On Spherical Harmonics Based Numerical Quadrature Over the Surface of a Sphere

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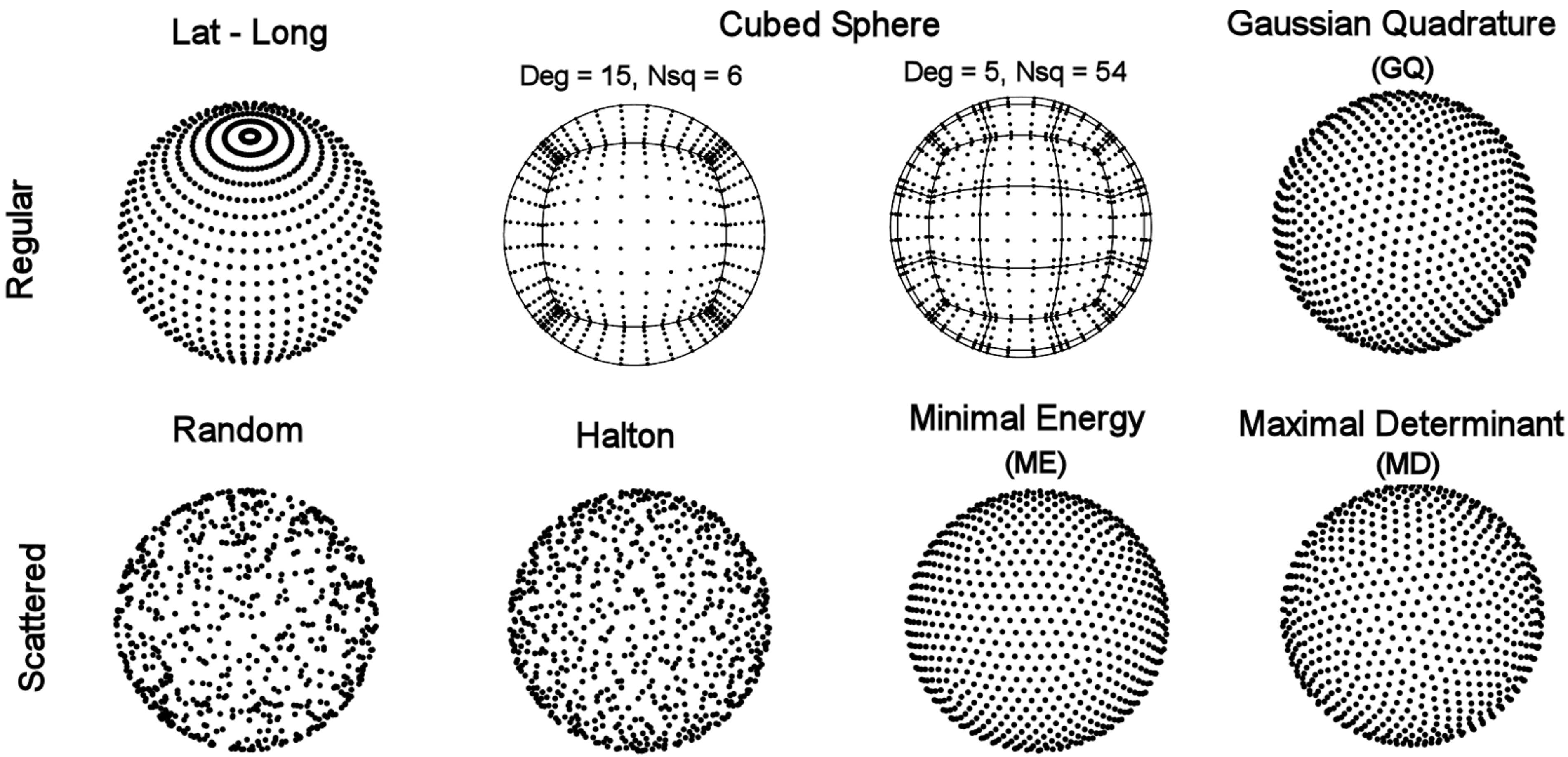
Examples of node layouts over the surface of a sphere



