Week 7: Deterministic Chemical Kinetics

(You are at the halfway point of CAAM 210!)

Skeletal Outline

`mca2driver`

[this is where the majority of the work is]

`dx=mcaode(t,x,k)` `(x=[R Pr RPr P D I])`

[write down ODEs]

`[t, xout]= mygill(tfin, rtab, x, c)`

[edit last week's mygill to return all reactants, not just dimer]

`h=update(x)`

[same as last week]

mca2driver

1. Set parameters: tfin, tinc, nr, x0, c (nr=4)
2. Hard code rtab (same as last week)
3. Call mygill nr times, interpolating and storing the time and concentration [t, xout], the outputs of mygill, for run=1:nr

…

First we look only at what happens to dimer, to create figure 1.

However, next we will look at all 6 chemicals, so we need to edit mygill so that it stores information for chemicals other than dimer. How do we do this?

mca2driver

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2. Hard code rtab (same as last week)
3. Call mygill nr times, interpolating and storing the time and concentration [t, xout], the outputs of mygill, for run=1:nr
4. Plot mean and standard deviation, hold on [Stochastic]

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5. Call ode23, which calls mcaode [Deterministic]
6. Superimpose deterministic dimer count on plot 1 to make first figure
7. Now run mygill only once (nr=1), and make the second figure with all the subplots by comparing stochastic to deterministic for each reactant

Task 1: write dx=mcaode(t,x,k)

Reactions are the same as last week. We're calling the propensities, k now (not c), with no necessary transformation.

R + Pr → RPr	(k1)
RPr → R + Pr	(k2)
RPr → 10P + R + Pr	(k3)
P + P → D	(k4)
D → P + P	(k5)
P →	(k6)
Pr + D → I	(k7)
I → Pr + D	(k8)

The first one has already been done dx(1,1) = $-c_1 x_1 x_2 + c_2 x_3 + c_3 x_3$

Ode23

- [t,x]=ode23(function handle, timespan, initial values)
  - Each element of the solution (and output) x is the solution at the time corresponding to that element in t.
  - Solves from start time to end time (specified in timespan)
  - Example: [t,y]=ode23(@vdp1,[0 20],[2 0]); (in MATLAB help)
- Our times are from 0 to tfin
- Our initial values are in x0, which we set earlier in the driver (make sure it's a row vector)
- Function handles are tricky animals. Remember, our functions are hidden in mcaode. You have to call mcaode *within* ode23 to pull out the functions you need. Then you need to tell ode23 for which values to solve the ODE by using @(t,x).

Task 2: ode23

- Let's write the one line of code that calls ode23 (and mcaode).
- You only need to call this once in your driver. You just access the different parts of its output (t, x) depending on which reactant you're considering.

mca2driver

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5. Call ode23, which calls mcaode [Deterministic]
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