Chemical reaction-diffusion systems with boundary equilibria

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Symmetry and Perturbative Theory
Chemical Reaction Networks

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Dynamics of chemical reaction networks

Global Attractor Conjecture: Trajectories of complex balanced CRNs are globally attracted to positive equilibria in each compatibility class.

Many partial results (Craciun, Dickenstein, Shiu, Sturmfels '09; Anderson '11; Angeli, de Leenheer, Sontag '11; Craciun, Nazarov, Pantea '13; Gopalkrishnan, Miller, Shiu '14; Balázs, Hopfbauer '22) and a potential full proof (Craciun '15).

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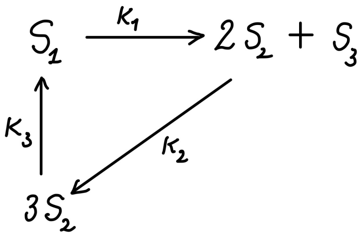
Our goals are to

- study mass action systems in PDE setting
- obtain *quantitative* convergence to equilibrium.

A specific reaction network...

We consider the following reaction network



The corresponding mass-action reaction-diffusion system reads as

$$\begin{cases} \partial_t u_1 - d_1 \Delta u_1 = -k_1 u_1 + k_3 u_2^3 \\ \partial_t u_2 - d_2 \Delta u_2 = 2k_1 u_1 + k_2 u_2^2 u_3 - 3k_3 u_2^3 \\ \partial_t u_3 - d_3 \Delta u_3 = k_1 u_1 - k_2 u_2^2 u_3 \end{cases} \quad \text{s.t.} \quad \begin{cases} \nabla u_i \cdot \nu = 0, & x \in \partial\Omega \\ u_i(x,0) = u_{i,0}(x), & x \in \Omega \end{cases}$$

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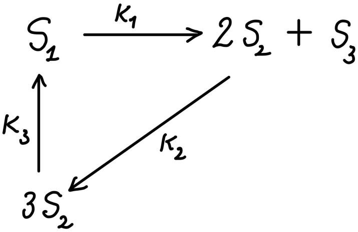

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The system has one conservation law of total mass

$$\int_\Omega (u_1(x,t) + u_2(x,t) + u_3(x,t)) = M := \int_\Omega (u_{1,0}(x) + u_{2,0}(x) + u_{3,0}(x)), \ \forall t > 0.$$

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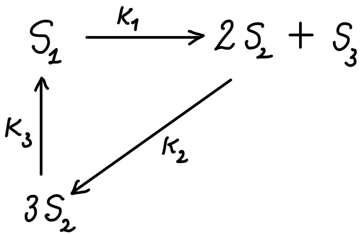

The reaction network is complex balanced.

Lemma

For $M > 0$, there exists a unique positive equilibrium $u_\infty \in (0,\infty)^3$ and one boundary equilibrium $u_* = (0, 0, M)$.

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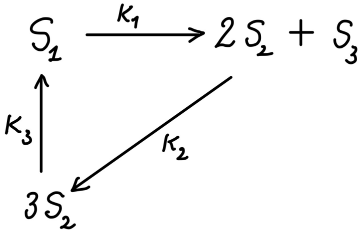

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In the ODE setting: the positive equilibrium u_∞ is globally attracting, see [Anderson '11, Gopalkrishnan & Miller & Shiu '14, Balázs & Hopfbauer '22]. These proofs are essentially *geometrical* and seem difficult to extend to the PDE setting!

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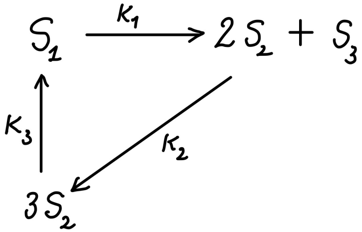

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This talk: We approach this problem by **entropy method**.

Relative entropy & Entropy dissipation

For the *relative entropy*

$$\mathscr{E}(u|u_\infty) = \sum_{i=1}^{3} \int_\Omega \left(u_i \ln \frac{u_i}{u_{i,\infty}} - u_i + u_{i,\infty} \right) dx$$

we know that

$$\frac{d}{dt}\mathscr{E}(u(t)|u_\infty) \le 0, \quad \forall t \ge 0.$$

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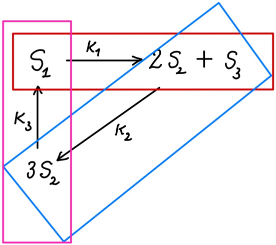
Moreover, we have the *entropy dissipation*

$$\begin{aligned} \mathscr{D}(u) &= -\frac{d}{dt}\mathscr{E}(u|u_\infty) \\ &= \sum_{i=1}^{3} d_i \int_\Omega \frac{|\nabla u_i|^2}{u_i} dx + \int_\Omega \left[k_1 \Psi\left(\frac{u_1}{u_{1,\infty}}; \frac{u_2^2 u_3}{u_{2,\infty}^2 u_{3,\infty}} \right) \right. \\ &\qquad \left. + k_2 \Psi\left(\frac{u_2^2 u_3}{u_{2,\infty}^2 u_{3,\infty}}; \frac{u_2^3}{u_{2,\infty}^3} \right) + k_3 \Psi\left(\frac{u_2^3}{u_{2,\infty}^3}; \frac{u_1}{u_{1,\infty}} \right) \right] dx \end{aligned}$$

where $\Psi(x; y) = x\ln(x/y) - x + y \ge 0$.

