

# Improved predictive sampling using quasi-Monte Carlo with application to neutron-cross-section evaluation

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This presentation available at  
<http://www.lanl.gov/home/kmh/>

April 14, 2005

Center for Devices and Radiological Health, FDA

LA-UR-05-3096

# Collaborators and counselors

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# Overview

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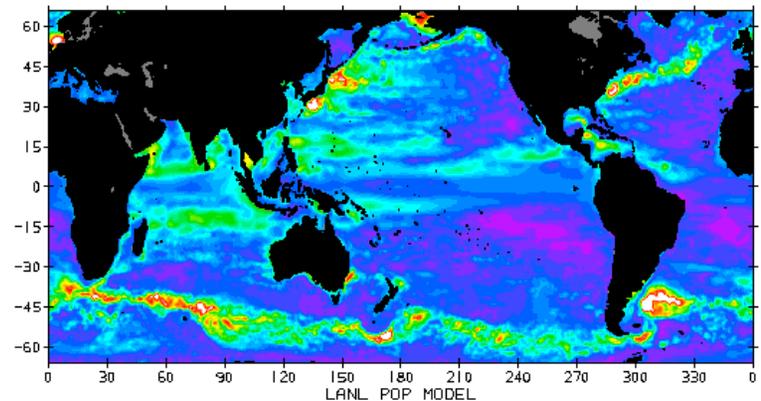
- Quasi-Monte Carlo (QMC) – purpose
- Digital halftoning – purpose and constraints
- New approaches to generating sample sets with uniform spacing
  - ▶ halftoning algorithm provides good point sets for QMC
  - ▶ leads to Repulsive Particle Model (RPM) and Centroidal Voronoi Tessellation (CVT)
- Point sets for sampling distributions in high dimensions
  - ▶ predictive sampling – estimate prediction mean and uncertainty
- Neutron cross-section evaluation
  - ▶ combine directly measured neutron cross sections for fission of  $^{239}\text{Pu}$  with a high-accuracy criticality measurement
  - ▶ Bayesian update
  - ▶ objective – to characterize prediction uncertainty using 30 samples for 30 input parameters

# Context – big physics simulation codes

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- Computer simulation codes
  - ▶ many input parameters, many output variables
  - ▶ very expensive to run; days to weeks on super computers
- Important to assess uncertainties in predictions - thus need to
  - ▶ compare codes to experimental data; make inferences
  - ▶ use advanced methods to estimate sensitivity of simulation outputs to inputs
    - Latin square (hypercube), stratified sampling, quasi-Monte Carlo, CVT
- Examples of complex simulations
  - ▶ nuclear-reactor design
  - ▶ ocean and atmosphere modeling
  - ▶ aircraft design; space shuttle design
  - ▶ casting of metals

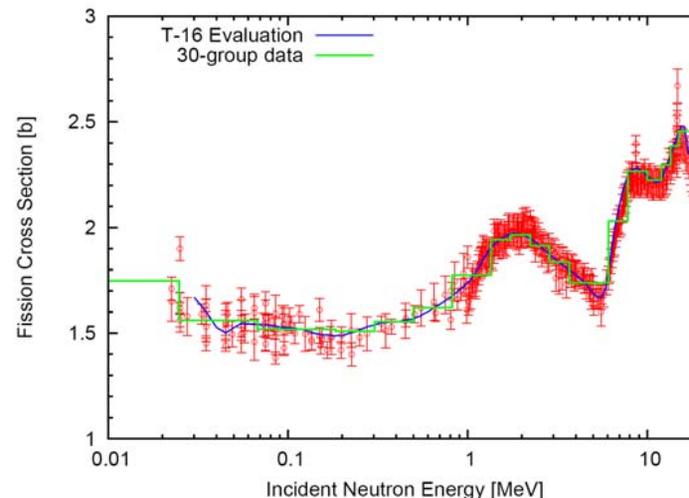
**calculations can take 3 months!**



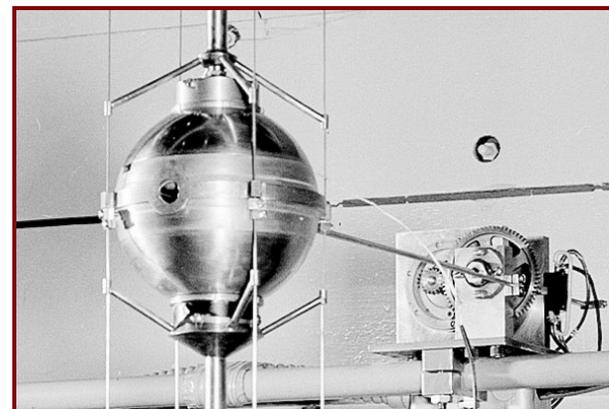
# Our application

- Focus on neutron cross sections
- Aim to improve our knowledge of the cross sections by incorporating a high-precision criticality measurement; integral constraint
- Criticality experiment simulated with a discrete-ordinate code, based on 30 energy bins
- Ultimate goal is to use the improved cross sections to predict other similar physical situations
- Need to characterize prediction uncertainties; 30-D parameter space

## Neutron fission cross section



## Criticality experiment



# Monte Carlo integration techniques

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- Generic purpose of Monte Carlo
  - ▶ estimate integral of a function over a specified region  $R$  in  $m$  dimensions, based on evaluations at  $n$  sample points

$$\int_R f(\mathbf{x}) d\mathbf{x} = \frac{V_R}{n} \sum_{i=1}^n f(\mathbf{x}_i)$$

- Constraints
  - ▶ integrand not available in analytic form, but calculable
  - ▶ function evaluations may be expensive, so minimize number
- Algorithmic approaches – want best accuracy with fixed number of function evaluations  $n$ 
  - ▶ simple quadrature (Riemann) – good for few dimensions; rms err  $\sim n^{-1}$
  - ▶ Monte Carlo – useful for many dimensions; rms err  $\sim n^{-1/2}$
  - ▶ quasi-Monte Carlo – reduce number of evaluations; rms err  $\sim n^{-1}$

# Quasi-Monte Carlo

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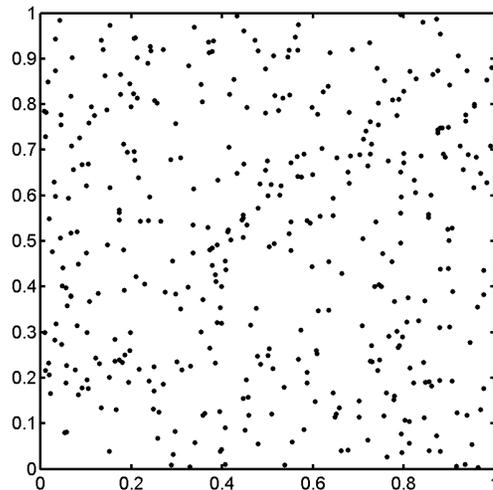
- Purpose
  - ▶ estimate integral of a function over a specified domain in  $d$  dimensions
  - ▶ obtain better rate of convergence of integral estimation than occurs in classic Monte Carlo
- Constraints
  - ▶ integrand function not available analytically, but calculable
  - ▶ function known (or assumed) to be reasonably well behaved, e.g. smooth
- Standard QMC approaches use low-discrepancy sequences; product space (Halton, Sobel, Faure, Hammersley, ...)
  - ▶ most studies usually involve many samples in a few dimensions
- Propose here new ways of generating sample point sets
  - ▶ our focus is on a few samples in high dimensions

# Point set examples

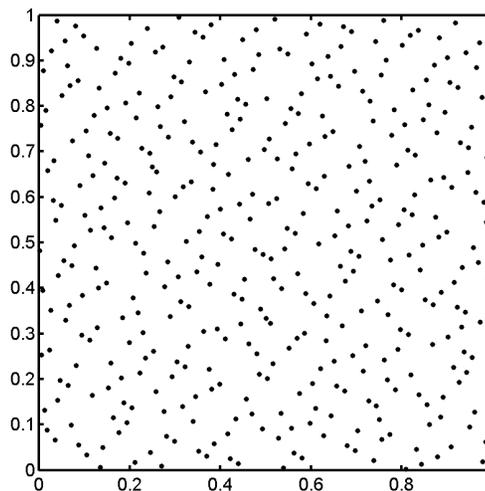
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- Scatter plots of different kinds of point sets (400 points)
- Halton sequence reduces clustering that occurs in random seqs.
- If quasi-MC sequences have better integration properties than random, is halftone pattern even better?

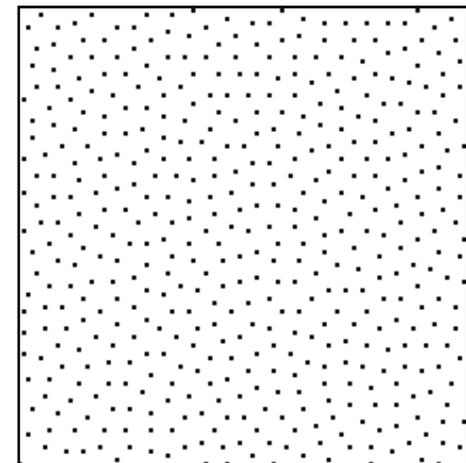
Random  
(independent)



Quasi-Random  
(Halton sequence)



Halftone  
(DBS sky)



