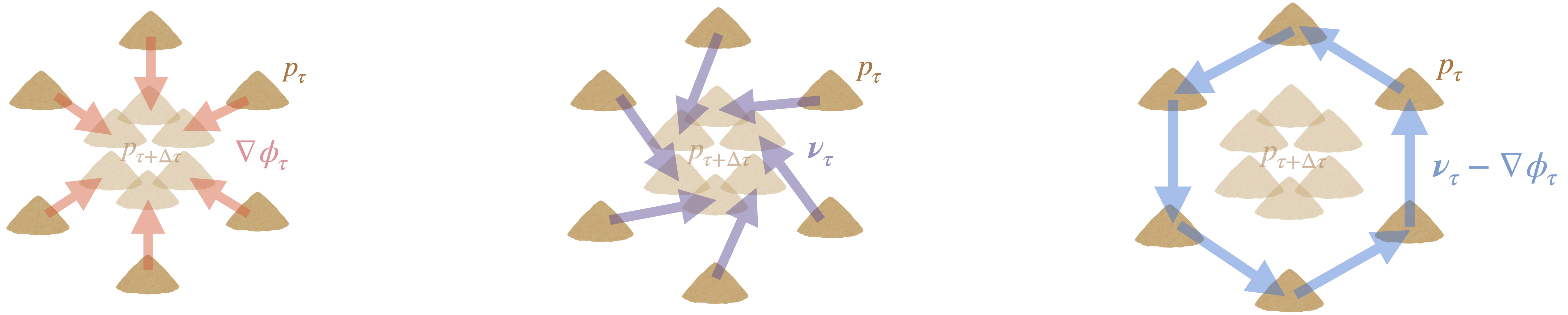
Geometric decomposition of entropy production rate:

Wisdom from optimal transport



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THE UNIVERSITY OF TOKYO SCHOOL OF SCIENCE THE UNIVERSITY OF TOKYO Universal Biology Institute

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M. Nakazato and SI. Phys. Rev. Res. **3**, 043093 (2021).
A. Dechant, S-I Sasa and SI. Phys. Rev. Res. **4**, L012034 (2022).
A. Dechant, S-I Sasa and SI. Phys. Rev. E **106**, 024125 (2022).
K. Yoshimura, A. Kolchinsky, A. Dechant and SI. Phys. Rev. Res. **5**, 013017 (2023).
A. Kolchinsky, A. Dechant, K. Yoshimura and SI. arXiv:2206.14599 (2022).
SI, Information Geometry, 1-42 (2023).

Decomposition of entropy production rate

The entropy production rate (EPR) at time t : $\sigma_t (\geq 0)$

Hatano-Sasa (nonadiabatic/adiabatic) decomposition: $\sigma_t = \sigma_t^{\mathrm{ex,HS}} + \sigma_t^{\mathrm{hk,HS}}$

$(\geq 0) \quad (\geq 0)$

T. Hatano and S-I. Sasa, Phys. Rev. Lett. **86**. 3463 (2001). M. Esposito and C. Van den Broeck, Phys. Rev. E **82**. 011143 (2010).

The EPR in a non-equilibrium steady state (NESS) σ^{st} is characterized by cycle flows.

J. Schnakenberg, Rev. of Mod. Phys. **48**, 571 (1976).

In a NESS

$$\sigma_t^{\mathrm{ex,HS}} = 0$$

$$\sigma_t^{\mathrm{hk,HS}} = \sigma^{\mathrm{st}}$$

A disadvantage of Hatano-Sasa decomposition

e.g.) Fokker-Planck equation $\partial_t p_t(\boldsymbol{x}) = -\nabla \cdot (\boldsymbol{\nu}_t(\boldsymbol{x}) p_t(\boldsymbol{x}))$ $\boldsymbol{\nu}_t(\boldsymbol{x}) = \mu \boldsymbol{F}_t(\boldsymbol{x}) - \mu T \nabla \ln p_t(\boldsymbol{x})$

NESS: $\partial_t p_t^{\mathrm{st}}(\boldsymbol{x}) = -\nabla \cdot (\boldsymbol{\nu}_t^{\mathrm{st}}(\boldsymbol{x}) p_t^{\mathrm{st}}(\boldsymbol{x})) = 0$ $\boldsymbol{\nu}_t^{\mathrm{st}}(\boldsymbol{x}) = \mu \boldsymbol{F}_t(\boldsymbol{x}) - \mu T \nabla \ln p_t^{\mathrm{st}}(\boldsymbol{x})$

$$\sigma_t = \frac{1}{\mu T} \int d\boldsymbol{x} \|\boldsymbol{\nu}_t(\boldsymbol{x})\|^2 p_t(\boldsymbol{x}) \qquad \sigma_t^{\mathrm{ex,HS}} = \frac{1}{\mu T} \int d\boldsymbol{x} \|\boldsymbol{\nu}_t(\boldsymbol{x}) - \boldsymbol{\nu}_t^{\mathrm{st}}(\boldsymbol{x})\|^2 p_t(\boldsymbol{x}) \qquad \sigma_t^{\mathrm{hk,HS}} = \frac{1}{\mu T} \int d\boldsymbol{x} \|\boldsymbol{\nu}_t^{\mathrm{st}}(\boldsymbol{x})\|^2 p_t(\boldsymbol{x})$$

The existence of a unique and asymptotically stable NESS is assumed implicitly.

For a nonlinear rate equation, mulitiple NESSs generally exist and these NESSs can be unstable.

In chemical thermodynamics, this decomposition is only defined for a complex-balanced system with an asymptotically stable NESS.

H. Ge and H. Qian, Chem. Phys. **472**, 241-248 (2016). R. Rao and M. Esposito, Phys. Rev. X **6**, 041064 (2016).

Proposition

We propose another decomposition "geometric decomposition" $\sigma_t = \sigma_t^{\mathrm{ex}} + \sigma_t^{\mathrm{hk}}$
without considering a NESS.

The excess EPR: σ_t^{ex} (≥ 0)

- The dissipation by the same time evolution driven by a potential

The housekeeping EPR: σ_t^{hk} (≥ 0)

- The dissipation by cycle flows which do not affect the time evolution

An idea of this geometric decomposition is originated from
geometry in optimal transport theory.

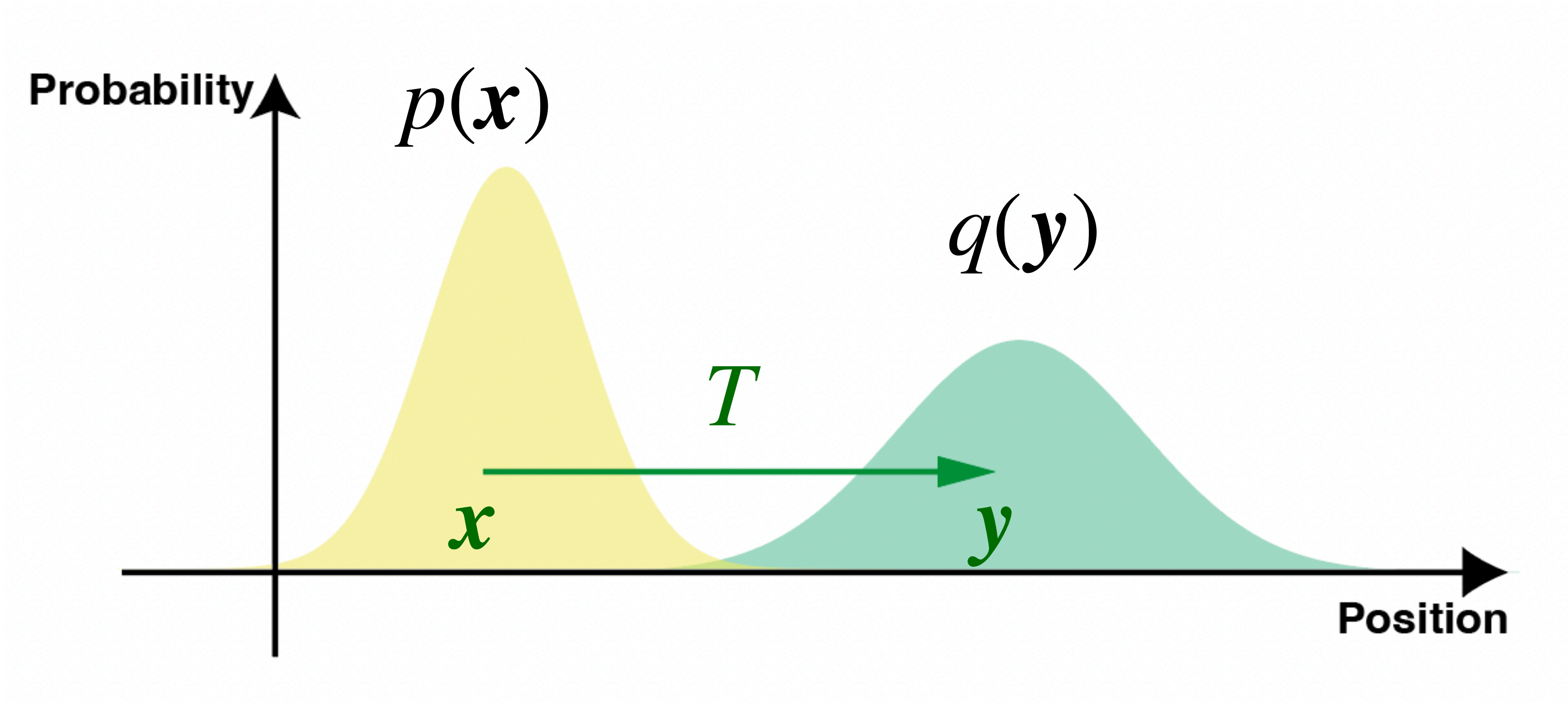
Optimal transport

<u>Optimal transport problem (Monge, 1781)</u> C. Villani, Optimal transport: old and new, (Springer 2009).

