Planar chemical reaction systems with algebraic and non-algebraic limit cycles

Gheorghe Craciun
University of Wisconsin-Madison

Radek Erban
University of Oxford

Chemical reaction networks and polynomial dynamical systems: mass action kinetics

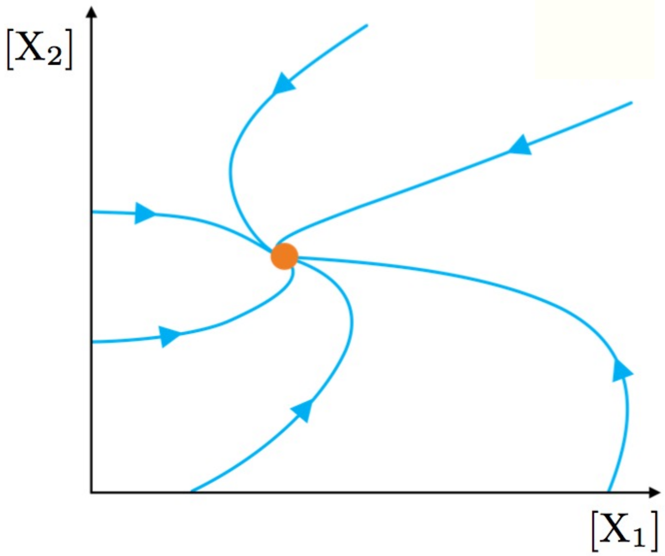
$$\varnothing \xrightarrow{k_1} X_1 \xrightarrow{k_2} X_1 + X_2 \xrightarrow{k_3} \varnothing$$

Chemical reaction networks and polynomial dynamical systems: mass action kinetics

$$\varnothing \xrightarrow{k_1} X_1 \xrightarrow{k_2} X_1 + X_2 \xrightarrow{k_3} \varnothing$$

$$\begin{aligned} \frac{dx_1}{dt} &= k_1 - k_3 x_1 x_2 \\ \frac{dx_2}{dt} &= k_2 x_1 - k_3 x_1 x_2 \end{aligned}$$

Chemical reaction networks and polynomial dynamical systems



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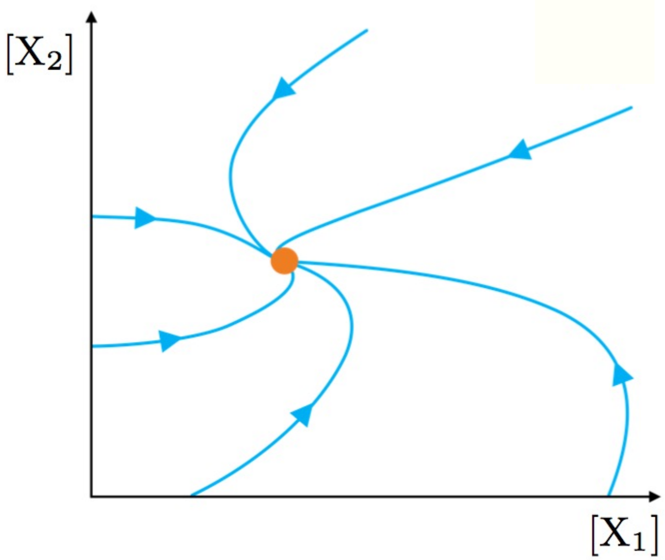

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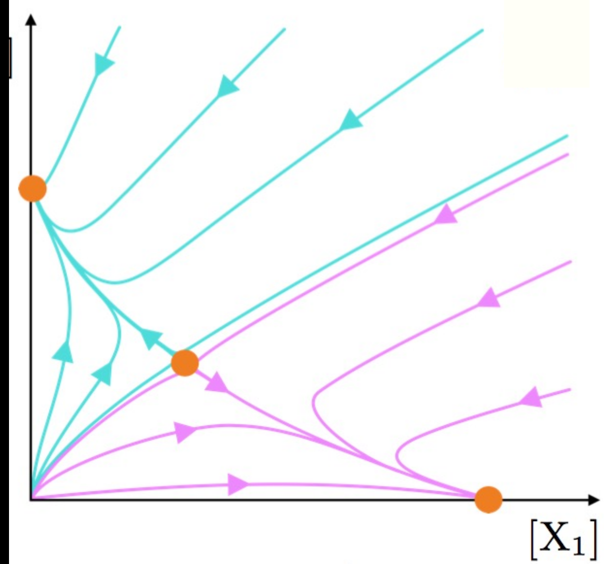

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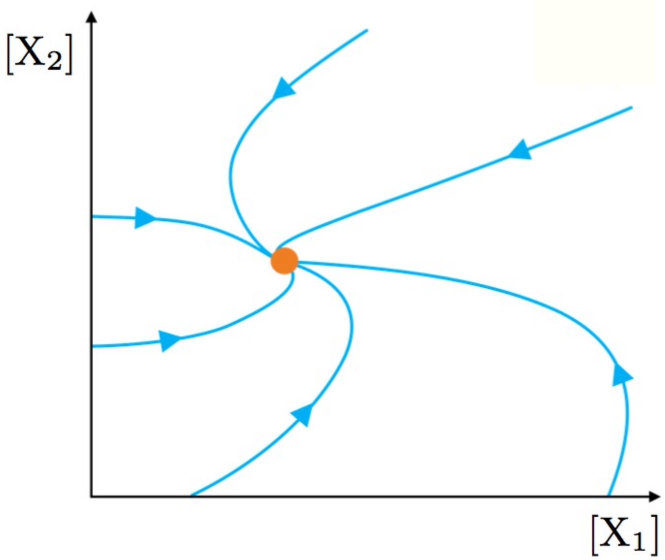

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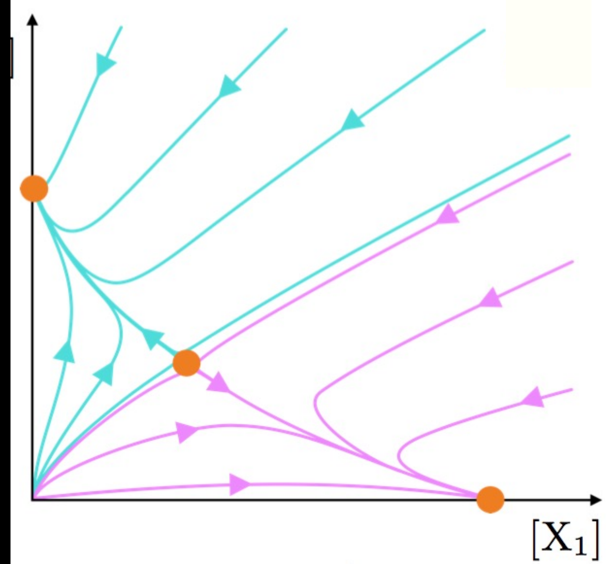