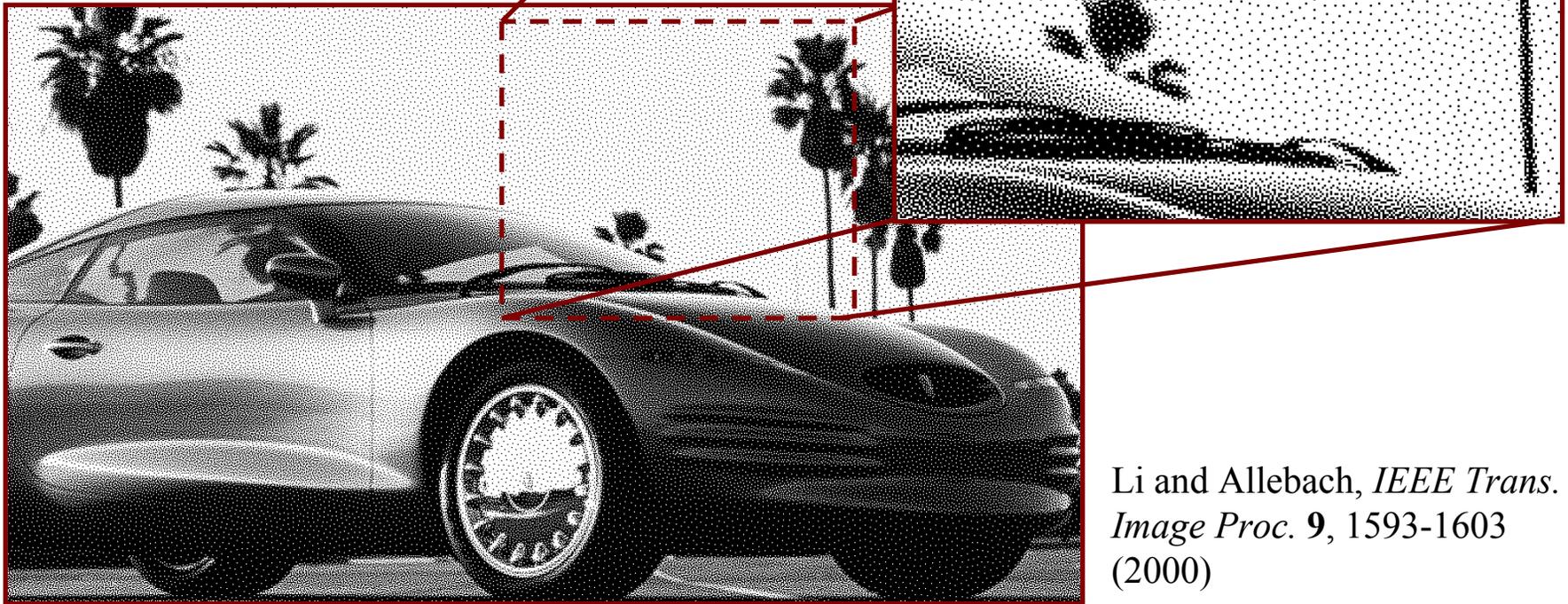
# Digital halftoning techniques

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- Purpose
  - ▶ render a gray-scale image by placing black dots on white background
  - ▶ make halftone rendering **look** like original gray-scale image
  - ▶ related to characteristics of human observer
  - ▶ important for laser printers
- Constraints
  - ▶ resolution – size and closeness of dots, number of dots
  - ▶ speed of rendering
- Various algorithmic approaches
  - ▶ error diffusion, look-up tables, blue-noise, ...
  - ▶ concentrate here on Direct Binary Search (Allebach et al.)

# Direct Binary Search example

- DBS produces halftone images with excellent visual quality
- Sky region has uniform density; quasi-random pattern
- Computationally intensive



Li and Allebach, *IEEE Trans. Image Proc.* **9**, 1593-1603 (2000)

# Direct Binary Search (DBS) algorithm

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- Consider digital halftone image to be composed of black or white pixels

- Cost function is based on perception of two images

$$\varphi = |\mathbf{h} * (\mathbf{d} - \mathbf{g})|^2$$

- ▶ where  $\mathbf{d}$  is the dot image,  $\mathbf{g}$  is the gray-scale image to be rendered, \* represents convolution, and  $\mathbf{h}$  is the image of the blur function of the human eye, for example,  $(w^2 + r^2)^{-3/2}$

- To minimize  $\varphi$

- ▶ start with a collection of dots with average local density  $\sim \mathbf{g}$

- ▶ iterate sequentially through all image pixels;

- ▶ for each pixel, swap value with neighborhood pixels, or toggle its value to reduce  $\varphi$

- Edge effects must be dealt with

- ▶ in above, dot image surrounded by field of uniform density

# Minimum Visual Discrepancy (MVD) algorithm

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Inspired by Direct Binary Search halftoning algorithm:

- Start with an initial set of points
- Goal is to create uniformly distributed set of points
- Cost function is variance in blurred point image

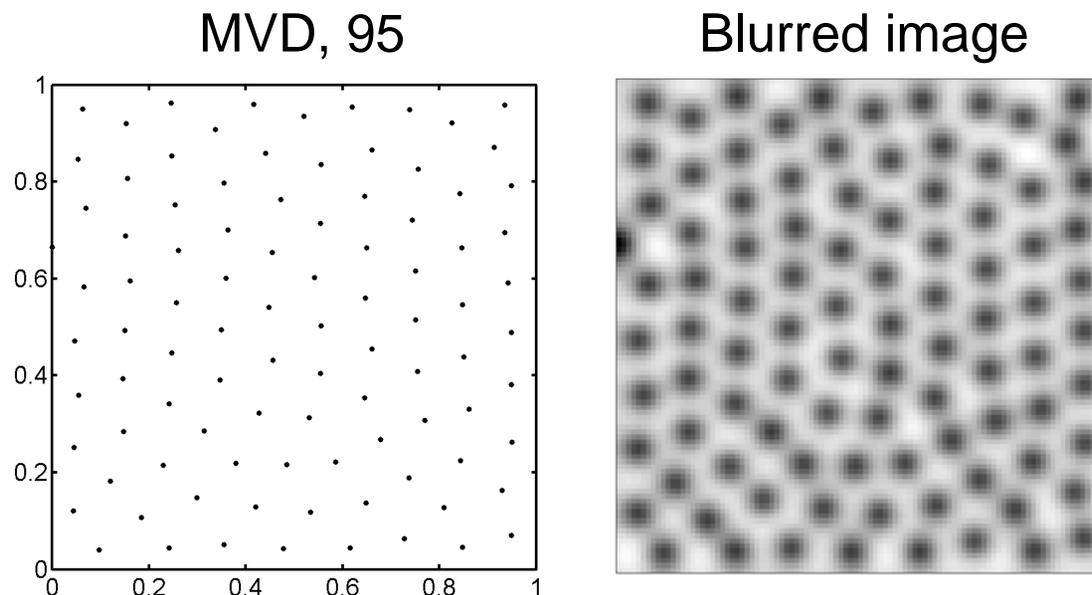
$$\psi = \text{var}(\mathbf{h} * \mathbf{d})$$

- ▶ where  $\mathbf{d}$  is the point (dot) image,  $\mathbf{h}$  is the blur function of the human eye, and  $*$  represents convolution
- Minimize  $\psi$  by
  - ▶ starting with some point set (random, stratified, Halton,...)
  - ▶ visiting each point in random order;
  - ▶ moving each point in 8 directions, and accept move that lowers  $\psi$  the most

# Minimum Visual Discrepancy (MVD) algorithm

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- MVD result; start with 95 points from Halton sequence
- MVD objective is to minimize variance in blurred image
- Effect is to force points to be evenly distributed, or as far apart from each other as possible
- Might expect global minimum is a regular pattern

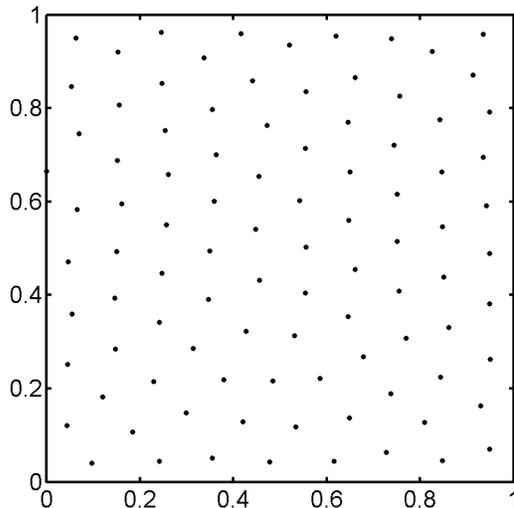


# MVD results

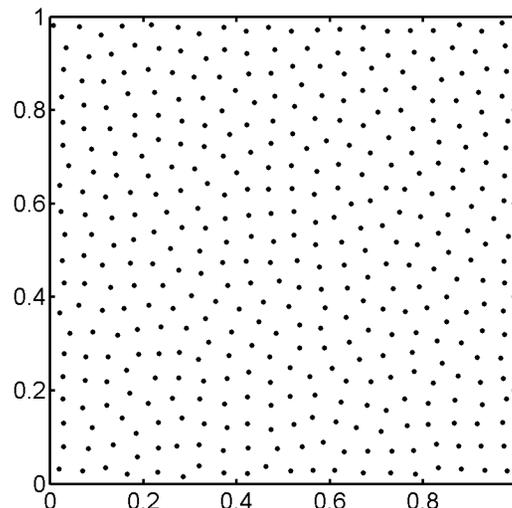
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- In each optimization, final pattern depends on initial point set
  - ▶ algorithm seeks local minimum, not global (as does DBS)
- Patterns somewhat resemble regular hexagonal array
  - ▶ similar to lattice structure in crystals or glass
  - ▶ however, lack long-range (coarse scale) order
  - ▶ best to start with point set with good long-range uniformity

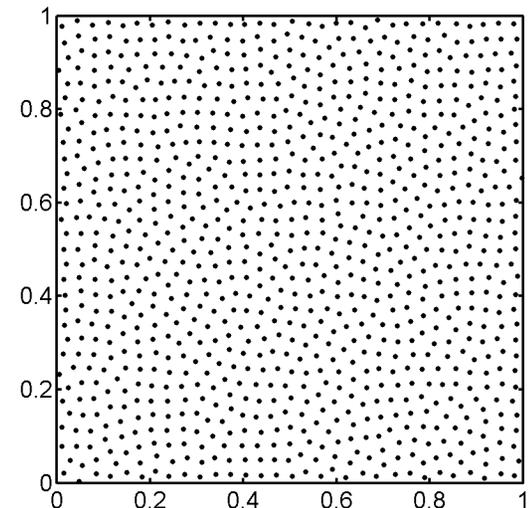
MVD, 95



MVD, 400



MVD, 1000



# Repulsive particle model

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- Model points as set of interacting (repulsive) particles
- Cost function is the potential

