Grid for Condensed Matter

Quantum Dots and Building Clusters Atom-by-Atom

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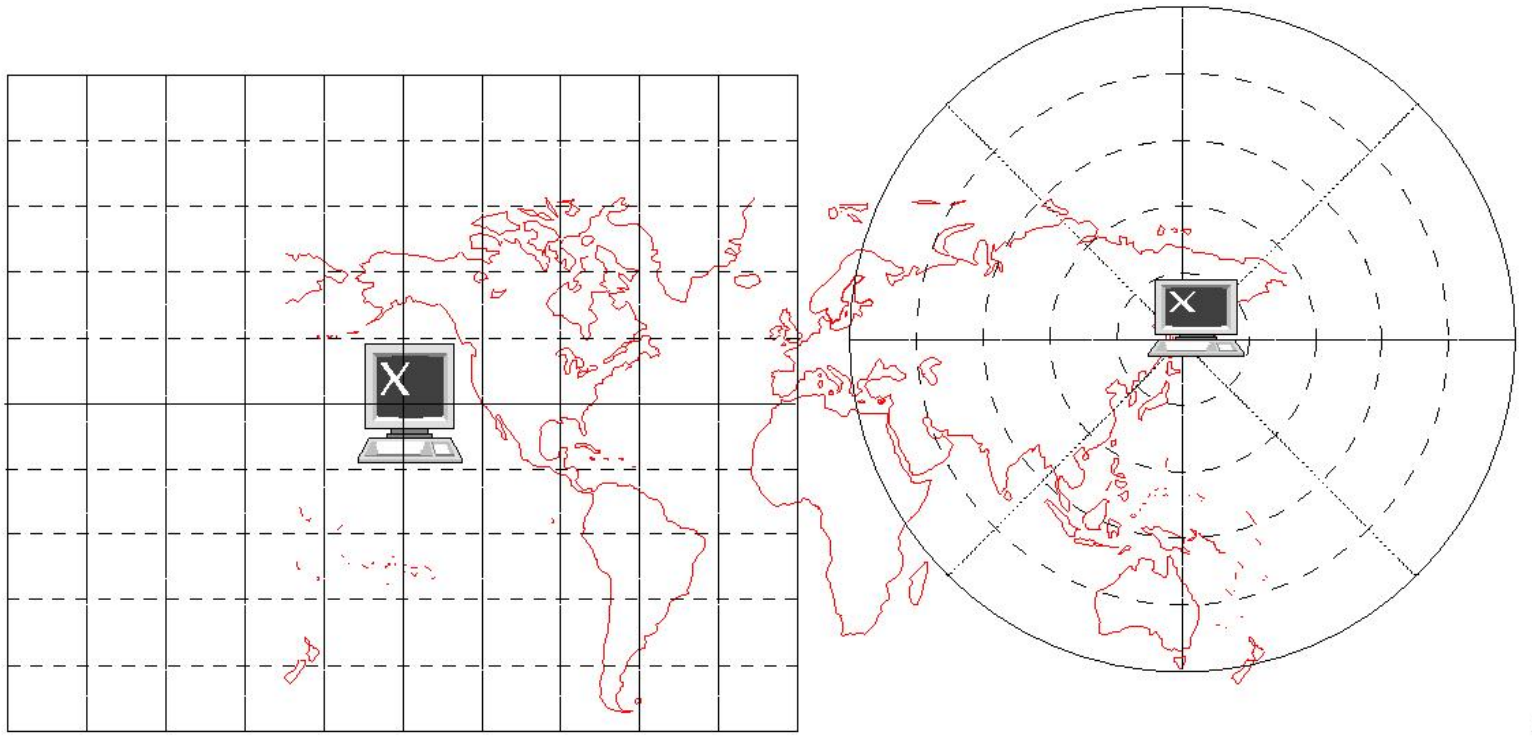
Pune University

User's point of view

.. actually layman's point of view ..

What is GRID? And where do you find it?



Where is the GRID??

National Grid Projects

- D-Grid (German)

Production Grids

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- Open Science Grid
- OurGrid
- Sun Grid
- Xgrid
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User's point of view

Shoot-and-forget

What is GRID?

- Collection of several (thousand) computing elements (heterogeneous)
- Geographically located at different places
- Connected by standard network
- Controlled by 'local' policies

In short, the GRID as a collection of a variety of independent computing platforms available to us with integrated, optimized management system.

User's point of view

When to use it?

Best suited for?

- Large number of jobs!
- Are they independent? (Preferably non-parallel)
- Independent of specific hardware
- Preferably 'static'!

MANTRA: Shoot and Forget

Physics of small scale

"There is plenty of room the bottom" -Feynman

Statements of the Problems

Problem 1: Quantum Dot

- What is the electronic structure of the quantum dot?
- How do the properties change as a function of size?
- Why Grids?

Problem 2: Atomic clusters

- What is the ground state geometry of the atomic clusters?
- How do clusters evolve as the size of number of atoms?
- Why Grids?

Problem 1

Quantum Dots

Quantum Dots

What are they?

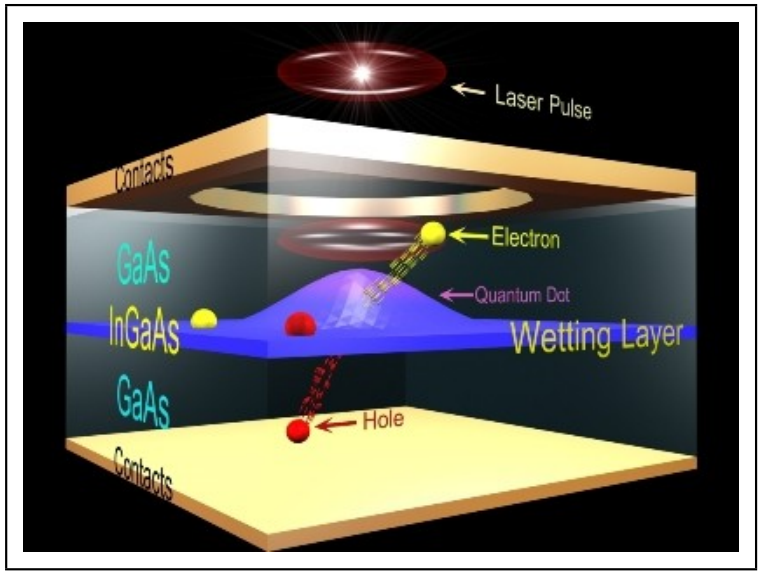
- Quantum Dots are the manifestation of *Confined electron systems*

Quantum Dots

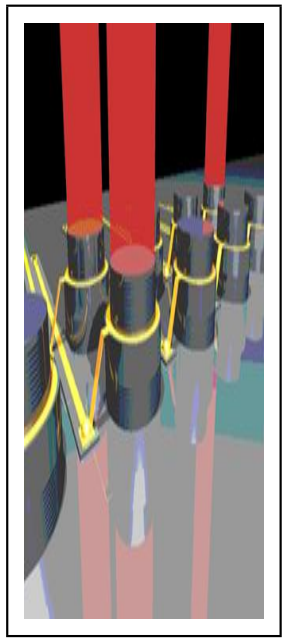
What are they?

