Towards a Qualitative Lagrangian Theory of Fluid Flow

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Abstract

Choosing between multiple ontological perspectives is crucial for reasoning about the physical world. Choosing the wrong perspective can make a reasoning task impossible. This paper introduces a *Lagrangian plug flow* ontology (PF) for reasoning about thermodynamic fluid flow. We show that this ontology captures continuously changing behaviors of flowing fluids not represented in currently implemented ontologies. These behaviors are essential for understanding thermodynamic applications such as power cycles, refrigeration, liquefaction, throttling and flow through nozzles. We express the ontology within the framework of *Qualitative Process* (QP) theory. To derive our QP theory for plug flow, we use the method of *causal clustering* to find causal interpretations of thermodynamic equations. We also incorporate qualitative versions of standard thermodynamic relations, including the second law of thermodynamics and Clapeyron's equation.

Introduction

The choice of ontology critically effects reasoning in a domain. In general, no single theory of a domain is adequate for every task because the underlying ontological choices may sometimes be inappropriate. Thus it has become widely recognized that the ability to switch ontological perspectives is crucial for expert physical reasoning (Collins & Forbus 1987), (Rajamoney & Koo 1990), (Amador & Weld 1990). This paper outlines a new ontology for fluid flow which captures behaviors essential for understanding many important thermodynamic phenomena such as power cycles, refrigeration, liquefaction, and throttling.

To demonstrate the importance of ontological choice, consider the phenomenon of fluid flow in a boiler tube (Figure 1). The thin slices in the figure represent fluid samples at different points along the fluid path. Subcooled liquid (i.e., liquid below its boiling temperature) enters the tube at point a. As liquid flows through the tube, heat flows into the liquid, warming it from its initial temperature at a to its boiling point at c, boiling it until e, and then superheating the gas above its boiling point until it exits at g. Fluid properties vary from inlet a to outlet g. Temperature T for example, rises smoothly from a to c, is constant from c to e during boiling, and rises again from e to g.

In many thermodynamic fluid flow problems, the spatial distribution of the fluid's properties must be recognized before an appropriate equation can be chosen or before a simplifying assumption can be made. For example, if our task is to calculate the heat Q absorbed by the boiler fluid based on values of fluid entropy S, it would be necessary to recognize the varying temperature and entropy profile of the fluid along the tube. Because of the spatial distribution, the appropriate equation (derived from an energy balance and the fundamental property relation) is

$$Q = \int_{S_a}^{S_g} T dS \qquad (1)$$

where S_a and S_g are the entropies of the entering and leaving fluid, respectively. A reasoner needs to know that temperature T varies along the integration path and so cannot be brought outside the integral sign. If our modeling ontology was incapable of representing spatially distributed properties, we could (as will be demonstrated) derive an oversimplified, inaccurate equation. In general, a thermodynamic reasoning system which cannot represent smooth, continuously changing behaviors through space lacks the wherewithal to make informed decisions about many commonly occurring fluid flow phenomena. The focus of this paper is how such spatially distributed phenomena can be represented within the framework of *Qualitative Process* (QP) theory (Forbus 1984).

Eulerian Viewpoint Models

Several ontologies have been proposed for modeling liquids and gases. At the macroscopic level, the *contained-stuff* (Forbus 1984) and *molecular collection* (Collins & Forbus 1987) ontologies describe fluid entities large enough to possess the traditional thermodynamic properties (temperature, pressure, etc.). At

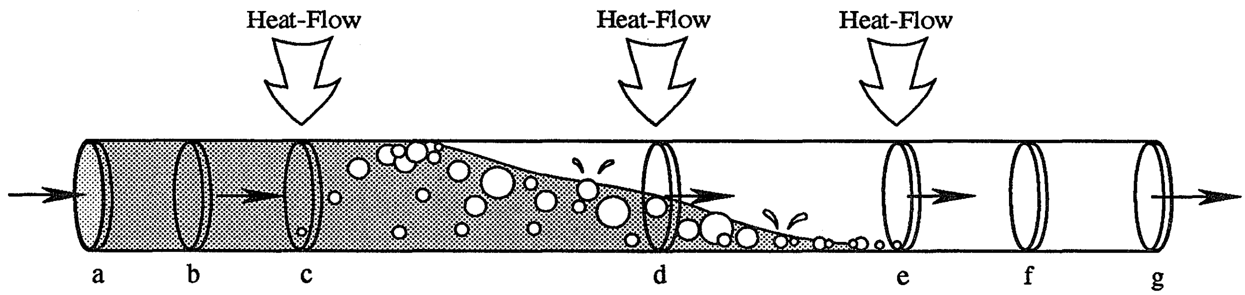

Figure 1: Water flow in a boiler tube

the microscopic level, the ontologies of (Rajamoney & Koo) and (Amador & Weld) describe the behavior of elementary fluid particles. In this paper we focus on macroscopic theories of fluids.

