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PARALLEL COMPUTATION AND MEASUREMENT UNCERTAINTY IN NONLINEAR DYNAMICAL SYSTEMS*

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Abstract

In certain physical systems measuring one variable of the system modifies the values of any number of other variables unpredictably. We show in this paper that under these conditions a parallel approach succeeds in carrying out the required measurement while a sequential approach fails. Specifically, we show that for a nonlinear dynamical system, namely, the Belousov-Zhabotinskii chemical reaction, measurement disturbs the equilibrium of the system and causes it to enter into an undesired state. If, however, several measurements are performed in parallel, the effect of perturbations seems to cancel out and the system remains in a stable state.

Keywords: nonlinear dynamical system, parallel computation, measurement, perturbation, Hopf bifurcation, Belousov-Zhabotinskii reaction.

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1 Introduction

Let $\mathcal{S}$ be a physical system, such as one studied by biologists (e.g., an ecosystem), or one maintained by engineers (e.g., a nuclear reactor). The system has n variables which are to be measured. One property of $\mathcal{S}$ is that measuring one of its variables modifies the values of any number of other variables of the system unpredictably. We show in this paper that under these conditions a parallel approach succeeds in carrying out the required measurement while a sequential approach fails.

Usually, the main purpose of parallelism is to speed up computations that would otherwise require an inordinate amount of time if performed sequentially (that is, using one processor). Thus, in parallel computation, n processors, $n > 1$, cooperate to solve a computational problem by working on it simultaneously. Theoretical and practical results have been obtained over the last twenty five years, demonstrating that parallelism yields significant improvements not only in the *speed* with which a solution is arrived at, but also in the *quality* of the solution itself. The level of improvement achieved through parallel computation in each case varied over a wide range depending on the problem being solved: from sublinear, to linear, or even superlinear in the number of processors used on the parallel computer. Furthermore, those results were obtained within conventional paradigms (such as, for example, when all the data required by a computation are available at the outset), as well as unconventional paradigms (such as, for example, when the data arrive in real time and the results must be delivered by a certain strict deadline). For surveys of these results, see [1, 2, 5, 18].

An important characteristic of traditional analyses of parallel computation is that the conditions governing the computational environment are, in a fashion, fully determined by the human in charge and the model of computation used. For example, in a real-time computation, if it is deemed that the arrival rate of the data is too high, it is possible for the people responsible for the computation to slow down the arrival rate, or to extend the deadline by which a solution is to be delivered, or to use a faster computer, and so on. A radical departure from this paradigm was taken recently. In [3], the focus is on computational environments in which a computation can succeed if and only if it is performed in parallel. In these environments, it is the laws of nature that prevail, rather than human-imposed computational circumstances or conditions on the computation. Specifically, it is shown that the principles governing such fields as physics, chemistry, and biology, are responsible for causing the inevitable failure of any sequential approach to solving the problem at hand, while at the same time allowing a parallel approach to succeed. A typical example of such principles is the uncertainty involved in measuring several related variables of a physical system. Another principle expresses the way in which the components of a system in equilibrium react when subjected to outside stress.

An example environment in which these phenomena manifest themselves is dynamical systems. In general, a *system* is a collection of elements that interact with one another. The system is characterized by a number of variables among which relationships of cause and effect hold. In particular, the system receives a number of inputs and produces a number of outputs based on these inputs. In a *static* system, the current values of the outputs depend only on the instantaneous values of the present inputs. If, on the other hand, the system has memory such that current outputs are based on present as well as past inputs, it is said to be a *dynamical* system. Here, variables are time-dependent. Excitations and responses vary with time. Moreover, the derivatives of variables with respect to time at any moment depend on the values of these variables at that moment [8]. Examples of dynamical systems include electrical systems, mechanical systems, thermal systems, fluid systems, and so on.

An illustration of how the ideas in [3] apply to dynamical systems is presented in [4]. There, it is shown that a resistance-inductance-capacitance (RLC) circuit certain variables of which are measured sequentially (in other words, one after the other), undergoes significant perturbations that affect its dynamical behavior. By contrast, these perturbations could be eliminated when the measurements are performed in parallel, that is, when the variables are measured simultaneously. This result confirmed the existence of physical systems with the property that certain operations on them can be performed successfully in parallel but not sequentially.

