Motion Algorithms

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Basic Question

Can two given points be connected by a path in a feasible space?
Configuration Space

Issues:
• Space dimensionality
• Geometric complexity
Any moving object maps to a point in its configuration space
Probabilistic Sampling

feasible space
Connectivity Issue

The $\beta$-lookout of a subset $X$ of $F$ is the set of all configurations in $X$ that see a $\beta$-fraction of $F\setminus X$

$$\beta\text{-lookout}(X) = \{ q \in X \mid \mu(V(q)\setminus X) \geq \beta \times \mu(F\setminus X) \}$$
$(\varepsilon, \alpha, \beta)$-Expansiveness of $F$

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$F$ is $(\varepsilon, \alpha, \beta)$-expansive if it is $\varepsilon$-good and each one of its subsets $X$ has a $\beta$-lookout whose volume is at least $\alpha \times \mu(X)$

[Hsu et al., 1997]
- Expansiveness only depends on **volumetric ratios**
- It is not directly related to the dimensionality of the configuration space

In 2-D the expansiveness of the free space can be made arbitrarily poor
Let $F$ be $(\varepsilon, \alpha, \beta)$-expansive, and $s$ and $g$ be two configurations in the same component of $F$. BasicPRM$(s, g, N)$ with uniform sampling returns a path between $s$ and $g$ with probability converging to 1 at an exponential rate as $N$ increases.

$$\gamma = Pr(\text{Failure}) \leq \left( \frac{c_1}{\varepsilon \alpha} \right) \exp\left( c_2 \varepsilon \alpha (-N + \frac{c_3}{\beta}) \right)$$
Most narrow passages in F are intentional ...

... but it is not easy to intentionally create complex narrow passages in F
Automatic robot programming

Reconfigurable robots

Assembly planning

Crowd simulation (egress)

Space robotics

Building code verification
Current projects

ai.stanford.edu/~latombe/projects/projects-www.html

- Development of a fully autonomous climbing robot

- Study of the long-timescale dynamics of protein
Autonomous Climbing Robots

Lemur

Capuchin
Motion of a Protein

<table>
<thead>
<tr>
<th>Bond/atomic vibration</th>
<th>Water dynamics</th>
<th>Helix forms</th>
<th>Fast anisotropic conf change</th>
<th>Slow conf change</th>
</tr>
</thead>
<tbody>
<tr>
<td>$10^{-15}$ femtosec</td>
<td>$10^{-12}$ picosec</td>
<td>$10^{-9}$ nanosec</td>
<td>$10^{-6}$ microsec</td>
<td>$10^{-3}$ millisec</td>
</tr>
<tr>
<td>MD step</td>
<td>one-day MD run</td>
<td>long MD run</td>
<td>where we need to be</td>
<td>where we’d love to be</td>
</tr>
</tbody>
</table>
Approaches

1. **Experimental approach:** Model discrete heterogeneity in proteins from X-Ray crystallography data

2. **Geometric/kinematic approach:** Explore reachable conformation space under geometric/kinematic constraints

3. **Markov model approach:** Model long timescale dynamics with Hidden Markov Models trained from Molecular Dynamics simulation trajectories
X-Ray Crystallography
Multiple states lead to ambiguous density
Multi-Conformer Approach

1. **Sample** a huge set $C$ of candidate conformers

2. Select the subset $M$ that collectively best models the electron density map (EDM)
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Multi-Conformer Approach was Used to produce PDB ID: 3eo6