Choice normally dictated by the preferred PDE solution strategy

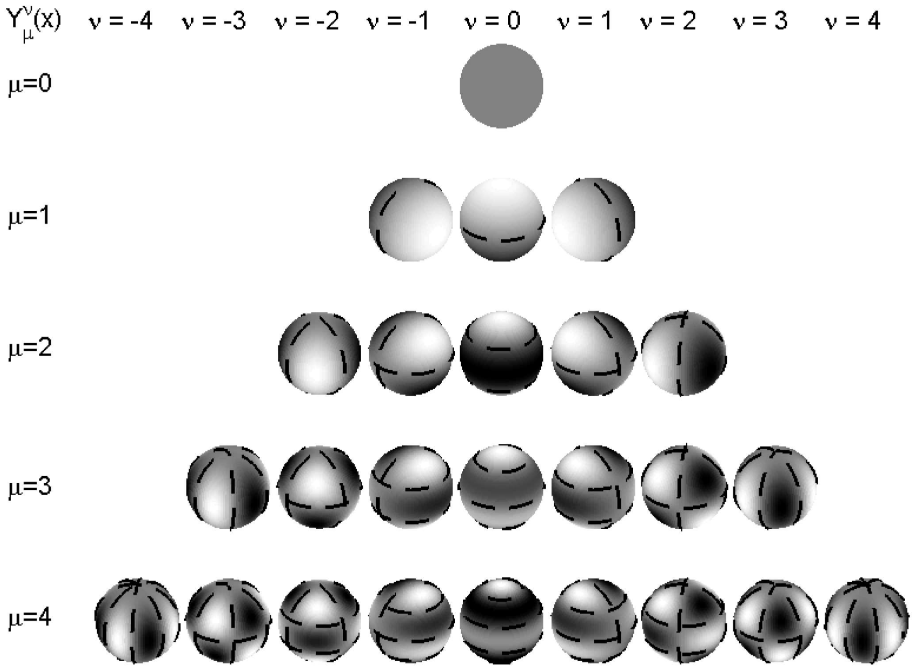
Questions:

1. **How accurately can quadrature be carried out if data is available only at these sets of nodes?**

2. **What is a practical procedure to obtain quadrature weights w_i at the individual node locations x_i such that $\iint f\, dS = \sum w_i f_i$ becomes a good approximation for as high degree spherical harmonic (SPH) functions as possible?**

Without spatial discretization: Continuous functions over the sphere

Any continuous function can be expanded in Spherical Harmonics



$\Leftarrow \quad \iint Y_0^0(\underline{x})\, dS = 1$

$\Leftarrow \quad \iint Y_\mu^\nu(\underline{x})\, dS = 0$ for all $\mu > 0,\ \nu = -\mu, \ldots, 0, \ldots, +\mu$

A general function $f(\underline{x})$ can be expanded

$$f(x) = \sum_{\mu=0}^{\infty} \sum_{\nu=-\mu}^{\mu} c_{\mu,\nu}\, Y_\mu^\nu(\underline{x})$$

To determine $\iint f\, dS$ is equivalent the coefficient $c_{0,0}$.

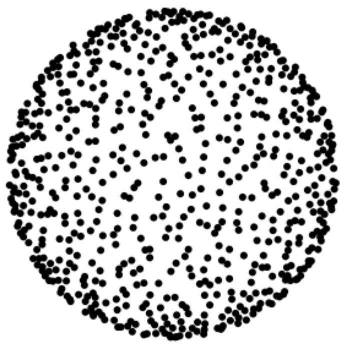
When the data is discrete in space:

Question: How well can the coefficient $c_{0,0}$ be 'pinned down' by the discrete data $f(x_i)$, available only at the node locations $x_i,\ i = 1, 2, \ldots, N$?

Extreme case: All nodes are placed along the equator. One cannot then distinguish even between Y_0^0 and Y_1^0.

