Symposium DEB2009

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Dynamic Energy Budget Theory

Reaching Consilience Between the Physical and the Biological Sciences through an Axiomatic Theory for Metabolism

Tiago Domingos

tdomingos@ist.utl.pt

Environment and Energy Scientific Area

Department of Mechanical Engineering

INSTITUTO SUPERIOR TÉCNICO

Overview

- The importance of scientific unification ...
  - ... through mathematics
  - ... respecting thermodynamic constraints
  - ... combining fundamental and applied science
- The fundamental principles of DEB
- Further developments in DEB
  - ... namely, the combination of general mathematical theory with massive statistical approaches

IST Research Towards Scientific Unification

- Unify the fields of
  - Thermodynamics,
  - Ecology (or, more generally, the natural sciences)
  - Economics (or, more generally, the social sciences)
- Formal analogy
  - The same mathematical/conceptual description and interpretation of different phenomena
    - e.g. wave equation, Malthusian ideas in Darwin and Wallace
  - Consistency within the same domain
  - Development of new theoretical results
- Substantive integration
  - Different mathematical/conceptual descriptions and interpretations of the same phenomenon
    - e.g., thermodynamic constraints
  - Consistency between different domains
  - Development of new theoretical results

Why is Scientific Unification Worthwhile?

- Curiosity
- Efficiency
  - Fast transfer of knowledge, insights and tools
- Consilience
  - But sometimes "capillarity" may be needed
- Falsifiability
- Simplicity
- Embedding
  - In a single (parameter) space
  - Able to deal with novelty (including the automatic generation of novelty)

Mathematical Theory in the Sciences

- In Physics and Economics, mathematical theory is paramount and there is a quest for a unified theory within each domain
  - However, in Physics there is also a paramount concern with empirical testing
- In contrast, in Biology mathematical theory has in general played a secondary role
  - Biology is frequently seen as a science of exception and particular cases, with no interest in abstraction and generalisation
- A minor group in Biology has developed "Theoretical Biology" and "Mathematical Biology"
  - One of the major schools for this has been the Netherlands
- However, Theoretical and Mathematical Biology have frequently been carried out without a concern for empirical testing
  - When this concern appears, models are of narrow application, reducing their theoretical breadth
- DEB
  - Builds on the Dutch tradition of Theoretical and Mathematical Biology, but couples it with a fundamental concern with producing general theory, subjected to careful empirical testing

Is (Mathematical) Theory Important in Science?

- "All models are wrong, but some are useful."
  George Box, statistician (c. 1980)
- "All models are wrong, and increasingly you can succeed without them."
  Peter Norvig, Google research director
- "Correlation supersedes causation, and science can advance even without coherent models, unified theories, or really any mechanistic explanation at all."
  Chris Anderson, editor of Wired (2009)
- "I just don't know very much about the field of economics. I'm not good at math, I don't know a lot of econometrics, and I also don't know how to do theory"
  Steve Levitt, author of *Freakonomics* (2003)

Anderson, C. (2009). What science can learn from Google? http://www.interdisciplines.org/liquidpub/papers/3

http://en.wikipedia.org/wiki/Steven_Levitt

A Refresher on the Philosophy of Science I

- Inductivism
  - "All swans are white"
  - The induction problem: black swans
- Falsificationism
  - Assymetry in truth:
    - I can prove that "All swans are white" is false, but I cannot prove that it is true
    - I can prove that "Some swans are black" is true, but I cannot prove that it is false
  - The assymetry is in "all" (universal quantifier) vs. "some" (existential quantifier)

Chalmers, A. F. (1999). What is this thing called science? (3rd. ed.) Open University Press, Buckingham.

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A Refresher on the Philosophy of Science II

- Kuhn’s paradigms
  - Paradigms: normal science (problem solving)
  - Revolutions: incommensurability
- Lakatos’s research programs
  - Hard core
  - Protective belt (auxiliary theory)
  - Negative and positive heuristics

  - ... so, theories are not just rejected based on specific “crucial” experiments
    - e.g.: Michelson-Morley experiment

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Occam's Razor:
The Epistemological and the Biological

