fixed length $L = 60$.

Course demo : Lorenz/Manifolds/Origin/Fixed-Length





Part of the Lorenz Manifold. Orbits have fixed length $L = 200$.

Heteroclinic Connections.

- The Lorenz Manifold helps understand the Lorenz attractor .
- Many orbits in the manifold depend sensitively on initial conditions .
- During the manifold computation one can locate heteroclinic orbits .
- These are also in the 2D unstable manifold of the nonzero equilibria.
- The heteroclinic orbits have a combinatorial structure [4].
- One can also continue heteroclinic orbits as ρ varies.

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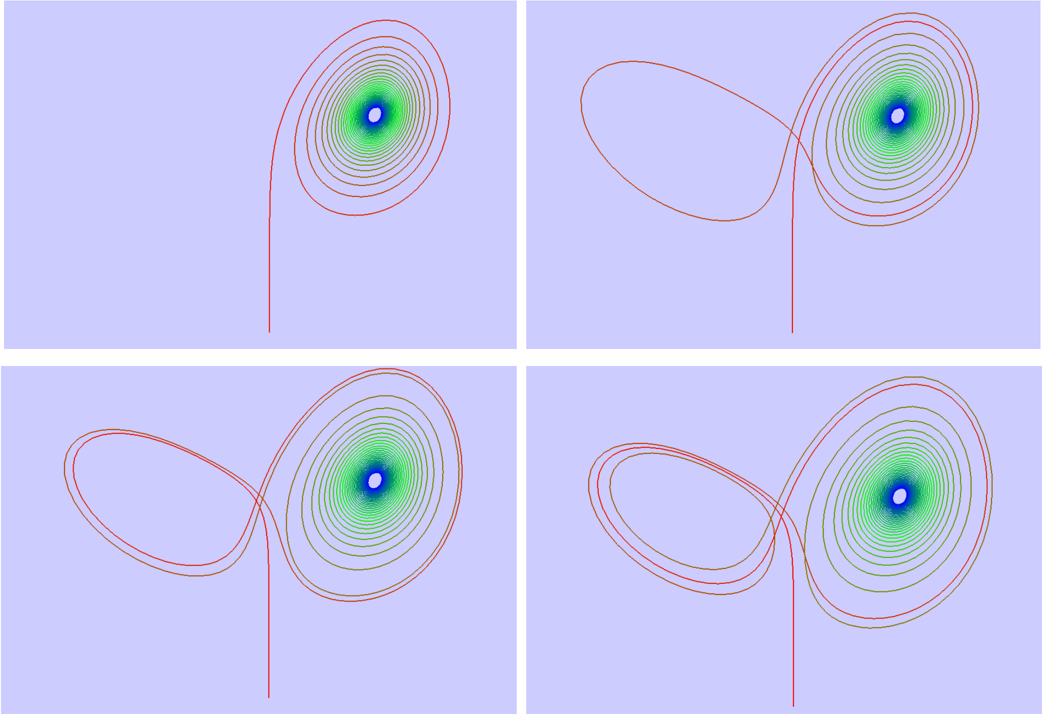
[4] Nonlinearity 19, 2006, 2947-2972.



Four heteroclinic orbits with very close initial conditions

One can also determine the intersection of the Lorenz manifold with a sphere .

The set-up is as follows :

$$
\begin{aligned}
x' &= T\,\sigma\,(y - x)\ , \\
y' &= T\,(\rho\, x \ - \ y \ - \ x\, z)\ , \\
z' &= T\,(x\, y \ - \ \beta\, z)\ ,
\end{aligned}
$$

which is of the form

$$\mathbf{u}'(t) \ = \ T\,\mathbf{f}(\ \mathbf{u}(t)\ )\ , \qquad \text{for} \quad 0 \le t \le 1\ ,$$

where

- T is the actual integration time , which is negative !

To this we add boundary and integral constraints .

The complete set-up consists of the ODE

$$\mathbf{u}'(t) \;=\; T\,\mathbf{f}(\,\mathbf{u}(t)\,)\;, \qquad \text{for} \quad 0 \le t \le 1\;,$$

subject to the following constraints :

$\mathbf{u}(0) - \epsilon\,(\cos(\theta)\;\mathbf{v}_1 - \sin(\theta)\;\mathbf{v}_2) \;=\; 0$	$\mathbf{u}(0)$ is on a small circle
$\mathbf{u}(1) \;-\; \mathbf{u}_1 \;=\; 0$	to keep track of the end point $\mathbf{u}(1)$
$\Vert\,\mathbf{u}_1\,\Vert \;-\; R \;=\; 0$	distance of $\mathbf{u}_1$ to the origin
$\langle\;\mathbf{u}_1/\Vert\,\mathbf{u}_1\,\Vert\;,\;\mathbf{f}(\mathbf{u}_1)/\Vert\,\mathbf{f}(\mathbf{u}_1)\,\Vert\;\rangle - \tau = 0$	to locate tangencies, where $\tau = 0$
$T\;\int_0^1\;\Vert\,\mathbf{f}(\mathbf{u})\,\Vert\;ds \;-\; L \;=\; 0$	to keep track of the orbit length
$(T - T_n)\;(L - L_n)\;-\;c\;=\;0\;.$	allows retraction into the sphere

The continuation system has the form

$$\mathbf{F}(\mathbf{X}_k) = 0 , \quad \text{where} \quad \mathbf{X} = (\mathbf{u}(\cdot) , \Lambda) .$$

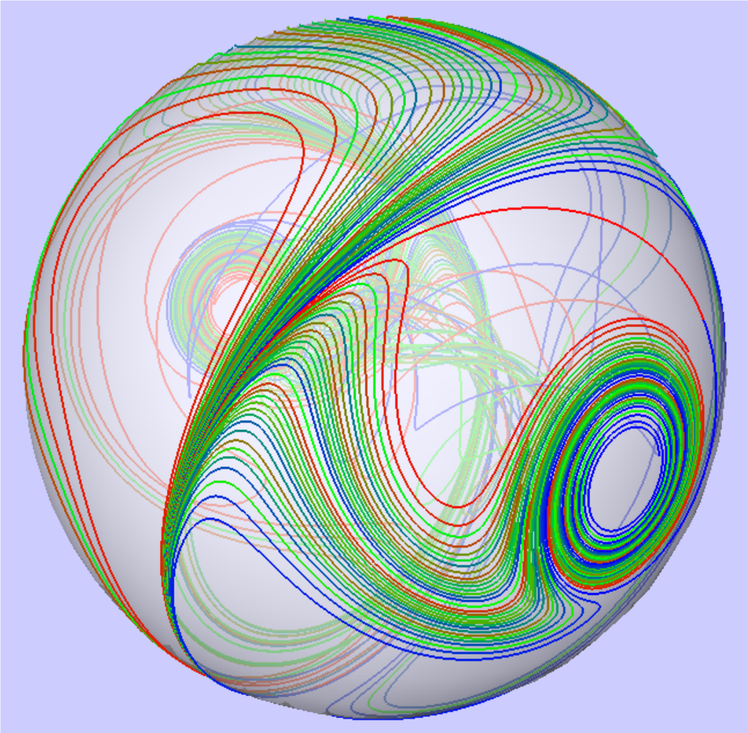
with continuation equation

$$\langle \mathbf{X}_k - \mathbf{X}_{k-1} , \dot{\mathbf{X}}_{k-1} \rangle - \Delta s = 0 , \qquad (\| \dot{\mathbf{X}}_{k-1} \| = 1) .$$

