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Sensitivity-Based Sampling and Other Approaches to Optimize New Well Locations

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Acknowledgements

- David Hart
- Arun Wahi
- Rick Beauheim

Goals

- "Better Understand" Culebra Hydrology
- Detect changes in head over time
- Detect changes in gradient over time
- Optimally locate new wells to meet first two goals
- Keep PA goals in mind when locating new wells
- Minimize the total number of wells that need to be monitored
- etc. ?

Goals - Refined

- Determine direction and magnitude of flow across site (NMED and EPA)
- Provide data from which causes of head changes can be inferred (EPA)
- Provide defensible boundary conditions and calibration data for PA calculations (PA)
  - Also examine areas to which PA calcs are sensitive
- Minimize total number of monitoring wells
- Address questions in conceptual model

Constraints

- Preserve existing locations of fiberglass wells
- Preserve existing locations of steel-cased wells
  - Minimize pad/road construction, survey costs
- Use up to date conceptual model of Culebra geology

Important Points

- Measuring *head* is not the same as measuring the *gradient*
  - Head is a scalar (magnitude)
  - Gradient is a vector (magnitude and direction)
- Head can be measured at a point
- In a 2-D aquifer, a minimum of 3 wells are necessary to measure gradient

Three Approaches

- **Geostatistical**
  - **Minimize limitations in the data set by locating wells to minimize the average estimation variance**
  - **Can be applied to scalar data sets (heads)**
- **Three Point Estimator**
  - **What does it take to accurately measure gradient?**
  - **Where are best places to locate new wells?**
- **Sensitivity Analysis**
  - **Determine locations where model outputs are most sensitive to model inputs (include PA performance measures)**
- **Combination of Approaches**

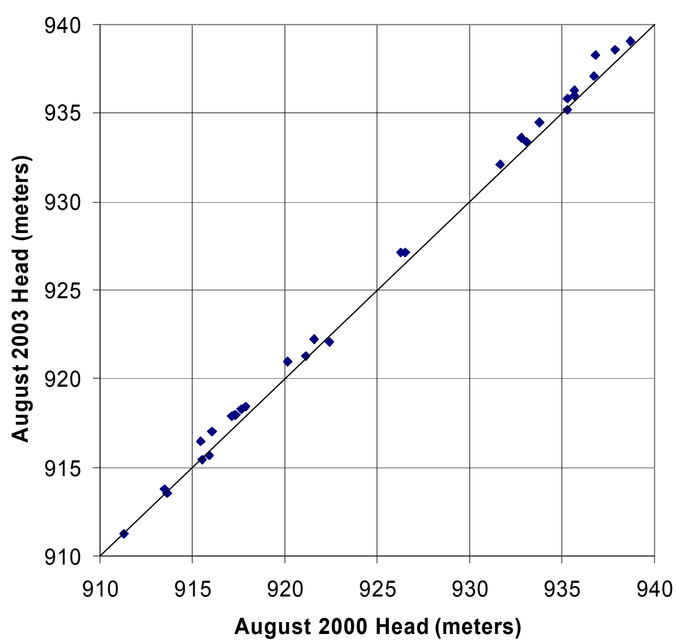
Monitoring Data

Intersection of August 2000 and 2003 Monthly Water Levels

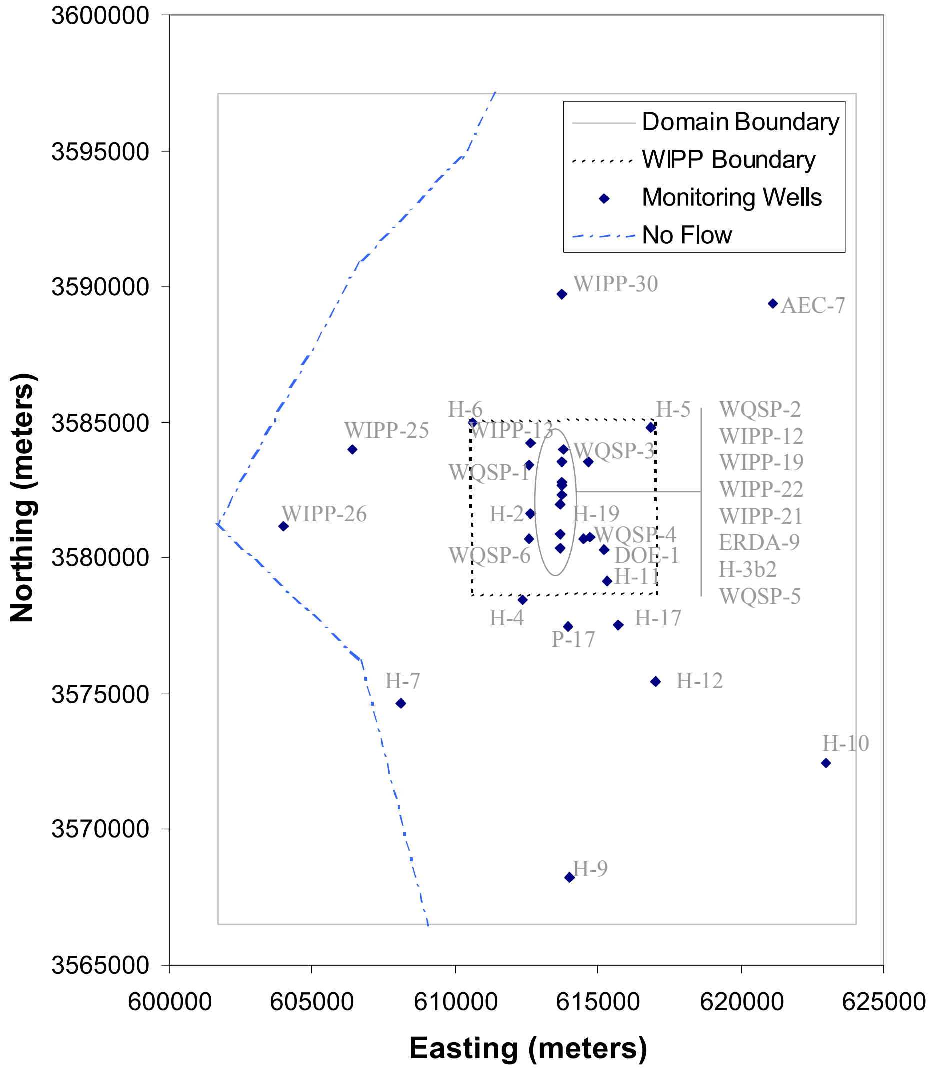
Integer ID	Well Name	X coordinate (m)	Y coordinate (m)	Adjusted 2000 Freshwater Head (m)	Adjusted 2003 Freshwater Head (m)	Difference 2003-2000 (meters)
1	AEC-7	621126	3589381	933.10	933.36	0.26
2	DOE-1	615203	3580333	915.42	916.49	1.07
3	ERDA-9	613696	3581958	921.56	922.25	0.69
4	H-2b2	612661	3581649	926.28	927.13	0.85
5	H-3b2	613701	3580906	917.28	917.93	0.66
6	H-4b	612380	3578483	915.90	915.66	-0.24
7	H-5b	616872	3584801	936.73	937.12	0.39
8	H-6b	610594	3585008	933.79	934.51	0.72
9	H-7b2	608117	3574620	913.64	913.59	-0.05
10	H-9b/c	613989	3568261	911.27	911.28	0.01
11	H-10b/c	622975	3572473	922.42	922.06	-0.36
12	H11b4	615301	3579131	915.52	915.45	-0.06
13	H-12	617023	3575452	916.10	917.02	0.92
14	H-17	615718	3577513	917.38	917.99	0.61
15	H-19b0	614514	3580716	917.65	918.30	0.65
16	P-17	613926	3577466	913.46	913.79	0.33
17	WIPP-12	613710	3583524	935.30	935.82	0.52
18	WIPP-13	612644	3584247	935.29	935.18	-0.11
19	WIPP-19	613739	3582782	937.88	938.59	0.70
20	WIPP-21	613743	3582319	926.55	927.12	0.57
21	WIPP-22	613739	3582653	932.83	933.59	0.76
22	WIPP-25	606385	3584028	931.66	932.14	0.49
23	WIPP-26	604014	3581162	921.14	921.25	0.12
24	WIPP-30	613721	3589701	936.79	938.23	1.43
25	WQSP-1	612561	3583427	935.69	936.29	0.60
26	WQSP-2	613776	3583973	938.75	939.05	0.30
27	WQSP-3	614686	3583518	935.70	935.97	0.27
28	WQSP-4	614728	3580766	917.87	918.45	0.58
29	WQSP-5	613668	3580353	917.12	917.88	0.76
30	WQSP-6	612605	3580736	920.16	920.95	0.79

30 wells total

Moderate and uniform rise in heads over 3 years



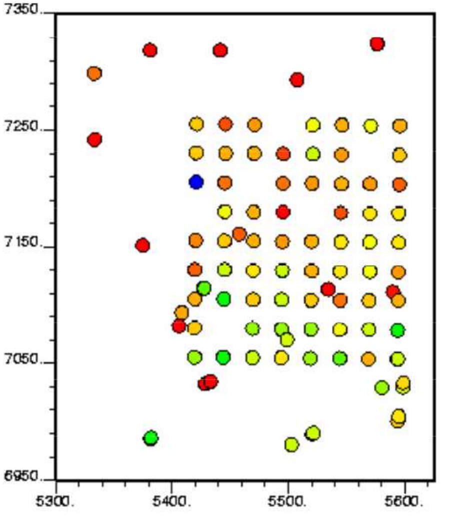
Monitoring Network Locations



Current Monitoring Network (August 2000 and 2003)

