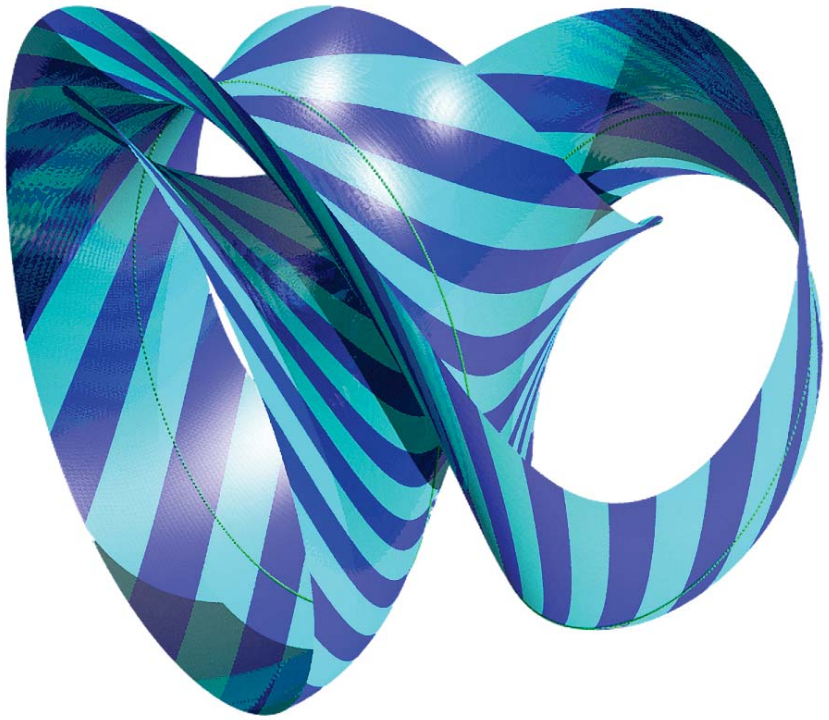
Computer assisted proofs in Nonlinear Dynamics



Jean-Philippe Lessard
McGill University

Many problems in differential equations can be reduced to questions about the zeros of some (possibly infinite dimensional) nonlinear function. Examples include equilibrium solutions, periodic solutions, their attached invariant manifolds, connecting orbits, invariant tori, etcetera. In many applications, especially when there are no small parameters, the resulting nonlinear equations are too difficult to solve by hand, and we resort to numerical simulations to better understand the problem.

Jay Mireles James
Florida Atlantic University

The main question addressed in this workshop is this: suppose we have computed a good numerical approximation -- can we establish the existence of a true solution nearby? Combining tools from functional analysis, complex analysis, numerical analysis, and interval computing, we see that for many of the problems mentioned above the answer is yes. Over the three days we will give a broad and example driven overview of the field of validated numerics.

1 de agosto 4-7pm
2 de agosto 4-7pm
3 de agosto 4-6pm

Salón 200
Edificio Anexo
IIMAS - UNAM

Formal Series Solutions: Initial Value Problems, Stable/Unstable Manifolds, And Automatic Differentiation

Computer Assisted Validation

Thm: (Henard) suppose that $f\colon \mathbb{R}^4 \to \mathbb{R}^4$ is a Hamiltonian vector field, with a saddle-focus equilibrium. If there exists transverse (relative to the energy section) homoclinic orbit then there is a cylinder of periodic orbits, parameterized by energy, accumulating to the homoclinic.

(Blue sky catastrophe)

Thm: (Devaney) suppose that $f\colon \mathbb{R}^4 \to \mathbb{R}^4$ is a Hamiltonian vector field, with a saddle-focus equilibrium. If there exists transverse (relative to the energy section) homoclinic orbit then f admits a chaotic horseshoe (near the homoclinic).

Computer Assisted Validation

Thm: (S. Kepley, MJ) the CRFBP with mass parameters $m_1 = 0.5, m_2 = 0.3$ and $m_3 = 0.2$ has a transverse homoclinic orbit to a saddle-focus equilibrium.

(to appear in JDE)

The proof is with substantial computer assistance.

- Prove the existence (with bounds) of a saddle focus equilibrium.
- Validated numerics for the stable/unstable manifolds.
- Prove that the stable/unstable manifolds intersect transversally.

Before we can validate these objects we must compute good representations of them. As J.P showed yesterday, Taylor series are well suited for computer assisted proof.

Initial Value Problems

Remarks/Notation

Recall that for two power series $f(z) = \sum_{n=0}^{\infty} a_n z^n \qquad g(z) = \sum_{n=0}^{\infty} b_n z^n$

the power series of the product is $(f \cdot g)(z) = \sum_{n=0}^{\infty} c_n z^n$ where $c_n = \sum_{k=0}^{n} a_{n-k} b_k$

For two infinite sequences $\{a_n\}_{n=0}^{\infty}$ and $\{b_n\}_{n=0}^{\infty}$ we define the *Cauchy product* $a * b$ by

$$(a * b)_n = \sum_{k=0}^{n} a_{n-k} b_k$$

Then $(f \cdot g)(z) = \sum_{n=0}^{\infty} (a * b)_n z^n$

Higher order products are similarly defined:

$$(a * b * c)_n = \sum_{k=0}^{n} \sum_{j=0}^{k} a_{n-k} b_{k-j} c_j \qquad (a * b * c * d)_n = \sum_{k=0}^{n} \sum_{j=0}^{k} \sum_{i=0}^{j} a_{n-k} b_{k-j} c_{j-i} d_i$$

$$(a * b * c * d * e)_n = \sum_{k=0}^{n} \sum_{j=0}^{k} \sum_{i=0}^{j} \sum_{\ell=0}^{i} a_{n-k} b_{k-j} c_{j-i} d_{i-\ell} e_\ell$$

and so on...

Initial Value Problems

Remarks/Notation

More generally if $f(x,y) = \sum_{m=0}^{\infty}\sum_{n=0}^{\infty} a_{mn} x^m y^n$ and $g(x,y) = \sum_{m=0}^{\infty}\sum_{n=0}^{\infty} b_{mn} x^m y^n$

then the power series for the product is given by

$$(f \cdot g)(x,y) = \sum_{m=0}^{\infty}\sum_{n=0}^{\infty} (a * b)_{mn} x^m y^n \quad \text{where} \quad (a*b)_{mn} = \sum_{j=0}^{m}\sum_{k=0}^{n} a_{m-j\, n-k} b_{jk}$$

Similarly

$$(a*b*c)_{mn} = \sum_{i=0}^{m}\sum_{j=0}^{n}\sum_{k=0}^{i}\sum_{\ell=0}^{j} a_{m-i\, n-j} b_{i-k\, j-\ell} c_{k\ell}$$

$$(a*b*c*d)_{mn} = \sum_{j_1=0}^{m}\sum_{k_1=0}^{n}\sum_{j_2=0}^{j_1}\sum_{k_2=0}^{k_1}\sum_{j_3=0}^{j_2}\sum_{k_3=0}^{k_2} a_{m-j_1\, n-k_1} b_{j_1-j_2\, k_1-k_2} c_{j_2-j_3\, k_2-k_3} d_{j_3 k_3}$$

and so forth...

These ideas extend naturally to series of more than two variables.

Initial Value Problems

Taylor Integrators

Initial Value Problems

Taylor Integrators

Let $F\colon \mathbb{R}^N \to \mathbb{R}^N$ be a vector field and let $\phi\colon \mathbb{R}^N \times \mathbb{R} \to \mathbb{R}^N$ denote the induced flow. Assume that F is real analytic.

- Given an initial condition $x_0 \in \mathbb{R}^N$ we are interested in the analytic solution curve $\gamma\colon (-\tau, \tau) \to \mathbb{R}^N$ having

$$\gamma(0) = x_0 \qquad \text{and} \qquad \gamma'(t) = F(\gamma(t))$$

- Let $\gamma(t) = \sum_{n=0}^{\infty} \gamma_n t^n \qquad \gamma_n \in \mathbb{R}^N \qquad \gamma_0 = x_0$

  denote the Taylor series for γ on $(-\tau, \tau)$. A Taylor integrator is an algorithm which, given an x_0 and a $K \in \mathbb{N}$ computes the coefficients $\gamma_1, \ldots, \gamma_K \in \mathbb{R}^N$.

Initial Value Problems

Taylor Integrators

See the Bibliography of my first day lecture.

Powerful software for rigorous Taylor integration is found at:

http://capd.ii.uj.edu.pl/

Computer Assisted Proofs in Dynamics group

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Initial Value Problems

Example: Consider the simple differential equation

$$x' = -x + \epsilon x^2 \qquad x(0) = x_0$$

We look for a power series solution $x(t) = \sum_{n=0}^{\infty} a_n t^n \qquad a_0 = x0$

Plugging in gives (left) $x'(t) = \sum_{n=0}^{\infty} (n+1) a_{n+1} t^n$

and (right) $-x(t) + \epsilon x(t)^2 = -\sum_{n=0}^{\infty} a_n t^n + \epsilon \sum_{n=0}^{\infty} \left(\sum_{k=0}^{n} a_{n-k} a_k \right) t^n$

$$= \sum_{n=0}^{\infty} \left(-a_n + \epsilon \sum_{k=0}^{n} a_{n-k} a_k \right) t^n$$

Initial Value Problems

Example: Consider the simple differential equation

$$x' = -x + \epsilon x^2 \qquad x(0) = x_0$$

We look for a power series solution $x(t) = \sum_{n=0}^{\infty} a_n t^n \qquad a_0 = x0$

Matching like powers:

$$(n+1)a_{n+1} = -a_n + \epsilon \sum_{k=0}^{n} a_{n-k} a_k$$

Or

$$a_{n+1} = \frac{1}{n+1}\left(-a_n + \epsilon \sum_{k=0}^{n} a_{n-k} a_k\right)$$

Or

$$a_n = \frac{1}{n}\left(-a_{n-1} + \epsilon (a * a)_{n-1}\right) \qquad n \geq 1$$

Initial Value Problems

Example:

- Given the initial condition x_0 the coefficients $a_1, \ldots, a_N$ are formally well defined to all orders.

- **Algorithm:** (for fixed approximation order N)
  - Let $a_0 = x_0$
  - For $n = 1$ to $n = N$

$$a_n = \frac{1}{n}\left(-a_{n-1} + \epsilon (a * a)_{n-1}\right)$$

  end

  - Return $a_0, a_1, \ldots, a_N$

Initial Value Problems

Example: Consider the simple differential equation

$$x' = -x + \epsilon x^2 \qquad x(0) = x_0$$

Consider

$$\phi(x_0 + x, t) = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} a_{mn} x^m t^n$$

Choose

$$a_{m0} = \begin{cases} x_0 & \text{if } m = 0 \\ s & \text{if } m = 1 \\ 0 & \text{if } m \geq 2 \end{cases}$$

So that

$$\phi(x_0 + x, 0) \subset [x_0 - s, x_0 + s]$$

$$x \in [-1, 1]$$

Initial Value Problems

Example: Consider the simple differential equation

$$x' = -x + \epsilon x^2 \qquad\qquad x(0) = x_0$$

Then

$$\frac{\partial}{\partial t}\phi(x_0 + x, t) = \sum_{m=0}^{\infty}\sum_{n=0}^{\infty}(n+1)a_{mn+1}x^m t^n$$

and

$$F(\phi(x_0 + x, t)) = \sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\left(-a_{mn} + \epsilon(a * a)_{mn}\right)x^m t^n$$

Initial Value Problems

Example: Consider the simple differential equation

$$x' = -x + \epsilon x^2 \qquad x(0) = x_0$$

Matching like powers leads to

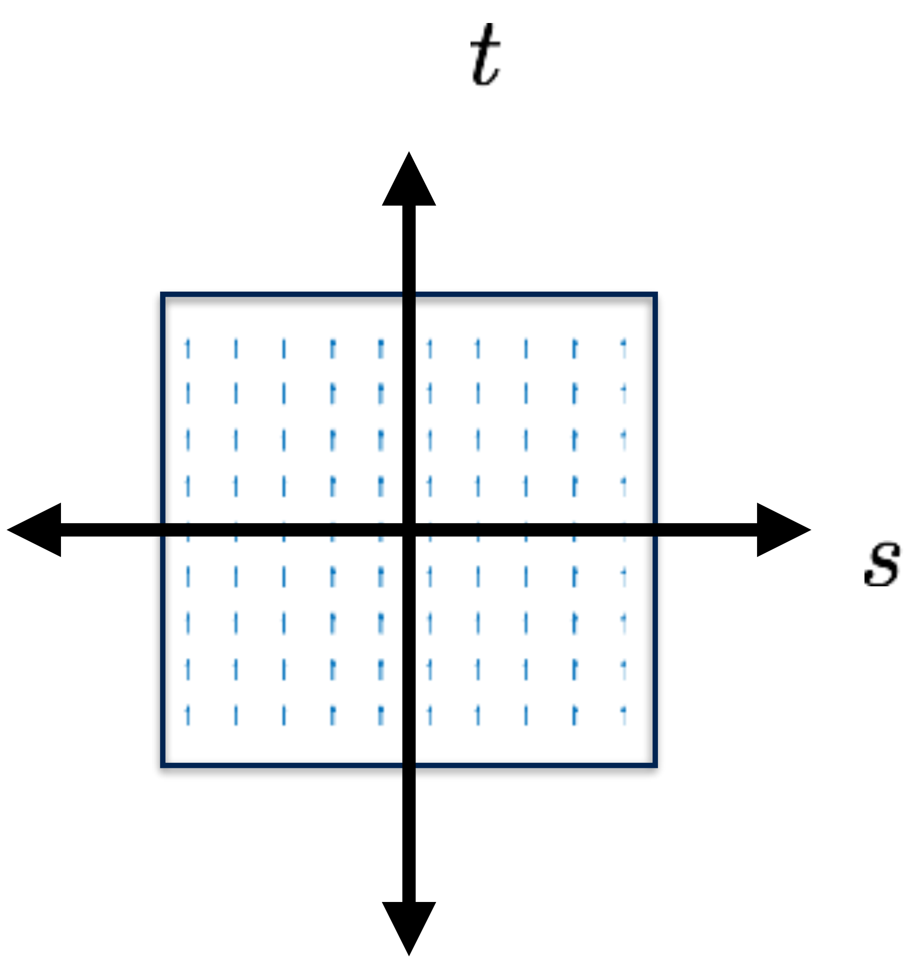
$$(n+1)a_{mn+1} = -a_{mn} + \epsilon(a * a)_{mn}$$

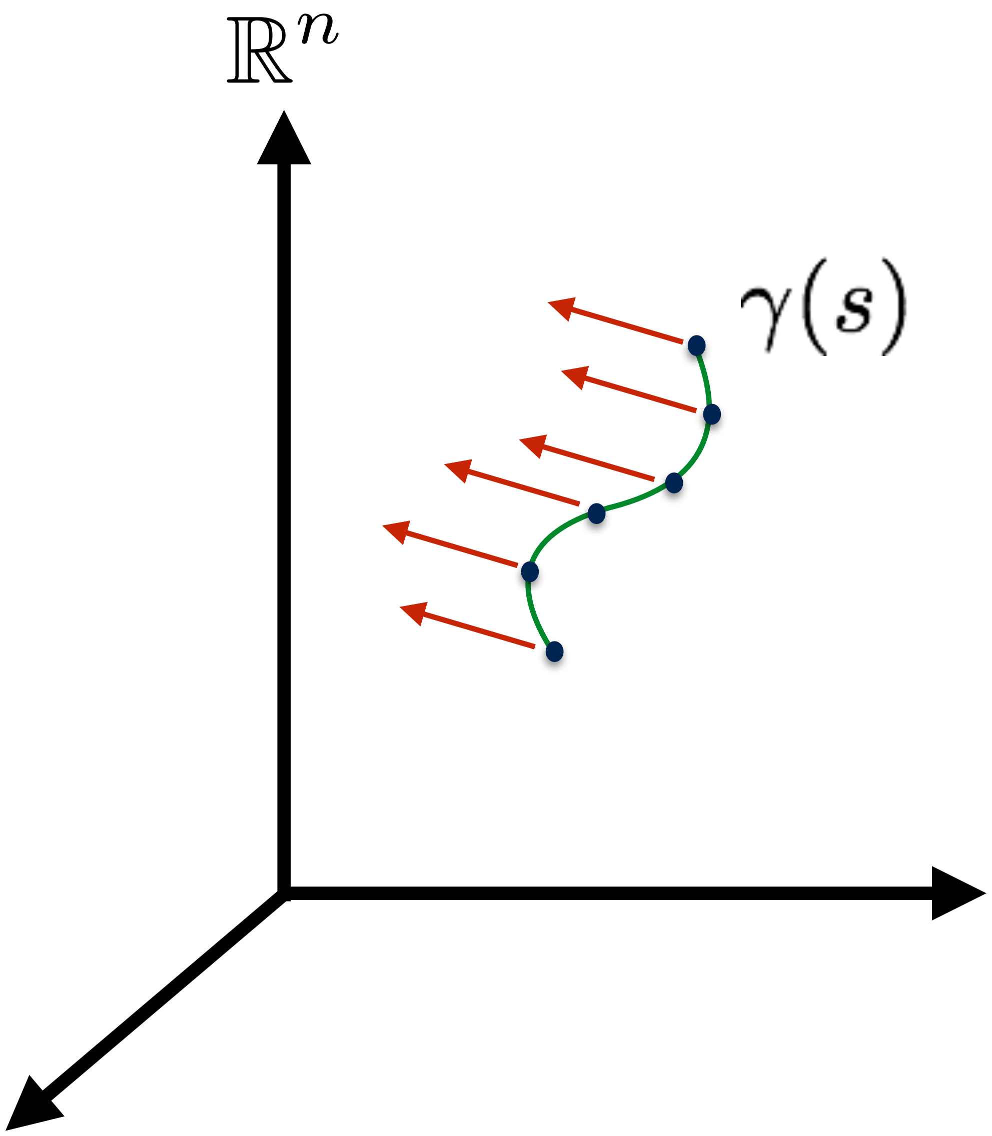
or
$$a_{mn} = \frac{1}{n}\left(-a_{mn-1} + \epsilon(a * a)_{mn-1}\right) \qquad n \geq 1, \quad m \geq 0$$

$$a_{m0} = \begin{cases} x_0 & \text{if } m = 0 \\ s & \text{if } m = 1 \\ 0 & \text{if } m \geq 2 \end{cases}$$

Initial Value Problems

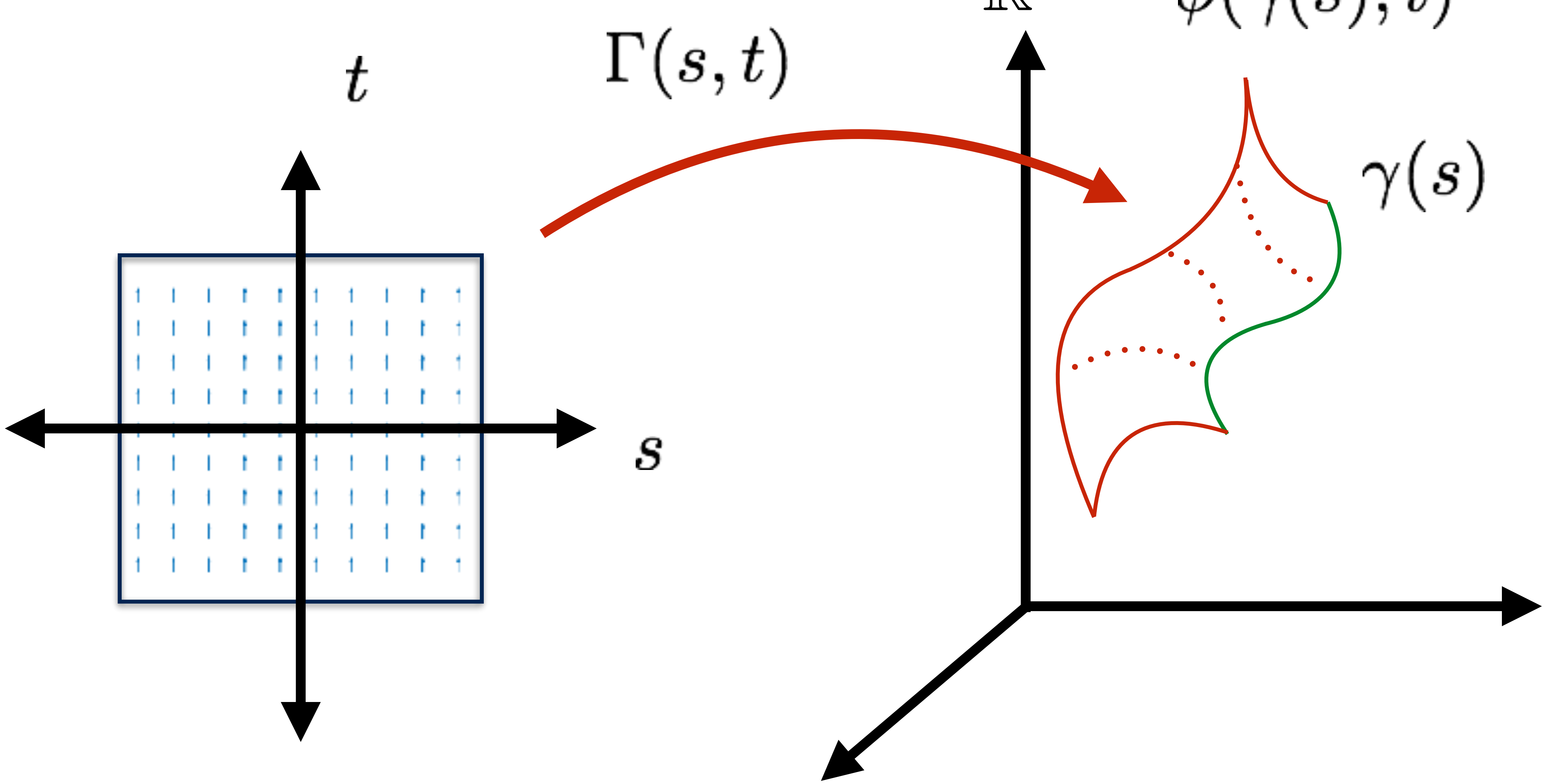
Advection of analytic curves:





Initial Value Problems

Advection of analytic curves:



Need

$$\frac{\partial}{\partial t}\Gamma(s, t) = F(\Gamma(s, t)) \qquad \Gamma(s, 0) = \gamma(s)$$

Initial Value Problems

Example:

$$F(x,y,z) = \begin{pmatrix} \sigma y - \sigma x \\ \rho x - y - xz \\ -\beta z + xy \end{pmatrix}$$

Consider a "material line" $\gamma\colon [-1,1] \to \mathbb{R}^3$ with power series

$$\gamma(s) = \sum_{m=0}^{\infty} \begin{pmatrix} a_m \\ b_m \\ c_m \end{pmatrix} s^m \qquad \langle \gamma'(s), f(\gamma(s)\rangle \neq 0 \text{ for all } s \in [-1,1]$$

Look for

$$\phi(\gamma(s),t) = \Gamma(s,t) = \sum_{m=0}^{\infty}\sum_{n=0}^{\infty} \begin{pmatrix} a_{mn} \\ b_{mn} \\ c_{mn} \end{pmatrix} s^m t^n$$

with

$$\begin{pmatrix} a_{m0} \\ b_{m0} \\ c_{m0} \end{pmatrix} = \begin{pmatrix} a_m \\ b_m \\ c_m \end{pmatrix} \quad m \geq 0$$

Initial Value Problems

Example:

$$F(x,y,z) = \begin{pmatrix} \sigma y - \sigma x \\ \rho x - y - xz \\ -\beta z + xy \end{pmatrix}$$