The computations are done in 2 stages :

- In the first run an orbit is grown by continuation :
  - The starting point is on the small circle of radius ϵ.
  - The starting point is in the strongly stable direction .
  - The free parameters are $\Lambda = (T , L , c , \tau , R , \mathbf{u}_1)$.
- In the second run the orbit sweeps the stable manifold.
  - The initial point is free to move around the circle :
  - The free parameters are $\Lambda = (T , L , \theta , \tau , R , \mathbf{u}_1)$.

Course demo : Lorenz/Manifolds/Origin/Sphere



Intersection of the Lorenz Manifold with a sphere

NOTE :

- We do not just change the initial point (*i.e.*, θ) and integrate !

- Every continuation step requires solving a boundary value problem .

- The continuation stepsize Δs controls the change in $\mathbf{X}$.

- $\mathbf{X}$ can only change a little in any continuation step.

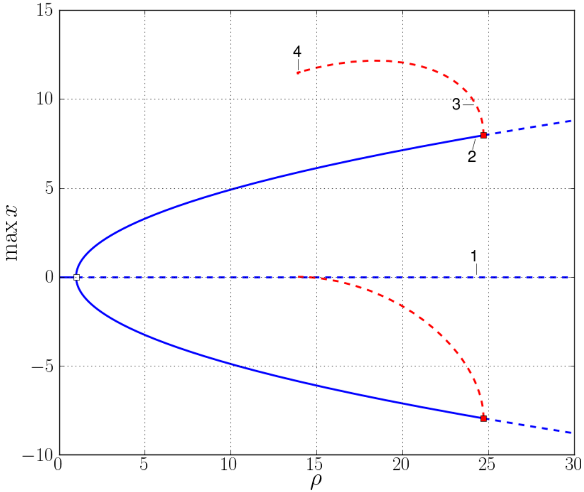
- This way the entire manifold (up to a given length L) is computed.

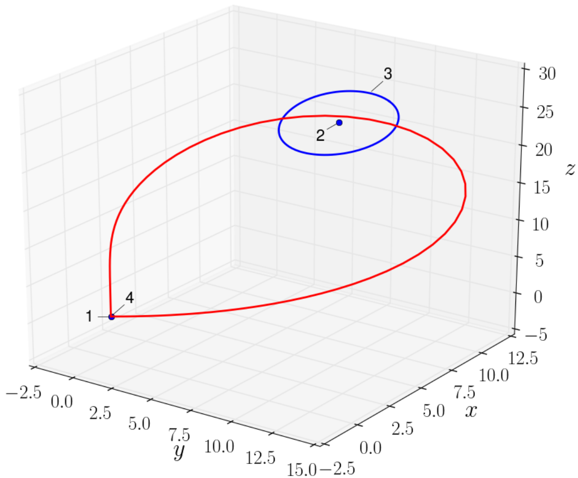
- The retraction constraint allows the orbits to retract into the sphere.

- This is necessary when heteroclinic connections are encountered.

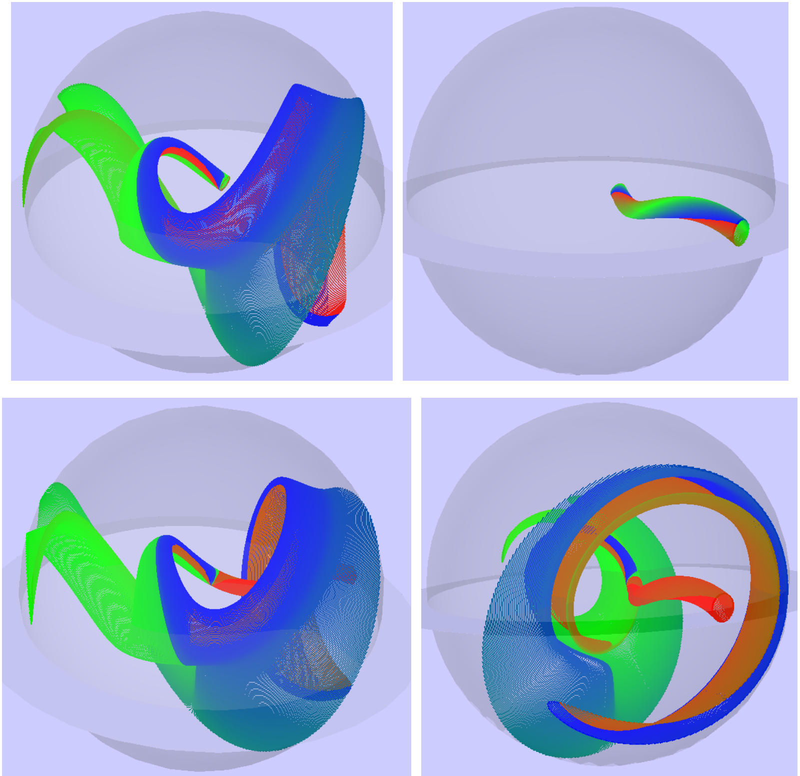
EXAMPLE : **Unstable Manifolds of a Periodic Orbit** .

(`Course demo` : `Lorenz/Manifolds/Orbits/Rho24.3`)





Left: Bifurcation diagram of the Lorenz equations. Right: Labeled solutions.



Both sides of the unstable manifold of periodic orbit 3 at $\rho = 24.3$.

EXAMPLE : **Unstable Manifolds in the CR3BP** .

(`Course demo` : `Restricted-3Body/Earth-Moon/Manifolds/H1`)

- "Small" Halo orbits have one real Floquet multiplier outside the unit circle.

