

Simulación de Sistemas a la Nanoescala

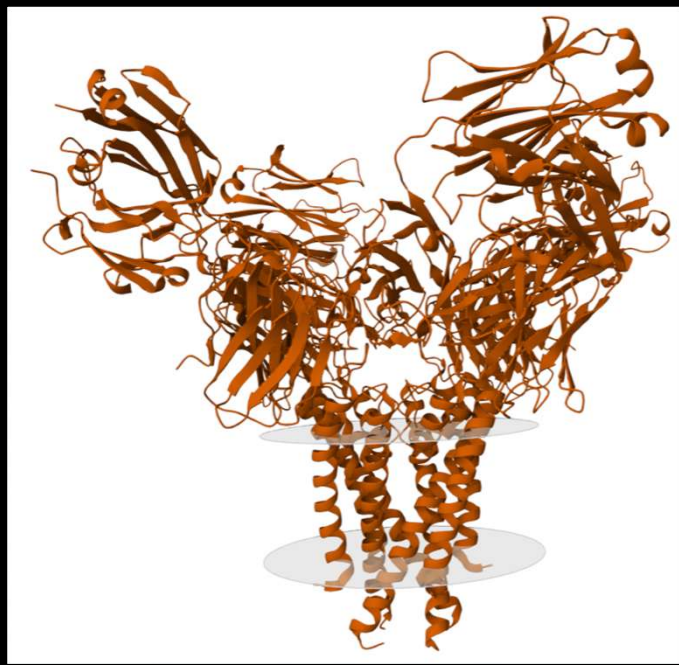
Formación de un canal proteico en una membrana

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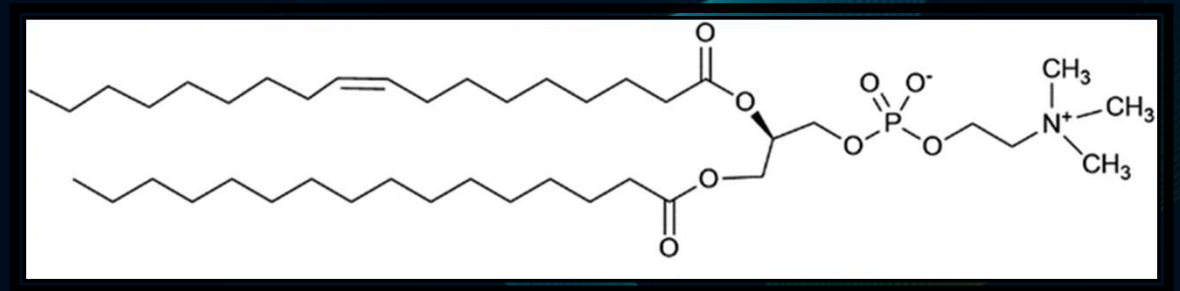
NIU: 1634788

