Tools and Techniques for Discrete Systems Analysis

Luca Cardelli

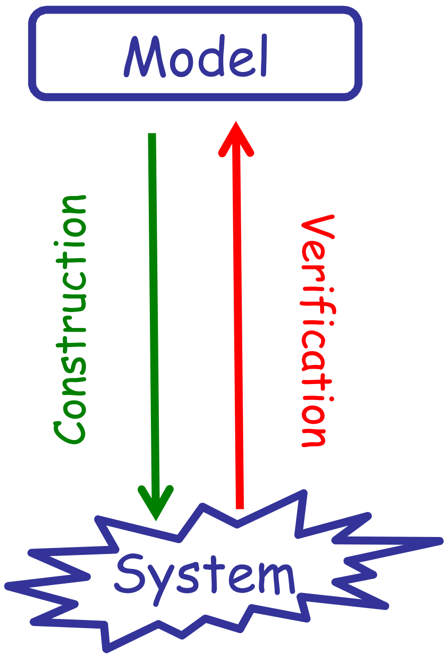
Microsoft Research

C.elegans Modelling Workshop
Cambridge, 2008-07-07

http://LucaCardelli.name

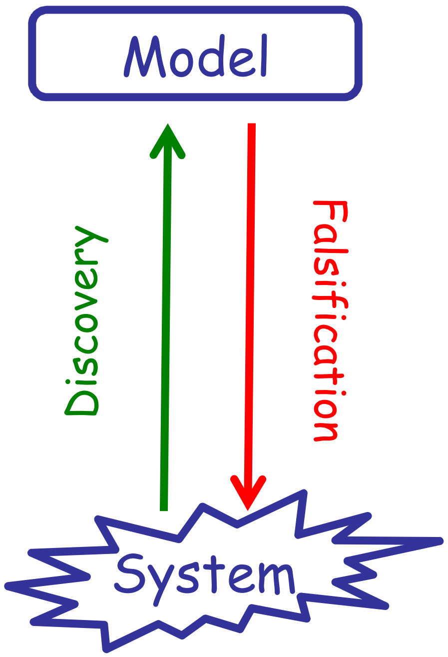
Scientific Method vs. Engineering Method