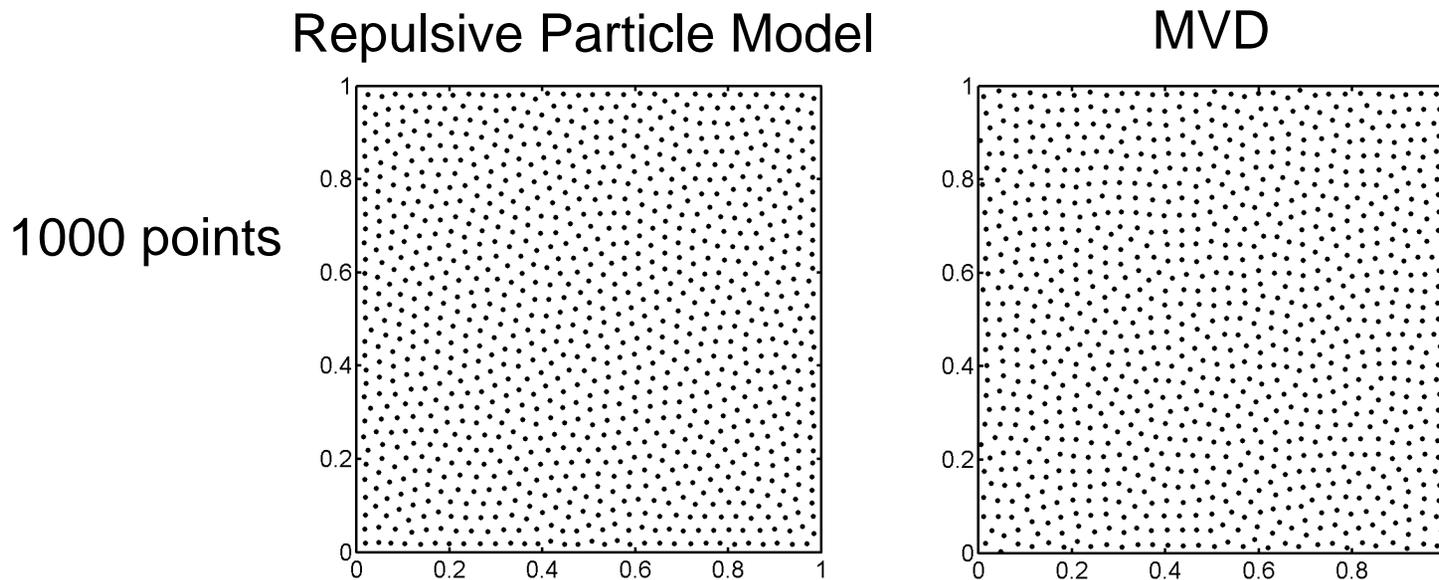
$$\psi = \sum_{i,j \geq i+1} V(\mathbf{x}_i, \mathbf{x}_j) + \sum_i U(\mathbf{x}_i)$$

- ▶ where  $V$  is a particle-particle interaction potential and  $U$  is a particle-boundary potential
  - ▶ particles are repelled by each other and from boundary
- Minimize  $\psi$  by moving particles by small steps
- This model is **analytically equivalent** to Minimum Visual Discrepancy ( $V$  and  $U$  directly related to blur function  $\mathbf{h}$ )
- Suitable for generating point sets in high dimensions

# Repulsive particle model

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- Equivalent to Minimum Visual Discrepancy algorithm
- Example of repulsive-particle results
  - ▶ resulting point pattern is visually indistinguishable from MVD pattern

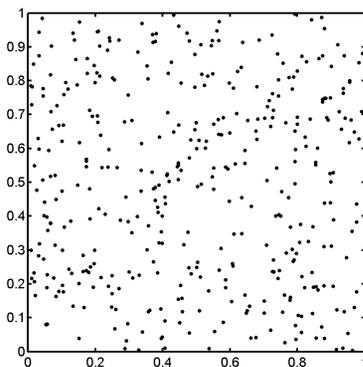


# Point set examples

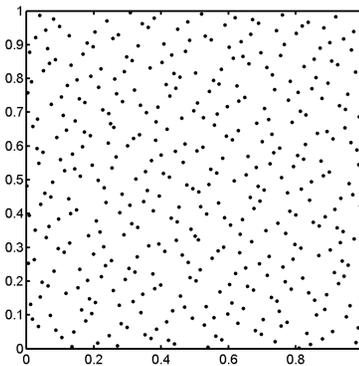
- Compare various kinds of point sets (400 points)
  - ▶ varying degrees of randomness and uniformity
- As the points become more uniformly distributed, the more accurate are the values of estimated integrals
- Example:

RMS relative accuracies of integral of  $\text{func2} = \prod_i \exp(-2|x_i - x_i^0|)$ ;  $0 < x_i^0 < 1$

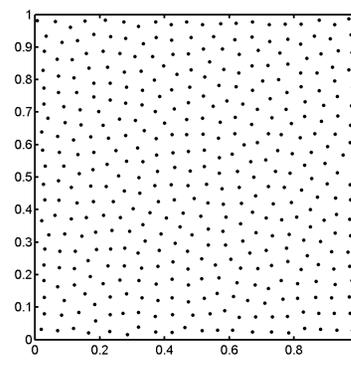
Random, 2.5%



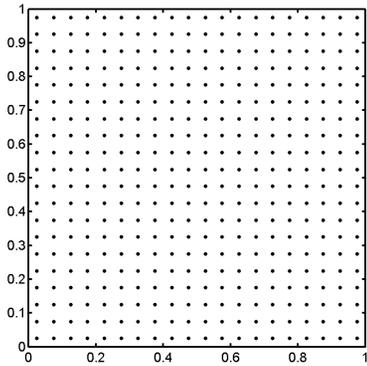
Halton, 0.5%



MVD, 0.14%

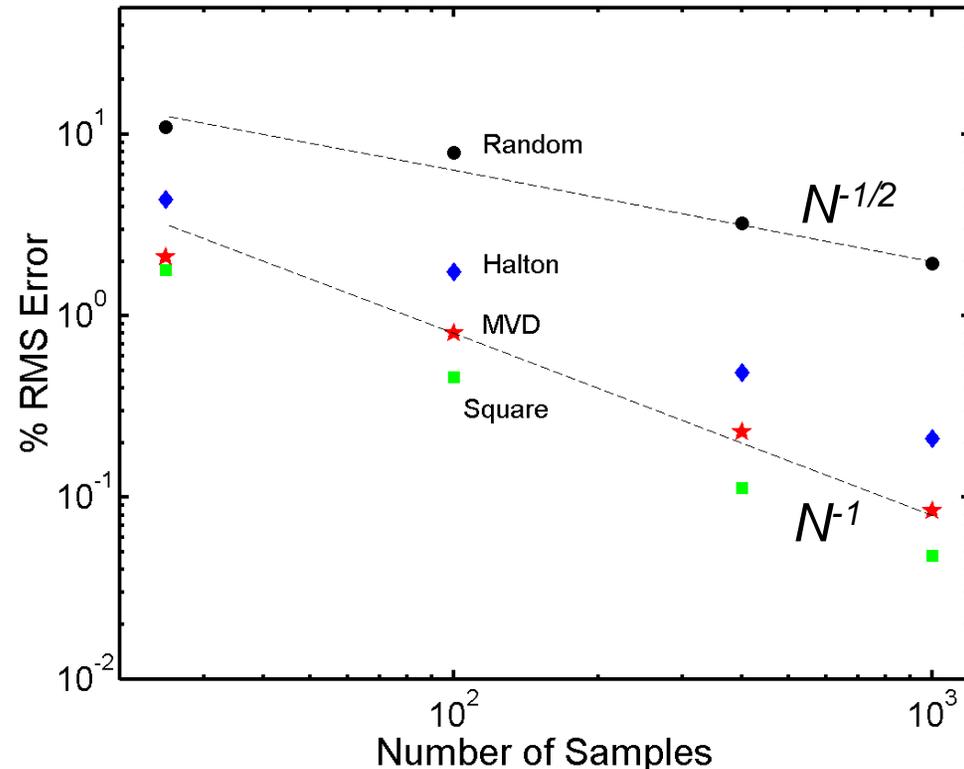


Grid, 0.09%



More Uniform, Higher Accuracy

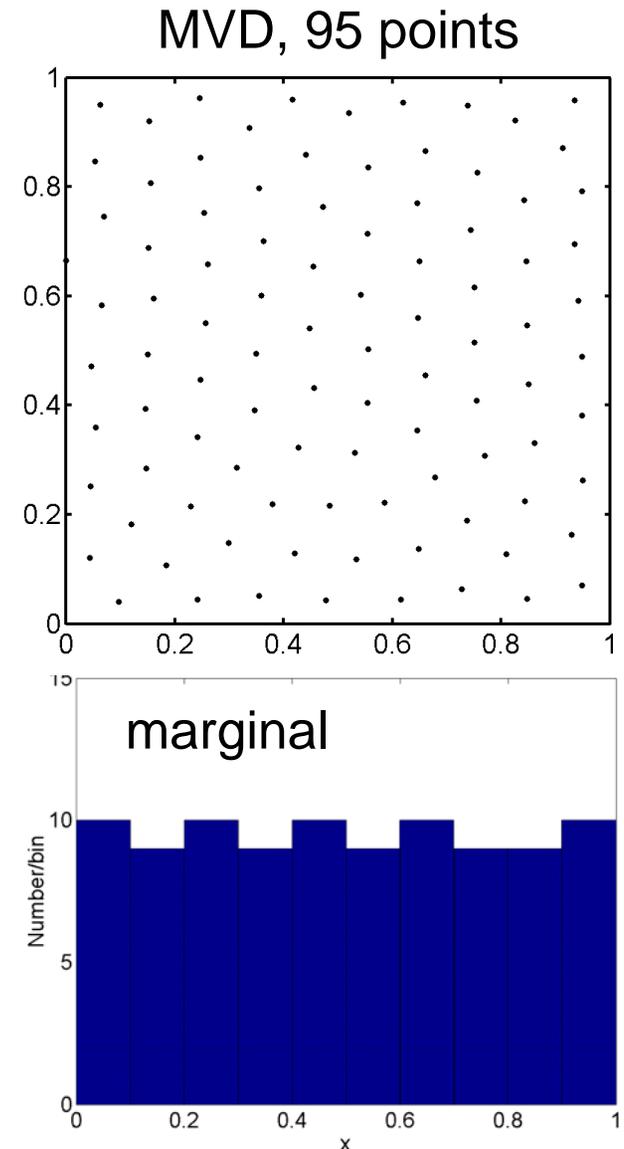
# Integration test problem



- RMS error for integral of  $\text{func2} = \prod_i \exp(-2|x_i - x_i^0|)$ ;  $0 < x_i^0 < 1$ 
  - ▶ integrate over  $x_i^0$  by using MC, drawing  $x_i^0$  from uniform distribution
  - ▶ from worst to best: random, Halton, MVD, square grid
  - ▶ lines show  $N^{-1/2}$  (expected for MC) and  $N^{-1}$  (expected for QMC)

