Version 2

# C2115 Practical introduction to supercomputing

Lesson 9

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# Batch systems (getting started)

# Batch processing

**Batch processing** is the execution of a series of programs (so-called batches) on a computer without the participation of the user. Batches are prepared in advance so that they can be processed without the participation of the user. All input data is prepared in advance in files (scripts) or entered using parameters on the command line. Batch processing is the opposite of interactive processing, where the user provides the required inputs only when the program is running.

**Advantages of batch processing**

- sharing computer resources between many users and programs
- postponing batch processing until the computer is less busy
- Eliminate delays caused by waiting for user input
- maximizing computer utilization improves investment utilization (especially for more expensive computers)

source: www.wikipedia.cz, modified

# Tools for batch processing

- **~~OpenPBS~~**
  ~~http://www.mcs.anl.gov/research/projects/openpbs/~~
- **Oracle Grid Engine**
  https://en.wikipedia.org/wiki/Oracle_Grid_Engine
- **~~Open Grid Scheduler~~**
  ~~http://gridscheduler.sourceforge.net/~~
  **open source**
- **Torque**
  https://en.wikipedia.org/wiki/TORQUE
  **open source**
- **PBSPro**
  https://www.openpbs.org/, https://www.altair.com/

PBSPro is used as a batch system on our local clusters (WOLF, …), in MetaCentrum VO, and IT4I