Engineering Method



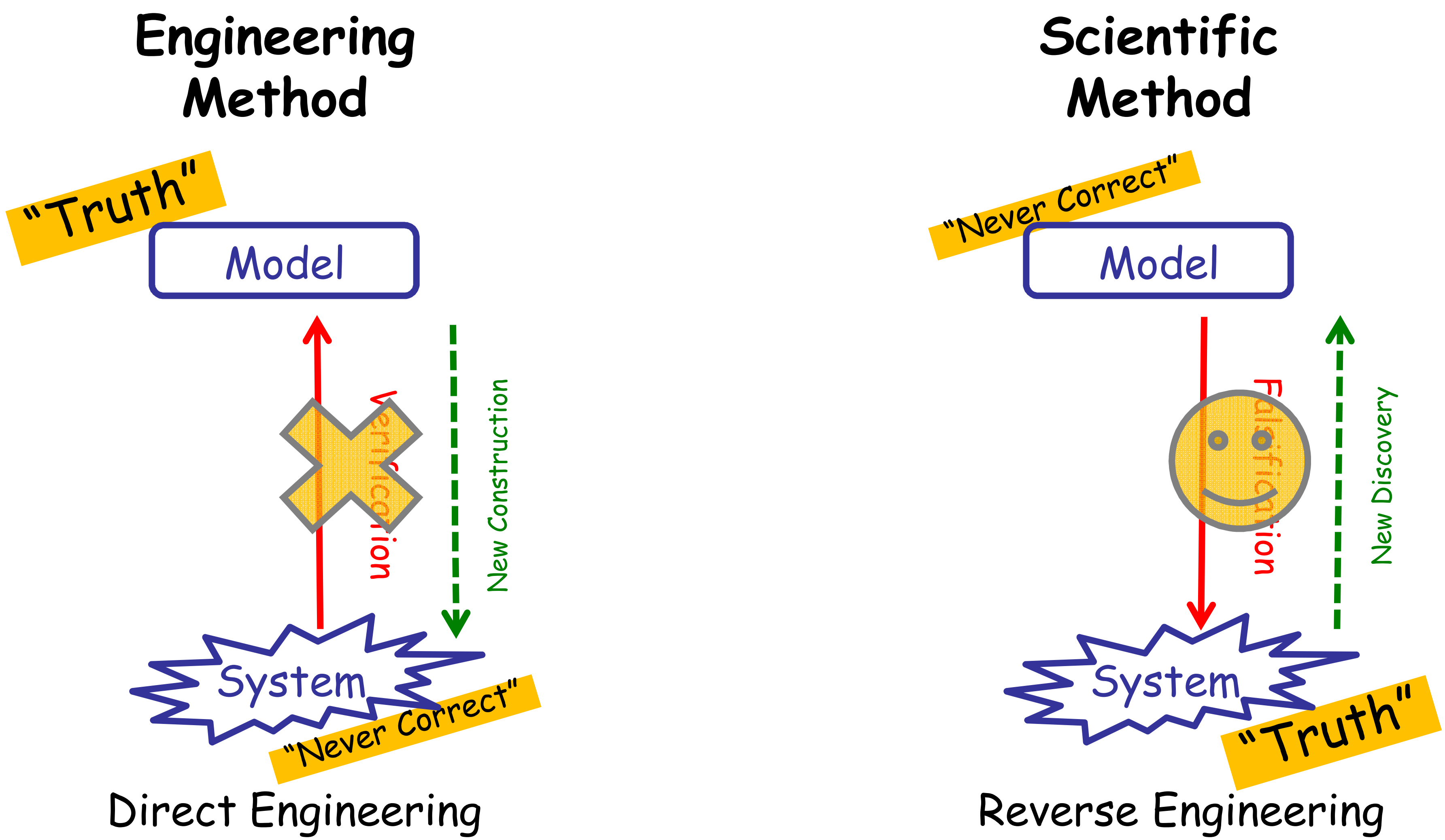
Direct Engineering

Scientific Method

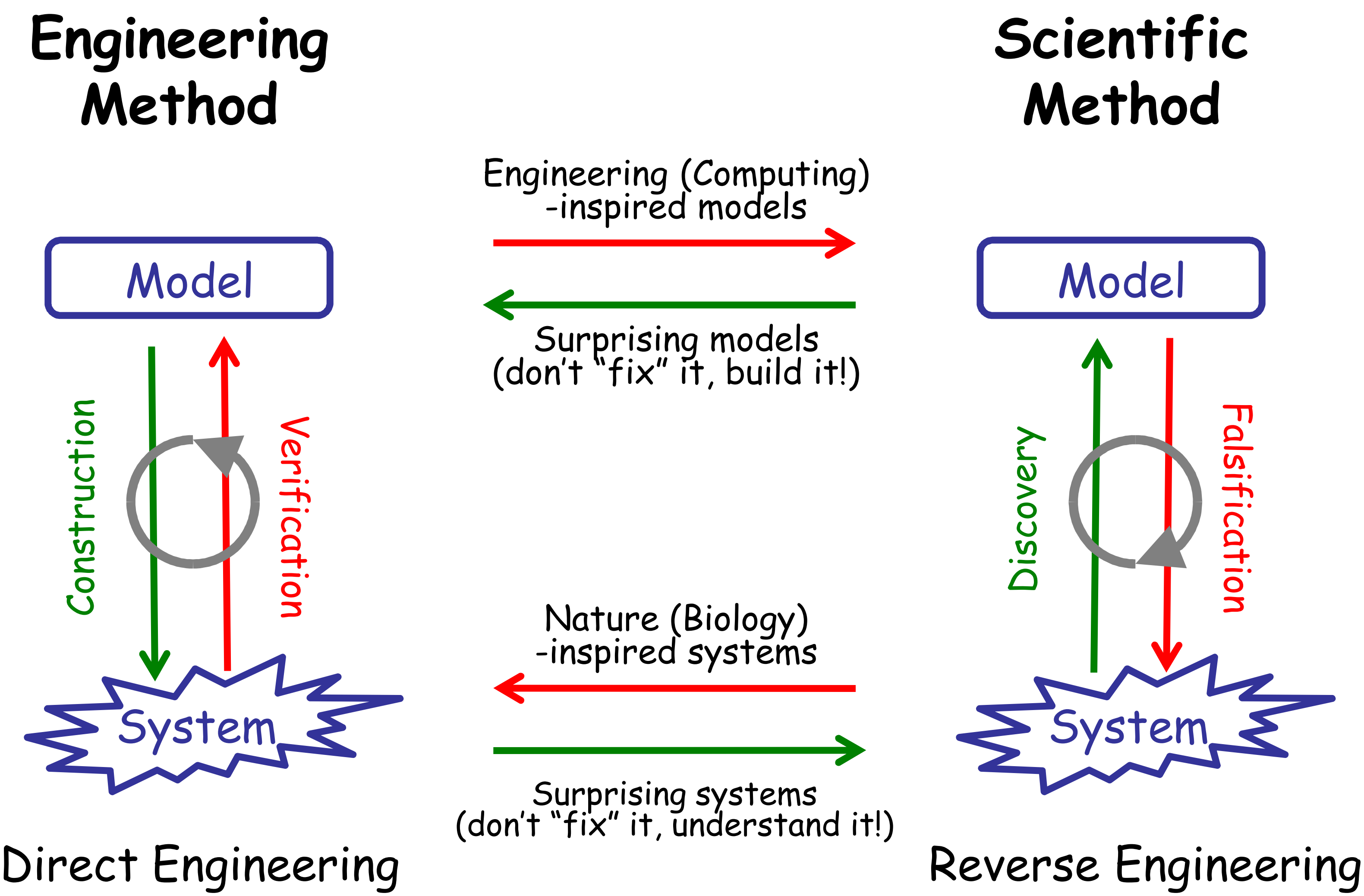