# Marginals for MVD points

- Sometimes desirable for projections of high dimensional point sets to sample each parameter uniformly
- Latin hypercube sampling designed to achieve this property (for specified number of points)
- Plot shows histogram of 95 MVD samples along x-axis, i.e., marginalized over y direction
- MVD points have relatively uniform marginal distributions

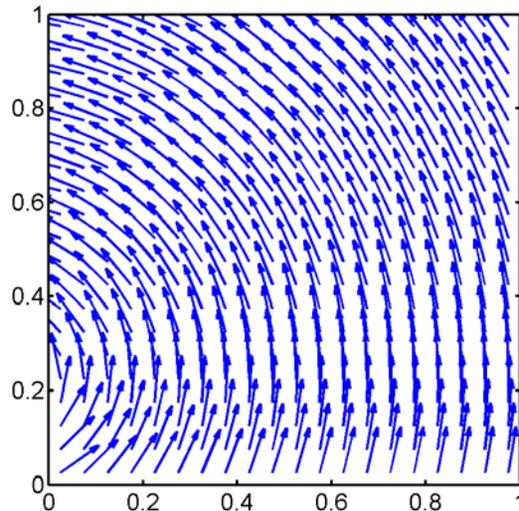


# Another use of MVD: visualization of flow field

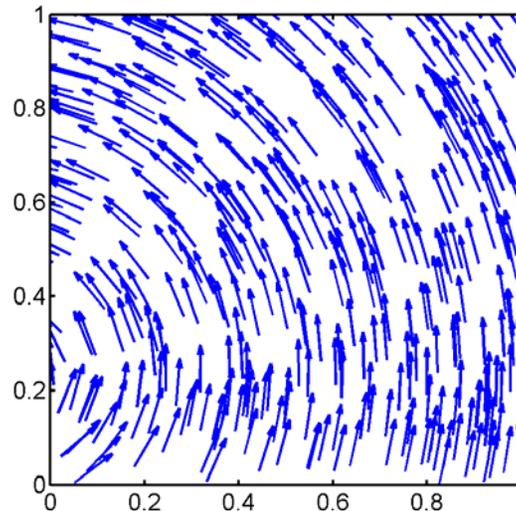
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- Fluid flow often visualized as field of vectors
- Location of vector bases may be chosen as
  - ▶ square grid (typical) - regular pattern produces visual artifacts
  - ▶ random points - fewer artifacts, but nonuniform placement
  - ▶ quasi-random - fewest artifacts and uniform placement

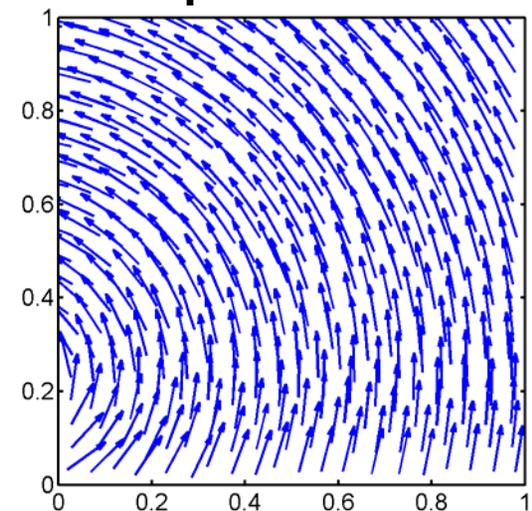
**Square grid**



**Random points**

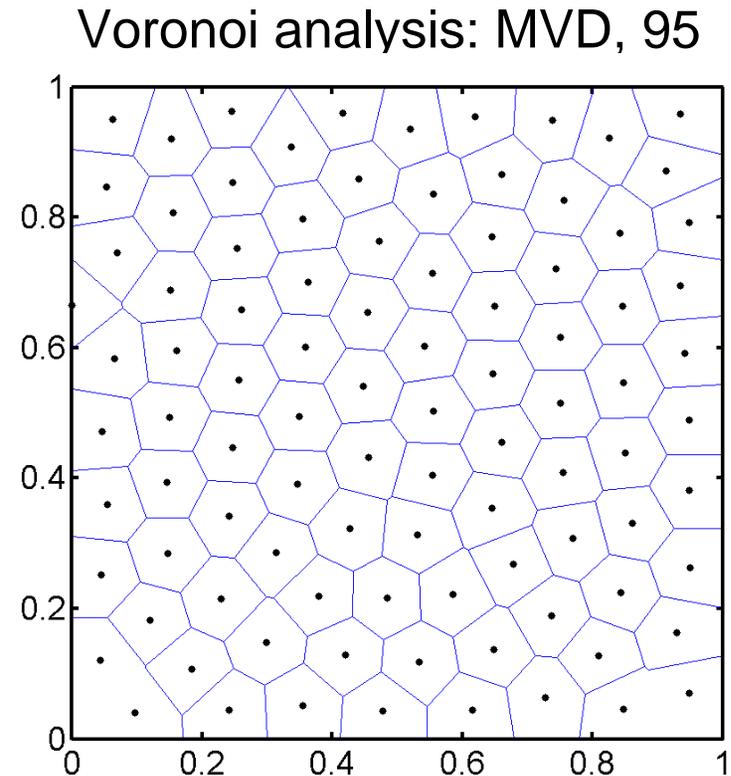


**Quasi-random (MVD)  
point set**



# Voronoi analysis

- Voronoi diagram (2D)
  - ▶ partitions domain into polygons
  - ▶ points in  $i$ th polygon are closest to  $i$ th generating point,  $\mathbf{x}_i$
  - ▶ boundaries shown are obtained by geometrical construction
- MC technique for Voronoi analysis
  - ▶ randomly throw large number of points  $\mathbf{z}_k$  into region
  - ▶ compute distance of each  $\mathbf{z}_k$  to all generating points  $\{\mathbf{x}_i\}$
  - ▶  $\mathbf{z}_k$  belongs to Voronoi region of closest  $\mathbf{x}_j$
  - ▶ can compute  $A_i$ , radial moments, identify neighbors, ...
- Readily extensible to high dimensions



# Voronoi analysis can improve classic MC

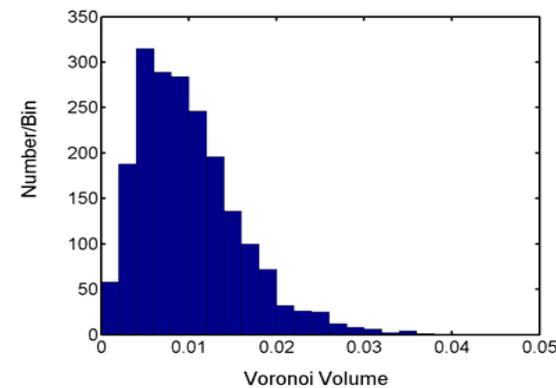
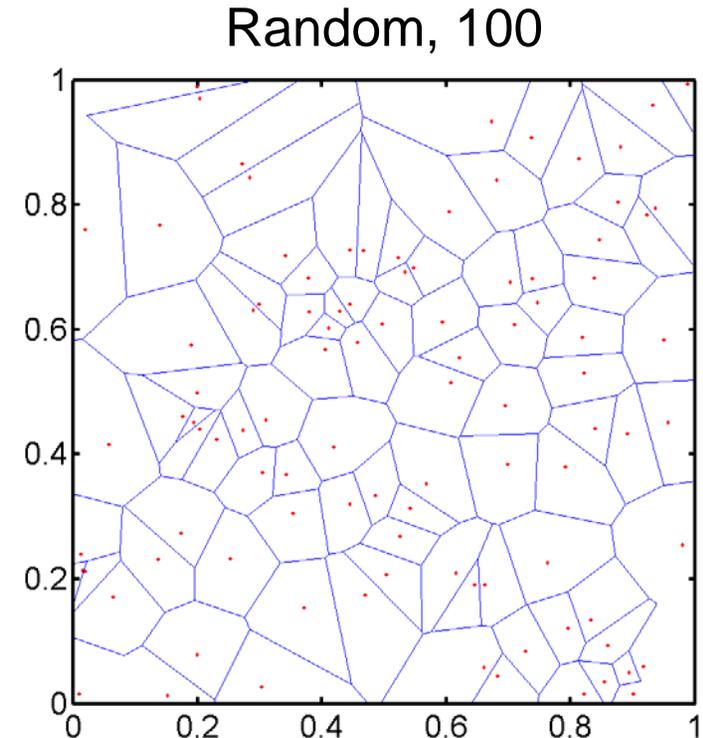
- Standard MC formula

$$\int_R f(\mathbf{x}) d\mathbf{x} = \frac{V_R}{n} \sum_{i=1}^n f(\mathbf{x}_i)$$

- Instead, use weighted average

$$\int_R f(\mathbf{x}) d\mathbf{x} = \sum_{i=1}^n f(\mathbf{x}_i) V_i$$

- ▶ where  $V_i$  is the volume of Voronoi region for  $i$ th point; Riemann integr.
- Accuracy of integral estimate dramatically improved in 2D:
  - ▶ factor of 6.3 for  $N = 100$  (func2)
  - ▶ factor of  $> 20$  for  $N = 1000$  (func2)
- Suitable for adaptive sampling
- Less useful in high dimensions (?)



qmc91

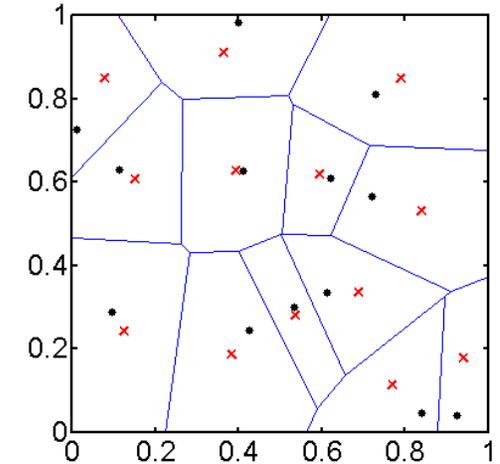
# Centroidal Voronoi Tessellation

- Plot shows 13 random points ( $\cdot$ ) and the centroids of their Voronoi regions ( $\times$ )
- A point set is called a Centroidal Voronoi Tessellation (CVT) when the generating points  $\mathbf{z}^j$  coincide with the centroids their Voronoi regions; a CVT minimizes

