Verified Numerics for ODEs in Isabelle/HOL

Fabian Immler

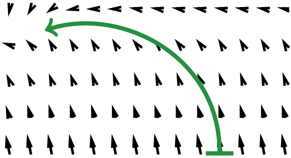
MAP 2016

Technische Universität München

Overview I

Ordinary Differential Equations

- modeling physics, biology, dynamical systems



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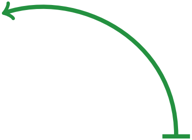

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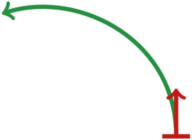

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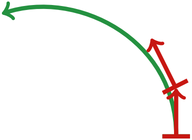

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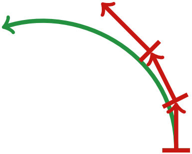

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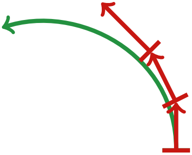

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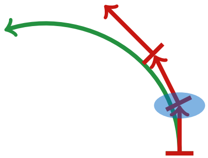

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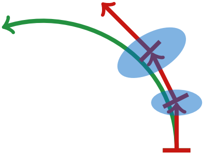

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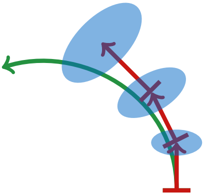

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Formalization and Verification

- formalization of $\mathbb{R}^n$ and ODEs in Isabelle

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Result

highly trusted code

Overview III

Applications/Challenges

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- Oil reservoir: stiff
- van-der-Pol: nonlinear
- Lorenz attractor: proof of topological properties based on computed enclosures

Content

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- Isabelle/HOL: interactive theorem prover

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In Isabelle/HOL

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```
class metric_space =
  fixes dist::"'a ⇒ 'a ⇒ real"
  assumes "dist x y = 0 ⟷ x = y"
  assumes "dist x y ≤ dist x z + dist y z"