We would like to transport a probability distribution from $p(\boldsymbol{x})$ to $q(\boldsymbol{y}) = \int d\boldsymbol{x}\delta(\boldsymbol{y} - T(\boldsymbol{x}))p(\boldsymbol{x})$.

A transport cost for each point depends on $||\boldsymbol{x} - \boldsymbol{y}||^2$.

What is T to minimize all the cost?



L2-Wasserstein distance

$$\mathscr{W}(p, q) = \sqrt{\inf_T \int d\boldsymbol{x}\,||\boldsymbol{x} - T(\boldsymbol{x})||^2\, p(\boldsymbol{x})}$$

<u>For the Fokker-Planck equation</u>, a relation between the free energy and L2-Wasserstein distance has been discussed.

R. Jordan, D. Kinderlehrer and F. Otto, SIAM journal on mathematical analysis, **29**, 1-17 (1998).

Optimal transport based on the continuity equation

Benamou-Brenier formula

J. D. Benamou and Y. Brenier, Y. Numerische Mathematik **84**, 375-393 (2000).

$$\mathscr{W}(p,q) = \sqrt{\inf_{(\boldsymbol{v}_t, P_t)_{\tau \le t \le \tau+\Delta\tau}} (\Delta\tau) \int_{\tau}^{\tau+\Delta\tau} dt \int d\boldsymbol{x} \, ||\boldsymbol{v}_t(\boldsymbol{x})||^2 P_t(\boldsymbol{x})}$$

such that $\partial_t P_t(\boldsymbol{x}) = -\nabla \cdot (\boldsymbol{v}_t(\boldsymbol{x}) P_t(\boldsymbol{x}))$, $\quad P_\tau(\boldsymbol{x}) = p(\boldsymbol{x})$, $P_{\tau+\Delta\tau}(\boldsymbol{x}) = q(\boldsymbol{x})$

An optimal solution:

$$\mathscr{W}(p,q) = \sqrt{(\Delta\tau) \int_{\tau}^{\tau+\Delta\tau} dt \int d\boldsymbol{x} \, ||\boldsymbol{v}_t^*(\boldsymbol{x})||^2 P_t(\boldsymbol{x})}$$

$$\partial_t P_t(\boldsymbol{x}) = -\nabla \cdot (\boldsymbol{v}_t^*(\boldsymbol{x}) P_t(\boldsymbol{x})),$$

$$\boldsymbol{v}_t^*(\boldsymbol{x}) = \nabla \phi_t(\boldsymbol{x})$$

$$\partial_t \phi_t(\boldsymbol{x}) + \frac{1}{2} \|\nabla \phi_t(\boldsymbol{x})\|^2 = 0$$

(Pressureless Euler equation in fluid mechanics without “vorticity”)

Minimum entropy production

Thermodynamic speed limit

E. Aurell *et al.* J. Stat. Phys. **147**, 487-505 (2012).

$$\int_{\tau}^{\tau+\Delta\tau} dt\sigma_t \geq \frac{\mathcal{W}(p_\tau, p_{\tau+\Delta\tau})^2}{\mu T \Delta\tau}$$

Infinitesimal time evolution

M. Nakazato and SI. Phys. Rev. Res. **3**, 043093 (2021).

$$\sigma_\tau \geq \frac{1}{\mu T}\left(\lim_{\Delta\tau\to 0}\frac{\mathcal{W}(p_\tau, p_{\tau+\Delta\tau})}{\Delta\tau}\right)^2$$

$$\sigma_\tau^{\rm rot} = \sigma_\tau - \frac{1}{\mu T}\left(\lim_{\Delta\tau\to 0}\frac{\mathcal{W}(p_\tau, p_{\tau+\Delta\tau})}{\Delta\tau}\right)^2$$

$$\sigma_\tau^{\rm rot} = 0 \;\; (\boldsymbol{\nu}_\tau(\boldsymbol{x}) = \boldsymbol{v}_\tau^*(\boldsymbol{x}) = \nabla\phi_\tau(\boldsymbol{x}))$$

$=: \sigma_\tau^{\rm hk}(\geq 0)$

Vortices (cycle flows)

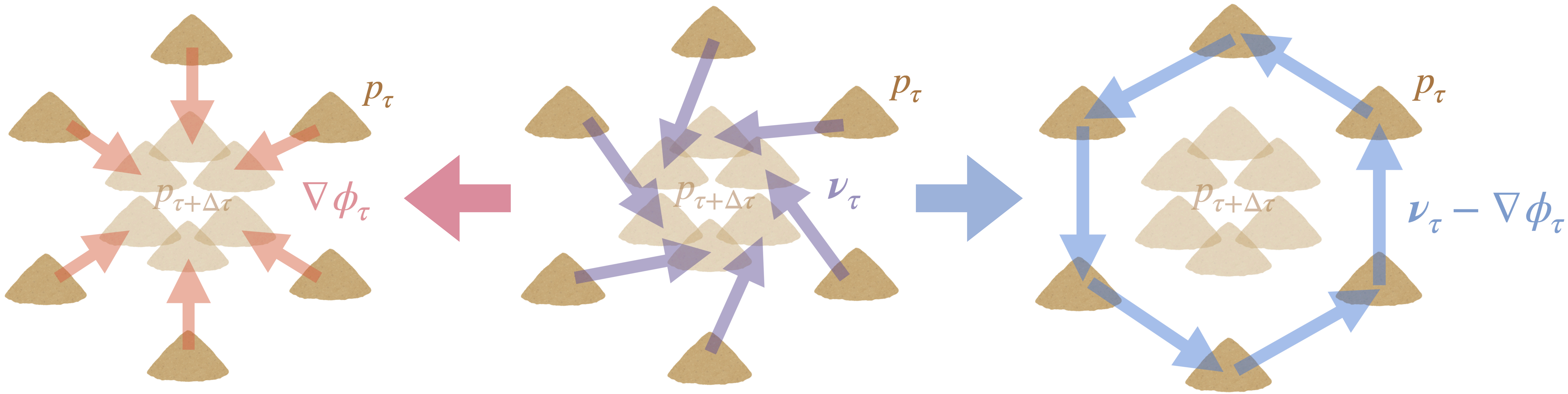
$=: \sigma_\tau^{\rm ex}(\geq 0)$

Optimal transport (potential)

Schematic of geometric decomposition

$(\Delta\tau \to 0)$

Optimal transport (potential) | (Non-optimal) time evolution | Vortices (cycle flows)



$$\partial_\tau p_\tau(\boldsymbol{x}) = -\nabla\cdot[(\nabla\phi_\tau(\boldsymbol{x}))p_\tau(\boldsymbol{x})]$$

$$\partial_\tau p_\tau(\boldsymbol{x}) = -\nabla\cdot[\boldsymbol{\nu}_\tau(\boldsymbol{x})p_\tau(\boldsymbol{x})]$$

$$\nabla\cdot[(\boldsymbol{\nu}_\tau(\boldsymbol{x}) - \nabla\phi_\tau)p_\tau(\boldsymbol{x})] = 0$$

