Solving the Contaminant Transport Problem Over a Random Conductivity Field

Michelle Hine

Advisor: Dr. Winter

Program in Applied Mathematics
University of Arizona
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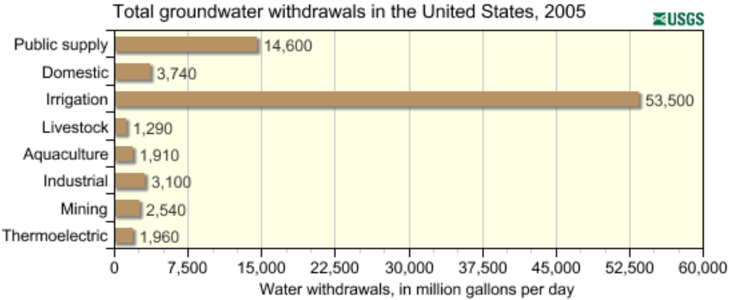
Outline

National Water Usage

- Water.
- In 2005, 23% of the United States national total freshwater usage came from groundwater



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Problem:

Many contaminants are water soluble

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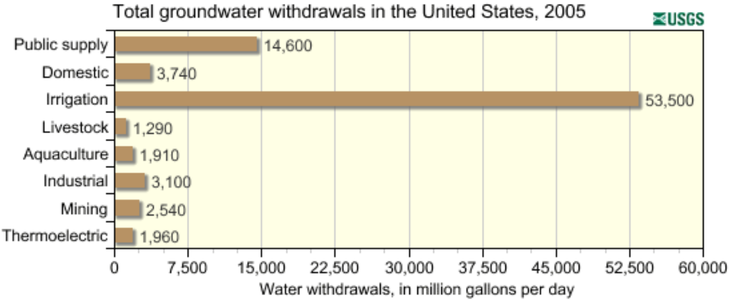

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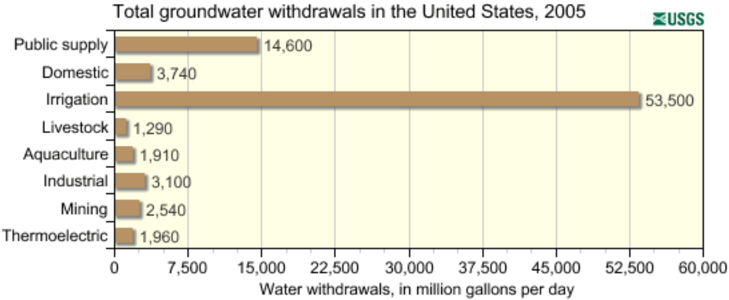

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Problem:

Many contaminants are water soluble

Motivational Example: Love Canal, New York

- 1920s – Love Canal becomes a dump site
- 1940s – Hooker Chemical buries 21,800 tons of chemical waste; seals off the dump site
- 1950s – Niagra Falls City School District wants to expand; tries to buy land from Hooker Chemical
- 1953 – Land sold for $1 to school district, with caveat explaining danger of building on the site

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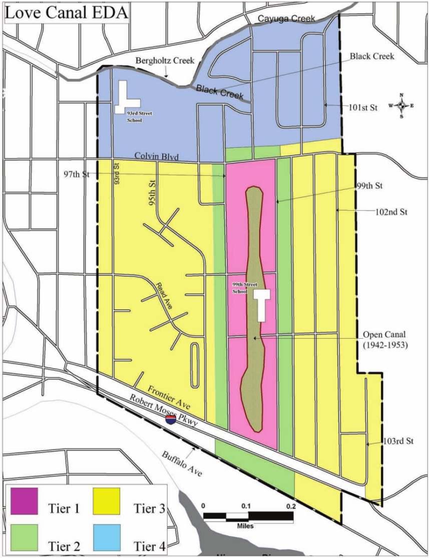
Love Canal, New York

- 1954-1955 – Schools built, school district sells extra land to developers
- 1958 – Clay cap on the waste site removed to use as fill dirt for developments
- 1960s-1970s – Waste containment measures failed, community exposed to hazardous chemicals
    - leaking into basements
    - oozing onto playgrounds [5]