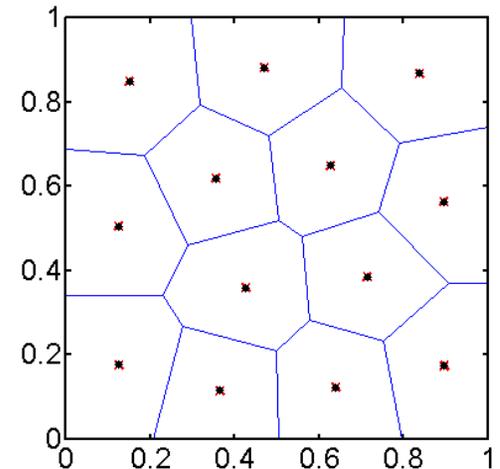
$$\sum_j \int_{V_j} |\mathbf{z}^j - \mathbf{x}|^2 d\mathbf{x}$$

- Algorithm (McQueen)
  - ▶ start with arbitrary set of generating points
  - ▶ perform Voronoi analysis using MC algorithm
  - ▶ move each generating point to its Voronoi centroid
  - ▶ iterate lasts two steps until convergence
- Final CVT points uniformly distributed

Start with random points



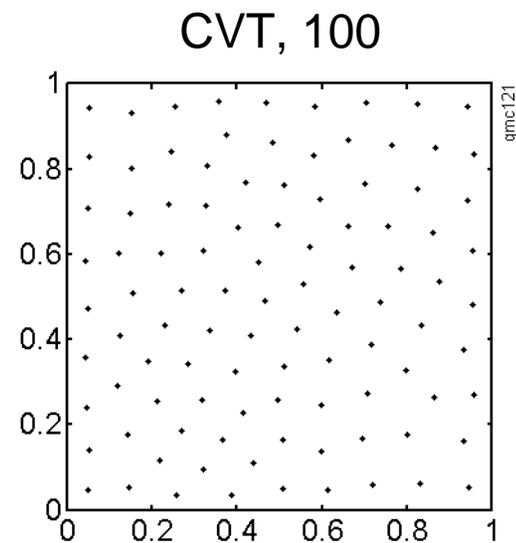
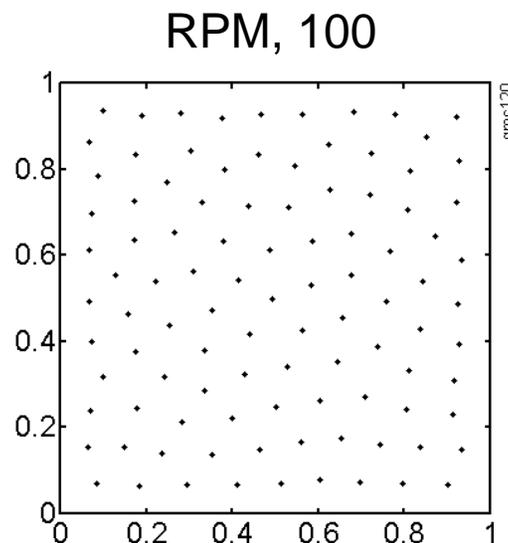
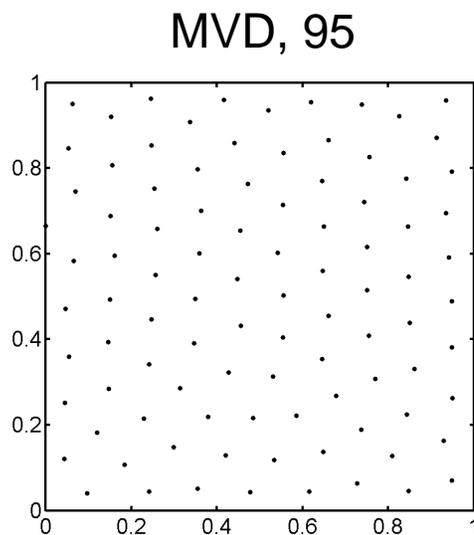
Final CVT point set



# Comparison of methods

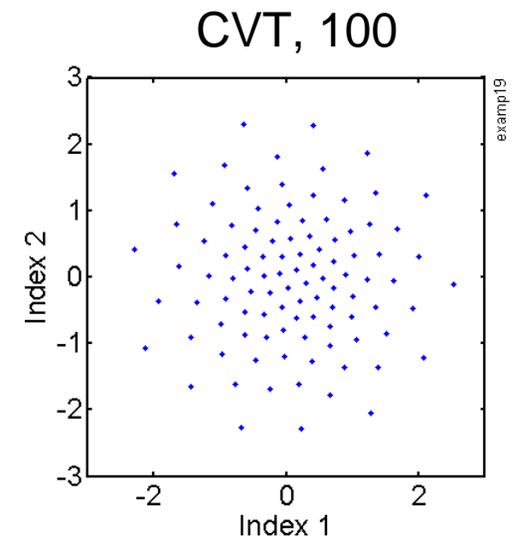
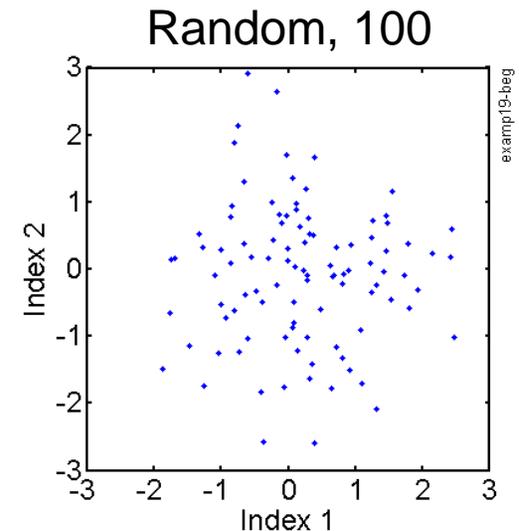
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- Preceding three algorithms provide uniformly-space points, have essentially equivalent patterns, and are useful for QMC
  - ▶ Minimum Visual Discrepancy (MVD)
  - ▶ Repulsive Particle Model (RPM)
  - ▶ Centroidal Voronoi Tessellation (CVT)
- For high dimensions: both CVT and RPM may be useful, RPM likely most efficient



# CVT for multi-variate normal distribution

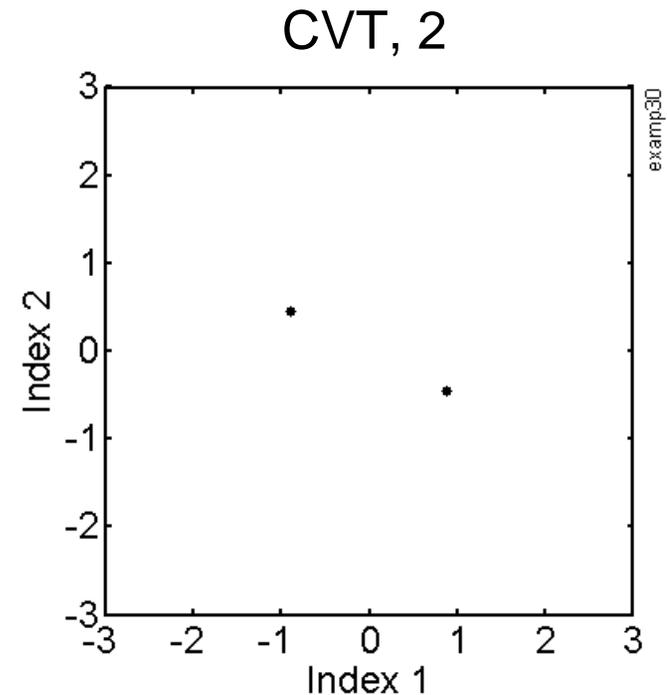
- CVT algorithm works for an arbitrary density function, e.g., a normal distribution
- In above MC algorithm for Voronoi analysis, simply draw random numbers from desired distribution
- Plots show starting random point set and final CVT set
- Radii of points are rescaled to achieve desired average variance along axes



# CVT: 2 points in 2 dimensions

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- Bi-variate normal distribution is rotationally symmetric
- Symmetry of situation means that the CVT points must be symmetric about origin; at the same radius
- This pattern is unique, up to a random rotation
- Both  $x_1$  and  $x_2$  values sampled (with near certainty), but there is a subspace, orthogonal to  $x_1$ - $x_2$  line, whose dependence is not sampled
- Generalizing, the  $d$ -D space is under-sampled when  $n < d + 1$



# Recall context

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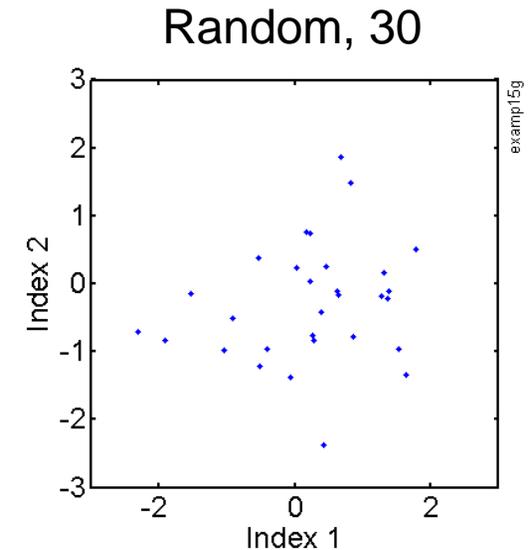
- Our interest is in characterizing the uncertainty in a simulation output, based on what we know about the uncertainties in the inputs



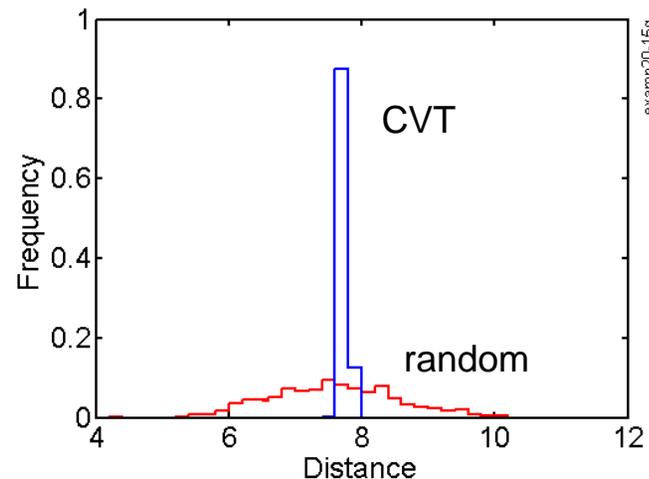
- But, the high cost of running the simulation limits how many samples can be drawn from a parameter distribution to obtain a predictive distribution
- We are often in a situation where the number of points is comparable to number of parameters ( $n \approx d$ )
- Our goal is to draw a modest number of points from a high-dimensional normal distribution
- Let's explore some of the characteristics of the problem by starting with the example of 2 sample points in 2D

