M-Pos615

A GENERAL FORMULATION OF CHEMICAL REACTIONS
IN COUPLED SYSTEMS. J.S. Shiner, Physiol.
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land. Chemical reactions are notorious in
that the formulation of their dynamics is
apparently fundamentally different from
that of other sorts of processes (mechani-
cal, electrical, e.g.). These other sorts
of processes share a common formalism,
which can be cast in terms of Lagrangian
dynamics extended to include a dissipation
function. It will be shown here how the
classical description of the dynamics of
chemical reactions, mass action kinetics,
can be reformulated so that they are given
by the Lagrangian formulation common to
other sorts of processes. This represents
a unification of the theory of the dynamics
of chemical reactions with that of other
sorts of processes and will simplify the
treatment of systems where chemical reac-
tions are coupled to other sorts of pro-
cesses (mechanochemical and electrochemical
systems, e.g.). The key to the reformula-
tion is the definitions of "resistances"
for chemical reactions, which allow mass
action kinetics to be recovered from the
formulation. The formulation is valid for
stationary and transient states arbitrarily
far from thermodynamic equilibrium.

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HIGHLY PARALLEL IMPLEMENTATION OF AUTONOMOUS
DIRECTION OPTIMIZER WITH COGNITION
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Musterle, B. Schapiro and P. Urban, Inst.Phys.
Theor. Chem., University of Tubingen, D-7400
The "relational" brain described in 1974
(Lect. Not. Biomath. 4, 342-369) can be impl-
emented in a highly parallel fashion. The
environment is represented in an "analogous"
(spatial) form, in the pseudosimultaneous cog-
nitive map of 1981 (BioSystems 13, 203-209).
n 2-D "stencil functions" serve to "lock" ev-
ery nearest source of type i into place, so
that automatically the right force field is
created at the center. A purely temporal"dis-
appointment/surprise" comparator records dev-
iations from the 2-D stencil functions, read-
justing them globally, during fast simulated
action. Real (slow) action gets disinhibited
only after the d/s output ceases. All of this
can be implemented with but a few types of
module. Several levels of spatiotemporal res-
olution ("tolerance") can be used simultane-
ously (cf. 1981 ACM Comp. Sci. Conf. St. Louis
p. 34). We claim that this is how our own
brain is organized functionally. The fish
pandaka pygmaea with its 1 mm^3 brain, and its
much larger close relative gobius niger, will
be natural candidates when testing the pres-
ent new design principle against reality (and
improving it) will be at stake.
Work supported in part by Humboldt and DFG.

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**THE THERMODYNAMICS OF LOCAL LINKAGE
EFFECTS** <u>Enrico Di Cera</u> Ist Fisica,
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Linkage effects occurring upon
ligand binding to biological
macromolecules can be cast in terms
of global or local descriptions.
The global dimension involves the
macromolecule as a whole and
complies with the principles of
thermodynamic stability [1]. The
local dimension refers to linkage
effects that can be monitored
specifically at individual sites
[2,3], such as redox equilibria of
cytochrome molecules or protein-DNA
interactions. In this dimension
paradoxical violations of the
second law can arise as a result of
local fluctuations of thermodynamic
variables. These local fluctuations
may have important implications in
biological systems at equilibrium
or steady state [4].

1. Di Cera et al. (1988) PNAS 85, 5077.
2. Ackers et al. (1983) J. Mol. Biol. 170, 223.
3. Di Cera, E. (1989) J. Theor. Biol. 136, 167.
4. Di Cera, E. (1989) J. Chem. Phys., in press.