- (Epistemological) Occam's razor (or Law of Parsimony), attributed to the 14th-century English logician William of Ockham, is the principle that, given two hypotheses consistent with the observed data, the simpler one should be preferred (Esmeir and Markovitch, 2007).
  - "Theories should be made as simple as possible, but not more"
    Albert Einstein
- In the context of machine learning, the widely accepted interpretation of Occam's razor is that given two consistent hypotheses, the simpler one is likely to have a lower error rate.
  - Empirical evidence both for and against (Esmeir and Markovitch, 2007)
- However, simplicity can be an aim in itself
- Karl Popper argued that simple theories are more falsifiable
- Simplicity in scientific theories?
  - e.g., is Copernicus simpler than Ptolomey?
    (No, namely before Galileo, Arthur Koestler, *The Sleepwalkers*)
- CONJECTURE (Biological Occam's Razor): *Ceteribus paribus*, organisms with simpler control models are evolutionarily favoured

Fundamental Principles of DEB Theory
Occam’s Razor

- Pragmatic Application of Occam’s Razor:
  - Minimum number of state variables
  - Minimum number of parameters
  - Constant functions instead of linear
  - Linear functions instead of non-linear
- Metabolic Control
  - Organisms increased their control over metabolism during evolution [Biological Occam’s Razor]
- Cell Universality:
  - Cells are metabolically very similar, independently of the organism [Epistemological Occam’s Razor] *or* its size [Biological Occam’s Razor]

Fundamental Principles of DEB Theory
Occam's Razor (cont.)

- Constant chemical composition (Strong Homeostasis) and conversion coefficients
- At constant food, one state variable and one forcing flow (Weak Homeostasis)
- At variable food, two state variables and one forcing flow (three independent flows)