Reverse Engineering

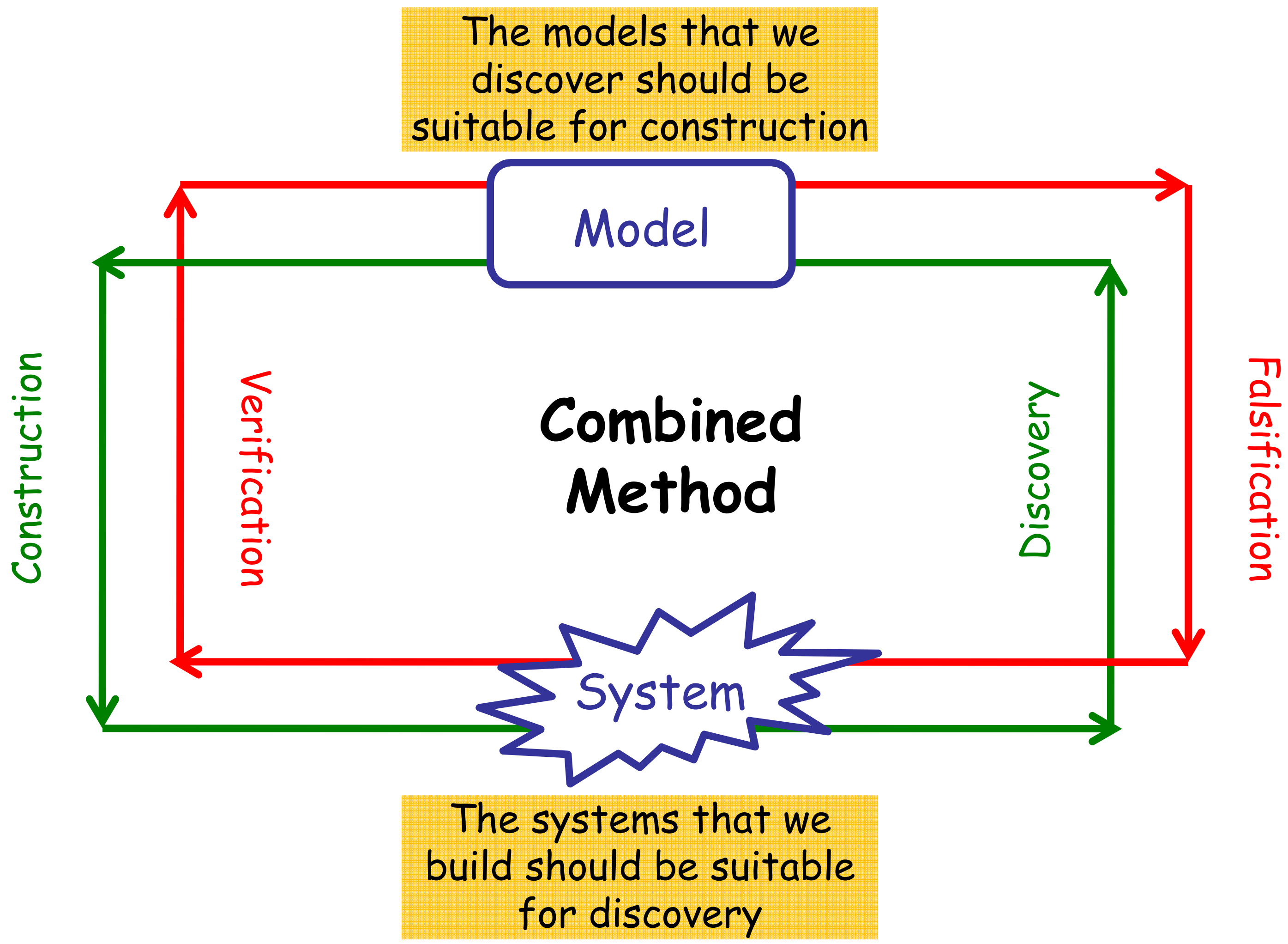
Scientific Method vs. Engineering Method



