Models of physical non-equilibrium (mass transfer) processes in structured porous media

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Two Scales of Interest

- Transfer between multiple pore domains within an REV
- Transfer between discrete hydrofacies in a geologically heterogeneous system

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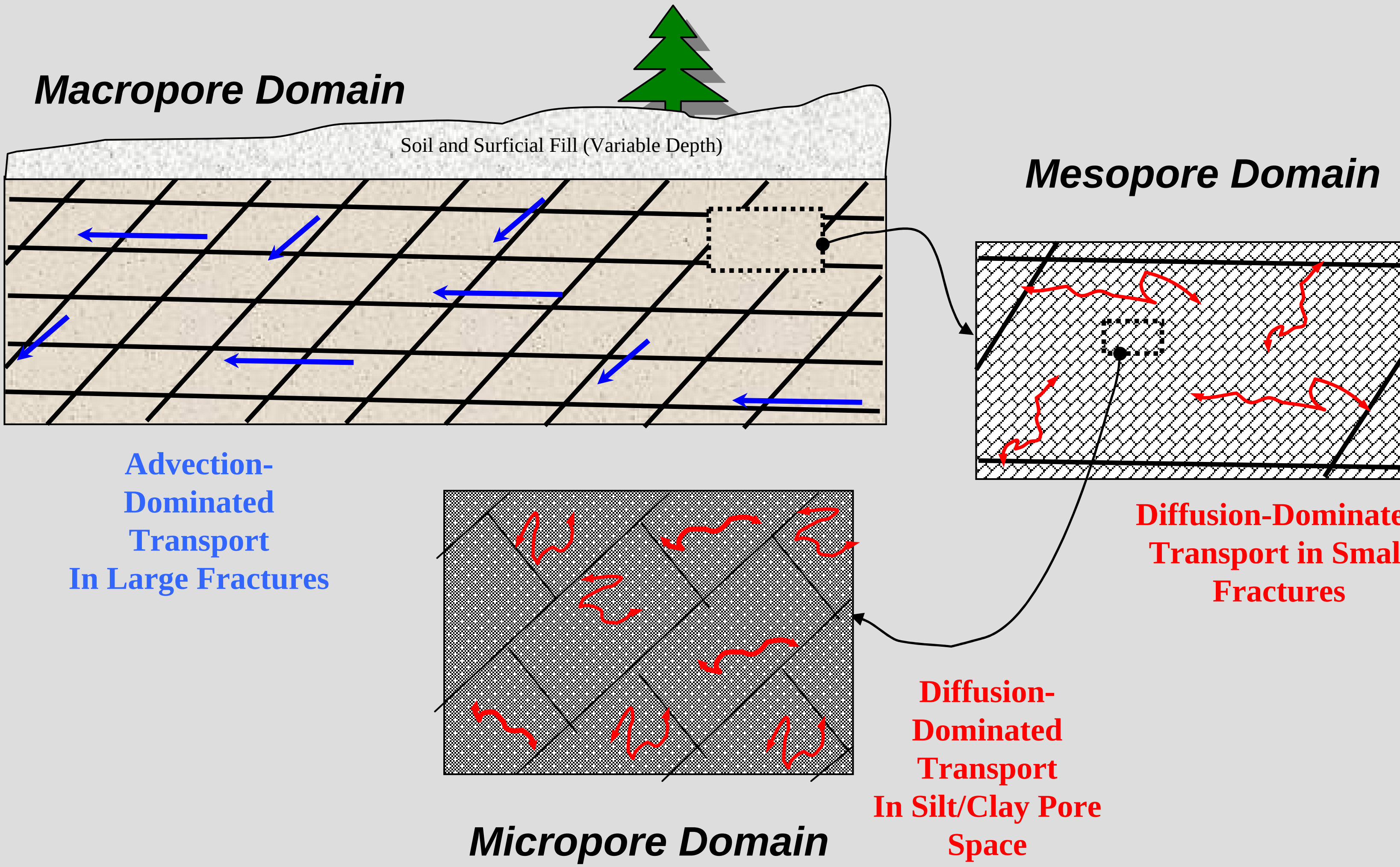
Fractured Saprolite