The contained-stuff (CS) ontology, a generalization of Hayes' *contained liquid* ontology (Hayes 1985), describes gases and multiple substances as well as liquids. The CS ontology uses the *Eulerian* viewpoint (Shapiro 1953), (Falkenhainer & Forbus 1991) which focuses on a particular region of space and specifies for each instant of time the properties of the fluid which happens to occupy the region. In the CS ontology, fluids are partitioned into individuals occupying regions delimited by containers.

A contained-stuff is a homogeneous *lumped parameter* (Coughanowr & Koppel 1965), (Throop 1989) model of fluid. Properties distributed over space (e.g., temperature) are "lumped" into a single value. In many cases, this modeling idealization is too inaccurate. For example, modeling a boiling tube with contained-stuffs is basically equivalent to viewing it as a well stirred boiling tank (Figure 2). Liquid enters the tank, boils and leaves as *saturated* gas (i.e., gas at its boiling temperature). The contained-liquid and contained-gas are both at the boiling temperature of the fluid. A thermodynamic reasoning system equipped with only the contained-stuff ontology can miss important distinctions needed to control further analyses. For example, to calculate heat flow Q, a contained-stuff model of the boiler tube suggests (with its constant temperature) that an appropriate equation is

$$Q = T\Delta S \qquad (2)$$

where ΔS is the change in entropy from liquid to gas. In contrast to equation (1), this equation is seriously inaccurate for the scenario shown in Figure 1.

Lagrangian Viewpoint Models

To model the changing conditions along a fluid path, we need a different perspective than that of a contained-stuff. A more promising approach is to use the *Lagrangian* viewpoint (Shapiro 1953), (Falkenhainer & Forbus 1991) in which a particular fluid par-

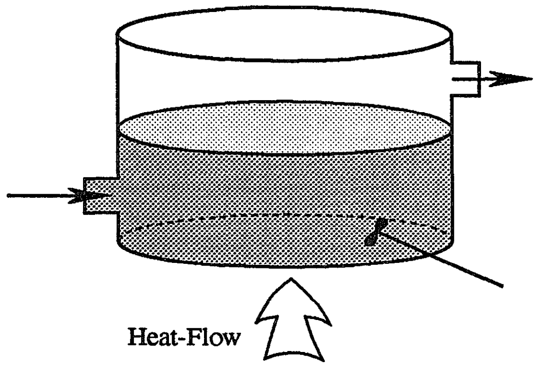

Figure 2: Contained-Stuff view of a boiler tube

ticle is modeled. As the particle travels through a system, it adjusts itself continuously to the new conditions encountered. Choosing a Lagrangian viewpoint means we view the fluid flow from the vantage point of a moving particle. In contrast, using the Eulerian viewpoint means picking a fixed path location to observe flow.

As a possible candidate ontology, we consider the molecular collection (MC) ontology developed by (Collins & Forbus 1987). The MC ontology is a tractable specialization of Hayes' *piece-of-stuff* (PoS) ontology. In the theory, an MC is a very small piece-of-stuff viewed as a collection of molecules. The ontology is said to be *parasitic* on the contained-stuff ontology because a contained-stuff description must be generated before an MC description is possible. When an MC enters a contained-stuff, equilibrating processes influence its properties to match those of the contained-stuff. For a phenomenon like fluid flow into a well mixed tank, this model is usually accurate enough. But, for phenomena where continuously changing properties along a path are important, the MC ontology suffers from the same problem as the contained-stuff ontology.

