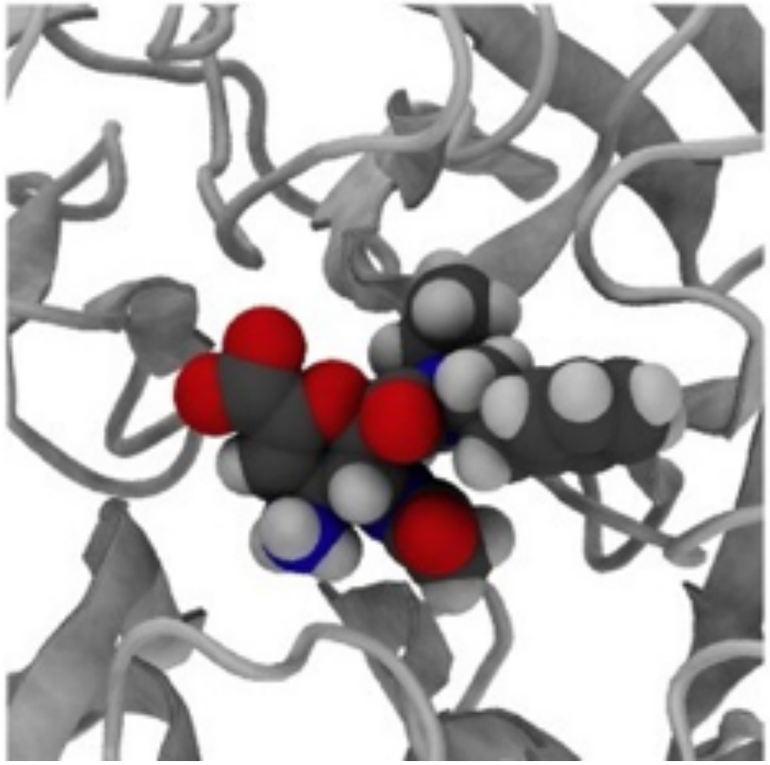
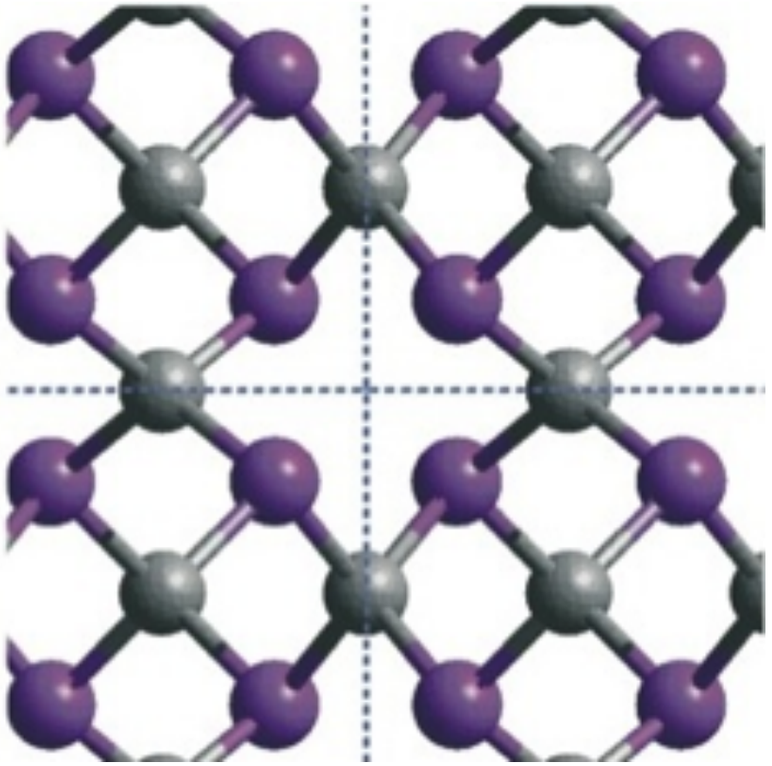
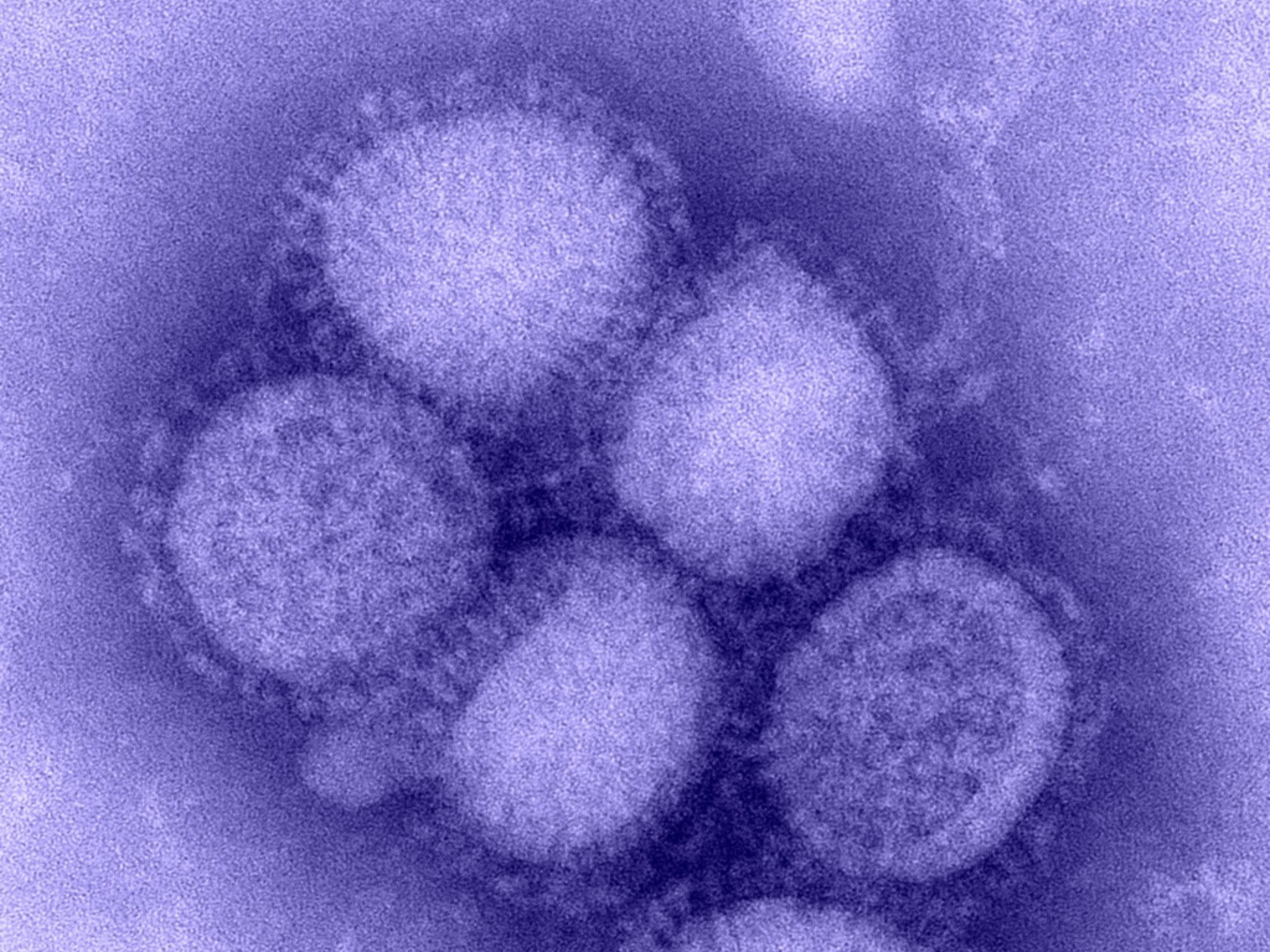
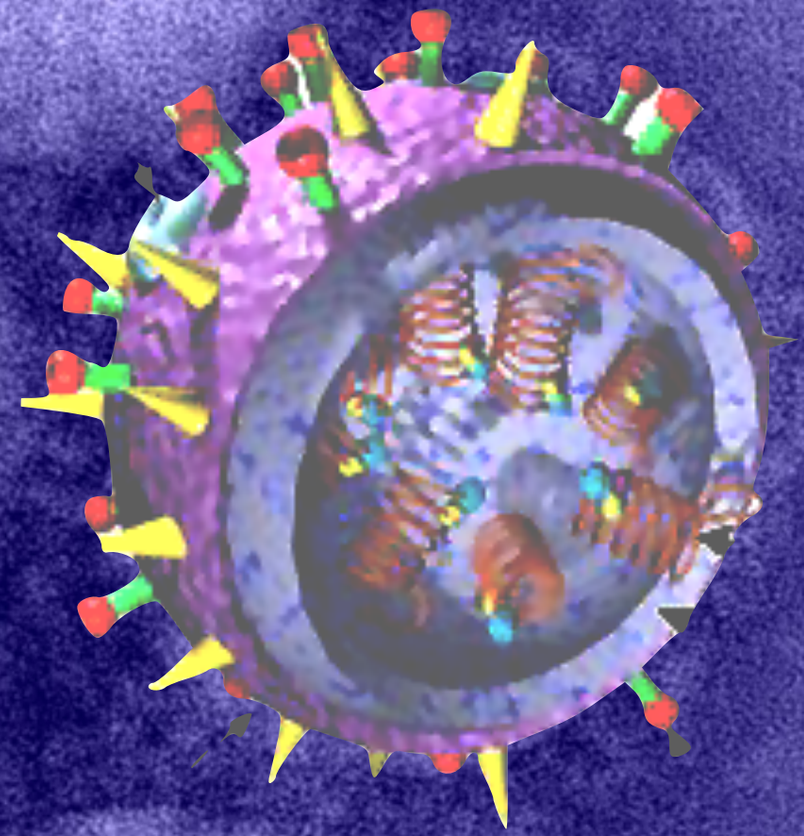
Computational Microscopes

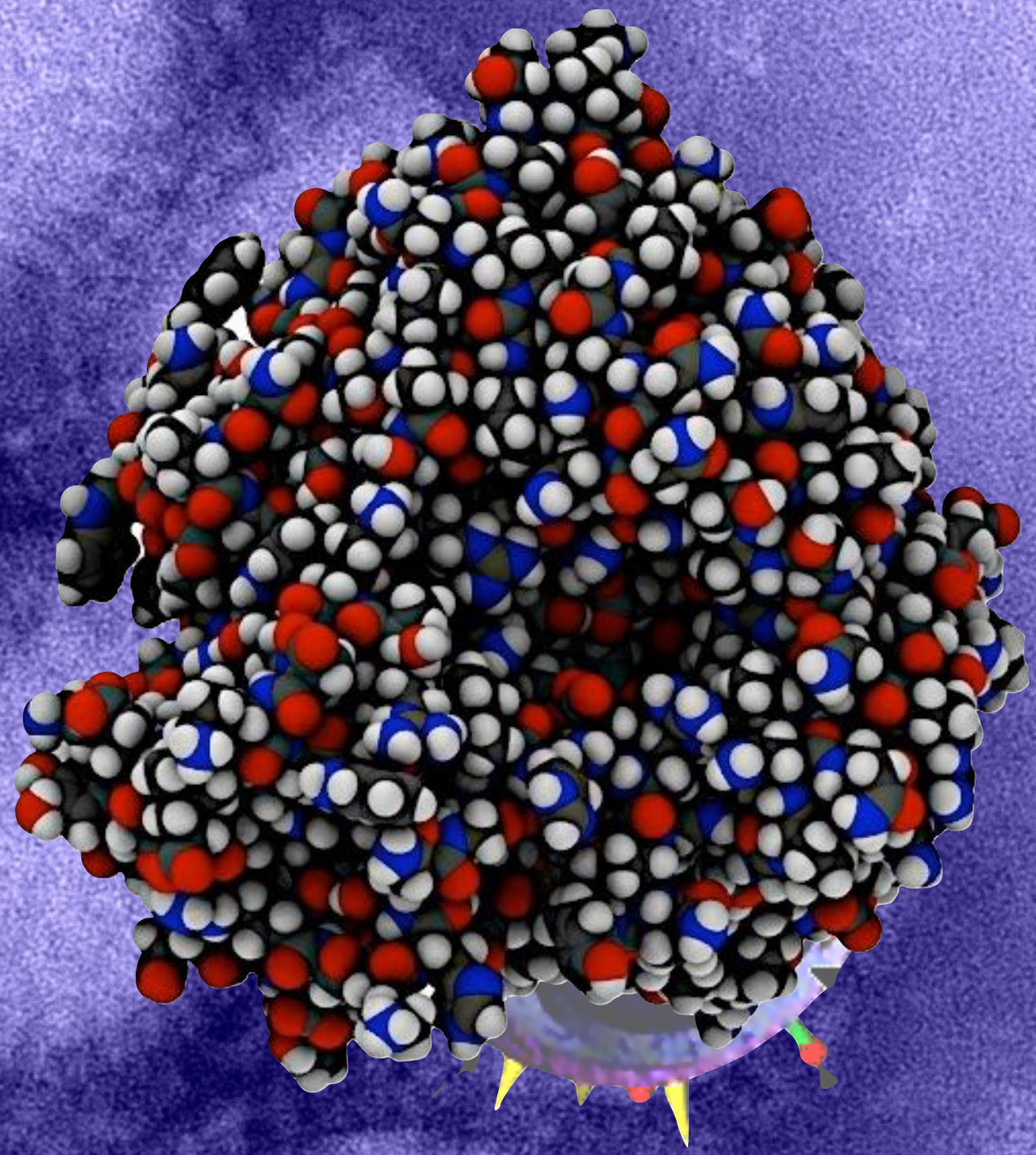
Christopher Woods
Research Software Engineer
Advanced Computing Research Centre





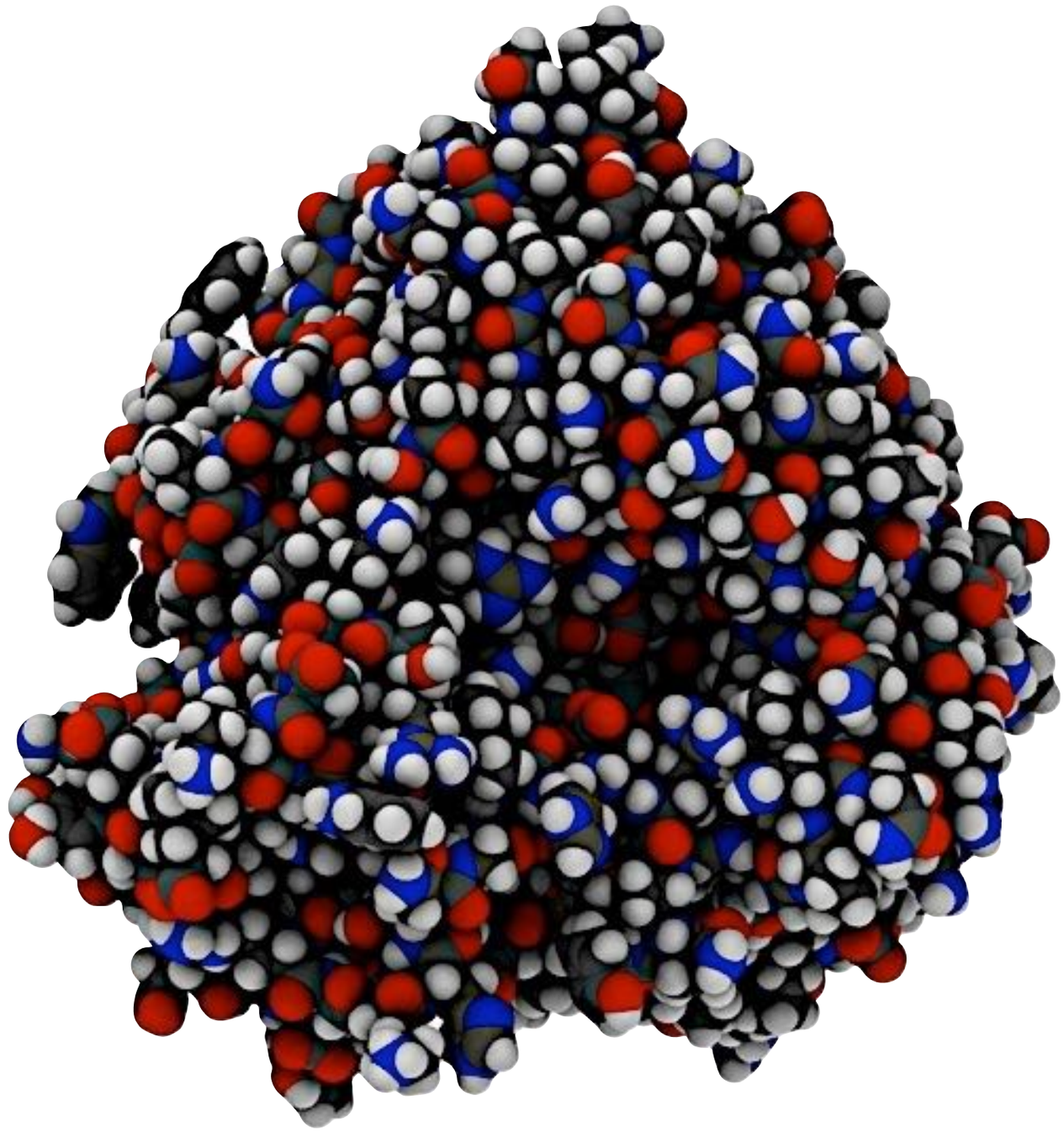






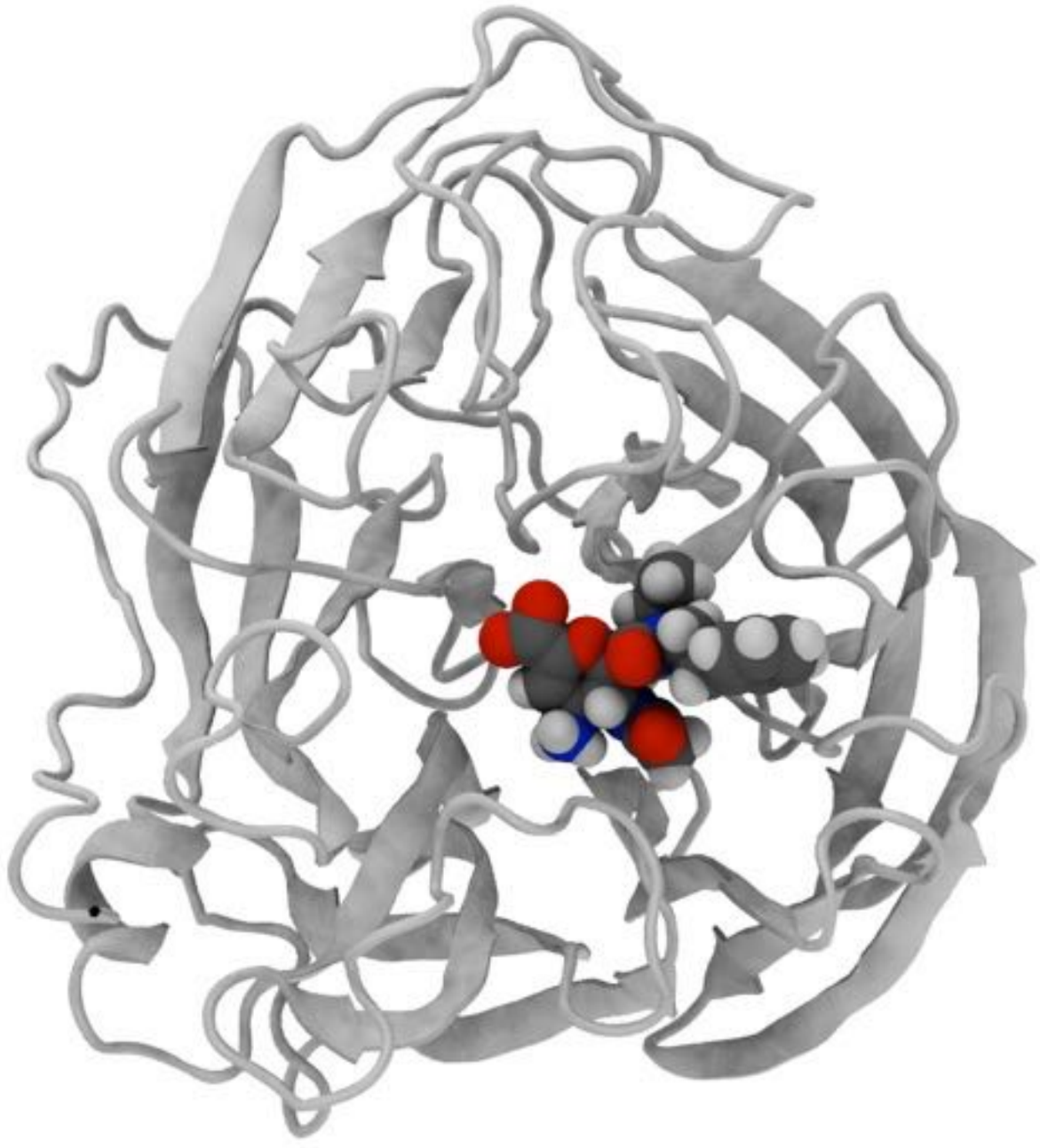
Protein

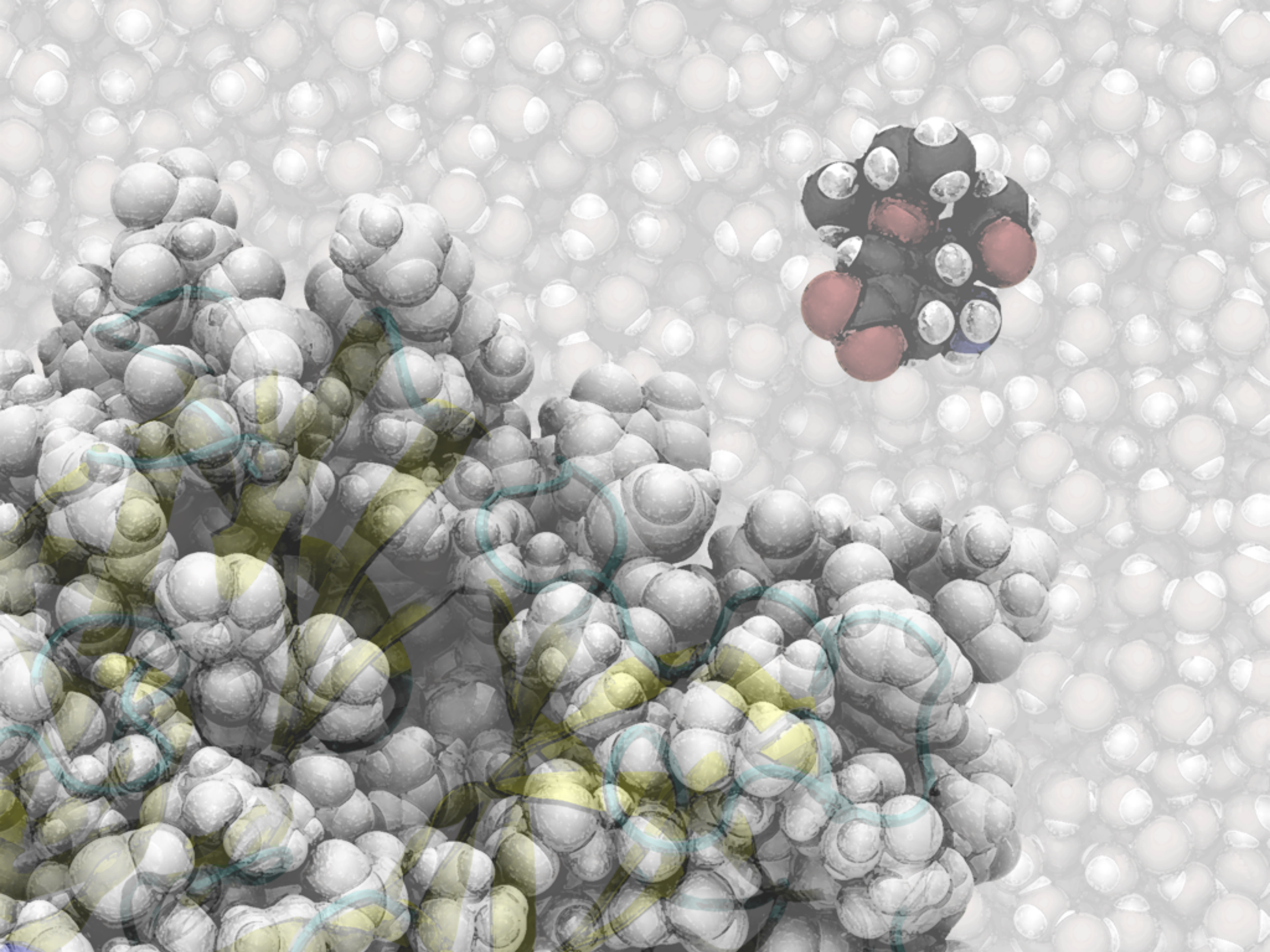
Neuraminidase



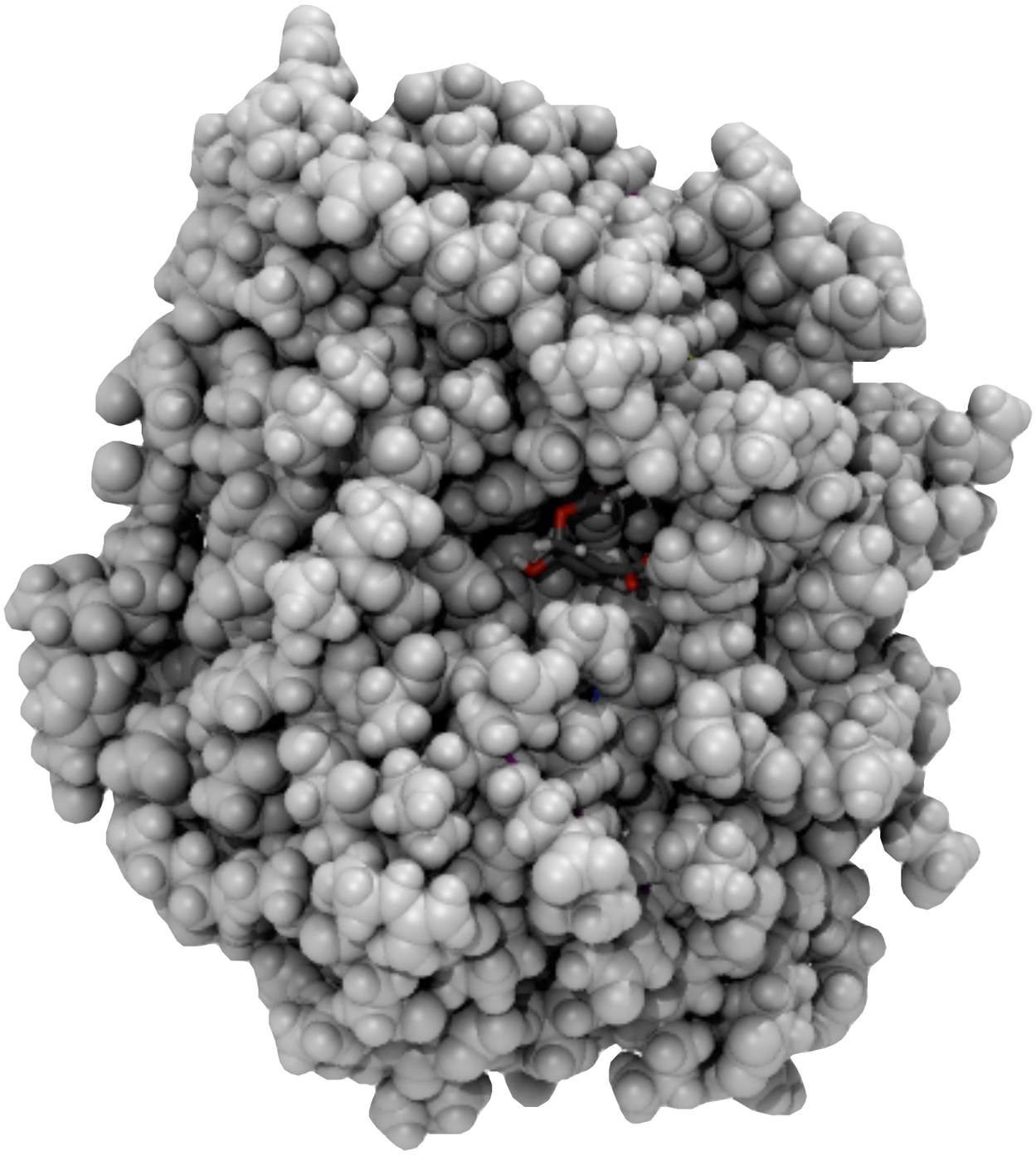
Protein

Neuraminidase





Molecular Mechanics
MM



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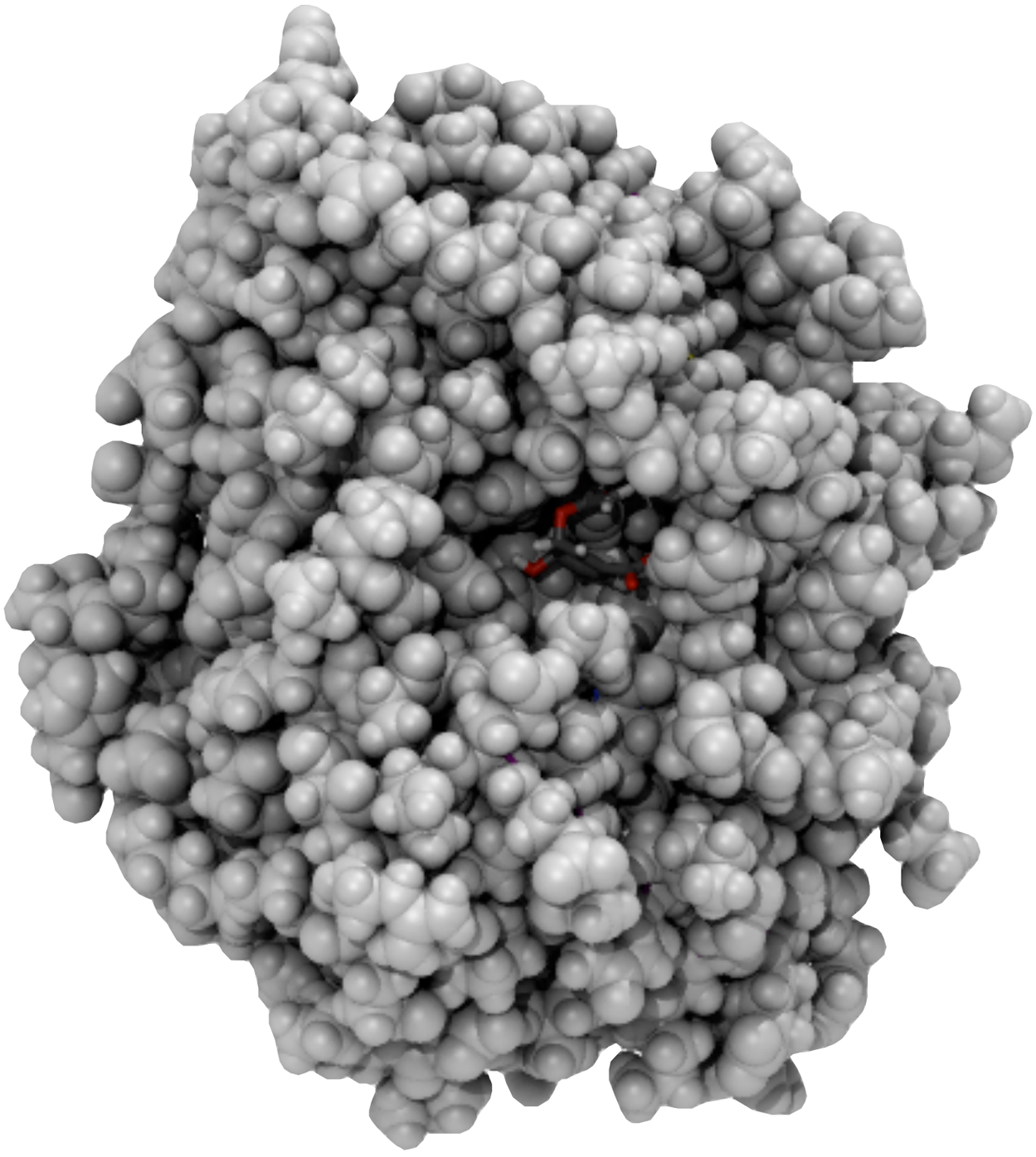

