Bioinformatics: Network Analysis

Modeling in Biology

COMP 572 (BIOS 572 / BIOE 564) - Fall 2013

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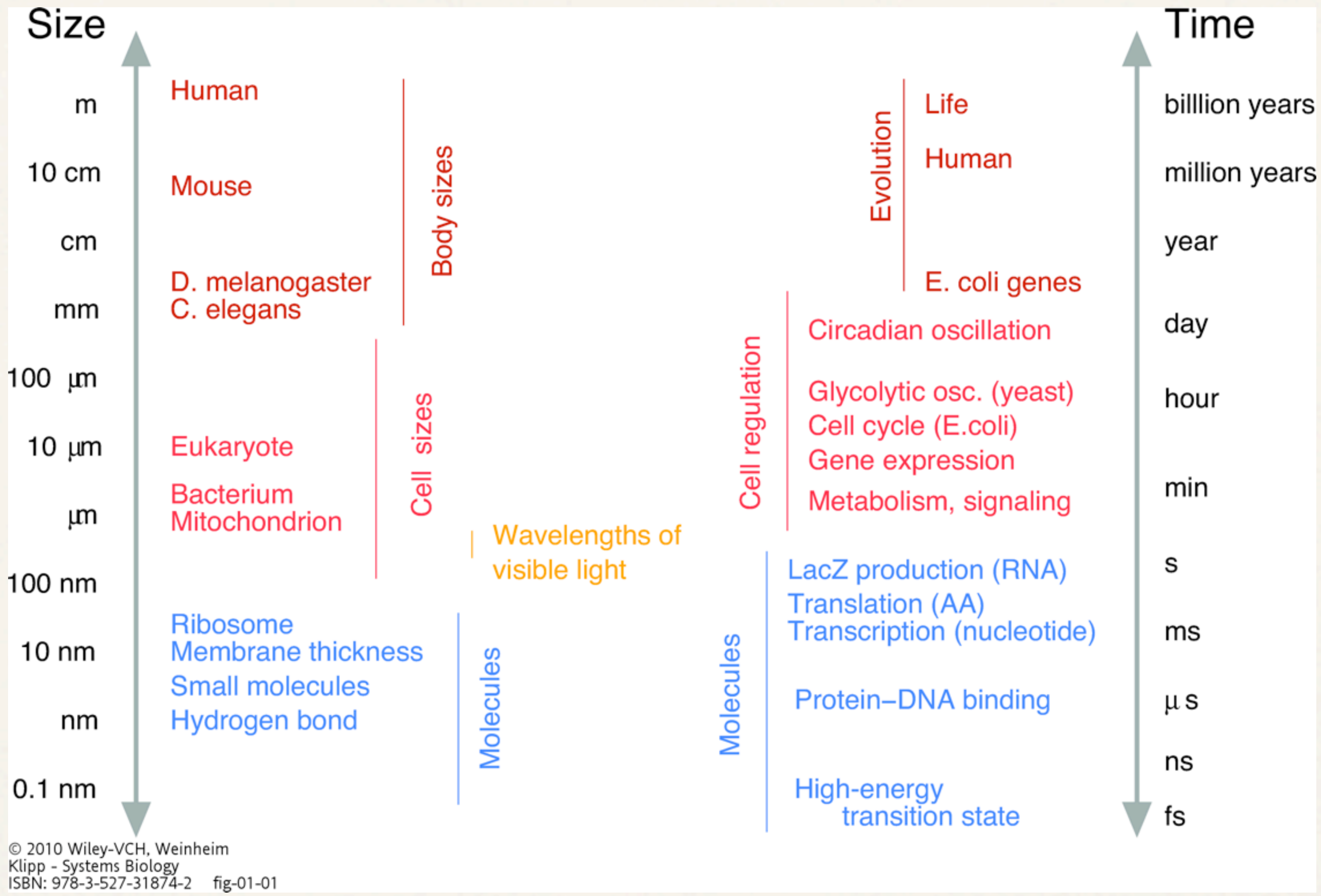
Biology in Time and Space