instance real::metric_space
sorry

instance complex::metric_space
sorry
```

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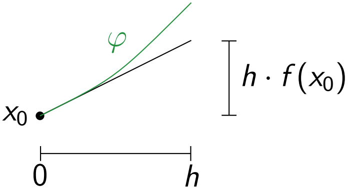
  - type of bounded continuous functions $\overline{\mathcal{C}}^{[\mathbb{R},\mathbb{R}^n]}$
- flow $\varphi(x_0, t)$ (solution for initial value x_0 at time t)

Euler Method



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  f ... slope given by ODE
  $\varphi(x_0, h) = x_0 + h \cdot f(x_0)$

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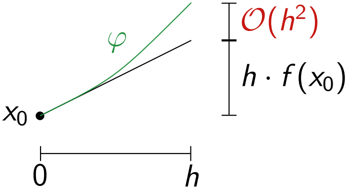

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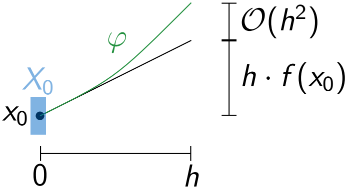

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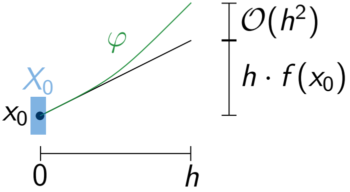

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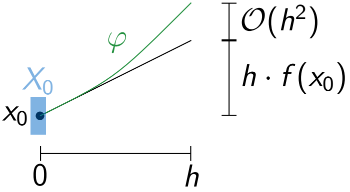

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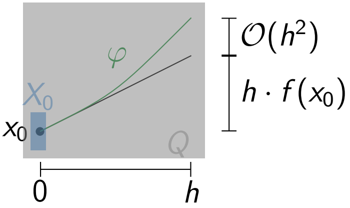

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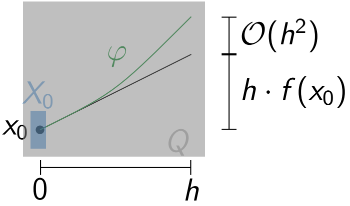

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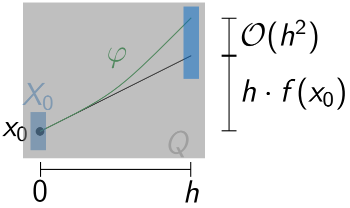

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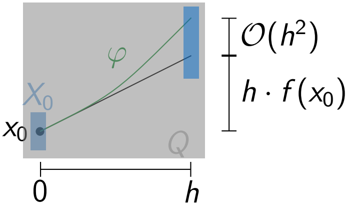

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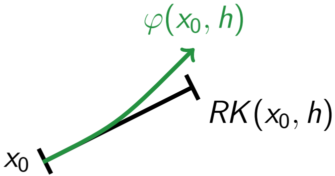
Theorem

$\varphi(X_0, h) \subseteq \mathrm{Euler}_h(X_0)$

Runge-Kutta methods



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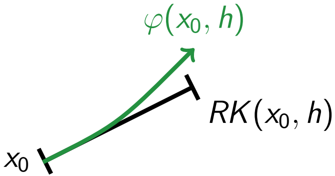

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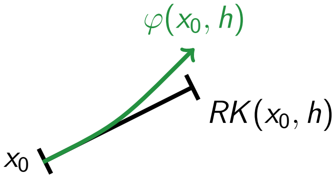

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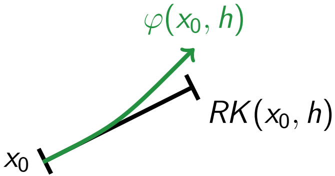

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- enclose errors (algorithm/finite precision)

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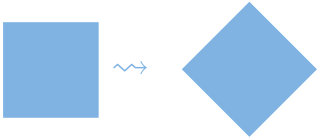

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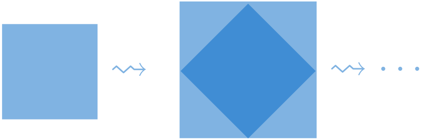

Affine Arithmetic

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$A : \mathbb{R}^n \to \mathbb{R}^m$