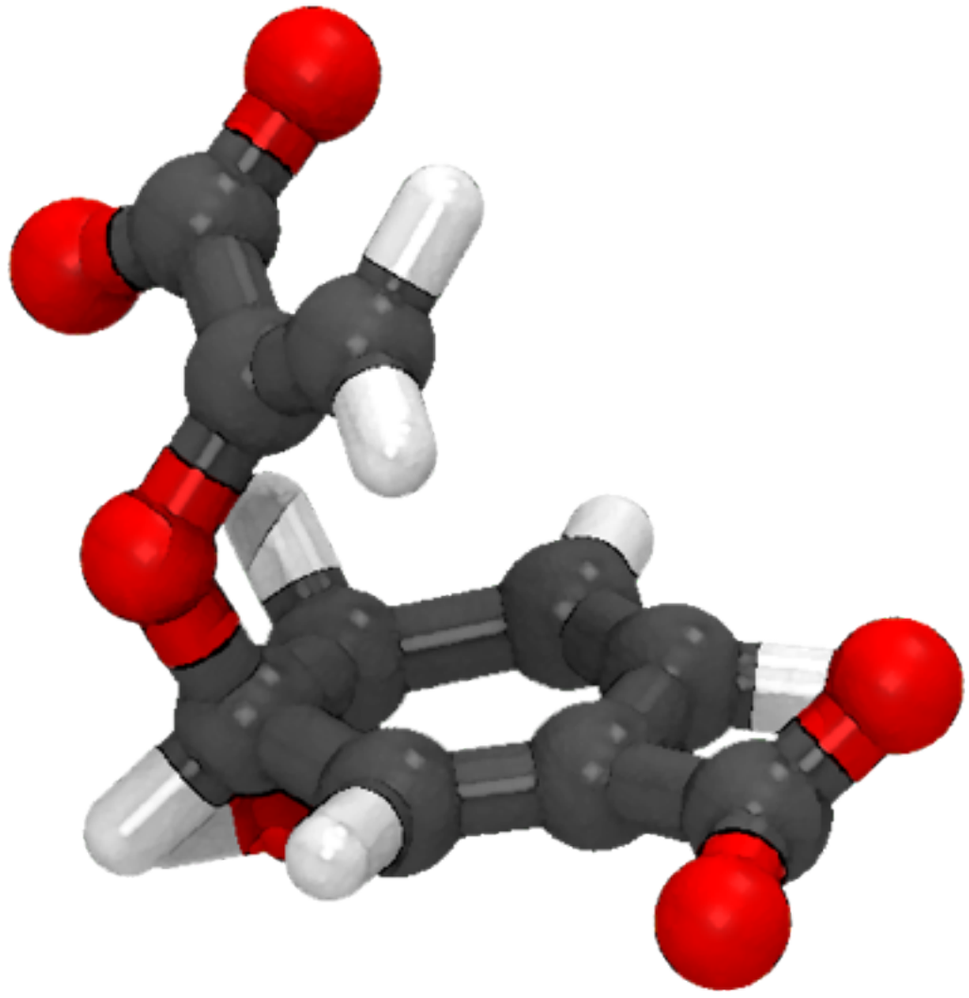

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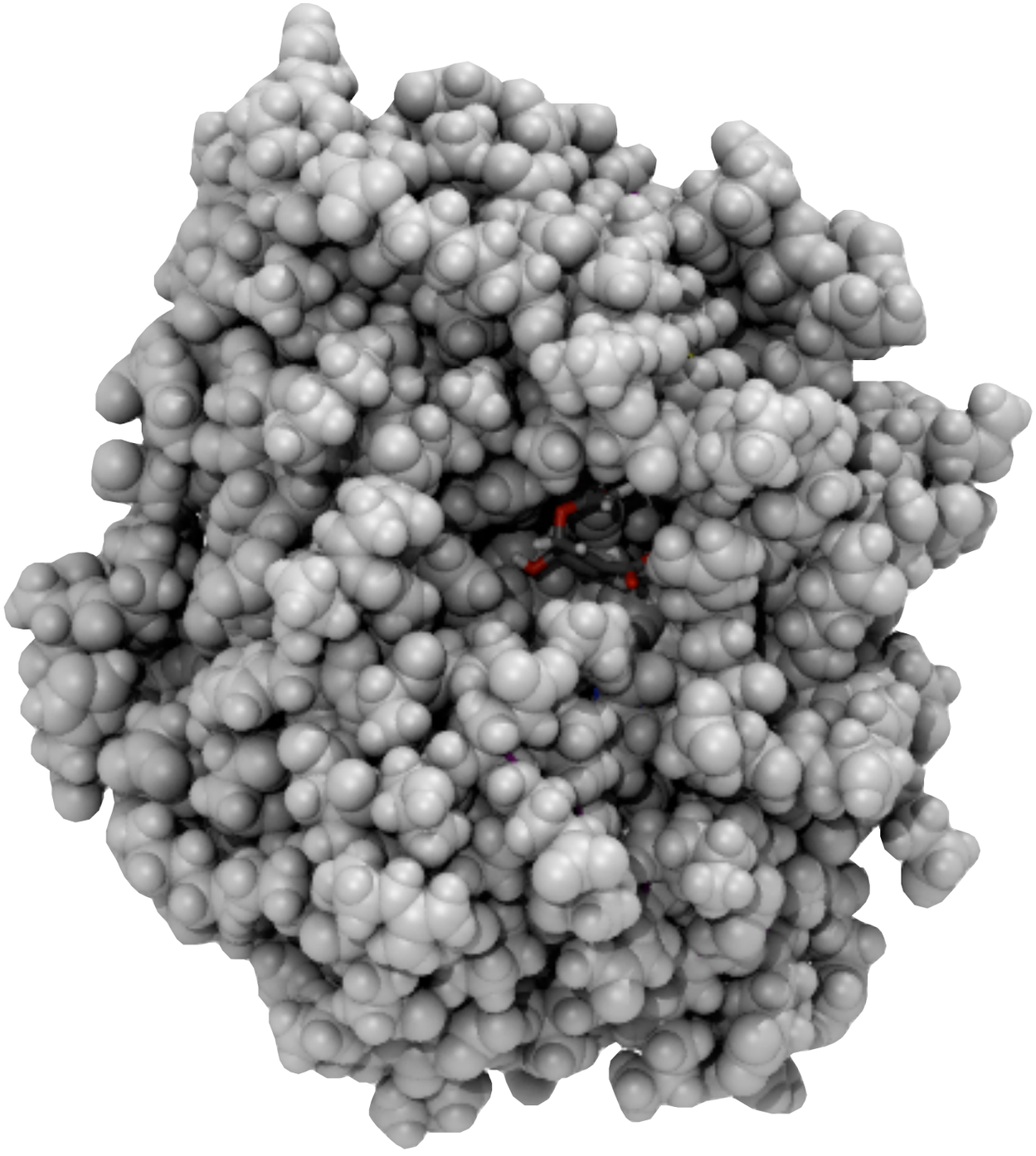
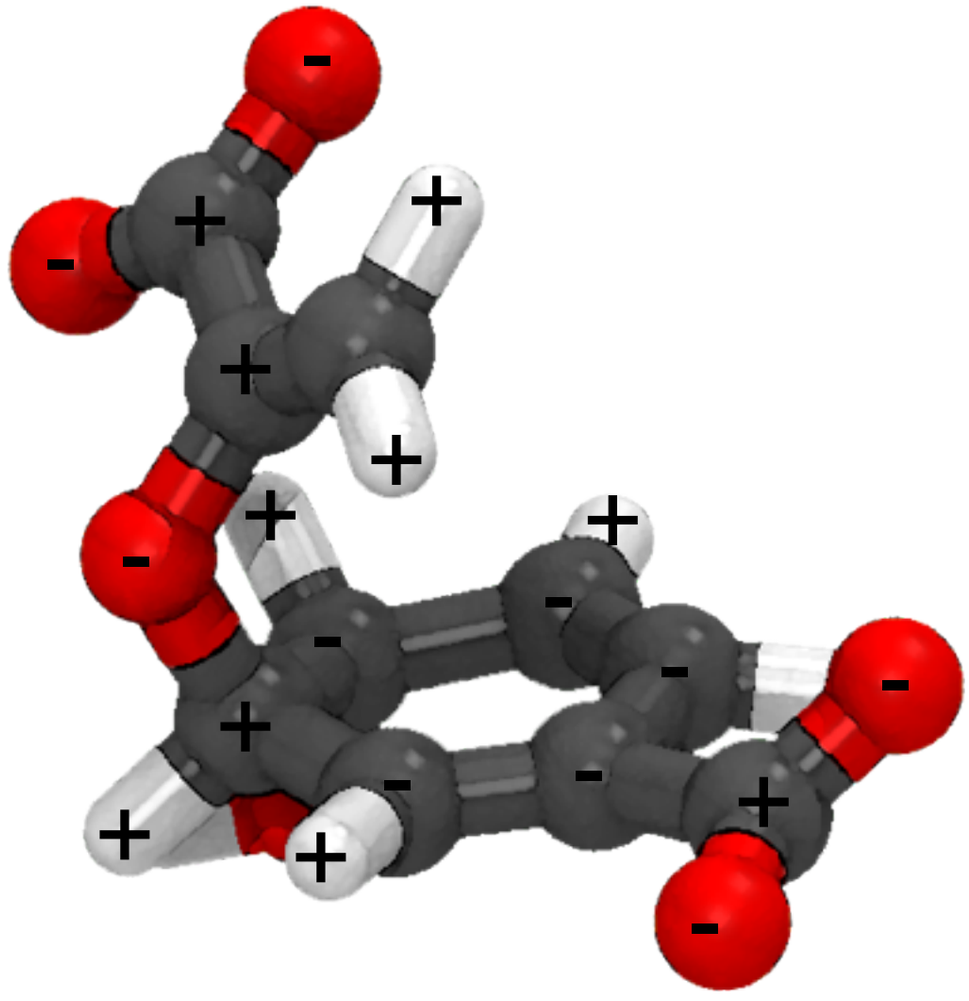
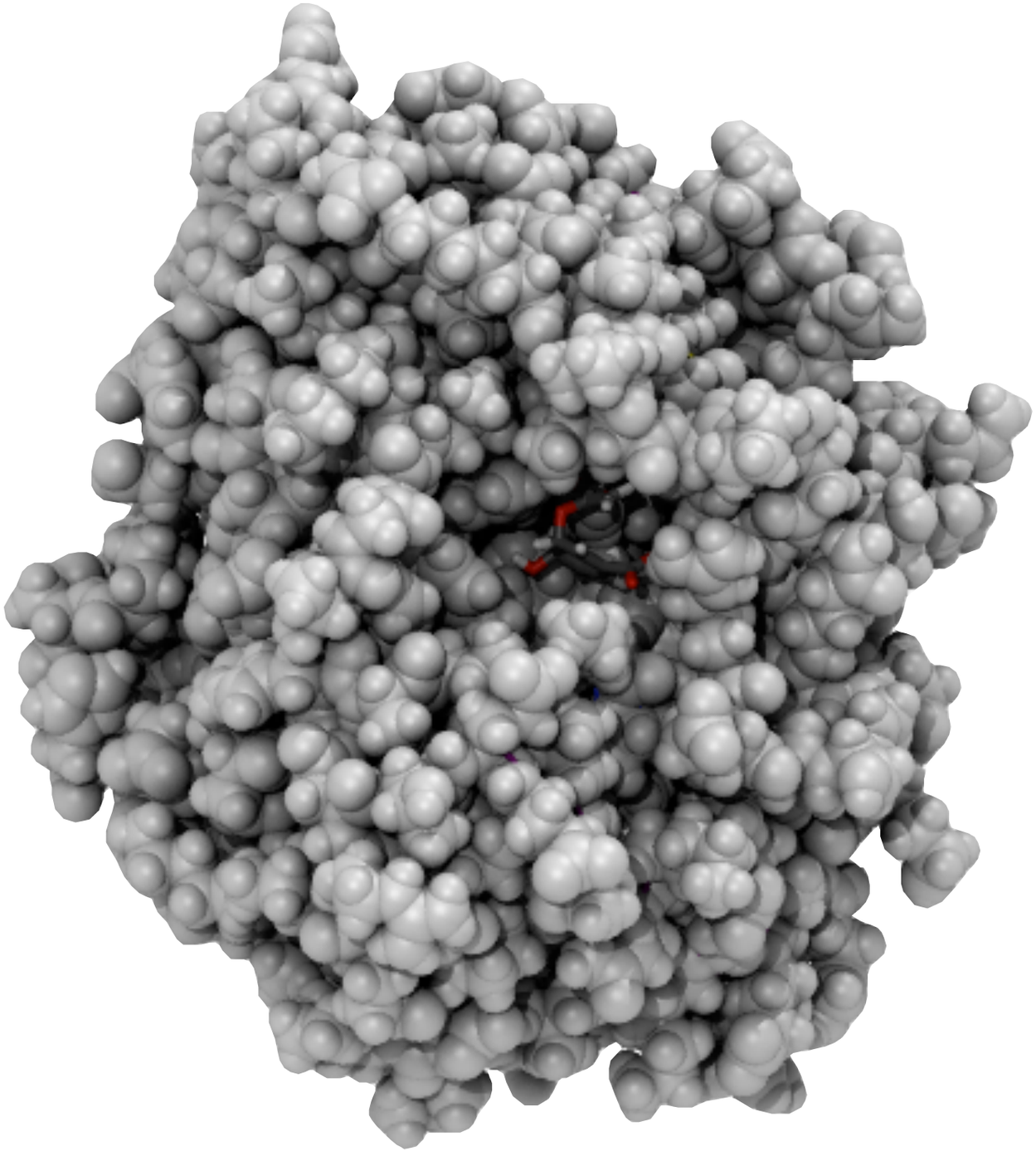
MM

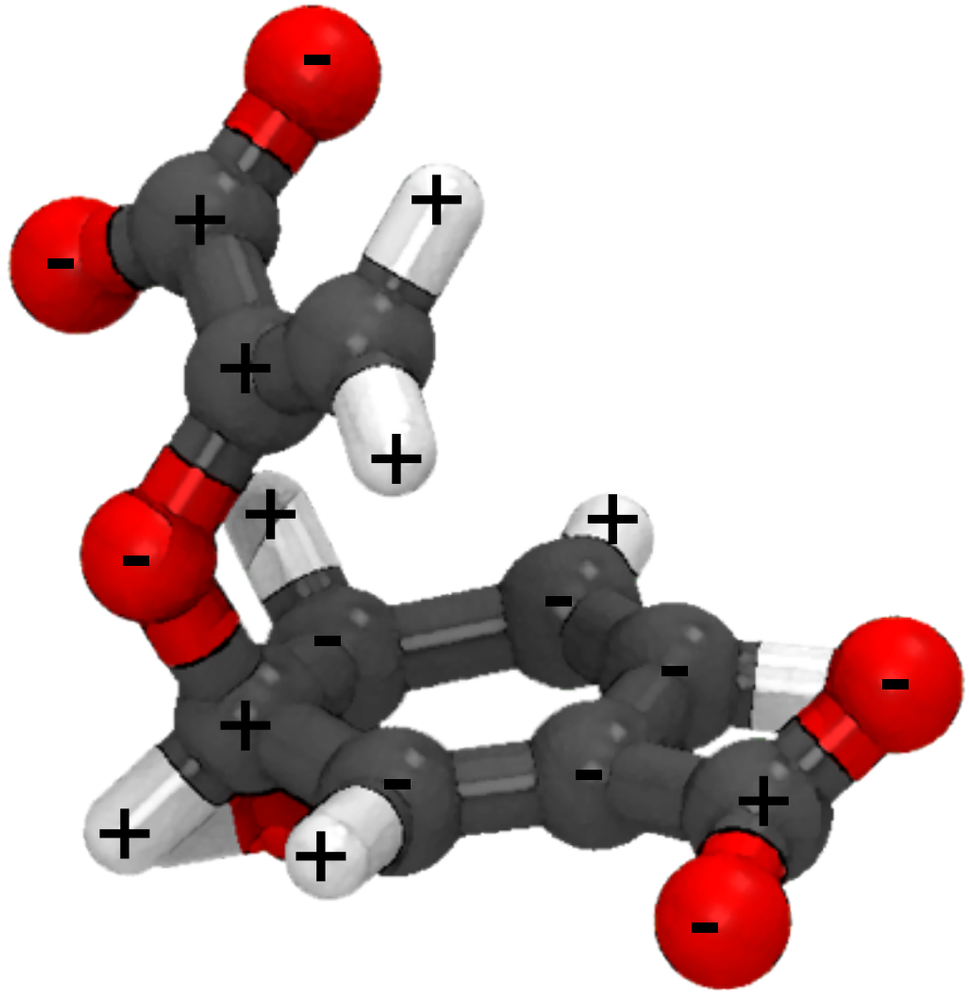




Molecular Mechanics
MM

$$E(r_{ij}) = \frac{q_i q_j}{4\pi\epsilon_0 r_{ij}}$$





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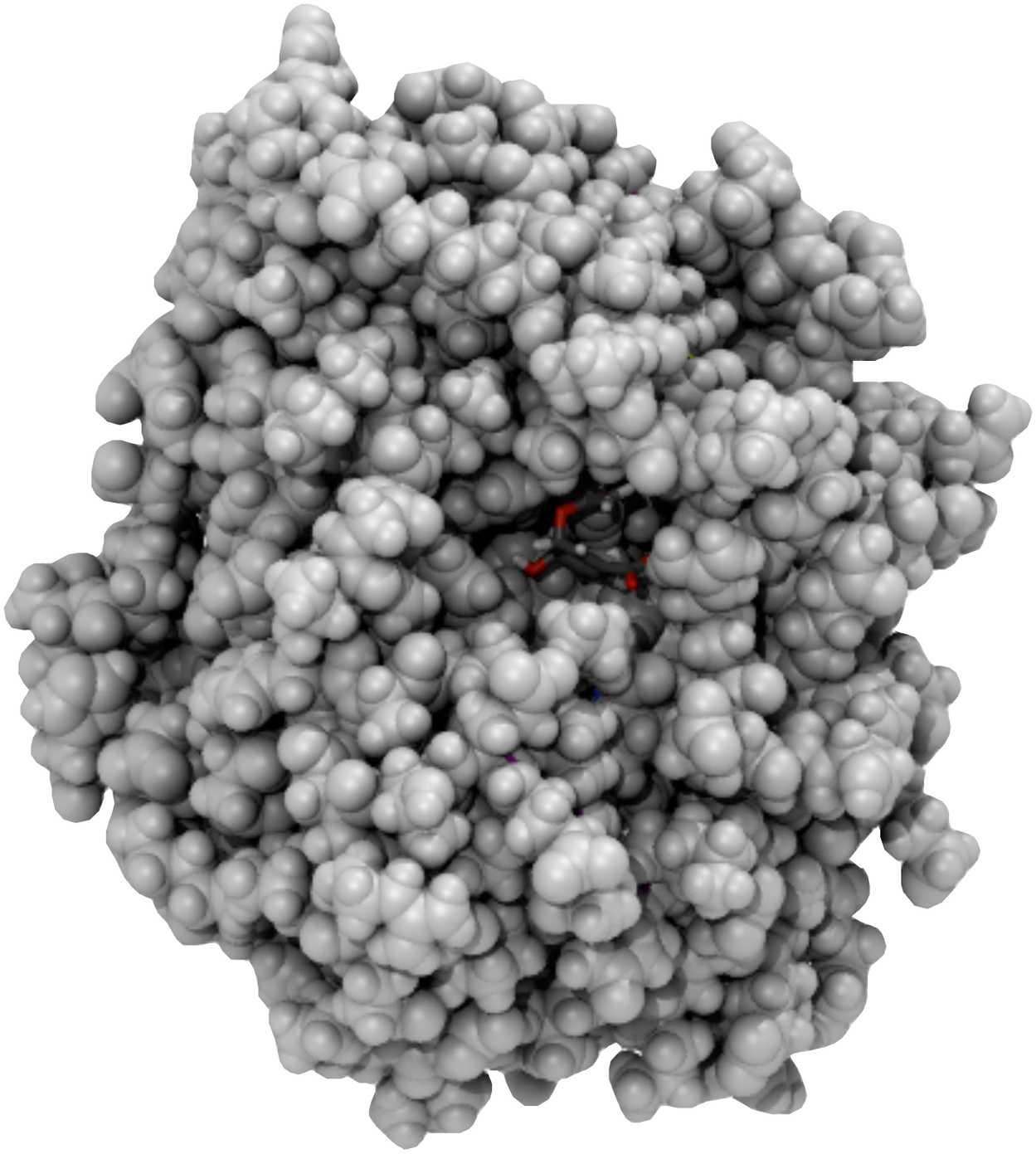

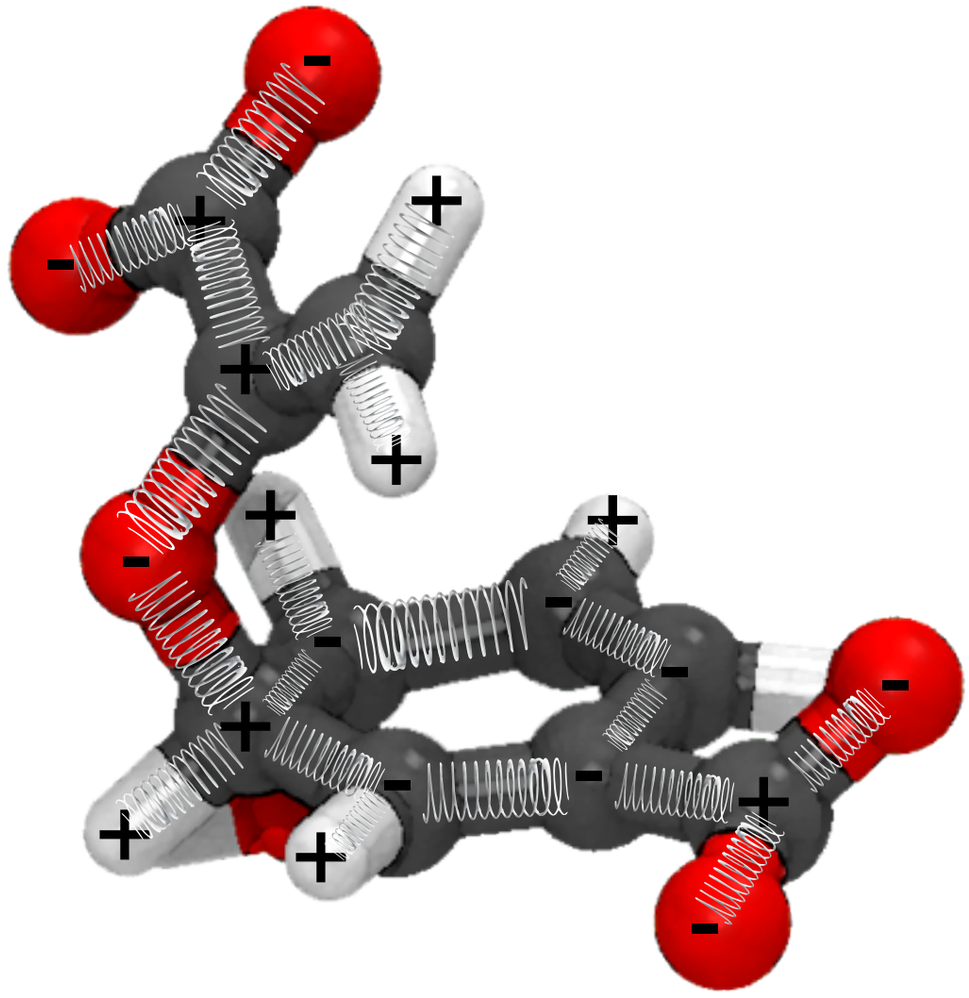

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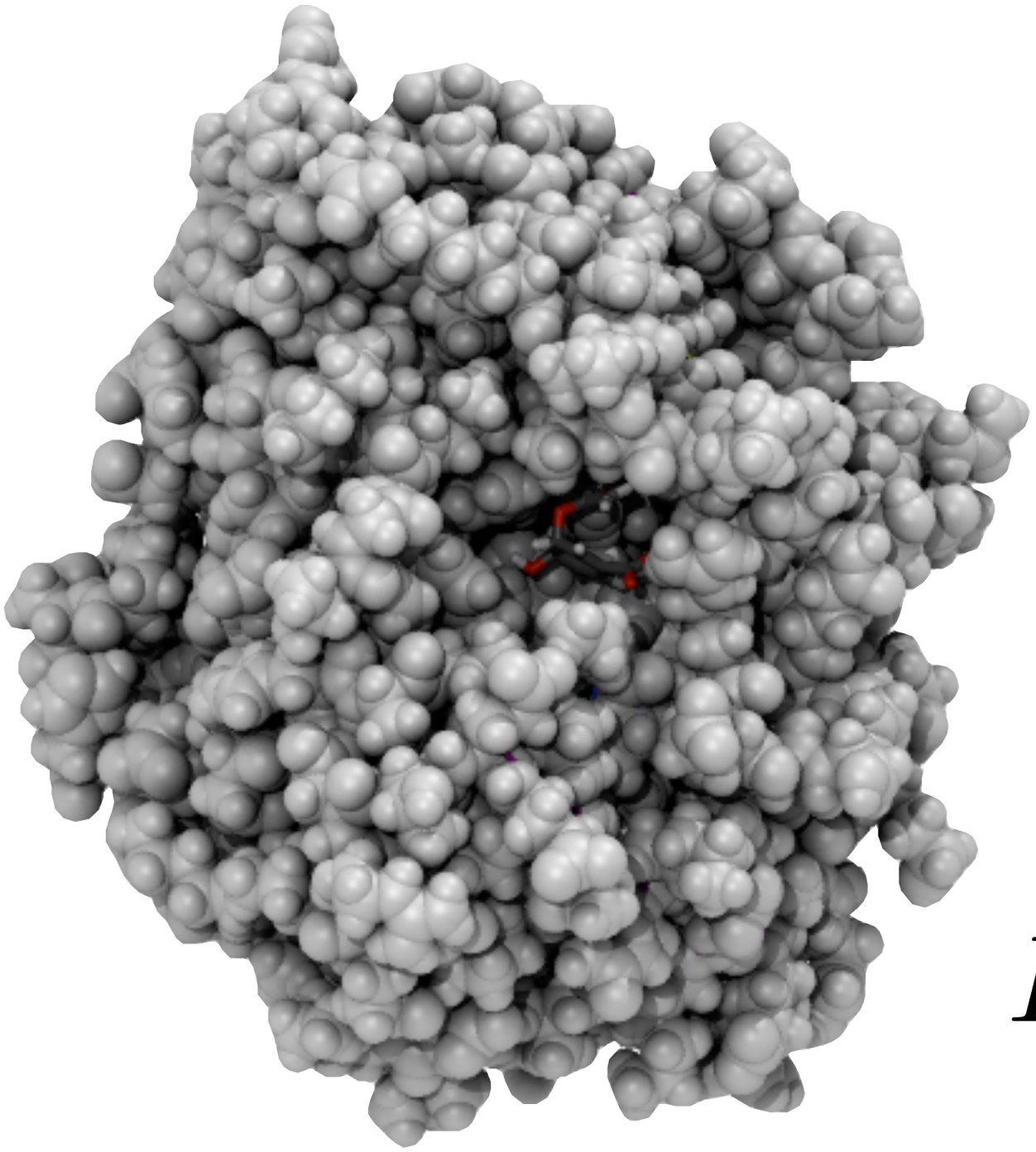

