Clustered Causal Ordering

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Abstract

Causal arguments are ubiquitous in human reasoning about physical phenomena. Formalization and computer modeling of these arguments is a major goal of qualitative physics. Building causal qualitative models of rich domains like classical thermodynamics has proven to be difficult. The most accessible and widely agreed upon source of knowledge is found in textbooks, usually in the form of noncausal mathematical equations. Iwasaki and Simon's causal ordering procedure addresses this problem by attempting to extract causality directly from mathematical equations. This paper examines the causal ordering procedure from the point of view of qualitative process theory. We illustrate how causal ordering is dependent on the choice of exogenous variables which in turn requires consideration of the many ways in which a system can interact with its surroundings. In other words, it suffers from environmental instability. This paper shows how directly influenced quantities can be used to find environmentally stable causal clusters. Because of their stability, causal clusters can be studied in isolation and used as building blocks in a broad range of environments. We demonstrate our ideas in the domain of thermodynamics by uncovering the causality of the Ideal Gas Law and Joule's temperature-internal energy relation.

1 INTRODUCTION

Causality plays a major role in human reasoning about physical phenomena. Since causality explains how a system achieves its behavior, it has been universally adopted as a means of explaining the happenings of nature. For the engineer, causal reasoning is important because it addresses the *attribution* problem [6]. Causality enables the engineer to attribute causes to observed effects in tasks such as diagnosis, design, and analysis. Formalizing and computer modeling of these and related tasks is a major goal of qualitative physics.

Forbus' qualitative process (QP) theory [2] may be viewed as a language in which the mechanisms of causally deterministic natural phenomena can be expressed. Processes are a key ontological primitive of the theory. They are the explicit causal mechanisms responsible for all changes. Examples are moving, accelerating, heating up, boiling and cooling. Processes cause changes by directly influencing quantities. Thus, they impose a direction of causality towards the directly influenced quantity. For example, an acceleration process directly influences an object's velocity. The object's velocity is causally dependent on the rate of that acceleration.

Unfortunately, building causal qualitative models of rich domains like classical thermodynamics is a difficult task. The most accessible and widely agreed upon source of knowledge is often found in textbooks in the form of noncausal mathematical equations. The equations concisely summarize what can happen but say nothing about underlying causality. Consider for example the Ideal Gas Law PV = mRT, where P, V, m and T represent gas pressure, volume, mass and temperature, respectively, and R is a constant. Is temperature causally dependent on pressure, or vice versa? Thermodynamics textbooks generally do not say. The qualitative modeler may try to resolve this problem by jumping to a finer level of detail, but this is often difficult. Scientific theories at that level may be difficult to find or hard to translate into a qualitative framework¹. The causal ordering procedure presented by Iwasaki and Simon [3,4] addresses this problem by attempting to extract causality directly from mathematical equations.

2 CAUSAL ORDERING

The causal ordering procedure begins with a mathematical model of a phenomenon in the form of n independent equations $\vec{f}(\vec{x}) = \vec{c}$ in n unknowns $\vec{x} = \{x_1, \ldots, x_n\}$. The equations must be *structural equations*; that is, each one must represent a fundamental mechanism or first principle of the phenomenon. Examples of fundamental mechanisms in thermodynamics are the conservation of mass and energy.

¹For example, one may be forced to consider statistical phenomena.



Figure 1: Structural equation matrices and (c) causal structure diagram

The procedure assigns causal dependencies between variables by propagation through a structural equation matrix (Figure 1a). Each a_{ij} term is either zero or one. Each row *i* designates which variables occur in equation $i : f_i(\vec{x}) = c_i$. If variable x_j appears in equation *i* then $a_{ij} = 1$. Each row must have at least one "1". In order for the procedure to work, the matrix must be expressible in upper triangular form (as in Figure 1a) with 1's along the diagonal. For some phenomena, such as those containing feedback, the procedure fails to find a unique ordering. In these cases the structural equation matrix cannot be expressed in upper triangular form. One or more terms below the diagonal has a "1" and the equations are underconstrained. In cases where all terms below the diagonal are zero and at least one of the diagonals is zero, the equations are overconstrained and may be inconsistent.

By definition, one or more rows of an upper triangular matrix must contain a single nonzero term a_{ii} . Each of these terms represents an *exogenous* variable x_i . The exogenous variables in \vec{x} are those which are causally dependent on factors outside the scope of the phenomenon under study. Exogenous variables are causal inputs to the phenomenon and are unaffected or negligibly affected by it. It is from these variables that causality is propagated to the other variables. The propagation is illustrated in Figure 1b for a simple 4x4 set of equations with exogenous variables x_3 and x_4 circled. The resulting causal structure or *influence* diagram is shown in Figure 1c. The diagram shows that x_2 is causally dependent on x_3 and x_4 , while x_1 is causally dependent on x_2 and x_4 .

