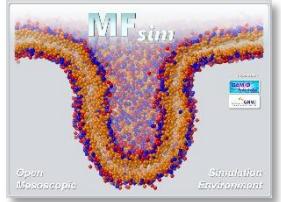


MF<sub>sim</sub>

2.2.4.0



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Simulation  
Environment

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[www.molecular-dynamics.de](http://www.molecular-dynamics.de)

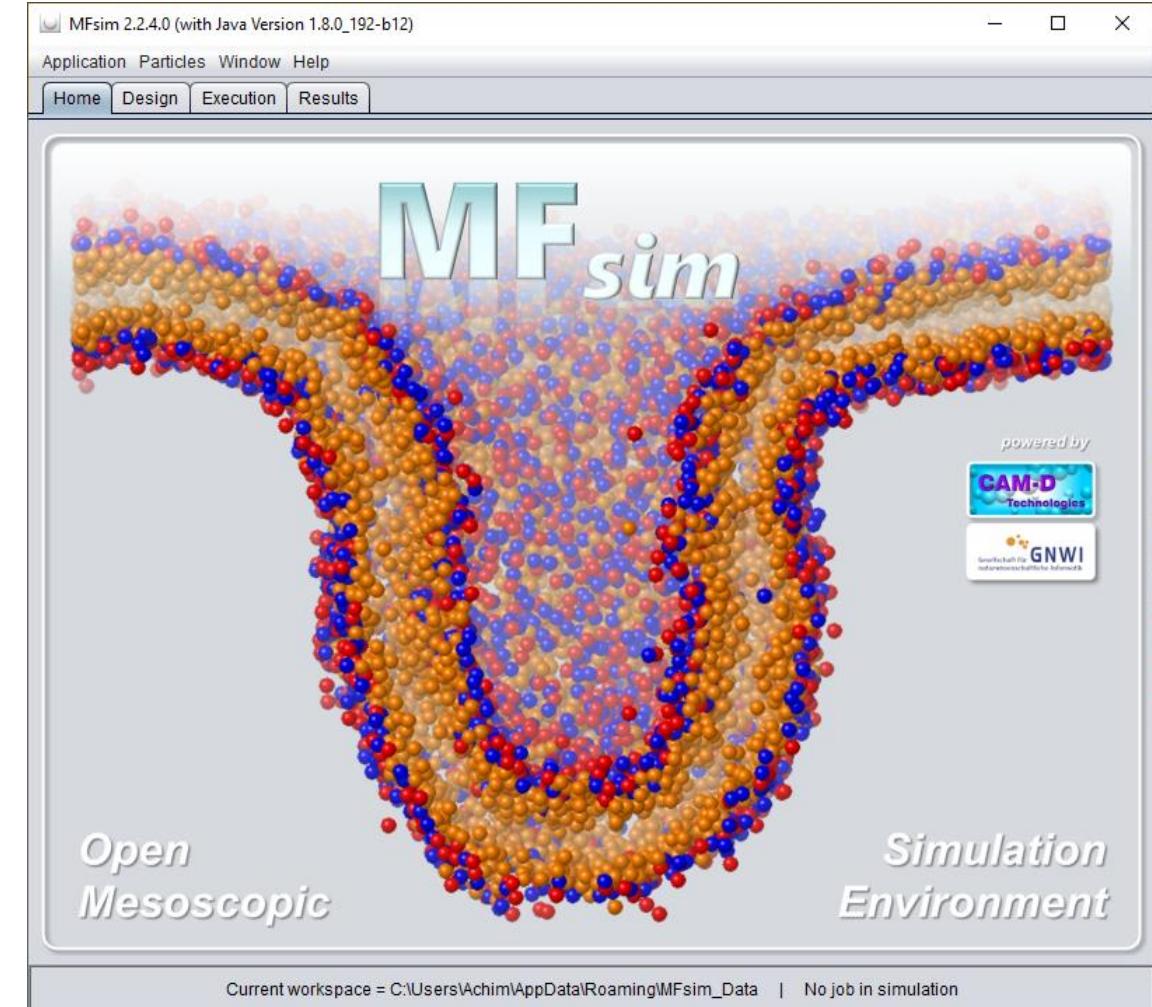


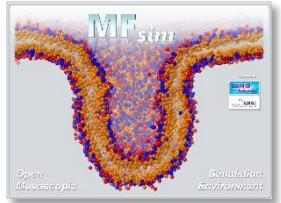
[www.gnwi.de](http://www.gnwi.de)

GitHub repository:  
<https://github.com/zieslesny/MFsim>

# Program Start

Start MFsim ...





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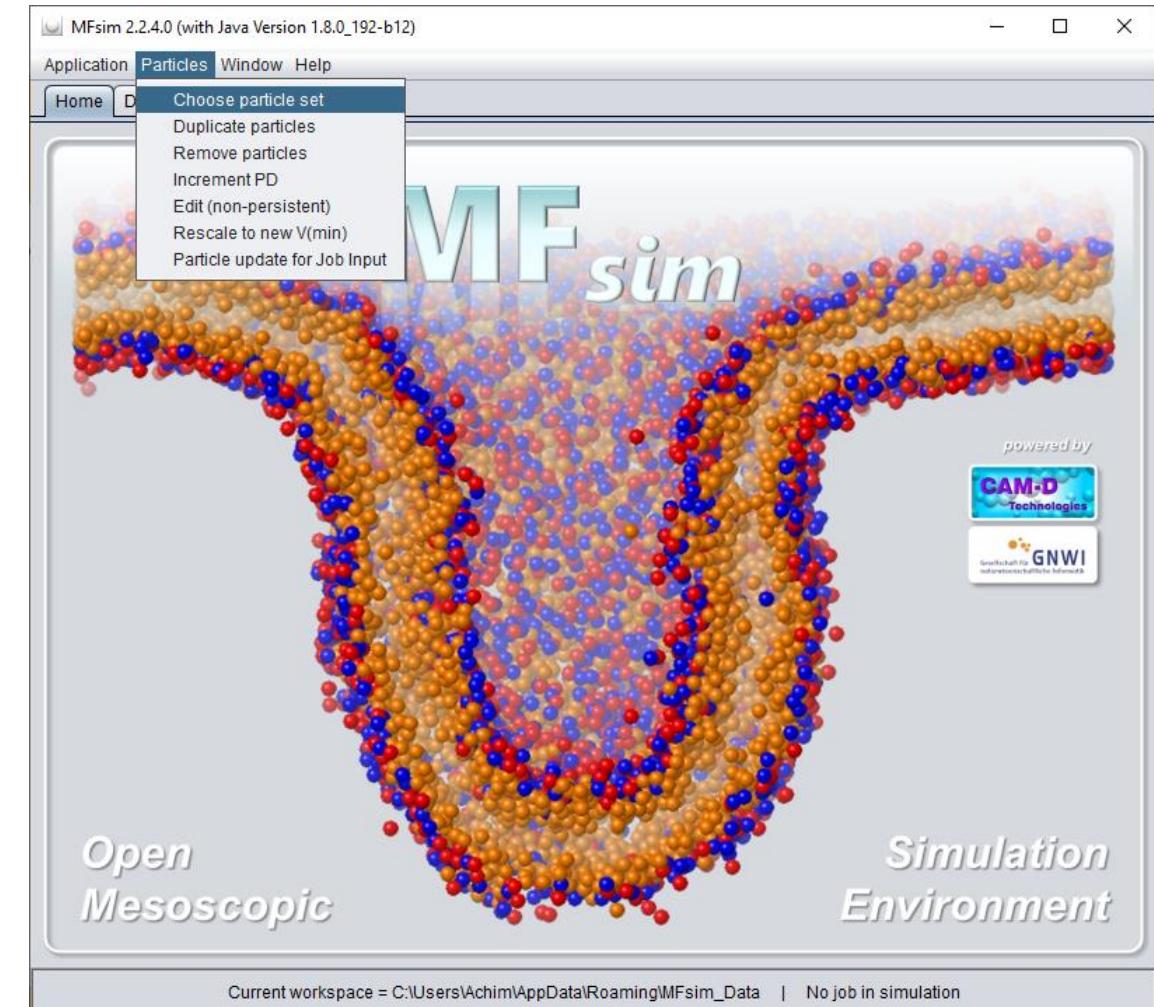
[www.molecular-dynamics.de](http://www.molecular-dynamics.de)

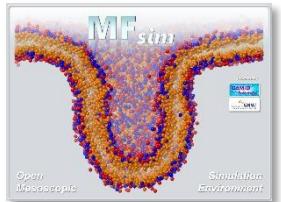


[www.gnwi.de](http://www.gnwi.de)

# Particle Set Choice

*... Choose particle set ...*





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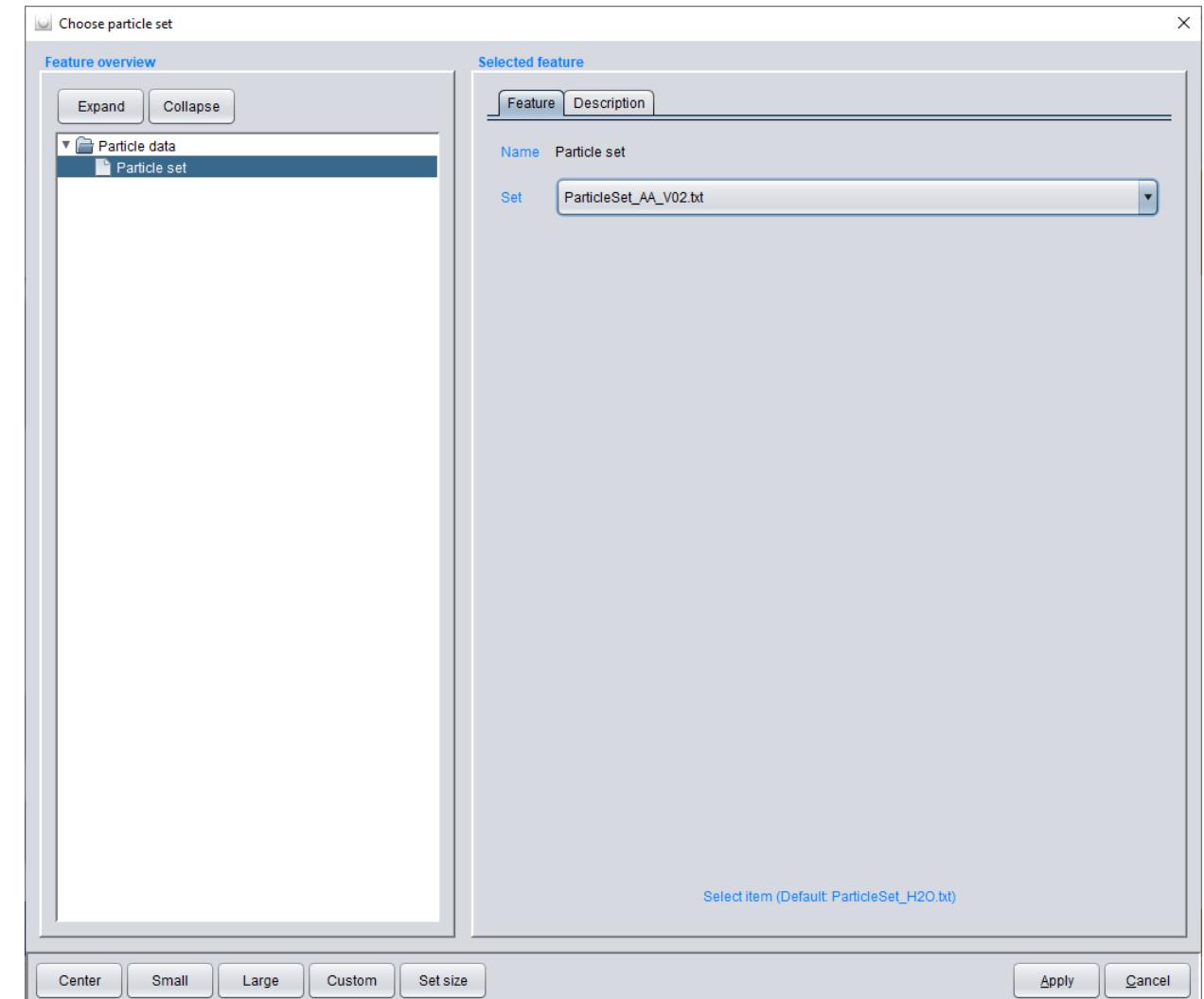
[www.molecular-dynamics.de](http://www.molecular-dynamics.de)

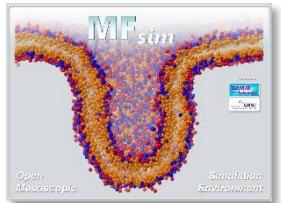


[www.gnwi.de](http://www.gnwi.de)

# Particle Set Choice

... *ParticleSet\_AA\_V02.txt* and **Apply**.





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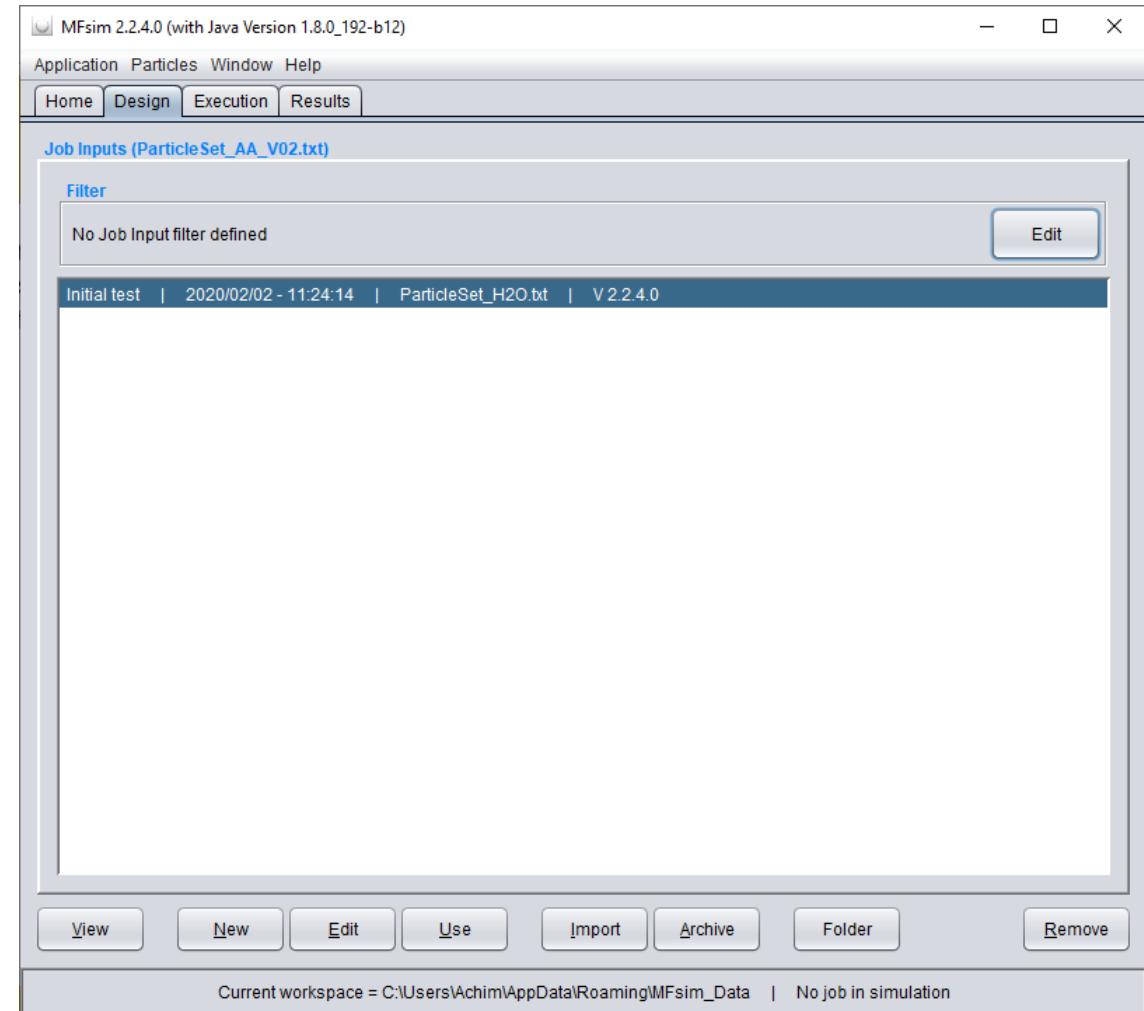
[www.molecular-dynamics.de](http://www.molecular-dynamics.de)

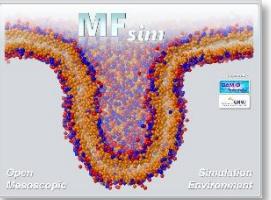


[www.gnwi.de](http://www.gnwi.de)

# Design of DMPC bilayer membrane Job Input

Select the **Design** tab (where the chosen particle set is displayed at the panel border) and hit the **New** button for a new Job Input.





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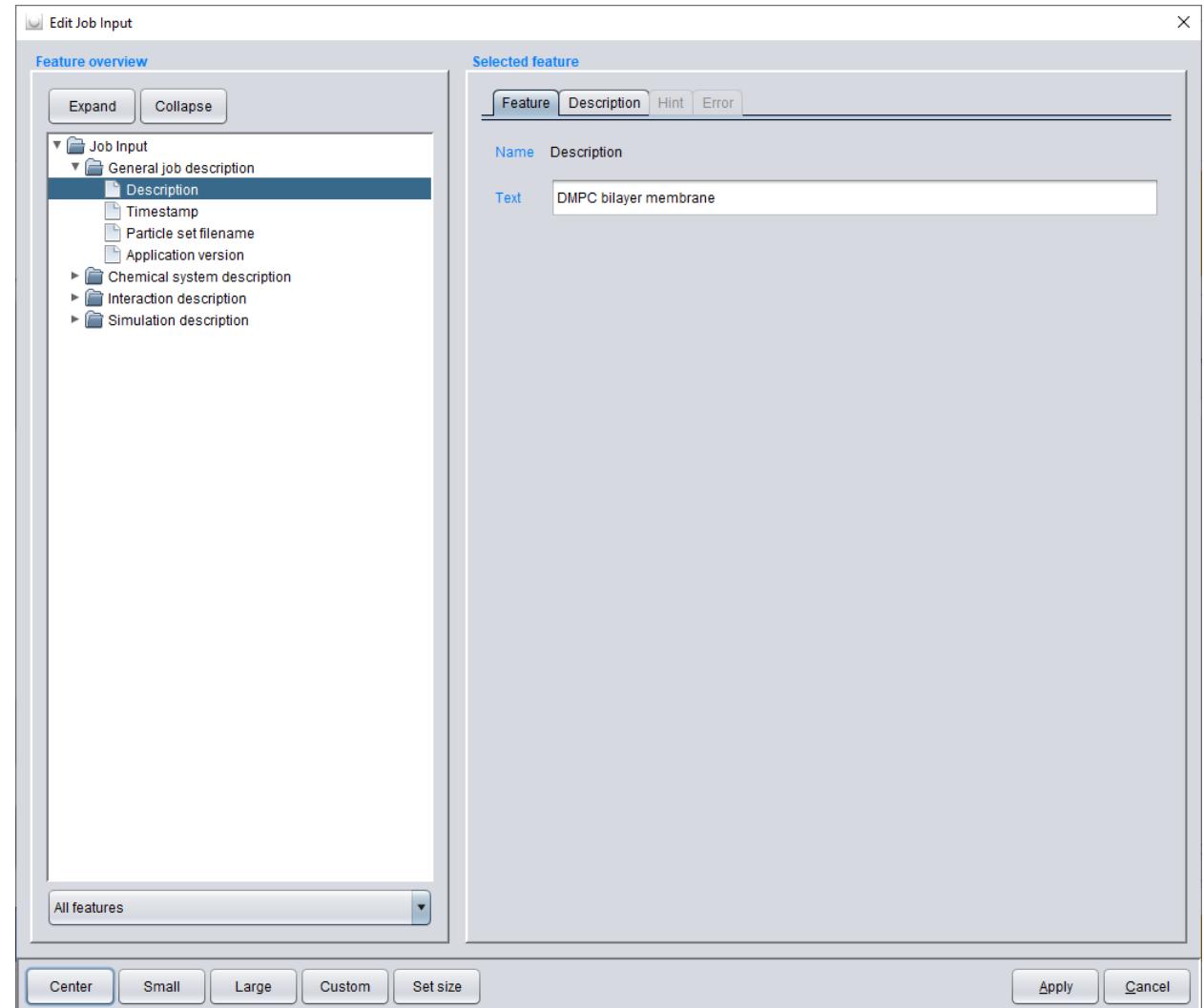


[www.gnwi.de](http://www.gnwi.de)

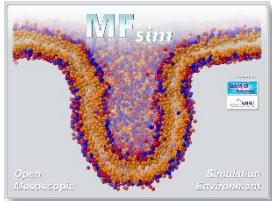
GitHub repository:  
<https://github.com/zieschny/MFsim>

# DMPC bilayer membrane Job Input – Description

Select **Job Input / General job description / Description** and change the description to *DMPC bilayer membrane*.



# DMPC bilayer membrane Job Input – Molecule Definition



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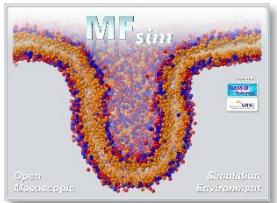


[www.gnwi.de](http://www.gnwi.de)

Select **Job Input / Chemical system description / Molecule definition**: The water molecule is already defined by default. To define the DMPC molecule hit the **Insert** button ...

Name	Molecular structure	Graphics color
Water	H2O	CYAN

# DMPC bilayer membrane Job Input – Molecule Definition



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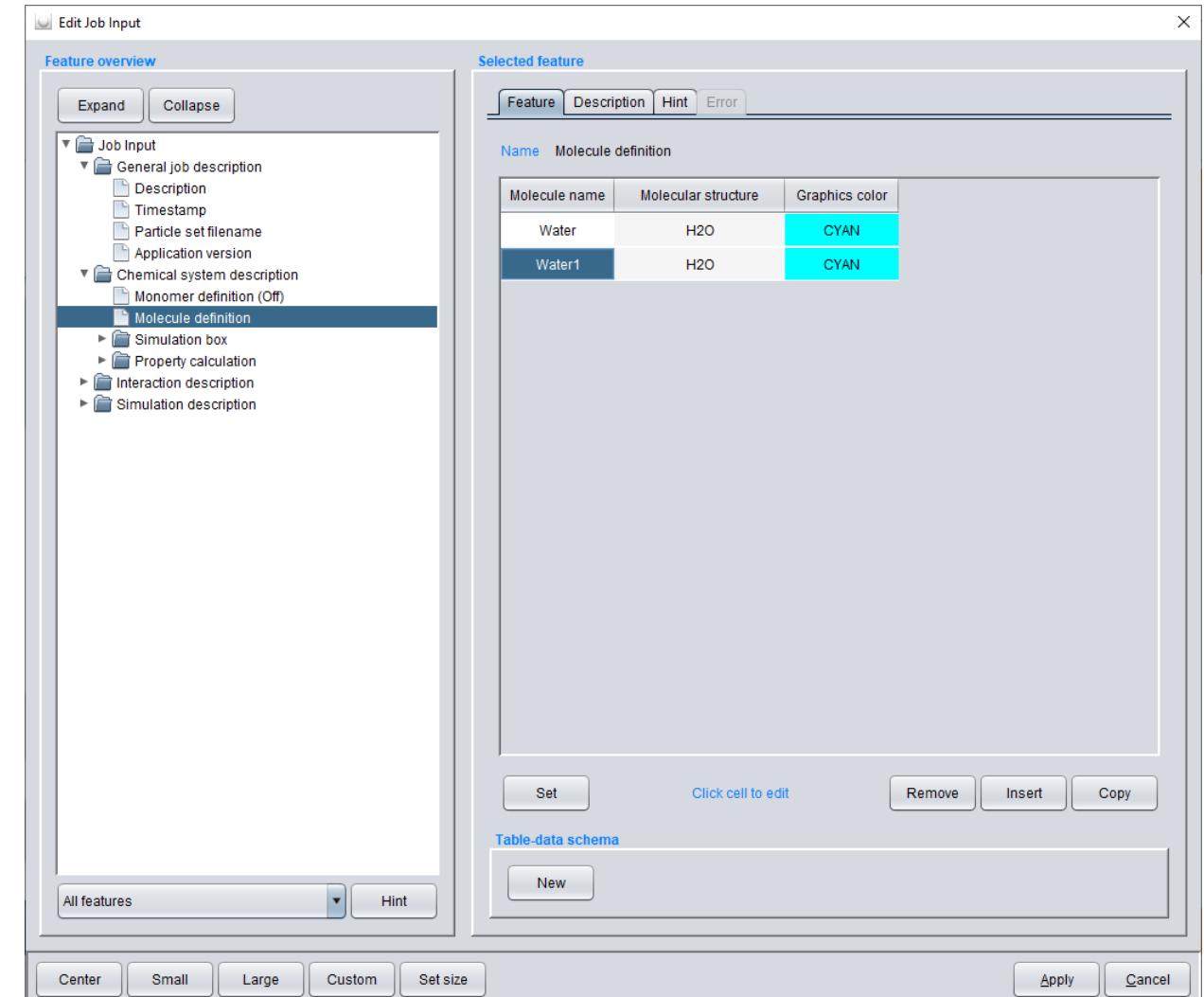


[www.molecular-dynamics.de](http://www.molecular-dynamics.de)



[www.gnwi.de](http://www.gnwi.de)

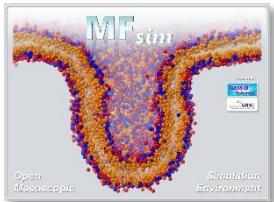
... for a new molecule row (again a water molecule by default) ...



The screenshot shows the 'Edit Job Input' dialog with the 'Selected feature' tab selected. Under 'Feature overview', the 'Job Input' section is expanded, showing 'General job description' and 'Chemical system description'. In 'Chemical system description', the 'Molecule definition' section is expanded, showing 'Monomer definition (Off)' and 'Molecule definition'. The 'Molecule definition' section is further expanded, showing 'Simulation box', 'Property calculation', 'Interaction description', and 'Simulation description'. On the right, the 'Selected feature' panel displays a table for 'Molecule definition'. The table has columns: 'Name', 'Molecular structure', and 'Graphics color'. It contains two rows: one for 'Water' (H<sub>2</sub>O, CYAN) and one for 'Water1' (H<sub>2</sub>O, CYAN). Buttons at the bottom include 'Set', 'Click cell to edit', 'Remove', 'Insert', and 'Copy'. At the bottom of the dialog are buttons for 'All features', 'Hint', 'Center', 'Small', 'Large', 'Custom', 'Set size', 'Apply', and 'Cancel'.

Name	Molecular structure	Graphics color
Water	H <sub>2</sub> O	CYAN
Water1	H <sub>2</sub> O	CYAN

# DMPC bilayer membrane Job Input – Molecule Definition



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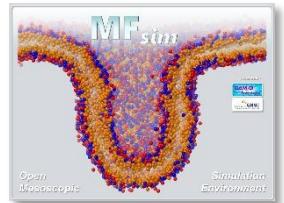
[www.gnwi.de](http://www.gnwi.de)

... change **Molecule name** to *DMPC*,  
**Graphics color** to *GREEN* and open the  
molecular structure editor dialog by double-  
click on **Molecular Structure** ...

The screenshot shows the 'Edit Job Input' dialog with the 'Selected feature' tab selected. Under 'Name' (Molecule definition), there are two rows:

Molecule name	Molecular structure	Graphics color
Water	H2O	CYAN
DMPC	H2O	GREEN

Buttons at the bottom include 'Set', 'Click cell to edit', 'Remove', 'Insert', 'Copy', 'New', 'Center', 'Small', 'Large', 'Custom', 'Set size', 'Apply', and 'Cancel'.



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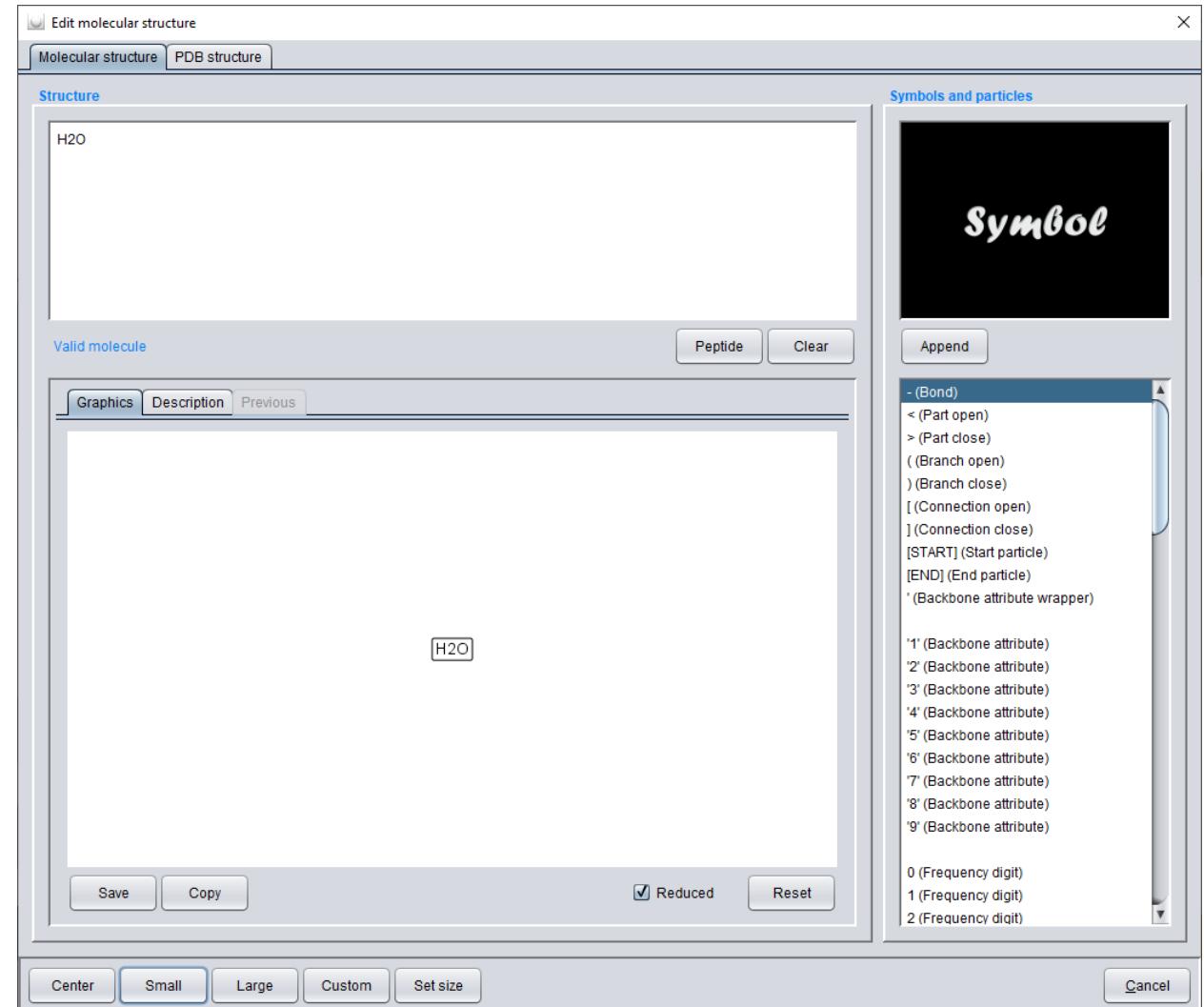
[www.molecular-dynamics.de](http://www.molecular-dynamics.de)



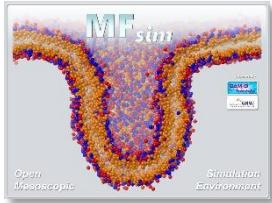
[www.gnwi.de](http://www.gnwi.de)

# DMPC bilayer membrane Job Input – Molecule Definition

... which displays the SPICES string and a topological depiction of the water molecule (represented by a single H<sub>2</sub>O particle).