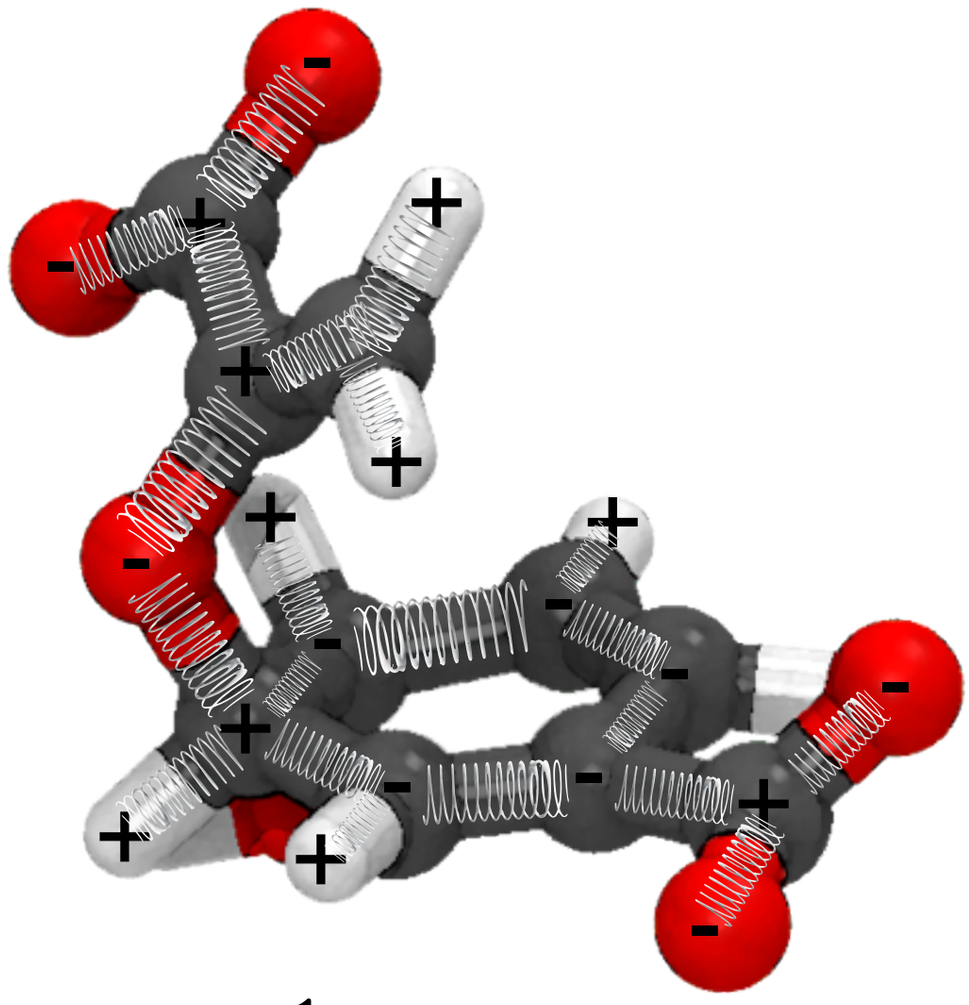

$$E(r) = \frac{1}{2}k(r - r_0)^2$$

Molecular Mechanics
MM

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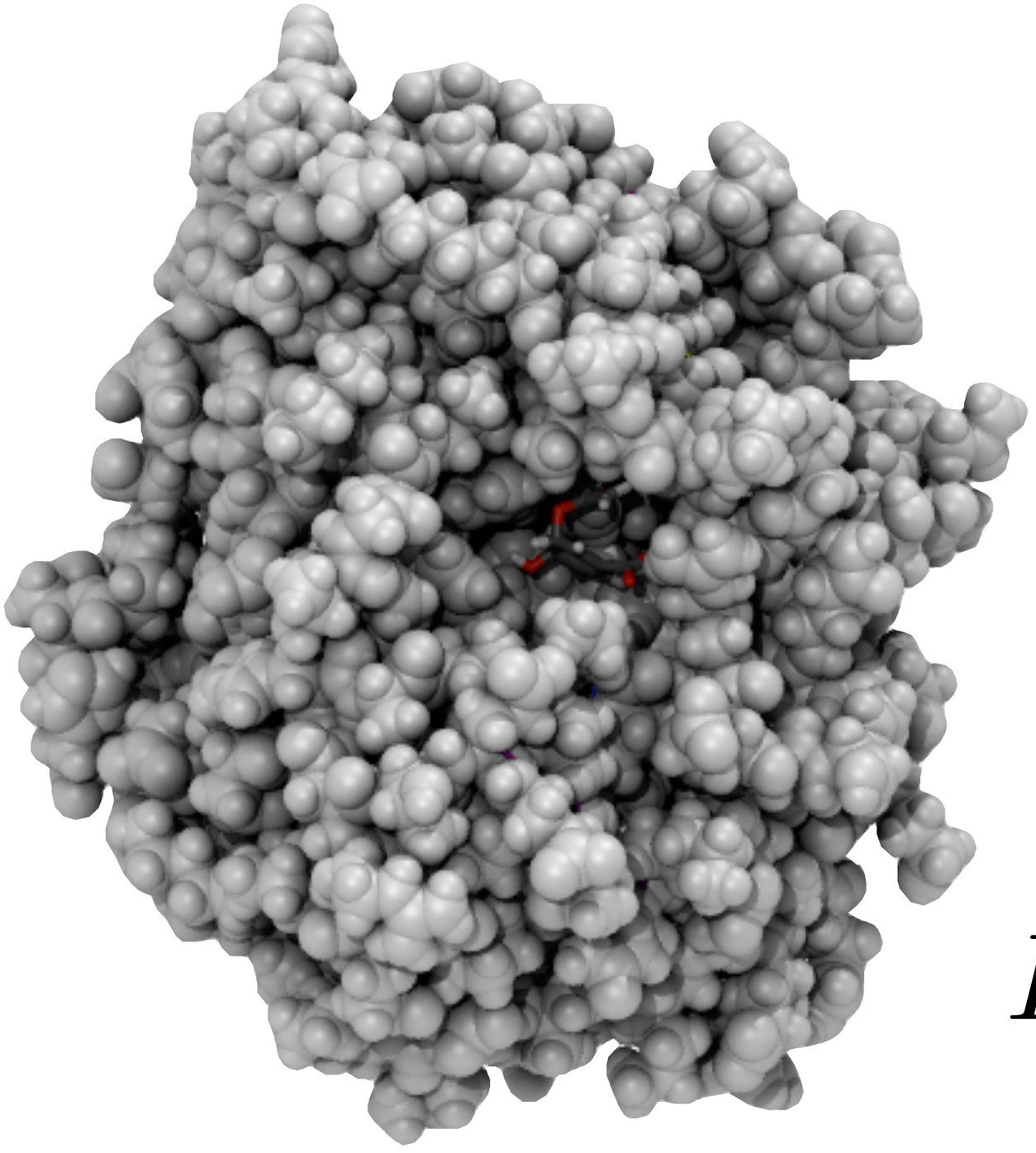
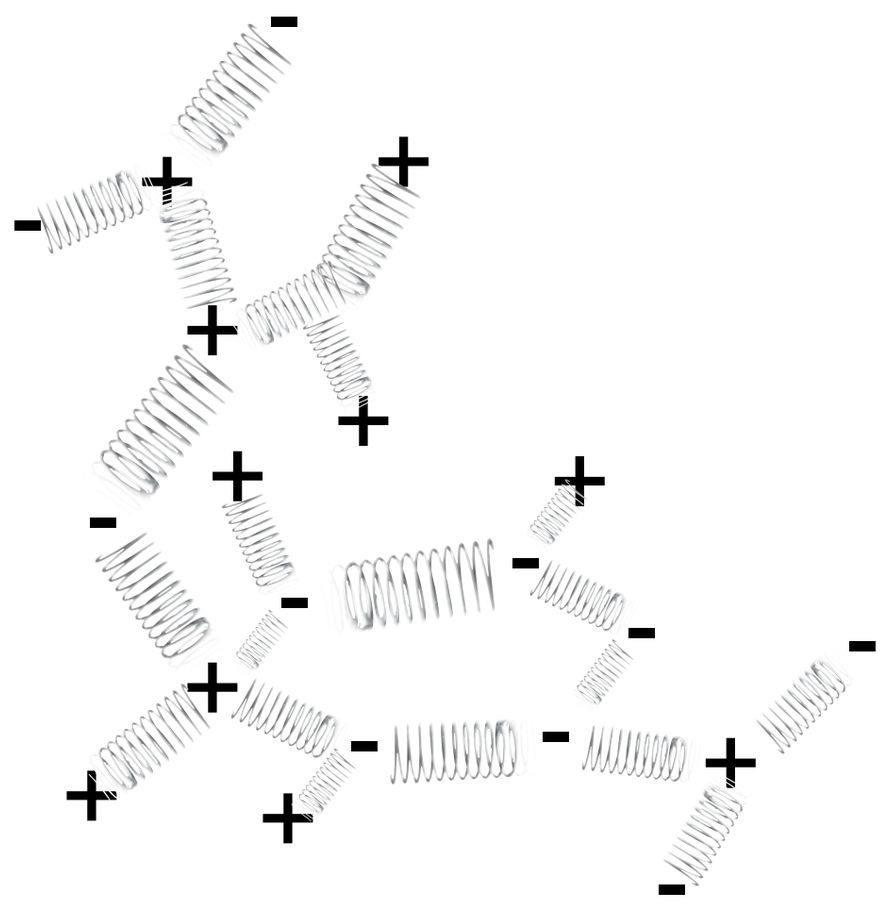
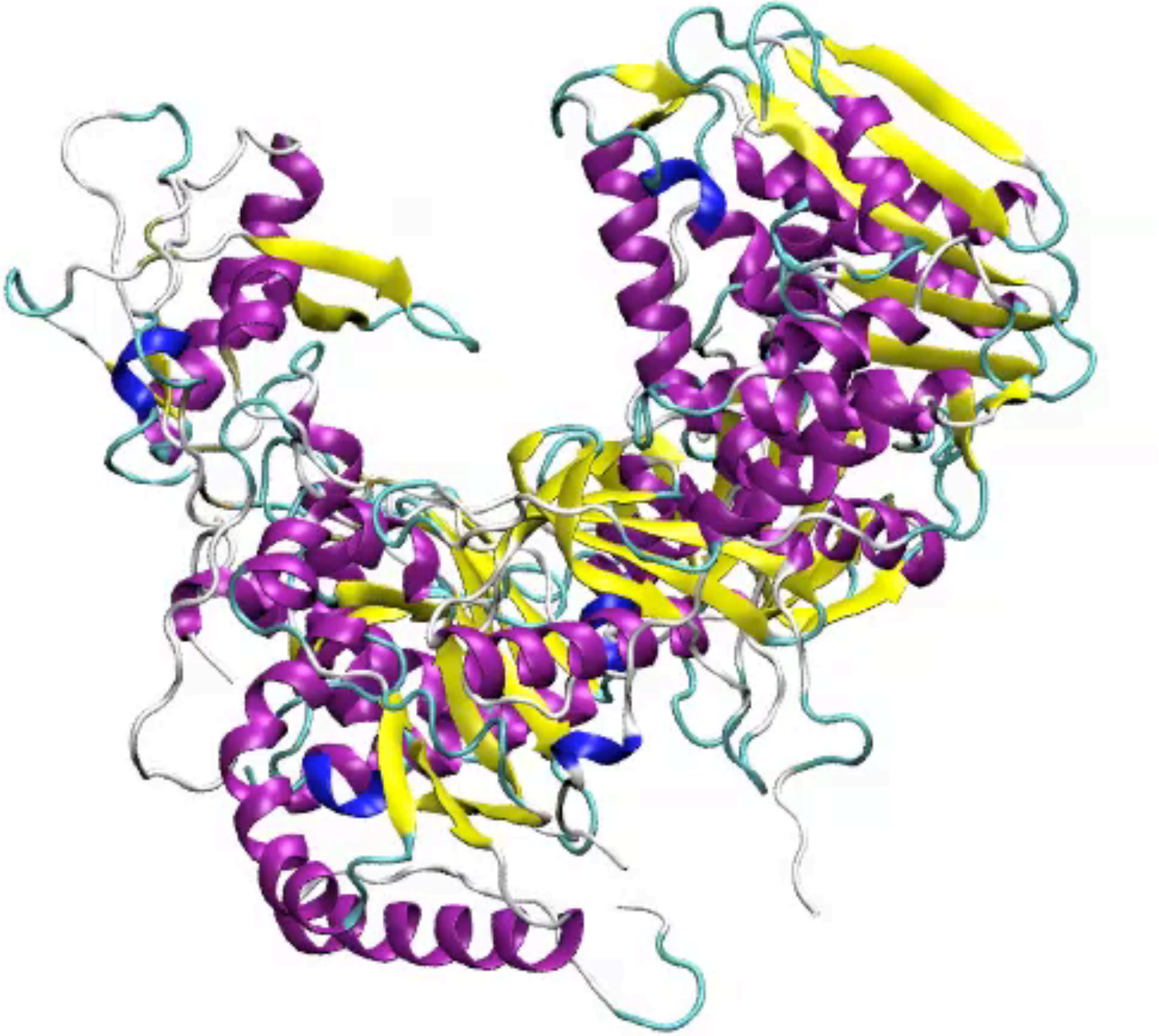


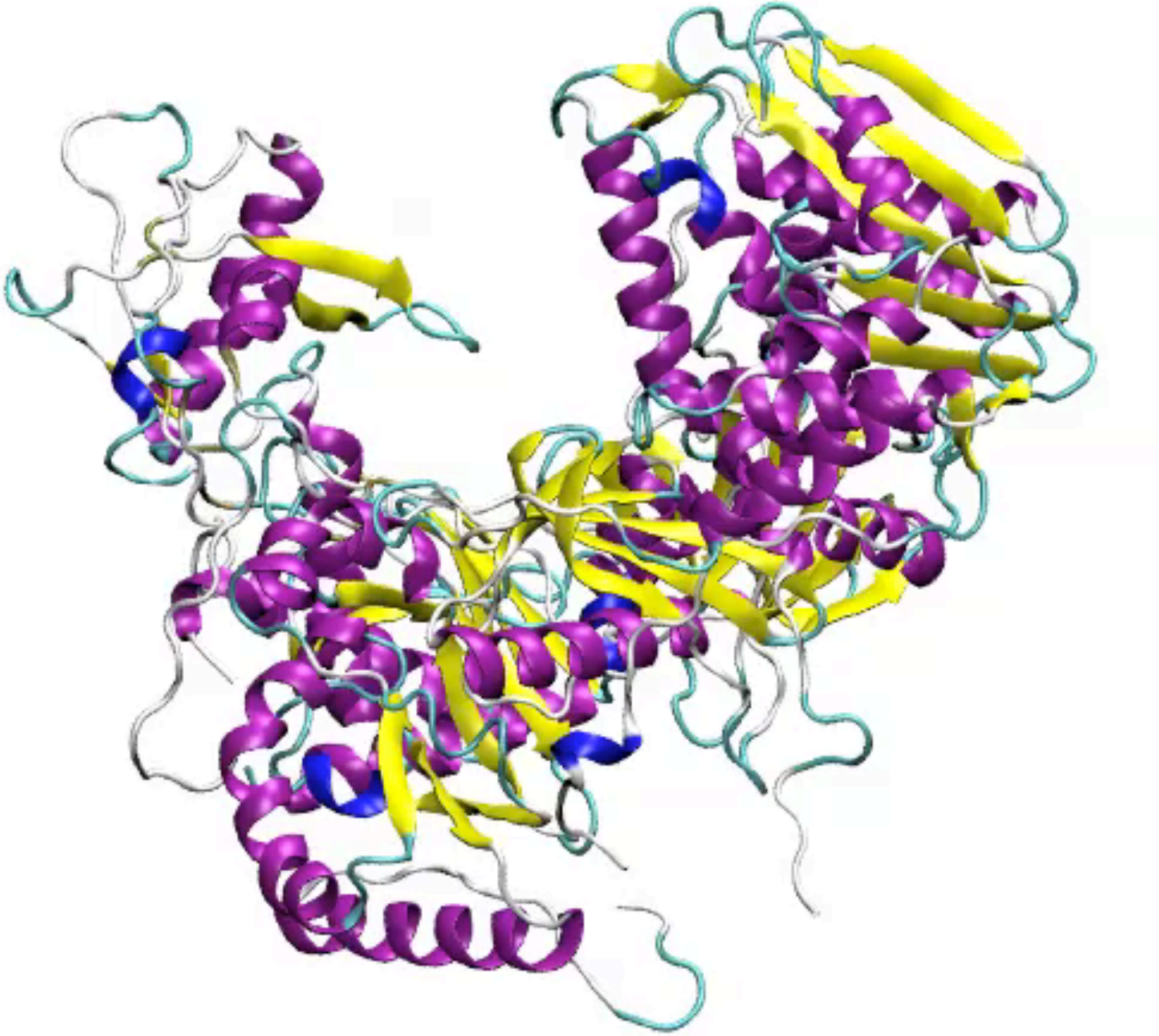


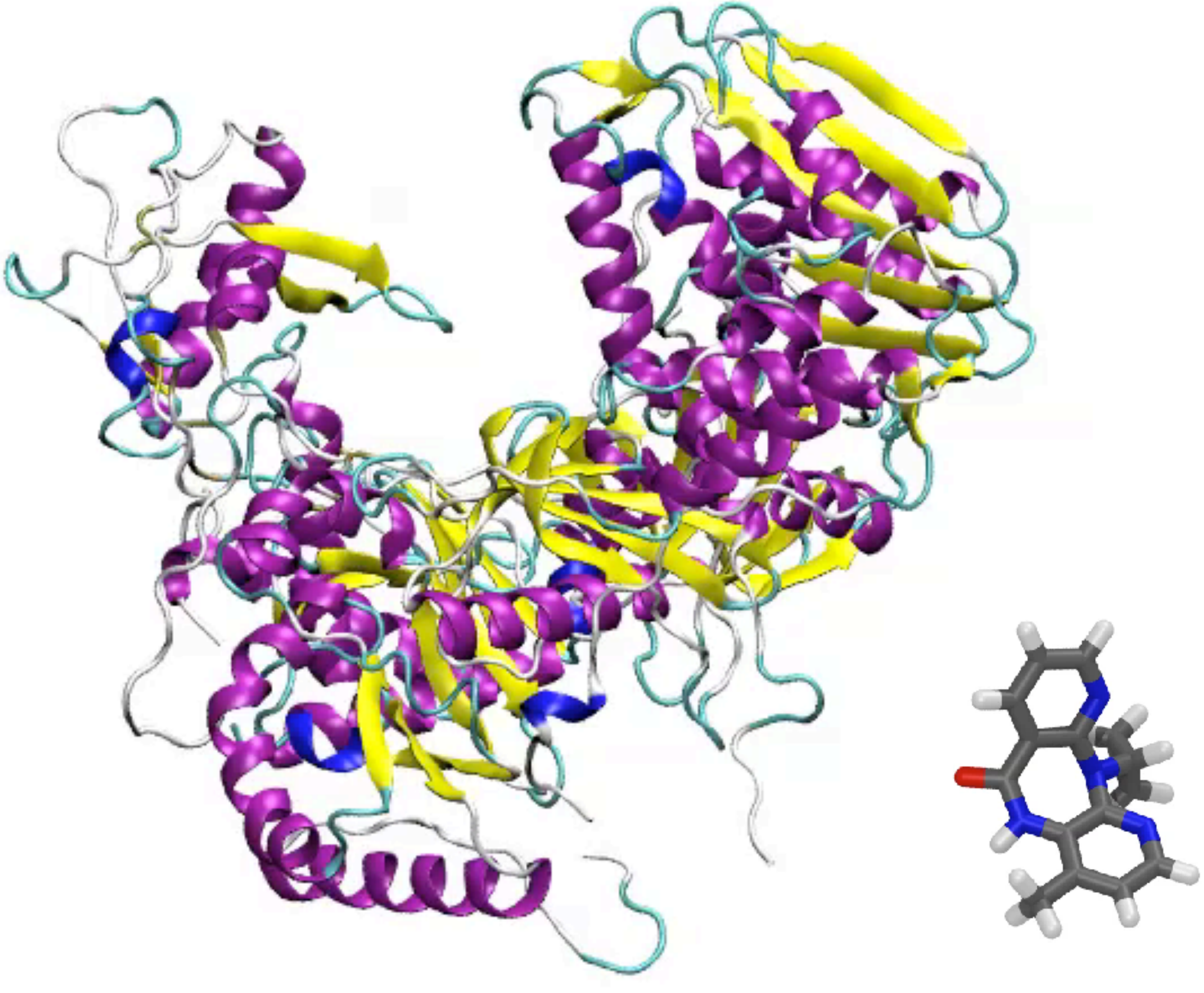
$$E(r) = \frac{1}{2}k(r - r_0)^2$$

Molecular Mechanics

- Atoms modelled as charged balls
- Bonds modelled as harmonic springs
- Allows energies of 10-100 000's of atoms to be evaluated rapidly
- MM - Balls on springs





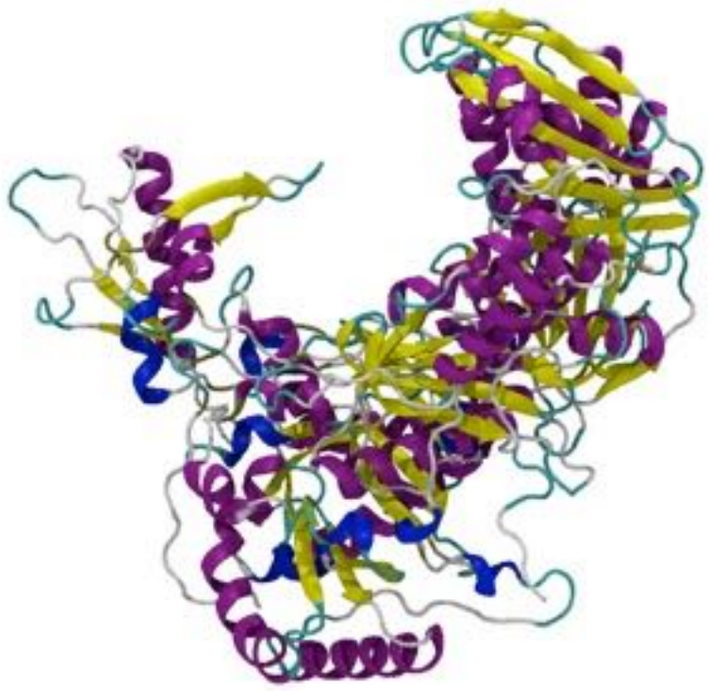


Molecular Dynamics

Molecular Dynamics

t

$x(t)$

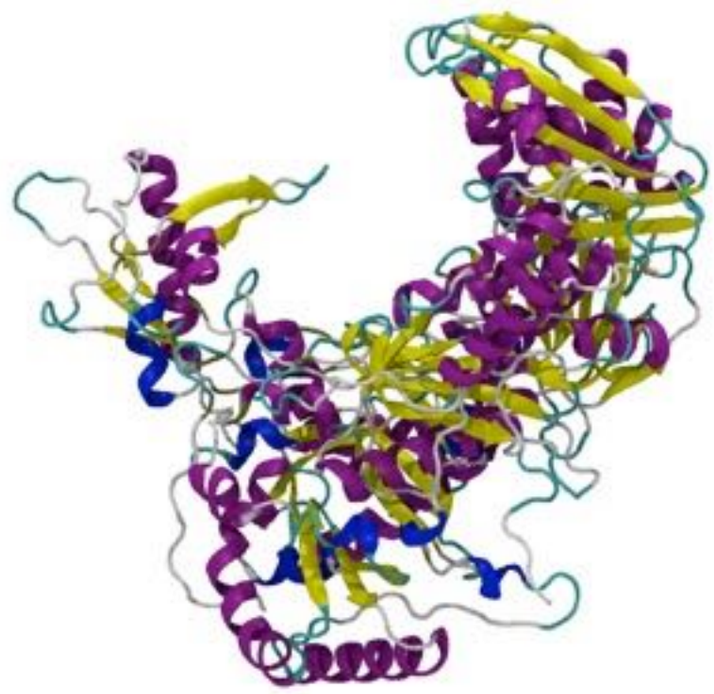


Molecular Dynamics

t

$x(t)$

$v(t)$



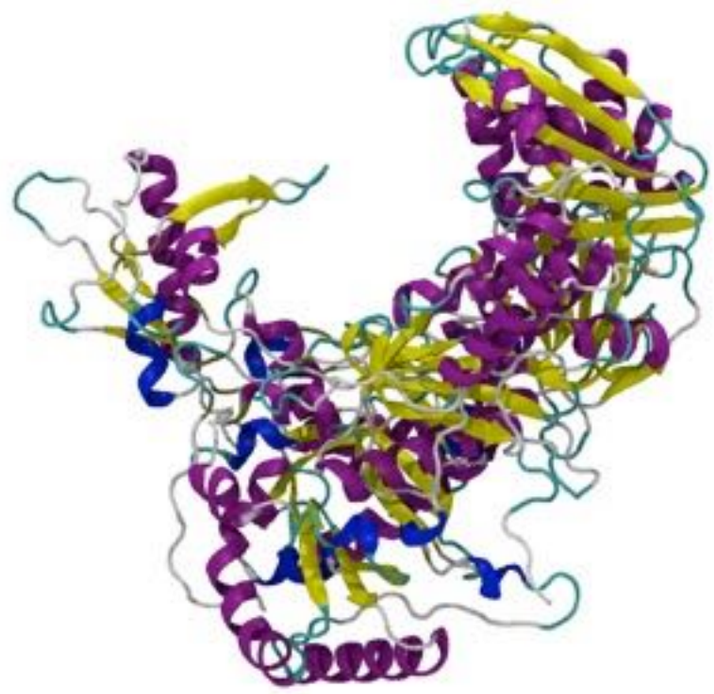
1. Assign velocities to all atoms

Molecular Dynamics

t

$x(t)$

$v(t)$



1. Assign velocities to all atoms

2. Calculate forces on all atoms

Force = Negative of the gradient of the potential

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$$E(r_{ij}) = \frac{q_i q_j}{4\pi\epsilon_0 r_{ij}}$$

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$$E(r_{ij}) = \frac{q_i q_j}{4\pi\epsilon_0 r_{ij}}$$

$$F(r_{ij}) = -\frac{dE(r_{ij})}{dr_{ij}}$$

Force = Negative of the gradient of the potential

$$E(r_{ij}) = \frac{q_i q_j}{4\pi\epsilon_0 r_{ij}}$$

$$F(r_{ij}) = -\frac{dE(r_{ij})}{dr_{ij}}$$

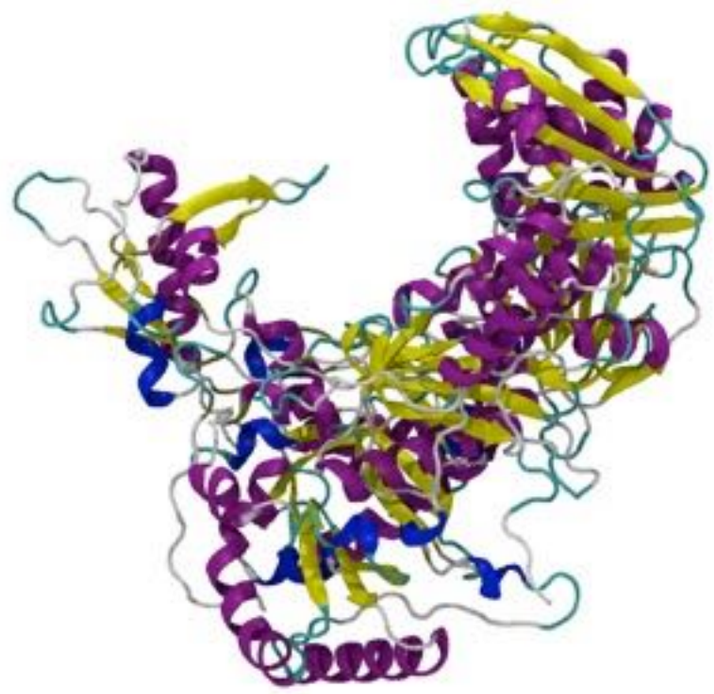
$$F(r_{ij}) = \frac{q_i q_j}{4\pi\epsilon_0 r_{ij}^2}$$