Consider again the example of fluid flow in a boiler tube. Figure 3 shows the envisionment describing MC's history. The MC enters the contained-liquid and begins equilibrating with it (state a). Once equilibrium

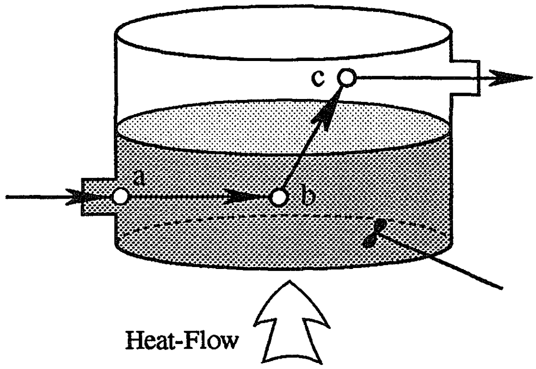

Figure 3: MC envisionment for a boiler tube

is reached, MC's properties match those of the boiling contained-liquid (state *b*). After loitering in the contained-liquid (To allow for MC's implicit motion through the contained-liquid), MC boils and enters the gas contained-stuff (state *c*) and eventually leaves. Because MC is parasitic on the piece-of-stuff ontology, its temperature is constant along the flow path.[1] Also, because MC is so small, the gradual vaporization along the fluid path is not represented. Instead, MC jumps from one state where it is completely liquid to another where it is completely vapor. This makes it impossible to directly represent scenarios where the exiting fluid is partially vaporized. Clearly, the MC ontology cannot represent the spatially distributed nature of flowing fluids.

Plug Flow Ontology

In this section, we introduce a new, nonparasitic *plug flow* ontology (PF) for reasoning about fluid flow. Like MC, the plug flow ontology is a macroscopic specialization of Hayes's piece-of-stuff ontology. The plug flow ontology describes a narrow slice or "plug" of fluid which travels along paths (see Figure 1). Unlike an MC which simply equilibrates with fluids it encounters, a plug is large enough to directly participate in the processes affecting the fluid. For example, when a plug is in a heat exchanger tube, it exchanges heat with entities outside the tube. When it is in a turbine, it pushes against the turbine blades and performs work.

Our plug flow ontology is restricted enough to avoid many of the problems associated with piece-of-stuff ontologies as described by Hayes (Hayes 1985). For example, a distinguishing feature of a plug is its physical contiguity. A plug completely fills a simply-connected region of space. In other words, it exists in one piece and has no holes. Thus we remove from consideration troublesome scenarios where flows branch or merge. Without this restriction, a plug could split into several subparts, each of which would require separate tracking as it moves to different locations and encounters varied conditions. Following the individual parts in such scenarios is impractical, both for human engineers and automated reasoners, and we make no allowances for it in our ontology.

[1] That is, temperature is constant after equilibrating.

Another distinguishing feature of a plug is its single thermodynamic state. A plug has a single set of thermodynamic properties (e.g., a single temperature). However, this does *not* mean a plug is homogenous. A plug is large enough to contain more than one phase. For example, a plug can be part water and part steam, as demonstrated by the partially vaporized plug at point *d* in Figure 1. Still, the plug has a single overall state which can be represented by a point in a thermodynamic diagram.

Although the plug flow ontology itself says nothing about when its viewpoint is appropriate or useful, it is intended for scenarios where fluid flow is orderly and steady-state. By orderly, we mean that no piece of fluid overtakes or mixes with any other fluid ahead or behind it. By steady-state, we mean that at any point along the fluid's path, conditions are constant with respect to time. In steady-state flow scenarios, all pieces of fluid act the same, allowing us to characterize their behaviors with a single representative plug.

Unlike MC, the plug flow ontology does not depend on a particular alternate ontology for deciding its appropriateness or for setting up the plug's global environment. Like all ontologies, the plug flow ontology is "pseudo-parasitic" in some sense. It is parasitic on an assumed state of the world. Only when an appropriate fluid flow is observed or inferred is PF appropriate. It is unimportant from PF's perspective whether the achievement of that flow was inferred using the piece-of-stuff ontology, an alternate ontology describing fluid pressure waves and gradients, or a set of partial differential equations.

An important class of entities in the plug flow ontology are paths. Paths are logical entities inferred from the structure of a scenario. For example, pipes, heat exchangers, turbines, pumps and nozzles provide paths for plug flow. It is worth noting that a path does not require the existence of a solid physical conduit. For example, a path can correspond to a *stream tube* (Shapiro 1953) of air flowing around an airplane wing. Such an application is a clear example of how parasitism on a contained-stuff ontology can be inappropriate for a piece-of-stuff ontology.