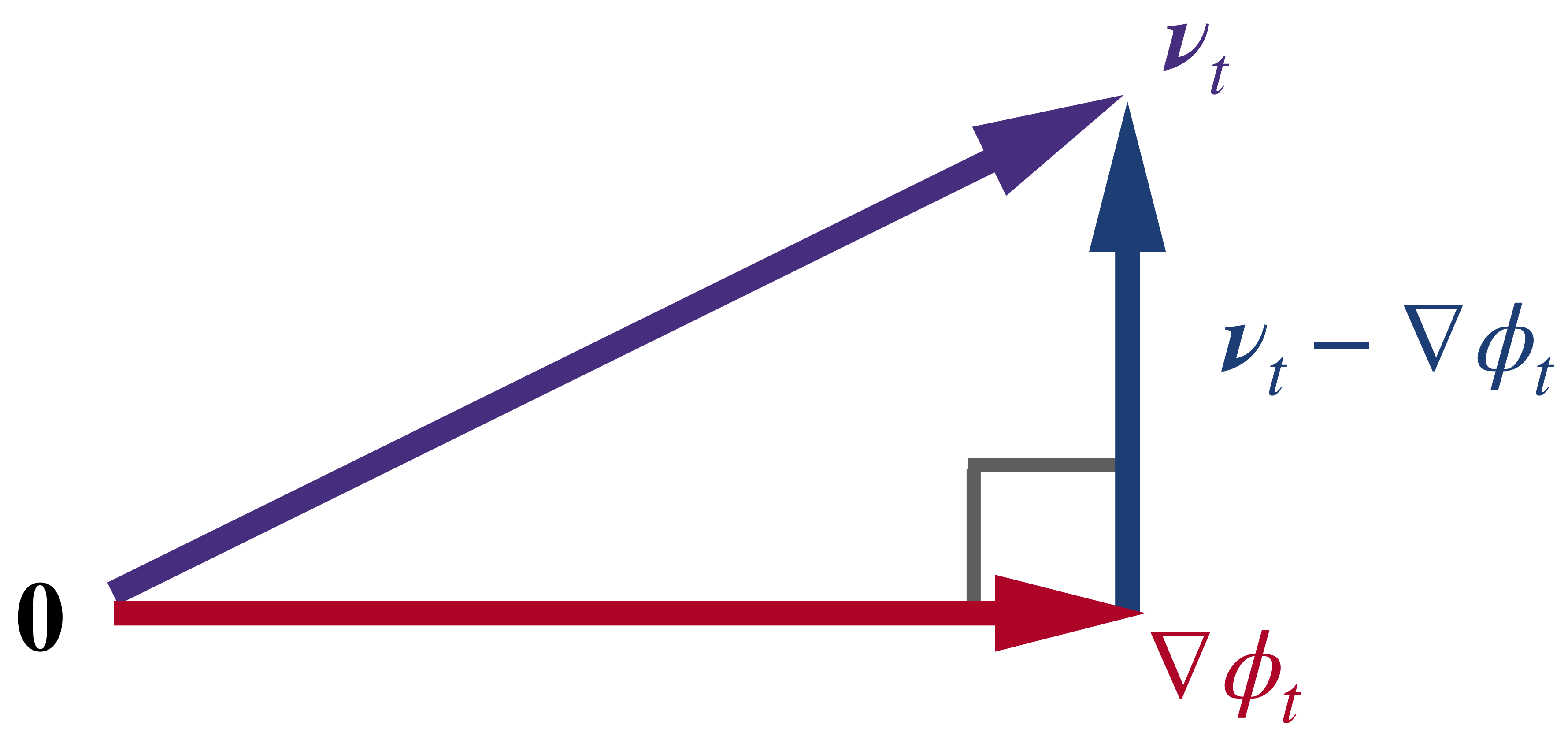
$$\sigma_\tau^{\mathrm{ex}} := \frac{1}{\mu T}\int d\boldsymbol{x}\|\nabla\phi_\tau(\boldsymbol{x})\|^2 p_\tau(\boldsymbol{x})$$

$$\sigma_\tau = \frac{1}{\mu T}\int d\boldsymbol{x}\|\boldsymbol{\nu}_\tau(\boldsymbol{x})\|^2 p_\tau(\boldsymbol{x})$$

$$\sigma_\tau^{\mathrm{hk}} := \frac{1}{\mu T}\int d\boldsymbol{x}\|\boldsymbol{\nu}_\tau(\boldsymbol{x}) - \nabla\phi_\tau(\boldsymbol{x})\|^2 p_\tau(\boldsymbol{x})$$

Inner product and orthogonality

Inner product: $\langle \boldsymbol{a}, \boldsymbol{b} \rangle_{\frac{p_t}{\mu T}} = \frac{1}{\mu T} \int d\boldsymbol{x} \boldsymbol{a}(\boldsymbol{x}) \cdot \boldsymbol{b}(\boldsymbol{x}) p_t(\boldsymbol{x})$



Pythagorean theorem:

$$\sigma_t = \langle \boldsymbol{\nu}_t, \boldsymbol{\nu}_t \rangle_{\frac{p_t}{\mu T}} = \underbrace{\langle \nabla \phi_t, \nabla \phi_t \rangle_{\frac{p_t}{\mu T}}}_{= \sigma_t^{\mathrm{ex}}} + \underbrace{\langle \boldsymbol{\nu}_t - \nabla \phi_t, \boldsymbol{\nu}_t - \nabla \phi_t \rangle_{\frac{p_t}{\mu T}}}_{= \sigma_t^{\mathrm{hk}}}$$

Orthogonality: $\langle \boldsymbol{\nu}_t - \nabla \phi_t, \nabla \phi_t \rangle_{\frac{p_t}{\mu T}} = 0$

$(\nabla \cdot [(\boldsymbol{\nu}_\tau(\boldsymbol{x}) - \nabla \phi_\tau) p_\tau(\boldsymbol{x})] = 0)$

A. Dechant, S-I Sasa and SI. Phys. Rev. Res. **4**, L012034 (2022).

Mathematically, the same decomposition had been proposed by Maes and Netočný based on $\nabla \cdot (\boldsymbol{u}_t p_t) = 0$.

$$\sigma_t \geq \sigma_t^{\mathrm{hk}} = \langle \boldsymbol{u}_t, \boldsymbol{u}_t \rangle_{\frac{p_t}{\mu T}}$$

C. Maes and K. Netočný, J. Stat. Phys. **154**, 188-203 (2014).

Orthogonal complement

Orthogonality in geometric decomposition:

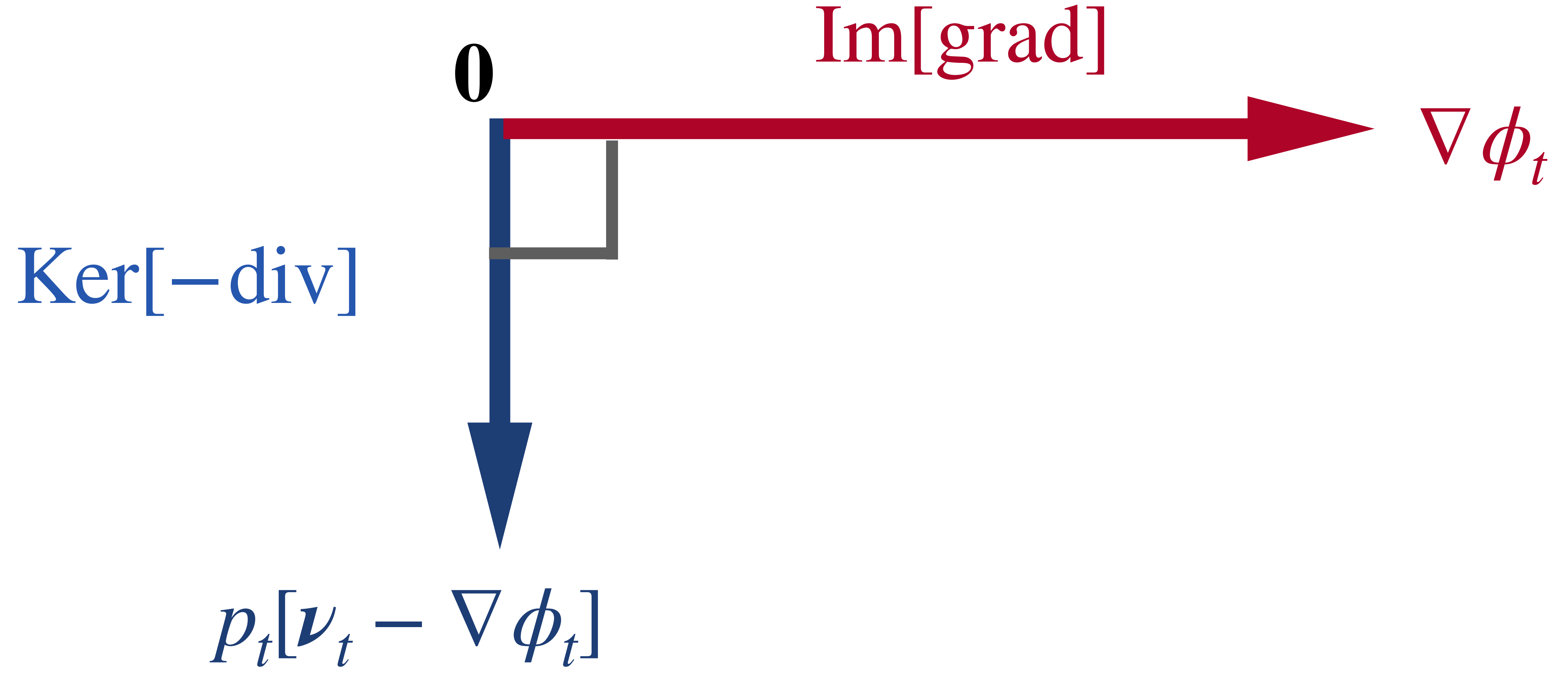
$$\langle \boldsymbol{\nu}_t - \nabla \phi_t, \nabla \phi_t \rangle_{\frac{p_t}{\mu T}} = 0$$

