Polygonal Approximation of Flows

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Multivalued maps on grids

Definition [Mrozek]: A **grid** on a compact space X is a finite collection of subsets $\mathcal{G}$ for which

- $\bigcup_{G \in \mathcal{G}} G = X$,
- $G = \mathrm{cl}(\mathrm{int}(G))$,
- $G \bigcap \mathrm{int}(H) = \emptyset$ if $G \neq H$.

A **multivalued map $\mathcal{F}$ on G** maps a point $G \in \mathcal{G}$ to a set of elements of $\mathcal{G}$ (and hence maps sets to sets), and we will write $\mathcal{F} : \mathcal{G} \rightrightarrows \mathcal{G}$. The geometric realizations of a subset of $\mathcal{S} \subset \mathcal{G}$ and the map $\mathcal{F}$ will be denoted by

$$|\mathcal{S}| = \bigcup_{G \in \mathcal{S}} G \quad \text{and} \quad F(\mathcal{S}) = |\mathcal{F}(\mathcal{S})|.$$

Outer approximations

A multivalued map $\mathcal{F}$ is an **outer approximation** to the dynamical system $\varphi : T \times X \to X$ if for some $k > 0$

$$\varphi((0,1], G) \subset \text{int}(F^{[0,k]}(G)) \text{ and } \varphi([-1,0), G) \subset \text{int}(F^{[-k,0]}(G))$$

where $\mathcal{F}^{[a,b]}(\mathcal{S}) = \cup_{n \in [a,b]} \mathcal{F}^n(\mathcal{S})$.

In the case of a map $f : X \to X$, there is a natural (minimal) outer approximation on any grid $\mathcal{G}$, namely $H \in \mathcal{F}(G)$ iff $f(G) \cap H \neq \emptyset$.

For flows one can of course use this approximation on the time-τ map to obtain an outer approximation. In practice, this may not be desirable in certain situations.

Dynamics of (combinatorial) multivalued maps

Definition: A set $\mathcal{A} \in \mathcal{G}$ is an **attractor** if $\mathcal{F}(\mathcal{A}) = \mathcal{A}$ and $\mathcal{B}$ is a **repeller** if $\mathcal{F}^{-1}(\mathcal{B}) = \mathcal{B}$. If $\mathcal{S} = \mathcal{A} \cap \mathcal{B}$ for some attractor $\mathcal{A}$ and some repeller $\mathcal{B}$, then $\mathcal{S}$ is a **Morse set**.

Theorem [K., Mischaikow, VanderVorst]: If $\mathcal{F}$ is an outer approximation of φ and $\mathcal{S}$ is a Morse set of $\mathcal{F}$, then $|\mathcal{S}|$ is an isolating block for a Morse set of φ.

Key fact: The combinatorics of finding Morse sets is easy. The complexity of the computation of the finest Morse decomposition of $\mathcal{F}$ is **linear** in the number of elements of $\mathcal{G}$ plus the number of images of $\mathcal{F}$.

Recurrence

Definition: The **recurrent set** is

$$\mathcal{R}(\mathcal{G}) = \{G : G \in \mathcal{F}^n(G) \text{ for some } n > 0\}.$$

On $\mathcal{R}(\mathcal{G})$, $G \sim H$ if $\exists m, n > 0$ such that $G \in F^m(H)$ and $H \in F^n(G)$.

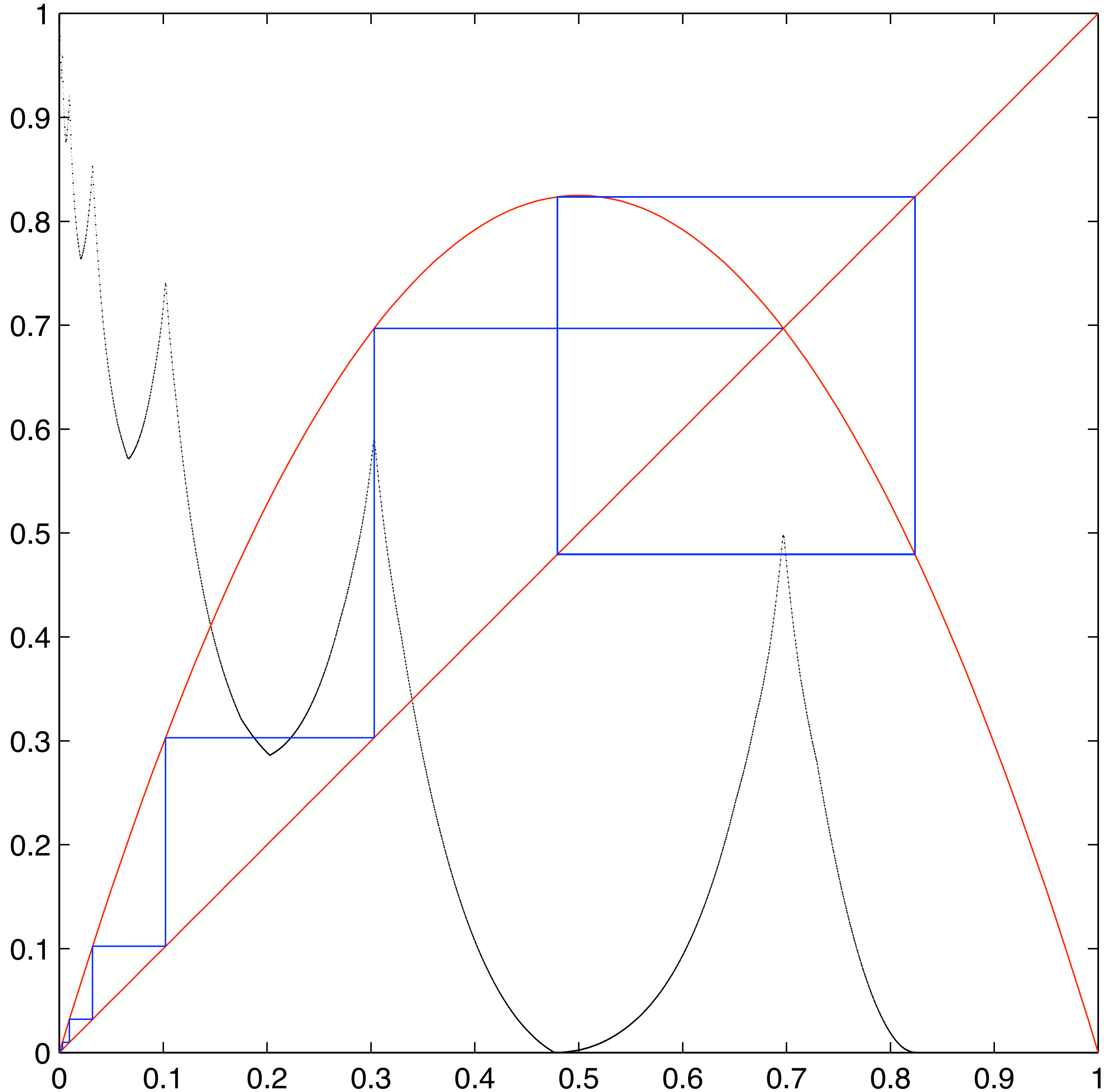
Equivalence classes of $\sim$ are the **recurrent components** of $\mathcal{F}$.

The recurrent components are the finest Morse decomposition for $\mathcal{F}$, i.e. the intersection of all attractor/repeller pairs.

Lyapunov functions

The graph algorithms also yield a discrete 'Lyapunov function' L for the graph, i.e. $L(G) = L(H)$ iff $G \sim H$ and $L(G) > L(H)$ whenever $H \in \mathcal{F}(G)$.

