Open Discussion of Plans for Spatially Structured Molecules in BioNetGen and MCell

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Diffusion: Fick's Second Law

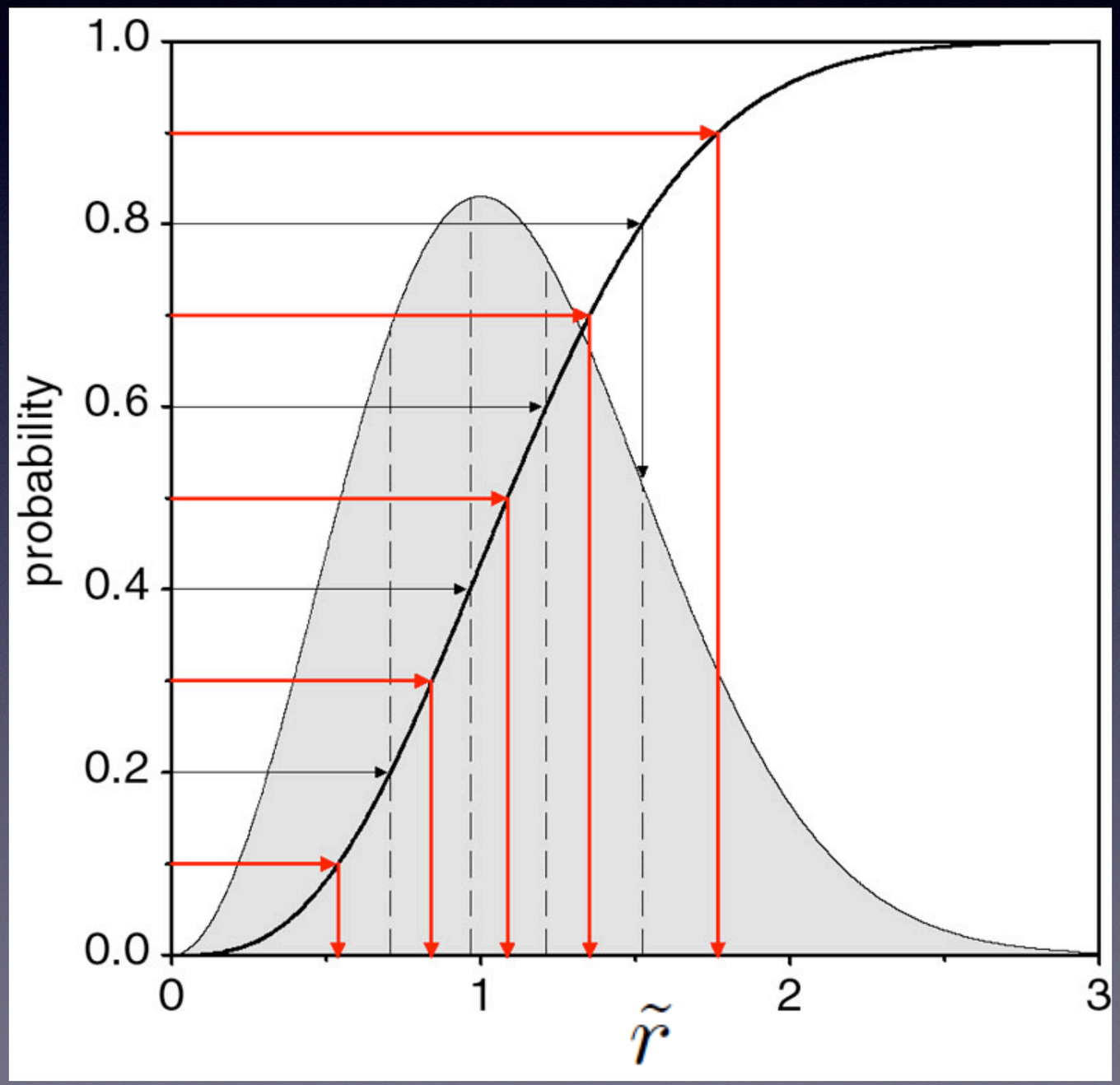
Applies when concentration in volume is changing in time (i.e. $J_{in} \neq J_{out}$)