Molecular Dynamics

t

$x(t)$

$v(t)$



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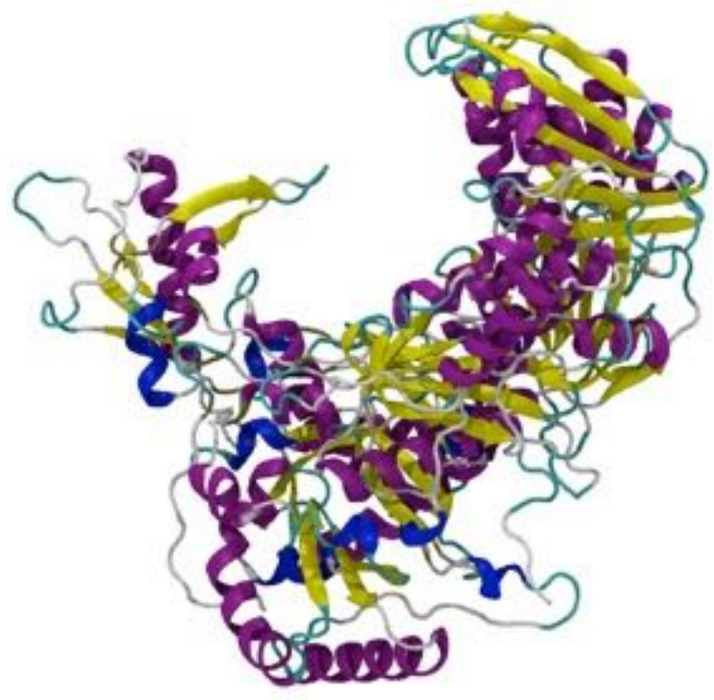
Molecular Dynamics

t

$x(t)$

$v(t)$



1. Assign velocities to all atoms

2. Calculate forces on all atoms

3. Use Newton's second law to calculate acceleration on each atom

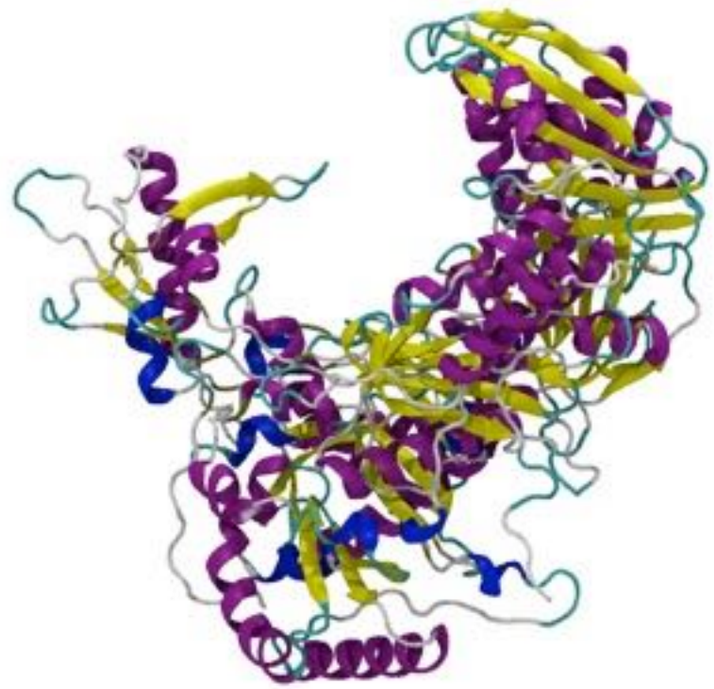
$$F = ma$$

Molecular Dynamics

t

$x(t)$

$v(t)$



1. Assign velocities to all atoms

2. Calculate forces on all atoms

3. Use Newton's second law to calculate acceleration on each atom

$$F = ma$$

4. Calculate velocities for the next timestep

$t + \Delta t$

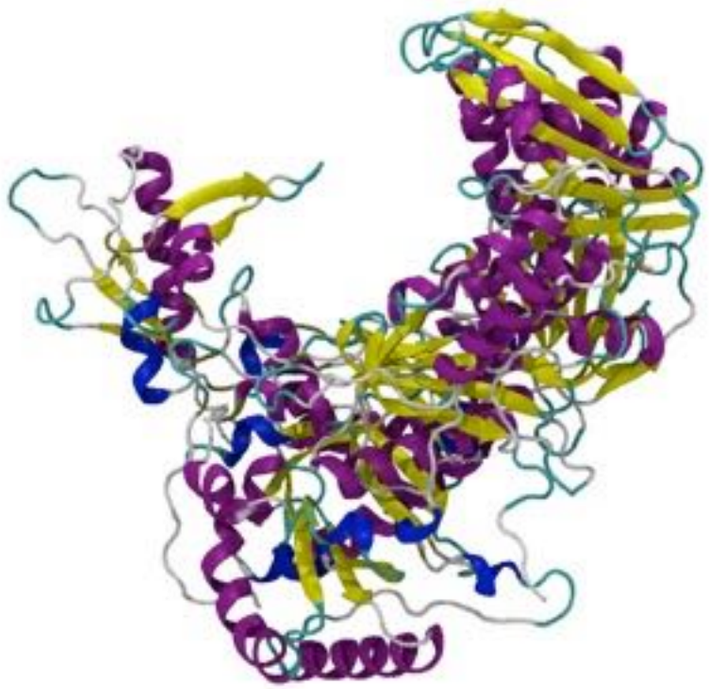
$v(t + \Delta t)$

Molecular Dynamics

t

$x(t)$

$v(t)$



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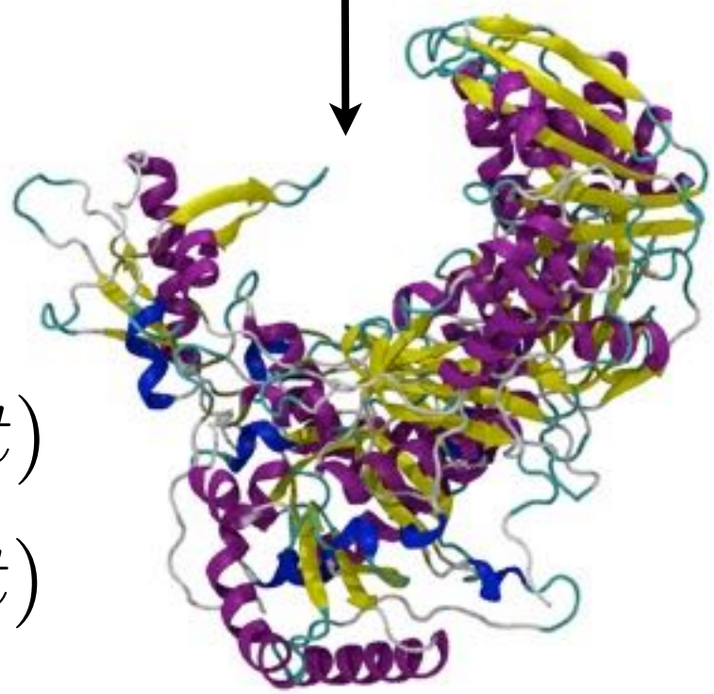


$t + \Delta t$

$x(t + \Delta t)$

$v(t + \Delta t)$

4. Calculate velocities for the next timestep

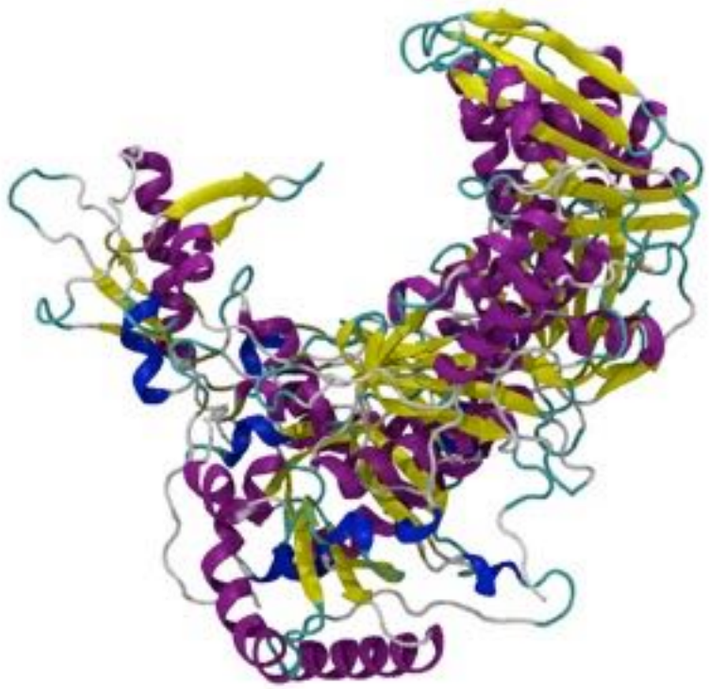
5. Use change of velocities to get coordinates for next timestep

Molecular Dynamics

t

$x(t)$

$v(t)$



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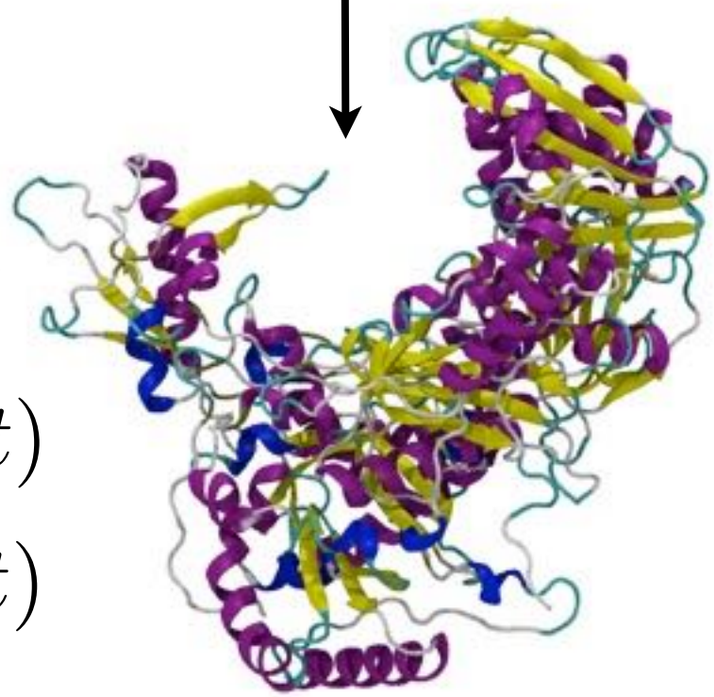
$t + \Delta t$

$x(t + \Delta t)$

$v(t + \Delta t)$



4. Calculate velocities for the next timestep

5. Use change of velocities to get coordinates for next timestep

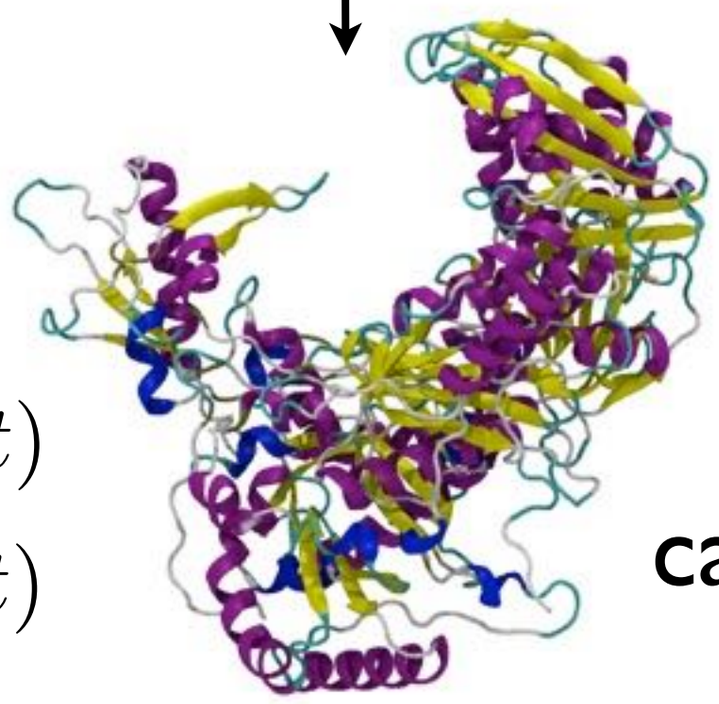
6. Go to step 2.

Molecular Dynamics

$t + \Delta t$

$x(t + \Delta t)$

$v(t + \Delta t)$



2. Calculate forces on all atoms

3. Use Newton's second law to calculate acceleration on each atom

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4. Calculate velocities for the next timestep

5. Use change of velocities to get coordinates for next timestep

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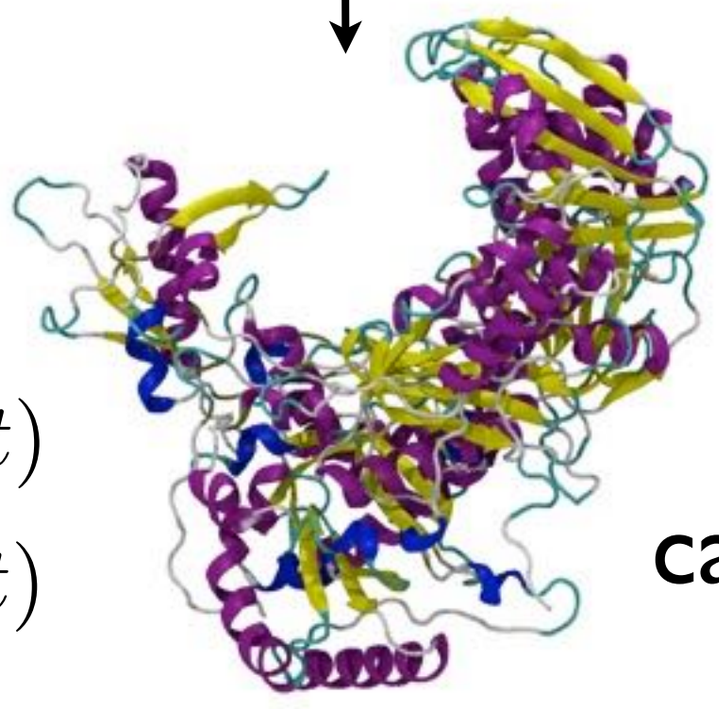
Molecular Dynamics

$t + \Delta t$

$x(t + \Delta t)$

$v(t + \Delta t)$



2. Calculate forces on all atoms

3. Use Newton's second law to calculate acceleration on each atom

$$F = ma$$

4. Calculate velocities for the next timestep

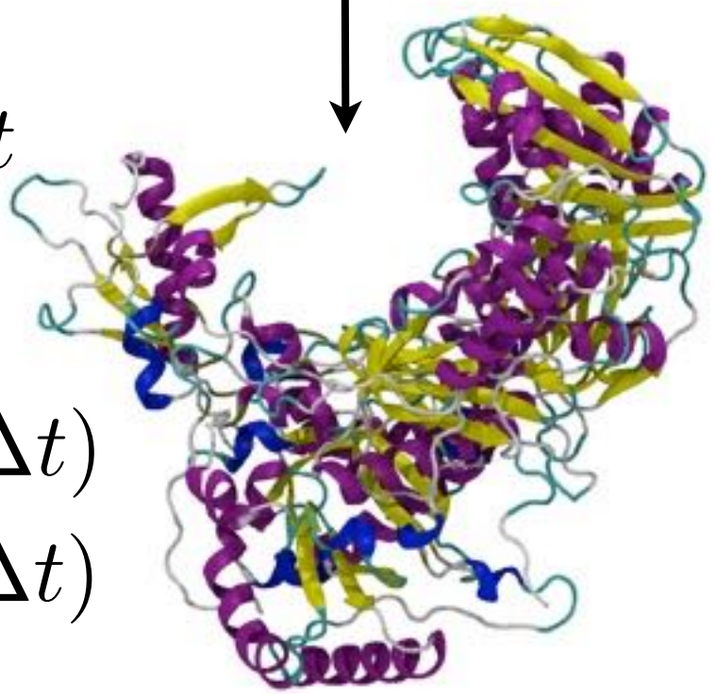
5. Use change of velocities to get coordinates for next timestep

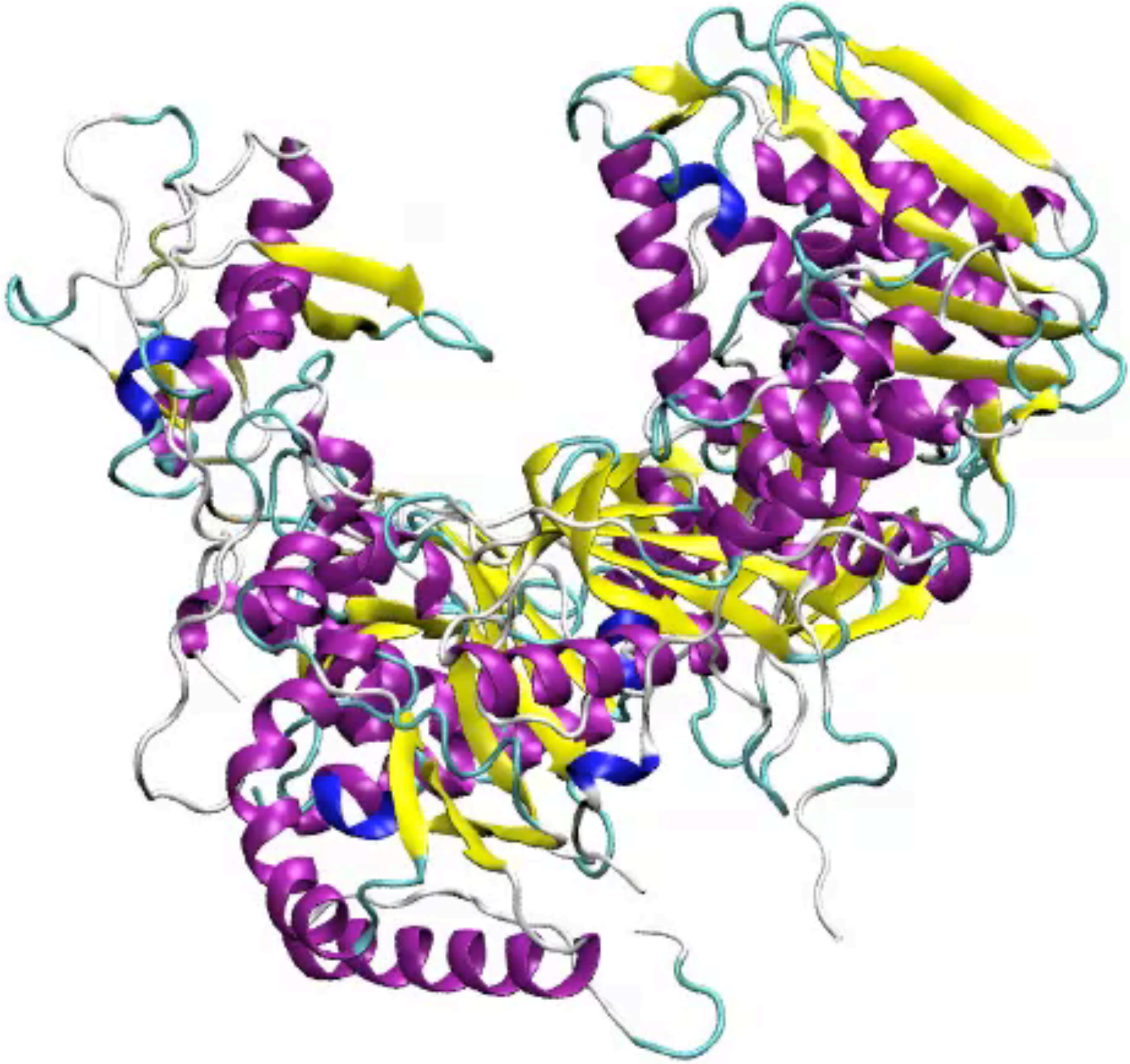
6. Go to step 2.

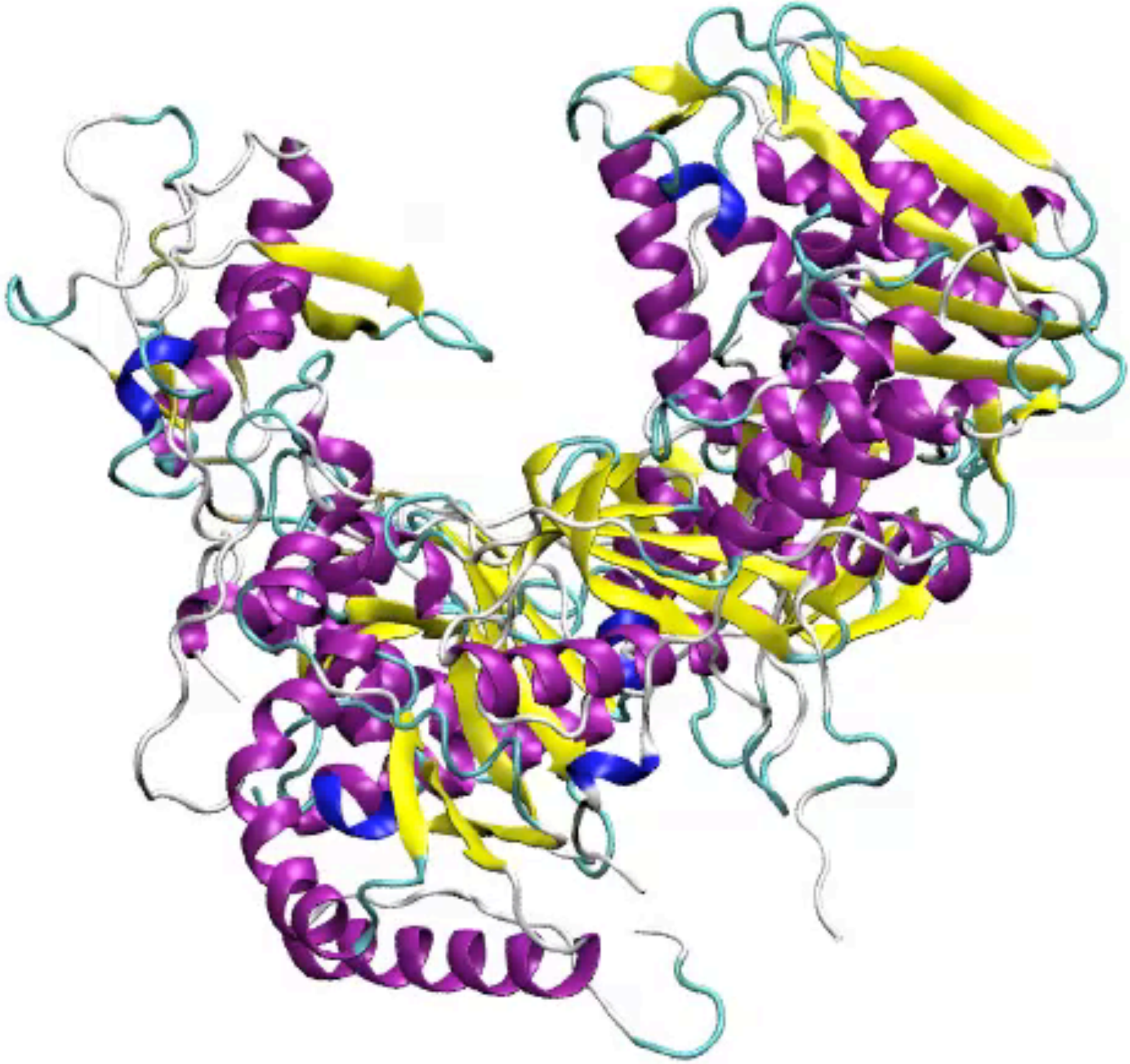
$t + 2\Delta t$

$x(t + 2\Delta t)$

$v(t + 2\Delta t)$







Physics gets in the way!

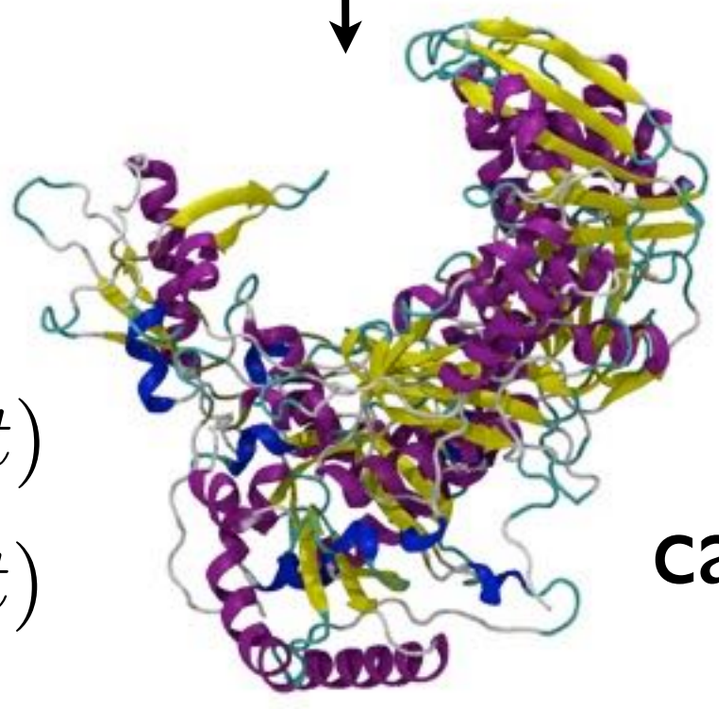
- Timestep Δt has to be less than the period of bond vibration otherwise the simulation will explode
- Frequency is ~10^{15} Hz
- Period, and so Δt is 1 femtosecond
- Need to repeat "Step 2-Step 5" 10^{15} times to simulate 1 second of motion of the protein
- 1 000 000 000 000 000 (thousand million million)

Molecular Dynamics

$t + \Delta t$

$x(t + \Delta t)$

$v(t + \Delta t)$



2. Calculate forces on all atoms

3. Use Newton's second law to calculate acceleration on each atom

$$F = ma$$

4. Calculate velocities for the next timestep

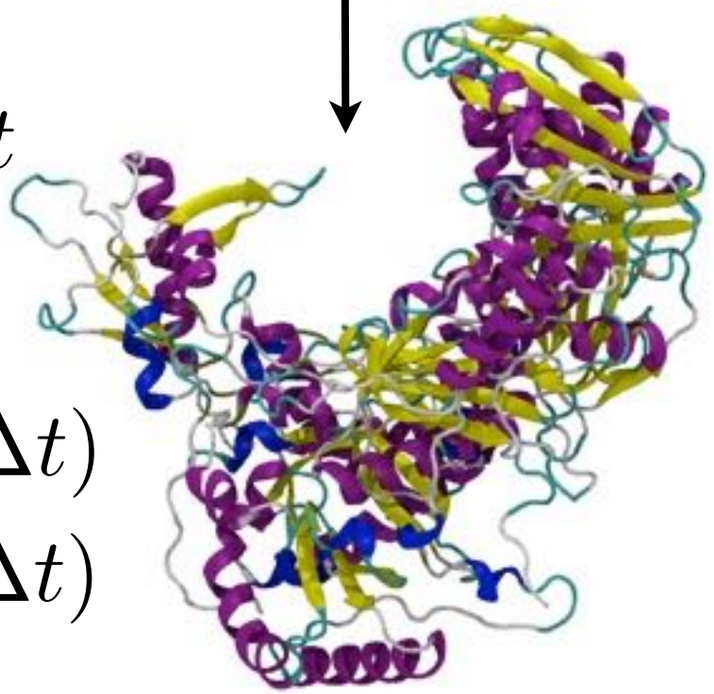
5. Use change of velocities to get coordinates for next timestep