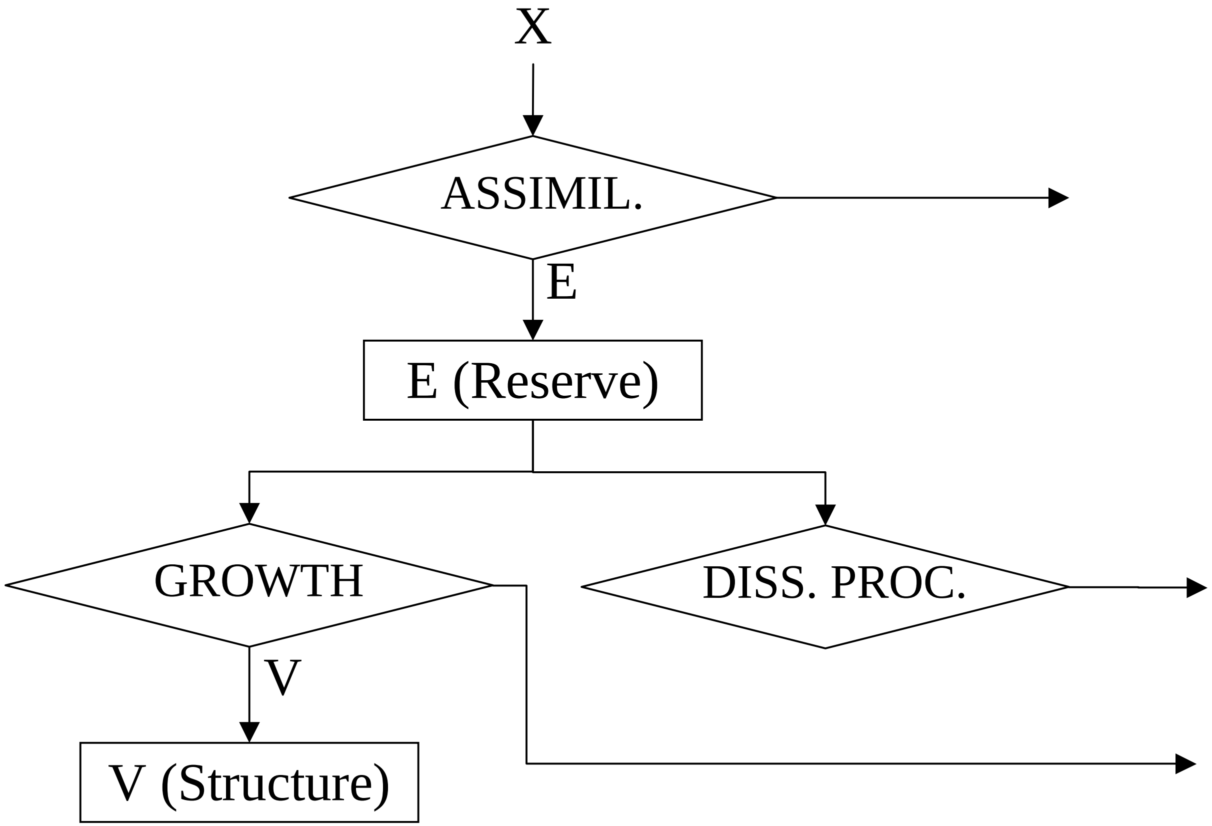
Thermodynamic Constraints

- Laws of thermodynamics
  - 1st Law: Conservation of mass and energy
  - 2nd Law: Entropy increase in adiabatic systems *or* entropy production in all processes
- Thermodynamic constraints must be obeyed, but are not enough to build theories in biological and social systems
- The major divide in Ecology:
  - Ecosystem and physiological ecology, based on energy and mass flows
  - Population and community ecology, based on the behaviour (fitness) of individuals
- An analogous divide in Economics:
  - Ecological economics (clear minority), based on energy and mass flows
  - Neoclassical economics (mainstream), based on the behaviour of humans (utility) and firms (profit)
- Optimisation requires trade-offs, for which thermodynamics is best

Fundamental Principles of DEB Theory
Thermodynamics

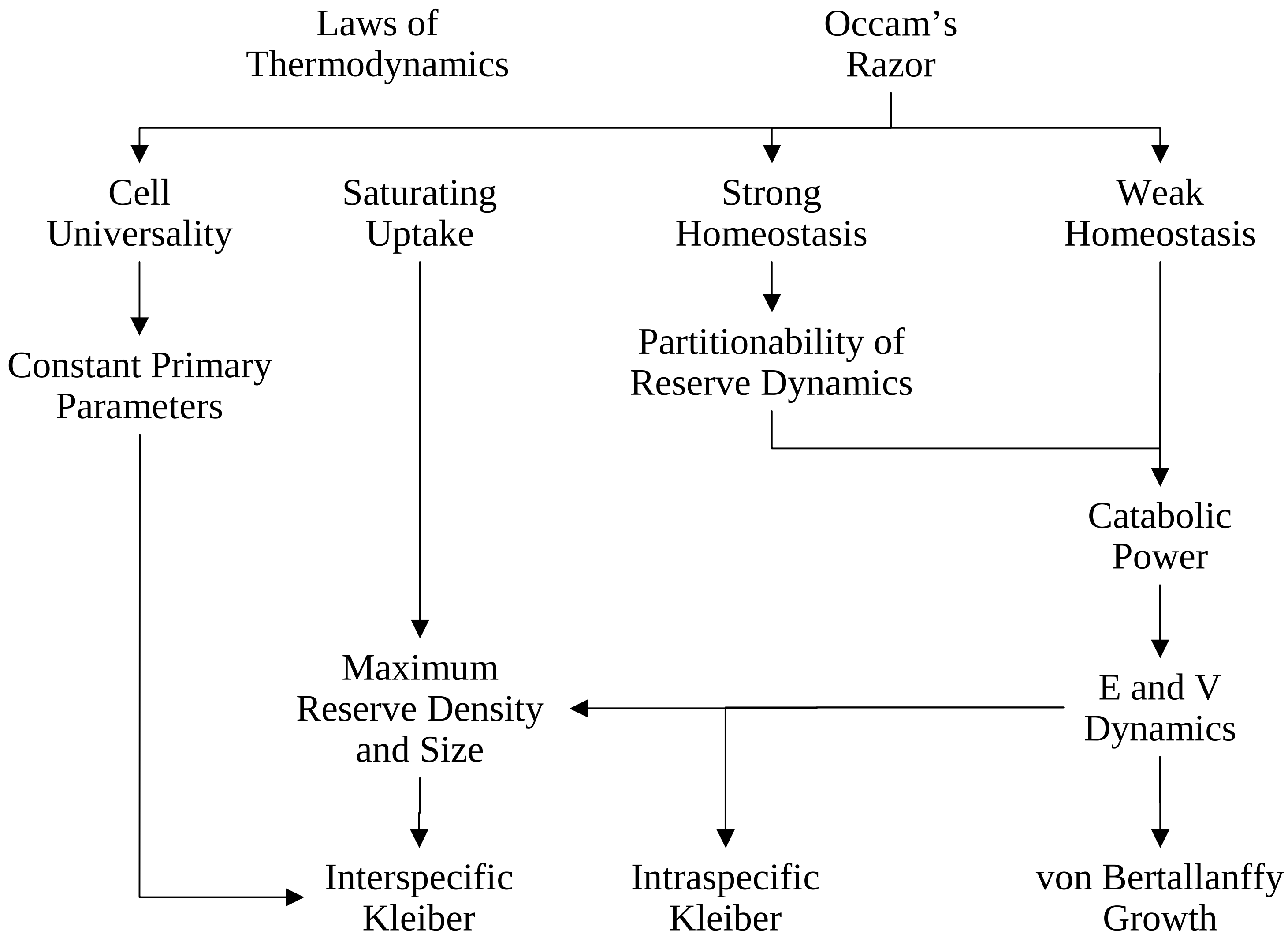
- First Law of Thermodynamics
  Mass and energy are conserved
- Second Law of Thermodynamics
  Energy and mass conversion leads to dissipation (entropy production)
  - [Biological and Epistemological Occam's Razor] Entropy production is (mass)volume-specific in maintenance, (mass)energy-specific in transformations
- Non-Equilibrium Thermodynamics
  Mass and energy flows per unit surface depend only on intensive properties
  - e.g., surface-dependent feeding and heating