- Quantum Dots are the manifestation of *Confined electron systems*
- **Fabrication:** Molecular Beam Epitaxy method, Electron Beam Lithography, Self assembly via Electrochemical means etc.

Molecular Beam Epitaxy



- **Basic Physics:**

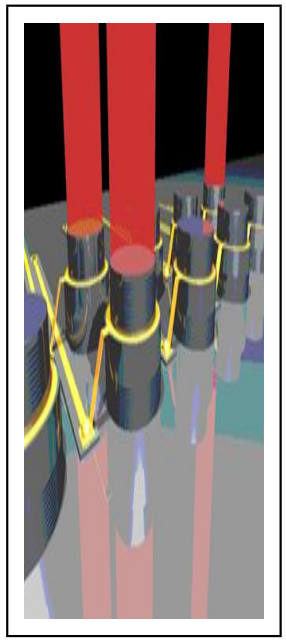


Quantum Dot Laser

Quantum Dots

Applications

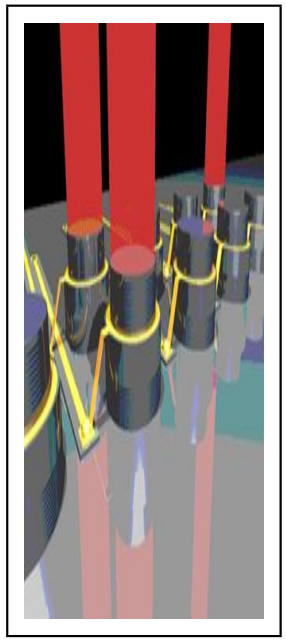
- **Basic Physics:**
- **Electronics:**



Quantum Dot Laser

Quantum Dots
Applications

- **Basic Physics:**
- **Electronics:**
- **Home appliances:**



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Applications

- **Basic Physics:**
- **Electronics:**
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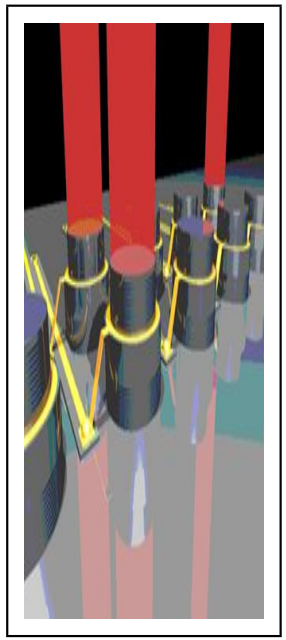
- **Computing:**



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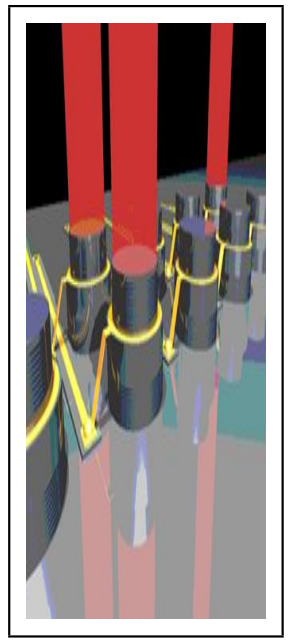
Applications

- **Basic Physics:**
- **Electronics:**
- **Home appliances:**
- **Computing:**
- **Fluorescence:**

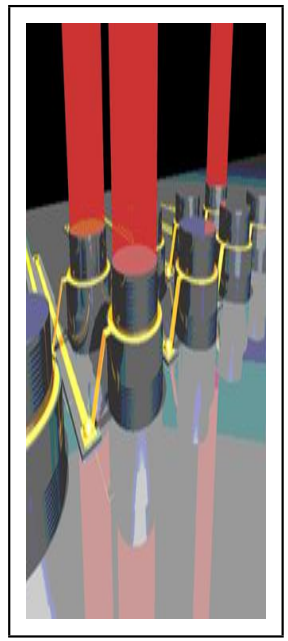


Quantum Dot Laser

QDs for location of a tumor

Quantum Dots
Applications

- **Basic Physics:**
- **Electronics:**
- **Home appliances:**
- **Computing:**
- **Fluorescence:**
- **Biological Dyes:**



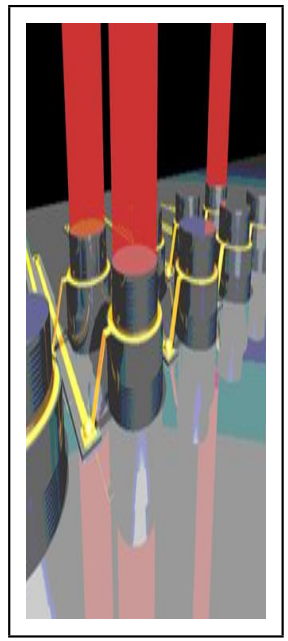
Quantum Dot Laser

QDs for location of a tumor

Quantum Dots
Applications

- **Basic Physics:**
- **Electronics:**
- **Home appliances:**
- **Computing:**
- **Fluorescence:**
- **Biological Dyes:**
- **Solar Panels:**

and lot more . . .

