Causodynamics of autowave patterns

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(Dated: July 8, 2005)

Perturbative dynamics of spiral and scroll waves involves the "response functions", i.e. critical eigenvectors of the adjoint lineaized operator, dual to the Goldstone modes. A well known method of calculating the Goldstone modes is time integration of the linearized equation. We suggest that backward time integration of the adjoint linearized equation, which we call causodynamics, can be used to calculate the response functions. This new method is more robust and easier to implement than existing methods. We illustrate how it works for propagating and rotating autowaves in reaction-diffusion systems. The method reveals unexpected qualitative difference between similarly looking regimes.

PACS numbers: 02.90.+p

Autowave vortices, i.e. spiral and scroll waves, are known as "organizing centres" in spatially extended dissipative nonlinear wave systems of various physical, chemical and biological origin[1–3]. But what does it mean to be an "organizing centre"? Here we introduce "causodynamics", a mathematical tool that gives a rigorous and quantitative meaning to this concept. We illustrate the usefulness of this tool for three examples of rotating spiral waves. It confirms that a spiral wave in excitable FitzHugh-Nagumo system[4], where waves propagate from the centre to the periphery, is an organizing centre. An "antispiral" in a complex Ginzburg-Landau equation [5], at parameter values where waves propagate from periphery towards the centre, nevertheless is also an organizing centre. However, a similarly looking, converging "antispiral" in a variant of FitzHugh-Nagumo equation with reflecting waves [6] is not an organizing centre.

More technically, causodynamics is a numerical procedure for computing *response functions (RFs)*, which are used in asymptotic theories of the movement of curved autowave fronts, as in the Kuramoto-Sivashinsky equation [7], and of the drift of spiral waves[8] and their three-dimensional relatives, scroll waves[9]. The RFs determine how the effects of an elementary perturbation onto the wave's location and/or phase depend on where the perturbation is applied.

The two uses of causodynamics are closely related. In the asymptotic theories, the integrals determining the drift of spirals and scrolls converge if the RFs are localized, as in known examples [10–13]. Hence a "wave-particle duality" of spiral waves: they fill the whole space, but behave as particle-like objects[14]. This localization can be identified with the concept of an "organizing centre", and correlates with the outward direction of the group velocity. Such correlation was hypothesized some time ago [9] and rigorous results about it have recently started to appear [15].

The suggested procedure answers two questions: whether a particular pattern is an organizing centre, and what are its RFs. The answers are: if solutions of the causodynamics equation converge to localized functions, this is an organizing centre, and the localized solutions provide the RFs; if not, this is not an organizing centre, and RFs do not make sense. The procedure does not use group velocity, so is applicable even if group velocity is not defined or its direction is not easily decided.

Formal setting: Lyapunov co-vectors of relative equilibria. Consider a continuous time dynamical system

$$\dot{\psi} = f(\psi) \tag{1}$$

symmetric with respect to a Lie group Γ of orthogonal linear transformations, $f(\Gamma\psi) \equiv \Gamma f(\psi)$. For instance, (1) can represent a reaction-diffusion system of equations, ψ spatial distribution of the concentrations of reagents, and Γ a group of rotations and translations of the spatial variables.

Consider also a one-parametric subgroup $\Gamma^t = \exp(\gamma_* t) \subset \Gamma$ with infinitesimal generator γ_*. This could be the subgroup of translations in a certain direction, or the subgroup of rotations around a certain axis. Let Ψ be ψ viewed in the moving frame of reference determined by Γ^t, $\psi(t) = \Gamma^t\Psi(t)$. Then Ψ satisfies $\dot{\Psi} = f(\Psi) - \gamma_*\Psi$. So a relative equilibrium $\psi_* = \Gamma^t\Psi_*$: $\dot{\Psi}_* = 0$, $\Gamma\Psi_* \neq \Psi_*$, i.e. a rotating or propagating wave, and corresponding γ_* satisfy the automodel equation

$$f(\Psi_*) - \gamma_*\Psi_* = 0. \tag{2}$$

The linearized equation, corresponding to (1), is

$$\frac{\mathrm{d}}{\mathrm{d}t}|\psi\rangle = F(\psi_*)|\psi\rangle \tag{3}$$

where $F = Df$ is the tangent operator (linearization) of f, and $|\psi\rangle$ is the perturbation of ψ (in general, we use ket-vectors to denote infinitesimal perturbations). Consider (3) in the moving frame of reference, $|\psi\rangle(t) = \Gamma^t|\Psi\rangle(t)$. This gives

