Uniform rotations

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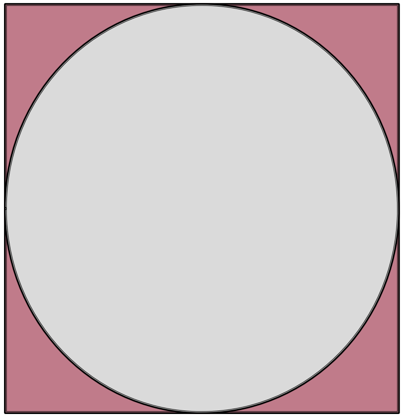
Uniform random unit vectors

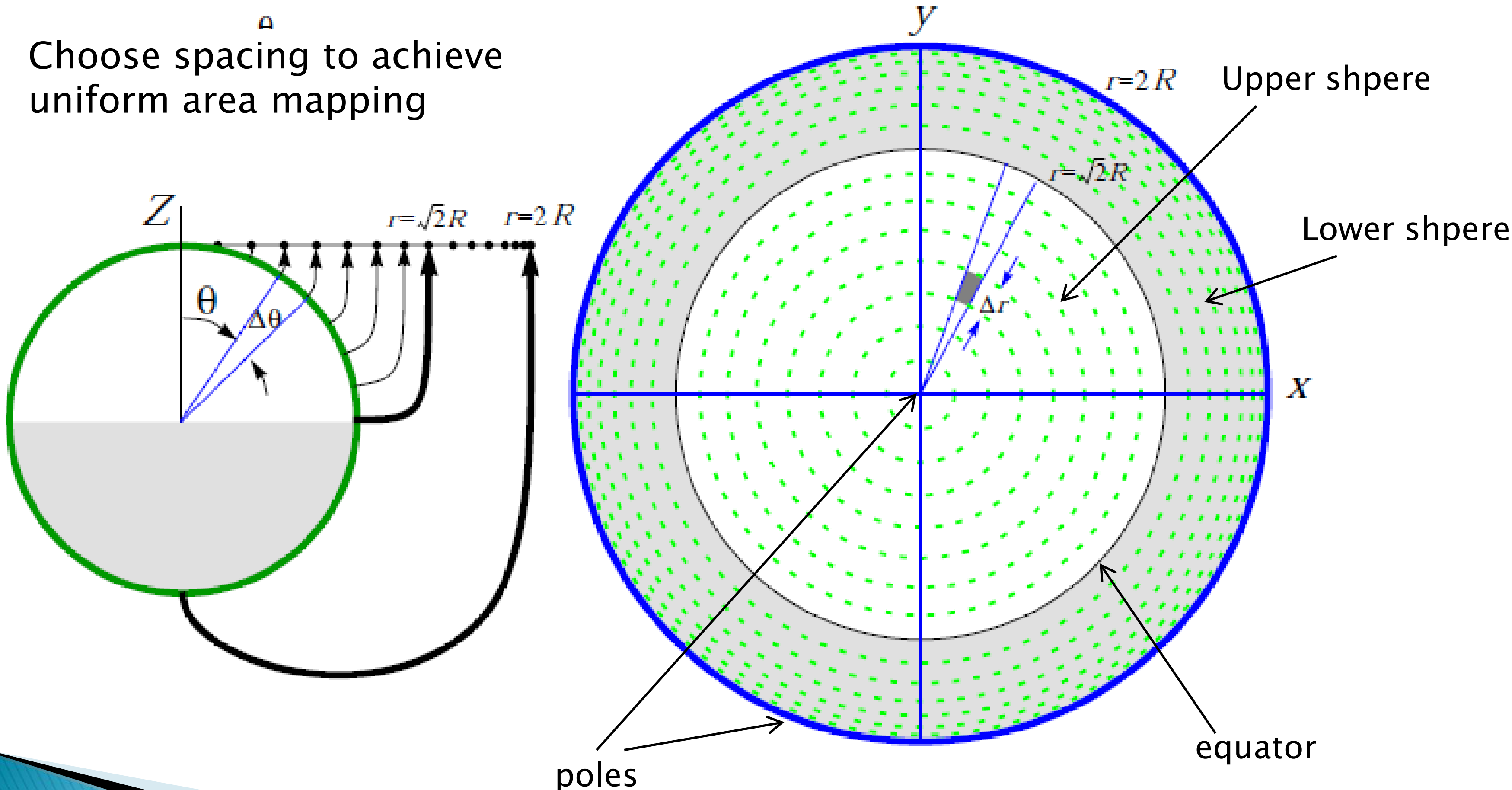
- Each point on unit sphere is equally likely
$$p(\vec{n}) = 1/4\pi$$
- The expected value is zero
- 3 random numbers in Cartesian coordinates & normalization favours corners
$$\vec{n} = \frac{(u_1, u_2, u_3)}{\|\vec{u}\|}$$
- Possible solution: reject coordinates which are outside of sphere

→ How to verify?