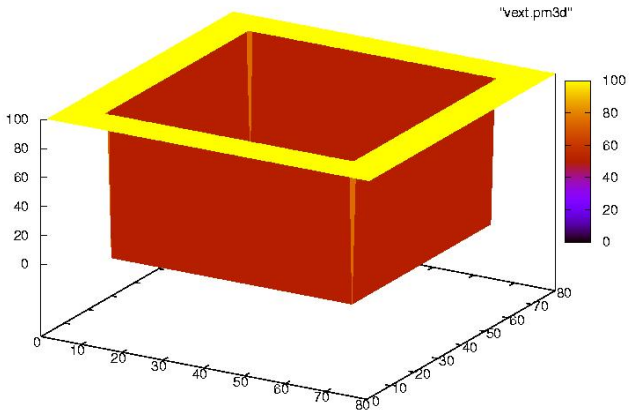


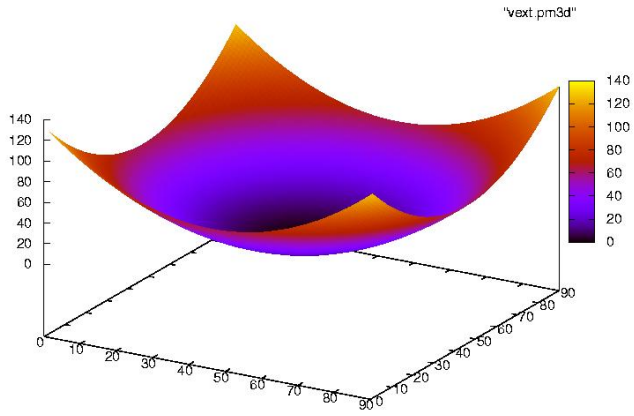
Quantum Dot Laser

QDs for location of a tumor

Computational Model

QDs are modeled as 2D interacting electrons confined by external potential.





- Equation of interacting electrons:

$$H\phi_{i,\sigma}(\mathbf{r}) = \left(-\frac{\hbar^2}{2m}\nabla_i^2 + V_{eff,\sigma}\right)\phi_{i,\sigma}(\mathbf{r}) = \epsilon_{i,\sigma}\phi_{i,\sigma}(\mathbf{r})$$

- Equation is in matrix form
- Hamiltonian H has to be diagonalized to get the energy *eigenvalues* ϵ's
- **Real Space** calculation: Finite difference method
- Typical grid $= 100 \times 100 \Rightarrow$ size of $H = 10000 \times 10000$

Calculation of properties

- The properties are obtained using the **Density Functional Theory** (DFT)
- According to DFT: there exists a unique charge density for the given *effective potential* of the system and vice versa.

- However *a priori*, we do not know the effective potential neither the density!
- So we guess!
- Self Consistency:
  1. From initial guess of density $\rightarrow$ effective potential
  2. Diagonalize DFT Hamiltonian and get new density
  3. Check if new density is same as the input density
  4. if not go to step 1 ; if yes exit!
- One may need hundreds of guesses to arrive at the lowest energy configuration!

Calculations Involved

Calculations for Quantum Dot

- The number of electrons vary for N=2 to 20
- Typical dot size varies in 5 steps of lengths
- Addition of impurity multiplies the calculation by 2!
- Shape of potential can also vary!

Example: For 10-electron quantum dot, with 5 values of spins and 100 initial guesses $\rightarrow$ No of calculations $\sim$ 5000!

Problem 2

Clusters

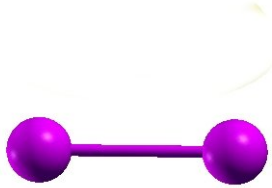
Clusters

Building blocks of nano-materials

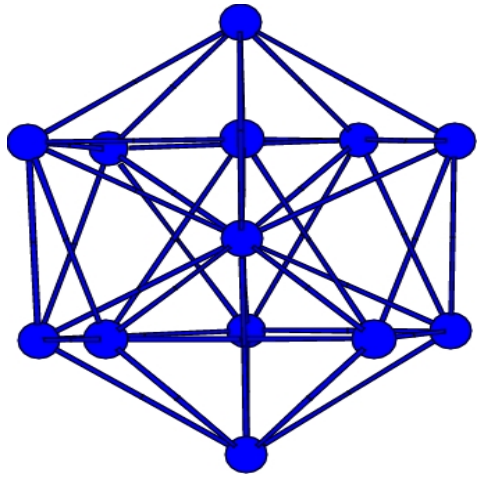
- Atomic clusters are aggregates of atoms!
  - Stable
  - Bound
  - Artificially formed in the lab
  - Any Size!

- Properties :
  - Shapes
  - Stability
  - Magnetic moments
  - Reactivity
  - and so on!