Structured Porous Media



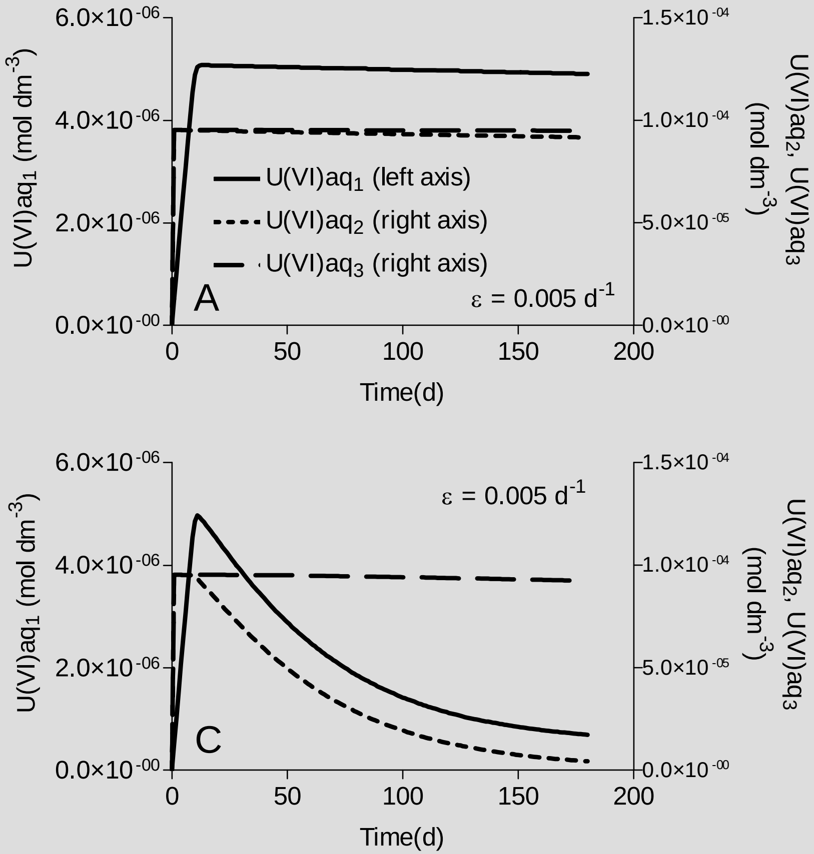
Model Approach

- Multiple Pore Region (MPR) model

$$\theta_1 \frac{\partial U(VI)aq_1}{\partial t} = -v_1\theta_1 \frac{\partial U(VI)aq_1}{\partial x} + \theta_1 D_{U(VI)1} \frac{\partial^2 U(VI)aq_1}{\partial x^2} + \theta_1 R_{12_{U(VI)}} + \theta_1 R_{13_{U(VI)}} - \theta_1 R_{U(VI)ads1} - \theta_1 R_{U(VI)bio1}$$

$$R_{12} = \varepsilon_{12}(C_2 - C_1)$$

Example Simulation



Breakthrough curves for aqueous U(VI) (A,C) in the macro (domain 1), meso (domain 2), and micro (domain 3) pores predicted by the MPR simulation model under abiotic (A) conditions (no enzymatic U(VI) reduction) or biotic (C) conditions.

(Roden and Scheibe, in revision)

Alternative Approach

- Treat multiple pore domains using surrogate “species” and treat mass transfer as a kinetic reaction
- Can use existing reactive transport codes (e.g. HBGC)