6. Go to step 2.

$t + 2\Delta t$

$x(t + 2\Delta t)$

$v(t + 2\Delta t)$

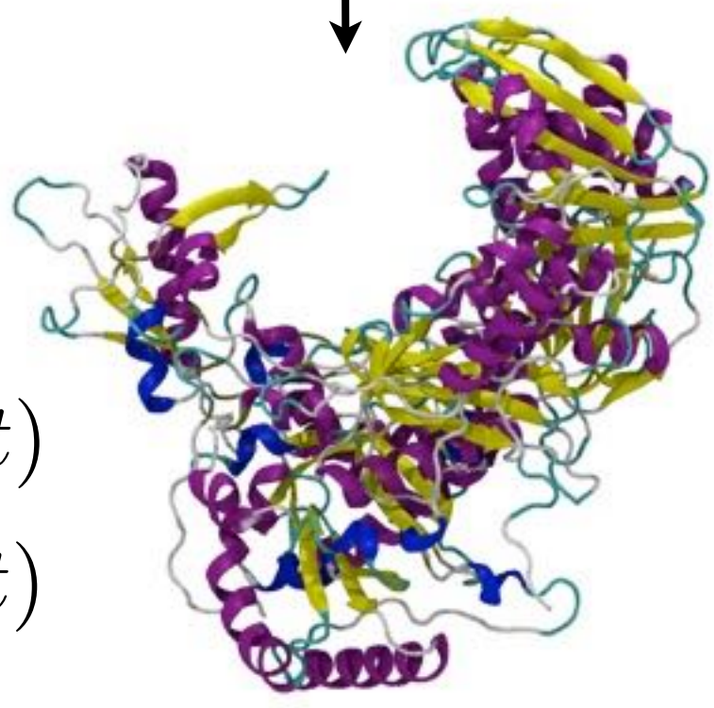


Molecular Dynamics

$t + \Delta t$

$x(t + \Delta t)$

$v(t + \Delta t)$



2. Calculate forces on all atoms

100,000 atoms ~ 10 M fp calcs

Single-core laptop (1 GHz)

1 step takes 100 ms

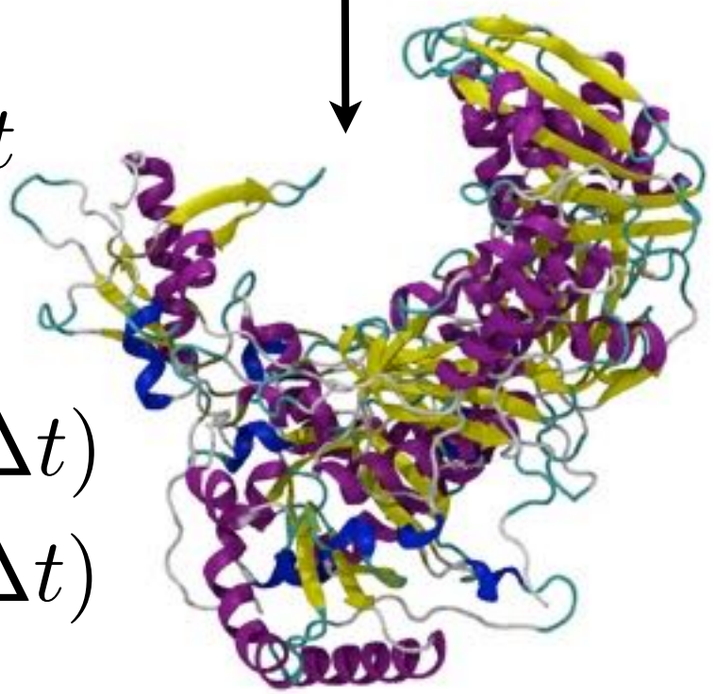
~ 1 nanosecond per day

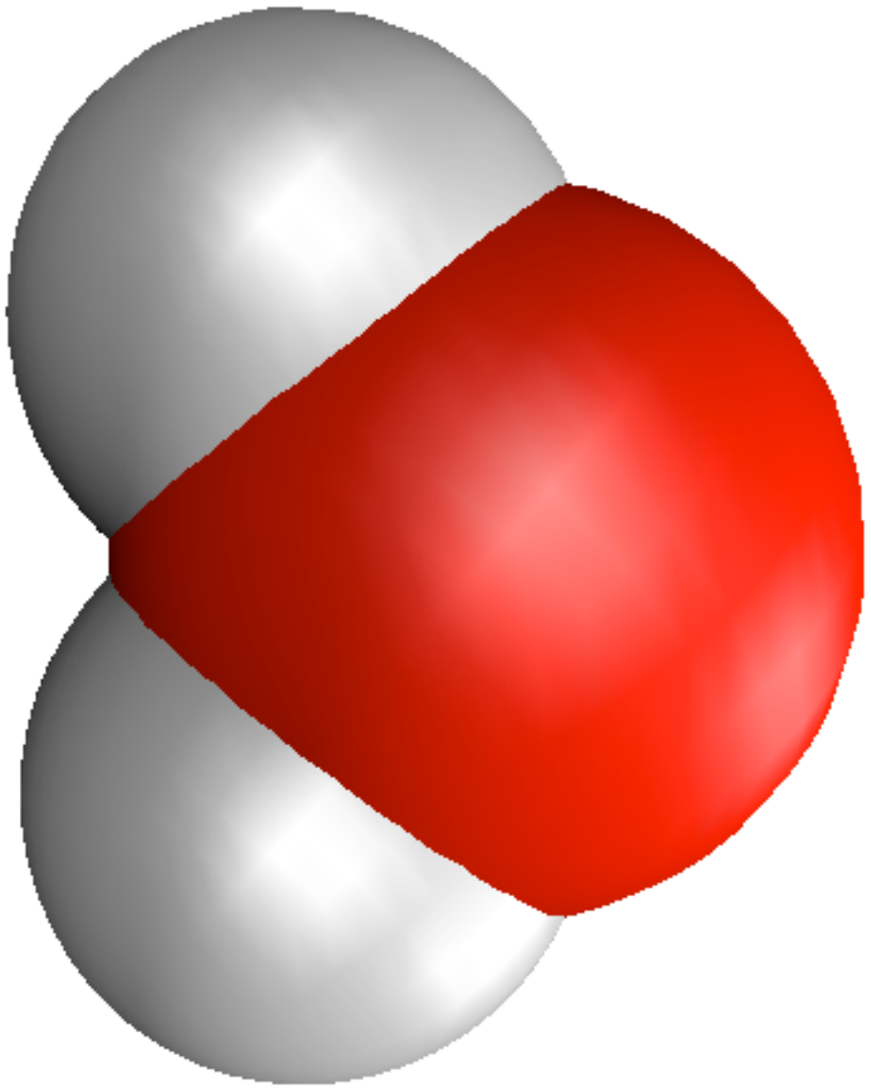
~ 1 second per 3000,000 years

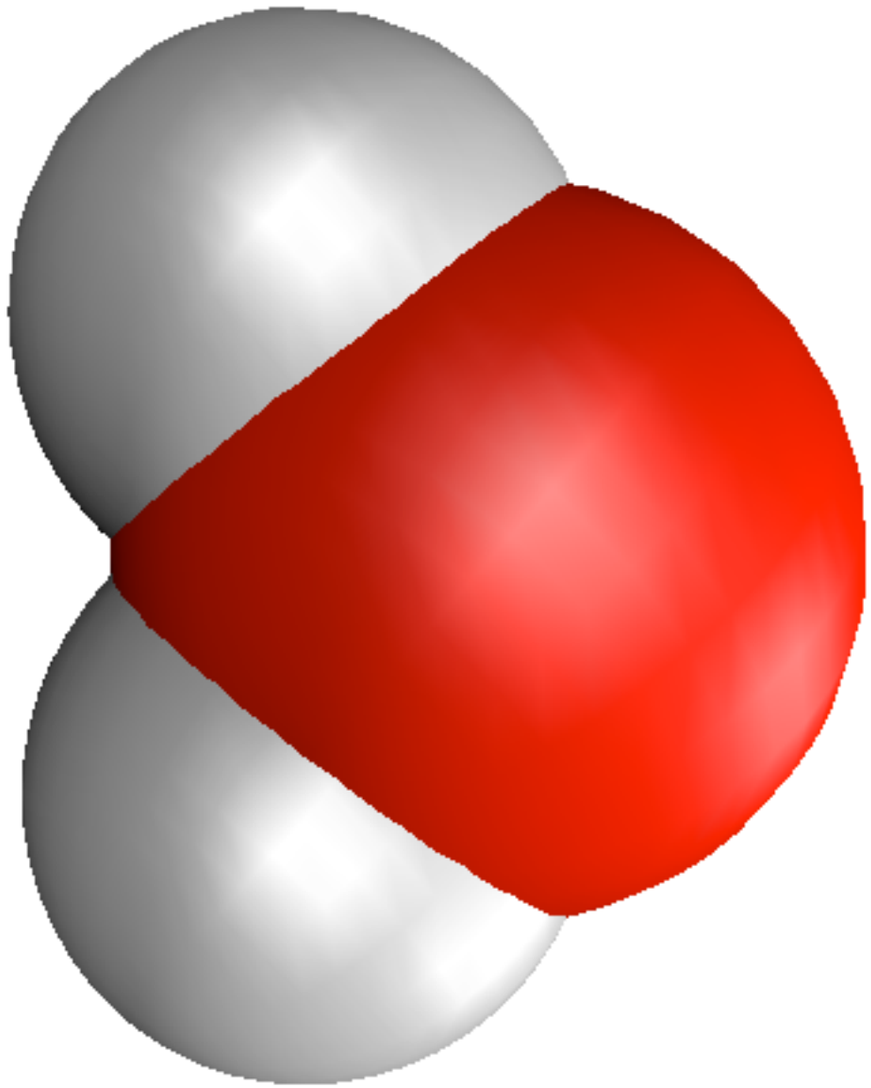
$t + 2\Delta t$

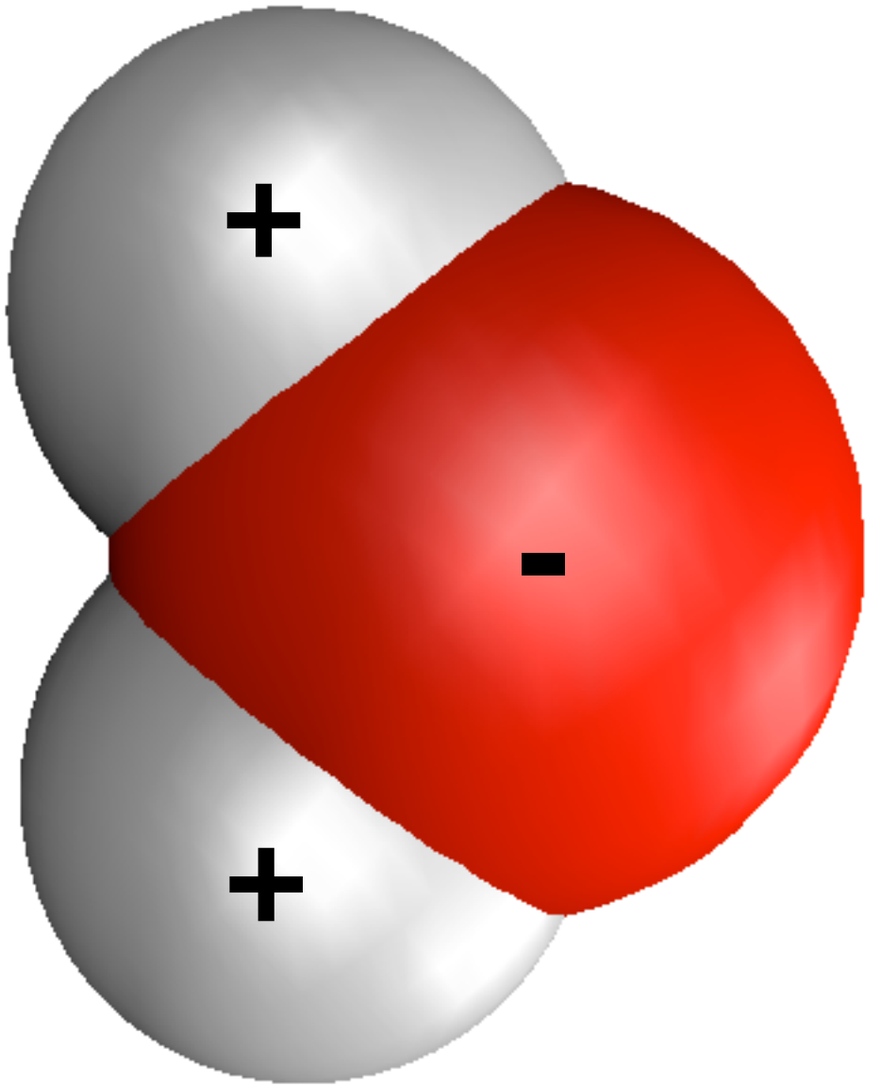
$x(t + 2\Delta t)$

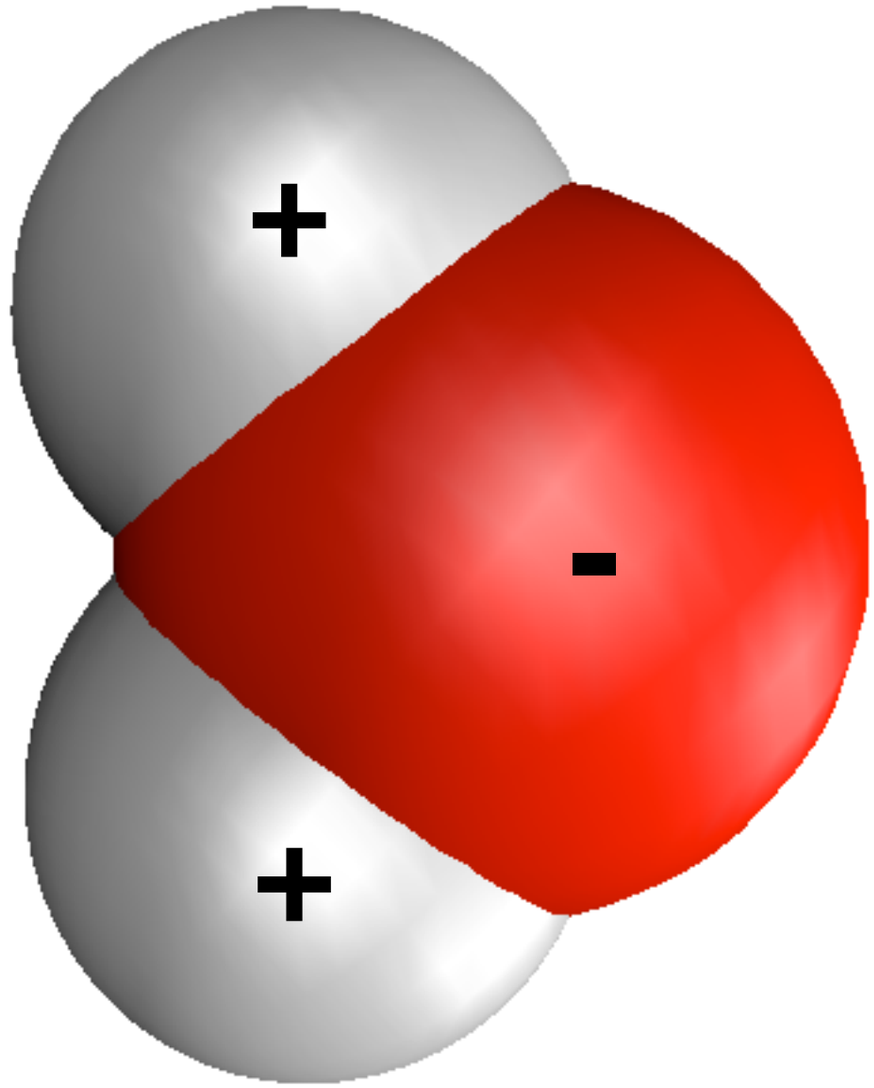
$v(t + 2\Delta t)$

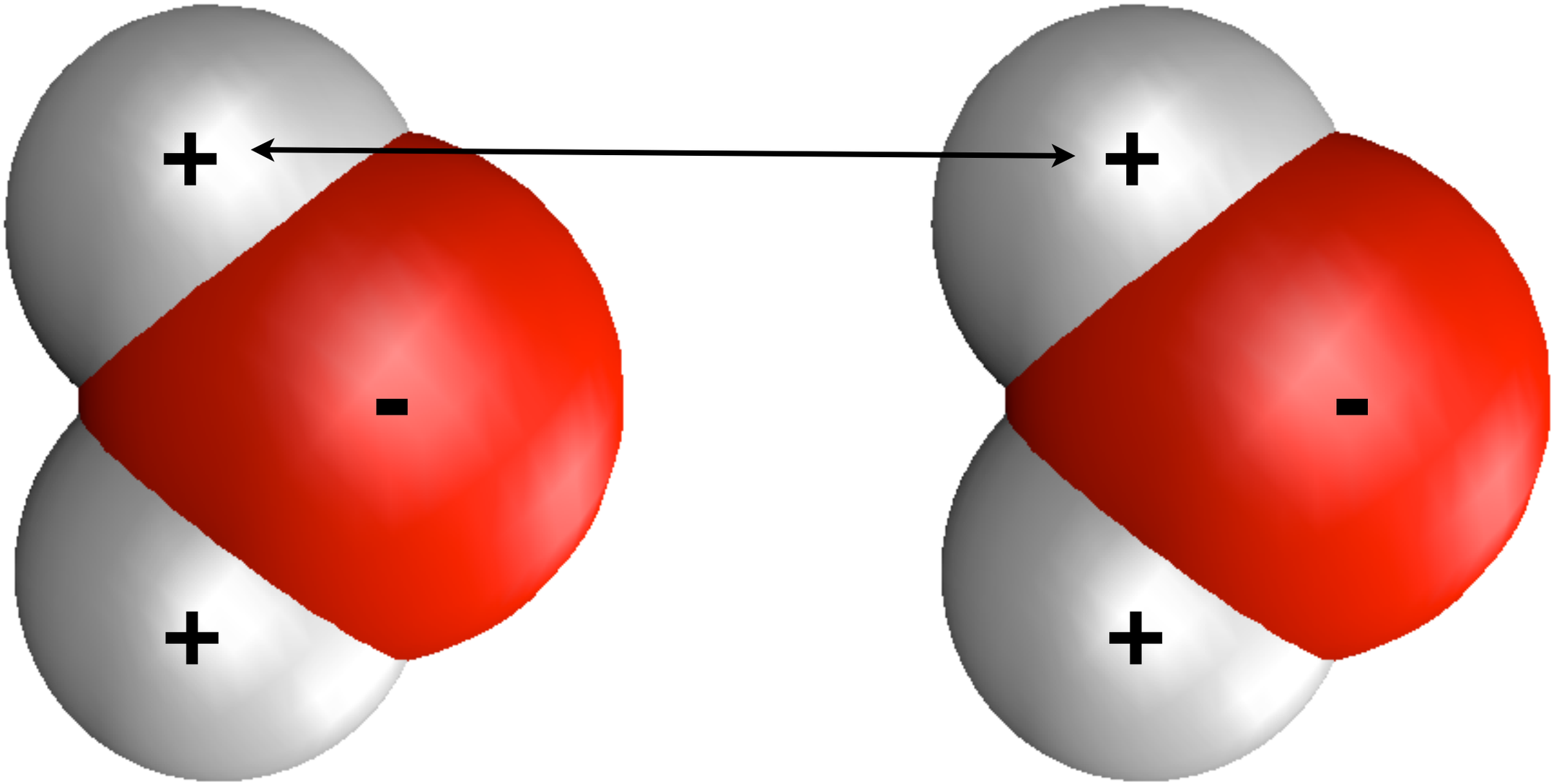


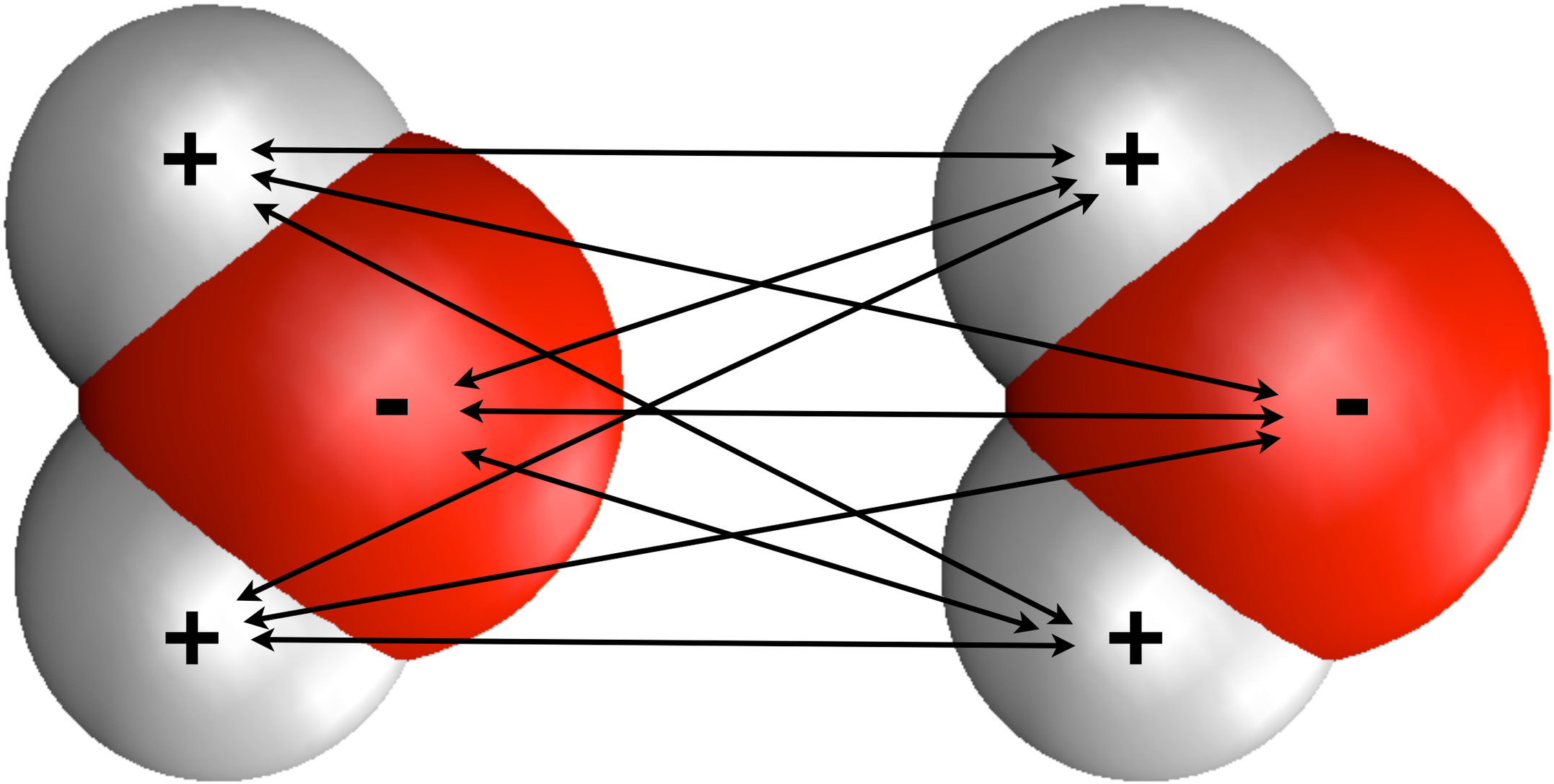


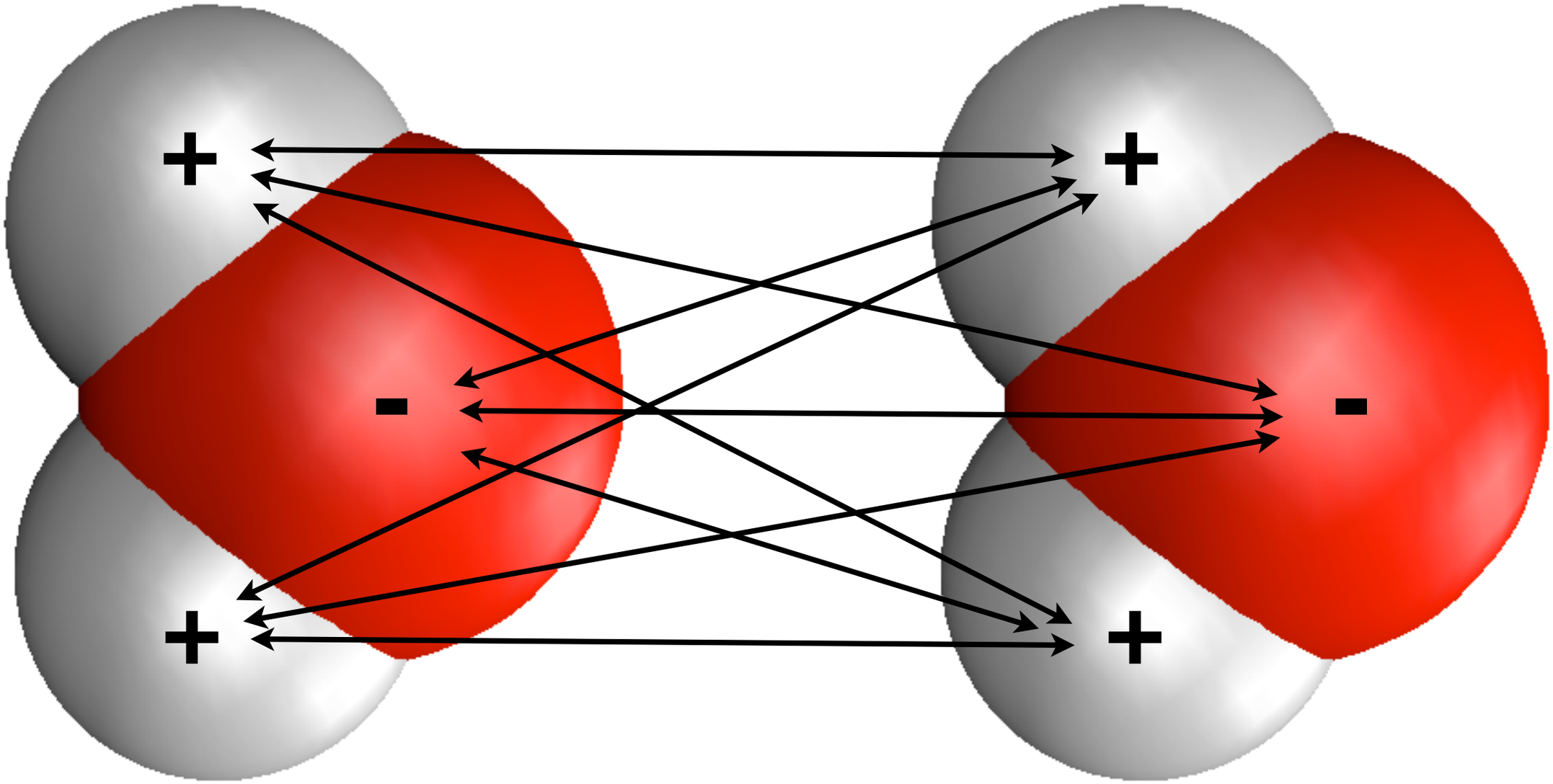












SSE (128 bit)