The RLC circuit considered in [4] is a *linear* dynamical system [7]. As such, the effect of the perturbations it experiences from measurement of its variables is, in general, relatively small. A natural question to ask therefore is whether dynamical systems that are *nonlinear* suffer more dramatically from sequential measurements of their attributes. In this paper we provide an example to illustrate the role played by parallelism when measurements are performed on nonlinear systems.

In general, most engineering systems, and in particular those chemical systems of interest in this paper, are required to stay in a stable equilibrium state. However, perturbations due to certain measurement operations may result in an instability known as a *Hopf bifurcation*. After the bifurcation, the equilibrium state will be unstable and the system will be in a new undesired state, such as periodic or chaotic. Thus, Hopf bifurcations should be avoided. On the other hand, it is usually required to know the detailed dynamical process of such systems, and a measurement near a Hopf bifurcation is needed. If a measurement causes a Hopf bifurcation, and the system, for example a chemical reaction, goes to a new state, the components and their quantity in the new state are very different from the old state [12]. Thus, in order to design a better measurement scheme, the perturbations caused by measurements should be considered.

In this paper, we extend our study begun in [4] to nonlinear dynamical systems. In such systems, the state variables, that is, the variables describing the behavior of the system, are related to one another by nonlinear functions. A specific nonlinear dynamical system is selected for this study, namely, the so-called Belousov-Zhabotinskii chemical reaction (BZ-reaction). The effect of measurements on the dynamical behavior of the BZ-reaction is analyzed. It is shown here that measurement disturbs the equilibrium of the system and causes it to enter into an undesired state. If, however, several measurements are performed in parallel, the effect of perturbations seems to cancel out and the system remains in a stable state.

It is important to note that the type of perturbations considered in this paper are caused by the instruments used in the measurement. When we say that measurements are performed *simultaneously*, we do not mean that the measuring instruments are applied "at the same time" to the system whose variables are to be measured. Instead, what is meant is that these instruments are permanently connected to the system and that the measurements are simultaneously recorded by the processors of a parallel computer. Further, these data should be dealt with in parallel because the system is dynamic. Thus, there are two reasons for which parallel computation is needed in dynamical systems:

1. It allows the perturbations caused by several permanently built-in measuring instruments to be cancelled out, and

2. It allows the dynamical behavior of the system to be better determined.

In contrast, sequential measurements could cause larger perturbations, and the dynamical behavior of the system could not be well determined because the state of the system is changing during the measurement events.

The remainder of this paper is organized as follows. In section 2, a hypothetical physical system is described whose behavior changes when measurements are performed on its variables. A concrete system with this property is described in section 3 along with an analysis of the effect of parallelism when measuring the system's variables. Some concluding remarks are offered in section 4.

2 Computational Problem

A physical system $\mathcal{S}$ possesses the following characteristics:

1. For $n > 1$, the system possesses a set of n variables (or properties), namely, $q_1, q_2, \ldots, q_n$. Each of these variables is a physical quantity (such as, for example, temperature, humidity, density, pressure, electric charge, and so on). These quantities can be measured and/or controlled independently, each at a given discrete location (or point) within $\mathcal{S}$. Henceforth, q_i, $1 \leq i \leq n$, is used to denote a variable as well as the discrete location at which this variable is measured and/or controlled.

2. The system is in a state of equilibrium, meaning that the values q_1, q_2, …, q_n satisfy a certain global condition $\mathcal{C}(q_1,\ q_2,\ \ldots,\ q_n)$.

3. At regular intervals, the state of the physical system is to be recorded. In other words, the values $q_1, q_2, \ldots, q_n$ are to be measured at a given moment in time where $\mathcal{C}(q_1,\ q_2,\ \ldots,\ q_n)$ is satisfied. Each interval has a duration of $\mathcal{T}$ time units; that is, the state of the system is measured every $\mathcal{T}$ time units.

