Nonlocal coupling among oscillators mediated by the diffusion of a chemical

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there are many problems in physical chemistry and biology involving the communication among individuals mediated by the diffusion of some chemical in the medium.

this chemical is both released and absorbed by the individuals, often depending on dynamical processes occurring within them.

the release, diffusion and absorption creates an effective coupling among individuals that affects their dynamics.

in this work we explore the consequences of this basic idea into models of non-locally coupled nonlinear oscillators.

coupling problems typically involve more than one timescale (difficulties in the computer simulations).
Ovarian cycles

- surge of luteinizing hormone from the anterior pituitary
- LH luteinizes several follicles in the ovary causing each to rupture and release its effective
- at the site of rupture a corpus luteum forms and secretes progesterone
- just after ovulation a new set of follicles begins to mature and releases estrogen (ovarian steroid)
- estrogen primes the system for another surge of LH
- cycle period = 28 days for humans
Synchronization of ovarian cycles


- McClintock effect: women that live together synchronize their ovarian cycles
- the synchronization of ovarian cycles is mediated by airborne chemosignals called pheromones
- two distinct chemicals: one advances and another delays the phase of the ovarian cycle
- pheromones diffuse in the atmosphere: there must be a common air supply
Chemotaxis of *Dictyostelium*

- chemotaxis: motion of an organism in response to a chemical stimulus
- *Dictyostelium*: amoeabae (“slime mold”)
- in absence of food about $10^5$ cells release signal molecules of chemoattractant cyclic adenosine monophosphate (cAMP) in the environment
- they can find other cells and move to create clusters (releasing every 6 min during periods reaching 5 to 6 hours after starvation)
Suprachiasmatic nucleus

- region of the brain (hypothalamus) responsible for controlling circadian rhythms
- receives input from specialized photosensitive ganglion cells in the retina
- maintains control by synchronizing their own near-24-hour rhythms and control circadian phenomena in local tissues
- it contains around 20,000 neurons (clock cells)
- collective rhythm possible because of frequency synchronization induced by coupling among clock cells
- coupling is mediated by a neurotransmitter (GABA) diffusing through intercell medium
Coupling model


- $N$ pointlike oscillator cells located at $\vec{r}_j$, $(j = 1, 2, \cdots N)$ in a $d$-dimensional Euclidean space
- each oscillator has an internal dynamics governed by the flux $\mathbf{F}(\mathbf{X}, t)$, where $\mathbf{X} = (x_1, x_2, \cdots x_M)^T$ in a $M$-dim. phase space
- the time evolution of each oscillator is affected by the local concentration of a chemical $A(\mathbf{r}, t)$

$$\frac{dX_j}{dt} = \mathbf{F}(X_j) + g(A(\vec{r}, t))$$
Coupling model in the adiabatic limit

- the concentration satisfies a inhomogeneous diffusion equation

\[
\varepsilon \frac{\partial A}{\partial t} = -\eta A + D \nabla^2 A + \sum_{k=1}^{N} h(\theta_k)\delta(\vec{r} - \vec{r}_k)
\]

- \( \eta \): coefficient of chemical degradation, \( D \): diffusion coefficient
- \( \varepsilon \approx 0 \): diffusion timescale much faster than oscillator period
- concentration fast-relaxes to a stationary value

\[
A(\vec{r}_j) = \sum_{k=1}^{N} \sigma(\vec{r}_j - \vec{r}_k)h(\theta_k)
\]

- \( \sigma(\vec{r}) \) is the Green function of the diffusion equation

\[
(\eta - D \nabla^2)\sigma(\vec{r}_j - \vec{r}) = \delta(\vec{r}_j)
\]

- chemical coupling in the adiabatic limit

\[
\frac{dX_j}{dt} = F(X_j) + \sum_{k=1}^{N} \sigma(\vec{r}_j - \vec{r}_k)g_h(\theta_k)
\]
Types of chemical coupling

- linear coupling: \( g(h(X_k)) = AX_k \)
- future coupling: \( g(h(X_k)) = AF(X_k) \)
- nonlinear coupling: \( g(h(X_k)) = AH(X_k) \)
- Green function for isotropic systems \( (r \equiv |r_j - r|) \)

\[
\sigma(r) = C \begin{cases} 
\exp(-\gamma r), & \text{if } d = 1, \\
K_0(\gamma r), & \text{if } d = 2, \\
\frac{\exp(-\gamma r)}{\gamma r}, & \text{if } d = 3
\end{cases}
\]