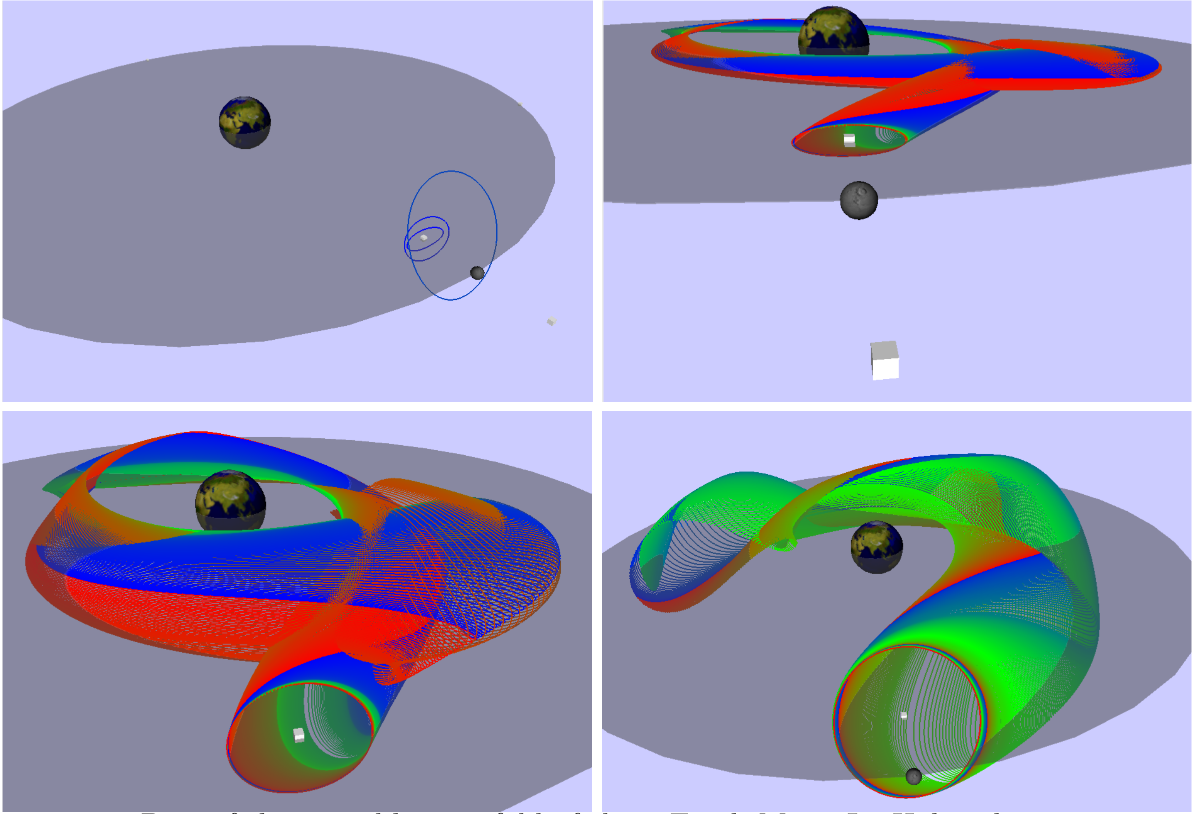
- Such Halo orbits are unstable .

- They have a 2D unstable manifold .

- The unstable manifold can be computed by continuation .

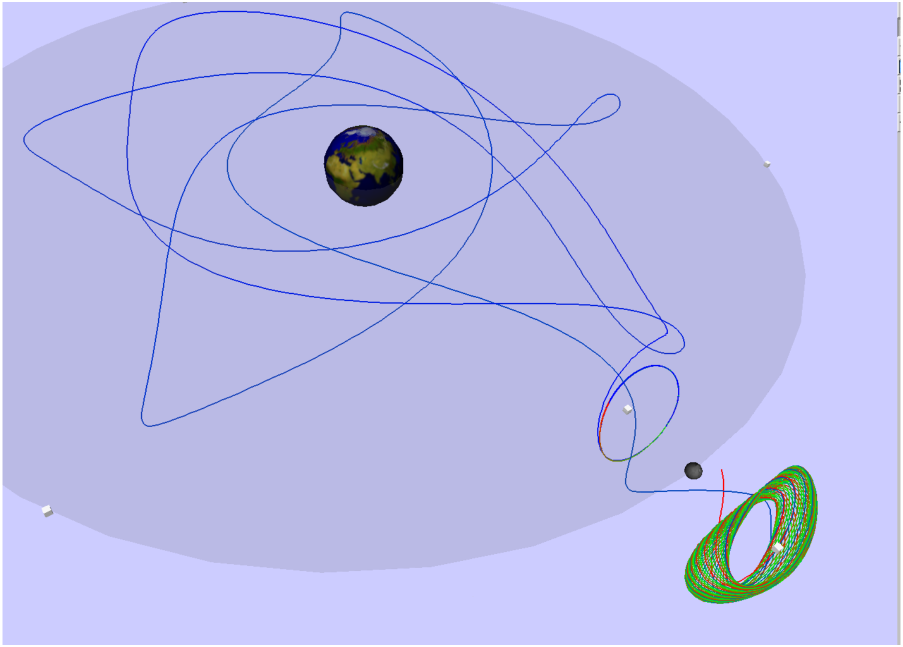
- First compute a starting orbit in the manifold.

- Then continue the orbit keeping, for example, $x(1)$ fixed .



Part of the unstable manifold of three Earth-Moon L1-Halo orbits.

- The initial orbit can be taken to be much longer · · ·
- Continuation with $x(1)$ fixed can lead to a Halo-to-torus connection!



- The Halo-to-torus connection can be continued as a solution to

$$\mathbf{F}(\ \mathbf{X}_k\ ) \quad = \quad \mathbf{0}\ ,$$

$$< \mathbf{X}_k - \mathbf{X}_{k-1}\ ,\ \dot{\mathbf{X}}_{k-1} > \quad - \quad \Delta s \quad = \quad 0\ .$$

where

$$\mathbf{X} \quad = \quad (\ \text{Halo orbit} \quad , \quad \text{Floquet function} \quad , \quad \text{connecting orbit})\ .$$

In detail , the continuation system is

$$\frac{du}{d\tau} - T_u f(u(\tau), \mu, l) = 0 \ ,$$

$$u(1) - u(0) = 0 \ ,$$

$$\int_0^1 \langle \ u(\tau) \ , \ \dot{u}_0(\tau) \ \rangle \ d\tau = 0 \ ,$$

$$\frac{dv}{d\tau} - T_u D_u f(u(\tau), \mu, l) v(\tau) + \lambda_u v(\tau) = 0 \ ,$$