As a plug flows through a path, the plug's width in the direction of flow is small enough that it can be considered to have a single location or position along the path. In QP theory terms, we define a quantity-type `(position ?plug ?path)` which defines a one-dimensional coordinate system for a `?plug` along the arc of a `?path`. When a plug's `position` in a particular path has a value in the range between zero and the length of the path `(length ?path)` inclusive, a QP view `(in ?plug ?path)` becomes active, indicating that the plug is in the path. When a plug is in a path, a quantity (velocity ?plug ?path) exists. If the velocity of a plug in a path is nonzero, a Path-Motion process becomes active, influencing the plug's position.

If a plug's position quantity for a particular ?path is nonexistent, the (in ?plug ?path) view for that plug and path is inactive, indicating that the plug is not in the path. If a series of paths are connected end to end, continuous flow from one to another can be modeled. As a plug leaves one path and enters another, its previous position quantity ceases to exist and a new position quantity for the next path becomes defined. These motions from place to place appear as transitions in the plug's total envisionment.

Modeling Thermodynamic Behavior

To make the plug flow ontology useful for thermodynamic applications, we must represent the plug's thermodynamic properties and the processes that affect them. The processes we model are heat-flow, work-flow (and its accompanying volume expansion/contraction), boiling, condensation, and throttling. Conspicuously absent from our list is mass-flow. Since a plug is a closed system, no mass enters or leaves it. In an Eulerian ontology, mass-flow at a location can be directly represented, but not in a Lagrangian ontology. The closest concept to mass-flow in the Lagrangian viewpoint is Path-Motion.

The nine basic thermodynamic plug properties we model are pressure P, temperature T, volume V, vapor pressure Vp, internal energy U, enthalpy H, entropy S, vapor fraction y, and mass m. To model the interactions between these properties, we use QP theory's causally directed connectives (basic knowledge of QP theory is assumed): direct influences (I), and qualitative proportionalities (qprop's). Because these connectives have a fixed causal direction, we are compelled to decide a priori which way causation will flow in all circumstances. Using the *causal clustering* technique (Skorstad 1992), an extension of Iwasaki and Simon's *causal ordering* procedure (Iwasaki & Simon 1986), we can uncover stable causal interpretations for some thermodynamic equations. As shown in (Skorstad 1990), the Ideal Gas Law $PV = RT$ and Joule's temperature-internal energy relation $U = c_v T$ have a stable causal interpretation. These causal dependencies among P, V, T, and U are shown in the *influence* diagram of Figure 4. This diagram represents our causal theory for thermodynamics. Notice the causal dependency of pressure on temperature. A change in temperature causes a change in pressure, but not vice versa. This asymmetry may seem odd. However, experiments done since Joule's time have shown that a drop in pressure without an accompanying work or heat flow has no effect on temperature.

Although the causal dependencies between P, V, and T were derived from the ideal gas law, these same

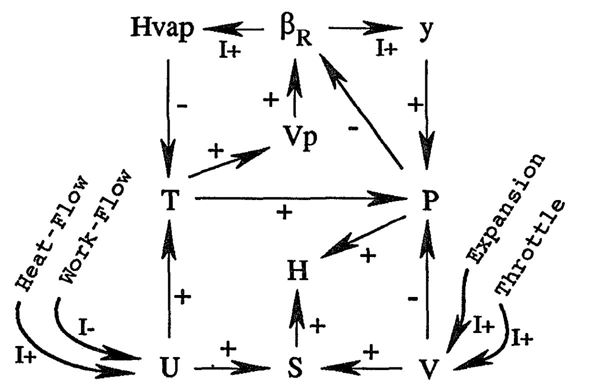

Figure 4: Causal theory for thermodynamic properties

dependencies also hold for liquids. This is true even though the ideal gas law does not hold for liquids; the properties P, V, and T are linked together in *some* equation of state which also describes liquids. It is an article of faith in thermodynamics that the relationship between these properties can be described mathematically. (Even van der Waals equation does a qualitatively good job modeling liquids and gases.) The causal clustering technique does not require knowing the exact form of an equation, only which variables are involved.

