An Application of Uncertainty Quantification to MPM

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THE UNIVERSITY of NEW MEXICO

What is Uncertainty Quantification?

- Characterize the likely outcomes of a particular simulation scenario
- Example: for a Gaussian distribution of ultimate tensile strength, how often will this bar break?
- Yes: feasible
- Discover and control “known unknowns” and “unknown unknowns” - the Rumsfeld doctrine
- Example: UQ can compensate for my bad model.
- No: garbage-in, garbage-out still applies

Types of Uncertainty

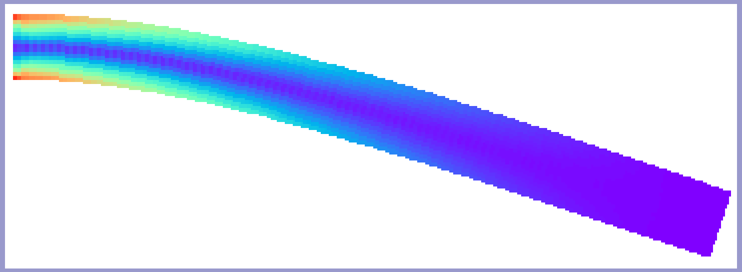
Aleatoric

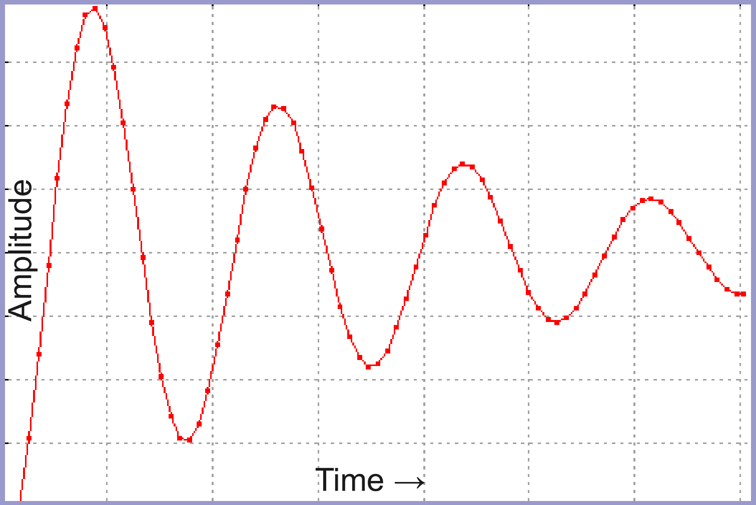
- Not reducible
- Example: natural fluctuations of air temperature or soil composition
- The air or soil cannot be improved

Epistemic

- Is reducible
- Example: a cheap thermometer with scatter and bias.
- Buy a better thermometer

Vibration of a cantilever beam modeled with MPM





<u>Inputs</u>

- Young's modulus
- Poisson's ratio
- Density
- Length
- Thickness
- CFL

<u>Outputs</u>

- Amplitude A
- Decay σ
- Frequency ω
- Phase Φ

$$A e^{-\sigma t} \cos(\omega t + \phi)$$

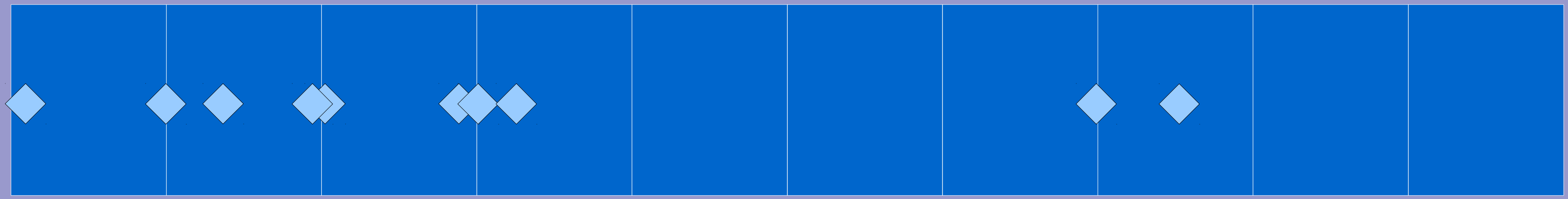
UQ methods

- Random: choose inputs randomly from a range; samples=thousands
- Latin Hypercube Sampling (LHS): to be described; samples=hundreds
- Response Surface: choose samples from Smolyak or factorial schemes; samples=tens-hundreds
- Stochastic Galerkin: add extra uncertainty dimension to the solution space via operator overloading; samples=one

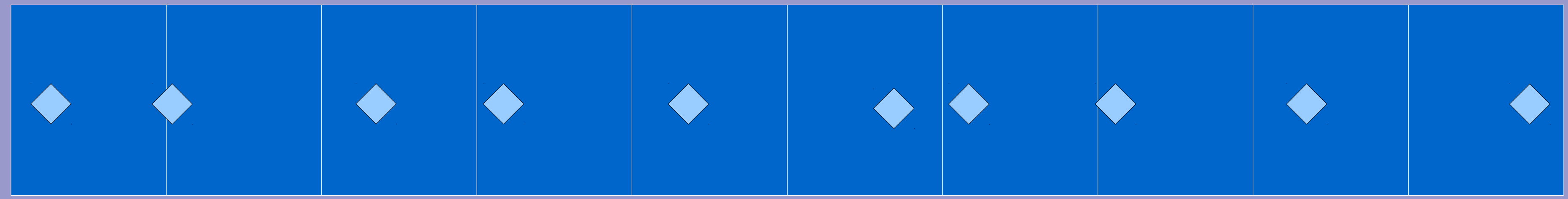
Response Surface methods may suffer from curse of dimensionality; sampling methods less so.