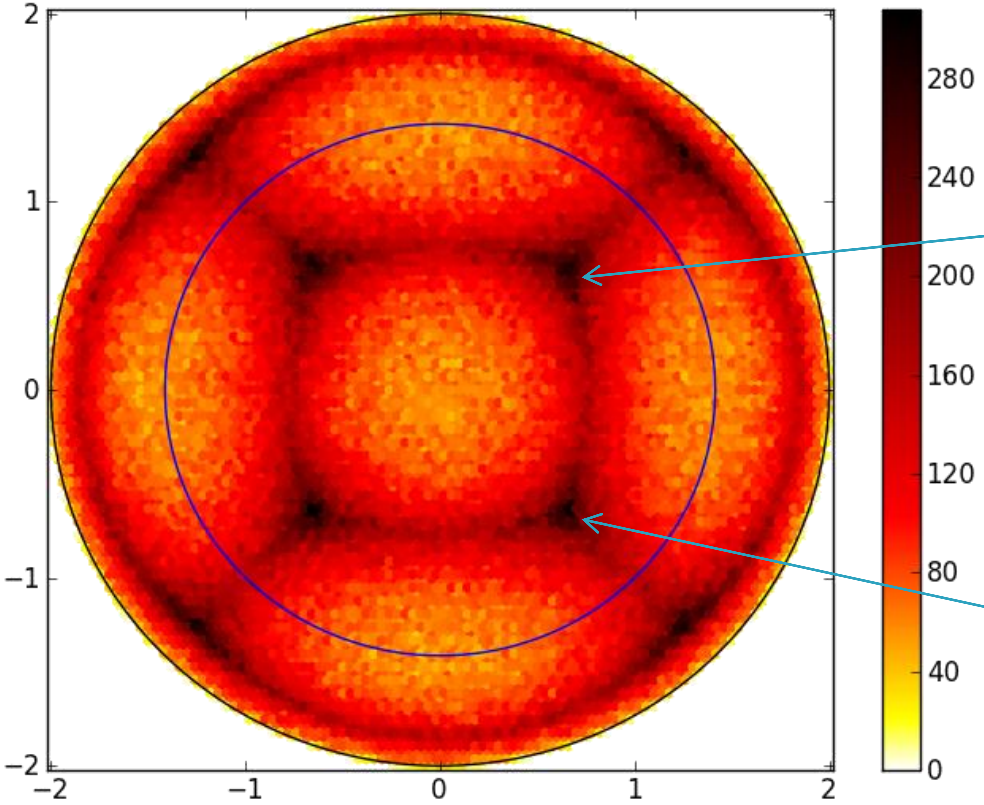


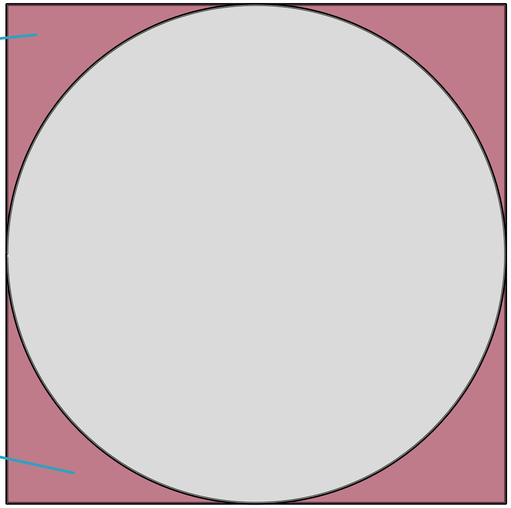
Visualization – stereographic projection

- Map surface to plane with equal area mapping



Visualization for non-uniform sampling





Spherical coordinates

$$\vec{n} = \sin\theta\cos\varphi\,\vec{e}_1 + \sin\theta\sin\varphi\,\vec{e}_2 + \cos\theta\,\vec{e}_2$$