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Explicit Round-Off Operation

round every generator
collect errors in fresh noise symbols ε_i

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  - enclosure of solution $\rightsquigarrow$ Euler/RK2

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  - set $\rightsquigarrow$ list
  - set of $\mathbb{R}^n \rightsquigarrow$ list of affine forms
  - enclosure of solution $\rightsquigarrow$ Euler/RK2
- code generation (Standard ML)

Refinement

- abstract specification of ODEs/algorithms
- refinement towards executable structures
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Up Next

applications/optimizations

Oil Reservoir Problem

Oil reservoir problem

$y'(t) = z(t)$

$z'(t) = z(t)^2 - \frac{1}{10^{-3}+y(t)^2}$

$y(0) = 10; z(0) = 0$

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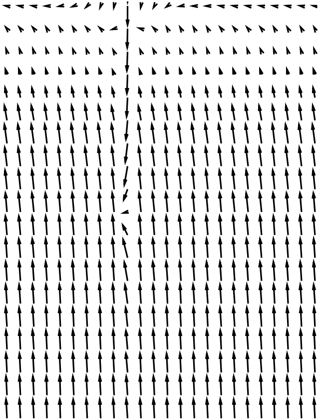

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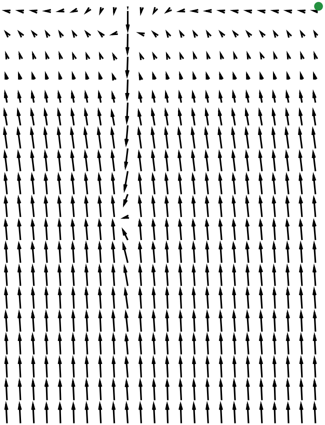

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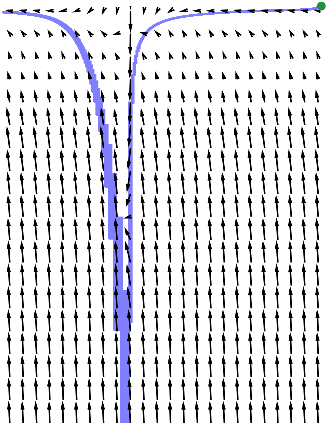

Content

Problems

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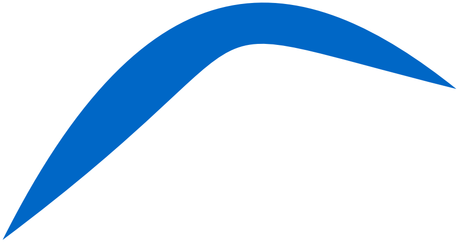

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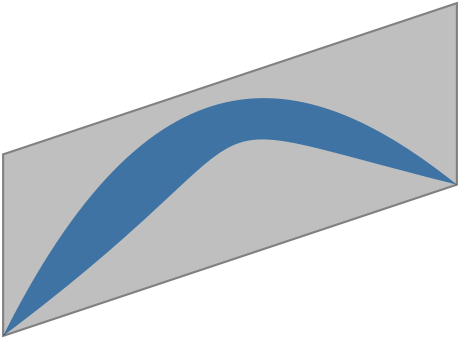

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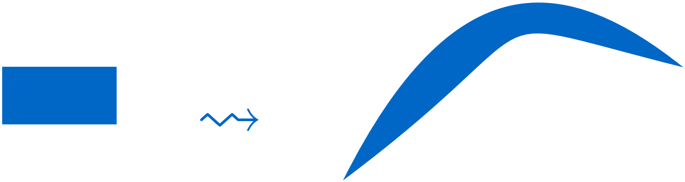

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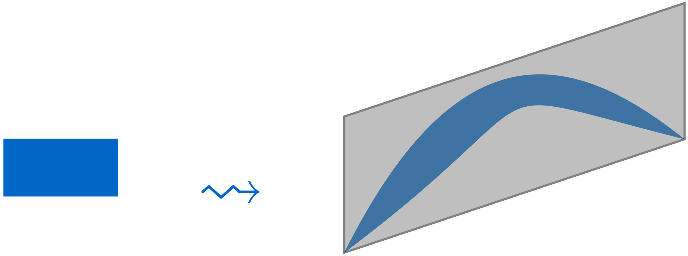

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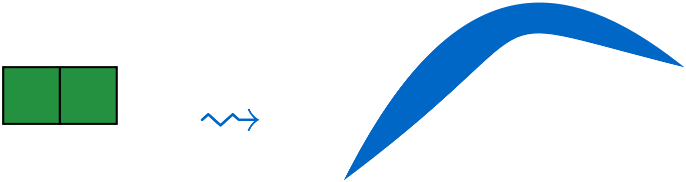

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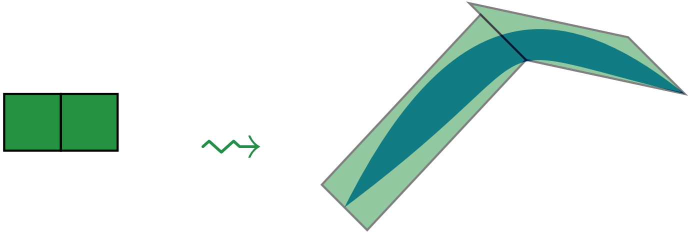

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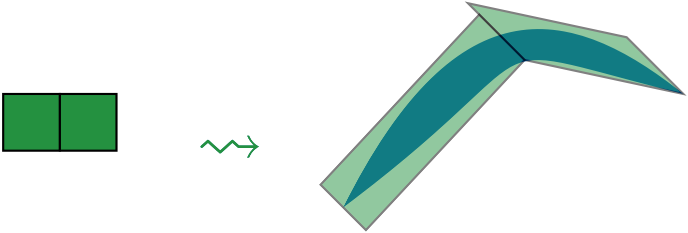
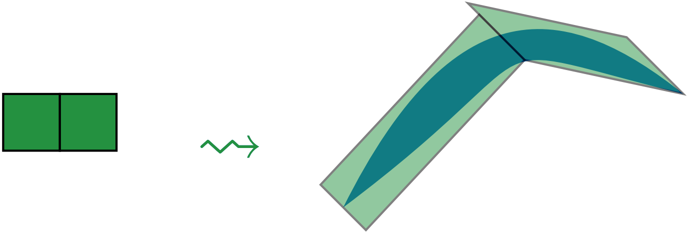


Heuristics

- split largest generator of affine form

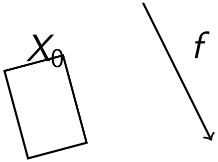
Splitting



Heuristics

- split largest generator of affine form
- split when diameter exceeds threshold