Then

$$\frac{\partial}{\partial t}\Gamma(s,t) = \sum_{m=0}^{\infty}\sum_{n=0}^{\infty}(n+1)\begin{pmatrix} a_{mn+1} \\ b_{mn+1} \\ c_{mn+1} \end{pmatrix} s^m t^n$$

and

$$F(\Gamma(s,t)) = \sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\begin{pmatrix} \sigma b_{mn} - \sigma a_{mn} \\ \rho a_{mn} - b_{mn} - (a*c)_{mn} \\ -\beta c_{mn} + (a*b)_{mn} \end{pmatrix} s^m t^n$$

Initial Value Problems

Example:

$$F(x,y,z) = \begin{pmatrix} \sigma y - \sigma x \\ \rho x - y - xz \\ -\beta z + xy \end{pmatrix}$$

Matching like powers gives

$$(n+1)\begin{pmatrix} a_{mn+1} \\ b_{mn+1} \\ c_{mn+1} \end{pmatrix} = \begin{pmatrix} \sigma b_{mn} - \sigma a_{mn} \\ \rho a_{mn} - b_{mn} - (a*c)_{mn} \\ -\beta c_{mn} + (a*b)_{mn} \end{pmatrix}$$

or

$$\boxed{\begin{pmatrix} a_{mn} \\ b_{mn} \\ c_{mn} \end{pmatrix} = \frac{1}{n}\begin{pmatrix} \sigma b_{mn-1} - \sigma a_{mn-1} \\ \rho a_{mn-1} - b_{mn-1} - (a*c)_{mn-1} \\ -\beta c_{mn-1} + (a*b)_{mn-1} \end{pmatrix}} \quad \begin{pmatrix} a_{m0} \\ b_{m0} \\ c_{m0} \end{pmatrix} = \begin{pmatrix} a_m \\ b_m \\ c_m \end{pmatrix}$$

$$n \geq 1, \quad m \geq 0.$$

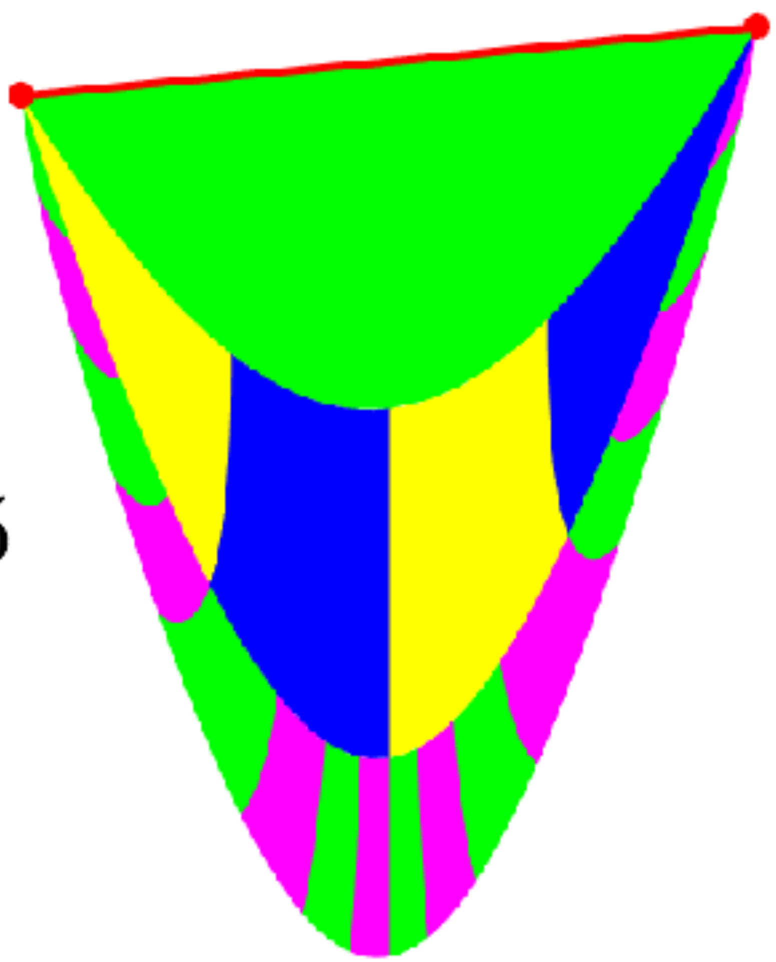
Initial Value Problems

39 modes in space

24 modes in time

Example:

$T = 0.25$

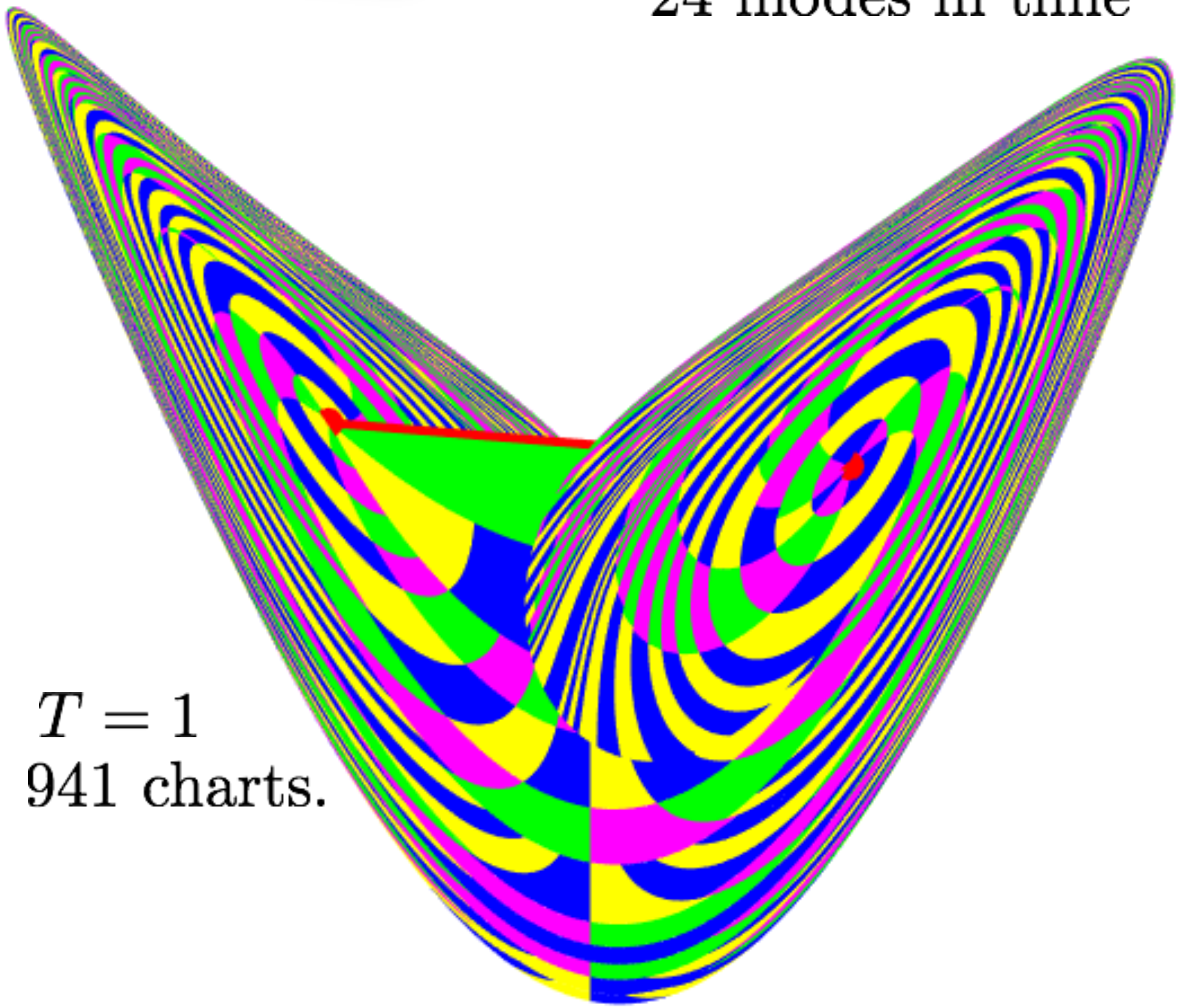


Initial Value Problems

39 modes in space

24 modes in time

Example:



$T = 1$

941 charts.

See:

SIAM J. Appl. Dyn. Syst., 17(1), 157–202. (46 pages)

Analytic Continuation of Local (Un)Stable Manifolds with Rigorous Computer Assisted Error Bounds

The Parameterization Method

High Order Taylor Parameterization of Stable/Unstable Manifolds

The Parameterization Method

Let $F\colon \mathbb{R}^N \to \mathbb{R}^N$ be a vector field and p_0 be an equilibrium point. Suppose that $DF(p_0)$ is diagonalizable with stable eigenvalues

$\lambda_1, \ldots, \lambda_m \in \mathbb{C}$

We would like to find a parameterization $P\colon B^m \to \mathbb{R}^N$ having that

$$P(0) = p_0 \qquad \text{and that} \qquad P(B^m) \subset W^s(p_0)$$

that is: P should parameterize a local stable manifold attached to p_0.

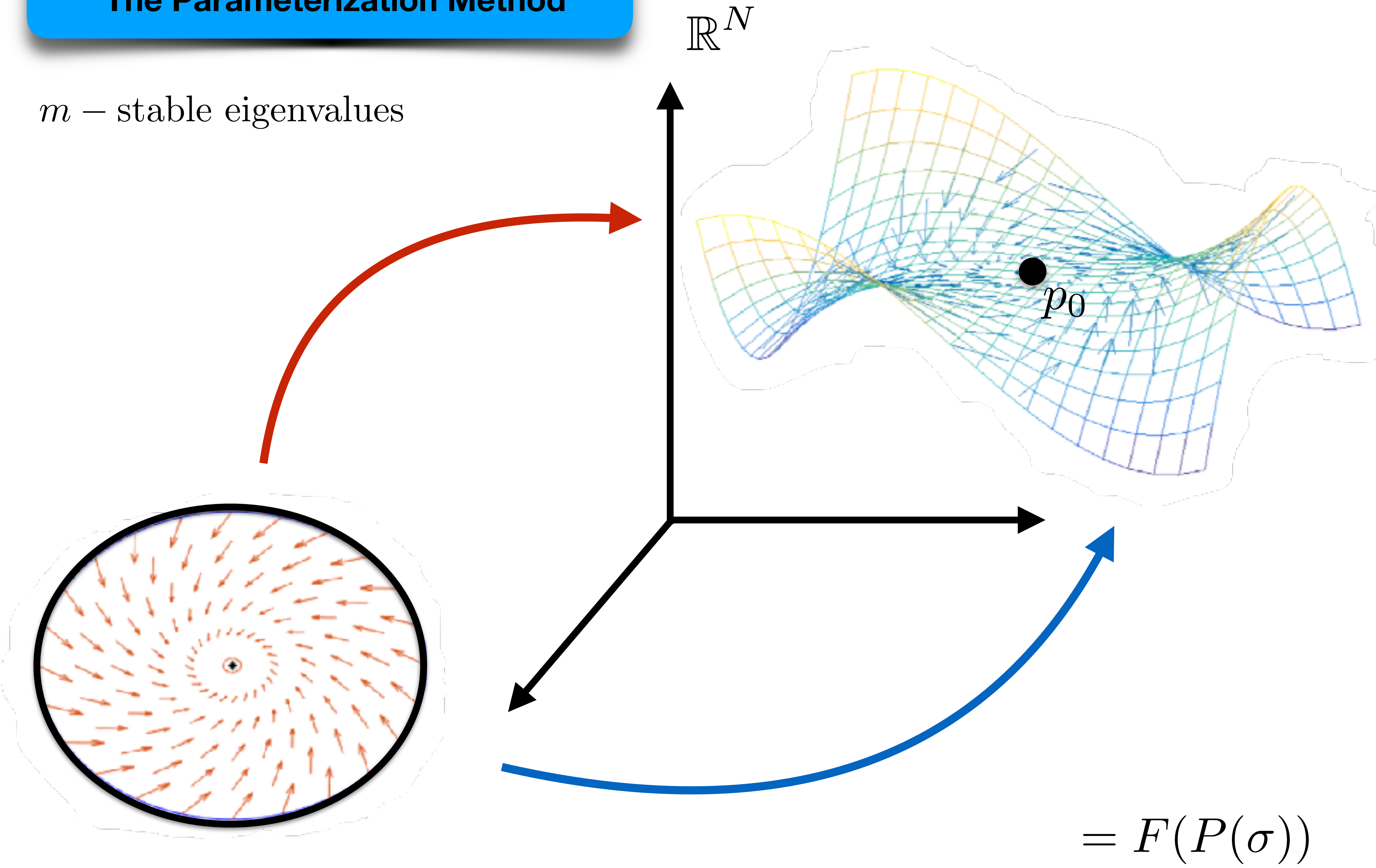
We use the *parameterization method*...

Cabré, Fontich, and de la Llave

(See the bibliography at the end of these slides)

The Parameterization Method

$m-$ stable eigenvalues



The Parameterization Method

Let

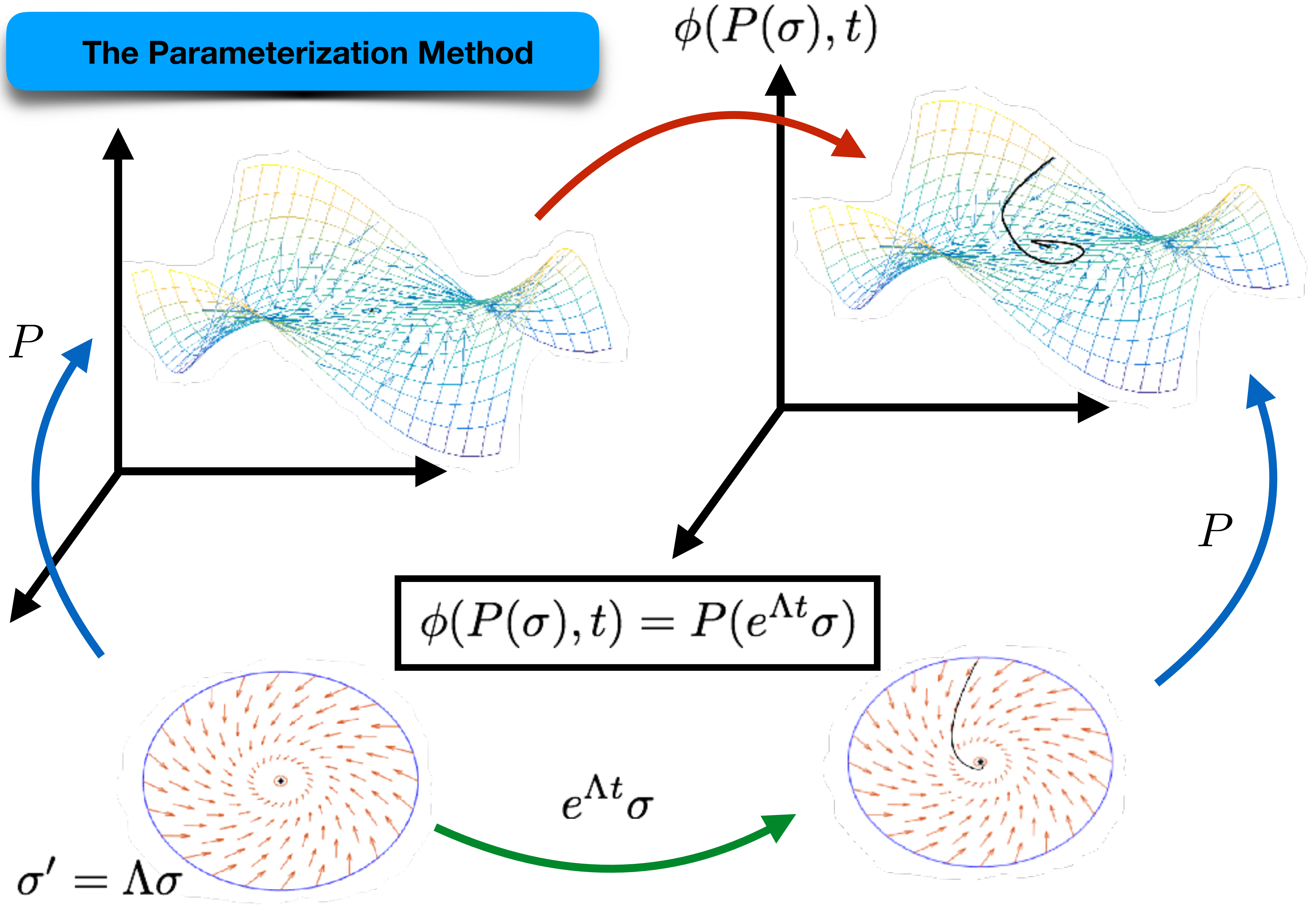
$$\Lambda = \begin{pmatrix} \lambda_1 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \lambda_m \end{pmatrix} \qquad \Lambda\sigma = \begin{pmatrix} \lambda_1\sigma_1 \\ \vdots \\ \lambda_m\sigma_m \end{pmatrix}$$

Then $DP(\sigma)\Lambda\sigma = \lambda_1\sigma_1 \frac{\partial}{\partial\sigma_1}P(\sigma) + \ldots + \lambda_m\sigma_m \frac{\partial}{\partial\sigma_1}P(\sigma)$

$$\begin{array}{|c|} \hline \lambda_1\sigma_1 \frac{\partial}{\partial\sigma_1}P_1(\sigma) + \ldots + \lambda_m\sigma_m \frac{\partial}{\partial\sigma_m}P_1(\sigma) = F_1(P(\sigma)) \\ \vdots \\ \lambda_1\sigma_1 \frac{\partial}{\partial\sigma_1}P_N(\sigma) + \ldots + \lambda_m\sigma_m \frac{\partial}{\partial\sigma_m}P_N(\sigma) = F_N(P(\sigma)) \\ \hline \end{array}$$

$$P(0) = p_0$$

The Parameterization Method



The Parameterization Method

Claim: if $P\colon B^m \to \mathbb{R}^N$ has

$$DP(\sigma)\Lambda\sigma = F(P(\sigma))$$

for all $\sigma \in B^m$ with $P(0) = p_0$ and $DP(0) = [\xi_1, \ldots, \xi_m]$ then

$$\phi(P(\sigma), t) = P(e^{\Lambda t}\sigma)$$

(or $t \leq 0$ in the unstable case)

Proof: Choose a $\sigma \in B^m$. Note that $e^{\Lambda t}\sigma \in B^m$ for all $t \geq 0$. Define

$$\gamma(t) = P(e^{\Lambda t}\sigma)$$

Then for any fixed $t > 0$

$$\begin{aligned} \gamma'(t) &= DP(e^{\Lambda t}\sigma)e^{\Lambda t}\Lambda\sigma \\ &= DP(\tilde{\sigma})\Lambda\tilde{\sigma} \\ &= F(P(\tilde{\sigma})) \\ &= F(P(e^{\Lambda t}\sigma)) \\ &= F(\gamma(t)) \end{aligned}$$

letting $\tilde{\sigma} = e^{\Lambda t}\sigma$

as $\tilde{\sigma} \in B^m$

The Parameterization Method

Claim: if $P\colon B^m \to \mathbb{R}^N$ has

$$DP(\sigma)\Lambda\sigma = F(P(\sigma))$$

for all $\sigma \in B^m$ with $P(0) = p_0$ and $DP(0) = [\xi_1, \ldots, \xi_m]$ then

$$\phi(P(\sigma), t) = P(e^{\Lambda t}\sigma)$$

for all $\sigma \in B^m$ and all $t \geq 0$.

Proof: Choose a $\sigma \in B^m$. Note that $e^{\Lambda t}\sigma \in B^m$ for all $t \geq 0$. Define

$$\gamma(t) = P(e^{\Lambda t}\sigma)$$

Then $\gamma(t)$ is the solution curve with $\gamma(0) = P(\sigma)$. By uniqueness we have that

$$\phi(P(\sigma), t) = \gamma(t) = P(e^{\Lambda t}\sigma)$$

as desired.

Since $\sigma \in B^m$, and $t > 0$ were arbitrary, we have the claim.

The Parameterization Method

Corollary: $P\colon B^m \to \mathbb{R}^N$ parameterizes a local stable manifold.

Proof:

The condition $P(0) = p_0$ gives that P parameterizes a disk containing the equilibrium.

The condition $DP(0) = [\xi_1, \ldots, \xi_m]$ gives that P is tangent to the appropriate eigenspace at p_0.

Now choose $\sigma \in B^m$ and consider $P(\sigma)$. Using the flow conjugacy gives

$$\begin{aligned}\lim_{t\to\infty} \phi(P(\sigma), t) &= \lim_{t\to\infty} P\left(e^{\Lambda t}\sigma\right) \\ &= P\left(\lim_{t\to\infty} e^{\Lambda t}\sigma\right) \qquad \text{continuity of } P. \\ &= P(0) \\ &= p_0\end{aligned}$$

Since $\sigma \in B^m$ was arbitrary we have that every orbit on the image of P accumulates in backward time to the equilibrium. Then

$$P(B^m) = W^s_{\text{loc}}(p_0)$$

as desired.

The Parameterization Method

Example:

$$F(x,y,z) = \begin{pmatrix} \sigma y - \sigma x \\ \rho x - y - xz \\ -\beta z + xy \end{pmatrix}$$

For a one dimensional stable/unstable manifold invariance equation is

$$\lambda \sigma \frac{d}{d\sigma} P(\sigma) = F(P(\sigma))$$

Look for a solution

The Parameterization Method

Example:

$$F(x,y,z) = \begin{pmatrix} \sigma y - \sigma x \\ \rho x - y - xz \\ -\beta z + xy \end{pmatrix}$$

Then left hand side of the invariance equation is

and on the right

The Parameterization Method

Example:

$$F(x,y,z) = \begin{pmatrix} \sigma y - \sigma x \\ \rho x - y - xz \\ -\beta z + xy \end{pmatrix}$$

Matching like powers gives that

for $n \geq 2$.

Need to extract terms of order n from the convolutions.

The Parameterization Method

Example:

Note that

Similarily

The Parameterization Method

Then

Example:

But

The Parameterization Method

Example:

Matching like powers gives

which becomes

This can be written as

where

The Parameterization Method

Example:

- as $n\lambda$ is not an eigenvalue.

  So the parameterization is formally well defined.