$$\frac{\mathrm{d}}{\mathrm{d}t}|\Psi\rangle = F(\Psi_*)|\Psi\rangle - \gamma_*|\Psi\rangle = L|\Psi\rangle, \tag{4}$$

where $L = F(\Psi_*) - \gamma_*$ is a constant operator. Appropriately chosen infinitesimal generators γ_j of Γ produce the "symmetry modes", or *"Goldstone modes" (GMs)* , $|\Psi_j\rangle = \gamma_j \Psi_*$, which are eigenvectors of L, $L|\Psi_j\rangle = \lambda_j|\Psi_j\rangle$, with $\mathrm{Re}\lambda_j = 0$ (the term descends from particle physics [16]). Thus, if solution $\psi_*(t)$ of (1) is linearly stable modulo symmetry Γ, then a solution of (4) or equivalently (3) with typical initial conditions in the limit $t \to +\infty$ will be a linear combination of GMs. That is, GMs can be calculated as leading Lyapunov vectors (LVs), via long-time limits of solutions to (4) or (3) with arbitrarily chosen initial conditions, a method often used in generic systems [17]. Finding GMs as $|\Psi_j\rangle = \gamma_j \Psi_*$ is trivial; yet if it wasn't, equation (3) is conceptually simpler than (4) as its solution does not require explicit knowledge of Γ^t.

The perturbation theory for the drift as in [7–9] requires the RFs, which are defined as eigenvectors of L^+,

$$\bar{\lambda}_j \langle \Psi_j| = L^+ \langle \Psi_j| = (F^+(\Psi_*) - \gamma_*^+)\langle \Psi_j| \tag{5}$$

(we use bra-vectors for linear functionals in the space of infinitesimal perturbations), dual to the GMs $|\Psi_j\rangle$. Problem (5) is overdetermined, as γ_*^+ is fixed by the automodel solution (2). Hence a straightforward approach requires very accurate knowledge of (Ψ_*, γ_*), otherwise the results are unusable[10–13]. However, by the analogy with $|\Psi_j\rangle$, vectors $\langle \Psi_j|$ can be calculated in the comoving frame of reference, as LVs of

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle \Psi| = L^+\langle \Psi| = (F^+(\Psi_*) - \gamma_*^+)\langle \Psi|$$

("Lyapunov co-vectors"). By using $\gamma_*^+ = -\gamma_*$ and introducing $\langle \psi| = \Gamma^{-t}\langle \Psi|$, we obtain, via elementary transformations, *the causodynamics equation*

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle \psi| = F^+(\psi_*(-t))\langle \psi| \tag{6}$$

which allows calculation of the Lyapunov co-vectors without explicit recourse to (Ψ_*, γ_*).

So, eigenvectors of the adjoint linarized operator L^+ can be calculated as principal LVs of (6), the adjoint linearized problem in the stationary frame of reference, on the solution *turned backwards in time*. The advantage of this method is that (Ψ_*, γ_*) are not required, it is enough to know $\psi_*(t)$, which is achieved by direct numerical simulation of (1).

To follow up the effects and to trace back the causes. The need for backward integration is in fact a very general issue, not restricted to systems with continuous symmetries[17]. The solution of a linear problem $\frac{\mathrm{d}}{\mathrm{d}t}|\psi\rangle = F(t)|\psi\rangle$, $t \ge 0$, $|\psi\rangle(0) = |\psi_0\rangle$, could be symbolically written via a time-ordered exponential $|\psi\rangle(t) = \exp\left(\int_0^t F(\tau)\,\mathrm{d}\tau\right)|\psi_0\rangle$. For such exponentials we have the following identity:

$$\left[\exp\left(\int_0^t F(\tau)\,\mathrm{d}\tau\right)\right]^+ = \exp\left(\int_0^t F^+(t-\tau)\,\mathrm{d}\tau\right), \tag{7}$$

since the exponential of the operator integral is, in fact, a continuous product, i.e. a limit of a product of a near-identical operators corresponding to different intervals of a partition of $[0, t]$, and adjugation swaps the order of multiplication of these near-identical operators.

Let $G(t_1, t_2) = \exp\left(\int_{t_1}^{t_2} F(\tau)\,\mathrm{d}\tau\right)$ be the propagator (tangent map) along a particular trajectory with tangent operator $F(t)$, so the LVs are the eigenvectors of G for large $(t_2 - t_1)$. LVs with largest real part eigenvalues designate the directions of the perturbations that grow the fastest or decay the slowest, for typical, randomly chosen initial perturbations.