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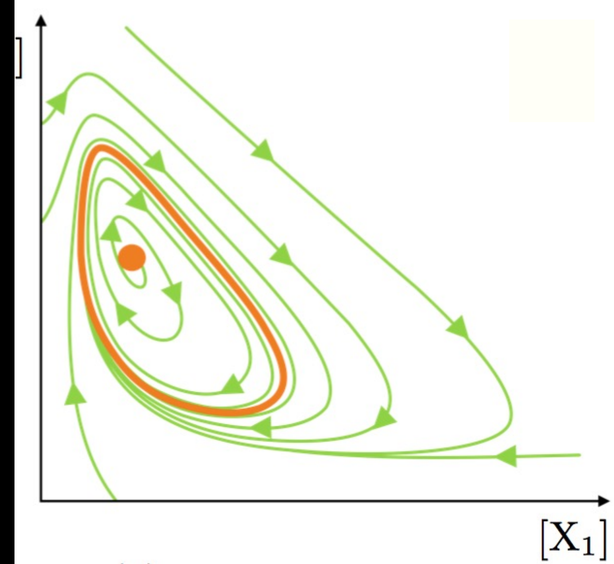

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Polly Yu, G. Craciun, Mathematical analysis of chemical reaction systems, Isr. J. Chem. 2018.

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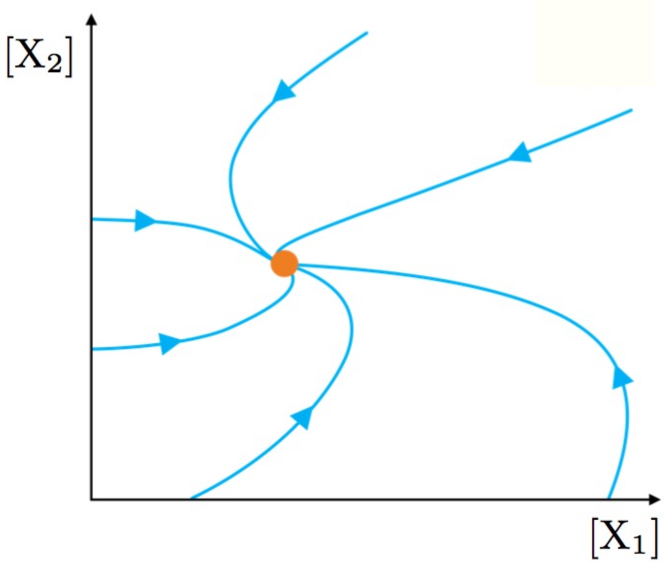

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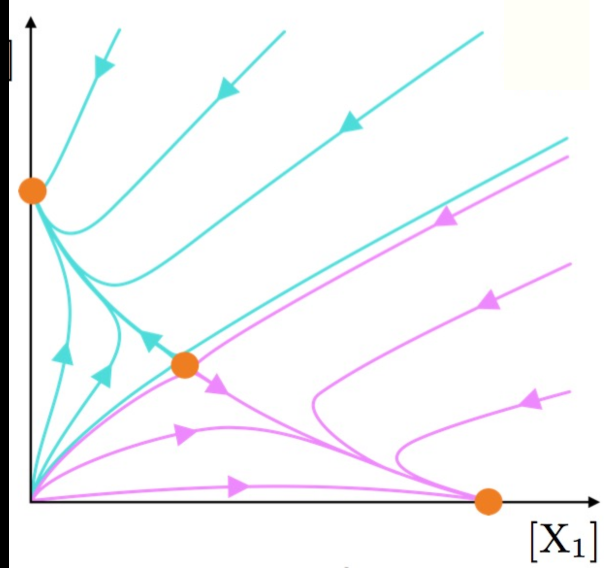

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$$\frac{dx_1}{dt} = -k_1 x_1 x_2 + k_2 x_1 - k_3 x_1^2$$

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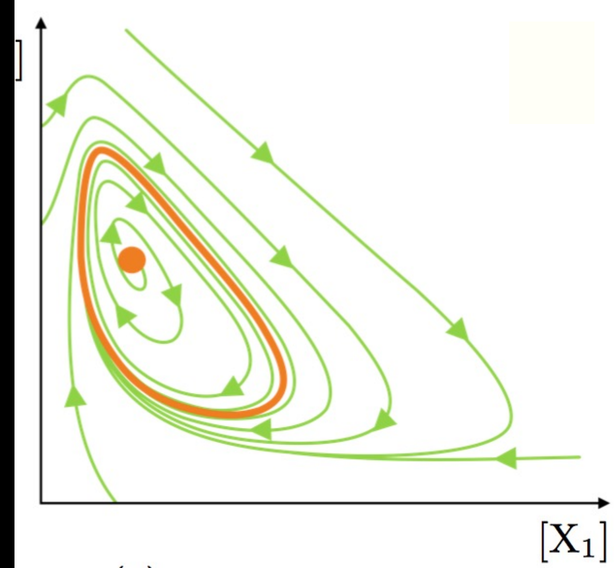