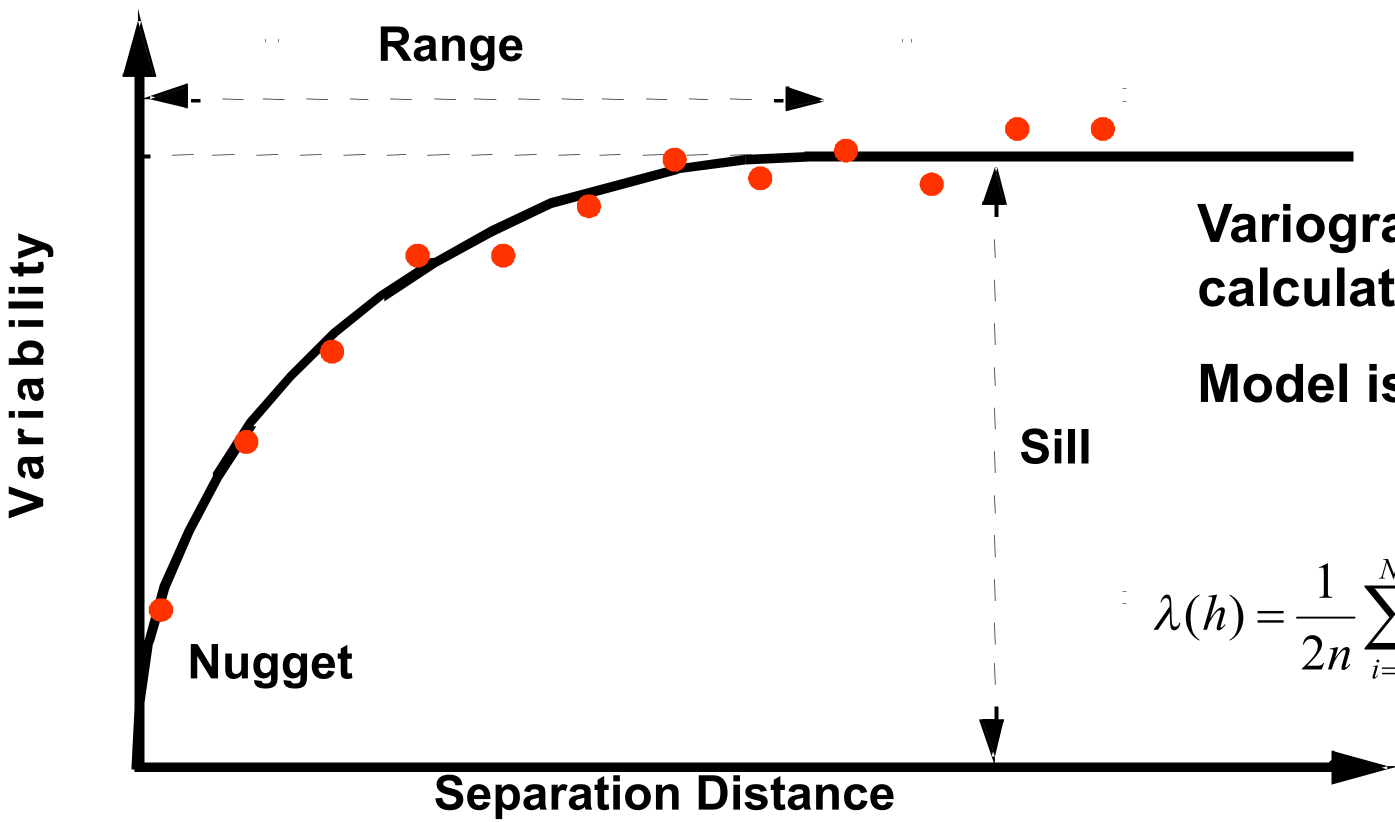
Geostatistics

- **Study of spatially and/or temporally correlated data**
  - **Differs from traditional statistics where theory is generally based on *independence* of observations**
- **Techniques for quantifying the style and amount of spatial continuity in a measured variable ("variogram")**
- **Tools for mapping parameters and *uncertainty* in spatial distribution**



Variogram

Variogram defines increase in variability between two samples as the distance between those points increases.



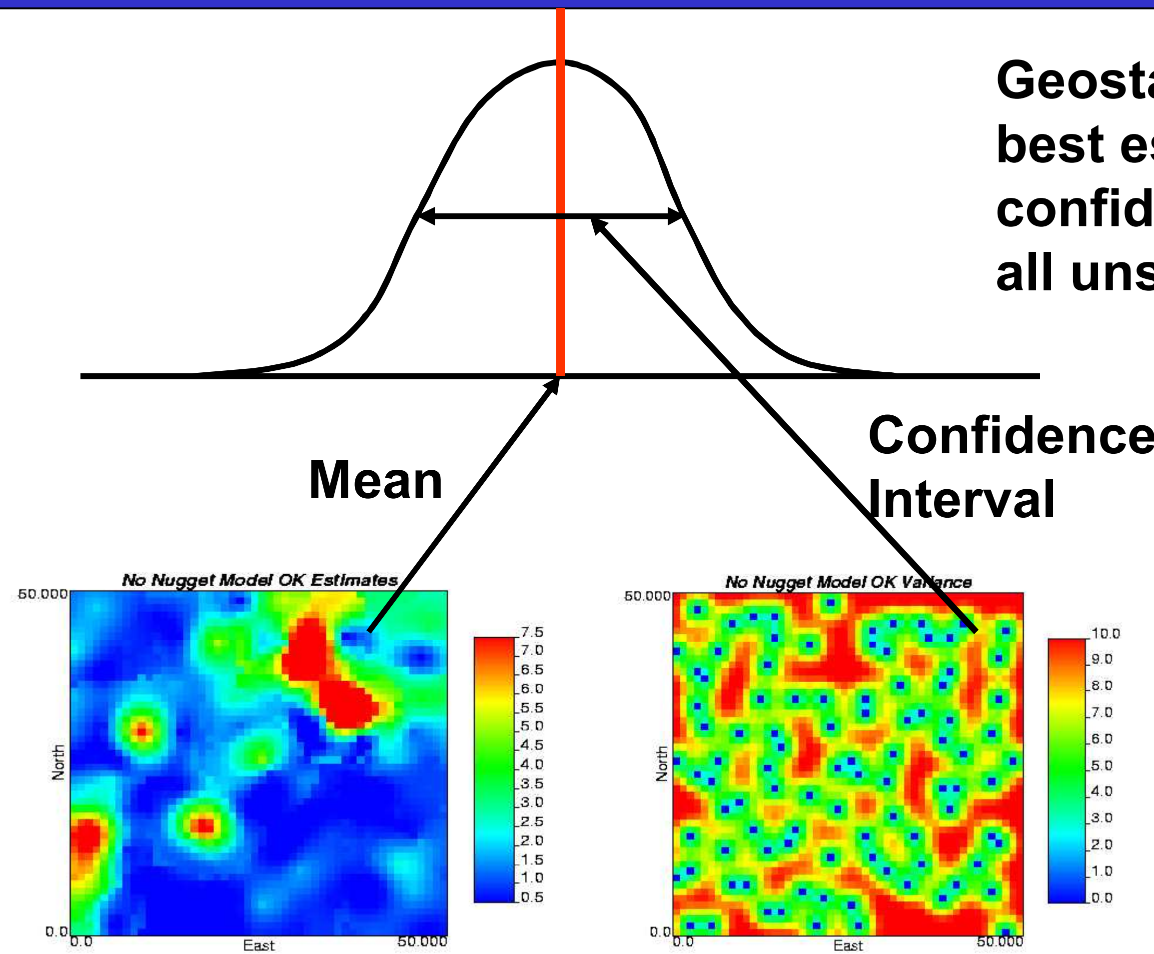
Variogram points are calculated from field data

Model is fit to points

$$\lambda(h) = \frac{1}{2n}\sum_{i=1}^{N}\left[Z_i(x) - Z_i(x+h)\right]^2$$

Estimate and Uncertainty

Geostatistics provides the best estimate and the confidence in that estimate at all unsampled locations



<u>Important Point:</u>
kriging variance (confidence interval) is only a function of data *locations*, not a direct function of data values

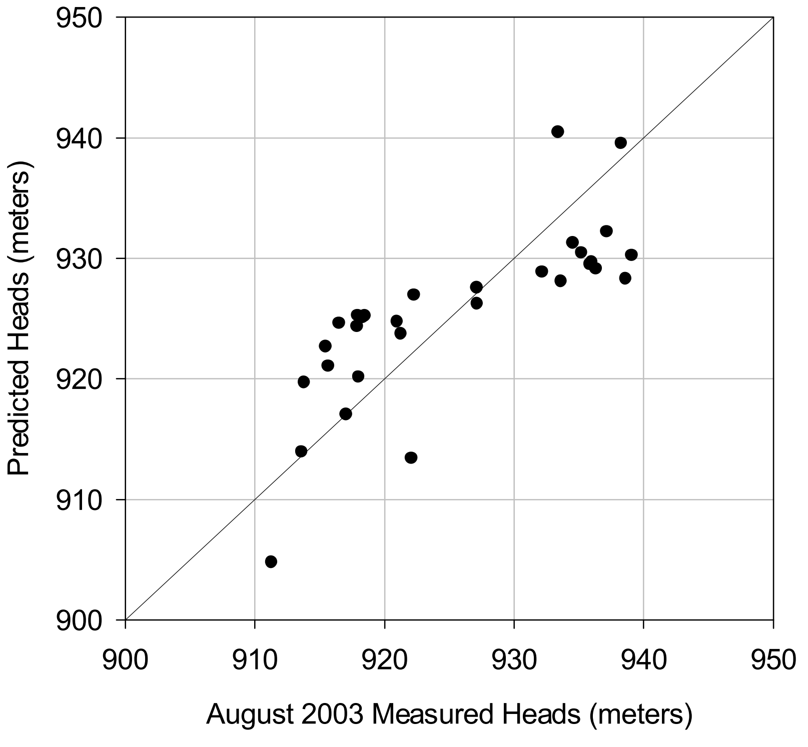
$$\sigma_{OK}^2(u) = Cov(0) - \sum_{i=1}^{N} \lambda_i Cov(u, u_i) - \mu$$

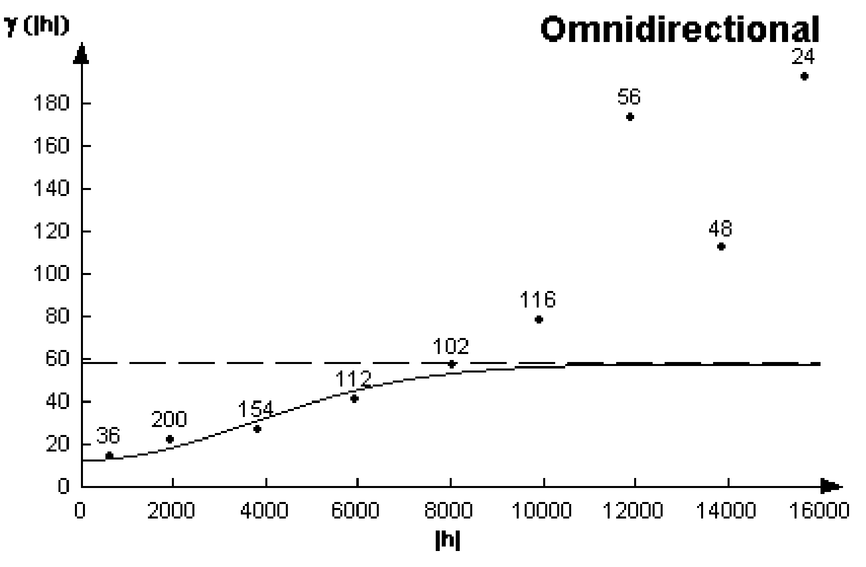
Monitoring with Geostatistics

- Set monitoring objective to be minimization of the hydraulic head estimation variance
  - Minimization of the average estimation variance across the domain
  - Minimization of the average estimation variance within the WIPP site
- Use most recent head measurements (August 2003)
  - Detrend the heads using a best-fit plane