This function obviously does not contain any topological information. However, a function V can be constructed which is piecewise constant on the grid and approximates a true Lyapunov function for the dynamics of φ, under certain conditions, **[K., Mischaikow, and VanderVorst; Ban].**



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Flows and polygons [Eidenschink and Mischaikow]

Given:

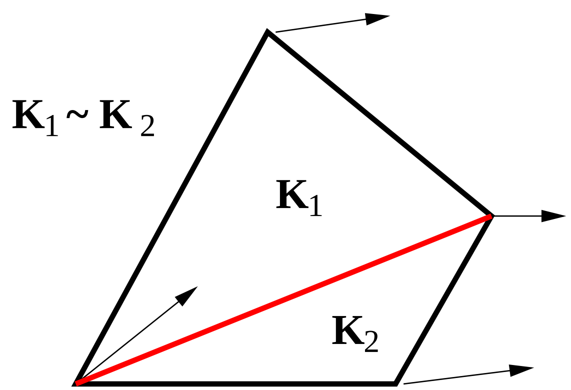
- $\Omega \in \mathbb{R}^d$ a polygonal (rectangular) region
- $f : \Omega \to \mathbb{R}^d$ a vector field on Ω

Find:

- $\mathcal{P}$ a polygonal decomposition of a full finite simplicial complex $\mathcal{K}$ with $|\mathcal{K}| = \Omega$
- $F : \mathcal{P} \rightrightarrows \mathcal{P}$ a multivalued map which is an outer approximation to the flow of $\dot{x} = f(x)$ on Ω

Definition: A simplex $L \in \mathcal{K}^{d-1}$ is a **flow transverse face** if $\nu(L) \cdot f(x) \neq 0$ for all $x \in L$ where $\nu(L)$ is normal to L. A polygon $P \in \mathcal{P}$ is a **flow transverse polygon** if every face $L \in \partial P$ is flow transverse.

Definition: Given a simplicial complex $\mathcal{K}$ the **minimal flow transverse polygonal decomposition** $\mathcal{P}$ of Ω consists of the equivalence classes of $\sim$ defined by $K_1 \sim K_2$ in $\mathcal{K}^d$ if $K_1 \cap K_2 = L \in \mathcal{K}^{d-1}$ and $\nu(L) \cdot f(x) = 0$ for some $x \in L$ and extended by transitivity.

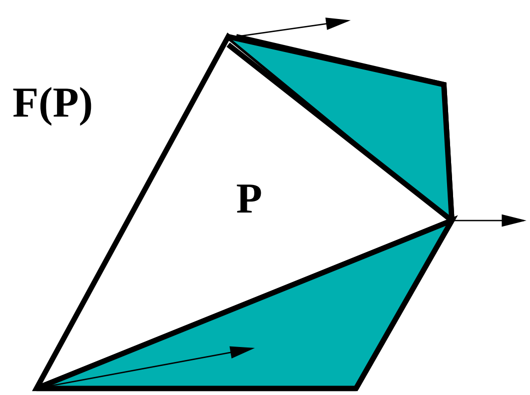


Flow induced multivalued map

Definition: The **flow induced multivalued map** $\mathcal{F} : \mathcal{P} \rightrightarrows \mathcal{P}$ is defined by:

• $P \in \mathcal{F}(P)$ iff P contains an equilibrium point (necessarily in its interior)

• $Q \in \mathcal{F}(P)$ if $P \cap Q = L \in \mathcal{K}^{d-1}$ and $\nu_P(L) \cdot f(x) > 0$ for $x \in L$ where $\nu_P(L)$ is normal to L pointing out of P, i.e. $Q \in F(P)$ if Q is *adjacent* to P along an **exit face** L of P.



Isolating blocks

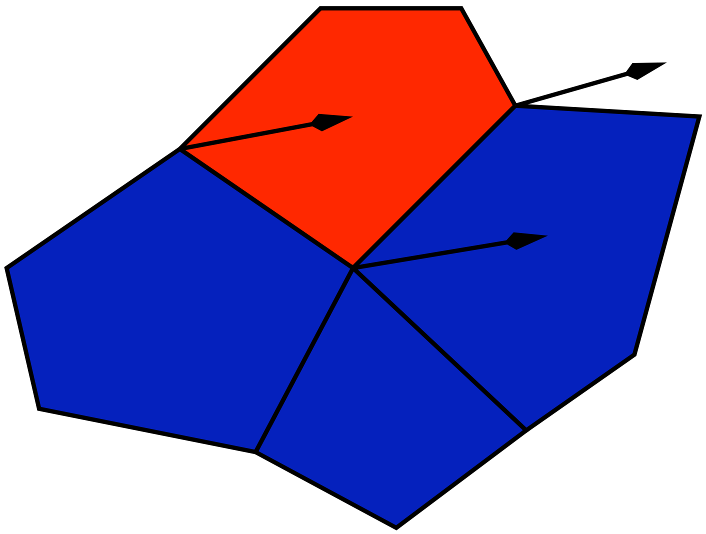
A compact set $N \subset \Omega$ is an **isolating block** if every point on $\partial|\mathcal{S}|$ immediately leaves $|\mathcal{S}|$ in either forward or backward time. Then an exit set for N can be taken as a subset of ∂N for computing the Conley index.

Theorem: If $\mathcal{S}$ is a Morse set of $\mathcal{F} : \mathcal{P} \rightrightarrows \mathcal{P}$ and either $|\mathcal{S}| \cap \Omega = \emptyset$ or Ω is an isolating block, then $|\mathcal{S}|$ is an isolating block.

Essentially, $\mathcal{F}$ is an outer approximation of the flow on the interior grid elements (after suitable rescaling of time).

In fact, $\varphi(t, x) \in \mathrm{int}(|\mathcal{F}^{\omega}(P)|)$ for any P containing x as long as $\varphi([0, t], x) \subset \Omega$.

Note: to be an isolating block a polygonal set must not only be flow transverse on its boundary (automatic), but it must also have no **re-entrant points** on its boundary.



Recap 1

[1] We have a license to start computing. **Any** simplicial complex will yield a multivalued map which can be made rigorous.

[2] The results of the computation can be arbitrarily bad. **However it will not give a wrong result.** If a Morse set is found which contains no invariant set for the flow, it will have trivial Conley index.

[3] The advantage of using the vector field directly is avoiding problems which can arise in approximating the time-τ map on a cubical grid: how long to integrate, large errors/ small cubes, lack of transversality...

[4] The disadvantage is of course the geometry of simplicial complexes can be complicated.

Outstanding issues 1

[1] How closely can we approximate the dynamics of the flow with this type of multivalued map?

[2] What (computable) properties of the base simplicial complex are sufficient to guarantee a close approximation?

[3] Does such an approximating complex always exist?

[4] What are the algorithms to compute such a complex?

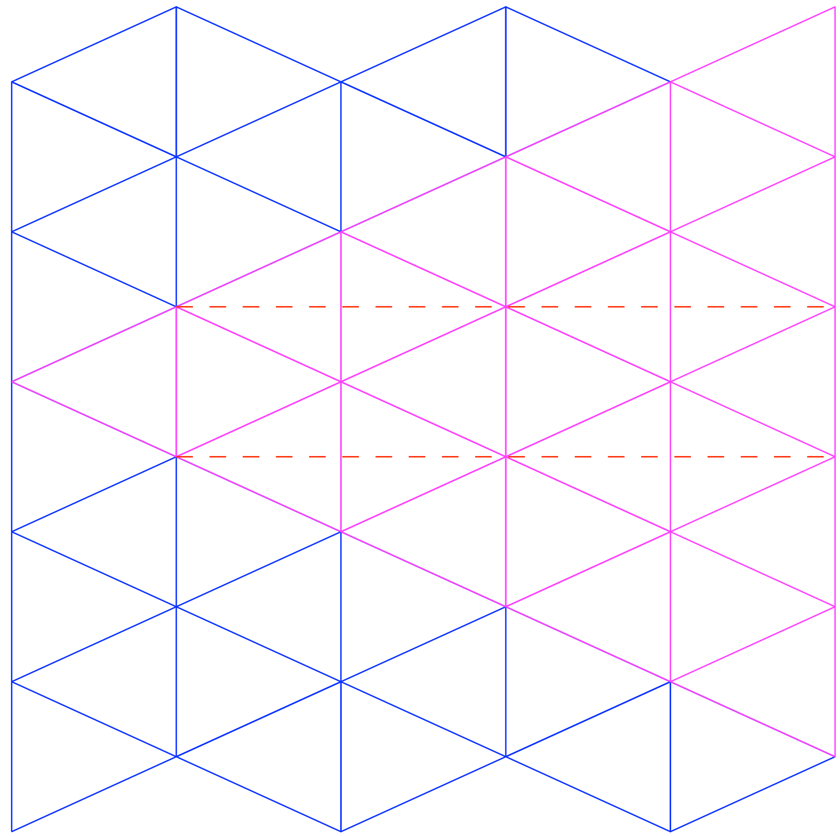
Parallel flow

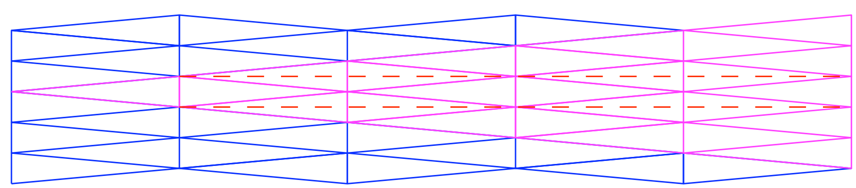
Consider the flow on $\mathbb{R}^d$ of $\dot{x} = \Pi = (1, 0, \ldots 0)$.