Fundamental Principles of DEB Theory (cont.)



- Specific Biological Assumptions
  - Negligible maintenance needs for reserve (E)
    - Empirically substantiated if reserve turnover is high
  - Substrate uptake is a saturating function of structural volume (V)

Implications of the Fundamental Principles



Sousa, T., T. Domingos, S.A.L.M. Kooijman (2008). From empirical patterns to theory: a formal metabolic theory of life. *Phil. Trans. R. Soc. B* 363: 2453-2464.

DEB as a Generalised (Non-Linear) Regression Mechanism

- Many successful theories in science are dependent on a simple formulation, with a systematic perturbation scheme (mathematically, e.g., Taylor expansions, moment expansions):
  - Thermodynamics of gases
    - Virial expansion for real gases
  - Classical mechanics
  - Quantum mechanics
    - Only the hydrogen and helium atom can be exactly calculated

- Along this path, DEB would in fact become a non-falsifiable theory (as all major scientific theories ☺)

Massive Scientific Problem Solving

- Automated fitting with massive distributed computer resources:
  - Seti@home
  - Protein structures
  - “Robot scientists”
- Massive human resources:
  - MMPORPG: Massive Multi-Player Online Role Playing Games
  - Mechanical Turk
  - USA Ecological Monitoring Network
- Education
  - More relevant learning, more demanding assessment

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General Theory and Complex Scientific Modelling Systems

- Complex Models: knowledge management systems
- Software maintenance
- Parameter estimation
- Current models as particular cases of DEB
  - e.g. ERSEM (Mateus et al., in prep.)
- Project deb.org
  - Simple "blackbox tool" for DEB models
  - Integrated with MoHid and MoHidLand for transport processes

Fundamental vs. Applied Science

- In the 19th and 20th centuries fundamental science was pursued for its own sake, in general with no motivation from applications
- In the late 20th and the 21st centuries the priority is for scientific research to be eminently applicable, downgrading the status of fundamental research
- A synthesis: Scientific research motivated by pratical concerns but builds new theory built on general principles
  - e.g, thermodynamics is a theory with the deepest fundamental implications in many fields that was generated from the engineering concern with the optimisation of heat engines
  - e.g., DEB is a general theory applicable to all organisms that was motivated by the interpretation of standardised toxicity tests.
  - e.g., the computer revolution allowed engineering to go from an art to a science: computers allow the application of fundamental principles to complicated (or even complex) systems
- Applied projects have the potential to generate resources for massive research efforts; “ongoing activities” implicitly generate massive amounts of information, which, if adequately organised (as is possible with current information technology) have enormous fundamental and applied significance

Conclusions

- DEB theory is built on a set of fundamental epistemological, physical and biological principles
- DEB has the characteristics of a robust research program
- One way forward for DEB is its development as a general pertubation theory, coupled with systematic statistical fitting procedures (preferably automatic)

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