# CVT: 30 points in 30 dimensions

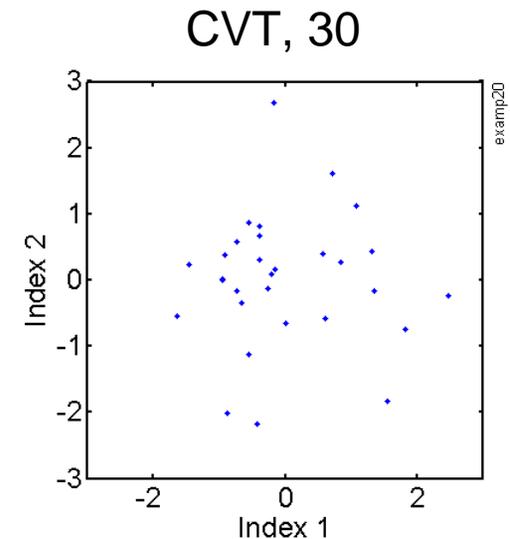
- 30 dimensional normal distribution
- Projected onto 2D plane, CVT result doesn't look much different than random sample set
- However, CVT points are uniformly separated in  $d$ -D, while random points are not



Point separation histogram

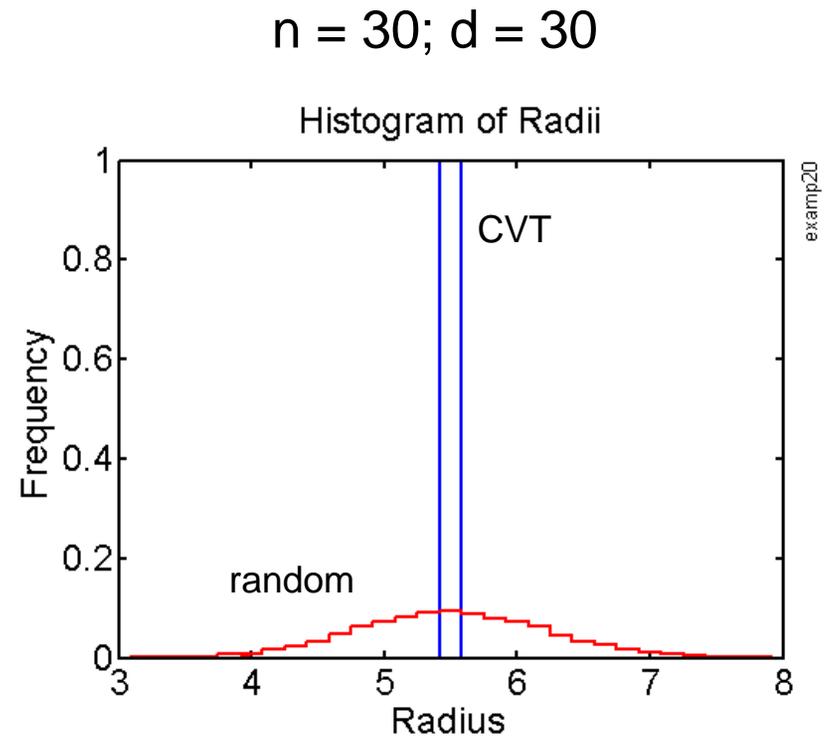


All points are nearest neighbors!



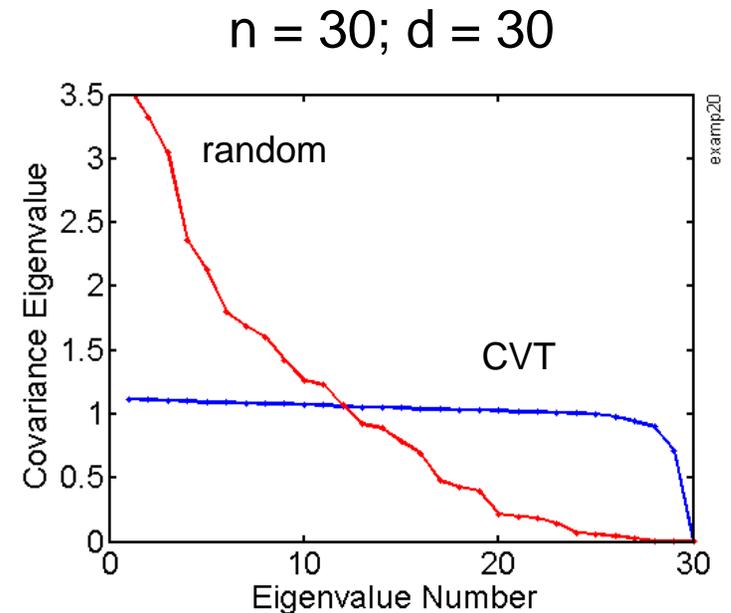
# CVT radial distribution: 30 points in 30D

- As with 2 points in 2D, all 30 CVT points in 30D are at the same radius
  - ▶ lie on the surface of a hypersphere
- As seen in last slide, the inter-point distances for CVT are essentially identical
  - ▶ regular point pattern (unique?)
- Rotation is only degree of freedom between different realizations of CVT
- One can generate new CVT patterns by randomly rotating an existing one



# Covariance analysis of point set

- Let  $\mathbf{x}^j$  be vector for  $j$ th point;  
point set is represented by matrix
$$\mathbf{X} = (\mathbf{x}^1; \mathbf{x}^2; \mathbf{x}^3; \cdots \mathbf{x}^n)^T$$
- Covariance of point set along the axes is  $\mathbf{X}\mathbf{X}^T$
- Eigenanalysis of  $\mathbf{X}\mathbf{X}^T$  yields the covariance spectrum
  - ▶ the  $i$ th eigenvalue is the variance of the points projected onto the  $i$ th eigenvector
- Conclude that spectrum for CVT point set is much more uniform than for random set, which is quite variable (the Wishart distribution)
- Last eigenvalue is zero; rank = 29



# Linear response model

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- Assume outputs of a simulation are linearly related to perturbations in the inputs,  $\delta \mathbf{y} = \mathbf{S}_y^T \delta \mathbf{x}$  where  $\mathbf{S}_y$  is sensitivity matrix  $\partial \mathbf{y} / \partial \mathbf{x}$



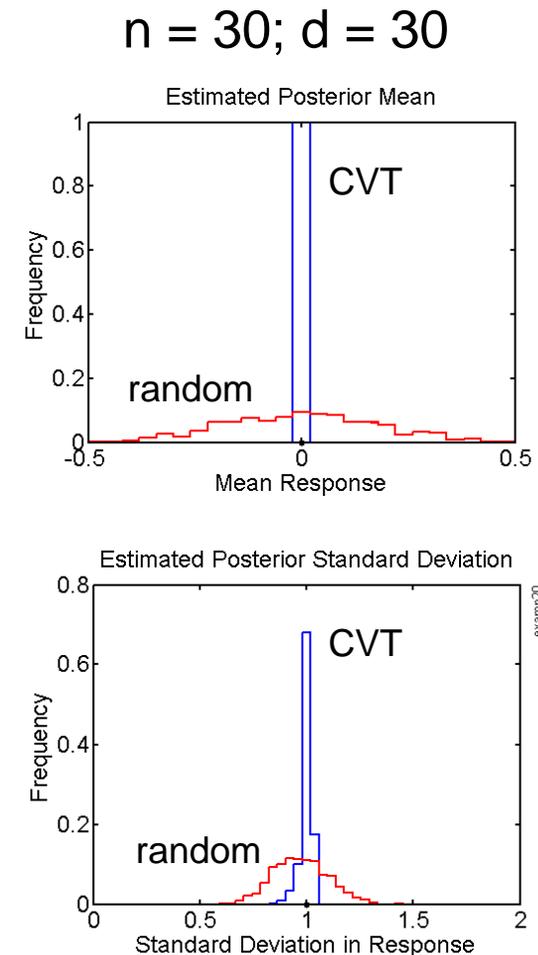
- The covariance in the output  $\mathbf{y}$  is

$$\mathbf{C}_y = \mathbf{S}_y^T \mathbf{C}_x \mathbf{S}_y$$

- ▶ when output  $y$  is a scalar, the covariance  $\mathbf{C}_y$  is a scalar (variance), and  $\mathbf{S}_y$  is a vector
- If linear model is sufficient and one knows the sensitivity matrix, then predictive distribution is easily characterized
- However, for large simulations, the sensitivity matrix is often unknown

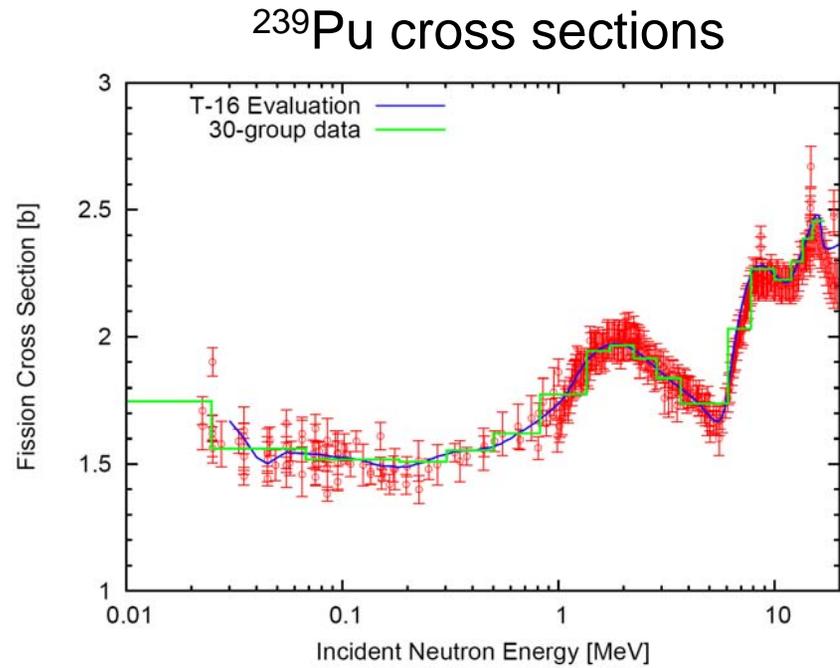
# Test single point set using random sensitivities