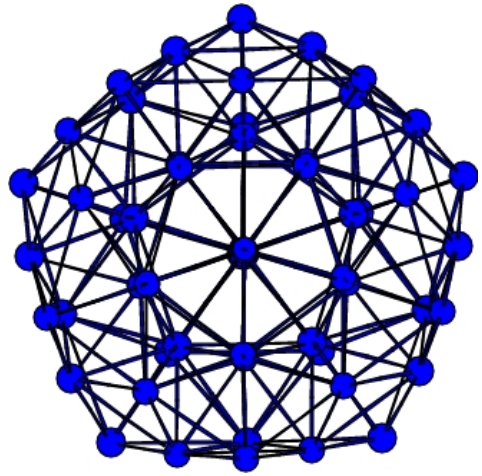
Clusters



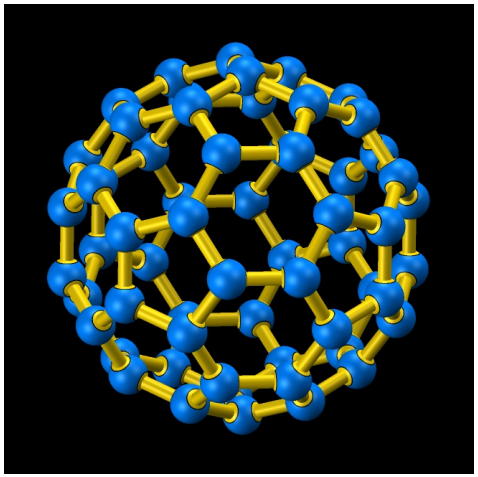
2 atom cluster



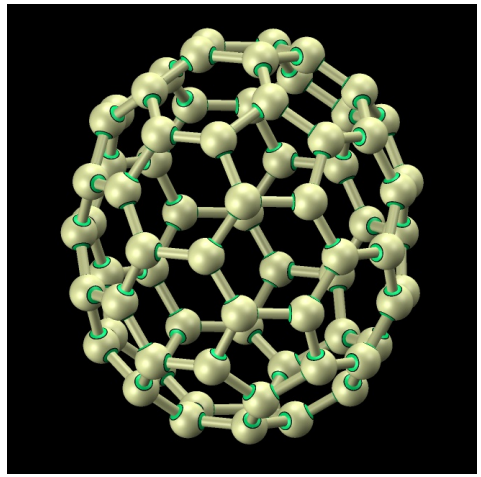
13 atom cluster



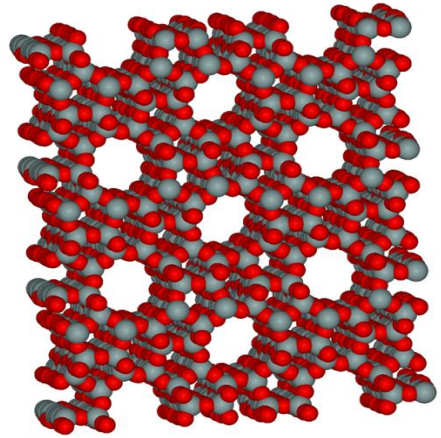
55 atom cluster



60 atom cluster



70 atom cluster



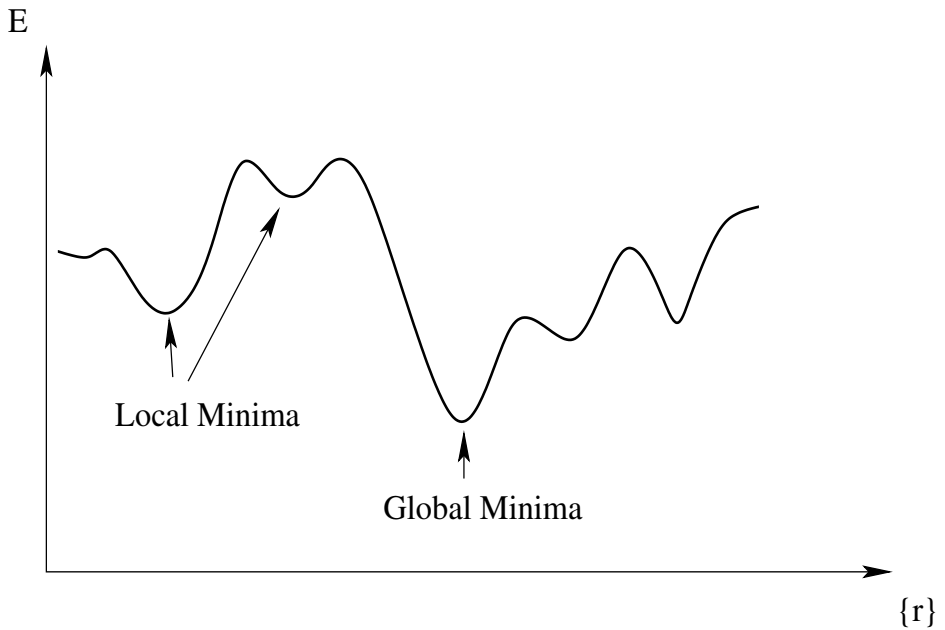
Zeolite

Clusters

- Clusters: Collection of N atoms interacting with each other via some potential $V(\vec{r})$.
- The total energy of the cluster

$$E = \sum_{i<j} V_{ij}(r_{ij})$$

A typical E looks like:



Quest for ground state structure

Non-linear optimization

- Simulated annealing at finite temperature for up to 50000 iterations (1000 iterations $\sim$ 3 picosec.)
- A *few hundred to a few thousand* structures to be searched and quenched
- Global optimization problem
- Each minimization may take up to 100-300 CPU hours on say, single Xeon processor.

The problem is complicated as the explicit form of the potential is not known *a priori* and the dynamics of the system is mixed: the electrons are treated quantum mechanically and the ions are treated classically. Number of variational parameters are ($3N$-6)

Example

Aluminium Cluster with 100 atoms

- Number of ions 100
- Ionic degrees of freedom $\sim$ 300
- Number of electrons 300
- The electronic wavefunction

$$\Psi_i = \sum_G C_G e^{-iGr}$$

- Number of terms in this expansion $\sim$ **200000**
- Total number of such Ψ's $\sim$ 150.
- Total variational parameters 200000 X 150 !

Calculations Involved

Calculations for Clusters

- At least 10 clusters in a series of calculations
- Hundreds of geometries are required for each
- Two charge states (typically 2) for each case
- Very large number of variational parameters involved

Example: For a series of 10 clusters, with 400 geometries and 2 states: total number of jobs = 10*400*2 = 8000!

Why grid?

Shoot-and-Forget!

- Break the problem into several separate pieces
  - Hundreds of initial guesses required for Quantum dots
  - Hundreds and thousands of geometries to be quenched
- Each of the piece can then be run independently
- Require standard computing node (Xeon/P4/Itanium)
- No specific requirement of parallelism

Nature of the problems make them ideal for the Grid!

Management of the jobs!

- Several thousand jobs to fire!
- How to shoot them and retrieve them? One by one? (naaah!)
- How to check the status of the jobs?
- What about those certificate?
- How many jobs to shoot at once??
- How to sort out the answers?

The answer is:

Management of the jobs!

- Several thousand jobs to fire!
- How to shoot them and retrieve them? One by one? (naaah!)
- How to check the status of the jobs?
- What about those certificate?
- How many jobs to shoot at once??
- How to sort out the answers?

The answer is:

Scripts!