Boiling and Condensing

Traditionally, qualitative models of boiling/condensing have relied on the concept of a boiling point constant. The temperature of a liquid must be raised to its boiling point before boiling can begin. We build a more general model based on the observation that the boiling point of a liquid is the temperature at which the liquid's *vapor pressure, Vp*, equals the pressure P distributed throughout the fluid.[2] The vapor pressure of a liquid is the pressure exerted by the vapor molecules that escape from the liquid. When a substance is in the liquid state, its vapor pressure is less than the liquid's pressure. As the liquid's temperature rises, more molecules escape and vapor pressure rises. A liquid must be heated until its vapor pressure reaches the opposing pressure P before boiling can begin. Alternately, if the liquid's pressure is decreased (e.g., by lowering the external confining pressure), boiling can begin once the liquid's vapor pressure is reached.

The causal dependencies for boiling are represented in the top half of Figure 4. Vapor pressure Vp is causally dependent on temperature T. β_R represents the rate of a boiling (or condensation) process. H_{vap} is the *heat of vaporization*, which is the energy expended when a liquid boils. In our theory, boiling and condensing can only become active when Vp and P are

[2] We ignore the fact that pressure increases with depth.

equal. In reality, there is evidence that vapor pressure must exceed fluid pressure, if only infinitesimally, in order to provide a driving force for boiling (Bohren 1989). Normally this disequilibrium is imperceptible and is ignored. In our theory, we follow the example of thermodynamic texts and idealize boiling/condensing by assuming that Vp and P are in equilibrium.[3]

Since our model excludes a disequilibrium driving force for boiling, what is to be the cause of boiling? This problem is more difficult than may be realized at first. Boiling does not occur simply because a liquid at its boiling point is heated. In fact, if a liquid at its boiling point ($Vp = P$) is heated at constant volume (e.g., in a sealed container), it moves *away* from its boiling point. To model boiling, we make use of a qualitative version of *Clapeyron's* equation: $dP/dT = \Delta H/(T\Delta V)$. Clapeyron's equation constrains the behavior of temperature T and pressure P during boiling and condensation. ΔH and ΔV are the change in enthalpy and volume, respectively, that occur when a liquid boils. Both are positive numbers. Thus, if pressure increases during boiling, temperature must also increase, and vice versa. It can also be shown that if pressure is constant during boiling, temperature must also be constant. In QP terminology we have $D_s[P] = D_s[T]$, where D_s is the sign of a derivative. Using this qualitative Clapeyron constraint, we state our boiling conditions:

> Boiling (or condensation) occurs when y (gas fraction) < 1 (or $0 < y$ for condensation), $Vp = P$, and it is required to satisfy Clapeyron's constraint.

To complete our theory of boiling/condensing, we must describe its effect on other fluid properties. It is well known that when a liquid converts to the higher energy vapor form (i.e., when it boils), the fluid cools.[4] We represent this with a qprop from boiling's heat of vaporization H_{vap} to temperature T, as shown in Figure 4. Also, it is known that when a liquid vaporizes, the more energetic vapor molecules increase the force of collisions in the entire fluid.[5] In other words, pressure increases. We represent this with a qprop from gas fraction y to pressure P.

Thermodynamic Constraints

The qualitative influence diagram of Figure 4 will sometimes yield behavioral ambiguity that can be reduced by adding global thermodynamic constraints. One useful constraint is a corollary of the second law of thermodynamics. The entropy S of an adiabatic system (i.e., engaged in no heat flow) must increase or remain constant. To further constrain behavior, there are a number of qualitative constraints which can be gleaned by examining thermodynamic diagrams of substances. For example, it can be shown that for fluids, $(\partial V/\partial S)_P > 0$. In other words, when a fluid's pressure is constant, volume V and entropy S change in the same direction: $D_S[V] = D_S[S]$. Similarly, it can be shown that $(\partial T/\partial V)_S < 0$. That is, when a fluid's entropy is constant, temperature T and volume V change in opposite directions: $D_S[T] = -D_S[V]$. For a justification of these constraints, see (Skorstad 1992).

[3]Nonequilibrium boiling models built by the author also yielded very complex behaviors.

[4]For a microscopic level explanation of this, see (Rajamoney & Koo 1990) and (Amador & Weld 1990).

[5]This can be demonstrated by boiling a liquid in a cylinder fitted with a piston. As the liquid boils, the piston rises.

