# **Download and Install (MS Windows)**







powered by



www.molecular-dynamics.de



www.gnwi.de

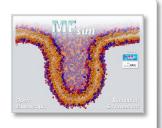
Download Windows OS installer executable *Install MFsim 2-2-4-0.exe* from folder *Installer for Windows OS* at MFsim GitHub repository *https://github.com/zielesny/MFsim.* 

Start the installer executable by a double-click and follow the instructions.

MFsim is installed by default in the Windows *Program Files* directory at *C:\Program Files\GNWIWFsim 2.2.4.0*: Open that folder with several MFsim start batch files named *Start\_MFsim\_64bit\_<memory>GB.bat* where <memory>defines the memory consumption of the Java virtual machine (JVM). Create a shortcut to an appropriate MFsim *start batch file* on your desktop that best fits your hardware resources and needs (e.g. for a computer with 16 gigabyte of available RAM the batch file *Start\_MFsim\_64bit\_8GB.bat* could be appropriate and would use up to 8 gigabyte of RAM).

MF<sub>sim</sub> 2.2.4.0

# **Program Start**



Start MFsim ...

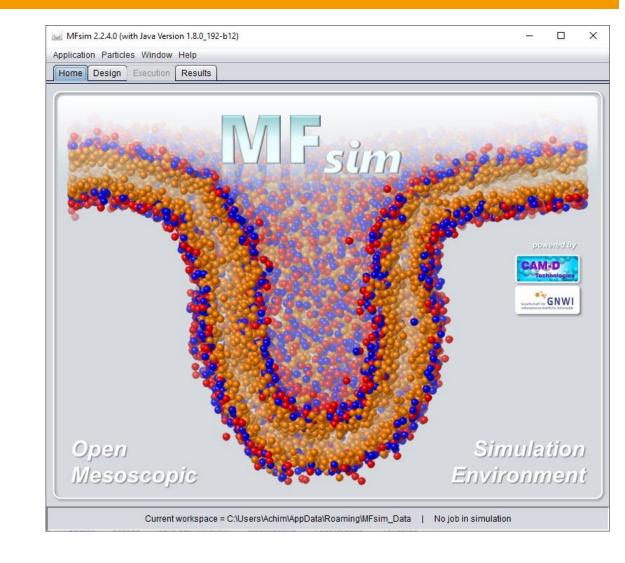
Open Mesoscopic

Simulation Environment

powered by







#### **Particle Set Choice**



Choose particle set ...