Scripts


```
#!/bin/bash

#################################################################
#    Script that :
# 1. Creates the directories by the index of geometries
# 2. Copies appropriate files required for the job to run on
#    the grid
# 3. Checks/Procures the validity of the proxy certificate
# 4. Submits the jobs at appropriate node on the grid
#    Script by --Vaibhav Kaware
#################################################################
function usage()
{
 echo "usage :"
 echo "${0} <beg> <end> <Name> <T> <remote_node>"
 echo "Where,"
 echo "beg : Index of geometry to begin with"
 echo "end : Index of geometry to end with"
 echo "Name : Name of cluster"
 echo "T : Temperature of cluster"
 echo "romote_node : Name of node, at which the job should"
 echo " : be submitted"
 echo
}
beg=${1}
end=${2}
name=${3}
T=${4}
node=${5}
```

..and scripts..


```
if [ $# -ne 5 ]
then
usage
exit 1
fi
echo
echo " **** PROXY CERTIFICATE INFO     ****   "
echo
voms-proxy-info --all
echo
echo "Should one procure a new certificate? [y/n]"
read x
if [[ "${x}" == Y* ]] || [[ "${x}" == y* ]]
then
   voms-proxy-init --voms euindia --hours 500 -vomslife 100:0
fi
echo
for i in `seq ${beg} ${end}`
do
 mkdir -v $i
 tar cjvf all.tar.bz2 INCAR* KPOINTS POSCAR.$i POTCAR \
 static.ser.x
 mv -v all.tar.bz2 $i
 cp ${name}.${T}.qnch.jdl run41.sh $i -v
 cd ${i}
 glite-wms-job-submit -o job.id -r ${node} \
 ${i}.${name}.${T}.jdl
 cd ..
done
exit 0
#################END OF SCRIPT#################
```

..and more scripts..


```
#!/bin/bash
# Script : submit.sh
# Script by --vaibhav
function usage()
{
 this_script=${1}
 echo
 echo Usage:
 echo "${this_script} <from> <to>"
 echo Script that displays the status of currently submitted jobs on the grid
 echo Directories must be named as numbers
 echo Resubmits the job in case the status is \'Aborted\'
 echo Retrieves the results, in case the status is \'Done\'
 echo " (Concerned parameters can be set in the script)"
 echo Displays the status as is, in case the status is anything else.
 echo
 echo "from : From which number to start checking the status"
 echo "to   : Upto which number should the checking of status done"
 echo
}

if [ $# -lt 2 ]
then
usage `basename ${0}`
exit 1
fi

from=${1}
to=${2}
```

..and scripts..


```
result_file="result.tar.bz2"
jobid_filename="job.id"
name="Ga41"
T="900"
basedir="/home/uipnp/vaibhav/quenches/${name}/${T}"
basedir="${PWD}"
archive="result.archive.${name}.${T}"

if [ ! -d ${archive} ]
then
mkdir -v ${archive}
fi

echo
echo " **** PROXY CERTIFICATE INFO     ****   "
echo
voms-proxy-info --all
echo
echo "Should one procure a new certificate? [y/n]"
read x
if [[ "${x}" == Y* ]] || [[ "${x}" == y* ]]
then
   voms-proxy-init --voms euindia --hours 500 -vomslife 100:0
fi
echo
```

..and scripts..


```
function submit()
{
 dir=${1}
 cd ${dir}
 if [ -f ${jobid_filename} ]
 then
     old_job_file=‘mktemp‘
     mv -vf ${jobid_filename} ${old_job_file}
     mv -fv ${old_job_file} .
 fi
 glite-wms-job-submit -a -o ${jobid_filename} -r ce01.unipune.ernet.in:2119/jobmanager-lcgpbs-eu
 sleep 60
 cd ..
}

function retrieve()
{
 dir=${1}
 result_file=${2}

 cd ${dir}
 echo ${PWD}
 result_dir=‘mktemp -d‘
 result_dir="${result_dir}/result"
 glite-wms-job-output --dir ${result_dir} -i ${jobid_filename}
 mv -v ${result_dir}/${result_file} ${basedir}/${archive}/result.qnch.${name}.${T}.${dir}.tar.bz
 cd ..
}
```

..and scripts..


```
aborted=0
running=0
other=0
done=0
ret=0

for i in `seq ${from} ${to}`
do
   echo -n "     "${i} : " "
   if [ -d ${i}.done ]
   then
echo "Data is already retrieved"
let ret+=1
   else
        somefile=`mktemp`
    glite-wms-job-status -i ${i}/${jobid_filename} 2>/dev/null 1>${somefile}

    status=`cat ${somefile} | grep "Current Status" | awk -F: '{print $2}'| awk '{print $1}'`
        destination=`cat ${somefile} | grep "Destination"| awk '{print $2}' | awk -F: '{print $1}`
        submitted=`cat ${somefile} | grep "Submitted"| awk -F"          " '{print $2}'`

    case ${status} in
   Aborted)
 let aborted+=1
 echo "ABORTED !!!! Hence resubmitting"
 submit ${i}
 ;;
   Cancelled)
 let aborted+=1
 echo Cancelled But not resubmitting
 rm -fv $i/job.id
 submit ${i}
 ;;
```

..and scripts..


```
Done)
 echo DONE :D !!!!  : ${destination}
 let done+=1
 retrieve ${i} ${result_file}
 mv -v ${i} ${i}.done
;;
Running)
 echo Running @ ======== ${destination} "    " Submitted on ${submitted}
 let running+=1
;;
Waiting)
 echo Waiting @ ======== ${destination} "    " Since ${submitted}
 let other+=1
   glite-wms-job-cancel --noint -i ${i}/${jobid_filename}
;;
Scheduled)
 echo Scheduled @ ======== ${destination} "    " Since ${submitted}
 let other+=1
   glite-wms-job-cancel --noint -i ${i}/${jobid_filename}
;;
Ready)
 echo Ready @ ======== ${destination} "    " Since ${submitted}
 let other+=1
   glite-wms-job-cancel --noint -i ${i}/${jobid_filename}
;;
*)
 echo ${status}
 let other+=1
;;
   esac
   fi
done
```

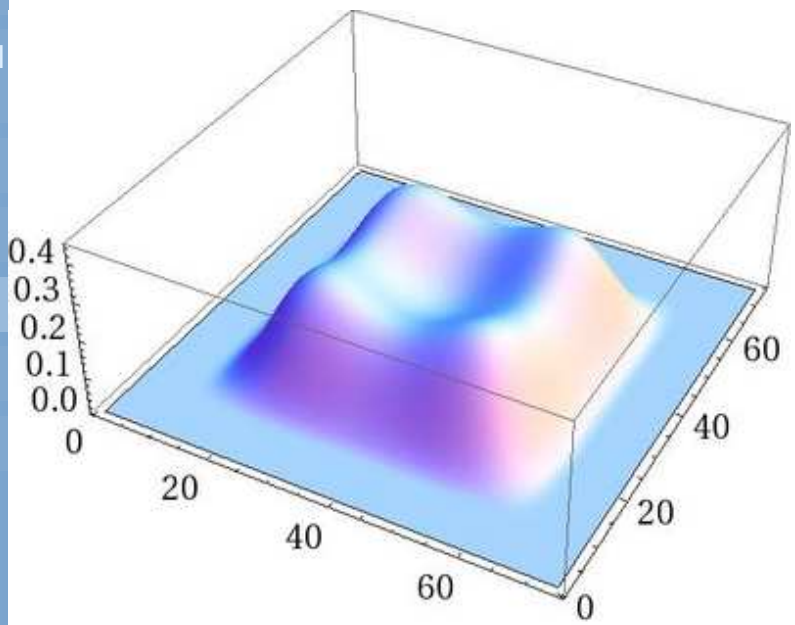
..and scripts..