# DMPC bilayer membrane Job Input – Molecule Definition



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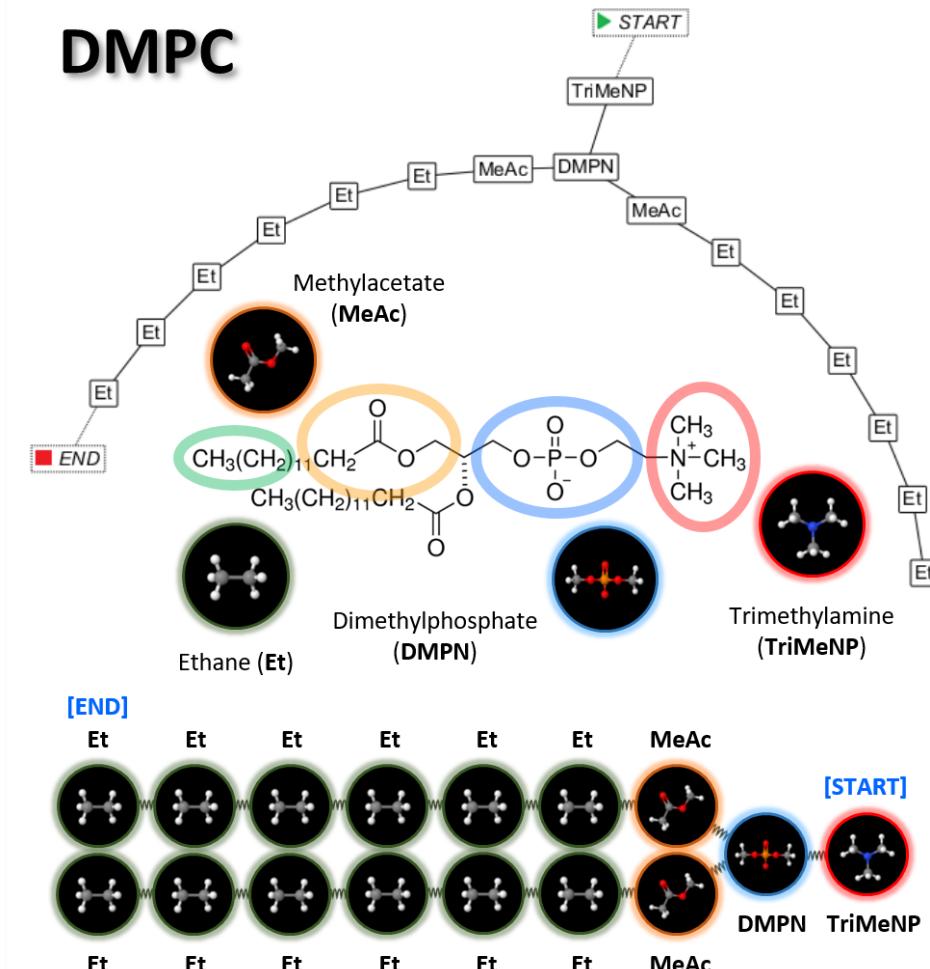
[www.gnwi.de](http://www.gnwi.de)

A SPICES string that may represent a DMPC molecule is

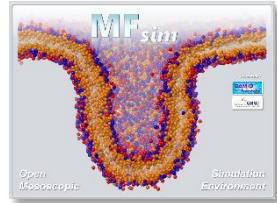
*TriMeNP[START]-DMPN(MeAc-6Et)(MeAc-6Et[END])*

where the [START]/[END] tag is inserted for later orientation in the simulation box compartment (see graphical illustration on the right).

## DMPC



*TriMeNP[START]-DMPN(MeAc-6Et)(MeAc-6Et[END])*



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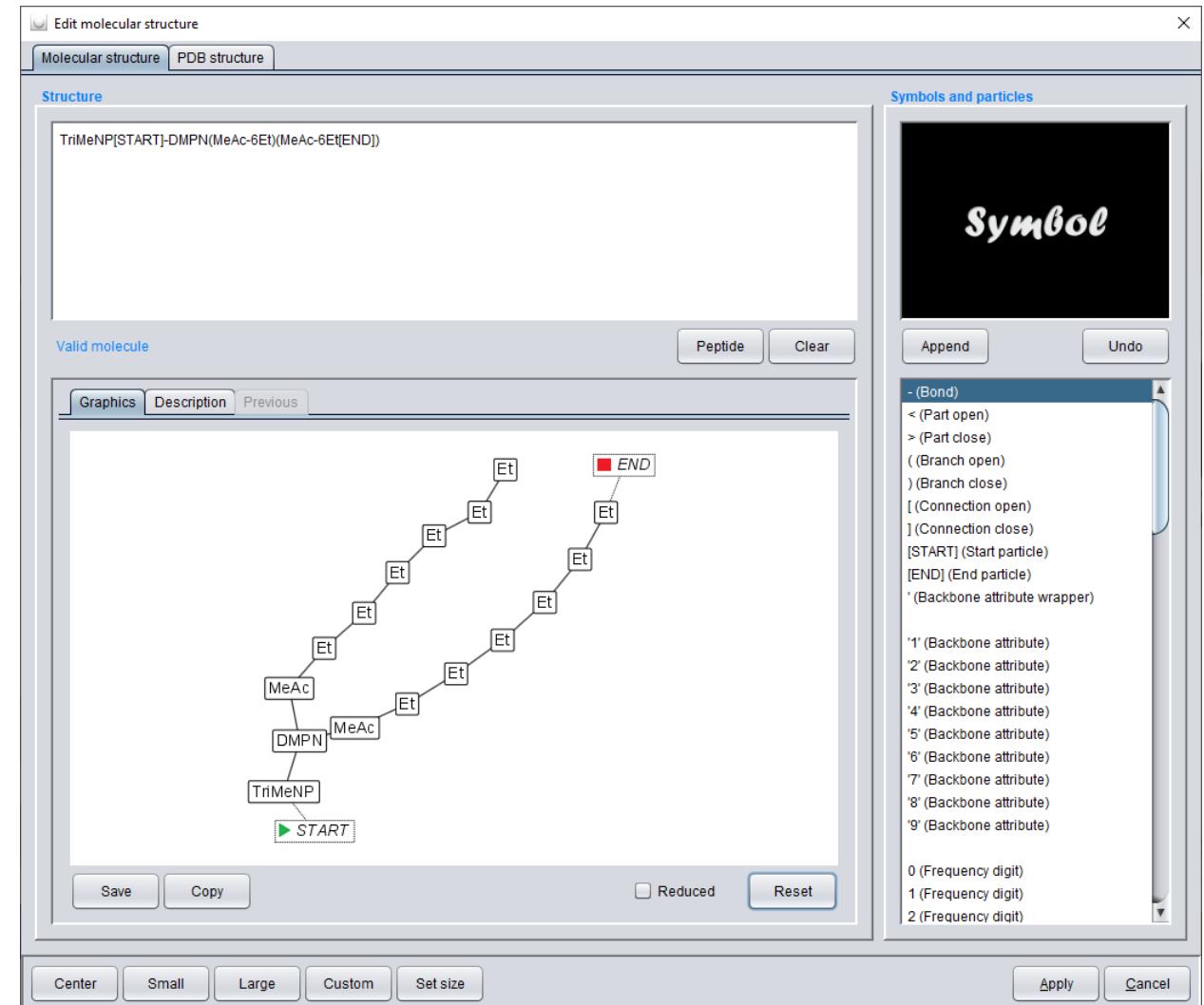
[www.molecular-dynamics.de](http://www.molecular-dynamics.de)



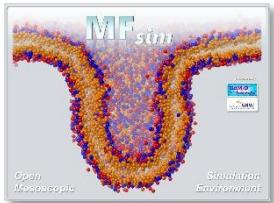
[www.gnwi.de](http://www.gnwi.de)

# DMPC bilayer membrane Job Input – Molecule Definition

Insert the SPICES string for DMPC into the **Structure** text box. For the **valid** SPICES string a topological depiction is automatically generated below which may be manually tailored for a non-overlapping view. Exit the structure editor dialog by hitting the **Apply** button.



# DMPC bilayer membrane Job Input – Molecule Definition



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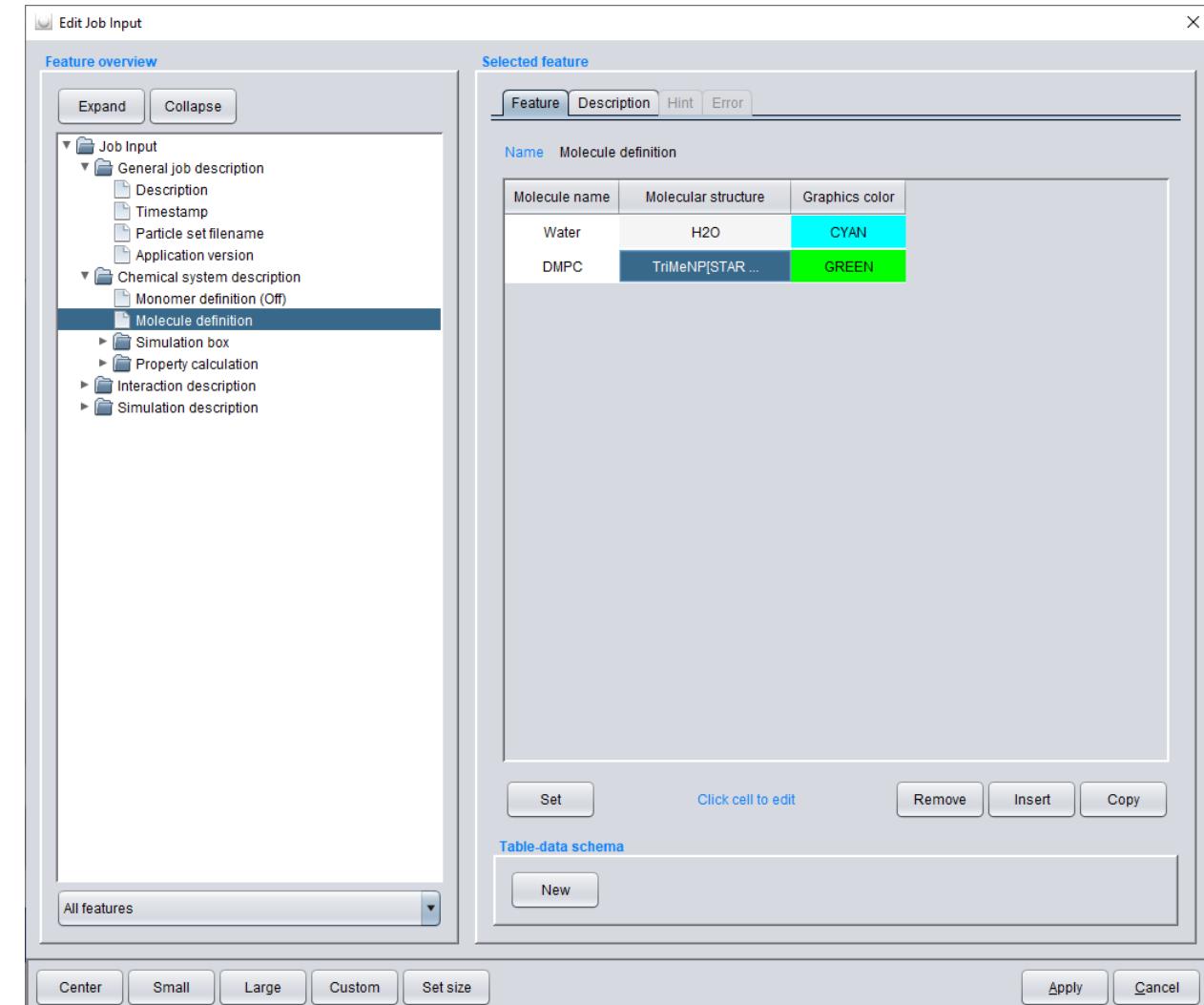


[www.molecular-dynamics.de](http://www.molecular-dynamics.de)

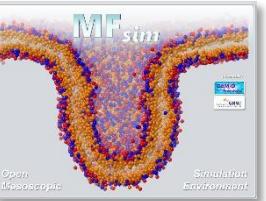


[www.gnwi.de](http://www.gnwi.de)

The DMPC molecule is successfully added to the molecule definitions.



Name	Molecular structure	Graphics color
Water	H2O	CYAN
DMPC	TriMeNP[STAR ...]	GREEN



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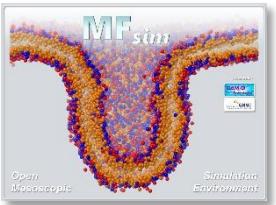


[www.gnwi.de](http://www.gnwi.de)

# DMPC bilayer membrane Job Input – Quantity

Select **Job Input / Chemical system description / Simulation box / Composition / Quantity** to fill the simulation box with 200.000 water and 1.600 DMPC molecules.

Name	Quantity
Water	200000
DMPC	1600



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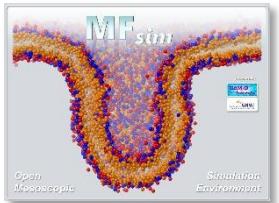


[www.gnwi.de](http://www.gnwi.de)

# DMPC bilayer membrane Job Input – Box Size

Select **Job Input / Chemical system description / Simulation box / Composition / Box size**: An area per DMPC molecule of  $50 \text{ \AA}^2$  and 800 DMPC molecules per layer lead to a total xy area of  $40.000 \text{ \AA}^2$ , i.e. to a *fixed* x and y simulation box size of  $200 \text{ \AA}$ . The size of the corresponding *flexible* z length according to DPD density and total particle number is automatically calculated.

ID	State x	x [Å]	State y	y [Å]	State z	z [Å]
01857	fixed	200	fixed	200	flexible	189.383611



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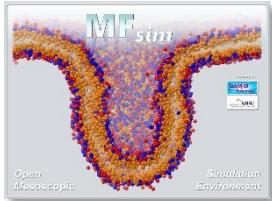
# DMPC bilayer membrane Job Input – Particle Display

Select **Job Input / Chemical system description / Simulation box / Particles and molecules display / Molecule particles**: Change **Display** of **H<sub>2</sub>O** particles to **Off** and **Graphics colors** of **DMPN** particles to **BLUE**, **Et** particles to **OLIVE**, **MeAc** particles to **ORANGE** and **TriMeNP** particles to **RED**.

The screenshot shows the 'Edit Job Input' dialog box for a 'DMPC bilayer membrane' simulation. The left pane, 'Feature overview', displays a hierarchical tree of simulation parameters. The right pane, 'Selected feature', shows a table of molecule definitions with their corresponding particle names, display settings, and graphics colors.

Name	Molecule name	Particle	Particle name	Display	Graphics color
DMPC	DMPN	Dimethylphosphate	On	BLUE	
DMPC	Et	Ethane	On	OLIVE	
DMPC	MeAc	MethylAcetate	On	ORANGE	
DMPC	TriMeNP	TriMethylamine	On	RED	
Water	H <sub>2</sub> O	Water	Off	CYAN	

# DMPC bilayer membrane Job Input – Table-Data Schemata



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[www.molecular-dynamics.de](http://www.molecular-dynamics.de)



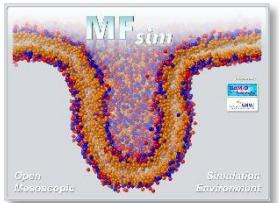
[www.gnwi.de](http://www.gnwi.de)

Save the DMPC display settings by hitting the **New** button for a new table-data schema (denoted *Schema 1* by default) and click the **Show** button ...

The screenshot shows the 'Edit Job Input' dialog box for a 'DMPC bilayer membrane' job. The left panel displays a tree view of job input features under 'Job Input'. The right panel shows a table for the selected feature 'Molecule particles'. The table lists molecule names, particle names, and display settings (On/Off) along with their corresponding graphics colors.

Name	Molecule name	Particle	Particle name	Display	Graphics color
DMPC	DMPN	Dimethylphosphate	On	BLUE	
DMPC	Et	Ethane	On	OLIVE	
DMPC	MeAc	MethylAcetate	On	ORANGE	
DMPC	TriMeNP	TriMethylamine	On	RED	
Water	H2O	Water	Off	CYAN	

# DMPC bilayer membrane Job Input – Table-Data Schemata



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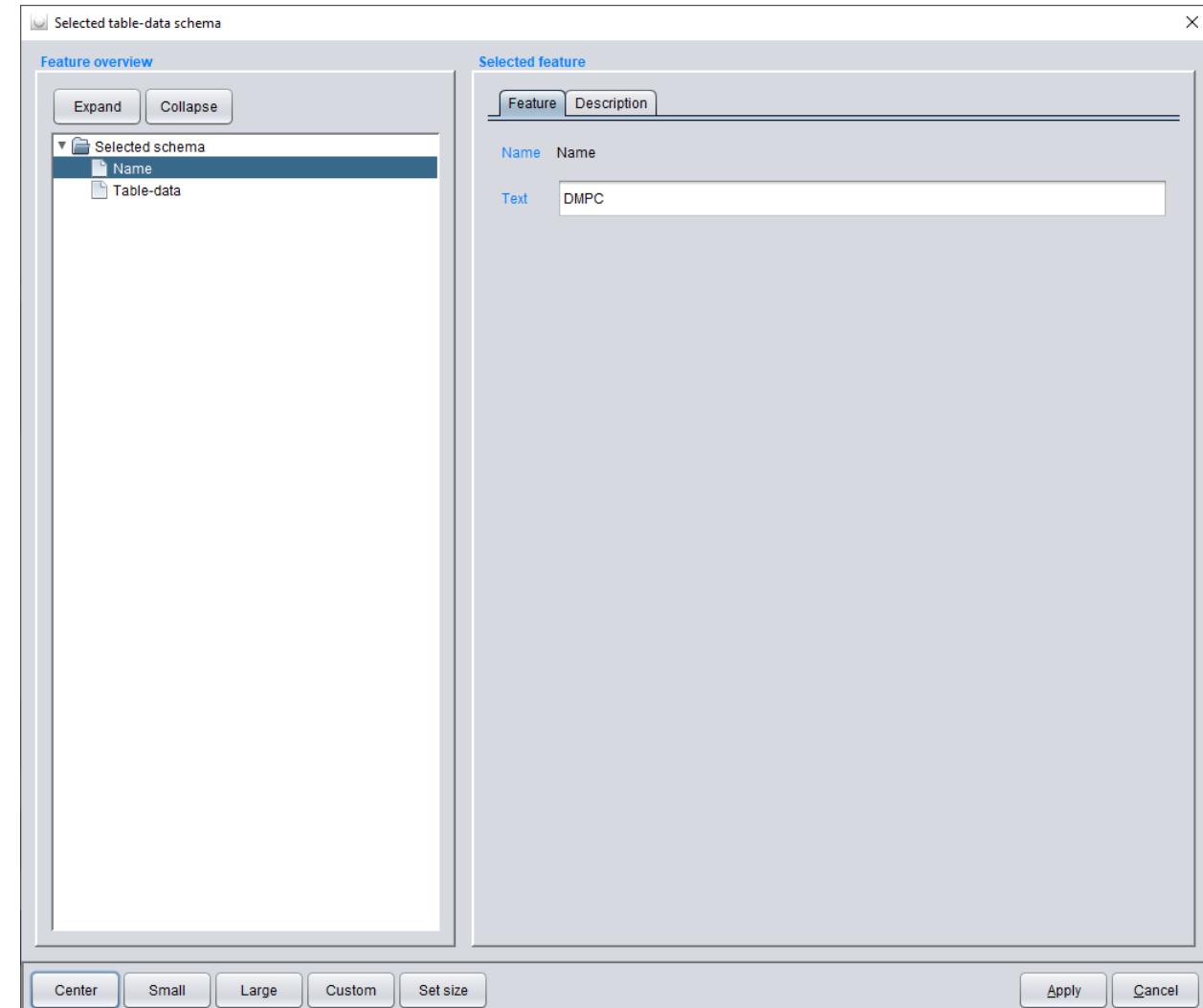


[www.molecular-dynamics.de](http://www.molecular-dynamics.de)

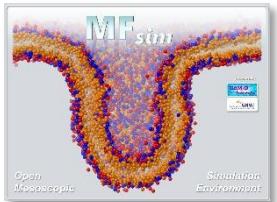


[www.gnwi.de](http://www.gnwi.de)

... for a schema name change to *DMPC* confirmed by hitting the **Apply** button ...



# DMPC bilayer membrane Job Input – Table-Data Schemata



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[www.gnwi.de](http://www.gnwi.de)

GitHub repository:  
<https://github.com/zieschny/MFsim>

... to complete the change.

Edit Job Input: "DMPC bilayer membrane"

Feature overview

Selected feature

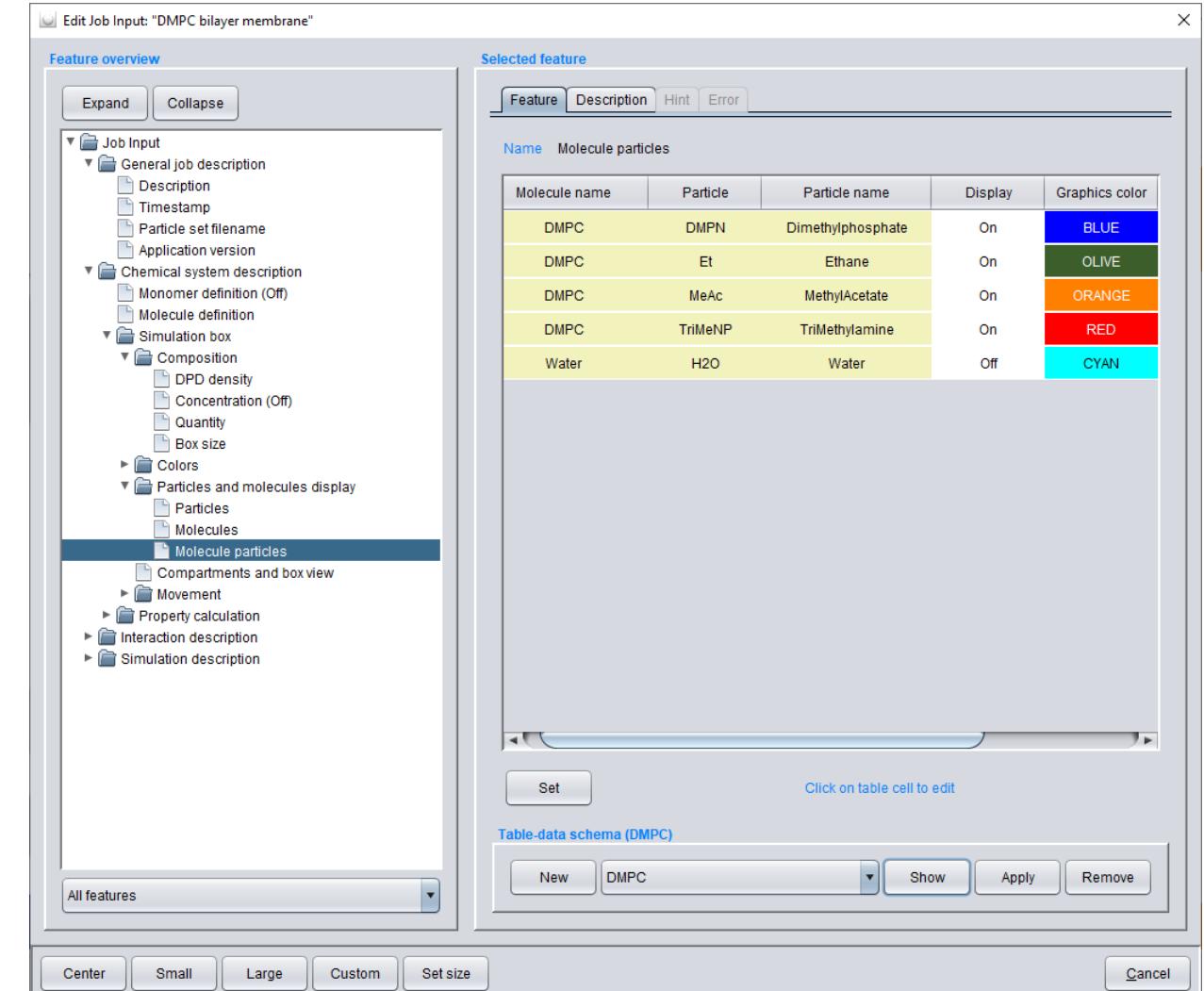
Molecule particles

Molecule name	Particle	Particle name	Display	Graphics color
DMPC	DMPN	Dimethylphosphate	On	BLUE
DMPC	Et	Ethane	On	OLIVE
DMPC	MeAc	MethylAcetate	On	ORANGE
DMPC	TriMeNP	TriMethylamine	On	RED
Water	H2O	Water	Off	CYAN

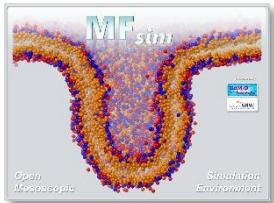
Table-data schema (DMPC)

New DMPC Show Apply Remove

Center Small Large Custom Set size Cancel



# DMPC bilayer membrane Job Input – Simulation Box



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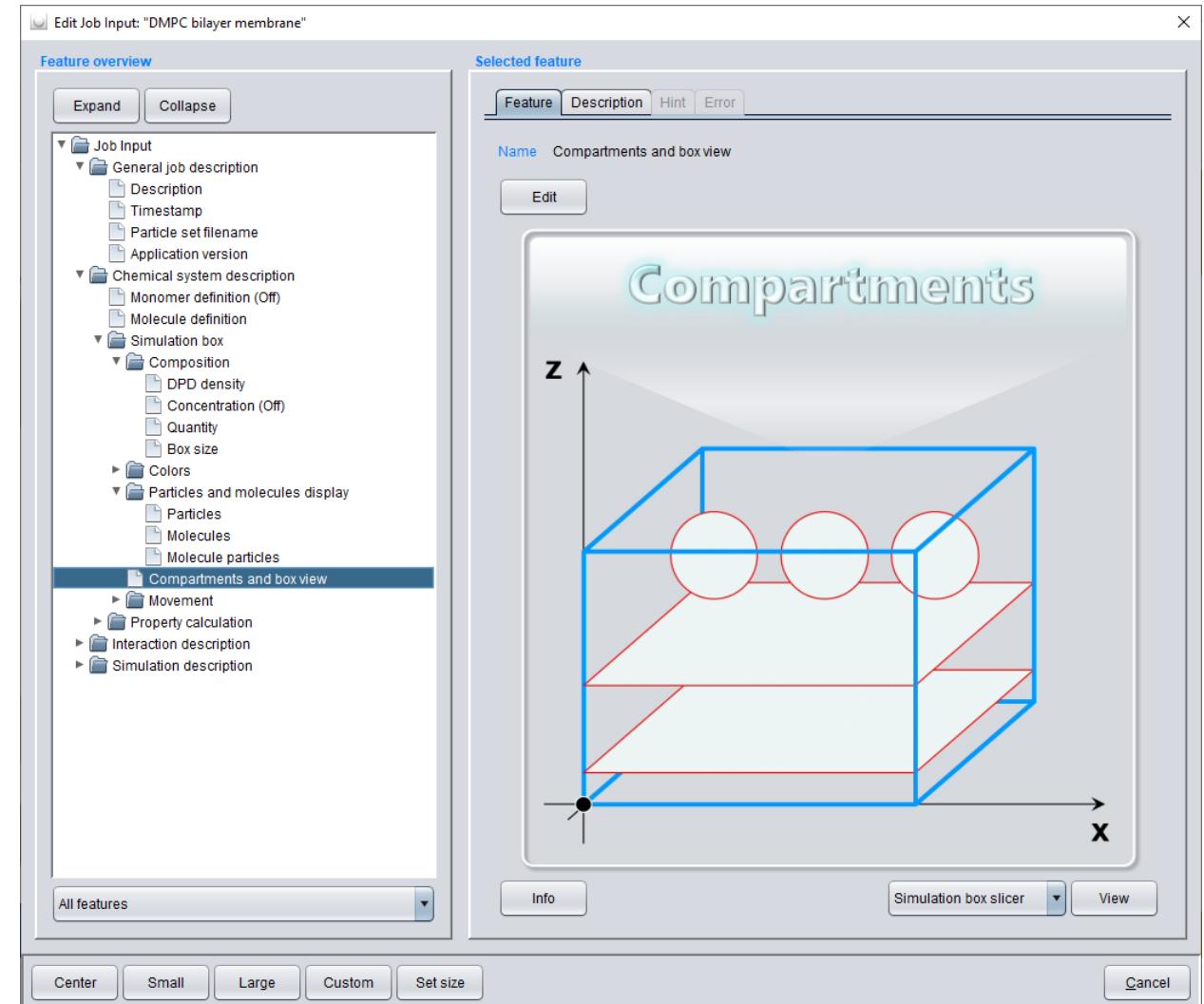


[www.molecular-dynamics.de](http://www.molecular-dynamics.de)

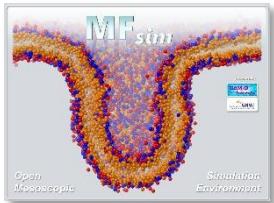


[www.gnwi.de](http://www.gnwi.de)

Select **Job Input / Chemical system description / Simulation box / Compartment and box view**: Click the **View** button ...



