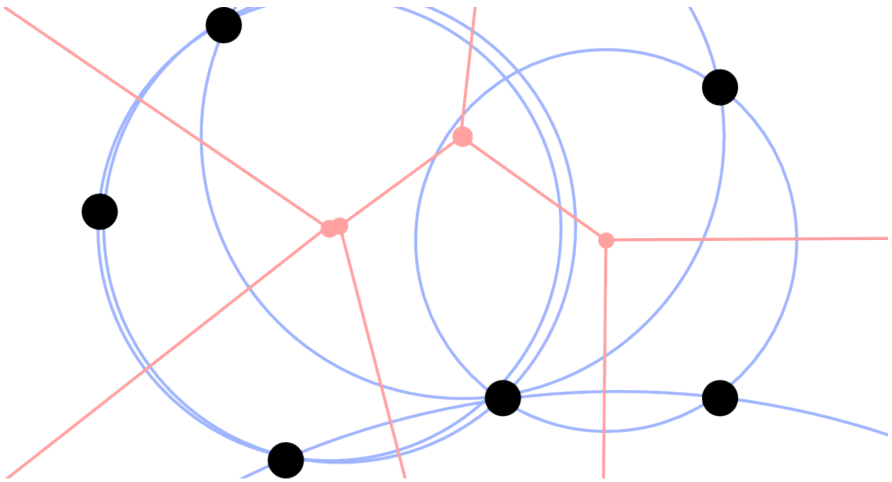
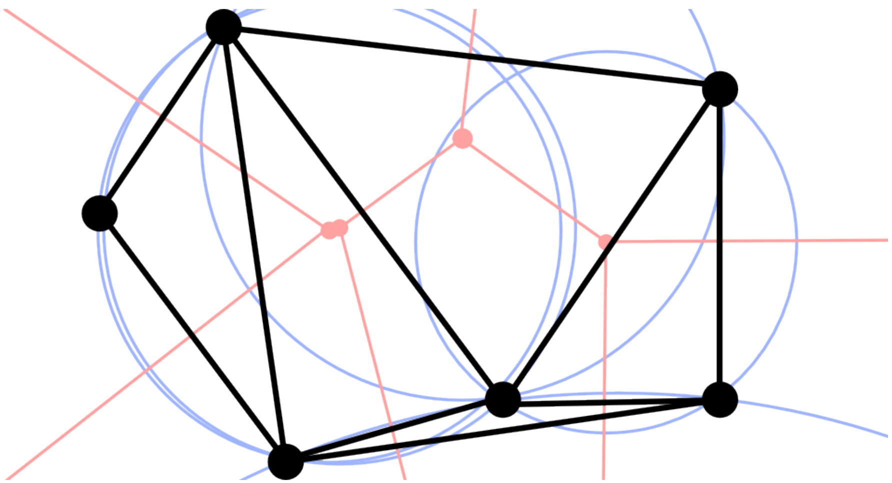
Voronoi Diagram



- Given a set *P* of *n* points in the plane (general position), its Voronoi diagram is a partition of the plane into *n* cells, each containing one point of *P* and everything closer to it than to any other point.