- For uniform distribution on sphere

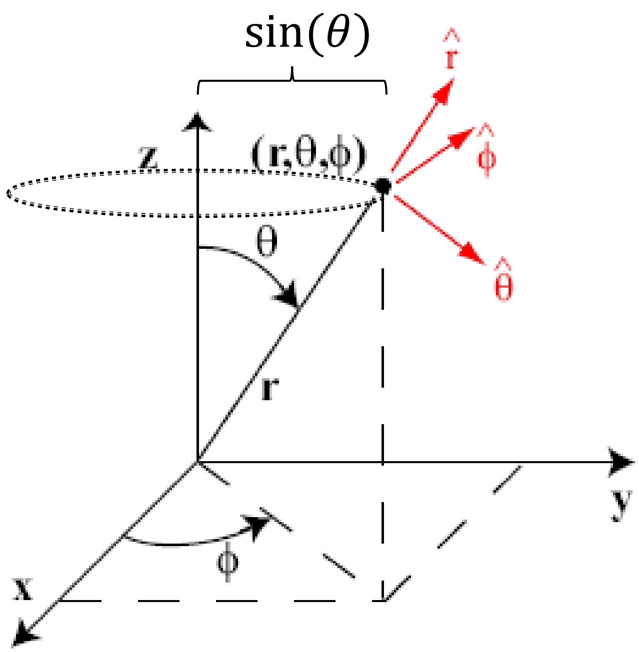
$$p_\theta(\theta) = \frac{1}{2}\sin\theta \qquad p_\varphi(\varphi) = 1/2\pi$$