$$R_{12} = \varepsilon_{12}(C_2 - C_1)$$

Show example (push-pull) with three different transfer rates

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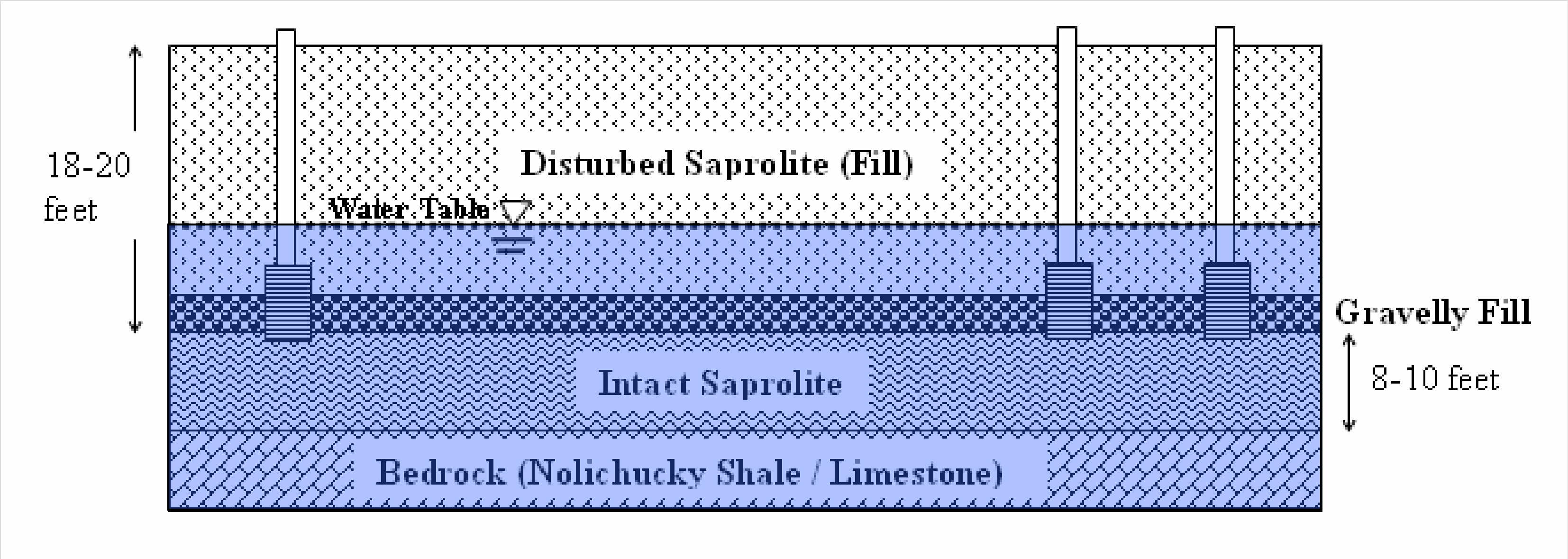
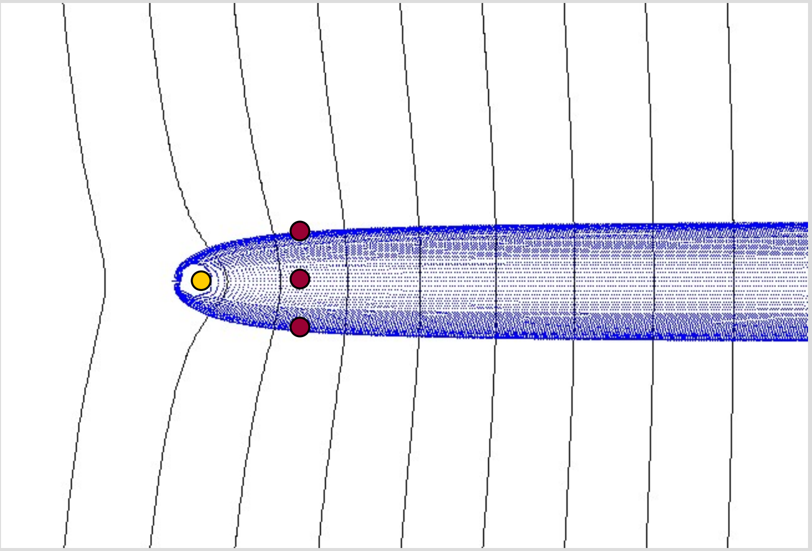
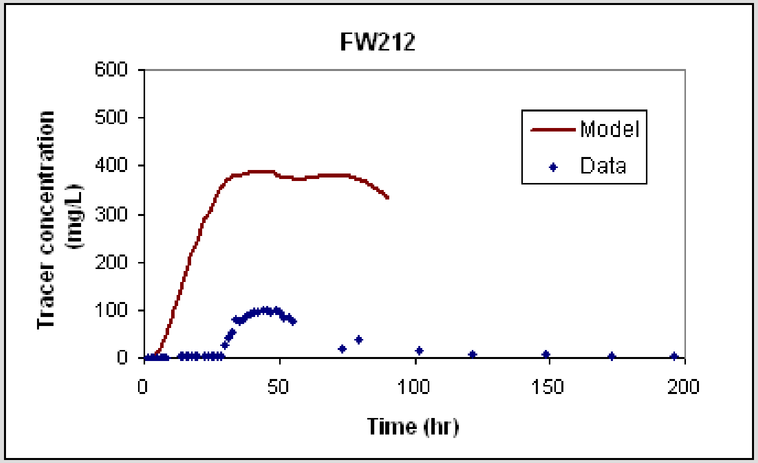
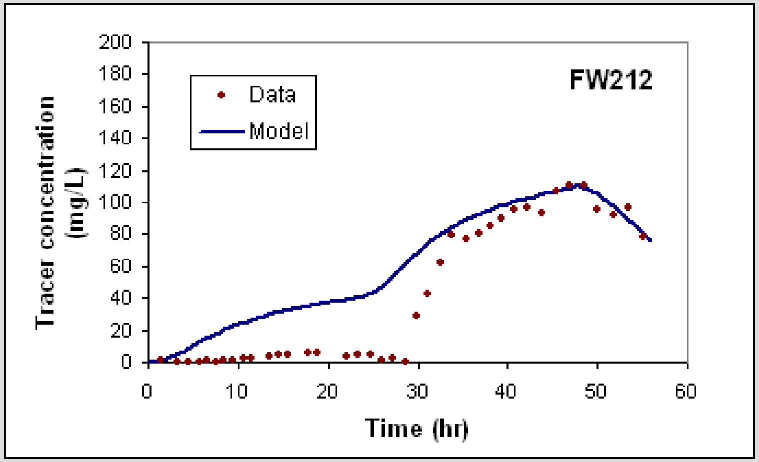