Delaunay Triangulation

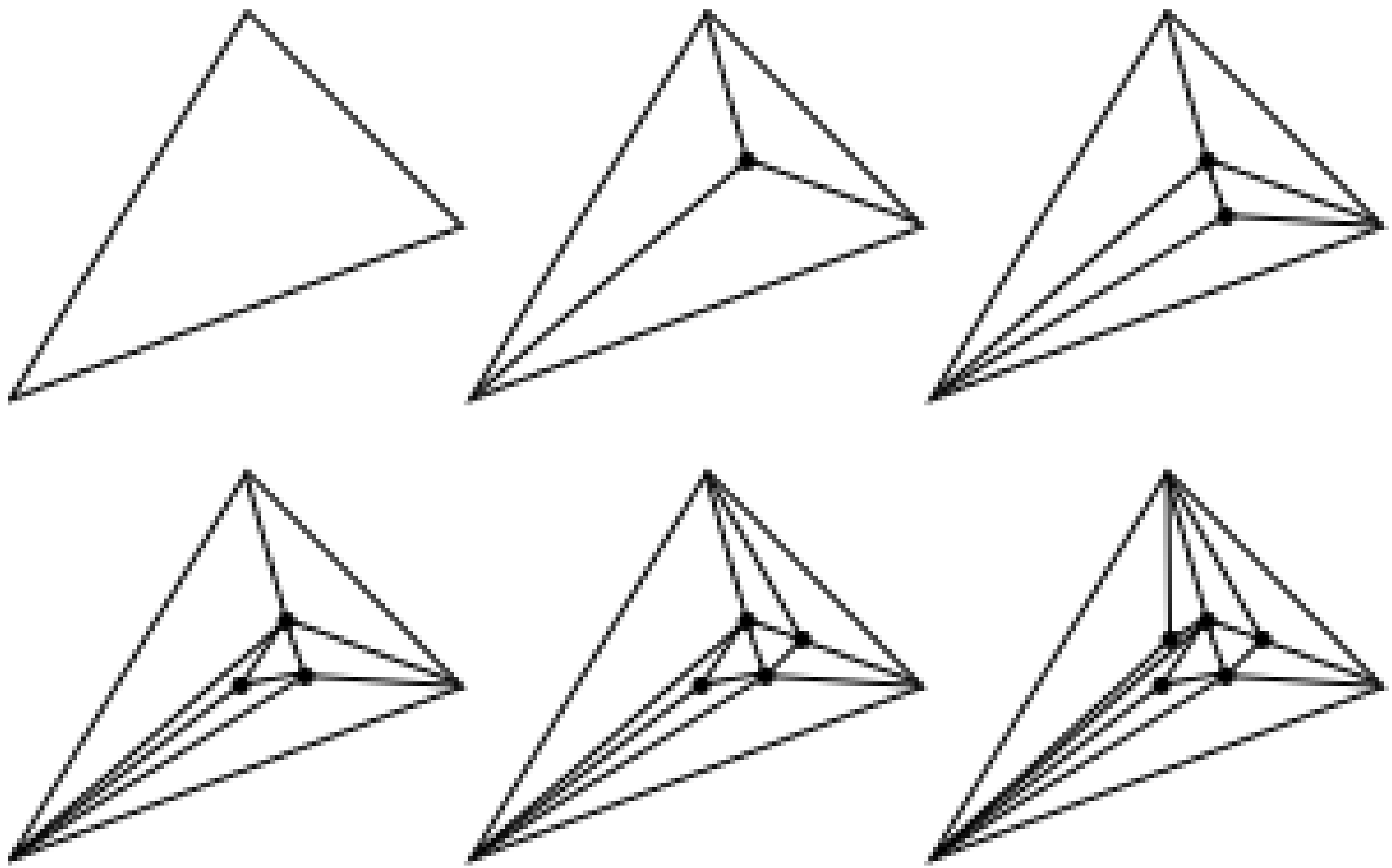


- 3 points p_i, p_j, p_k in P form a triangle in DT(P) iff the unique circle through p_i, p_j, p_k contains no other point from P.
- 2 points p_i, p_j in P form an edge in DT(P) iff there exists a circle through p_i and p_j that contains no other point from P.

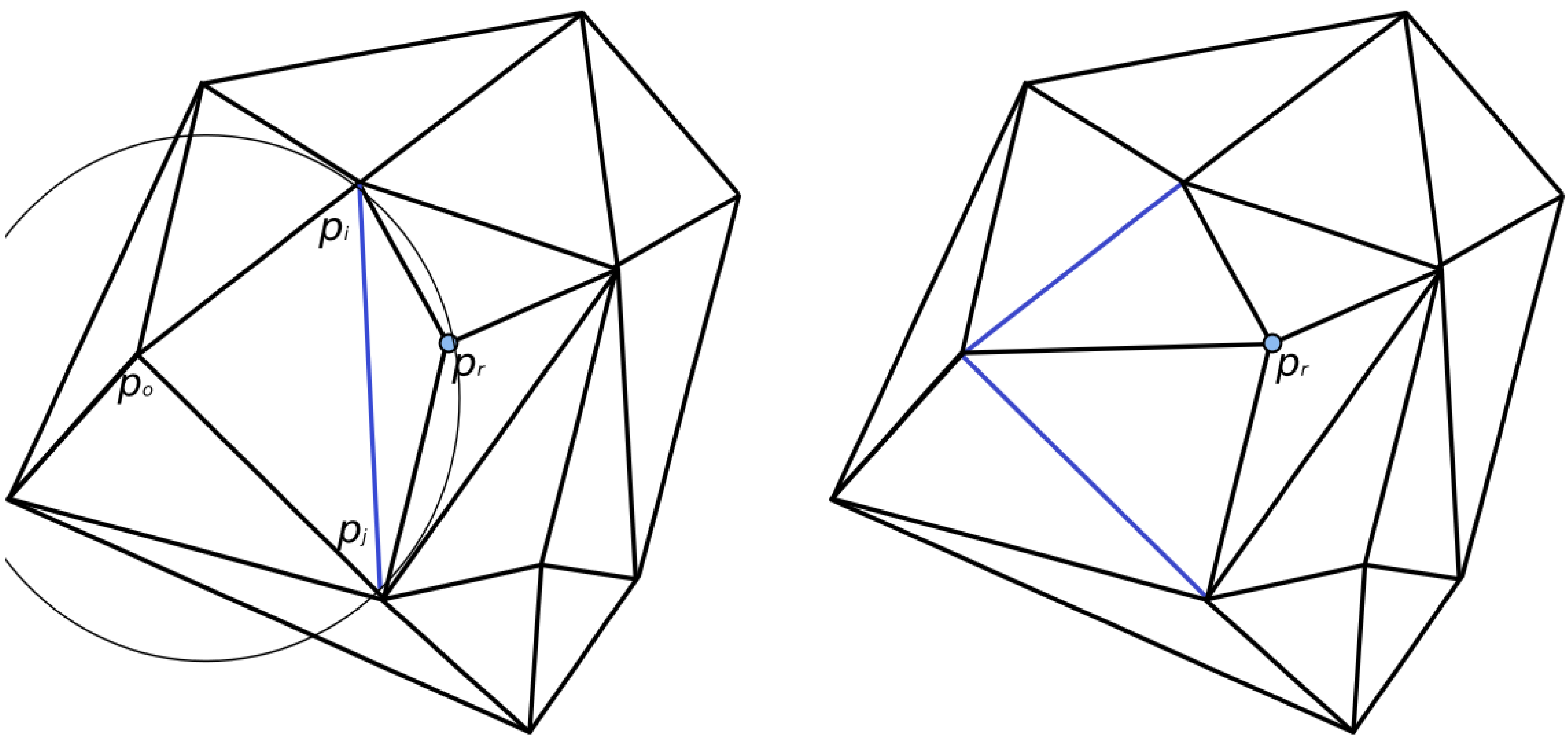
Constructing DT

- Construct VD(P) in O($n$log$n$) time and O(n) space and convert it to DT(P) in O(n) time.
- VD(P) algorithms are complex and can cause serious precision problems.
- DT(P) can be determined directly in O(n^2) time.
  - Randomized version O_e($n$log n).
  - Generalizes to 3D.