- inverse coupling length: \( \gamma = \sqrt{\eta/D} \),
- \( C \) is determined from the normalization condition

\[
\int d^d r \sigma(r) = 1
\]
Phase oscillators with chemical coupling

- for phase oscillators $\mathbf{X} \rightarrow \theta$ and $\mathbf{F} \rightarrow \omega$
- nonlinear coupling (extended Kuramoto model)

$$\dot{\theta}_j = \omega_j + K \sum_{k=1}^{N} \sigma(\vec{r}_j - \vec{r}_k) \sin (\theta_k - \theta_j)$$

- for $d = 1$ the Green function is $\sigma(x_i - x_j) = e^{-\gamma|x_i - x_j|}$ with $\gamma = \sqrt{\frac{\eta}{D}}$ (inverse coupling length), and normalization constant determined by $\int dx \sigma(x) = 1$
- one-dimensional lattice with periodic boundary conditions
- normalization factor $\kappa(\gamma) = 2 \sum_{\ell=1}^{N'} e^{-\gamma\ell}$

$$\dot{\theta}_j = \omega_j + \frac{K}{\kappa(\gamma)} \sum_{\ell=1}^{N'} e^{-\gamma\ell} [\sin (\theta_{j-\ell} - \theta_j) + \sin (\theta_{j+\ell} - \theta_j)].$$
Frequency synchronization


- frequency without coupling: $\omega_j$, randomly chosen according to a zero-mean gaussian PDF $g(\omega)$
- frequency after coupling: $\Omega_j = \dot{\theta}_j$
- small $\gamma$: nearly global coupling = complete synchronization
- intermediate $\gamma$: partial synchronization
- large $\gamma$: nearly local coupling = no synchronization
Partial frequency synchronization

- $N_i$: length of $i$th sync plateau
- $N_p$: number of plateaus
- average plateau size: 
  \[ \langle N \rangle = \frac{1}{N_p} \sum_{i=1}^{N_p} N_i \]
- sync degree: 
  \[ P = \frac{\langle N \rangle}{N} \]
- completely sync state: $P = 1$
- completely non-sync state: $P \approx 0$
- critical $\gamma$ for increasing $K$
- small $K$: no sync for any $\gamma$
- global coupling ($\gamma = 0$): sync after 
  \[ K_c = \frac{2}{\pi g(0)} = 0.08 \]
- local coupling (large $\gamma$): no sync, even with large $K$
Phase synchronization

- equality of phases (stronger than frequency sync)
- complex order parameter

\[ z(t) = R(t)e^{i\varphi(t)} = \frac{1}{N} \sum_{j=1}^{N} e^{i\theta_j(t)} \]

- completely synchronized state: \( R = 1, \rightarrow \text{small } \gamma \) (global)
- non-synchronized state: \( R \approx 0, \rightarrow \text{intermediate } \gamma \)
- partially synchronized state: \( 0 < R < 1, \rightarrow \text{large } \gamma \) (local)
Transition to phase synchronization

- $\bar{R}$: time-averaged order parameter magnitude
- synchronization transition for a critical $\gamma_c$ (fixed $K$)
- $\gamma_c$ decreases with increasing lattice size $N$
- thermodynamical limit ($N \to \infty$): $\gamma_c = 0.00025$
- coupling parameter plane: deep blue: no phase sync, red: complete phase sync
Spatial recurrence matrix

- one-dimensional spatial pattern with $N$ sites: $\{x_k\}_{k=0}^{N}$
- spatial recurrence: two sites $i$ and $j$ have the same height, up to some precision $\varepsilon$
- spatial recurrence matrix: $R_{ij} = 1$ if $|x_i - x_j| \leq \varepsilon$, and 0 otherwise

$$R_{ij} = \Theta(|x_i - x_j| - \varepsilon)$$

- spatial recurrence plot is a graphical representation of the spatial recurrence matrix with elements $R_{ij}$. 
Spatial recurrence plot

- spatial recurrence plot: graphical representations of the spatial recurrence matrix with elements $R_{ij}$
- characterizes the existence of spatially homogeneous (synchronized) states in phase and frequency
- characterizes the existence of spatially inhomogeneous states (chimeras)
Recurrence quantification analysis