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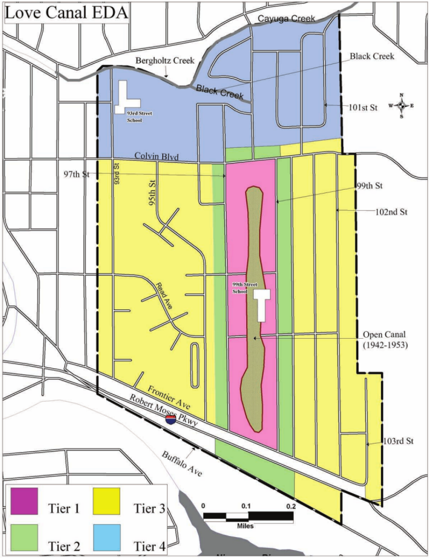

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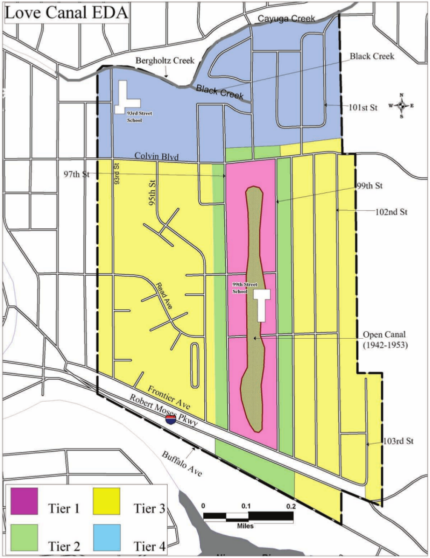

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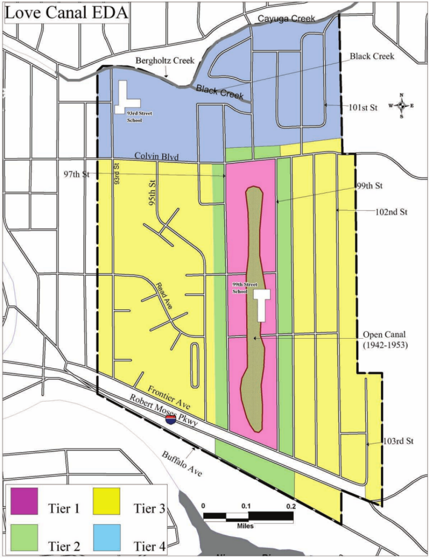

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Groundwater Hydrology

- Fluid flows through a saturated porous media
- Uncertainty: pore structures

Definition: Porosity

n is a number between 0 and 1, the fraction of permeable volume:

$$n = \frac{V_V}{V_T}$$

Lower porosity indicates that less fluid can travel through the medium at any given time.

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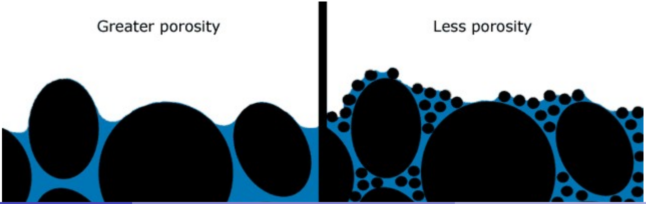

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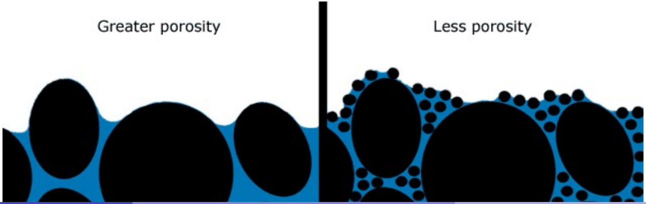


Groundwater Hydrology

Definition: Hydraulic conductivity

K describes the ease of water traveling through the pore space.

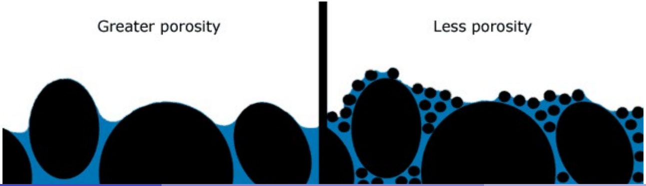
Definition: Hydraulic flux

q is the specific discharge of a fluid at a single point.