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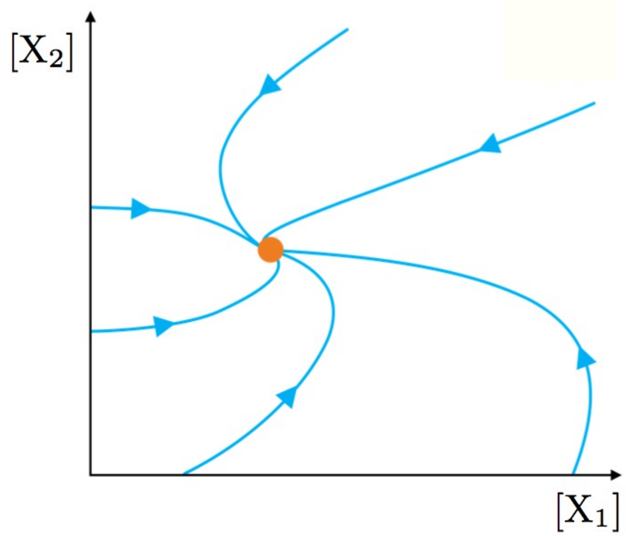
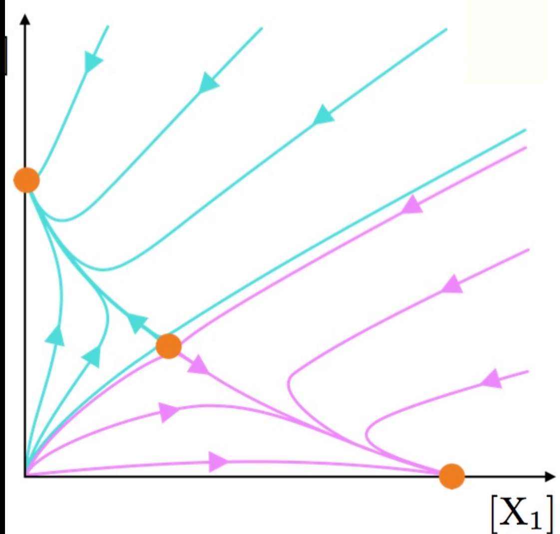
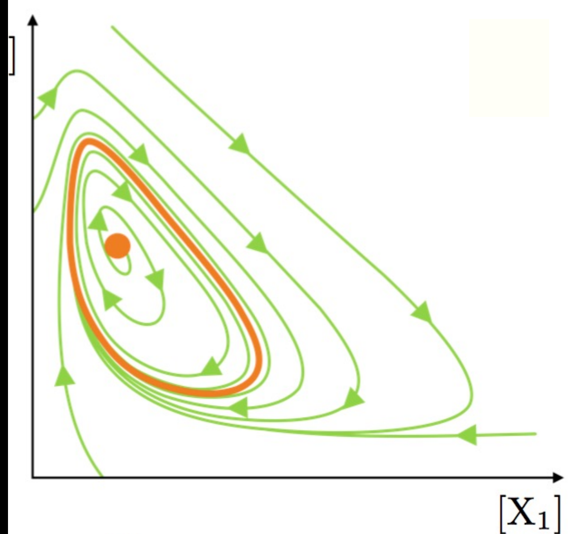
$$\frac{dx_2}{dt} = k_7 - k_8 x_2 + k_3 x_1 - k_4 x_2 - k_5 x_1^2 x_2 + k_6 x_1^3$$

Chemical reaction networks and polynomial dynamical systems







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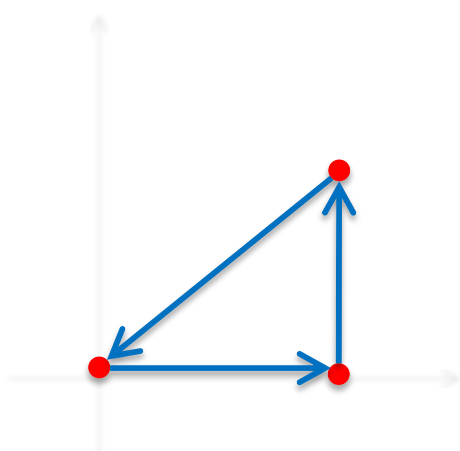

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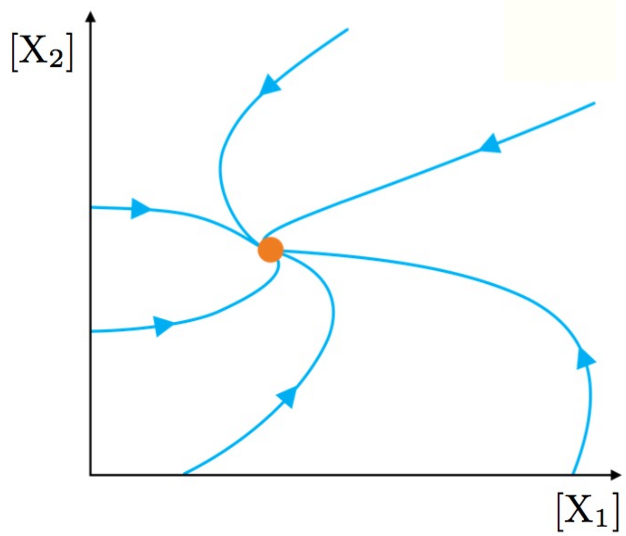

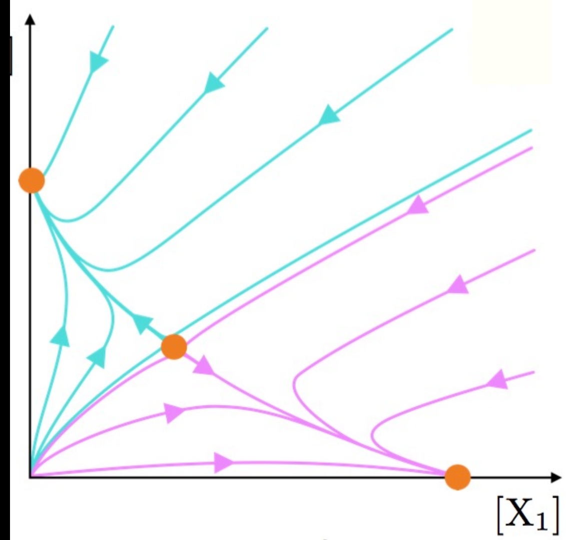

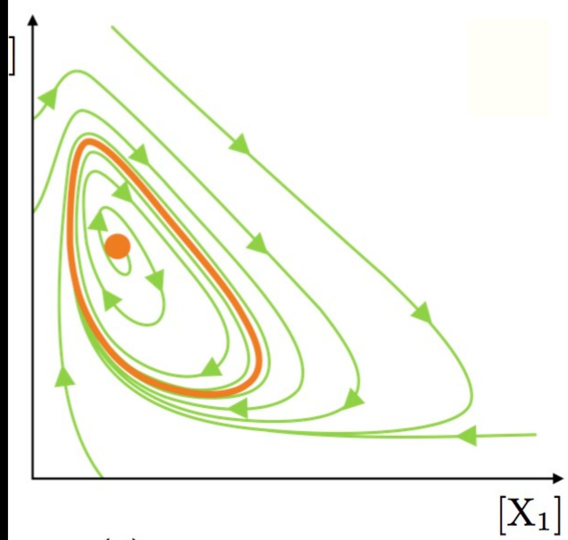

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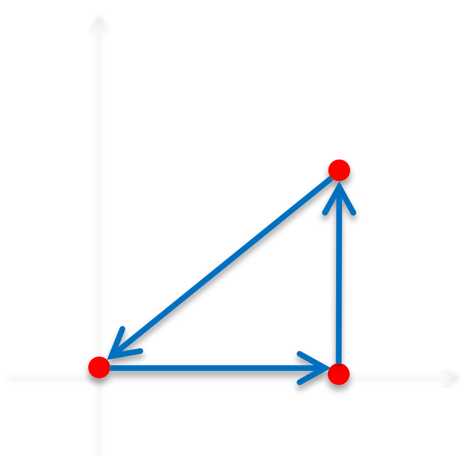