- Choose random numbers with non-uniform distribution

$$\theta = \cos^{-1}(1-2u)$$

and use

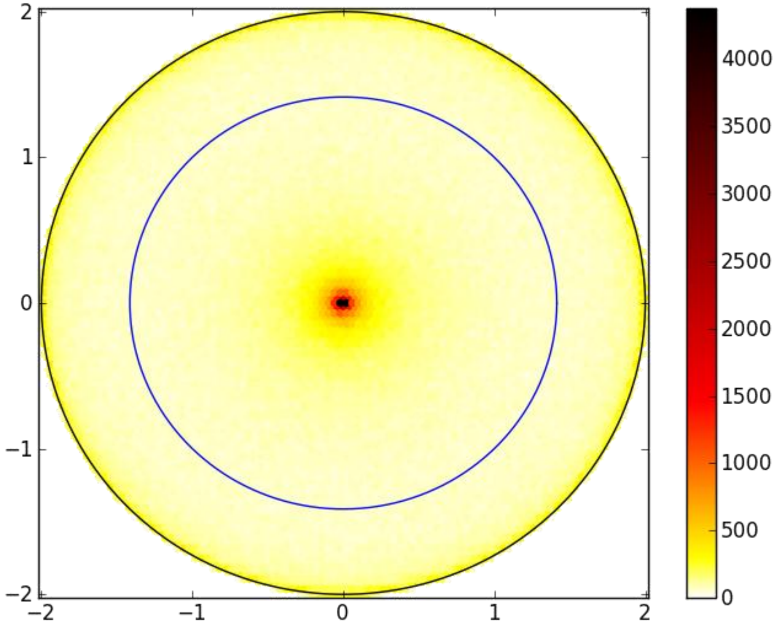
$$\sin\cos^{-1}x = \sqrt{1-x^2}$$



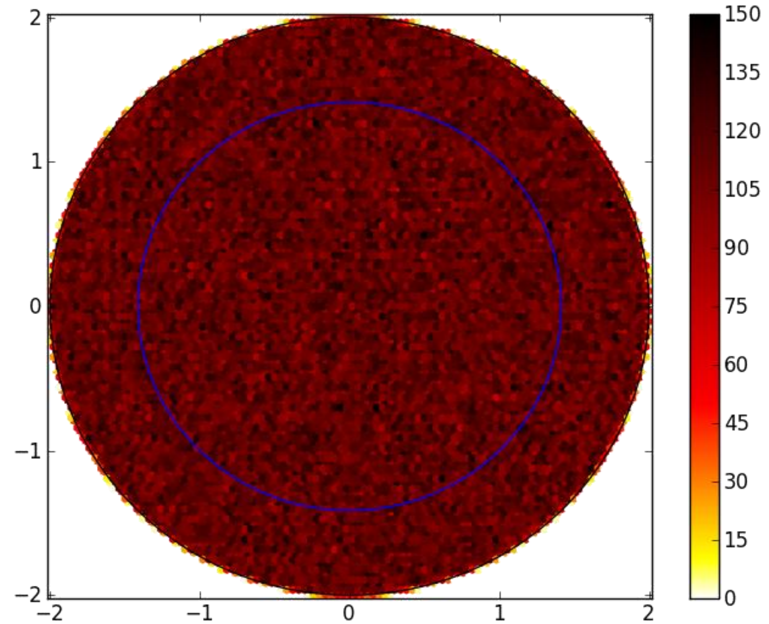
Spherical coordinates visualization

- Uniform distribution of θ favors the poles
  - Nematic order in system

$$p_\theta(\theta) = 1$$

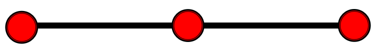


$$p_\theta(\theta) = \frac{1}{2}\sin\theta$$



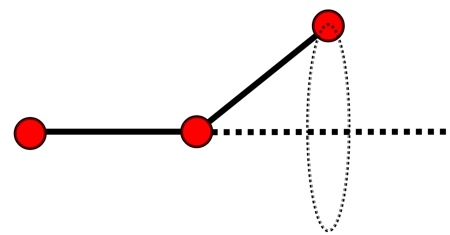
Monte Carlo with internal coordinates

- Correct acceptance ratio or use non-uniform random numbers

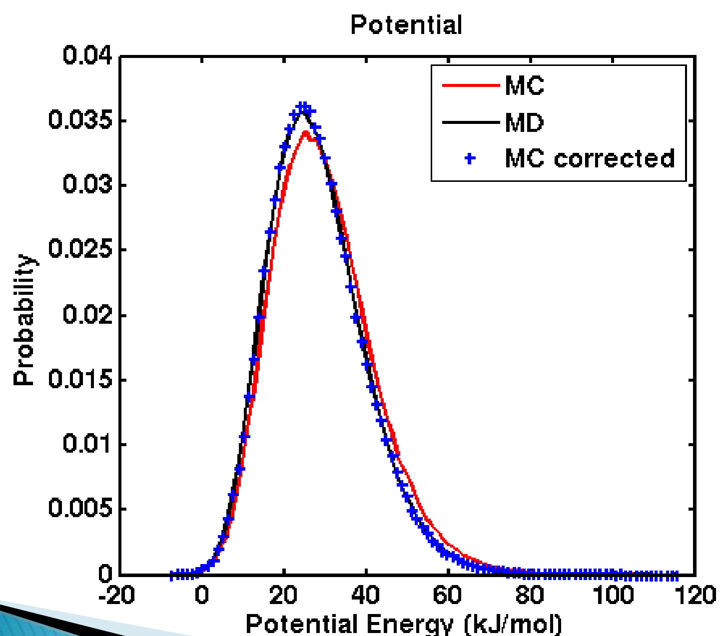