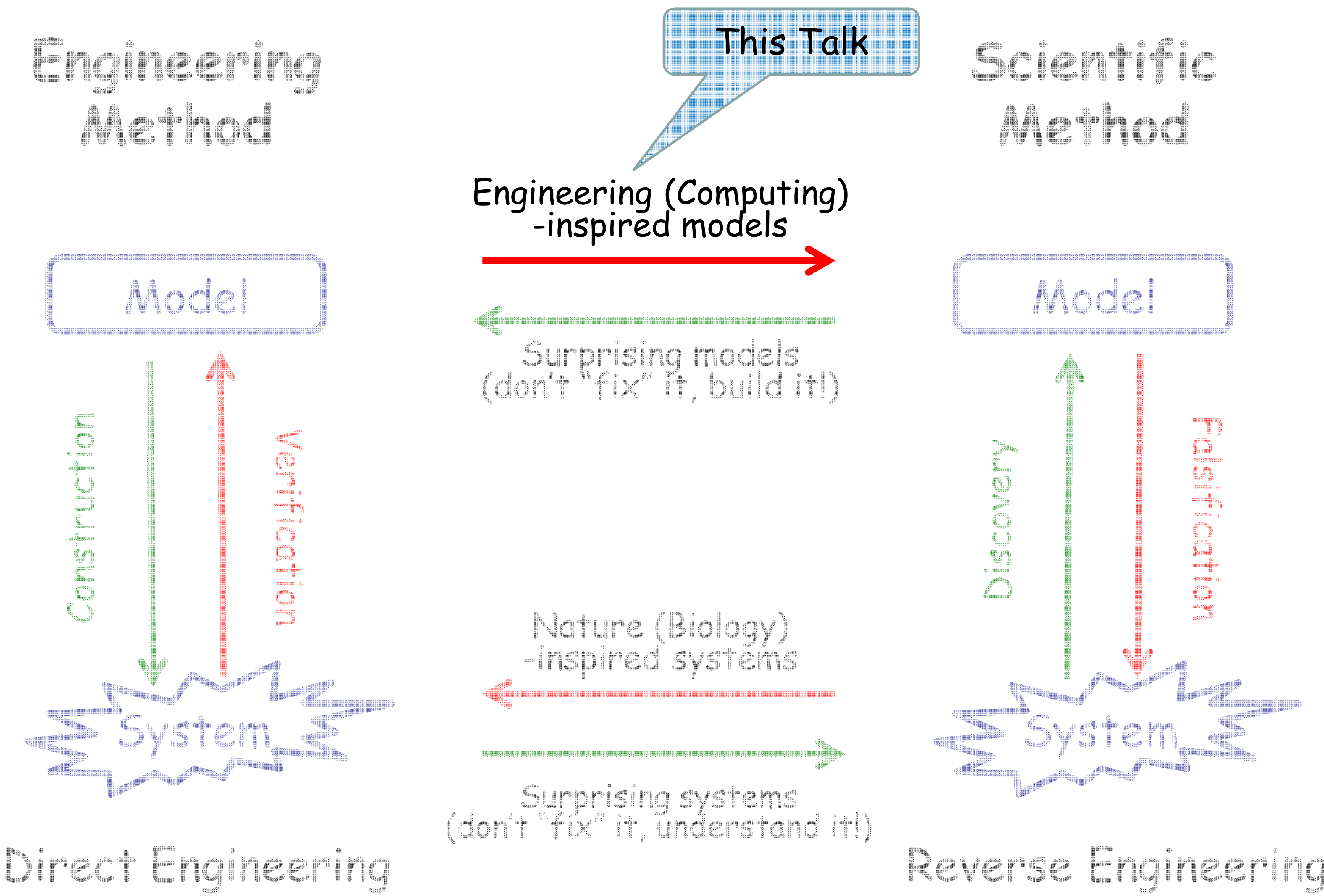
Scientific Method vs. Engineering Method



Scientific Method vs. Engineering Method

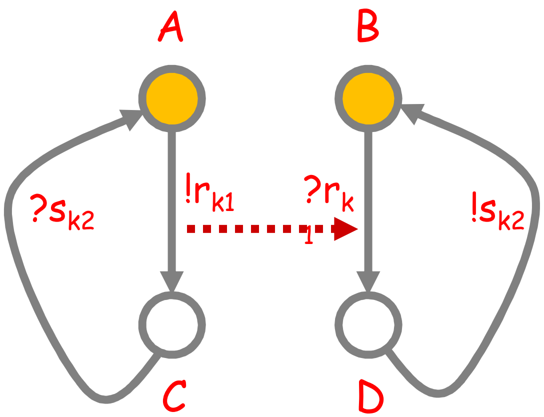


Scientific Method vs. Engineering Method

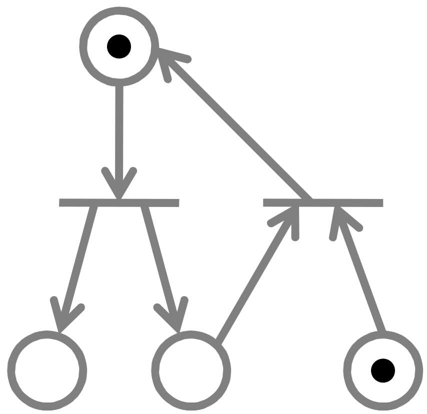


The Program and the State Space

The "program":