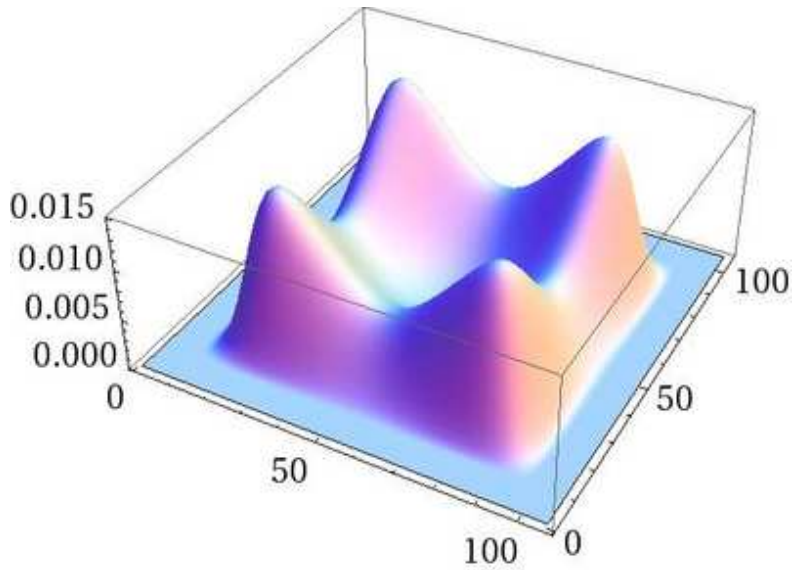

```
echo
echo "Done : ${done} | Aborted : ${aborted} | Already retrieved : ${ret} | Running : ${running}
echo

exit 0
```

With special thanks to Mr. Vaibhav Kaware.

Results for Quantum Dot

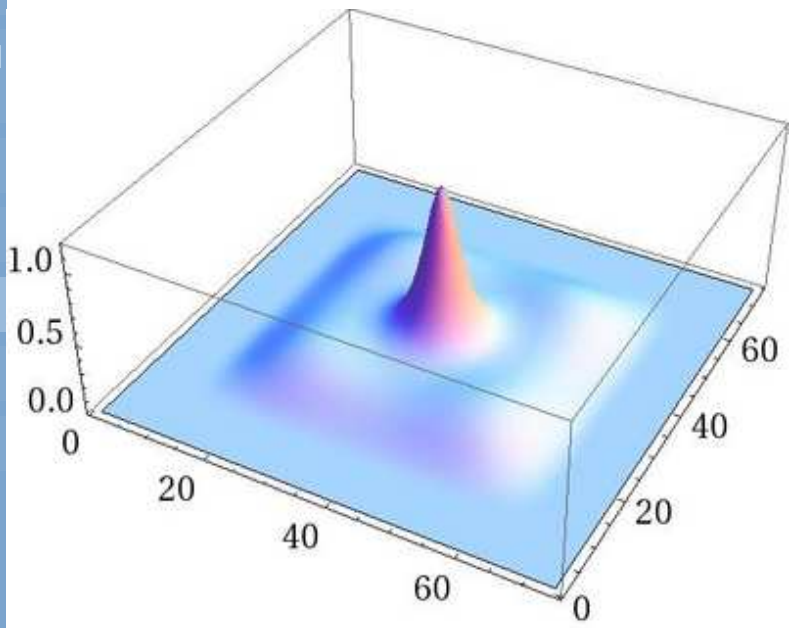
Charge density of 4-electron quantum dot. With dot size ∼40 nm and ∼ 200 nm

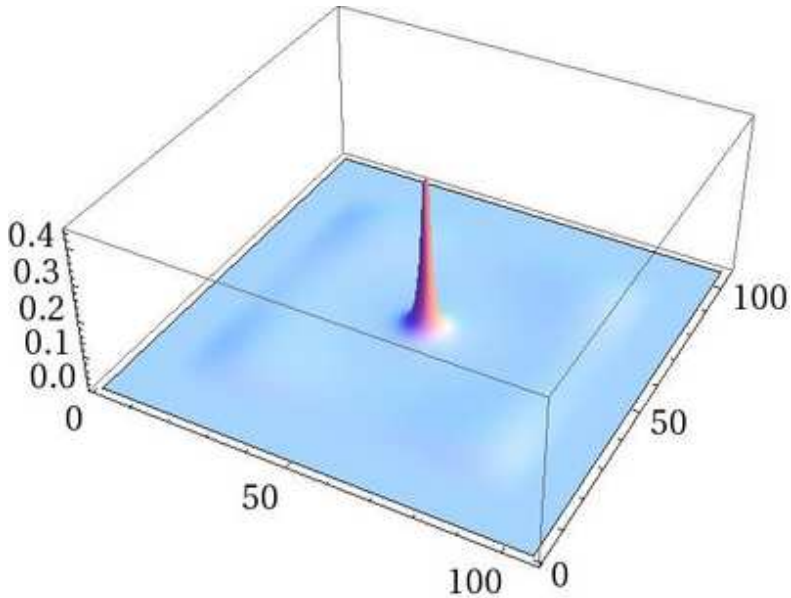




Results for Quantum Dot

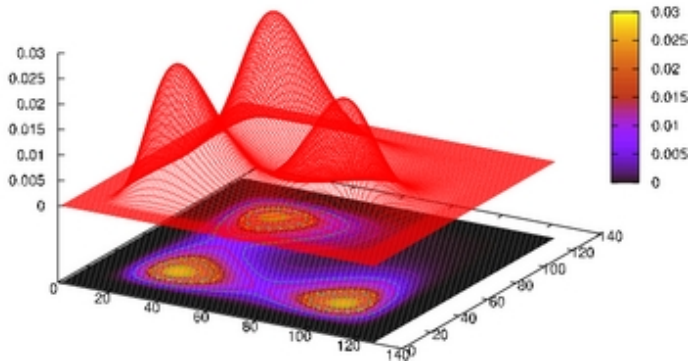
Charge density of 4-electron quantum dot with an impurity at the center. Dot size ∼40 nm and ∼ 200 nm

