

MCDiff

(Monte Carlo Diffusion)

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FADD

(Fluorescence Accumulation after DNA Damage)

Procedure Objective: measure rate of accumulation of proteins

Problem: guess and check

Solution: simulate cellular dynamics to determine governing parameters

D: *diffusion coefficient*, governs movement

F: *mobile fraction* - proportion of proteins in motion

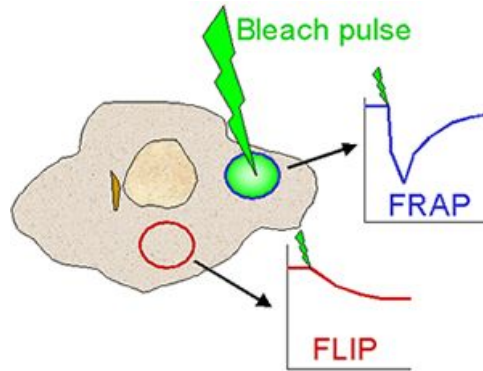
Simulation Assumptions

- Particles move according to random walk
 - Proteins always move at each time step
 - Movement distance obeys gaussian
 - Movement direction is uniform around circle
 - Movement is in 2 dimensions
 - No interaction between molecules
 - “Escaping molecules” bounce back to same position
- Modeled as 1D points
- Trapping is permanent



Additional Considerations

- “Bleaching effect”
 - Percent of fluorescence is bleached*
 - No molecules revert



Functions

- Parse 3 input files
- Generate nucleus and roi regions
- For each trial:
 - Populate nucleus
 - Simulate laser
 - Bleach points
 - Move points
 - Get D and F
- After X trials, generate heat map and move towards best parameter set