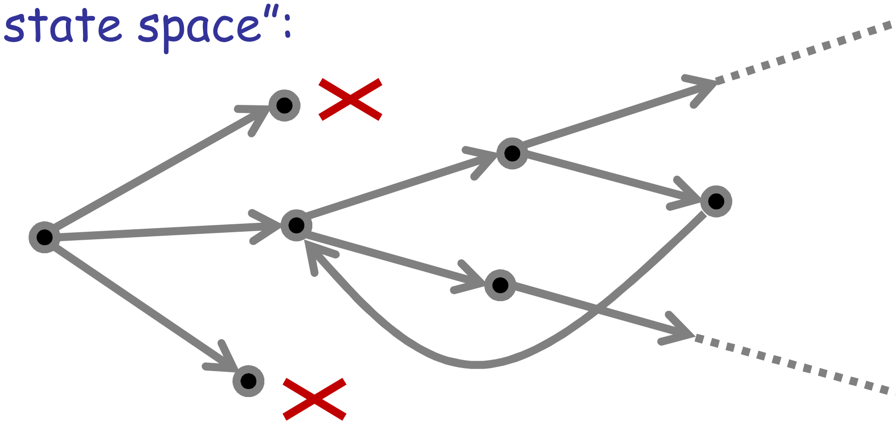


Or



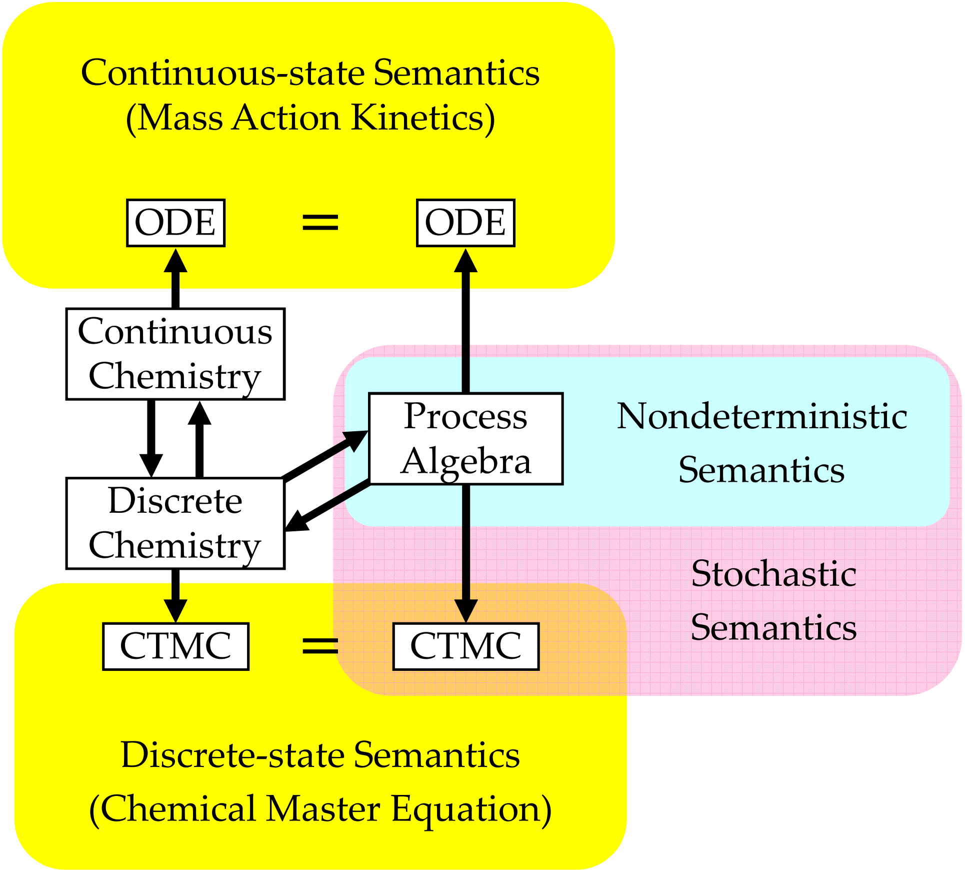
Finite

The "state space":