- **Algorithm:** (for fixed approximation order N)
  - Compute the equilibrium p_0 and eigendata λ, p_1.
  - For $n = 2$ to $n = N$

    Solve

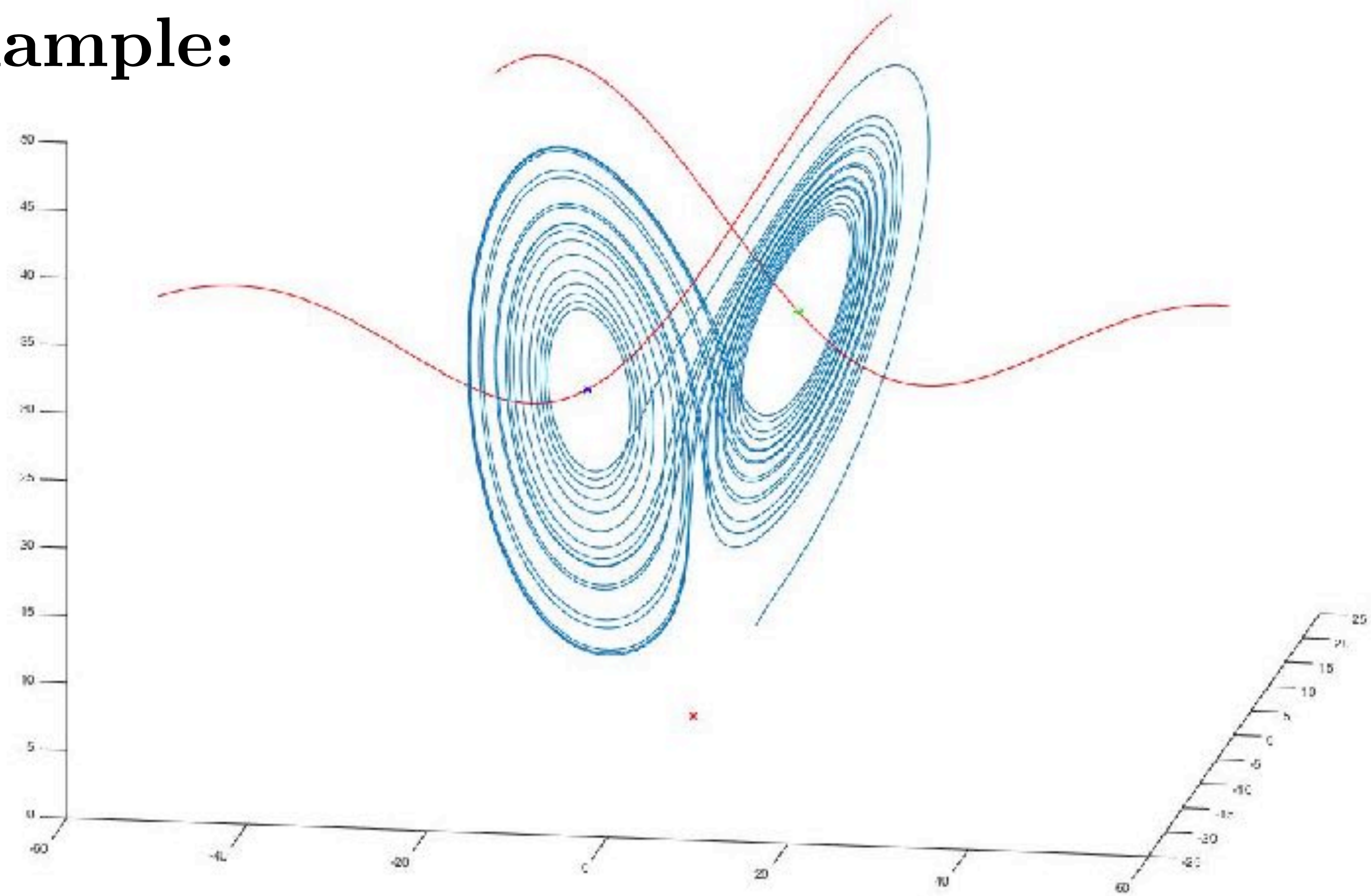
    Store p_n

    end
  -

The Parameterization Method

Classic parameter values.

Example:



Approximation order $N = 50$.

$P^N([-1,1])$

Eigenvector scaled to length 58.

The Parameterization Method

Example:

$$F(x,y,z) = \begin{pmatrix} \sigma y - \sigma x \\ \rho x - y - xz \\ -\beta z + xy \end{pmatrix}$$

Suppose there are two stable/unstable eigenvalues $\lambda_1, \lambda_2 \in \mathbb{C}$.
Invariance equation is:

$$\lambda_1 \sigma_1 \frac{\partial}{\partial \sigma_1} P(\sigma_1, \sigma_2) + \lambda_2 \sigma_2 \frac{\partial}{\partial \sigma_2} P(\sigma_1, \sigma_2) = F(P(\sigma_1, \sigma_2))$$

Look for a solution

$$P(\sigma_1, \sigma_2) = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \begin{pmatrix} a_{mn} \\ b_{mn} \\ c_{mn} \end{pmatrix} \sigma_1^m \sigma_2^n$$

with

$$\begin{pmatrix} a_{00} \\ b_{00} \\ c_{00} \end{pmatrix} = p_0 \qquad \begin{pmatrix} a_{10} \\ b_{10} \\ c_{10} \end{pmatrix} = \xi_1 \qquad \begin{pmatrix} a_{01} \\ b_{01} \\ c_{01} \end{pmatrix} = \xi_2$$

The Parameterization Method

Example: Then

$$\lambda_1\sigma_1\frac{\partial}{\partial\sigma_1}P(\sigma_1,\sigma_2)+\lambda_2\sigma_2\frac{\partial}{\partial\sigma_2}P(\sigma_1,\sigma_2)=\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}(m\lambda_1+n\lambda_2)\begin{pmatrix}a_{mn}\\ b_{mn}\\ c_{mn}\end{pmatrix}\sigma_1^m\sigma_2^n$$

and

$$F(P(\sigma_1,\sigma_2))=\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\begin{pmatrix}\sigma b_{mn}-\sigma a_{mn}\\ \rho a_{mn}-b_{mn}-(a*c)_{mn}\\ -\beta c_{mn}+(a*b)_{mn}\end{pmatrix}\sigma_1^m\sigma_2^n$$

As before:

$$[DF(p_0)-(m\lambda_1+n\lambda_2)\mathrm{Id}]\,p_{mn}=-R_{mn}$$

where

$$R_{mn}=\begin{pmatrix}0\\ -(a\hat{*}c)_{mn}\\ (a\hat{*}b)_{mn}\end{pmatrix}$$

$$(a\hat{*}b)_{mn}=(a*b)_{mn}-a_{00}b_{mn}-b_{00}a_{mn}$$

$$(a\hat{*}c)_{mn}=(a*c)_{mn}-a_{00}c_{mn}-c_{00}a_{mn}$$

The Parameterization Method

Example:

- The matrix $DF(p_0) - (m\lambda_1 + n\lambda_2)\mathrm{Id}$ is invertible as as long as $(m\lambda_1 + n\lambda_2) \notin \mathrm{spec}(DF(p_0))$
- **Algorithm:** (for fixed approximation order N)
  - Compute equilibrium p_0, and eigendata $\lambda_1, p_1, \lambda_2, p_2$
  - Check that λ_1, λ_2 non-resonant. If resonant return.
  - For $m + n = 2$ to m+n = N

    Compute R_{mn} (depends on lower order terms).

    Solve $[DF(p_0) - (m\lambda_1 + n\lambda_2)\mathrm{Id}]p_{mn} = -R_{mn}$

    Store p_{mn}

    end
  - return all p_{mn} with $0 \leq m + n \leq N$

The Parameterization Method

Example:

Unstable manifolds of eyes: computed to order $N = 150$, scale $= 3.6$

Unstable manifolds of origin: computed to order $N = 50$, scale slow $= 20$ scale fast $= 2$.

Combining the Parameterization Method with Taylor Integration of Material Lines

(Charts and Atlases for Attached Invariant Manifolds)

Chart maps and atlases

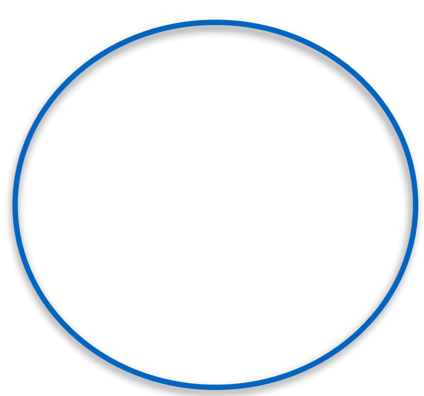
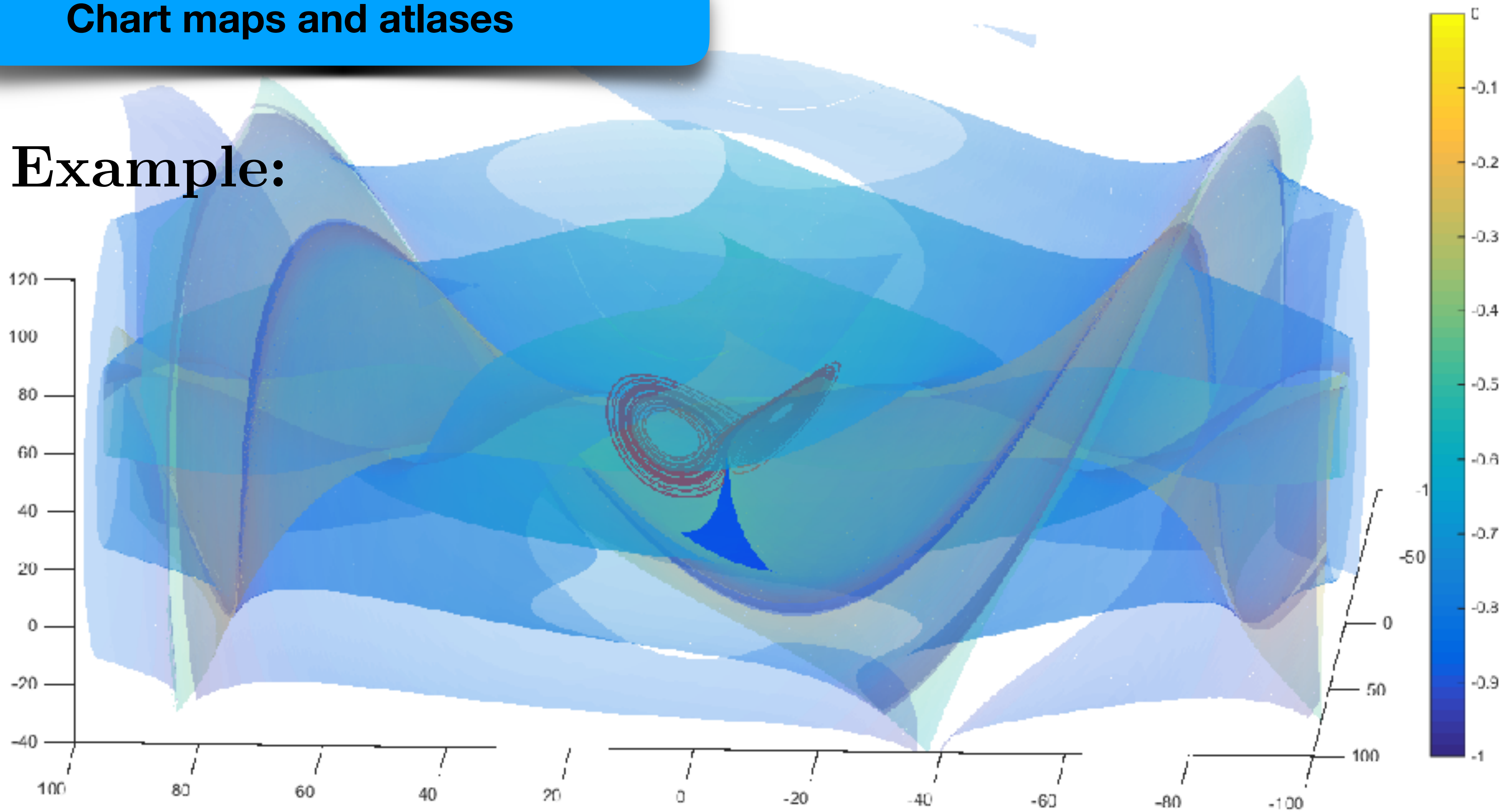


Chart maps and atlases

Example:

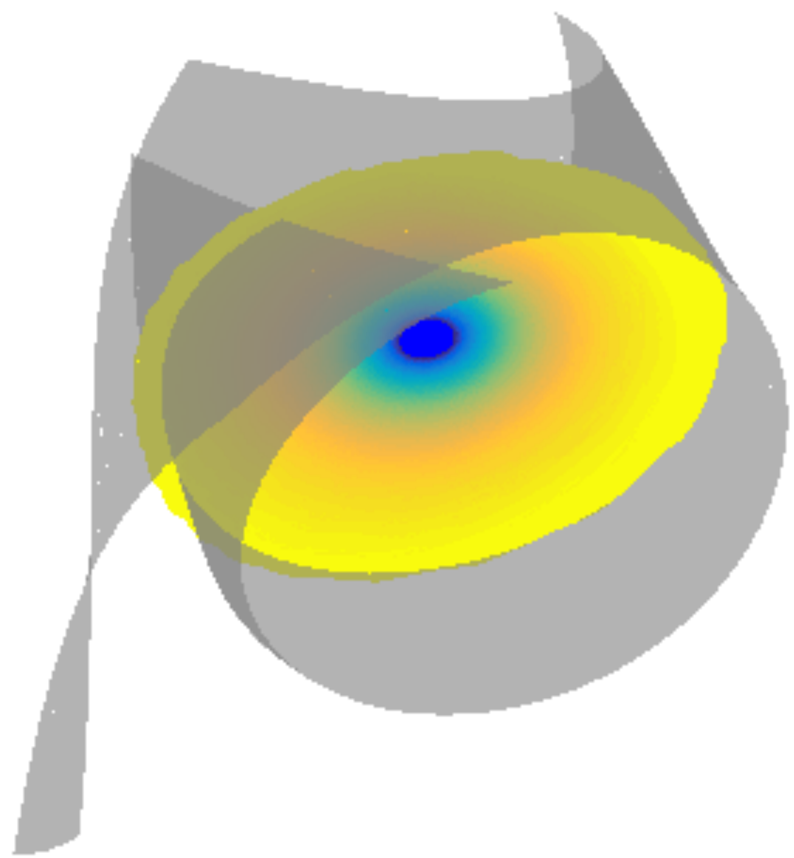


Backward integration of the boundary of the stable manifold attached to the origin: minus one time unit. 4,674 polynomial chart maps and the local parameterization.

See:
SIAM J. Appl. Dyn. Syst., 17(1), 157–202. (46 pages)
Analytic Continuation of Local (Un)Stable Manifolds with Rigorous Computer Assisted Error Bounds
Approximation order 24 in time and 39 in space.

Chart maps and atlases

Example



Backward integration of the boundary of the stable manifold attached to the origin: minus one time unit.
4, 674 polynomial chart maps and the local parameterization.
Approximation order 24 in time and 39 in space.

Chart maps and atlases

Non-polynomial vector fields

and

Automatic Differentiation

Automatic Differentiation

Suppose that F is not polynomial but is composed of elementary functions. Then we use *automatic differentiation* to re-write F in polynomial form. The drawback is that we will increase the dimension of the system.

The idea is that functions like $e^x, \sin(x), \cos(x), \sqrt{x}, x^{3/2}, \ldots$ solve simple differential equations.

... and ...

Differentiation turns composition into multiplication.

Automatic Differentiation

Example: Consider the equation

$$x' = -x + \epsilon x e^{-x}$$

Let

$$y = e^{-x}$$

Then

$$\begin{aligned} y' &= -e^{-x} x' \\ &= -y(-x + \epsilon x y) \\ &= xy - \epsilon x y^2 \end{aligned}$$

Now we want to solve the system:

$$\begin{aligned} x' &= -x + \epsilon x y & \qquad x(0) &= x_0 \\ y' &= xy - \epsilon x y^2 & \qquad y(0) &= e^{-x_0} \end{aligned}$$

Automatic Differentiation

Example: Consider the equation

$$x' = -x + \epsilon x y \qquad x(0) = x_0$$
$$y' = xy - \epsilon x y^2 \qquad y(0) = e^{-x_0}$$

$$x(t) = \sum_{n=0}^{\infty} a_n t^n \qquad y(t) = \sum_{n=0}^{\infty} b_n t^n$$

$$x'(t) = \sum_{n=0} (n+1) a_{n+1} t^n \qquad y'(t) = \sum_{n=0} (n+1) b_{n+1} t^n$$

$$a_{n+1} = \frac{1}{n+1}[-a_n + \epsilon (a * b)_n]$$

$$b_{n+1} = \frac{1}{n+1}[(a * b)_n - \epsilon (a * b * b)_n]$$

This costs twice as much memory...

Automatic Differentiation

Why does it work?

$U \subset \mathbb{R}^N$ and open set.

$F: U \subset \mathbb{R}^N \to \mathbb{R}^N$ a non-polynomial vector field.

Let M be the number of non-polynomial terms in F.

We look for $R: U \to \mathbb{R}^{M+N}$, $H: U \to \mathbb{R}^M$, and a polynomial vector field $G: \mathbb{R}^{N+M} \to \mathbb{R}^{N+M}$ so that

$$R(x,y) = \begin{pmatrix} x \\ H(x) \end{pmatrix}$$

and

$$DR(x)F(x) = G(R(x))$$

Then orbits of G "project down" to orbits of F.

Automatic Differentiation

Why does it work?

Suppose that $\Gamma(t)$ is a solution of $\Gamma'(t) = G(\Gamma(t))$ with $\Gamma(0) = R(x_0)$.

Let $\gamma(t)$be the solution of $x' = F(x)$ with $\gamma(0) = x_0$.

Consider the curve $R(\gamma(t))$. We have

$$\frac{d}{dt}R(\gamma(t)) = DR(\gamma(t))\,\gamma'(t)$$
$$= DR(\gamma(t))\,F(\gamma(t))$$
$$= G(R(\gamma(t)))$$

So $R(\gamma(t))$ is the solution curve of G associated with the initial condition $R(x_0)$.

By uniqueness $\Gamma(t) = R(\gamma(t))$. Then:

- $R(x)$ parameterizes an invariant manifold.
- The projection of an orbit on $R(x)$ is an orbit for F.

Automatic Differentiation

Example: Consider the equation $x' = -x + \epsilon x e^{-x}$

$$R(x) = \begin{pmatrix} x \\ e^{-x} \end{pmatrix}$$

Check that:

$$DR(x)F(x) = G(R(x))$$

$$G(x, y) = \begin{pmatrix} -x + \epsilon x y \\ xy - \epsilon x y^2 \end{pmatrix}$$

If we start with an initial condition having

$$(x_0, y_0) = R(x_0) = (x_0, e^{-x_0})$$

Then the solution curve $\Gamma' = G(\Gamma)$ with $\Gamma(0) = R(x_0)$ has

- $\Gamma(t) = (x(t), e^{-x(t)})$ as long as its defined.
- $x(t)$ solves the original ODE as long as it is defined.

The CRFBP

$$r_j(x,y) = \sqrt{(x-x_j)^2 + (y-y_j)^2}$$

$$j = 1,2,3$$

$$m_1 + m_2 + m_3 = 1$$

$$\begin{aligned}
x' &= v \\
v' &= 2w + x - m_1 \frac{x - x_1}{r_1(x,y)^3} - m_2 \frac{x - x_2}{r_2(x,y)^3} - m_3 \frac{x - x_3}{r_3(x,y)^3} \\
y' &= w \\
w' &= -2v + y - m_1 \frac{y - y_1}{r_1(x,y)^3} - m_2 \frac{y - y_2}{r_2(x,y)^3} - m_3 \frac{y - y_3}{r_3(x,y)^3}
\end{aligned}$$

The CRFBP

The vector field is:

$$F(x,v,y,w) = \begin{pmatrix} v \\ 2w + x - m_1 \frac{x-x_1}{r_1^3} - m_2 \frac{x-x_2}{r_2^3} - m_3 \frac{x-x_3}{r_3^3} \\ w \\ -2v + y - m_1 \frac{y-y_1}{r_1^3} - m_2 \frac{y-y_2}{r_2^3} - -m_3 \frac{y-y_3}{r_3^3} \end{pmatrix}$$

Introduce the variables

$$z_1 = \frac{1}{r_1} = \frac{1}{\sqrt{(x-x_1)^2 + (y-y_1)^2}}$$

$$z_2 = \frac{1}{r_2} = \frac{1}{\sqrt{(x-x_2)^2 + (y-y_2)^2}}$$

$$z_3 = \frac{1}{r_3} = \frac{1}{\sqrt{(x-x_3)^2 + (y-y_3)^2}}$$

The CRFBP

Take

$$z_1 = \frac{1}{r_1} = \frac{1}{\sqrt{(x - x_1)^2 + (y - y_1)^2}}$$

Then for example

$$z_1' = \frac{-1}{2((x - x_1)^2 + (y - y_1))^{3/2}} \left(2(x - x_1)x' + 2(y - y_1)y'\right)$$

$$= -\left(\frac{1}{((x - x_1)^2 + (y - y_1))^{1/2}}\right)^3 ((x - x_1)v + (y - y_1)w)$$

$$= -z_1^3 ((x - x_1)v + (y - y_1)w)$$

So

$$z_j' = -(x - x_1)vz_j^3 - (y - y_1)wz_j^3 \qquad j = 1, 2, 3.$$

So: replace r_j^{-1} with z_j in F and append the equations for z_j' to the vector field.

The CRFBP

$$F(x,v,y,w) = \begin{pmatrix} v \\ 2w + x - m_1 \frac{x-x_1}{r_1^3} - m_2 \frac{x-x_2}{r_2^3} - m_3 \frac{x-x_3}{r_3^3} \\ w \\ -2v + y - m_1 \frac{y-y_1}{r_1^3} - m_2 \frac{y-y_2}{r_2^3} - -m_3 \frac{y-y_3}{r_3^3} \end{pmatrix}$$

expands to the polynomial field

$$G(x,v,y,w,z_1,z_2,z_3) = \begin{pmatrix} v \\ 2w + x - m_1(x-x_1)z_1^3 - m_2(x-x_2)z_2^3 - m_3(x-x_3)z_3^3 \\ w \\ -2v + y - m_1(y-y_1)z_1^3 - m_2(y-y_2)z_2^3 - -m_3(y-y_3)z_3^3 \\ -(x-x_1)vz_1^3 - (y-y_1)wz_1^3 \\ -(x-x_2)vz_2^3 - (y-y_2)wz_2^3 \\ -(x-x_3)vz_3^3 - (y-y_3)wz_3^3 \end{pmatrix}$$

The CRFBP

For

$$F(x,v,y,w) = \begin{pmatrix} v \\ 2w + x - m_1 \frac{x-x_1}{r_1^3} - m_2 \frac{x-x_2}{r_2^3} - m_3 \frac{x-x_3}{r_3^3} \\ w \\ -2v + y - m_1 \frac{y-y_1}{r_1^3} - m_2 \frac{y-y_2}{r_2^3} - -m_3 \frac{y-y_3}{r_3^3} \end{pmatrix}$$

$$U = \mathbb{R} \backslash \{(x_1,y_1),(x_2,y_2),(x_3,y_3)\} \qquad R(x,v,y,w) = \begin{pmatrix} x \\ v \\ y \\ w \\ \frac{1}{\sqrt{(x-x_1)^2+(y-y_1)^2}} \\ \frac{1}{\sqrt{(x-x_2)^2+(y-y_2)^2}} \\ \frac{1}{\sqrt{(x-x_3)^2+(y-y_3)^2}} \end{pmatrix}$$

$$G(x,v,y,w,z_1,z_2,z_3) = \begin{pmatrix} v \\ 2w + x - m_1(x-x_1)z_1^3 - m_2(x-x_2)z_2^3 - m_3(x-x_3)z_3^3 \\ w \\ -2v + y - m_1(y-y_1)z_1^3 - m_2(y-y_2)z_2^3 - -m_3(y-y_3)z_3^3 \\ -(x-x_1)vz_1^3 - (y-y_1)wz_1^3 \\ -(x-x_2)vz_2^3 - (y-y_2)wz_2^3 \\ -(x-x_3)vz_3^3 - (y-y_3)wz_3^3 \end{pmatrix}$$

we can check that $F, R,$ and G satisfy $DR(x)F(x) = G(R(x))$.