To predict or to control the system, it is important to know consequences of particular perturbations. To determine those, one needs to know the components of a given perturbation along the eigenvectors of G. Such components are obtained by projecting the perturbation to the eigenvectors of G^+. According to (7), $G^+(t_1, t_2)$ is the propagator of the equation with adjoint and *time-inverted* operator, i.e. of equation (6).

The leading Lyapunov vectors $|\psi_j\rangle$ indicate the most important *effects* achievable by small perturbations. They can be found by calculating the linarized *"effectodynamics"* equation (3) forward in time.

The leading Lyapunov co-vectors $\langle \psi_j|$ indicate the most important *causes*, i.e. what is needed to achieve those effects. They can be found by calculating the adjoint linearized *"causodynamics"* equation (6) backward in time.

Causodynamics of excitation waves. Now we illustrate how this works for excitation waves in FitzHugh-Nagumo reaction-diffusion system of equations,

$$\partial_t u = \frac{1}{\epsilon}\left(u - \frac{u^3}{3} - v\right) + \nabla^2 u, \quad \partial_t v = \epsilon(u - \alpha v + \beta), \tag{8}$$

where $\alpha = 0.5$, $\beta = 0.75$, $\epsilon = 0.3$, $u = u(\vec{r}, t)$, $v = v(\vec{r}, t)$, $\vec{r} \in \mathbb{R}^d$, $d = 1$ or 2, and $t \in [0, T]$. Here Γ is the connected component of the Euclidean group of $\mathbb{R}^d$. The linearized "effectodynamics" problem for perturbations $|u\rangle$, $|v\rangle$ is

$$\partial_t|u\rangle = \frac{1}{\epsilon}(1-u^2)|u\rangle - \frac{1}{\epsilon}|v\rangle + \nabla^2|u\rangle, \quad \partial_t|v\rangle = \epsilon|u\rangle - \epsilon\alpha|v\rangle, \tag{9}$$

and the adjoint linearized "causodynamics" problem is

$$\partial_t\langle u| = \frac{1}{\epsilon}(1-\tilde{u}^2)\langle u| + \epsilon\langle v| + \nabla^2\langle u|, \quad \partial_t\langle v| = -\frac{1}{\epsilon}\langle u| - \epsilon\alpha\langle v|, \tag{10}$$

where $u = u(\vec{r}, t)$ is a self-similar solution (relative equilibrium) of (8), and $\tilde{u} = u(\vec{r}, T-t)$ is the same solution reversed in time. Figure 1 illustrates solutions of these three problems for $d = 1$, for a single propagating pulse, and fig. 2 the same for $d = 2$, for a spiral wave.

The curvature-velocity coefficient in Kuramoto-Sivashinsky theory[7], which determines whether a convex

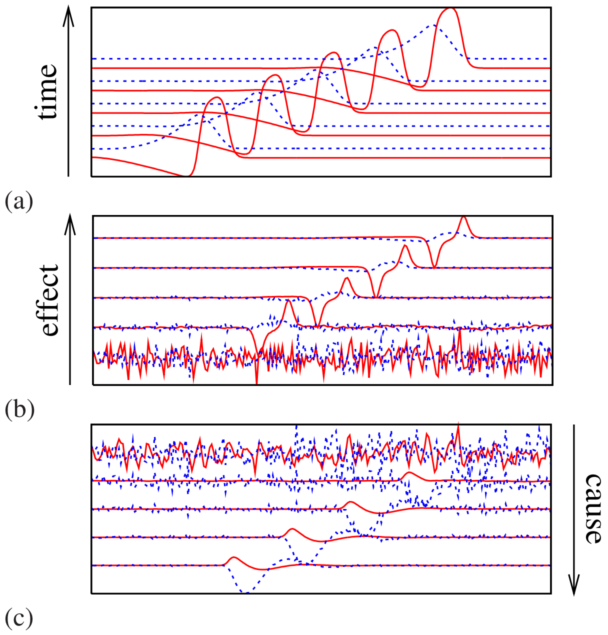

FIG. 1: (color online) Solutions of (a) FitzHugh-Nagumo system (8) ("dynamics"), (b) linearized system (9) ("effectodynamics") and (c) backward adjoint linearized system (10) ("causodynamics") in one spatial dimension. Solutions of linear problems are normalized, $\max_{x\in\mathbb{R}}(||u\rangle|, ||v\rangle|) = 1$ and similarly for $\langle u|$, $\langle v|$. Initial conditions for the linear problems are white noise. Red solid lines: u-components, blue dashed lines: v-components. Space scale 70, time interval between profiles 5, time goes from bottom to top, arrows by the sides indicate direction of calculation. Numerics: cental difference in space, $h_x = 0.5$, forward Euler in time, $h_t = 0.1$.