Definition: Pore velocity

v is the velocity experienced by the fluid.

$$v(x) = \frac{q(x)}{n}$$



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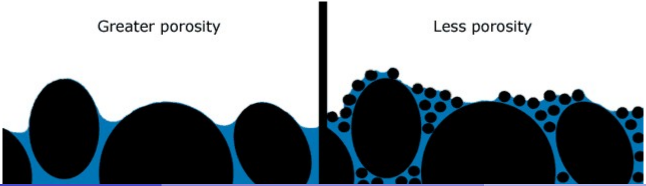

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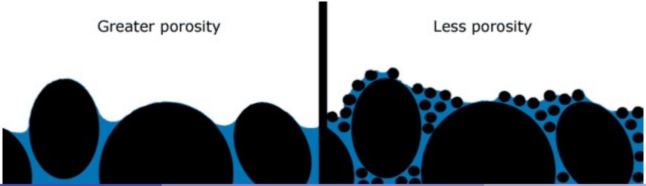


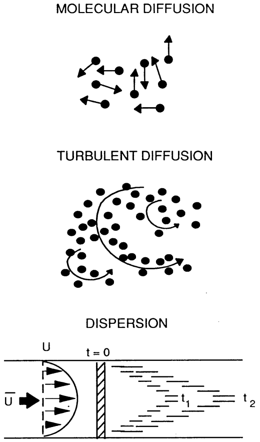
Diffusion and Dispersion

Definition: Diffusion

Motion or mixing of particles; particles move from high to low concentration
microscopic scale

Definition: Dispersion

Mixing caused by physical processes, such as varying velocities
continuum scale



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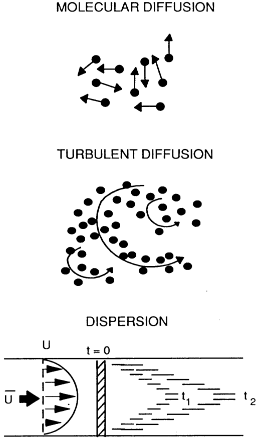

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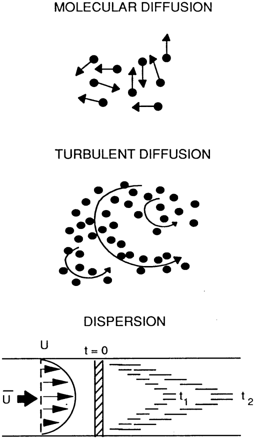

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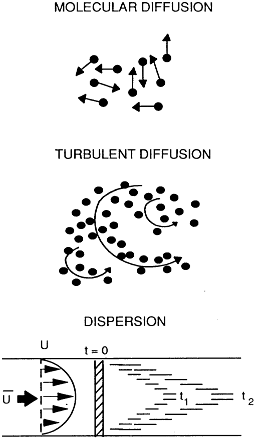

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Advection-Dispersion Equation

- Want to model the flow of contaminants through groundwater transport
- Governing equation: advection dispersion equation
  c=concentration of contaminant, D=dispersion coefficient, v=pore velocity

$$\frac{\partial c}{\partial t} = \nabla \cdot (D \nabla c) - v \nabla c$$

- In one dimension, with D constant:

$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} - v \frac{\partial c}{\partial x}$$

- We want to solve over a random conductivity field, so $v = v(x)$ and varies at every point.
- How do we obtain $v(x)$?