How to obtain SPH coefficients from discrete data:

Interpolation:



The SPH expansion agrees with function values f_i at nodes $\underline{x}_i$ when

$$\sum_{\mu=0}^{\mu_{\max}} \sum_{\nu=-\mu}^{\mu} c_{\mu,\nu}\, Y_\mu^\nu(\underline{x}_i) = f(\underline{x}_i) \quad , \quad i=1,2,\ldots,N=(\mu_{\max}+1)^2$$

The SPH coefficients $c_{\mu,\nu}$ then follow from solving the square linear system

$$\begin{bmatrix} & & \\ & A & \\ & & \end{bmatrix}\begin{bmatrix} c_{0,0} \\ \vdots \\ \vdots \end{bmatrix} = \begin{bmatrix} f_1 \\ \vdots \\ f_n \end{bmatrix} \quad \Rightarrow \quad \begin{bmatrix} c_{0,0} \\ \vdots \\ \vdots \end{bmatrix} = \begin{bmatrix} & & \\ & A & \\ & & \end{bmatrix}^{-1}\begin{bmatrix} f_1 \\ \vdots \\ f_n \end{bmatrix}$$

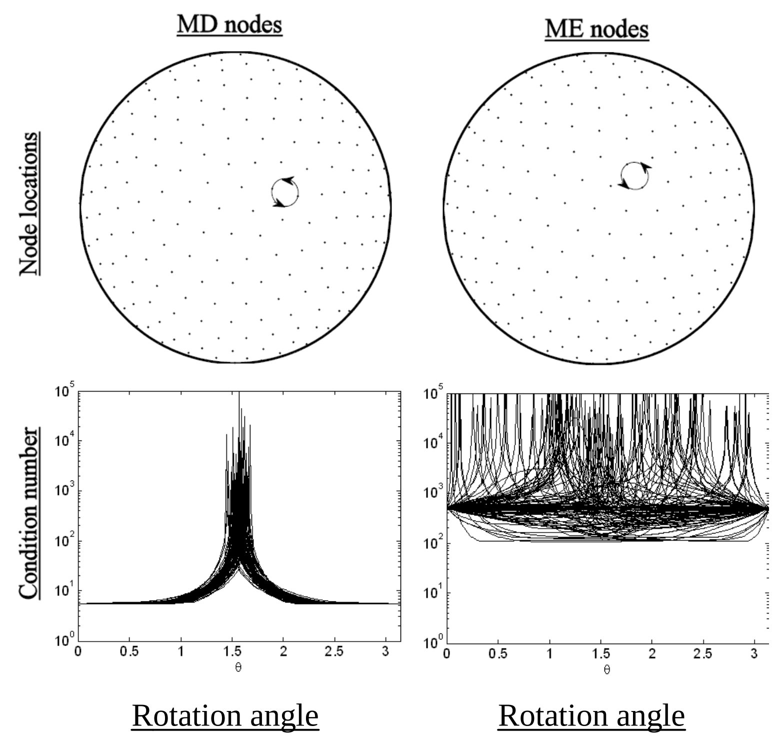
Since $c_{0,0} = \iint f\, dS$ and $\iint f\, dS = \sum w_i f_i$, we can read off the quadrature weights from the top row of A^{-1}.

Any problems with this?

Take any two nodes and move them so they end up interchanged. Two rows of the A-matrix have changed places, so its determinant has changed sign. It must have been zero somewhere in between.

Even 'innocent' looking node sets may be on the brink of singularity or extreme ill-conditioning.

MD sets are constructed - *at great computational expense* - to be as well conditioned as possible. ME nodes are just 'pushed away' from each other.

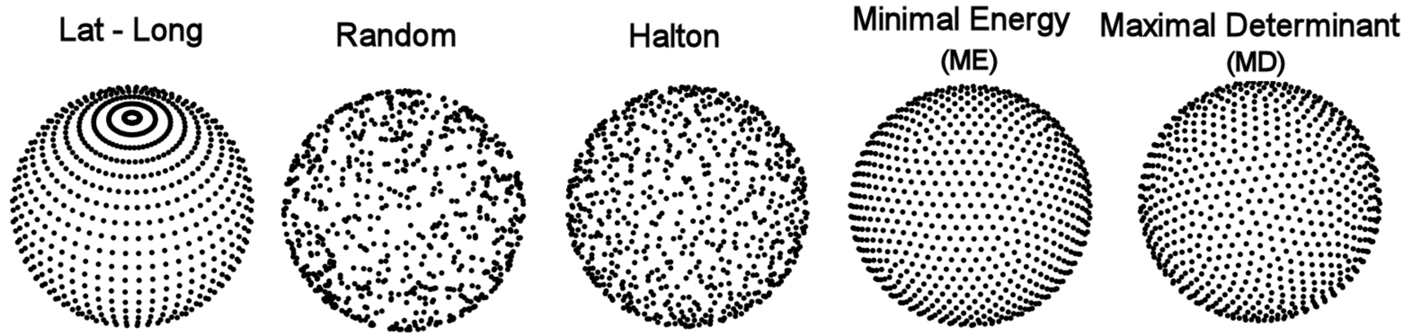


Present novelties:

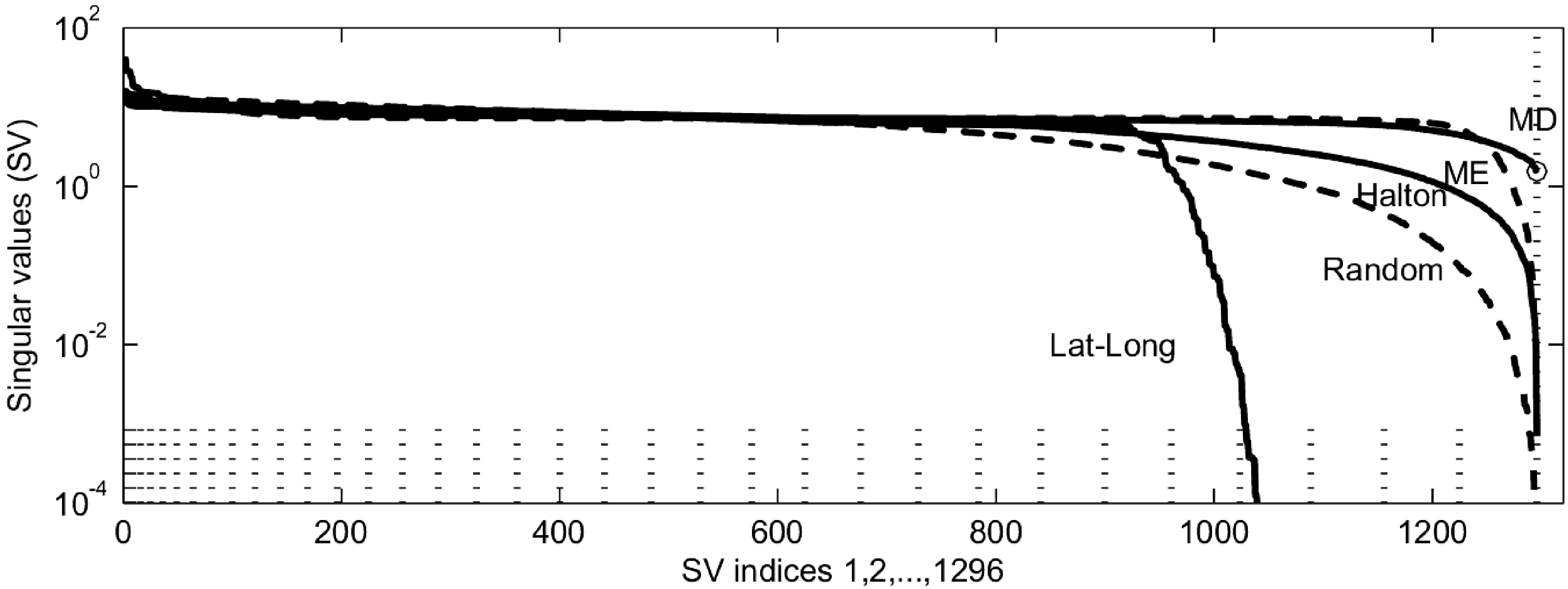
- This conditioning issue can be bypassed - ME nodes are every bit as good as MD nodes for quadrature.
- However, there are still genuine differences between the other types of node sets.

SVD factorization of the *A*-matrices for different node sets

Five of the node distributions, all with $N = 36^2 = 1296$ nodes:



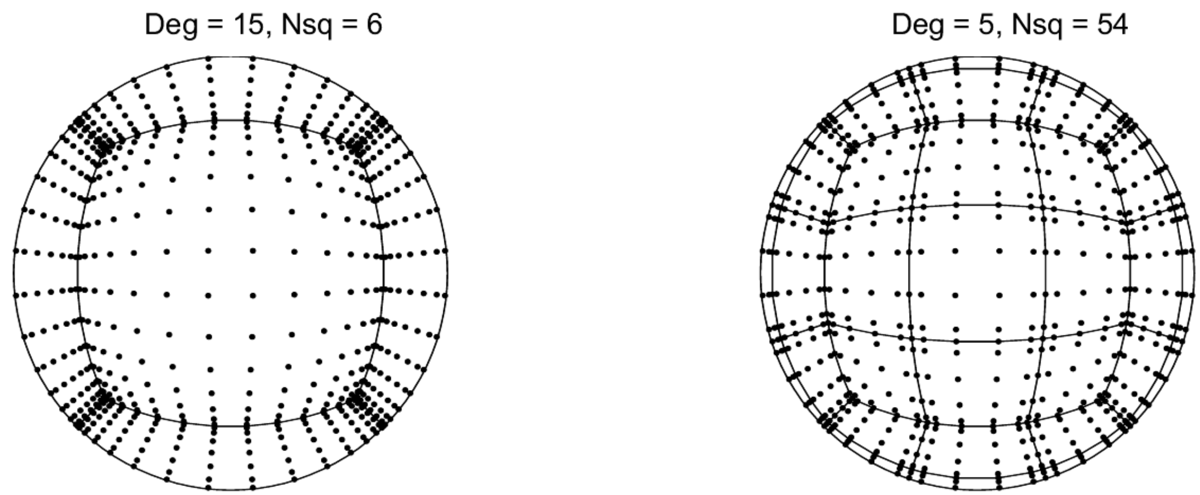
The size of the $N = 1296$ singular values of the corresponding *A*-matrices:

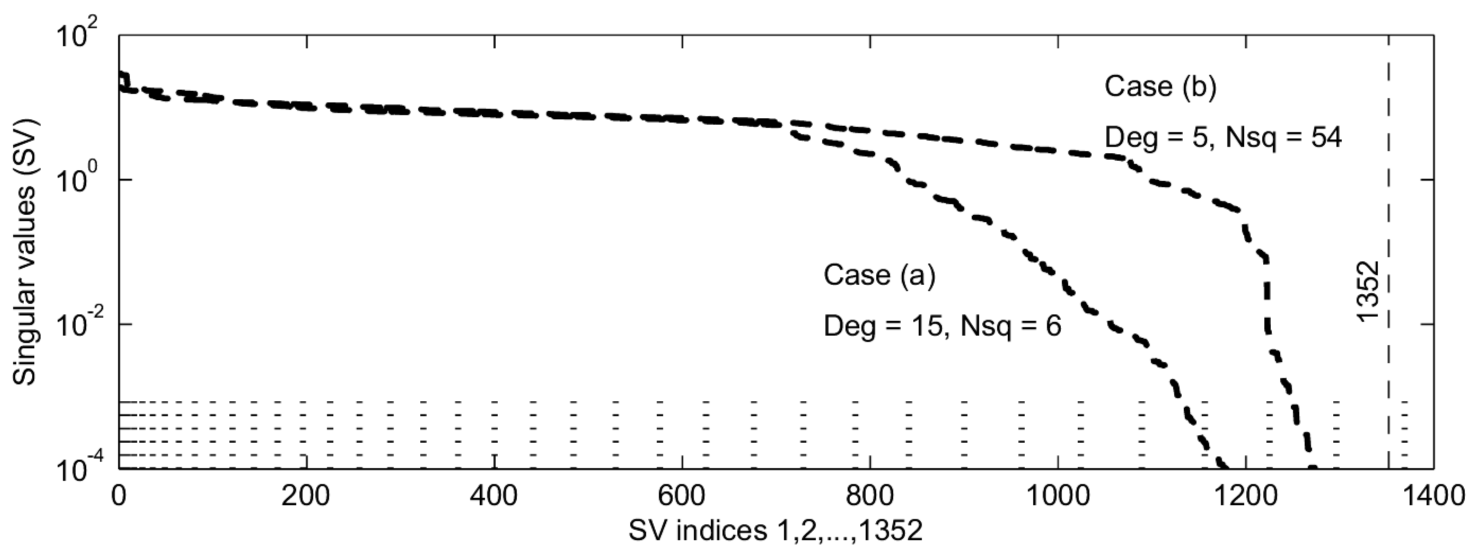


- The Lat-Long node set is incapable of distinguishing many of the SPHs from each other.
- If one omits very few of the last singular values ("pinv" instead of "inv" for *A*-martrix), the irregular node layouts fare a lot better, and ME doing just as well as ME.