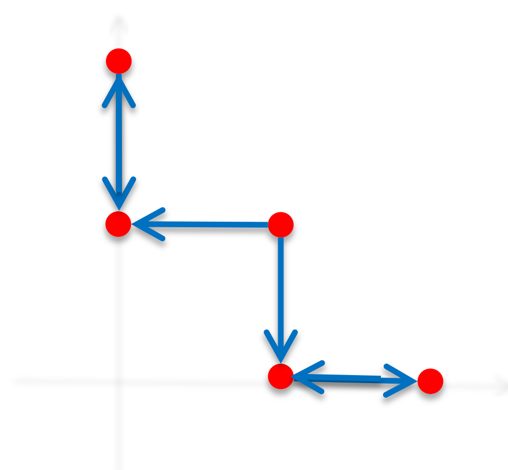

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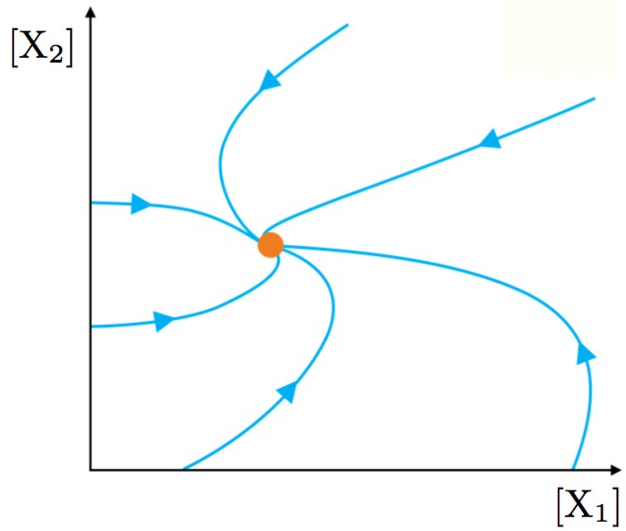

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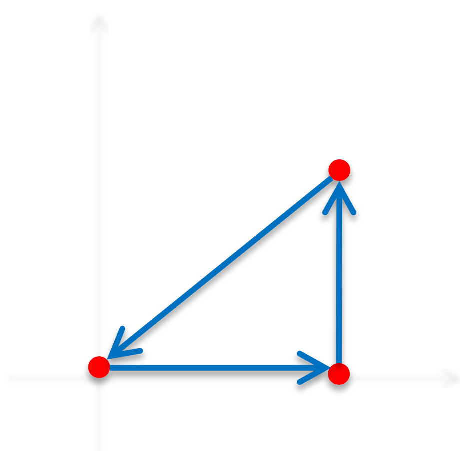

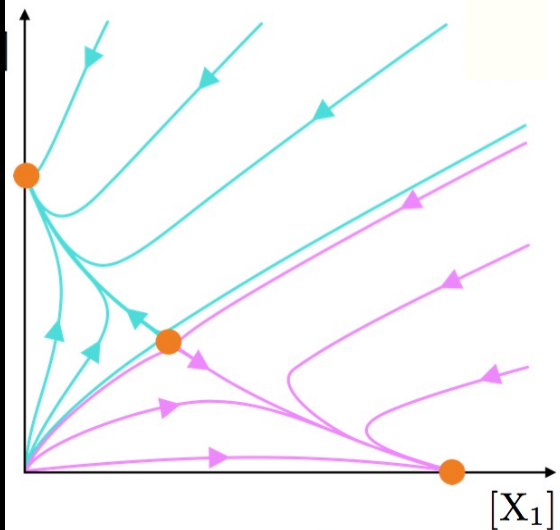

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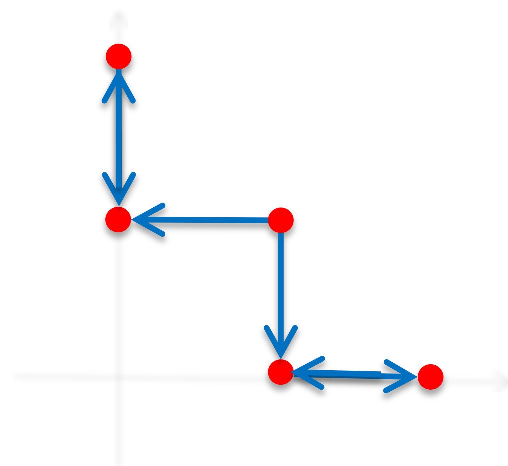

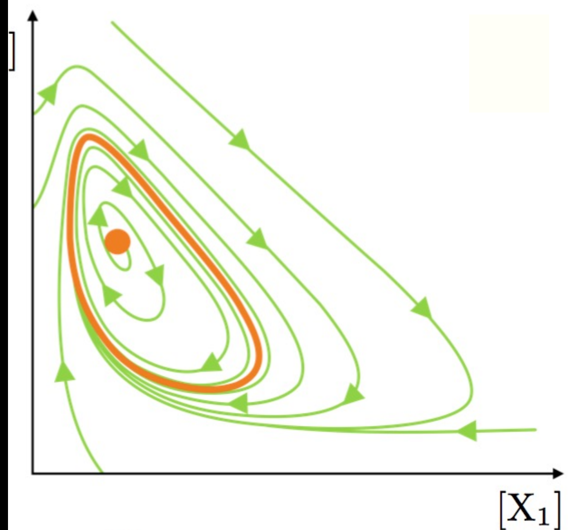

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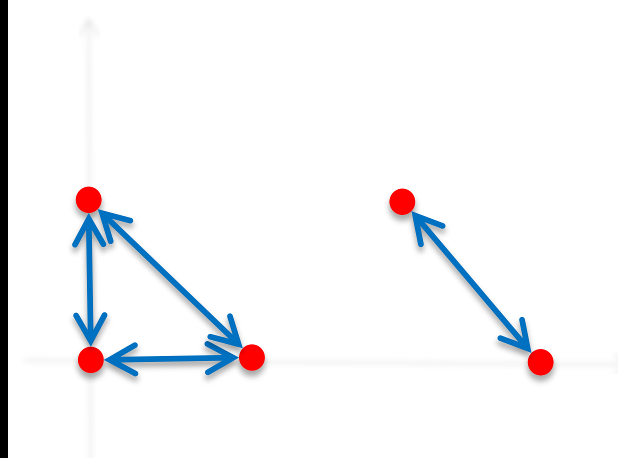