Potentially infinite

Chemistry vs. Process Algebra



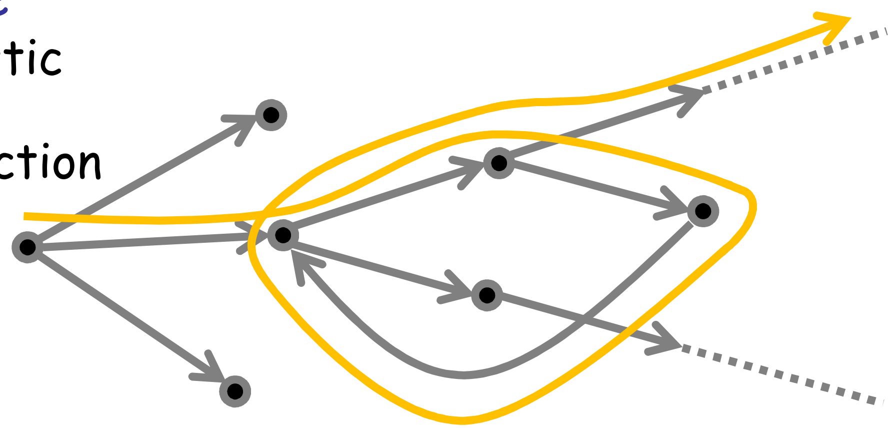
These diagrams commute via appropriate maps.

L. Cardelli: "On Process Rate Semantics" (TCS)

L. Cardelli: "A Process Algebra Master Equation" (QEST'07)

Simulation

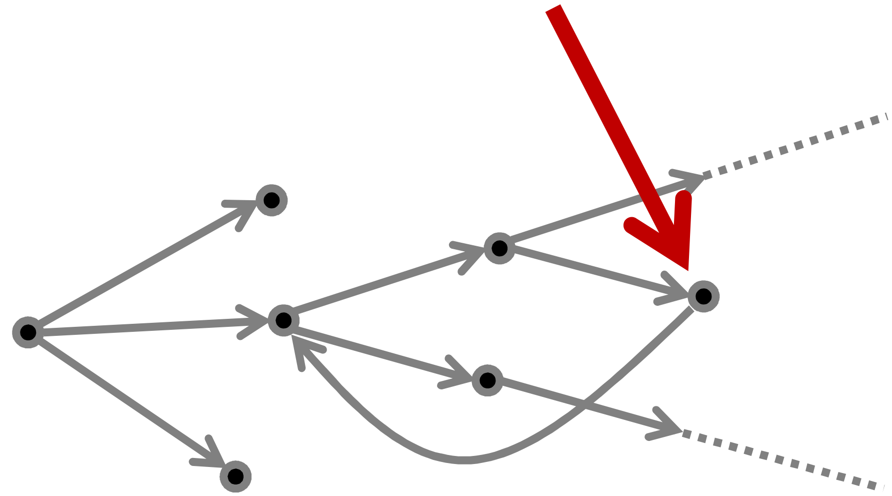
- Run "the program" through a walk in states space.
- Basic stochastic algorithm: Gillespie
  - Exact (i.e. based on physics) stochastic simulation of chemical kinetics.
  - Can compute concentrations and reaction times for biochemical networks.
- Stochastic Process Calculi
  - Now may [BioSPi, SPiM, BioPEPA, BetaBinders, …]
- Hybrid approaches
  - Continuous + discrete/stochastic switching



Control Flow Analysis

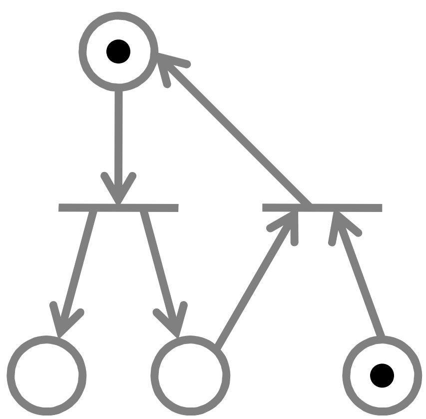
- Who called who?
  - Overapproximation of behavior used to answer questions about what "cannot happen".