The CRFBP

A CRFBP Taylor Integrator for advecting analytic arcs is given by:

$$\Gamma(t, s) = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \Gamma_{mn} s^m t^n, \qquad \text{where } \gamma(s) = \sum_{m=0}^{\infty} \gamma_m s^m$$

is the arc of initial conditions

$\Gamma_{m0} = \gamma_m$ and

$$\Gamma_{mn+1} = \frac{1}{n+1} \begin{pmatrix} \Gamma^2_{mn} \\ 2\Gamma^4_{mn} + \Gamma^1_{mn} + N(\Gamma^1, \Gamma^5, \Gamma^6, \Gamma^7)_{mn} \\ \Gamma^4_{mn} \\ -2\Gamma^2_{mn} + \Gamma^3_{mn} + M(\Gamma^3, \Gamma^5, \Gamma^6, \Gamma^7)_{mn} \\ -(\Gamma^1 - x_1 * \Gamma^2 * \Gamma^5 * \Gamma^5 * \Gamma^5)_{mn} - (\Gamma^3 - y_1 * \Gamma^4 * \Gamma^5 * \Gamma^5 * \Gamma^5)_{mn} \\ -(\Gamma^1 - x_2 * \Gamma^2 * \Gamma^6 * \Gamma^6 * \Gamma^6)_{mn} - (\Gamma^3 - y_2 * \Gamma^4 * \Gamma^6 * \Gamma^6 * \Gamma^6)_{mn} \\ -(\Gamma^1 - x_3 * \Gamma^2 * \Gamma^7 * \Gamma^7 * \Gamma^7)_{mn} - (\Gamma^3 - y_3 * \Gamma^4 * \Gamma^7 * \Gamma^7 * \Gamma^7)_{mn} \end{pmatrix}$$

Here

$$N(\Gamma^1, \Gamma^5, \Gamma^6, \Gamma^7)_{mn} = -m_1(\Gamma^1 - x_1 * \Gamma^5 * \Gamma^5 * \Gamma^5)_{mn} - m_2(\Gamma^1 - x_2 * \Gamma^6 * \Gamma^6 * \Gamma^6)_{mn} - m_3(\Gamma^1 - x_3 * \Gamma^7 * \Gamma^7 * \Gamma^7)_{mn}$$

$$M(\Gamma^3, \Gamma^5, \Gamma^6, \Gamma^7)_{mn} = -m_1(\Gamma^3 - y_1 * \Gamma^5 * \Gamma^5 * \Gamma^5)_{mn} - m_2(\Gamma^3 - y_2 * \Gamma^6 * \Gamma^6 * \Gamma^6)_{mn} - m_3(\Gamma^3 - y_3 * \Gamma^7 * \Gamma^7 * \Gamma^7)_{mn}$$

The first four components give the advected arc in the CRFBP.

The CRFBP

Let p_0 be an equilibrium for CRFBPF with stable/unstable eigenvalues λ_1, λ_2 and eigenvectors ξ_1, ξ_2.

- $R(p_0)$ is an equilibrium for G with eigenvalues λ_1, λ_2.
- $DR(p_0)\xi_{1,2}$ are the associated eigenvectors.
- the homological equations are:

$$[DG(R(p_0)) - (m\lambda_1 + n\lambda_2)\mathrm{Id}_7]p_{mn} = -R_{mn}$$

where

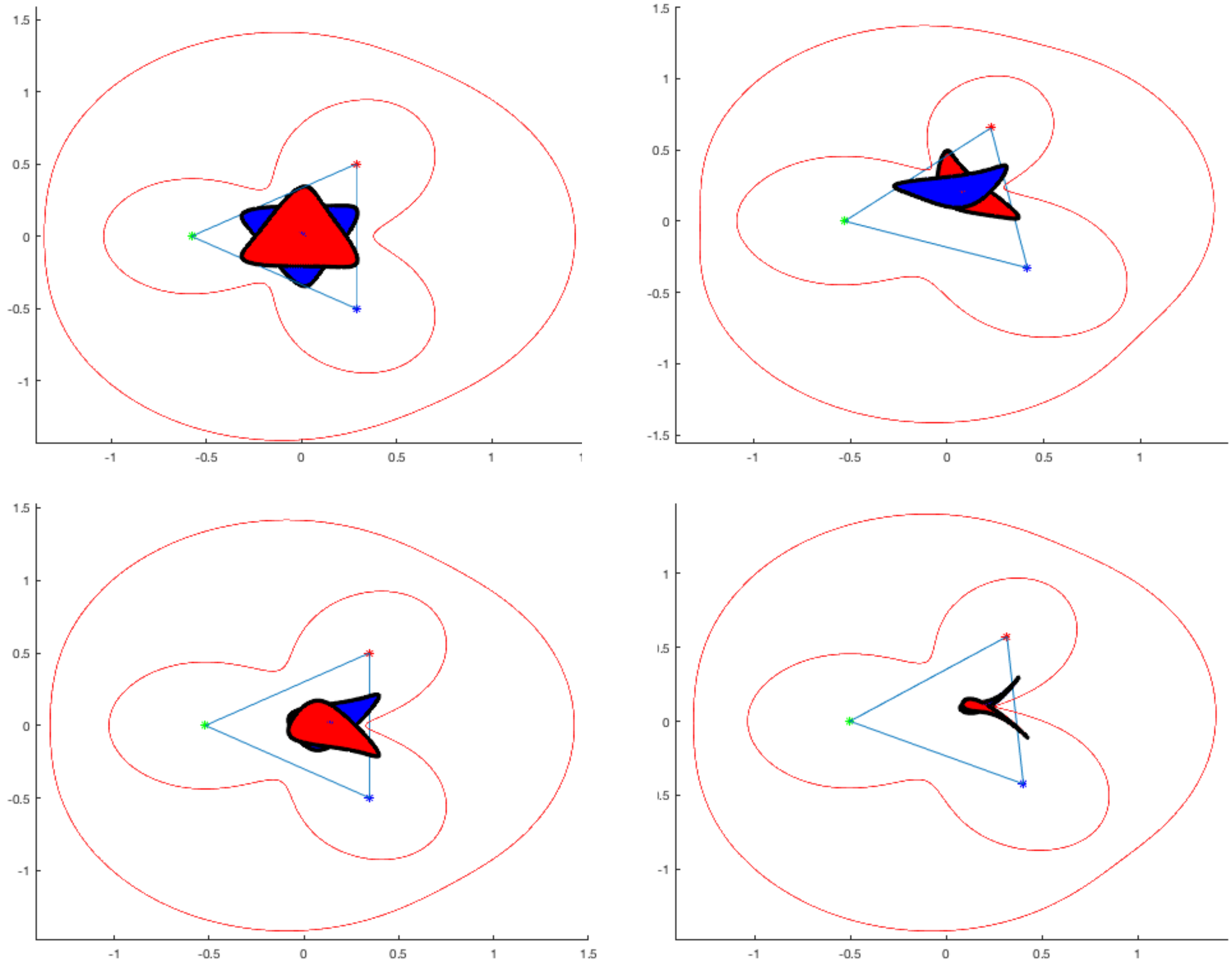
$$R_{mn} = \begin{pmatrix} 0 \\ -m_1(\Gamma^1 - x_1 \hat{*} \Gamma^5 \hat{*} \Gamma^5 \hat{*} \Gamma^5)_{mn} - m_2(\Gamma^1 - x_2 \hat{*} \Gamma^6 \hat{*} \Gamma^6 \hat{*} \Gamma^6)_{mn} - m_3(\Gamma^1 - x_3 \hat{*} \Gamma^7 \hat{*} \Gamma^7 \hat{*} \Gamma^7)_{mn} \\ 0 \\ -m_1(\Gamma^3 - y_1 \hat{*} \Gamma^5 \hat{*} \Gamma^5 \hat{*} \Gamma^5)_{mn} - m_2(\Gamma^3 - y_2 \hat{*} \Gamma^6 \hat{*} \Gamma^6 \hat{*} \Gamma^6)_{mn} - m_3(\Gamma^3 - y_3 \hat{*} \Gamma^7 \hat{*} \Gamma^7 \hat{*} \Gamma^7)_{mn} \\ -(\Gamma^1 - x_1 \hat{*} \Gamma^2 \hat{*} \Gamma^5 \hat{*} \Gamma^5 \hat{*} \Gamma^5)_{mn} - (\Gamma^3 - y_1 \hat{*} \Gamma^4 \hat{*} \Gamma^5 \hat{*} \Gamma^5 \hat{*} \Gamma^5)_{mn} \\ -(\Gamma^1 - x_1 \hat{*} \Gamma^2 \hat{*} \Gamma^6 \hat{*} \Gamma^6 \hat{*} \Gamma^6)_{mn} - (\Gamma^3 - y_1 \hat{*} \Gamma^4 \hat{*} \Gamma^6 \hat{*} \Gamma^6 \hat{*} \Gamma^6)_{mn} \\ -(\Gamma^1 - x_1 \hat{*} \Gamma^2 \hat{*} \Gamma^7 \hat{*} \Gamma^7 \hat{*} \Gamma^7)_{mn} - (\Gamma^3 - y_1 \hat{*} \Gamma^4 \hat{*} \Gamma^7 \hat{*} \Gamma^7 \hat{*} \Gamma^7)_{mn} \end{pmatrix}$$

The first four components parameterize the stable/unstable manifold in the CRFBP.