# PBSPro

**Documentation:**

https://www.altair.com/pbs-works-documentation/

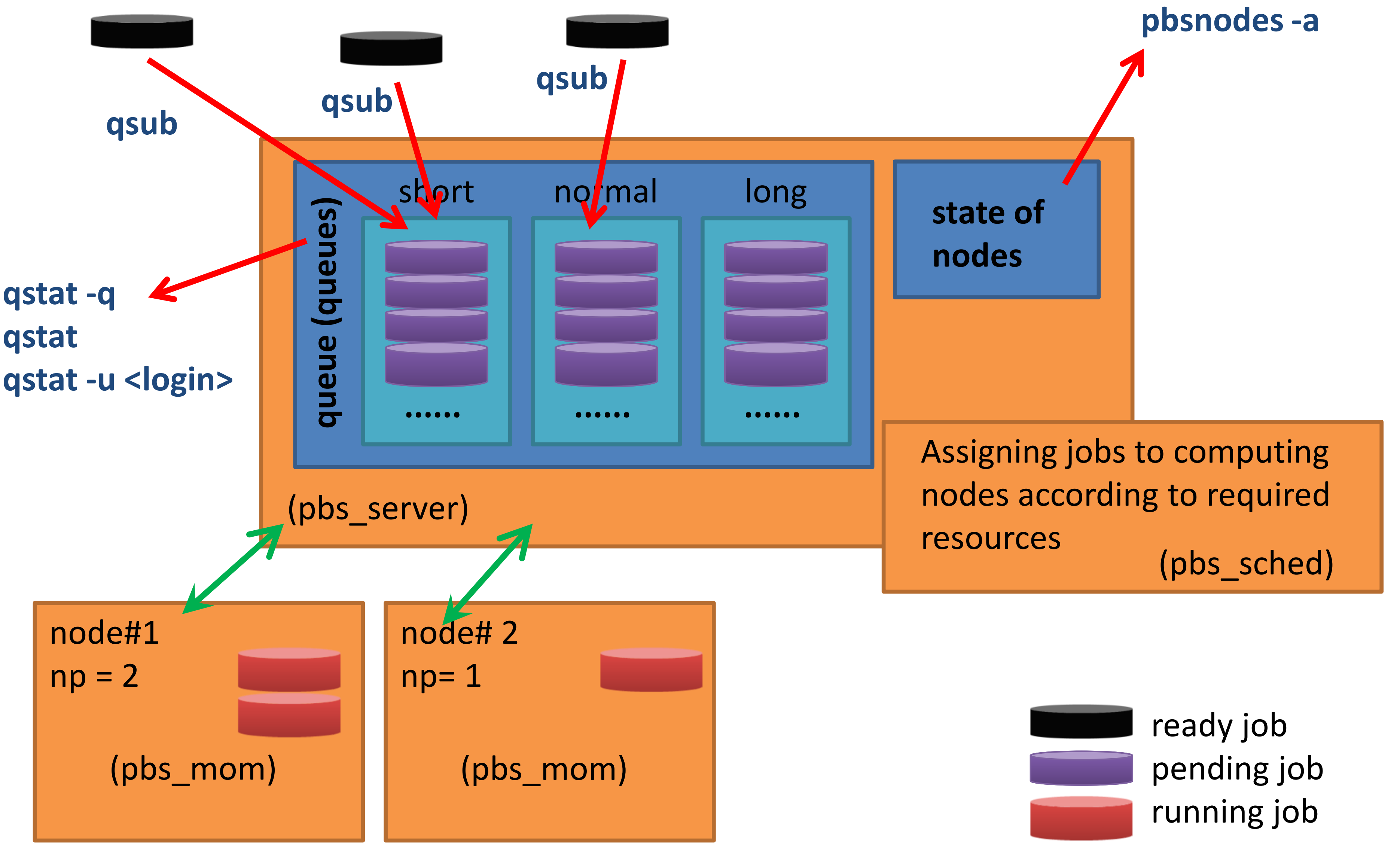
# Necessary condition

## Second authentication without password

It is necessary to set up login between compute nodes and the server (and vice versa) using ssh without explicit entry of password.

- **our local clusters (WOLF, ...), MetaCentrum** – you must have a valid Kerberos ticket during job submission by the qsub command into the batch system
- **IT4I** - using ssh authorized keys

# Architecture



# Torque - commands, job states

| | |
|---|---|
| **qsub** | submits job to the batch system |
| **qstat** | prints information about the batch system (job list, queue list) |
| **pbsnodes** | prints information about computing nodes |
| **qrls** | releases job from the state **holded** (if circumstances allow) |

**Job states:**

| | |
|---|---|
| **Q** (queued) | job is waiting in queue to run on computing node |
| **R** (running) | job is running on computing nodes |
| **C** (completed) | job has been completed (information about completed tasks is displayed only for a limited time - most often 24 hours) |
| **H** (holded) | job has been paused, job can be released with command **qrls** |
| **E** (exiting) | job is ending |
| **F** (finished) | job is completed: successful or unsuccessful termination |

# We assign tasks

Command **qsub** is used to submit jobs into the batch system.

```
$ qsub -q default job.sh
1.ubuntu
```

task script, e.g.

```
#!/bin/bash
echo "Hello world from `hostname`!"
```

queue name to which we want to submit the task

command prints job ID if submission is successful

```
$ ls
job.sh job.sh.o1 job.sh.e1
```

files are not available until the job is completed

standard job output

standard job error output

# Exercise 1

1. What queues of batch system are available on the WOLF cluster. Use the command qstat and selection according to the documentation.
2. What is the difference between -Q and -q options of qstat command?
3. What jobs are already submitted to the WOLF cluster batch system?
4. Place the job script from the previous example in a separate directory and submit it into the batch system. Use queue default.
5. On which computing node did the task run?
6. Create a new job script that you place in a different directory. The script prints the name of the computing node and pauses its operation for 10 minutes. Submit the job into queue default.
7. Monitor the state of the batch system with commands qstat and pbsnodes.
8. On which compute node did the task run this time?

# Exercise 2

1. Log in to MetaCentrum front node perian.ncbr.muni.cz.
2. What batch system queues are available. Use the command qstat.
3. How many jobs are currently included in the batch system?
4. Place job script from the previous example into a separate directory and submit it to the batch system. Use queue default.
5. On which computing node did the task run? How long did it take for the task to start?

# Exercise 3

1. Log in to MetaCentrum front node zuphux.cerit-sc.cz.
2. What batch system queues are available. Use qstat command. Why is it different from the queues you saw on the perian.ncbr.muni.cz?
3. How many jobs are currently included in the batch system?
4. Place the job script from the previous sample into a separate directory and submit it to the batch system. Use queue default. How does the job identifier differ from the job identifier submitted from the front node onyx.ncbr.muni.cz?
5. On which compute node did the task run? How long did it take for the task to start?