$$v(1) - s v(0) = 0 \quad (s = \pm 1) \ ,$$

$$\langle \ v(0) \ , \ v(0) \ \rangle - 1 = 0 \ ,$$

$$\frac{dw}{d\tau} - T_w f(w(\tau), \mu, 0) = 0 \ ,$$

$$w(0) - (u(0) + \varepsilon v(0)) = 0 \ ,$$

$$w(1)_x - x_\Sigma = 0 \ .$$

The system has

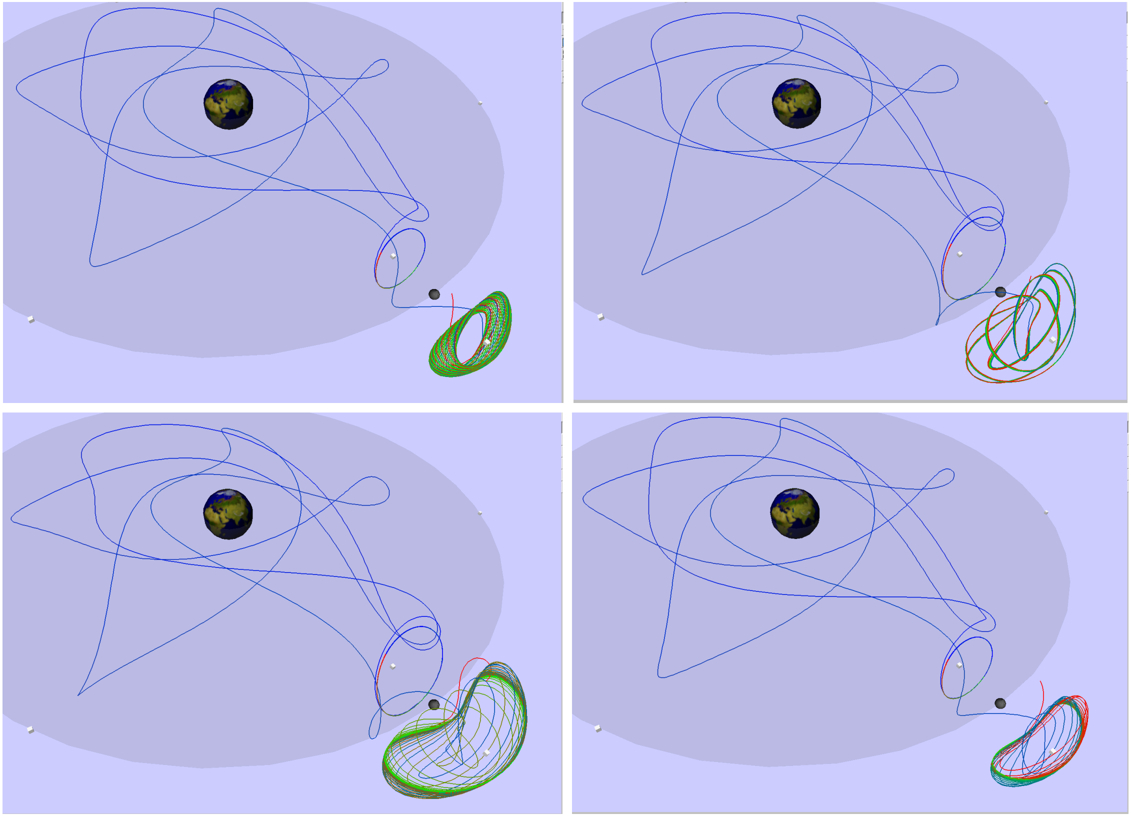
18 ODEs , 20 boundary conditions , 1 integral constraint .