$$\nabla \phi_t \in \mathrm{Im}[\mathrm{grad}] = \{ \nabla \psi \,|\, \psi(\boldsymbol{x}) \in \mathbb{R} \}$$

$$p_t[\boldsymbol{\nu}_t - \nabla \phi_t] \in \mathrm{Ker}[-\mathrm{div}] = \{ \boldsymbol{j}(\boldsymbol{x}) \in \mathbb{R}^{\mathrm{d}} \,|\, -\nabla \cdot \boldsymbol{j} = 0 \}$$

$$(-\nabla \cdot [(\boldsymbol{\nu}_\tau(\boldsymbol{x}) - \nabla \phi_\tau) p_\tau(\boldsymbol{x})] = 0)$$

$$\mathrm{Ker}[-\mathrm{div}] \perp \mathrm{Im}[\mathrm{grad}]$$



Information-geometric orthogonality (Path probability)

SI, Information Geometry, 1-42 (2023)

Path probability for modified dynamics

$$\mathbb{P}_{\boldsymbol{\nu}'}(\boldsymbol{x}_t, \boldsymbol{x}_{t+dt}) = \mathbb{T}_{\boldsymbol{\nu}'}(\boldsymbol{x}_{t+dt} | \boldsymbol{x}_t) p_t(\boldsymbol{x}_t)$$

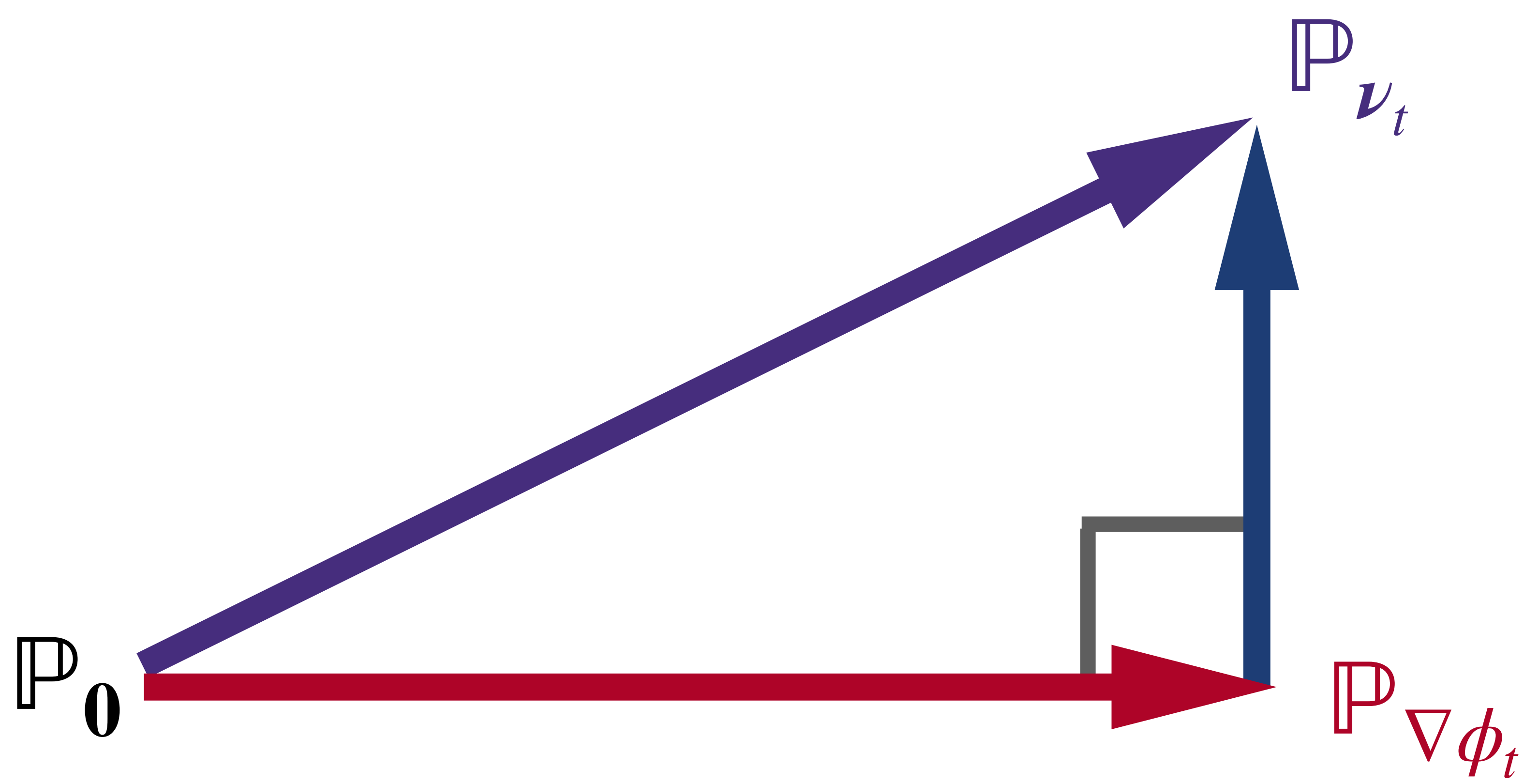
$$\mathbb{T}_{\boldsymbol{\nu}'}(\boldsymbol{x}_{t+dt} | \boldsymbol{x}_t) \propto \exp\left[-\frac{\|\boldsymbol{x}_{t+dt} - \boldsymbol{x}_t - (\mu \boldsymbol{F}_t(\boldsymbol{x}_t) + \boldsymbol{\nu}'(\boldsymbol{x}_t) - \boldsymbol{\nu}_t(\boldsymbol{x}_t))dt\|^2}{4\mu T dt}\right]$$

$$\partial_t p_t(\boldsymbol{x}) = -\nabla \cdot (\boldsymbol{\nu}'(\boldsymbol{x}) p_t(\boldsymbol{x}))$$

Kullback-Leibler divergence: $D_{\mathrm{KL}}(\mathbb{P}_{\boldsymbol{\nu}'} \| \mathbb{P}_{\boldsymbol{\nu}''}) = \int d\boldsymbol{x}_t d\boldsymbol{x}_{t+dt} \mathbb{P}_{\boldsymbol{\nu}'}(\boldsymbol{x}_t, \boldsymbol{x}_{t+dt}) \ln \frac{\mathbb{P}_{\boldsymbol{\nu}'}(\boldsymbol{x}_t, \boldsymbol{x}_{t+dt})}{\mathbb{P}_{\boldsymbol{\nu}''}(\boldsymbol{x}_t, \boldsymbol{x}_{t+dt})}$

Generalized Pythagorean theorem (Information-geometric orthogonality):

$$\underbrace{D_{\mathrm{KL}}(\mathbb{P}_{\boldsymbol{\nu}_t} \| \mathbb{P}_{\boldsymbol{0}})}_{= \sigma_t dt/4} = \underbrace{D_{\mathrm{KL}}(\mathbb{P}_{\boldsymbol{\nu}_t} \| \mathbb{P}_{\nabla \phi_t})}_{= \sigma_t^{\mathrm{hk}} dt/4} + \underbrace{D_{\mathrm{KL}}(\mathbb{P}_{\nabla \phi_t} \| \mathbb{P}_{\boldsymbol{0}})}_{= \sigma_t^{\mathrm{ex}} dt/4}$$



(Ker[−div] ⊥ Im[grad])

Rate/master equation

Chemical reaction: $$\sum_{i=1}^{N} \kappa_{i\rho}^{+} \mathrm{X}_i \underset{k_\rho^-}{\overset{k_\rho^+}{\rightleftharpoons}} \sum_{i=1}^{N} \kappa_{i\rho}^{-} \mathrm{X}_i$$

Rate equation (nonlinear): $d_t c_i = \sum_\rho \mathsf{S}_{i\rho} J_\rho$ Stoichiometric matrix: $\mathsf{S}_{i\rho} = \kappa_{i\rho}^{-} - \kappa_{i\rho}^{+}$

Flow: $J_\rho = J_\rho^{+} - J_\rho^{-}$ e.g., (Ideal dilute solution) $J_\rho^{\pm} = k_\rho^{\pm} \prod_i (c_i)^{\kappa_{i\rho}^{\pm}}$

Master equation: $d_t p_i = \sum_\rho \mathsf{S}_{i\rho} J_\rho = \sum_j [W_{ij} p_j - W_{ji} p_i]$