Let $\mathcal{K}$ be a full finite simplicial complex and $\Omega = |\mathcal{K}|$.

What type of triangulation gives the best approximation?

Intuitively, triangles should be long in the direction of the vector field and thin in directions orthogonal to it.



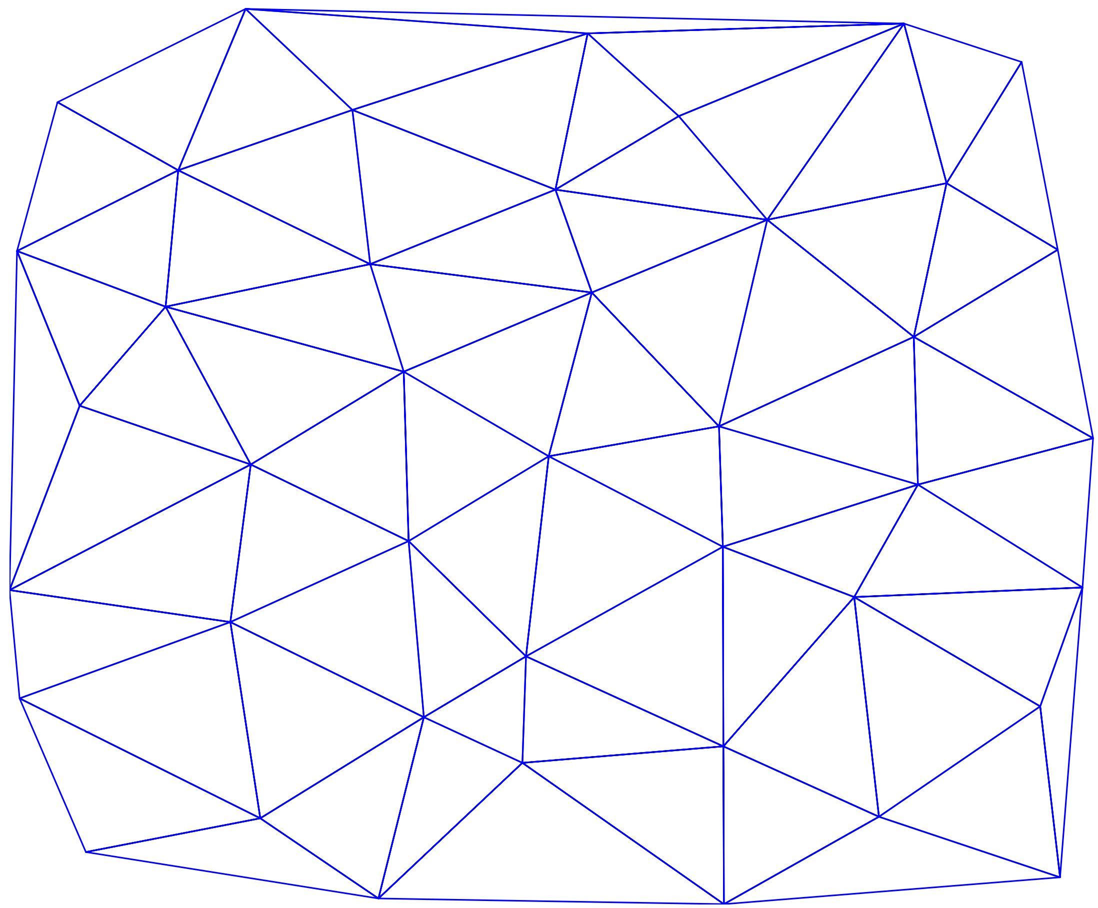


Delaunay triangulations

Definition: A d-simplex satisfies the **Delaunay property** if its open circumball contains no vertices. A simplicial complex in which every d-simplex satisfies the Delaunay property is a **Delaunay complex (triangulation).**

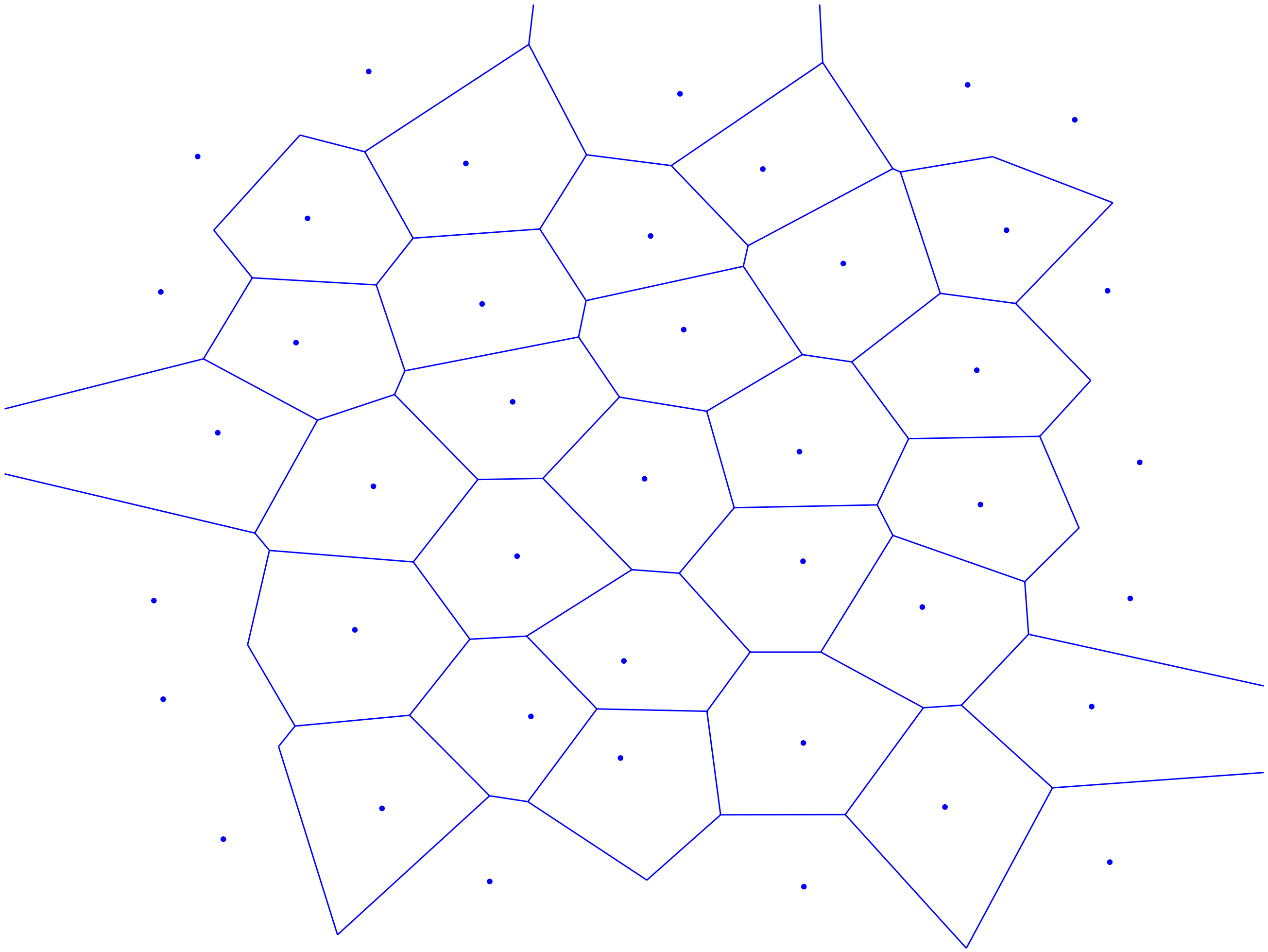
Theorem: Given any finite set $S \subset \mathbb{R}^d$, there exists a triangulation of the convex hull of S which is a Delaunay complex. Moreover, if no set of $d+2$ points in S lie on a $d-1$ sphere, the Delaunay complex of S is unique.