Latin Hypercube Sampling (LHS)

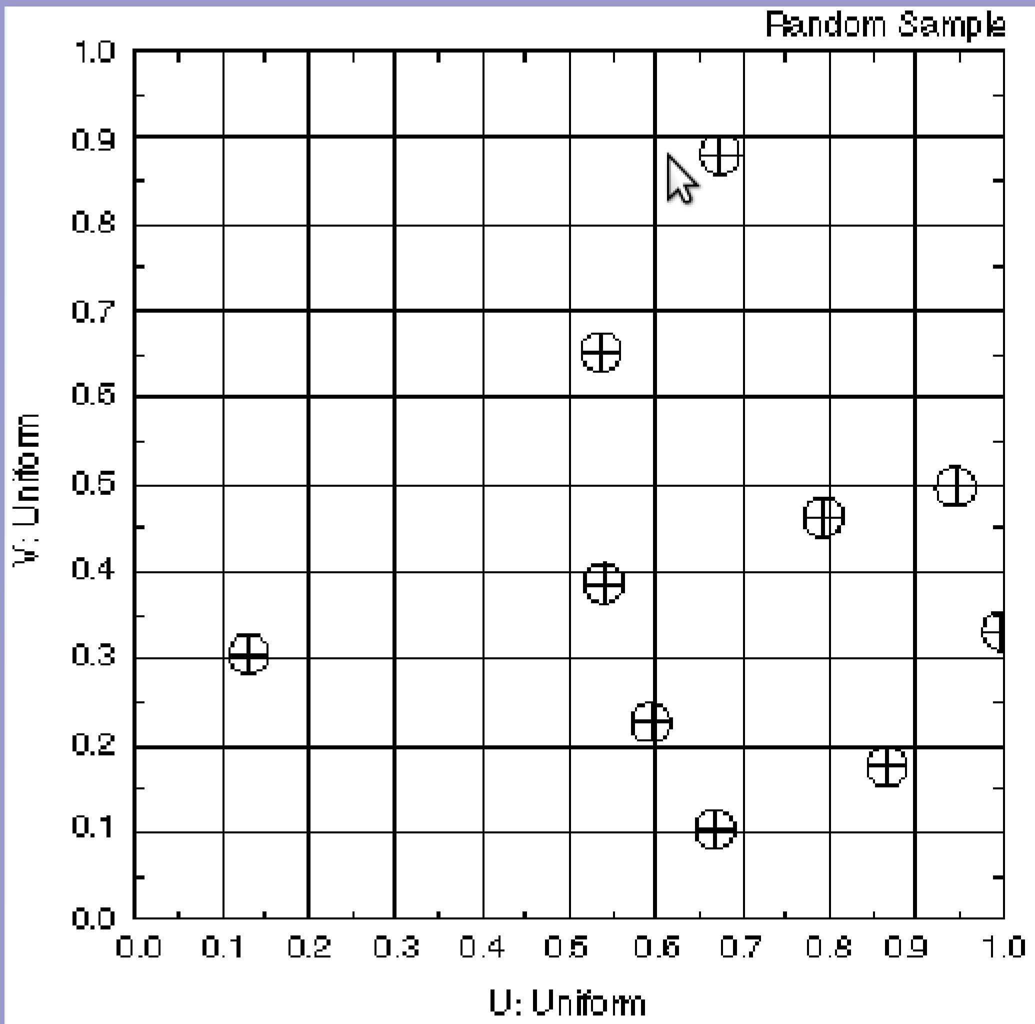
- Consider ten random samples within a range:

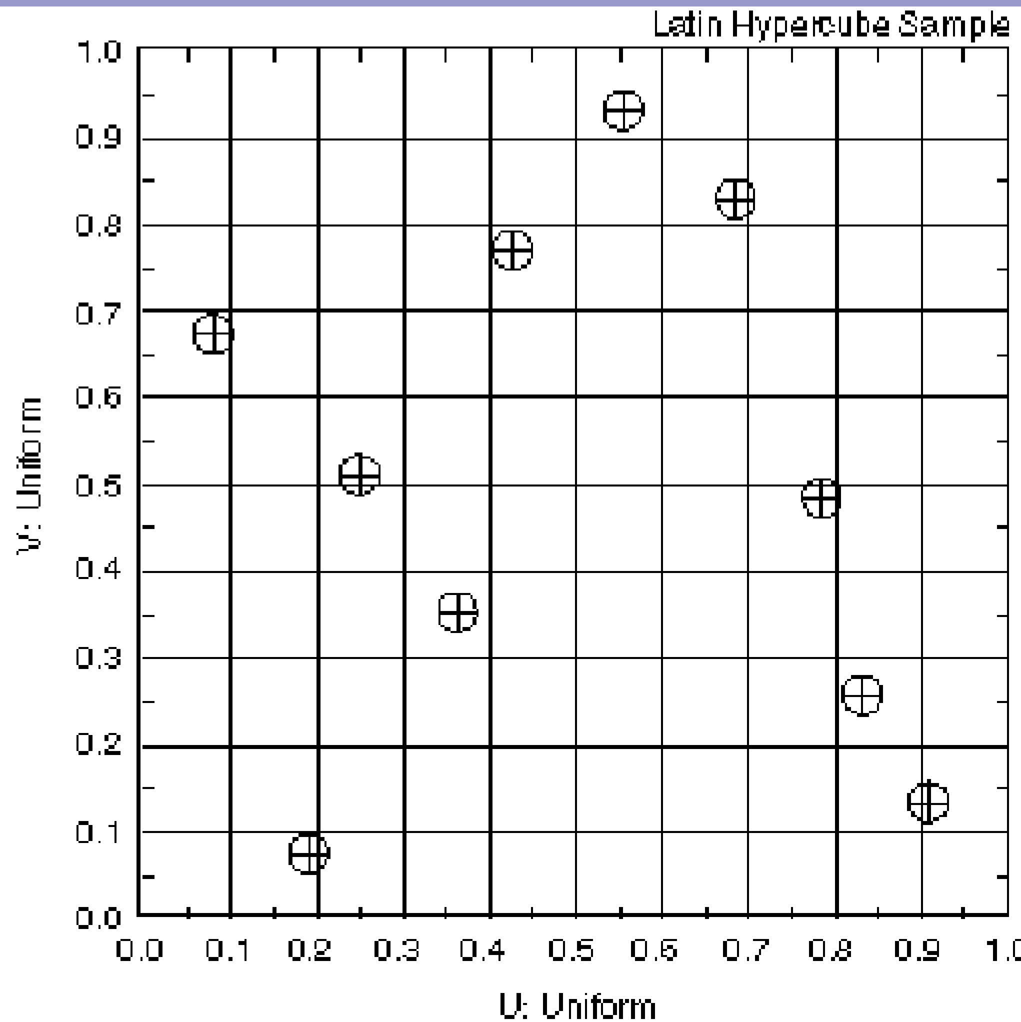


- Unsatisfying sample set due to gaps and clusters
- Now restrict each random sample to fall within a sub-interval:



2D sample space





Gaps and clusters

Every interval has a sample

Jon C. Helton and Cedric J. Sallaberry, lecture notes, 2010, Sandia National Laboratory and the University of New Mexico

Extend to N dimensions

- Choose number of samples M
- For each of the N inputs (six in our cantilever beam example) define a range with M intervals and an array with M elements
- Randomly choose a value that falls within each interval and store in the array
- Shuffle the elements of each input array randomly and differently
- Select first element of each input array – this is your first sample. Similarly for M samples.

Run the samples

Sampling methods are embarrassingly parallel

End up with six input arrays and four output arrays of N samples each

How can we analyze the data and find useful information?

Output Analysis with R

The (free) R language and statistics package:

http://www.r-project.org/

Form a correlation matrix:

as.dist(cor(uq))

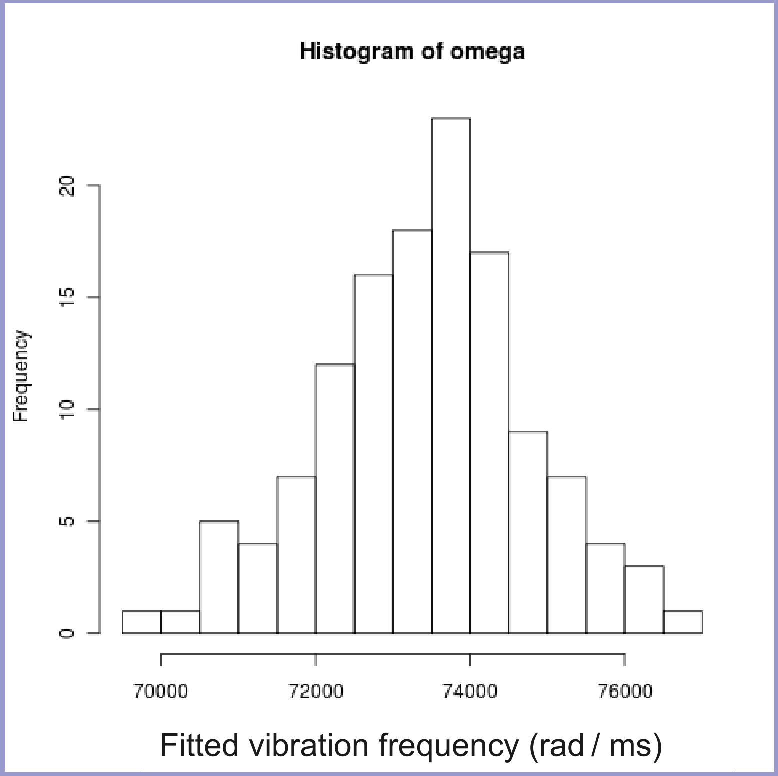
	Ymod	dens	pois	beamH	beamL	CFL	amp	sigma	omega
dens	0.03								
pois	-0.02	0.02							
beamH	-0.00	0.00	-0.02						
beamL	-0.20	-0.05	-0.12	-0.07					
CFL	0.03	0.11	0.04	-0.01	0.09				
amp	0.03	0.10	0.07	0.51	-0.19	0.01			
sigma	0.12	-0.01	-0.43	0.54	-0.32	-0.15	-0.09		
omega	0.41	-0.25	0.13	0.61	-0.69	-0.08	0.43	0.49	
Phi	-0.13	-0.06	0.23	-0.63	0.23	-0.27	-0.39	-0.64	-0.51