# DMPC bilayer membrane Job Input – Simulation Box



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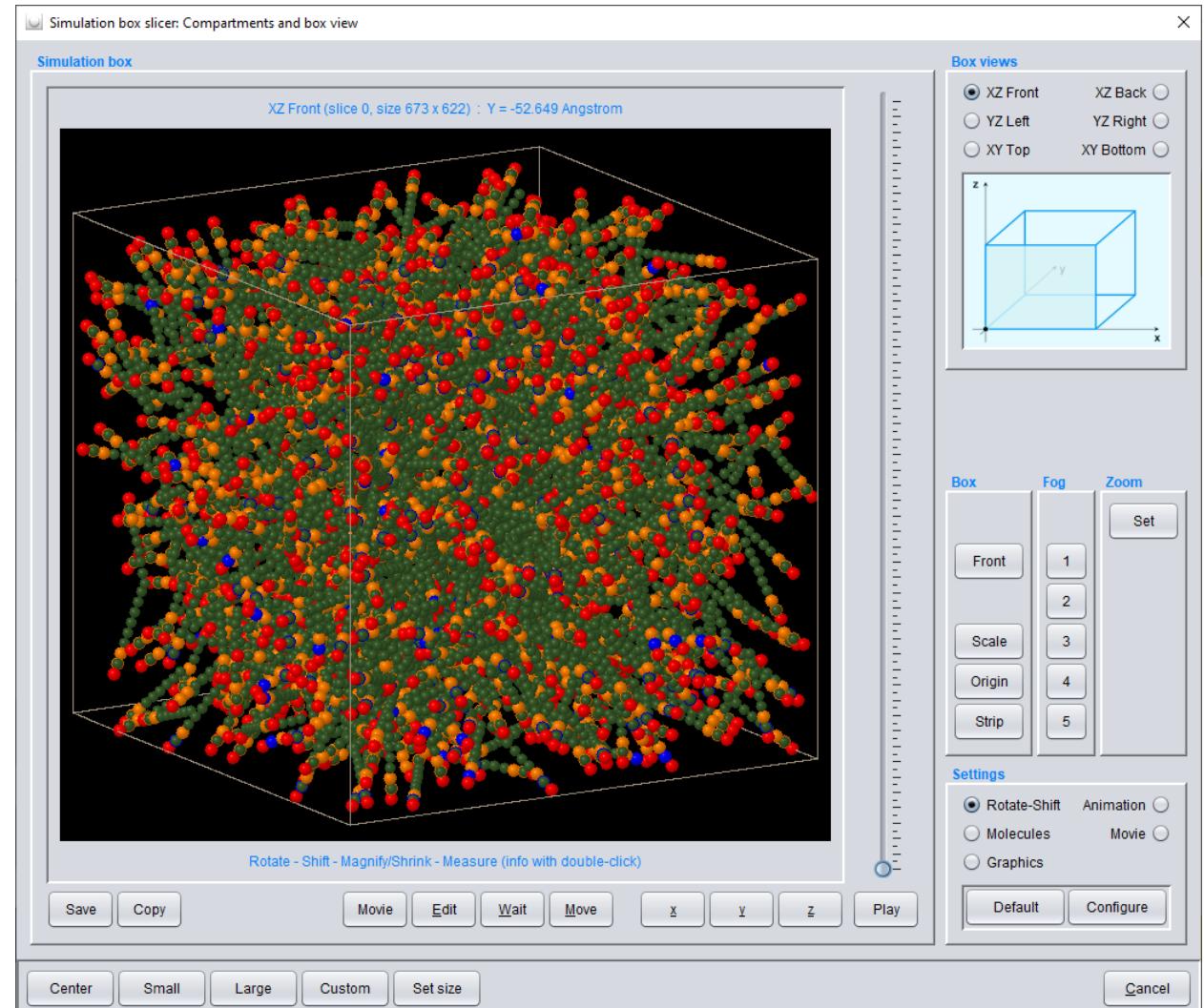
[www.molecular-dynamics.de](http://www.molecular-dynamics.de)



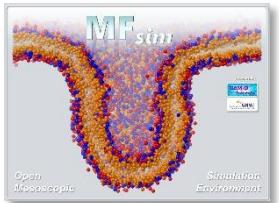
[www.gnwi.de](http://www.gnwi.de)

GitHub repository:  
<https://github.com/zieschny/MFsim>

... to view the default random distribution of DMPC molecules in form of linear SPICES tubes in the simulation box. **Cancel** the dialog ...



# DMPC bilayer membrane Job Input – Compartments



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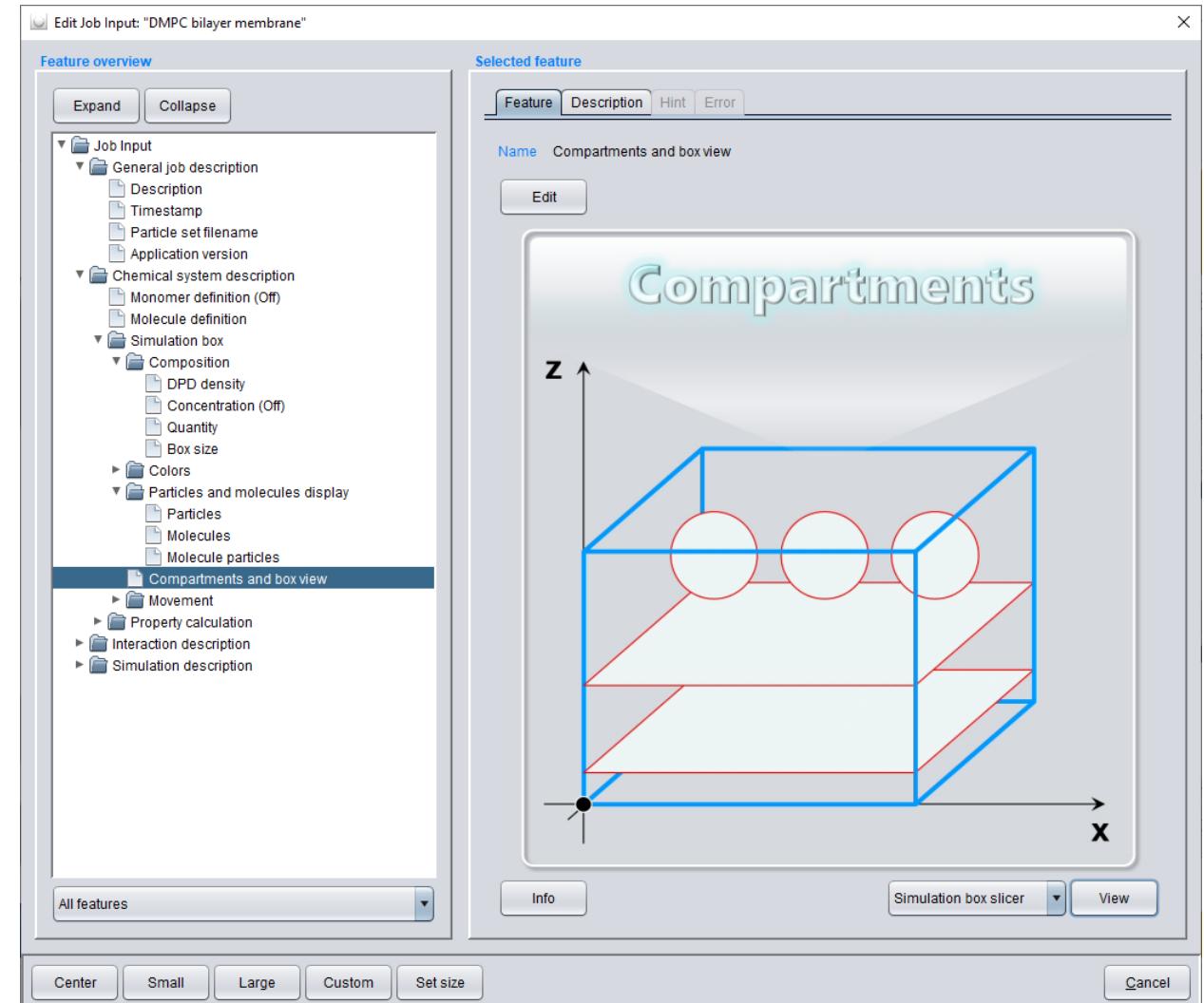


[www.molecular-dynamics.de](http://www.molecular-dynamics.de)

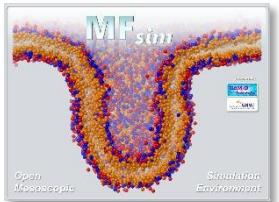


[www.gnwi.de](http://www.gnwi.de)

... and hit the **Edit** button for compartment definition ...



# DMPC bilayer membrane Job Input – Compartments



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... with all molecules in the bulk volume at startup. Hit the **Name** button ...

Edit compartments of simulation box

Compartments Geometry

Feature overview

Selected feature

Name Chemical composition

Molecule name	Molecular structure	%	Quantity	Orientation
Water	H <sub>2</sub> O	100	200000	Random
DMPC	TriMeNP[STAR ...	100	1600	Random

Set

Click on table cell to edit

Table-data schema

New

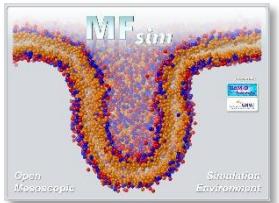
All features

Name Add sphere Add xy-layer

Center Small Large Custom Set size

Cancel

# DMPC bilayer membrane Job Input – Compartments



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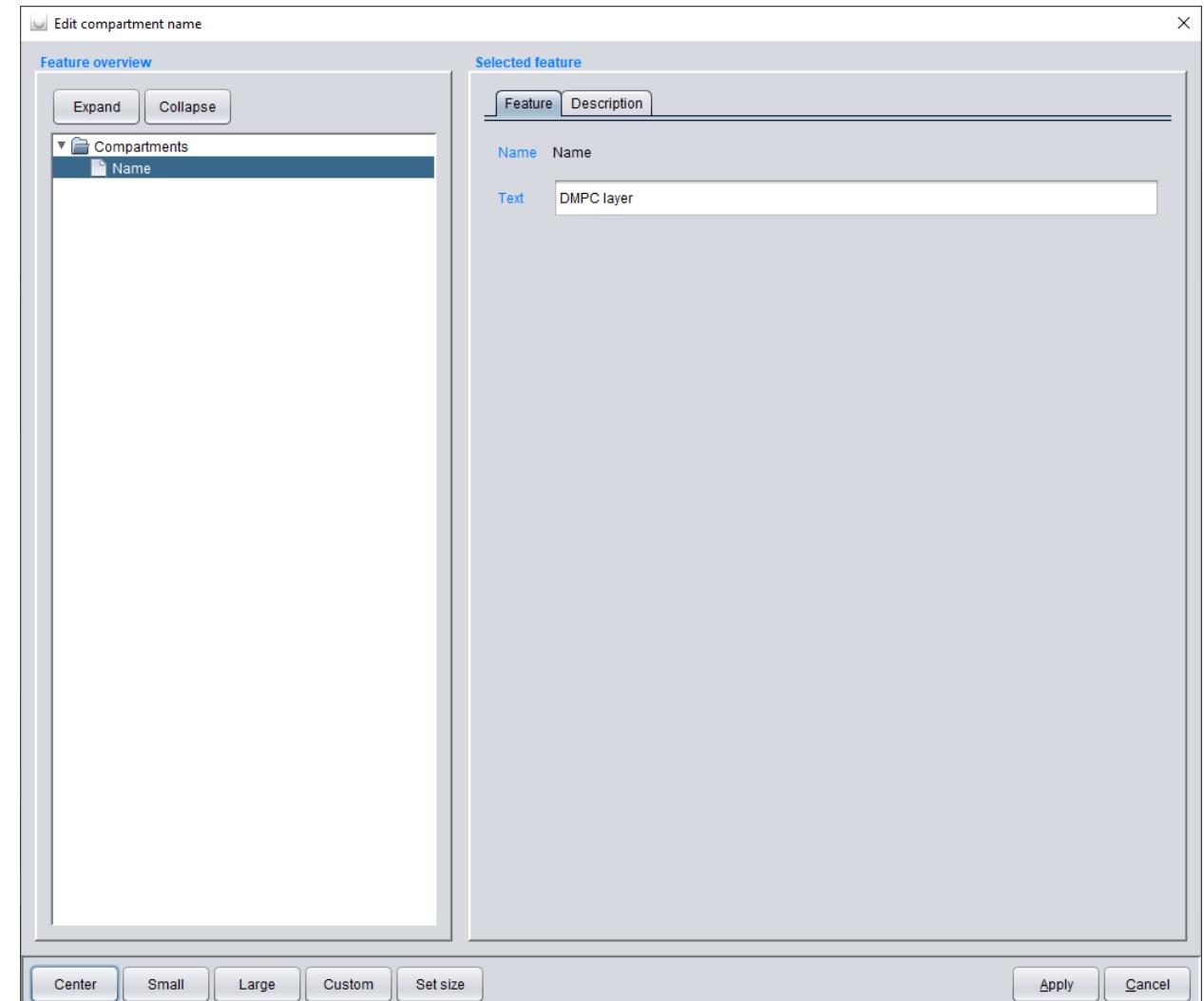


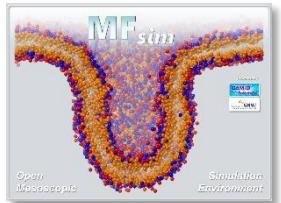
[www.molecular-dynamics.de](http://www.molecular-dynamics.de)



[www.gnwi.de](http://www.gnwi.de)

... to specify the *DMPC layer* name and exit the dialog with a confirmative **Apply**.





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# DMPC bilayer membrane Job Input – Compartments

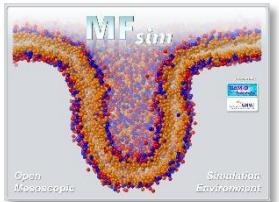
Hit button **Add xy-layer: DMPC layer ...**

Screenshot of the 'Edit compartments of simulation box' dialog. The 'Compartments' tab is selected. In the 'Feature overview' tree, 'Chemical composition' is selected under 'Bulk'. On the right, the 'Selected feature' panel shows the 'Chemical composition' table. The table lists molecules: Water (H2O) and DMPC (TriMeNP[STAR]). The table includes columns for Molecule name, Molecular structure, %, Quantity, and Orientation.

Molecule name	Molecular structure	%	Quantity	Orientation
Water	H2O	100	200000	Random
DMPC	TriMeNP[STAR ...	100	1600	Random

Buttons at the bottom include 'Set', 'Table-data schema', 'New', 'Center', 'Small', 'Large', 'Custom', 'Set size', and 'Cancel'.

# DMPC bilayer membrane Job Input – Compartments



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... to create a new xy-layer in the middle of the simulation box.

Edit compartments of simulation box

Compartments Geometry

Feature overview

Selected feature

Chemical composition

Molecule name	Molecular structure	%	Quantity	% Surface	Quantity
Water	H <sub>2</sub> O	0	0	0	0
DMPC	TriMeNP[STAR ...]	0	0	0	0

Set

Click on table cell to edit

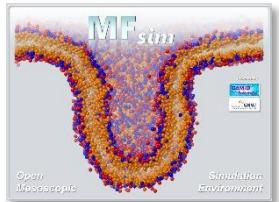
Table-data schema

New

All features

Name Add sphere: DMPC layer Add xy-layer: DMPC layer Remove

Center Small Large Custom Set size Apply Cancel



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# DMPC bilayer membrane Job Input – Compartments

Fill the layer with 100% of the **DMPC** molecules and choose 100% surface orientation to properly align the [START]/[END] tagged particles ...

Edit compartments of simulation box

Compartments Geometry

Feature overview

Selected feature

Name Chemical composition

Molecule name	Molecular structure	%	Quantity	% Surface	Quantity
Water	H <sub>2</sub> O	0	0	0	0
DMPC	TriMeNP[STAR ...]	100	1600	100	1600

Set Click cell to edit

Table-data schema

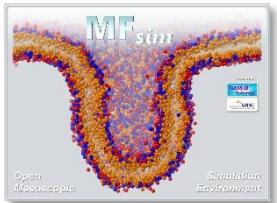
New

All features

Name Add sphere: DMPC layer Add xy-layer: DMPC layer Remove

Center Small Large Custom Set size Apply Cancel

# DMPC bilayer membrane Job Input – Compartments



Open  
Mesoscopic

Simulation  
Environment

powered by



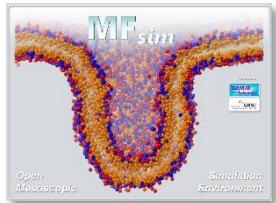
[www.molecular-dynamics.de](http://www.molecular-dynamics.de)



[www.gnwi.de](http://www.gnwi.de)

... in *Random xy top/bottom* fashion with the [START] tagged DMPC particles at the layer's top and bottom surfaces.

ity	% Surface	Quantity in volume	Quantity on surface	Orientation
0	0	0	0	None
600	100	0	1600	Random xy top/bottom



Open  
Mesoscopic

Simulation  
Environment

powered by



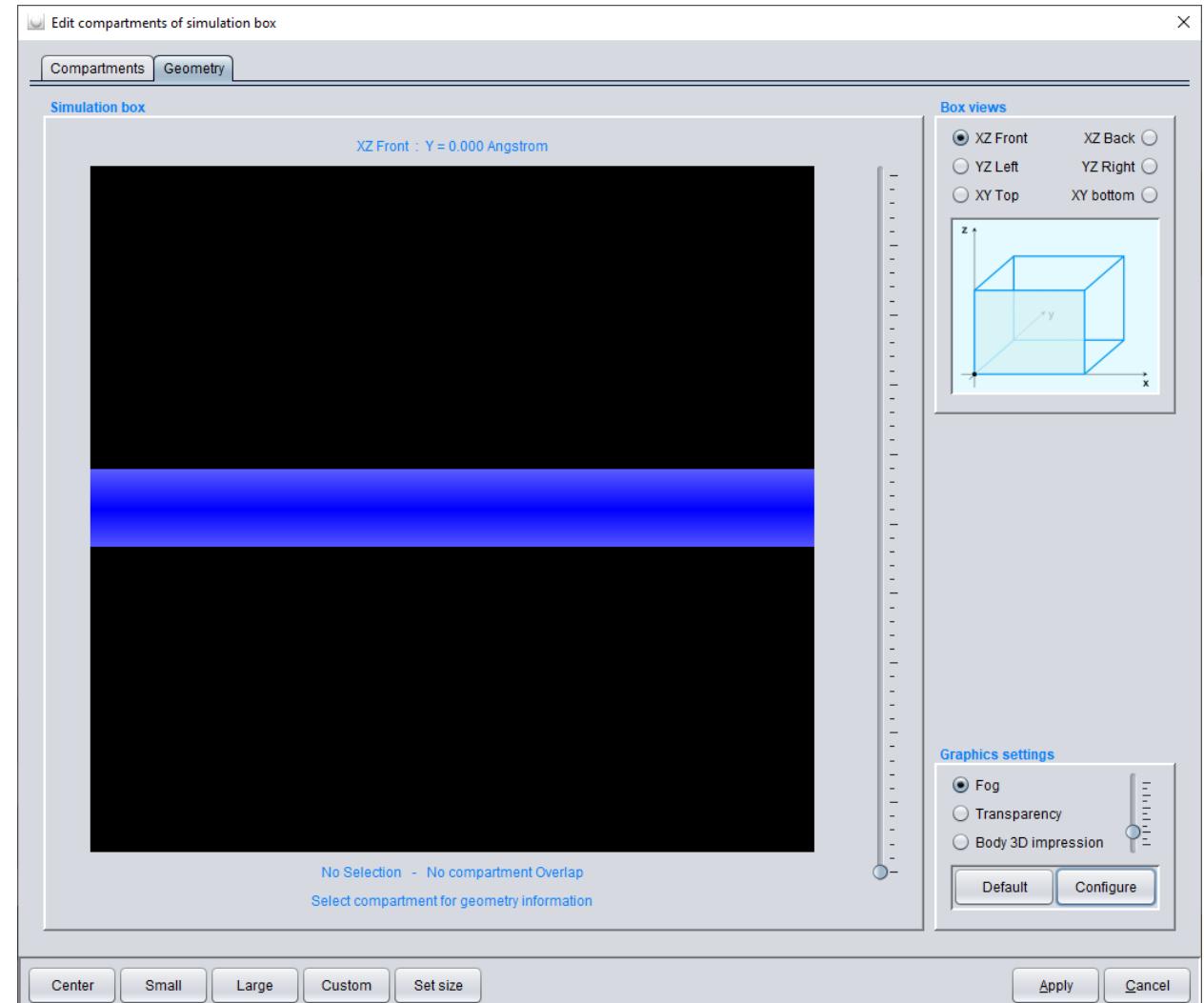
[www.molecular-dynamics.de](http://www.molecular-dynamics.de)



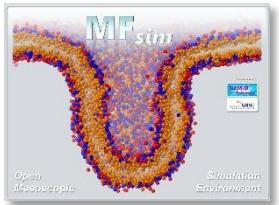
[www.gnwi.de](http://www.gnwi.de)

# DMPC bilayer membrane Job Input – Compartments

Select the **Geometry** tab to view (and possibly manipulate) the compartment position (not necessary in this tutorial since the default compartment position is in the z-middle of the box). Confirm the compartment definition by **Apply** ...



# DMPC bilayer membrane Job Input – Simulation Box



Open  
Mesoscopic

Simulation  
Environment

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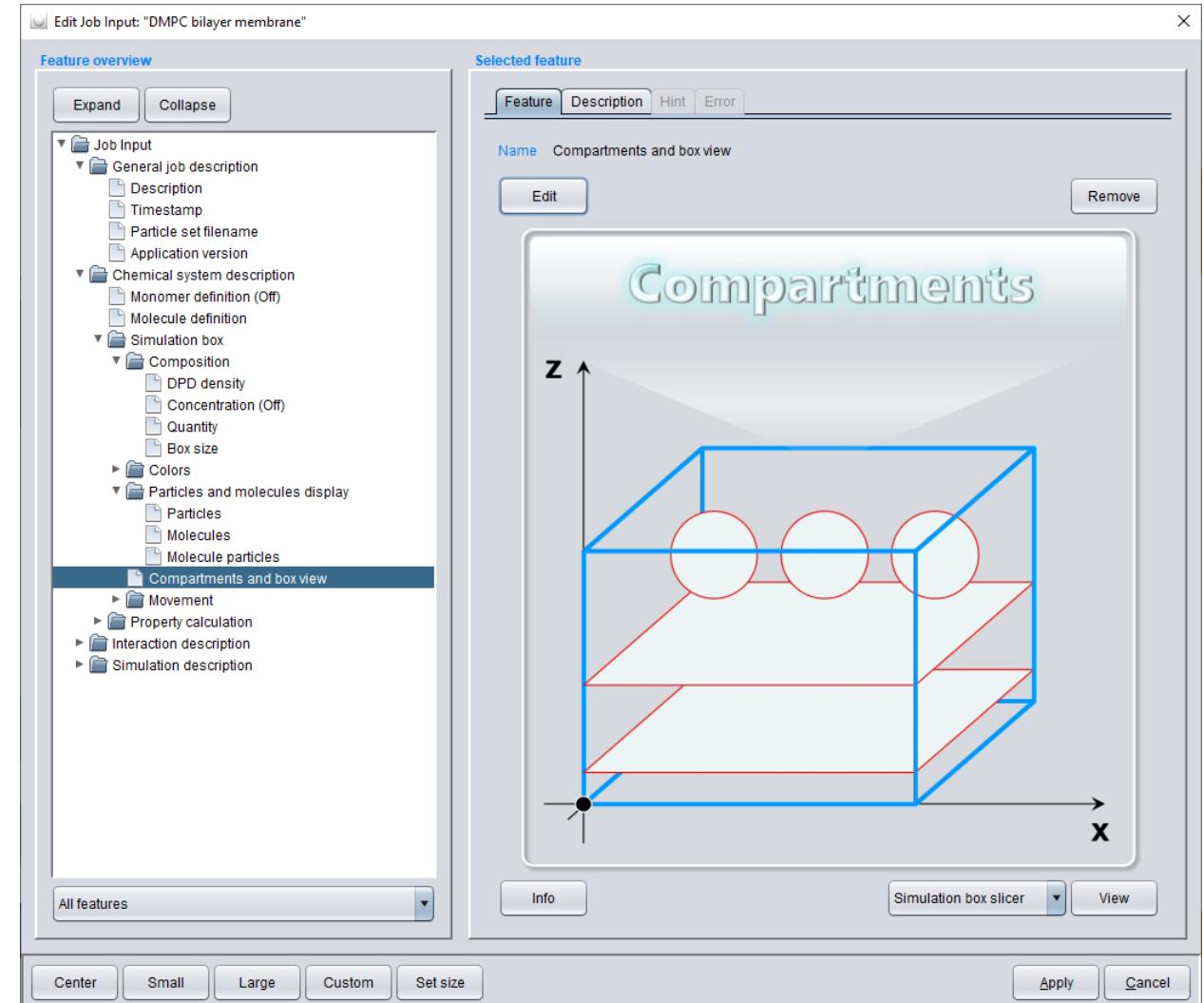


[www.molecular-dynamics.de](http://www.molecular-dynamics.de)

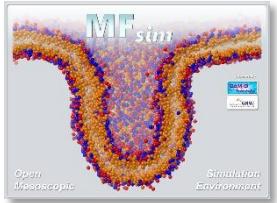


[www.gnwi.de](http://www.gnwi.de)

... to return to the Job Input feature dialog  
and hit again **View** ...



# DMPC bilayer membrane Job Input – Simulation Box



Open  
Mesoscopic

Simulation  
Environment

powered by

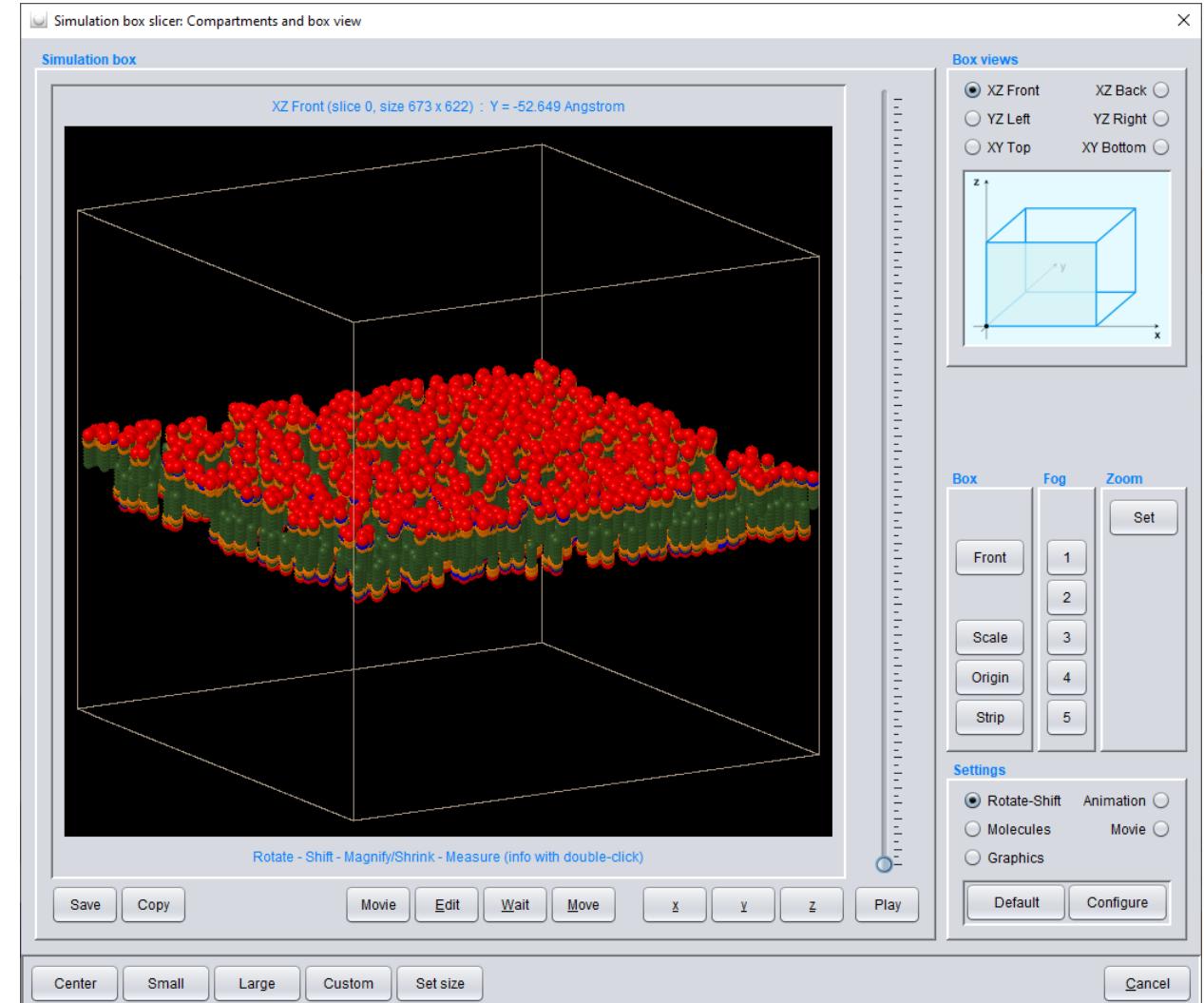


[www.molecular-dynamics.de](http://www.molecular-dynamics.de)

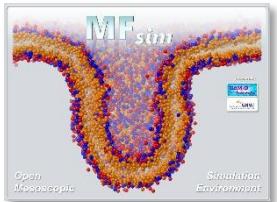


[www.gnwi.de](http://www.gnwi.de)

... to inspect the DMPC layer with the top/bottom aligned DMPC molecules.