Tracer Interpretation

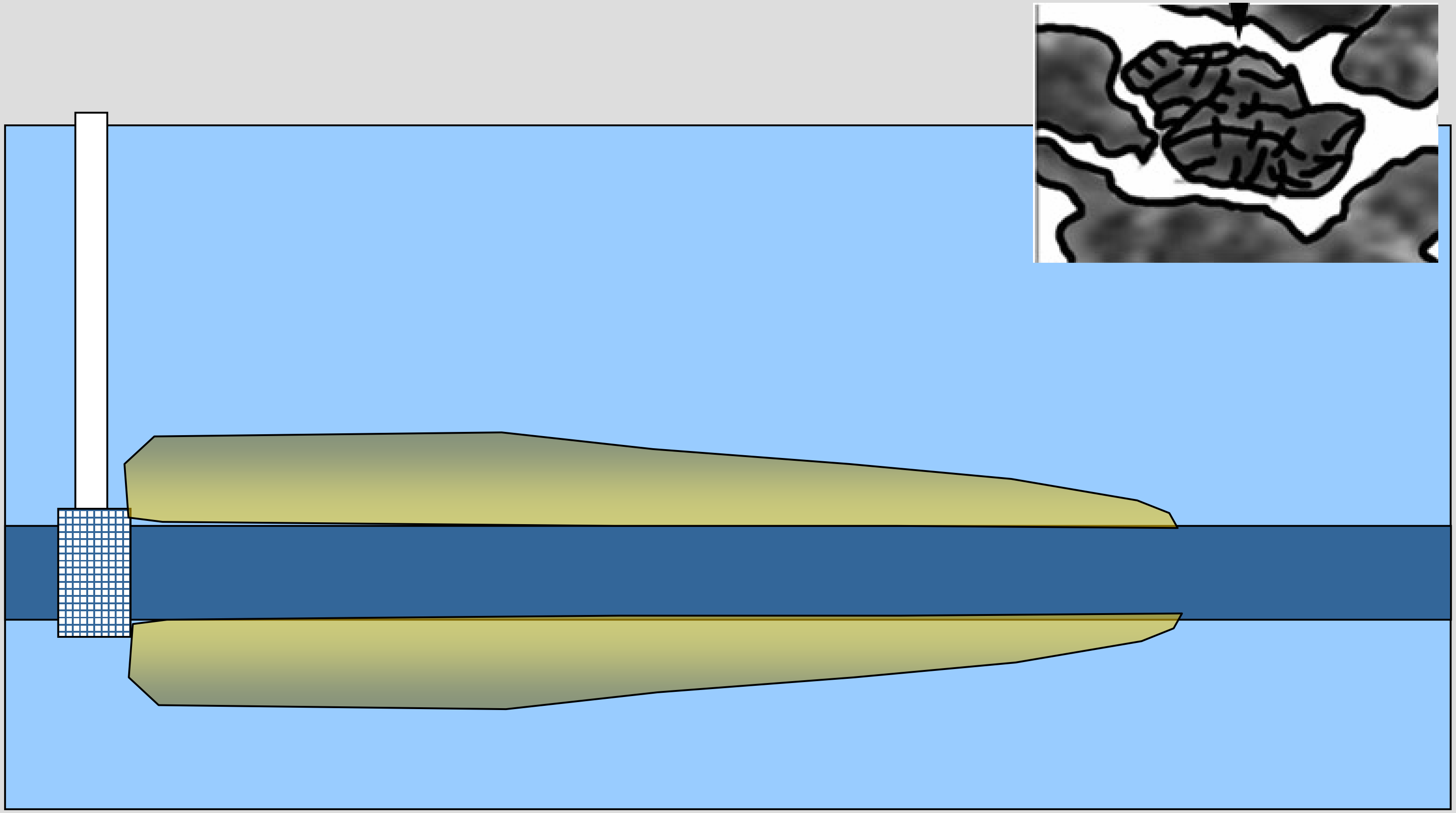
- Gravel layer dominates flow
- Mass transfer gravel ←→ fill and gravel ←→ saprolite is a significant process







