Stochastic kinetics, game theory, and octave

James B. Rawlings

Department of Chemical and Biological Engineering

THE UNIVERSITY of WISCONSIN MADISON

May 28, 2009

Outline

Introduction to stochastic kinetics

Stochastic kinetics

- Small species populations
- Species numbers are integers, reactions cause integer jumps
- Large fluctuations in species numbers and reaction rates
- Biological networks and catalyst particles

Introduction to stochastic kinetics

Stochastic kinetics

- Small species populations
- Species numbers are integers, reactions cause integer jumps
- Large fluctuations in species numbers and reaction rates
- Biological networks and catalyst particles

Model reduction

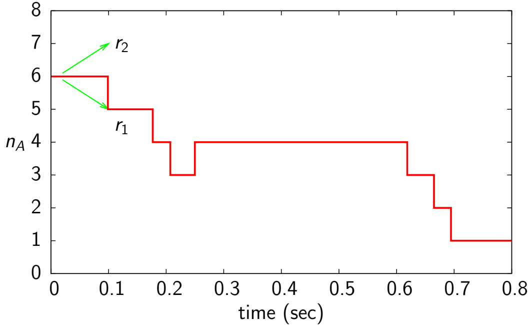
Develop reduced models from stochastic chemical reactions. These models must meet the following requirements:

- Simpler than the full model (fewer reactions, fewer parameters, or faster simulation times)
- Converge to the full model as a specified parameter goes to zero

Stochastic simulation method — kinetic Monte Carlo

$$A \underset{k_2}{\overset{k_1}{\rightleftharpoons}} B \qquad \begin{array}{ll} k_1 = 2 & k_2 = 1 \\ n_{A0} = 6 & n_{B0} = 3 \end{array}$$

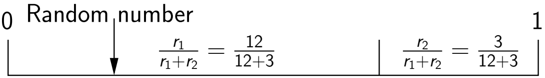
$$A \underset{k_2}{\overset{k_1}{\rightleftharpoons}} B \qquad k_1 = 2 \quad k_2 = 1 \qquad n_{A0} = 6 \quad n_{B0} = 3$$



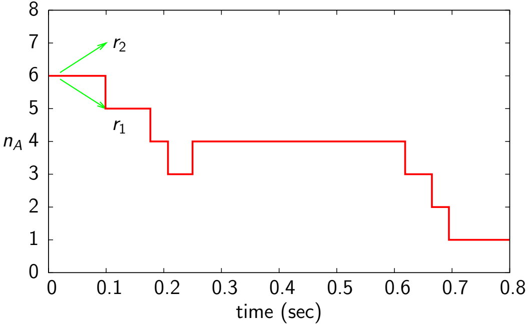
KMC Algorithm

1. Choose which reaction

- Which reaction:



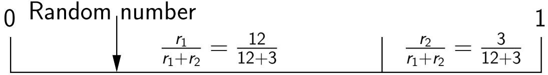
$$A \underset{k_2}{\overset{k_1}{\rightleftharpoons}} B \qquad k_1 = 2 \quad k_2 = 1 \qquad n_{A0} = 6 \quad n_{B0} = 3$$



KMC Algorithm

1. Choose which reaction
2. Choose time step

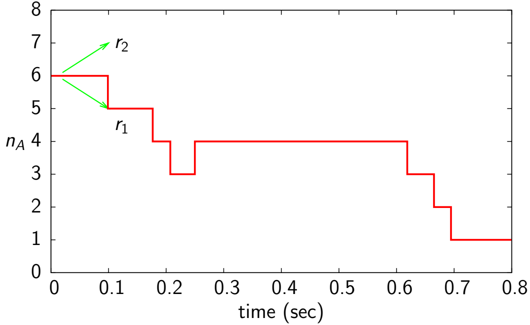
- Which reaction:



- Time step: Sample from an exponential distribution where the distribution mean is the sum of reaction rates.