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Diffusion Equation

- The pore velocity v is generated by a pressure gradient across the media
- Described by the diffusion equation for K hydraulic conductivity, h pressure

$$\frac{\partial h}{\partial t} = \nabla \cdot (K \nabla h)$$

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Finding the pressure field

- First, we generate a random conductivity field, so $K = K(x)$ is inhomogeneous
- Solve for the hydraulic head $h(x)$, using the diffusion equation to solve for the steady state pressure

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- In one dimension:

$$\begin{aligned} 0 &= \frac{\partial}{\partial x}\left(K(x)\frac{\partial h(x))}{\partial x}\right) \\ &= \frac{\partial K(x)}{\partial x}\frac{\partial h(x)}{\partial x} + K(x)\frac{\partial^2 h(x)}{\partial x^2} \end{aligned}$$

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Calculating the velocity

- The flux of water $q(x)$ though a random conductivity field is described by Darcy's Law:

$$q(x) = -K(x)\nabla h(x)$$

  for K the conductivity and h the pressure
- Calculate the pore flow v by dividing the flux q by the porosity n.

$$v(x) = \frac{q(x)}{n}$$

- Finally, we can run the advection-dispersion equation

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Recap: The Big Idea

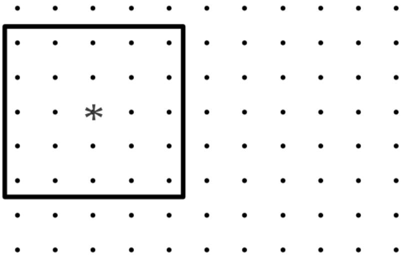
1. Generate random conductivity field $K(x)$
2. Calculate pressure field $h(x)$
3. Use pressure field to calculate hydraulic flux $q(x)$
4. Use hydraulic flux to calculate pore velocity $v(x)$
5. Run advection-dispersion equation to calculate $c(t, x)$

Generating a Random Conductivity Field

- Create a random conductivity field of size $n_x \times n_y$
- Idea: use convolution with 1 to smooth out an underlying field uniformly distributed random variables.
- Use a traveling window of size L to sum $L \times L$ random variables
  - Start with underlying field $(n_x + L - 1) \times (n_y + L - 1)$
  - Use a traveling window to sum a certain number of the variables

$$\sum_{i=1}^{L^2} X_i 1 = \sum_{i=1}^{L^2} X_i$$

  - Voilà! A correlated, random field



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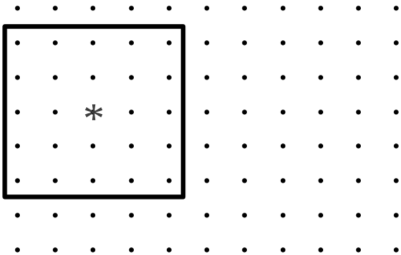

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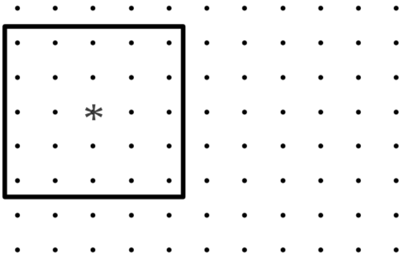

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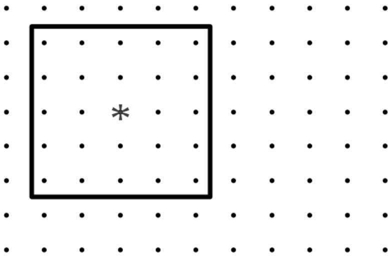

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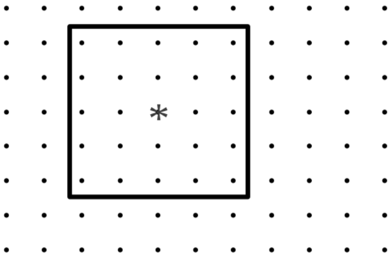

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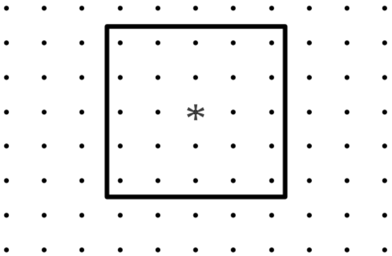

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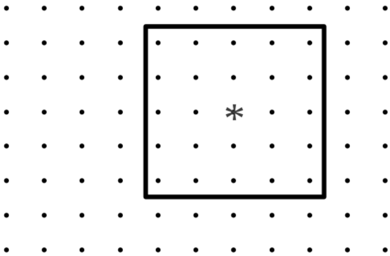