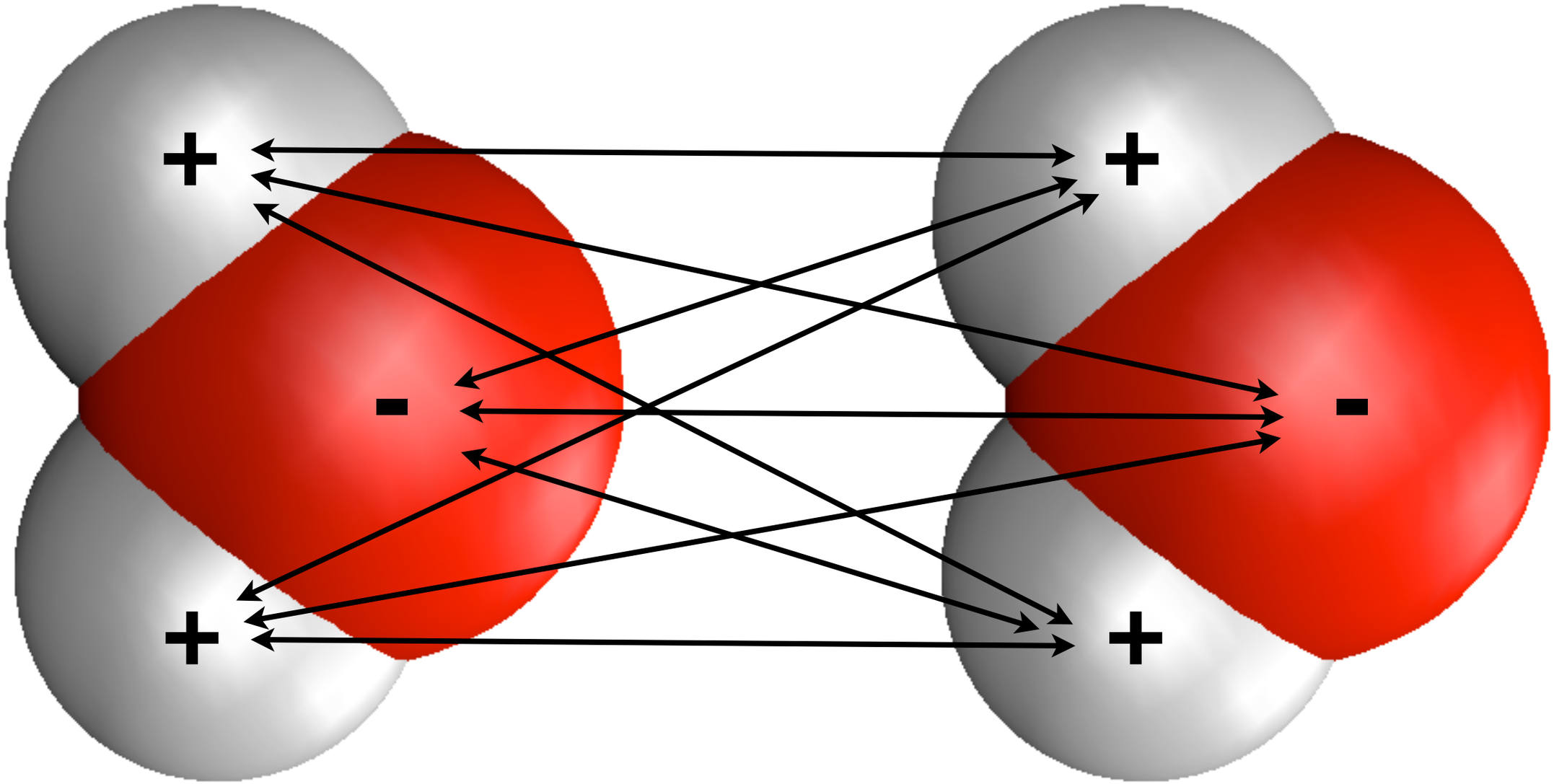
A	B

x

X	Y

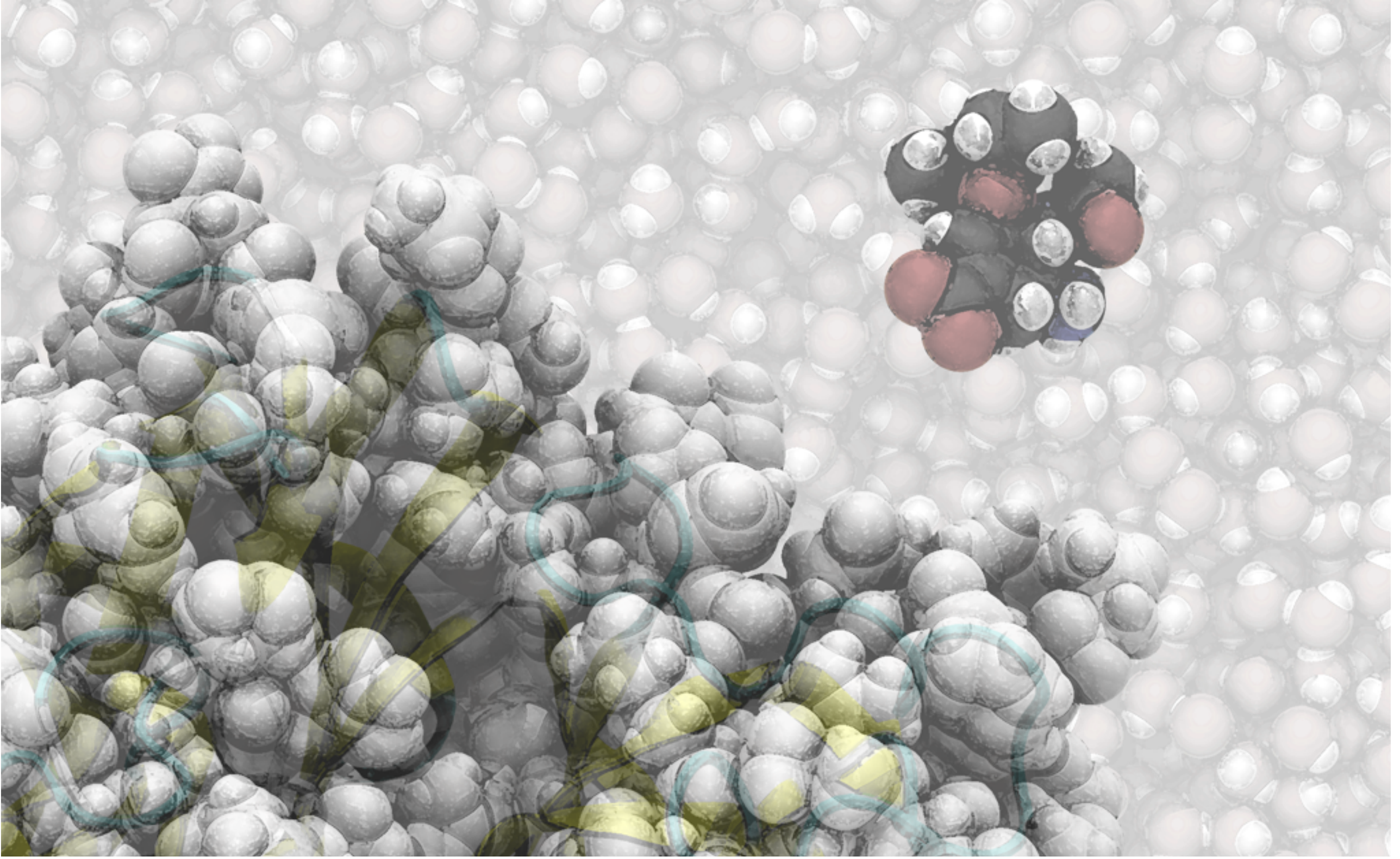
=

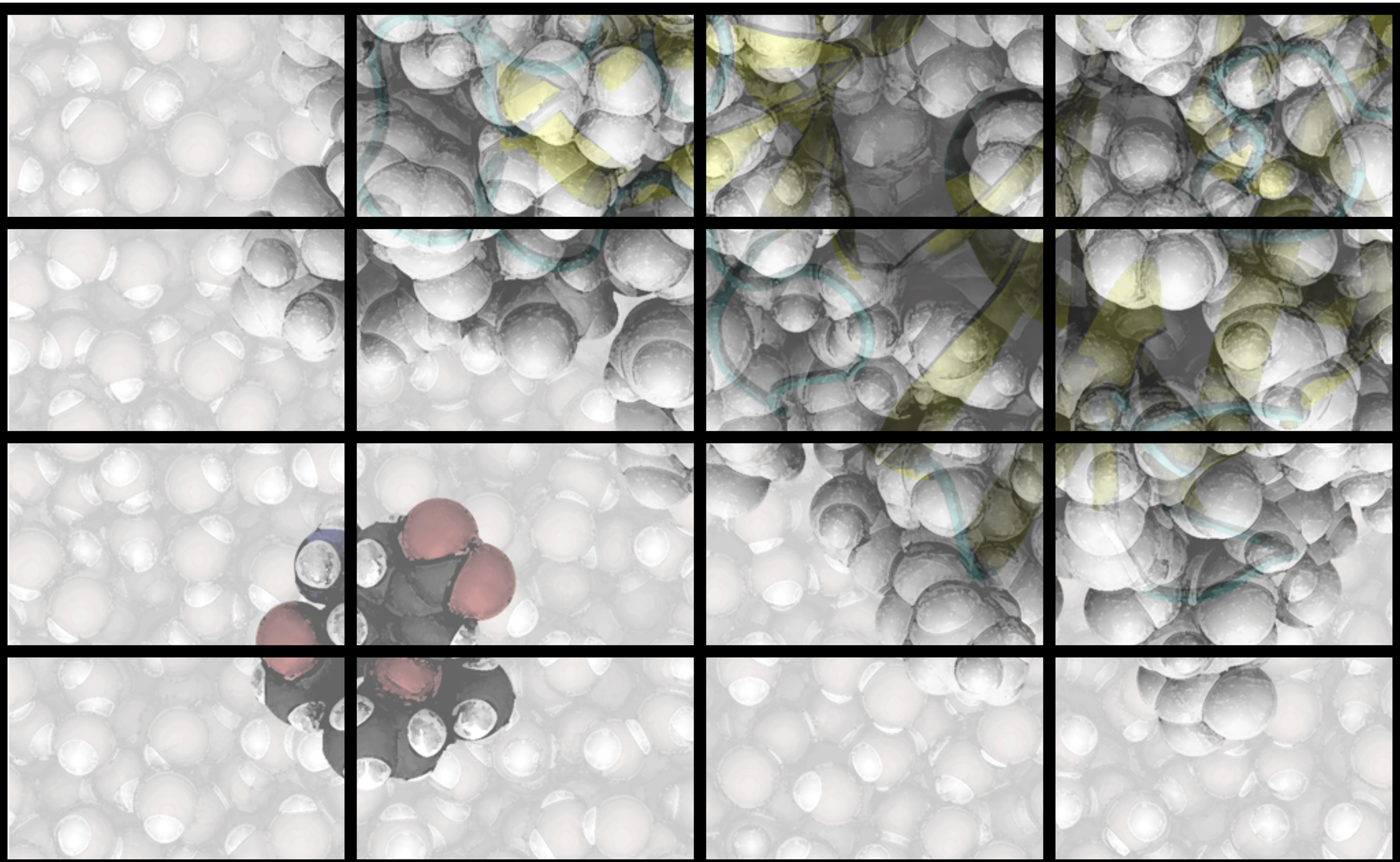
A*X	B*Y

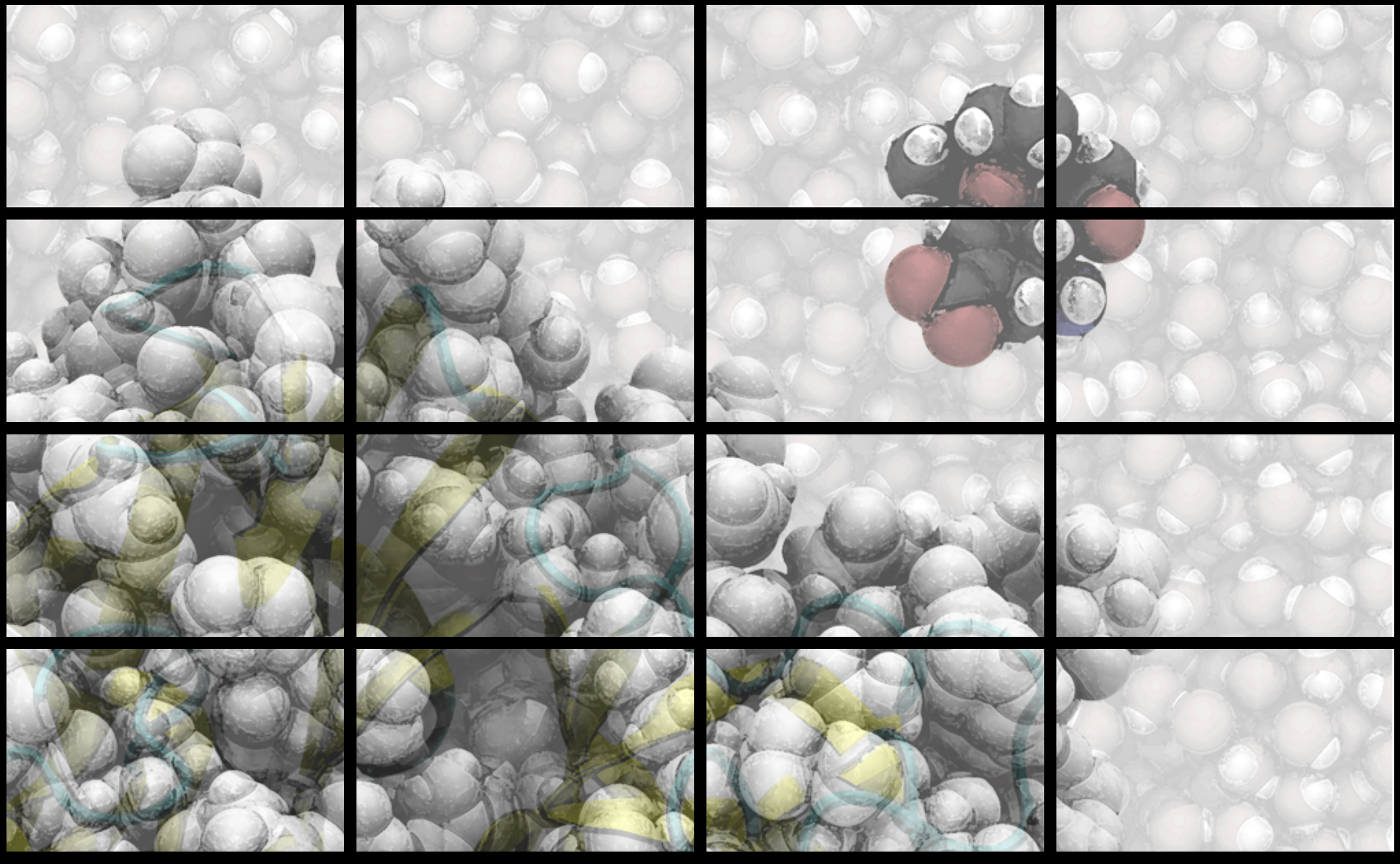


AVX (256 bit)

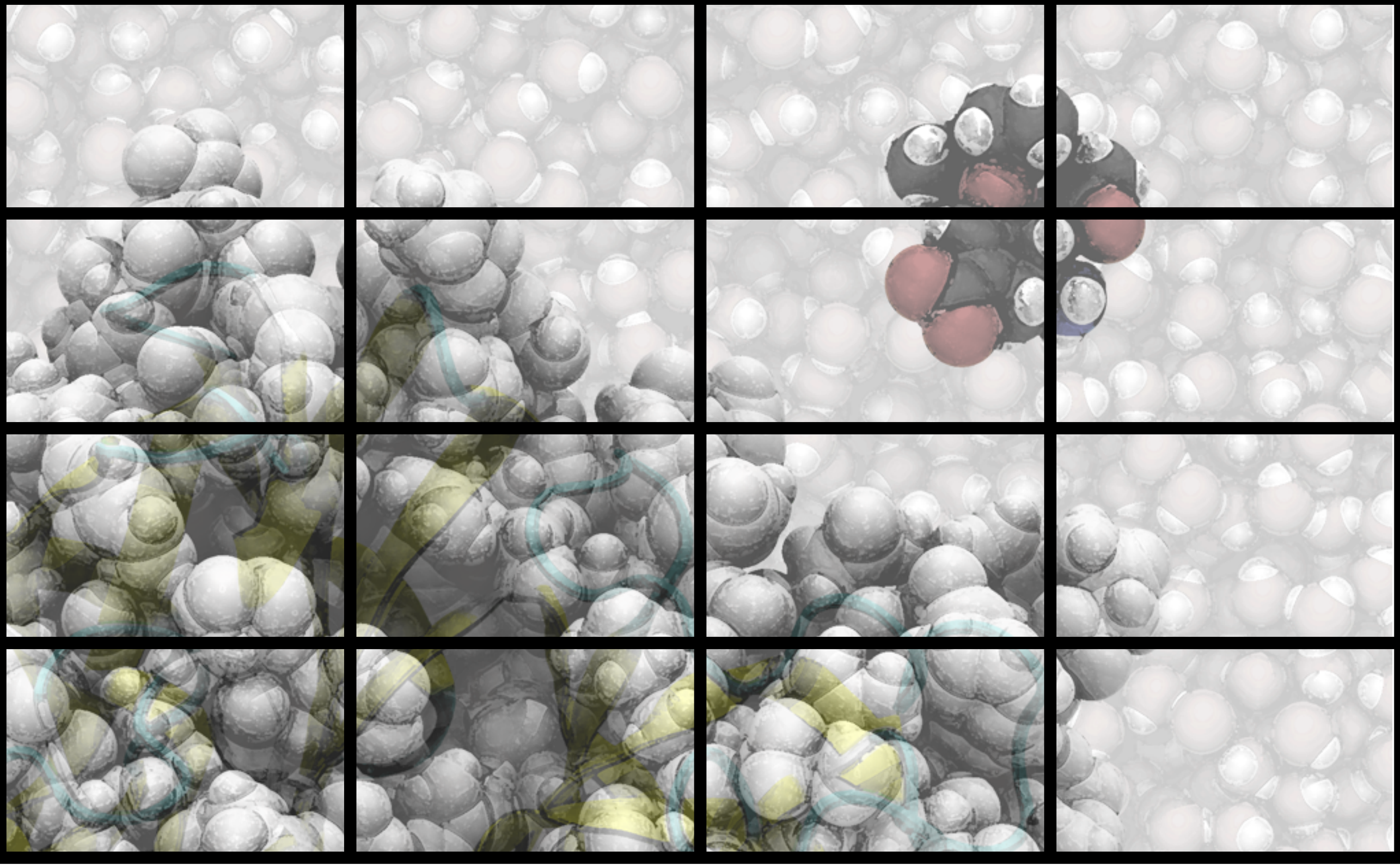
A	B	C	D
x		x	
X	Y	Z	W
=		=	
A*X	B*Y	C*Z	D*W



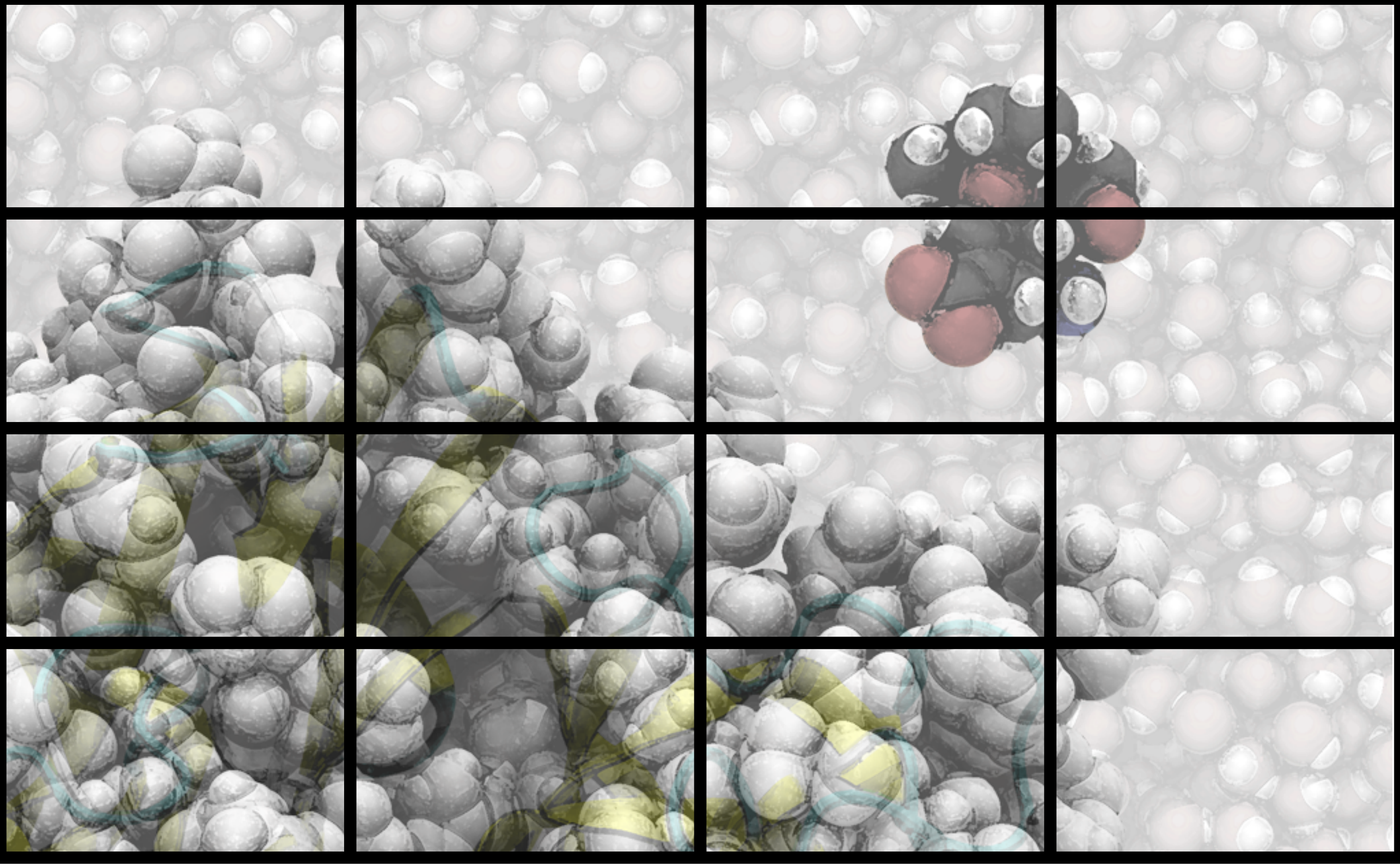




4x4x4 boxes



4x4x4 boxes 2016 box pairs!



OpenMP/TBB 4x4x4 boxes 2016 box pairs!

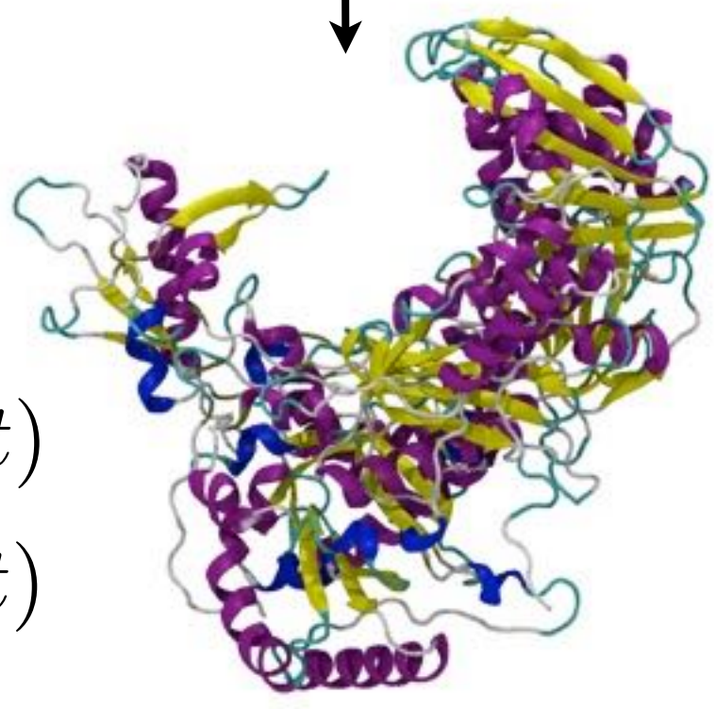
Big task queue of independent box pairs

Molecular Dynamics

$t + \Delta t$

$x(t + \Delta t)$

$v(t + \Delta t)$



2. Calculate forces on all atoms

100,000 atoms ~ 10 M fp calcs

Multi-core laptop (AVX)

1 step takes 20 ms

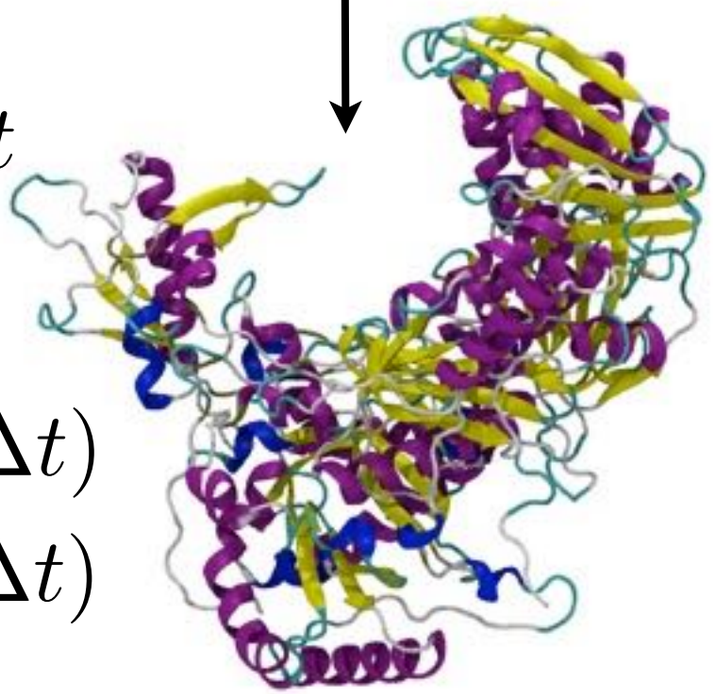
~ 5 nanoseconds per day

~ 1 second per 600,000 years

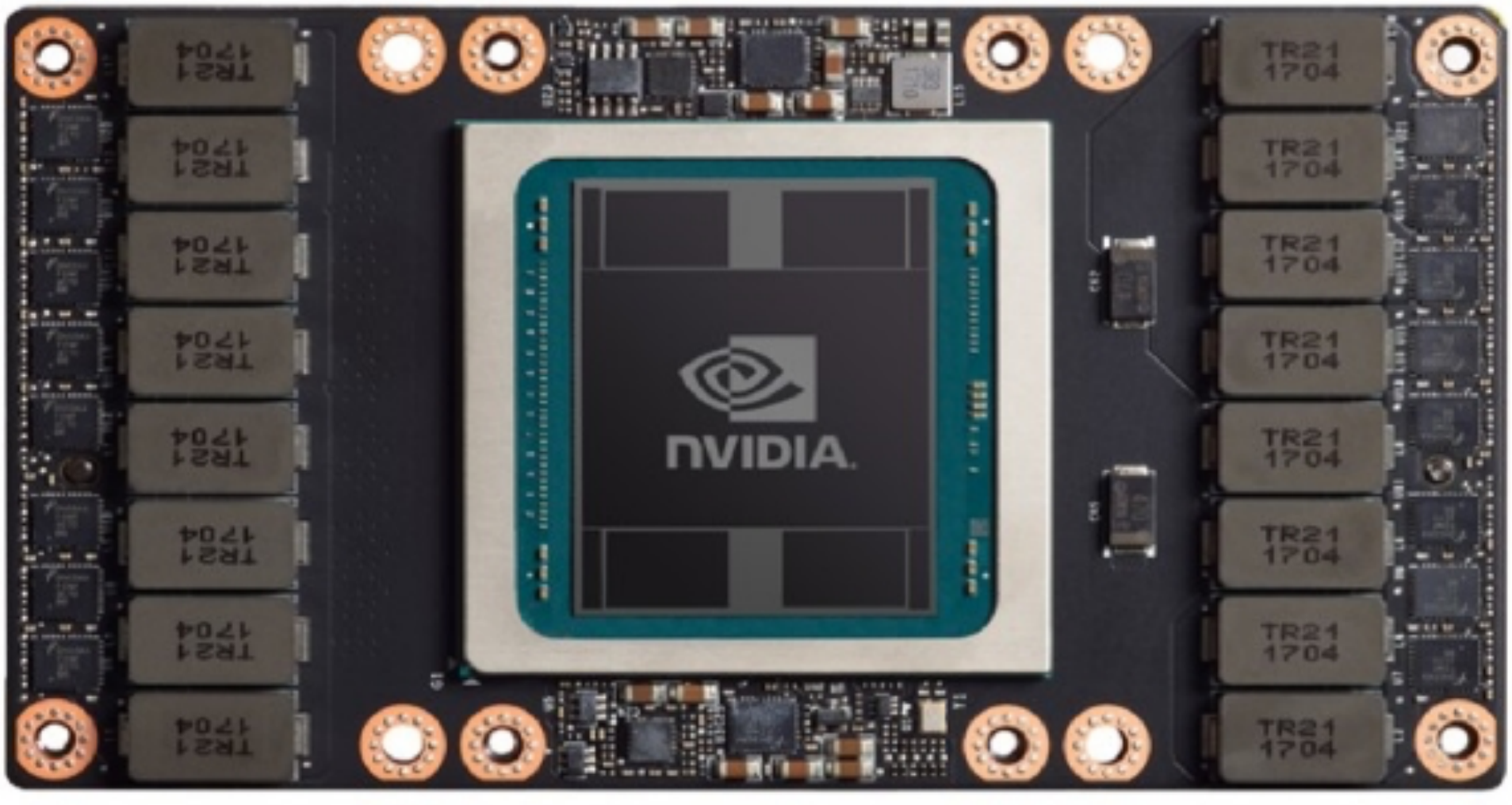
$t + 2\Delta t$

$x(t + 2\Delta t)$

$v(t + 2\Delta t)$

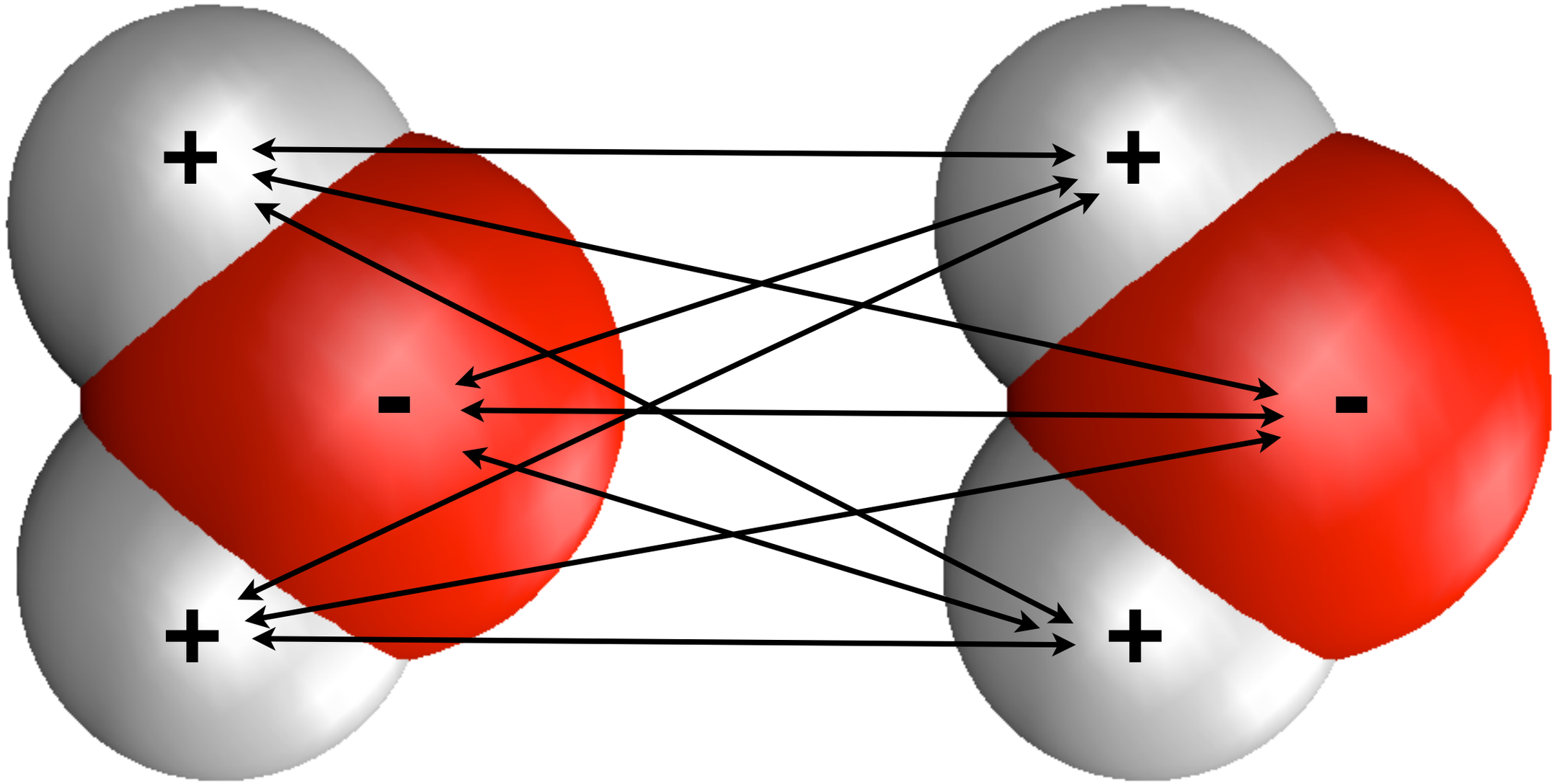


Graphic Processors (GPGPUS)