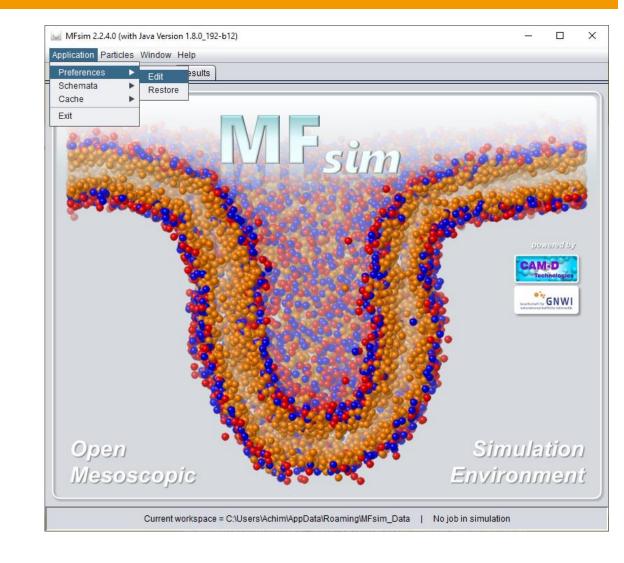
Open Mesoscopic

Simulation Environment

powered by

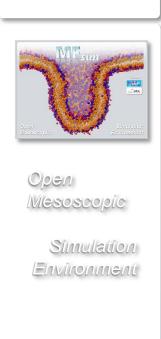






기기도<sup>21m</sup>

#### **Particle Set Choice**



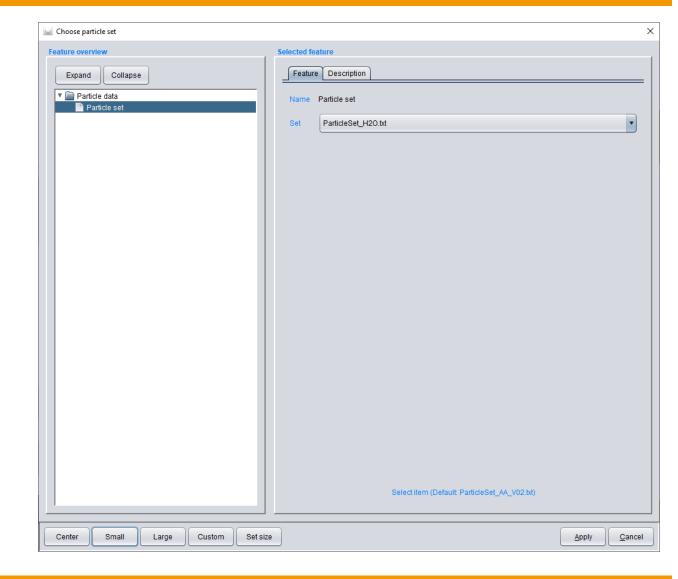
powered by

CAM-D

www.molecular-dynamics.de

**Technologies** 

... ParticleSet\_H2O.txt and Apply (note, that this minimum particle set with just one water particle is to be used for test purposes only).