In [4], Iwasaki extended the procedure to include differential as well algebraic equations. The procedure requires that differential equations be translated into "canonical form". That is, each differential equation must contain only one derivative, as in $\dot{x_i} = f_i(\vec{x})$, and each derivative must appear in only one equation. A variable whose derivative appears in a differential equation is said to be causally dependent on the other variables in the equation. For those variables which do not appear as derivatives in any equations, causal dependencies are found, as before, by propagation through a structural equation matrix.

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(1)	Dynamic $f_1(x_1, x_2, x_4) = c_1$	Equilibrated $f_1(x_1, x_2, x_4) = c_1$			x ₂	<i>x</i> ₃	×4	X5
(2)	$f_2(x_2,x_3,x_4)=c_2$	$f_2(x_2, x_3, x_4) = c_2$			1	-①		
(3)	$\dot{x_3} = f_3(x_2, x_5)$	(3')	$x_3 = c_3$		2%-	(1)		
(4)	$\dot{x}_4 = f_4(x_5)$	(4')	$X_4 = C_4$				(1)	
(5)	$X_5 = C_5$		$x_5 = c_5$				-	1
	(a)		(b)			(C)		
	(×5)-	x ₃ - x x ₄ - x	3 X2 X1	(d)				

Figure 2: Causal ordering in a dynamic system

The matrix is formed by "equilibrating" the differential equations, that is, by replacing each differential equation $\dot{x}_i = f_i(\vec{x})$ with the constant equation $x_i = c_i$. Causal propagation then proceeds from exogenous variables and the newly introduced constants to the remaining variables.

An example will help clarify the procedure. Consider the mathematical model defined by the equations in Figure 2a. Because of equation (3), \dot{x}_3 is causally dependent on both x_2 and exogenous x_5 as shown in Figure 2d. Similarly, \dot{x}_4 is causally dependent on x_5 because of equation (4). The edges marked with an *i* in the causal structure diagram (Figure 2d) are causal integration links between a derivative of a variable and the variable itself. In QP theory terms, the variables x_3 and x_4 are the *directly influenced* quantities and they are directly influenced by *processes*.

Figures 2b and c show the equilibrated version of the differential equations and the corresponding structural equation matrix. The intuition behind constant equations (3') and (4') is that directly influenced quantities x_3 and x_4 change so slowly compared to x_1 and x_2 that they can be regarded as constant. x_3 and x_4 are influenced by integration links and integration requires finite time to cause a change. In contrast, algebraic equations (1) and (2) respond instantly to any changes in their variables. Thus they represent fast mechanisms which are instantaneous in comparison. Notice that the differential equations provided two more seeds, x_3 and x_4 , at which propagation through the matrix can begin. These "quasi-exogenous" variables are circled with dotted lines in Figure 2c. Notice also that exogenous variable x_5 was not needed for causal propagation through the equilibrated equations.





Figure 3: Contained gas examples

3 CAUSAL CLUSTERS

As we have seen, the causal ordering procedure usually requires finding exogenous variables that act as starting points for the propagation of causal influence to other variables. Choosing exogenous variables requires knowing how the outside world behaves relative to the system of interest. In general, the causal ordering of system S in world W_1 does not hold in world W_2 . We illustrate this problem by considering the classic thermodynamics example of a gas inside a cylinder with a movable piston (Figure 3a). The gas can be cooled or heated by the environment. The gas can also expand or contract by movement of the piston. In other words, the gas can exchange energy with its surroundings through the flow of heat or work. The mass of the contained gas can also be changed by gas flowing into and out of the cylinder. If the cylinder is in thermal contact with an extremely large body such as a lake, the thermal partner's temperature T_0 is negligibly affected by heat exchanges with the contained gas and can be considered exogenous, $T_0 = c_i$. However, if the heat capacity of the thermal partner is of the same order of magnitude as the gas, T_0 will not remain constant but will change as it equilibrates with the gas at temperature T. T_0 is then no longer exogenous and can not be used as a starting point for causal propagation. As a consequence, the causal ordering of the contained gas variables may change. Any causal ordering uncovered by the procedure for the internal gas variables thus seems less convincing since it apparently depends on factors *outside* the gas cylinder. It would seem strange, for example, if switching the thermal partner from a large lake to a car radiator would change the direction of influence between gas temperature and pressure.