# DMPC bilayer membrane Job Input – Simulation Box



Open  
Mesoscopic

Simulation  
Environment

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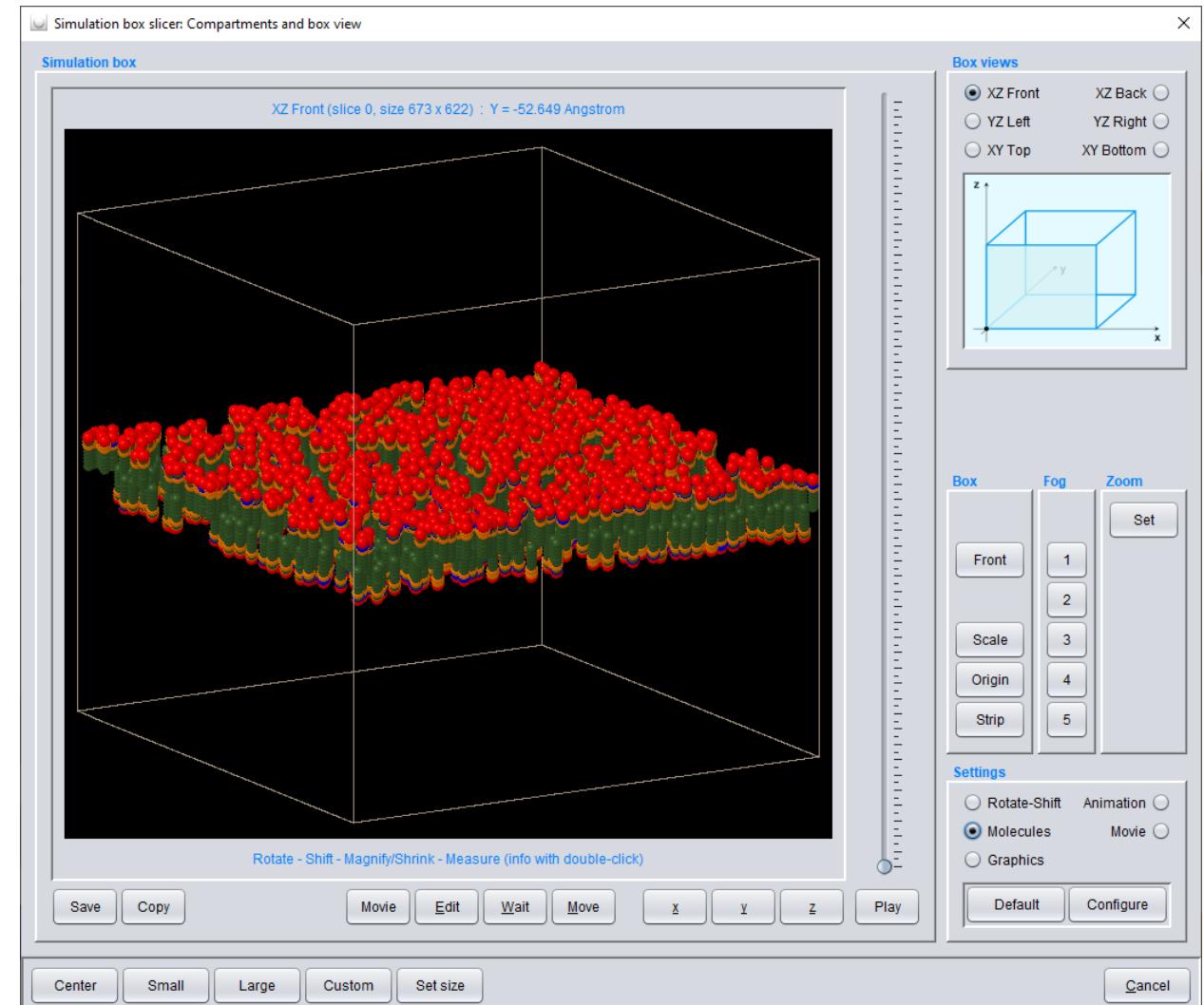


[www.molecular-dynamics.de](http://www.molecular-dynamics.de)

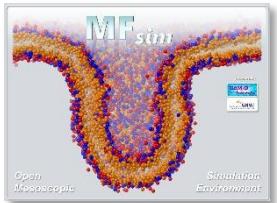


[www.gnwi.de](http://www.gnwi.de)

Select **Molecules** in the **Settings** panel  
and hit the **Configure** button ...



# DMPC bilayer membrane Job Input – Simulation Box



Open  
Mesoscopic

Simulation  
Environment

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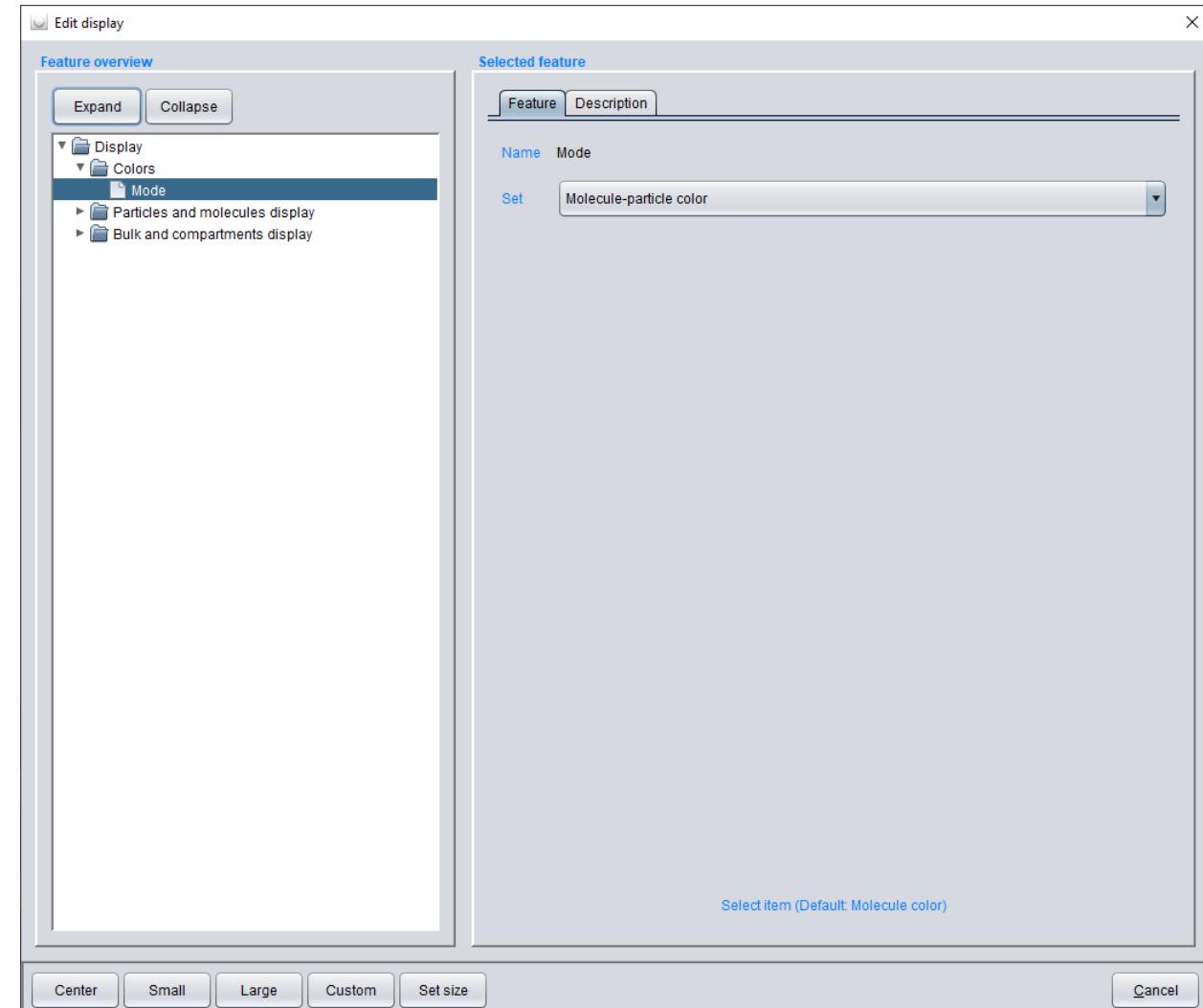


[www.molecular-dynamics.de](http://www.molecular-dynamics.de)

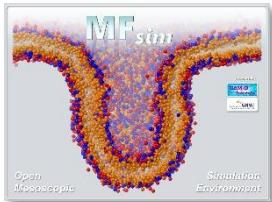


[www.gnwi.de](http://www.gnwi.de)

... to open the *Edit display* dialog.



# DMPC bilayer membrane Job Input – Simulation Box



Open  
Mesoscopic

Simulation  
Environment

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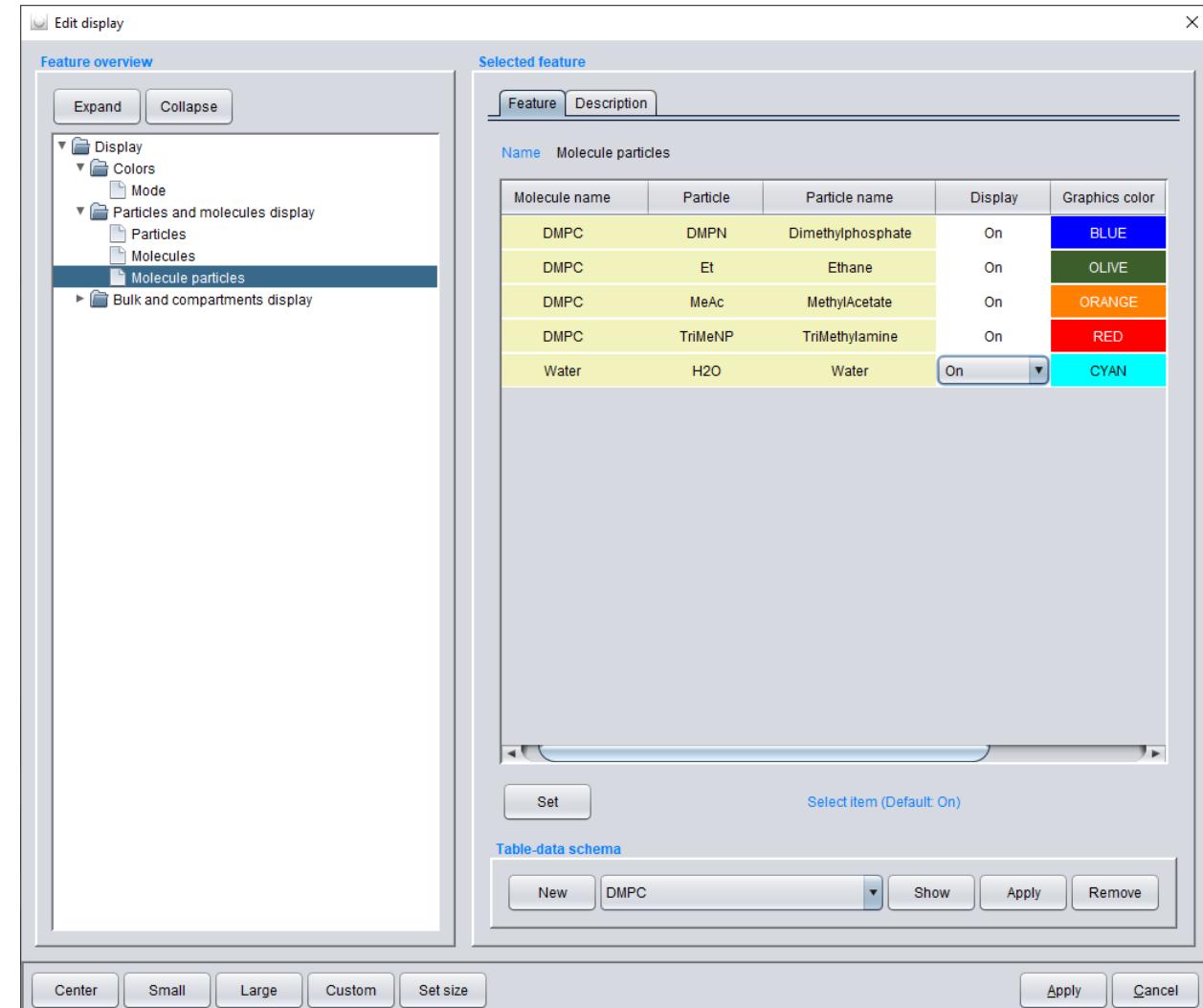
[www.molecular-dynamics.de](http://www.molecular-dynamics.de)



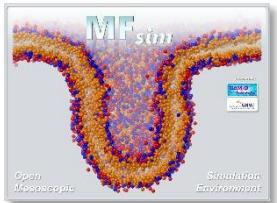
[www.gnwi.de](http://www.gnwi.de)

GitHub repository:  
<https://github.com/zieschny/MFsim>

Select **Display / Particles and molecules display / Molecule particles** and set the **Display** of the **H<sub>2</sub>O** particles to **On**. Confirm the setting by hitting the **Apply** button to leave the dialog ...



# DMPC bilayer membrane Job Input – Simulation Box



Open  
Mesoscopic

Simulation  
Environment

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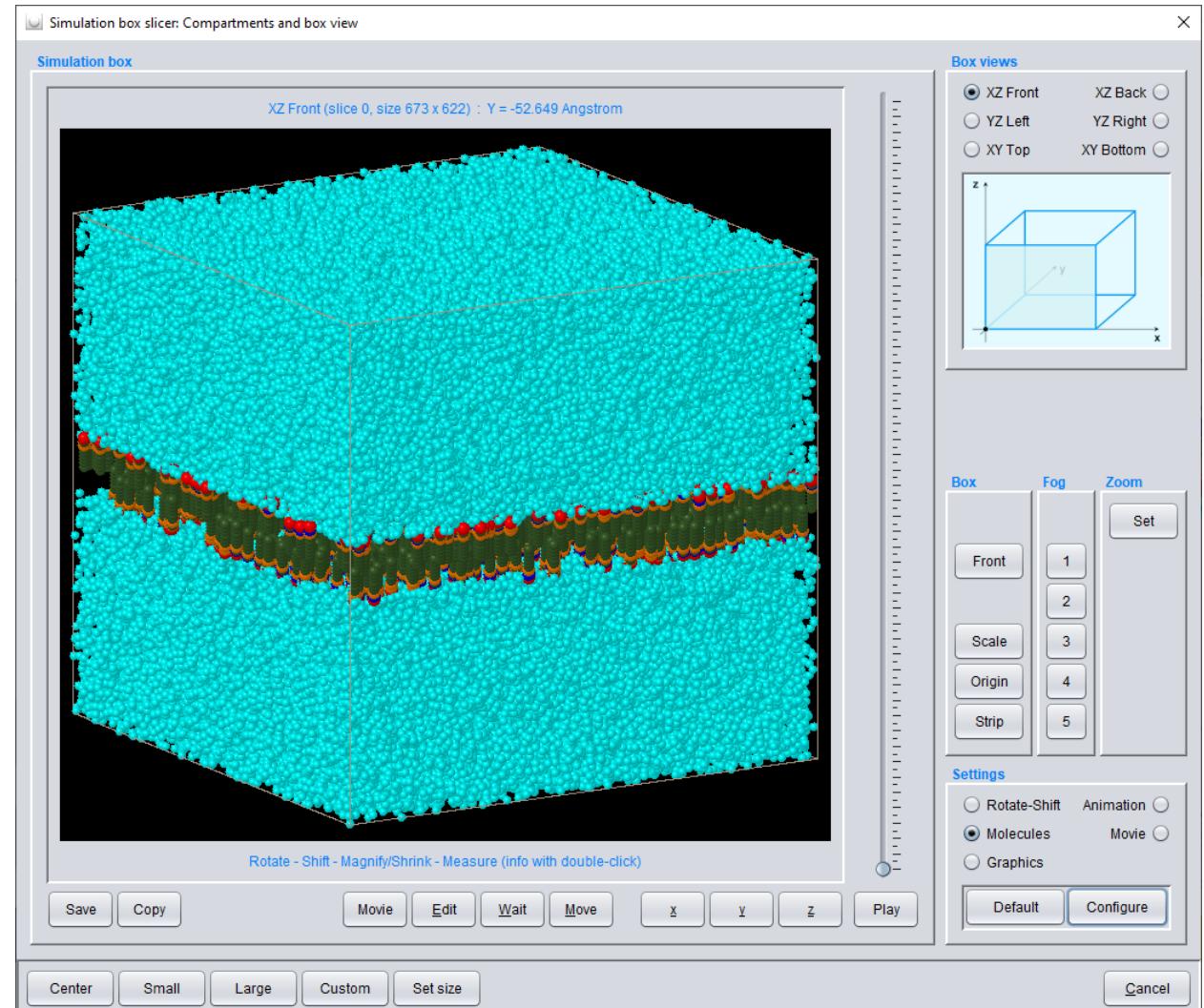


[www.molecular-dynamics.de](http://www.molecular-dynamics.de)

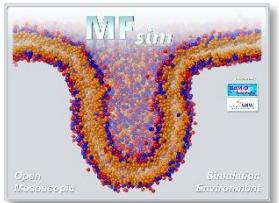


[www.gnwi.de](http://www.gnwi.de)

... to view the simulation box with all molecules including water. **Cancel** the simulation box view dialog.



# DMPC bilayer membrane Job Input – Simulation Box



Open  
Mesoscopic

Simulation  
Environment

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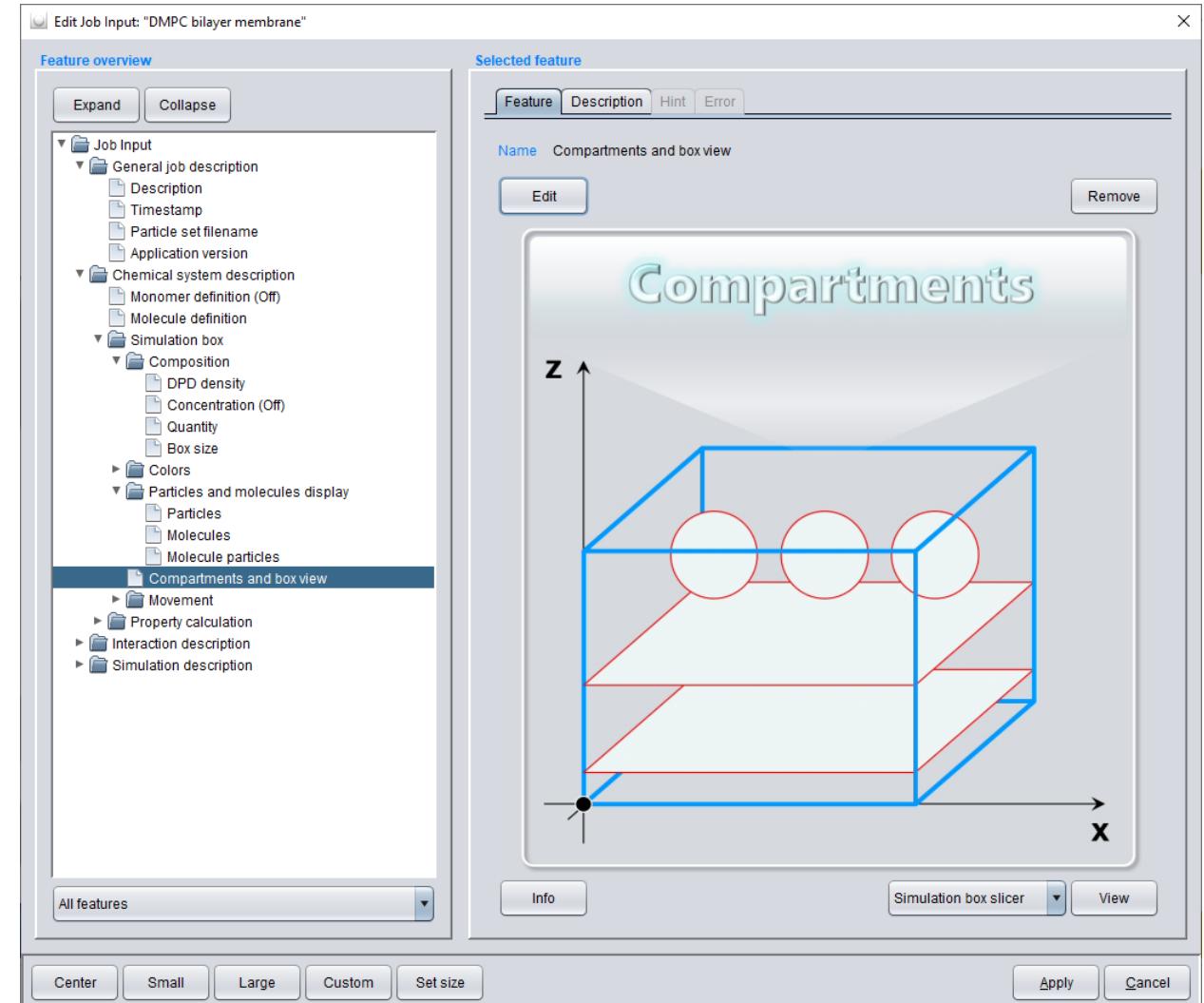


[www.molecular-dynamics.de](http://www.molecular-dynamics.de)

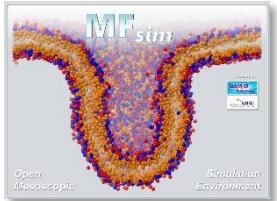


[www.gnwi.de](http://www.gnwi.de)

... to return to the Job Input feature dialog.



# DMPC bilayer membrane Job Input – Simulation Steps



Open  
Mesoscopic

Simulation  
Environment

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[www.gnwi.de](http://www.gnwi.de)

The number of **Simulation steps** at **Job Input / Simulation description** is set to 1.000 which corresponds to a simulation time of about 50 nanoseconds. This default setting is not changed.

Edit Job Input: "DMPC bilayer membrane"

Feature overview

Selected feature

Feature	Description	Hint	Error
Name	Simulation steps		
Number of steps	1000	0.055	54.512

Click on table cell to edit

Table-data schema

New

Cancel

Center Small Large Custom Set size

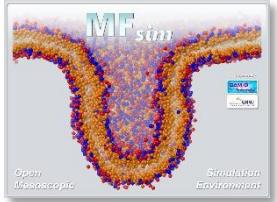
Expand Collapse

Job Input

- General job description
  - Description
  - Timestamp
  - Particle set filename
  - Application version
- Chemical system description
  - Monomer definition (Off)
  - Molecule definition
- Simulation box
  - Composition
    - DPD density
    - Concentration (Off)
    - Quantity
    - Box size
  - Colors
  - Particles and molecules display
    - Particles
    - Molecules
    - Molecule particles
    - Compartments and box view
    - Movement
  - Property calculation
  - Interaction description
  - Simulation description
    - Simulation steps
    - Time step length
    - Output frequency
    - Integration type
    - Initial minimization steps
    - Minimization step output
    - Periodic boundaries
    - DPD unit mass
    - Initial velocity scaling steps

All features

# DMPC bilayer membrane Job Input – Integration Type



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Mesoscopic

Simulation  
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[www.gnwi.de](http://www.gnwi.de)

Select **Job Input / Simulation description** / **Integration type** and change **Type** to **S1MVV**.

Edit Job Input: "DMPC bilayer membrane"

Feature overview

Selected feature

Feature	Description	Hint	Error
Name	Integration type		
Type	S1MVV	true	none

General job description

- Description
- Timestamp
- Particle set filename
- Application version

Chemical system description

- Monomer definition (Off)
- Molecule definition

Simulation box

- Composition

  - DPD density
  - Concentration (Off)
  - Quantity
  - Box size

- Colors
- Particles and molecules display

  - Particles
  - Molecules
  - Molecule particles
  - Compartments and box view
  - Movement

- Property calculation
- Interaction description

Simulation description

- Simulation steps
- Time step length
- Output frequency
- Integration type

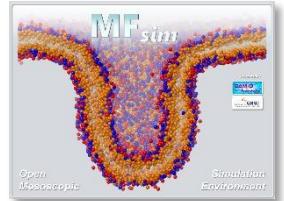
  - Initial minimization steps
  - Minimization step output
  - Periodic boundaries
  - DPD unit mass
  - Initial velocity scaling steps
  - Random number generator

All features

Table-data schema

New

Center Small Large Custom Set size Apply Cancel



Open  
Mesoscopic

Simulation  
Environment

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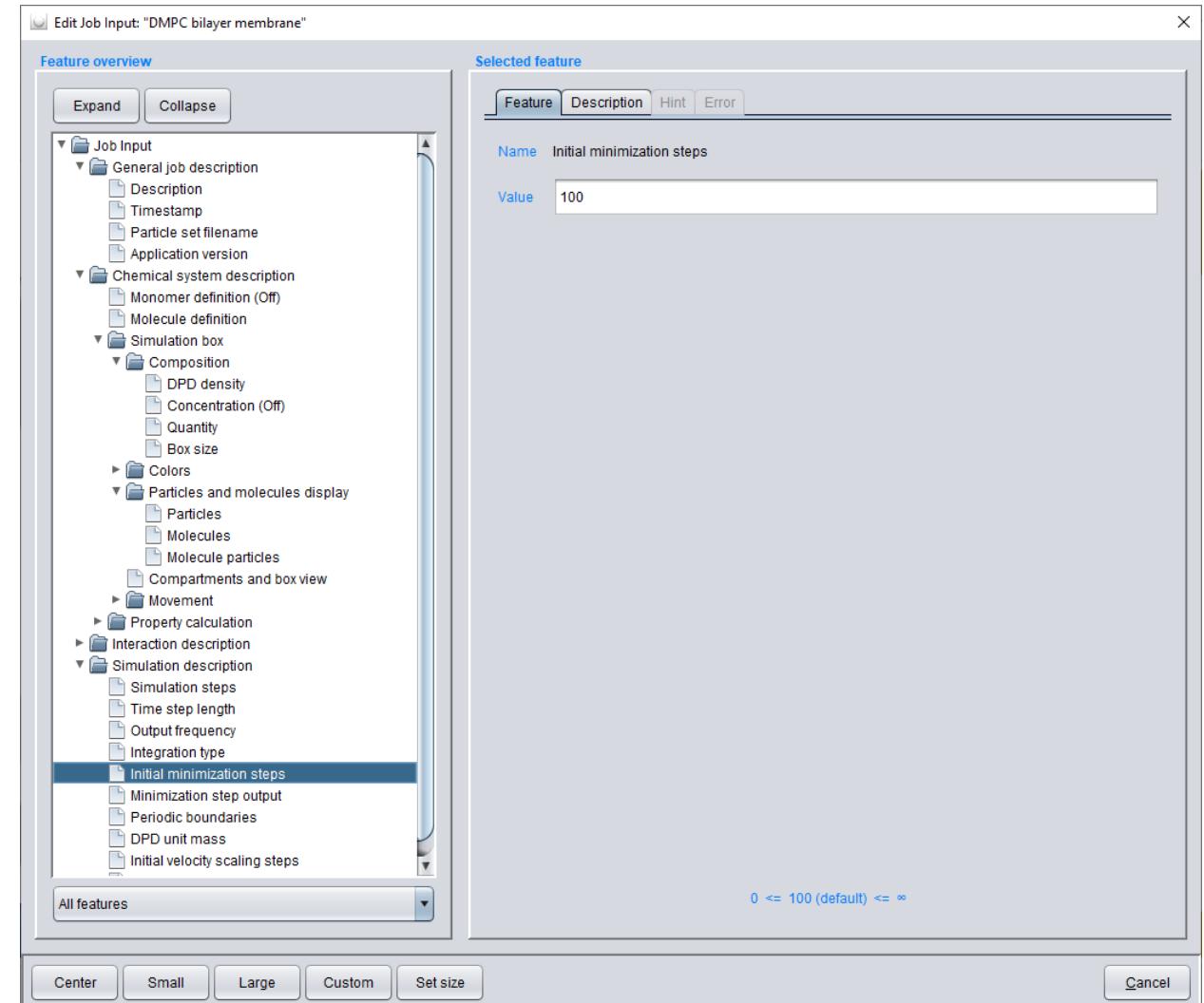
[www.molecular-dynamics.de](http://www.molecular-dynamics.de)

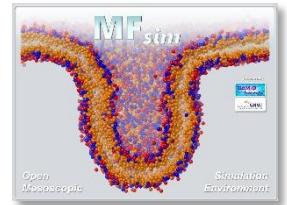


[www.gnwi.de](http://www.gnwi.de)

# DMPC bilayer membrane Job Input – Minimization Steps

Select **Job Input / Simulation description / Initial minimization steps** which specifies 100 steps by default and is not changed.





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Simulation  
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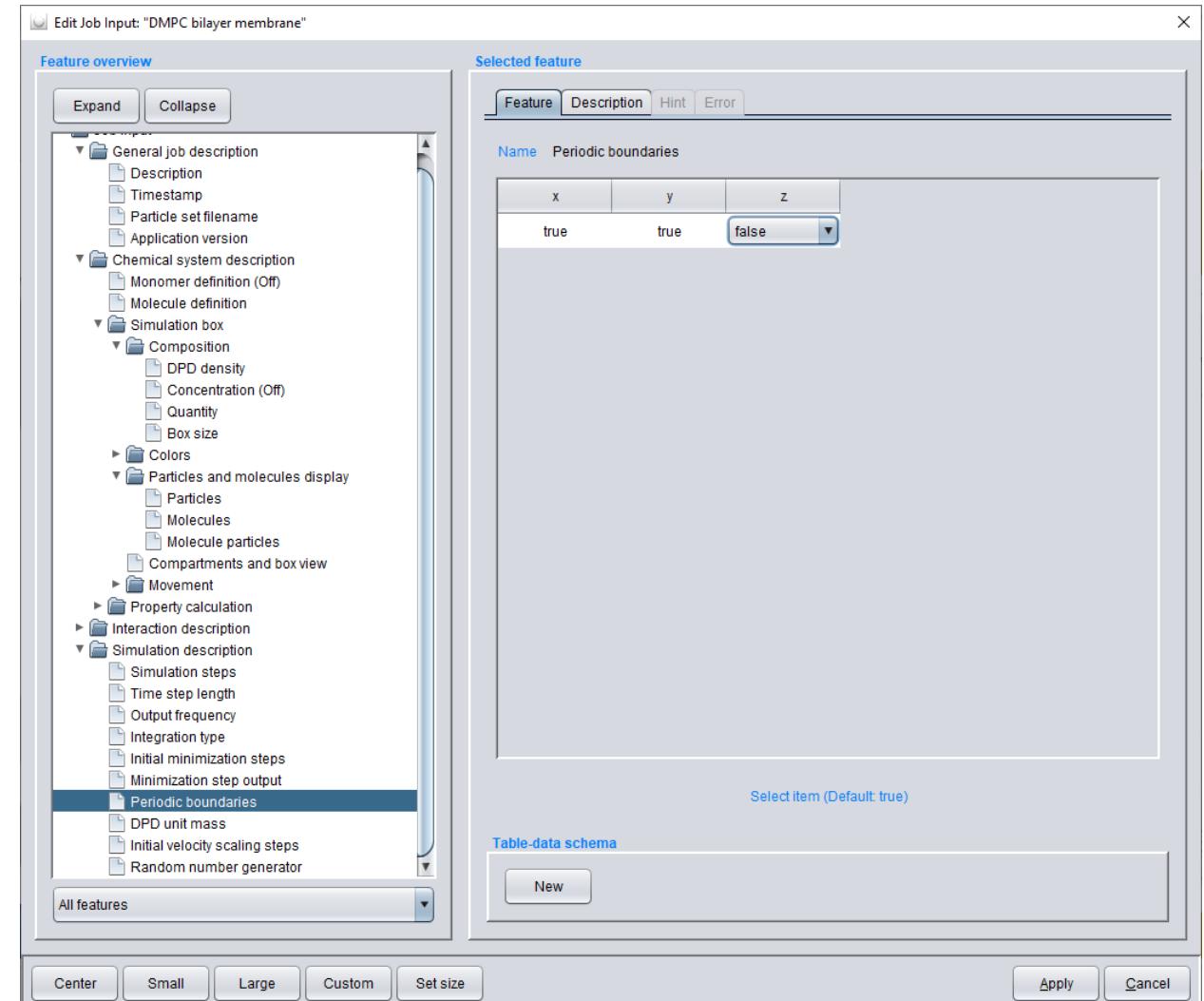


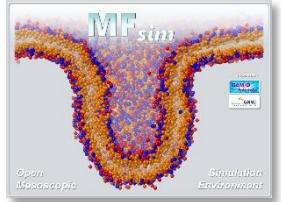
[www.gnwi.de](http://www.gnwi.de)

# DMPC bilayer membrane Job Input – Periodic Boundaries

Select **Job Input / Simulation description** / **Periodic boundaries** and change periodic boundaries in **z** direction to *false* (i.e. no periodic boundary but reflective walls).

Finally confirm all Job Input settings by hitting the **Apply** button to leave the dialog.