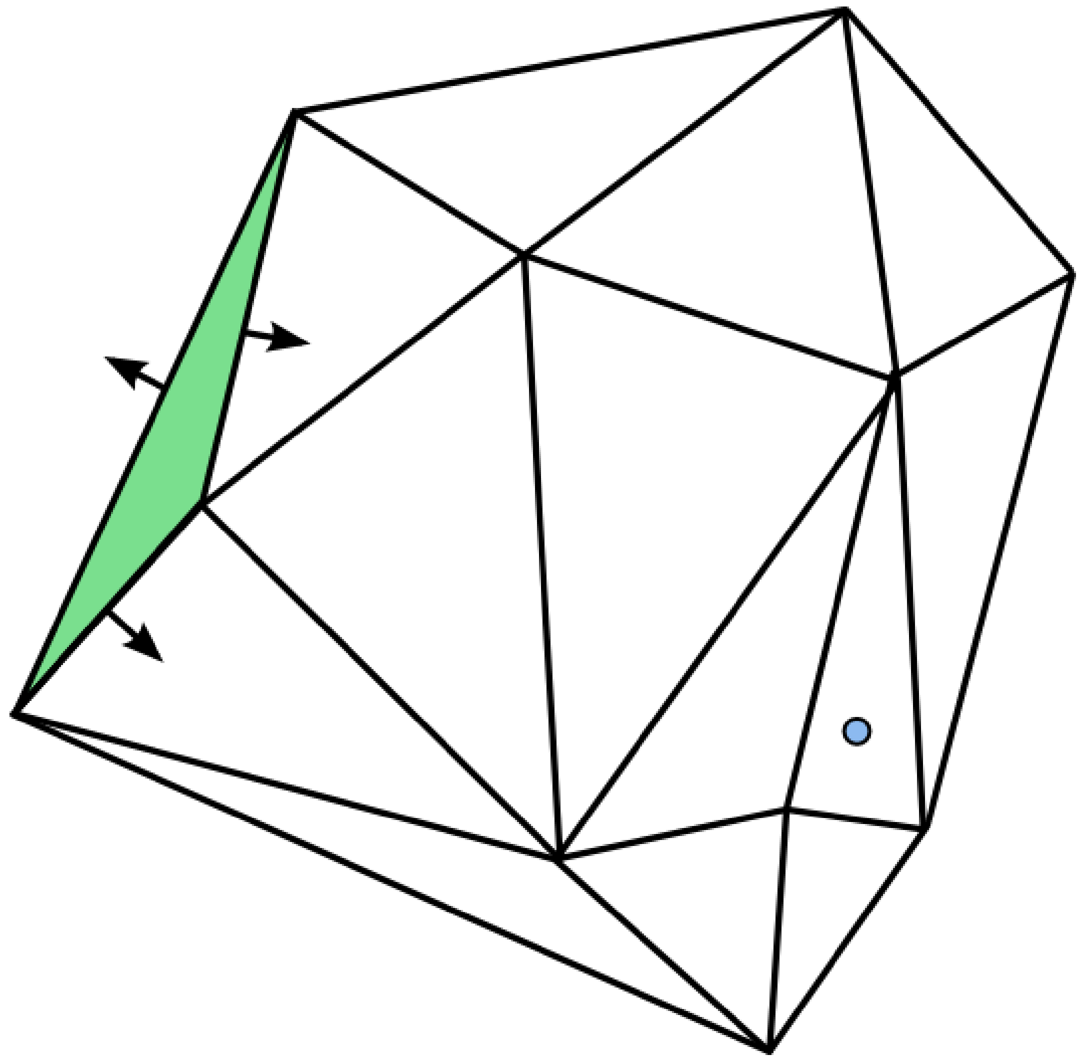
Constructing DT



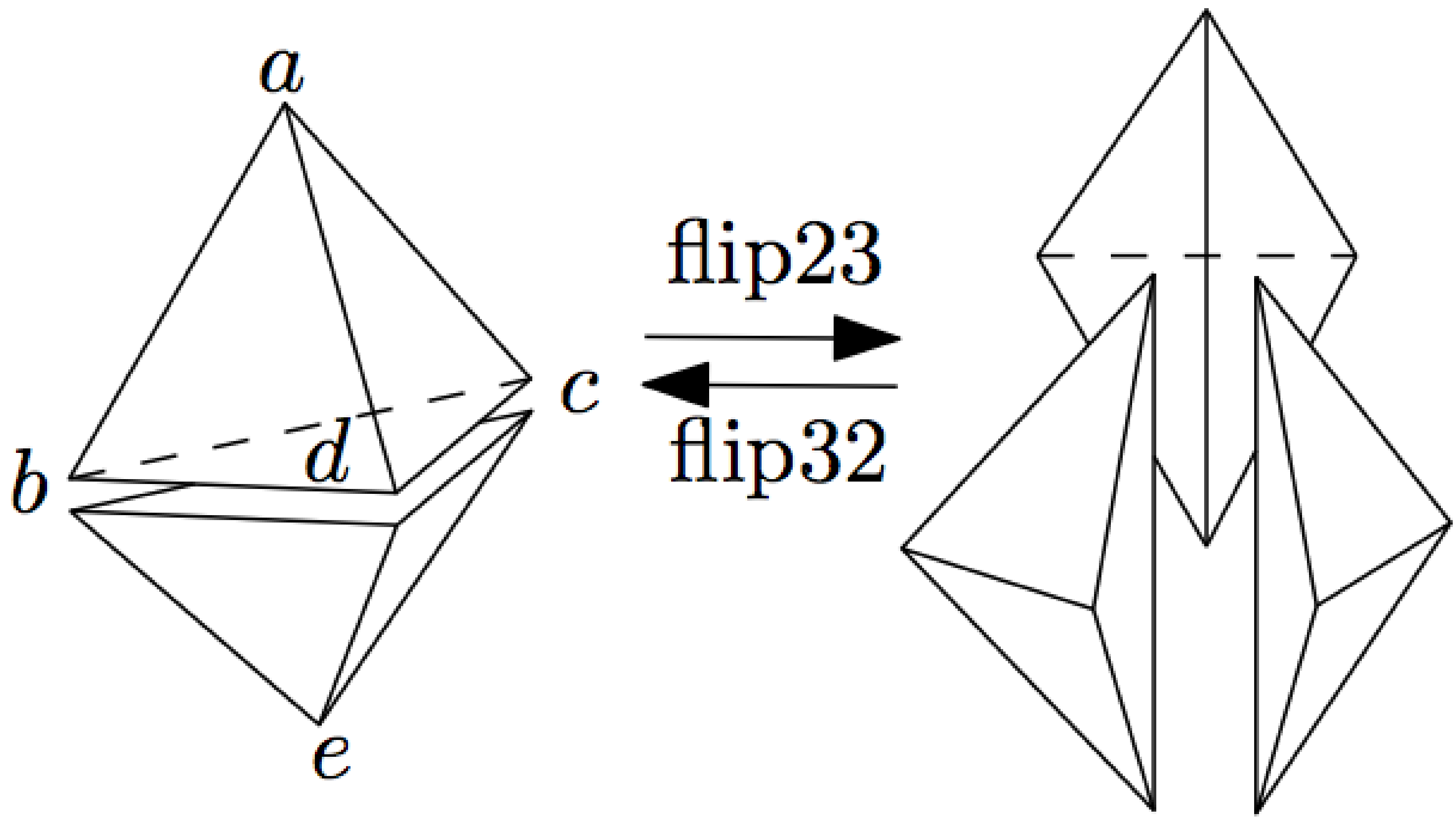
O(n) Flips pr. Added Point



Locating a Triangle in O(n) Time



Flips in R^3



Kinetic Delaunay Triangulation in R^2

- *n* points with (piecewise) linear trajectories.
- Events:
  - Insertion and deletion (disregarded in the following).
  - Trajectory and/or speed change events (deletion followed by insertion).
  - Circle events: 4 points on a common circle.
  - Side events: 3 points on a common line where one half-plane contains no points. Can be considered as a special case of circle events (imagine everything inside a huge triangle with stationary corners).
- Simplifying assumption: No collisions, no pair of events occurs at the same time.

Incircle test

$$\begin{vmatrix} a_x & a_y & a_x^2 + a_y^2 & 1 \\ b_x & b_y & b_x^2 + b_y^2 & 1 \\ c_x & c_y & c_x^2 + c_y^2 & 1 \\ d_x & d_y & d_x^2 + d_y^2 & 1 \end{vmatrix}$$

- If this determinant is 0 then point *d* is inside the circle through points *a*, *b*, and *c*?
- Why?
- Assuming linear trajectories, roots of a 4-th degree polynomial need to be determined to find time *t* where these 4 points are cocircular.