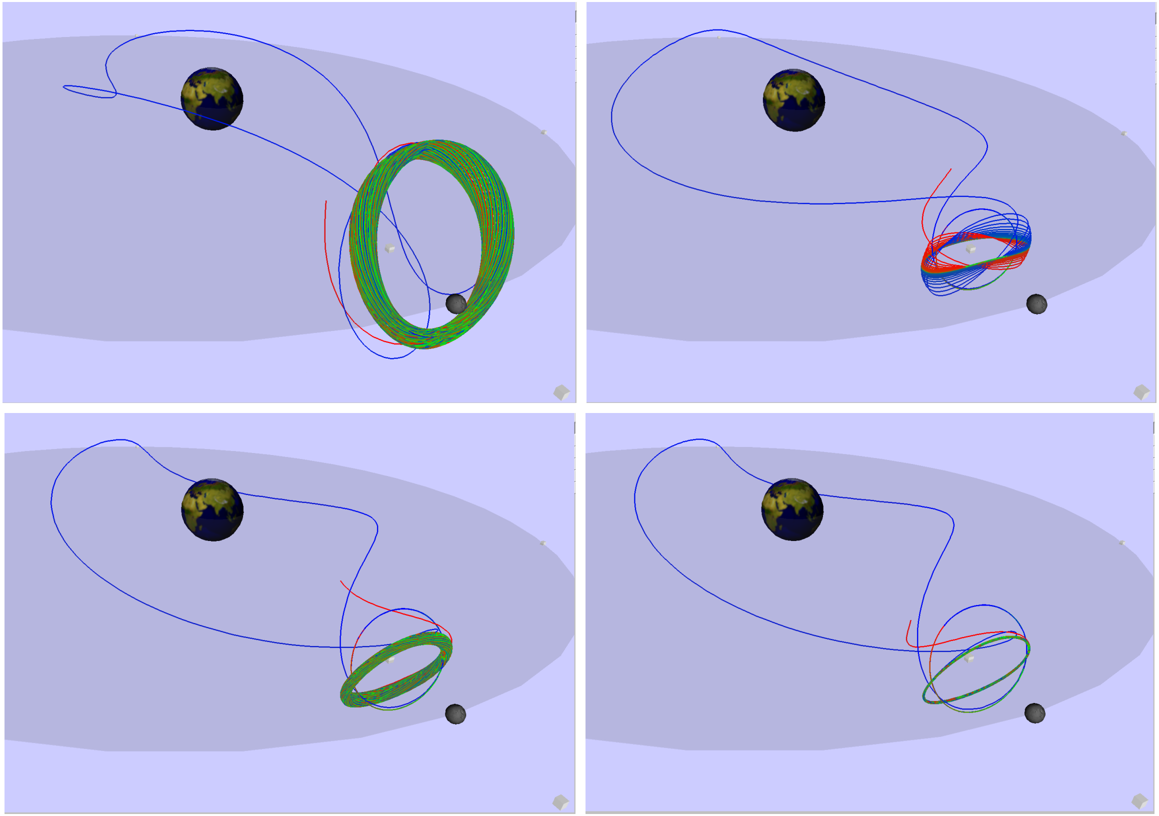
We need

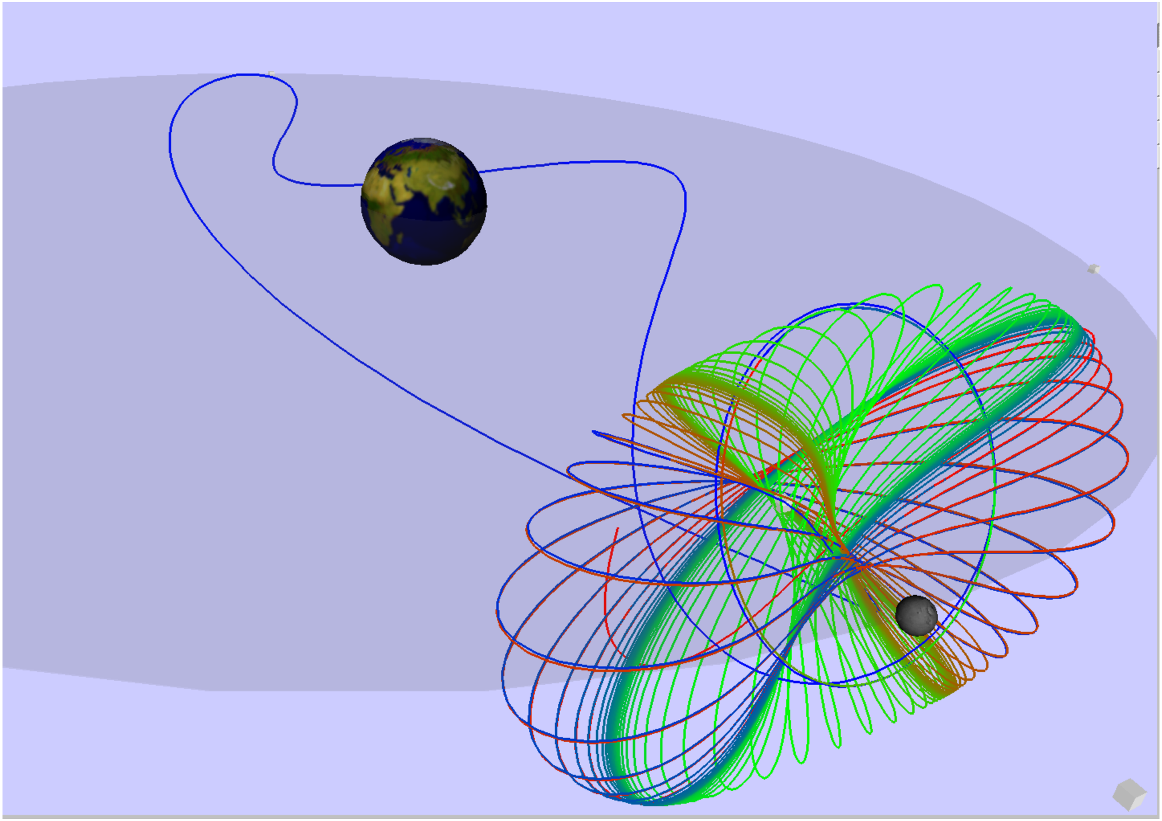
20 + 1 + 1 - 18 = 4 free parameters .

Parameters :

- An orbit in the unstable manifold: T_w , l , T_u , x_Σ
- Compute the unstable manifold: T_w , l , T_u , ε
- Follow a connecting orbit: λ_u , l , T_u , ε







The Solar Sail Equations

The equations in `Course demo : Solar-Sail/Equations/equations.f90` :

$$x'' = 2y' + x - \frac{(1-\mu)(x+\mu)}{d_S^3} - \frac{\mu(x-1+\mu)}{d_P^3} + \frac{\beta(1-\mu)D^2 N_x}{d_S^2}$$

$$y'' = -2x' + y - \frac{(1-\mu)y}{d_S^3} - \frac{\mu y}{d_P^3} + \frac{\beta(1-\mu)D^2 N_y}{d_S^2}$$

$$z'' = -\frac{(1-\mu)z}{d_S^3} - \frac{\mu z}{d_P^3} + \frac{\beta(1-\mu)D^2 N_z}{d_S^2}$$

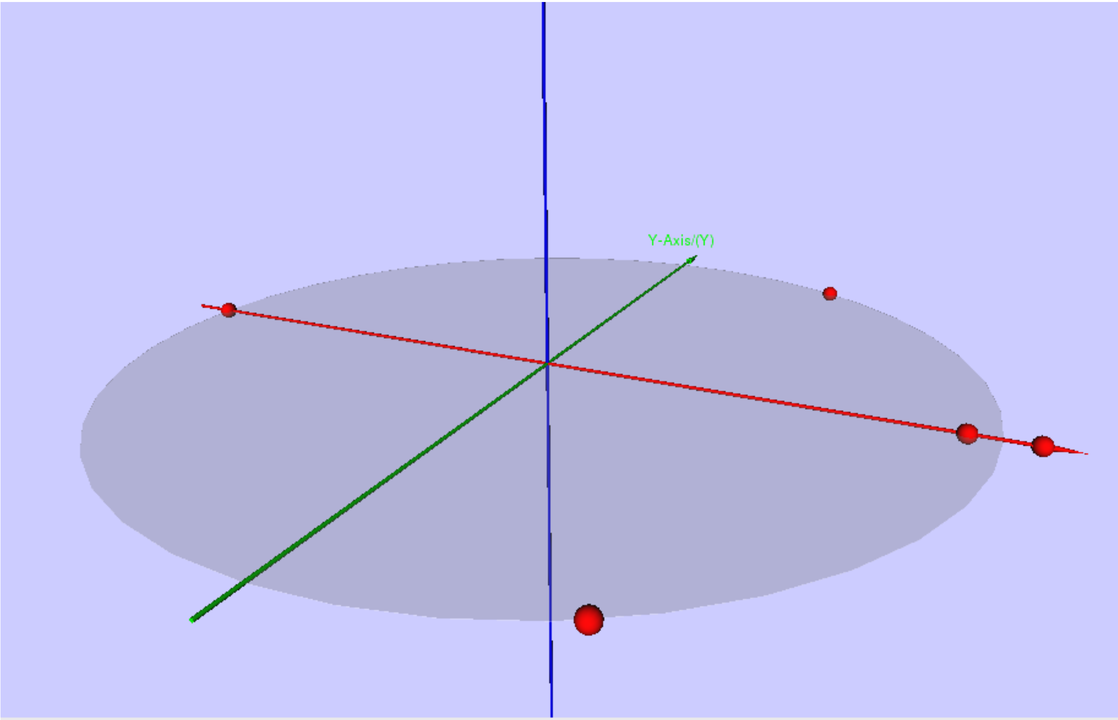
where

$$d_S = \sqrt{(x+\mu)^2 + y^2 + z^2}\,,\ d_P = \sqrt{(x-1+\mu)^2 + y^2 + z^2}\,,\ r = \sqrt{(x+\mu)^2 + y^2}$$

