

Aspects of Qualitative Physics of Diffusional Processes.

Extended abstract

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The study of the qualitative physics of diffusional processes gives rise to challenging problems in cognitive modeling and in simulation. As is the case with qualitative physics in general, when compared with the science of physics, questions related to the nature of scientific thought emerge. In particular, the issue of the difference, whether qualitative or quantitative, between the scientific (mathematical) models of reality and the cognitive models. The formal tools offered by mathematics to extract the knowledge which is captured in the mathematical formulation of a process seem to be different in scope, logical economy and power from the cognitive inferencing tools. The work reported here provides an opportunity to compare the two approaches and gain some insight into their nature.

The physics of diffusion is close enough to everyday life physics that we can use vocabulary borrowed from the latter to describe the former. At the center of our attention here is the process of diffusional drift of particles that are enclosed by containers with irregular boundaries and compositions. We are interested in reasoning about the effect of the size and shape of the container and the composition of its medium on the diffusion transit time over a certain distance. For example, in the case illustrated in the figure below, we are interested to know by how much should the time to diffuse from a to b be influenced by the size of the opening d. Is the dependency of the time on d linear, or is there no dependency at all? The answer is that the diffusion transit time becomes sensitive to d only when d is less than 5% of the total cross section of the container. To grasp this argument we have to flip between levels of description of the process and say that for a large enough d, even though the flux of particles forward to the target is blocked, the flux of particles back, away from the target region, is blocked as well, resulting in no real net effect on the overall diffusion time. However, if d is "very" small (the exact figure has to be determined from a quantitative model), the particles will have hard time finding the small opening during their random search, and the diffusional flow will be inhibited.



This should remind us that the physics of diffusion is different from the physics we encounter in everyday life in one important sense. Its underlying dynamics is governed by random movements of particles. Although to the naked eye there may be an observed flow of particles from regions of high concentration to regions of low concentrations, there is no real driving force behind it, and its only fuel is the thermal energy of particles. Coincidentally, an elegant derivation of some of the fundamental features of diffusion was aided by the introduction of a *virtual force* that is responsible for the drift (Einstein 1906). This derivation was rejected by the physicists community at the time and then later re-proved by others using a more "realistic" mental model. This example may serve as a clue to the power of imagination that is going on and which gives intuitive-physics its computational effectiveness.

The mathematical formulation for the process of diffusion is known for centuries. It is based on the division of the diffusion medium into infinitesimal volume elements and the monitoring of the change of concentration as a function of time in these elements (see for example Lin and Segel 1974 and Hardt 1980b). This results in the diffusion equation which is a second order partial differential equation, which in the case of diffusion along one dimension has the form:

$$\partial P / \partial t = D \partial^2 P / \partial x^2$$

with the fundamental (point release at the origin into an infinite space) solution:

$$P(x, t) = (1/4 \pi D t)^{-1/2} e^{-\frac{x^2}{4Dt}}$$

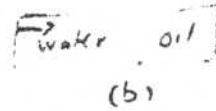
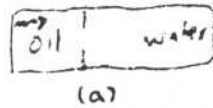
Initial and boundary conditions do not affect the equation, they only affect the solution. These conditions are formulated as equations that have to be solved simultaneously with the original diffusion equation. This fact implies that in order to reason about the effect of boundary geometry on the solution, one has to solve a different set of equations for each unscaled variation in the size and the shape of the system. This is an exceedingly difficult task for irregular boundaries and inhomogeneous compositions.

Here we are after a different formulation of the model of the process which will facilitate the estimation of the pace of diffusion and of other features of interest. Such model has to be based on a set of concepts that are not visible in the classical mathematical formulations but that can be viewed as combinations of behavioral and structural features of the system. A clear distinction between structure and behavior, such as the one made in the mathematical formulation above, is not too effective in supporting inferences because the dynamics of the flow process is not simply related to the geometry of the system. Part of the problem solving expertise in this domain is to determine the structure which is relevant for a particular problem set-up. Namely, to know which regions in the system should be ignored since the diffusing particles get in and out of them quickly, and which regions have a strong effect on the time it takes the diffusing particles to approach their target. The above observation implies that in our case, the problem domain has no natural structure and therefore, a structure has to be imposed by the problem solver. Hence, a major part of the problem solving task is to invent a structure which can be appropriately imposed upon the domain. We have developed an expertise in manipulating relevant structures for problems in this domain. To illustrate some of the expert knowledge used to answer questions about diffusion times consider the following:

Molecules released from the surface on the left diffuse to, and are trapped by the surface on the right. The molecules are slightly soluble in water, and highly soluble in oil. In case (a)

they diffuse through the layer of oil before reaching the layer of water. In case (b) the thickness of each layer is unchanged but the order is reversed so the molecules diffuse first through the water and then the oil. Compare the transit times.