Residual Variogram

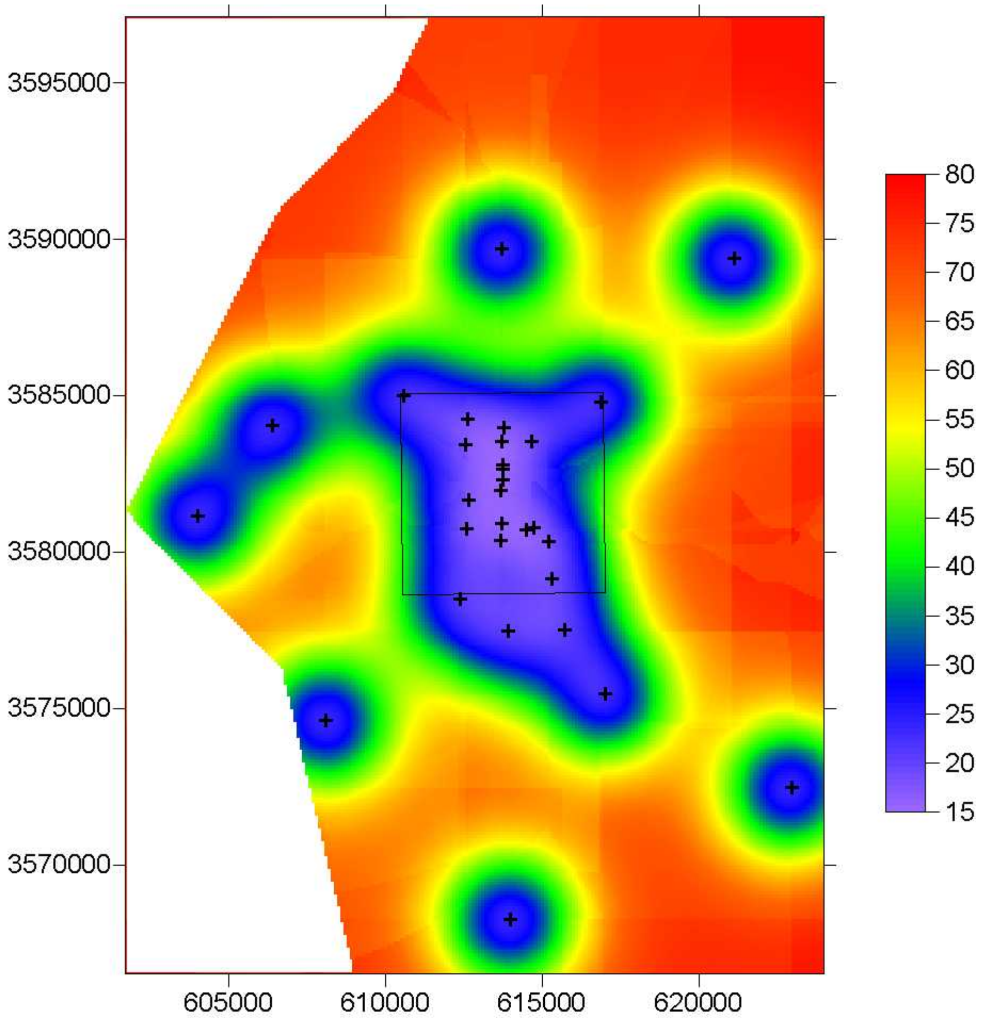
Residuals (differences) between best fit plane and measurements are used in geostatistical estimation





Isotropic, Gaussian variogram with range of 9000m. Nugget value is approximately 22% of total variance

Estimation Variance



- Estimation variance map shows gaps in data
- Little control (high variance) on boundary conditions to north, east and southeast
- Strong predictability of heads within WIPP site (low variance)

Geostatistics: Network Design

- **Estimation variance is only a function of the data locations, <u>not the data values</u>**
  - **Data values are used to determine the variogram**
- **Determine reduction in variance due to any proposed well location, *before that well is drilled!***

$$\sigma^2_{OK}(x_0) = Cov(0) - \sum_{i=1}^{N} \lambda_i Cov(x_0, x_i) - \mu$$

Well Removal

Well Removed	Domain Average	Percent Increase	WIPP Average	Percent Increase
None	50.84	NA	23.3	NA
AEC-7	53.87	6	23.34	0.2
DOE-1	50.83	0	23.75	1.9
ERDA-9	50.84	0	23.31	0
H-2	50.85	0	23.74	1.9
H-3	50.84	0	23.33	0.1
H-4	51.08	0.5	24.29	4.2
H-5	51.94	2.2	25.37	8.8
H-6	51.46	1.2	24.06	3.3
H-7	52.09	2.5	23.33	0.1
H-9	52.93	4.1	23.3	0
H-10	53.11	4.5	23.34	0.2
H-11	50.84	0	23.69	1.6
H-12	51.97	2.2	23.33	0.1
H-17	50.83	0	23.45	0.6
P-17	50.96	0.2	23.4	0.4
WIPP-12	50.83	0	23.32	0.1
WIPP-13	50.8	-0.1	23.59	1.2
WIPP-19	50.84	0	23.3	0
WIPP-22	50.84	0	23.3	0
WIPP-25	52.14	2.6	23.32	0.1
WIPP-26	51.99	2.3	23.32	0.1
WIPP-30	53.44	5.1	23.32	0

Remove one well at a time from network and examine changes in estimation variance calculations

Well Removal (WIPP-12 & 22)

Well Removed	Domain Average	Percent Increase	WIPP Average	Percent Increase
W-12 & W-22	50.83	NA	23.32	NA
AEC-7	53.86	6	23.35	0.2
DOE-1	50.83	0	23.77	1.9
ERDA-9	50.83	0	23.32	0
H-2	50.84	0	23.75	1.8
H-3	50.83	0	23.34	0.1
H-4	51.07	0.5	24.3	4.2
H-5	51.91	2.1	25.35	8.7
H-6	51.45	1.2	24.08	3.3
H-7	52.08	2.5	23.34	0.1
H-9	52.93	4.1	23.32	0
H-10	53.1	4.5	23.35	0.1
H-11	50.83	0	23.7	1.6
H-12	51.96	2.2	23.34	0.1
H-17	50.82	0	23.47	0.6
P-17	50.95	0.2	23.41	0.4
WIPP-13	50.79	-0.1	23.64	1.4
WIPP-19	50.83	0	23.33	0.1
WIPP-25	52.13	2.6	23.34	0.1
WIPP-26	51.98	2.3	23.33	0.1
WIPP-30	53.42	5.1	23.33	0.1

First remove WIPP-12 and WIPP-22

Then remove one well at a time from network and examine changes in estimation variance calculations

Well Removal (WIPP-22, 12, H-12 and P-17)

Well Removed	Domain Average	Percent Increase	WIPP Average	Percent Increase
W-12, W-22, H-12, P-17	52.01	NA	23.43	NA
AEC-7	55.07	5.9	23.48	0.2
DOE-1	51.97	-0.1	23.89	1.9
ERDA-9	52	0	23.43	0
H-2	52.02	0	23.86	1.8
H-3	52	0	23.46	0.1
H-4	52.46	0.9	24.8	5.8
H-5	53.13	2.2	25.52	8.9
H-6	52.63	1.2	24.19	3.2
H-7	53.35	2.6	23.46	0.1
H-9	54.3	4.4	23.43	0
H-10	54.55	4.9	23.48	0.2
H-11	51.87	-0.3	23.84	1.7
H-17	52.59	1.1	23.65	0.9
WIPP-13	51.97	-0.1	23.75	1.4
WIPP-19	52	0	23.45	0.1
WIPP-25	53.31	2.5	23.45	0.1
WIPP-26	53.16	2.2	23.45	0.1
WIPP-30	54.62	5	23.45	0.1

First remove WIPP-12, WIPP-22, H-12, P-17

Then remove one well at a time from network and examine changes in estimation variance calculations

Geostatistical Approach: Summary

- Geostatistics can be used to identify gaps in data
  - North, East and SW boundaries of WIPP domain
- Necessary but not sufficient result for identifying new well locations
- Well Removal
  - Removing WIPP-12 and WIPP-22 has negligible effect on ability of monitoring network to predict heads
  - Removal of WIPP-12, WIPP-22, P-17 and H-12 does effect predictive ability of network
  - Some combination of WIPP-19, ERDA-9 and H-3 are candidates for removal

Approach 2: Three-Point Estimator

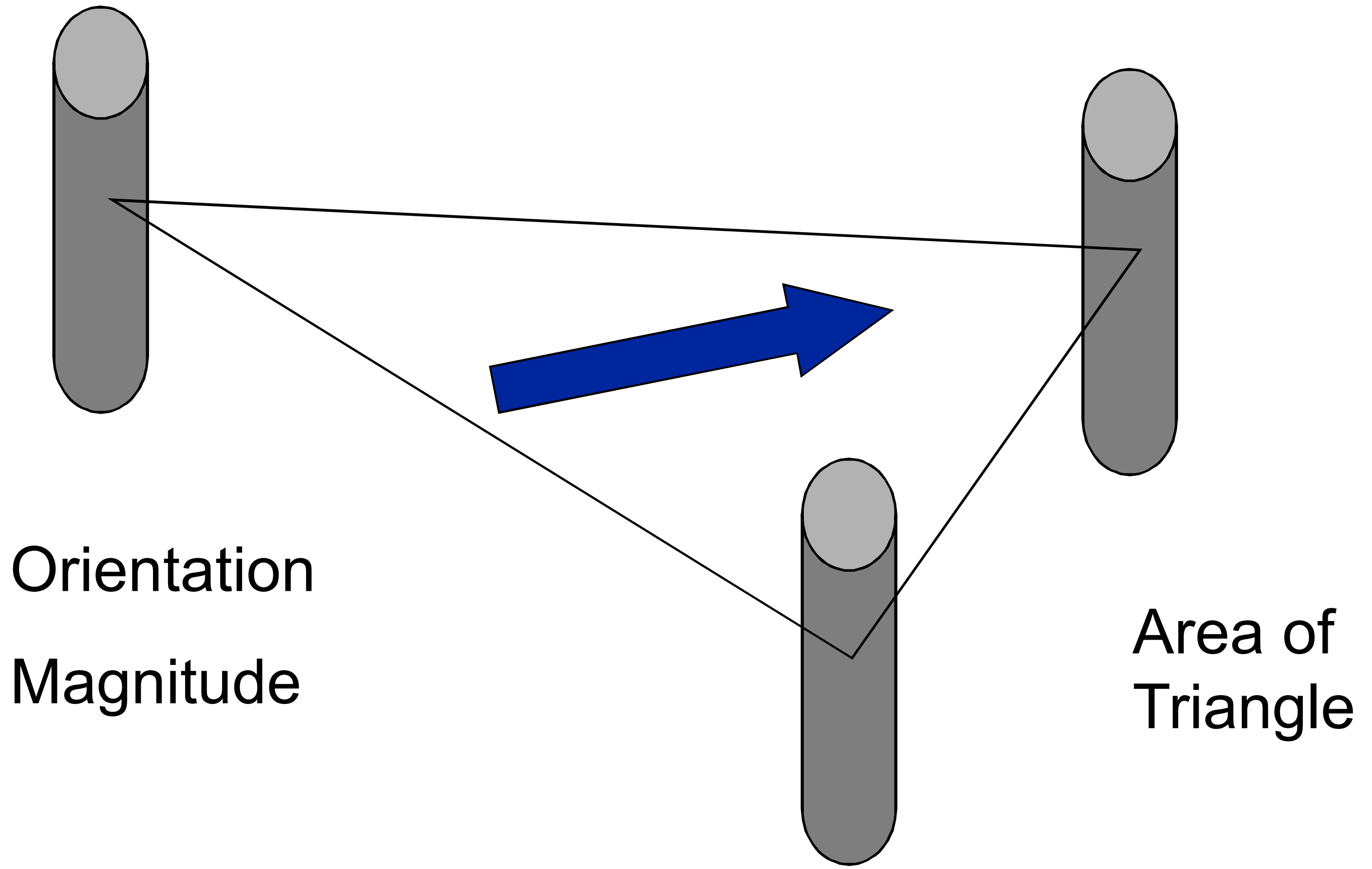
- Focused on determining the best locations for new wells given the objective of more accurately defining the magnitude and orientation of the gradient
- Apply regionally (multipoint) and locally (three-point)
- Eventually use to detect changes over time
- Currently, a work in progress

Three-Point Estimator (Cont).