- Assume linear model,  $\delta \mathbf{y} = \mathbf{S}_y^T \delta \mathbf{x}$   
where  $\mathbf{S}_y$  is sensitivity matrix  $\partial y / \partial \mathbf{x}$
- Test predictive response of a single sample set for an ensemble of random sensitivity vectors  $\mathbf{S}_y$  :
  - ▶  $\mathbf{S}_y = N_d(0,1)$ ;  $\text{mean}(\mathbf{S}_y) = 0$  ,  $\text{var}(\mathbf{S}_y) = 1$
  - ▶ assume input  $\mathbf{x}$  distribution is uncorrelated, unit-variance  $d$ -dimen. normal distribution,  $N_d(0,1)$ ;  $\mathbf{C}_x = \mathbf{1}$
  - ▶ then expect:  $\text{mean}(\mathbf{y}) = 0$  ,  $\text{var}(\mathbf{y}) = 1$
- Plots show CVT (blue) predicts mean and standard deviation of predictive distribution more accurately than random Monte Carlo (red)



# Neutron cross sections

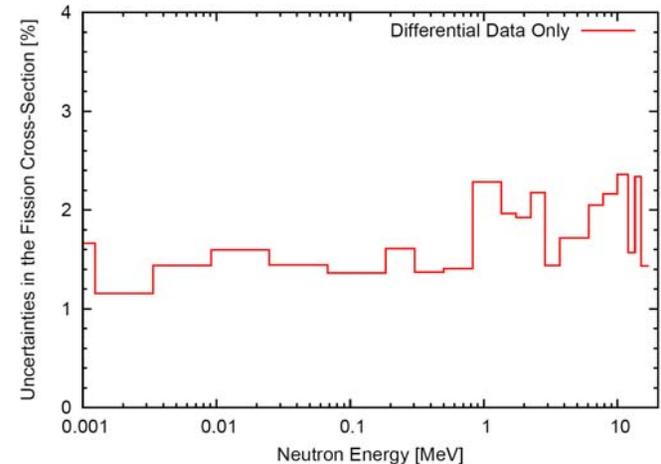
- Plot shows
  - ▶ measured fission cross sections for neutrons on  $^{239}\text{Pu}$ ; red data points
  - ▶ inferred cross sections; blue line
  - ▶ weighted average in 30 energy bins (groups); green histogram
- PARITSN code simulates neutron transport based on multigroup, discrete-ordinates method
  - ▶ uses 30 energy bins
  - ▶ calculates criticality for specified configuration of fissile-material
  - ▶ establish dependence of criticality experiment to cross sections



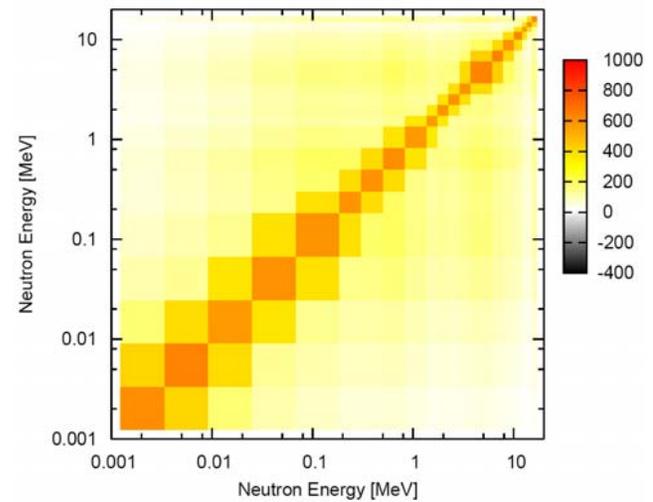
# Neutron cross sections - uncertainties

- Analysis of measured cross sections yields a set of evaluated cross sections
- Uncertainties in evaluated cross sections are  $\sim 1.4\text{-}2.4\%$
- Covariance matrix important
- Strong positive correlations caused by normalization uncertainties in each experiment

standard error in cross sections



correlation matrix

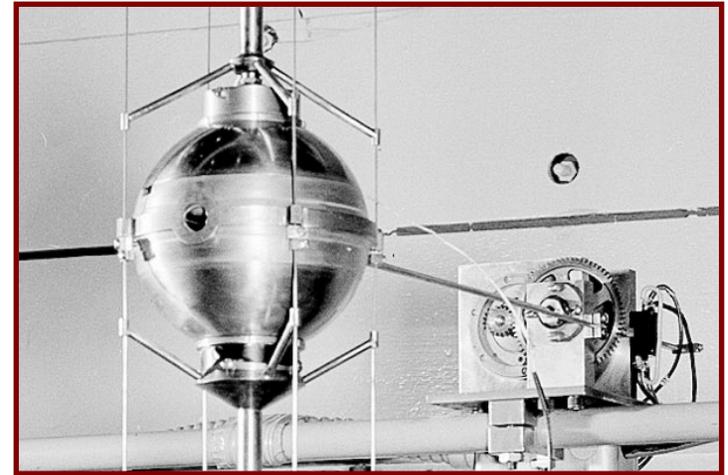


# JEZEBEL – criticality experiment

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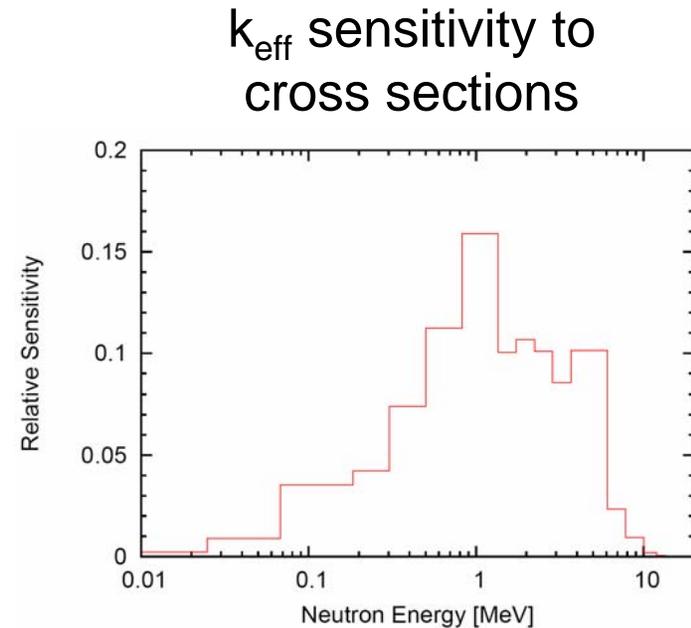
- JEZEBEL experiment (1950-60)
  - ▶ fissile material  $^{239}\text{Pu}$
  - ▶ measure neutron multiplication as function of separation of two hemispheres of material
  - ▶ summarize criticality with neutron multiplication factor,  $k_{\text{eff}} = 0.9980 \pm 0.0019$
  - ▶ very accurate measurement
- Our goal – use highly accurate JEZEBEL measurement to improve our knowledge of  $^{239}\text{Pu}$  cross sections

JEZEBEL set up



# JEZEBEL – sensitivity analysis

- PARITSN code relates  $k_{\text{eff}}$  to neutron cross sections
- Sensitivity of  $k_{\text{eff}}$  to cross sections found by perturbing cross section in each energy bin by 1% and observing increase in  $k_{\text{eff}}$
- Observe that 1% increase in all cross sections results in 1% increase in  $k_{\text{eff}}$ , as expected



# Bayesian update

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- For data linearly related to the parameters, the Bayesian (aka Kalman) update is

$$\mathbf{C}_1^{-1} \mathbf{x}_1 = \mathbf{C}_0^{-1} \mathbf{x}_0 + \mathbf{S}_y^T \mathbf{C}_y^{-1} \mathbf{S}_y (\mathbf{y} - \mathbf{y}_0)$$

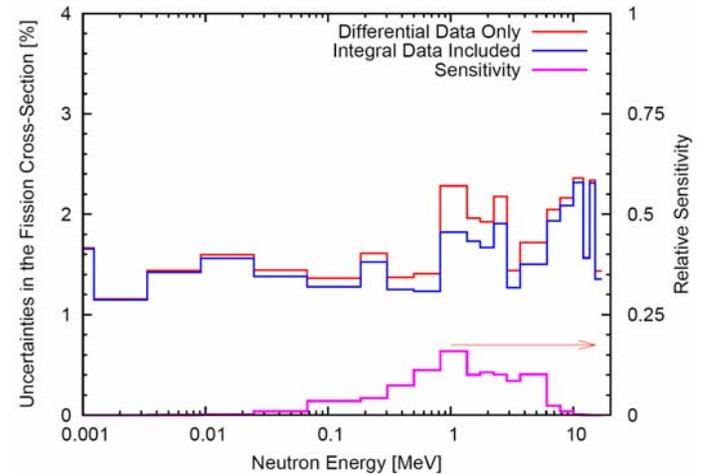
$$\mathbf{C}_1^{-1} = \mathbf{C}_0^{-1} + \mathbf{S}_y^T \mathbf{C}_y^{-1} \mathbf{S}_y$$

- ▶  $\mathbf{x}_0$  and  $\mathbf{x}_1$  are parameter vectors before and after update
  - ▶  $\mathbf{C}_0$  and  $\mathbf{C}_1$  are their covariance matrices
  - ▶  $\mathbf{y}$  and  $\mathbf{C}_y$  are the measured data vector and its covariance
  - ▶  $\mathbf{y}_0$  is the value of  $\mathbf{y}$  for  $\mathbf{x}_0$
  - ▶  $\mathbf{S}_y$  is the matrix of the sensitivity of  $\mathbf{y}$  to  $\mathbf{x}$ ;  $\partial \mathbf{y} / \partial \mathbf{x}$
- For the JEZEBEL case,  $\mathbf{y}$  is a scalar ( $k_{\text{eff}}$ ),  $\mathbf{C}_y$  is a scalar (variance), and  $\mathbf{S}_y$  is a vector