# Resource allocation

https://wiki.metacentrum.cz/wiki/PBS_Professional

resources are specified using the option **-l** of command qsub, you can enter multiple specifications at the same time, e.g.:

```
$ qsub -l select=1:ncpus=1:mem=400mb:scratch_local=10gb \
       script.sh
```

or

```
$ qsub -l select=1:ncpus=1:mem=400mb:scratch_local=10gb \
       -l walltime=10:00 script.sh
```

# Number and type of nodes and CPUs

```
select=[N1]chunk_specification1[+[N2]chunk_specification1]
```

Number of blocks (chunks)

Example:

```
select=1:ncpus=1:mem=400mb:scratch_local=10gb
```

block specification

**It is only used to reserve computing resources. However, this does not mean that job will run automatically on allocated computing resources. This must be ensured by job script.**

# Number and type of nodes and CPUs, II

List of allocated CPUs is available as a list of compute nodes listed in the file whose name is specified in the system variable **PBS_NODEFILE**. This variable is available in running job:

```
#!/bin/bash
echo $PBS_NODEFILE
cat $PBS_NODEFILE
```

**Example:**

```
$ qsub -l select=1:ncpus=2+1:ncpus=1 script.sh
```

Result:

```
/var/spool/torque/aux//10312644.arien-pro.ics.muni.cz
zubat2.ncbr.muni.cz
zubat2.ncbr.muni.cz
mandos2.ics.muni.cz
```

List of CPU slots is then available in the full job description, item **exec_host**:

```
$ qstat -f <job_number>
```

# Number and type of nodes and CPUs, III

**Properties:**

Computing nodes can have specified properties. These are short strings whose meaning depends on the system administrators. The properties of nodes are listed by the command **pbsnodes** item **resources_available**.

In the specification of computing resources, user can only request such computing nodes that have the specified properties.

**Examples:**

```
select=1:ncpus=1:brno=True
select=1:ncpus=1:os=debian80
select=1:ncpus=1:cl_tarkil=True
select=1:ncpus=1:cluster=tarkil
select=1:ncpus=1:vnode=zubat1
select=1:ncpus=1:vnode=^zubat1
```

exclusion

# Additional resource specification

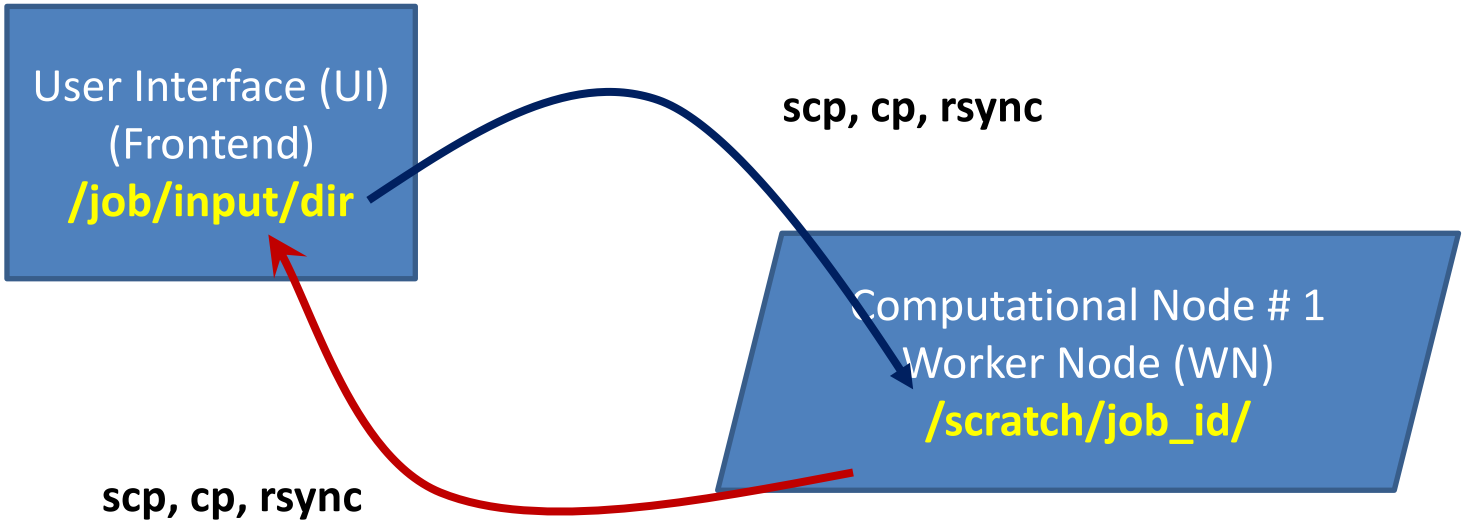
| Resource | | Description |
|---|---|---|
| **mem** | | memory size, units mb, gb |
| **scratch_local** | | size of local data storage, unit mb, gb |
| **scratch_ssd** | | size of local data storage on SSD, units mb, gb |
| **walltime** | | maximum job run time in conjunction with the queue **default** |

**Job with insufficiently specified resource requirements may be terminated prematurely in MetaCentrum.**

# Copying files

# Copying files

Torque/PBSPro has internal support for copying files using stagein and stageout directives. However, this method is practically unusable, and the user should provide all operations related to copying data to the local data storage within the job (commands cp, scp, rsync). This method is described in the documentation of MetaCentrum VO.