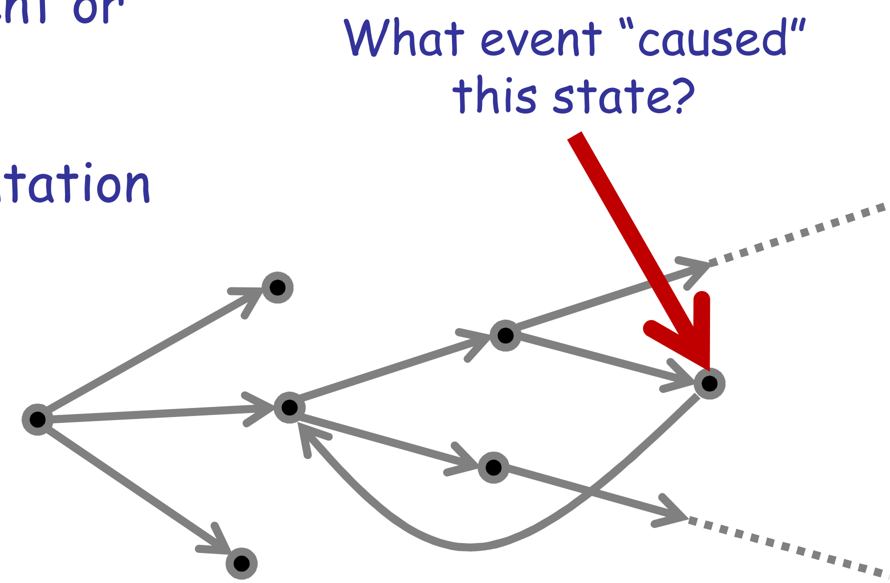
What event may (or may not) have been involved in reaching this state?



Causality Analysis

- What event caused what other event or state to happen?
- Need a different level of representation (the "event space")
  - Petri Nets
  - Event Structures