$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2}$$

$$\frac{\partial c}{\partial t} = D \nabla^2 c$$

Free Diffusion: Concentration in Space and Time

$$\rho(r,t) = \frac{1}{\pi^{d/2}\lambda^d} e^{-r^2/\lambda^2}$$



$$\lambda = \sqrt{4Dt}$$

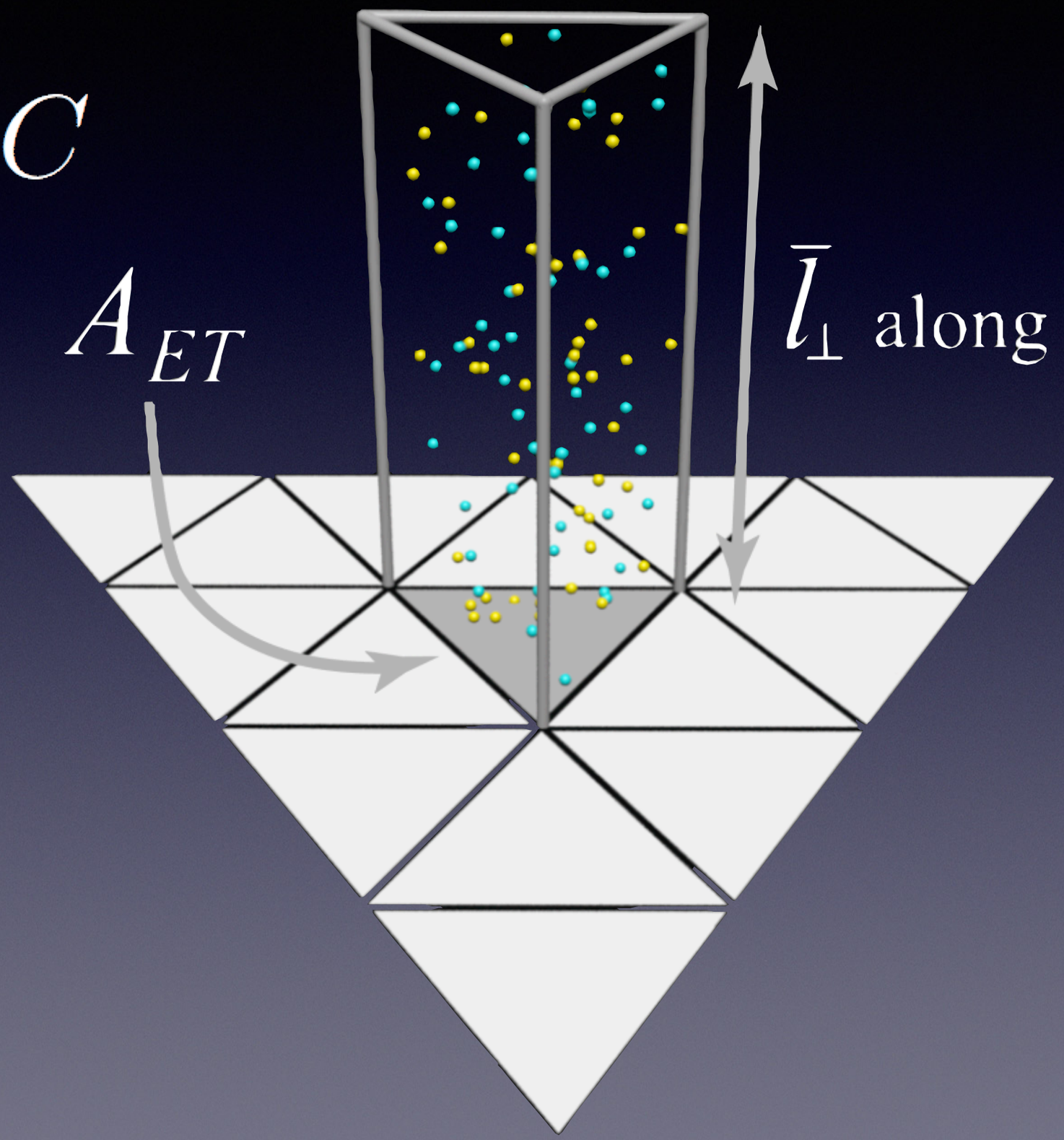
$$\tilde{r} = r/\lambda$$

$$\bar{l}_r = 2\sqrt{\frac{4D\Delta t}{\pi}}$$

$$\bar{l}_\perp = \sqrt{\frac{4D\Delta t}{\pi}}$$

Bimolecular Reactions:
Rate of Encounter of Particles with Collision Cross-section

$$A + B \xrightarrow{k} C$$



Bimolecular Reactions:
Derivation of probability of reaction per collision

$$A + B \xrightarrow{k} C$$

Probability of reaction between diffusing volume molecule and a surface molecule:

From rate of encounter:

$$p_{bt} = 1 - (1 - p_b)^{N_H} \approx N_H p_b$$

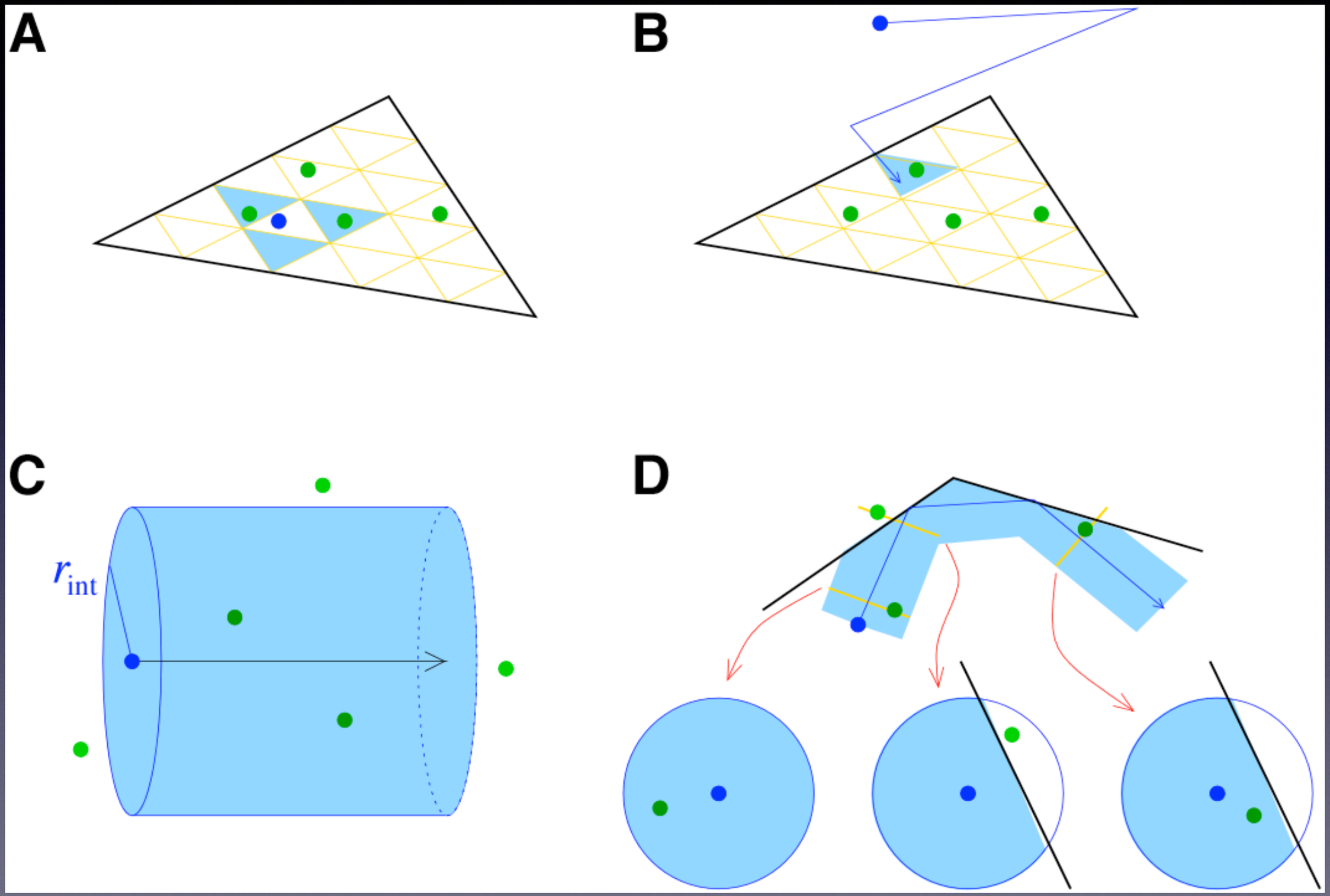
$$N_H = N_A \bar{l}_\perp A_{ET} [A]_o$$