User Interface (UI)
(Frontend)
**/job/input/dir**

**scp, cp, rsync**

Computational Node # 1
Worker Node (WN)
**/scratch/job_id/**

**scp, cp, rsync**

On MetaCentrum VO and NCBR clusters, the local working directory is setup by the batch system. The path to the local storage is available in the **SCRATCHDIR** environment variable.

# MetaCentrum

# Batch systems

MetaCentrum VO consists of three separate batch systems:

- **meta-pbs.metacentrum.cz** handles computing nodes from MetaCentrum, default on all front nodes except **zuphux.cerit-sc.cz**
- **cerit-pbs.cerit-sc.cz** handles computing nodes from CERIT-SC, default on the front node **zuphux.cert-sc.cz**
- **elixir-pbs.elixir-czech.cz** handles the computing nodes of the ELIXIR project to which tasks can be moved from arien or wagap if the nodes are not busy

Both systems are user compatible (same options), differences can be found in the documentation of MetaCentrum VO.

Default Torque server can be changed by setting the PBS_SERVER variable, e.g.

list tasks from CERIT-SC

```
[kulhanek@zuphux ~]$ qstat
[kulhanek@zuphux ~]$ export PBS_SERVER=meta-pbs.metacentrum.cz
[kulhanek@zuphux ~]$ qstat
```

list tasks from MetaCentrum

# Running the gaussian program in MetaCentrum

**http://gaussian.com/**

**https://wiki.metacentrum.cz/wiki/Gaussian-GaussView**

# Exercise 4

Goal of this exercise is to create a model of $C_{60}$ molecule and calculate its molecular vibrations with semiempirical quantum-chemical method PM6 in gaussian program version 16.

Into the protocol, report the results of the following exercise in summary, provide only important information.

1. Load the structures of the C60 molecule into Nemesis (File → Import structure from → XYZ).
2. Create an input file for the program gaussian (File → Export Structure as ... → Gaussian Input). Choose the PM6 method and geometry optimization. Then add the keyword FREQ (after the keyword Opt) and save the file with an .com extension.
3. Move the created input file to MetaCentrum front node, prepare the job script and include the job in the batch system. Follow the documentation of MetaCentrum, **the job must use local data storage on the computing node.**
4. Transfer the result of the task (file extension .log) to your workstation and display the calculated molecular vibrations in the Nemesis program, following the instructions below.