4. If the values $q_1, q_2, \ldots, q_n$ are measured *one by one*, each separately and independently of the others, this disturbs the equilibrium of the system. Specifically, suppose (without loss of generality) that $q_1, q_2, \ldots, q_{i-1}$ have already been measured, for some i, $1 < i < n$. Now, when q_i is subsequently measured, *at least one* other value q_j, $1 \leq j \leq n$ and $j \neq i$, will change unpredictably shortly thereafter (within one time units), such that $\mathcal{C}(q_1,\ q_2,\ \ldots,\ q_n)$ is no longer satisfied. Most importantly, the values of $q_{i+1}, q_{i+2}, \ldots, q_n$, none of which has yet been registered, may be altered irreparably.

This last property of $\mathcal{S}$ is reminiscent of a number of well-known principles that manifest themselves in many subfields of the physical and natural sciences and engineering, as illustrated in what follows.

Uncertainty in measurement

The phenomenon of interest here occurs in systems where measuring one variable of a given system affects, interferes with, or even precludes the subsequent measurement of another variable of the system. It is important to emphasize that the kind of uncertainty of concern in this context is in no way due to any errors that may be introduced by an imprecise or not sufficiently accurate measuring apparatus.

1. In quantum mechanics, *Heisenberg's uncertainty principle* puts a limit on our ability to measure simultaneously pairs of 'complementary' variables. Thus, the *position* and *momentum* of a subatomic particle, or the *energy* of a particle in a certain state and the *time* during which that state existed, cannot be defined at the same time to arbitrary accuracy [6]. In fact, what this principle says is that once *one* of the two variables is measured (however accurately, but independently of the other), the act of measuring itself introduces a disturbance that affects the value of the *other* variable. For example, suppose that at a given moment in time t_0 the position p_0 of an electron is measured. Assume further that it is also desired to determine the electron's momentum m_0 at time t_0. When the momentum is measured, however, the value obtained is not m_0, as it would have been changed by the previous act of measuring p_0.

2. In digital signal processing the *uncertainty principle* is exhibited when conducting a Fourier analysis. Complete resolution of a signal is possible either in the time domain t or the frequency domain w, but not both simultaneously. This is due to the fact that the Fourier transform is computed using e^{iwt}: Since the product wt must remain constant, narrowing a function in one domain, causes it to be wider in the other [10, 14]. For example, a pure sinusoidal wave has no time resolution, as it possesses nonzero components over the infinitely long time axis. Its Fourier transform, on the other hand, has excellent frequency resolution: It is an impulse function with a single positive frequency component. By contrast, an impulse (or *delta*) function has only one value

in the time domain, and hence excellent resolution. Its Fourier transform is the constant function with nonzero values for all frequencies and hence no resolution.

Other examples in this class include image processing, sampling theory, spectrum estimation, image coding, and filter design [17].

Each of the phenomena discussed typically involves *two* variables in equilibrium. Measuring one of the variables has an impact on the value of the other variable. The system $\mathcal{S}$, however, involves *several* variables (two or more). In that sense, its properties, as listed at the beginning of this section, are extensions of these phenomena.

3 Measurement in Dynamical Systems

The dynamical system of concern here consists of at least two variables and two system parameters. The system's behavior, namely, equilibrium, periodic, or chaotic, is determined by the parameters and the initial values of the variables. When one or more parameters change, the dynamical system may experience a phase transition, that is, a change of state (equilibrium point, period, chaos). Near the critical points, any perturbations, such as those arising when performing measurements on the variables, may cause a phase transition. The old state is unstable, and a new state appears.

Often, such as in chemical reactions, it is desirable that the system be in a stable equilibrium point state. Further, the state close to the phase transition critical point may be chosen in order, for example, to speed up the reaction. In this case, some perturbations caused by measurements may lead to undesired phase transitions. Simultaneous measurements on two or more variables, on the other hand, can prevent the phase transition as shown in what follows.

In dynamics, the phase transition is studied by a so-called *bifurcation analysis*. When the form of the system equations is known, we can obtain the condition and stability of the phase transition (bifurcation) as a function of the system parameters. The pertubations caused by measurements are usually equivalent to modifying the values of the parameters. Therefore, an analytical form of the bifurcation is useful to analyze the perturbations caused by measurements.

A simple but common bifurcation from equilibrium point to period or chaos is Hopf bifurcation. When a system is in Hopf bifurcation, the eigenvalues of the Jacobian have zero real part but nonzero imaginary part, and the first derivative of the real part with respect to the state variables is not zero. With these conditions, one can determine when the system is in Hopf bifurcation.