Introducción

Sistema que simular



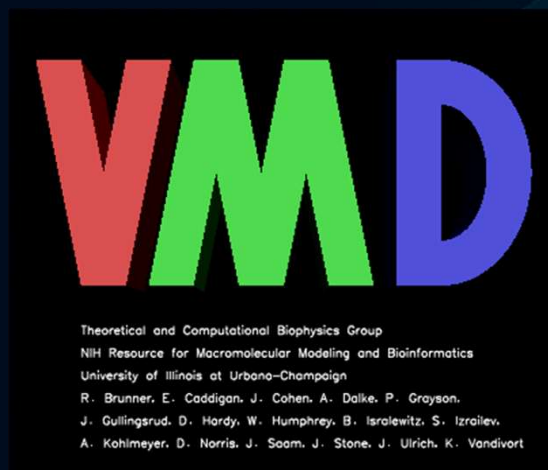
Canal específico de K



Componente de la membrana lipídica

Introducción

Principales herramientas

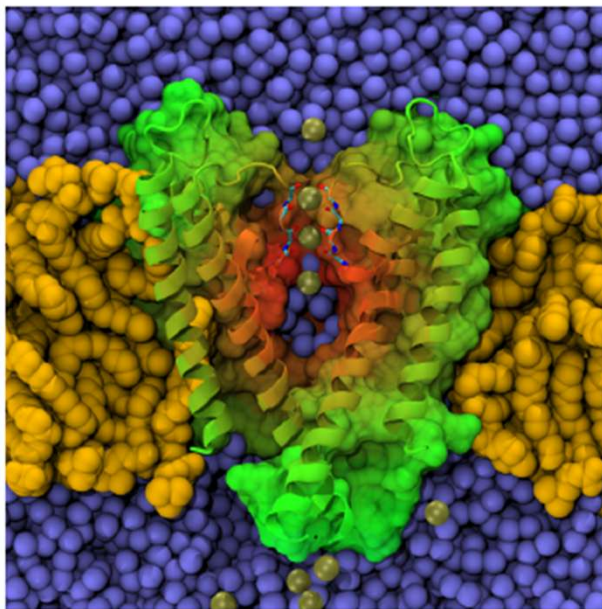


NAMD

Introducción

Fuente de apoyo

University of Illinois at Urbana-Champaign
Beckman Institute for Advanced Science and Technology
Theoretical and Computational Biophysics Group
Computational Biophysics Workshop



Alek Aksimentiev

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Código

Obtención de ficheros .pdb y .psf

Código 1

```
# Primero abrir VMD
# Cargar y guardar segmento A

mol new 1k4c.pdb
set sel [atomselect top "all"]
$sel set segname A
$sel writepdb KCSA-A.pdb

# Hacemos segmento B

set sel [atomselect top "all and not name K"]
$sel set segname B
$sel move {{-1.0 0.0 0.0 310.66}} {0.0 -1.0 0.0 310.66}
{0.0 0.0 1.0 0.0} {0.0 0.0 0.0 1.0}}
$sel writepdb KCSA-B.pdb
```

Código 2

```
# Proteínas

foreach S { A B C D } {

set seg [atomselect top "segname $S and
chain C and protein"]

$seg writepdb seg$$S.pdb

$seg delete

}

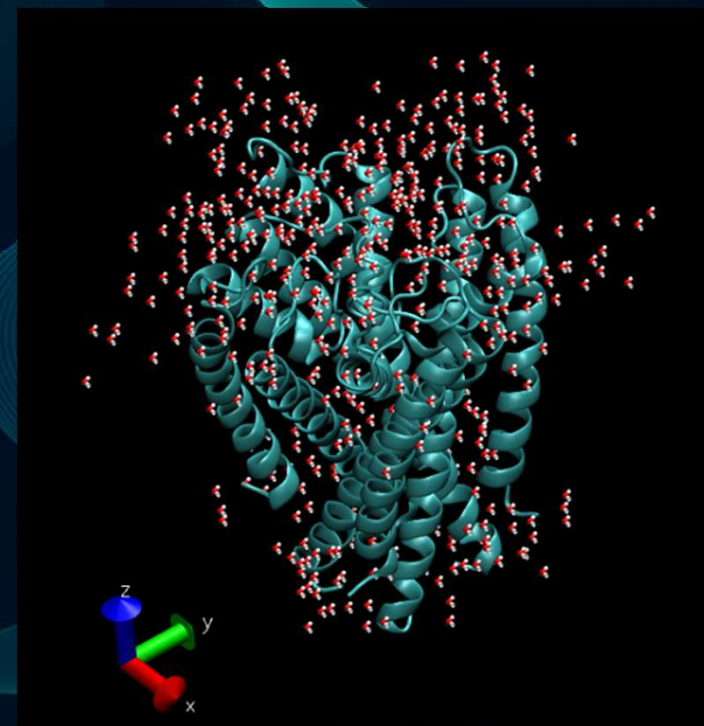
# Iones

set pot [atomselect top "name K and resid
3001 3003 3005 3006"]

$pot set name POT

$pot set resname POT

$pot writepdb pot.pdb
```