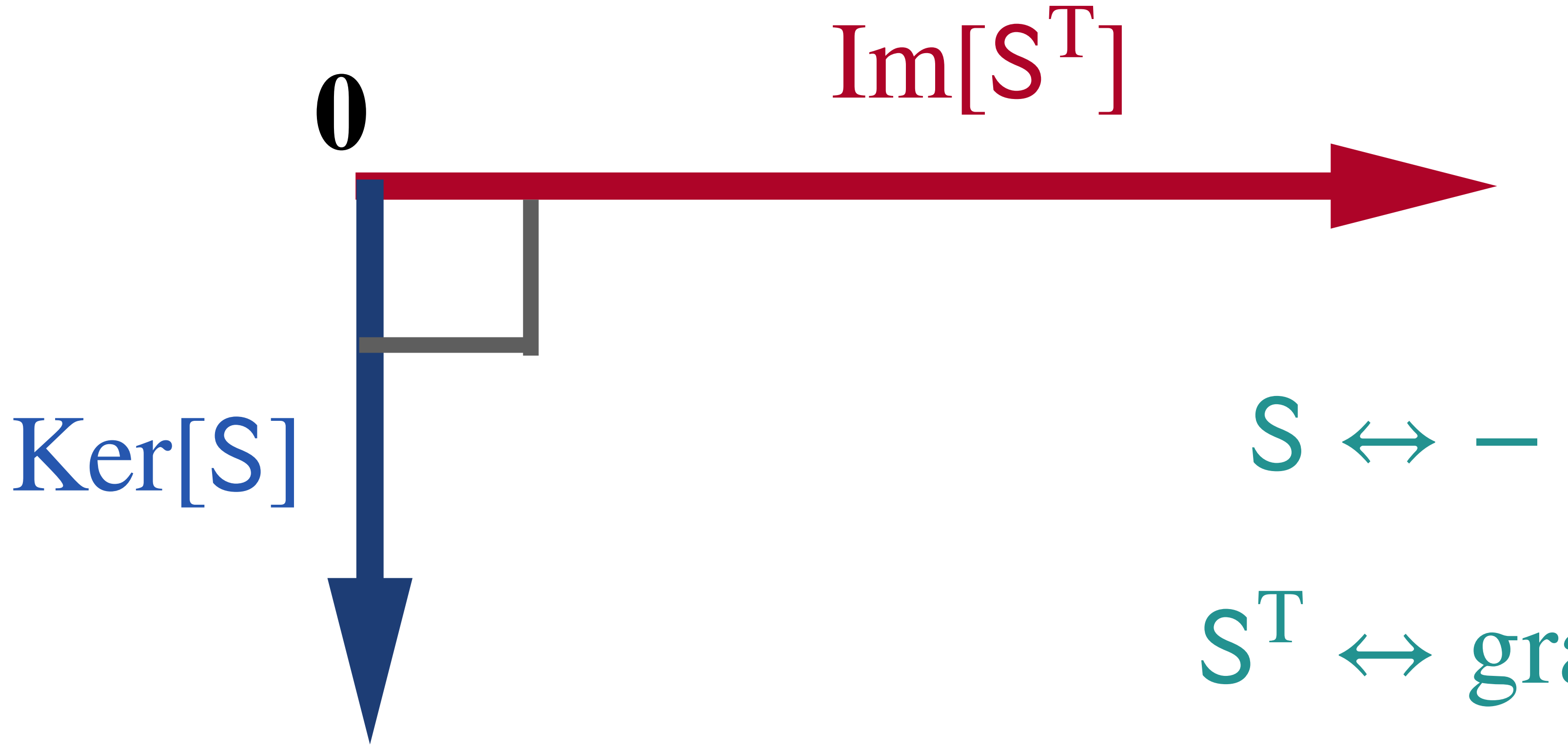
Flow: $J_\rho = W_{ij} p_j - W_{ji} p_j \ (\rho = (i, j), W_{ij} \neq 0, W_{ji} \neq 0)$

Incidence matrix: $\mathsf{S}_{k\rho} = \delta_{ki} - \delta_{kj} \ (\rho = (i, j))$

Geometric decomposition for rate/master equation

EPR: $\sigma_t = \sum_\rho F_\rho J_\rho = \sum_\rho (J_\rho^+ - J_\rho^-) \ln \frac{J_\rho^+}{J_\rho^-}$

Orthogonality: $\mathrm{Ker}[\mathsf{S}] \perp \mathrm{Im}[\mathsf{S}^\mathsf{T}]$



$\mathsf{S} \leftrightarrow -\mathrm{div}$

$\mathsf{S}^\mathsf{T} \leftrightarrow \mathrm{grad}$

Geometry I (Inner product given by the Onsager matrix):

$\sigma_t = \langle \boldsymbol{F}, \boldsymbol{F} \rangle_{\mathsf{L}}$ $\quad\quad$ $\langle \boldsymbol{F}, \boldsymbol{F} \rangle_{\mathsf{L}} \leftrightarrow \langle \boldsymbol{\nu}_t, \boldsymbol{\nu}_t \rangle_{\frac{p_t}{\mu T}}$

K. Yoshimura, A. Kolchinsky, A. Dechant and SI. Phys. Rev. Res. **5**, 013017 (2023).

Geometry II (generalized Kullback-Leibler divergence):

$\sigma_t = D(\boldsymbol{j}(\boldsymbol{f}) \| \boldsymbol{j}(\boldsymbol{0}))$ $\quad\quad$ $D(\boldsymbol{j}(\boldsymbol{f}) \| \boldsymbol{j}(\boldsymbol{0})) \leftrightarrow 4 D_{\mathrm{KL}}(\mathbb{P}_{\boldsymbol{\nu}_t} \| \mathbb{P}_{\boldsymbol{0}}) / dt$

A. Kolchinsky, A. Dechant, K. Yoshimura and SI. arXiv:2206.14599 (2022).

Geometry I: Onsager-projective excess/housekeeping EPR

K. Yoshimura, A. Kolchinsky, A. Dechant and SI. Phys. Rev. Res. **5**, 013017 (2023).

Inner product: $\langle \boldsymbol{A}, \boldsymbol{B} \rangle_{\mathsf{L}} = \boldsymbol{A}^{\mathrm{T}} \mathsf{L} \boldsymbol{B}$

Onsager matrix: $\mathsf{L}_{\rho\rho'} = \dfrac{J_\rho^+ - J_\rho^-}{\ln J_\rho^+ - \ln J_\rho^-} \delta_{\rho\rho'}$ $\quad \mathsf{L}_{\rho\rho'} = J_\rho^+ \delta_{\rho\rho'}$ $(J_\rho^+ = J_\rho^-)$

EPR: $\sigma_t = \langle \boldsymbol{F}, \boldsymbol{F} \rangle_{\mathsf{L}}$

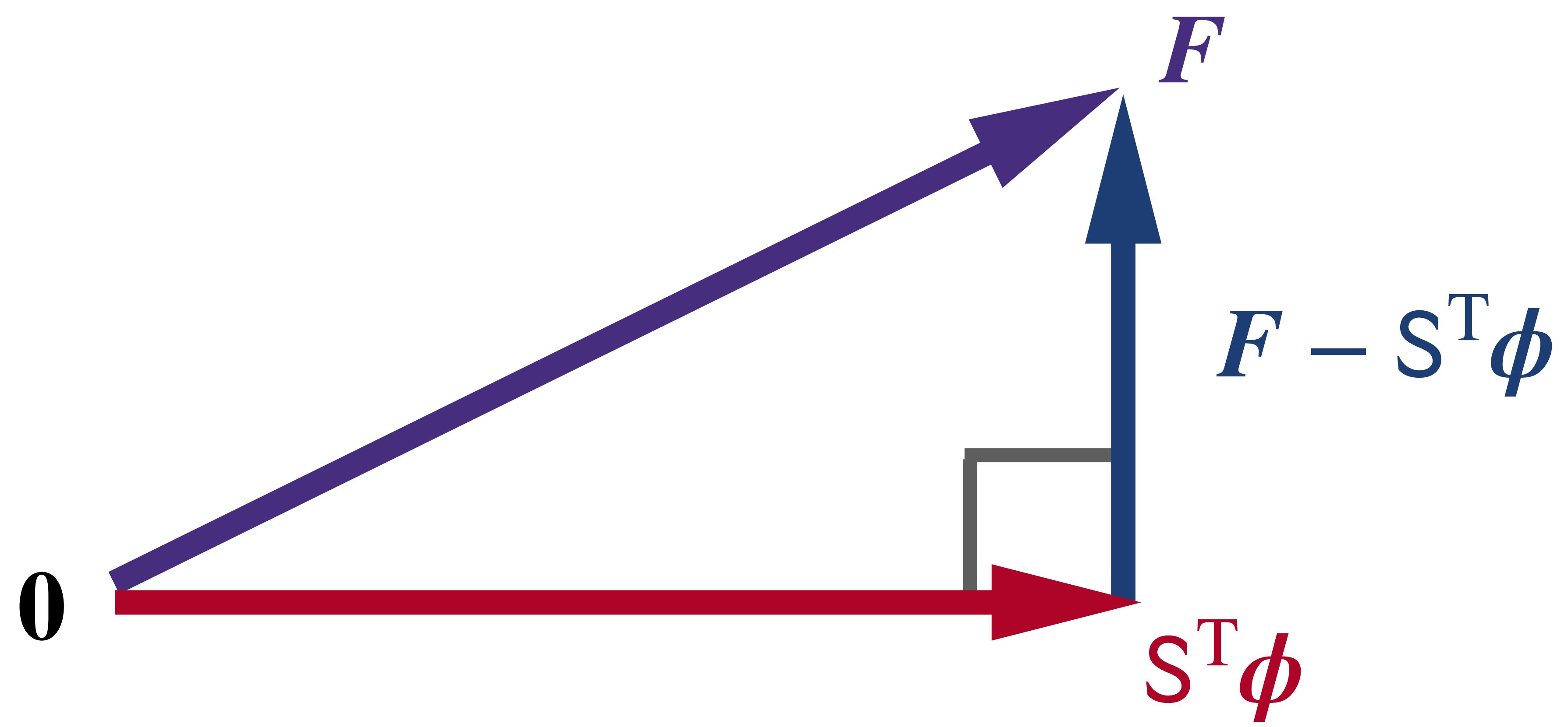
"Optimal transport": $d_t \boldsymbol{c} = \mathsf{S}\boldsymbol{J} = \mathsf{S}\boldsymbol{J}^*$ $\quad \boldsymbol{J} - \boldsymbol{J}^* \in \mathrm{Ker}[\mathsf{S}]$