Ymod: Young's modulus
Dens: Density
Pois: Poisson's ratio
BeamH: Beam thickness
BeamL: Beam length
CFL: Critical time step ratio
Amp: Fitted vibration amplitude
Sigma: Fitted decay
Omega: Fitted vibration frequency
Phi: Fitted phase shift

Consider the strongest correlations

Typical Results

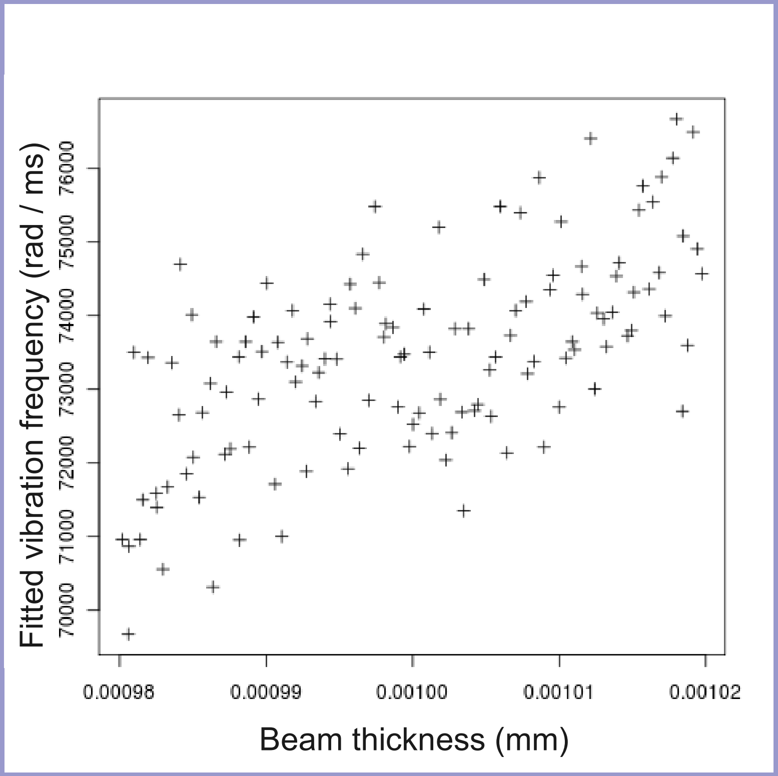
Observed output: Probability Distributions (4 histograms)



png("hist_omega.png")
plot(hist(omega,breaks=12))

No surprise here – the output is clustered around a “popular” value

Input/output correlations (45 scatter plots)

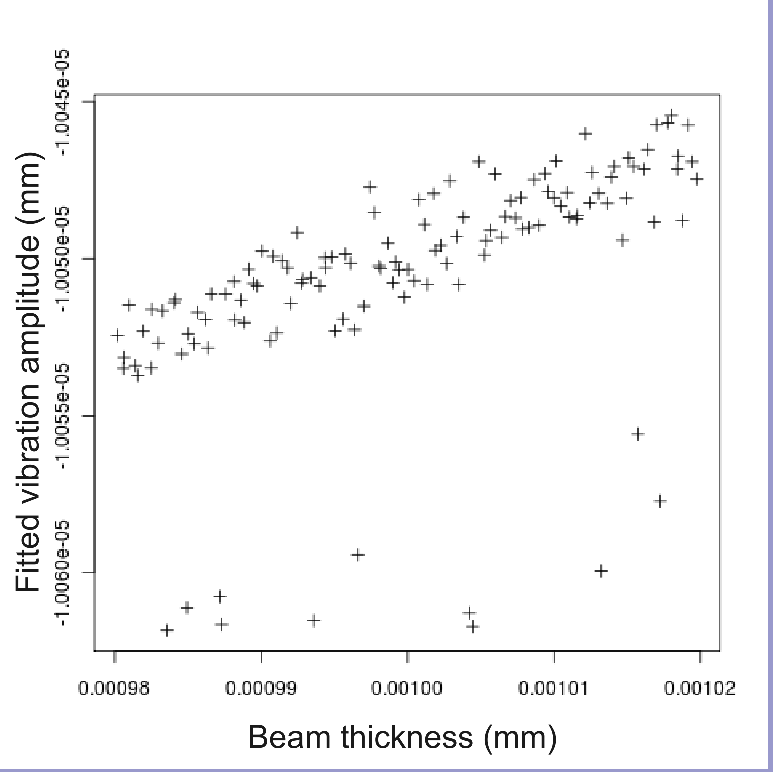


png("corr_beamH-omega.png")
plot(beamH,omega,pch=3)