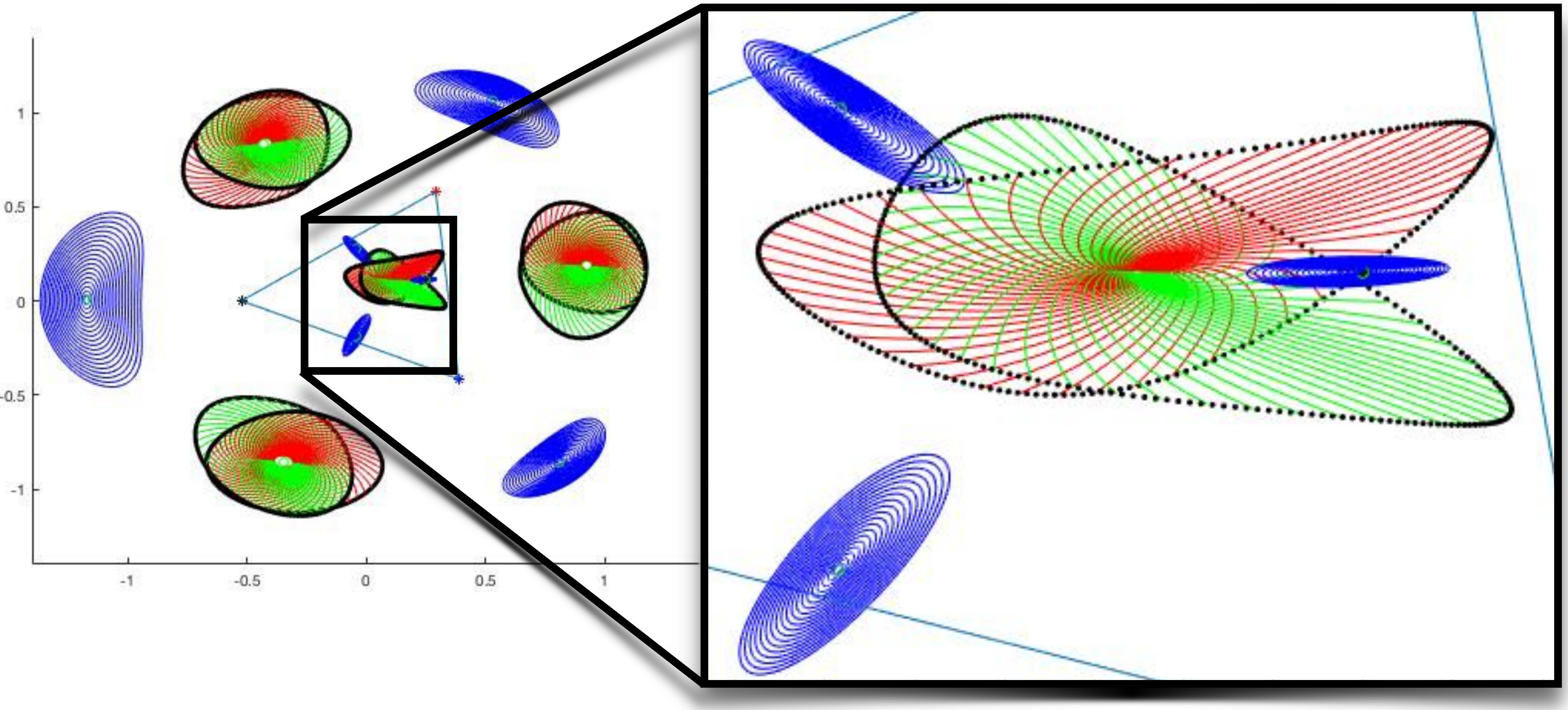
The CRFBP

The CRFBP

Parameterized to order 45



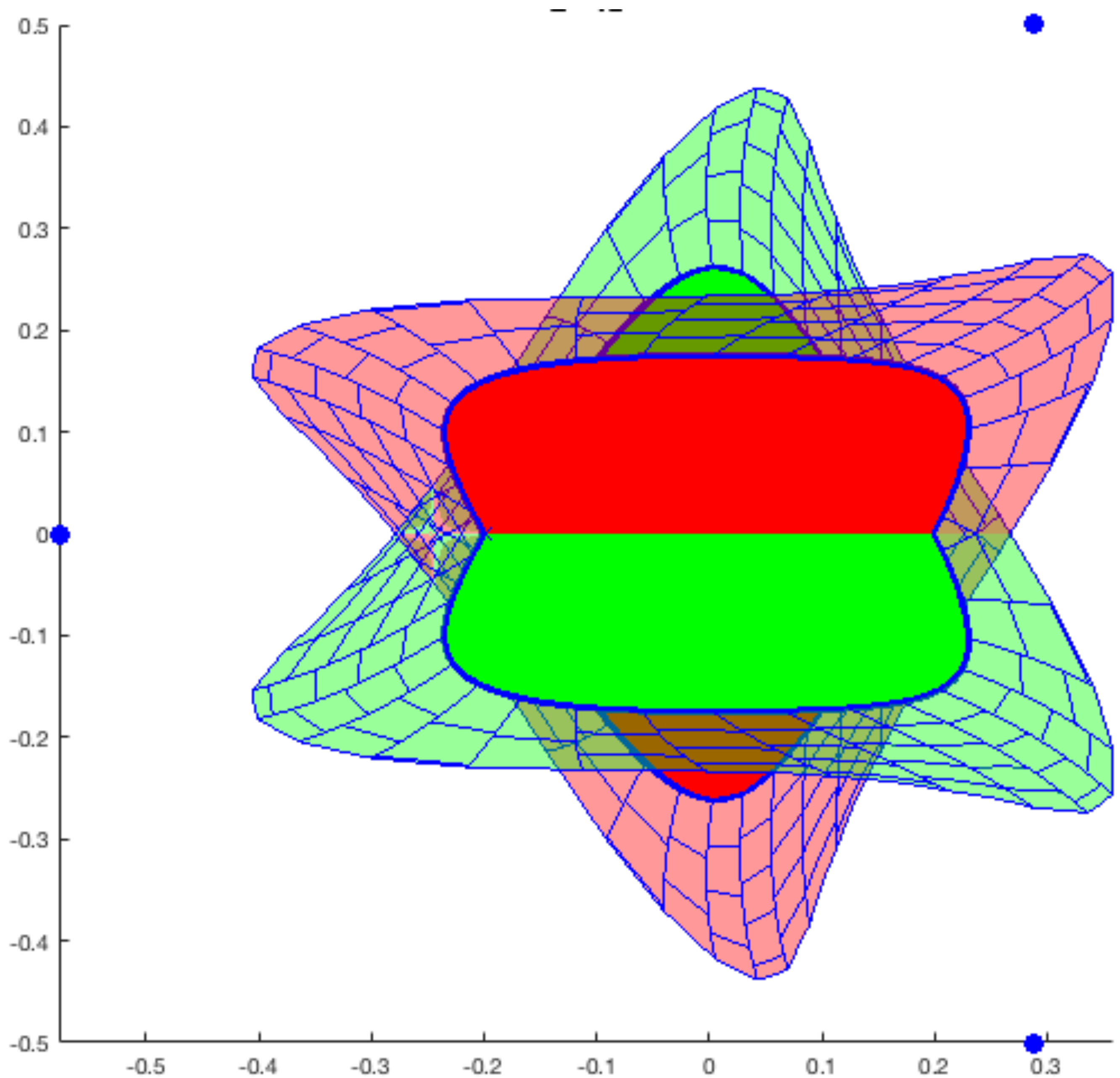
The CRFBP



The CRFBP

30 initial boundary arcs

$\mathcal{L}_0$

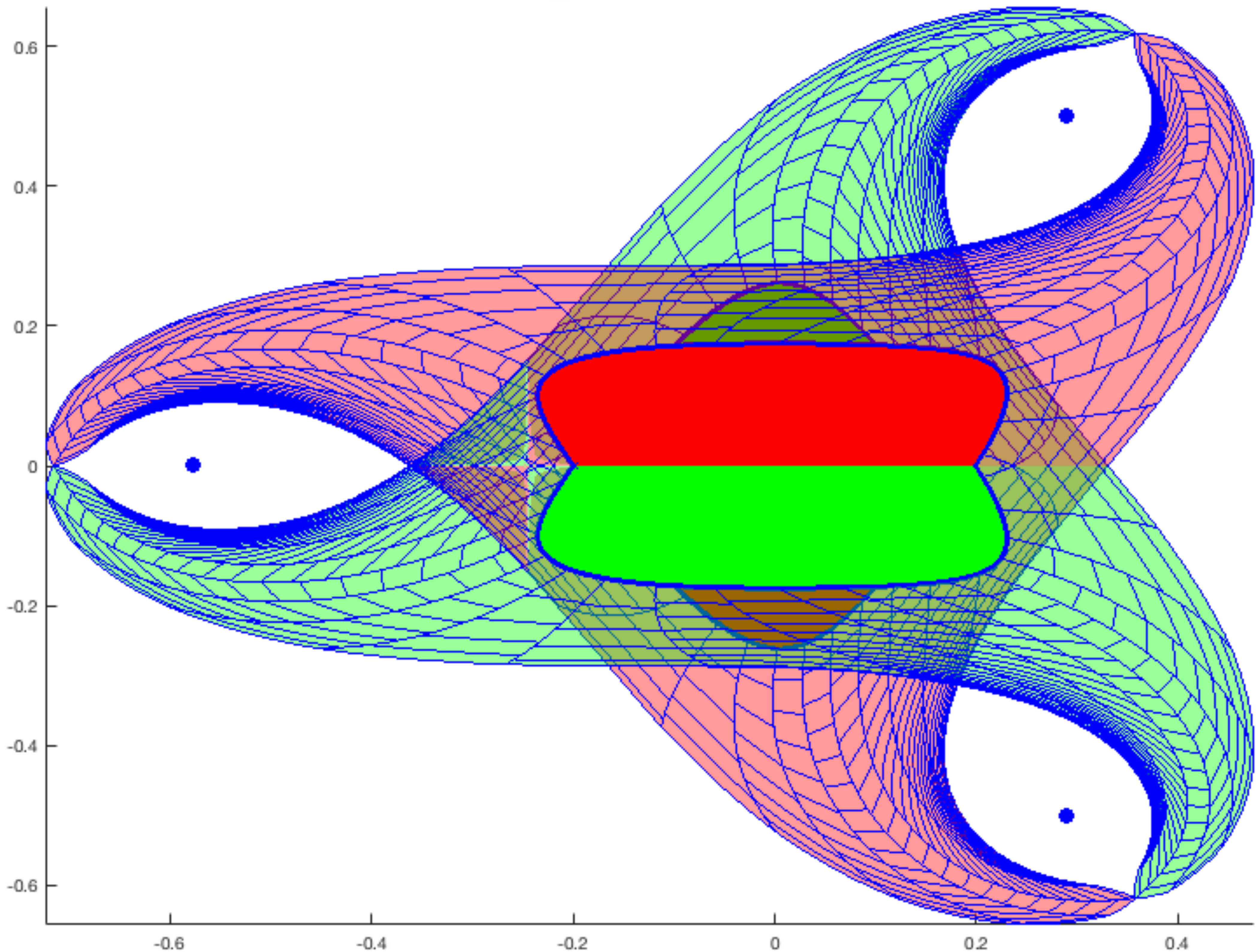


$T = \pm 0.25$

The CRFBP

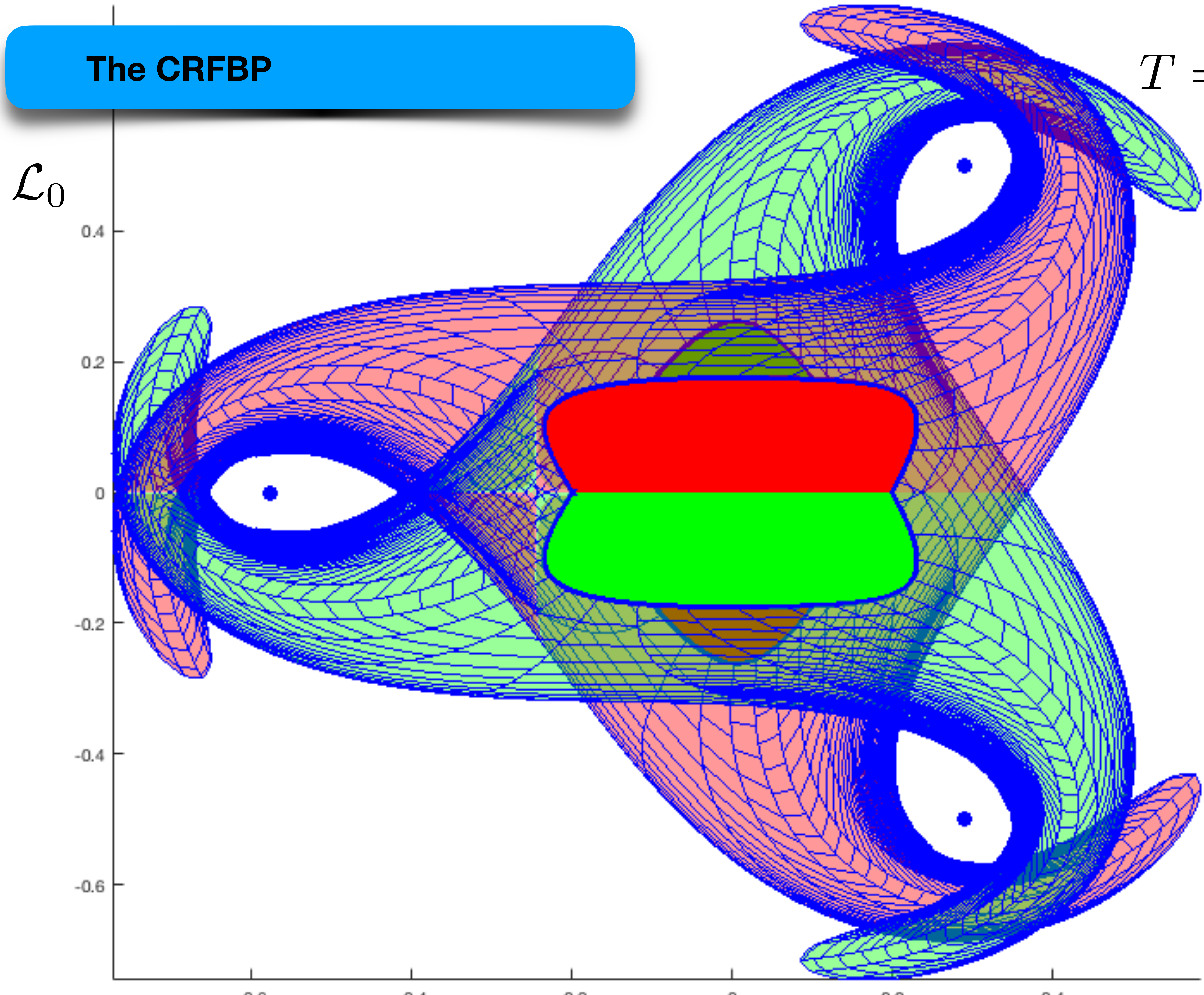
$T = \pm 0.75$

$\mathcal{L}_0$



The CRFBP

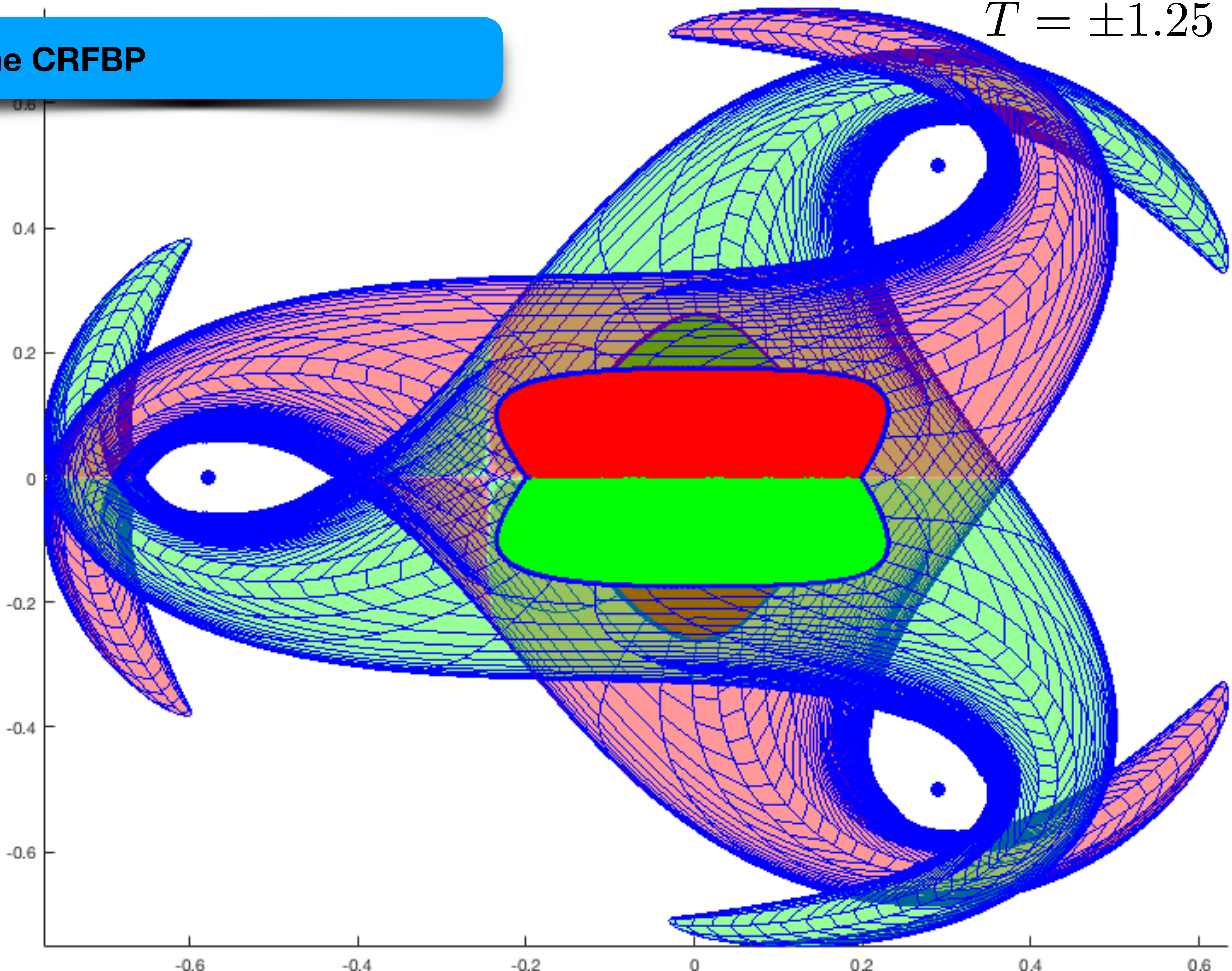
$T = \pm 1$



The CRFBP

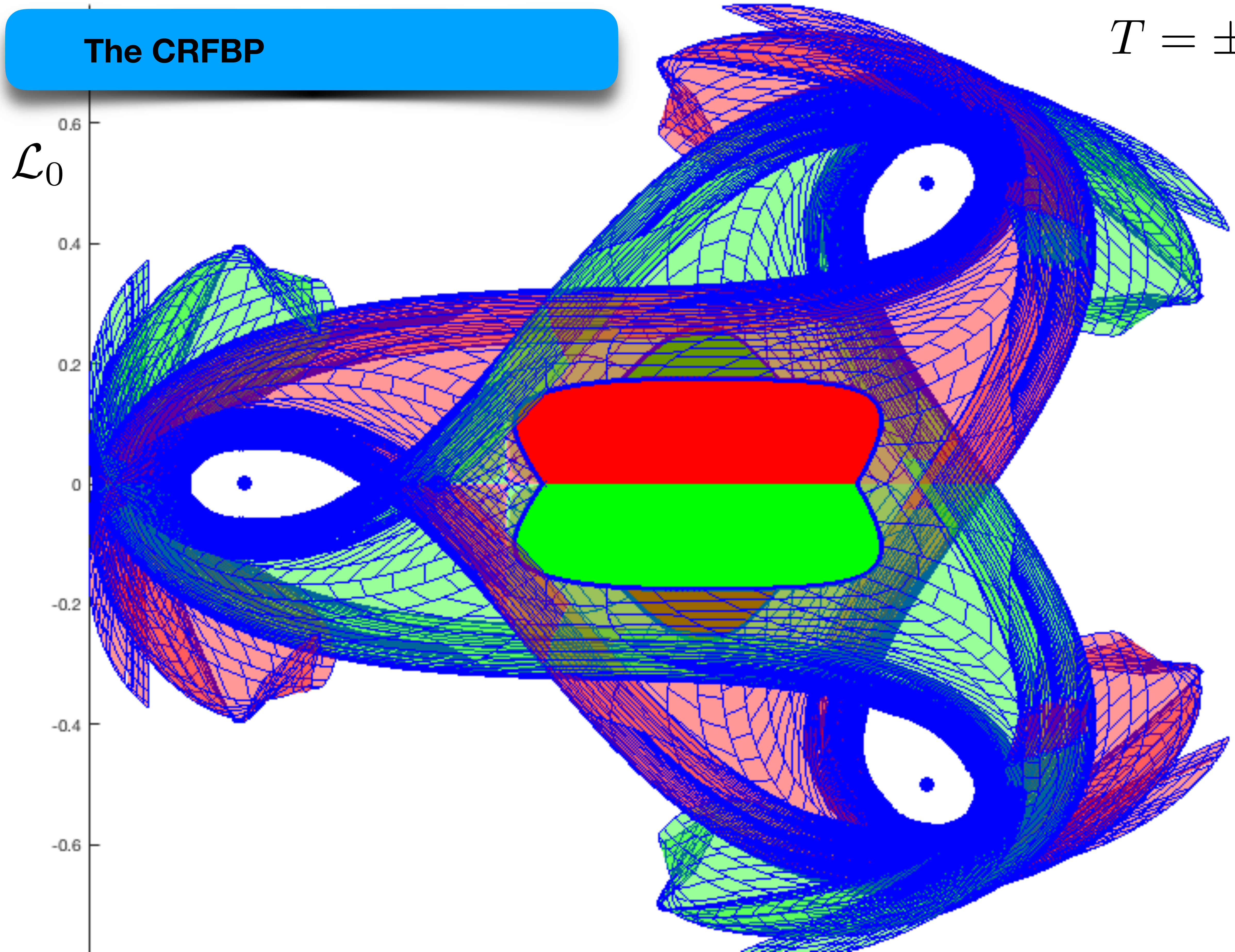
$\mathcal{L}_0$

$T = \pm 1.25$

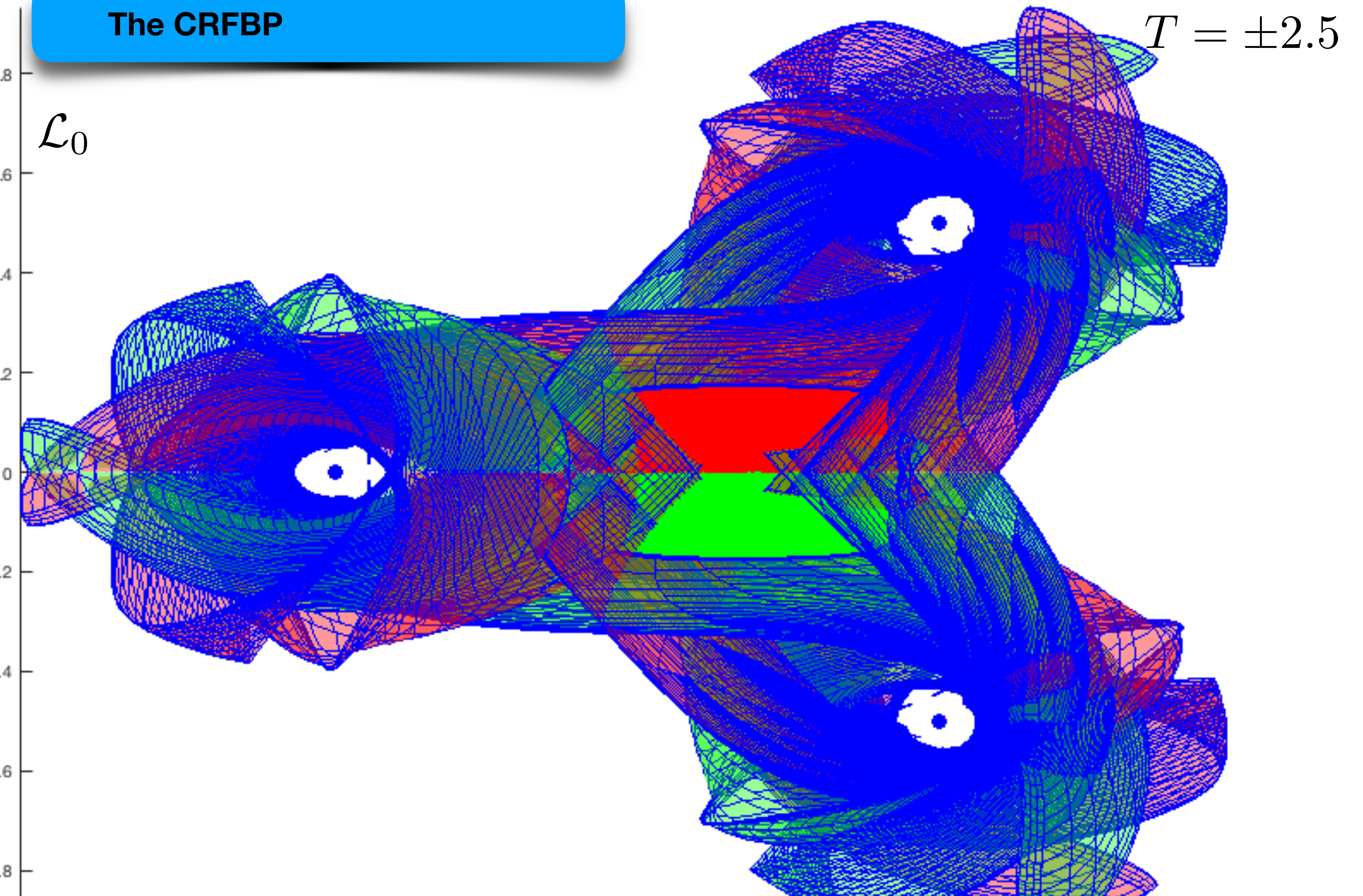


The CRFBP

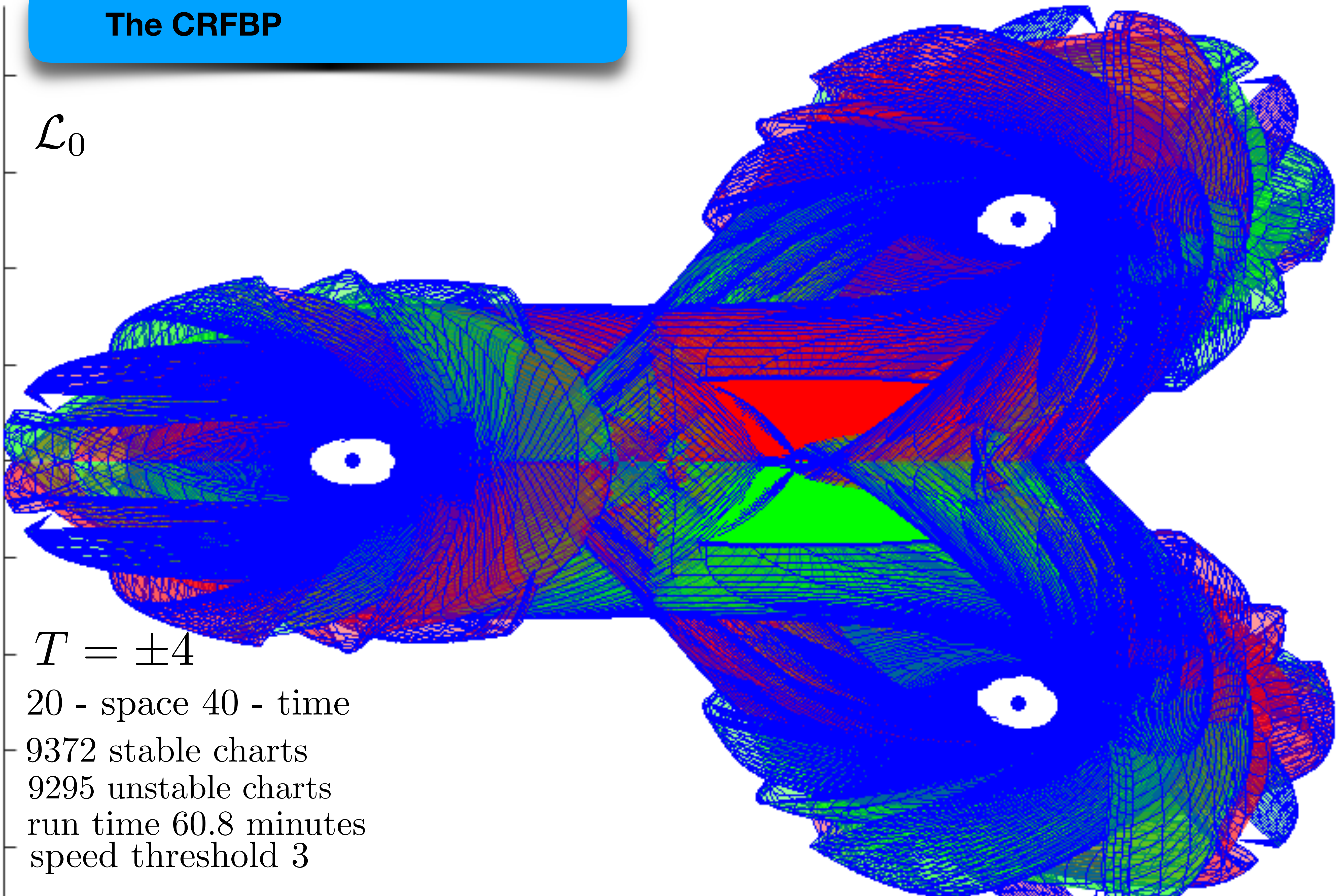
$T = \pm 1.5$



The CRFBP

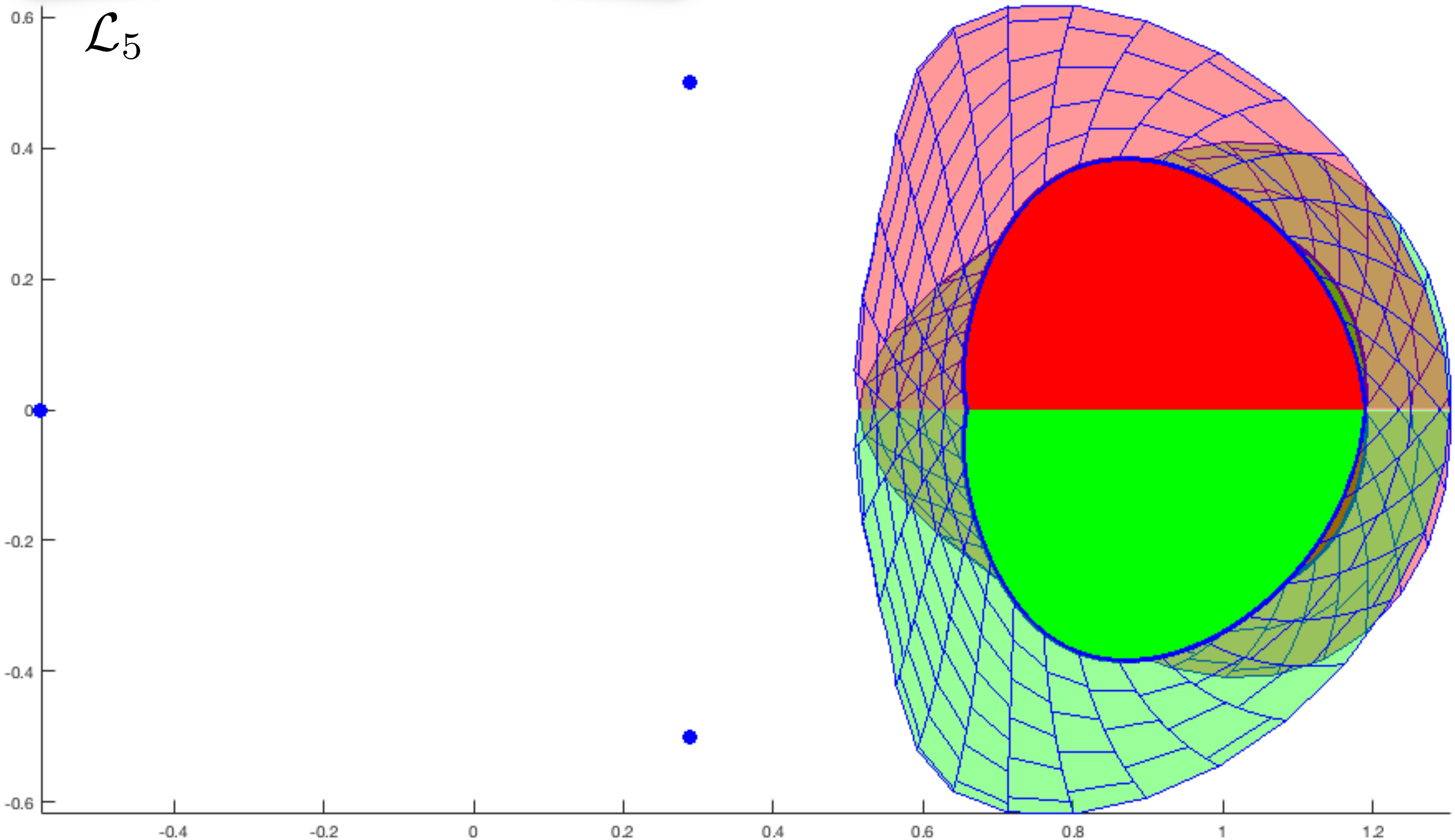


The CRFBP


$\mathcal{L}_0$
$T = \pm 4$
20 - space 40 - time
9372 stable charts
9295 unstable charts
run time 60.8 minutes
speed threshold 3

