# The 2D Gel Electrophoresis Simulator: *SimGel*

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## 1 Introduction

2-dimensional (2D) gel electrophoresis has been a popular and useful protein/DNA analysis method for a long time because of its ease of examination. Although the procedure of this method is relatively easier than other molecular biological experiments, it has several physically caused limitations such as random distortion of gel, spot smears and quasi-spots (artifacts), and uneven intensity of each spot.

In order to alleviate these difficulties and help practitioners with computational aids, we developed the *SimGel*, an interactive 2D gel electrophoresis simulator. *SimGel* helps you to analyze ordinary electrophoresis quantitatively, interactively, and in details of single nucleotide/amino-acid of every spot with pin-point accuracy.

*SimGel* allows practitioners to:

- try many kind of restriction enzymes and examine optimal experimented condition in advance
- pin-point the approximate location of the focused spots
- view the location of spots without any smear and gel distortion
- trace the location of spots(labeled/unlabeled) in arbitrary time-scale and physical scale
- measure the spots in one nucleotide/amino-acid wise
- review the nucleotide/amino-acid sequence interactively

So we believe that this new application program will not only help practitioners of molecular biological experiment but also change the way to practice the experiments in biology laboratory. And additionally, combination of *SimGel* and automated RLGS (Restriction Landmark Genomic Scanning) electrophoretogram processing method [1] will promote the highly computational functional analysis of genes that is very crucial for *post*-Genome Project research activities.

## 2 Method and Results

2D gel electrophoresis simulation naturally requires the modeling of behavior of molecules in a gel with electoric potential gradient. Simulation of protein electrophoresis needs prediction of isoelectric points, denoted as $pI$, for every tested proteins. Although the prediction of $pI$ is expected to be built in *SimGel*, current implementation employs simulation of DNA electrophoresis only. We wanted to find mobility dependency on molecular size to compute the location of every spot at arbitrary moment. We measured the mobility of every spot that has different molecular size from our examination results of electrophoresis for *E. coli* genome. As Figure 2 shows, the measurement found that, in a certain range of molecular size ($m$), the mobility ($M$) can be denoted in the equation; $M(m) = \exp^{a \log(m)+b}$.

However too small/large molecules do not follow the equation and such molecules are almost invisible on the electrophoretogram. Besides, the mechanism of micro/macro molecular behavior in a gel

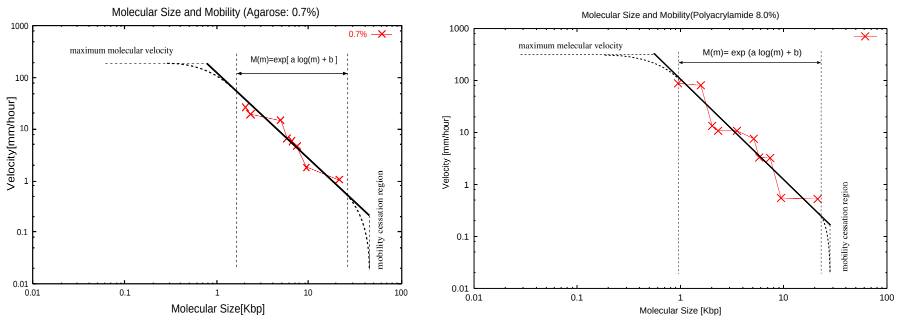


Figure 1: Measured data are plotted as cross-hairs. Solid line represents molecular mobility depends on molecular size. Dotted arcs represent unknown but expected molecular mobility for very small/large molecules.

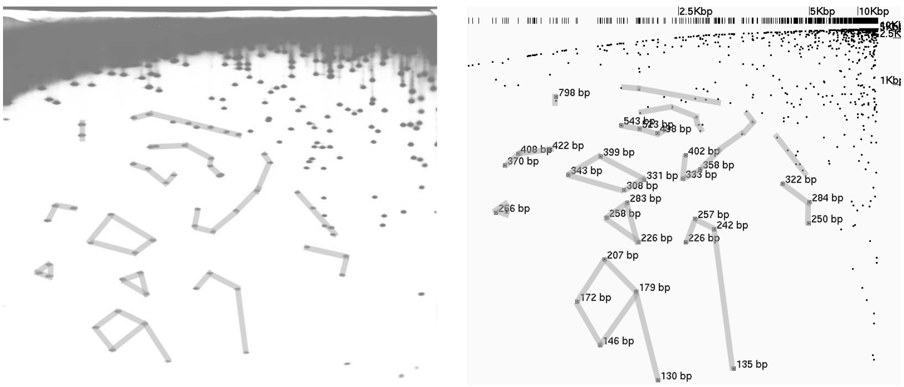


Figure 2: Side by side comparison between 2D electrophoretogram (left) and *SimGel* simulated image (right) with base-size tags for *E. coli* DNA. The stripe patters are added to provide at-a-glance correspondence between spots.

has definitely non-linear characteristics. In addition, it is well known that molecular mobility strongly depends on DNA bending caused by adenine-thymine tacts [2]. So it is very hard to compute the behavior from a fine mathematical model and such computation gets simply beyond the performance of personal computers. Thus we need to focus on a certain range of molecular size which allows us to take try-and-error approach to construct a model to simulate the electrophoresis with reasonable precision. Our preliminary implementation attained fairly identical spot images that is obtained by 2D electrophoresis experiments (see Figure 2).

# References


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