- Regional estimates assume a homogeneous aquifer
- Reduce the number of wells needed to the minimum – three
  - Still an assumption of homogeneity, but much less restrictive on the local scale
- Apply to all possible combinations of three wells

Three-Point Estimator

Measurement of Head at 3 locations uniquely defines gradient for a confined aquifer



WIPP Example

Monitoring Well network locations

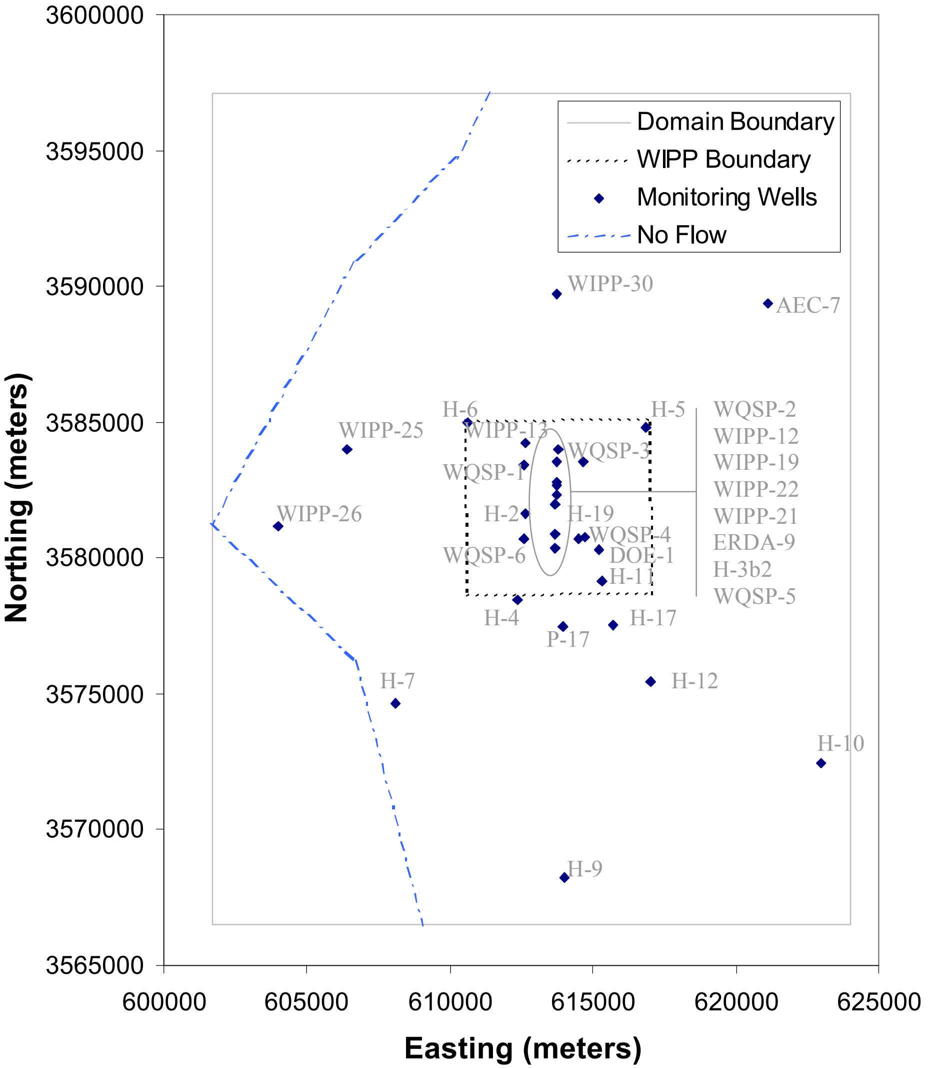
How many three-point estimators?

$$mCn = \frac{m!}{n!(m-n)!}$$

m = 30

n = 3

mCn = 4060



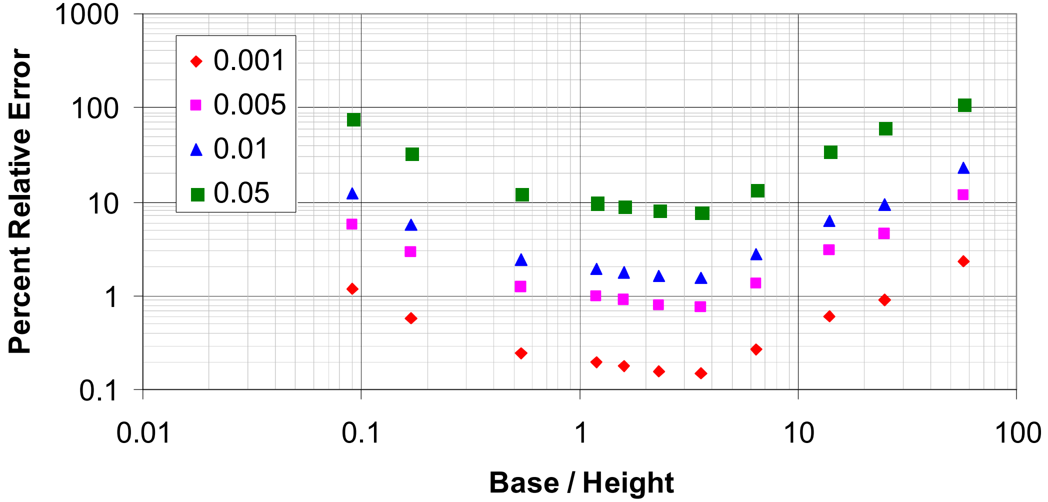
Measurement Error

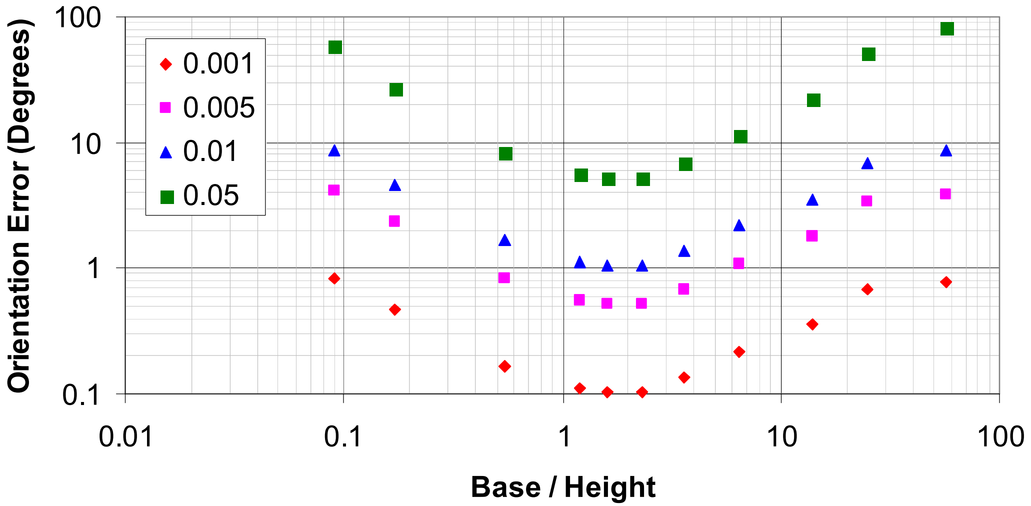
- **Measurement error has different effects on estimates depending on the gradient**
- **Same amount of measurement error in an area of low gradient is worse than in high gradient areas**
- **Determine relative head measurement error (RHME) as a function of measurement error and expected head drop across estimator**

$$RHME = \frac{\sigma}{head \quad drop}$$

σ = standard deviation of normally distributed measurement error (10 cm in Culebra)

Acceptable Estimators





Estimators with base to height ratios between 0.5 and 5.0 produce best results

Different levels of RHME produce different amounts of error in estimating the magnitude and orientation of the gradient

How to Monitor?

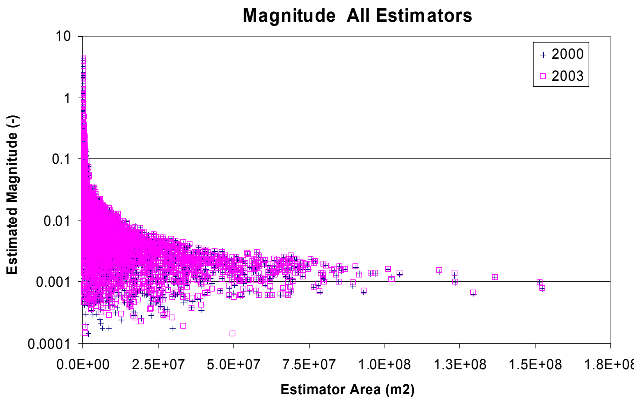
- The calculations in the previous slides give us two "rules of thumb" to weed out poor estimators
  - Measurement error relative to head drop
  - Shape of triangle (Base to height ratio)
- Apply to WIPP data set with the same number of wells across different time periods
  - CCA and 2000 have 25 wells in common
  - Use measurement error data and allow for a msmt error to head drop ratio of 0.025
  - Limit base to height ratio to [0.5,5.0]

Magnitude Estimates

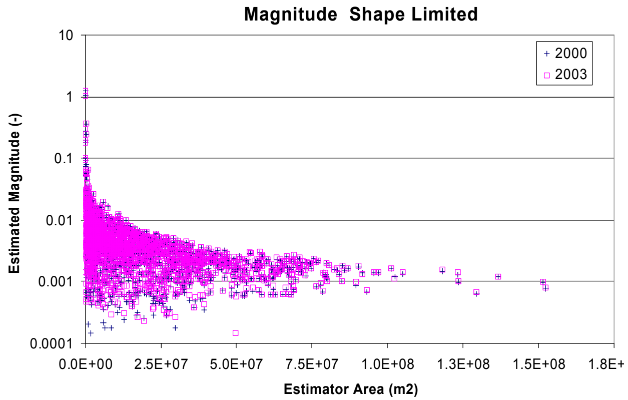
Estimates of magnitude as a function of estimator size