Reaction networks and polynomial dynamical systems

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Remark. *Any dynamics that can be obtained using polynomial dynamical systems on the positive orthant can also be obtained using mass-action systems.*

In particular: *if one could solve Hilbert's 16th problem for mass-action systems, then this would solve the problem in general.*

Polynomial dynamical systems in 2D: Hilbert's 16^{th} problem

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Hilbert's 16th problem: What can be said about the number and location of limit cycles (isolated closed orbits) of a planar polynomial vector field with components of degree n?

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$$\frac{\mathrm{d}x}{\mathrm{d}t} = f(x,\ y), \qquad \frac{\mathrm{d}y}{\mathrm{d}t} = g(x,\ y)$$

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$$\frac{\mathrm{d}x}{\mathrm{d}t} = f(x,\ y), \qquad \frac{\mathrm{d}y}{\mathrm{d}t} = g(x,\ y)$$

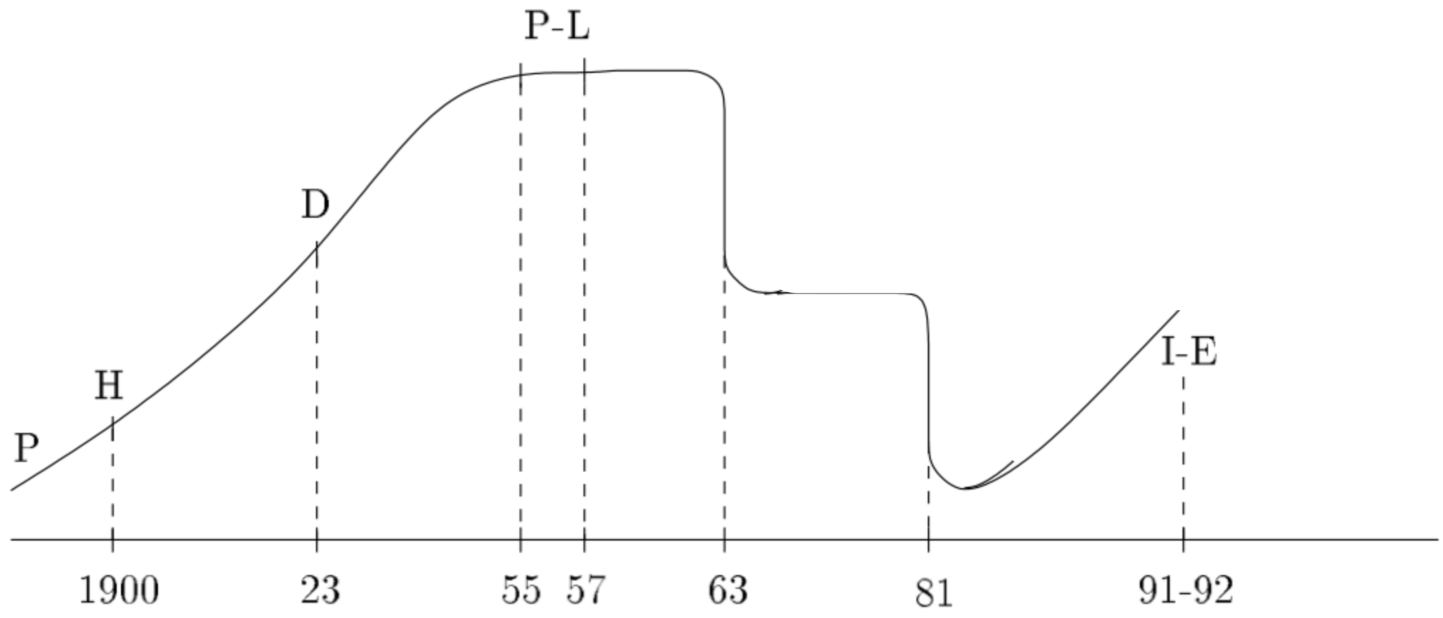
Problem 1. *Is it true that a planar polynomial vector field has but a finite number of limit cycles?*

Problem 2. *Is it true that the number of limit cycles of a planar polynomial vector field is bounded by a constant depending on the degree of the polynomials only?*

The bound on the number of limit cycles in Problem 2 is denoted by $H(n)$ and known as the *Hilbert number*. Linear vector fields have no limit cycles; hence $H(1) = 0$. It is still unknown whether or not $H(2)$ exists.

Yulij Ilyashenko, Centennial history of Hilbert's 16th problem, Bull. AMS ***2002****.*

A short history of Hilbert's 16th problem



P—Poincaré; H—Hilbert, D—Dulac, P-L—Petrovskii-Landis, E—Ecalle, I—Ilyashenko;

Yulij Ilyashenko, Centennial history of Hilbert's 16th problem, Bull. AMS ***2002****.*

Reaction networks and limit cycles: some recent work

Erban, R., Kang, H.: Chemical systems with limit cycles. Bulletin of Mathematical Biology **85**, 76 (2023)

Boros, B., Craciun, G., Yu, P.: Weakly reversible mass-action systems with infinitely many positive steady states. SIAM Journal on Applied Mathematics **80**(4), 1936–1946 (2020)

Banaji, M., Boros, B., Hofbauer, J.: Oscillations in three-reaction quadratic mass-action systems. Studies in Applied Mathematics **152**(1), 249–278 (2024)

Boros, B., Hofbauer, J.: Limit cycles in mass-conserving deficiency-one mass-action systems. Electronic Journal of Qualitative Theory of Differential Equations **2022**(42), 1–18 (2022)

Boros, B., Hofbauer, J.: Some minimal bimolecular mass-action systems with limit cycles. Nonlinear Analysis: Real World Applications **72**, 103839 (2023)