**https://wiki.metacentrum.cz/wiki/Gaussian-GaussView**

# Nemesis

**Starting the program:**

```
$ module add nemesis
$ nemesis
```

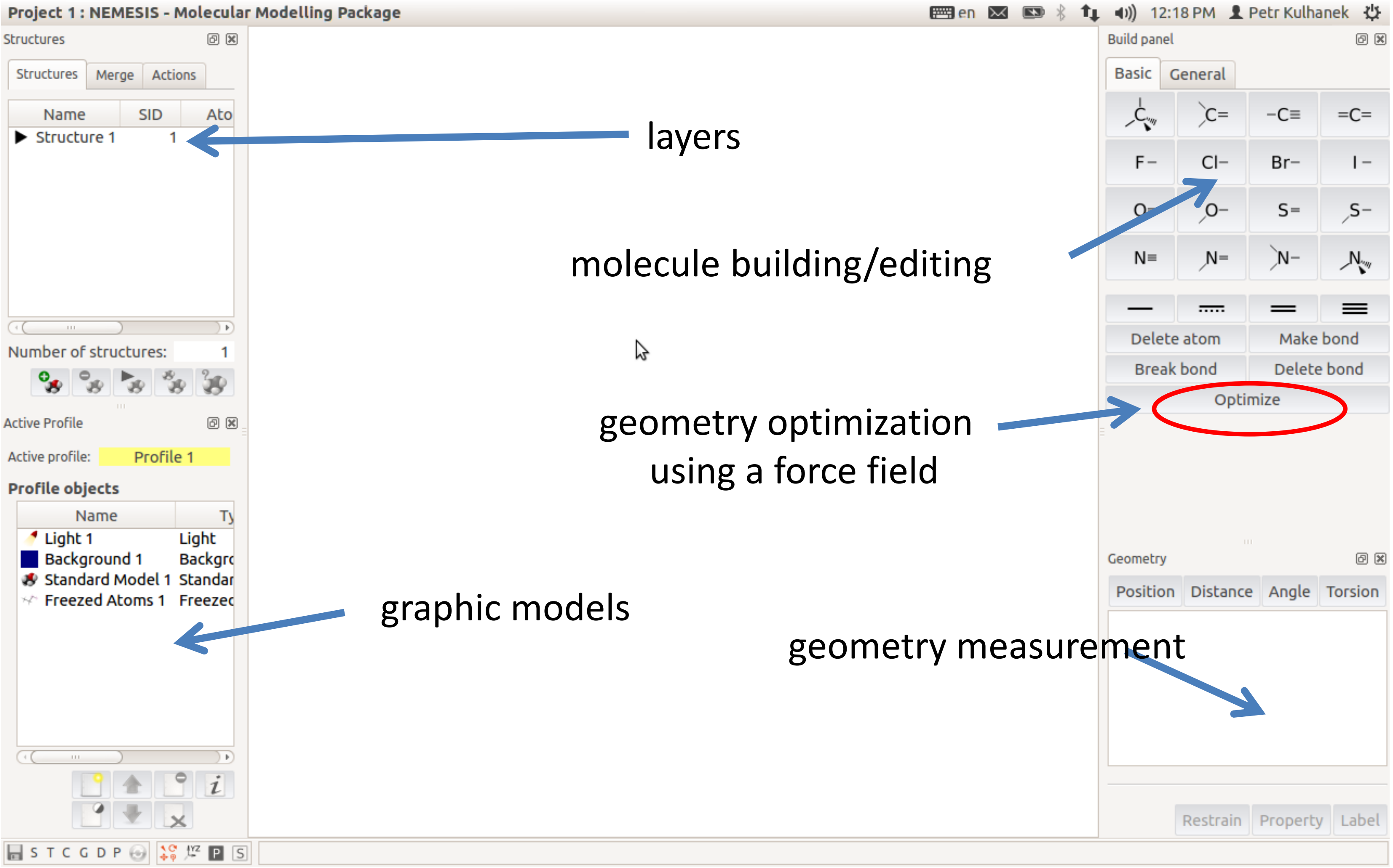
**Mouse:**

| | |
|---|---|
| Left button | selection |
| Middle button | rotation |
| Right button | translation |
| Wheel | zoom |

**Modifiers:**

| | |
|---|---|
| Shift | XZ -> Y moves |
| Ctrl | toggles between secondary and primary manipulator |

# Build Project



| Name | Ty |
|---|---|
| Light 1 | Light |
| Background 1 | Backgro |
| Standard Model 1 | Standar |
| Freezed Atoms 1 | Freezec |

