

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.

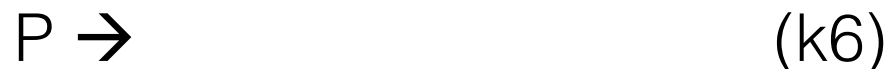
However, next we will look at all 6 chemicals, so we need to edit mygill so that it stores information for chemicals other than dimer. How do we do this?

mca2driver

1. Set parameters: t_{fin} , t_{inc} , nr , x_0 , c ($nr=4$)
2. Hard code r_{tab} (same as last week)
3. Call `mygill` nr times, interpolating and storing the time and concentration $[t, x_{out}]$, the outputs of `mygill`, for $run=1:nr$
4. Plot mean and standard deviation, hold on [Stochastic]
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 $\text{dx}=\text{mcaode}(t,x,k)$

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



The first one has already been done $\text{dx}(1,1) = -c_1x_1x_2 + c_2x_3 + c_3x_3$

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

1. Set parameters: t_{fin} , t_{inc} , nr , x_0 , c ($nr=4$)
2. Hard code r_{tab} (same as last week)
3. Call `mygill` nr times, interpolating and storing the time and concentration $[t, x_{out}]$, the outputs of `mygill`, for $run=1:nr$
4. Plot mean and standard deviation, hold on [Stochastic]
5. Call `ode23`, which calls `mcaode` [Deterministic]
6. Superimpose deterministic dimer count on plot 1 to make first figure [Stochastic]
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