Código

Tratamiento del Sistema

Código 3

Membrana

```
$popc moveby [vecinvert [measure center  
$popc weight mass]]
```

```
$popc writepdb PT.pdb
```

Canal, primera línea es seleccionar el centro de la proteína

```
set vest [atomselect $mol "protein and resid  
97 to 106"]
```

```
$k moveby [vecinvert [measure center $vest  
weight mass]]
```

```
$k writepdb KT.pdb
```

Código 4

```
mol delete all
```

```
resetpsf
```

```
readpsf Mb.psf
```

```
coordpdb PT.pdb
```

```
readpsf ../2Solvatacion/ProtSol.psf
```

```
coordpdb KT.pdb
```

```
writesf K_Mb_Raw.psf
```

```
writepdb K_Mb_Raw.pdb
```

Código 5

Selección de lípidos

```
set bl [atomselect top "name P1 and beta > 0"]
```

```
set segll [$bl get segid]
```

```
set resll [$bl get resid]
```

Selección de aguas

```
set bw [atomselect top "name OH2 and beta > 0"]
```

```
set seglw [$bw get segid]
```

```
set reslw [$bw get resid]
```

Creación del Sistema (después de cargar el sistema de nuevo y reseteado los psf

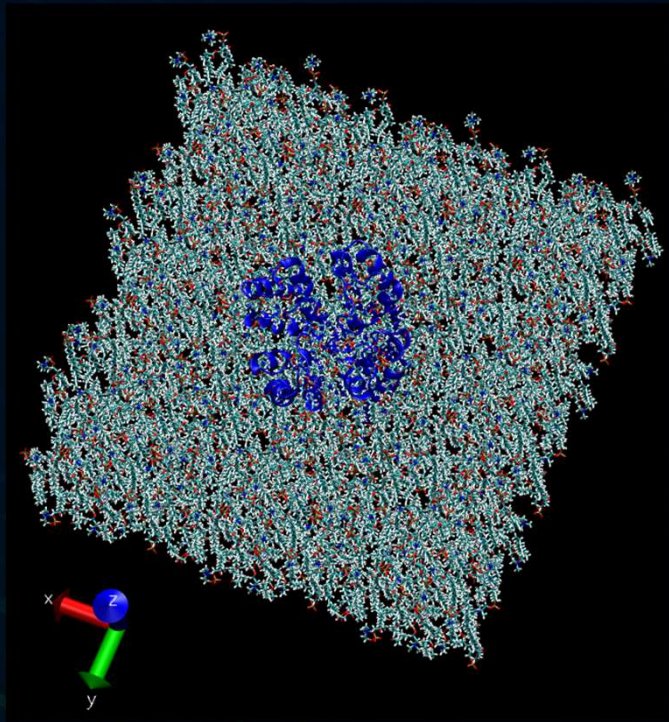
```
foreach segid $segll resid $resll {delatom $segid  
$resid}
```

```
foreach segid $seglw resid $reslw {delatom $segid  
$resid}
```