Reduction



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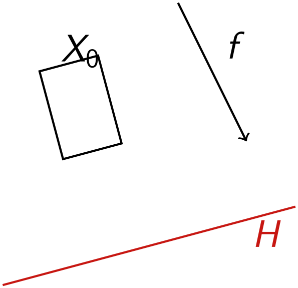

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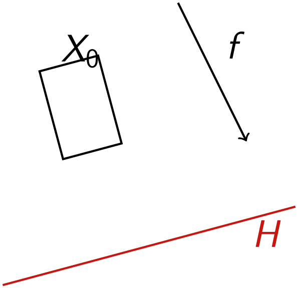

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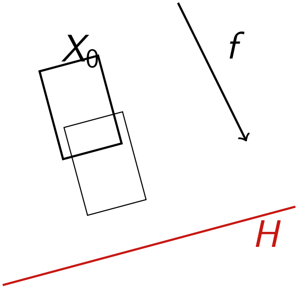

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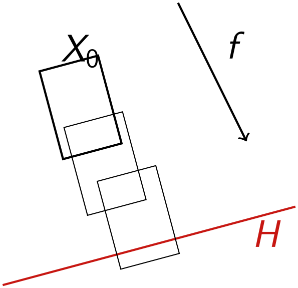

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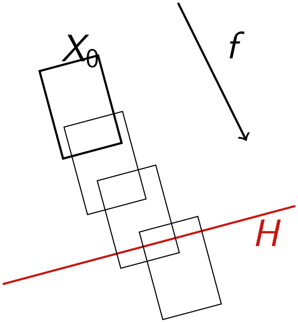

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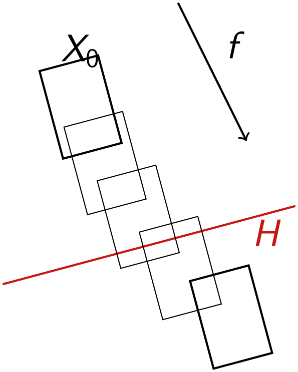

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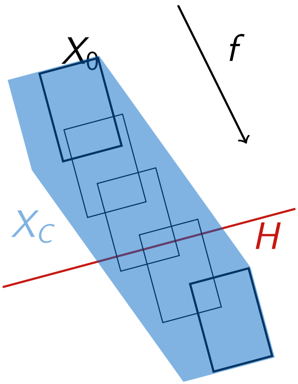

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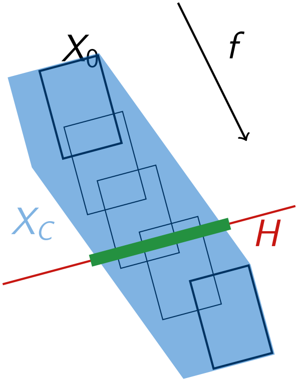

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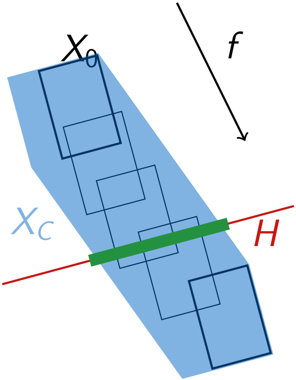
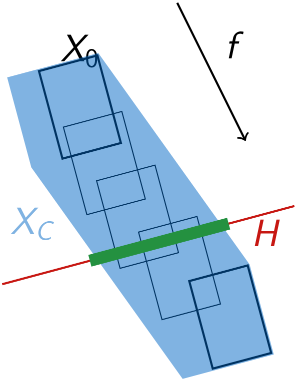


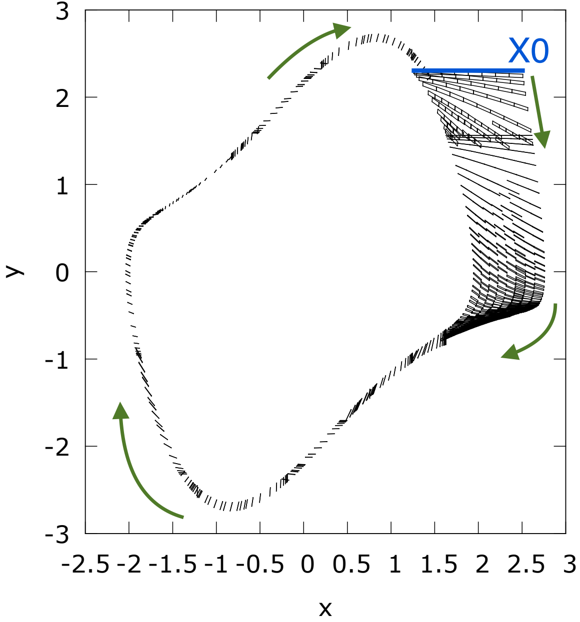
- $X_C \cap H$ can be smaller

Reduction

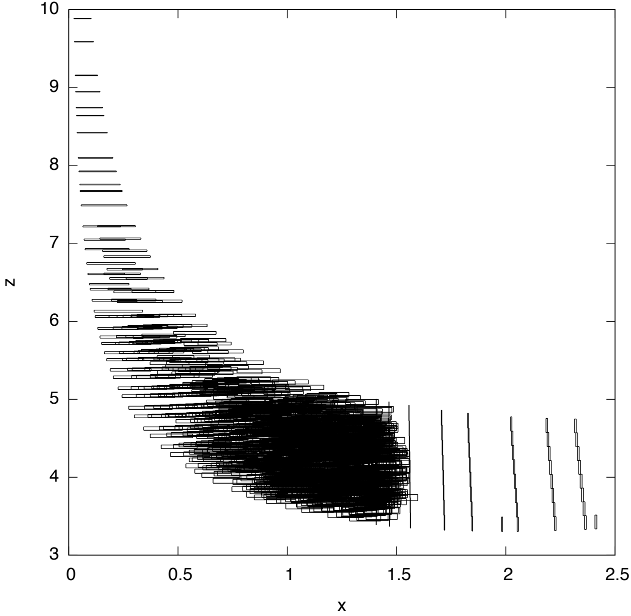


- $X_C \cap H$ can be smaller
- geometric zonotope/hyperplane intersection

Van-der-Pol Oscillator

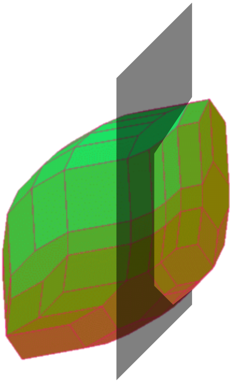


Lorenz attractor (reduction)



Verification of Geometric Algorithms

$\Bigg($



[Boldo, MAP 2016]

Enclosures in Affine Arithmetic

Zonotope

$$\gamma\langle a_0, \ldots, a_k\rangle = \left\{ a_0 + \sum_{i=1}^{k} \varepsilon_i \cdot a_i \middle| \varepsilon_i \in [-1; 1], a_i \in \mathbb{R}^n \right\}$$

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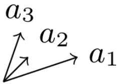

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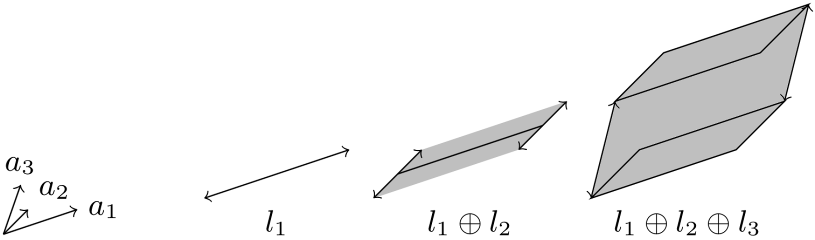

Zonotope ∩ Hyperplane

- approximate geometric algorithm [Girard/Le Guernic 2008]
- "proof" not at all formal!
- but similar to convex hull [Knuth: Axioms and Hulls, 1992]

Girard and le Guernic's Algorithm

- reduction to two-dimensional problem

Proposition 1. *Let G be a hyperplane, $G = \{x \in \mathbb{R}^d : x \cdot n = \gamma\}$, Z a set, and ℓ a vector. Let $\Pi_{n,\ell}$ be the following linear transformation:*