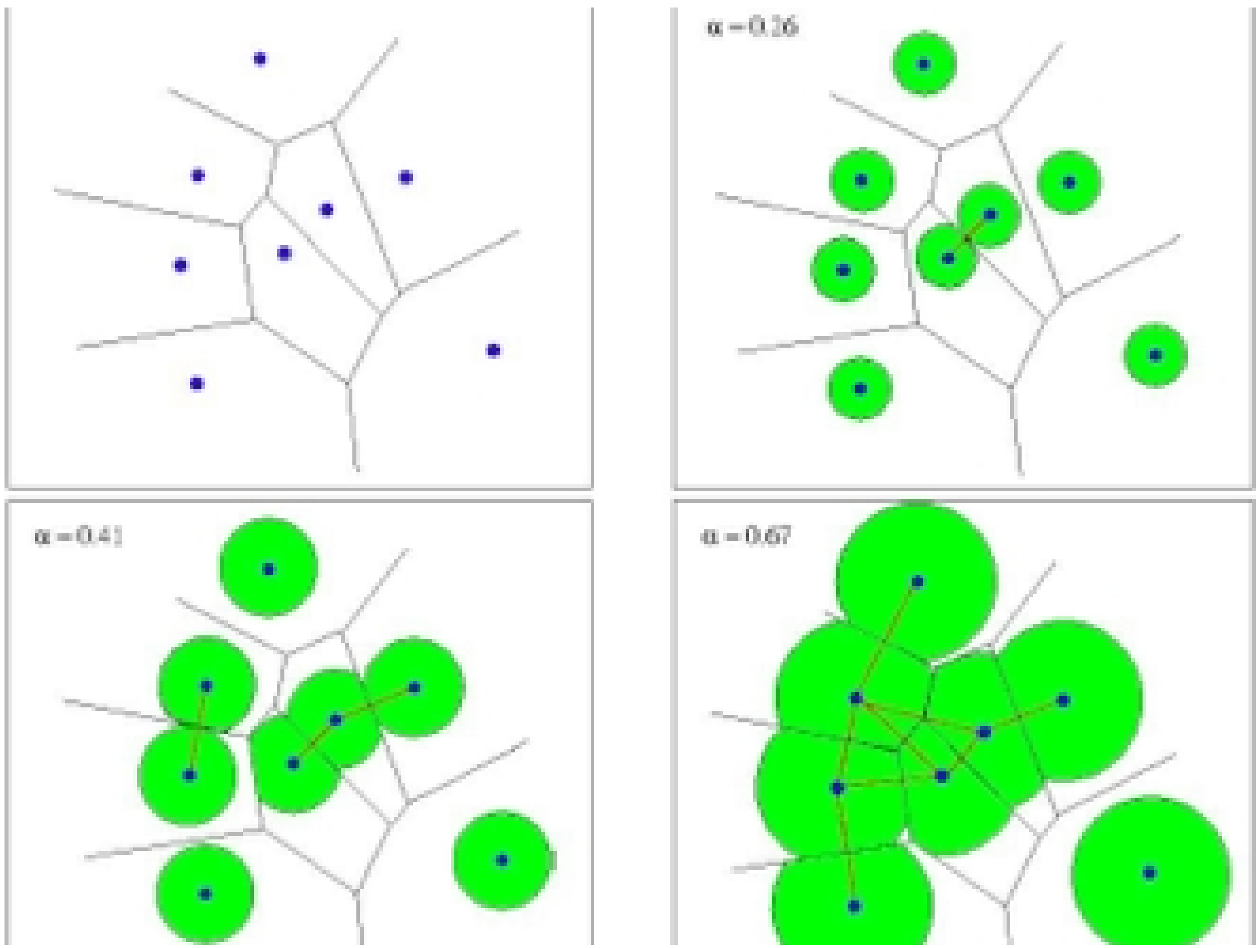
Events – Kinetic DT in R^2

- Determine DT at $t = 0$.
- Identify times for flip events for pairs af triangles sharing an edge and place these events on a heap. One certificate pr. edge.
- Repeat:
  - Remove top flip events from the heap and flip.
  - Delete future events involving one of the two deleted triangles (or use lazy deletion).
  - Identify times for up to 5 new flip events and place them on the heap.
- until the heap is empty or $t > t_{\text{end}}$

Kinetic DT in R^2

- Responsive: Well, flips require O(1) time, 5 new certificates need to be added. Computing their failure time depends on trajectories. Linear trajectories involve finding roots of polynomials of at most 4-th degree.
- Compact: Yes, O(*n*) certificates at any time since DT is planar.
- Local: No, but expected degree of a vertex in DT is 6, so this is the expected number of certificates involving it.
- Efficient: Unsure. Some scheduled events can become inactive due to neighboring flips

α-Complexes via Voronoi Diagrams



α-Complexes via Delaunay Triangulations

- 0-simplex=vertex, 1-simplex=edge, 2-simplex = triangle, 3-simplex = tetrahedron (in R^3)
- *k*-simplex is short iff its smallest circumcircle has radius at most α.
- *k*-simplex is Gabriel iff its smallest circumcircle contains no other points.
- *k*-simplex of DT is in αC iff it short and Gabriel, or it is a face of another DT-simplex that is short and Gabriel.
- A face of a short simplex is short but a face of a Gabriel simplex is not necessarily Gabriel.

Events – Kinetic αC in R^2

- Determine DT at $t = 0$.
- Short triangles of DT are automatically Gabriel. They and their faces are in αC.
- If an edge is not already in αC, it is checked if it is short and Gabriel. If so, it is added to αC.
- Times for flip and radius events are determined and stored in a heap.
- What about Gabriel events for edges? They are actually redundant.

Redundancy of Gabriel Events

- Any triangle of αC in R^2 is automatically Gabriel (otherwise it would not be in DT).
- Consider an edge *ab* of DT that is about to change from Gabriel to non-Gabriel or vice versa.
- At the time of transition, its smallest circumcircle goes through *a* and *b* and through a third vertex *c*.
- Δabc is short and Gabriel and therefore in αC. Hence, all faces of Δ*abc* (including *ab*) are in αC.