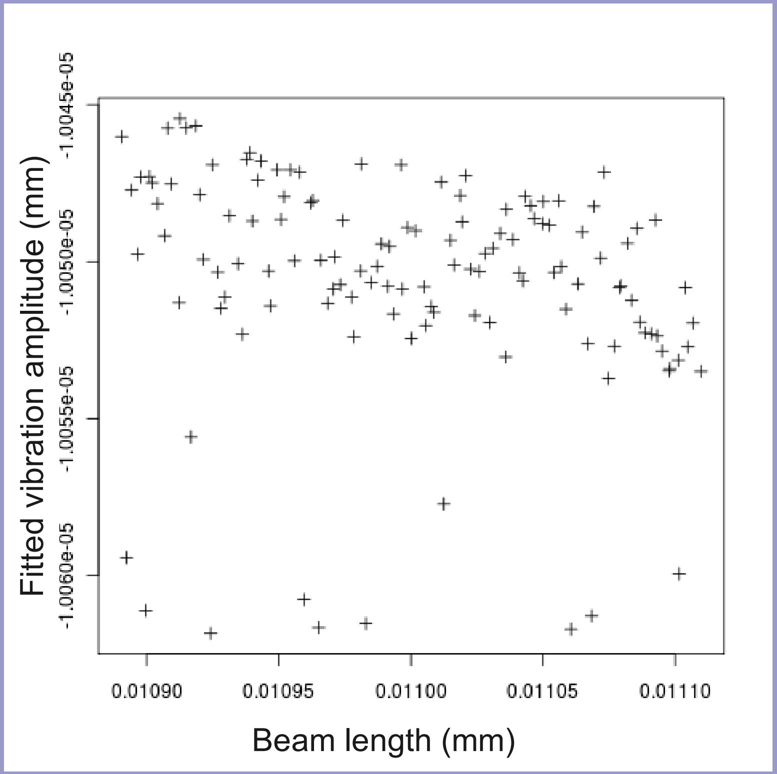
A thicker beam vibrates faster – did we really need all this UQ just to explain the obvious?

Pop Quiz:

Vibration amplitude with respect to beam thickness



Vibration amplitude with respect to beam length



Is anything unexpected?

Code Mistake

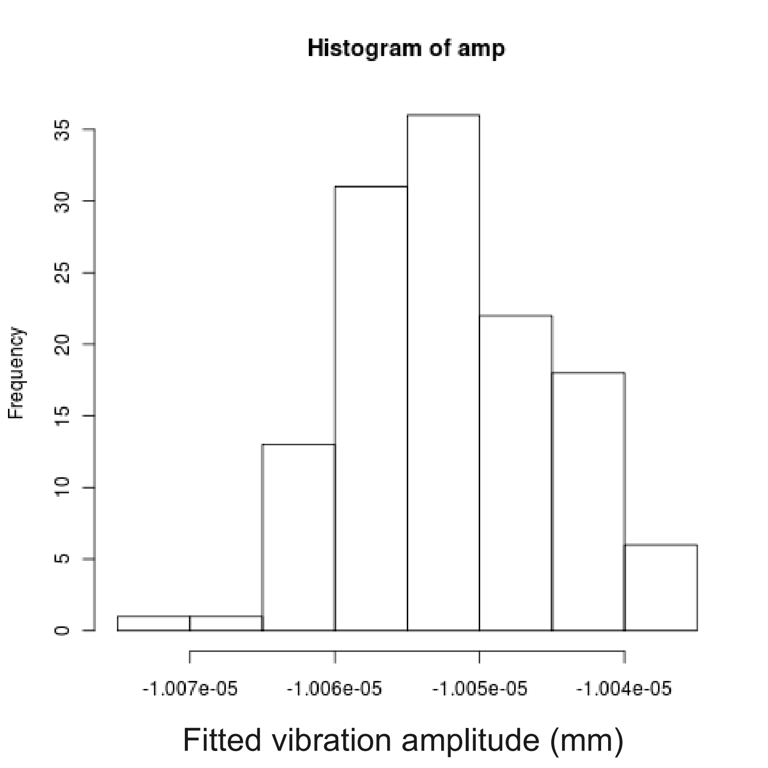
Improper use of the ceiling function:

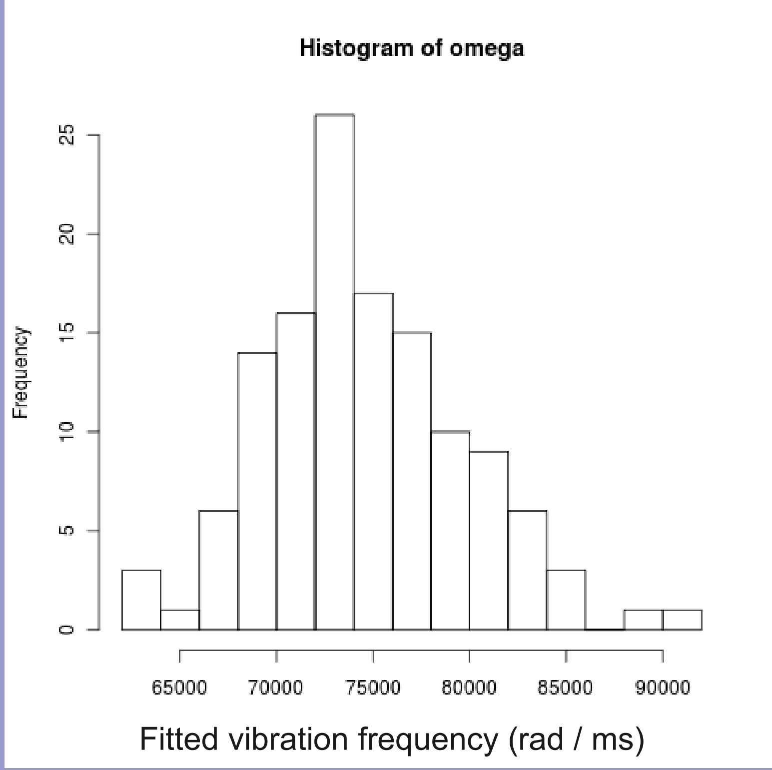
```
const int nx=int(ceil((e.x-b.x)/(pch.dx/ppe.x)));
const int ny=int(ceil((e.y-b.y)/(pch.dy/ppe.y)));
const int nz=int(ceil((e.z-b.z)/(pch.dz/ppe.z)));
```

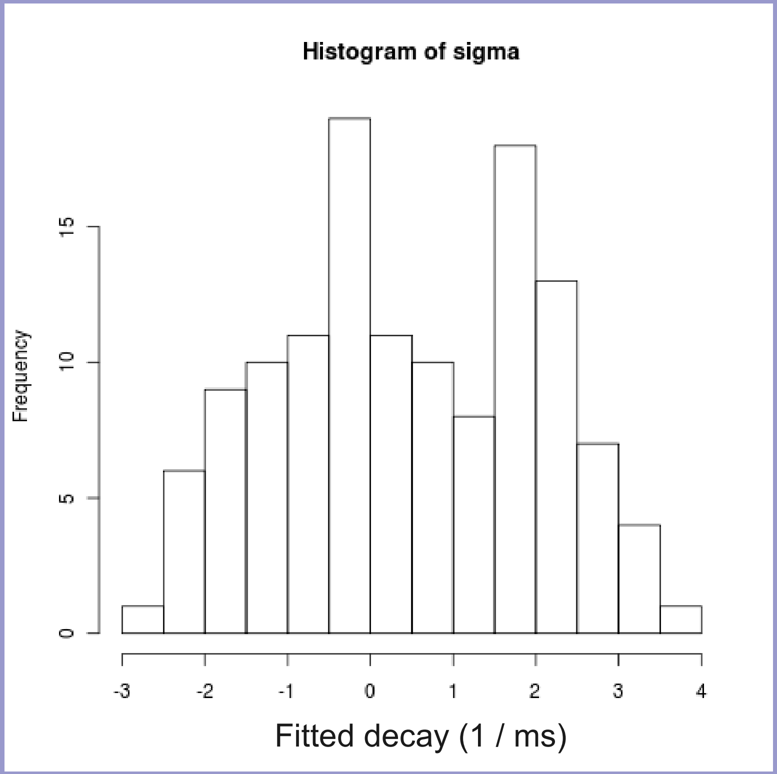
Should be:

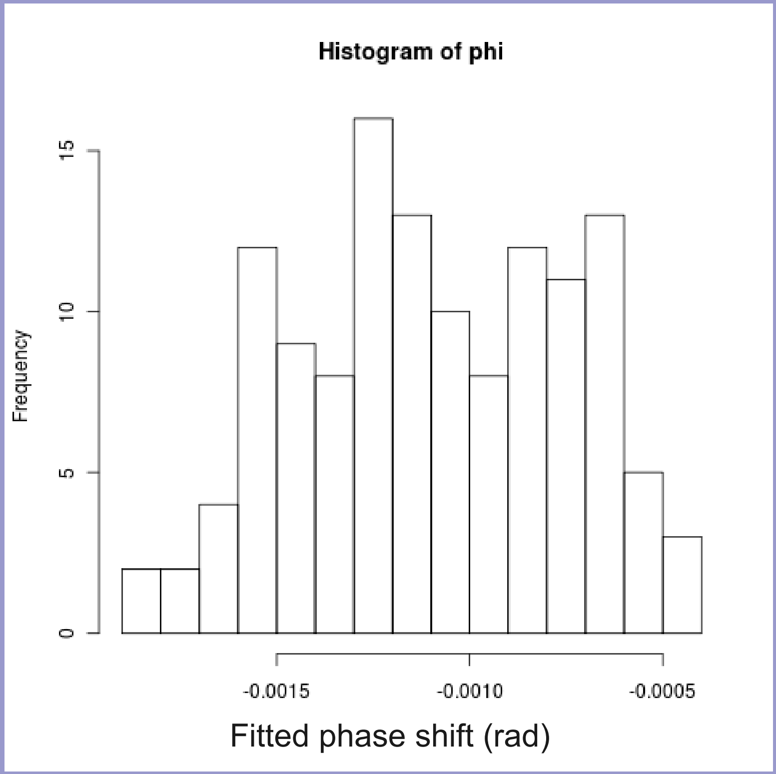
```
const int nx=int(round((e.x-b.x)/(pch.dx/ppe.x)));
const int ny=int(round((e.y-b.y)/(pch.dy/ppe.y)));
const int nz=int(round((e.z-b.z)/(pch.dz/ppe.z)));
```

Fix the mistake and run the samples again.
Generate the corrected correlation matrix.