Remark: In $\mathbb{R}^2$, the Delaunay triangulation maximizes the minimum angle over all possible triangulations.



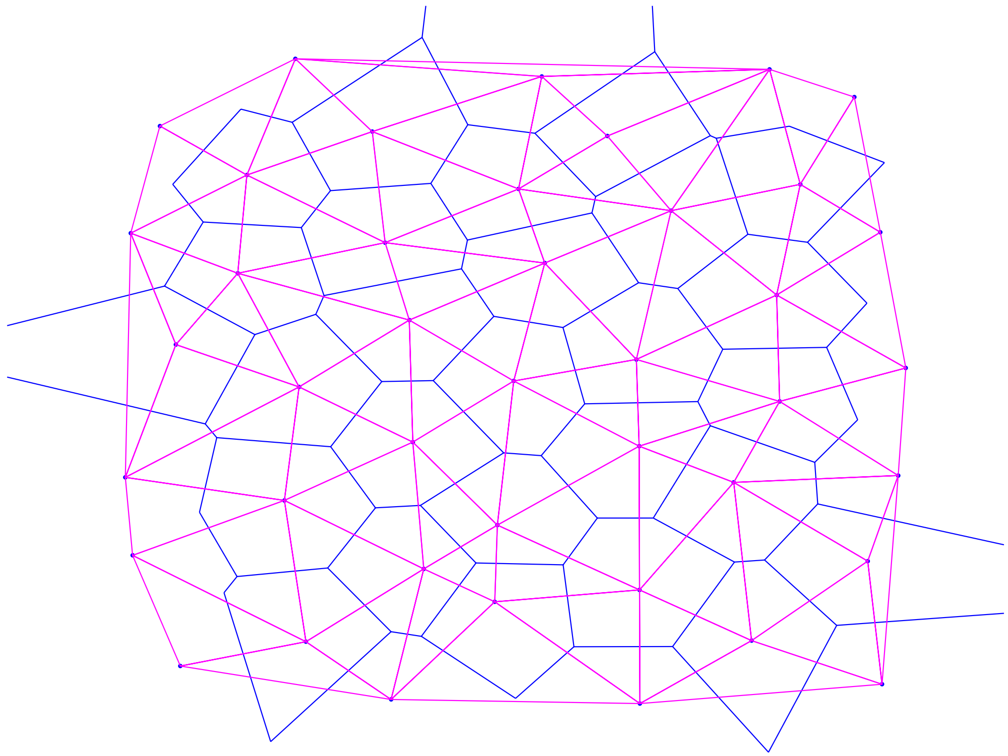
Voronoi diagrams

Definition: Given a finite set $S \subset \mathbb{R}^d$, the locus of the set of all points in $\mathbb{R}^d$ which are closer to $x_0 \in S$ than any other point in S is called the **Voronoi polygon at** x_0. The collection of all Voronoi polygons is a polygonal decomposition of the plane called the **Voronoi diagram**.



Delaunay-Voronoi duality

Remark: The Delaunay triangulation is dual to the Voronoi diagram of a generic set of points.



Computing Delaunay triangulations

There are many methods for computing a Delaunay triangulation (or Voronoi diagram) especially in 2 dimensions:

- **Delaunay (or Bowyer-Watson) (or Incremental) insertion**
- Bistellar flip methods
- Polytope methods. . .

The Delaunay insertion method works in any dimension and is readily generalizable to our situation.

Delaunay insertion

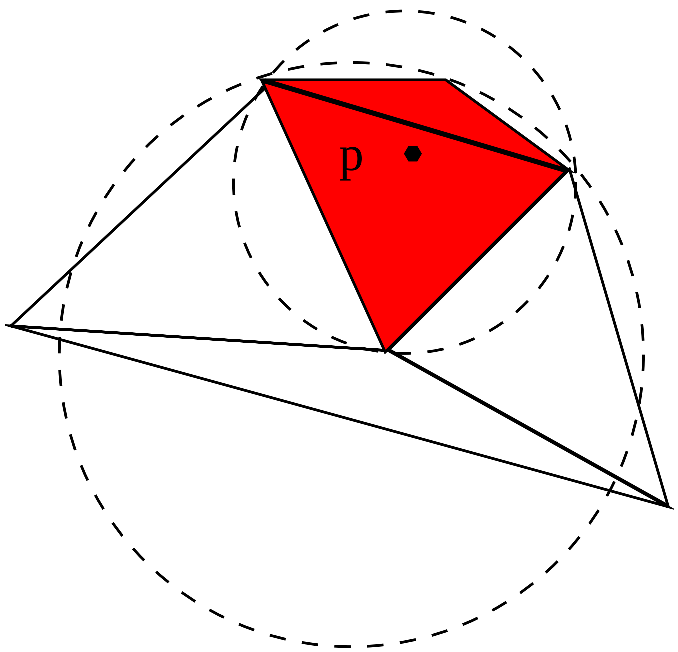
Given $\mathcal{K}$ the Delaunay triangulation of a finite set $S \subset R^d$, a new point p in the convex hull of S can be inserted to compute the Delaunay triangulation of $S \cup \{p\}$ as follows:

[1] Delete all simplices of $\mathcal{K}$ whose open circumball contains p.

[2] The union of all such simplices, called the **Delaunay kernel,** is a polygon which is star-shaped at p.

[3] Retriangulate the Delaunay kernel by simplices composed of a face of the boundary and p.

[4] The new complex is a Delaunay triangulation of $S \cup \{p\}$.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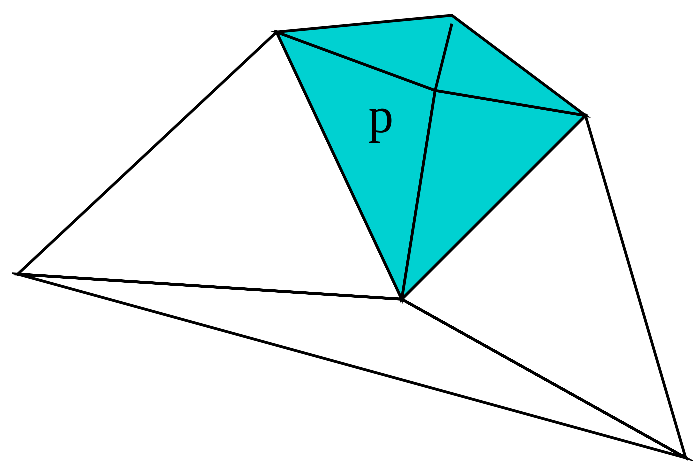
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Anisotropic Delaunay triangulations

Implementation of Delaunay insertion requires only the circumscription test:

Does point p lie inside the circumball of simplex K?

Let M be a symmetric, positive definite matrix and

$$g_M(u,v) = \langle Mu, v\rangle$$

the corresponding bilinear form.

The circumballs in this metric are ellipsoids, and the circumscription test is just linear algebra.

Theorem: If $S \subset \mathbb{R}^d$ is a finite set of points. Then generically there is a unique triangulation of the convex hull of S which satisfies the Delaunay property using circumballs in $(\mathbb{R}^d, g_M)$, which therefore can properly be called an (anisotropic) Delaunay complex in (R^d, g_M).

This **constant** metric situation will work for parallel flow with

$$M = \Lambda(\mu) = \begin{bmatrix} 1 & 0 & 0 & \ldots & 0 \\ 0 & \mu^{-1} & 0 & \ldots & 0 \\ \ldots & & & & \\ 0 & 0 & 0 & \ldots & \mu^{-1} \end{bmatrix}$$

but what about arbitrary flows?