Results for both 2000 and 2003 data are shown

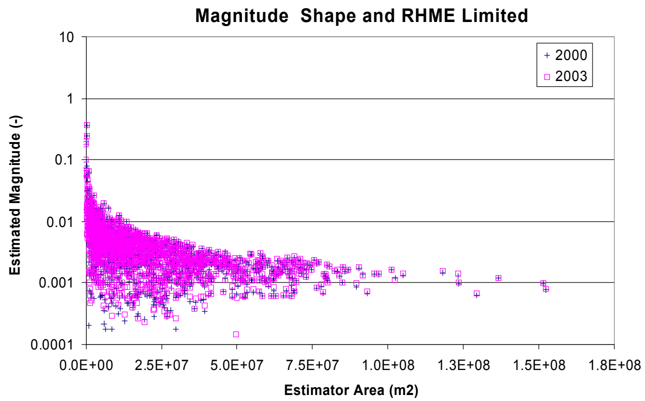
All



Shape



RHME and Shape



Large estimators return magnitude of regional gradient

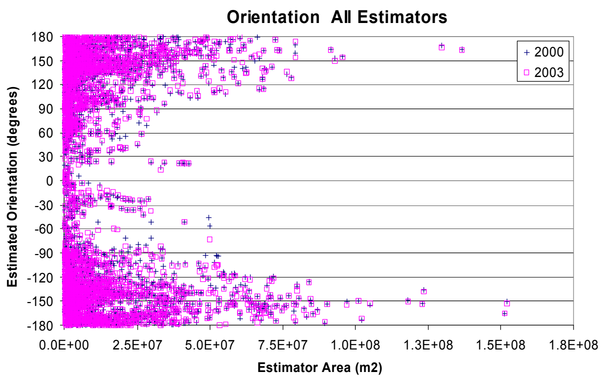
Variability in small estimators decreases as shape and RHME constraints are applied

Orientation Estimates

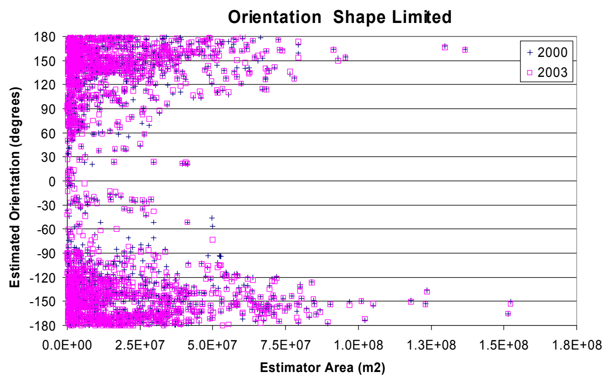
Estimates of orientation as a function of estimator size

Results for both 2000 and 2003 data are shown

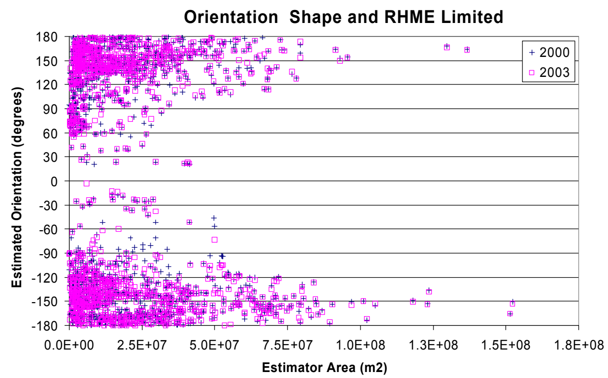
All



Shape



RHME and Shape



Large estimators return orientation of regional gradient – more variable than magnitude

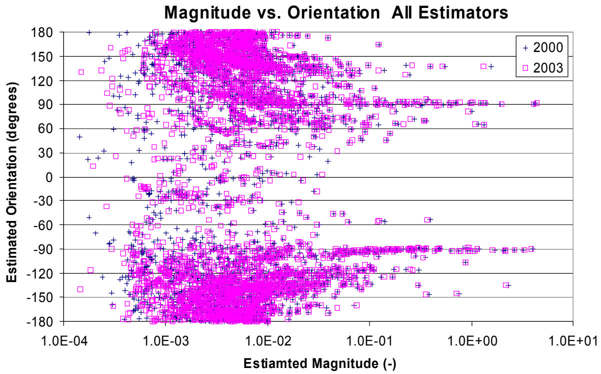
Variability in small estimators decreases as shape and RHME constraints are applied

Orientation vs. Magnitude

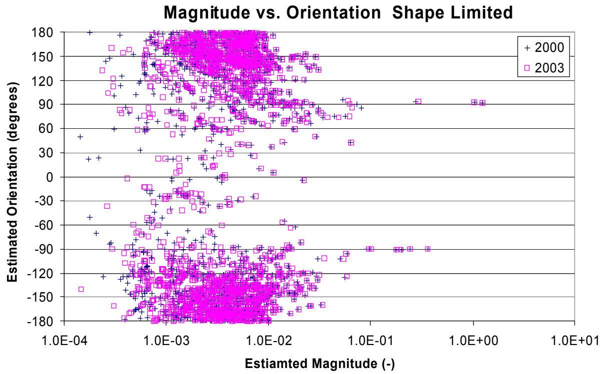
Orientation as a function of magnitude shows that strongest gradients are not aligned with the regional flow direction

Results for both 2000 and 2003 data are shown

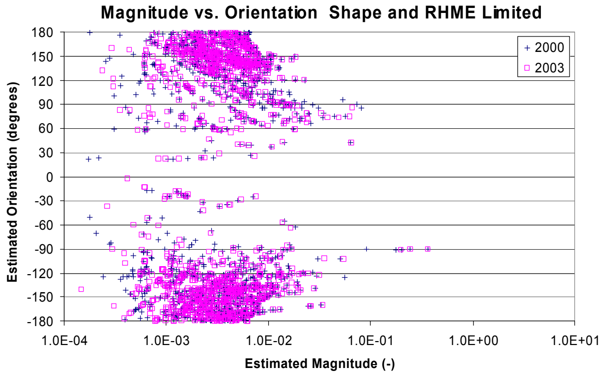
All



Shape



RHME and Shape

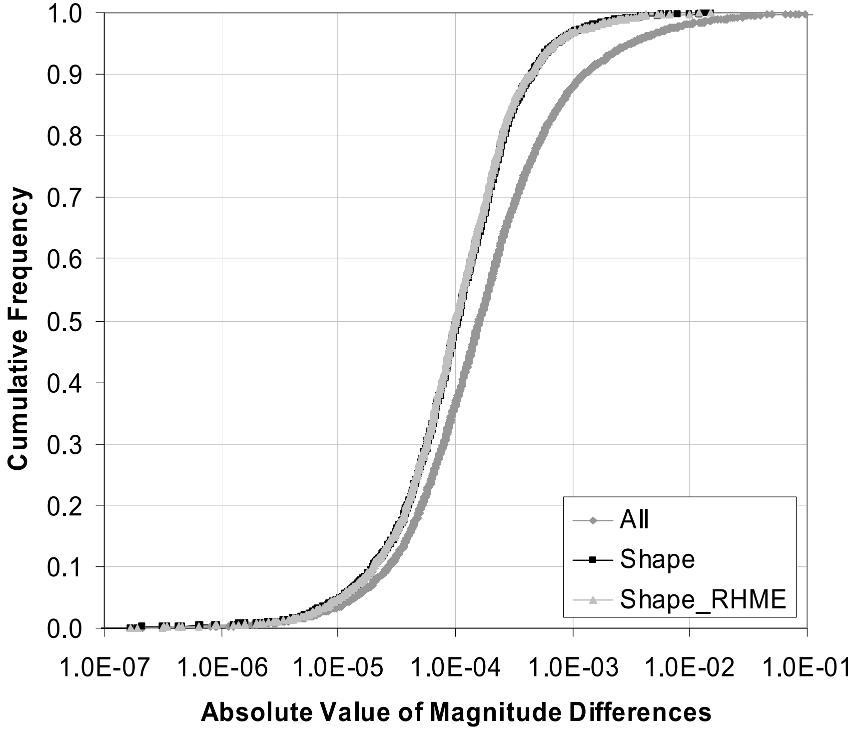


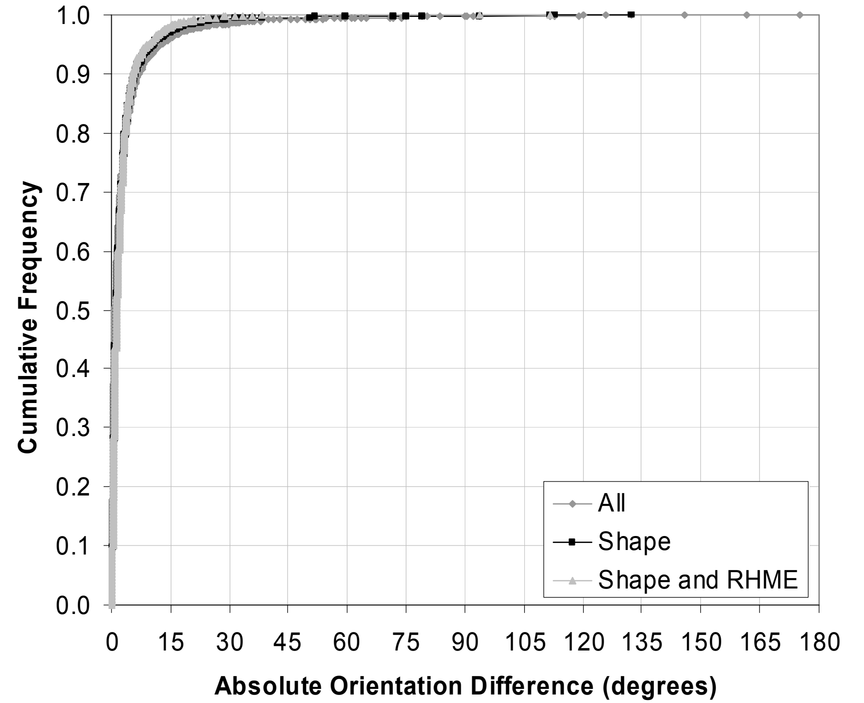
Strong magnitudes are flows going across low T zones

Strongest magnitudes along +/- 90 degree orientations are removed as as shape and RHME constraints are applied

Final 2000-2003 Comparison

Distributions of absolute differences between individual estimators between 2000 and 2003