From Mass Action:

$$p_{bt} = k[A]_o \Delta t$$

$$p_b = \frac{k}{N_A A_{ET}} \sqrt{\frac{\pi \Delta t}{D}}$$

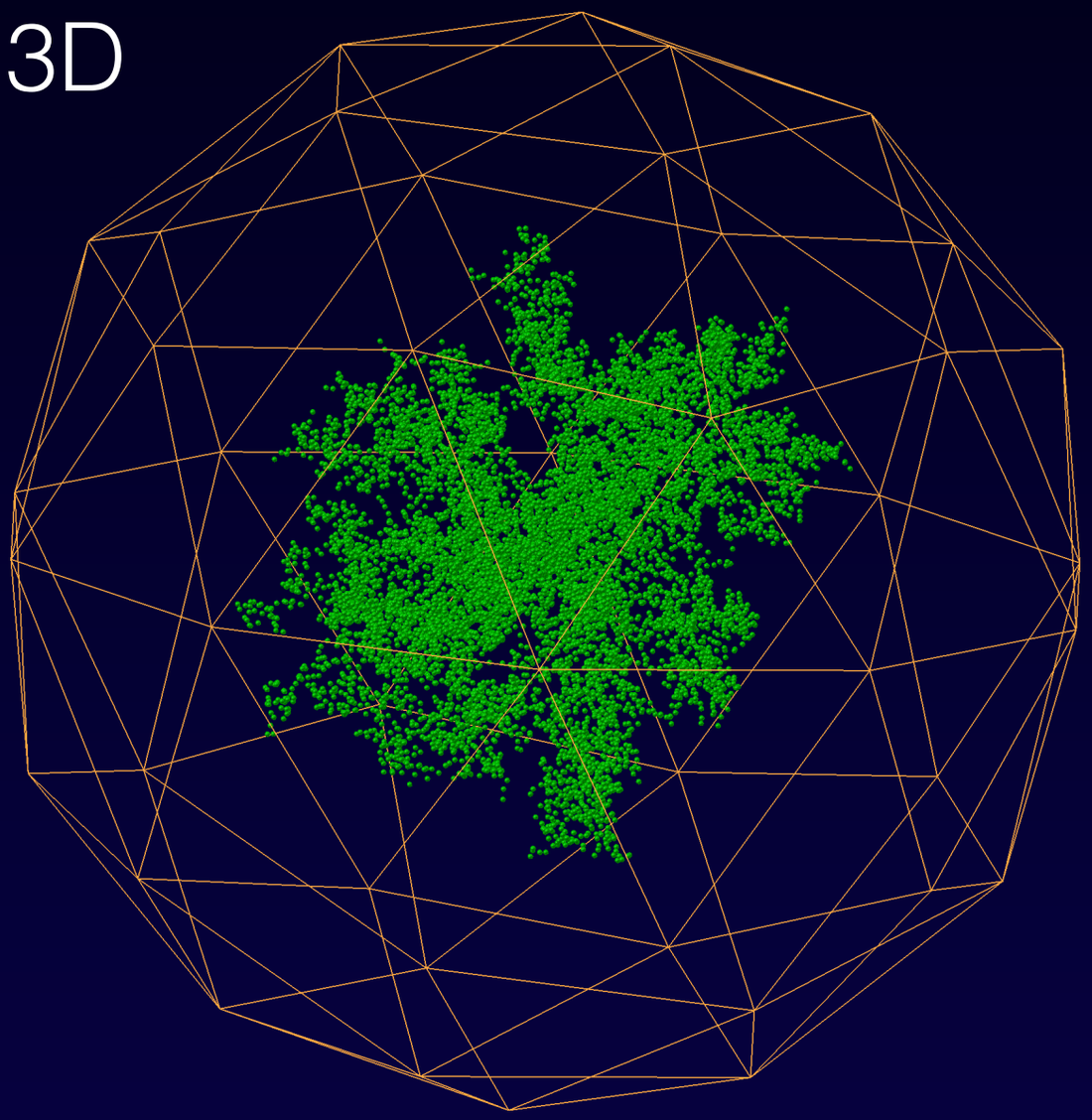
Bimolecular Reactions: Collision Detection