- recurrence rate: fraction of recurrent points: $RR = \frac{1}{N^2} \sum_{i,j} R_{ij}$
- determinism: fraction of points belonging to diagonal structures
- $P(\ell)$: probability distribution function of diagonal lengths
\[
DET = \frac{\sum_{\ell=2}^{N} \ell P(\ell)}{\sum_{i,j\neq i} R_{ij}}
\]
- laminarity: fraction of points belonging to horizontal structures
Synchronization of biological clock cells

- model for coupled circadian clock cells in the SCN
- each clock cell with its own period $\tau_j \approx 24h$ (Gaussian distribution)
- Van der Pol-Kronauer oscillator describing the clock cell dynamics

$$\mathbf{X}_j = \frac{12}{\pi} \begin{pmatrix} x_j \\ y_j \end{pmatrix}, \mathbf{F}(\mathbf{X}_j, t) = \begin{pmatrix} y_j + \epsilon \left( x_j - \frac{4}{3} x_j^3 \right) + B(t) - C_x x_j \\ - \left( \frac{24}{\tau_j} \right)^2 x_j + B(t)y_j - C_y y_j \end{pmatrix}$$

- $C_{x,y}$ are coupling parameters
- photic stimulation: $B(t) = C \left( 1 - m\langle x \rangle \right) \left[ I(t) \right]^{1/3}$
- spatial average: $\langle x \rangle = \left( 1/N \right) \sum_{i=1}^{N} x_i$
Phase and frequency of clock cells

- oscillator dynamics displays a limit cycle encircling the origin \((x_{k0} = 0, y_{k0} = 0)\)
- geometrical phase
  \[ \theta_k(t) = \arctan \left( \frac{y_k(t) - y_{k0}}{x_k(t) - x_{k0}} \right) \]
- oscillator frequency and period
  \[ \Omega_k = \frac{2\pi}{T_k} = \lim_{T \to \infty} \frac{\theta_k(T) - \theta_k(0)}{T} \]
Synchronization of clock cells under constant darkness

- protocol I: the system is evolved in constant darkness ($I = 0$)
- top: (a) distribution of periods of SCN cells with $\gamma = 1$ for $D_x = 1.91 \times 10^{-1}$ (red circles) and $7.64 \times 10^{-1}$ (open circles)
- (b) time series for the $x$ and $y$ variables of one typical SCN cell (dashed and full thin lines, respectively) and mean field $\langle x \rangle$ (full thick line)
- bottom: $D_x$ increased to $7.64 \times 10^{-1}$ (open circles)
Synchronization of clock cells under dark-bright cycles

- protocol II: the system experiences dark-bright cycles of duration $\Delta t = 12h$ and constant light intensity $I_0 = 1000$
- top: (a) time series for the $x$ variables of three SCN cells selected out of a lattice with 10201 cells with $\gamma = 1$ for $D_x = 7.64 \times 10^{-3}$
- (b) power spectra of the response of the three cells depicted in (a)
Transition to period synchronization of clock cells

- top: dependence of the period dispersion (black), order parameter magnitude (blue) and synchronization degree (red) with the coupling strength
- $D_x^*$: critical coupling strength for onset of period synchronization
- bottom: critical coupling strength vs. exponent $\gamma$ considering the behavior of the period variance (black) and synchronization degree (red).
Chemical coupling of chaotic maps

• if the local dynamics is governed by a one-dimensional map $x \mapsto f(x)$ we have (future coupling)

$$x_{n+1}^{(i)} = (1 - \varepsilon)f(x_n^{(i)}) + \varepsilon \sum_{j=1}^{N} \sigma(\vec{r}_i - \vec{r}_j)f(x_n^{(j)}).$$

• non-locally coupled map lattice in one spatial dimension (where $N' = (N - 1)/2$ for $N$ odd)

$$x_{n+1}^{(i)} = (1-\varepsilon)f\left(x_n^{(i)}\right) + \frac{\varepsilon}{\kappa(\gamma)} \sum_{s=1}^{N'} e^{-\gamma s} \left[ f\left(x_{n-\gamma s}^{(i-s)}\right) + f\left(x_{n+\gamma s}^{(i+s)}\right) \right],$$