Is there such a concept as a Delaunay complex on an arbitrary Riemannian manifold (X, g)? How can it be computed?

Riemannian-Delaunay triangulations

Theorem/Conjecture: Let (X, g) be a compact Riemannian manifold. Let $S \subset X$ be a finite set satisfying the density condition that every ball of sufficiently small radius (some fraction of the convexity radius) contains a point of S. Then there exists a triangulation of $\mathcal{K}$ of (M, g) with $\mathcal{K}^0 = S$ and every $K \in \mathcal{K}^d$ has a (unique?) strongly convex (minimal radius?) circumball which contains no points of S. Generically, this Delaunay triangulation is unique.

Proved for 2-dimensional manifolds. **[Libon]**

Proof for any dimension?

Flow-induced Riemannian metric

Let $\mathcal{E}$ be the equilibrium set in Ω.

Choose a vector field $f^{\perp}(x)$ orthogonal to $f(x)$ on $\Omega \setminus \mathcal{E}$ and let $Dh(x) = [f(x)|f^{\perp}(x)]$.

For $R(x) \neq 0$, define

$$M_{\mu}^{f}(x) = \frac{1}{R(x)\|f(x)\|^2} Dh(x) \cdot \Lambda(\mu) \cdot Dh^T(x).$$

Let $g_{\mu}^{f}(x)(u,v) = \left\langle M_{\mu}^{f}(x)u, v \right\rangle$ be the corresponding bilinear form.

Then $(\Omega \setminus \mathcal{E}, g_{\mu}^{f})$ is a Riemannian manifold.

Fix $M_\mu^f(x_0)$ at some x_0 and $\mu < 1$.

Then the unit ball in the metric determined by this constant matrix is an ellipsoid with:

- major axis in the direction of the vector field $f(x_0)$,
- the eccentricity determined by μ,
- and the size determined by $R(x_0)$.

Remark: The function $R(x)$ is related to the curvature of the vector field at x_0.

Practical Riemannian-Delaunay triangulations

In practice a triangulation can be constructed from approximations by constant metrics. [Borouchaki, George, Hecht, Laug, and Saltel]

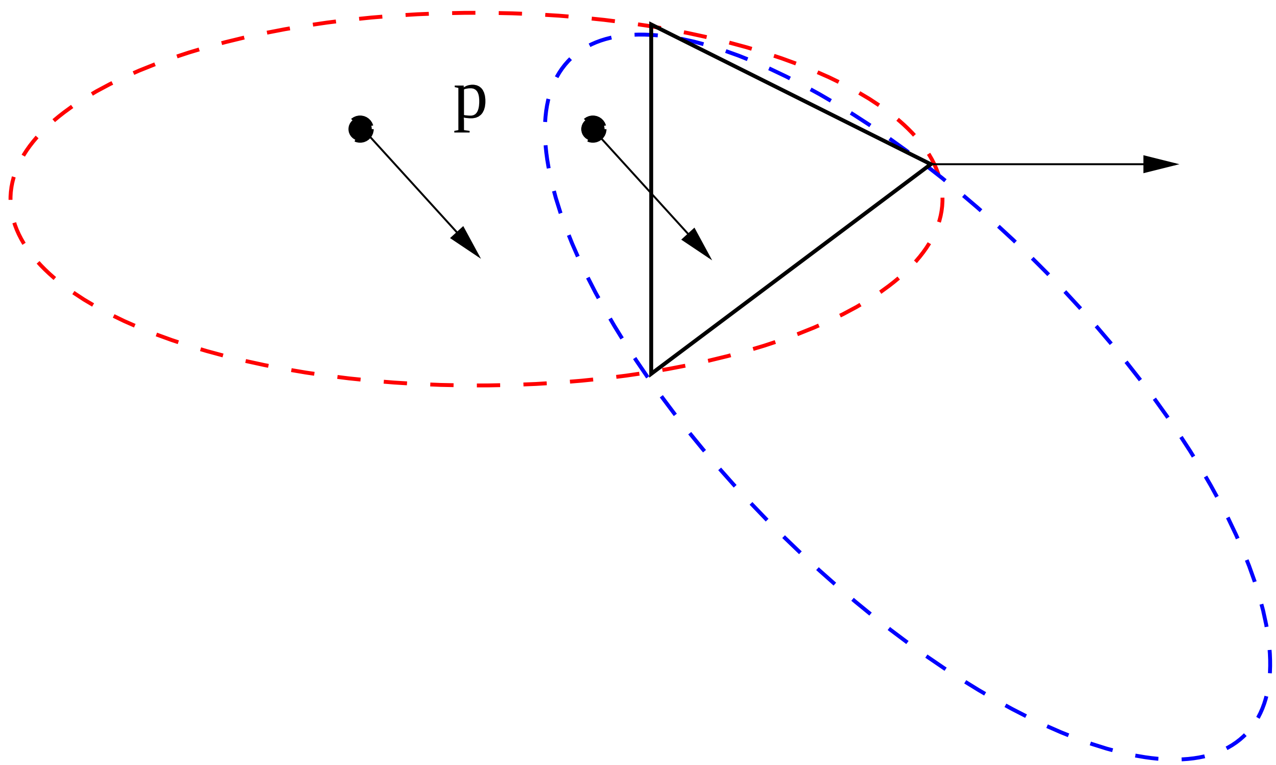
Using the constant metrics determined by p and the vertices of K, a star-shaped kernel can be constructed by modifying the circumscription condition to require that p lie inside one or all such circumballs or satisfy some average condition.

Example: Let

$$\alpha_p = d_p(p, O_p)/d_p(v, O_p) \quad \text{and} \quad \alpha_v = d_v(p, O_v)/d_v(v, O_v)$$

be the ratios of the distances from p to the circumcenter of K to the circumradii of K measured in the constant metrics at p and at some vertex v of K.

Then K is in the Delaunay kernel of p if $\alpha_p + \alpha_v < 2$.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Recap 2

[1] Given any finite set of vertices S in $\Omega \backslash \mathcal{E}$ we can (in principle) compute a Riemannian-Delaunay triangulation of the convex hull of S which is aligned to the flow.

[2] The insertion algorithm is dimension independent and computational geometers have developed very fast algorithms.

[3] There are a number of computational issues:

- Early in the insertion, the metric approximation is bad.
- In dimensions higher than 2, the Delaunay kernel must be reduced to ensure that it is star-shaped with respect to the insertion point.
- If simplices get too thin, then multiple precision arithmetic may be needed.

Outstanding issues 2

[1] If the location of the vertices is bad, then the triangulation can be bad.

[2] Is there an algorithm to choose the vertices?

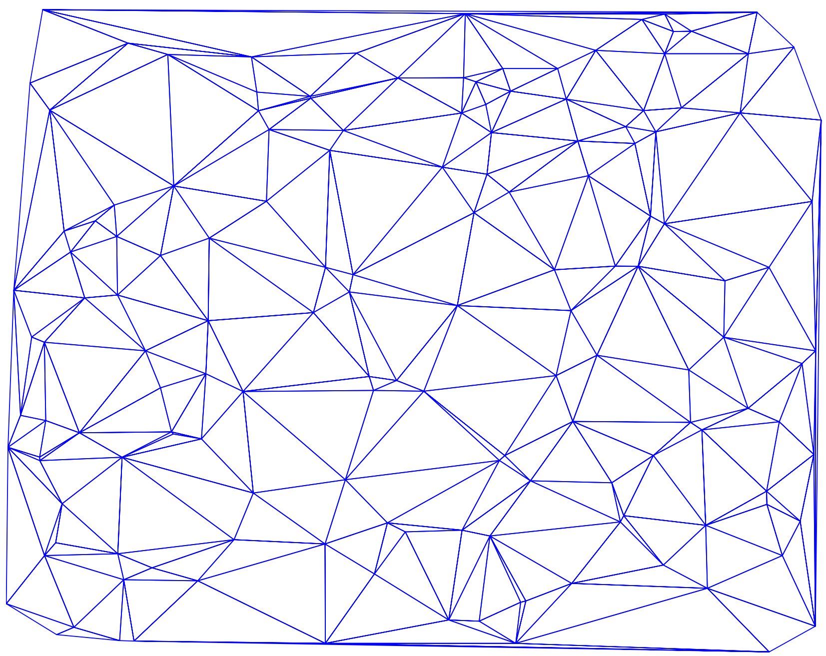
[3] How closely can we approximate the dynamics of the flow?