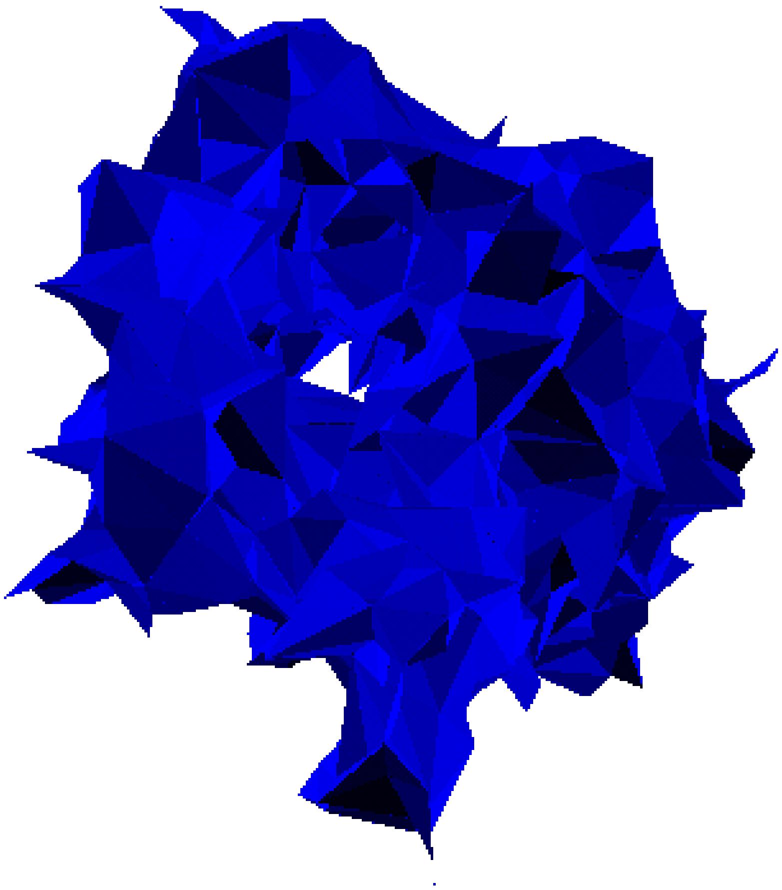
Kinetic αC in R^2

- Place flip events for pairs of edge-sharing DT-triangles and radius events for DT-triangles and DT-edges on a heap.
- Repeat:
  - If next is a flip event, flip. If the original pair of triangles was short so is the new pair. If it was non-short, check if the new edge is short. Create 5 new flip events.
  - If it is a radius event and its simplex σ is to become
    - short: If σ is Gabriel, σ and all its faces are added to αC.
    - non-short: all faces of σ are short. Remove σ from αC (if it is in αC). If a face of σ is not Gabriel and has no other coface in αC, σ has to be removed from αC.
- until the heap is empty or $t > t_{end}$

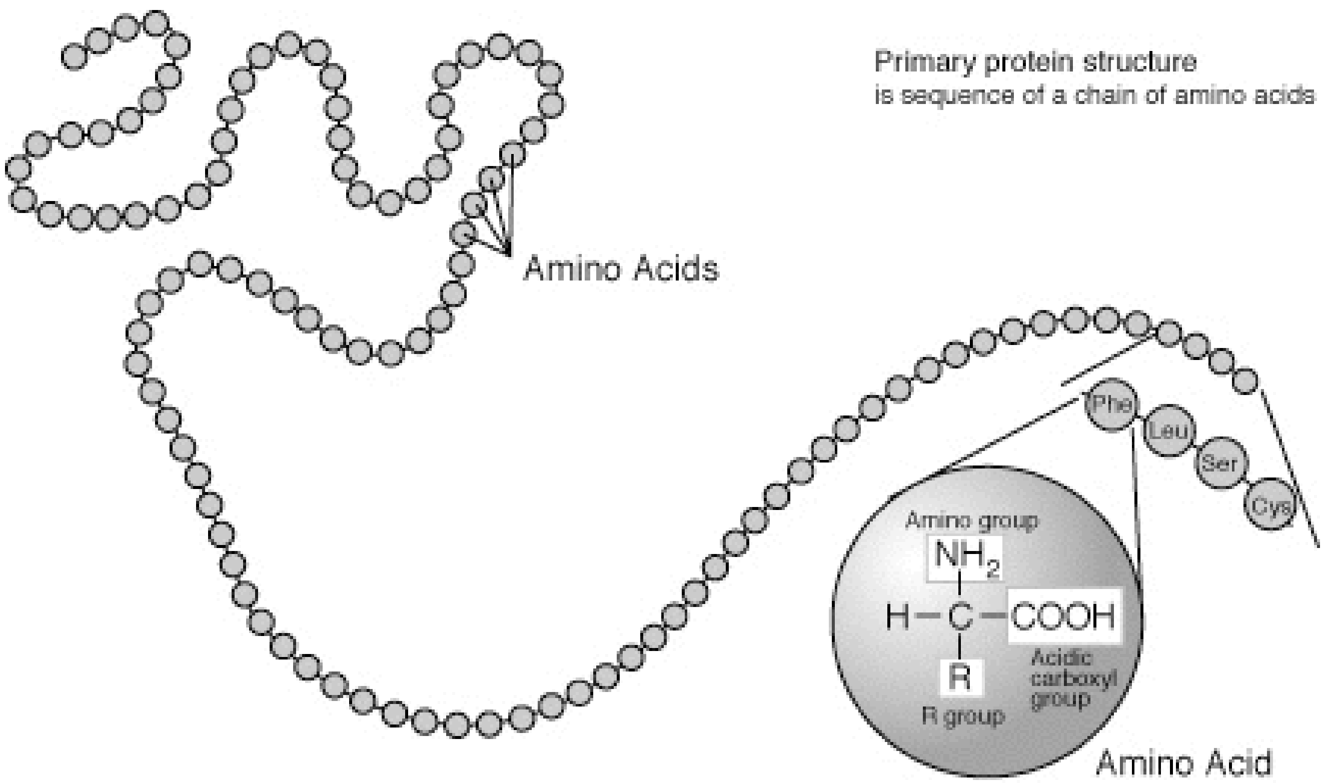
Certificate Failures

- Assuming piecewise-linear trajectories, finding the time when a radius certificate of an
  - Edge-sharing pair of DT-triangles fails, requires finding a root of a polynomial of degree 2.
  - triangle fails, requires finding a root of a polynomial of degree 5.
  - tetrahedron fails, requires finding a root of a polynomial of degree 8 (this is R^3 case).