3.1 An Example of A Nonlinear Dynamical System

The Oregonator model of the BZ reaction is as follows [9, 13, 16]:

$$\begin{aligned} \dot{\alpha} &= s(\eta - \eta\alpha + \alpha - q\alpha^2) \\ \dot{\eta} &= s^{-1}(-\eta - \eta\alpha + f\rho) \\ \dot{\rho} &= w(\alpha - \rho) \end{aligned} \tag{1}$$

where $\alpha \propto [HBrO_2]$, $\eta \propto [Br^-]$, $\rho \propto$ [Ce(IV)], and s, w, q, and f are parameters. All variables and parameters are nonnegative.

The equilibrium point $(\bar{\alpha}, \bar{\eta}, \bar{\rho})$ of the system is the solution of equation (1) by letting $\dot{\alpha} = \dot{\eta} = \dot{\rho} = 0$:

$$\begin{aligned} \bar{\alpha} &= [-q + 1 - f + \sqrt{(q - 1 + f)^2 + 4q(1 + f)}]/2q \\ \bar{\eta} &= f\bar{\alpha}/(1 + \bar{\alpha}) \\ \bar{\rho} &= \bar{\alpha}. \end{aligned} \tag{2}$$

The Jacobian of the system is

$$J = \begin{bmatrix} s(-\bar{\eta} + 1 - 2q\bar{\alpha}) & s(1 - \bar{\alpha}) & 0 \\ -s^{-1} + \bar{\eta} & s^{-1}(-1 - \bar{\alpha}) & s^{-1}f \\ w & 0 & -w \end{bmatrix}. \tag{3}$$

By letting

$$|J - I\lambda| = 0, \tag{4}$$

we can obtain a form of the eigenvalue λ and the system variables. Rather than solving the equation for λ, which would be complicated, we search instead for Hopf bifurcations using the Hopf bifurcation conditions. Let $\lambda = a + ib$, where a and b are real, and substitute it into equation (4). This

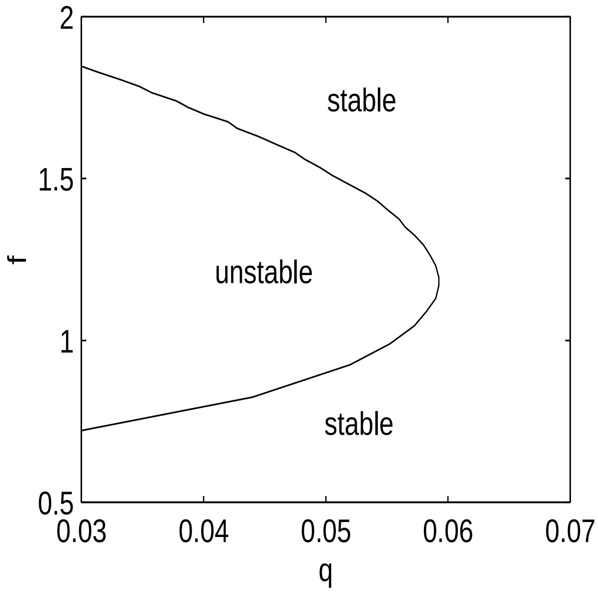

Figure 1: The system in Hopf bifurcation.

yields two equations for the real and imaginary parts. Letting $a = 0$ and $b \neq 0$, we obtain the following two equations:

$$w - s - sb^2 + s^2\bar{\eta}w + 2sq\bar{\alpha} + 2sq\bar{\alpha}^2 + 2s^2q\bar{\alpha}w + 2s\bar{\eta} - s\bar{\alpha} - s^2w + \bar{\alpha}w = 0 \quad (5)$$

$$s^2\bar{\eta}b^2 + wfs - wfs\bar{\alpha} - 2sq\bar{\alpha}w - 2sq\bar{\alpha}^2w - 2s\bar{\eta}w + s\bar{\alpha}w + sw + b^2 + \bar{\alpha}b^2 \\ -s^2b^2 + 2s^2q\bar{\alpha}b^2 + swb^2 = 0. \quad (6)$$

Solving equation (5) for b^2 and substituting in equation (6), we obtain the expression for the Hopf bifurcation. The condition $\frac{\partial a}{\partial c}|_{a=0} \neq 0$ can also be checked, where c stands for s, f, q, or w.