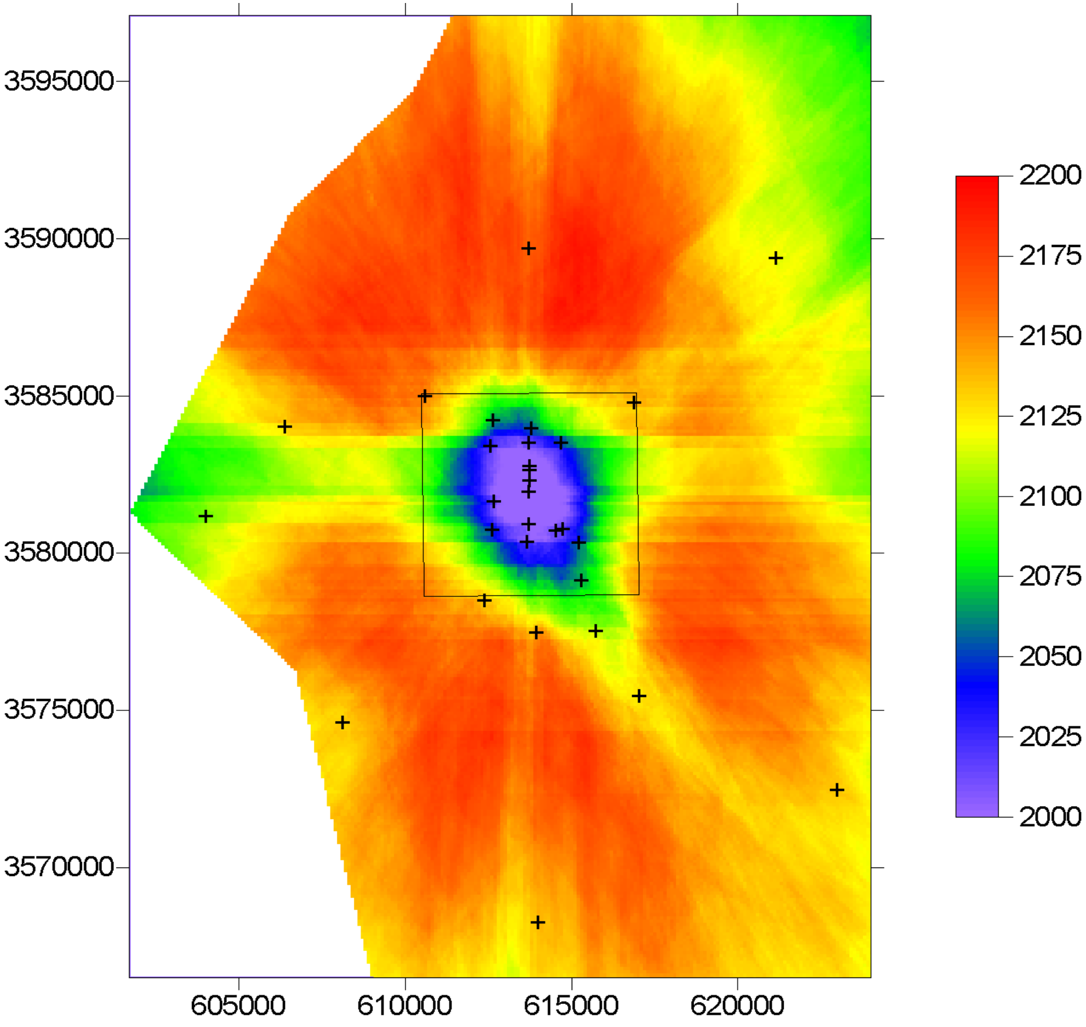
Significant differences occur in only a small fraction of the estimators

Locate New Wells

- **New idea:**
  - **Use groundwater flow model results to provide estimate of head at every location**
  - **Consider every location as a potential new well location**
  - **Calculate additional number of <u>acceptable</u> estimators created by each new well**
  - **Locate well(s) in areas of greatest efficiency**

- **Inverse of this idea to determine which wells to remove from network**

Estimator Efficiency



Map shows total number of acceptable estimators with the addition of a new well at each location in the domain.

Well Removal

Removed Well	Remaining Acceptable Estimators	Absolute Decrease	Percent Decrease	Percent of Maximum Decrease
AEC-7	1650	229	-11.2	56.4
DOE-1	1683	196	-9.4	48.3
ERDA-9	1765	114	-5.1	28.1
H-2b2	1722	157	-7.4	38.7
H-3b2	1736	143	-6.6	35.2
H-4b	1644	235	-11.5	57.9
H-5b	1625	254	-12.5	62.6
H-6b	1650	229	-11.2	56.4
H-7b2	1620	259	-12.8	63.8
H-9b/c	1696	183	-8.7	45.1
H-10b/c	1672	207	-10	51
H11b4	1665	214	-10.4	52.7
H-12	1634	245	-12	60.3
H-17	1642	237	-11.6	58.4
P-17	1653	226	-11	55.7
WIPP-12	1737	142	-6.6	35
WIPP-13	1696	183	-8.7	45.1
WIPP-19	1752	127	-5.8	31.3
WIPP-21	1766	113	-5	27.8
WIPP-22	1757	122	-5.5	30
WIPP-25	1618	261	-12.9	64.3
WIPP-26	1650	229	-11.2	56.4
WIPP-30	1634	245	-12	60.3

Remove <u>one well at a time</u> from network and examine reduction in the total number of acceptable estimators as well as relative changes

Well Removal (WIPP-12 & 22)

Removed Well	Remaining Acceptable Estimators	Absolute Decrease	Percent Decrease	Percent of Maximum Decrease
AEC-7	1414	202	-11.5	57.5
DOE-1	1448	168	-9.4	47.9
ERDA-9	1505	111	-5.9	31.6
H-2b2	1473	143	-7.8	40.7
H-3b2	1487	129	-7	36.8
H-4b	1414	202	-11.5	57.5
H-5b	1390	226	-13	64.4
H-6b	1410	206	-11.7	58.7
H-7b2	1385	231	-13.3	65.8
H-9b/c	1448	168	-9.4	47.9
H-10b/c	1432	184	-10.4	52.4
H11b4	1433	183	-10.3	52.1
H-12	1397	219	-12.6	62.4
H-17	1410	206	-11.7	58.7
P-17	1416	200	-11.4	57
WIPP-13	1440	176	-9.9	50.1
WIPP-19	1491	125	-6.7	35.6
WIPP-21	1503	113	-6	32.2
WIPP-25	1383	233	-13.4	66.4
WIPP-26	1409	207	-11.8	59
WIPP-30	1401	215	-12.3	61.3

First remove WIPP-12 and WIPP-22

Remove one well at a time from network and examine reduction in the total number of acceptable estimators as well as relative changes

Well Removal (WIPP-12 & 22, H-12 and P-17)

Removed Well	Remaining Acceptable Estimators	Absolute Decrease	Percent Decrease	Percent of Maximum Decrease
AEC-7	1052	164	-12.5	54.7
DOE-1	1076	140	-10.5	46.7
ERDA-9	1134	82	-5.7	27.3
H-2b2	1104	112	-8.2	37.3
H-3b2	1112	104	-7.6	34.7
H-4b	1046	170	-13	56.7
H-5b	1032	184	-14.1	61.3
H-6b	1038	178	-13.6	59.3
H-7b2	1028	188	-14.5	62.7
H-9b/c	1074	142	-10.7	47.3
H-10b/c	1066	150	-11.3	50
H11b4	1058	158	-12	52.7
H-17	1029	187	-14.4	62.3
WIPP-13	1064	152	-11.5	50.7
WIPP-19	1117	99	-7.1	33
WIPP-21	1127	89	-6.3	29.7
WIPP-25	1025	191	-14.7	63.7
WIPP-26	1049	167	-12.7	55.7
WIPP-30	1032	184	-14.1	61.3

First remove WIPP-12 and WIPP-22, H-12 and P-17

Remove one well at a time from network and examine reduction in the total number of acceptable estimators as well as relative changes