• normalization condition

$$\sum_{k=1}^{N} \sigma(|\vec{r}_j - \vec{r}|) = 1 \Rightarrow \kappa(\gamma) = 2 \sum_{s=1}^{N'} e^{-\gamma s},$$

• periodic boundary conditions: $x_n^{(i \pm N)} = x_n^{(i)}$
Lyapunov spectrum

- Lyapunov exponents of a coupled map lattice: $\lambda_k = \ln \Lambda_k$, where $\{\Lambda_k\}_{k=1}^N$ are the eigenvalues of the matrix

$$\hat{\Lambda} = \lim_{n\to\infty} \left( \tau_n^T \tau_n \right)^{1/2n},$$

- where we define the ordered product of the jacobian matrices

$$\tau_n = T_{n-1} T_{n-2} \cdots T_1 T_0, \quad T_n^{(ij)} = \frac{\partial x_{n+1}^{(i)}}{\partial x_n^{(j)}},$$

- for the chemical coupling in one spatial dimension

$$T_n^{(ik)} = (1-\varepsilon)f' \left(x_n^{(i)}\right) \delta_{ik} + \frac{\varepsilon}{\kappa(\gamma)} \exp (-\gamma r_{ik}) f' \left(x_n^{(k)}\right) (1-\delta_{ik}),$$

- where $r_{ij} = \min_\ell |i - j + \ell N|$
Lyapunov spectrum of Bernoulli maps

- $f(x) = \beta x \mod 1$, strongly chaotic for $\beta > 1$
- Lyapunov spectrum
  \[ \lambda_k = \ln \beta + \ln \left| (1 - \varepsilon) + \frac{\varepsilon}{\kappa(\gamma)} b_k \right| \]
- periodic boundary conditions
  $\rightarrow$ jacobian matrices are circulant

\[ b_k = 2 \sum_{m=1}^{N'} e^{-\gamma m} \cos \left( \frac{2\pi km}{N} \right) , \]
Stability of a completely synchronized state

- \( x_n^{(1)} = x_n^{(2)} = \ldots = x_n^{(N)} = x_n^* \): defines a synchronization manifold \( S \) in the phase space

- Lyapunov spectrum of the completely synchronized state

  \[
  \lambda_k^* = \lambda_U + \ln \left| (1 - \varepsilon) + \frac{2\varepsilon}{\kappa(\gamma)} \sum_{m=1}^{N'} e^{-\gamma m} \cos \left( \frac{2\pi km}{N} \right) \right|
  \]

- \( \lambda_U \): Lyapunov exponent of the uncoupled map

- the completely synchronized state is transversely stable if \( \lambda_2^* \leq 0 \), such that \( \varepsilon_c \leq \varepsilon \leq \varepsilon'_c \), where

  \[
  \varepsilon_c = \left( 1 - e^{-\lambda_U} \right) \left( 1 - \frac{b_1}{\kappa(\gamma)} \right)^{-1}, \quad \varepsilon'_c = \left( 1 + e^{-\lambda_U} \right) \left( 1 - \frac{b_{N'}}{\kappa(\gamma)} \right)^{-1}
  \]
Synchronization of Ulam maps

- Ulam map
  \[ f(x) = 4x(1 - x), \ x \in [0, 1), \]
  strongly chaotic (\( \lambda_U = \ln 2 \))

- completely synchronized state is transversely stable if
  \[ \varepsilon_c \leq \varepsilon \leq \varepsilon'_c, \]
  \[ \varepsilon_c = \frac{1}{2\Delta}, \varepsilon'_c = \frac{3}{2\Delta'} \]

\[ \Delta = 1 - \frac{b_1}{\kappa(\gamma)}, \ \Delta' = 1 - \frac{b_{N'}}{\kappa(\gamma)} \]
Conclusions

- oscillator coupling mediated by a diffusing substance reduces, in the one-dimensional case, to an exponentially decaying (non-local) coupling (in the adiabatic limit)
- it allows to pass from a global (all-to-all) to a local (laplacian) coupling by varying a single parameter
- frequency and phase synchronization were analyzed in terms of the coupling parameter plane (strength vs. range)
- transition to frequency and phase synchronization in terms of both $K$ and $\gamma$
- recurrence quantification analysis used to characterize phase and frequency spatial patterns
- Lyapunov spectrum can be obtained and it is possible to study the transversal stability of the completely synchronized state
Thank you very much