For convenience, we set $s = 1.27$ and $w = 0.161$. Figure 1 plots the relation between the other two parameters f and q when the system is in Hopf bifurcation. When the values of f and q are taken in the regime marked by 'stable', the system is in a stable equilibrium point state as shown in Fig. 2(a). When the values are taken in the region marked by 'unstable', the equilibrium point is unstable, and a new stable periodic state appears

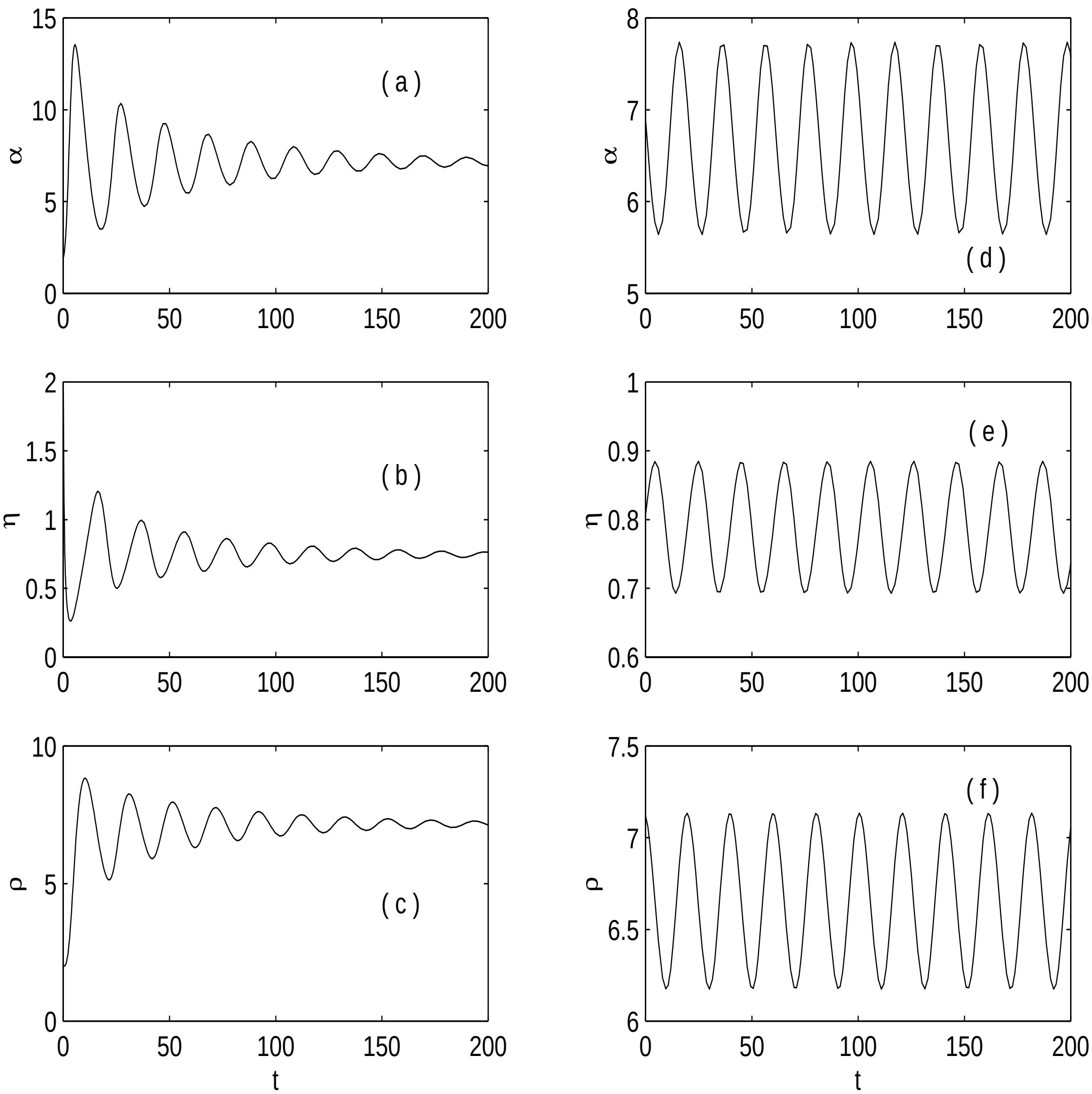

Figure 2: Time series of the BZ reaction, when the parameters are chosen in the stable regime (a,b,c), and unstable regime (d,e,f), respectively.