$$\begin{aligned} \Pi_{n,\ell} : \mathbb{R}^d &\to \mathbb{R}^2 \\ x &\mapsto (x \cdot n, x \cdot \ell) \end{aligned}$$

Then, we have the following equality

$$\{x \cdot \ell : x \in Z \cap G\} = \{y : (\gamma, y) \in \Pi_{n,\ell}(Z)\}$$

Proof. Let y belongs to $\{x \cdot \ell : x \in Z \cap G\}$, then there exists x in $Z \cap G$ such that $x \cdot \ell = y$. Since $x \in G$, we have $x \cdot n = \gamma$. Therefore $(\gamma, y) = \Pi_{n,\ell}(x) \in \Pi_{n,\ell}(Z)$ because $x \in Z$. Thus, $y \in \{y : (\gamma, y) \in \Pi_{n,\ell}(Z)\}$. Conversely, if $y \in \{y : (\gamma, y) \in \Pi_{n,\ell}(Z)\}$, then $(\gamma, y) \in \Pi_{n,\ell}(Z)$. It follows that there exists $x \in Z$ such that $x \cdot n = \gamma$ and $x \cdot \ell = y$. Since $x \cdot n = \gamma$, it follows that $x \in G$. Thus, $y = x \cdot \ell$ with $x \in Z \cap G$ and it follows that $y \in \{x \cdot \ell : x \in Z \cap G\}$. ∎

Girard and le Guernic's Algorithm

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lemma inter_proj_eq:
  fixes n g l
  defines "G ≡ {x. x • n = g}"
  shows "(λx. x • l) ` (Z ∩ G) =
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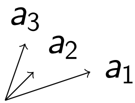

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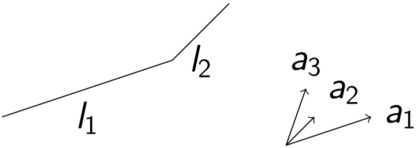

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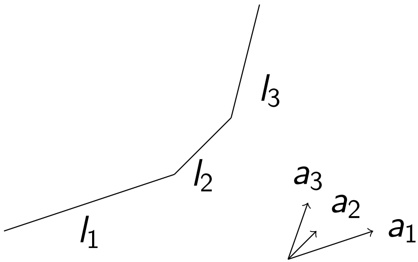

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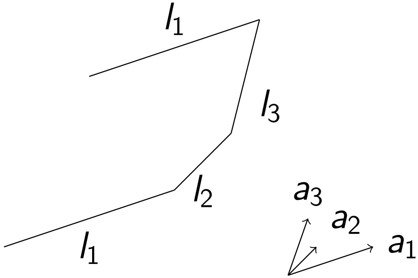

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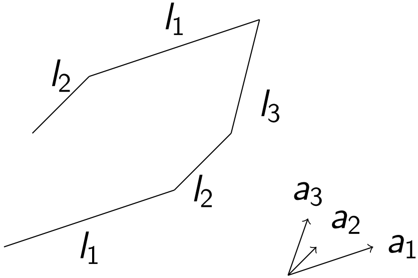

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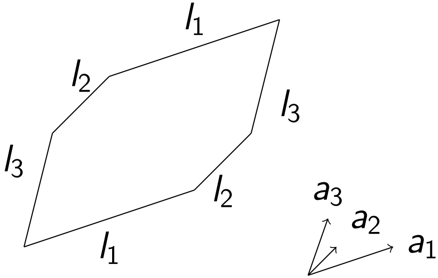

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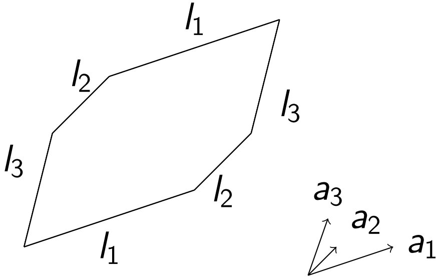

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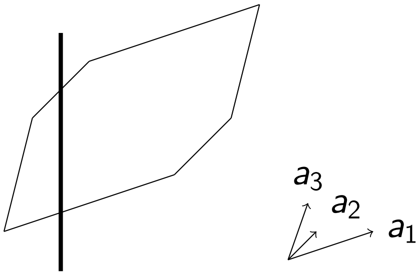

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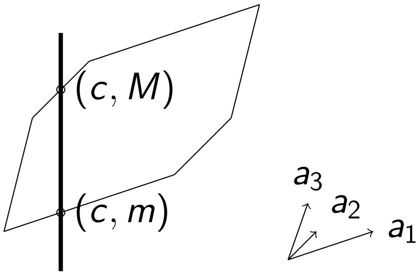