SVD factorization of the *A*-matrices for Cubed Sphere node sets

Both cases shown have N = 1352 nodes



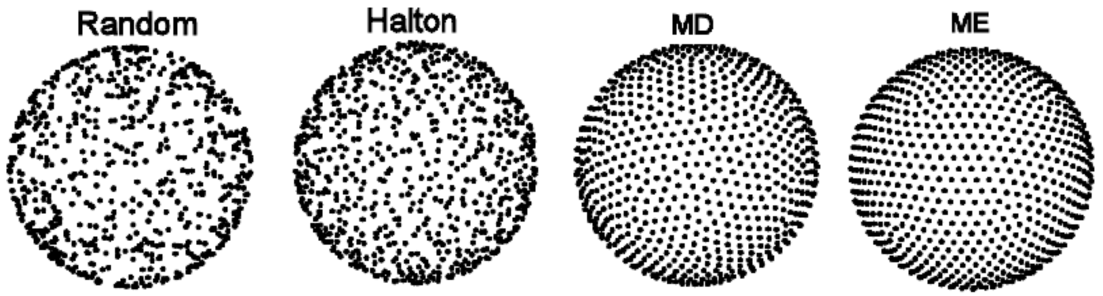


Conceptual reminiscence of Lat-Long;

Likely that both non-uniformity and lattice-like layout are disadvantages compared to quasi-uniform scattered node sets.

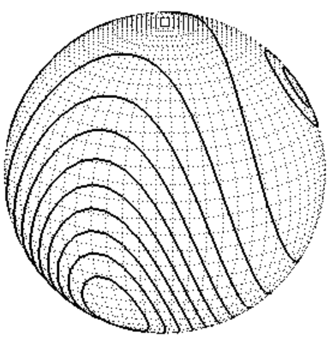
Quadrature errors when obtaining weights with *pinv* instead of *inv*

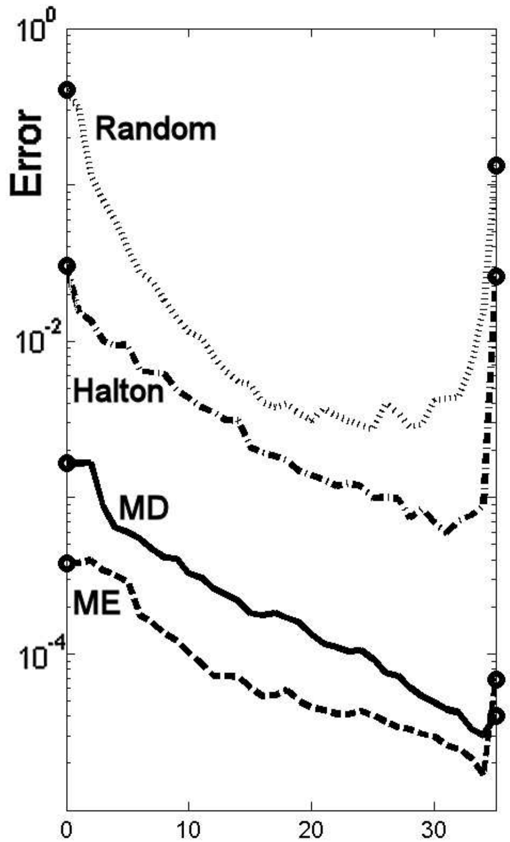
Focus on four scattered node cases, all with $N = 36^2 = 1296$ nodes