Stochastic simulation method — kinetic Monte Carlo

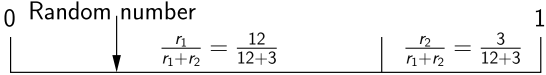
$$A \underset{k_2}{\overset{k_1}{\rightleftharpoons}} B \qquad \begin{array}{ll} k_1 = 2 & k_2 = 1 \\ n_{A0} = 6 & n_{B0} = 3 \end{array}$$



KMC Algorithm

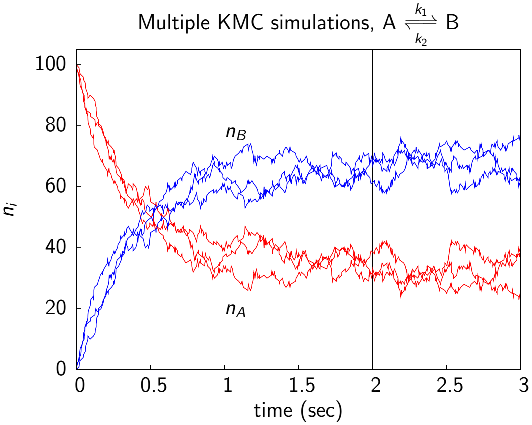
1. Choose which reaction
2. Choose time step
3. Repeat

- Which reaction:

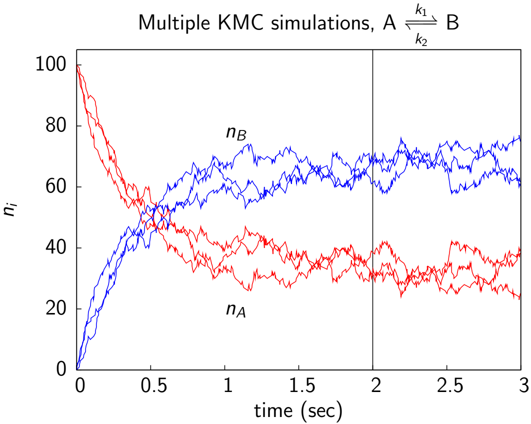


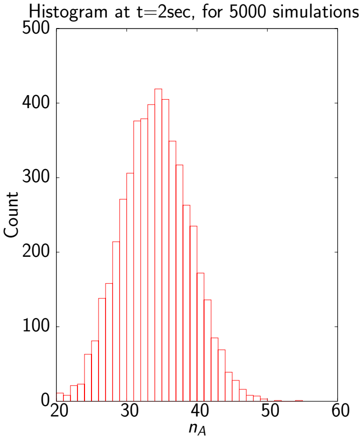
- Time step: Sample from an exponential distribution where the distribution mean is the sum of reaction rates.

KMC simulations and probability



KMC simulations and probability

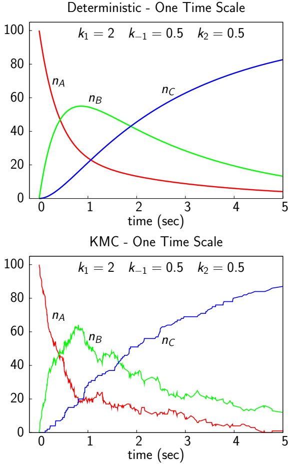




- KMC simulations are samples of a probability distribution that evolves in time.
- We can write the evolution equation for the probability density (master equation).

Kinetics of multiple time scales

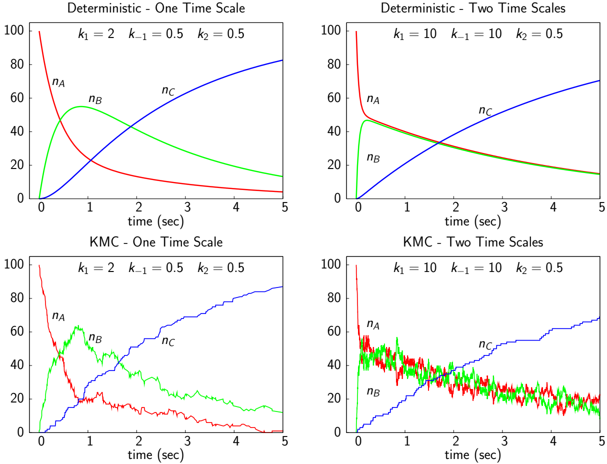
$$A \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} B \xrightarrow{k_2} C$$