Open  
Mesoscopic

Simulation  
Environment

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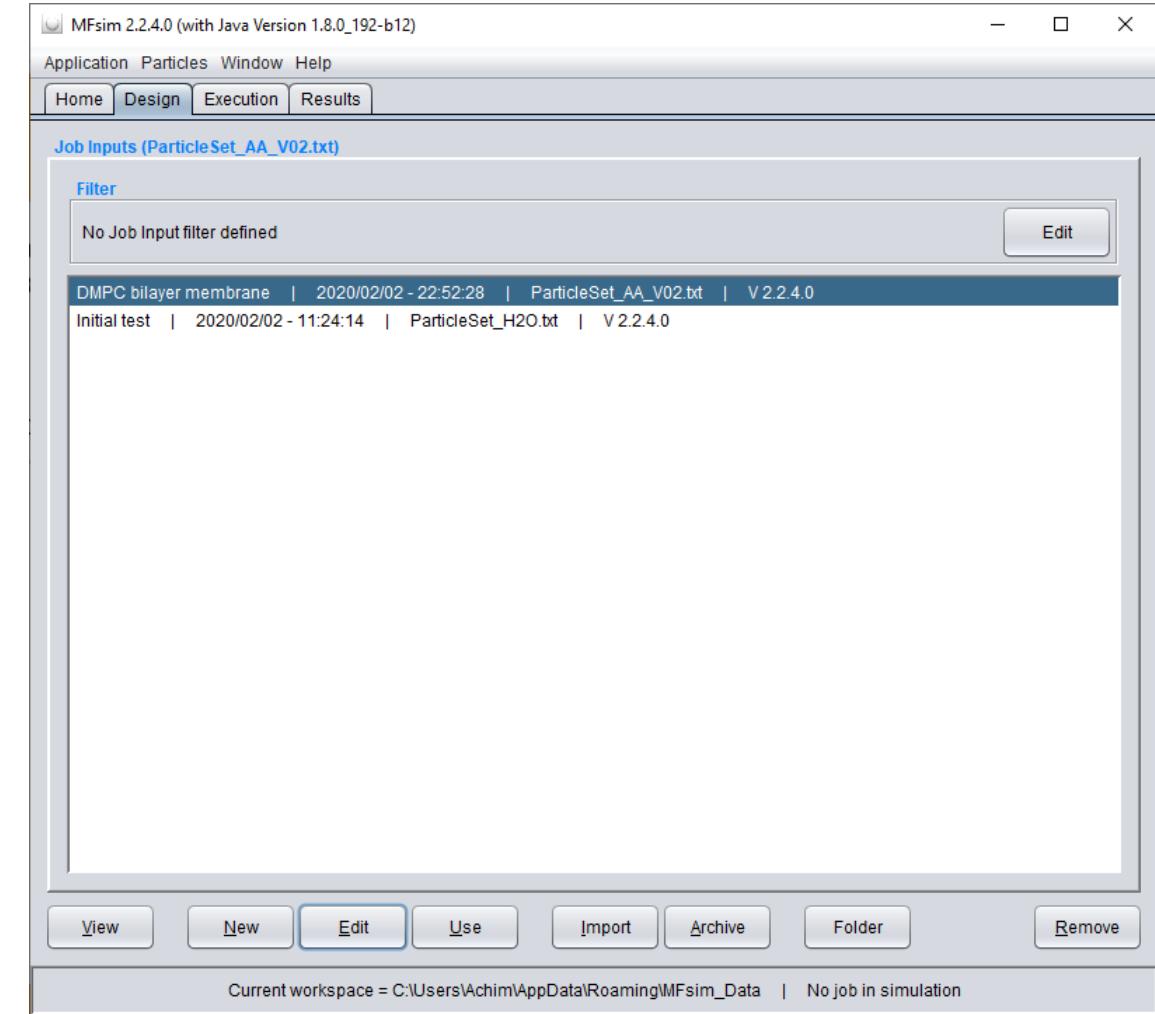
[www.molecular-dynamics.de](http://www.molecular-dynamics.de)

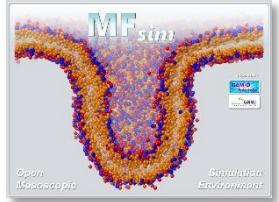


[www.gnwi.de](http://www.gnwi.de)

# DMPC bilayer membrane Job Input

The new Job Input appears in the list.





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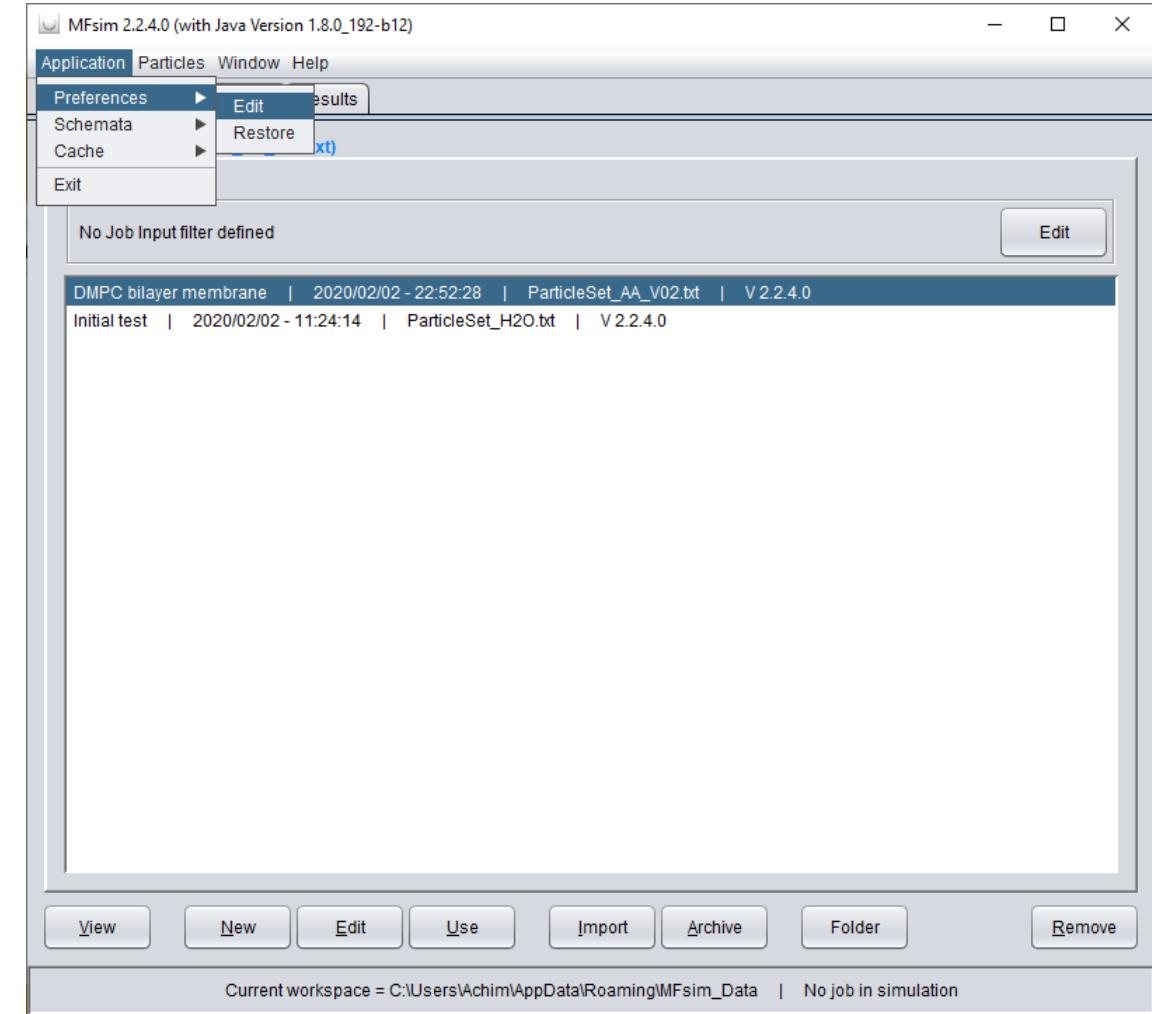
[www.molecular-dynamics.de](http://www.molecular-dynamics.de)

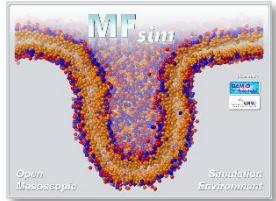


[www.gnwi.de](http://www.gnwi.de)

# DMPC bilayer membrane – Preferences

Select menu item **Application** /  
**Preferences / Edit ...**





Open  
Mesoscopic

Simulation  
Environment

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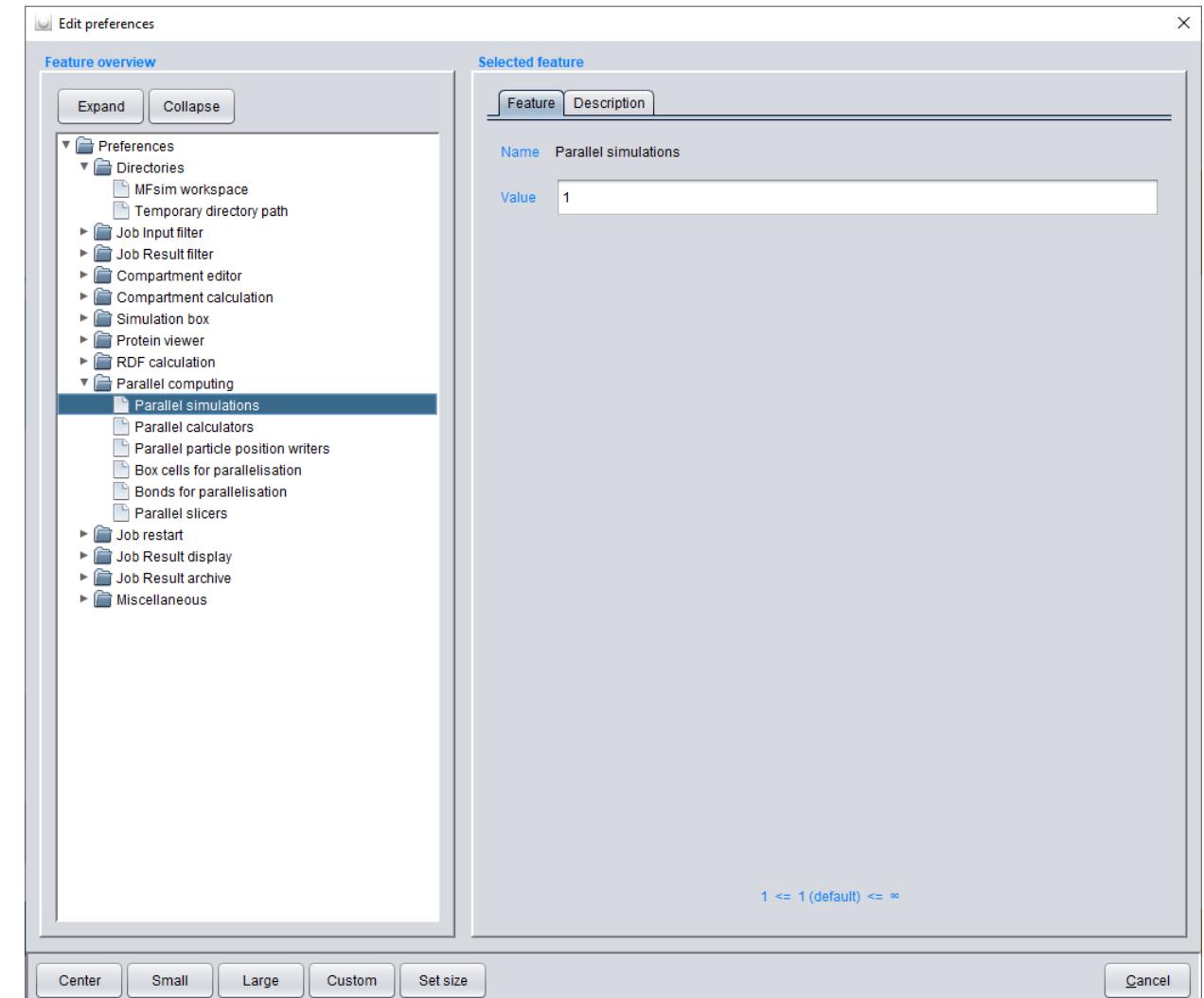
[www.molecular-dynamics.de](http://www.molecular-dynamics.de)



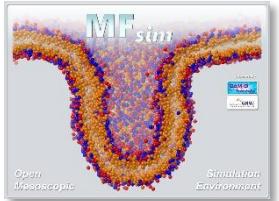
[www.gnwi.de](http://www.gnwi.de)

# DMPC bilayer membrane – Preferences

... and select **Preferences / Parallel computing** for adequate parallelization settings to exploit the performance of your multi-core processor in an optimum manner. For an octa-core processor do not change the **Parallel simulations** ...



# DMPC bilayer membrane – Preferences



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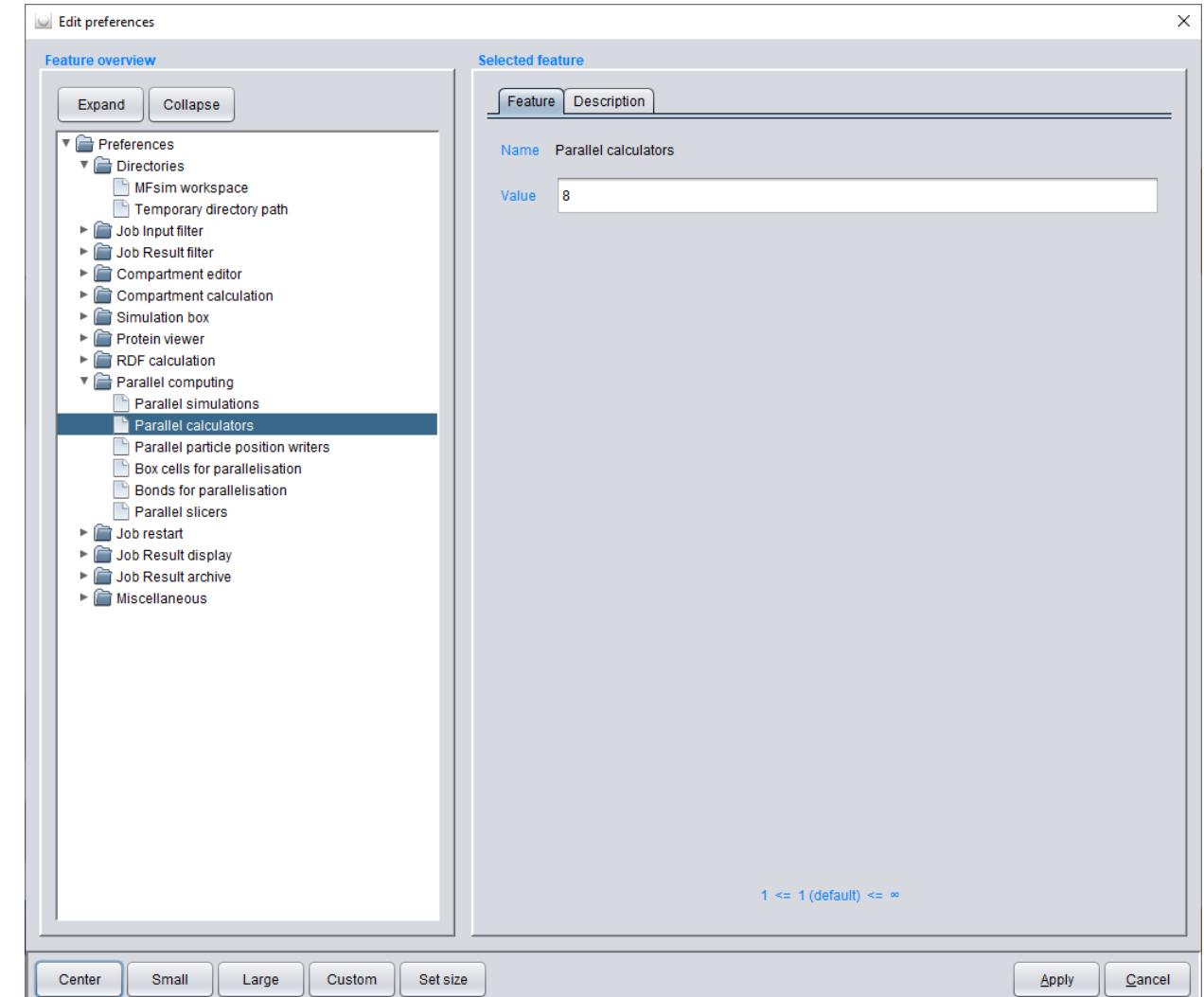
[www.molecular-dynamics.de](http://www.molecular-dynamics.de)

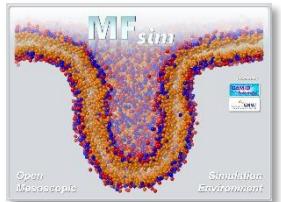


[www.gnwi.de](http://www.gnwi.de)

GitHub repository:  
<https://github.com/zieslesny/MFsim>

... but set **Parallel calculators** to 8 ...





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Simulation  
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[www.molecular-dynamics.de](http://www.molecular-dynamics.de)

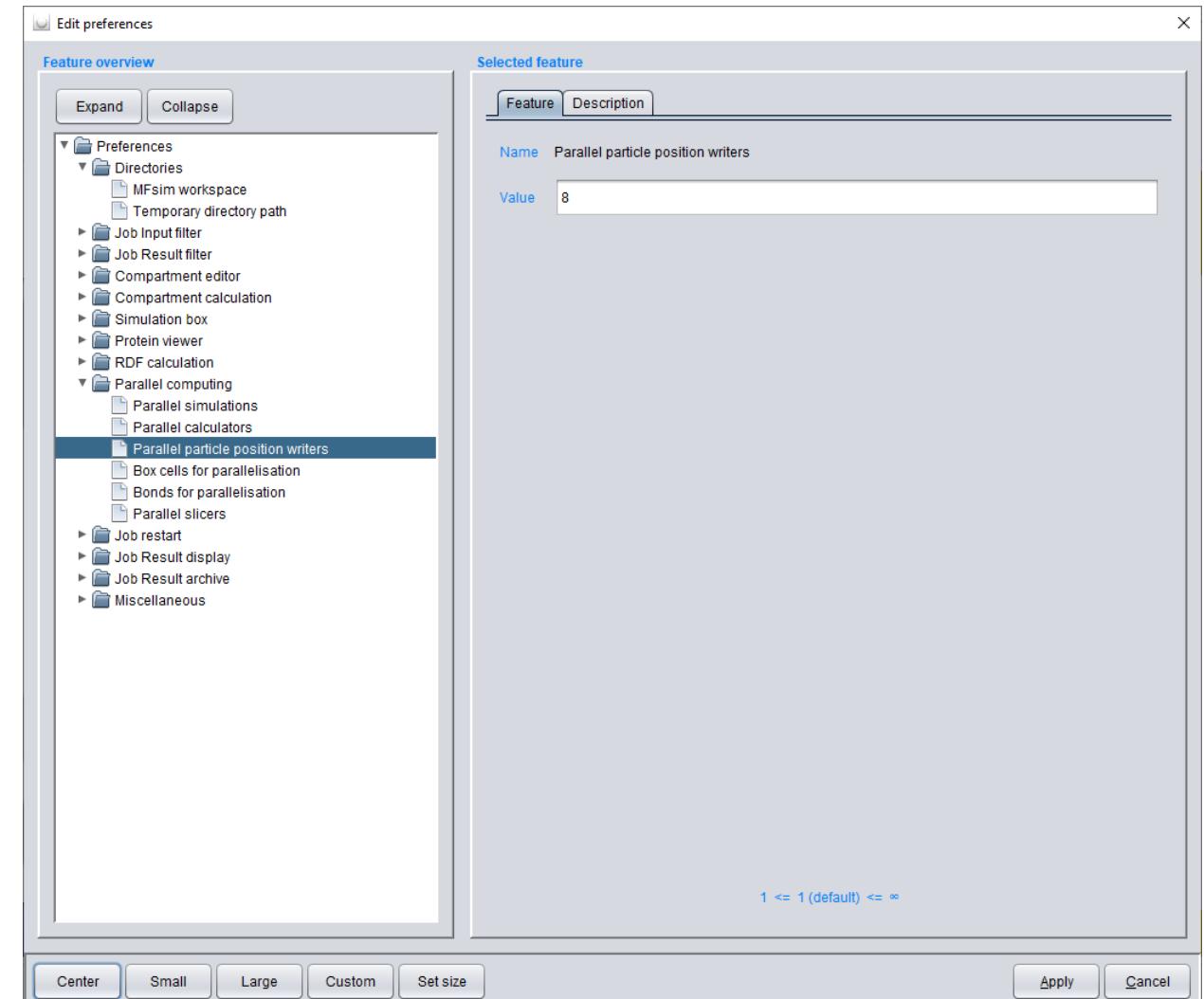


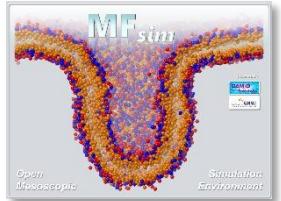
[www.gnwi.de](http://www.gnwi.de)

# DMPC bilayer membrane – Preferences

... **Parallel particle position writers** to 8

...





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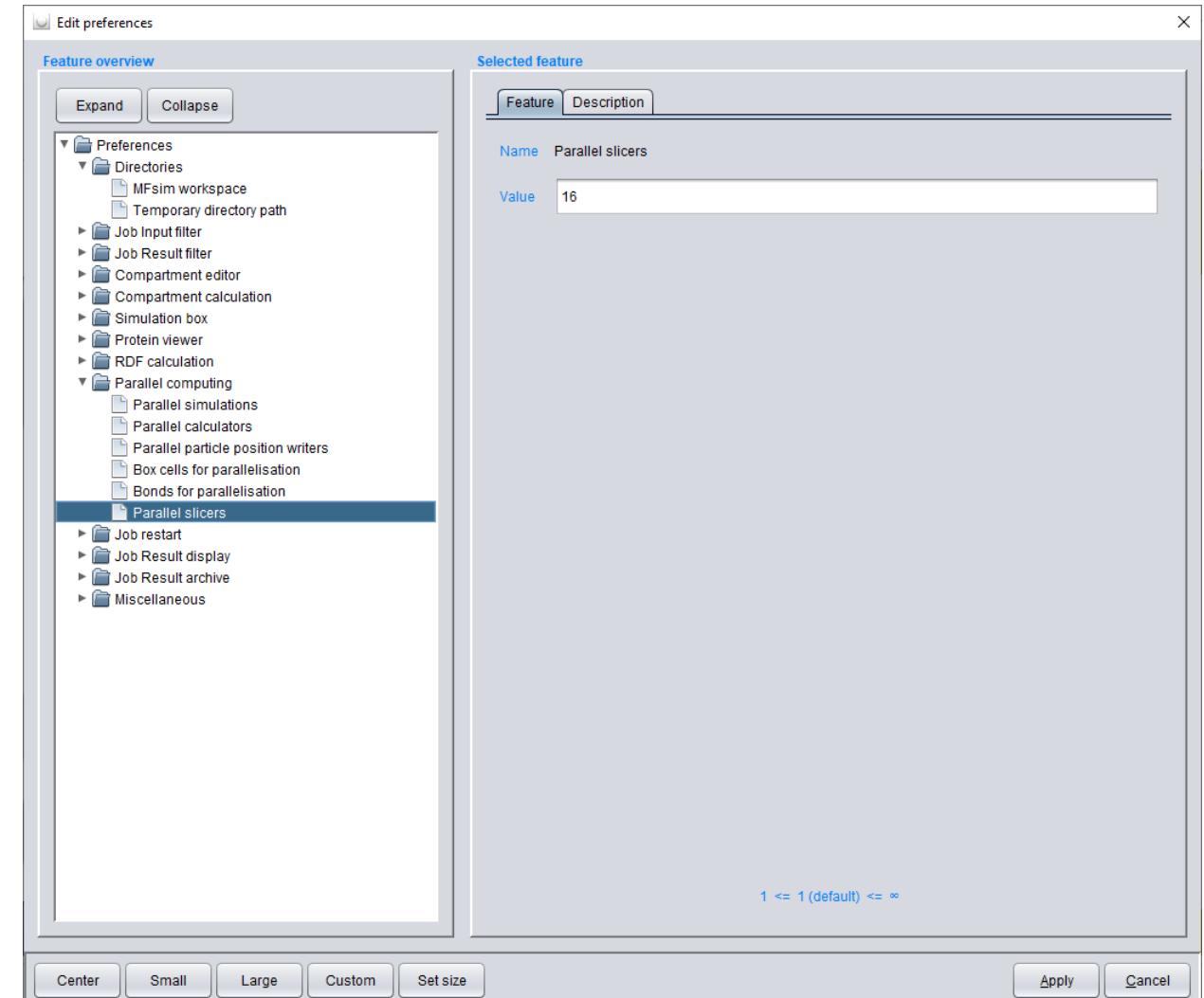
[www.molecular-dynamics.de](http://www.molecular-dynamics.de)

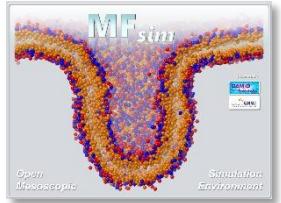


[www.gnwi.de](http://www.gnwi.de)

# DMPC bilayer membrane – Preferences

... and **Parallel slicers** to 16. Then leave the dialog with **Apply**.





Open  
Mesoscopic

Simulation  
Environment

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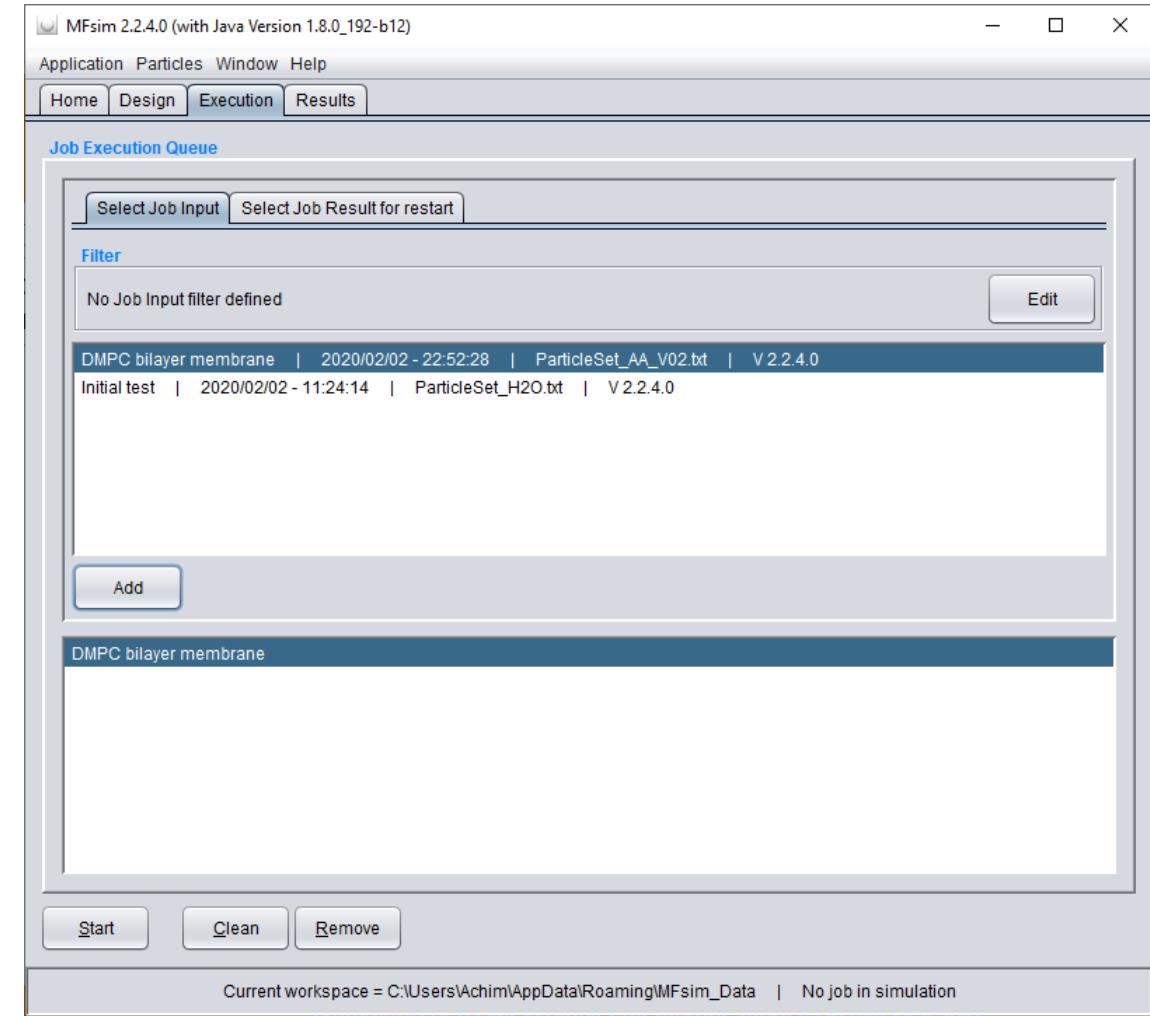
[www.molecular-dynamics.de](http://www.molecular-dynamics.de)

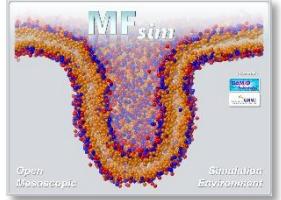


[www.gnwi.de](http://www.gnwi.de)

# DMPC bilayer membrane – Job Execution

Select the **Execution** tab and **Add** the *DMPC bilayer membrane* job to the **Job execution queue**.