$\mathsf{L}\mathsf{S}^{\mathrm{T}}\boldsymbol{\phi} \leftrightarrow p_t(\boldsymbol{x})(\nabla \phi_t(\boldsymbol{x}))$

$\mathsf{L}\mathsf{S}^{\mathrm{T}}\boldsymbol{\phi} = \boldsymbol{J}^*$ $\quad \mathsf{S}^{\mathrm{T}}\boldsymbol{\phi} \in \mathrm{Im}[\mathsf{S}^{\mathrm{T}}]$ $(\perp \mathrm{Ker}[\mathsf{S}])$

Onsager-projective decomposition:

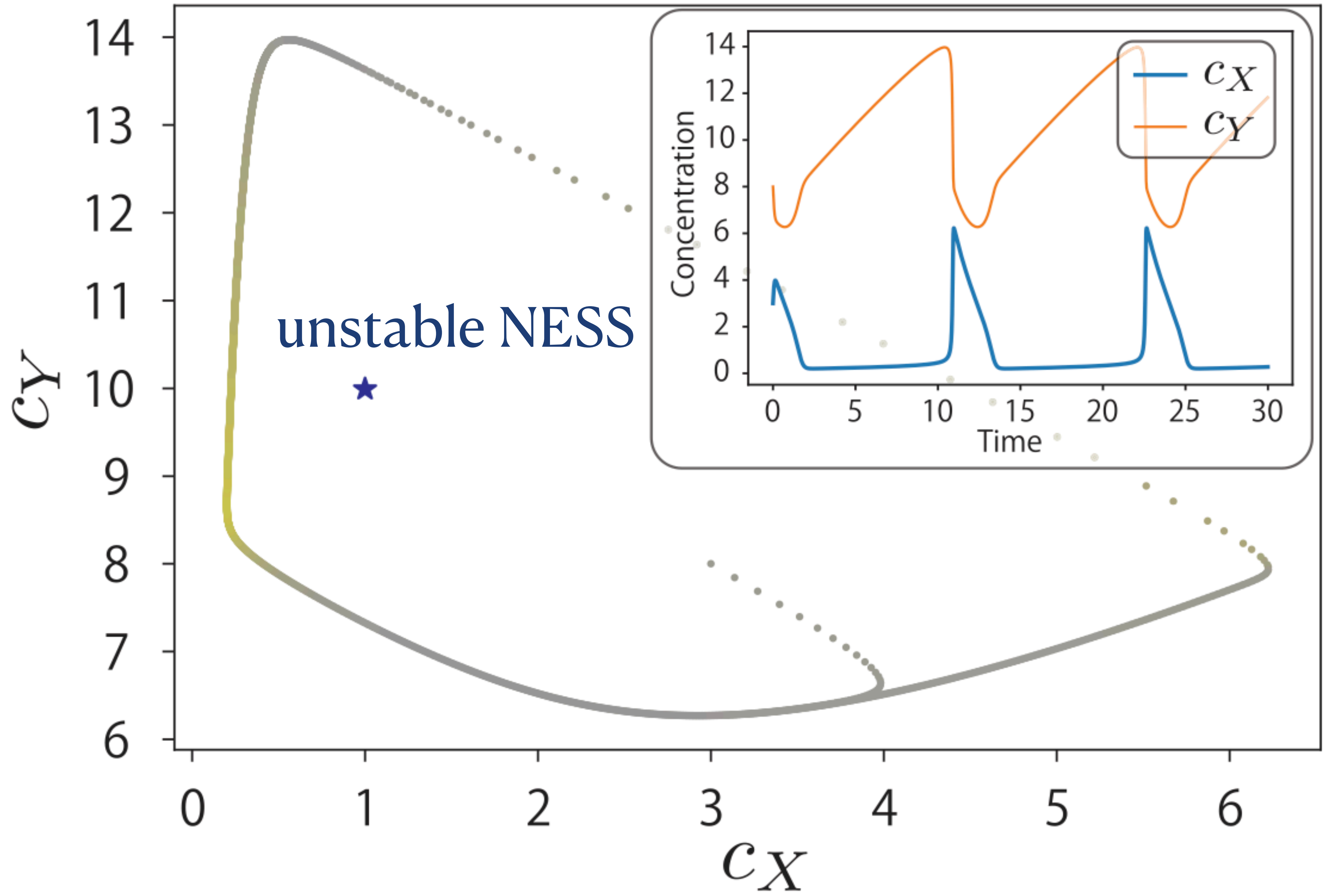
$$\sigma_t = \langle \boldsymbol{F}, \boldsymbol{F} \rangle_{\mathsf{L}} = \underbrace{\langle \mathsf{S}^{\mathrm{T}}\boldsymbol{\phi}, \mathsf{S}^{\mathrm{T}}\boldsymbol{\phi} \rangle_{\mathsf{L}}}_{=: \sigma_t^{\mathrm{ex;ons}} (\geq 0)} + \underbrace{\langle \boldsymbol{F} - \mathsf{S}^{\mathrm{T}}\boldsymbol{\phi}, \boldsymbol{F} - \mathsf{S}^{\mathrm{T}}\boldsymbol{\phi} \rangle_{\mathsf{L}}}_{=: \sigma_t^{\mathrm{hk;ons}} (\geq 0)}$$