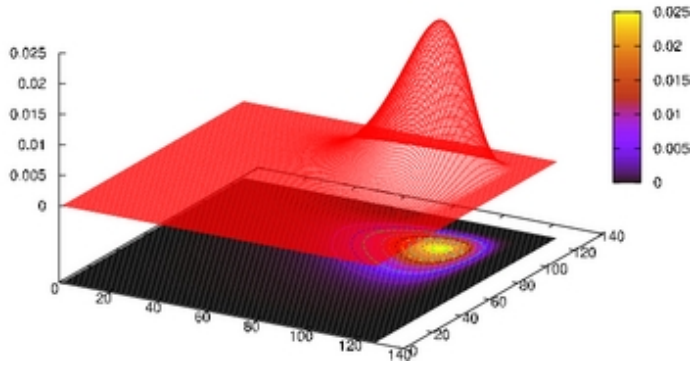




Results for Quantum Dot

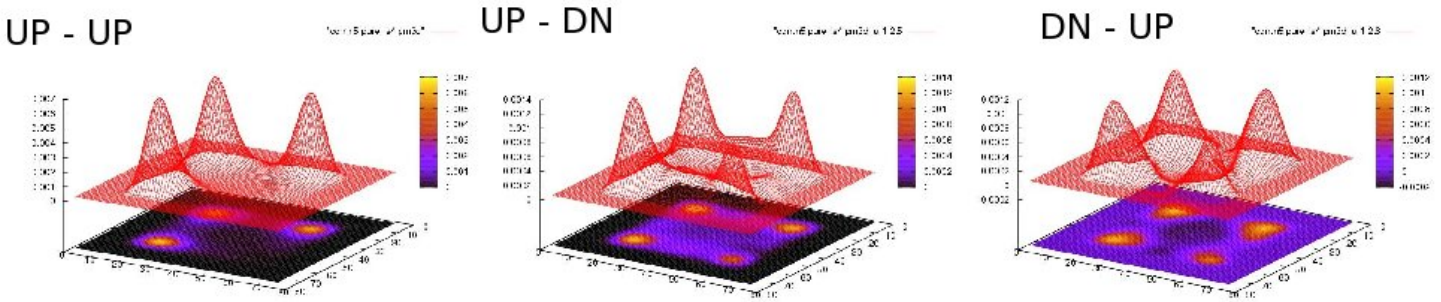
Problems with Density Functional Theory

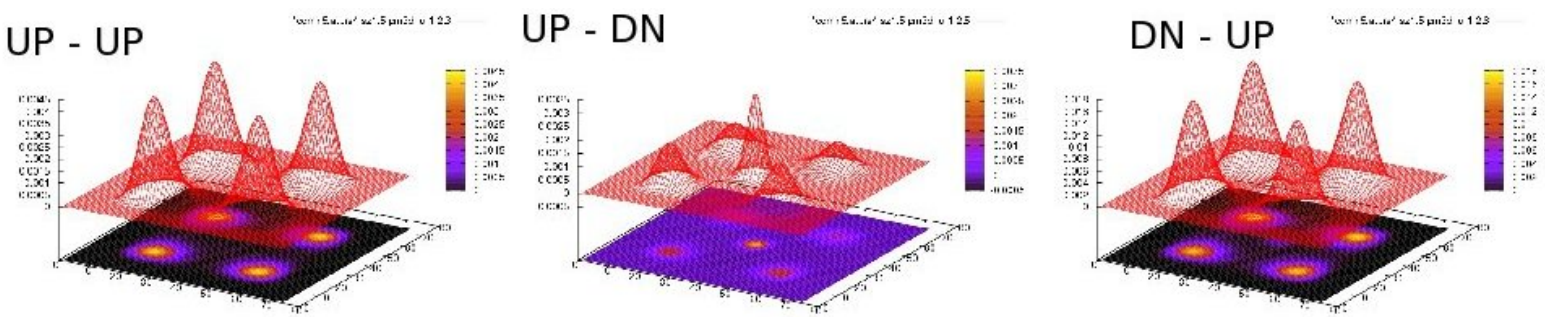




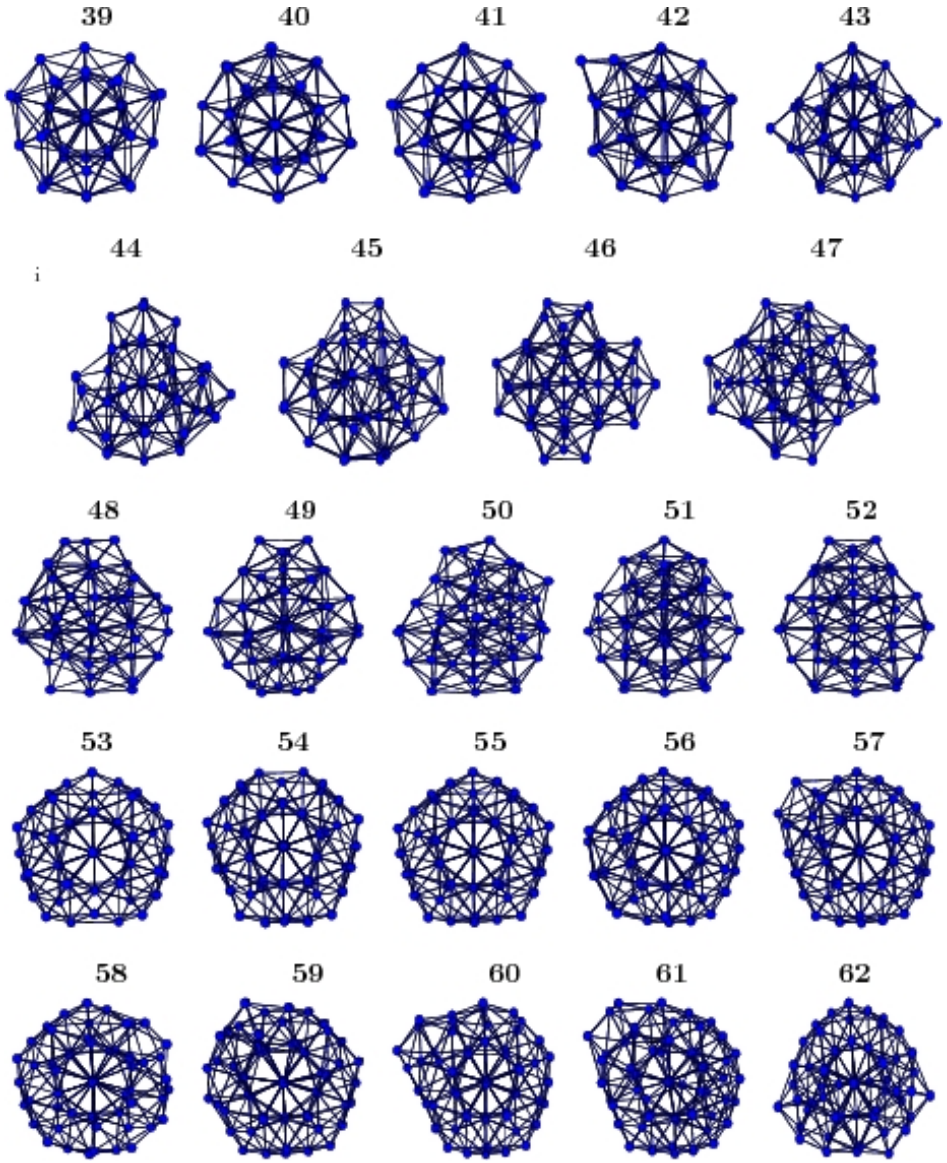
Correlations using Configuration Interaction Method