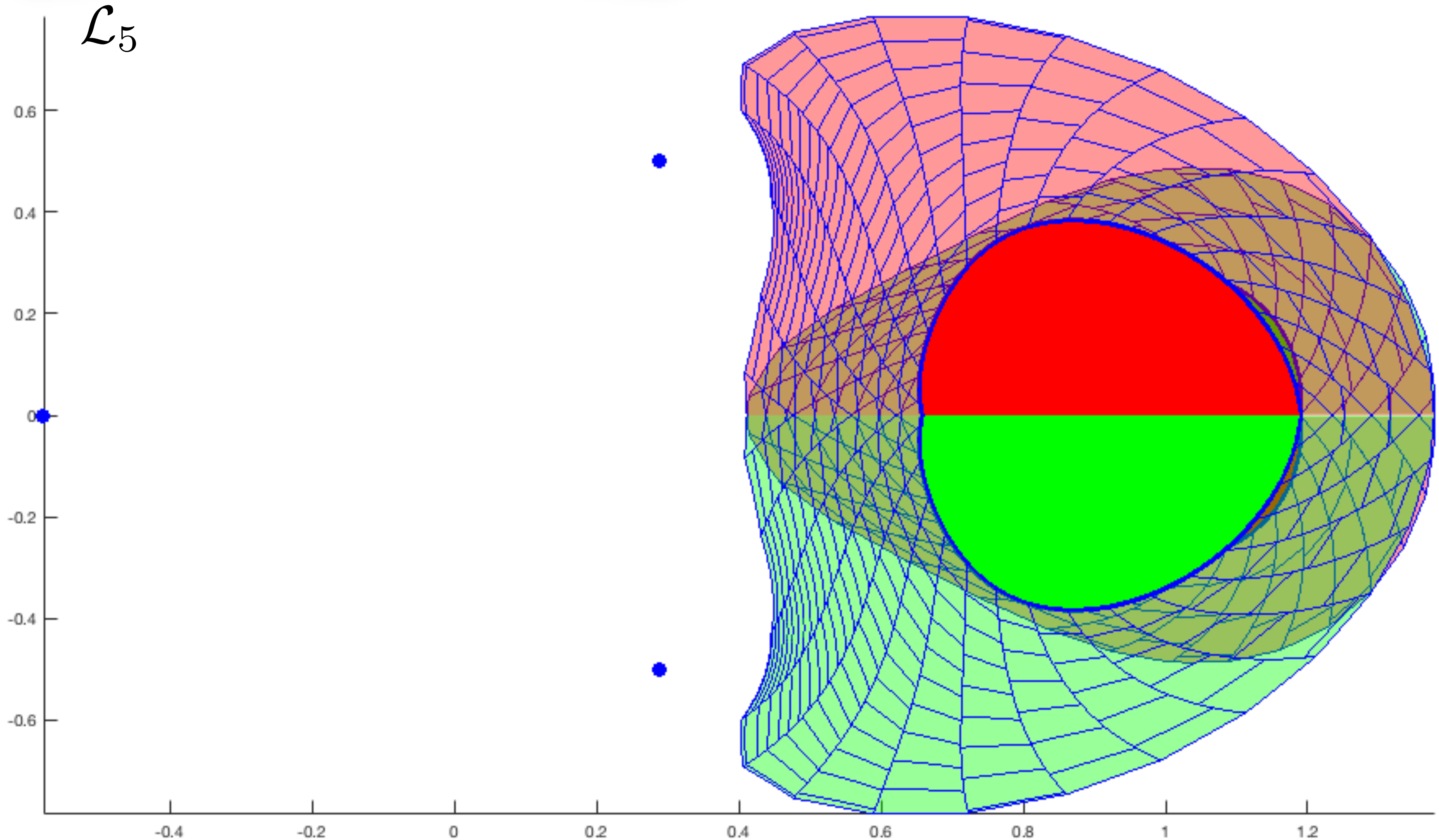
The CRFBP

30 initial boundary arcs



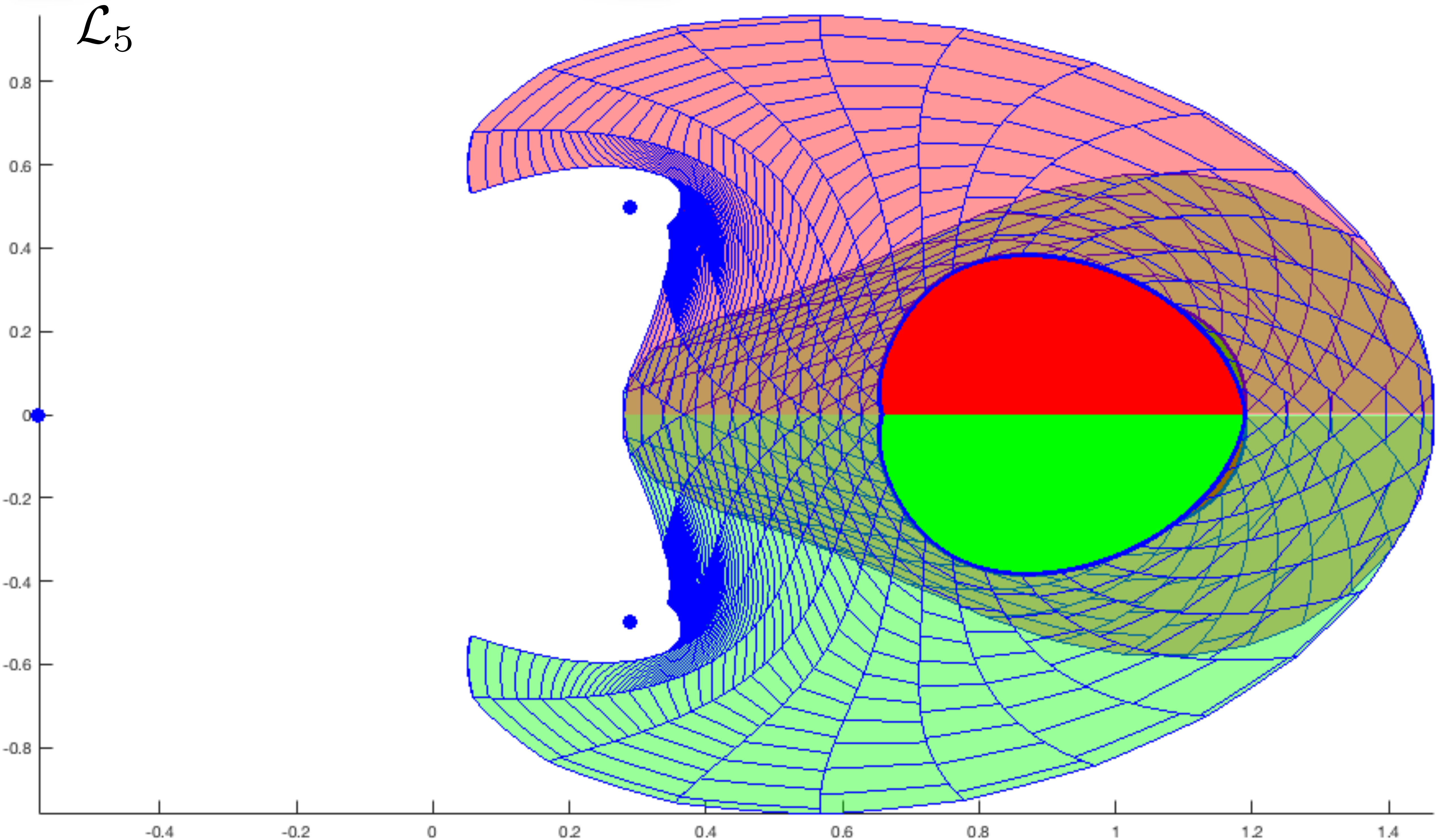
$T = \pm 0.5$

The CRFBP



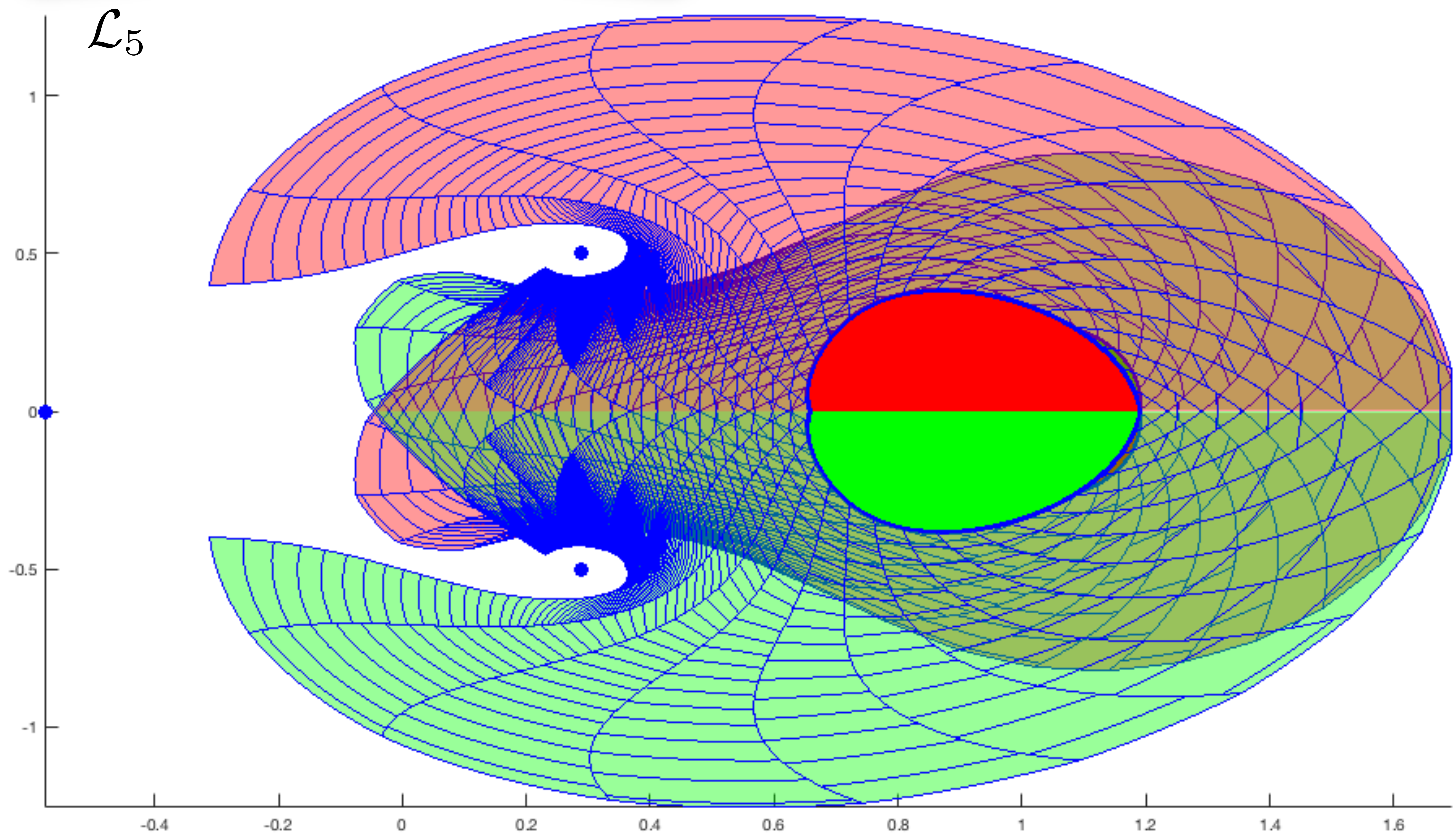
$T = \pm 0.75$

The CRFBP



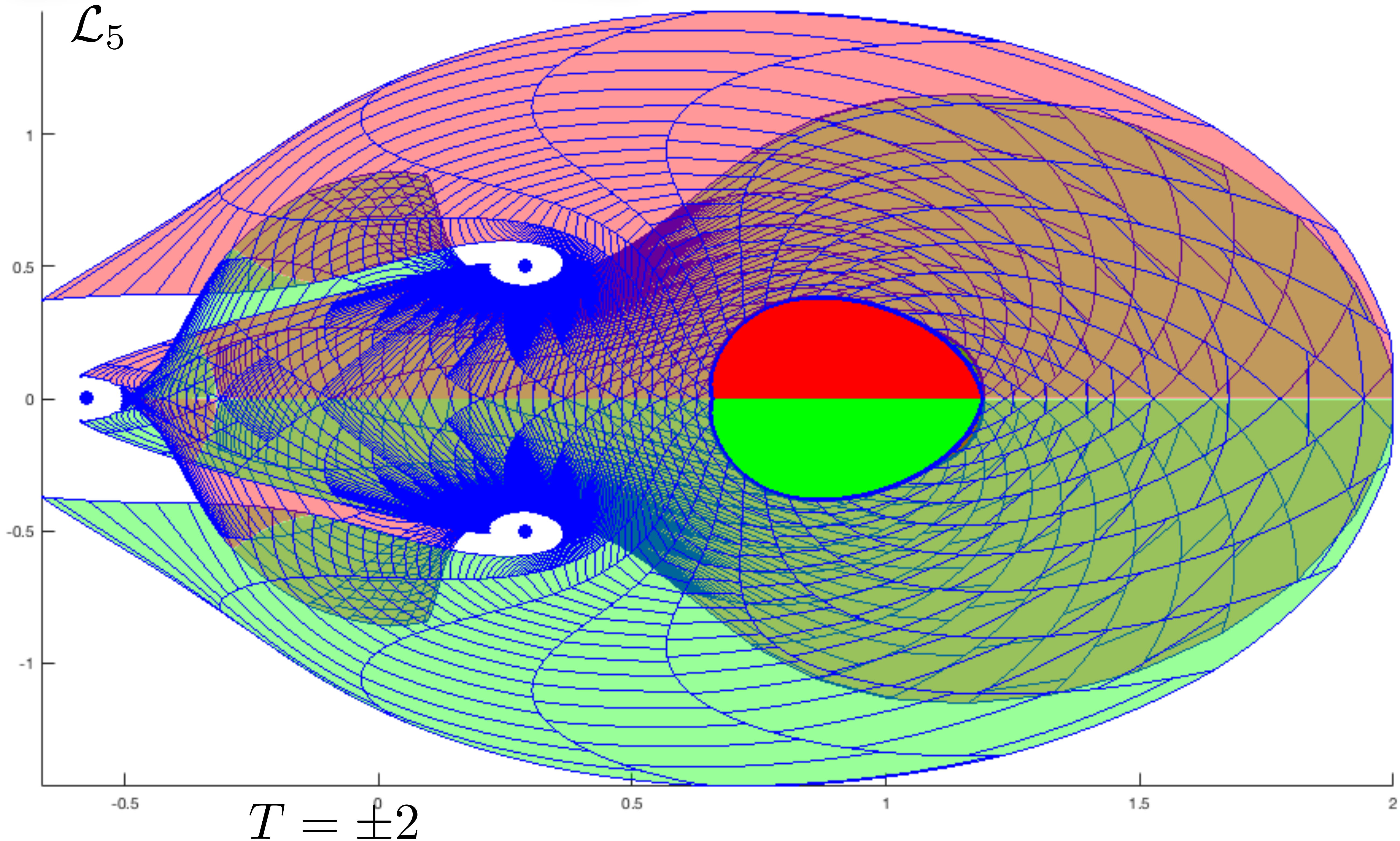
$T = \pm 1.15$

The CRFBP

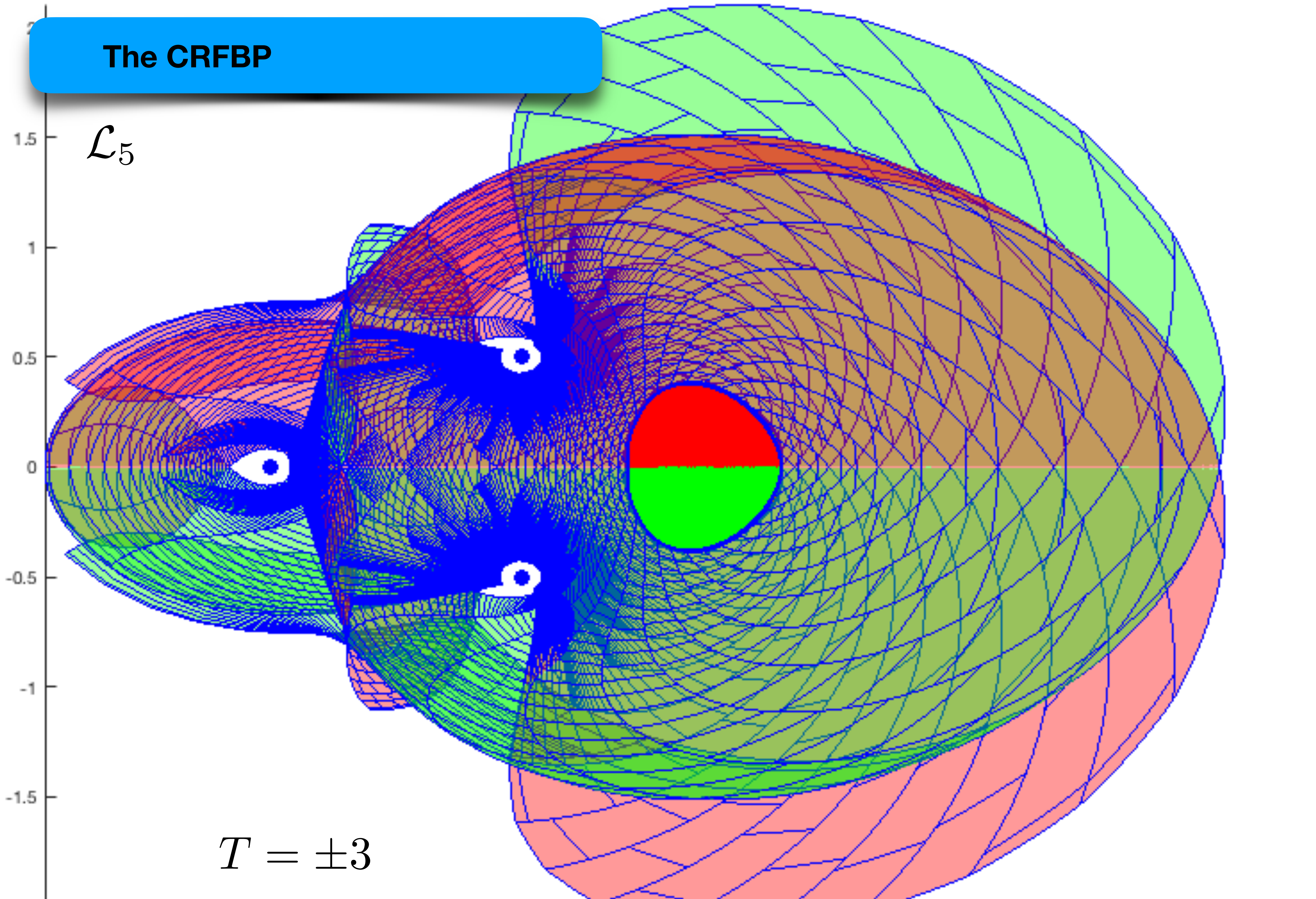


$T = \pm 1.5$

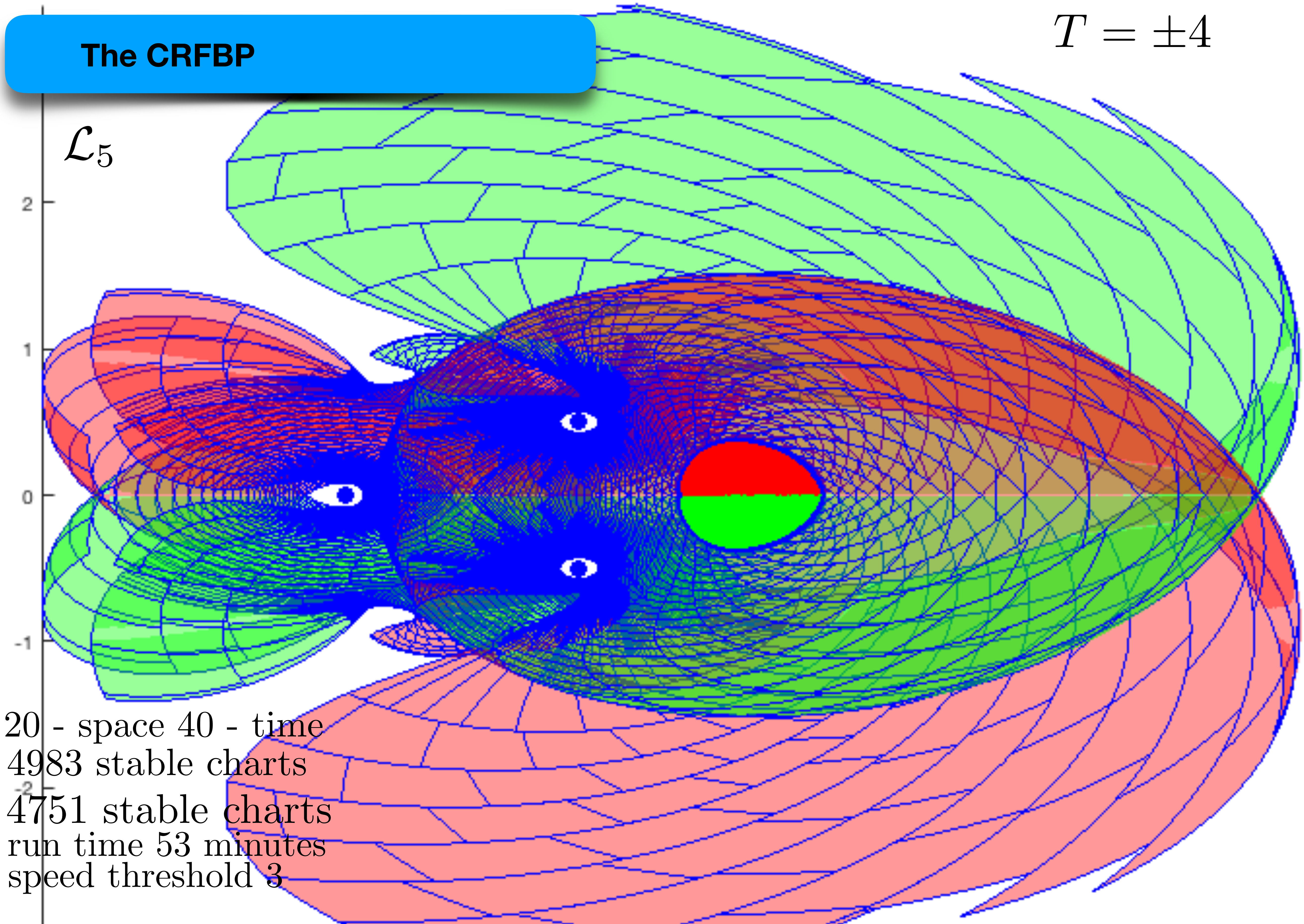
The CRFBP



The CRFBP



The CRFBP



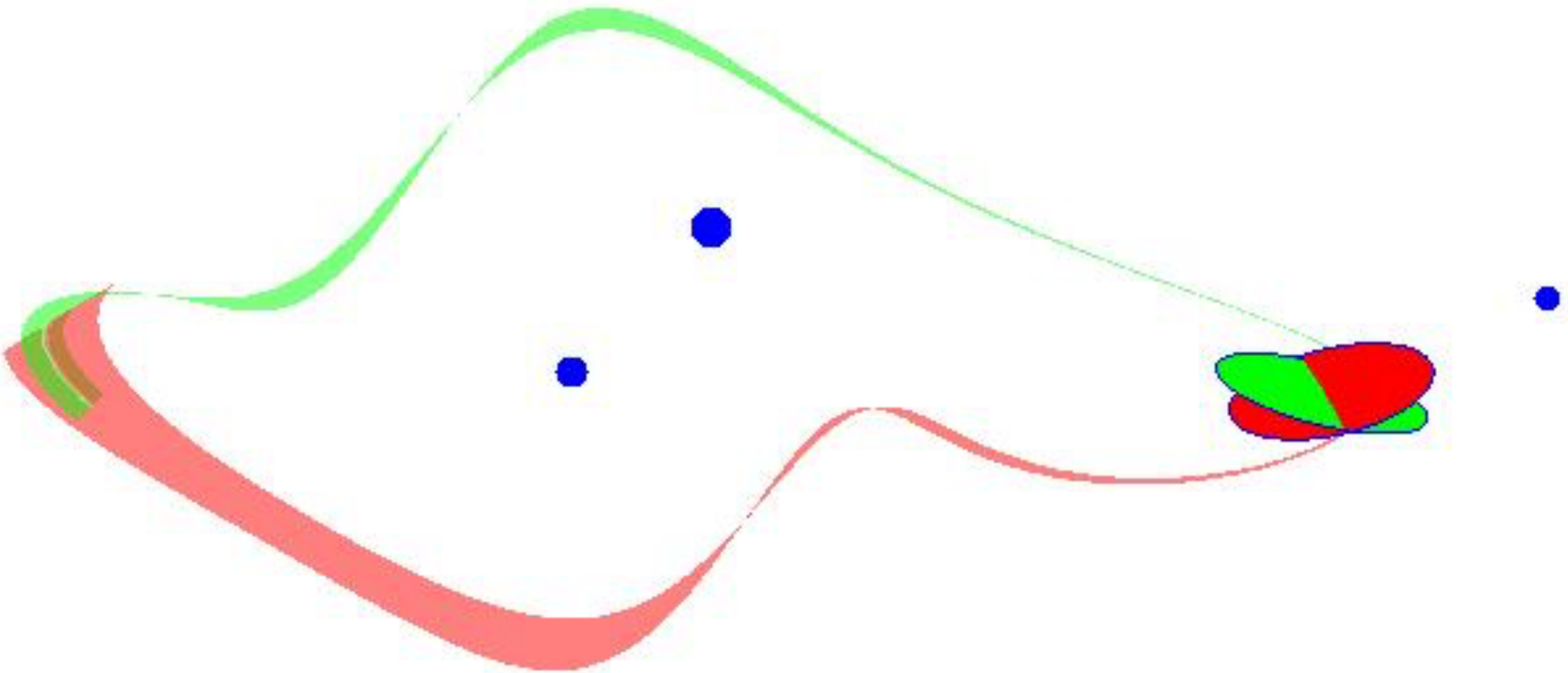
$T = \pm 4$

20 - space 40 - time
4983 stable charts
4751 stable charts
run time 53 minutes
speed threshold 3