Example

Using the plug flow theory outlined above, QPE (an implementation of QP theory) produces envisionments which explicitly describe the continuously changing nature of fluid flow along paths. For example, in a typical boiler tube scenario, QPE generates the 11 state total envisionment shown in Figure 5. The QPE input for this scenario includes a description of the entities involved (a plug, pipe and furnace) and constraints imposed to limit the size of the envisionment. In this scenario, we constrain behavior by asserting that the plug enters as subcooled liquid. Also, motion through the tube is asserted to be in the positive direction, pressure is constant,[6] and the furnace is always hotter than the plug.

The plug history from state a to g corresponds to a fluid behavior already described (see Figure 1). In addition, the envisionment describes alternative histories. For example, the plug may exit the boiler partially vaporized as shown at point j. Many aspects of the fluid's behavior have been captured which are impossible to represent in a contained-stuff or MC ontology. The plug flow envisionment makes explicit the fact that: (*i*) gas exiting the boiler may be superheated, as shown at state g, (*ii*) fluid temperature rises from a to c, and from e to g, (*iii*) fluid temperature is constant from c to e, and (*iv*) internal energy U, entropy S and enthalpy H rise continuously from inlet a to outlet g.

Discussion

Recognizing the spatially distributed behaviors of fluid flow is important for many reasoning tasks in thermodynamics. Our work in this area is most similar to (Throop 1989) who describes extensions to Kuiper's QSIM that permit spatial qualitative simulation. While his work focuses on the qualitative simulation task, ours deals mainly with model building.

Spatially distributed behaviors are so important that diagrams of them in the form of *state trajectories* are standard thermodynamic tools in the analysis of many systems. As a piece of fluid travels through a system, its changing properties describe a continuous trajectory through thermodynamic space. Engineers routinely use these thermodynamic trajectories to qualitatively describe and reason about power cycles, refrig-

[6]This is a standard assumption in boiler analyses.

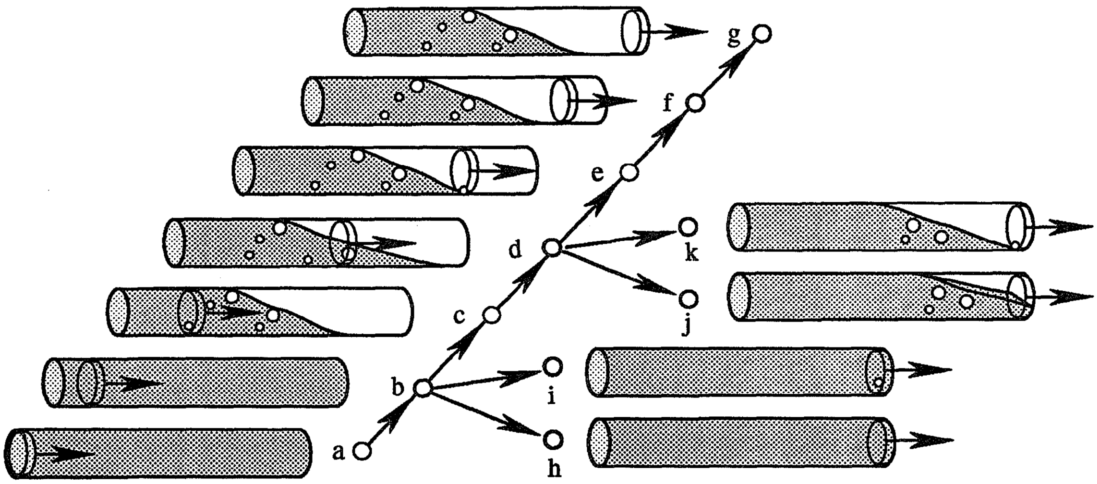

Figure 5: Plug flow envisionment for boiler

eration, liquefaction, throttling, flow through nozzles and many other phenomena. For example, by comparing the trajectory of a simple steam plant with a hypothetical Carnot cycle, an engineer can easily see why the steam plant is less efficient. We view the plug flow ontology as a first step towards building a qualitative representation of fluid flow trajectories. Besides the heat exchanger example shown above, we have also used the plug flow ontology to model the trajectory of fluid flow through a turbine. We believe that qualitative representations of such behaviors will provide an important framework for automated reasoning about thermodynamic systems.

Acknowledgments: Thanks to Ken Forbus, John Collins and Janice Skorstad for insightful discussions. This work is supported by the Office of Naval Research.

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