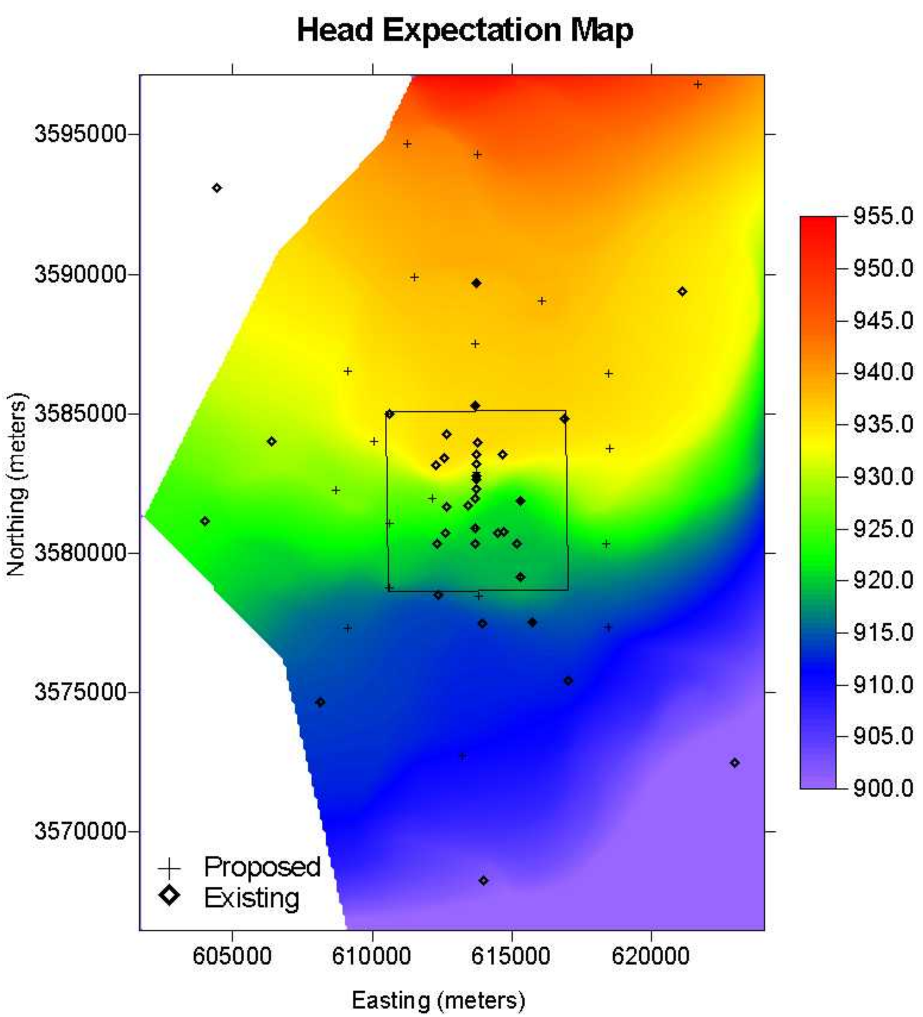
Three-Point Summary

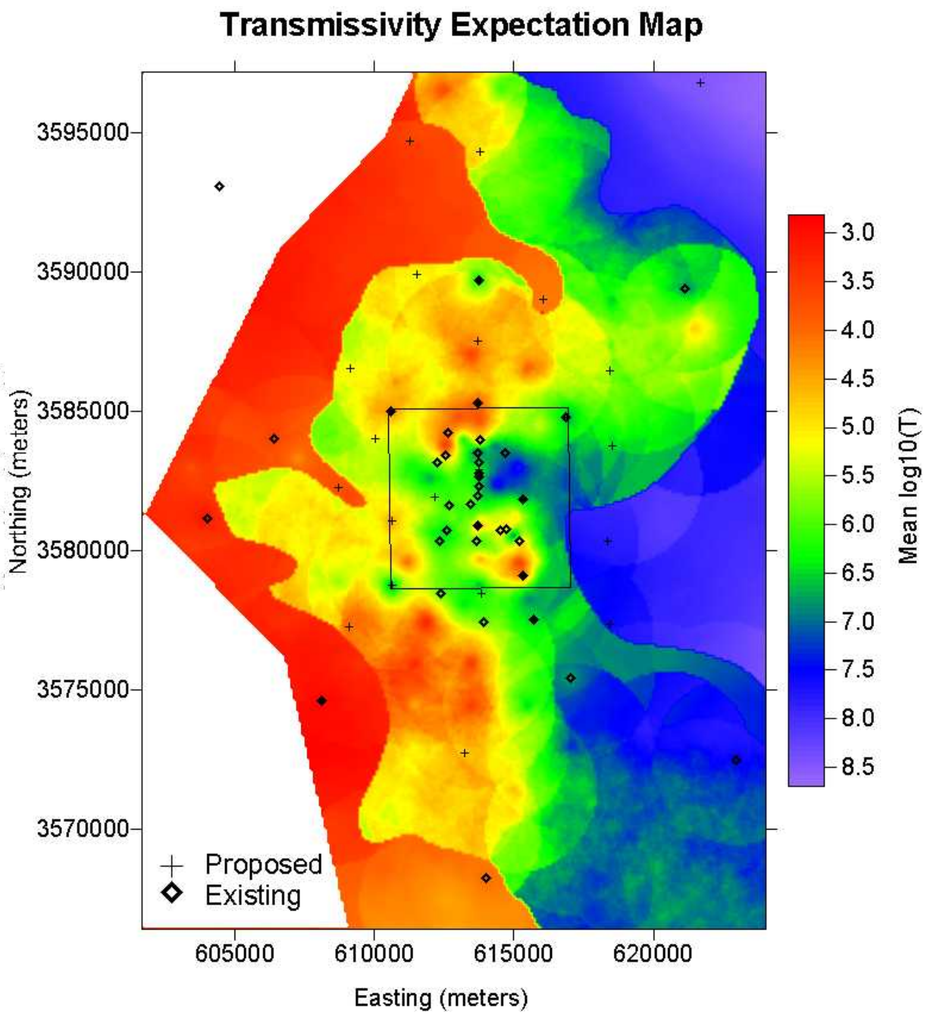
- Used simulation to refine three-point approach
  - Relative measurement error
  - Triangle shape
- Applied three-point estimator to temporal monitoring
  - This can be "operationalized" to quickly detect changes
- Developed and demonstrated approach for determining best locations to locate new monitoring wells
- Examined changes in gradient monitoring network due to well removal

Approach 3: Sensitivity-Based

- **Use recent results of stochastic transmissivity field calibration**
- **Consider the estimated head and transmissivity at each model cell to be a stochastic input parameter to the transport model**
  - **Estimated parameters are drawn independently *across realizations***
- **Rank Correlation Coefficient provides measure of sensitivity**
  - **Sensitivity of integrated performance (travel time) measure influenced by all parameters (all estimated T's or heads)**

Calibration Results: Head & T

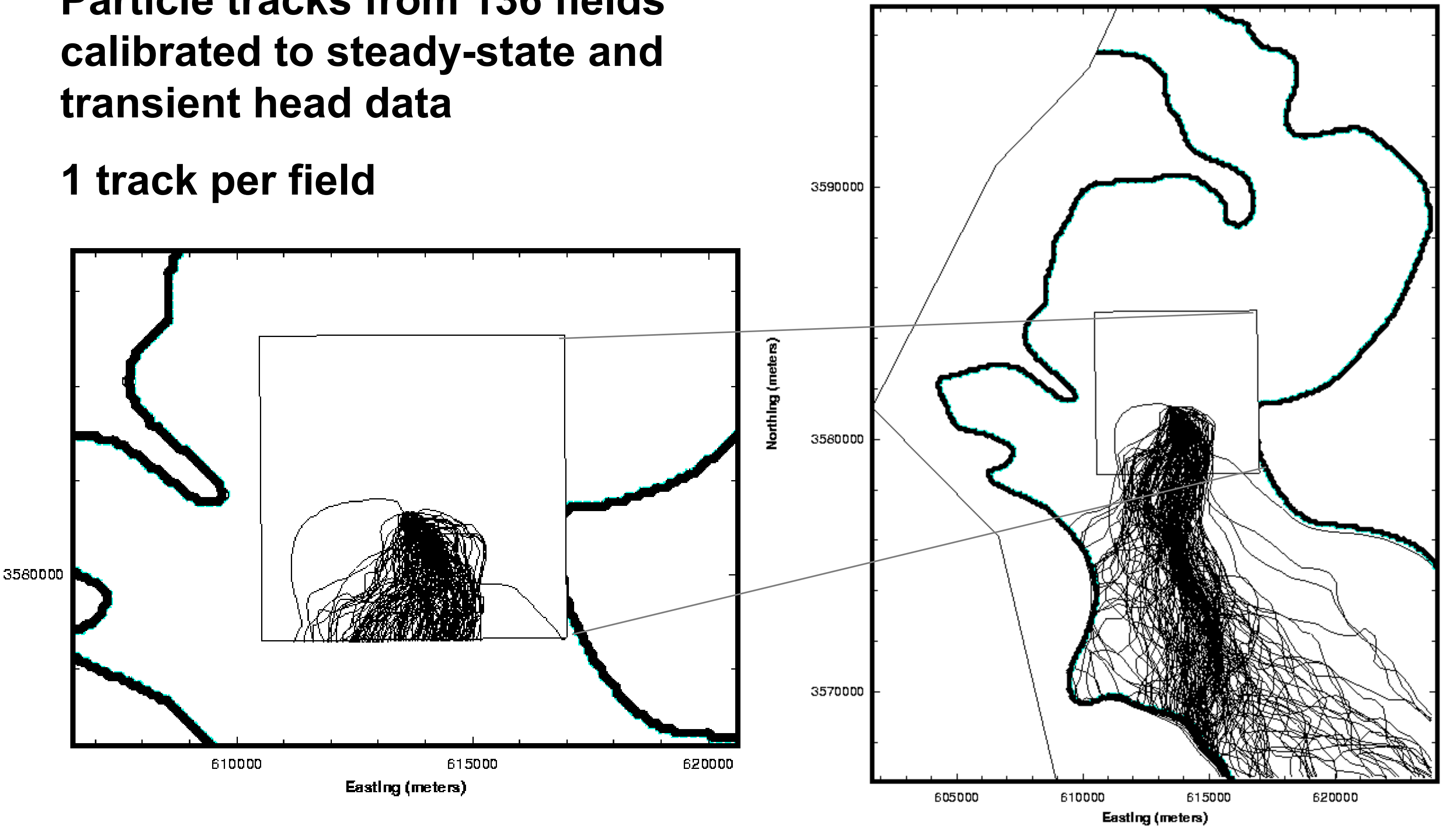




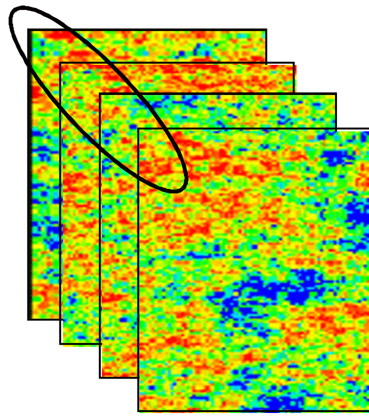
Particle Tracking Results

Particle tracks from 136 fields calibrated to steady-state and transient head data

1 track per field



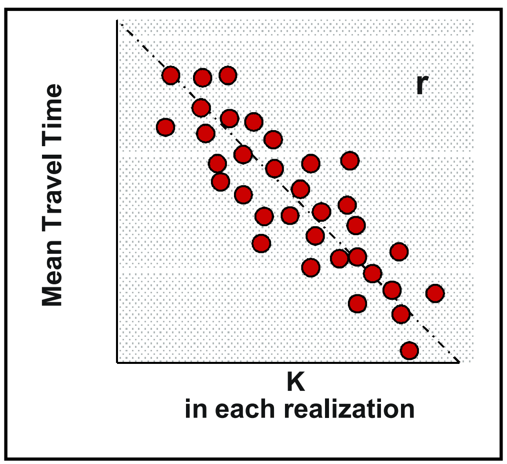
Sensitivity Analysis Approach



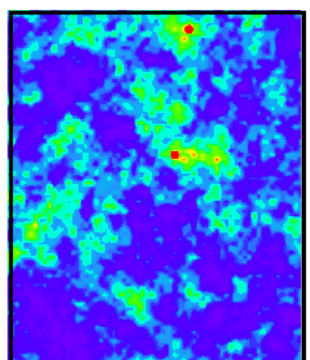
T or Head at Every Grid Block

Groundwater Flow and Particle Tracking Model

Mean Travel Time for Every Realization



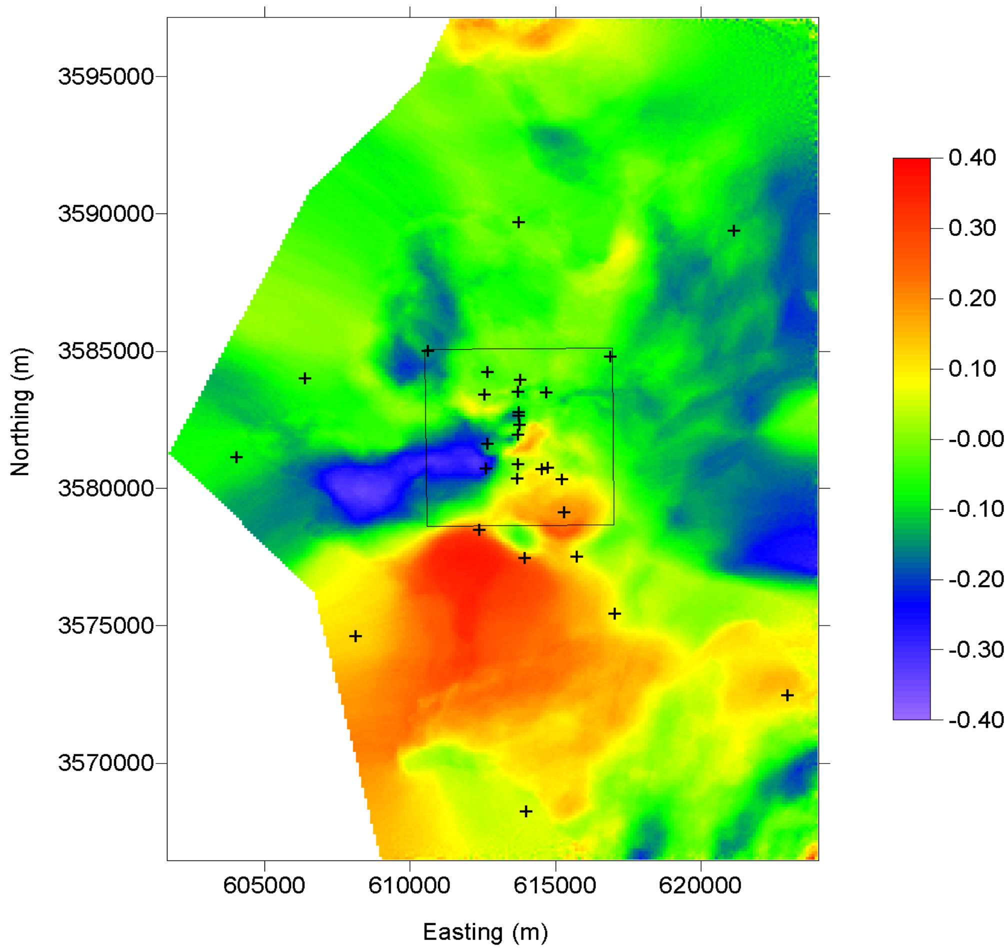
Map of r Values



$$r(\mathbf{x})_s = \frac{\sum_{i=1}^{n}(R_i - \overline{R})(S_i - \overline{S})}{\sqrt{\sum_{i=1}^{n}(R_i - \overline{R})^2}\sqrt{\sum_{i=1}^{n}(S_i - S)^2}}$$