layers

molecule building/editing

geometry optimization using a force field

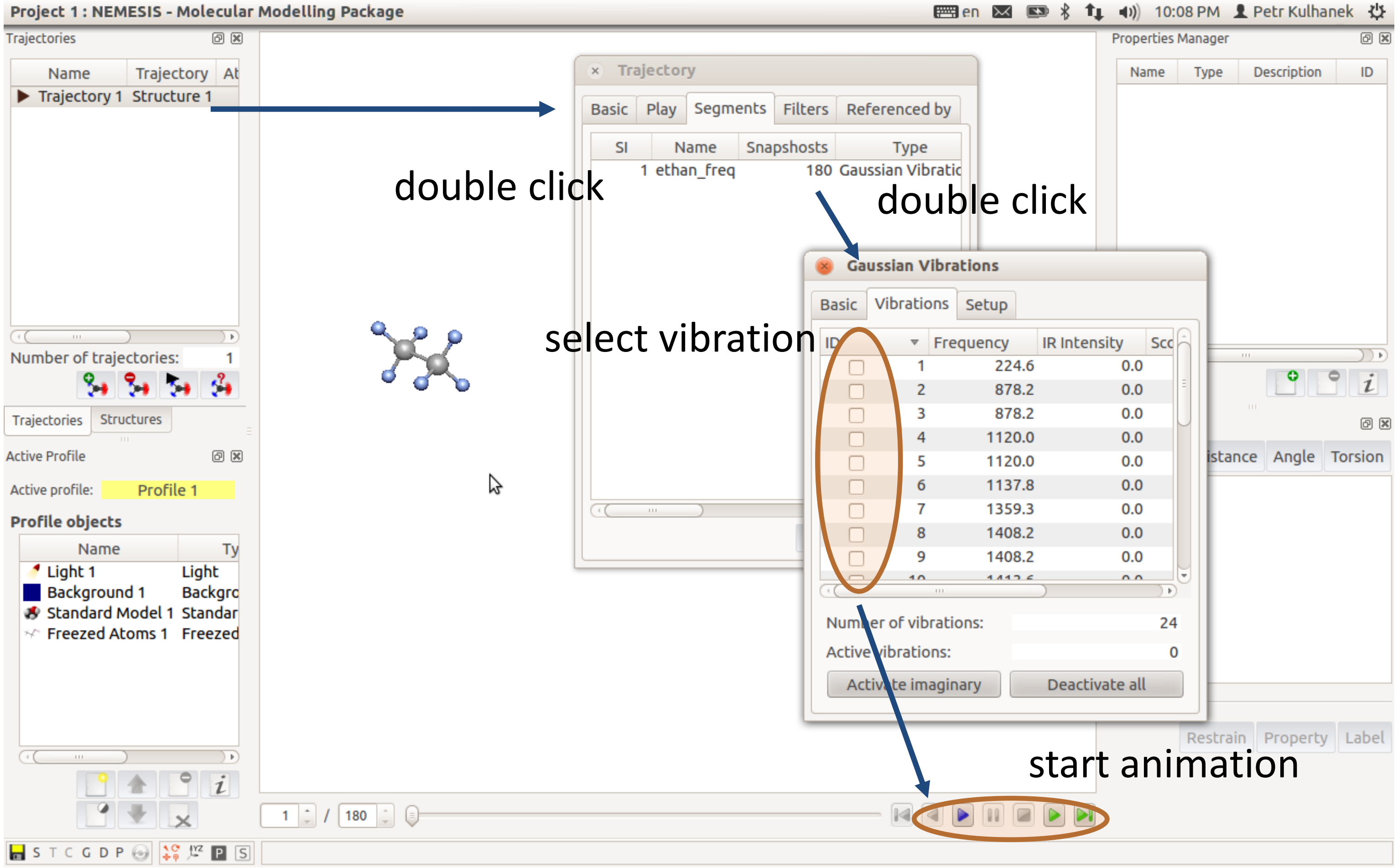
graphic models

geometry measurement

**Force field settings for optimization:** menu Geometry-> Optimizer Setup

# Trajectory: Vibration visualization

1) Project: Trajectory
2) File -> Import Trajectory as -> Gaussian Vibrations



Project 1 : NEMESIS - Molecular Modelling Package

en 10:08 PM Petr Kulhanek

Trajectories

| Name | Trajectory | At |
|---|---|---|
| Trajectory 1 | Structure 1 | |

Number of trajectories: 1

Trajectories | Structures

Active Profile

Active profile: Profile 1

**Profile objects**

| Name | Ty |
|---|---|
| Light 1 | Light |
| Background 1 | Backgrc |
| Standard Model 1 | Standar |
| Freezed Atoms 1 | Freezed |

Trajectory

Basic | Play | Segments | Filters | Referenced by

| SI | Name | Snapshosts | Type |
|---|---|---|---|
| 1 | ethan_freq | 180 | Gaussian Vibratic |

Gaussian Vibrations

Basic | Vibrations | Setup

| ID | Frequency | IR Intensity | Sco |
|---|---|---|---|
| □ 1 | 224.6 | 0.0 | |
| □ 2 | 878.2 | 0.0 | |
| □ 3 | 878.2 | 0.0 | |
| □ 4 | 1120.0 | 0.0 | |
| □ 5 | 1120.0 | 0.0 | |
| □ 6 | 1137.8 | 0.0 | |
| □ 7 | 1359.3 | 0.0 | |
| □ 8 | 1408.2 | 0.0 | |
| □ 9 | 1408.2 | 0.0 | |

Number of vibrations: 24

Active vibrations: 0

Activate imaginary | Deactivate all

Properties Manager

| Name | Type | Description | ID |
|---|---|---|---|

istance | Angle | Torsion

Restrain | Property | Label

1 / 180

double click

double click

select vibration

start animation