Modified Hypothesis



Continuum Approach

- Treat as enhanced vertical “diffusion” or “dispersion” (may require code modification to account for full dispersion tensor)

Show example using HBGC

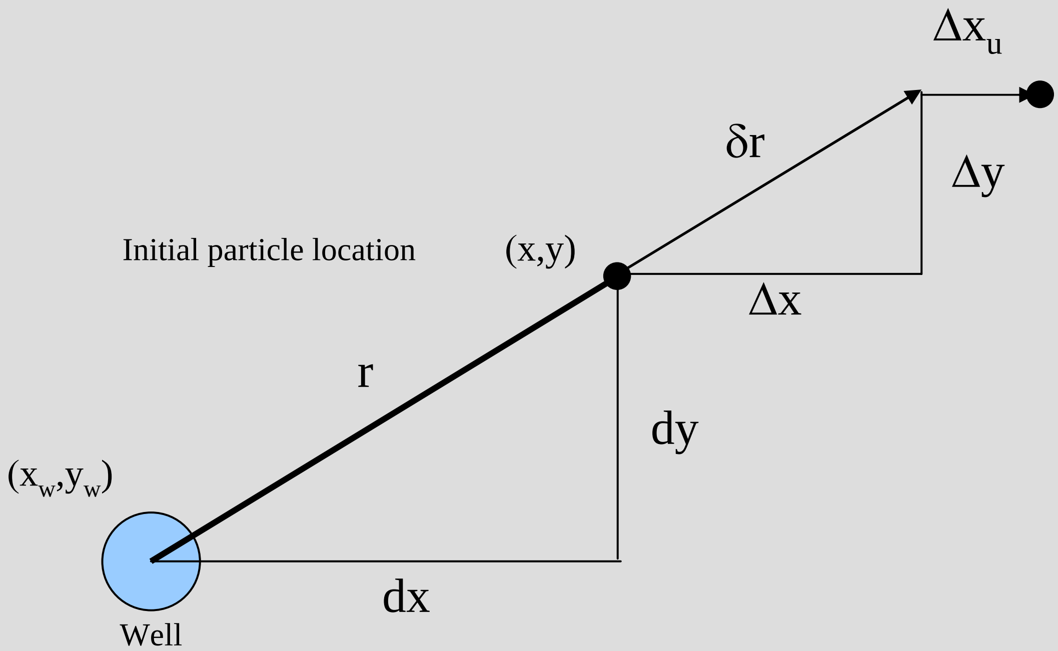
Discrete (Particle) Approach

- Simulate solute transport using random-walk equivalent of advection-dispersion model
- Simulate mass transfer using transition probabilities

