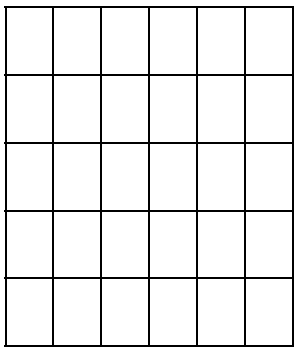
This research group created a software tool called the COMETS, Computation of Microbial Ecosystems in Time and Space. The novelty of this tool is it takes into account time and space (spacetime!), not like static FBA where everything is a bulk. The software source is available at

http://www.bu.edu/segrelab/comets/

This is a Java application, which runs on all platforms. But it does ask you to install a dependency, which I couldn't get it to work. The dependency is a licensed software. I got a free license for academic use, but seems like it's not accepted by COMETS. Anyways, here is what they did...

So image the following is a Petri dish. In the software, they break this area to many small boxes, like how images are made up of pixels. Then they model this Petri dish with those boxes. (Go to the link above and watch the picture, it gives you an intuitive sense)



Each box has the following properties:

1. biomass for each species (in grams, dry cell weight).
   if there are n species, there will be n biomasses
2. the amount of metabolite (chemical) for each metabolite (in mmoles)
   if there are n metabolites, there will be n numbers representing all metabolites
3. the concentration of each metabolite. this is just property 3 divided by the volume

Note that these properties are both functions of **space** and **time**. This way, we can track, say, how much toluene is present at (2 cm, 3 cm), after 5 minutes is passed.

Biomass in each box can increase due to cellular growth, or decrease due to death.

Everything after this point is pretty much what Naveen told us the other day. We are essentially solving an optimization problem. We want to maximize the biomass for each species while making sure none of the constraints are violated.

There is one main difference, however. While static FBA considers everything as a whole, this model considers it as many little boxes. Therefore, they also take into account diffusion. So, a species may decrease/increase due to:

1. generation/depletion from chemical reactions (also considered in static FBA)
2. conversion to/from biomass (also considered in static FBA)
3. diffusion into/out of the neighbouring areas (**not** considered in static FBA)
    a. for this part, Fick's Law is used to model diffusion

Based on everything above, the model is completely described. Then there is the lengthy math, and a whole set of notations which threw me off… I will take a closer look later.

The results: A number of tests they run match experimental observations. They have run up to three bacteria species in a culture, and the results seem good. And there is this discussion on "metabolic eclipse dilemma" which COMETS also seems to verify successfully.