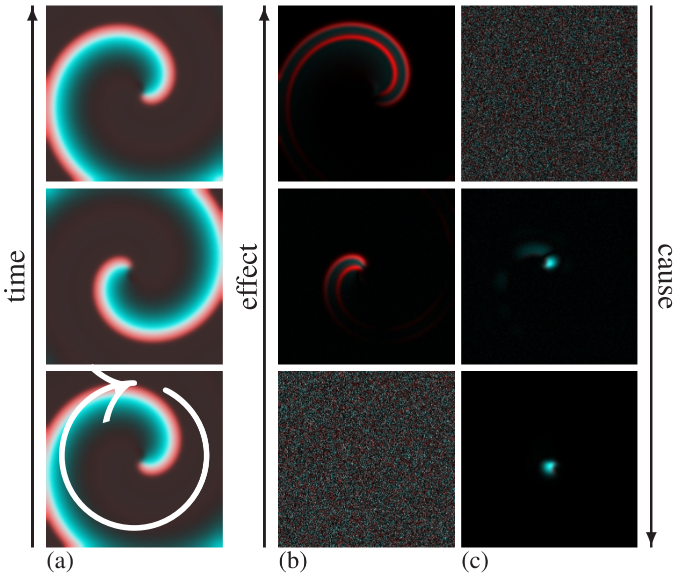

FIG. 2: (color online) (a) Dynamics, (b) effectodynamics and (c) causodynamics of a spiral wave in FitzHugh-Nagumo system (8) in two spatial dimensions. Solutions of linear problems are normalized as for fig. 1. Red colour component: absolute value of u-components, cyan colour component: absolute value of v-components. Space scale 40×40, snapshots with time interval 10, time goes from bottom to top, $h_x = 0.5$, $h_t = 0.03$.

autowave front is delayed or accelerated compared to a plane front, is the matrix element of the diffusion operator between the GM and the RF of the pulse solution of (8) for $d = 1$, fig. 1(a). Here $\Gamma \sim \mathbb{R}^1$, $\gamma_1 = -\partial_x$, and there is only one GM and one RF. Figures 1(b,c) illustrate how easily the GM and RF are found numerically. The solution of (9), fig. 1(b), converges, as it should, to the GM, the spatial derivative of the pulse. Solution of (10), fig. 1(b) converges to the RF of the pulse on the same timescale, but backwards in time. These results are enough to find the curvature-velocity coefficient.

The situation with the spiral wave, fig. 2, is more complicated. The Euclidean group of $\mathbb{R}^2$ is three dimensional, with two directions of translations and the rotation. So a typical solution of effectodynamics equation (9) converges to a linear combination of the three GMs, i.e. of a gradient of the spiral wave solution in some direction, and the angular derivative, fig. 2(b). Different initial conditions, set with a different seed of the pseudorandom number generator, produce similar pictures. Solution of the causodynamics equation (10) converges to a combination of the three RFs, fig. 2(c). In our numerics, this combination *is always localized* in the vicinity of the tip of the spiral. So, this spiral wave is a true organizing centre.

In these and further calculations, the empirical $|\mathrm{Re}(\lambda_j)|$ did not exceed 0.03, so the method is reasonably accurate. Individual RFs can be extracted from their mixture in the causodynamics solutions, using the biorthogonality of the set of RFs to the set of GMs [13].

Different kinds of "antispirals". We have done a similar "causodynamic analysis" for the complex Ginzburg-Landau equation

$$\partial_t z = (1 - (1 - i\alpha)|z|^2)z + (1 + i\beta)\nabla^2 z \qquad (11)$$

where $z = u + iv \in \mathbb{C}$, for $\alpha = -0.2$, $\beta = -1$, and for a modification of the FitzHugh-Nagumo system with quasi-soliton regimes, described in [6]. These two models admit solutions in the form of converging, concave spirals, which look like sinks rather than sources of waves, "antispirals", see fig. 3(a) and fig. 4(a). Are they organizing centres or not?

The effectodynamics solutions in both cases converge to gradients of the of the nonlinear solutions, which are delocalized, fig. 3(b) and fig. 4(b). No difference here.