Boros, B., Hofbauer, J.: Oscillations in planar deficiency-one mass-action systems. Journal of Dynamics and Differential Equations **36**(Suppl 1), 175–197 (2024)

Reaction networks and limit cycles

Degree	*Weakly reversible*	*Source and target*	*Mass action*	*Fully general (not mass action)*
n	$W(n)$	$M(n)$	$S(n)$	$H(n)$
2	$= 0$	$= 0$	≥ 3	≥ 4
3	≥ 3	≥ 3	≥ 6	≥ 13
4	≥ 6	≥ 6	≥ 13	≥ 28
as $n \to \infty$	$\geq \mathcal{O}(n)$	$\geq \mathcal{O}(n^2 log(n))$	$\geq \mathcal{O}(n^2 log(n))$	$\geq \mathcal{O}(n^2 log(n))$

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Reaction networks and algebraic limit cycles

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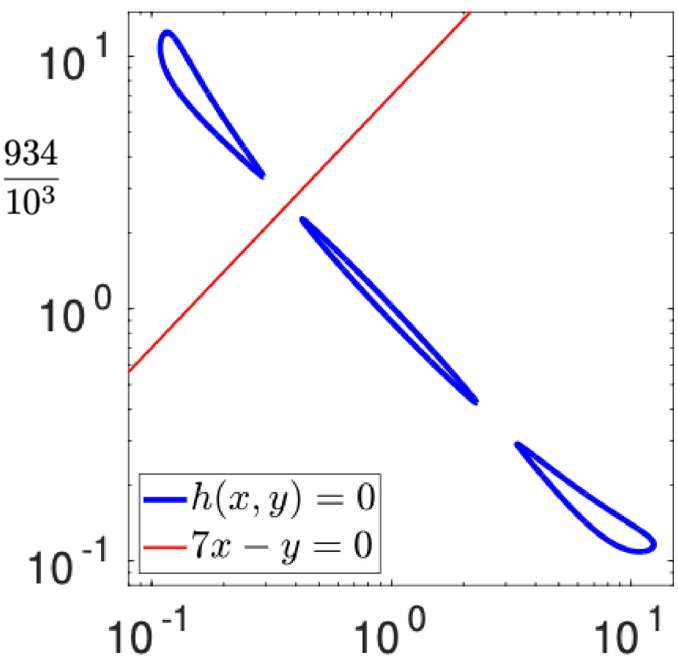
$$h(x,y) = x^2y^2 - \frac{9}{10^3}\left(x^3y + xy^3\right) + \frac{6}{10^4}\left(x^3 + y^3\right) + \frac{2}{50}\left(x^2y + xy^2\right) - 2xy + \frac{934}{10^3}$$

$$\frac{dx}{dt} = h(x,y) + (y - 7x)\frac{\partial h}{\partial y}(x,y)$$

$$\frac{dy}{dt} = h(x,y) + (7x - y)\frac{\partial h}{\partial x}(x,y)$$



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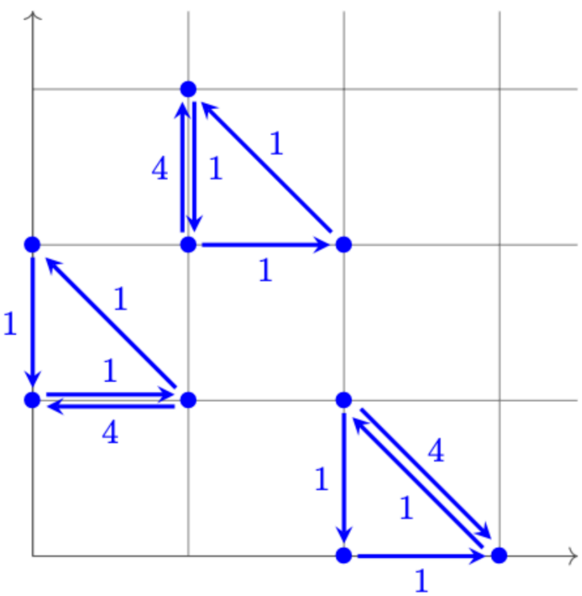

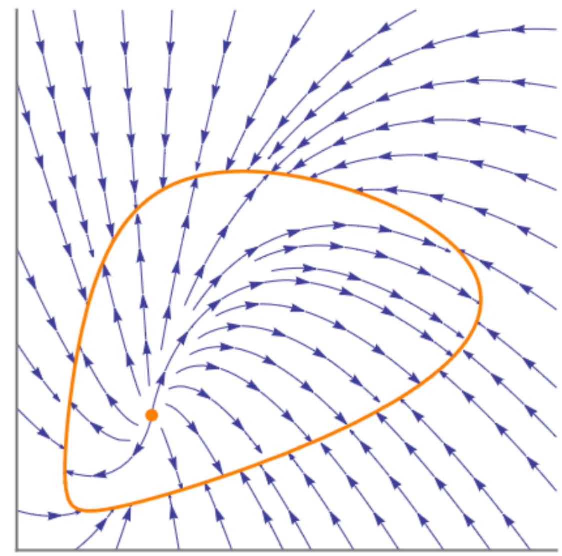

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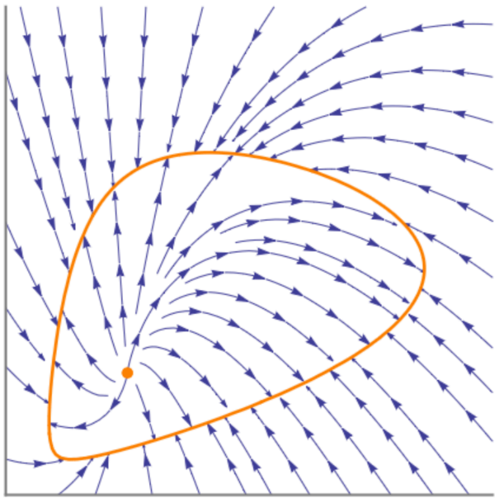

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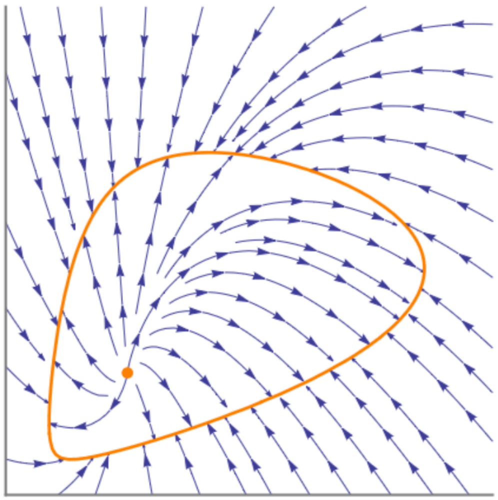