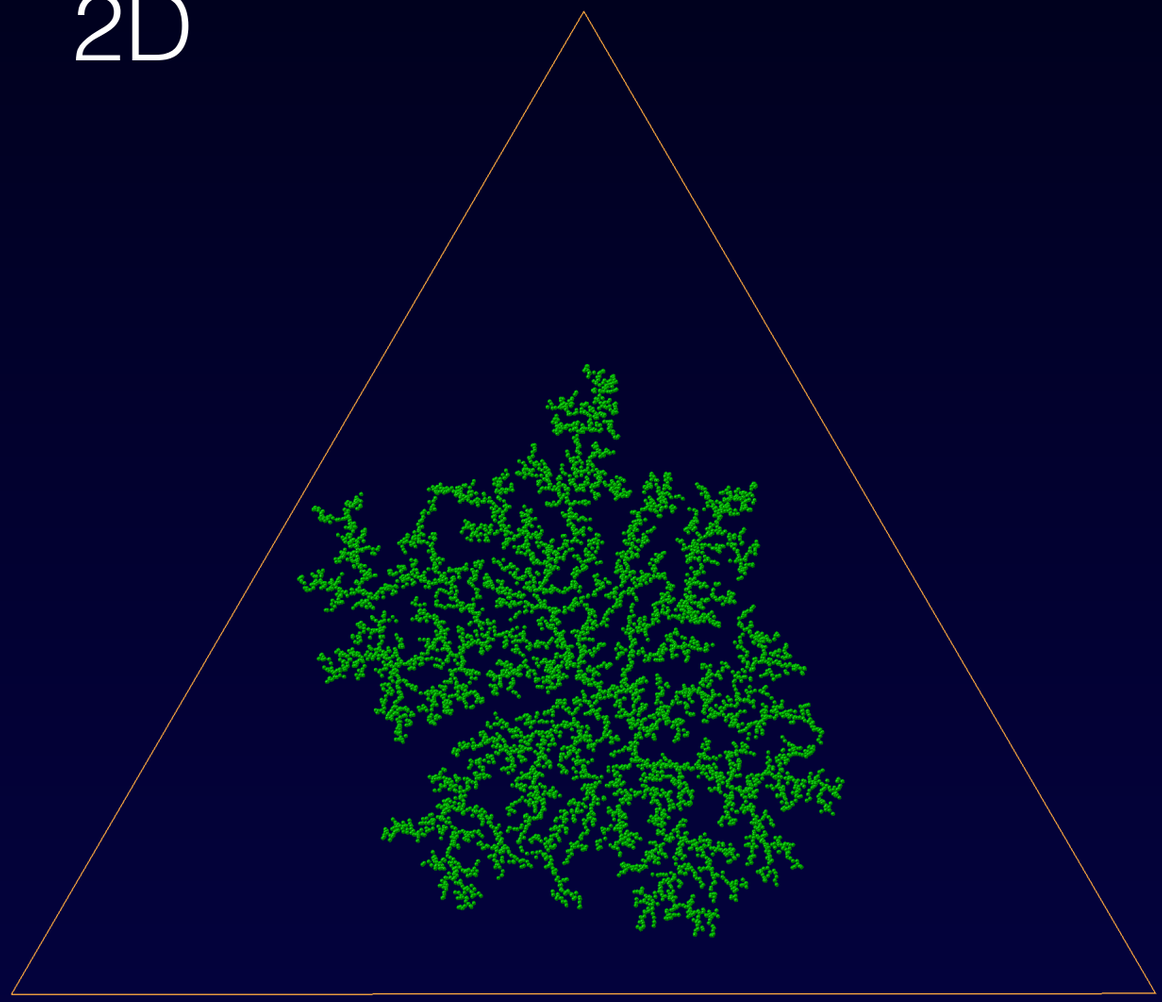
Fractal Filigree Spatial Structure Emerges From Unordered Diffusion-Limited Aggregation