Test Function 1

Combination of four Gaussians

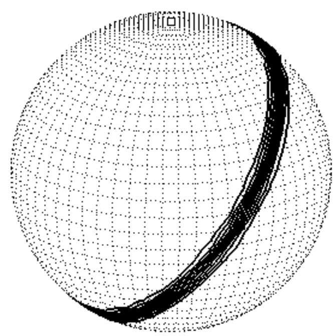


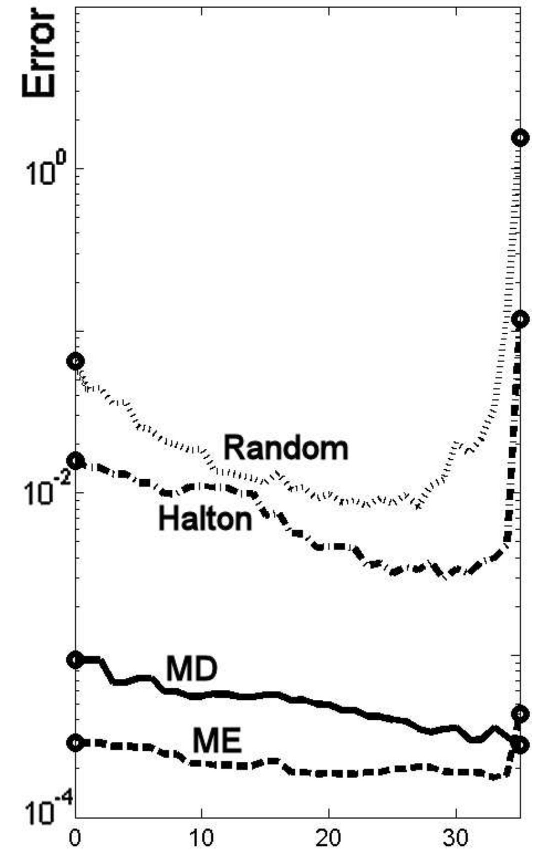


pinv truncation order

Test Function 2

tanh function: sharp transition between 0 and 1



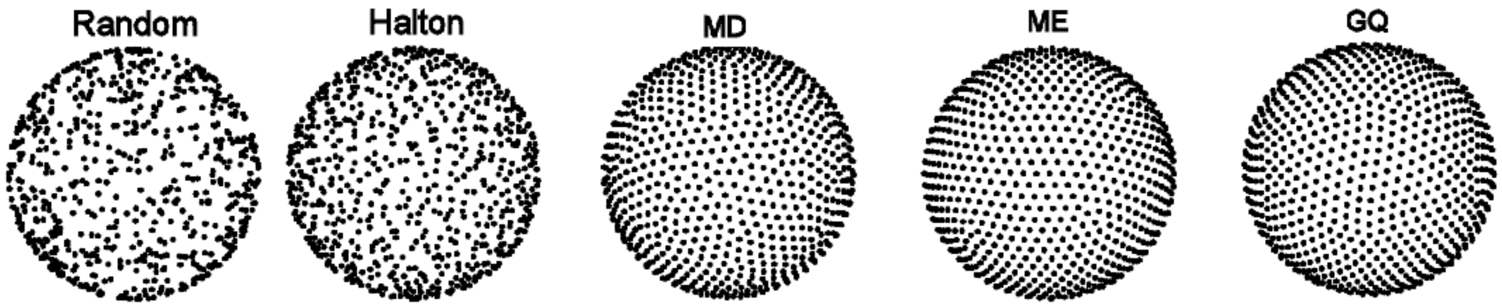


pinv truncation order

Easy to create rule-of-thumb for how many degrees of freedom to eliminate when using pinv to calculate quadrature weights.

Applying 'rule of thumb', convergence rates under node refinement

Include here also Gaussian Quadrature (GQ)

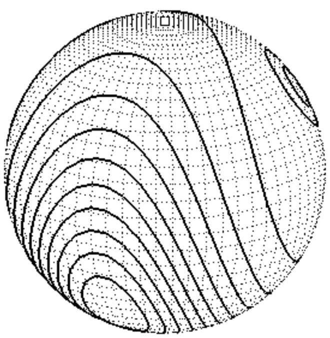


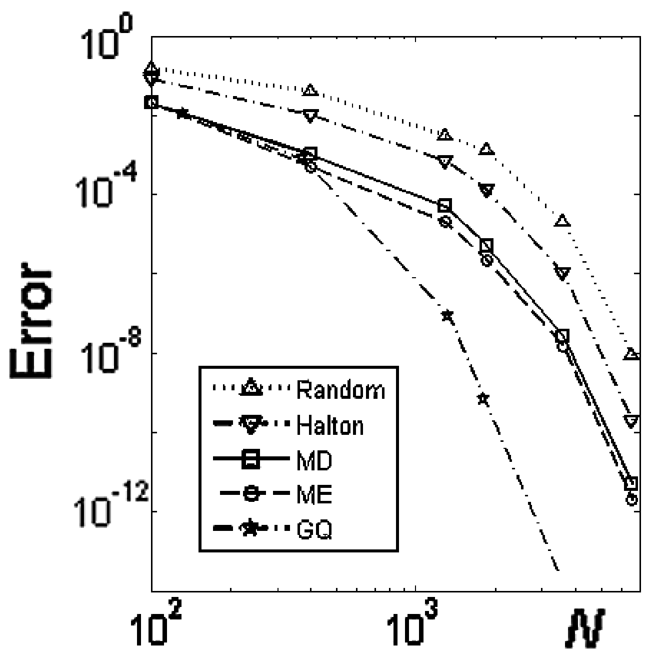
In 1-D, one needs data at N nodes to 'pin down' uniquely a polynomial $p_{N-1}(x)$, of degree N-1. By placing the nodes at the GQ locations, one can exact quadrature result for all polynomials up through degree 2N-1.