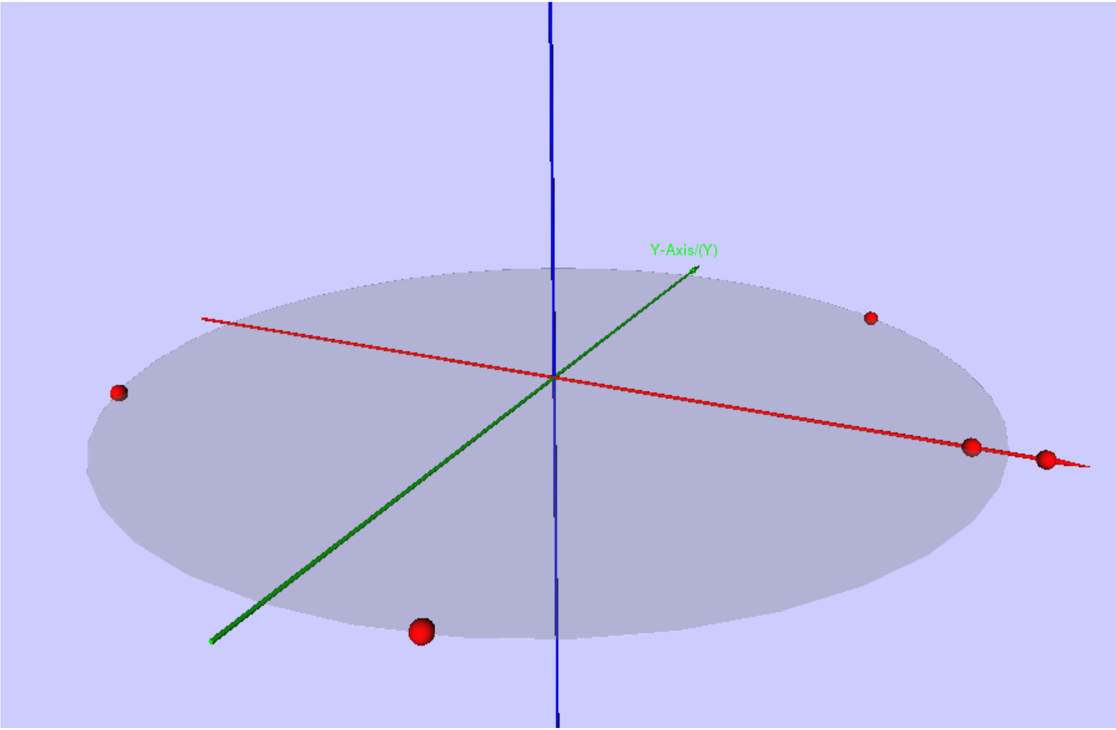
$$N_x = [\cos(\alpha)(x+\mu) - \sin(\alpha)y]\ [\cos(\delta) - \frac{\sin(\delta)z}{r}]/d_S$$

$$N_y = [\cos(\alpha)y + \sin(\alpha)(x+\mu)]\ [\cos(\delta) - \frac{\sin(\delta)z}{r}]/d_S$$

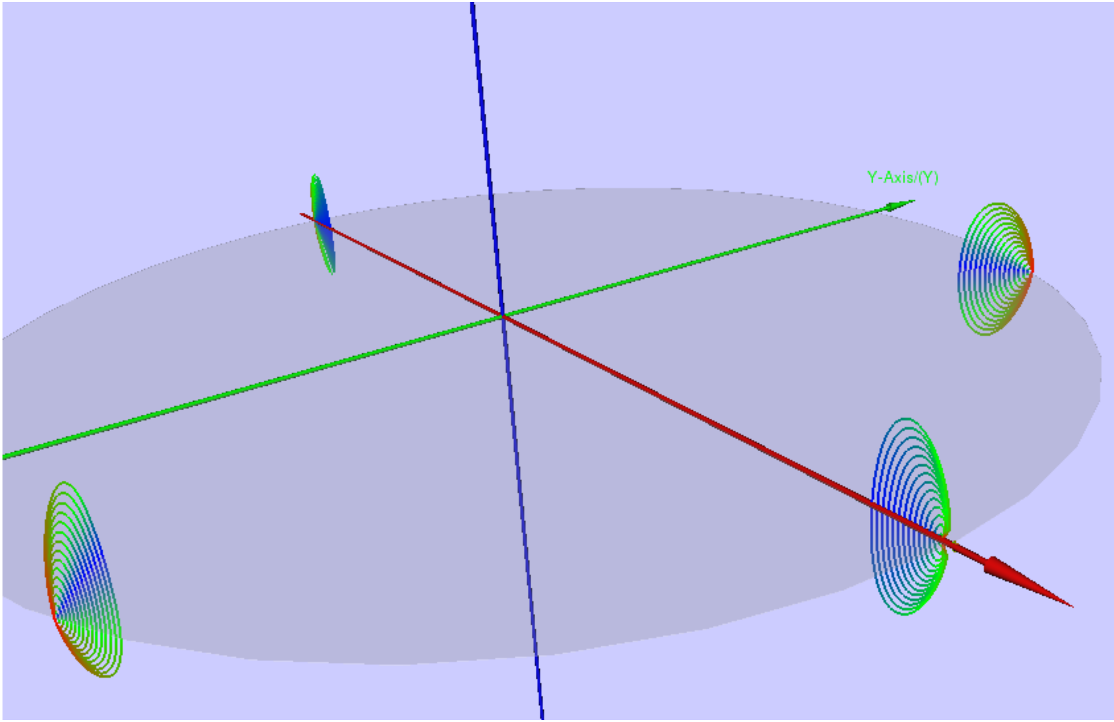
$$N_z = [\cos(\delta)z + \sin(\delta)r]/d_S\ ,\ \ D = \frac{x+\mu}{d_S}N_x + \frac{y}{d_S}N_y + \frac{z}{d_S}N_z$$



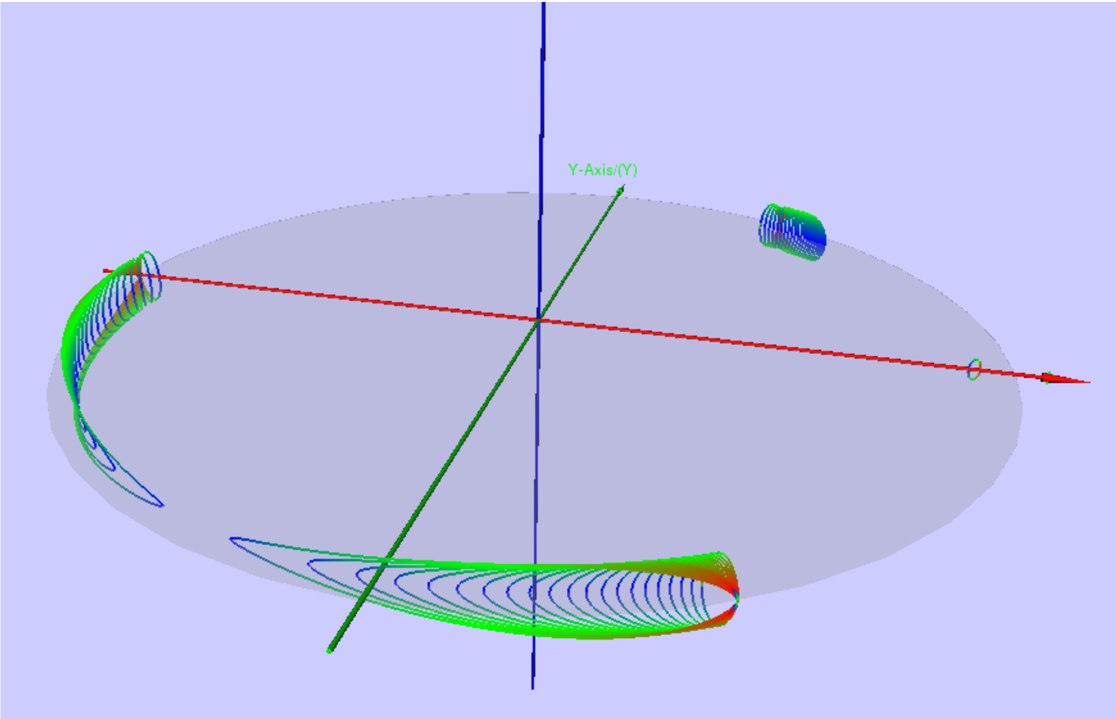
Sun-Jupiter libration points, for $\beta = 0$, $\alpha = 0$, $\delta = 0$.