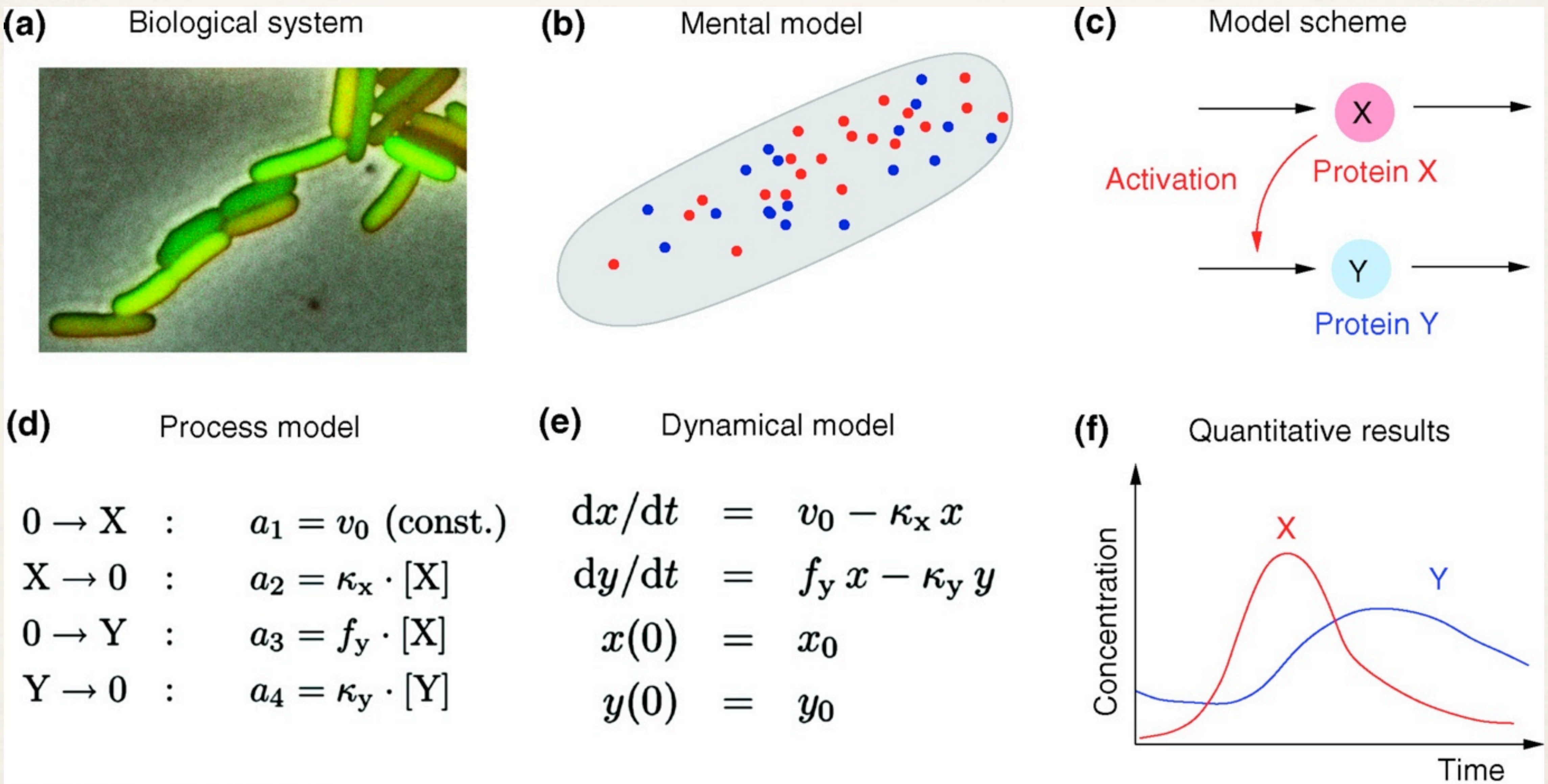


A description of biological entities and their properties encompasses different levels of organization and different time scales.

Models and Modeling

- A model is an abstract representation of objects or processes that explains features of these objects or processes.

Models and Modeling



Klipp - Systems Biology
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Models and Modeling

- Mathematical modeling and computer simulations can help us understand the internal nature and dynamics of processes and to arrive at predictions about their future development and the effect of interactions with the environment.

Models and Modeling

- Modeling is a subjective and selective procedure.
- A model represents only specific aspects of reality that are relevant to the question under consideration.
- How detailed a model is does not make it right or wrong; it just determines whether the model is appropriate to the problem to be solved.
- In fact...

Models and Modeling

"Essentially, all models are wrong, but some are useful."

- George E.P. Box

Models and Modeling

- Modeling drives conceptual clarification.
- Modeling highlights gaps in knowledge or understanding.
- Modeling can assist experimentation.
- Model results can often by presented in precise mathematical terms that allow for generalization.
- Modeling allows for making well-founded and testable predictions.

Basic Notions for Computational Models

- Model scope
  - Models consist of mathematical elements (variables, parameters, constants)
  - A model describe certain aspects of the system, and simplifies/ neglects all others

Basic Notions for Computational Models

- Model statements
  - Statements and equations describe facts about the model elements
  - Examples include ODEs, inequalities, probabilistic statements, etc.

Basic Notions for Computational Models

- System state
  - The state of a system is a snapshot of the system at a given time.
  - The state is described by the set of variables that must be kept track of in a model.

Basic Notions for Computational Models

- Variables, parameters, and constants
  - A constant is a quantity with a fixed value.
  - Parameters are quantities that have a given value.
  - Variables are quantities with a changeable value for which the model establishes relations.

Basic Notions for Computational Models

- Model behavior
  - Two fundamental factors that determine the behavior of a system are
    - influences from the environment (input), and
    - processes within the system.
  - Measurements of the system output often do not suffice to choose between alternative models, as different system structures may still produce similar system behavior.

Basic Notions for Computational Models

- Model classification

  - A *structural* or *qualitative* model specifies the interactions among model elements. A *quantitative* model assigns values to the elements and to their interactions.

  - In a *deterministic* model, the system evolution through all following states can be predicted from the knowledge of the current state. *Stochastic* descriptions give instead a probability distribution for the successive states.

Basic Notions for Computational Models

- Model classification
  - The nature of values that time, state, or space may assume distinguishes a *discrete* model (where values are taken from a discrete set) from a *continuous* model (where values belong to a continuum).

Basic Notions for Computational Models

- Model classification
  - *Reversible* processes can proceed in a forward and backward direction.
  - *Irreversibility* means that only one direction is possible.
  - *Periodicity* indicates that the system assumes a series of states in the time interval $\{t, t+\Delta t\}$ and again in the time interval $\{t+i\Delta t, t+(i+1)\Delta t\}$ for $i=1,2,...$

Basic Notions for Computational Models

- Steady states
    - *Steady* (or, stationary) states are determined by the fact that the values of all state variables remain constant in time.
    - The asymptotic behavior of dynamic systems, that is, the behavior after a sufficiently long time, is often stationary.
    - Other types of asymptotic behavior are *oscillatory* or *chaotic* regimes.

Acknowledgments

- Materials in this lecture are mostly based on Chapter 1 in the textbook by Klipp et al.