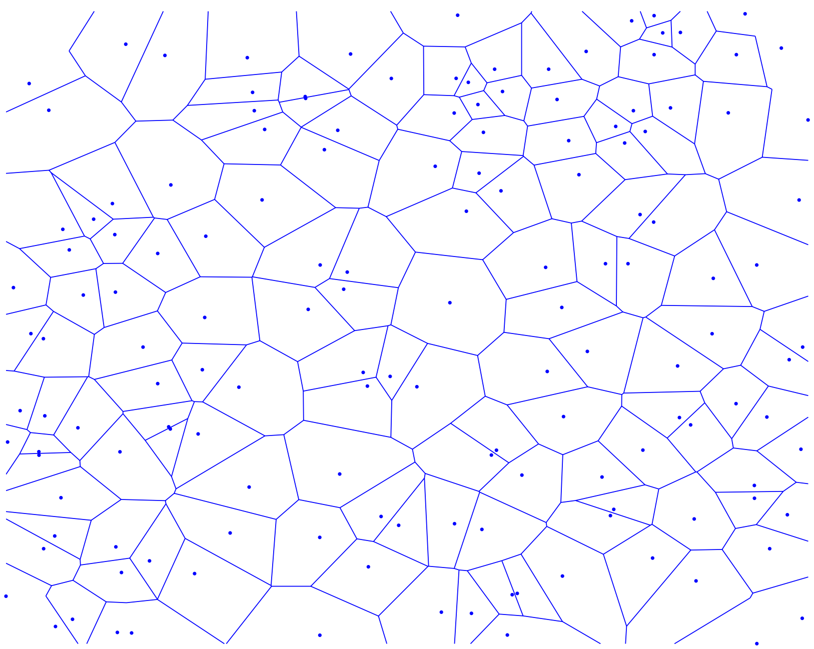
[4] Are there computable properties of the base simplicial complex are sufficient to guarantee a close approximation?

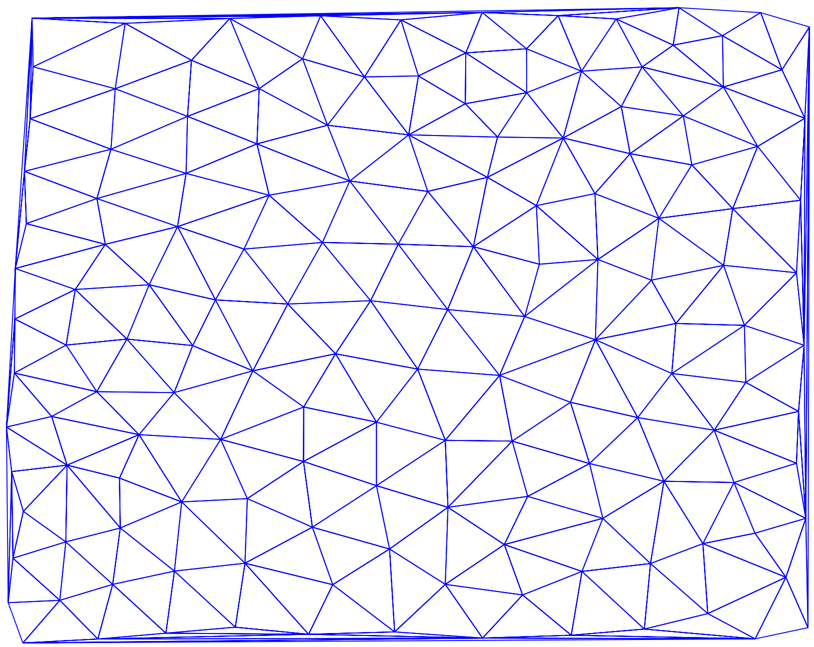
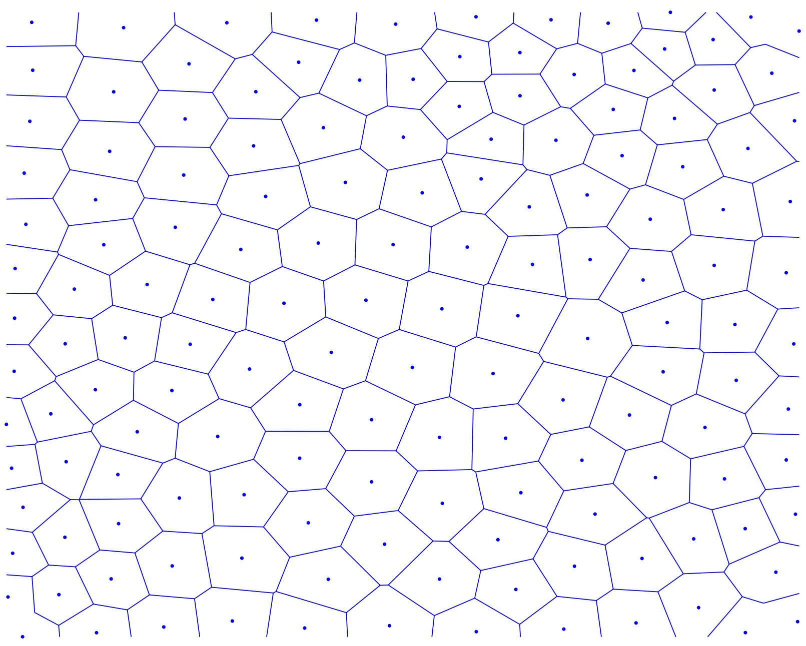
[5] Does such an approximating complex always exist/ can always be computed?

Centroidal Voronoi diagrams

Strategy: Place vertices so that each vertex is located at the centroid of its Voronoi region. **[Du, Faber, Gunzberger, and Ju]**





• Resulting elements are high quality, i.e. close to equilateral.

• There are naturally parallelizable algorithms involving probabilistic averaging.

Overall procedure

[1] Choose a set of initial vertices randomly with respect to the curvature density $R(x)$.

[2] Perform probablistic centroidal averaging using distances in the Riemannian metric to obtain a final set of vertices.

[3] Compute Riemannian-Delaunay triangulation.

[4] (Rigorously) compute the flow transverse polygonal decomposition and multivalued map.