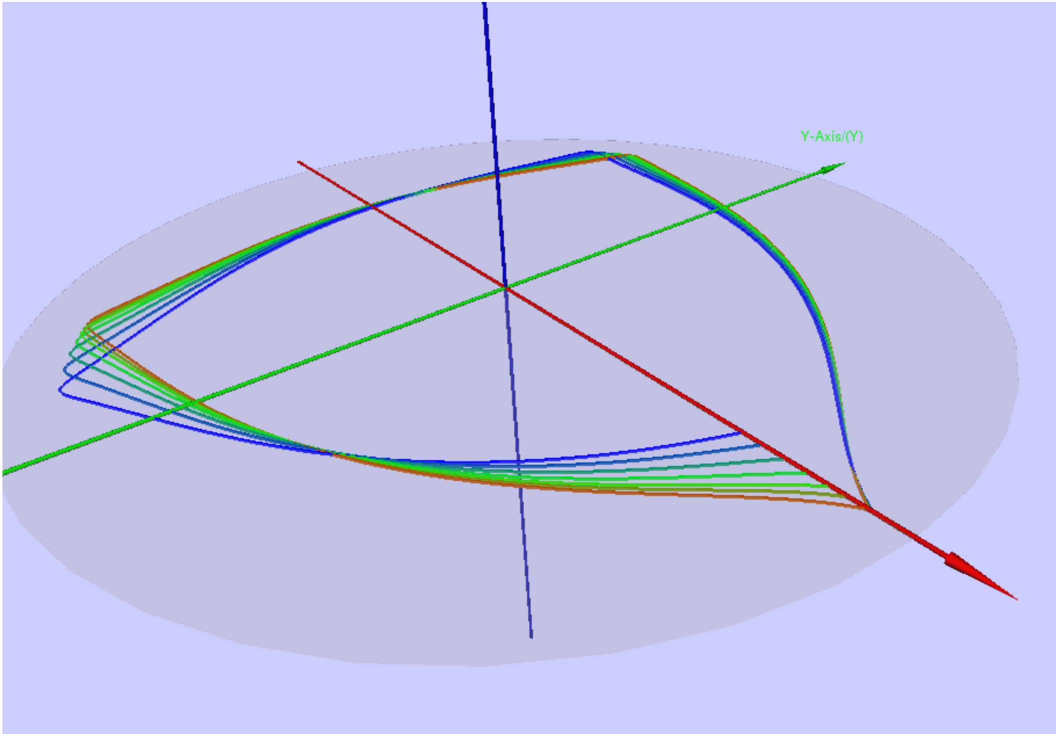
Sun-Jupiter libration points, for $\beta = 0.02$, $\alpha = 0.02$, $\delta = 0$.



Sun-Jupiter libration points, with $\delta \in [-\frac{\pi}{2}, \frac{\pi}{2}]$, for various β, with $\alpha = 0$.

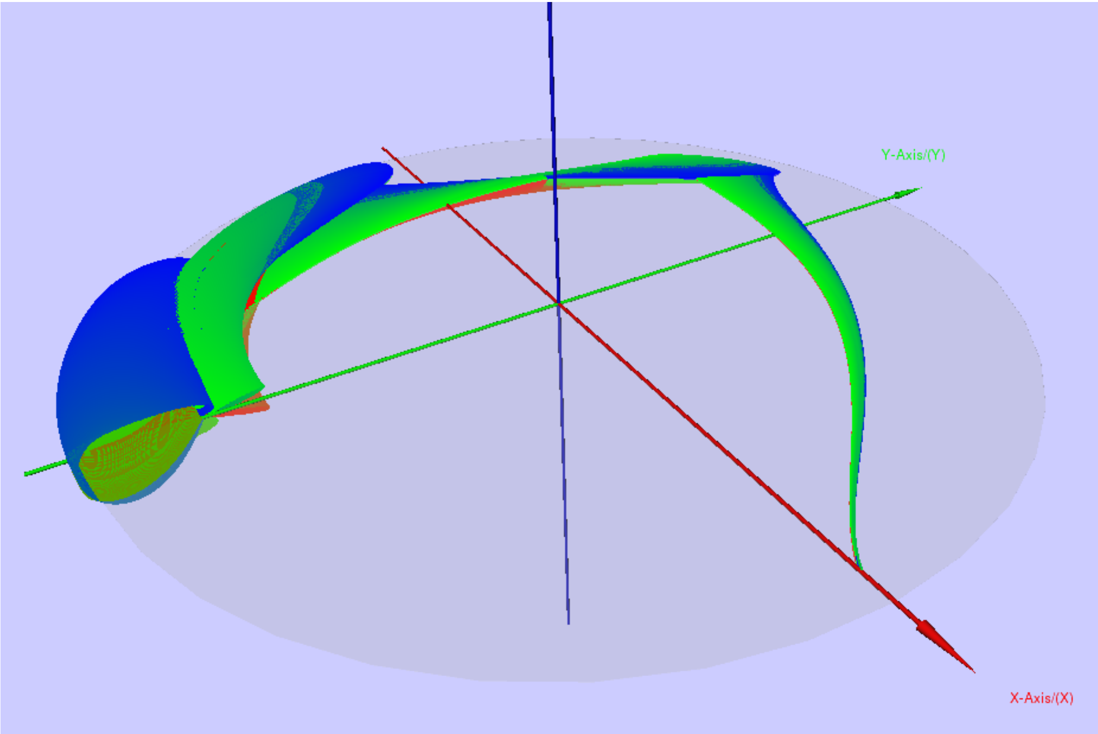


Sun-Jupiter libration points, with $\delta \in [-\frac{\pi}{2}, \frac{\pi}{2}]$, for various α, with $\beta = 0.15$.



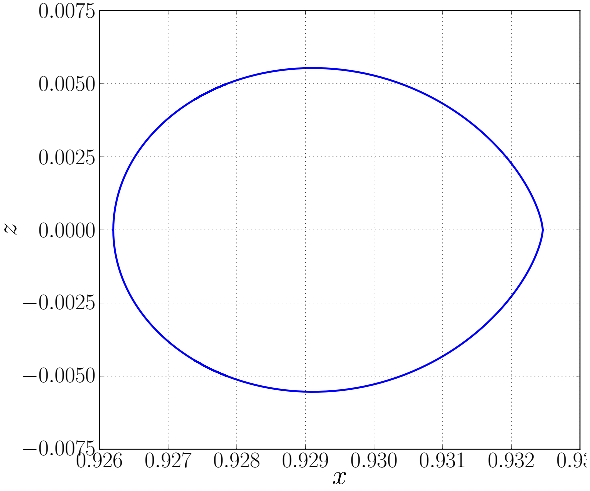
Sun-Jupiter: detection of a homoclinic orbit at $\beta = 0.050698$, with $\alpha = 0$, $\delta = 0$.