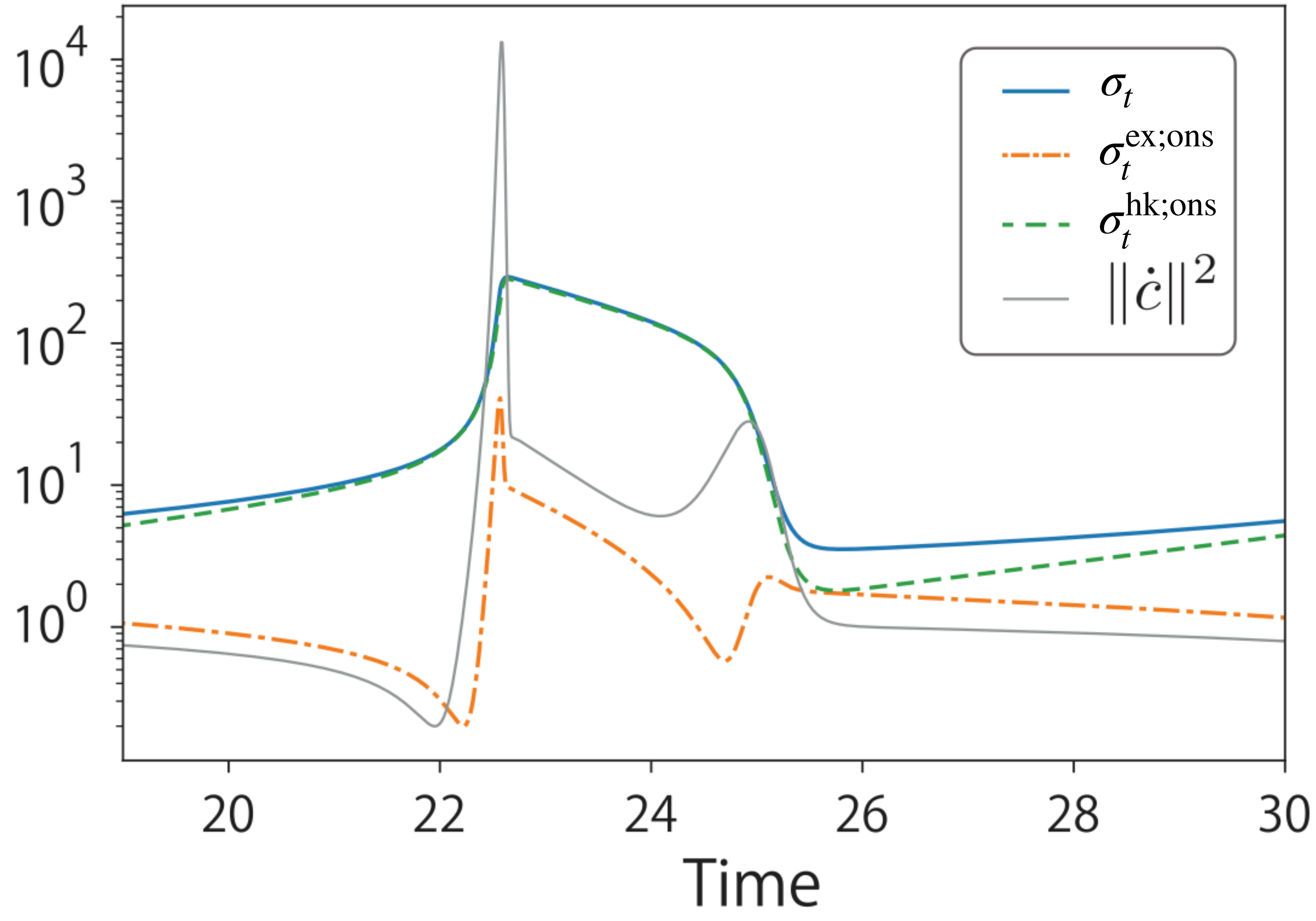


$\langle \mathsf{S}^{\mathrm{T}}\boldsymbol{\phi}, \boldsymbol{F} - \mathsf{S}^{\mathrm{T}}\boldsymbol{\phi} \rangle_{\mathsf{L}} = 0$ $\quad (\mathrm{Ker}[\mathsf{S}] \perp \mathrm{Im}[\mathsf{S}^{\mathrm{T}}])$

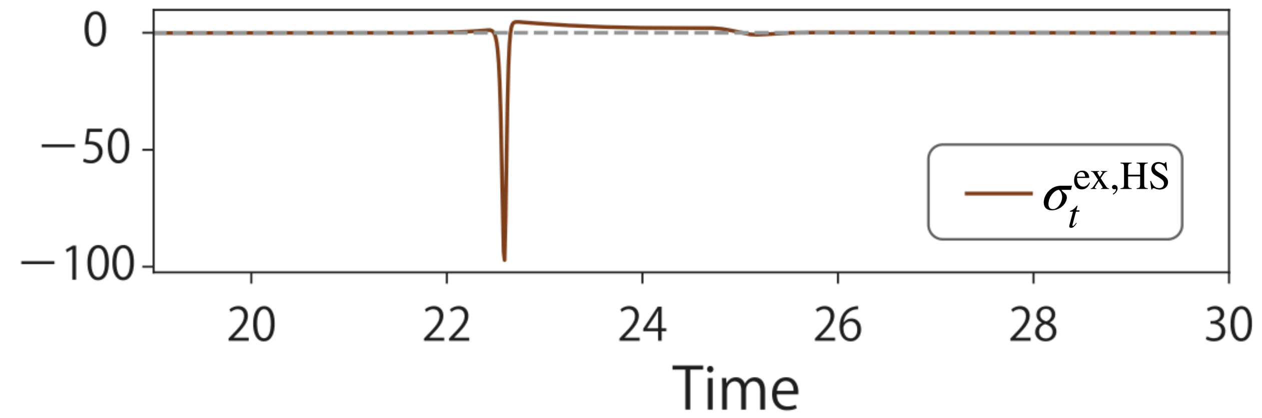
Numerics: Brusselator

K. Yoshimura, A. Kolchinsky, A. Dechant and SI. Phys. Rev. Res. **5**, 013017 (2023).





The Hatano-Sasa excess EPR can be negative.



$$\varnothing \underset{k_1^-}{\overset{k_1^+}{\rightleftharpoons}} X \qquad X \underset{k_2^-}{\overset{k_2^+}{\rightleftharpoons}} Y \qquad 2X + Y \underset{k_3^-}{\overset{k_3^+}{\rightleftharpoons}} 3X \qquad \|\dot{c}\|^2 = (d_t c_X)^2 + (d_t c_Y)^2$$

Geometry II: Information-geometric excess/housekeeping EPR

A. Kolchinsky, A. Dechant, K. Yoshimura and SI. arXiv:2206.14599 (2022).

Generalized KL divergence:

$$D(\boldsymbol{j}(\boldsymbol{f}')\|\boldsymbol{j}(\boldsymbol{f}'')) = \sum_e \left[j_e(\boldsymbol{f}')\ln\frac{j_e(\boldsymbol{f}')}{j_e(\boldsymbol{f}'')} - j_e(\boldsymbol{f}') + j_e(\boldsymbol{f}'') \right]$$

$$\boldsymbol{j}^+ = (J_1^+, \cdots, J_{|\rho|}^+, J_1^-, \cdots, J_{|\rho|}^-)^{\mathrm{T}}$$

$$\boldsymbol{j}^- = (J_1^-, \cdots, J_{|\rho|}^-, J_1^+, \cdots, J_{|\rho|}^+)^{\mathrm{T}}$$

$$j_e(\boldsymbol{\theta}) = j_e^+ \exp(\theta_e - f_e)$$

$$f_e = \ln[j_e^+/j_e^-]$$

EPR: $\sigma_t = D(\boldsymbol{j}(\boldsymbol{f})\|\boldsymbol{j}(\boldsymbol{0}))$

"Optimal transport": $d_t\boldsymbol{c} = \mathsf{S}\boldsymbol{J} = \tilde{\mathsf{S}}\boldsymbol{j}(\boldsymbol{f}) = \tilde{\mathsf{S}}\boldsymbol{j}(\tilde{\mathsf{S}}^{\mathrm{T}}\boldsymbol{\varphi})$ $\quad \boldsymbol{j}(\boldsymbol{f}) - \boldsymbol{j}(\tilde{\mathsf{S}}^{\mathrm{T}}\boldsymbol{\varphi}) \in \mathrm{Ker}[\tilde{\mathsf{S}}]$ $\quad \boldsymbol{j}(\tilde{\mathsf{S}}^{\mathrm{T}}\boldsymbol{\varphi}) \leftrightarrow \mathbb{P}_{\nabla\phi_t}$

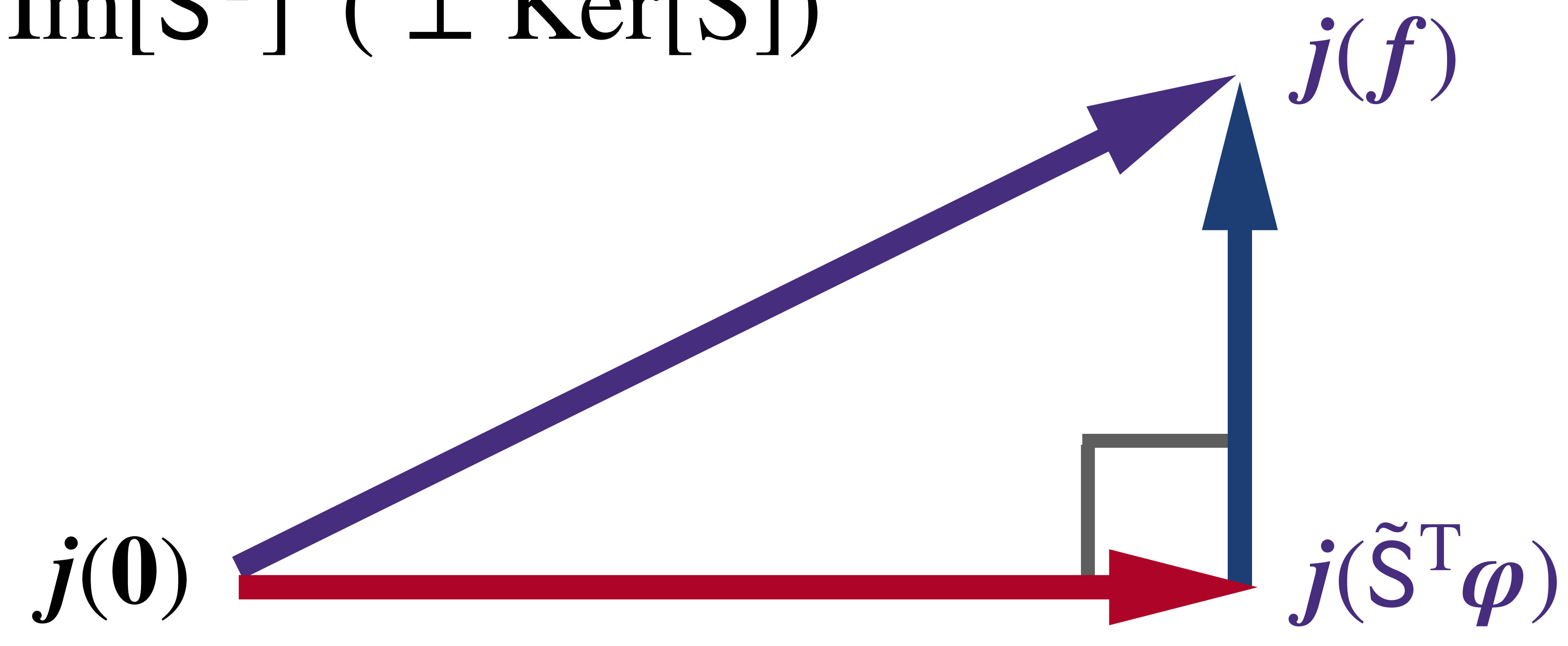
$$\tilde{\mathsf{S}}^{\mathrm{T}}\boldsymbol{\varphi} \in \mathrm{Im}[\tilde{\mathsf{S}}^{\mathrm{T}}] \;\; (\perp \mathrm{Ker}[\tilde{\mathsf{S}}])$$