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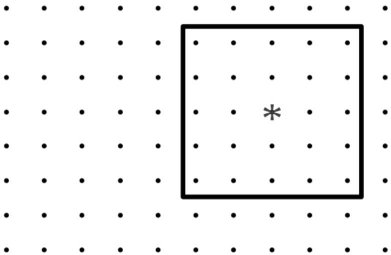
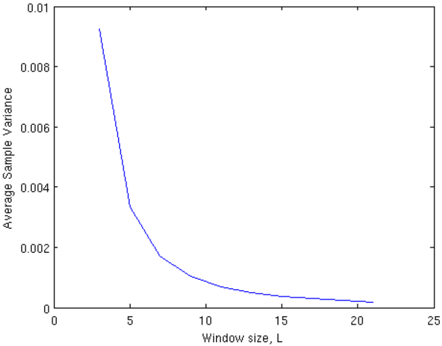


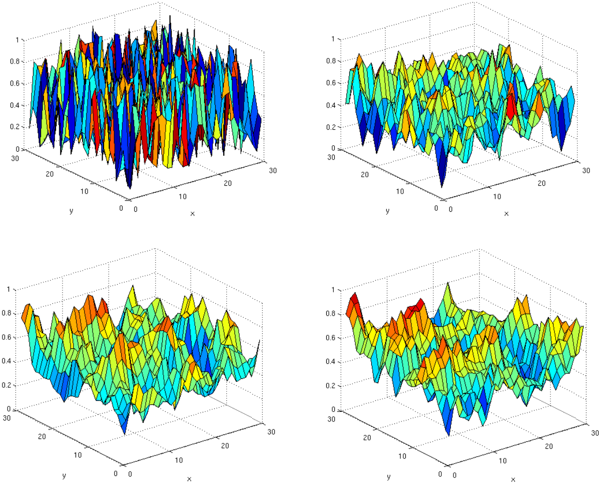
Different Window Sizes

- Increasing the window size decreases the sample variance
- 100 iterations of a 1000×1000 point vector field with window sizes ranging from $L = 3$ to $L = 21$



Different Window Sizes

- 30×30 point conductivity fields generated from the same underlying field; $L = 1, 3, 5, 7$



Solving the Diffusion Equation

- Options: finite difference methods, finite element methods
- Because we are solving for the steady-state solution, we can use an implicit method $\rightarrow$ Backward Euler
- Boundary conditions:
  - Left & right—constant
  - Top & bottom—no-flow

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Discretizing the Diffusion Equation

- Formulate the equation as a matrix using implicit discretized diffusion equation (for simplicity, shown with homogeneous K):

$$\frac{h_{i,j}^{(m+1)} - h_{i,j}^{(m)}}{\Delta t} = K\left(\frac{h_{i+1,j}^{(m+1)} - 2h_{i,j}^{(m+1)} + h_{i-1,j}^{(m+1)}}{(\Delta x)^2} + \frac{h_{i,j+1}^{(m+1)} - 2h_{i,j}^{(m+1)} + c_{i,j-1}^{(m+1)}}{(\Delta y)^2}\right)$$

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Solving the Diffusion Equation

- Rewrite 3 dimensions as 2 dimensions—space and time

$$H = \begin{pmatrix} h_{1,1} & & & \\ h_{2,1} & & & \\ h_{3,1} & & & \\ h_{4,1} & & & \end{pmatrix} \quad \Leftrightarrow \quad H = \begin{pmatrix} h_{1,1} \\ h_{2,1} \\ h_{3,1} \\ h_{4,1} \\ \\ \\ \\ \\ \\ \end{pmatrix}$$

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$$H = \begin{pmatrix} h_{1,1} & h_{1,2} & & \\ h_{2,1} & h_{2,2} & & \\ h_{3,1} & h_{3,2} & & \\ h_{4,1} & h_{4,2} & & \end{pmatrix} \quad \Leftrightarrow \quad H = \begin{pmatrix} h_{1,1} \\ h_{2,1} \\ h_{3,1} \\ h_{4,1} \\ h_{1,2} \\ h_{2,2} \\ \vdots \\ \\ \end{pmatrix}$$