Course demo : Solar-Sail/Sun-Jupiter/Libration/Manifolds

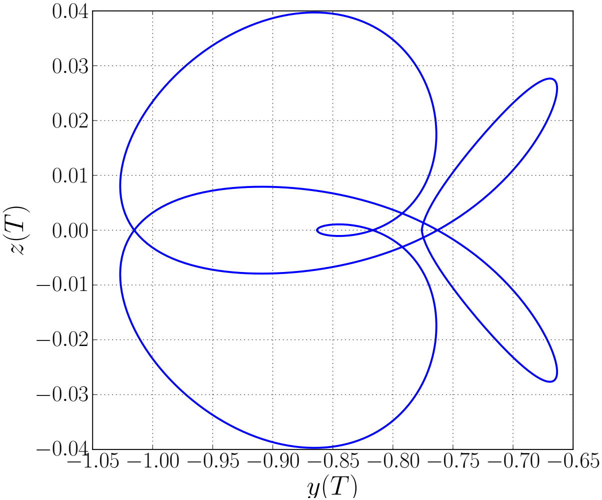


Sun-Jupiter: unstable manifold orbits for $\delta \in [-\frac{\pi}{2}, \frac{\pi}{2}]$, with $\beta = 0.05$, $\alpha = 0.1$.

Course demo : Solar-Sail/Sun-Jupiter/Libration/Manifolds

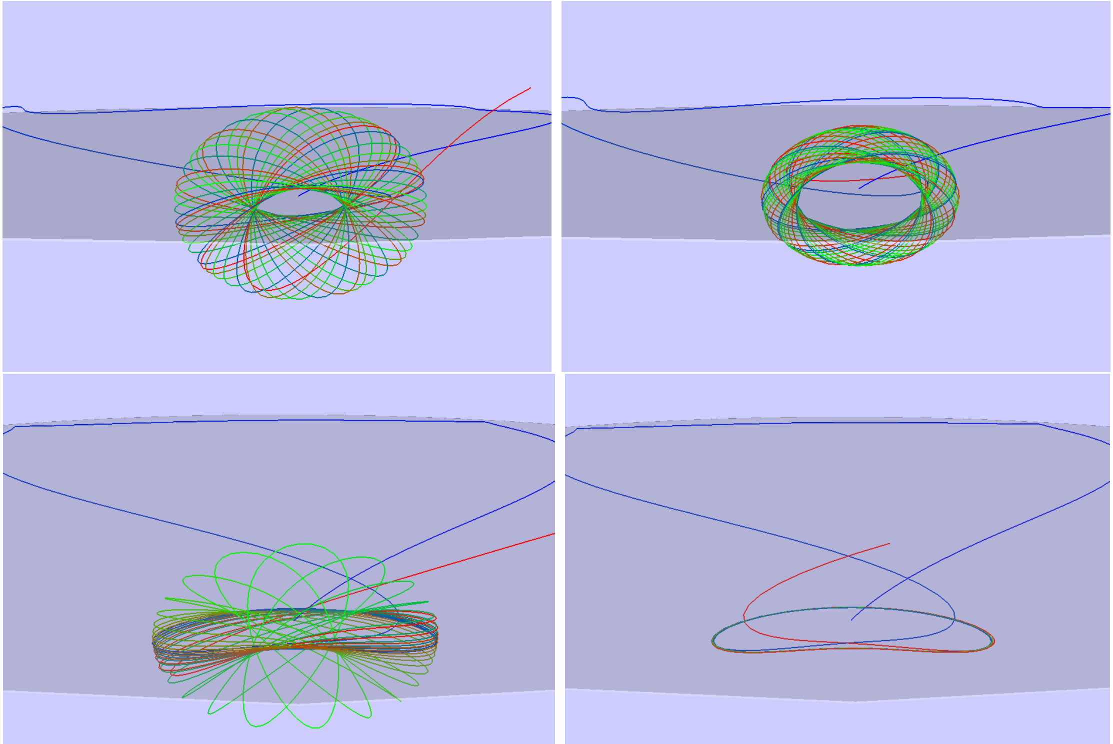


The libration points

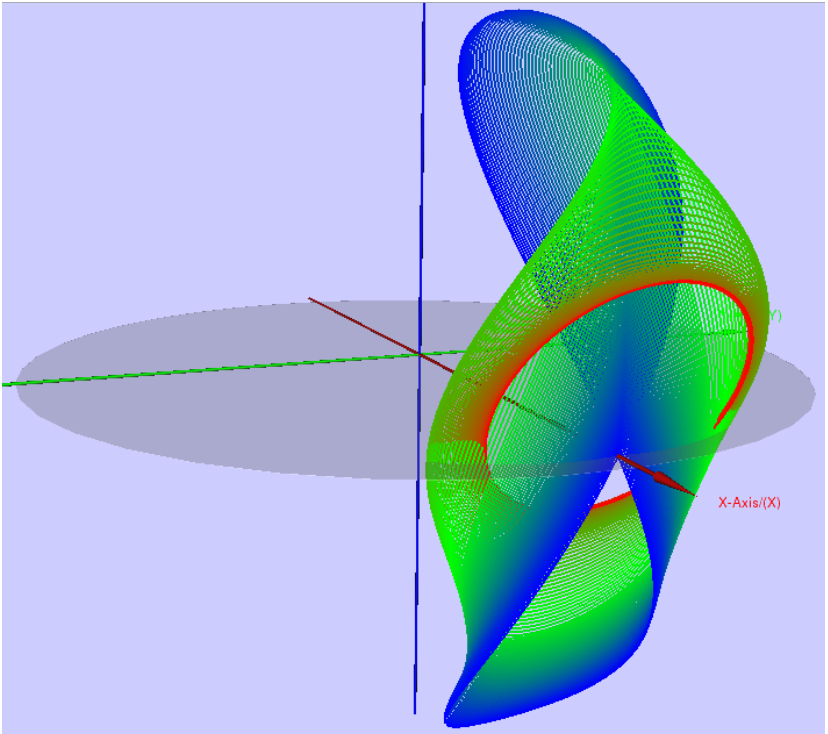


The end points

Course demo : Solar-Sail/Sun-Jupiter/Libration/Manifolds



Some connecting orbits for $\alpha = 0.07$ and varying β and δ.



V_1-orbits with $\beta = 0.15$, $T = 6.27141$, $\delta \in [0\ ,\ 0.6415]$.