$$A + B \rightarrow B + B$$

3D

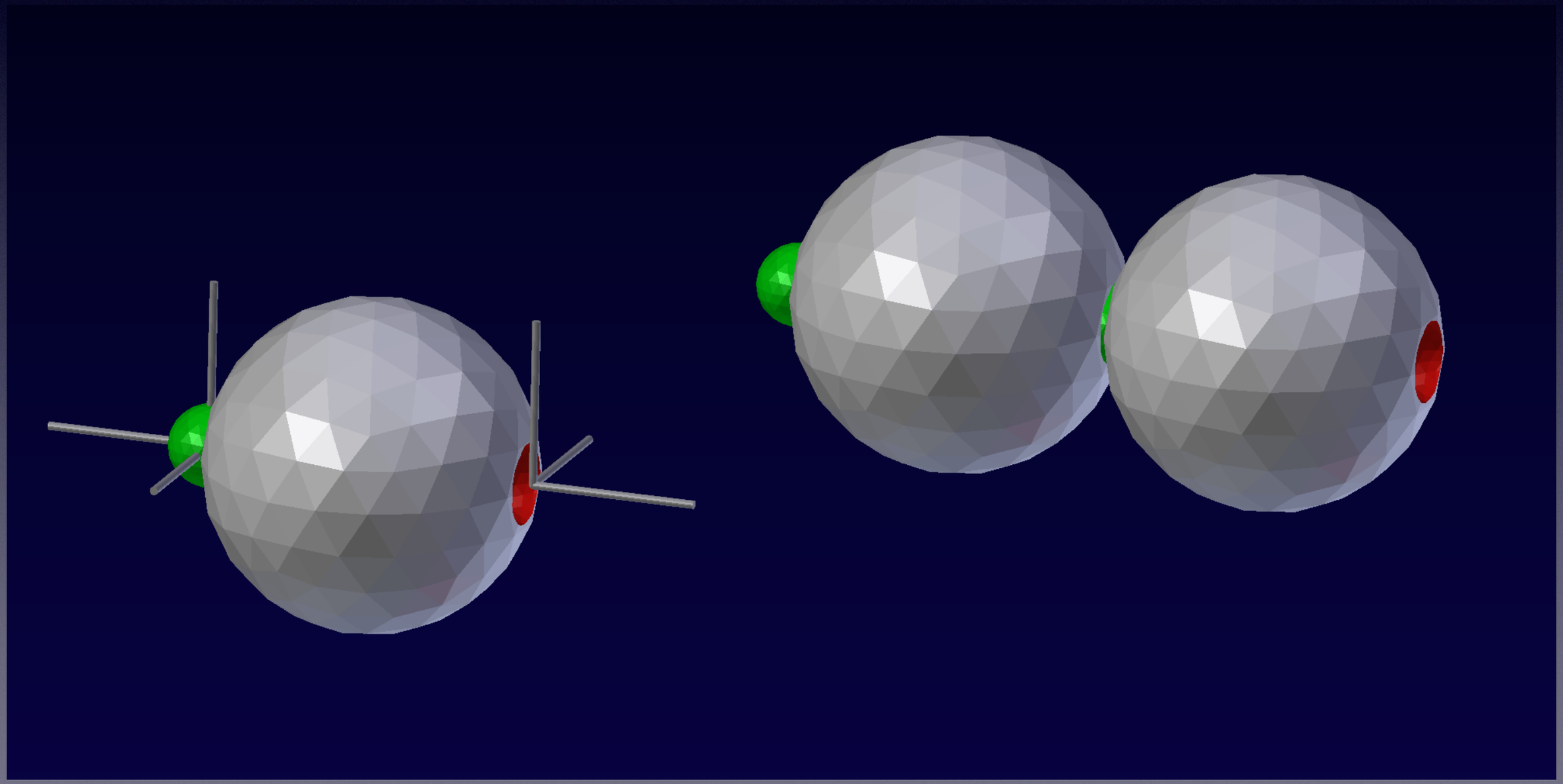


2D