Correlations: 5 atom quantum dot ($S_z = 1.5$) at $r_a \sim 4$



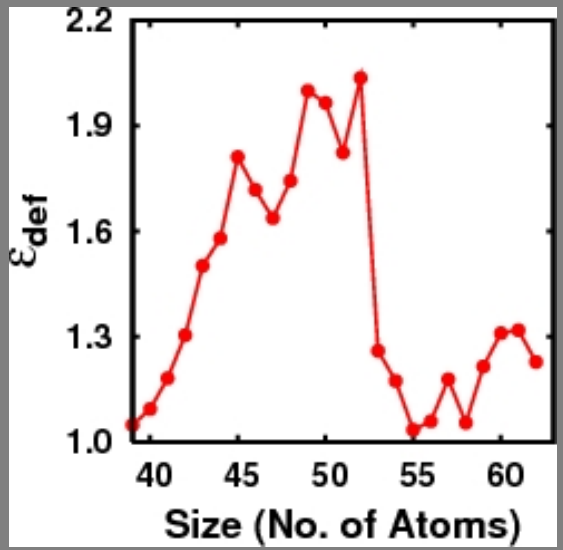


Results for Clusters



Atomic cluster of Sodium (Na)

Deformation parameter

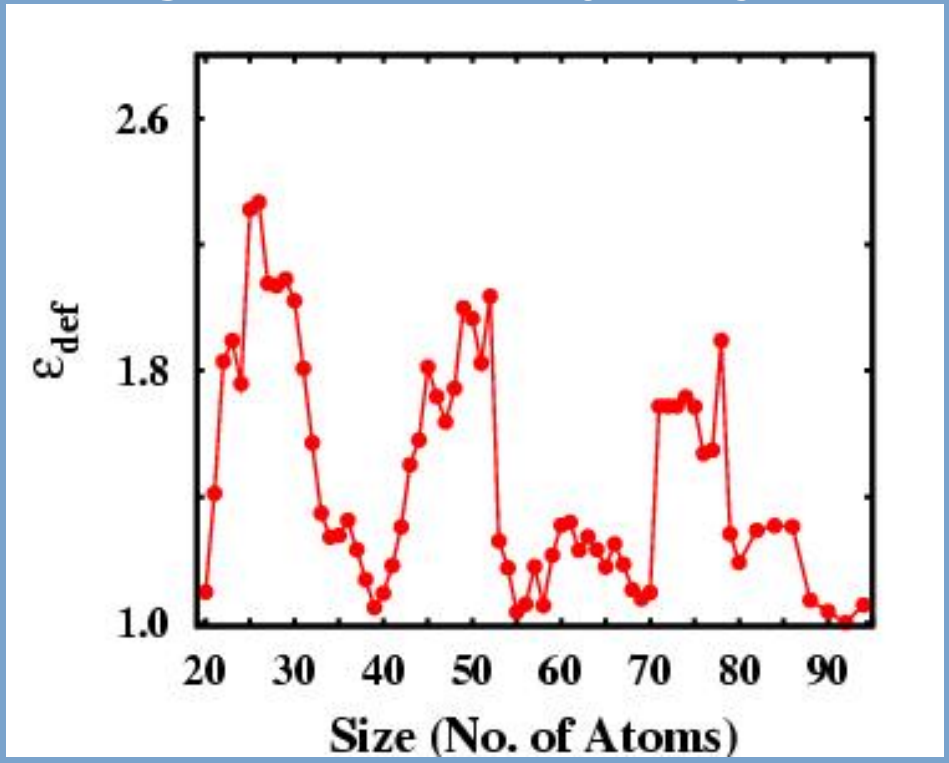


$\epsilon_{def} = 1 \Rightarrow$ Sphere

Results for Clusters

Building cluster atom-by-atom

Sodium N=20 to 92



$\epsilon_{def} = 1 \Rightarrow$ Sphere

Summary

- Both the problems involve hundreds of independent calculation
- All these jobs can be fired with shoot-and-forget strategy!
- Grid can be harnessed for such Condensed matter physics application

- Issues
  - Slow network connectivity between India-Europe.
  - Efficient MPI/SMP implementation would be desirable

Contributors

Quantum Dots

- Bhalchandra Pujari
- Kavita Joshi
- D. G. Kanhere

Clusters

- Shahab Zorriasatein
- Seyed Mohammad Ghazi
- Vaibhav Kaware
- Kavita Joshi
- D. G. Kanhere

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- Dr. Stefano Cozzini, Italy - Technical Manager
- Neeta, Mangesh and others - Local system administrators.

Thank You!

```
echo ${COMMENTS} | mail bspujari@unipune.ernet.in
```