Sensitivity of Travel Time to Head

- The sign of the RCC indicates the sign of the correlation between head and travel time
- Regions of greatest sensitivity are to south of WIPP site and to west of WIPP site
- Values near boundaries are strongly influenced by fixed head boundary conditions

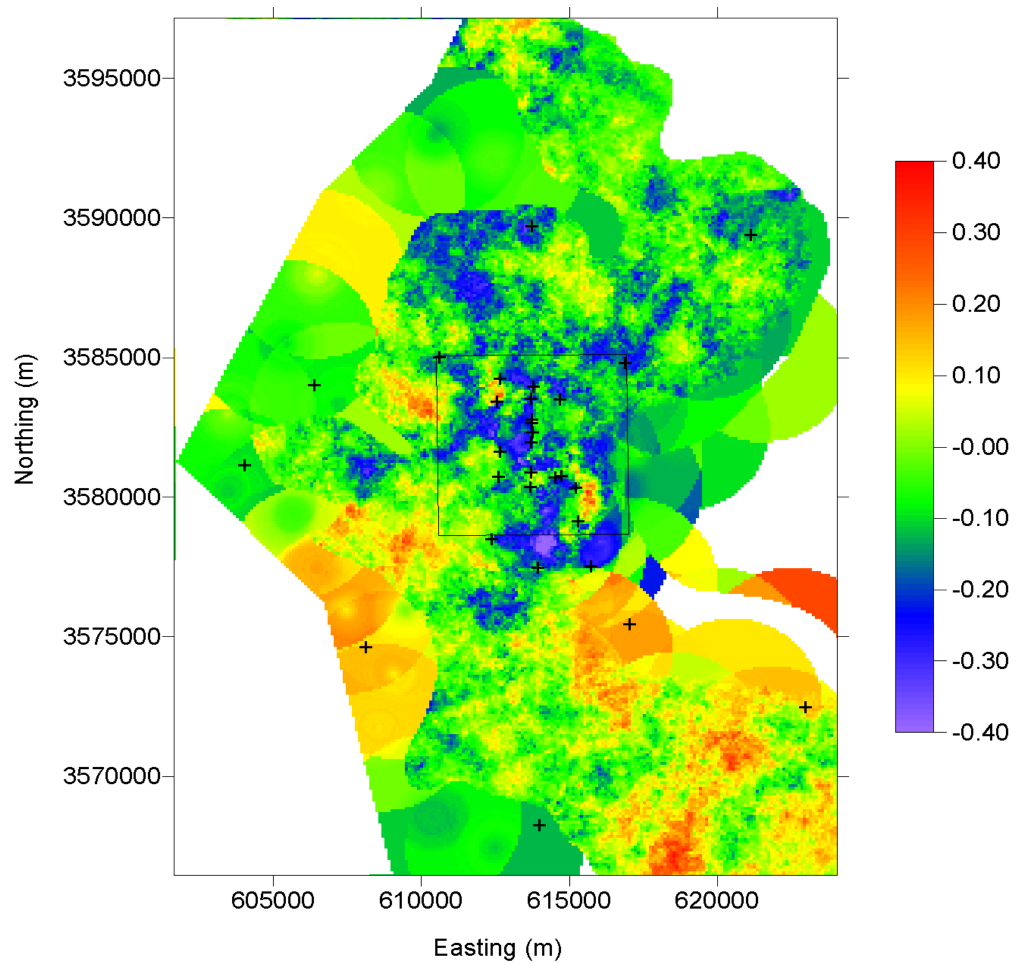


Sensitivity of Travel Time to T

Sign of the RCC indicates the sign of the correlation between T and travel time

Sensitivity is more localized relative to head sensitivity map (diffusive vs. convective forcing)

Regions of greatest sensitivity are directly south of WIPP site, to NW of WIPP site and southern boundary (?)



Sensitivity Approach: Summary

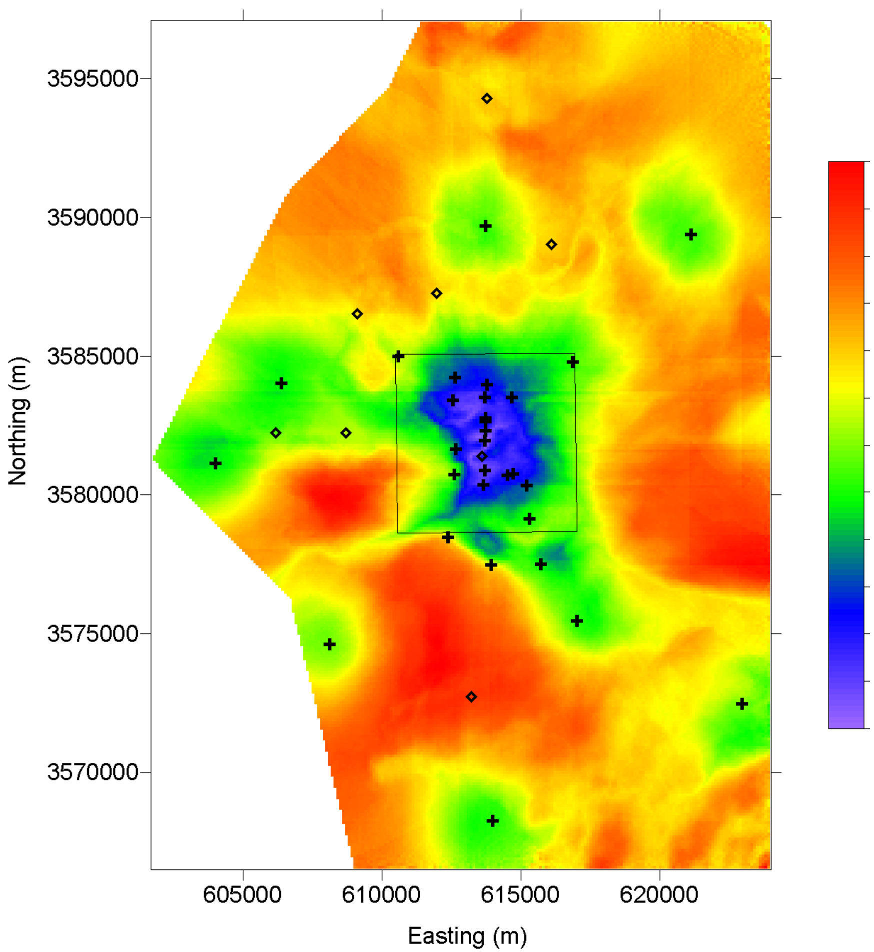
- **Performance measure (travel time) is more or less sensitive to head and T at different parts of the aquifer**
  - **Target regions of high sensitivity for monitoring wells.**
- **Advantages:**
  - **Direct link between monitoring and PA**
- **Disadvantages:**
  - **Computationally intense to calculate**

Combined Approach

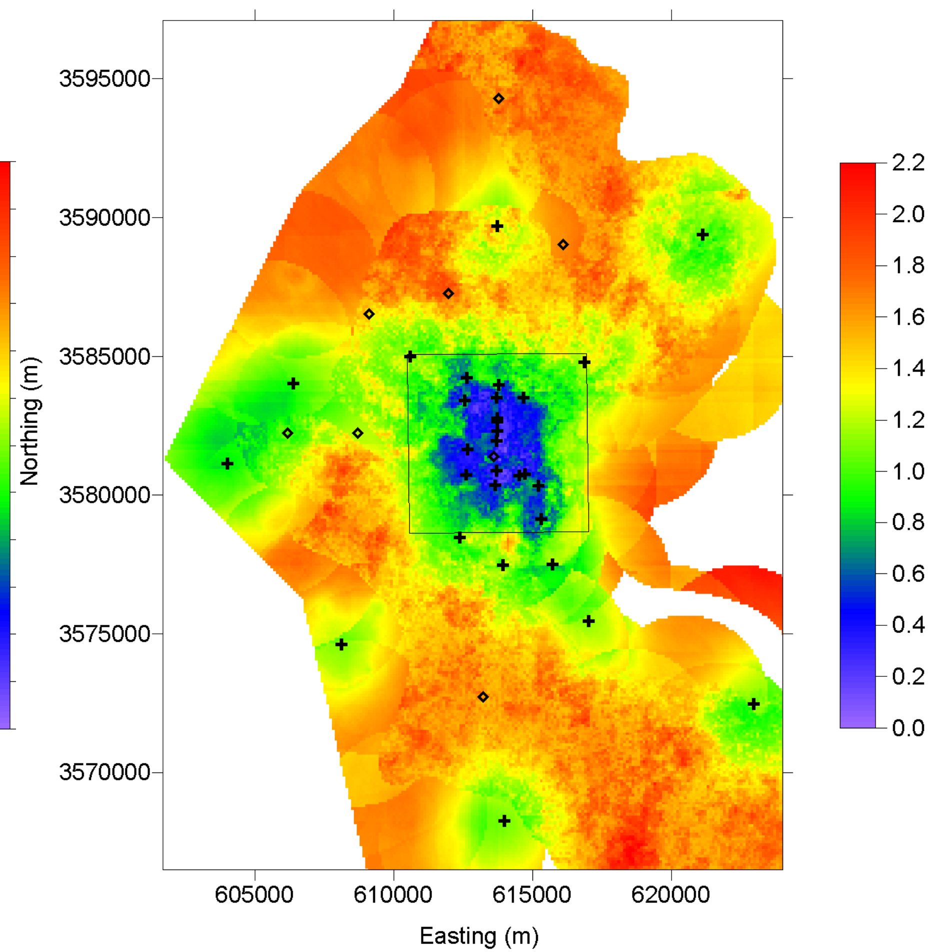
- **Only combine approaches to determine locations for new wells**
- **Rescale each different result to scale from 0.0 to 1.0**
  - **Rescale the *absolute values* of the sensitivities**
- **Sum the three rescaled results to get a final combined score [0.0,3.0]**
  - **The higher the score, the better the location for a new well**

Combined Score Maps

Includes Sensitivity to Head



Includes Sensitivity to T



New/Proposed well locations are shown

Combination Summary

- Different approaches summed to get combined score
  - Maps including sensitivity to head or T are roughly the same
- New/Proposed Wells are generally in high score locations
  - C-2737 is in a low score location
  - IMC-461 and SNL-9 could be moved south

Final Wrap Up

- Three approaches to monitoring
- Geostatistical:
  - Identifies data gaps in <u>head</u> measurements
  - Wells can be removed from WIPP site area
  - Wells needed to meet goal of identifying boundary condition heads
- Three Point Estimator
  - Technique to improve <u>gradient</u> estimates (direction and magnitude of flow across site)
  - Wells in WIPP site can be removed
  - Wells needed in area surrounding WIPP site

Final Wrap Up (Cont.)

- **Sensitivity Based Monitoring**
  - Direct connection between monitoring and PA
  - Considers sensitivity to both head and T
  - Wells needed south and west of WIPP site
- **Combining Approaches**
  - Majority of new/planned monitoring wells in high score locations
  - Improved network can provide data to infer causes of head/gradient changes