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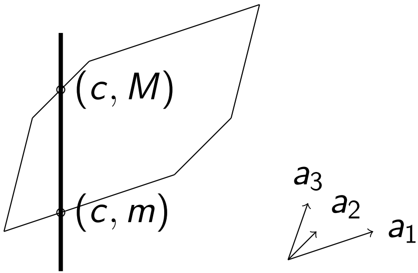

Knuth's Theory of CCW Systems

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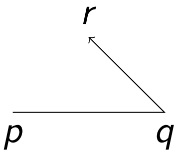
  $pqr \implies qrp$



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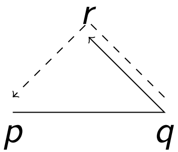

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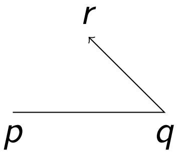

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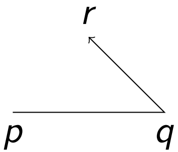
- nondegeneracy: $pqr \vee prq$



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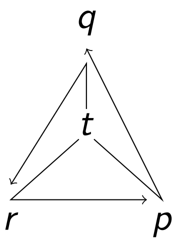

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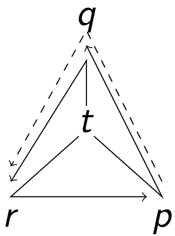

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$$t \longrightarrow s$$

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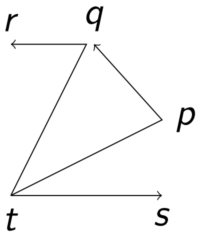

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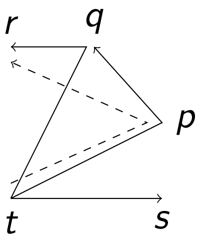

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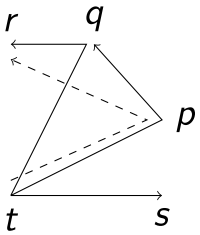

total order in halfplane left of ts

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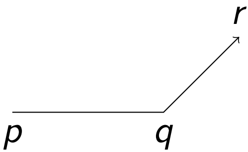
total order in halfplane left of ts
sorted$[p, q, r]$

Extensions for Vector Spaces

- translation:
  $(p + s)(q + s)(r + s) \Leftrightarrow pqr$



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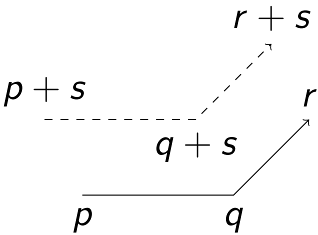

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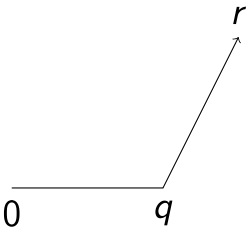

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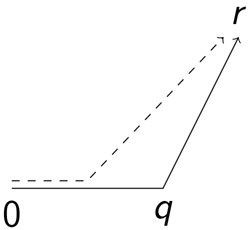

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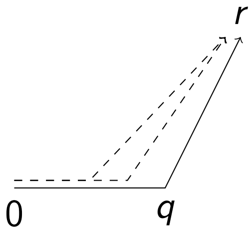

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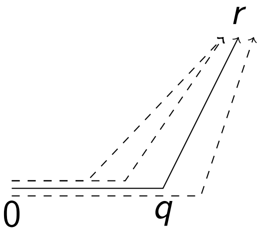

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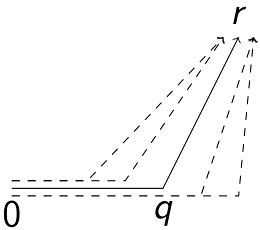

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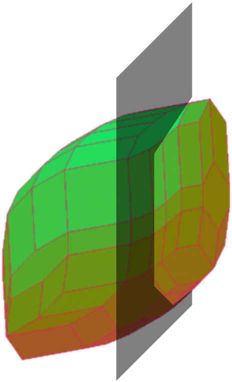
- reflection: $0(-p)q \iff 0qp$