Histogram of amp
Frequency
0
5
10
15
20
25
30
35
-1.007e-05
-1.006e-05
-1.005e-05
-1.004e-05
Fitted vibration amplitude (mm)

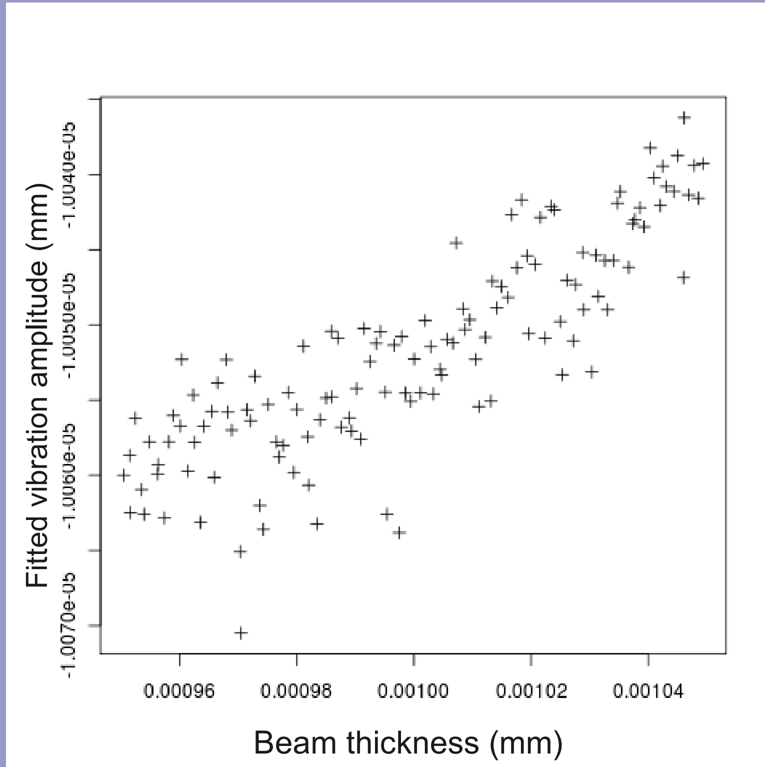

Histogram of omega
Frequency
0
5
10
15
20
25
65000
70000
75000
80000
85000
90000
Fitted vibration frequency (rad / ms)

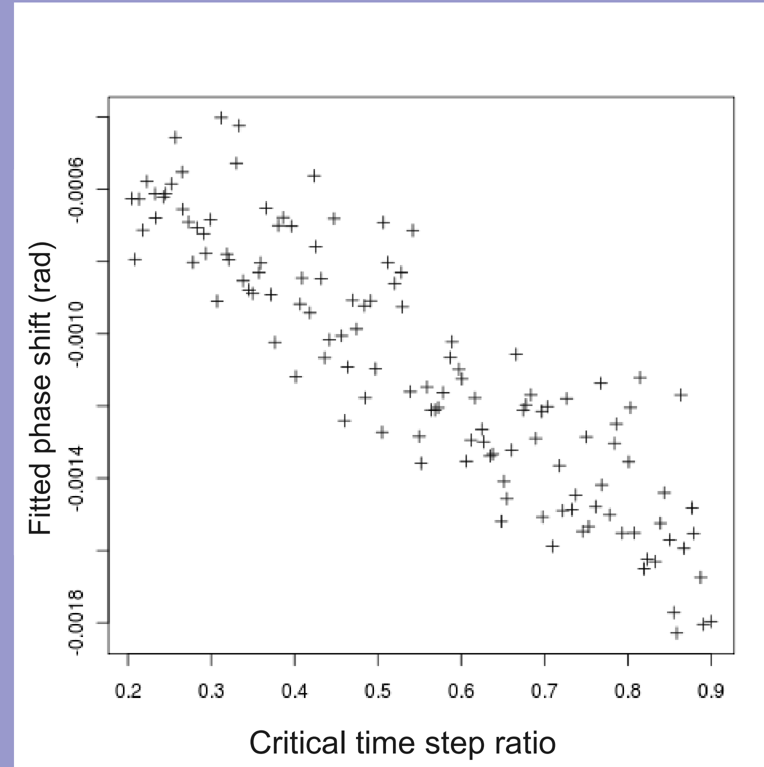

Histogram of sigma
Frequency
0
5
10
15
-3
-2
-1
0
1
2
3
4
Fitted decay (1 / ms)


Histogram of phi
Frequency
0
5
10
15
-0.0015
-0.0010
-0.0005
Fitted phase shift (rad)