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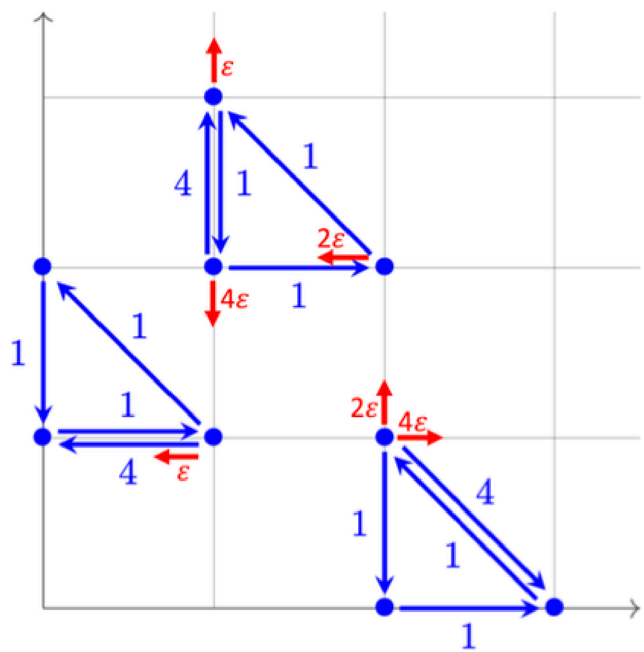

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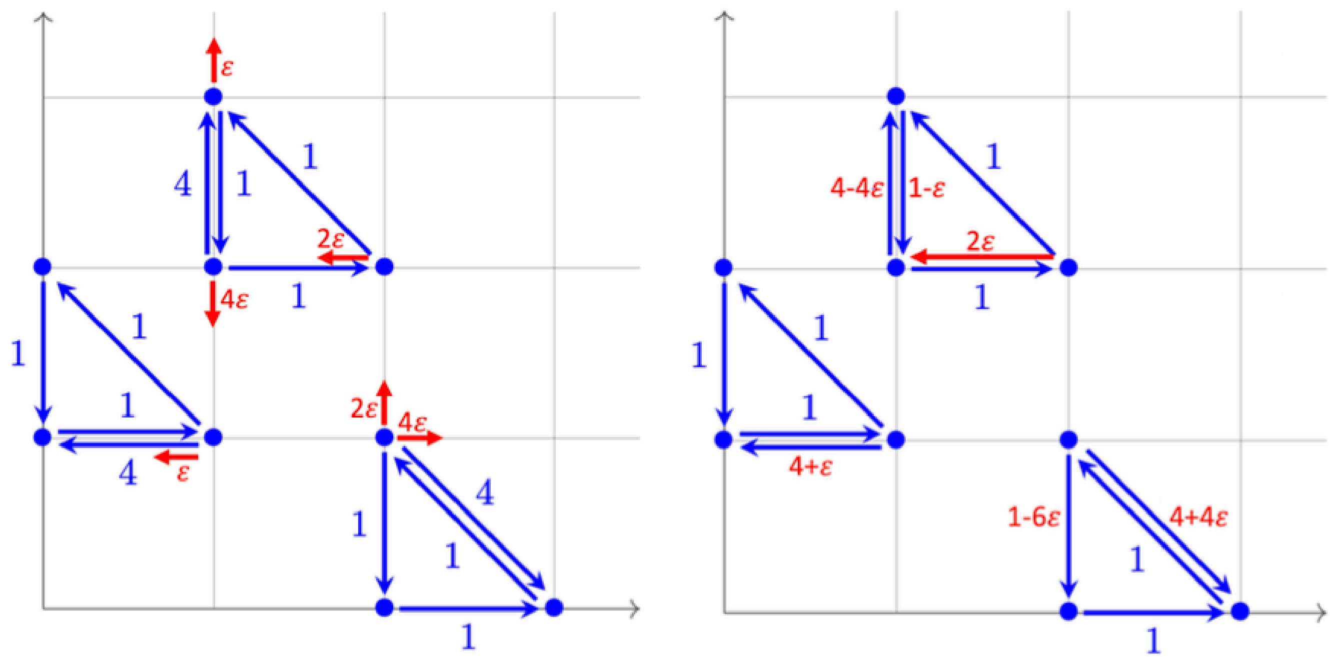

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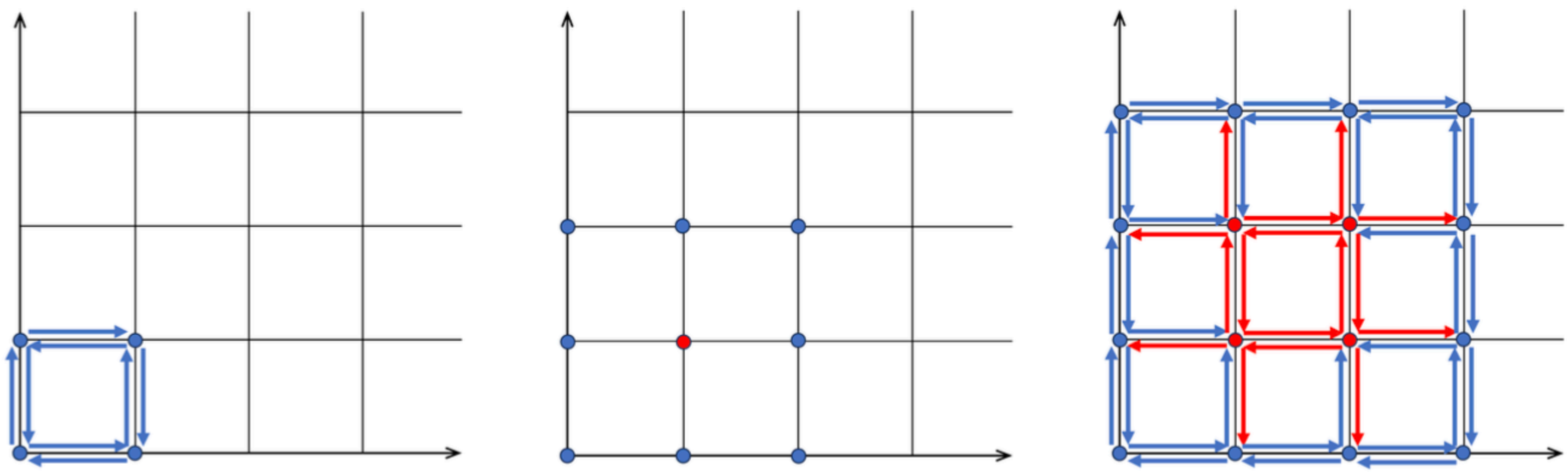