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$$H = \begin{pmatrix} h_{1,1} & h_{1,2} & h_{1,3} & h_{1,4} \\ h_{2,1} & h_{2,2} & h_{2,3} & h_{2,4} \\ h_{3,1} & h_{3,2} & h_{3,3} & h_{3,4} \\ h_{4,1} & h_{4,2} & h_{4,3} & h_{4,4} \end{pmatrix} \quad \Leftrightarrow \quad H = \begin{pmatrix} h_{1,1} \\ h_{2,1} \\ h_{3,1} \\ h_{4,1} \\ h_{1,2} \\ h_{2,2} \\ \vdots \\ h_{3,4} \\ h_{4,4} \end{pmatrix}$$

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- Rewrite 3 dimensions as 2 dimensions—space and time
- Obtain a sparse, tridiagonal matrix with fringes

$$
\left[\begin{array}{cccc|cccc|cccc|cccc}
1 & & & & -4 & 2 & & & 1 & & & & & & & \\
 & 1 & & & 1 & -4 & 1 & & & 1 & & & & & & \\
 & & 1 & & & 1 & -4 & 1 & & & 1 & & & & & \\
 & & & 1 & & & 2 & -4 & & & & 1 & & & & \\
\hline
 & & & & 1 & & & & -4 & 2 & & & 1 & & & \\
 & & & & & 1 & & & 1 & -4 & 1 & & & 1 & & \\
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\hline
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& & & & & & & 1 & & & 2 & -4 & & & & 1
\end{array}
$$

Solving the Diffusion Equation

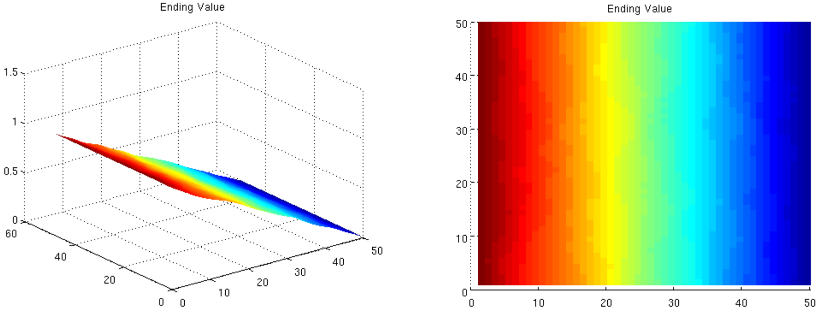

Figure: Pressure field generated for 50×50 grid using window L=3, left boundary fixed at 1.0, right boundary fixed at 0.0 and no-flow conditions top and bottom. $\Delta x = \Delta y = 0.01$.

Solving the Advection-Dispersion Equation

- Similarly, use the finite differences on the advection-dispersion equation
- Not steady state, so cannot use Backward Euler
- Instead, use Adams-Bashforth 2, Adams-Moulton 3

$$y_2 = y_1 + \frac{h}{2}(3f_1 - f_0)$$
$$y_3 = y_1 + \frac{h}{2}(5f_2 + 8f_1 - f_0)$$

- Use for-loops to calculate concentration of contaminant at each point

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Numerical Solution of ADE

- Numerical solution of advection dispersion equation with point mass initial conditions.