Open  
Mesoscopic

Simulation  
Environment

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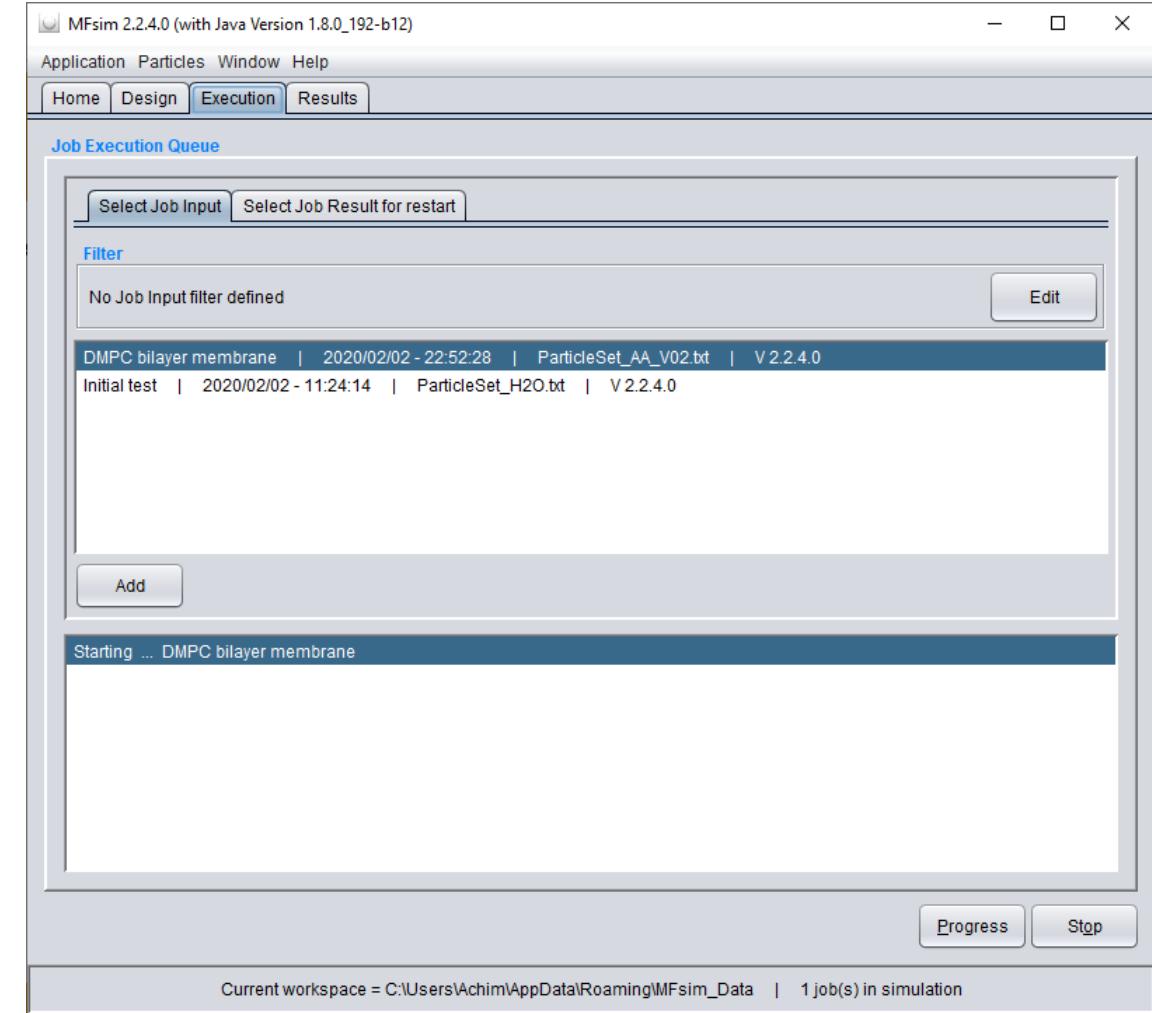
[www.molecular-dynamics.de](http://www.molecular-dynamics.de)

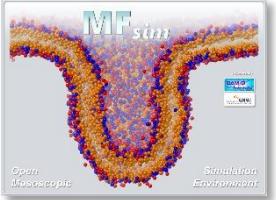


[www.gnwi.de](http://www.gnwi.de)

# DMPC bilayer membrane – Job Execution

Start the job execution by hitting the **Start** button ...





Open  
Mesoscopic

Simulation  
Environment

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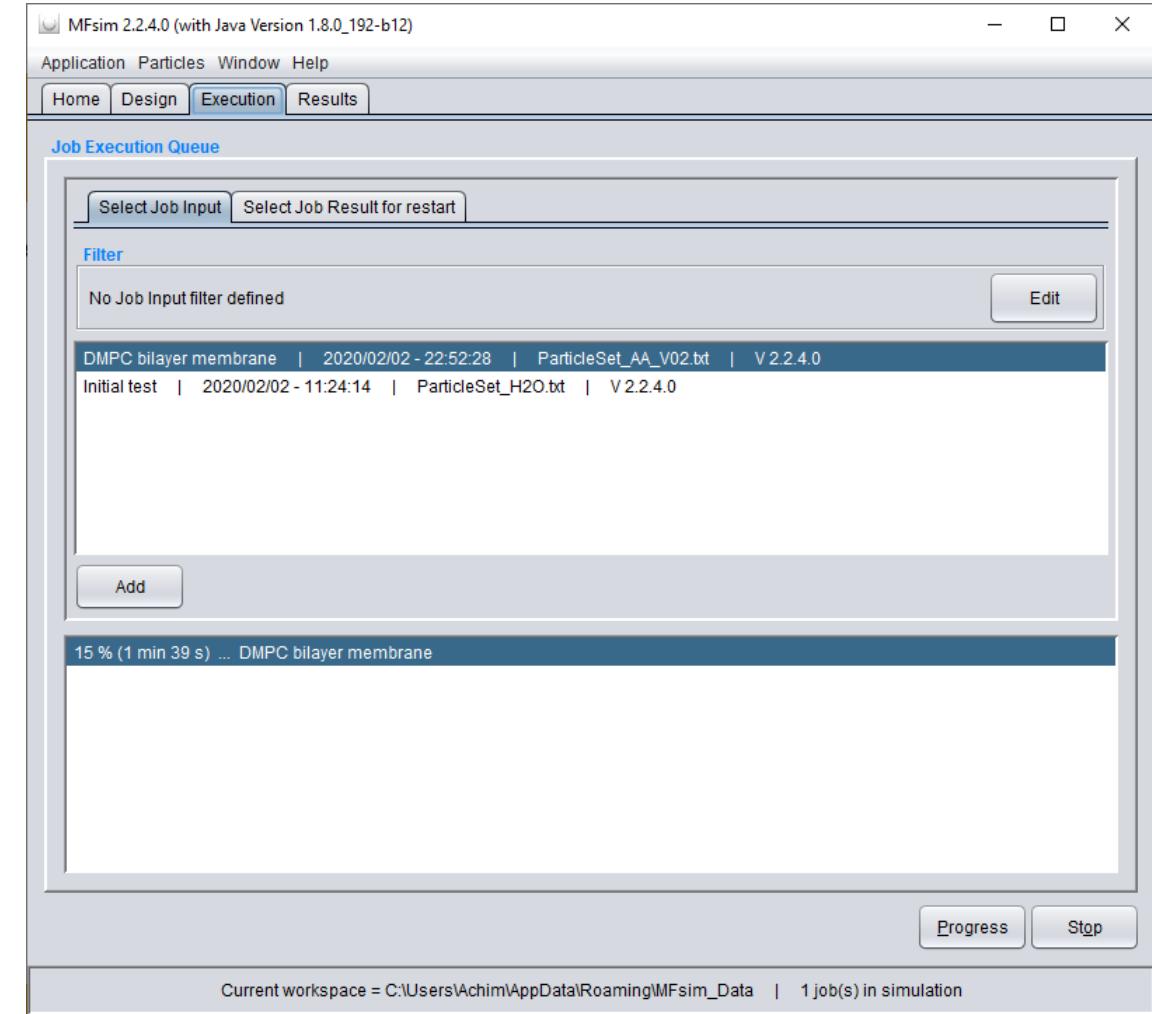
[www.molecular-dynamics.de](http://www.molecular-dynamics.de)

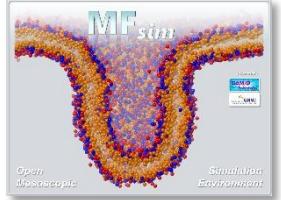


[www.gnwi.de](http://www.gnwi.de)

# DMPC bilayer membrane – Job Execution

... and wait for the job to finish within a few minutes.





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Simulation  
Environment

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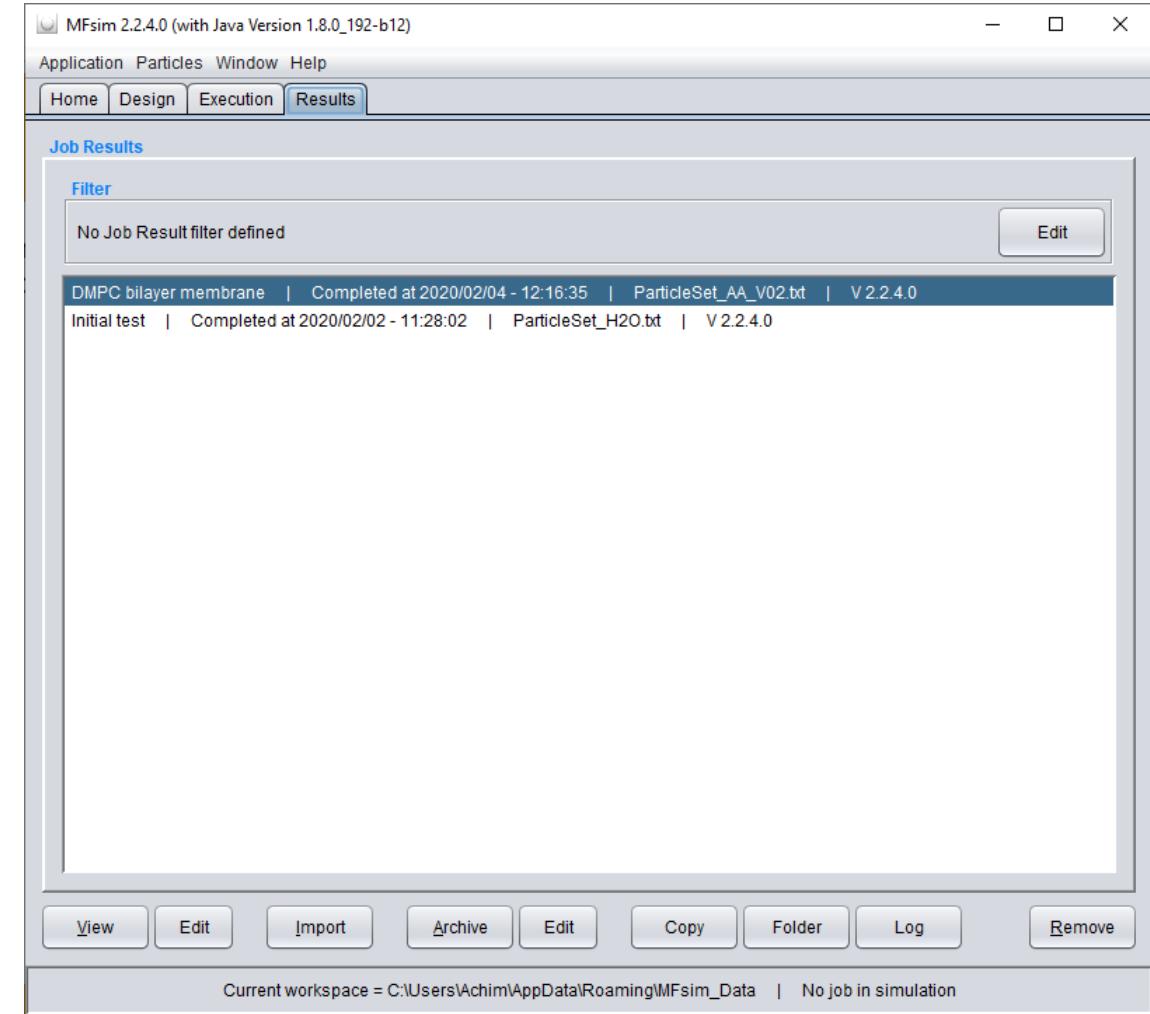
[www.molecular-dynamics.de](http://www.molecular-dynamics.de)

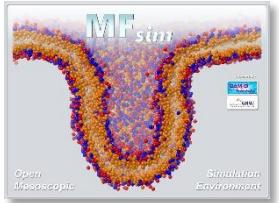


[www.gnwi.de](http://www.gnwi.de)

# DMPC bilayer membrane Job Result

Select the **Results** tab which now contains the new (selected) Job Result. Hitting the **View** button ...





Open  
Mesoscopic

Simulation  
Environment

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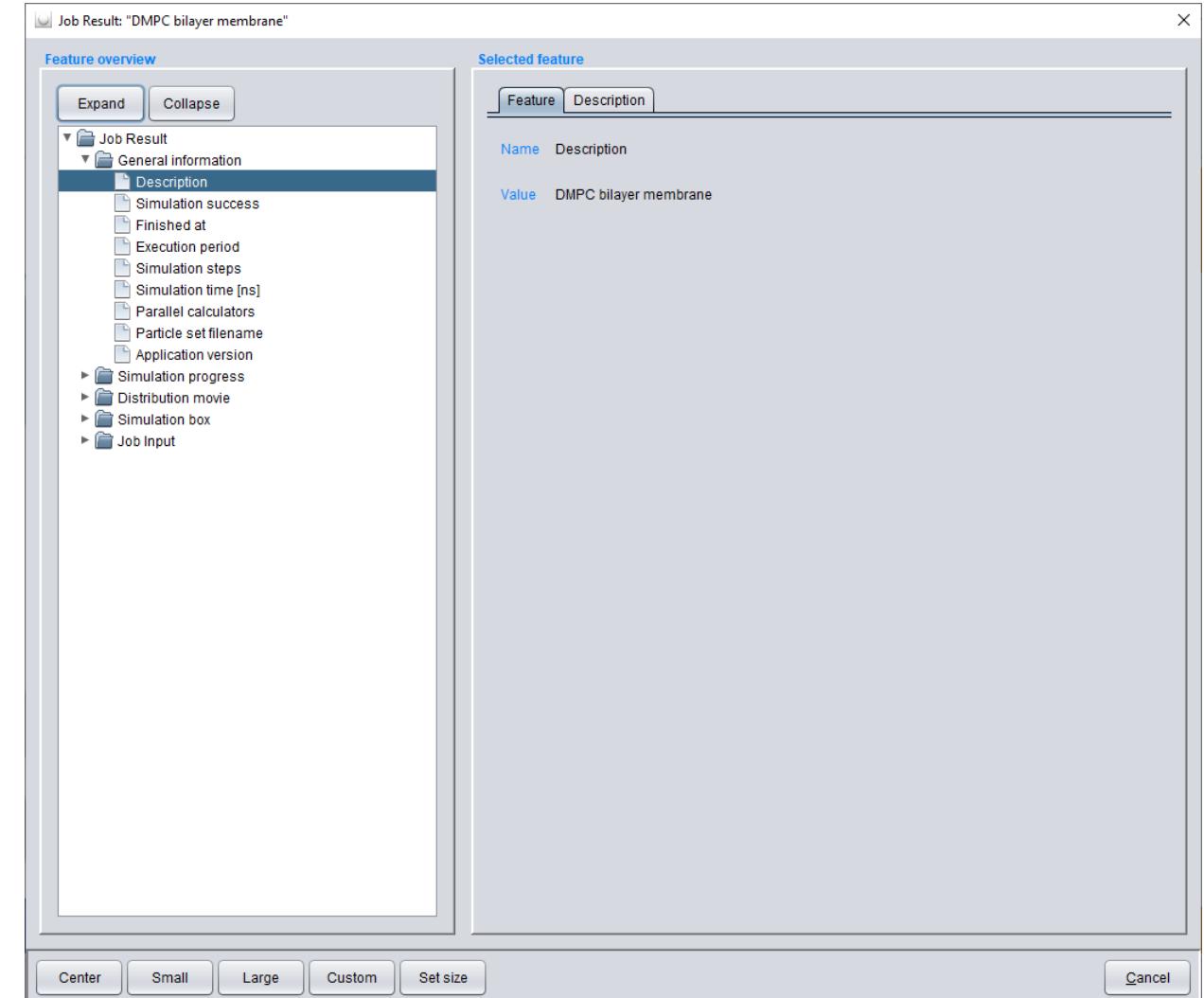
[www.molecular-dynamics.de](http://www.molecular-dynamics.de)



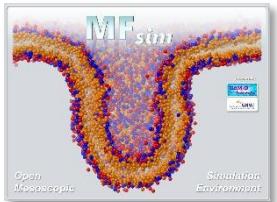
[www.gnwi.de](http://www.gnwi.de)

# DMPC bilayer membrane Job Result

... opens the Job Result dialog:



# DMPC bilayer membrane Job Result – Simulation Box



Open  
Mesoscopic

Simulation  
Environment

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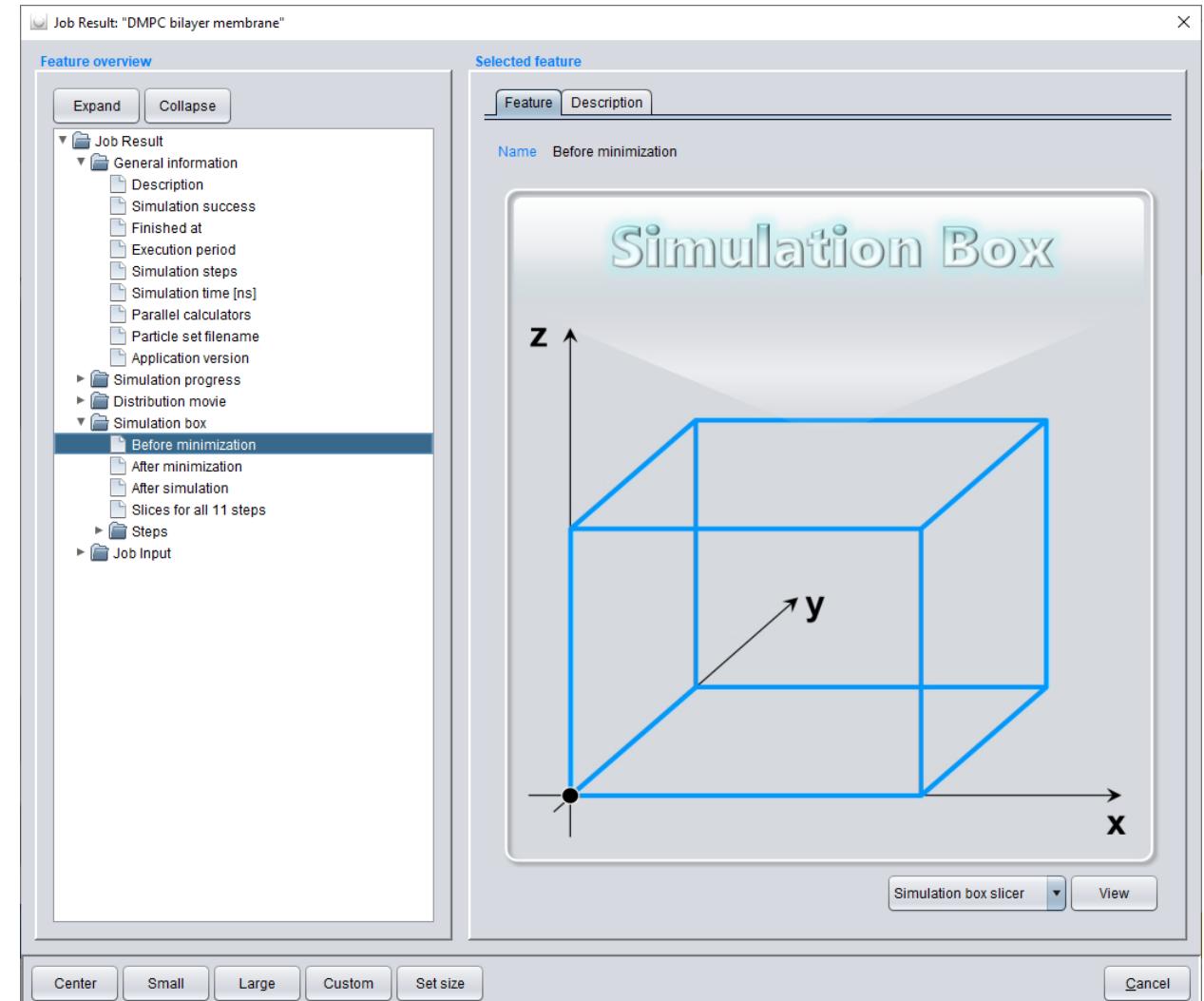


[www.molecular-dynamics.de](http://www.molecular-dynamics.de)

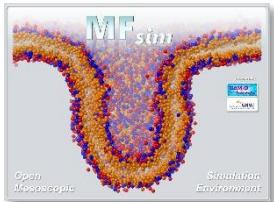


[www.gnwi.de](http://www.gnwi.de)

Select **Job Result / Simulation box / Before minimization** and hit the **View** button ...



# DMPC bilayer membrane Job Result – Simulation Box



Open  
Mesoscopic

Simulation  
Environment

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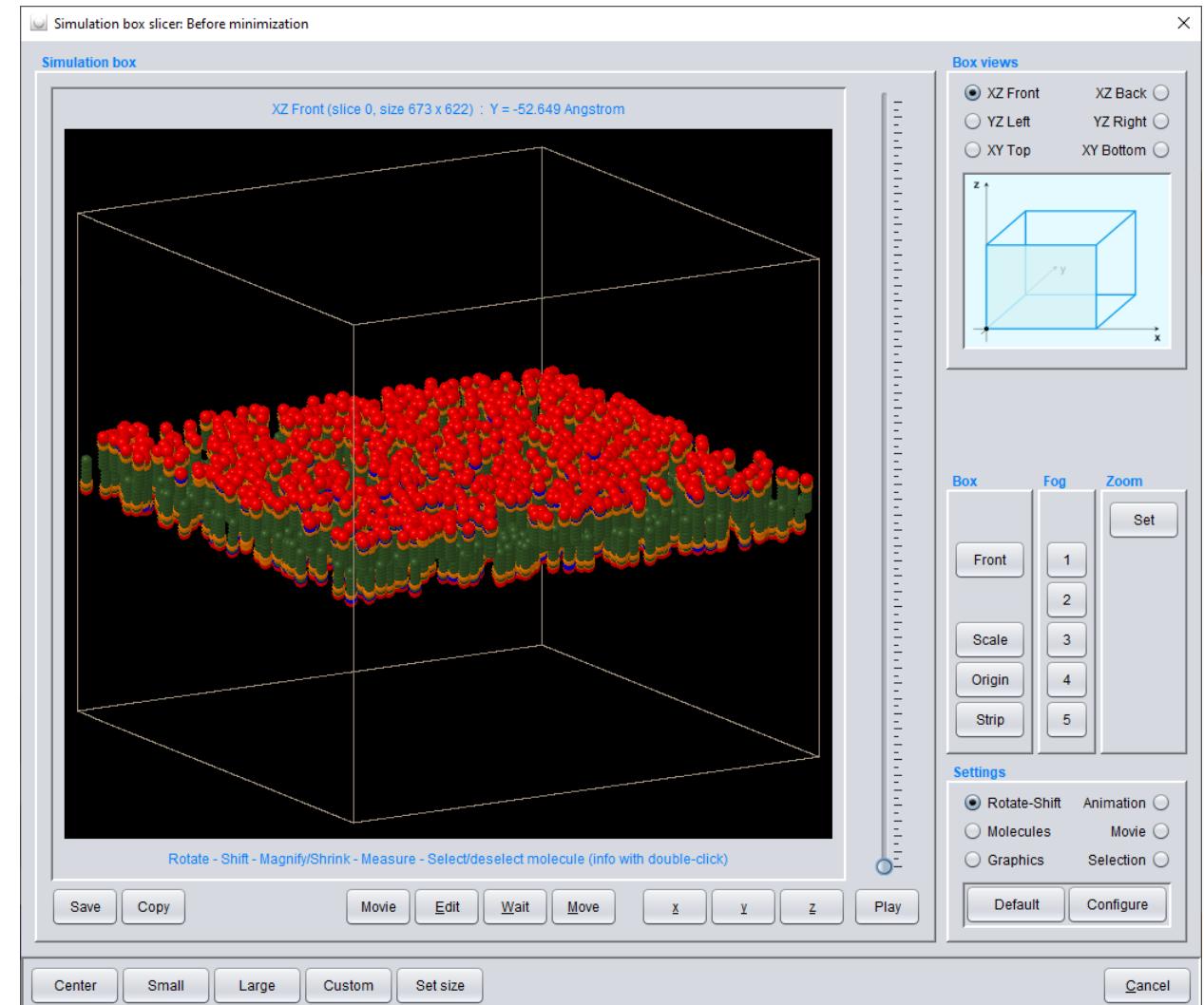


[www.molecular-dynamics.de](http://www.molecular-dynamics.de)

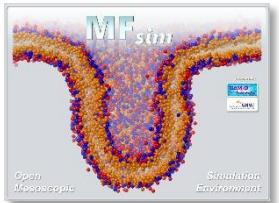


[www.gnwi.de](http://www.gnwi.de)

... to inspect the initial simulation box.  
**Cancel** the dialog ...



# DMPC bilayer membrane Job Result – Simulation Box



Open  
Mesoscopic

Simulation  
Environment

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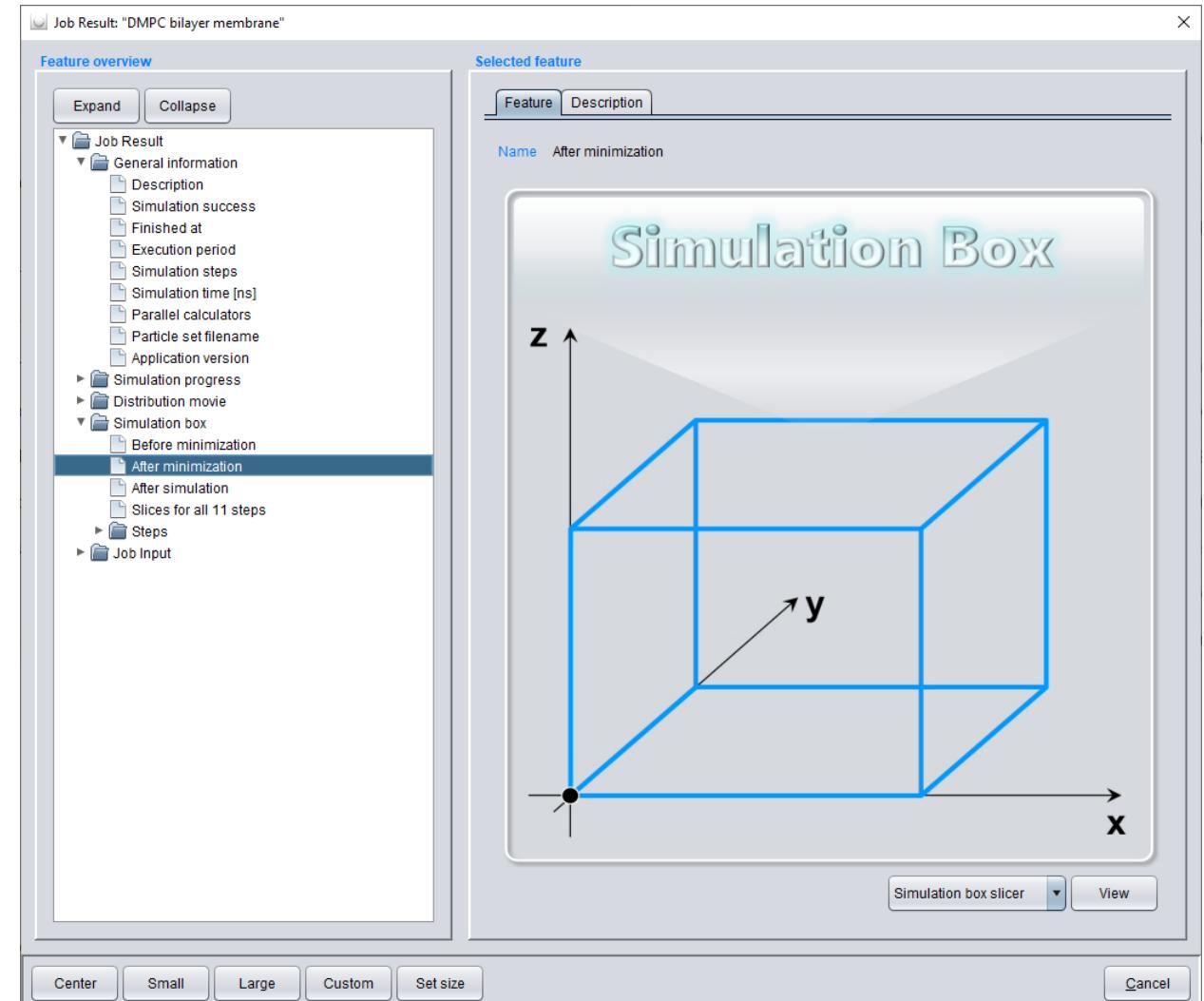
[www.molecular-dynamics.de](http://www.molecular-dynamics.de)



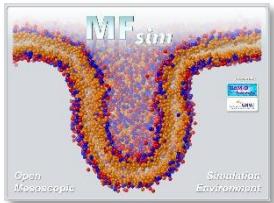
[www.gnwi.de](http://www.gnwi.de)

... and select **Job Result / Simulation box**  
**/ After minimization**. Hit the **View** button

...



# DMPC bilayer membrane Job Result – Simulation Box



Open  
Mesoscopic

Simulation  
Environment

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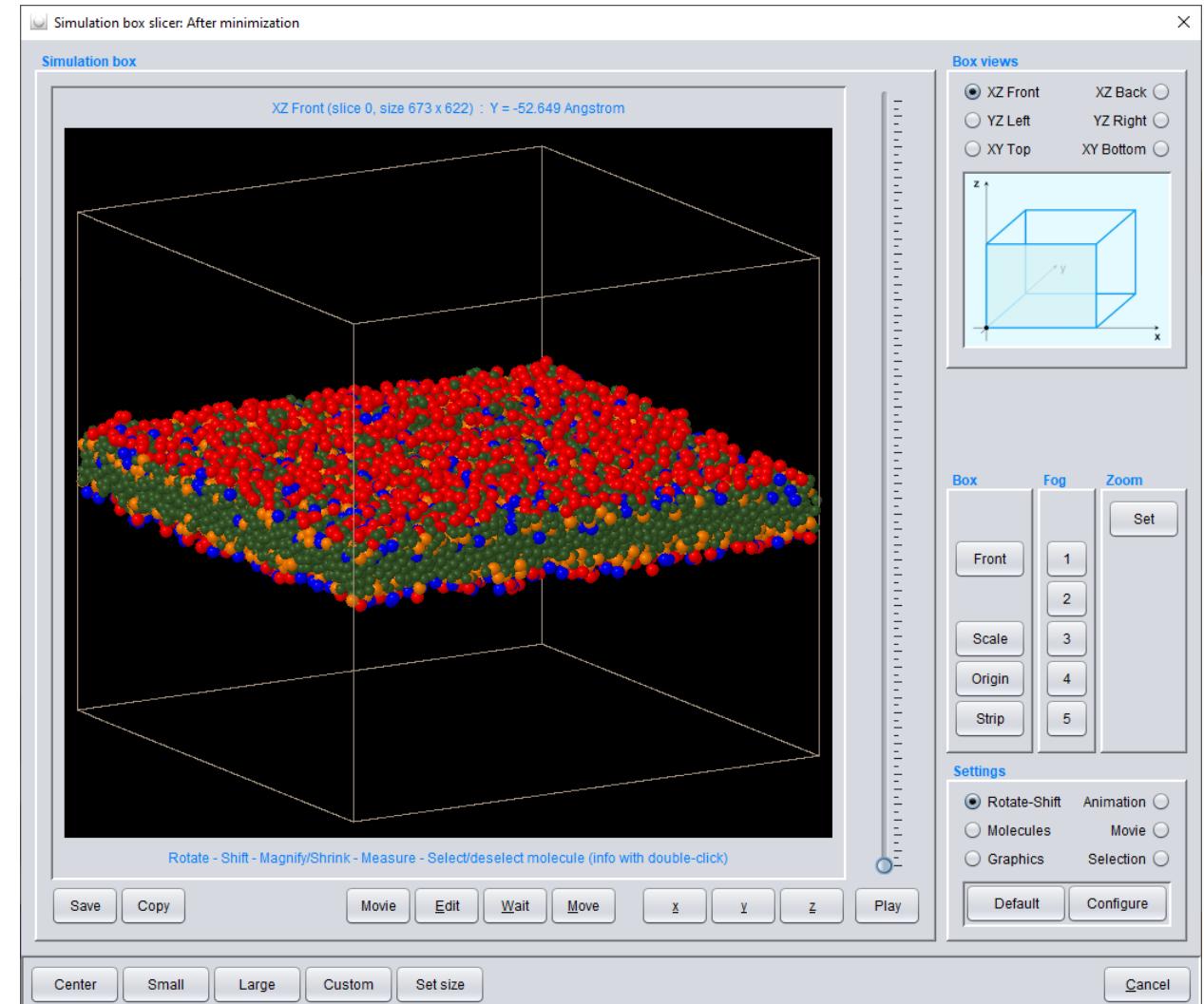


[www.molecular-dynamics.de](http://www.molecular-dynamics.de)

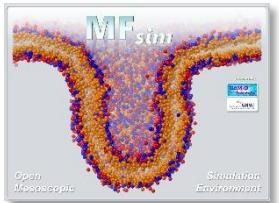


[www.gnwi.de](http://www.gnwi.de)

... to inspect the simulation box after the minimization steps are performed. **Cancel** the dialog ...