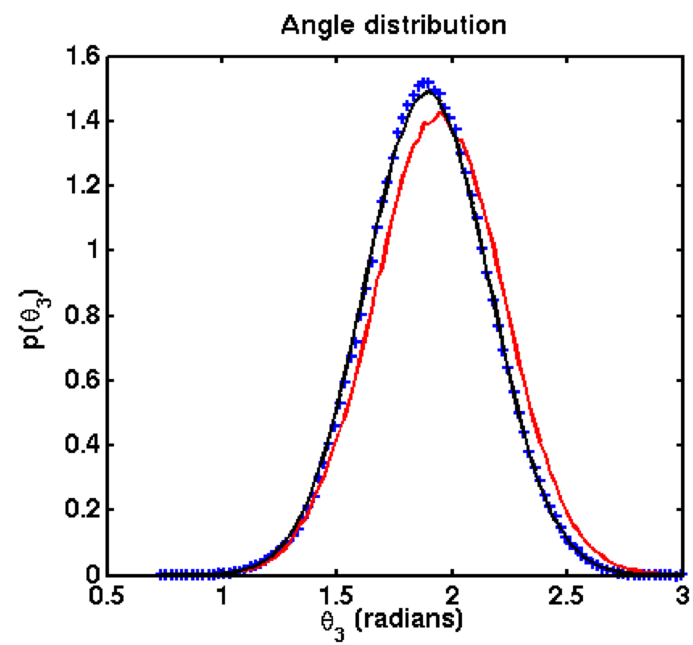
$$p_{12} = p(\theta)p(\varphi)$$

$$p_{22} = p(\theta)$$



$$\frac{p_{21}}{p_{12}} = \sin(\theta)$$



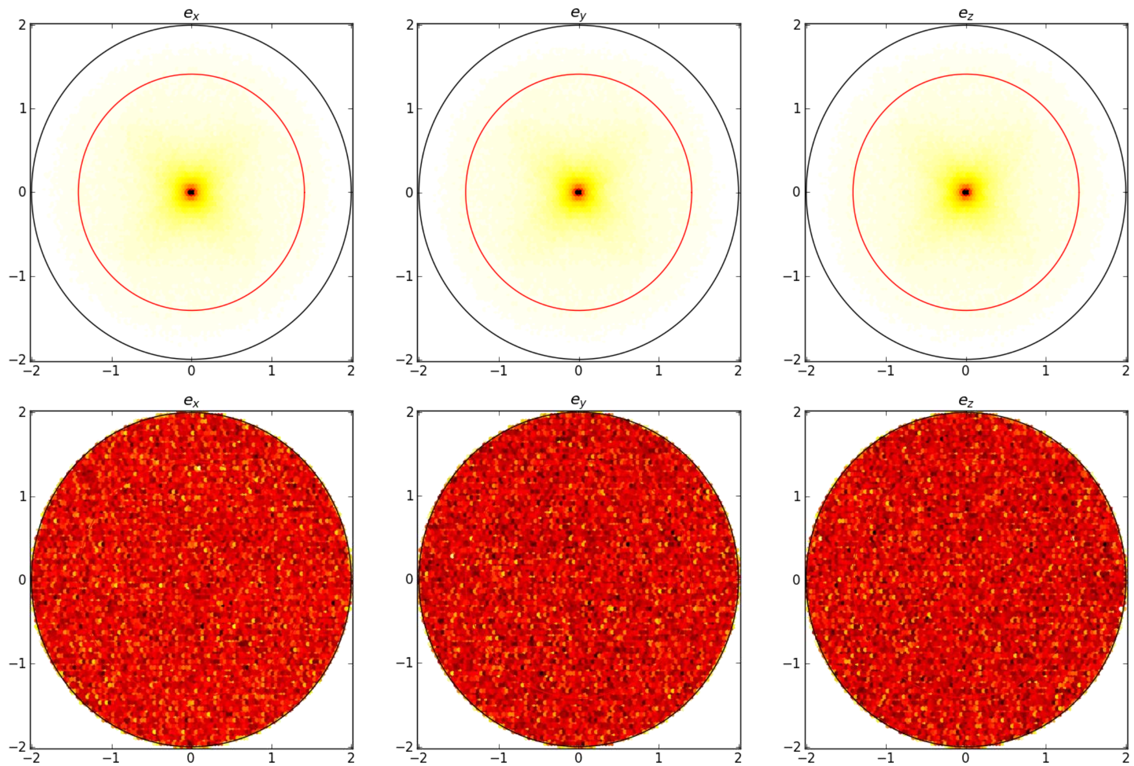


Uniform Random Rotations

- Rotation angle θ around random axis is not uniformly distributed
- Stereographic projection for all 3 unit vectors

$$p_\theta(\theta) \propto 1, \theta \in [0, \pi]$$

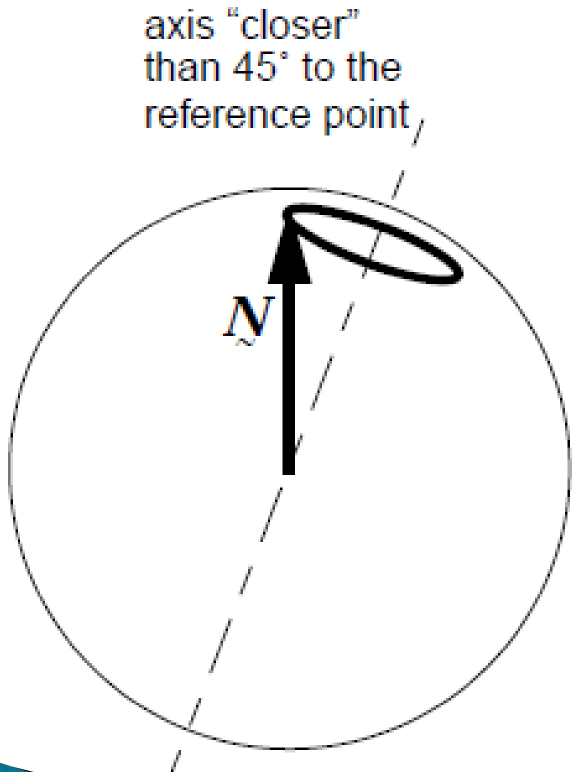
$$p_\theta(\theta) \propto \left(\sin\frac{\theta}{2}\right)^2$$



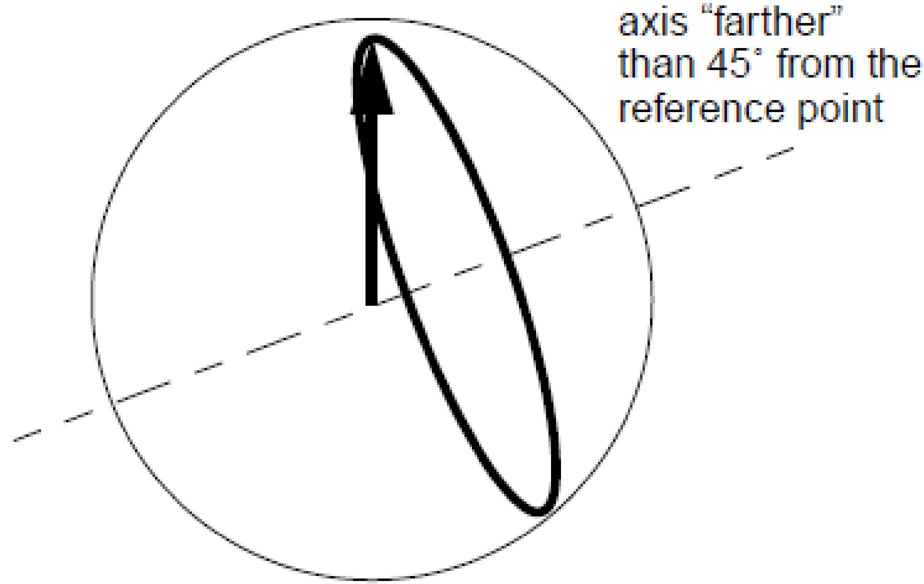
* Shoemake, K., Uniform random rotations, in: D. Kirk (Ed.), Graphics Gems III, Academic Press, London, 1992, pp. 124–132.

