Charged Containers for Optimal 3D Q-space Sampling

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Introduction: In the effort of extracting meaningful microstructural properties from diffusion weighted MRI (dMRI) it becomes clear that a large number of acquisitions are required to get the full extent of the information [1]. The discussion concerning optimal q-space sampling strategies has been lively from the very start of diffusion imaging [2-5]. Among the most well known approaches is the electrostatic repulsion algorithm suggested by Jones et. al. [6]. Jones algorithm finds a 'uniform' distribution of q-space sample points by finding the lowest electrostatic energy of a system consisting of N antipodal charge pairs distributed on the surface of a sphere, equation (1). This approach works well as long as the relation between samples in different q-shells is not taken into account. However, when aiming for a full 3-dimensional reconstruction of the diffusion propagator the sample points should preferably be evenly distributed in the targeted 3-dimensional q-space. The present work demonstrates how this can be achieved by extending the electrostatic charge distribution model. The extension is as elegant as it is simple: Add a volume of the desired shape having an evenly distributed total charge equal to the negative of the sum of the moving point charges.

$$E = k\,q^2 \sum_{i=1}\sum_{j\neq i} \|\mathbf{x}_i - \mathbf{x}_j\|^{-1} + \|\mathbf{x}_i + \mathbf{x}_j\|^{-1} \qquad (1)$$

Theory: To add the energy term corresponding to the uniformly charged volume we need to find the added potential inside the volume. Equation (2) gives the potential for a sphere of radius one having a constant density of negative charges. Equation (3) gives the electrostatic energy of the total system. While the energy definition of equation (1) works well in the intended context a different definition is natural for a fully 3-dimensional q-space sampling system. The first term in equation (3) is the interaction energy from outer product tensor charges representing the q-space samples. Thus, each charge is positioned in a higher dimensional space that can naturally represent the concept of orientation [7]. The reason for normalizing the first x-vector in the outer product is to keep a linear radial scale. The second term is the energy from the point charges interaction with the uniform negative charge volume. Minimizing the energy will result in a distribution of point charges that cancels the continuous potential field as much as possible resulting in a 3-dimensional distribution that is uniform in the same sense as the original charge repulsion results. It is possible to specify any shape of the negatively charged volume as long as a reasonable and differentiable function can be given for the interior potential. There is no need to find an expression for the exterior potential as minimum energy solutions always have all point charges inside. In the result section below two examples of distributions attained using a uniformly charged cube as the negative volume are shown. The second term of equation (3) was here replaced by a sixth order polynomial to approximate the interior potential [8].

$$V = -\frac{1}{2}\,k\,Q\,(3 - r^2) \qquad (2)$$

$$E = k\,q^2 \sum_{i=1}\sum_{j\neq i} \|\,\hat{\mathbf{x}}_i\mathbf{x}_i^T - \hat{\mathbf{x}}_j\mathbf{x}_j^T\|^{-1} \; - \; \frac{kq}{2}\underbrace{Q}_{=\sum q}\sum_i (3 - \|\mathbf{x}_i\|^2\,) \qquad (3)$$

Method: The energy minimization was performed using a simulated annealing inspired gradient search algorithm. Search times are roughly proportional to the square of the number of tensor charges, higher accuracy will of course require longer search times. Typically finding a low energy point for a 100-charges system can be done in less than a minute using a standard laptop.

Results: Figure 1 shows the result for 7 tensor charges. Tensor charges are visualized as diametrically positioned pairs of colored spheres. It has one charge at the origin (red) and 6 charges in an icosahedral arrangement (blue). The transparent half-sphere indicates the outer surface of the negative uniformly charged sphere. Figure 2 shows the result for 37 charges. It also shows one in the center and 6 arranged as an icosahedron (green), the outer 'shell' have the remaining 30 charges. The colors of the charge markers indicate the distance from the center. The smaller transparent sphere (r=0.5) was added purely to provide extra visual cues for the charge positions. Figure 3 shows the result for 110 charges. It shows the same behavior: One charge in center – 1:st 'shell' is an icosahedron (dark green) - 2:nd 'shell' has 29 charges (bright green) - the outer shell has 74 charges.

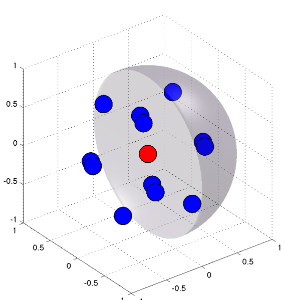

Figure 1

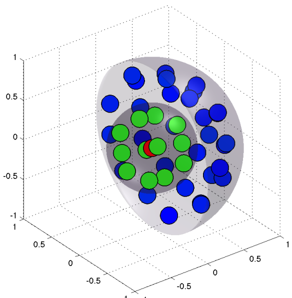

Figure 2

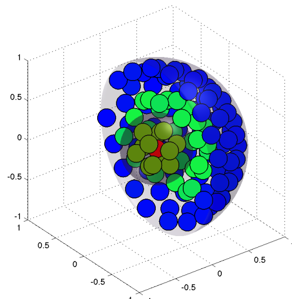

Figure 3

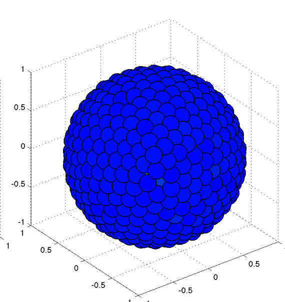

Figure 4

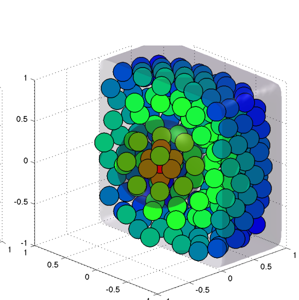

Figure 5

The 'shelling' behavior displayed in these examples is a consistent and compelling feature of the low energy level solutions regardless of the number of charges used. Figure 4 shows the outer shell result for 500 charges. Figures 5 and 6 shows the results using a uniformly charged cube for the 'capture potential'. The cube-ness of the charge distribution is clearly visible although there is a relatively marked rounding of the corners. Interestingly, as can be seen from the 200-charge distribution in figure 5, the forming of spherical shells is also present for the inner parts of the cube. From the center out the first three shell-like groupings contain 3, 5, and 45 charges. Figure 6 shows a 500-charge cube optimization.

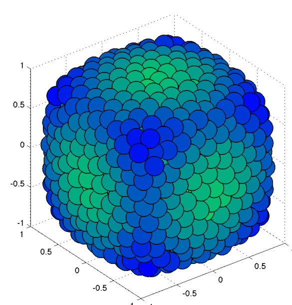

Figure 6

Conclusions: We have presented a novel method for generating evenly distributed samples in a part of q-space that can be pre-specified in a general way. We have demonstrated the feasibility for two shapes, a sphere and a cube. The results are interesting from several points of view. There is a market tendency for the samples to group in shells indicating that the present work may provide a preferable alternative to recently proposed shell-interaction schemes [9]. The distributions attained for the cube case are far from Cartesian, this may be an advantage in a sparse reconstruction, e.g. compressed sensing, setting.

References: [1] Wiegell et al., Radiology 217, 2000. [2] Assaf et al., MRM 52, 2004, [3] Wu et al., Neuroimage 36, 2007. [4] Alexander, MRM 60, 2008. [5] Westin et al, ISMRM, 2012. [6] Jones et al., MRM 42, 1999. [7] Knutsson, SCIA, 1989. [8] Hummer, Electrostatics 36, 1995. [9] Caruyer, CDMRI, 2011.