The CRFBP

Looking for intersections

The CRFBP

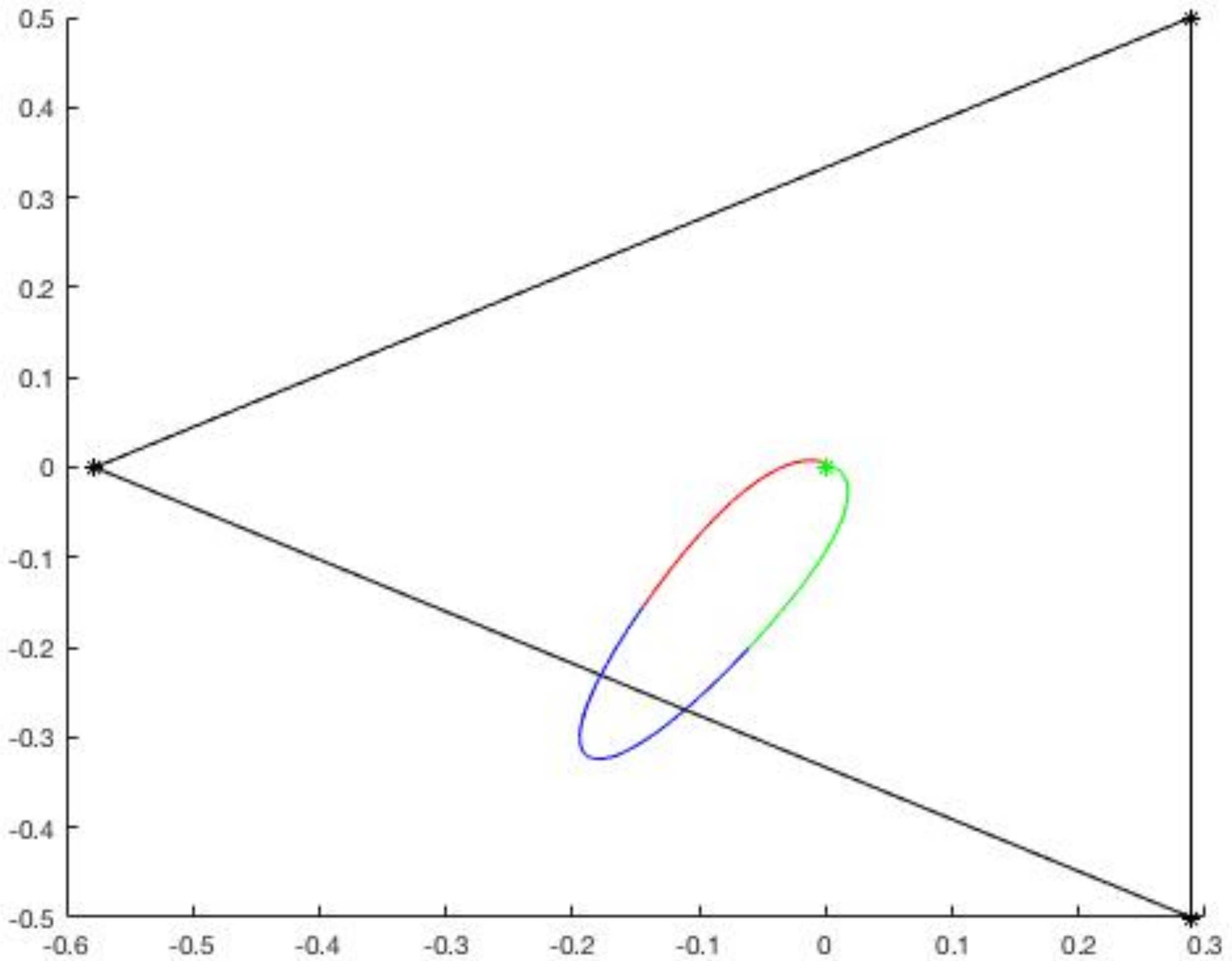


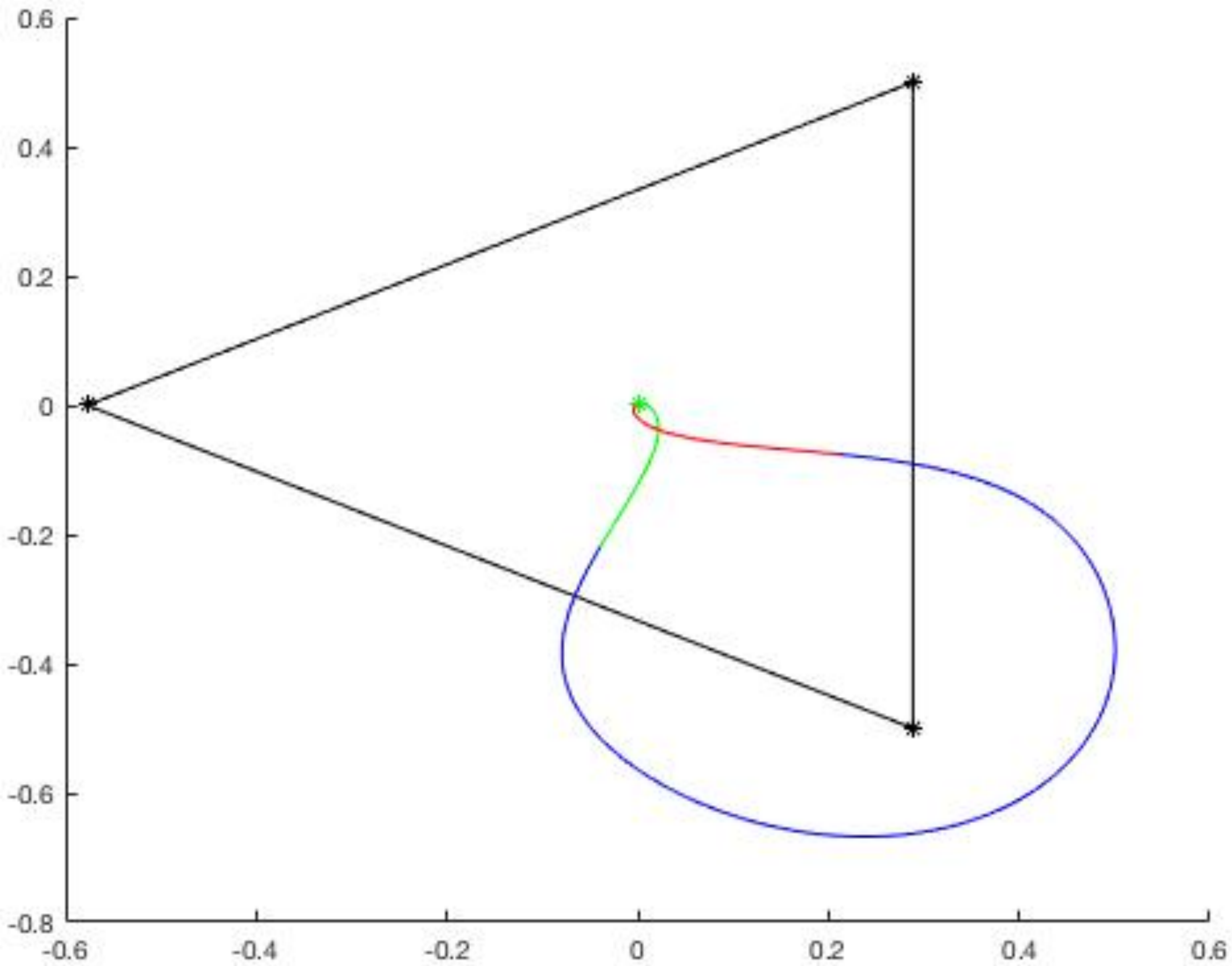
The CRFBP

42 homoclinic connections at $\mathcal{L}_0$

23 homoclinic connections at $\mathcal{L}_5$

The CRFBP

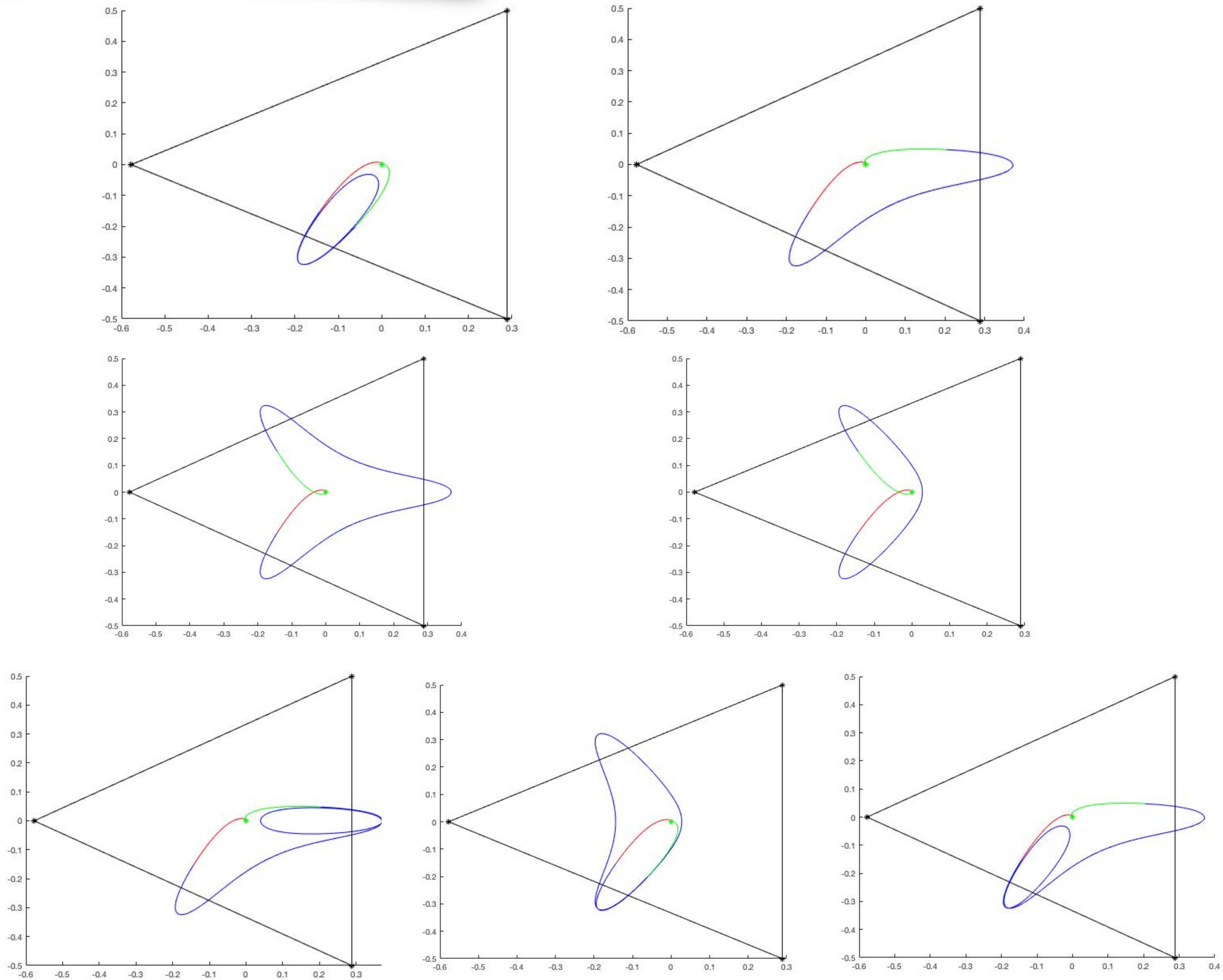




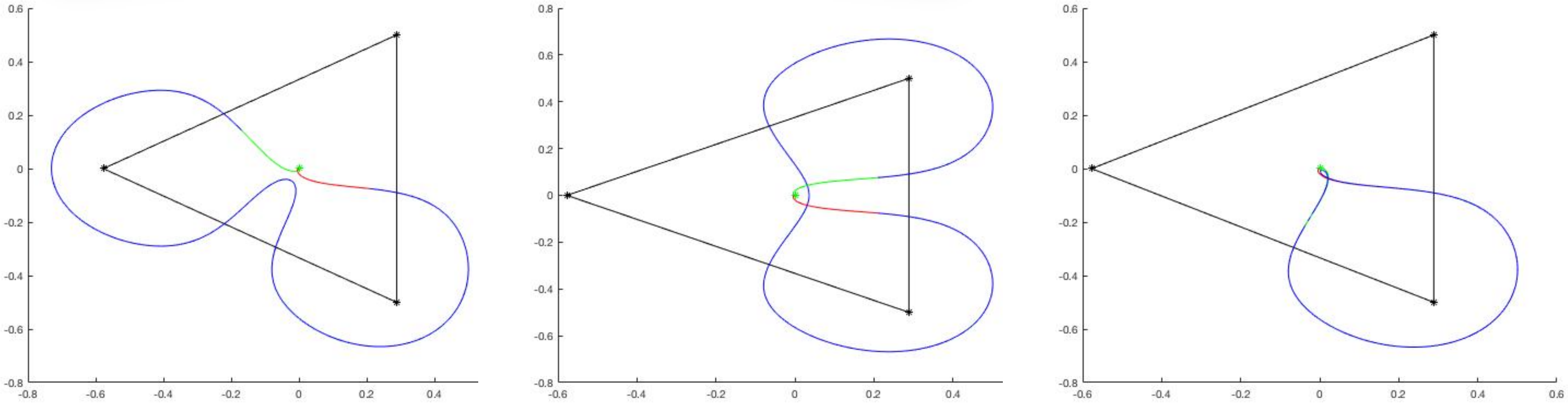
Shortest connections at $\mathcal{L}_0$

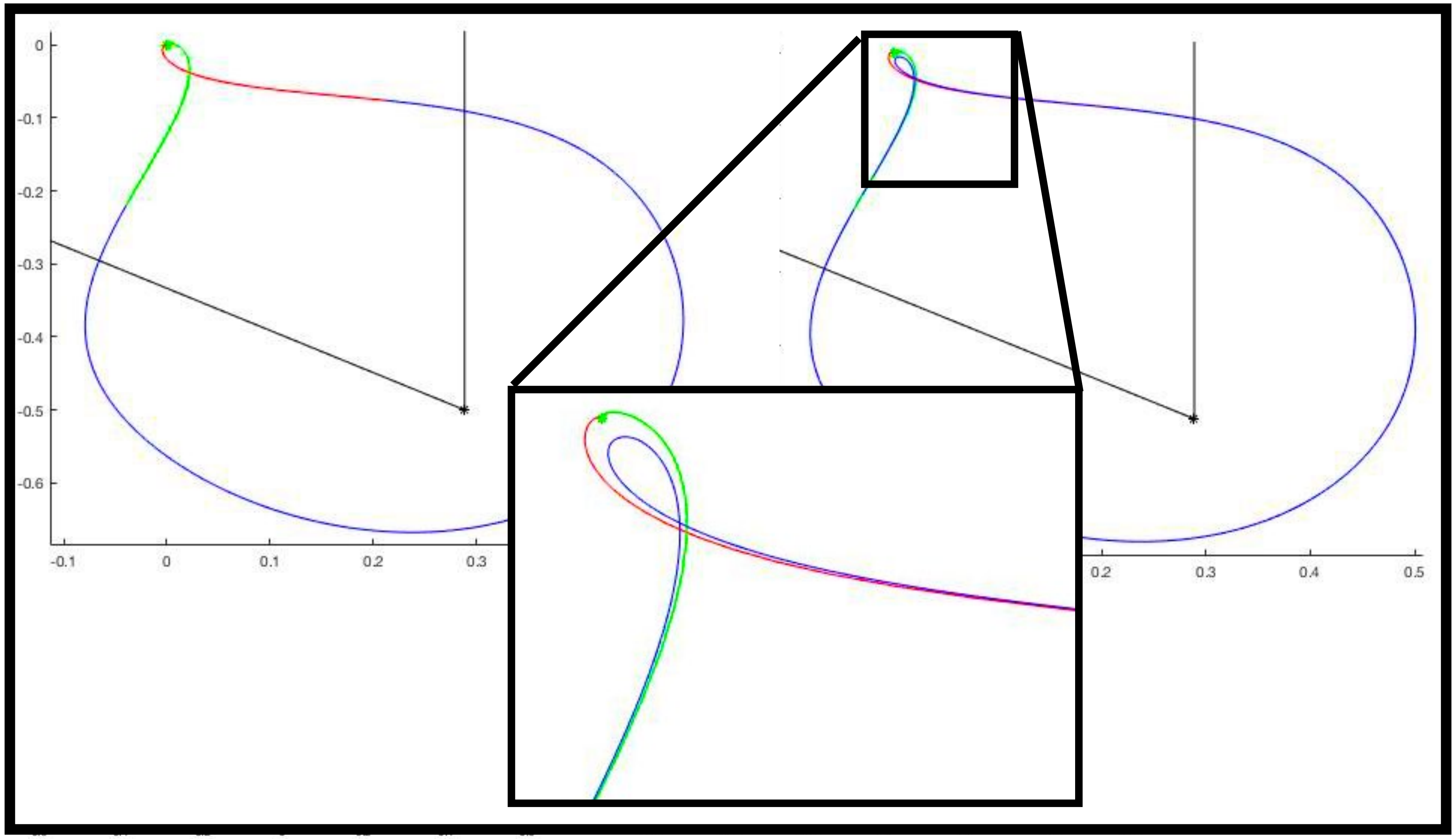
Basic "letters in the alphabet"