as displayed in Fig. 2(b). From the stable equilibrium point state to the periodic state, the system experiences a Hopf bifurcation.

As mentioned previously, it is desired that the system be in a stable equilibrium point. When measurement is performed sequentially, the perturbations, on q for example, may lead the system from the stable regime to an unstable regime. Now if we measure simultaneously, the perturbations may change the values of f and q simultaneously, and it is possible for f and q still to be located in the stable regime. In this case, simultaneous measurement keeps the system stable. We elaborate this point more formally in what follows.

3.2 Analysis

For the Oregonator model of the BZ reaction, the condition for the system in Hopf bifurcation is expressed by equation 6 (after substituting for b^2 from equation 5 and for $\bar{\alpha}$, $\bar{\eta}$, and $\bar{\rho}$ from equation 2). In this equation, the system's four parameters are related nonlinearly. For simplicity, let us assume that the measurement disturbs only two of them. When $f = 1.0$ and $q = 0.05$, we obtain w as a function of s,

$$\begin{aligned} w \approx & (2\sqrt{0.013s^8 + 0.453s^6 + 16.043s^4 + 110.565s^2 + 755.289} \\ & -0.225s^4 - 1.356s^2 - 54.965)/(1.028s^3 + 16.062s)\,, \end{aligned} \tag{7}$$

where s and w are not less than zero.

Fig. 3(a) displays w changing with s. When the values of w and s are on the curve, the system is in Hopf bifurcation. Above the curve, the system is in stable equilibrium state. Under the curve, the equilibrium is unstable. It is seen from the figure that the unstable parameter regime increases rapidly as w decreases. If before the measurement, w and s are near 0.5 and 5, respectively, the system is in a stable equilibrium state. In this case, a measurement that causes w to decrease will easily lead the system to an undesired state.

If we perform several measurements *simultaneously*, when w is perturbed, s may be perturbed too *simultaneously*. It is easy to see from Fig. 3(a) that the perturbation on s is helpful to decrease the effect of the perturbation on w. For example, if initially $w = w_0 = 0.5$ and $s = s_0 = 5.0$, the system is in the stable regime. Now, if a measurement disturbs $\Delta w = -0.06$ and $\Delta s > 1$ or < -1, the system is still located in the stable regime at $(w, s) = (w_0 + \Delta w, s_0 + \Delta s)$.