Spherical coordinates – angle distribution

Many different rotation axes can bring the pole to a point on the upper part of the sphere but only a few rotate it to the lower one.



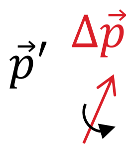
$$p_\theta(\theta) \propto \left(\sin\frac{\theta}{2}\right)^2$$

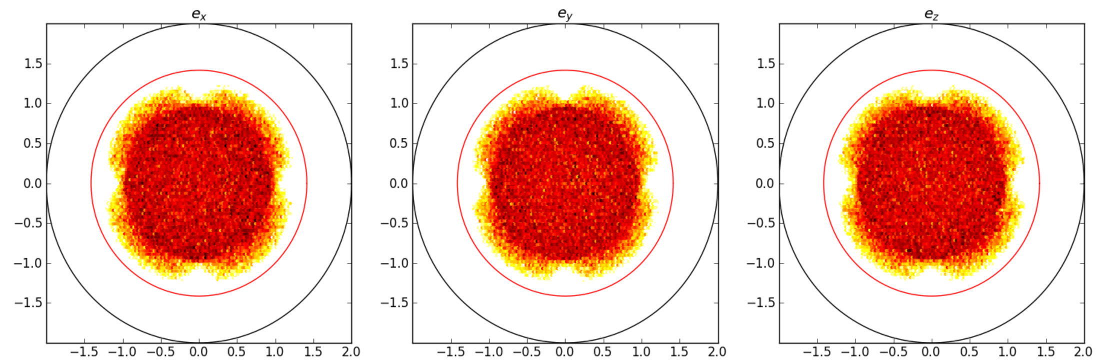


Random displacements with non-zero p

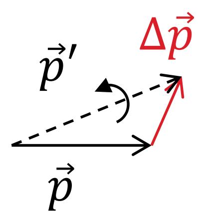
$$\Delta\vec{p} = (u_1, u_2, u_3), \qquad u_i \in [0,1]$$