- addition
  $0pq \implies 0pr \implies 0p(q+r)$

Close Parenthesis



)

Content

The Lorenz Attractor

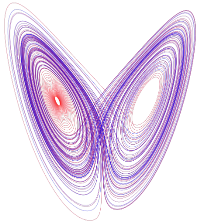
- Lorenz equations (1963)

$$\begin{aligned}\dot{x} &= 10(y - x)\\ \dot{y} &= x(28 - z) - y\\ \dot{z} &= xy - \frac{8}{3}z\end{aligned}$$

Edward N. Lorenz

The Lorenz Attractor

- Lorenz equations (1963)
- numerical simulations



Lorenz attractor

The Lorenz Attractor

- Lorenz equations (1963)
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- conjecture: chaos
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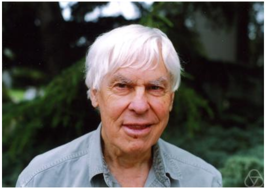

Smale's 14th problem

The Lorenz Attractor

- Lorenz equations (1963)
- numerical simulations
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Warwick Tucker

The Lorenz Attractor

- Lorenz equations (1963)
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- conjecture: chaos (strange attractor)
- proof: Tucker (1999), relying on C++-program
- correctness of program?

Sketch of Tucker's Proof

1. attracting set (numerically enclose ODE)

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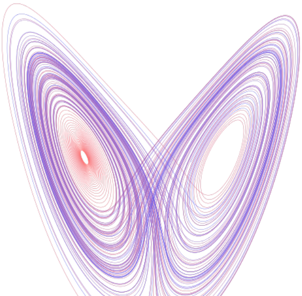
Contribution

part 1. using *verified* ODE solver

return map

- 3D continuous dynamics



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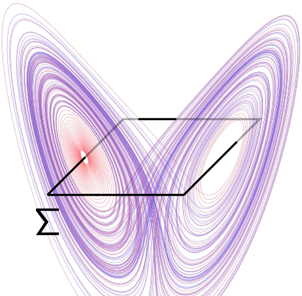

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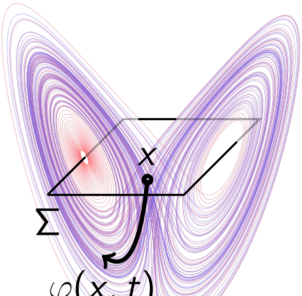

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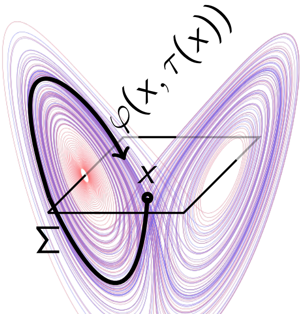

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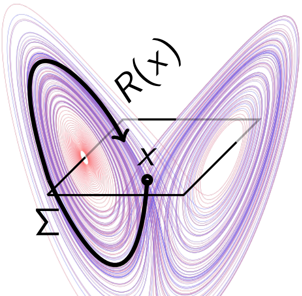

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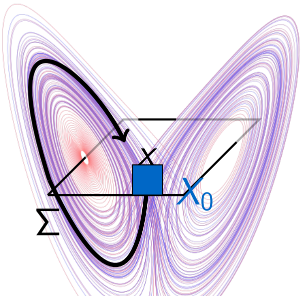

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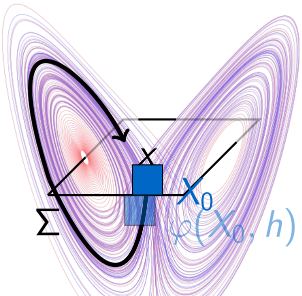

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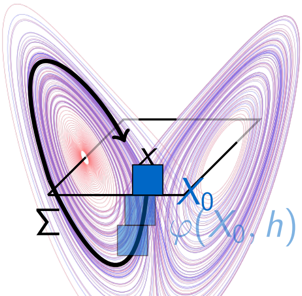

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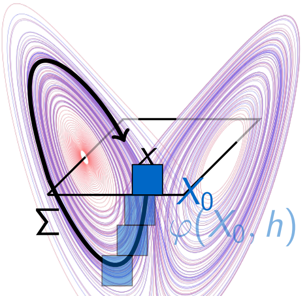