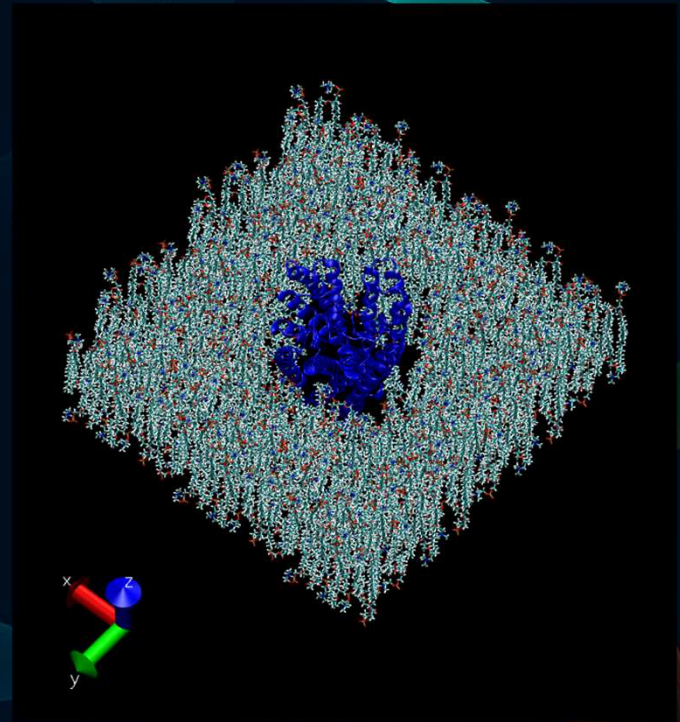
```
writesf K_Mb.psf
```

```
writepdb K_Mb.pdb
```


Código



Tratamiento del Sistema



Código

Código 6

Indicar ficheros

```
mol new ../input/K_Mb.psf
```

```
mol addfile ../input/K_Mb.pdb
```

```
set all [atomselect top "all"]
```

```
$all set beta 0
```

```
set fixed [atomselect top "water or name CLA POT or protein or (chain L /  
and name O2 P1 O3 O4 O1 C15 H52 H51 H11 C11 H12 N C14 H42 H43 H41 /  
C12 H22 H23 H21 C13 H33 H31 H32)"]
```

```
$fixed set beta 1
```

```
$all writepdb K_Mb.fix
```

Simulaciones

Fichero melting.conf

Encontrar el origen de la celda

```
set all [atomselect top all]
```

```
measure center $all
```

Encontrar Vectores de la base

```
set all [atomselect top all]
```

```
measure minmax $all
```

Los valores que nos dan los restos y obtienes el valor total del vector



Valor de la red de un sistema periódico electrostático: Debe ser mayor al vector de la red y múltiplo de 2, 3 o 5.

Código

Error

```
ERROR: Constraint failure in RATTLE algorithm for atom 37189!  
ERROR: Constraint failure; simulation has become unstable.  
ERROR: Constraint failure in RATTLE algorithm for atom 36408!  
ERROR: Constraint failure; simulation has become unstable.  
ERROR: Constraint failure in RATTLE algorithm for atom 17627!  
ERROR: Constraint failure; simulation has become unstable.  
ERROR: Constraint failure in RATTLE algorithm for atom 17210!  
ERROR: Constraint failure; simulation has become unstable.  
ERROR: Constraint failure in RATTLE algorithm for atom 13913!  
ERROR: Constraint failure; simulation has become unstable.  
ERROR: Constraint failure in RATTLE algorithm for atom 3828!  
ERROR: Constraint failure; simulation has become unstable.  
FATAL ERROR: Exiting prematurely; see error messages above.  
FATAL ERROR: Exiting prematurely; see error messages above.  
[Partition 0][Node 0] End of program
```

Conclusiones

Estado Final del Trabajo	
 <p>No he conseguido efectuar las simulaciones propuestas del flujo de iones por temas de tiempo y errores.</p>	 <p>He aprendido comandos nuevos y métodos de trabajo en el campo de las simulaciones de sistemas nanométricos diferentes a los vistos en clase.</p>

Gracias por vuestra atención



(aplausos)



The background is a dark navy blue. On the left side, there are faint, concentric, wavy lines in a slightly lighter shade of blue. On the right side, there are more prominent, flowing, wavy shapes in shades of teal and light blue. A large, solid orange question mark is centered on the page. The text "Espacio de Preguntas" is written in a white, serif font, positioned horizontally across the middle of the question mark.

Espacio de Preguntas