The same in both
 Much longer in (a)
 Much longer in (b)



The following relations will suffice to answer the above question. These relations are part of a larger set of rules that have been formulated for this domain (Hardt 1987b). In all these relations the following is true:

(and (is-region ?a) (is-region ?b) (is-homogeneous ?a) (is-homogeneous ?b) (is-particle ?p) (is-position ?x) (is-position ?y) (is-source ?source) (is-target ?target) (is-time ?t) (is-time ?ta) (is-time ?tb) (is-time ?ti) (is-interface ?interface))

Relation 7: Symmetry

This relation states that the transit time between two points in an homogeneous space is independent of the direction of the motion.

IF
 ((equal (transit-time of ?p from (?x in ?a) to (?y in ?a)) ?t)
 THEN
 (equal (transit-time of ?p from (?y in ?a) to (?x in ?a)) ?t))

Relation 8: Accessibility

This relation states that the transit time is inversely proportional to the accessibility of the target.

IF
 ((greater (accessibility of ?p to ?a) (accessibility of ?p to ?b))
 THEN
 (greater (duration of ?p at ?a) (duration of ?p at ?b)))

Relation 9: Interference

This relation states that the time spent going back and forth before being captured by a target in one region is inversely proportional to the duration spent at that region.

IF
 (greater (duration of ?p at ?a) (duration of ?p at ?b))
 THEN
 (greater (interference-time of ?p from (?source in ?a) to (?target in ?b))
 (interference-time of ?p from (?source in ?b) to (?target in ?a))))

Relation 10: Time Decomposition

This relation states that the transit time across two regions is the sum of the times to cross each region separately plus the interference time.

IF
 ((and (equal (transit-time of ?p from (?source in ?a) to (?interface in ?a)) ?ta)
 (equal (transit-time of ?p from (?interface in ?b) to (?target in ?b)) ?tb)
 (equal (interference-time of ?p from (?source in ?a) to (?target in ?b)) ?ta))
 THEN

(equal (transit-time from (?source in ?a) to (?target in ?b)) (plus ?ta ?tb ?ti)))

Affinity

Given that all geometrical parameters are the same for the two regions, this relation states that the accessibility of a region to a particle is proportional to its affinity to that region.

IF

((greater (affinity of ?p to ?a) (affinity of ?p to ?b)))

THEN

((greater (accessibility of ?p to ?a) (accessibility of ?p to ?b)))

To answer the question we realize that in case b, the sink is more accessible to the particles and hence the transit time in this case is shorter. Consider now another problem:

Molecules released from one spherical surface diffuse to, and are trapped by a second, concentric, spherical surface. The radius of the inner surface is much less than the radius of the outer surface. Case (a): the molecules are released from the outer surface and diffuse inward. Case (b): the molecules are released from the inner surface and diffuse outward. Compare the transit times.

Longer in (a)

The same in both

Longer in (b)



This problem can be answered using the relations mentioned above and by adding a relation that states that the outer target has the greater accessibility. Also, this problem can be solved using a more complete description of sink parameters and their influence on sink accessibility. The problem of recognizing problem features that are relevant for computing high level features such as accessibility is addressed by this research but will not be discussed here (see Hardt 1986c, 1987b).

It becomes apparent from looking at these relations that the knowledge captured in them provides a way to structure the diffusion domain, estimate the diffusion time in each part of the structure, and combine the individual times. A mathematically exact solution method which is based on a model which is a combination of the mathematical and conceptual models presented above is given in (Hardt 1980a,b).