Advection

$$r = \mathrm{sqrt}[(x - x_w)^2 + (y - y_w)^2]$$

$$\mathbf{dr = Q\Delta t / 2\pi r B\theta}$$



Mass Transfer

$$\frac{\partial C_1}{\partial t} = -R_{12}\,\frac{\partial C}{\partial x}$$

$$\frac{\Delta\left[\dfrac{Np_1\,M_p}{B_1\theta_1\Delta y^2}\right]}{\Delta t} = R_{12}\,\frac{\left[\dfrac{Np_2}{B_2\theta_2} - \dfrac{Np_1}{B_1\theta_1}\right]}{\dfrac{B_1 + B_2}{2}}\,\frac{M_p}{\Delta y^2}$$

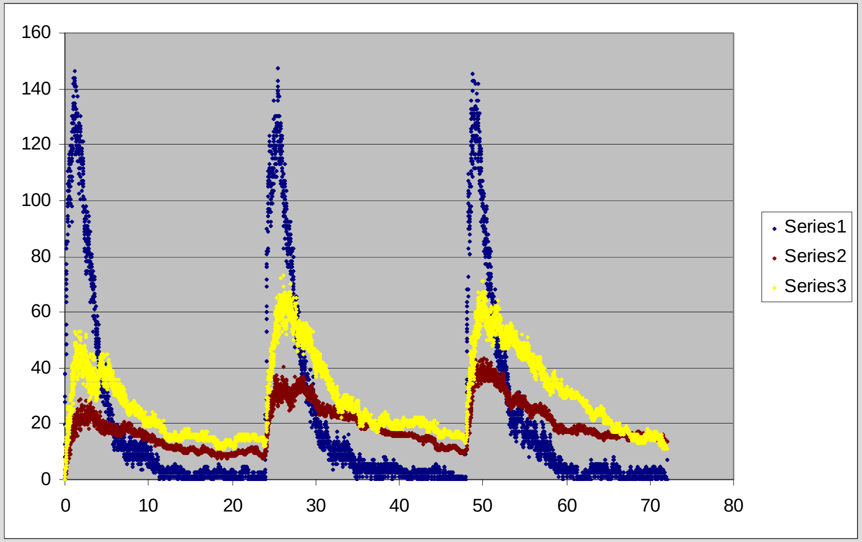
Transfer Probabilities

$$\Delta Np_1 = \frac{-2R_{12}\Delta t Np_1}{B_1 + B_2} + \frac{2R_{12}\Delta t Np_2}{B_1 + B_2}\left(\frac{B_1\theta_1}{B_2\theta_2}\right)$$

$$\Pr\{transfer\}_{12} = \frac{2R_{12}\Delta t}{B_1 + B_2}$$

$$\Pr\{transfer\}_{21} = \frac{2R_{12}\Delta t}{B_1 + B_2}\left(\frac{B_1\theta_1}{B_2\theta_2}\right)$$

Example Run


160
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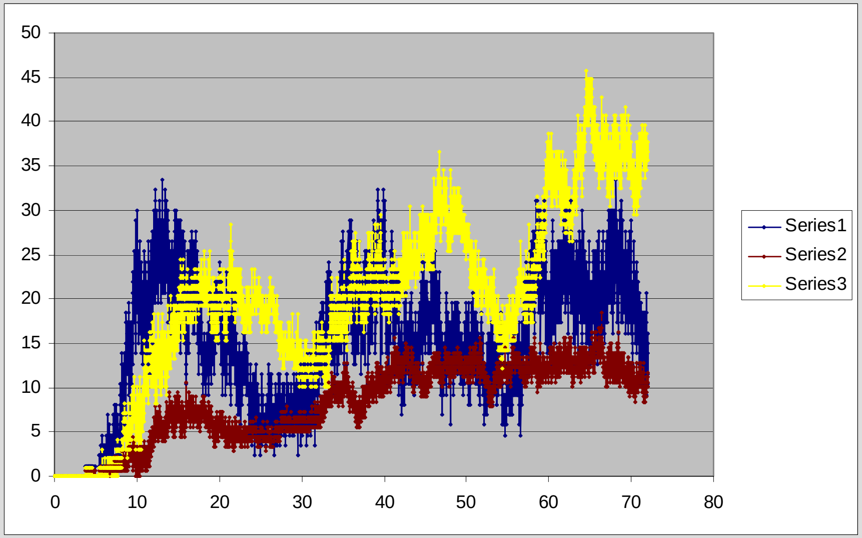
Series1
Series2
Series3


50
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Series1
Series2
Series3