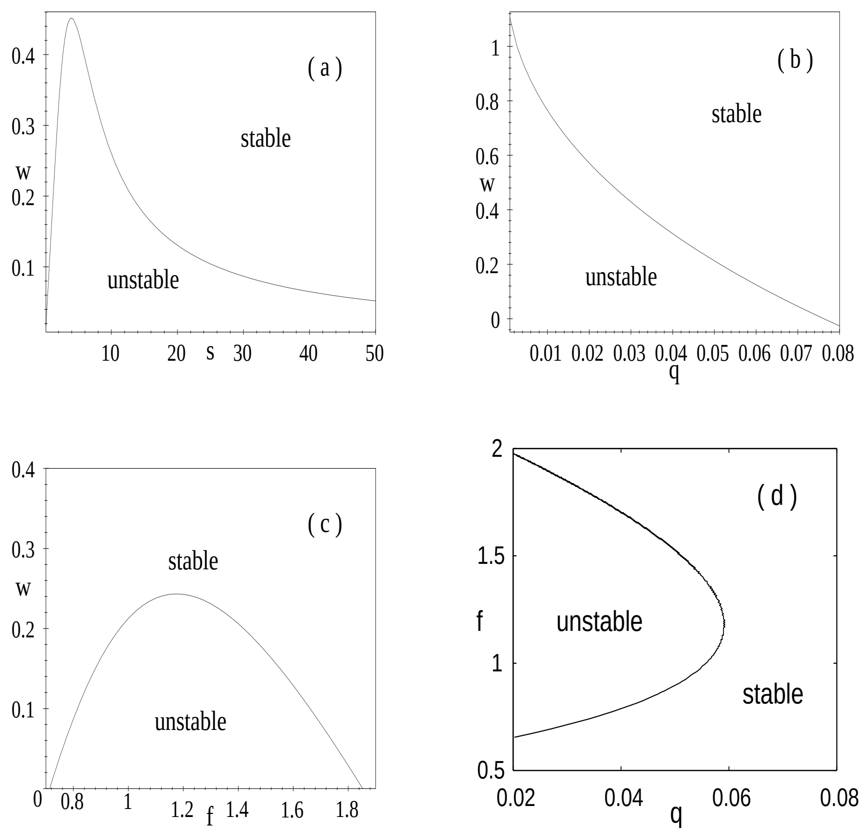

Figure 3: Hopf bifurcation diagrams of the B-Z reaction. (a) $f = 1.0$ and $q = 0.05$; (b) $f = 1.0$ and $s = 1.27$; (c) $s = 1.27$ and $q = 0.05$; (d) $w = 0.161$ and $s = 1.27$.

Similarly, when we fix $f = 1.0$ and $s = 1.27$, the Hopf bifurcation condition is expressed by w and q as shown in Fig. 3(b). Here, only the perturbation causing q to increase is useful for releasing the effect from the perturbation on w. Again, Fig. 3(c) is the Hopf bifurcation diagram when $s = 1.27$ and $q = 0.05$. The perturbation on both w and f can be better than on w or f alone. The same conclusion can be drawn from Fig. 3(d) where $w = 0.161$ and $s = 1.27$ are fixed.

4 Conclusion

A hypothetical physical system is described in [3] with the property that certain operations on its variables can only succeed if performed in parallel. Instances of these operations include measuring or setting a number of physical attributes of the system, such as temperature, pressure, voltage, and so on. Success or failure of these operations is determined by the laws of nature governing the behavior of the system. Examples of these laws are *Heisenberg's uncertainty principle* in quantum mechanics, which puts a limit on our ability to measure with a high degree of accuracy pairs of 'complementary' variables, *Le Châtelier's principle* of chemical systems in equilibrium, and the *homeostatic principle* in biology which is concerned with the behavior displayed by an organism under stress.

A concrete example of such a system was presented in [4]. There, a simple RLC circuit is described whose dynamical behavior is significantly affected by sequential measurements of its variables. A parallel measurement approach, on the other hand, greatly mitigates these perturbations and often eliminates them altogether. It should be noted that our interest in [4] was in the *short-term* dynamical behavior of the RLC circuit. Such behavior is important in the context of real-time control applications, where the variables of a system need to be monitored on a permanent basis and measured at regular intervals [11]. By contrast, it is clear that the *long-term* behavior of the RLC circuit (a *linear* dynamical system) is very simple: The circuit settles into a stable equilibrium state.

In this paper, we extended our study to nonlinear dynamical systems. The effect of measurements on the dynamical behavior of the Belousov-Zhabotinskii chemical reaction was analyzed using Hopf bifurcation theory. We showed that measurement disturbs the equilibrium of the system and causes it to enter into an undesired state. Therefore, both the short and long term behaviors of the system could be changed by perturbations. If, however, several measurements are performed in parallel, the effect of perturbations seems to cancel out and the system remains in a stable state. We note in passing, for its historical interest, the fact that one of pioneers in the field of computation, Alan Turing, did some important work in chemistry during the early 1950's, particularly on chemical reactions with nonlinear kinetic laws [15]. We feel that revisiting this subject from a *computational* viewpoint fittingly closes the scientific cycle (as well as the historical one).

The example of [4] and that of this paper are both of systems that are affected by *measurements*, in the sense that measuring one of their variables (or several sequentially) disturbs their equilibrium. An open question for further investigation is to study the role of parallelism in systems whose equilibrium is disturbed when the values of their variables are deliberately *modified* (rather than merely *measured*) by an external operator.

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