## **Design of new Job Input**



Mesoscopic

Simulation Environment

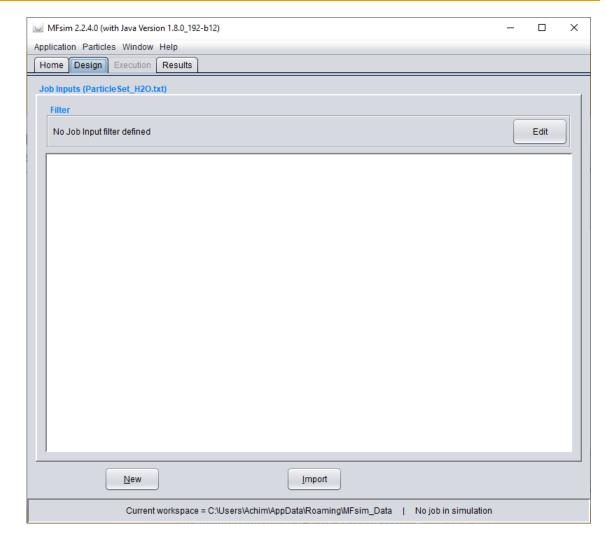
powered by





www.gnwi.de

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



# Design of new Job Input



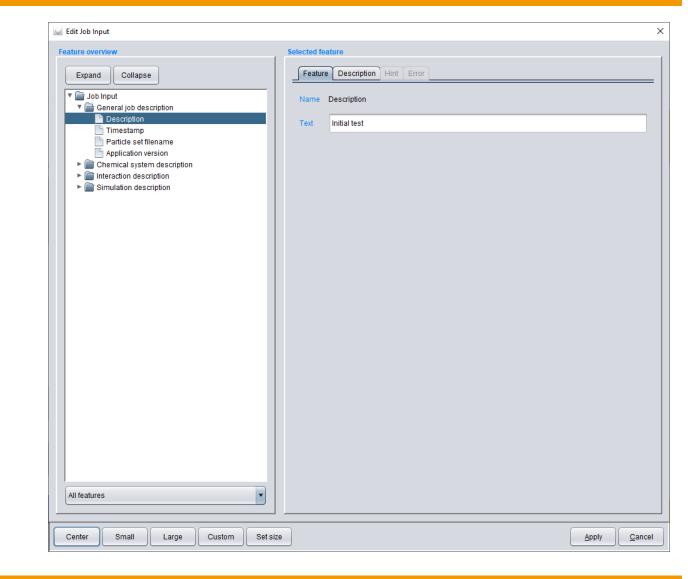
Open Mesoscopic

Simulation Environment

powered by









# Design of new Job Input



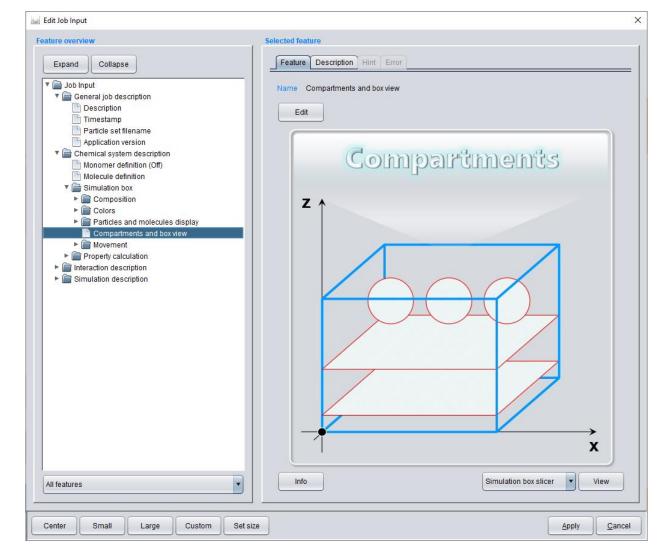
Open Mesoscopic

Simulation Environment

powered by









기가 3.2.4.0 2.2.4.0

# **Design of new Job Input**



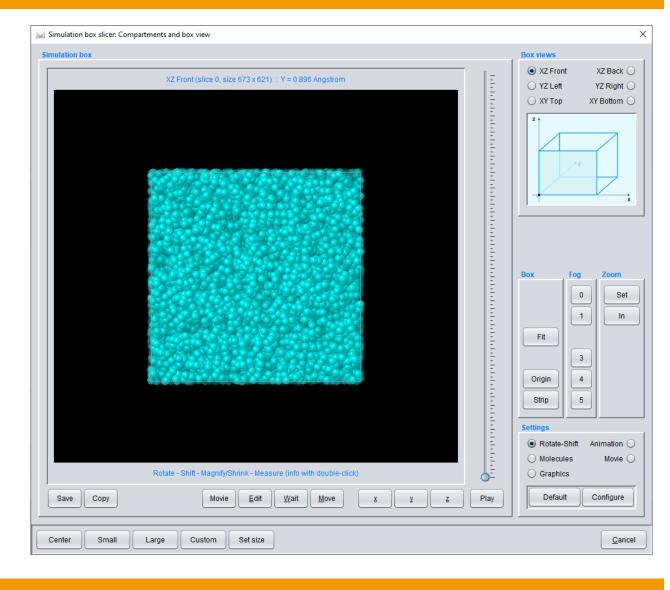
Open Mesoscopic

Simulation Environment

powered by

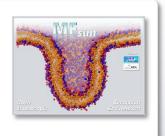


... to display the simulation box filled (randomly) with (24.000) water particles (the default Job Input that is automatically generated). *Cancel* the dialog ...



기기구. 기기구. 기기구. 기기구.

# **Design of new Job Input**



... and *Apply* the Job Input settings.