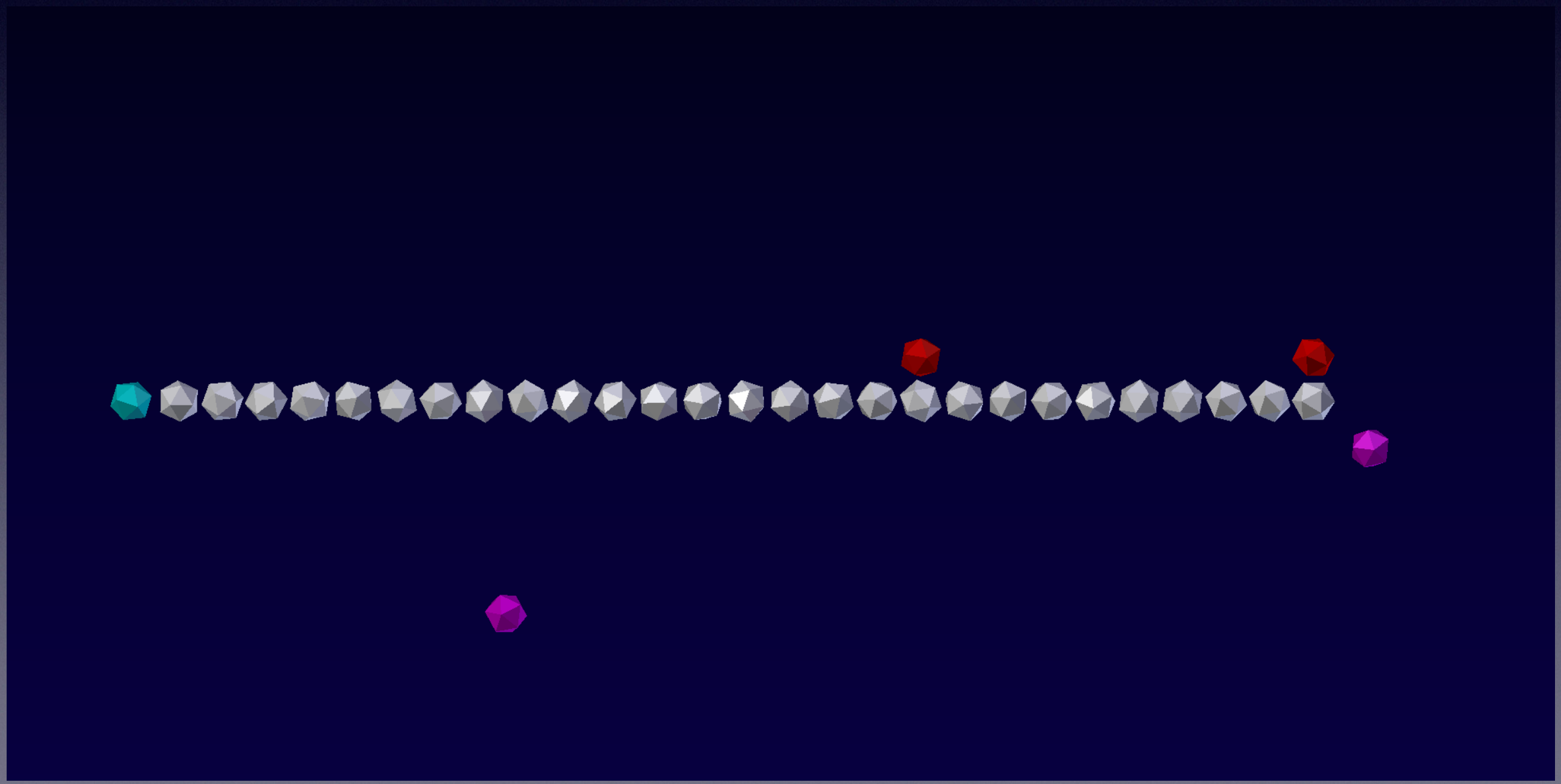
Large-Scale Ordered Spatial Structure Emerges From Simple Local Assembly Rules