One time scale

Kinetics of multiple time scales

$$\mathrm{A} \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} \mathrm{B} \xrightarrow{k_2} \mathrm{C}$$

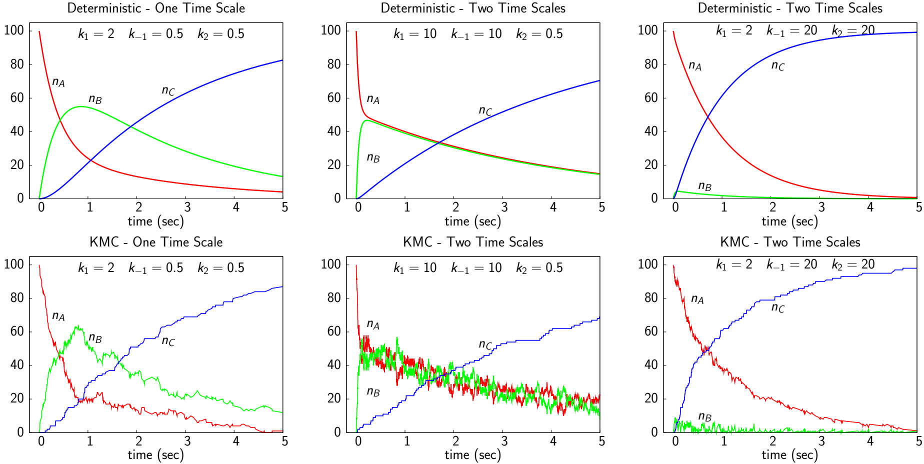


One time scale

Reaction equilibrium

Kinetics of multiple time scales

$$A \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} B \xrightarrow{k_2} C$$



One time scale | Reaction equilibrium | Reactive intermediate

Game theory: example

- Player 1 wants to optimize his profit function V_1. He gets to make decision u_1.

Game theory: example

- Player 1 wants to optimize his profit function V_1. He gets to make decision u_1.
- Player 2 wants to optimize his profit function V_2. He gets to make decision u_2.

Game theory: example

- Player 1 wants to optimize his profit function V_1. He gets to make decision u_1.
- Player 2 wants to optimize his profit function V_2. He gets to make decision u_2.
- The problem is both players' decisions affect both players' profit functions

$$V_1(u_1, u_2) \qquad V_2(u_1, u_2)$$

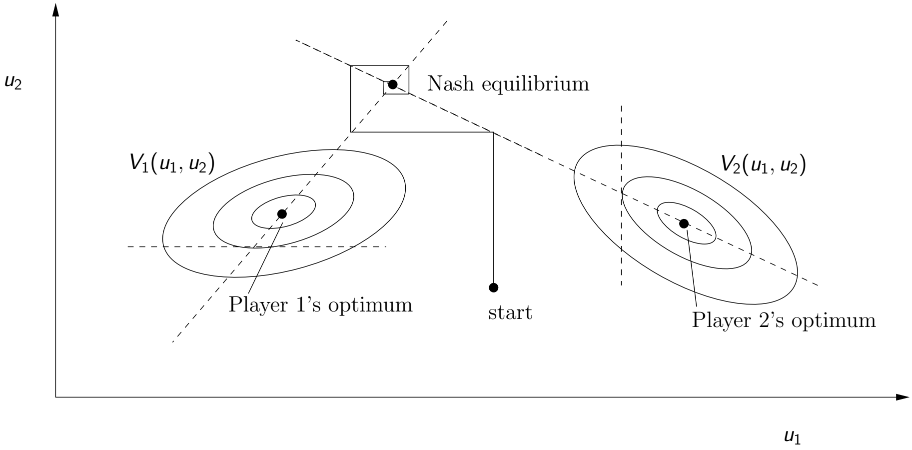
Game theory: example

- Player 1 wants to optimize his profit function V_1. He gets to make decision u_1.
- Player 2 wants to optimize his profit function V_2. He gets to make decision u_2.
- The problem is both players' decisions affect both players' profit functions