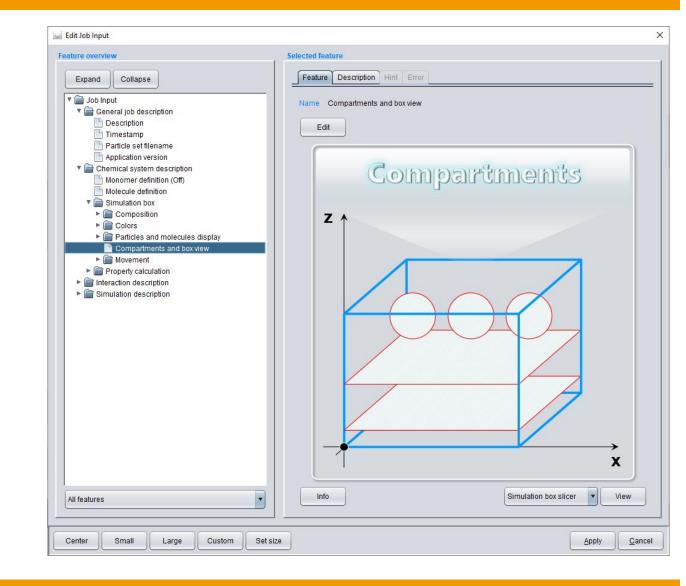
Open Mesoscopic

Simulation Environment

powered by







## **Design of new Job Input**



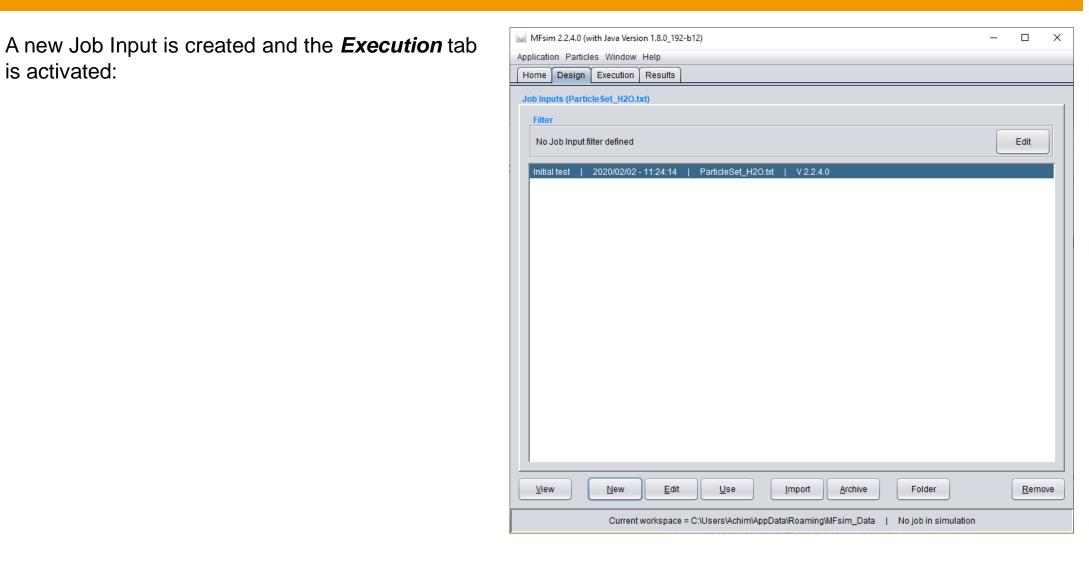
is activated:

Simulation Environment

powered by







#### **Job Execution**



Open Mesoscopic

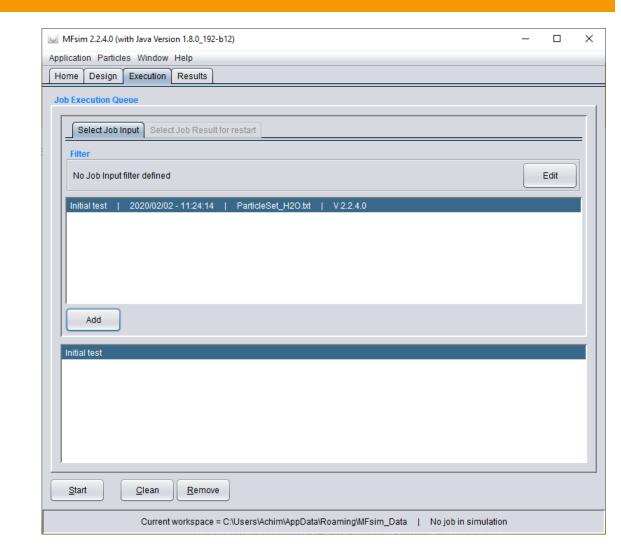
Simulation Environment

powered by





www.gnwi.de



Click the **Execution** tab and **Add** the new Job Input to the job execution queue:

기기도<sup>21m</sup>

#### **Job Execution**



Open Mesoscopic

Simulation Environment

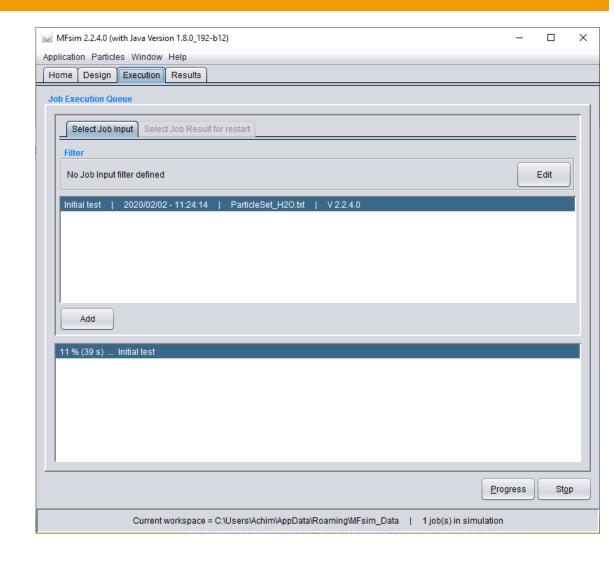
powered by



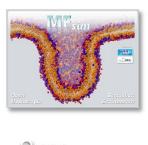


www.gnwi.de

**Start** job execution (simulation) and wait until the simulation is finished.



# Job Result Inspection



Open Mesoscopic

Simulation Environment

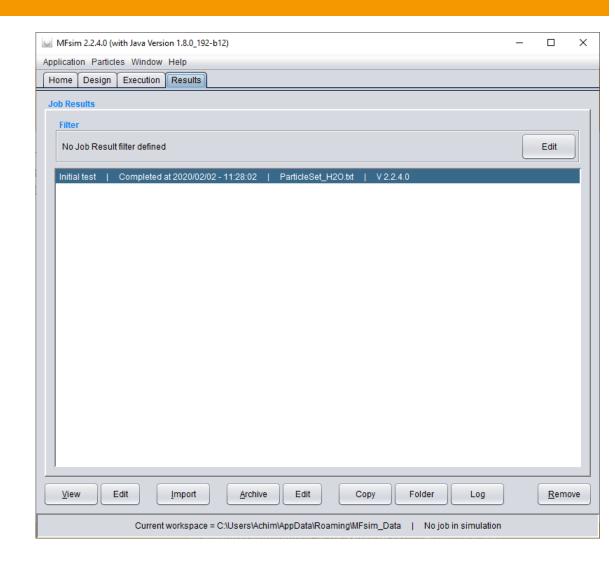
powered by



Gesellschaft für GNWI naturwissenschaftliche Informatik

www.gnwi.de

Select the **Results** tab that now contains the (successfully *Completed*) Job Result. Hit the **View** button ...



## **Job Result Inspection**



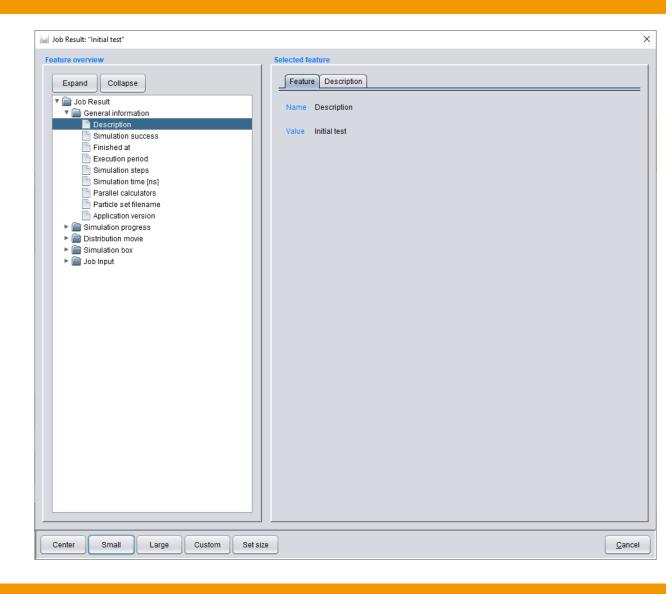
Open Mesoscopic

Simulation Environment

powered by



... to inspect the Job Result features ...