Explicit form of entropy dissipation



Entropy dissipation contains all reactions

$$\mathscr{D}(u) = -\frac{d}{dt}\mathscr{E}(u|u_\infty)$$

$$= \sum_{i=1}^{3} d_i \int_\Omega \frac{|\nabla u_i|^2}{u_i}dx + \int_\Omega \left[k_1 \Psi\left(\frac{u_1}{u_{1,\infty}}; \frac{u_2^2 u_3}{u_{2,\infty}^2 u_{3,\infty}}\right) + k_2 \Psi\left(\frac{u_2^2 u_3}{u_{2,\infty}^2 u_{3,\infty}}; \frac{u_2^3}{u_{2,\infty}^3}\right) + k_3 \Psi\left(\frac{u_2^3}{u_{2,\infty}^3}; \frac{u_1}{u_{1,\infty}}\right)\right] dx$$

Entropy method

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we obtain *exponential convergence to equilibrium* with rate $\lambda/2$

$$\sum_{i=1}^{3} \|u_i(t) - u_{i,\infty}\|^2_{L^1(\Omega)} \leq C_{\mathrm{CKP}}^{-1}\mathscr{E}(u(0)|u_\infty)e^{-\lambda t}.$$

In case of no boundary equilibria, the exponential convergence to equilibrium is well proven! (Desvillettes, Fellner, T. SIAM 2017; Fellner, T. ZAMP 2018)

The problem of boundary equilibria...

In this case, the inequality

$$\boxed{\mathscr{D}(u) \geq \lambda \mathscr{E}(u|u_\infty)}$$

is unfortunately not true as a functional inequality, because $(u_* = (0, 0, M))$

$$\lim_{u \to u_*} \mathscr{D}(u) = 0 \quad \text{but} \quad \liminf_{u \to u_*} \mathscr{E}(u|u_\infty) > 0.$$

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We first estimate $\mathscr{D}(u)$ using $\Psi(x,y) \geq (\sqrt{x} - \sqrt{y})^2$

$$\mathscr{D}(u) \gtrsim \sum_{i=1}^{3} \int_\Omega \frac{|\nabla u_i|^2}{u_i} dx + \int_\Omega \left[\sqrt{\frac{u_1}{u_{1,\infty}}} - \frac{u_2}{u_{2,\infty}}\sqrt{\frac{u_3}{u_{3,\infty}}}\right]^2 dx$$
$$+ \int_\Omega \frac{u_2^2}{u_{2,\infty}^2} \left[\sqrt{\frac{u_3}{u_{3,\infty}}} - \sqrt{\frac{u_2}{u_{2,\infty}}}\right]^2 dx + \int_\Omega \left[\frac{u_2}{u_{2,\infty}}\sqrt{\frac{u_2}{u_{2,\infty}}} - \sqrt{\frac{u_1}{u_{1,\infty}}}\right]^2 dx$$

If u_2 nicely behaves...

$$\mathscr{D}(u) \gtrsim \sum_{i=1}^{3}\int_\Omega \frac{|\nabla u_i|^2}{u_i}dx + \int_\Omega \left[\sqrt{\frac{u_1}{u_{1,\infty}}} - \frac{u_2}{u_{2,\infty}}\sqrt{\frac{u_3}{u_{3,\infty}}}\right]^2 dx$$

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If we have

$$u_2(x,t) \geq c_0 > 0 \quad \forall (x,t)$$

Then

$$\mathscr{D}(u) \gtrsim \min\{c_0^2, 1\}\widehat{\mathscr{D}}(u) \quad \text{with} \quad \widehat{\mathscr{D}}(u) = \text{Diffusion part} + \mathscr{H}(u)$$

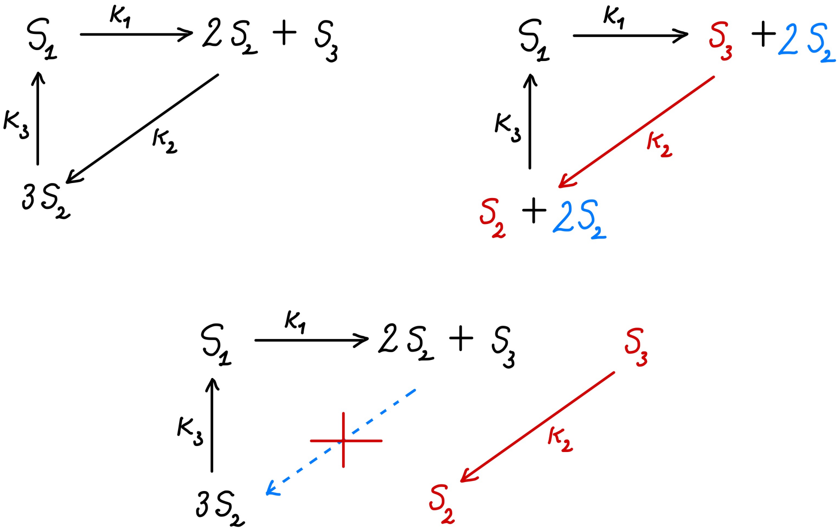
It is important that

$$\widehat{\mathscr{D}}(u) = 0 + \text{conservation laws} \quad \Leftrightarrow \quad u = u_\infty.$$