Similarly, the external force against which the gas expands (or is compressed by) may or may not be independent of the gas variables. In many instances the external force is just the weight of the piston and can be treated as an exogenous variable. However, in Figure 3b we see a system where the external force increases proportionally to gas volume. Figure 3c shows an environment in which the thermal partner's temperature T_0 is affected by the gas pressure. The point of these examples is to illustrate how environmental variables may be affected in any number of unforeseeable ways by the system. In general, there are no safe exogenous variable choices for a system that may be placed in varied environments. The standard causal ordering procedure is environmentally unstable.

Fortunately, for certain phenomena it is possible to identify sets of equations whose internal causal order is stable. A causal cluster is a set of n structural algebraic equations in n unknowns such that (1) its equilibrated structural matrix can be expressed in upper triangular form, and (2) its variables are affected by external variables solely through derivative causal links. In QP terminology, the environment can affect the cluster's variables only through the direct influence of processes. The usefulness of this definition is that it allows us to avoid exogenous variables as the starting points for causal propagation. Instead, propagation begins at directly influenced variables only. As a consequence, the causal dependencies within the cluster are environmentally stable. In Figure 2b, equations $\{1, 2, 3', 4'\}$ would form a causal cluster if it was known that they were always affected by external variables solely through *i* links. When found, clusters can be studied separately and used as causal building blocks in many systems. In the next section we present an example of a causal cluster in thermodynamics.

4 AN EXAMPLE

Consider again the contained gas examples of Figure 3. Thermodynamics defines several properties for the gas, including temperature T, pressure P, volume V, mass m and internal energy U. The hundreds of equations typically appearing in a thermodynamics textbook are all derived from relatively few fundamental principles such as the first and second laws of thermodynamics, conservation of mass, equations of state, and so forth. The number of first principles that we need to consider is not large. We assume the gas is at a low enough pressure so that it behaves "ideally" and the Ideal Gas Law holds:

$$PV = mRT \tag{1}$$

For an ideal gas, the internal energy is a function of temperature and mass only²:

$$U = m \cdot c_v(T) \cdot T \tag{2}$$

where c_v is the heat capacity of the gas and is a function of temperature only. The contained gas can interact with its surroundings through assorted heat, work and mass flow processes. The gas is affected by its surroundings *solely* through the direct influence of such processes. This is true in standard thermodynamic scenarios, where the system

²This was first noticed by Joule in 1843 for a fixed quantity of gas.

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changes smoothly and continuously. For example, the mass of any contained gas is directly influenced by mass flow processes only. In differential equation form, the environmental influences on the sample gas are constrained by the conservation of mass principle:

$$\dot{m} = m_{R,in} - m_{R,out} \tag{3}$$

where the m_R 's are the rates of mass flow processes into and out of the cylinder. The internal energy U of a contained gas is directly influenced by all three kinds of processes. A heat flow process from the surroundings into the gas positively influences its internal energy. A work process which lifts the piston decreases the gas' internal energy. A mass flow process into the gas increases its internal energy. In differential equation form, all environmental influences on internal energy are constrained by the conservation of energy principle³:

$$\dot{U} = Q_R - W_R + U_{R,in} - U_{R,out} + P_0 V_{R,in} - P V_{R,out}$$
(4)

where Q_R and W_R are the rates of heat and work flow respectively, the U_R 's and V_R 's are the rates at which internal energy and volume flow into and out of the cylinder through its portals, and P_0 is the pressure of the gas entering the cylinder. Finally, the gas volume is directly influenced by the environment through motion processes acting on the piston (or, more generally, at the gas boundary). The motion processes are due in turn to Newton's law of motion.

Equations (1), (2) and constant equations for m, U and V define a causal cluster with quasiexogenous variables V, m, and U (see Figure 4). The cluster's internal causal dependencies remain the same regardless of the thermodynamic environment of the gas. In other words, the causality of the Ideal Gas Law and Joule's relation has been determined. Pressure is causally dependent on volume, mass, and temperature. Temperature is causally dependent on internal energy and mass. In fact, the causality of these equations holds in any situation for which the Ideal Gas Law applies. This is because the conditions under which the Ideal Gas Law holds are sufficient for the causal cluster to exist. The Ideal Gas Law applies only

³We use rate forms of the standard thermodynamics differential equations.

to gases which have an single identifiable *state* at a given point in time. In other words, the gas must be homogeneous, or close to it. For a gas undergoing a thermodynamic change, this homogeneity constraint implies that the environment must influence the gas slowly in comparison to the processes which restore the gas to a homogeneous state. As a consequence, the environmentally influenced variables in the Ideal Gas Law (and Joule's equation) can be replaced with constant equations to form the equilibrated causal cluster of Figure 4. Thus, in any ideal gas scenario, the Ideal Gas Law, Joule's relation and the constant equations of Figure 4a satisfy the causal cluster definition and their causality is as shown in Figure 4c.