720 GB/s memory bandwidth, 5.3 TF DP, 10.6 TF SP

Multi-precision Calculations



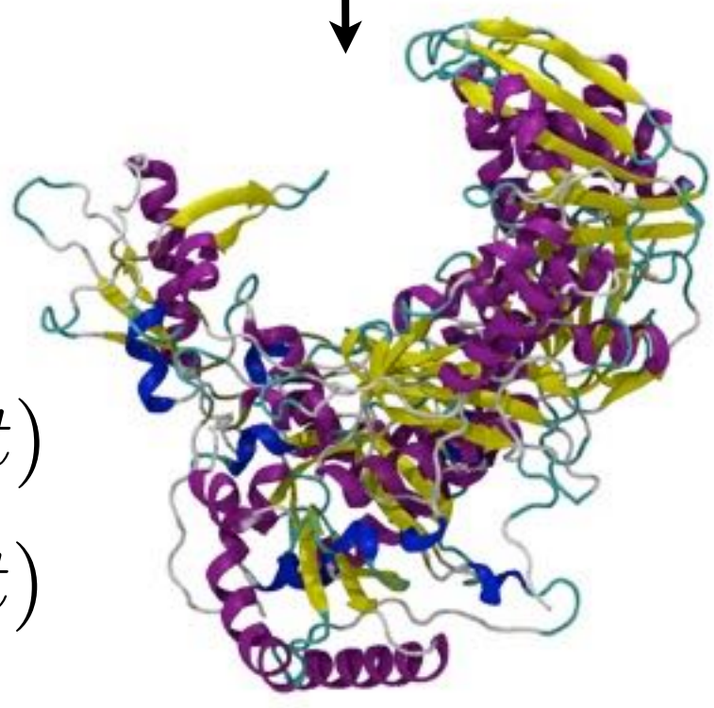
Calculate individual forces using single-precision floats
Accumulate sum of forces into double-precision doubles

Molecular Dynamics

$t + \Delta t$

$x(t + \Delta t)$

$v(t + \Delta t)$



2. Calculate forces on all atoms

100,000 atoms ~ 10 M fp calcs

GPGPU (P100)

1 step takes 1 ms

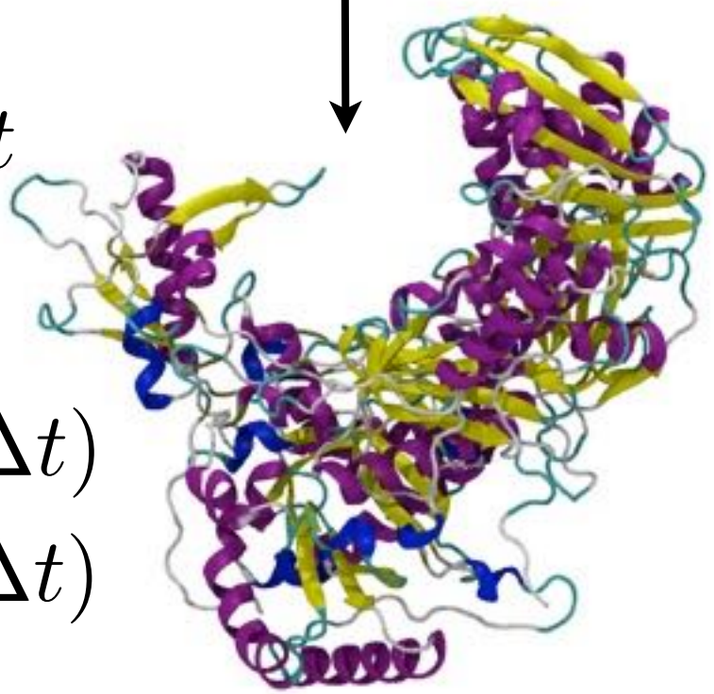
~ 90 nanoseconds per day

~ 1 second per 30,000 years

$t + 2\Delta t$

$x(t + 2\Delta t)$

$v(t + 2\Delta t)$

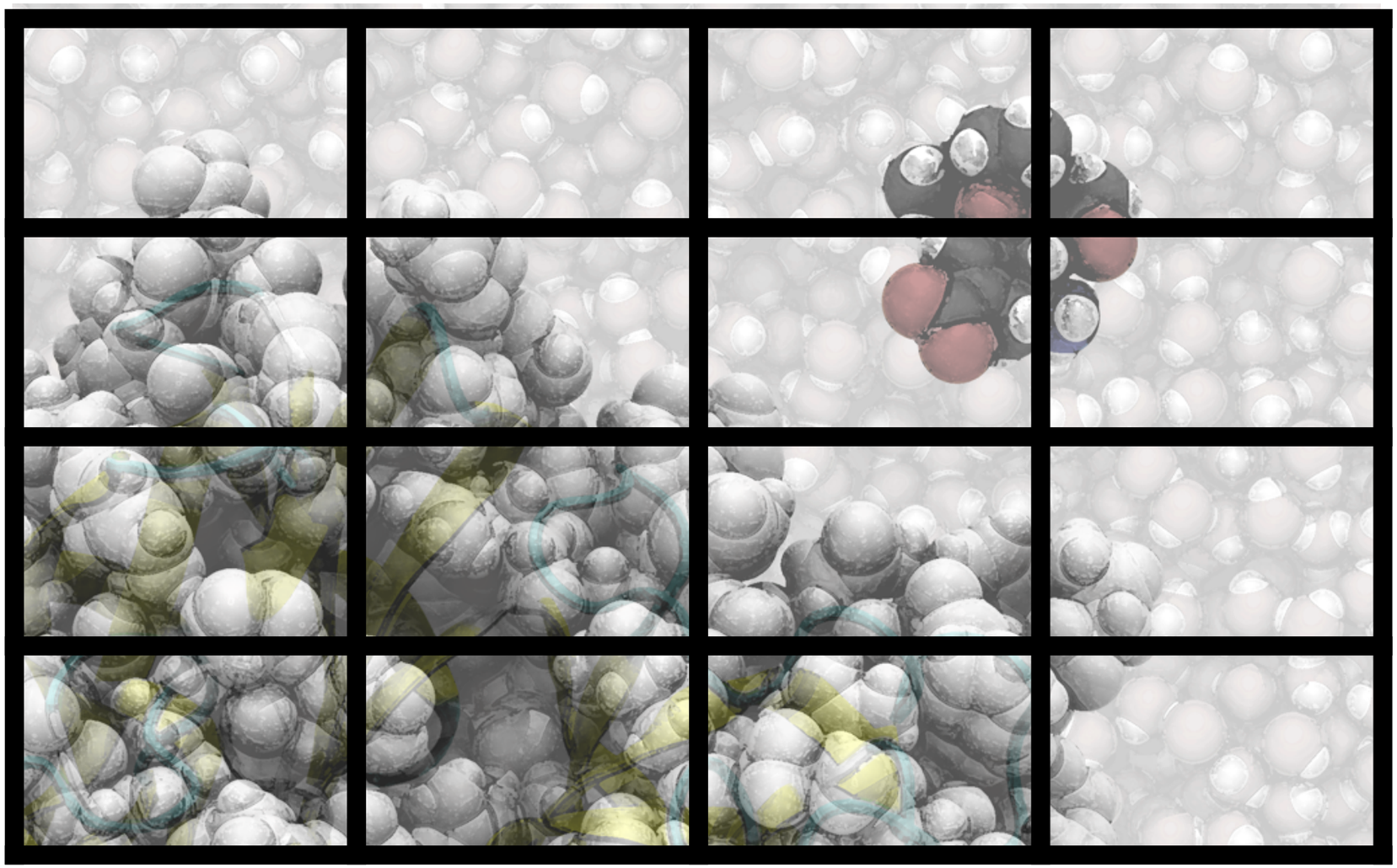


HPC Supercomputer

BlueCrystal Phase 4
15,000 CPU cores
64 P100s

Intel Omnipath
Interconnect

Multi-node (MPI)



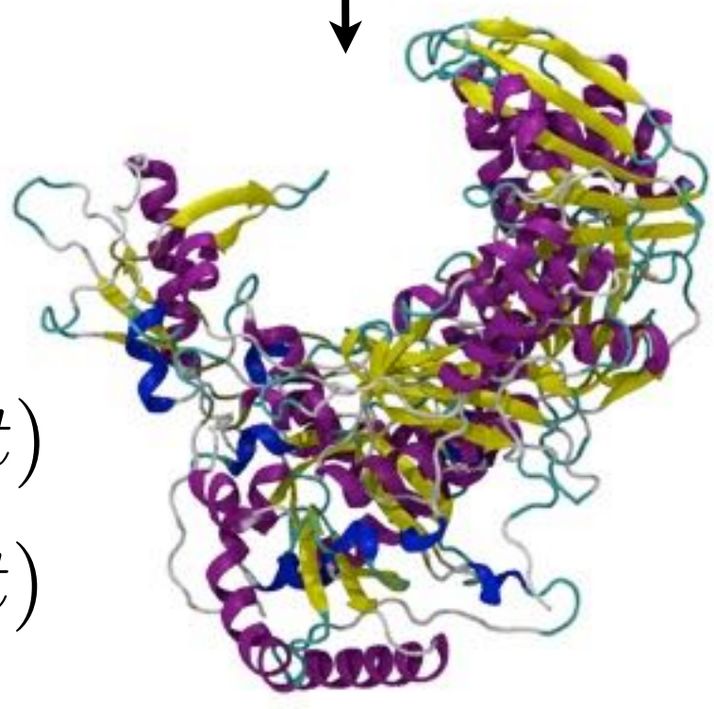
Disperse boxes over nodes.
Use MPI to communicate between nodes
(need low-latency interconnect)

Molecular Dynamics

$t + \Delta t$

$x(t + \Delta t)$

$v(t + \Delta t)$



2. Calculate forces on all atoms

100,000 atoms ~ 10 M fp calcs

BC4 (128 nodes)

1 step takes 0.3 ms

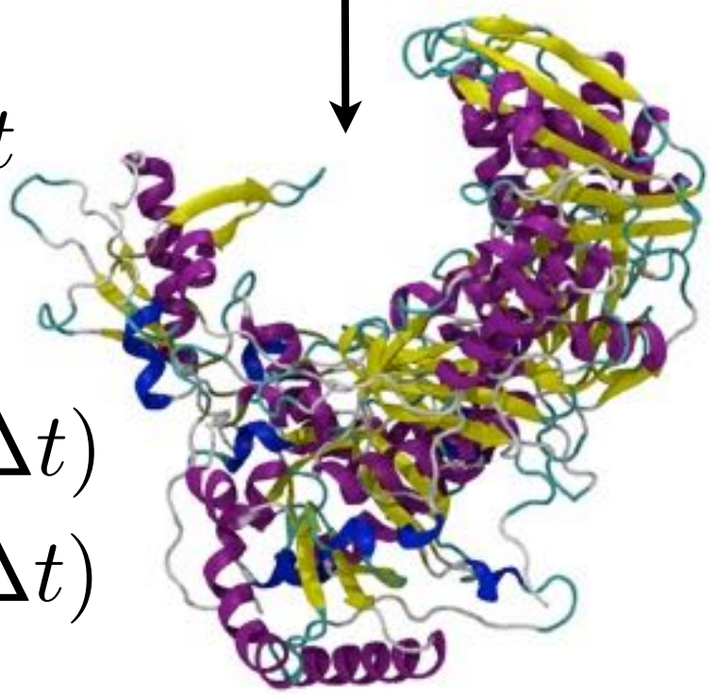
~ 300 nanoseconds per day

~ 1 second per 9,000 years

$t + 2\Delta t$

$x(t + 2\Delta t)$

$v(t + 2\Delta t)$



Anton 2

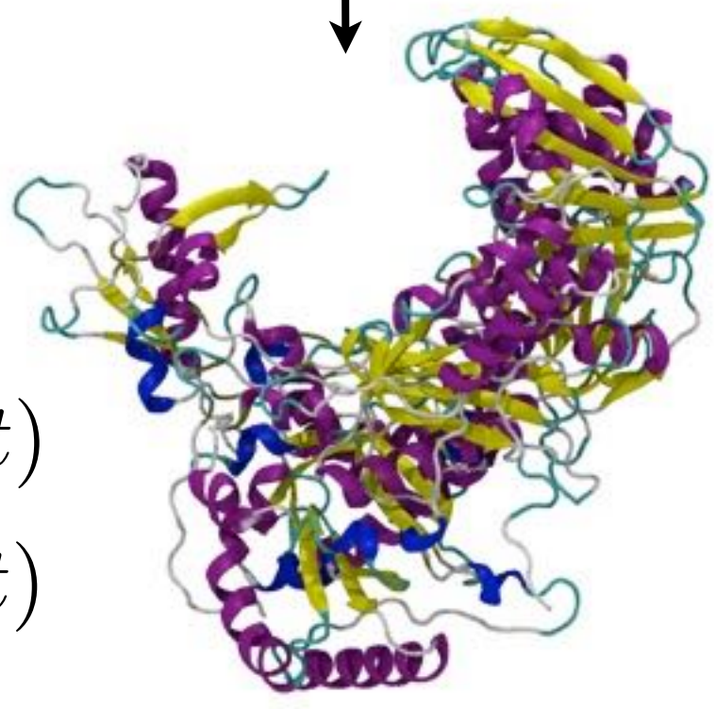
Custom Molecular Dynamics Supercomputer
Completely custom chip (force calculation in hardware!)
Designed and built by a billionaire
https://www.deshawresearch.com

Molecular Dynamics

$t + \Delta t$

$x(t + \Delta t)$

$v(t + \Delta t)$



2. Calculate forces on all atoms

100,000 atoms ~ 10 M fp calcs

Anton 2

1 step takes 1.5 µs

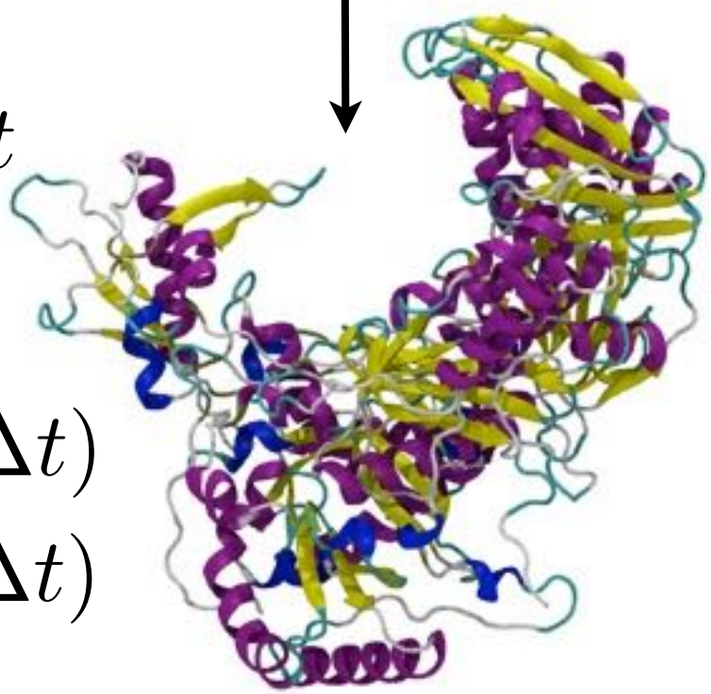
~ 60,000 nanoseconds per day

~ 1 second per 45 years

$t + 2\Delta t$

$x(t + 2\Delta t)$

$v(t + 2\Delta t)$

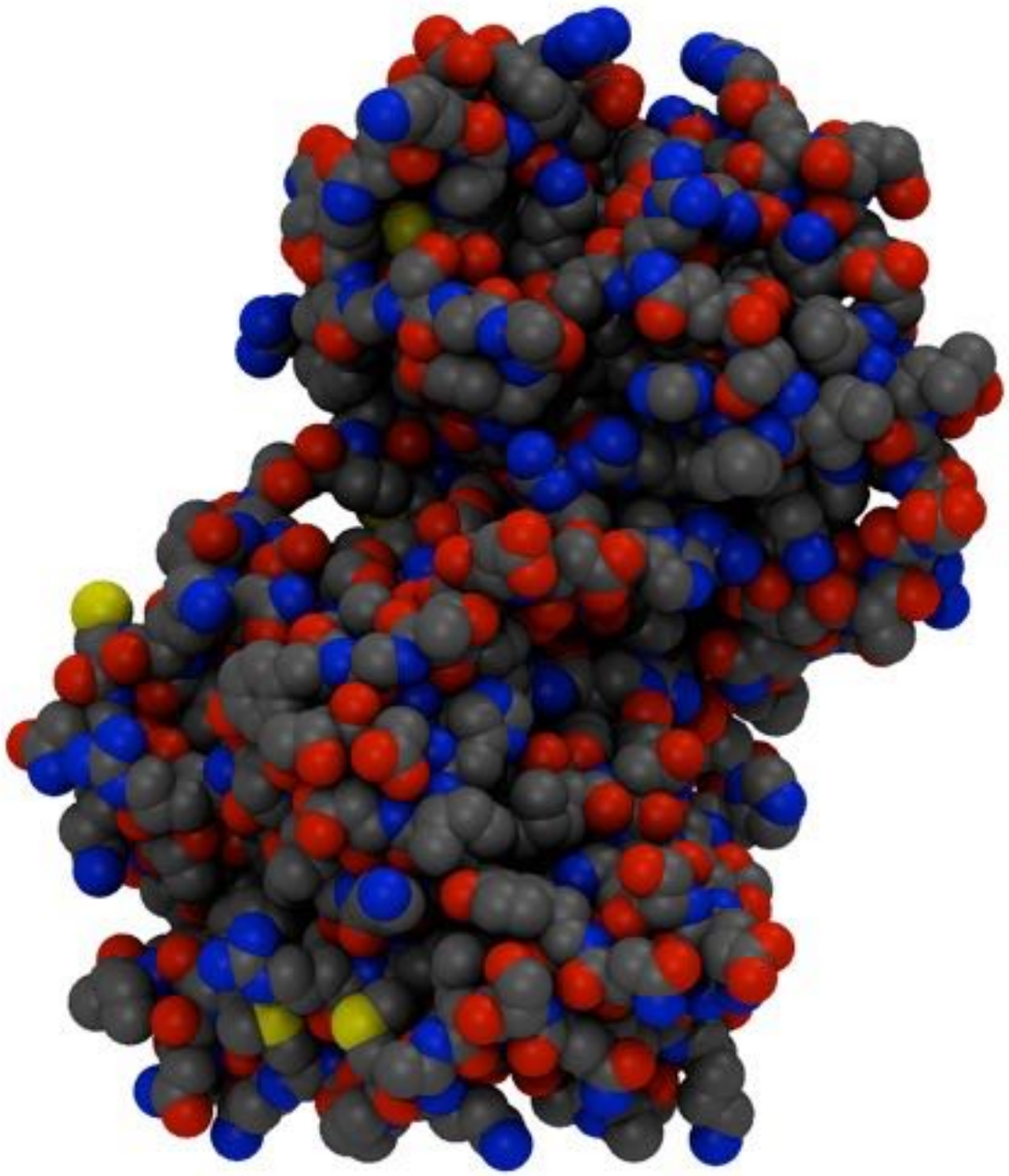


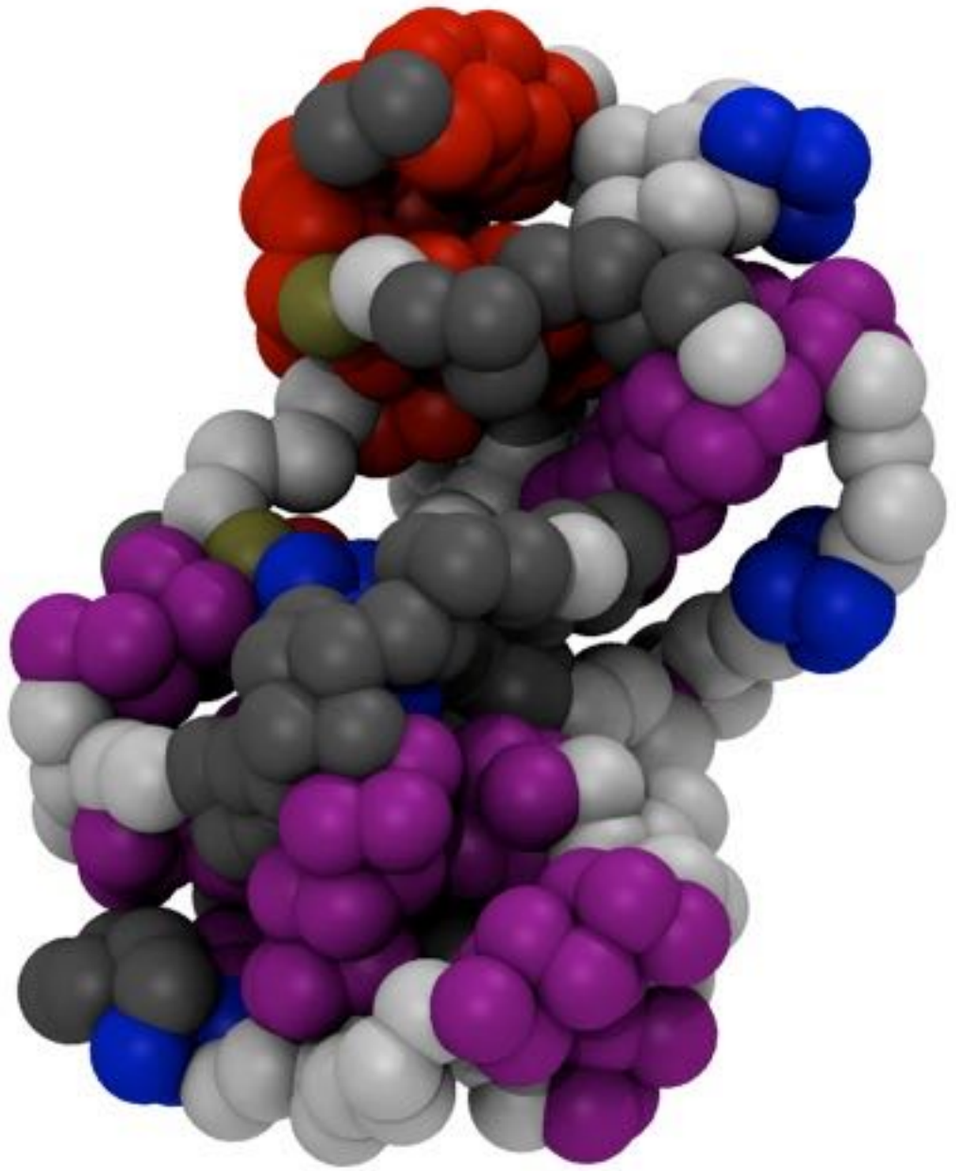
Speed Comparison

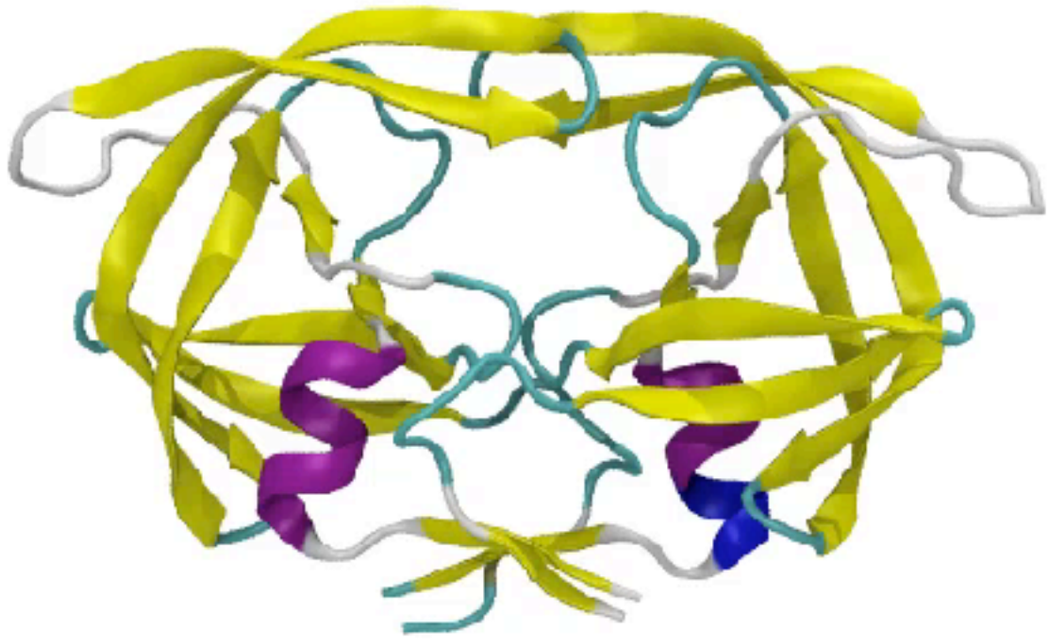
	Serial	Laptop	GPU	Cluster	Anton 2
Time per step	100 ms	20 ms	1 ms	300 μs	1.5 μs
nanoseconds per day	1	5	90	300	60,000
Years per second	3000,000	600,000	30,000	9000	45
Speedup	**1**	**5**	**90**	**300**	**60,000**