Information-geometric decomposition:

$$\sigma_t = D(\boldsymbol{j}(\boldsymbol{f})\|\boldsymbol{j}(\boldsymbol{0})) = \underline{D(\boldsymbol{j}(\boldsymbol{f})\|\boldsymbol{j}(\tilde{\mathsf{S}}^{\mathrm{T}}\boldsymbol{\varphi}))} + \underline{D(\boldsymbol{j}(\tilde{\mathsf{S}}^{\mathrm{T}}\boldsymbol{\varphi})\|\boldsymbol{j}(\boldsymbol{0}))}$$

$$=: \sigma_t^{\mathrm{hk;IG}} (\geq 0) \qquad =: \sigma_t^{\mathrm{ex;IG}} (\geq 0)$$

$$(\sigma_t^{\mathrm{hk;IG}} \neq \sigma_t^{\mathrm{hk;ons}}, \sigma_t^{\mathrm{ex;IG}} \neq \sigma_t^{\mathrm{ex;ons}})$$



$(\mathrm{Ker}[\tilde{\mathsf{S}}] \perp \mathrm{Im}[\tilde{\mathsf{S}}^{\mathrm{T}}])$

Applications of geometric decompositions to TURs

Thermodynamic uncertainty relations (TURs):

$R(\boldsymbol{x}), \boldsymbol{R}$: Observable

For Fokker-Planck Eq.: $$\sigma_t^{\mathrm{ex}} = \langle \nabla \phi_t, \nabla \phi_t \rangle_{\frac{p_t}{\mu T}} \geq \frac{|\langle \nabla \phi_t, \nabla R \rangle_{\frac{p_t}{\mu T}}|^2}{\langle \nabla R, \nabla R \rangle_{\frac{p_t}{\mu T}}} = \frac{|d_t \langle R \rangle_{p_t}|^2}{\langle \nabla R, \nabla R \rangle_{\frac{p_t}{\mu T}}} \quad \langle R \rangle_{p_t} = \int d\boldsymbol{x} R(\boldsymbol{x}) p_t(\boldsymbol{x})$$

A. Dechant, S-I Sasa and SI. Phys. Rev. E **106**, 024125 (2022).

For rate Eq.: $$\sigma_t^{\mathrm{ex;ons}} = \langle \mathsf{S}^{\mathrm{T}} \boldsymbol{\phi}, \mathsf{S}^{\mathrm{T}} \boldsymbol{\phi} \rangle_{\mathsf{L}} \geq \frac{|\langle \mathsf{S}^{\mathrm{T}} \boldsymbol{R}, \mathsf{S}^{\mathrm{T}} \boldsymbol{\phi} \rangle_{\mathsf{L}}|^2}{\langle \mathsf{S}^{\mathrm{T}} \boldsymbol{R}, \mathsf{S}^{\mathrm{T}} \boldsymbol{R} \rangle_{\mathsf{L}}} = \frac{|d_t(\boldsymbol{c}^{\mathrm{T}} \boldsymbol{R})|^2}{\langle \mathsf{S}^{\mathrm{T}} \boldsymbol{R}, \mathsf{S}^{\mathrm{T}} \boldsymbol{R} \rangle_{\mathsf{L}}}$$

K. Yoshimura, A. Kolchinsky, A. Dechant and SI. Phys. Rev. Res. **5**, 013017 (2023).

$\sigma_t^{\mathrm{ex;IG}}$ also provides a TUR for a highly irreversible process.

$$\sigma_t^{\mathrm{ex;IG}} \geq 2|d_t(\boldsymbol{c}^{\mathrm{T}} \boldsymbol{R})| \tanh^{-1} \frac{|d_t(\boldsymbol{c}^{\mathrm{T}} \boldsymbol{R})|}{\sum_e j_e^+ |(\tilde{\mathsf{S}}^{\mathrm{T}} \boldsymbol{R})_e|} \qquad \left(\sup_e |(\tilde{\mathsf{S}}^{\mathrm{T}} \boldsymbol{R})_e| \leq 1 \right)$$

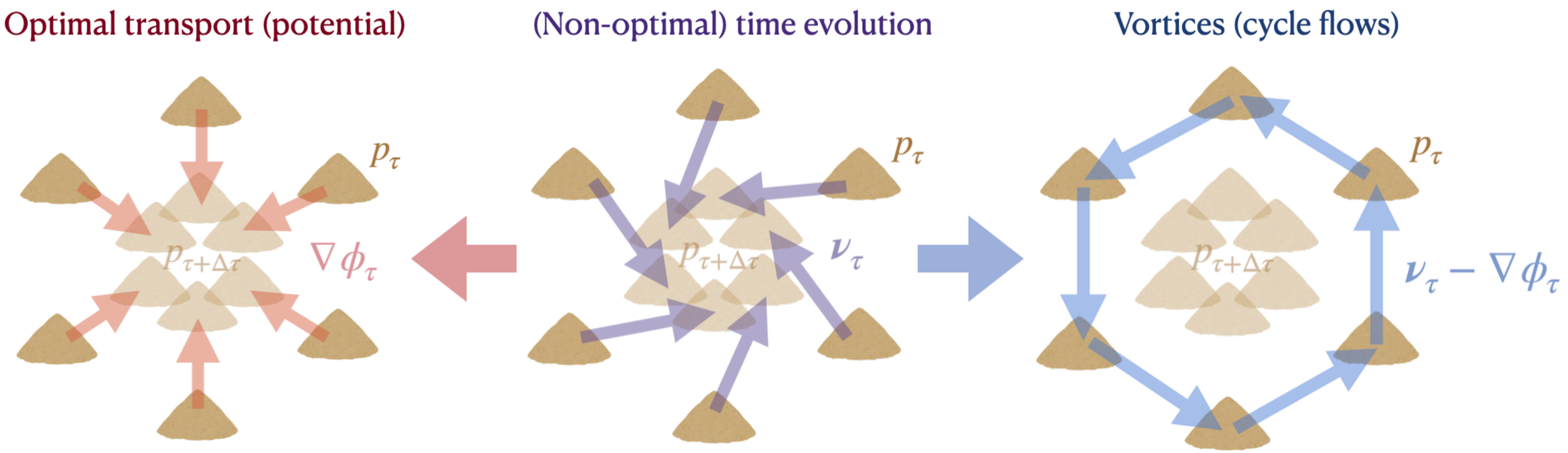
A. Kolchinsky, A. Dechant, K. Yoshimura and SI. arXiv:2206.14599 (2022).

Summary

We propose geometric decompositions of EPR $\sigma_t = \sigma_t^{\mathrm{ex}} + \sigma_t^{\mathrm{hk}}$. ($\sigma_t = \sigma_t^{\mathrm{ex;ons}} + \sigma_t^{\mathrm{hk;ons}}$, $\sigma_t = \sigma_t^{\mathrm{ex;IG}} + \sigma_t^{\mathrm{hk;IG}}$)

- The excess EPR σ_t^{ex} means the dissipation by the same time evolution driven by a potential.

- The housekeeping EPR σ_t^{hk} means the dissipation by cycle flows which do not affect the time evolution.



We generalize geometric decomposition for a nonlinear rate equation, where a unique and stable NESS does not exist generally. Geometric decompositions may be useful, at least, to derive TURs.