The CRFBP

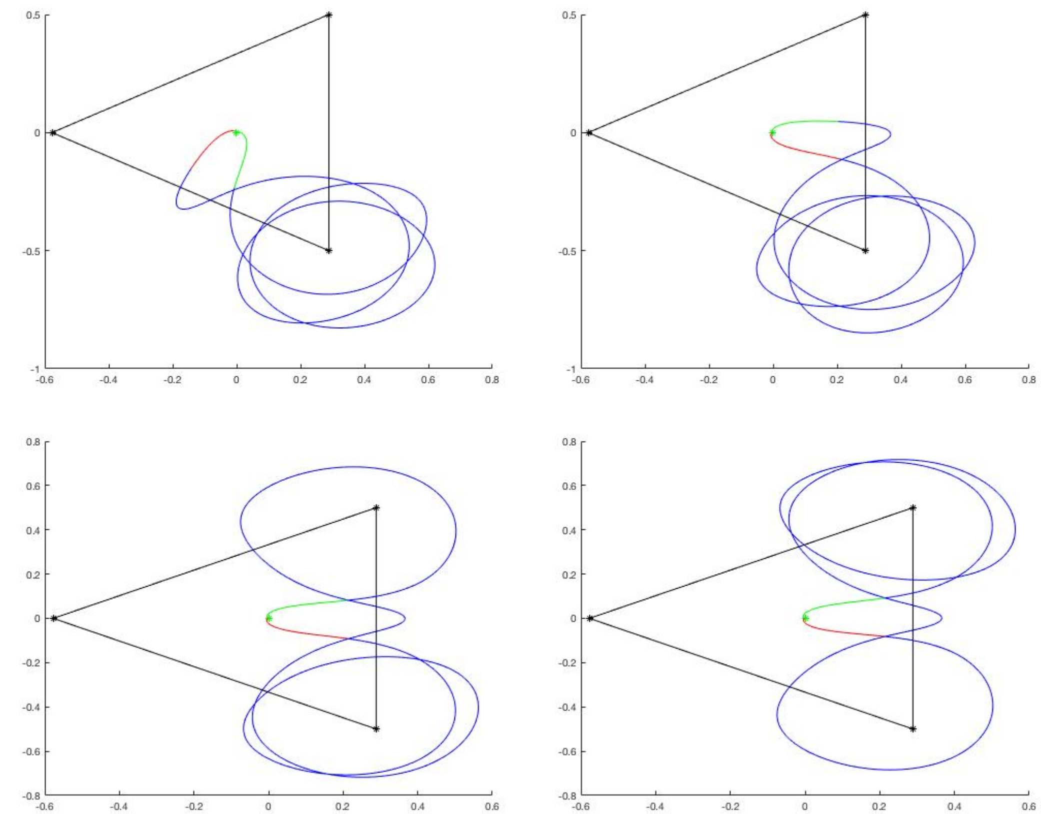


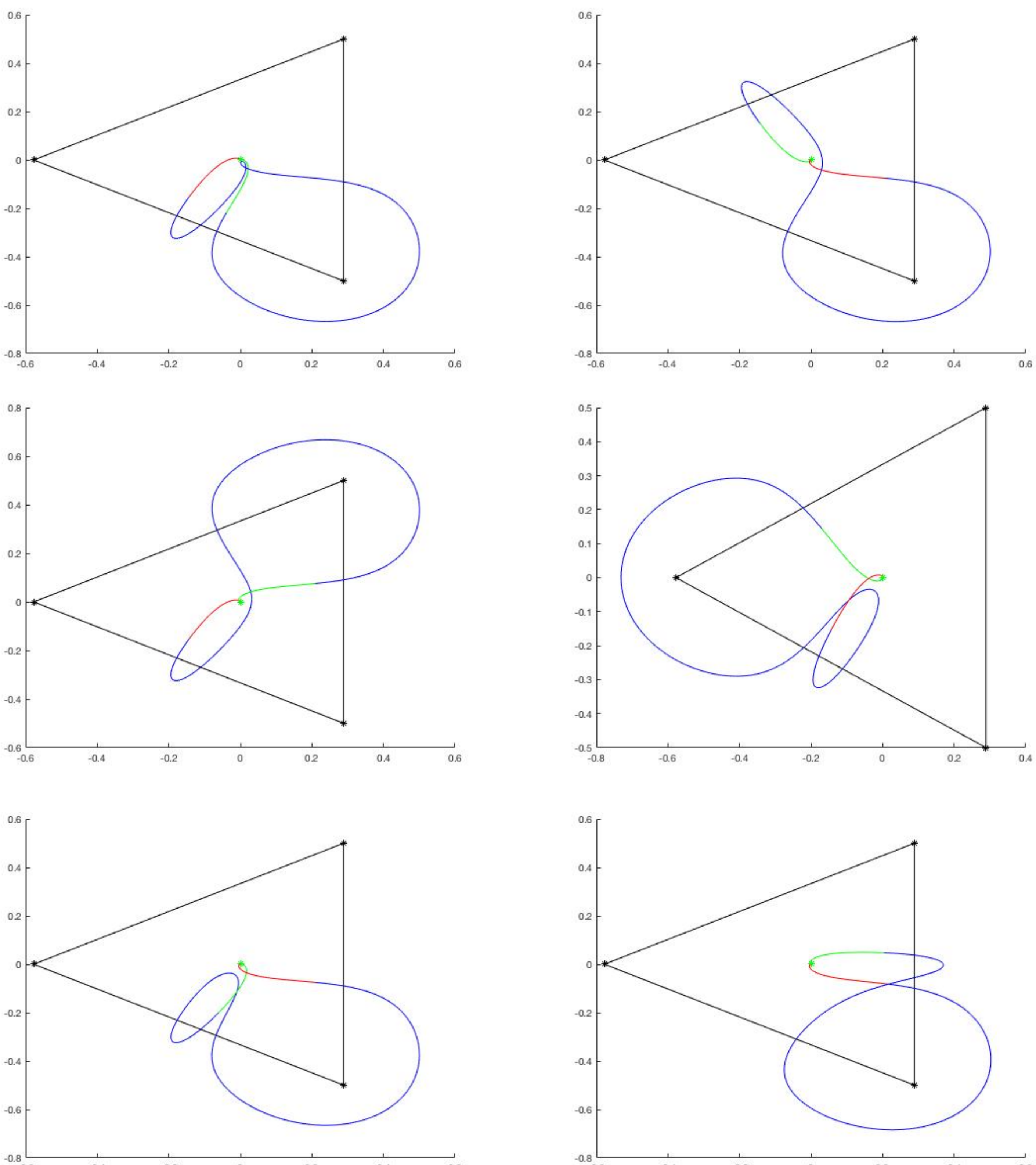
The CRFBP



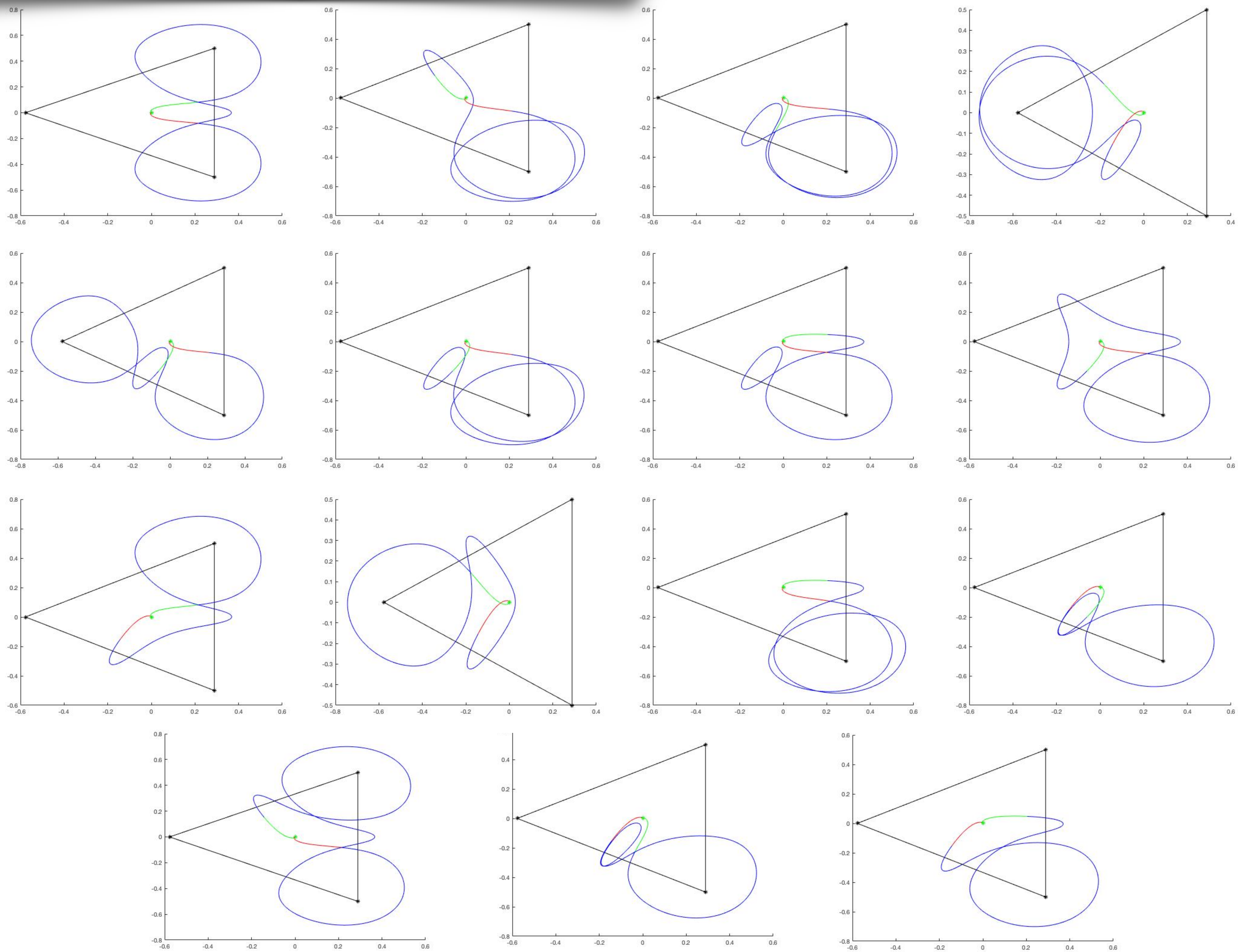


The CRFBP

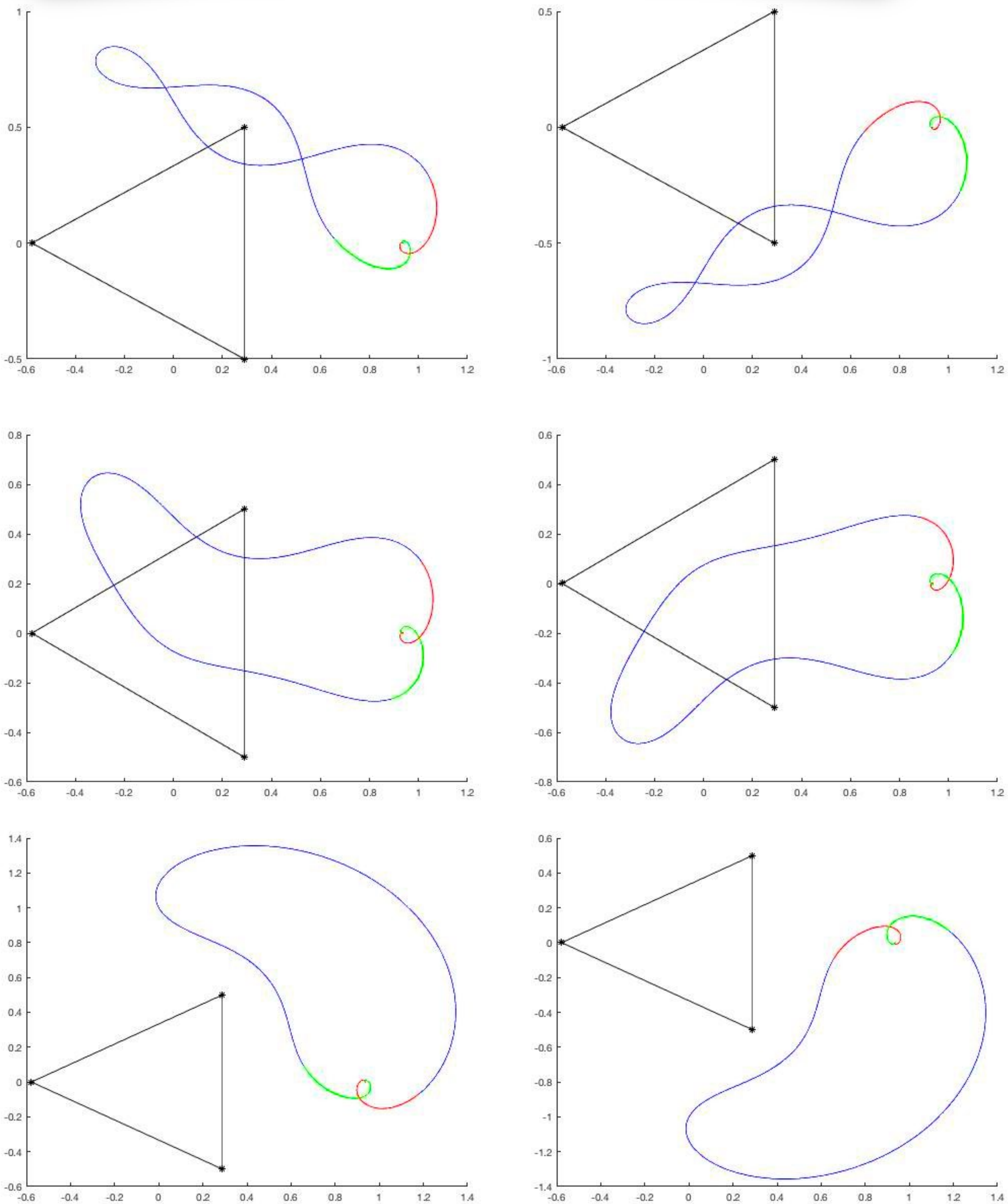


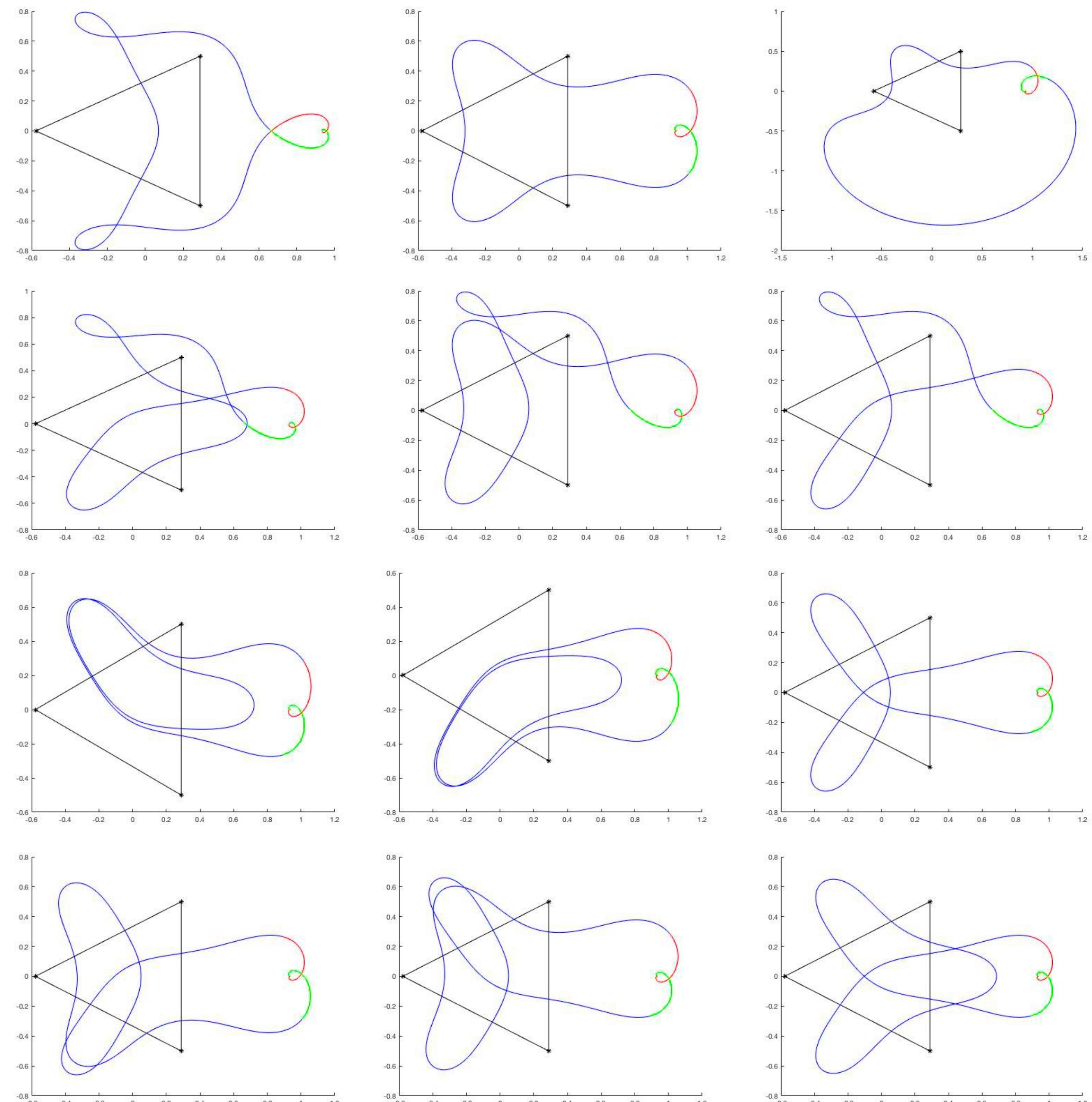


The CRFBP



The CRFBP

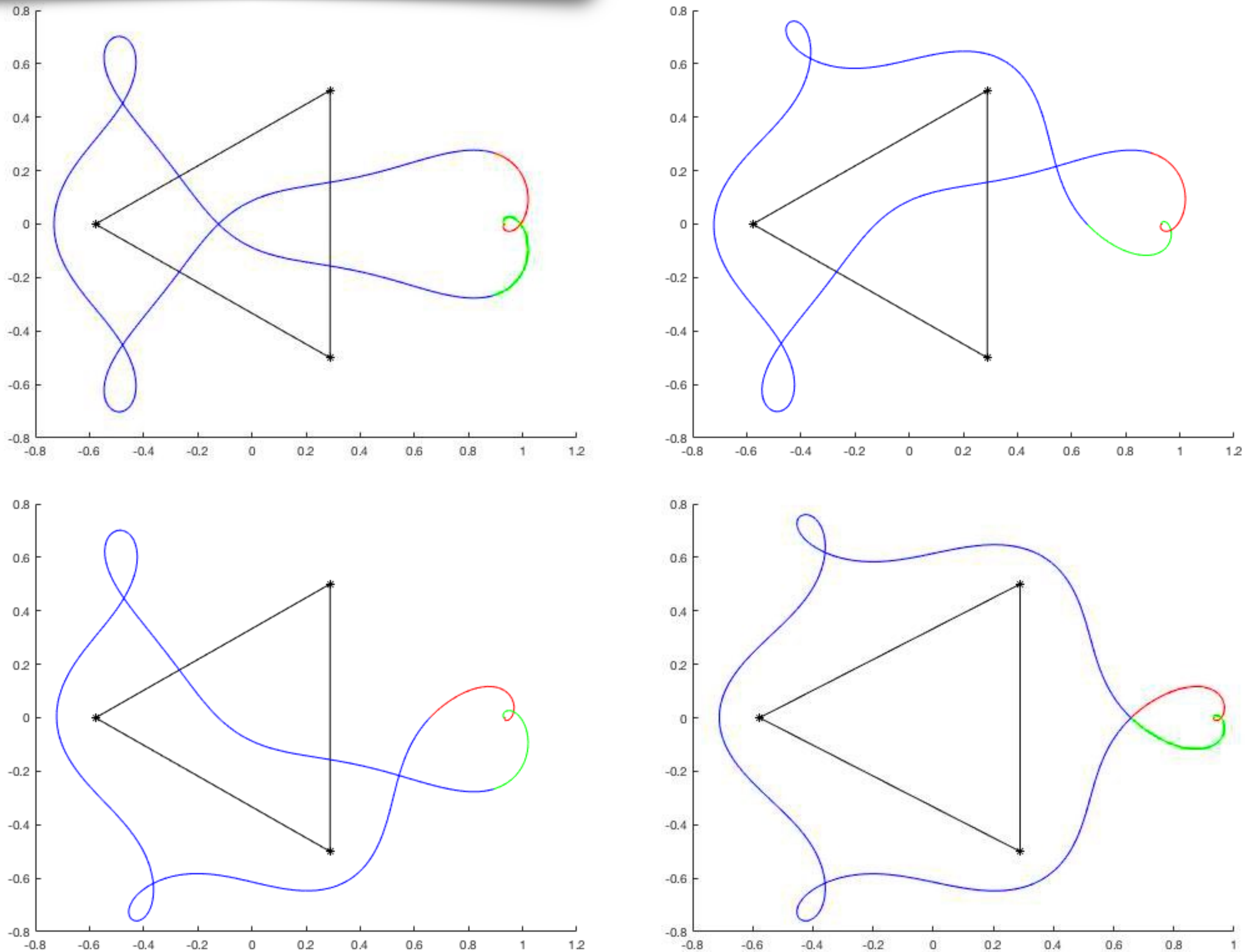




Shortest connections at $\mathcal{L}_5$

Basic "letters in the alphabet"

The CRFBP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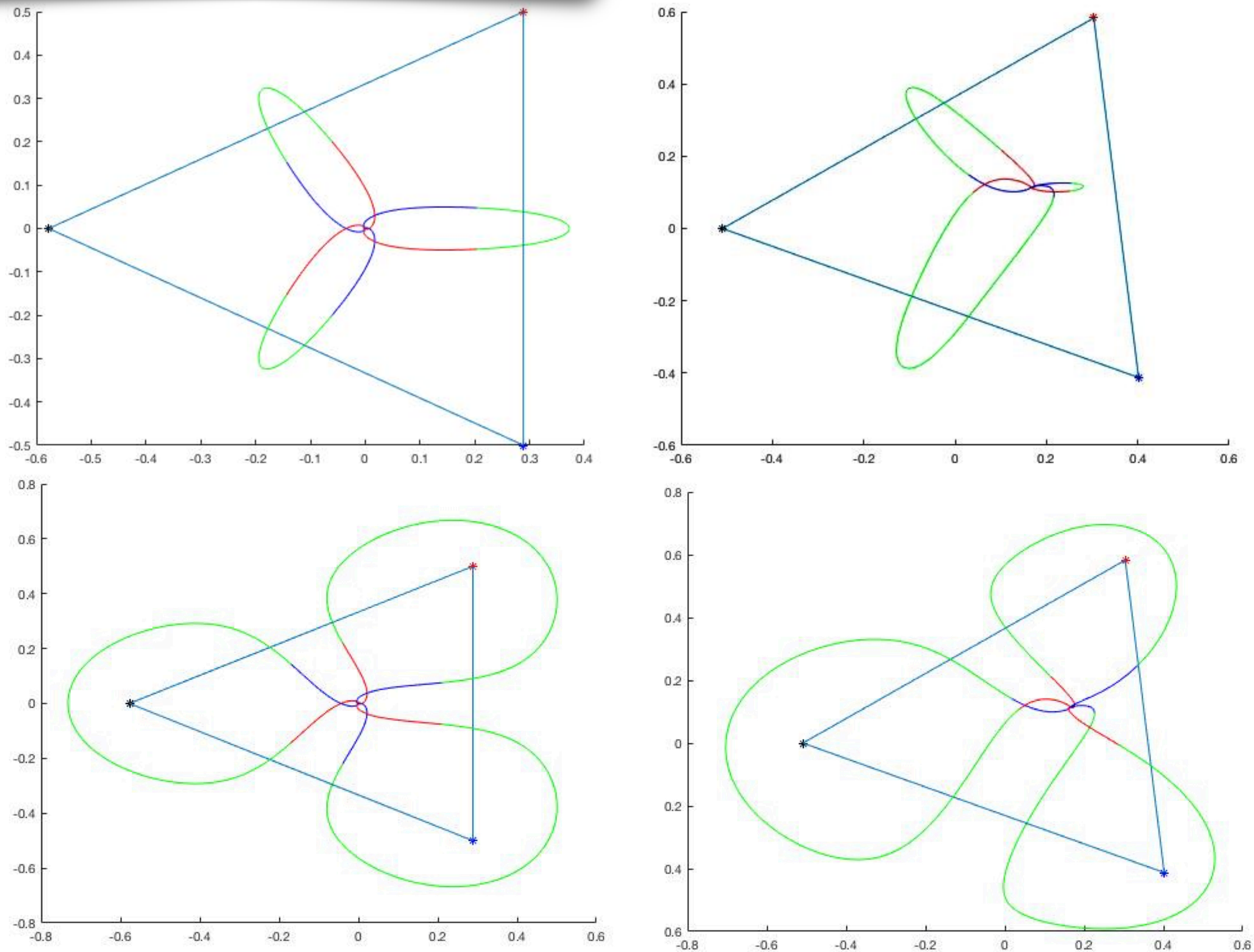
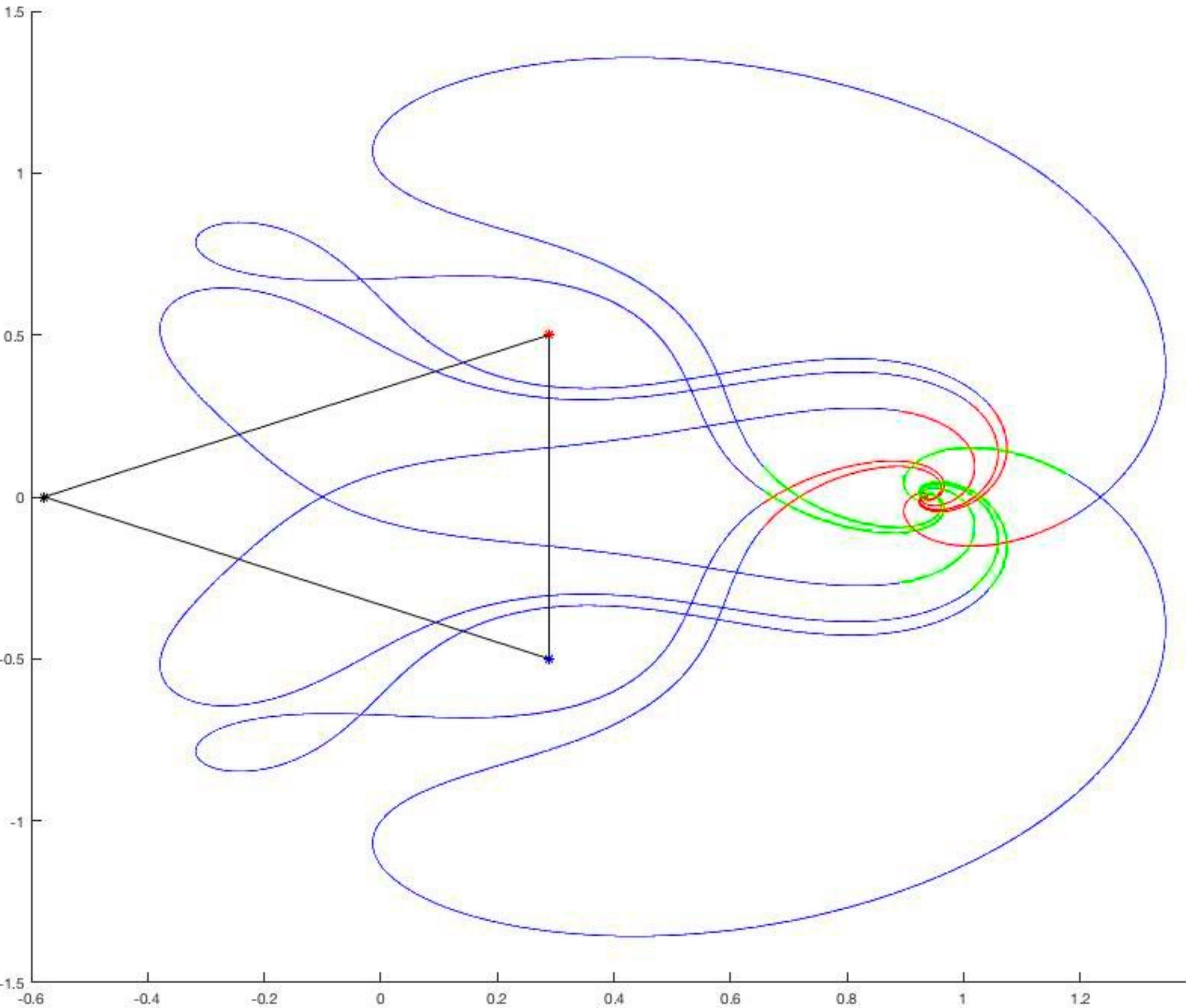
The CRFBP

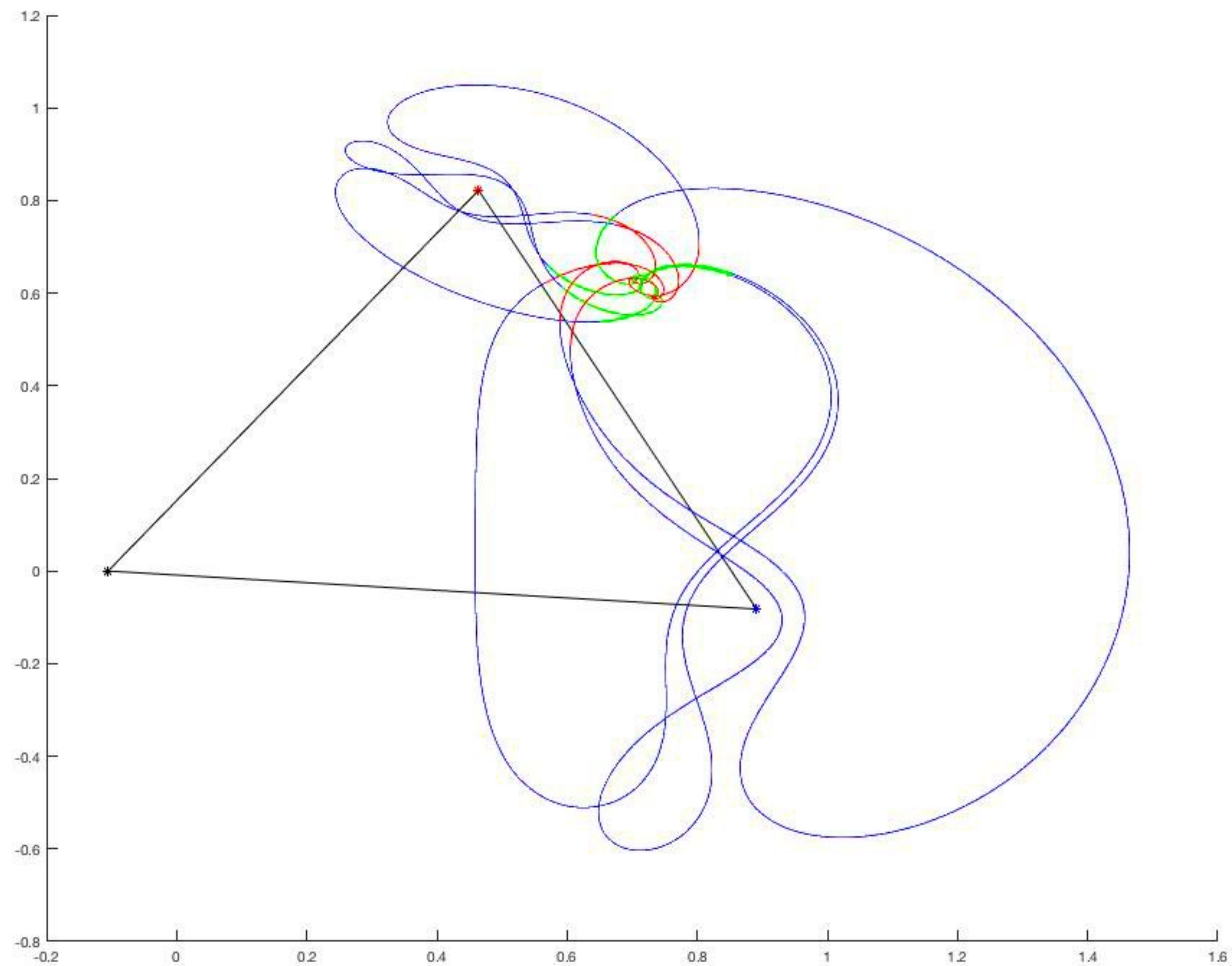
Continuation at $\mathcal{L}_0$



The CRFBP

Continuation at $\mathcal{L}_5$





The CRFBP

Question: how to validate these results?

- Need validated bounds on the parameterizations
- Need validated bounds on advected material lines

In both cases the Taylor series coefficients are given by nonlinear recurrence relations of the form

$$p_n = T(p_0, p_1, \ldots, p_n)$$

Tomorrow I will discuss an especially simple approach to validated numerics for problems of this kind.

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