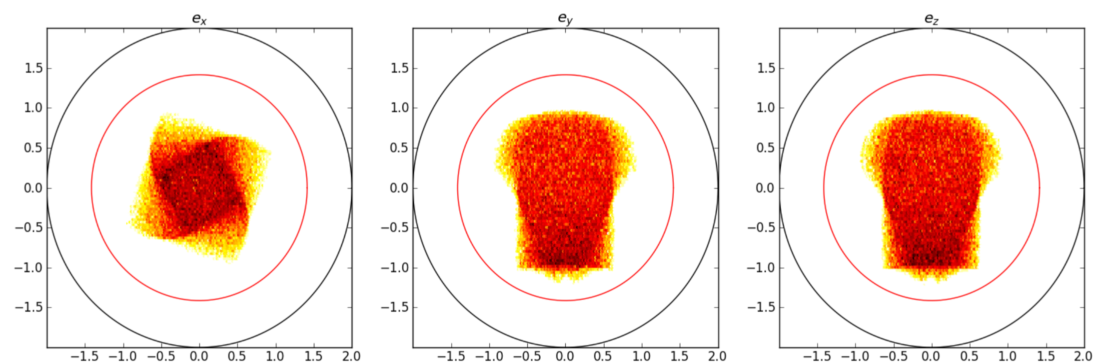
$$\vec{p} = (0,0,0)$$



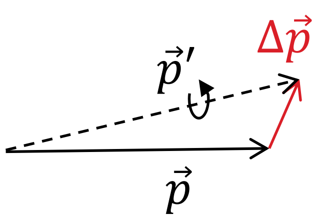


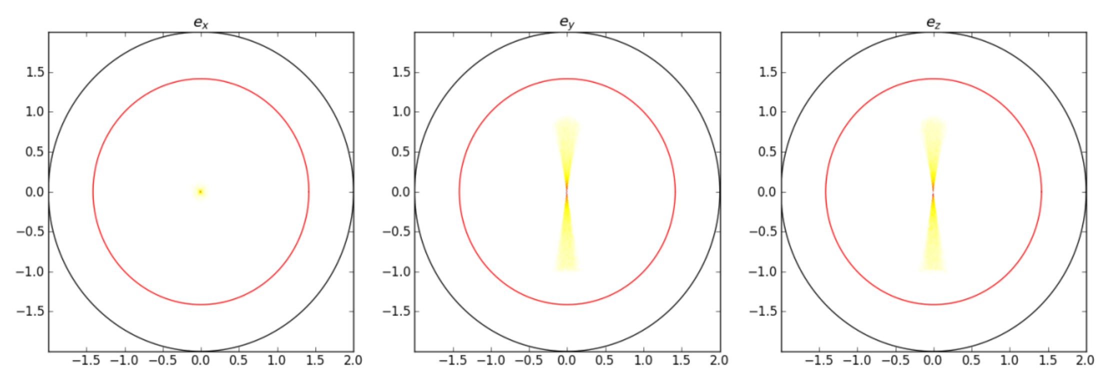
$$\vec{p} = (\pi, 0, 0)$$





$$\vec{p} = (2\pi, 0, 0)$$





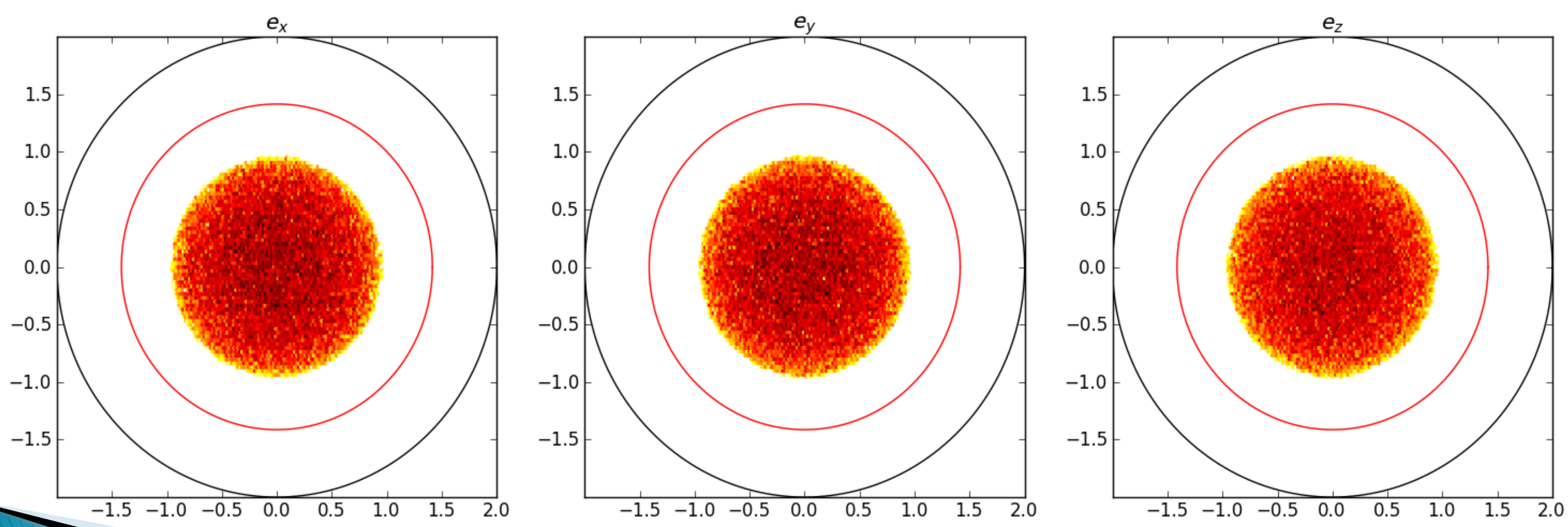
Improved takestep routine

- Choose random axis of rotation
- Choose random angle with

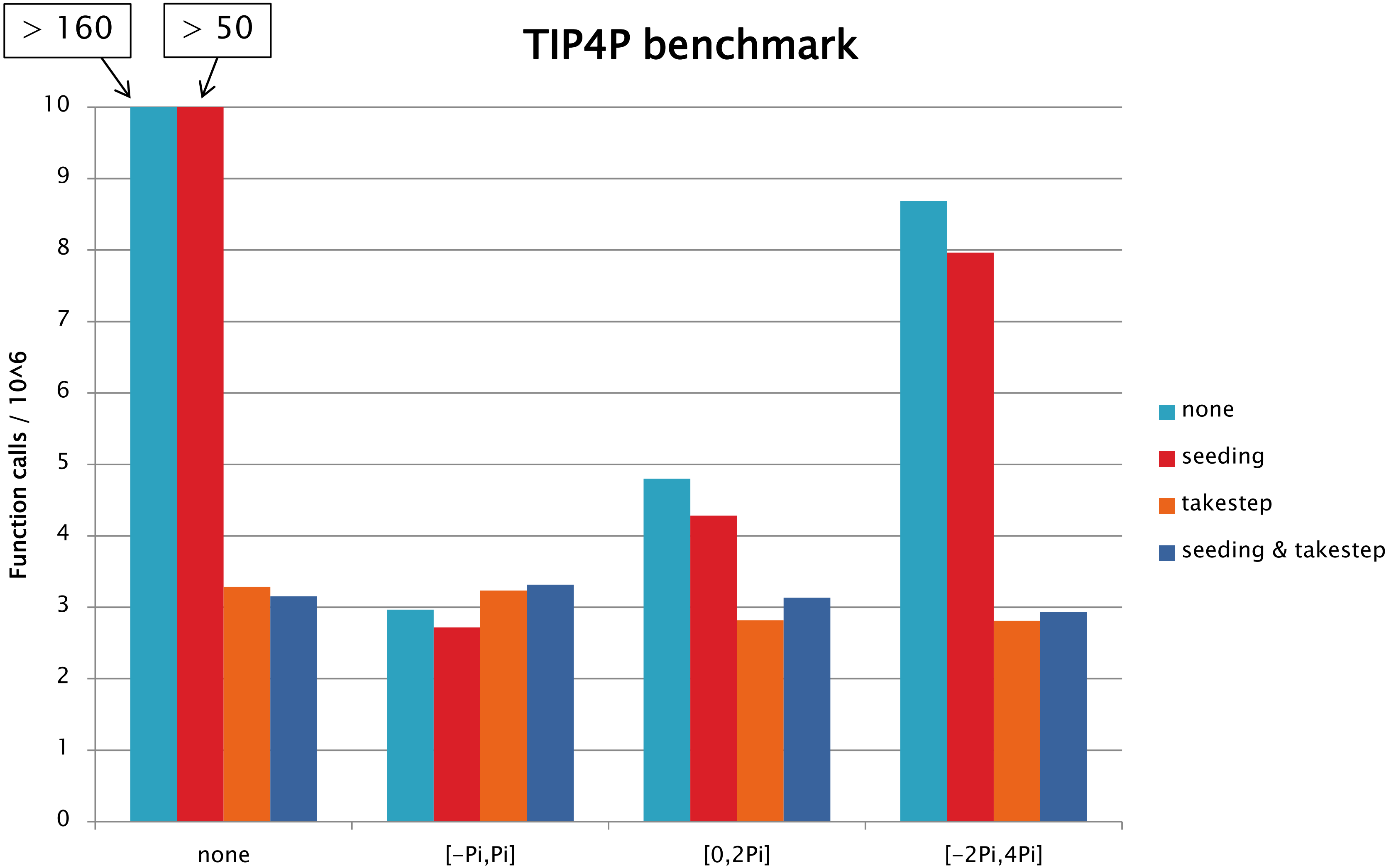
$$p_\theta(\theta) \propto \left(\sin\frac{\theta}{2}\right)^2$$

- Combine current angle axis vector and step using quaternions

rot_takestep_aa from rotations.f90



Effect of uniform rotations



Summary

- Know what you are doing when running benchmarks
  - Use proper random initial configurations
  - Use proper displacements when benchmarking quenching

- Performance does not depend on the definition of the angle-axis vector when using the new takestep routine (tested for TIP4P, benzene crystal)

- Similar problems in different context (see e.g. MC)
  - Take care for proper normalization when using non-carthesian coordinates!