# DMPC bilayer membrane Job Result – Simulation Box



Open  
Mesoscopic

Simulation  
Environment

powered by

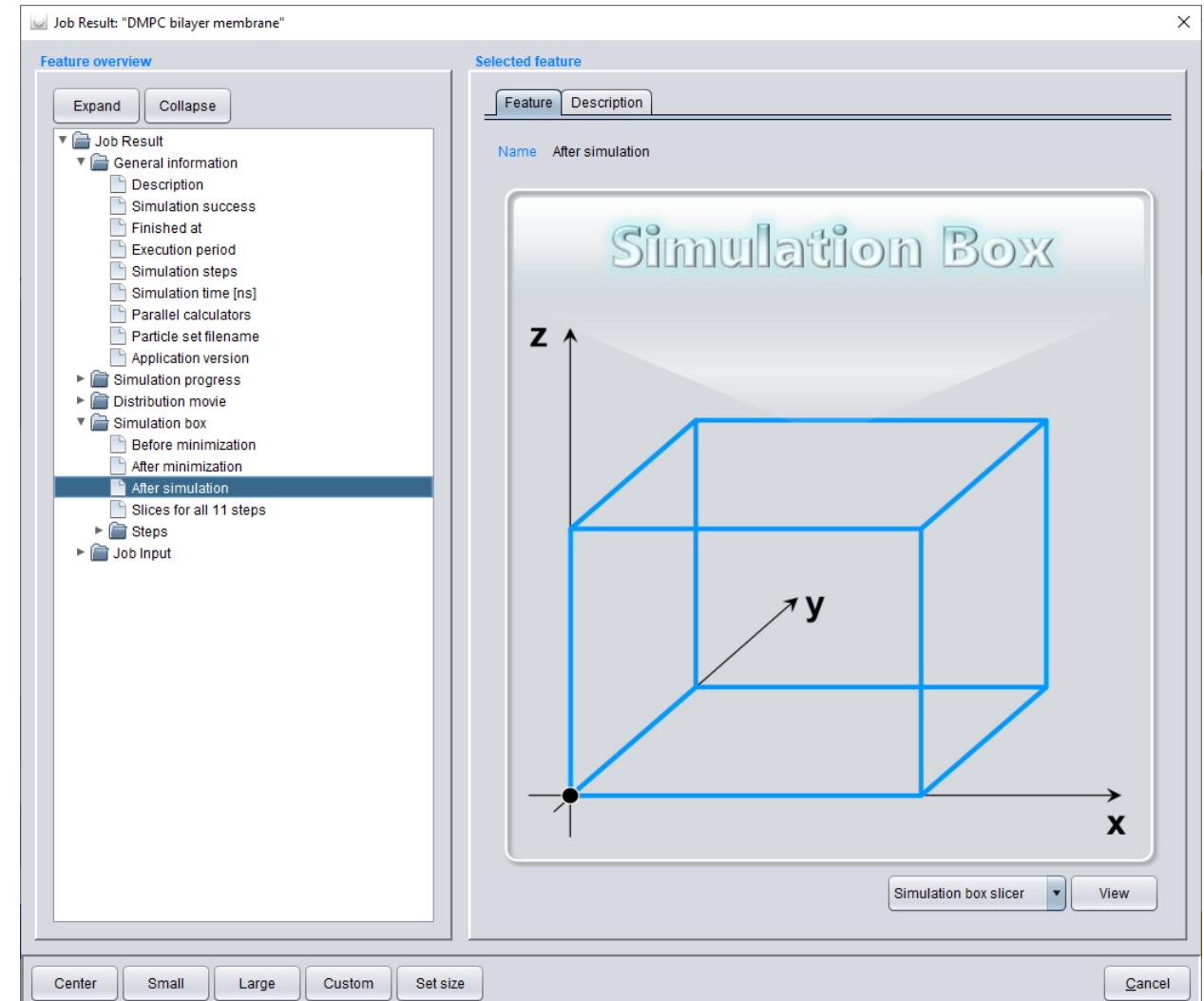


[www.molecular-dynamics.de](http://www.molecular-dynamics.de)

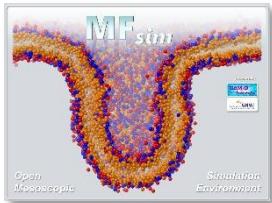


[www.gnwi.de](http://www.gnwi.de)

... and select **Job Result / Simulation box**  
**/ After simulation**. Hit the **View** button ...



# DMPC bilayer membrane Job Result – Simulation Box



Open  
Mesoscopic

Simulation  
Environment

powered by

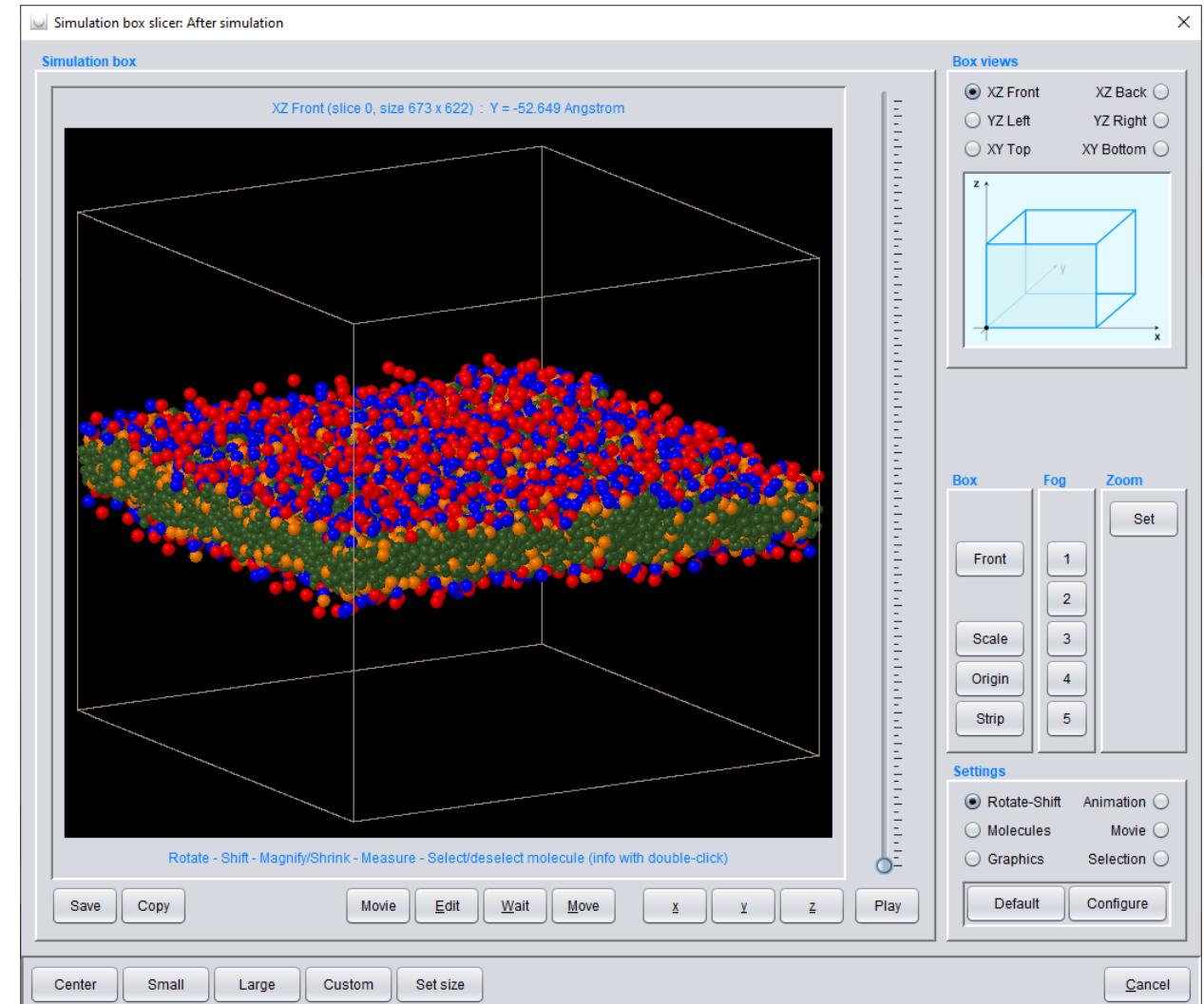


[www.molecular-dynamics.de](http://www.molecular-dynamics.de)

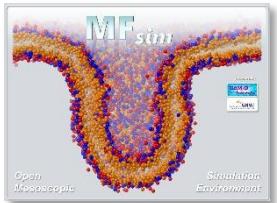


[www.gnwi.de](http://www.gnwi.de)

... to inspect the simulation box at the last simulation step. On the **Box** panel click the **Front** button and then the (appearing) **Fit** button ...



# DMPC bilayer membrane Job Result – Simulation Box



Open  
Mesoscopic

Simulation  
Environment

powered by

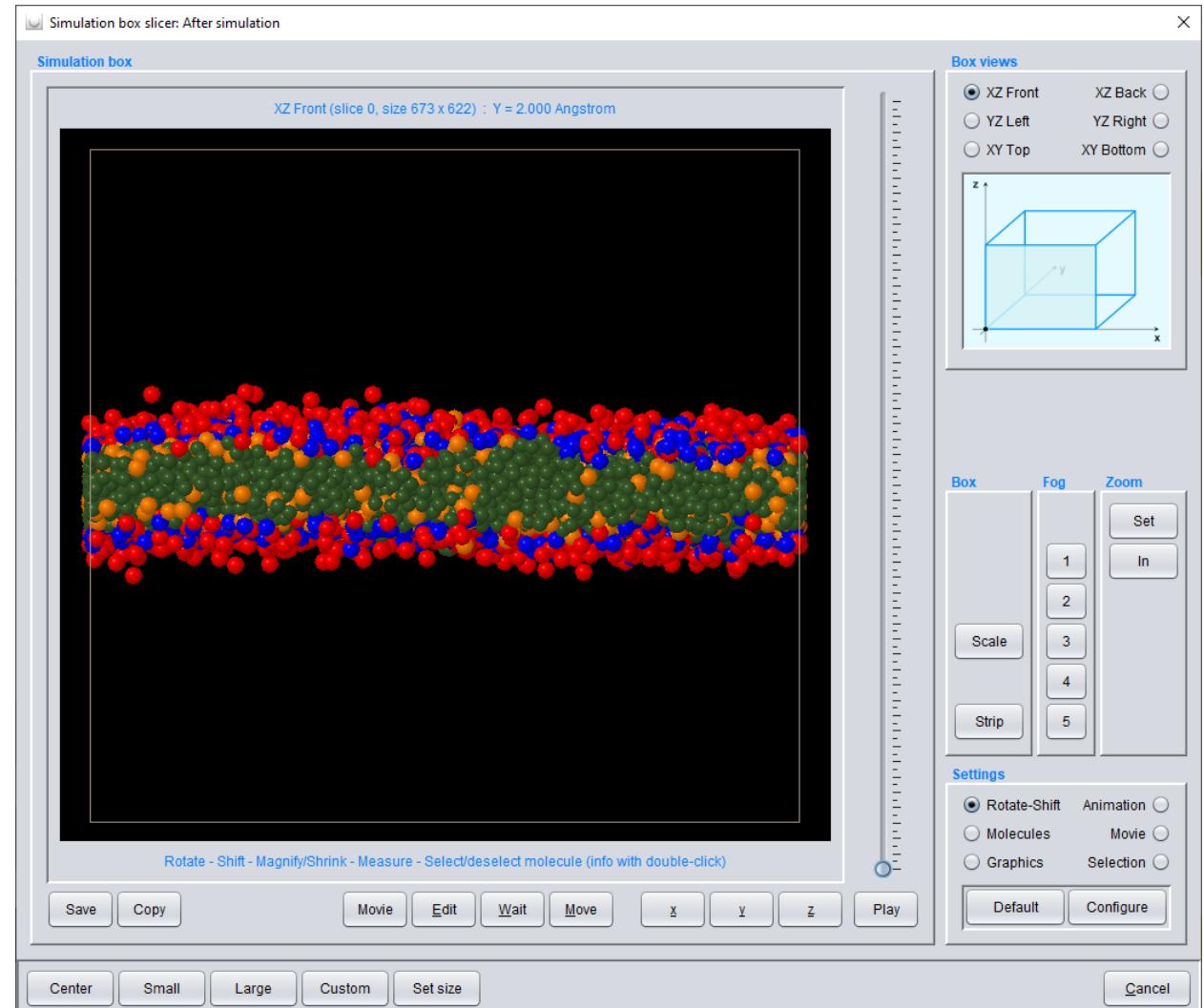


[www.molecular-dynamics.de](http://www.molecular-dynamics.de)

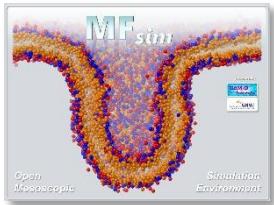


[www.gnwi.de](http://www.gnwi.de)

... to arrive at the optimized xz front view of the simulation box.



# DMPC bilayer membrane Job Result – Measurements



Open  
Mesoscopic

Simulation  
Environment

powered by

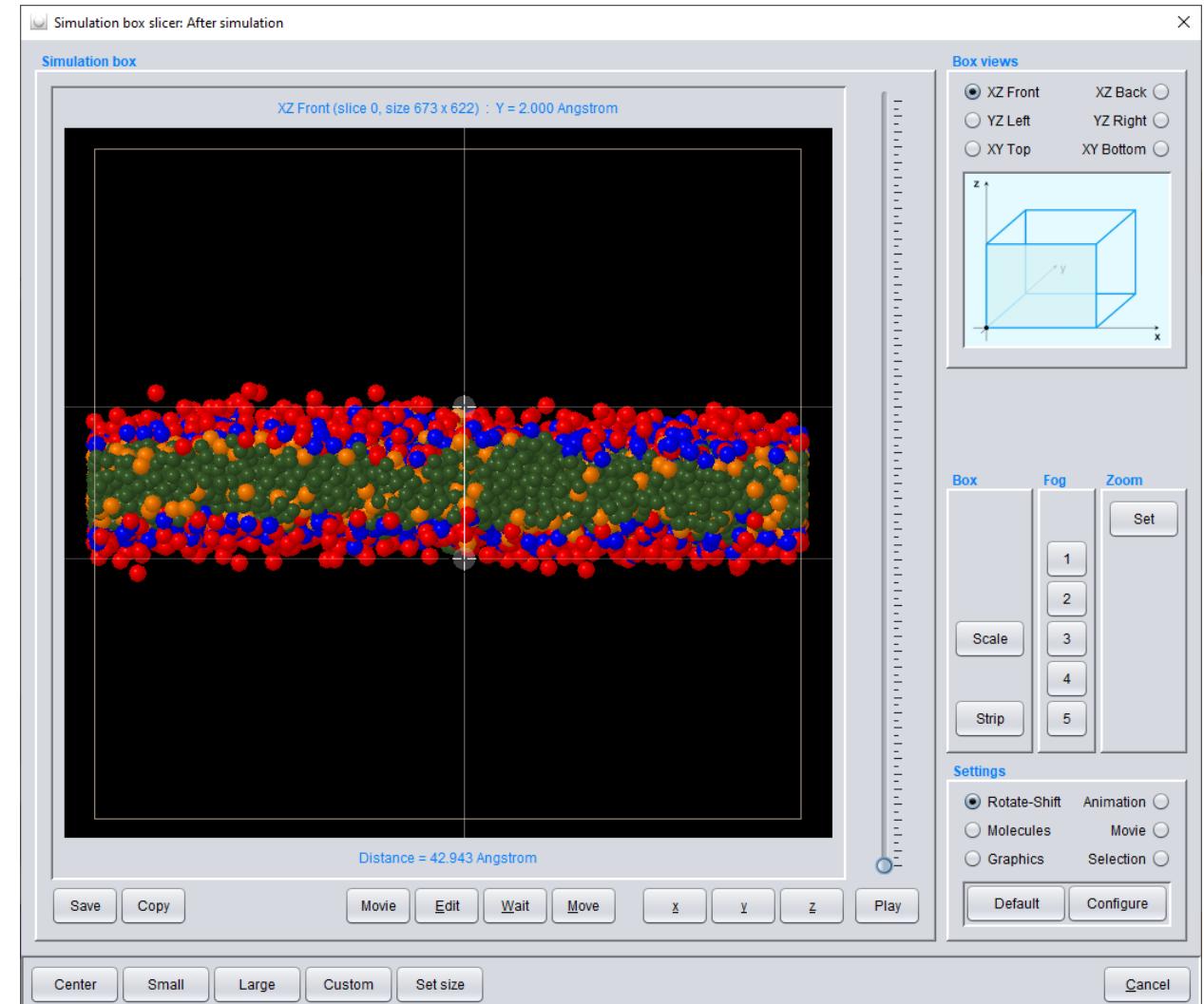


[www.molecular-dynamics.de](http://www.molecular-dynamics.de)

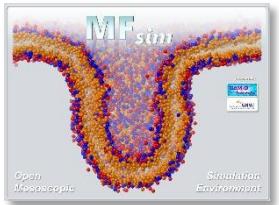


[www.gnwi.de](http://www.gnwi.de)

With **Ctrl-Shift mouse clicks** length measurements within the simulation box can be performed.



# DMPC bilayer membrane Job Result – Zoom



Open  
Mesoscopic

Simulation  
Environment

powered by

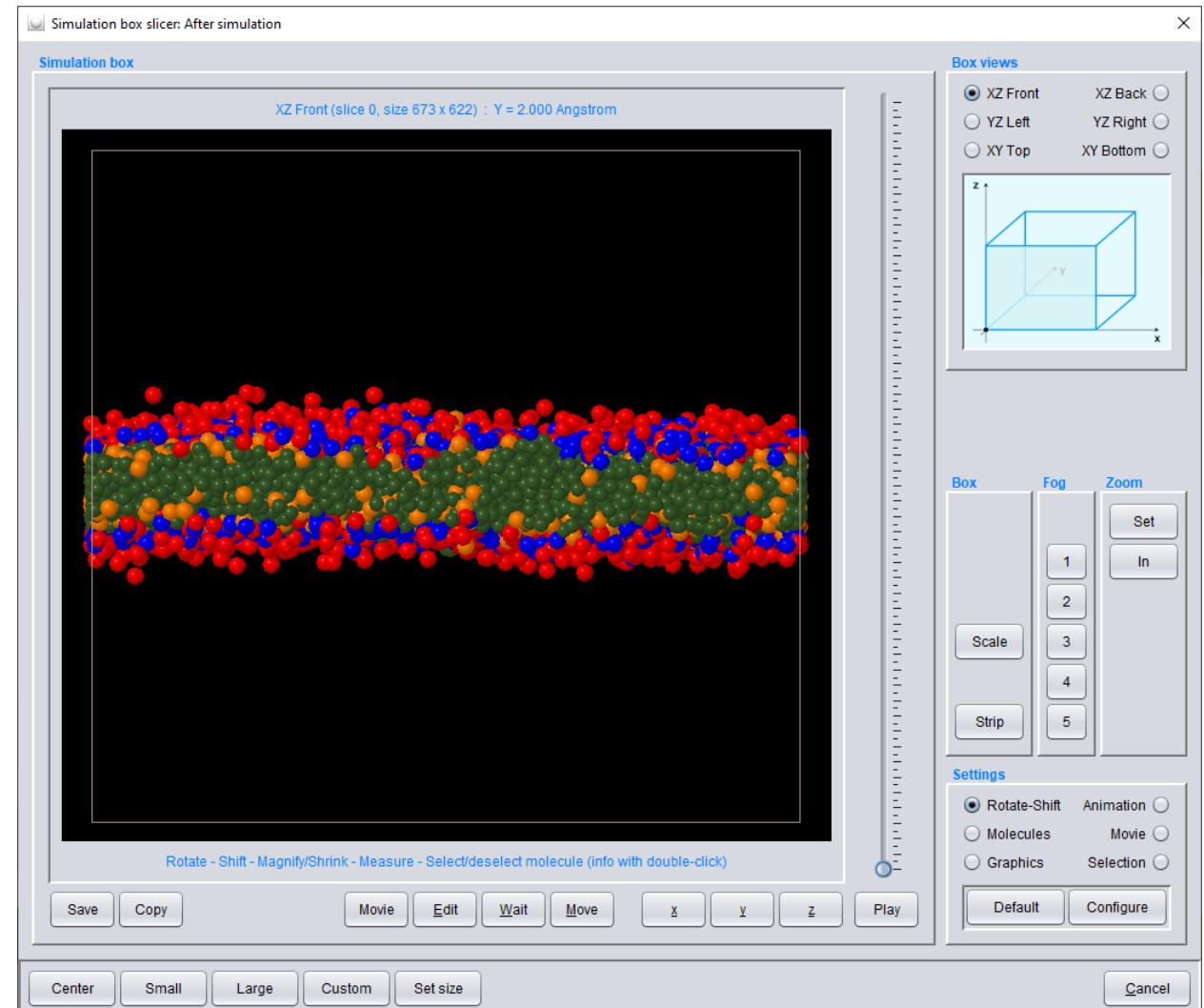


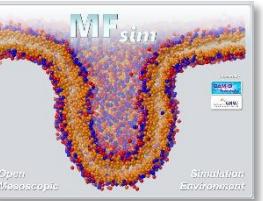
[www.molecular-dynamics.de](http://www.molecular-dynamics.de)



[www.gnwi.de](http://www.gnwi.de)

Hitting the **In** button on the **Zoom** panel ...





Open  
Mesoscopic

Simulation  
Environment

powered by



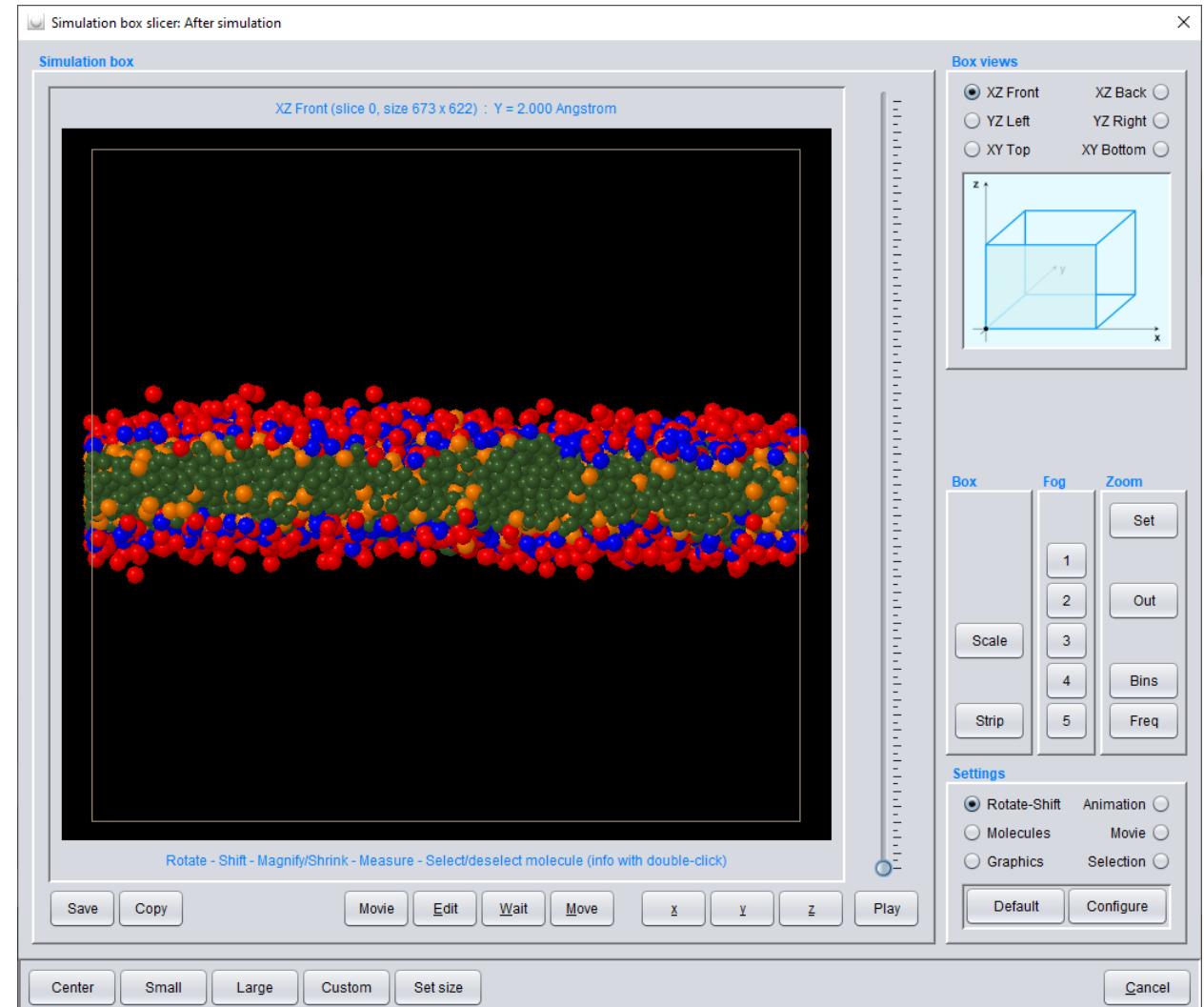
[www.molecular-dynamics.de](http://www.molecular-dynamics.de)



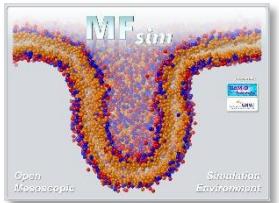
[www.gnwi.de](http://www.gnwi.de)

# DMPC bilayer membrane Job Result – Zoom

... defines the whole simulation box as a zoom volume which allows for the analysis of particle/molecules distributions. A click on the **Bins** button ...



# DMPC bilayer membrane Job Result – Zoom



Open  
Mesoscopic

Simulation  
Environment

powered by

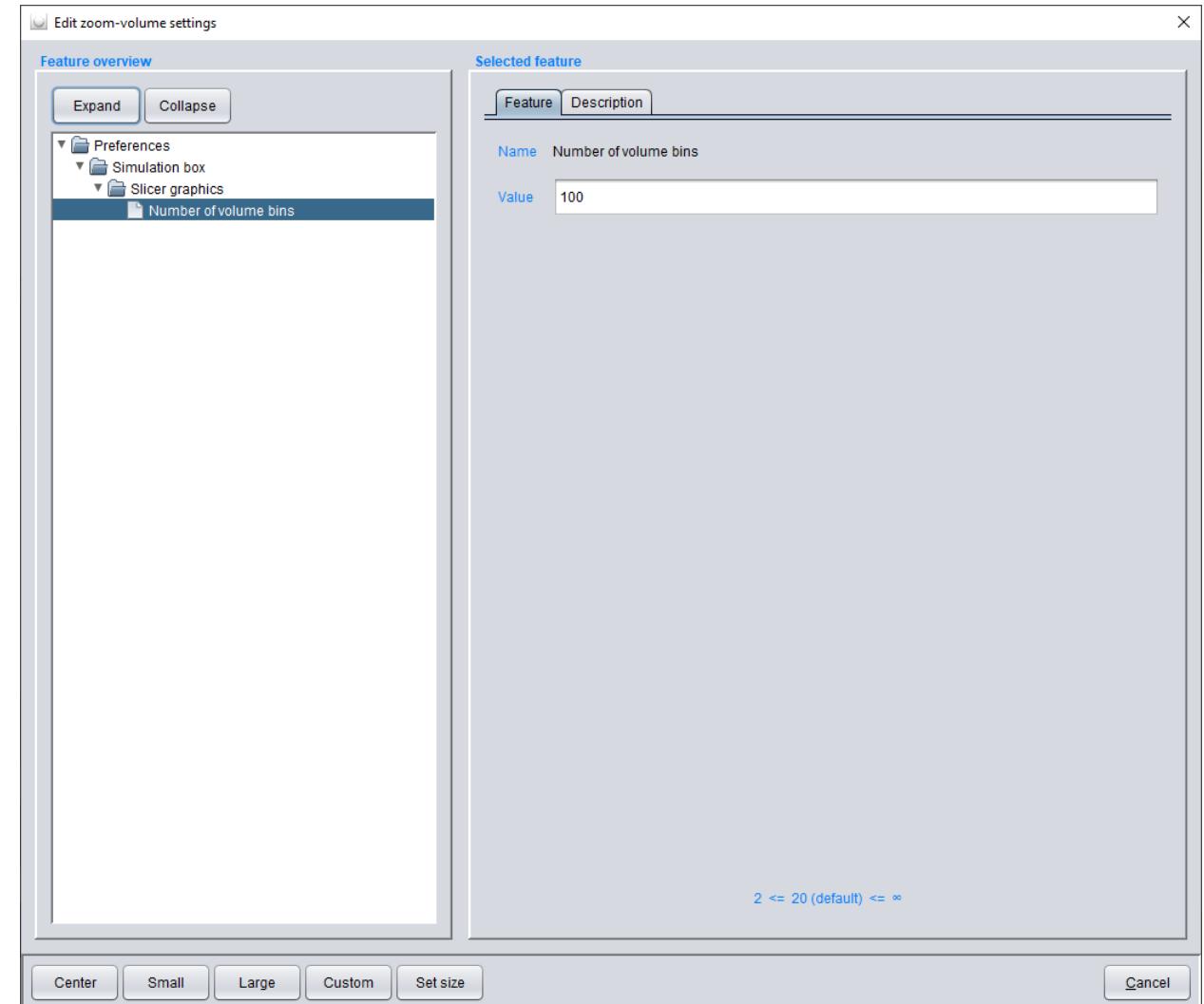


[www.molecular-dynamics.de](http://www.molecular-dynamics.de)

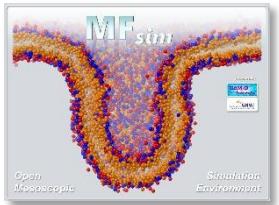


[www.gnwi.de](http://www.gnwi.de)

... allows for the definition of 100 volume bins along a simulation box axis. **Cancel** the dialog ...