By examining the algebraic equations, the signs of the causal dependencies in the cluster can also be determined. From the Ideal Gas Law PV = mRT, it is clear that all else being equal, pressure and temperature must change in the same direction. In other words, when mass and volume are constant, increasing temperature must be accompanied by increasing pressure. Therefore pressure is causally dependent on temperature in the *positive* sense. Likewise, the signs of the other dependencies can be found, yielding the edge labels shown in Figure 4c.

5 ALTERNATE MECHANISMS

Within the ideal gas cluster, causal ordering is independent of the environment. But the question remains—how can one be certain that the equations in the cluster represent fundamental mechanisms? Consider the Ideal Gas Law. It is an equation of state containing four variables P, V, m, and T. Assigning values to any three variables uniquely defines the fourth and the state of the gas. But in fact, other properties could be chosen to characterize its state. For example, by using Joule's relation (2) to replace m and T in the Ideal Gas Law (1), we get an alternate equation of state containing the four variables P, V, U, and T:

$$PV = RU/c_{v}(T) \tag{5}$$

Does this more accurately reflect the mechanism underlying ideal gas behavior? The question has merit since the new equation yields a new cluster with a different causal structure (Figure 5).

The author has never seen the alternate equation of state (5) in any textbook. Thermodynamics textbooks always prefer the Ideal Gas Law. This may be due to its reflecting a basic, underlying mechanism. Or it may simply be due to the fact that all of its variables are directly measurable properties while those of (5), are not (because of internal energy). It seems that to resolve the question of fundamental equations, one must examine the phenomenon of contained gases at a finer level of detail. The algebraic nature of the Ideal Gas Law is a consequence of the level at which thermodynamics views the world. Con-



tained gases are viewed as homogenous entities having macroscopic properties. A result of modeling at such a coarse grain size is that the processes underlying the Ideal Gas Law are concealed. According to the *kinetic theory*⁴ of gases [1], pressure, volume, temperature, and mass interact through processes operating at a molecular level.

By dropping to the level of the kinetic theory of gases, the processes responsible for the aggregate behavior of gases can be found. In this way one can confirm that the Ideal Gas Law and Joule's equation correspond to fundamental mechanisms and hence that the causal ordering of Figure 4 is valid. According to the kinetic theory, internal energy is the *total* molecular energy stored in the gas. This energy is in the form of intermolecular translational motion and atomic vibrations and rotations within molecules. Temperature is a measure of the average translational motion of individual gas molecules. Thus internal energy, temperature and mass are tightly bound together at the molecular level and Joule's equation would destroy this correspondence. The kinetic theory provides further evidence for the causal dependencies between U, T, and m shown in Figure 4c.

According to the kinetic theory, pressure is a measure of the forces due to collisions of gas molecules with each other and their container. In a constant volume container, pressure varies directly with the product of the number of molecules and their mean square velocity. Mass is a measure of the number of molecules and temperature is a measure of molecular velocity. Thus pressure, mass, and temperature are in an intimate and direct causal relationship. This is reflected by the Ideal Gas Law but not the alternate equation of state (5). Thus, the equations in our cluster (Figure 4) represent fundamental mechanisms and the resulting causal ordering is confirmed.

⁴The kinetic theory was developed between 1850 and 1880 by Maxwell, Boltzmann, Clausius and others.

6 DISCUSSION

The casual ordering procedure of Iwasaki and Simon provides a useful tool for uncovering causality which may be difficult to determine otherwise. We have shown how clusters of equations can be found whose internal causal dependencies hold in a broad range of environments. In QP theory terms, it is the set of possible *processes* in a domain which provides the means for partitioning it into stable clusters. The processes impose a direction of causality into the cluster and dictate which of its variables are gateways for causal propagation. The stable causal ordering within a cluster satisfies an intuitive sense that causality should be a property of a system that reflects the underlying physics, and should not be due to particular configurations of the outside world.

This work is similar to [5], where Iwasaki describes how the behavior of a large system can be determined from the behavior of independent internal aggregates and how increased modeling detail in the aggregates does not affect the entire system. In other words, she shows that in certain cases (1) disjoint subsystems are mutually independent, and (2) the system is independent of the components. Our work shows how one of the ontological primitives of QP theory, processes, defines clusters which are stable across large classes of environments. In other words, the components are independent of their systems. As an illustration, we have shown how all classical thermodynamic systems having contained gases are decomposable and possess the causal cluster of Figure 4 as an independent component.

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