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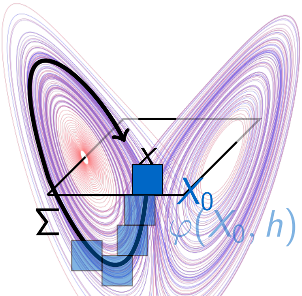

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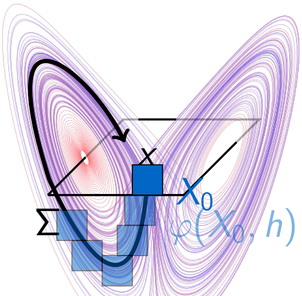

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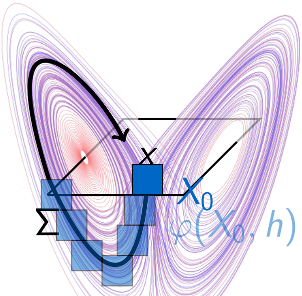

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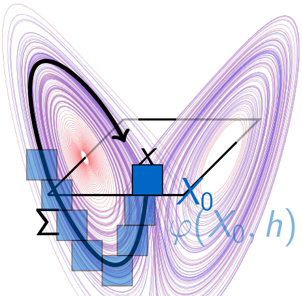

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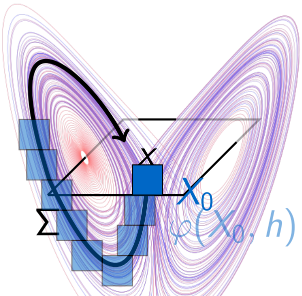

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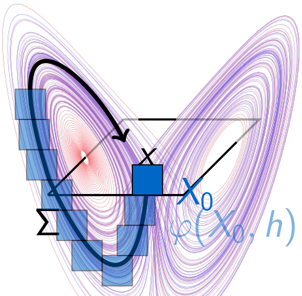

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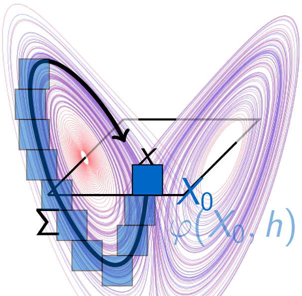

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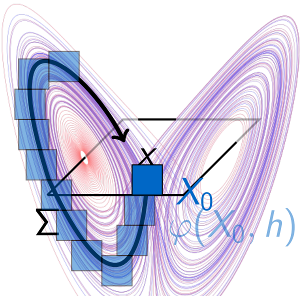

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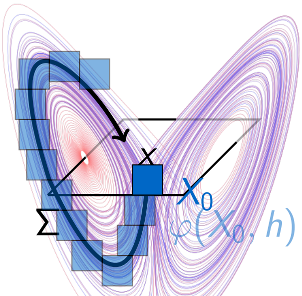

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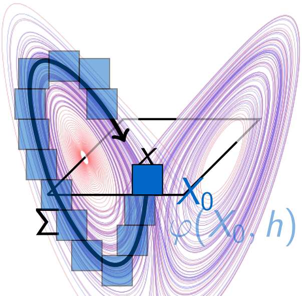

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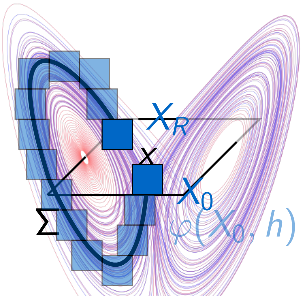

Certify attracting set N

Goal

- given N
- show: $R(N) \subseteq N$

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Parallelization

Certify attracting set N

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Parallelization

- subdivision: $N = \bigcup_{i=0}^{14000} N_i$

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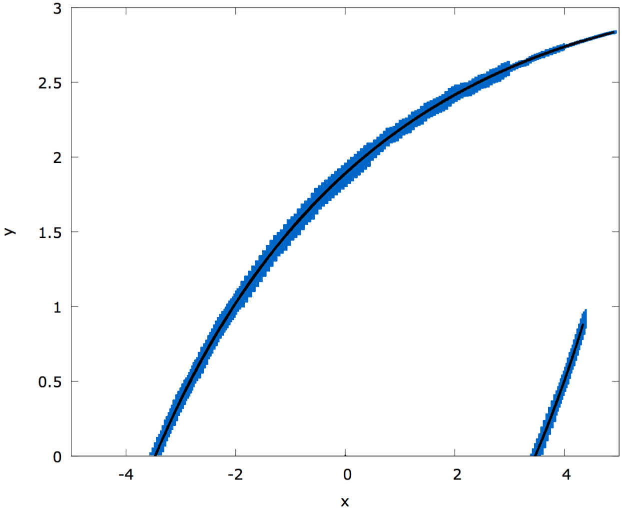
Result

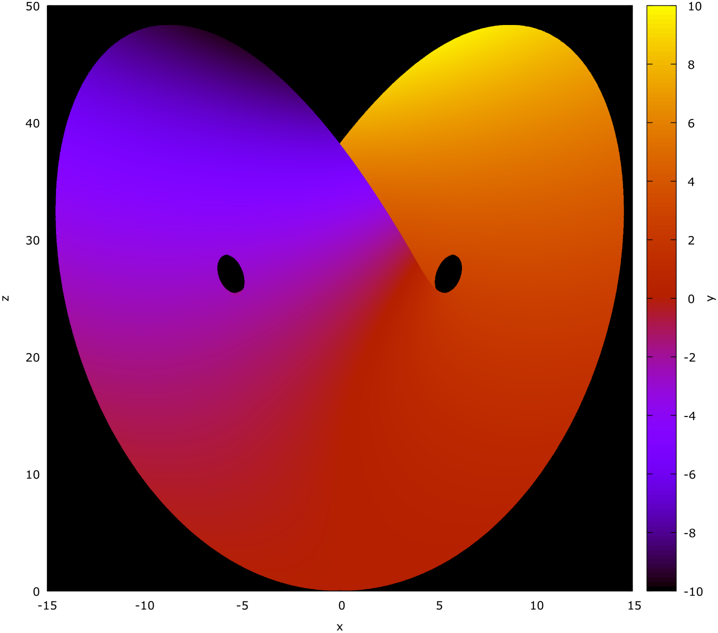
verified a sufficiently precise N

Bound on N

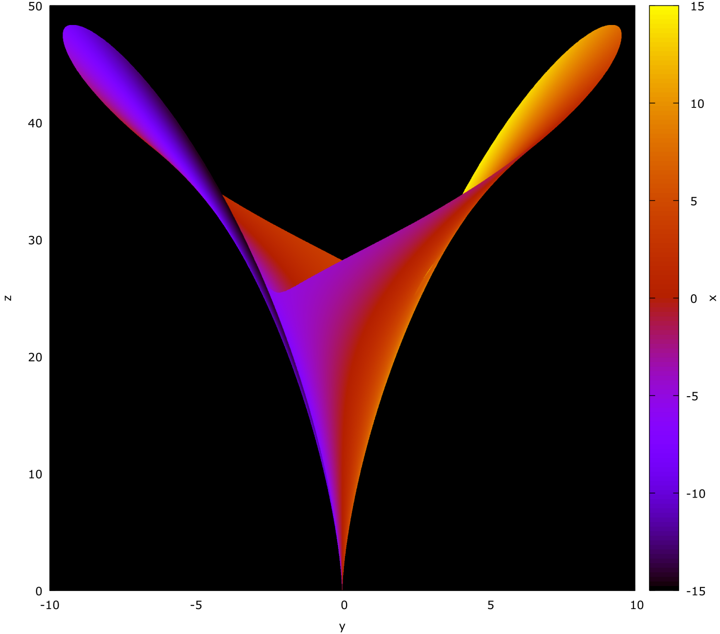


- blue: N_{Tucker}, black: $N_{Isabelle}$

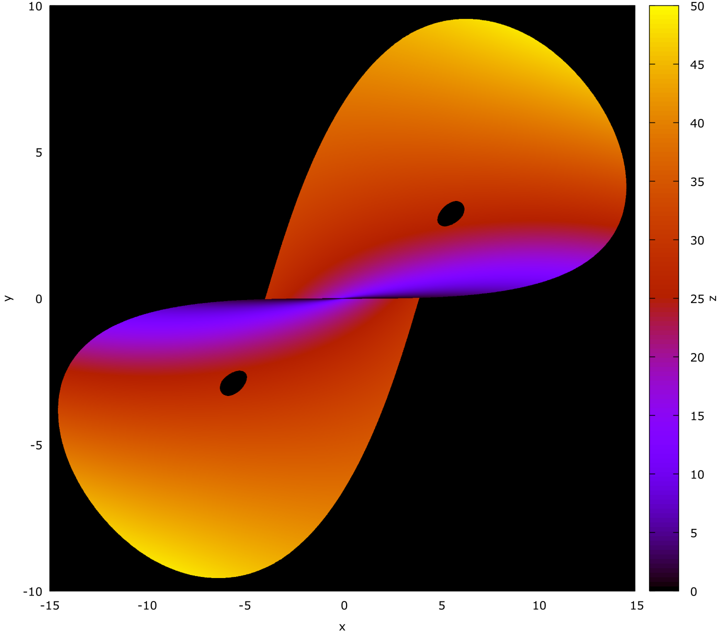
Lorenz Attractor (Front)



Lorenz Attractor (Left)



Lorenz Attractor (Bottom)



Conclusion

verification is feasible and useful:

- verified computation as part of proof

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- verified computation as part of proof
- novel combination of affine arithmetic/Runge-Kutta methods/reduction

Verified Numerics for ODEs in Isabelle/HOL

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