.85

Tiny amplitude error related to beam thickness



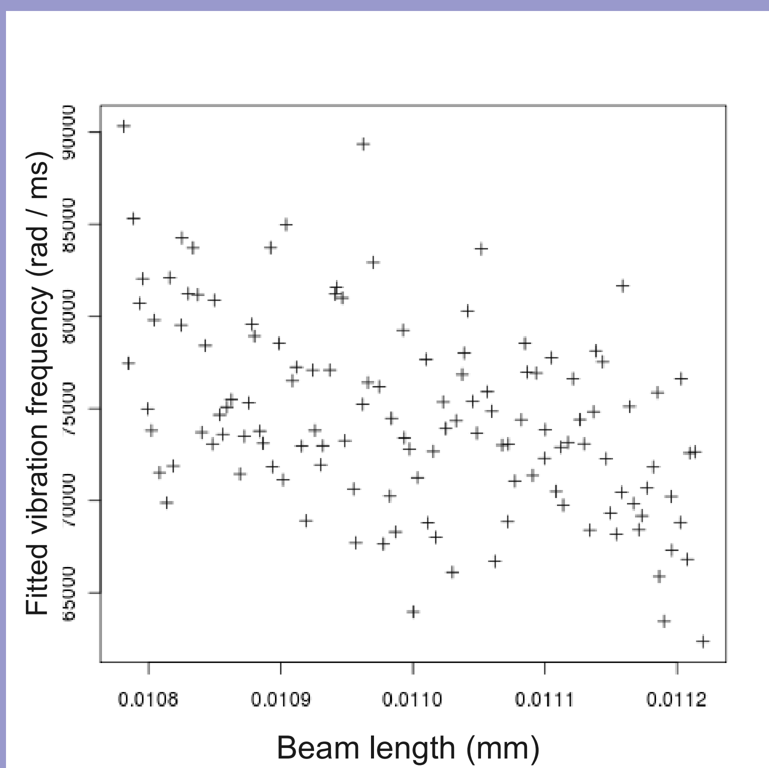


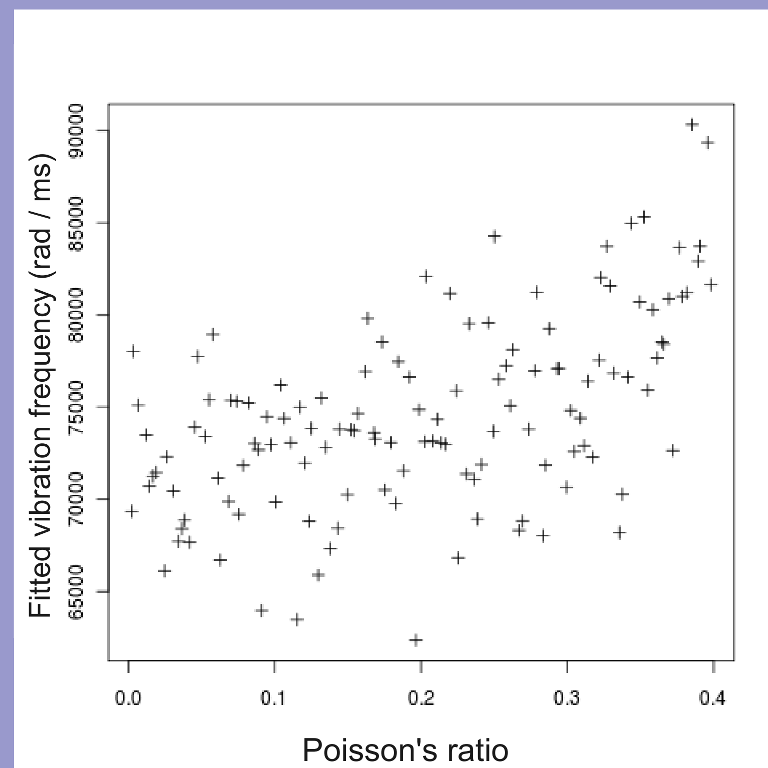
-.89

Significant phase shift due to CFL – new information

-.46

Expected frequency change related to beam length





.53

Major frequency change related to Poisson's ratio – new information

References

- J.C. Helton, F.J. Davis “Latin hypercube sampling and the propagation of uncertainty in analyses of complex systems”
- J.C. Helton, J.D. Johnson, C.J. Sallaberry, C.B. Storlie “Survey of sampling-based methods for uncertainty and sensitivity analysis” Reliability Engineering and System Safety 91 (2006) 1175–1209
- Dongbin Xiu “Fast Numerical Methods for Stochastic Computations: A Review” Communications in Computational Physics, Vol. 5, No. 2-4, 242-272
- P. J. Roache “Quantification of Uncertainty in Computational Fluid Dynamics” Annu. Rev. Fluid. Mech. 1997, 29:123-60

Acknowledgements

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```
# UQ for a cantilever in MPM
# run as: R -f thisFile.R

# Import the ten columns of data; each starts with a header label
uq = as.data.frame(read.table(file("mydata"),header=T))

options(width=200) # wider screen for correlation matrix
as.dist(cor(uq)) # form the correlation matrix

# name each column, just for convenience
Ymod=uq[,1]
dens=uq[,2]
pois=uq[,3]
beamH=uq[,4]
beamL=uq[,5]
CFL=uq[,6]
amp=uq[,7]
sigma=uq[,8]
omega=uq[,9]
phi=uq[,10]

png("density_omega.png")
plot(density(omega))

png("hist_omega.png")
plot(hist(omega,breaks=12))

png("corr_beamH-omega.png")
plot(beamH,omega,pch=3)
```