GQ Concept: The polynomial space that is not 'pinned down' integrates to exactly zero.

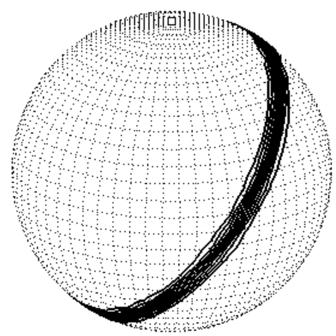
GQ Counterpart on the sphere: When placed at perfect positions, N nodes suffice for exact quadrature of about the first 3N spherical harmonics.

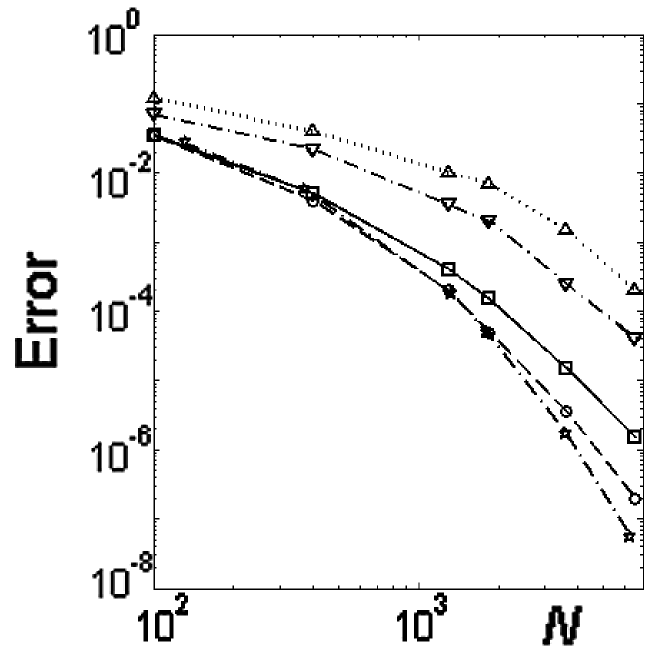
Test function 1





Test function 2





For practical quadrature: ME node sets come very close to theoretical perfection.

Conclusions

- **Lat-Long node sets conceptually flawed for the task of numerical quadrature**
  - Node density is too non-uniform for achieving best accuracy
  - Mismatch between node layout (on fixed latitude lines only) and SPH basis functions

- **No justification for using (difficult-to-calculate) MD or GQ node sets**
  - ME sets (or almost any quasi-uniform scattered node sets) work excellently well for quadrature

- **Node sets are typically decided on for effective solution of PDEs, and not for quadrature alone.**
  - Direct comparisons between RBF-FD on ME-like node sets and DG on Cubed Sphere are presented in:

    N. Flyer, E. Lehto, S. Blaise, G.B. Wright and A. St-Cyr, A guide to RBF-generated finite differences for nonlinear transport: Shallow water simulations on a sphere, J. Comput. Phys. 231 (2012), 4078-4095.

Publication on present quadrature discussion

BF and J.M. Martel, *On spherical harmonics based numerical quadrature over the surface of a sphere*, to appear in *Adv. Comput. Math.* (2014)

Future opportunities (BF and Jonah Reeger, USAF Institute of Technology)

- Bring down the cost of finding weights at N nodes from $O(N^3)$ to $O(N \log N)$.

- Develop an effective weight calculation algorithm also for cases when adaptive refinement have led to node sets of highly non-uniform density (with SPH then no longer applicable as 'reference')