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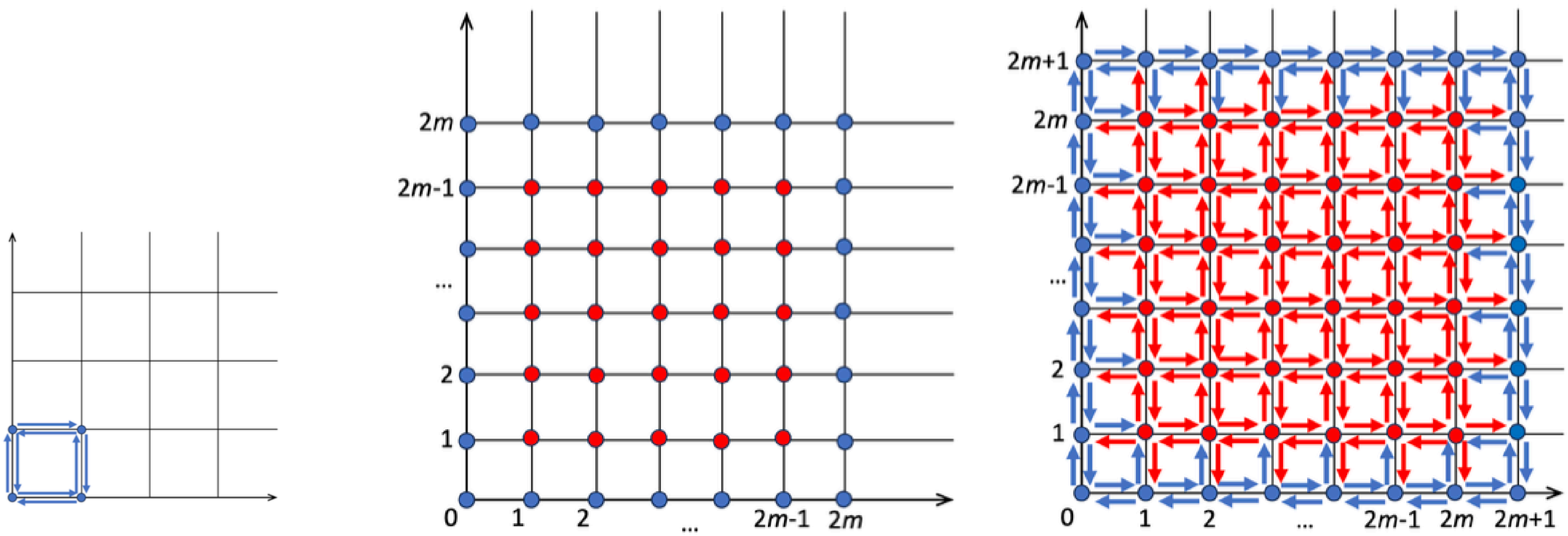

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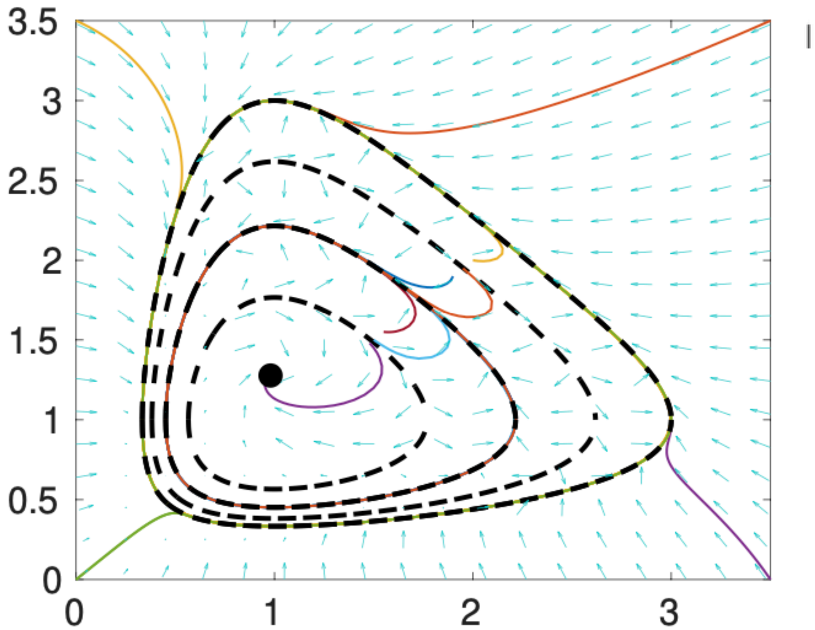

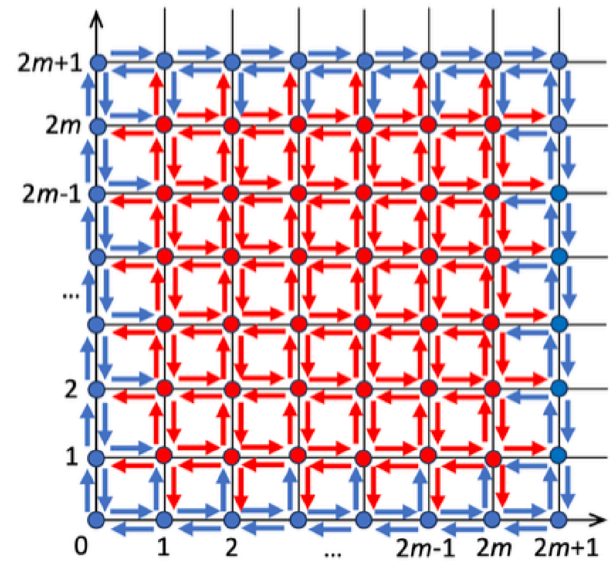

Theorem. *There exists a reversible chemical system of order $4N+2$ that has N algebraic limit cycles for all $N \in \mathbb{N}$. In particular, we have $W^a(4N+2) \geq N$.*

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