A-Complexes of Proteins



Amino Acid Chain

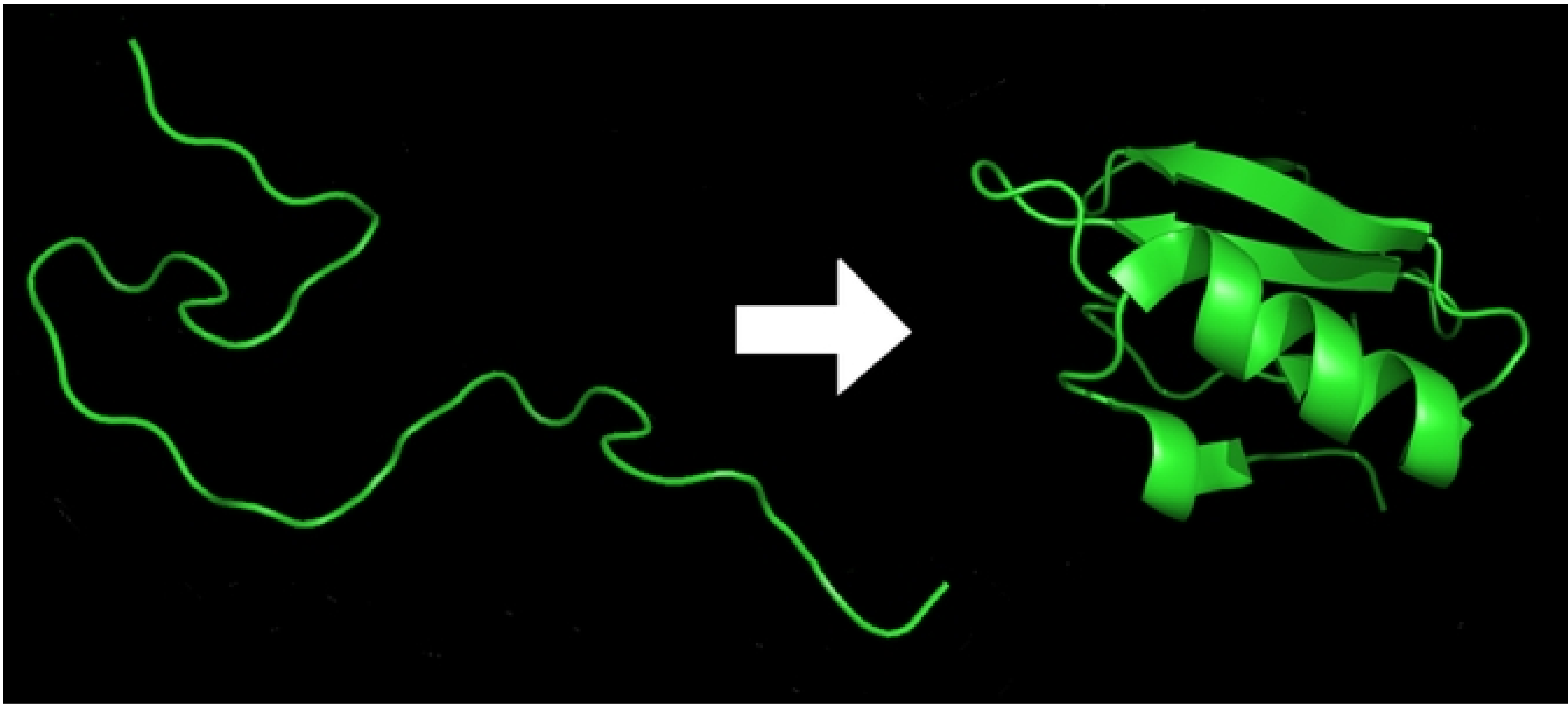


From wikipedia

Backbone: disregard side chains and hydrogens.