→ Don‘t code yourself, use existing modules!

Vector and rotation modules

module vec3
(vec3.f90)

vec_len
vec_angle
vec_cross
vec_dyad
vec_random
det3x3
invert3x3
identity3x3

All functions checked in testsuite that error is less than 10^{-8}

module rotations
(rotations.f90)

rot_aa2q
rot_aa2mx
rot_q2aa
rot_q2mx
rot_mx2q
rot_mx2aa

rot_q_multiply
rot_rotate_aa
rot_get_orientation_aa

rot_random_q
rot_random_aa
rot_small_random_aa
rot_takestep_aa

References

- Review on rotations
  www.mech.utah.edu/~brannon/public/rotation.pdf
- Uniform random quaternion
  Shoemake, K., Uniform random rotations, in: D. Kirk (Ed.), *Graphics Gems III*, Academic Press, London, 1992, pp. 124–132.
- Uniform random matrices
  James Arvo, "Fast Random Rotation Matrices", in *Graphics Gems III*, pages 117-120, edited by David Kirk, Academic Press, New York, 1992.
- Angle axis angle distribution
  Miles, Roger E. (December 1965), "On random rotations in R3", Biometrika (Biometrika, Vol. 52, No. 3/4) 52 (3/4): 636–639, doi:10.2307/2333716
- Wikipedia – Rotation matrix