기기도<sup>21m</sup>

# Job Result Inspection



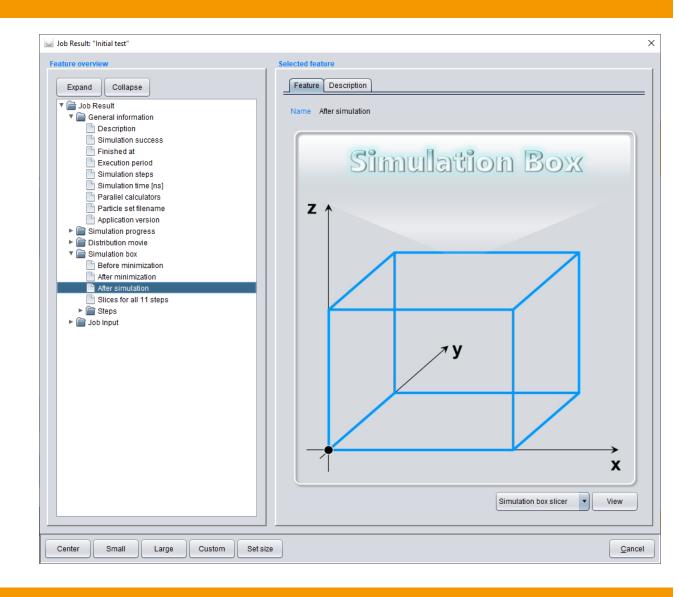
Open Mesoscopic

Simulation Environment

powered by



... e.g. *View* the simulation box *After simulation* ...



# Job Result Inspection



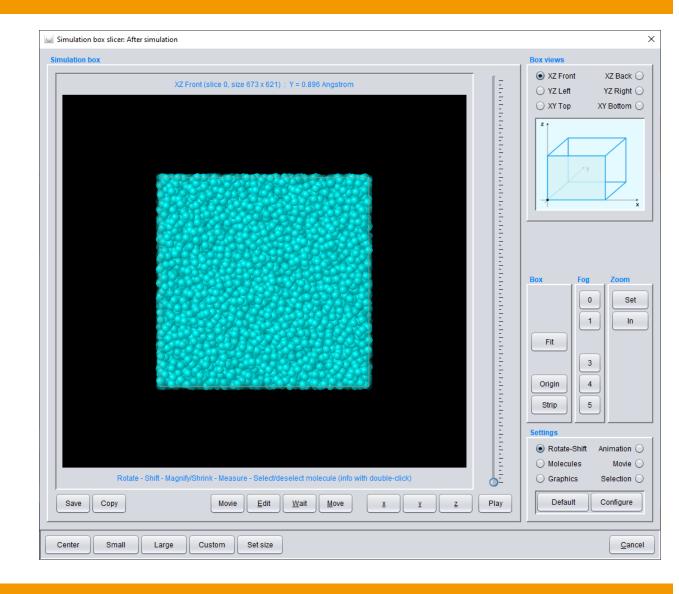
Open Mesoscopic

Simulation Environment

powered by



... where the initial graphical display may be changed ...



MF<sub>sim</sub> 2.2.4.0

## **Job Result Inspection**



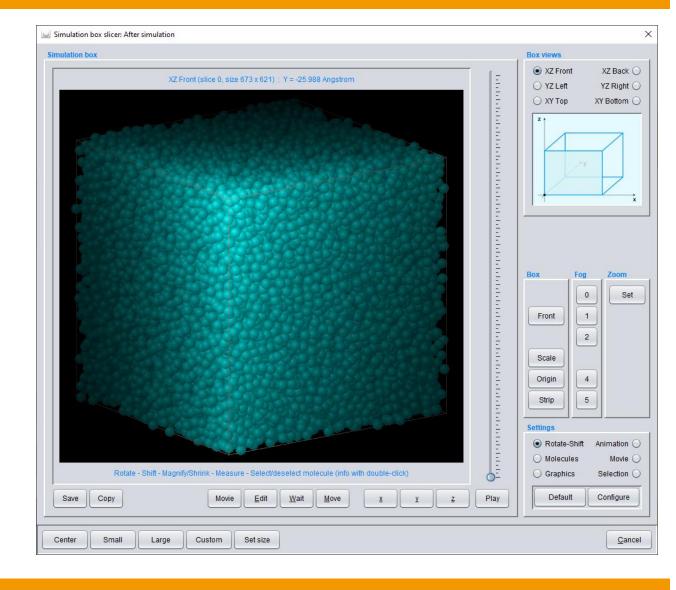
Open Mesoscopic

Simulation Environment

powered by



... to a more appealing one (not explained in this tutorial – but you may just play & explore ...). Return to the *Results* tab by cancelling all modal dialogs with the *Cancel* button.



#### **Preferences**







powered by



MFsim is initialized with numerous preference settings that may be changed with **Application**/*Preferences*/*Edit*.

The default preference settings may not adequately exploit a specific computer hardware thus the performance of MFsim may be considerably enhanced by an appropriate choice of e.g. parallelization or graphics settings (see corresponding tutorials).

**Exit** the application via menu item **Application/Exit** or simply close the window.