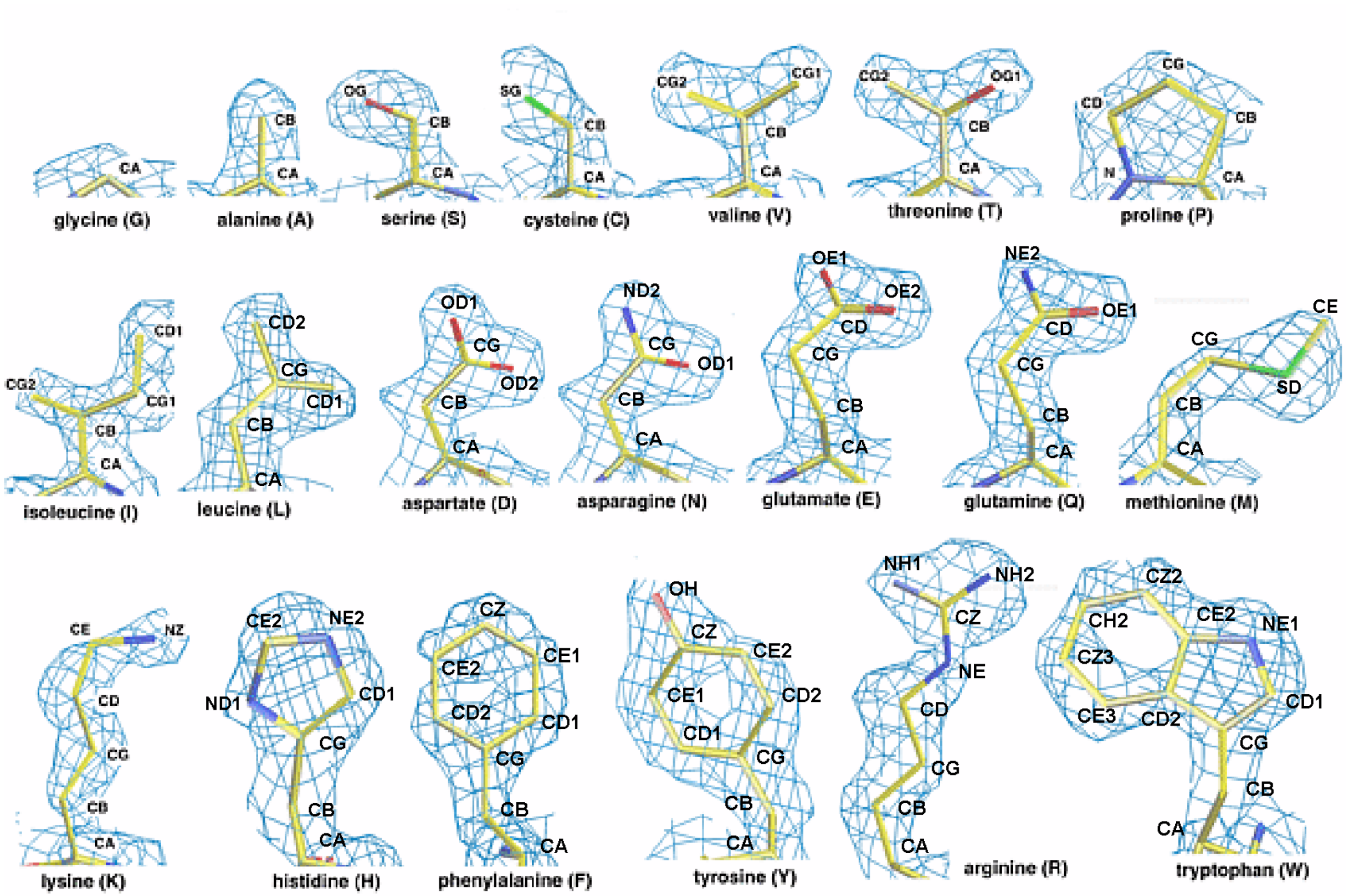
C_α-trace: disregard all but C_α-atoms.

Folding



From Wikimedia Commons

20 Different Side Chains



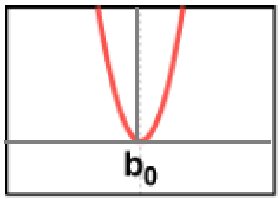
0-5 degrees of freedom pr. side chain

From http://www.doe-mbi.ucla.edu/Legacy/CHEM153BH/info2.htm

Potential Energy Function

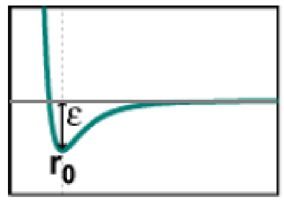
- U = Bond + Angle + Dihedral + van der Waals + Electrostatic[1,2,3]

Bonded interactions



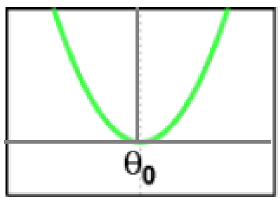
Bond

$$\sum_{i}^{bonds} K_{b,i}(b_i - b_{0,i})^2$$



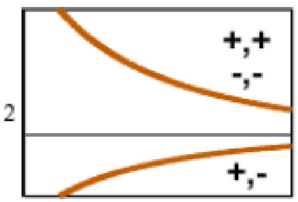
van der Waals

$$\sum_{pairs\text{-}i,j} [\varepsilon_{ij}\left(\frac{r_{0,ij}}{r_{ij}}\right)^{12} - 2\varepsilon_{ij}\left(\frac{r_{0,ij}}{r_{ij}}\right)^{6}]$$



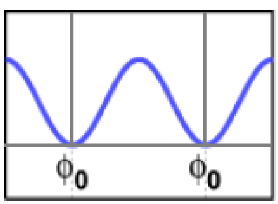
Angle

$$\sum_{i}^{bond\ angles} K_{\theta,i}(\theta_i - \theta_{0,i})^2$$



Electrostatic

$$332 \sum_{pairs\text{-}i,j} \left(\frac{q_i q_j}{r_{ij}}\right)$$



Dihedral

$$\sum_{i}^{torsion\ angles} K_{\phi,i}\{1 - \cos[n_i(\phi_i - \phi_{0,i})]\}$$

Nonbonded interactions

1. Levitt M. Hirshberg M. Sharon R. Daggett V. Comp. Phys. Comm. (1995) 91: 215-231
2. Levitt M. *et al.* J. Phys. Chem. B (1997) 101: 5051-5061
3. Dynameomics: Protein Mechanics, Folding and Unfolding through Large Scale All-Atom Molecular Dynamics Simulations. David A. C. Beck. Valerie Daggett Research Group

α-Complexes for Rotating R^2-Points

- Subset of points rotates around common point with the same circular velocity.
- Flip and radius events require solutions of second degree polynomials

α-Complexes for Rotating R^3-Points

- Subset of points rotates around common axis with the same circular velocity.
- Flip and radius events require solutions of fourth degree polynomials.
- Radius events for tetrahedra with 2 rotating and two stationary points still refuses to be solved analytically.