# DMPC bilayer membrane Job Result – Zoom



Open  
Mesoscopic

Simulation  
Environment

powered by

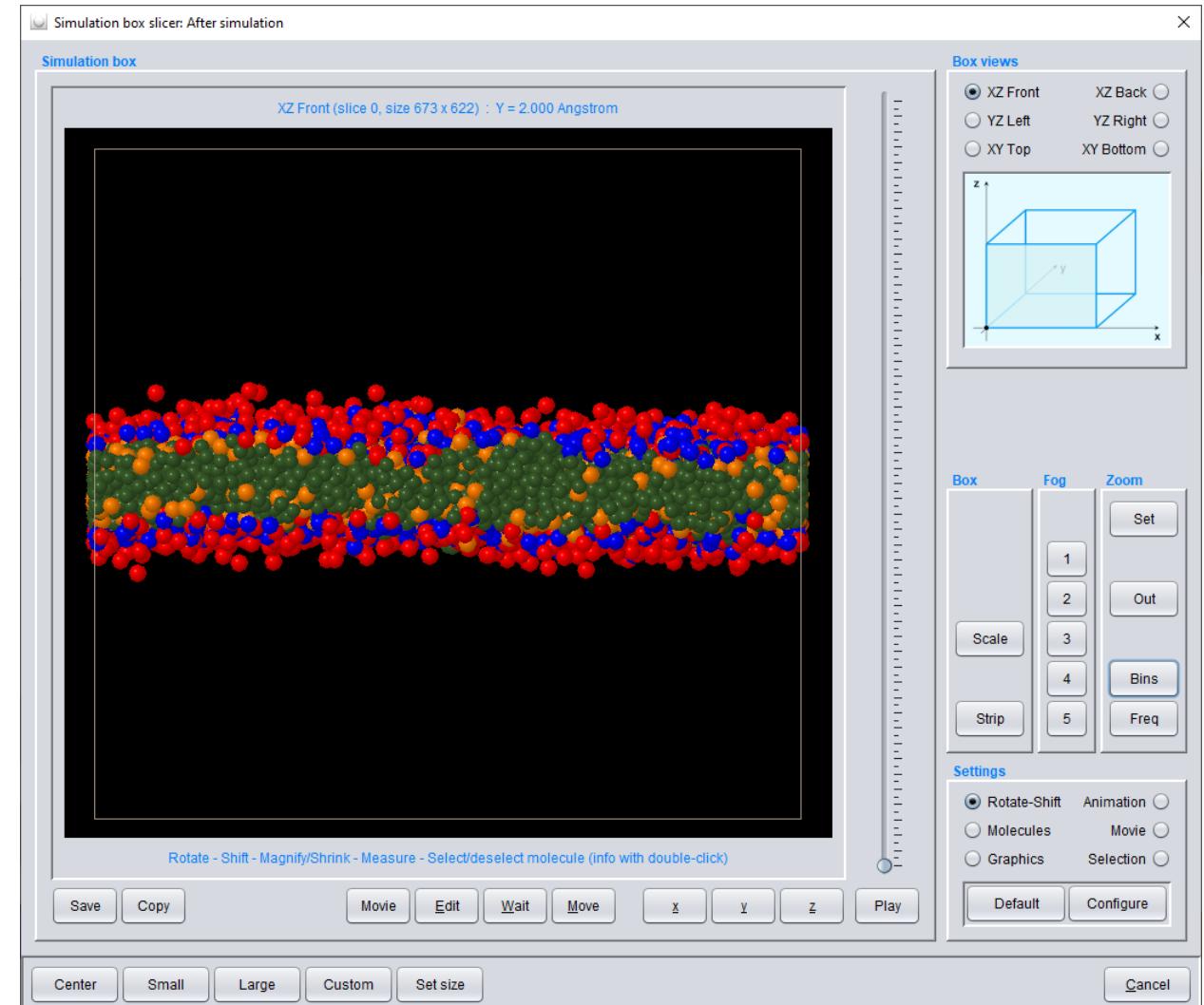


[www.molecular-dynamics.de](http://www.molecular-dynamics.de)

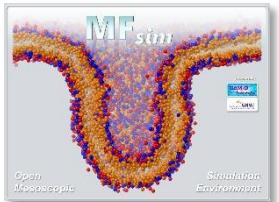


[www.gnwi.de](http://www.gnwi.de)

... and hit the **Freq(ueency)** button ...



# DMPC bilayer membrane Job Result – Frequencies



Open  
Mesoscopic

Simulation  
Environment

powered by

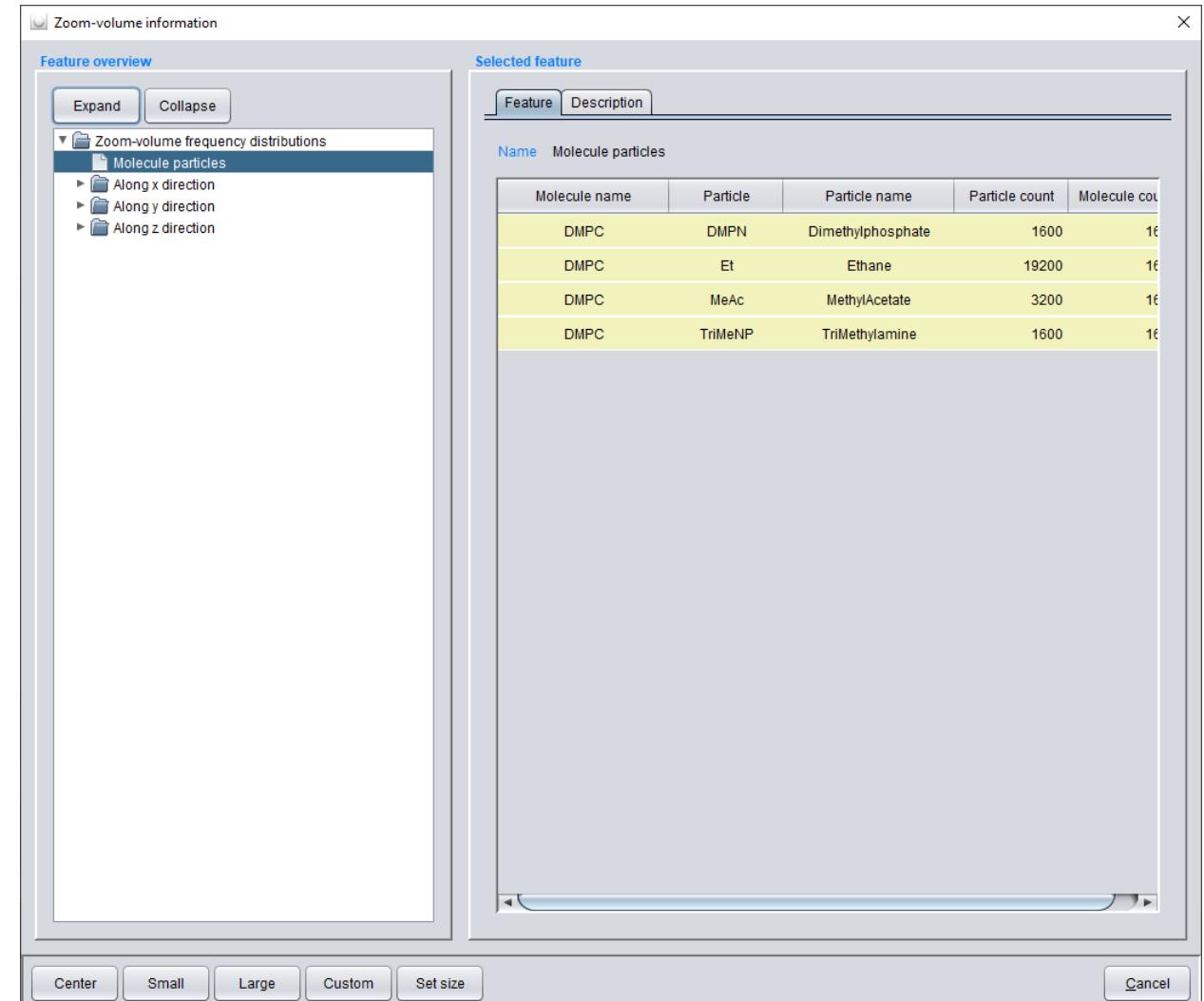


[www.molecular-dynamics.de](http://www.molecular-dynamics.de)

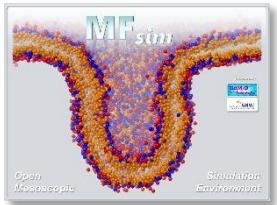


[www.gnwi.de](http://www.gnwi.de)

... to open the **Zoom-volume frequency distributions** dialog.



# DMPC bilayer membrane Job Result – Frequencies



Open  
Mesoscopic

Simulation  
Environment

powered by

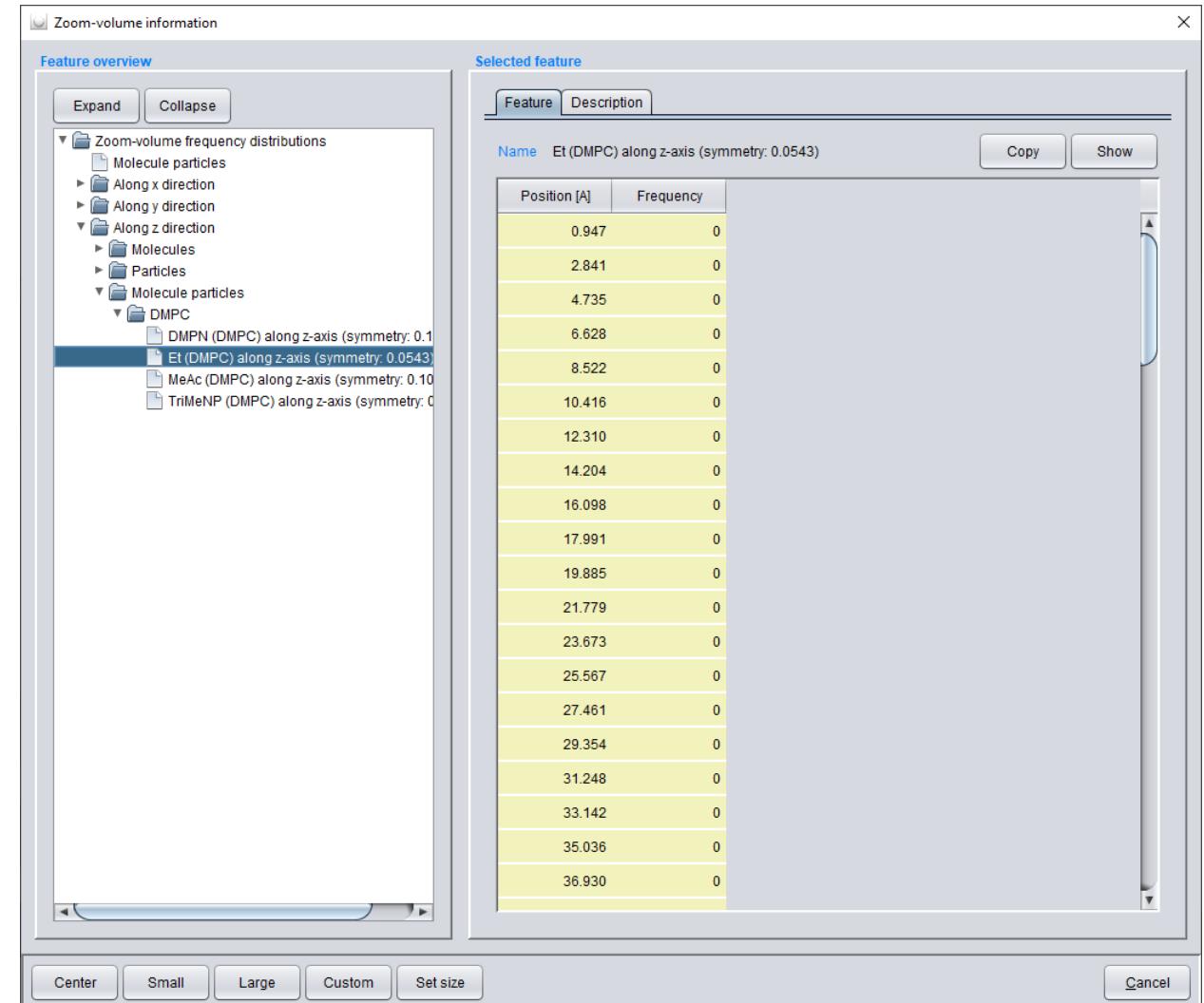


[www.molecular-dynamics.de](http://www.molecular-dynamics.de)

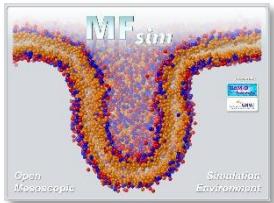


[www.gnwi.de](http://www.gnwi.de)

Select **Zoom-volume frequency distributions / Along z direction / Molecule particles / DMPC / Et ...** and hit the **Show** button ...



# DMPC bilayer membrane Job Result – Frequencies



Open  
Mesoscopic

Simulation  
Environment

powered by

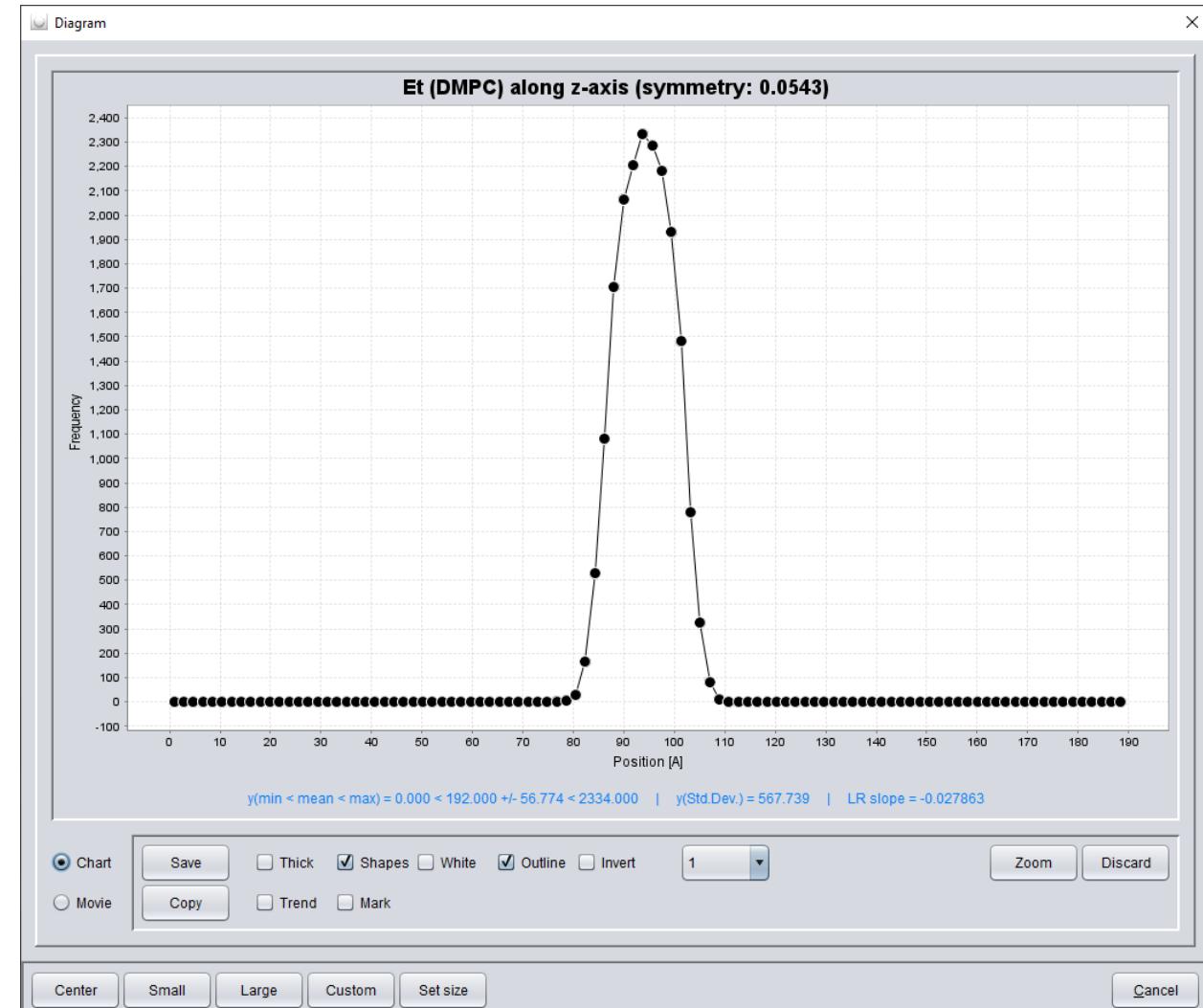


[www.molecular-dynamics.de](http://www.molecular-dynamics.de)

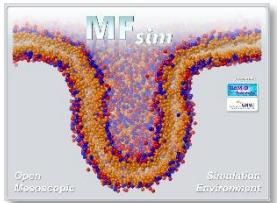


[www.gnwi.de](http://www.gnwi.de)

... to view the (binned) distribution of the Et particles of the DMPC molecules along the z-axis of the simulation box – the hydrophobic core of the bilayer membrane.  
**Cancel** the frequency dialogs ...



# DMPC bilayer membrane Job Result – Frequencies



Open  
Mesoscopic

Simulation  
Environment

powered by

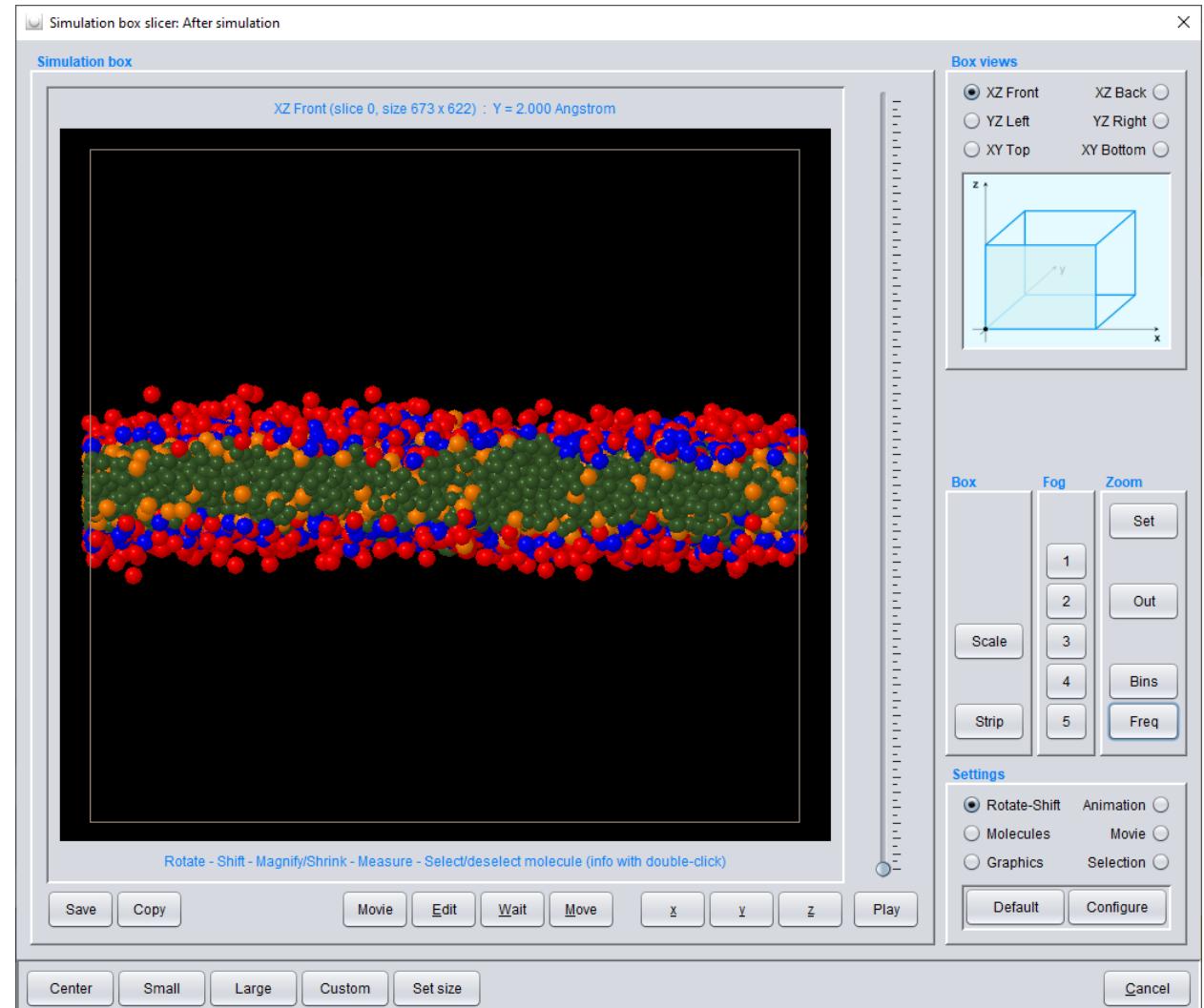


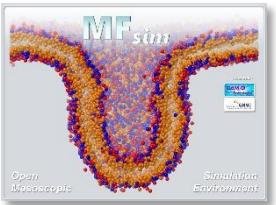
[www.molecular-dynamics.de](http://www.molecular-dynamics.de)



[www.gnwi.de](http://www.gnwi.de)

... to return to the simulation box view and  
**Configure** the **Molecules Settings** to  
include water ...





Open  
Mesoscopic

Simulation  
Environment

powered by



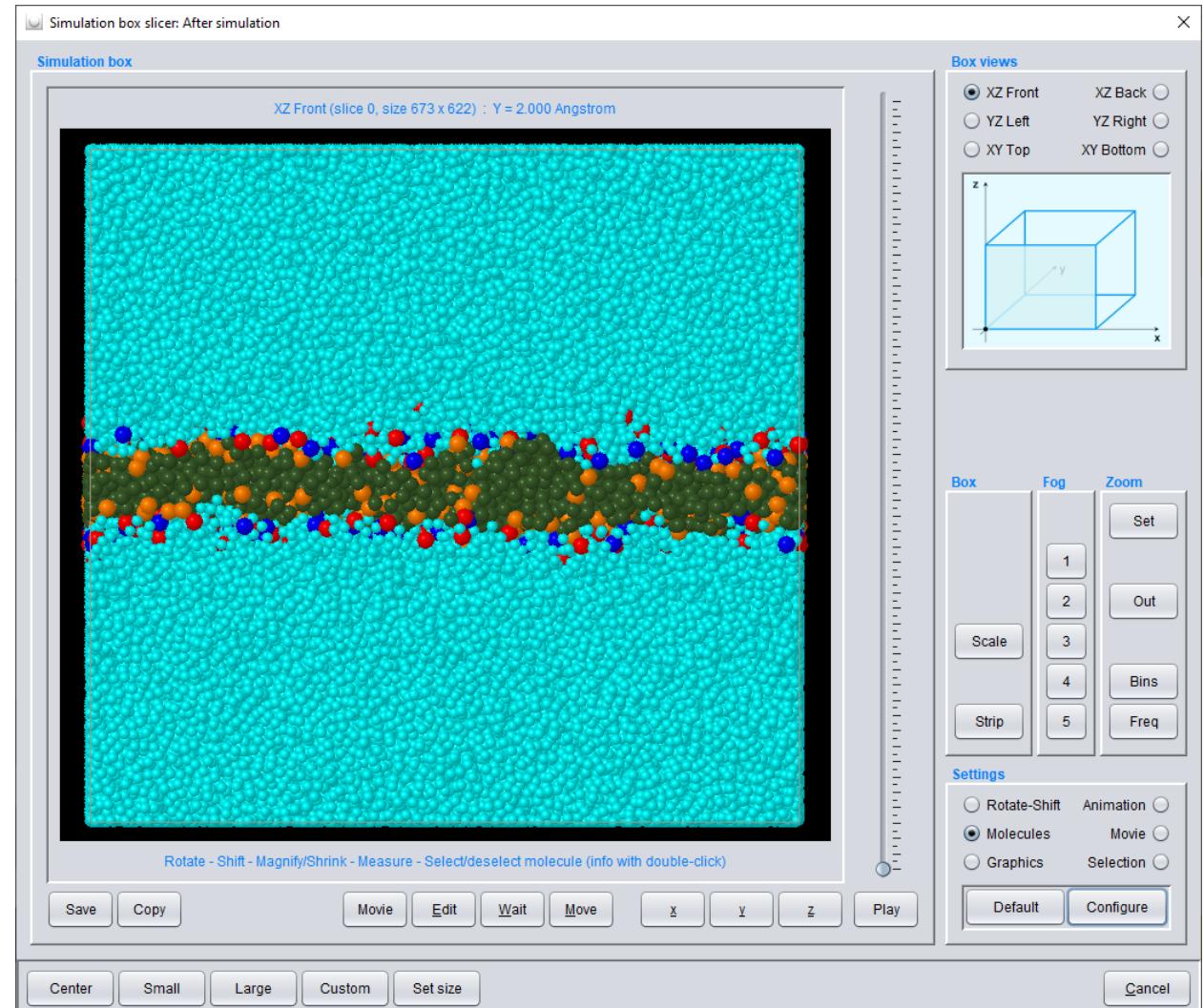
[www.molecular-dynamics.de](http://www.molecular-dynamics.de)



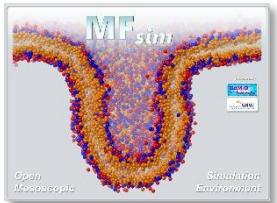
[www.gnwi.de](http://www.gnwi.de)

# DMPC bilayer membrane Job Result – Frequencies

... so that a frequency analysis of the water molecules becomes available by hitting again the *Freq(uency)* button ...



# DMPC bilayer membrane Job Result – Frequencies



Open  
Mesoscopic

Simulation  
Environment

powered by

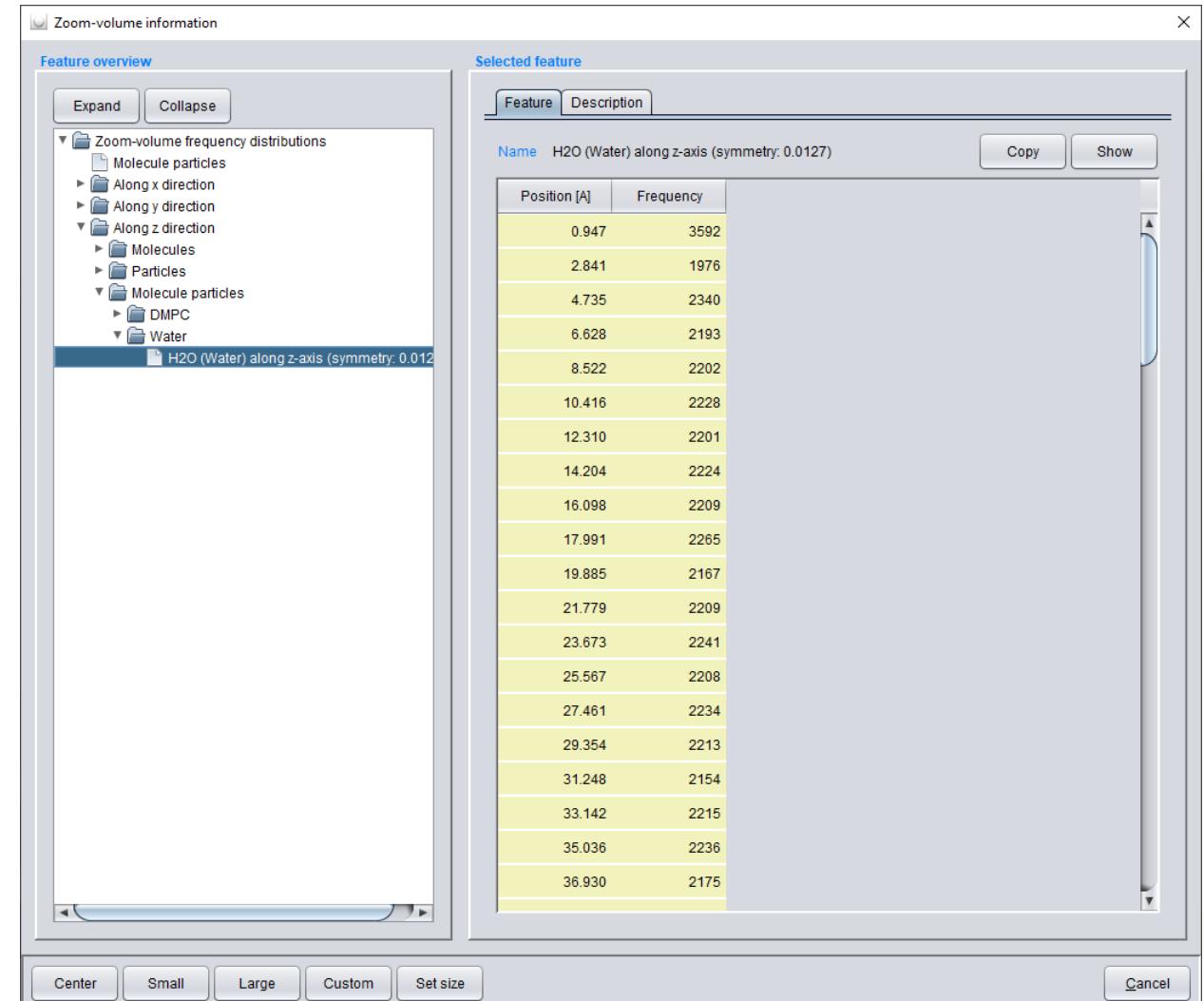


[www.molecular-dynamics.de](http://www.molecular-dynamics.de)

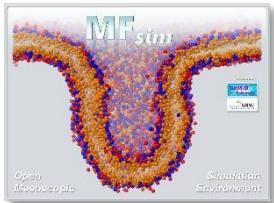


[www.gnwi.de](http://www.gnwi.de)

... selection of **Zoom-volume frequency distributions** / **Along z direction** / **Molecule particles** / **Water** / **H<sub>2</sub>O** ... and hitting the **Show** button ...



# DMPC bilayer membrane Job Result – Frequencies



Open  
Mesoscopic

Simulation  
Environment

powered by



[www.molecular-dynamics.de](http://www.molecular-dynamics.de)



[www.gnwi.de](http://www.gnwi.de)

... to view the (binned) distribution of the H<sub>2</sub>O particles (water molecules) along the z-axis of the simulation box with a minimum in the hydrophobic core of the bilayer membrane and characteristic fluctuations at the reflective walls.