The work discussed here is related in many interesting ways to work done by other researchers working on qualitative physics. The list of references at the end of the paper mentions some of them. Also, it may be mentioned that the problem solving task which concerns us here may be considered as an example of a more general class of cognitive processes where the processor has to impose its own (biased) structuring on the stream of inputs it has to deal with. In very few cases the chunking that appears in the pre-processed input such as single words in a sentence, individual objects in the visual field, sequence of events in a fixed time period etc., correspond in a one-one fashion to meaningful conceptual units.

Related Work:

Bylander T. and Chandrasekaran B. (1985). Understanding Behavior Using Consolidation. Proc. Ninth IJCAI, Los Angeles, 450-454.

Davis R. (1984). Diagnostic Reasoning Based on Structure and Behavior. *Artificial Intelligence*, 24.

De Kleer J. and Brown J.S. (1984). A Qualitative Physics Based on Confluences. *Artificial Intelligence*, 24,

Einstein A. (1906). In: *Investigations on the Theory of Brownian Movement*. Dover Publications Inc. 1956, pp. 36-62.

Forbus K.D. (1984). Qualitative Process Theory. *Artificial Intelligence*, 24,

Gentner D. and Gentner D.R. (1983). Flowing waters or teaming crowds: mental models of electricity. In: *Mental Models*. (D. Gentner and A.L. Stevens Eds.). Lawrence Erlbaum Associates Publishers, Hillsdale, New Jersey, 101-129.

Hardt S.L. (1979). Pace of Diffusion Through Membranes. *Journal of Membrane Biology*, 48, 299-330.

Hardt S.L. (1980a). The Diffusion Transit Time: A Simple Derivation. *Bull. Mathematical Biology*. 87, 1-7.

Hardt S.L. (1980b). *Diffusion in Structured Media*. Ph.D. Thesis, The Weizmann Institute of Science. To be published in Lecture Notes in Biomathematics, S. Levin editor, Springer Verlag.

Hardt S.L. (1984). *Naive physics and the physics of diffusion. Or: when Intuition fails*. Research Report number 211, Department of Computer Science University at Buffalo.

Hardt S.L. (1986a) On the Power of Qualitative Simulation. Winter Simulation Conference. ACM, Washington D.C.

Hardt S.L. (1986b) Qualitative Simulation for Estimating Diffusion Transit Times. AAAI-86 workshop on AI and Simulation. Philadelphia Pennsylvania.

Hardt S.L. (1986c) Flexible Interpretations: A Computational Model for Dynamic Uncertainty Assessment. Second workshop on Uncertainty and Artificial Intelligence. University of Pennsylvania, Philadelphia.

Hardt S.L. (1987a). Qualitative Reasoning and Simulation for Knowledge Intensive Explanations and Predictions. *Symposium on Modeling and Simulation Technology*. Tucson Az. Zeigler B.P. Oren T.I. Editors.

Hardt S.L. (1987b). Qualitative Reasoning About Diffusion Times. Manuscript in preparation.

Hardt S.L. (1987c). Bridging and Reduction During Multi-Level Qualitative Reasoning. Manuscript in preparation.

Hayes P. (1985). The Naive Physics Manifesto. In: *Formal Theories of the Commonsense World*, (J.R. Hobbs and R.C. Moore eds.). Ablex Publications, Norwood, New Jersey, 1-36.

Kuipers B.J. (1986). Qualitative Simulation. *Artificial Intelligence*, 29, 289-338.

Lin C.C. and Segel L.A. (1974). *Mathematics Applied to Deterministic Problems in the Natural Sciences* Macmillan Publishing Company, New York.

Riesbeck C.K. (1984). Knowledge reorganization and reasoning style. In: *Developments in Expert Systems*, (M.J. Coombs Ed.). Academic Press. 159-175.

Stanfill C. and Waltz D. (1986). Toward Memory Based Reasoning. *Communication of the ACM* vol. 29. 1213-1228.

Ullman S. (1985). Visual Routines. In: *Visual Cognition*, Pinker S. Editor. Bradford Books, MIT Press, Cambridge, Ma.

Walters D. (1987). Selection of Image Primitives for General Purpose Visual Processing. To appear in *Computer Vision Graphic and Image Processing* (February).

Weld D.S. (1986). The Use of Aggregation in Causal Simulation. *Artificial Intelligence*, 30,