Assembly by aligning and docking binding site coordinates

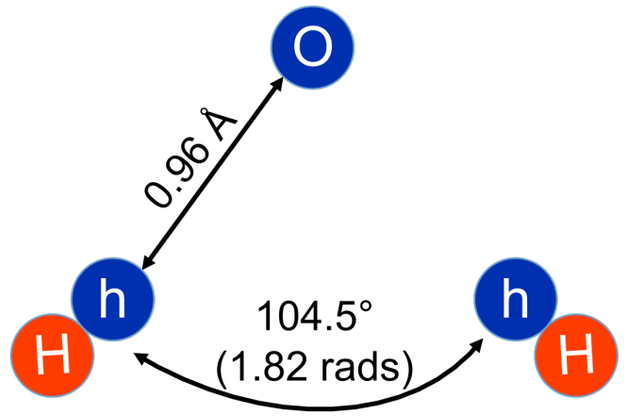


Directed Transport Along Assembled Structures

Simple example of transport on filament with MCell3-macromol



Subaim 1.1 Spatially structured, multi-state multi-component molecules

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molecule types
O[shape=sphere](h,h)
H(x)
seed species
O(h{0.96,0,0},h{0.96,1.82,0}) O_init
H(x) H_init
reaction rules
O(h) + H(x) -> O(h!b).H(x!b) k_OH
```

- Point particles
- 'h' components 0.96 Å from center of O atom
- 1.82 radians between 'h' components

Fig IV.5. Proposed syntax for spatially structured complexes in BNGL.

Issues for Discussion

1) How to get coordinates of components (i.e. binding sites)?
    a) from PDB?
2) How to do diffusion of small complexes?
    a) aggregation of macromolecule members/components?
3) How to do diffusion of large complexes?
    a) tumbling?
4) How to do collision detection?
    a) non-space-filling/non-crowding?
    b) space-filling/crowding?
5) Other issues?