Then we can prove

$$\widehat{\mathscr{D}}(u) \geq \lambda \mathscr{E}(u|u_\infty).$$

What it means on the network...



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Asking for a lower bound

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$$\partial_t u_2 - d_2 \Delta u_2 = 2k_1 u_1 + k_2 u_2^2 u_3 - 3k_3 u_2^3 \geq -3k_3 u_2^3$$

which gives

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which gives

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$\rightarrow$ Even if a trajectory would converge to the boundary equilibrium $u_* = (0,0,M)$, it cannot converge faster than $(1+t)^{-1}$.

Competing phenomena - Algebraic decay

Therefore, instead of $\mathscr{D}(u) \gtrsim \mathscr{E}(u|u_\infty)$ we can only prove

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This is nevertheless enough to get an **algebraic decay**

$$\frac{d}{dt}\mathscr{E}(u|u_\infty) \lesssim -\frac{1}{1+t}\mathscr{E}(u|u_\infty) \quad \Rightarrow \quad \mathscr{E}(u(t)|u_\infty) \lesssim \frac{1}{1+t}\mathscr{E}(u(0)|u_\infty)$$

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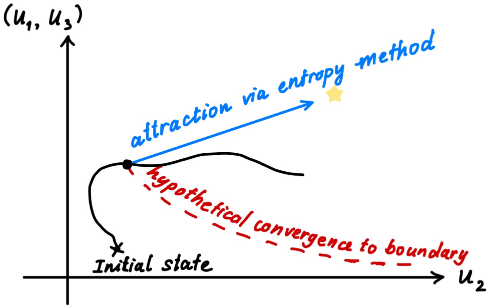

Recovering exponential decay...

From

$$\sum_{i=1}^{3} \|u_i(t) - u_{i,\infty}\|_{L^1(\Omega)}^2 \lesssim \frac{1}{1+t}\mathscr{E}(u(0)|u_\infty),$$

there is an *explicit* time $T_0 > 0$ such that

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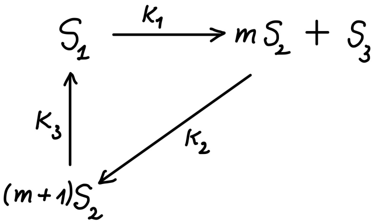
This is enough to show

$$\mathscr{D}(u(t)) \geq \min\{c_1, 1\}\mathscr{E}(u(t)|u_\infty) \quad \forall t \geq T_0$$

and we recover **exponential decay** towards to positive equilibrium.

The result...



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Theorem (Fellner, T. ZAMP 2018)

Assume that $\inf_\Omega u_{2,0}(x) > 0$*, then the solution to the reaction-diffusion system converges exponentially to the positive complex balanced equilibrium with* <u>*explicitly computable*</u> *rates and constants.*

Conditional exponential trend to equilibrium

Theorem (Fellner, T. ZAMP 2018)

Assume that the reaction network is complex balanced and possesses a boundary equilibrium. **Assume moreover** *that*

$$\mathscr{D}(u(t)) \geq \Lambda(t)\mathscr{E}(u(t)|u_\infty) \quad \forall t > 0,$$

where $\Lambda(t)$ *satisfies* $\int_0^\infty \Lambda(t)dt = +\infty$ *then*

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Related works

- Craciun, Jin, Pantea, Tudorascu (2021): $A + nB \leftrightarrows B + C$, $mA + nB \leftrightarrows pA + qB$.
- Jin (2019): $A + 2B \leftrightarrows B + C$, shows the **instability of boundary equilibria**.
- Pierre, Suzuki, Umakoshi (2018): $\alpha_1 S_1 + \ldots \alpha_m S_m \leftrightarrows \beta_1 S_1 + \ldots + \beta_m S_m$.

Conclusion and Future

Conclusion

- Entropy method gives *quantitative* convergence to equilibrium.
- For boundary equilibria, it is enough to control the (possible) decay rate to boundary.

Future

- Extending the ideas in the case of boundary equilibria. We already failed (have not succeeded) to apply it to the network[1]

$$\begin{array}{ccc} S_1 + S_2 & \longrightarrow & 3S_1 \\ \uparrow & & \downarrow \\ 2S_2 & \longleftarrow & 2S_1 + S_3 \end{array}$$

- Geometric techniques from the ODE setting?

[1] D. Anderson. SIAM J. Appl. Math. (2011)

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