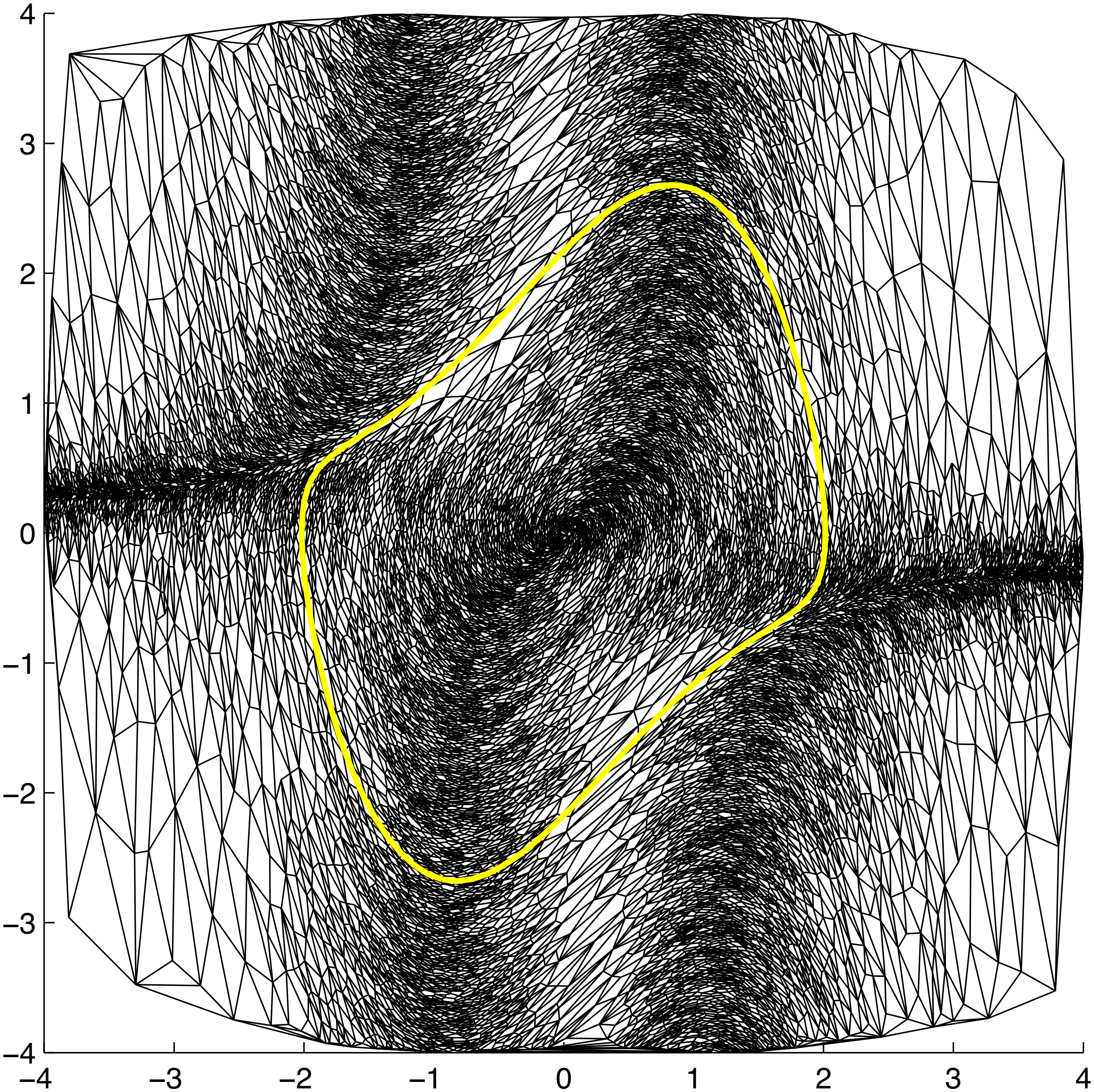
[5] Apply graph algorithms to obtain rigorous isolating blocks.

[6] Extract isolating blocks and repeat with a smaller μ if necessary.

Reverse Van der Pol

$$\begin{aligned} \dot{x} &= -y \\ \dot{y} &= (x^2 - 1)y + x. \end{aligned}$$

The next figure will show the minimal flow transverse decomposition of a triangulation containing $20,000$ vertices, $39,9940$ triangles, and $27,552$ polygons.



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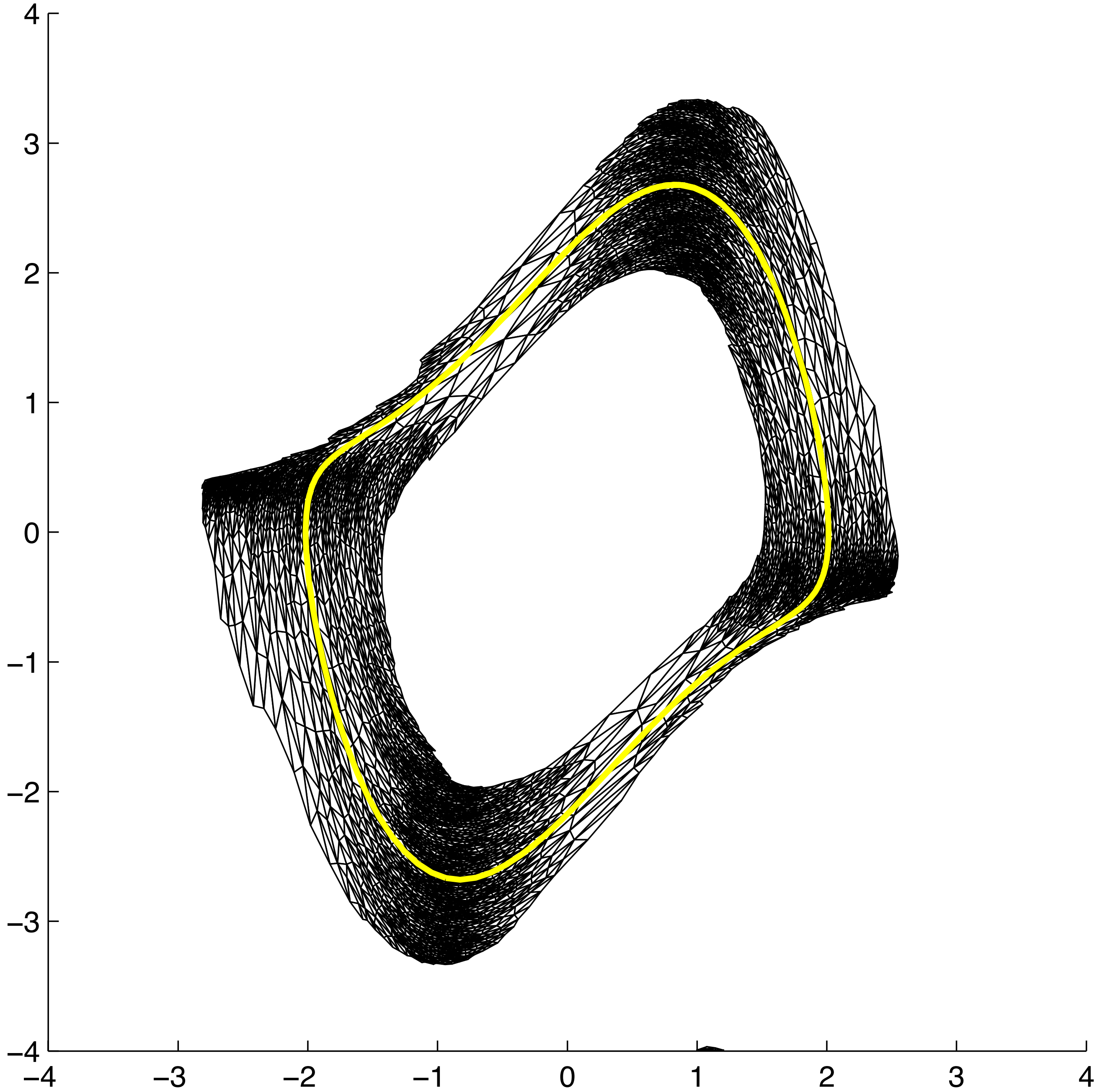
From this triangulation, we can extract the recurrent component the multivalued map which contains the periodic orbit. This set contains $8,093$ triangles in $5,812$ polygons.