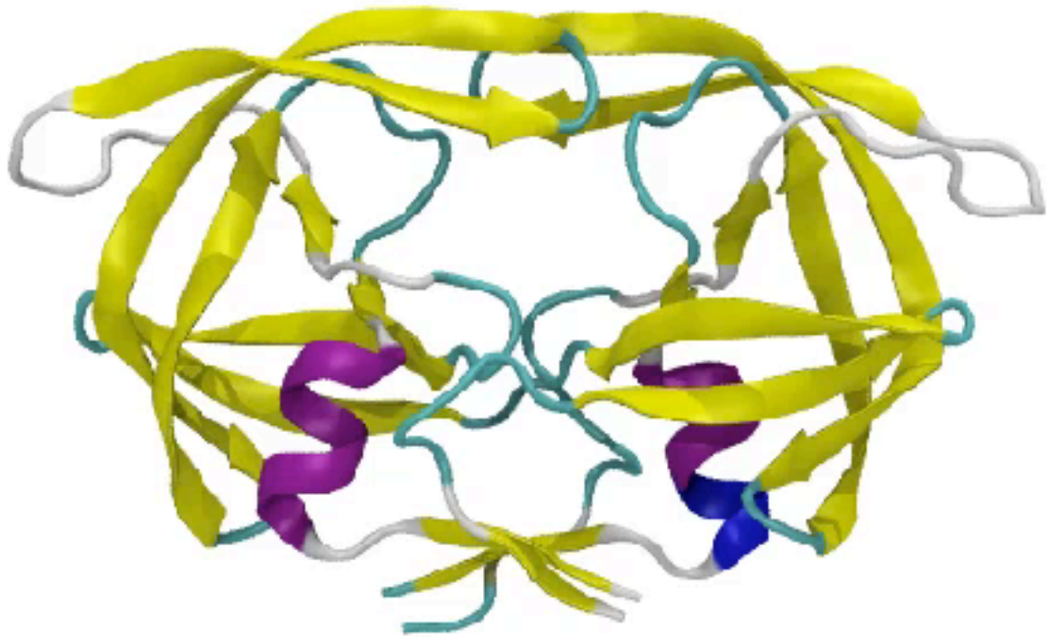
Change the Algorithm

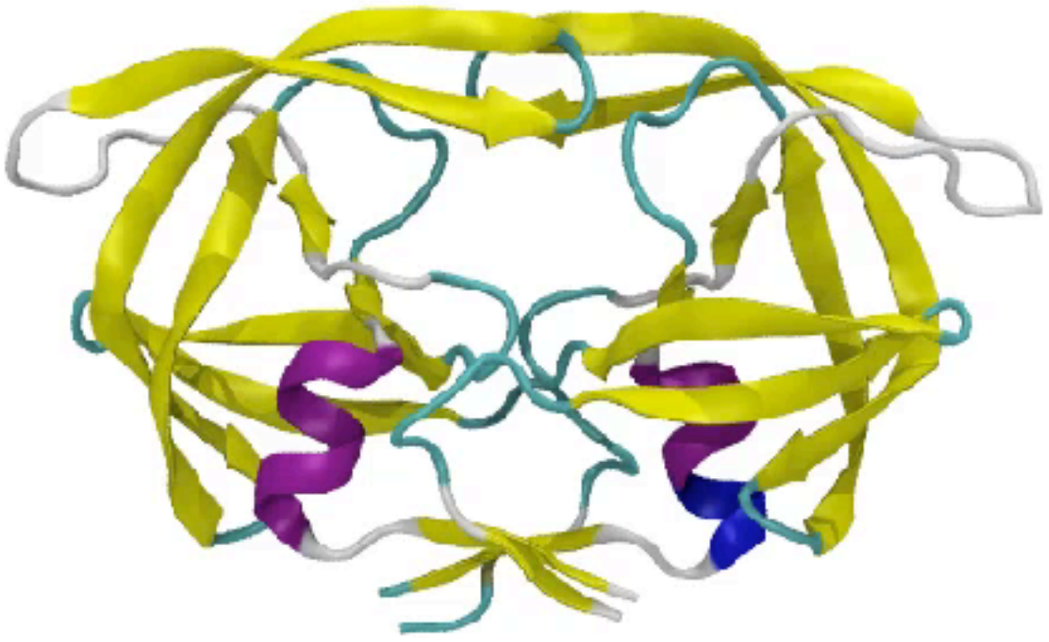
- Need to be clever to simulate more
  - Not just optimising the software/ hardware
  - Really examine the algorithm and approximations

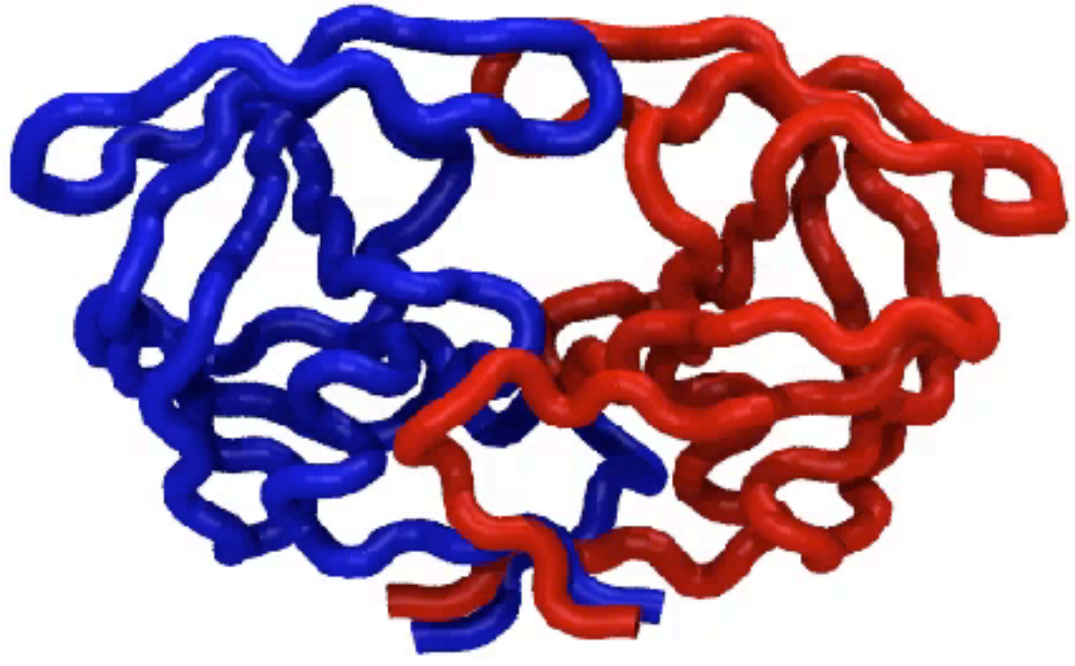


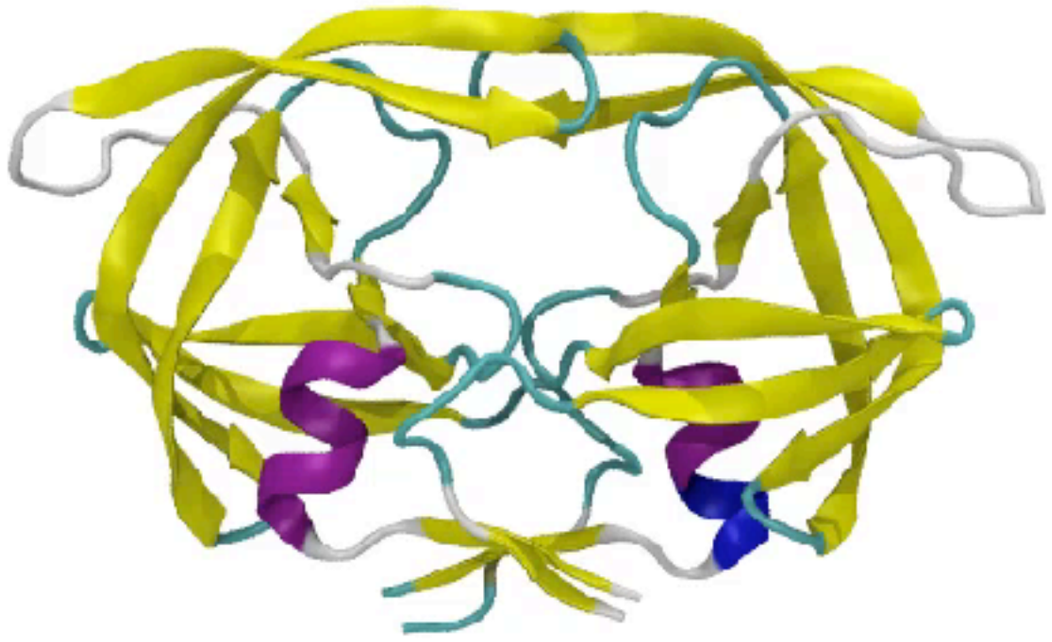


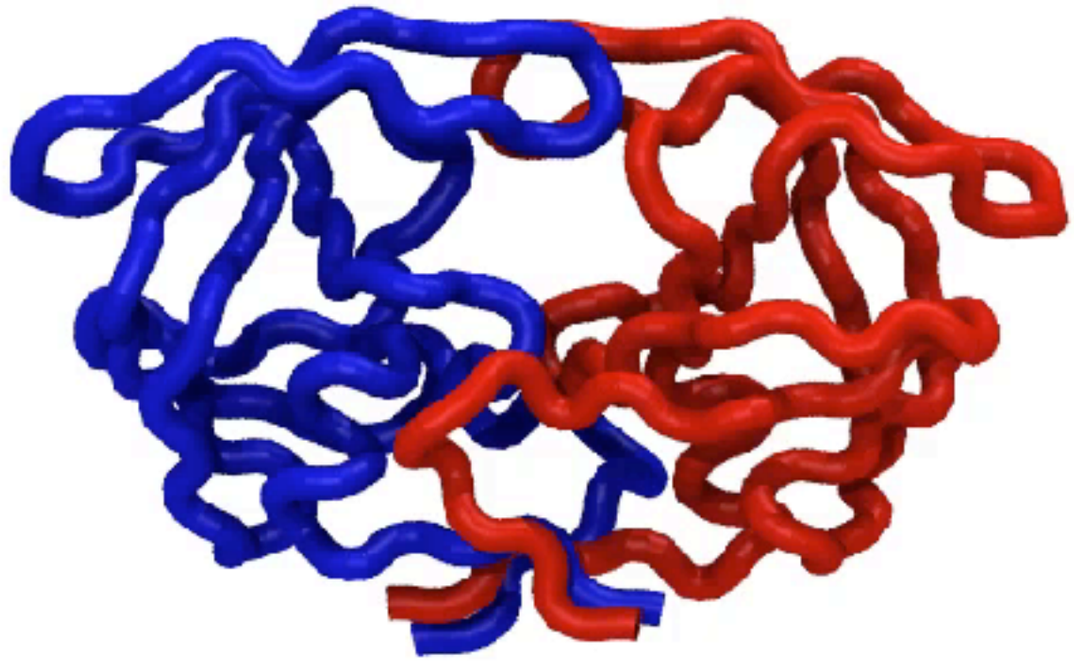


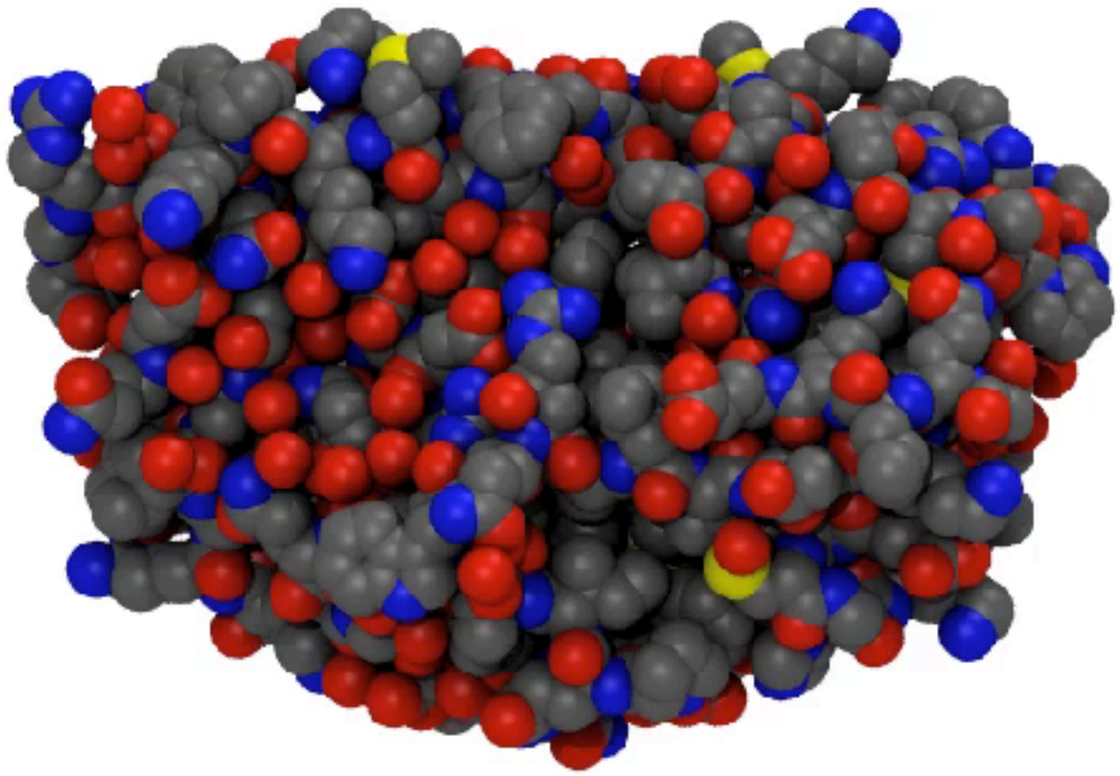


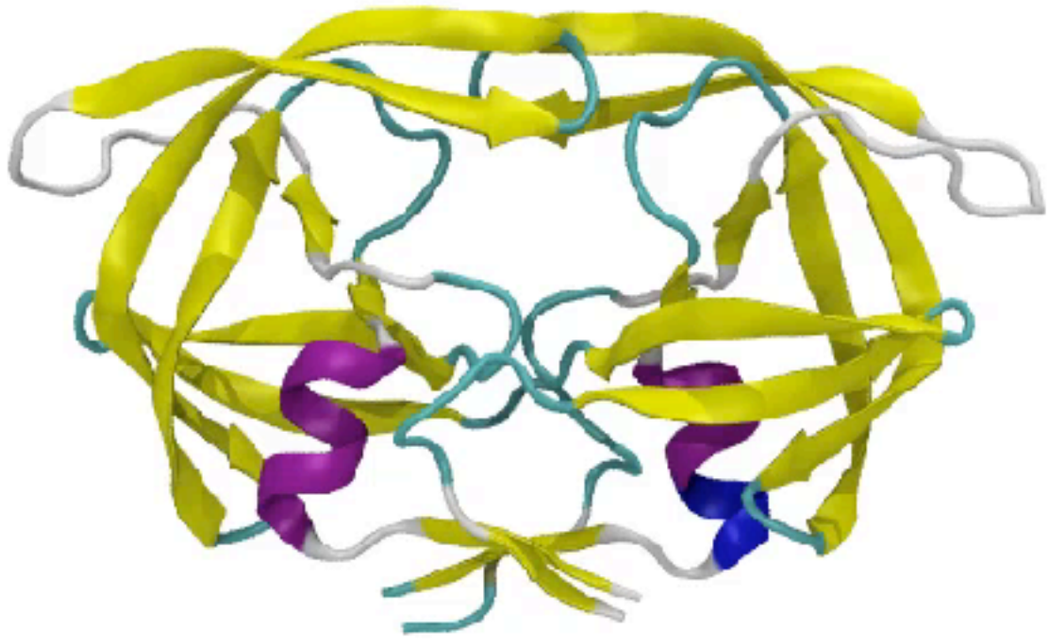


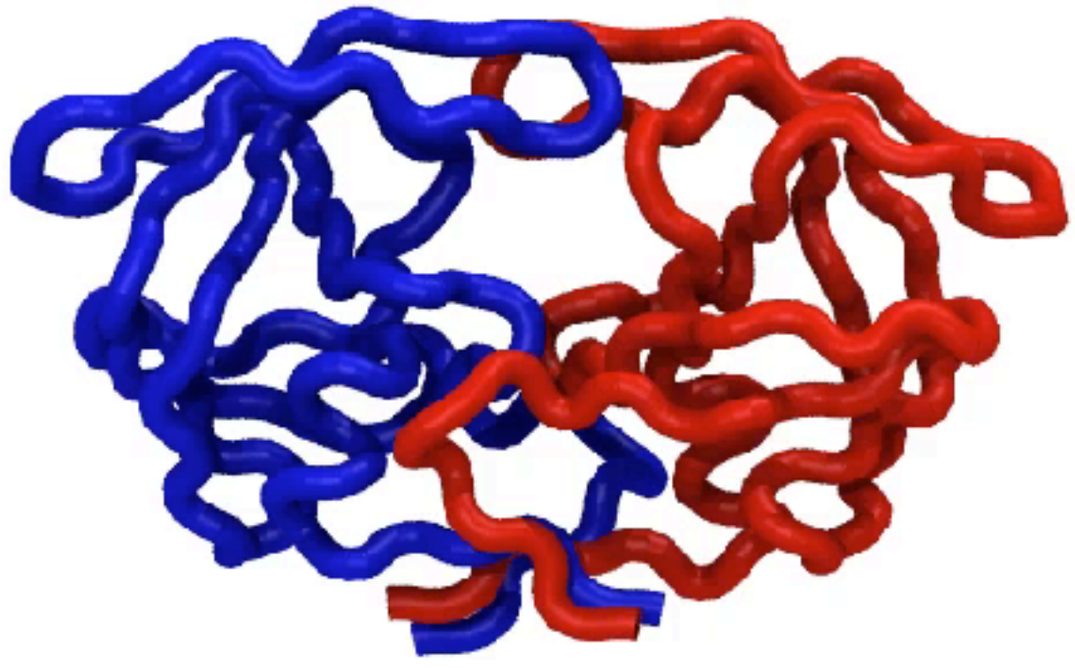


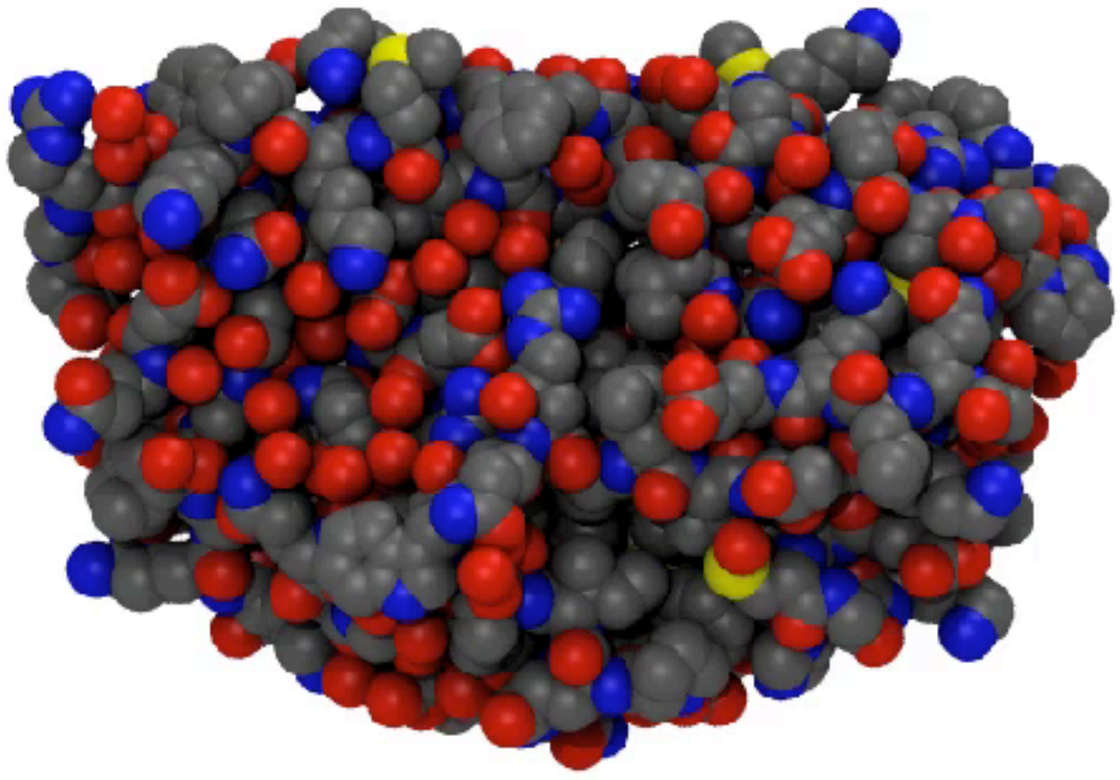


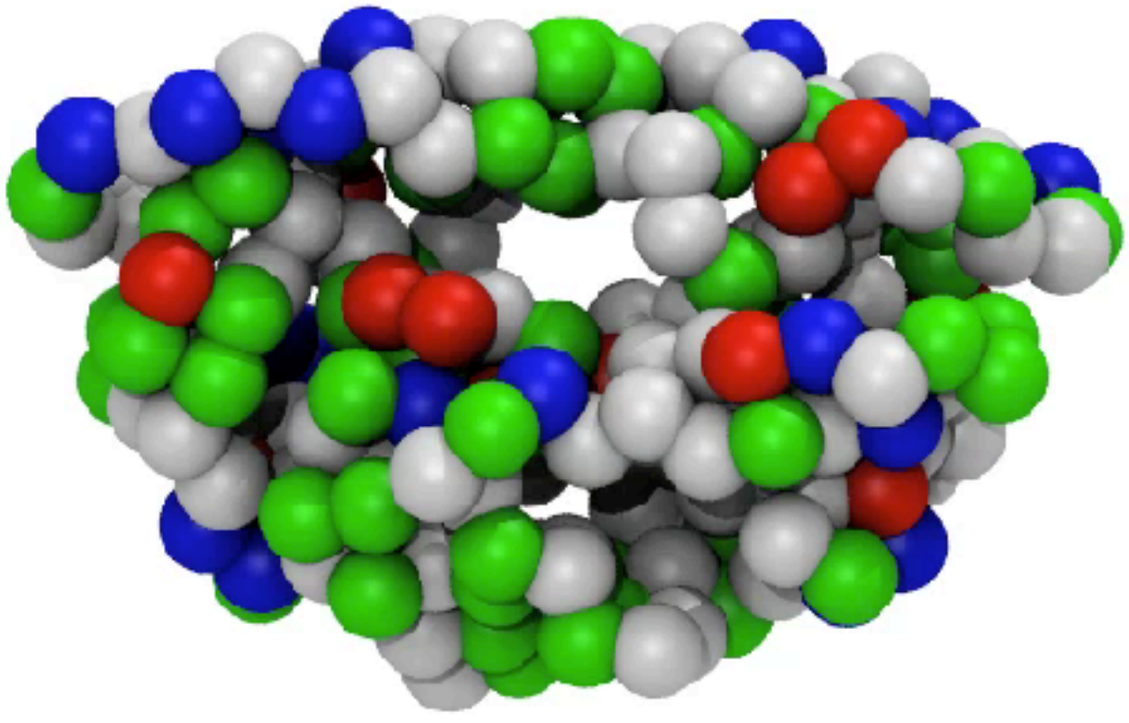


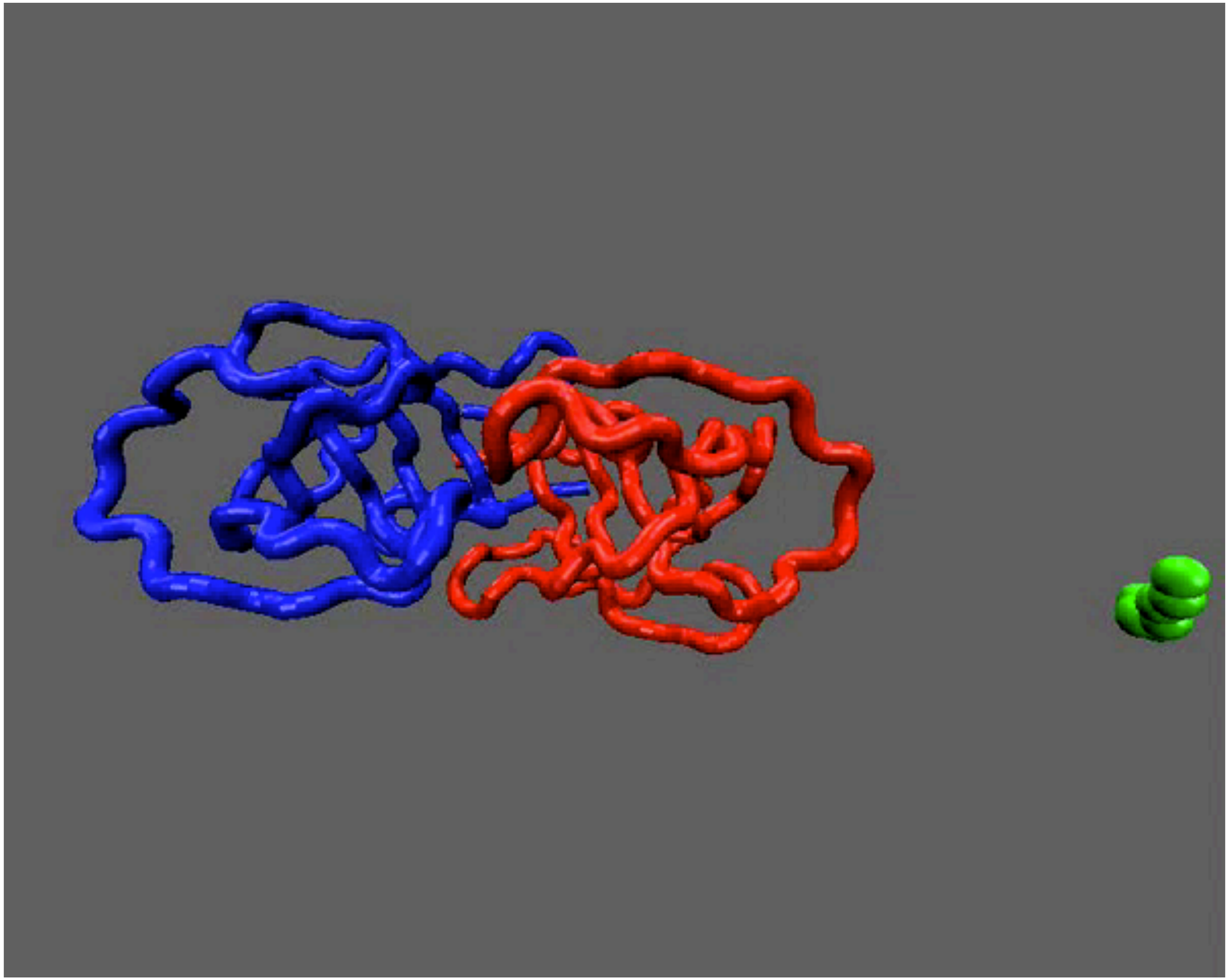












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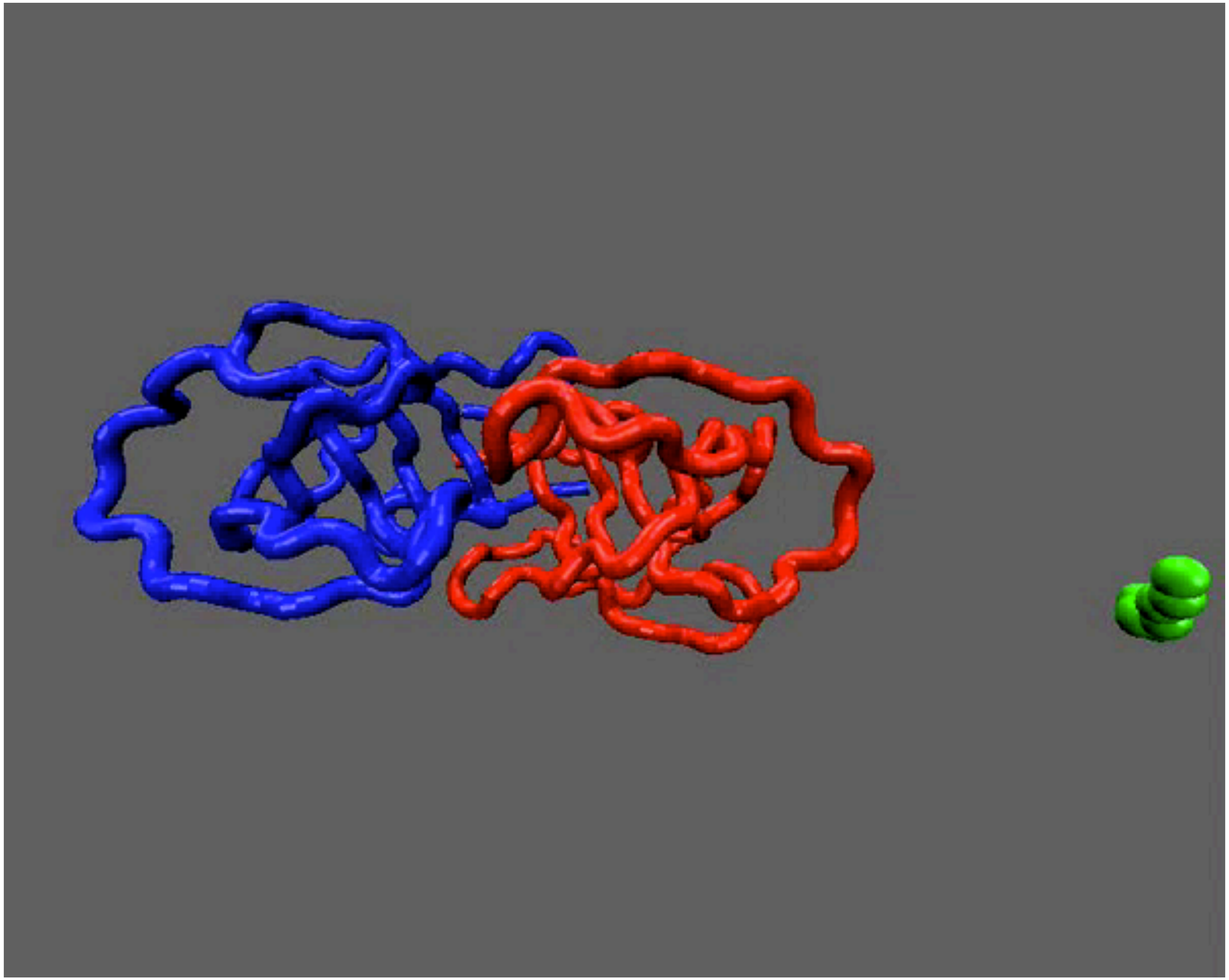

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Questions?