The difference is revealed by the causodynamics solutions. For model (11), such solution converges to a narrowly localized peak around the rotation centre, fig. 3(c). So although this spiral rotates "the wrong way", it still is an organizing centre,

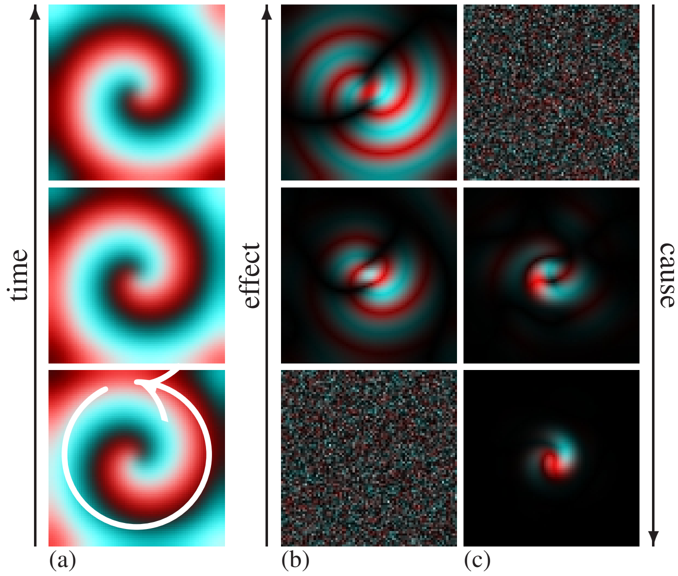

FIG. 3: Same, for a converging spiral in the complex Ginzburg-Landau equation (11). Space scale is 40×40, time interval between snapshots is 15, $h_x = 0.5$, $h_t = 0.025$.

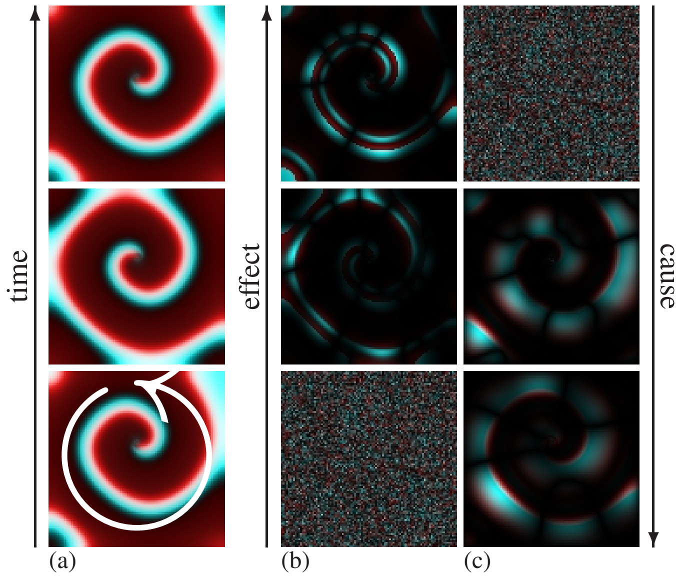

FIG. 4: Same, for a converging spiral in the Mornev et al. system [6]. Spatial scale 50×50, time interval between snapshots 10, spiral rotates inward with period about 6.8, $h_x = 0.5$, $h_t = 0.005$.

and will behave as an essentially localized, particle-like object, in its response to perturbations.

On the contrary, the causodynamics solution of model [6] shows no signs of localization near the core of the spiral. Instead, emphasized is the periphery of the spiral, fig. 4(c). So, this is not an organizing centre, and phenomenology of spirals and scrolls in this model will be entirely different from those in (8) and (11), and not described by asymptotics [8, 9].

Conclusions. Causodynamics, defined as backward-time integration of the adjoint linearized equation (6), provides a new method of calculating RFs, alternative to direct solution of the eigenvalue problem (5). The advantages of the new method are that it is easy to implement, although it may require large memory to store the solution of the nonlinear problem, and it is more robust as it does not need very accurate knowledge of the automodel solution.

On the qualitative level, this method allows to distinguish true organizing centres from those only looking so.

The considered examples are from a special area, but the mathematics involved is fairly generic. Lyapunov vectors are widely used in the analysis of complex systems. Lyapunov covectors, and causodynamics as a method of their calculation, can be at least as useful as Lyapunov vectors are already.

Author is grateful to I.V. Biktasheva for inspiring discussions and to M.A. Tsyganov for advice on model [6]. Support by EPSRC grants GR/S43498/01 and GR/S75314/01 is acknowledged.

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