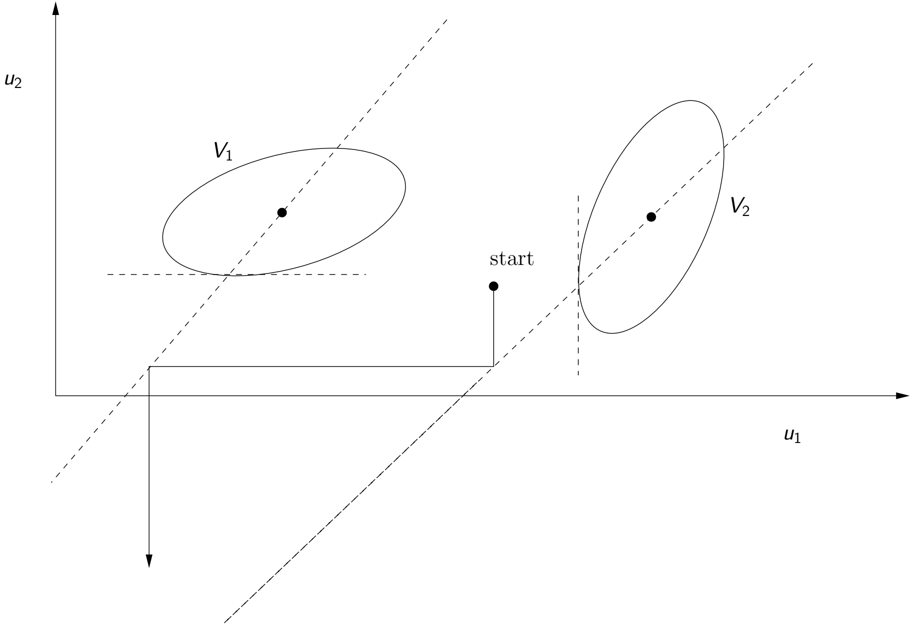
$$V_1(u_1, u_2) \qquad V_2(u_1, u_2)$$

- Here's the picture for quadratic functions

Two-player game



Unhappy outcome in two-player game



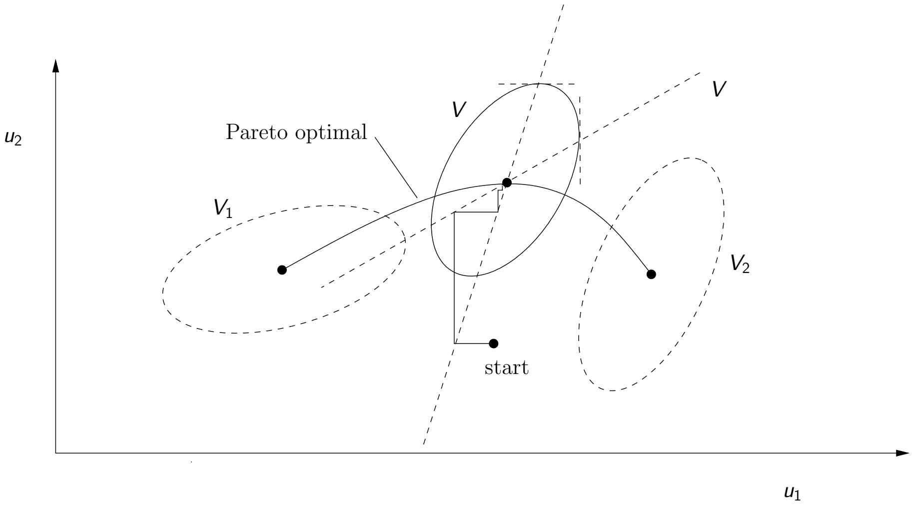
Cooperative game

- Define a common objective for both Player 1 and Player 2.

$$V(u_1, u_2) = \lambda V_1 + (1 - \lambda) V_2 \qquad 0 < \lambda < 1$$

- Both Players 1 and 2 agree to cooperate and maximize this common objective.
- Here's the picture for the unhappy Nash functions

Cooperative two-player game



What is Octave?

`www.octave.org`