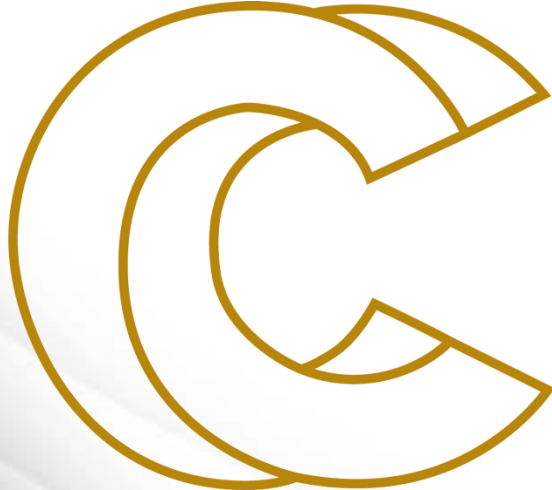




EURO²

Middle East Technical University, July 2025

Welcome to the Course

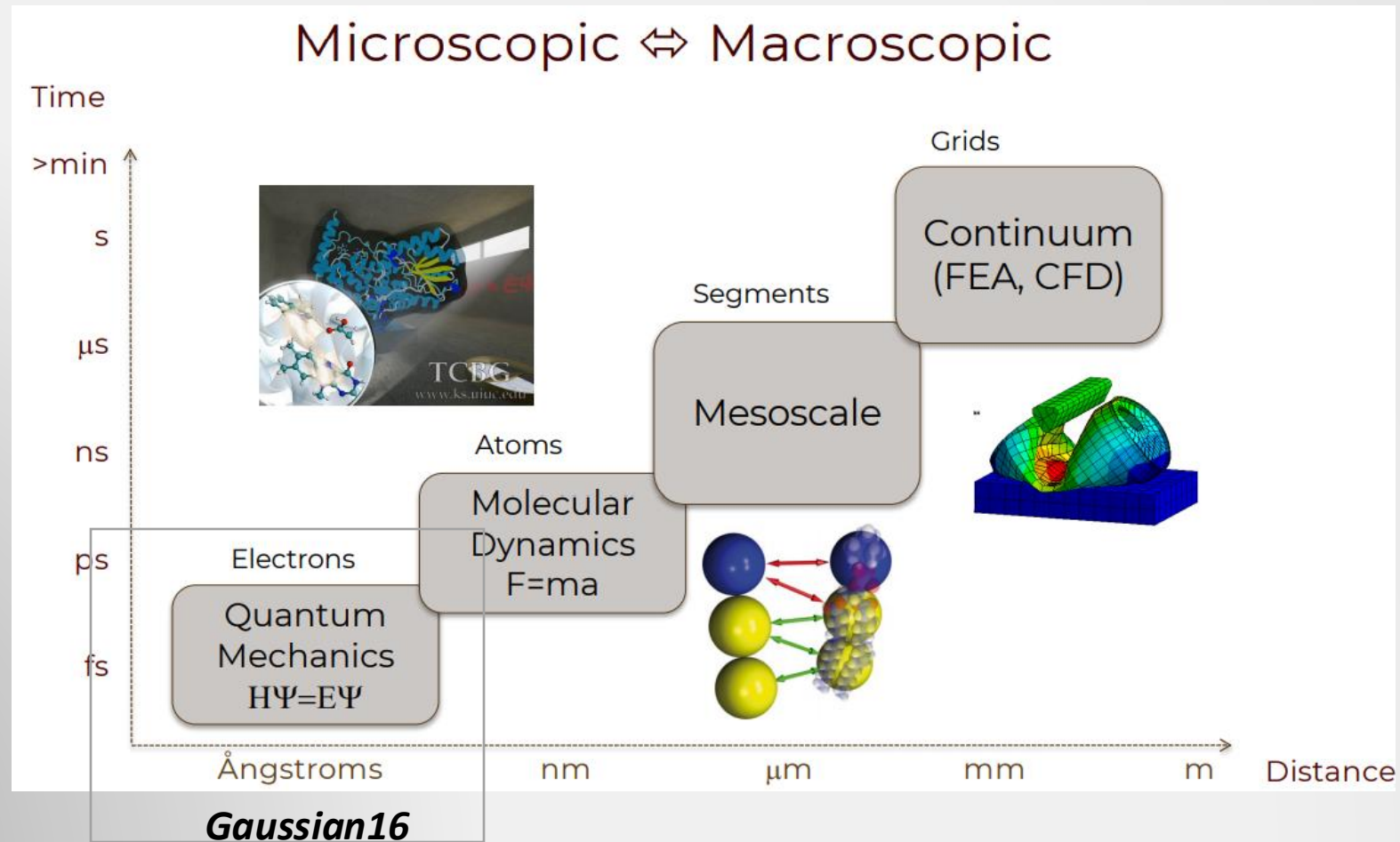
Electronic structure calculations by Gaussian 16

Welcome to the Course

Meet the Instructor

- Dr. Erol Yildirim
Department of Chemistry
Middle East Technical University

Lesson 1: Introduction



Preknowledge/Prerequisite(s)

- <https://openondemand.yonetim/>
- MobaXterm, WinSCP, puttyrequired
- <https://gaussian.com/gaussian16/>
- Gaussian 16, Revision C.01 installed at TRUBA

Preknowledge/Prerequisite(s)

- *Host name ARF: 172.16.6.11*
- *To use Gaussian ve Gaussview*
module load apps/gaussian/g16-avx
module load apps/gaussian/gview
- *Working Directory*
/arf/scratch/eyildirim
- *Your home directory*
/arf/home/eyildirim
- *Some other commands such as: To convert chk file to fchk :*
/arf/sw/apps/gaussian/avx/g16/formchk **xxxx.chk**

Preknowledge/Prerequisite(s)

commands in ARF

To run job: `sbatch xxx.slurm`

To check submitted jobs: `squeue -u username`

To kill a jobs: `scancel jobid`

```
#!/bin/bash
#SBATCH -p orfoz
#SBATCH -A eyildirim
#SBATCH -J HTM3a
#SBATCH -N 1
#SBATCH -n 1
#SBATCH -c 55 # orfoz sunucularinda node basina 55 veya 110 cekirdek talep edilebilir.
```

```
#SBATCH -C weka
#SBATCH --time=1-10:00:00
#SBATCH --output=HTM3a.log
#SBATCH --error=slurm-%j.err
```

```
module purge
```

```
module load apps/gaussian/g16-avx2
```

```
export GAUSS_SCRDIR=/tmp/$SLURM_JOB_ID
source $g16root/g16/bsd/g16.profile
```

```
if [ -d "$GAUSS_SCRDIR" ]
then
rm -rf $GAUSS_SCRDIR
else
mkdir -p $GAUSS_SCRDIR
fi
```

```
# Generate Linda nodes list
NODELIST=$(scontrol show hostnames $SLURM_JOB_NODELIST)
NODES=$(echo $NODELIST | tr ' ',)
LINDA_NODES=$(echo $NODES | sed 's/,/:55,/g')":55"
```

```
# Create the Gaussian input file with Linda workers
echo "%LindaWorkers=$LINDA_NODES" > HTM3a.com
cat HTM3a.gjf >> HTM3a.com
```

```
$g16root/g16/g16 < HTM3a.com
rm -rf $GAUSS_SCRDIR
```

```
exit
```

Gaussian 16 job script example

Thanks



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