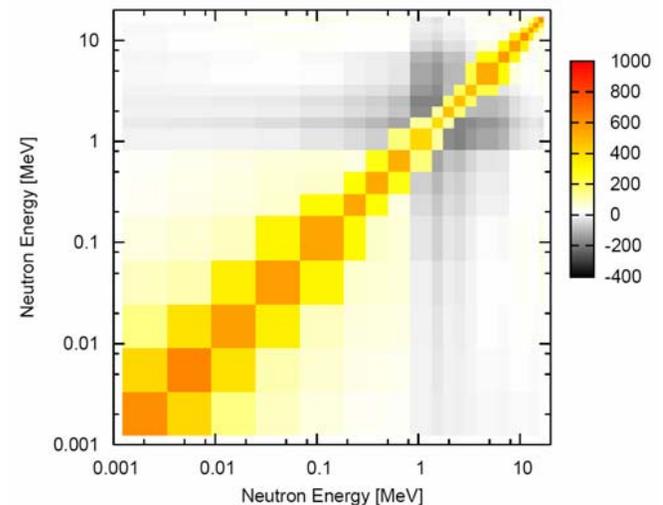
# Updated cross sections

- Plot shows uncertainties in cross sections before and after using JEZEBEL measurement
- Modest reduction in uncertainties; follows energy dependence of sensitivity
- Correlation matrix is significantly altered
- Strong negative correlations introduced by integral constraint of matching JEZEBEL's  $k_{\text{eff}}$

standard error in cross sections



correlation matrix



# Uncertainty in subsequent simulations

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- Intend to use updated cross sections in new calculations, with expectation that integral constraint will reduce uncertainties
- Next, demonstrate use of Monte Carlo sampling for estimating the uncertainty in new predictions; use random MC or qMC?
- Demonstrate usefulness of quasi-MC in form of CVT point sets by “predicting”  $k_{\text{eff}}$  measured in JEZEBEL
  - ▶ for this demo, assume linear model with known sensitivity vector
  - ▶ under these assumptions, we can calculate exact answer and compare to MC-style sampling to obtain predictive distribution
- For new physical scenario, we would not have sensitivity vector and we would have to do full simulation calculation, so only a modest number of function evaluations can be done

# Rotation matrix in high dimensions

- Given unit vectors  $\mathbf{a}$  and  $\mathbf{b}$ , want rotation matrix that map  $\mathbf{a}$  into  $\mathbf{b}$
- Algorithm (thanks to Mike Fitzpatrick)

- ▶ for matrix  $\mathbf{M}_1 = (\mathbf{a}; \mathbf{b})^T$

- ▶ Singular Value Decomposition (SVD) of:

$$\mathbf{M}_1 = \mathbf{U}\Sigma\mathbf{V}^T$$

- ▶ the bases of the subspace orthogonal to  $\mathbf{a}$  and  $\mathbf{b}$  are given by singular vectors in  $\mathbf{U}$ , except for first two

- ▶ then, do SVD on outer product matrix  $\mathbf{M}_2 = \mathbf{B}\mathbf{A}^T$

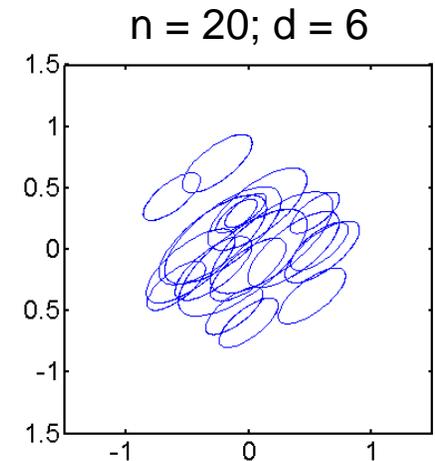
$$\mathbf{A} = (\mathbf{a}; \mathbf{u}^3; \mathbf{u}^4; \dots; \mathbf{u}^d)^T; \quad \mathbf{B} = (\mathbf{b}; \mathbf{u}^3; \mathbf{u}^4; \dots; \mathbf{u}^d)^T$$

- ▶ rotation matrix is  $\mathbf{R} = \mathbf{U}_2 \mathbf{D} \mathbf{V}_2^T$

where  $\mathbf{D}$  is identity matrix, except  $[\mathbf{D}]_{dd} = \det(\mathbf{U}_2 \mathbf{V}_2^T)$

- Random rotations – randomly choose directions of  $\mathbf{a}$  and  $\mathbf{b}$

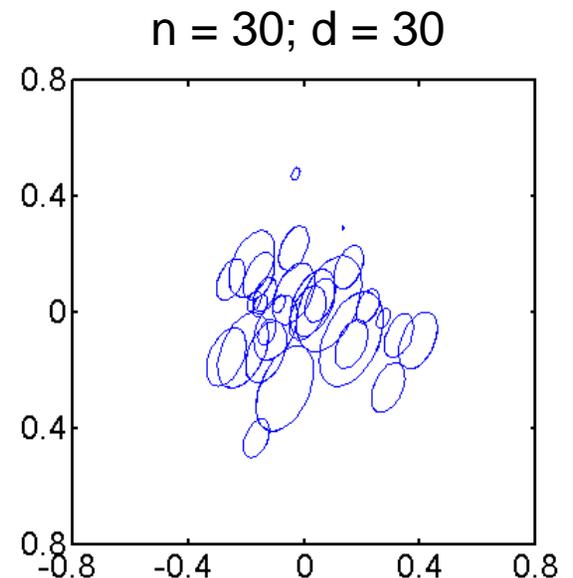
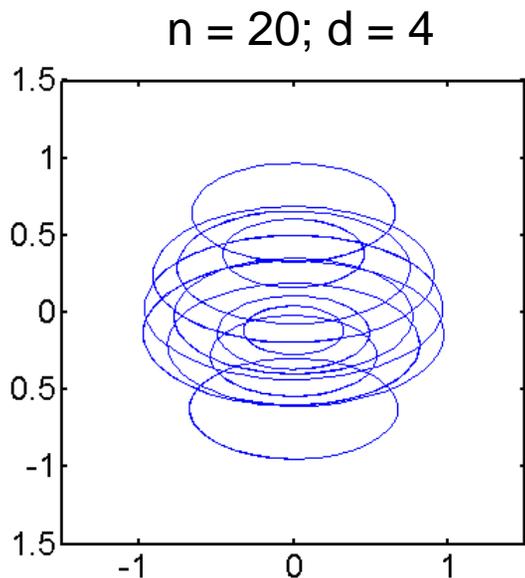
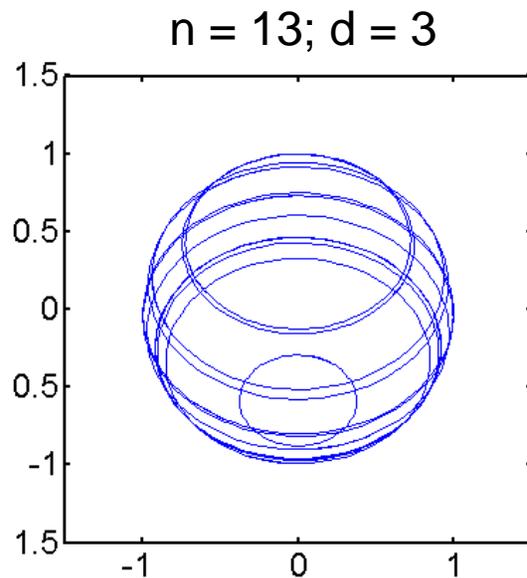
- ▶ simple algorithm: randomly draw vector from normal distribution and normalize it to unit length



# Examples of rotations in high dimensions

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- Random rotations in various dimensions
- All points have unit radius (on surface of unit hypersphere)



# Sampling from correlated normal distribution

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- Want to draw samples from multi-variate normal distribution with known covariance  $\mathbf{C}_x$
- Important to include correlations among uncertainties, i.e., off-diagonal elements
- Algorithm:
  - ▶ perform eigenanalysis of covariance matrix of  $d$  dimensions

$$\mathbf{C}_x = \mathbf{U}\mathbf{\Lambda}\mathbf{U}^T$$

where  $\mathbf{U}$  is orthogonal matrix of eigenvectors and  
 $\mathbf{\Lambda}$  is the diagonal matrix of eigenvalues

- ▶ draw  $d$  samples from unit variance normal distribution,  $\xi_i$
- ▶ scale this vector by  $\lambda_i^{1/2}$
- ▶ transform vector into parameter space using the eigenvector matrix
- ▶ to summarize:  $\mathbf{x} = \mathbf{U}\mathbf{\Lambda}^{1/2}\boldsymbol{\xi}$

# Accuracy of predicted $k_{\text{eff}}$ and its uncertainty

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- Check accuracy of predicted mean and standard deviation based on 30 samples; CVT vs. random sample sets
  - ▶ exact value from known sensitivity and linear model
- Conclude – CVT is more accurate here than random sampling

**Results from 1000 sample sets; ‘rot’ indicates single sample set randomly rotated to achieve each new one**

	est. mean $k_{\text{eff}}$		est. std. dev. $k_{\text{eff}}$	
	avg.	rms dev.	avg.	rms dev.
random	0.99788	0.00037	0.00191	0.00028
random-rot	0.99824	0.00010	0.00218	0.00010
CVT-rot	0.99796	0.00001	0.00197	0.00002
exact-linear	0.99796	-	0.00195	-

# Summary

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- CVT sampling is useful in predictive sampling for obtaining higher accuracy for a limited number of simulations
- CVT and repulsive particle model may be used to generate QMC point sets
  - ▶ particularly useful for modest number of points

# Future work

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- Need a way to estimate accuracy of results, a problem common to all QMC approaches
- Important to learn to cope with under-sampling ( $n < d + 1$ )
  - ▶ a parameter subspace dependence is not sampled so some aspects of uncertainty in input parameters may be missed
  - ▶ satisfactory solution requires careful thought, taking into account what is known about the influence of input parameters on the simulation output
- Sequential generation of point sets
  - ▶ add additional points, keeping previous points fixed
- Adaptive sampling – improve estimate by importance sampling, i.e., increasing density of points in selected regions
- Employ advanced analysis of outputs produced by input samples
  - ▶ weighted Monte Carlo
  - ▶ characterize output response as function of inputs

# Future work

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- Semi-random-quasi-Monte Carlo
  - ▶ partially randomize quasi-Monte Carlo
  - ▶ strike balance between random and deterministic patterns
  - ▶ try to achieve the benefits of each approach

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