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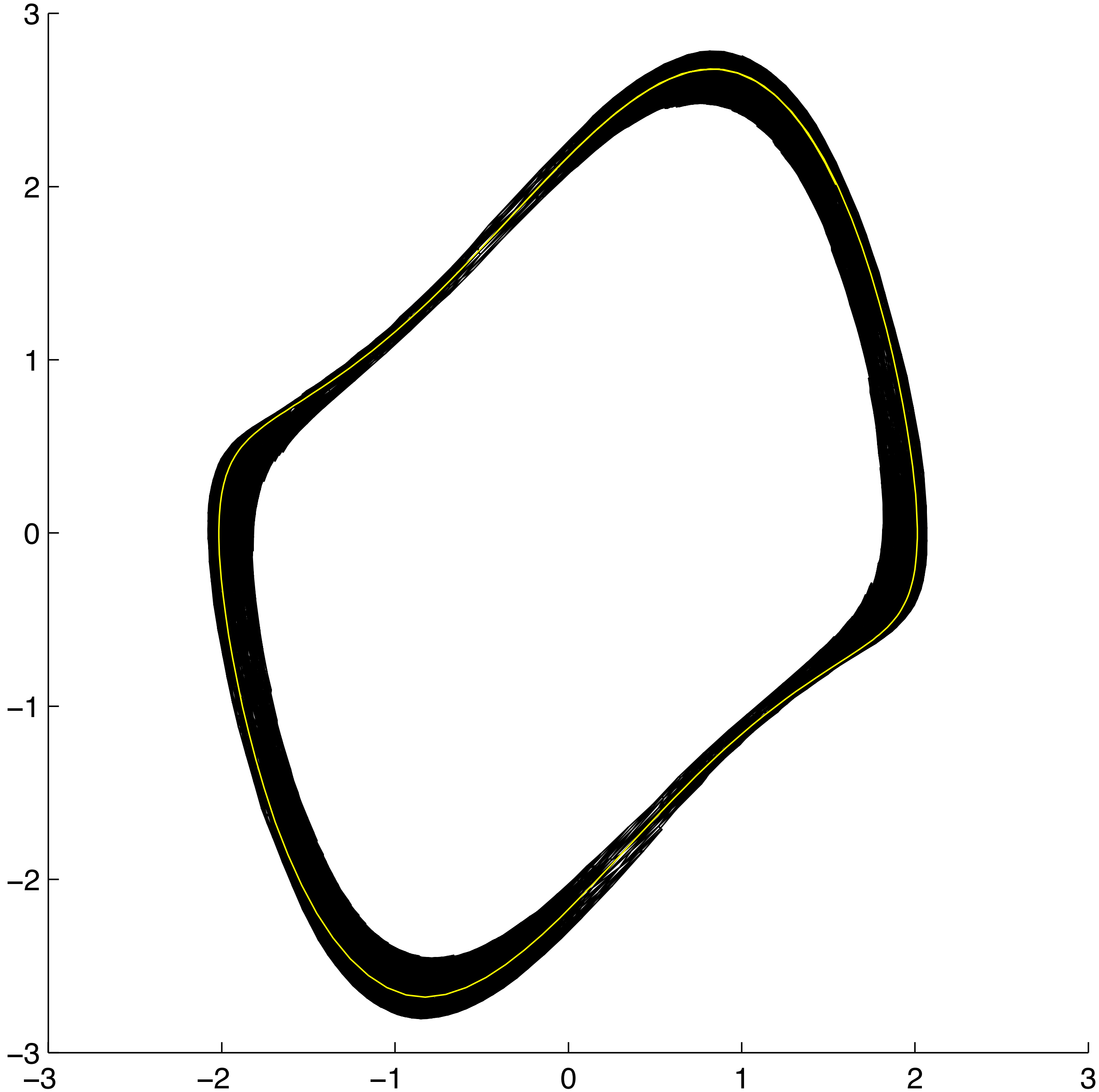
This triangulation can be refined to approximate the periodic orbit more closely. The next figure shows a recurrent set for the multivalued map containing $20,119$ triangles.



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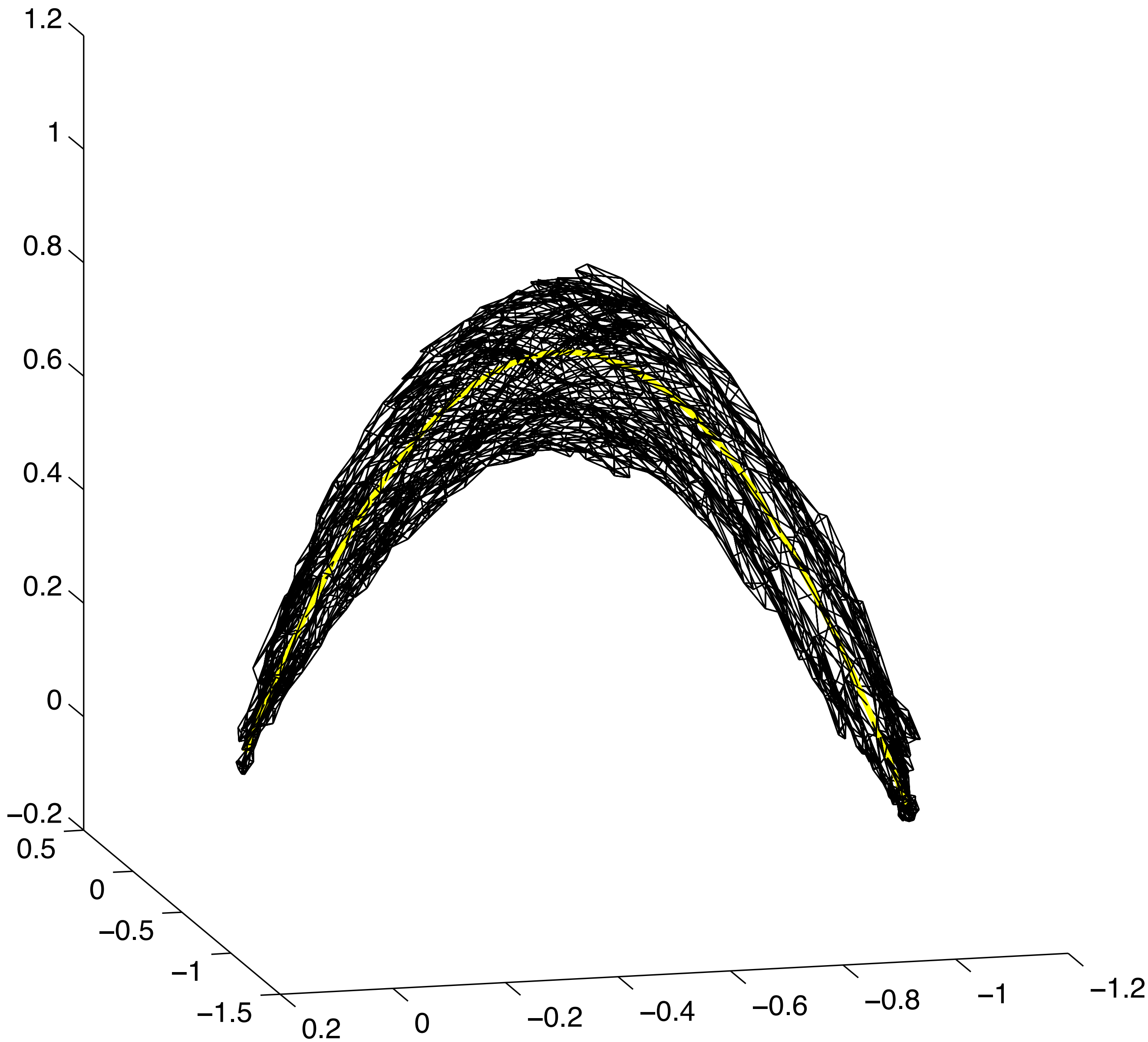
3-d connecting orbit

$$\begin{aligned}\dot{x} &= -x(x+1) - z \\ \dot{y} &= y(2+6x-y) + 3\left(x + \frac{z}{3}\right) \\ \dot{z} &= z(2-x+5y)\end{aligned}$$

This 3-dimensional system, related to the ground state problem for a system of coupled semilinear Poisson equations with critical exponents, has a connecting orbit between the equilibria $(0,0,0)$ and $(-1,-1,0)$ as the intersection of a 2-dimensional unstable manifold and a 2-dimensional stable manifold. The connecting orbit is also proven in **[Hulshof and VanderVorst]** to be a parabola over the line $x = y, z = 0$. An isolating neighborhood of this connecting orbit with $12,326$ simplices is shown in the next figure.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−1
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Current/ future work

- There are implementation, algorithmic, and parallelization issues to resolve.

- Automate the (human) choices to be made in performing any given computation: $R(x)$, μ, # vertices, # averaging points, metric approximation...

- 4-d fast/slow system [Gameiro and Mischaikow]

- PDE bifurcation diagrams [Day, Hiraoka, Junge, Mischaikow, Ogawa, Wanner]

- Theoretical results

Flow oriented triangulations and chain recurrence

Definition: A simplex K is **δ-oriented** to the flow if every **entrance face** L has the following property:

$\exists\, y \in L$ such that $v - y \in C(f(y), \delta) = \{w : w \cdot f(y) \geq \delta \|w\| \|f(y)\|\}$

where v is the vertex opposite L in K.

Theorem: For every $\epsilon > 0$, there exists $\delta > 0$ so that if $\mathcal{K}$ is δ-oriented and diam($\mathcal{K}$) is sufficiently small, then the recurrent set of the multivalued map $\mathcal{R}(\mathcal{P})$ is contained in $\mathcal{R}_\epsilon(|\mathcal{K}|, \varphi)$.