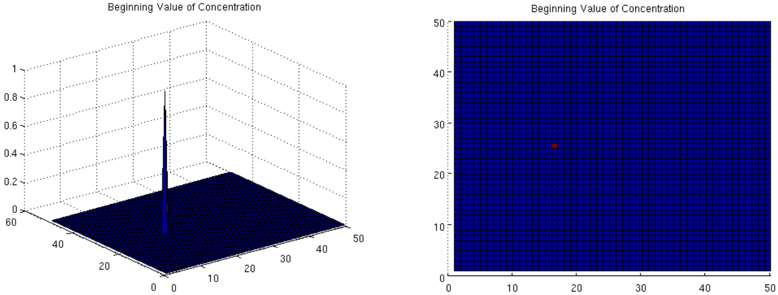

Figure: $t = 00.00e - 5$

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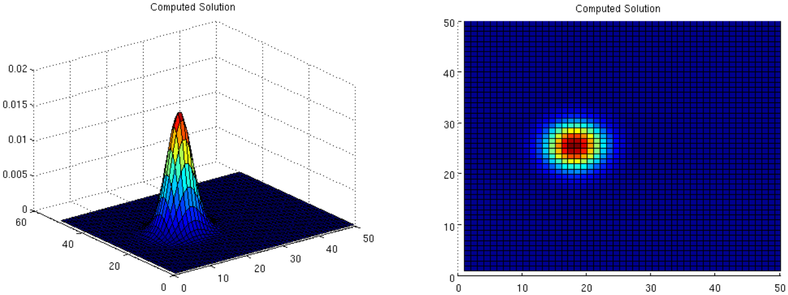

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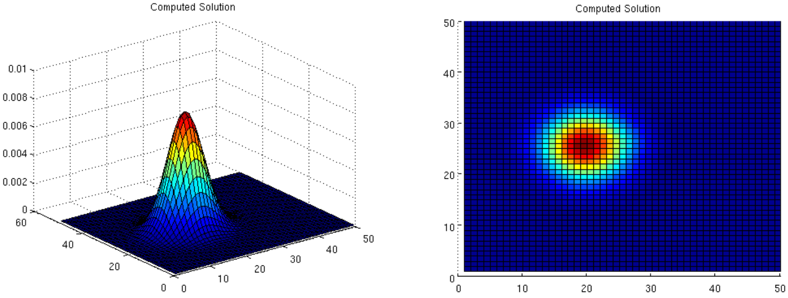

Figure: $t = 10.00e - 5$

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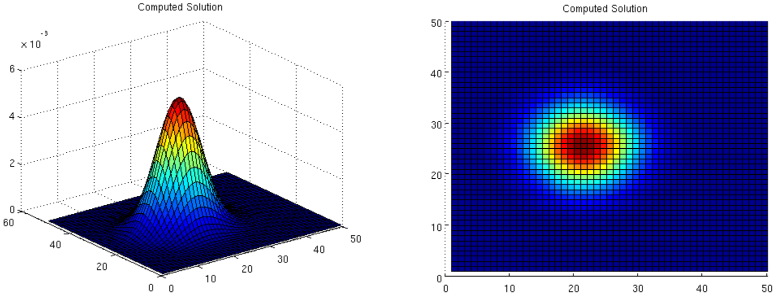

Figure: $t = 15.00e-5$

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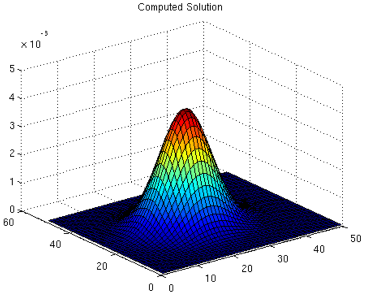

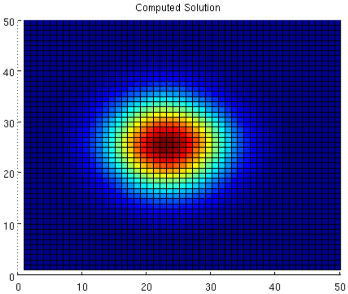

Figure: $t = 20.00e - 5$

Discussion of Results

- Generating random conductivity field using an underlying vector field of i.i.d. random variables
  - Can control both the average conductivity and the correlation of the generated field
  - Rapid calculation
- Using finite differences and Backward Euler to solve the steady-state diffusion equation seems to be an effective method of calculating the pressure gradient
  - Only a few iterations needed—rapid calculation
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- Comparison with exact Gaussian solution of point source with constant velocity
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Future Research Directions

- Implement volume conservative method
- Find out exactly how the conductivity field changes with window sizes
  - Fractal dimension
  - Quantification of the decrease in variance
- Experiment with different resolution
  - Changing Δx and Δy
  - Vary the two parameters independently

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Building a More Comprehensive Code

- Integrate actual site parameters
- Code in groundwater remediation methods, such as a contaminant sink
- Add probabilities of failure of remediation methods
- GOAL: Build up to code that would become a risk-assessment model, helping select the best remediation strategy given individual site parameters

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Acknowledgements

I would like to thank Dr. Larry Winter for his advice and support with this project.

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