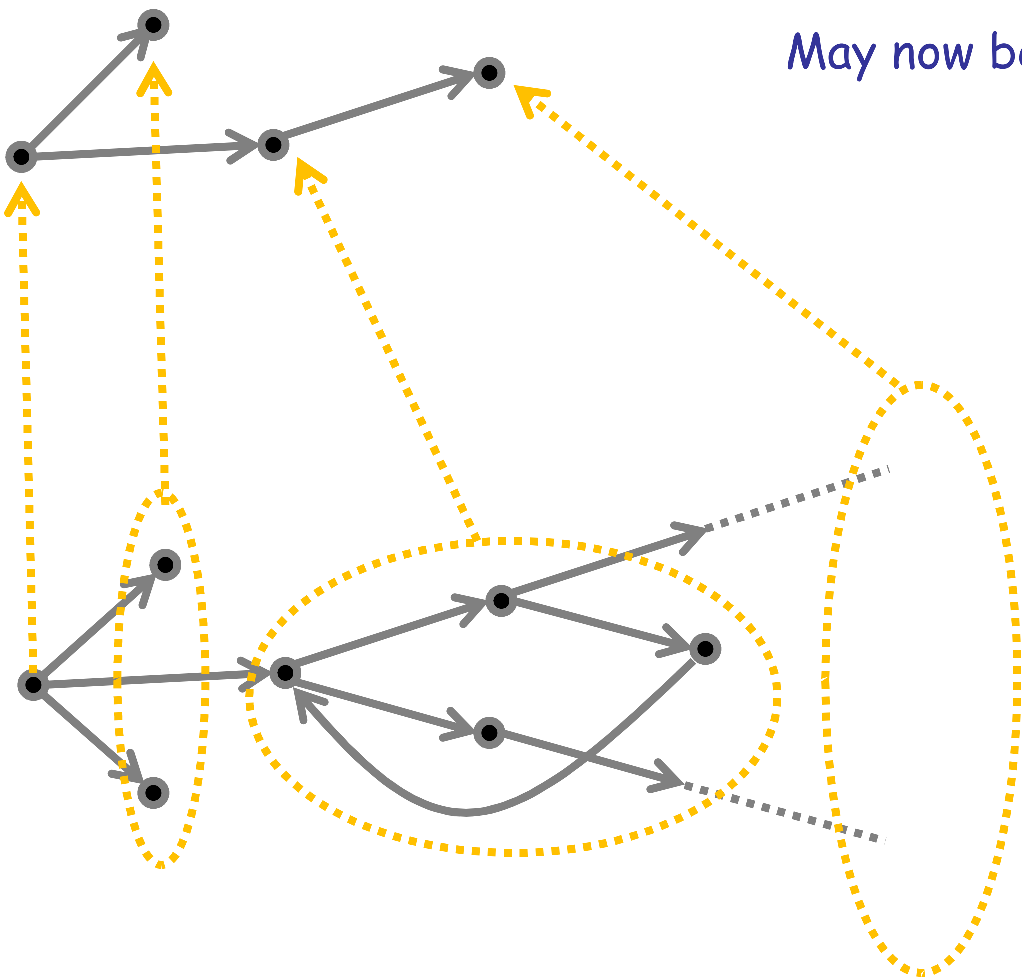




Abstract Interpretation

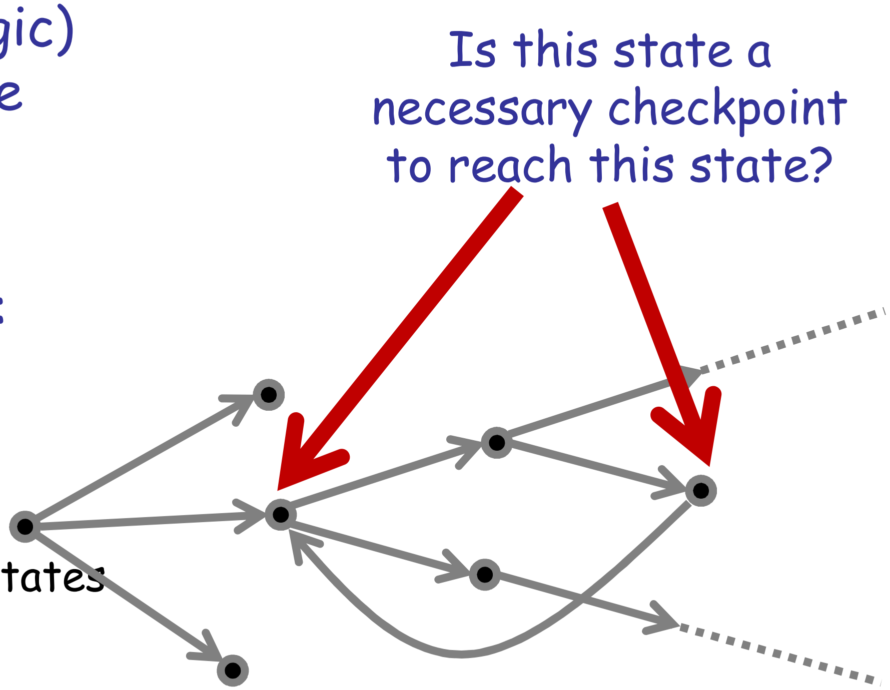
- Precisely relating abstract views to more concrete views of the system

May now be finite!



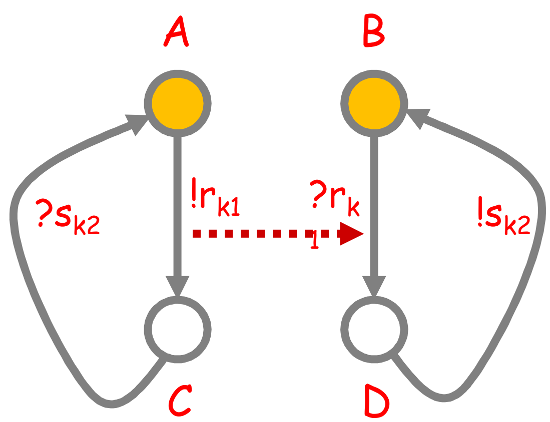
Modelchecking

- Asking questions (in Temporal Logic) about structure of a (finite) state space.
- Various flavors of modelchecking:
  - Temporal
    - About paths through state space
  - Quantitative
    - About quantitative measures of states
  - Probabilistyc/Stochastic
    - About probabilities of reaching states.

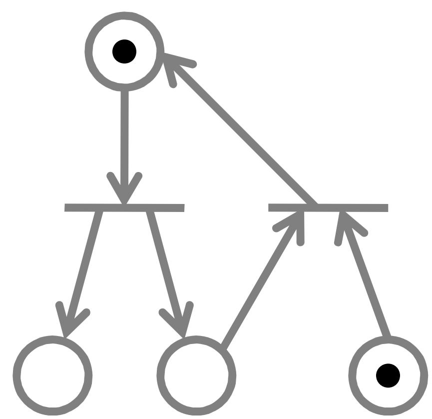


Model Maintenance

- Biology (unlike much of chemistry) is combinatorial
  - Biochemical systems have many regular repeated components
  - Components interact and combine in complex combinatorial ways
  - Components have local state
  - A biochemical system is vastly more compact that its potential state space
- One may expand the state space during analysis, but must not do it during description
- There is a good way:
  - Describe biochemical systems compositionally
  - Each component with its own state and interactions
  - ... as Nature intended...



Or



Or ...

Conclusions

- Connections between modeling approaches
  - Connecting the discrete/concurrent/stochastic/molecular approach
  - to the continuous/sequential/deterministic/population approach

- Connecting syntax with semantics
  - Syntax = model presentation (equations/programs/diagrams/blobs etc.)
  - Semantics = state space (generated by the syntax)

- Ultimately, connections between analysis techniques
  - We need (and sometimes have) good semantic techniques to analyze state spaces (e.g. calculus, but also increasingly modelchecking)
  - But we need equally good syntactic techniques to structure complex models (e.g. compositionality) and analyze them