

# Simulacije svojstava materijala na CRO-NGI

Treći dan CRO-NGI, SRCE, Zagreb

- Korisnički slučaj -

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Odjel za fiziku, Sveučilište J. J. Strossmayera, Osijek

14. prosinca 2011.



- 1 Problematika
- 2 ABINIT na CRO-NGI
- 3 Prednosti korištenja CRO-NGI

# Sadržaj

- 1 Problematika
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## Što proučavamo? I kako?

- svojstva materijala --→ elektroni
- kvantno-mehaničke jednadžbe
- broj varijabli

## Što proučavamo? I kako?

- svojstva materijala --> elektroni
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## Procesi prilikom izvođenja računa

```

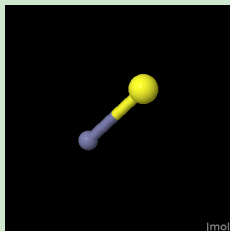
-----
- Total cpu          time (s,m,h):  -1717651.0  -28627.52  -477.125
- Total wall clock time (s,m,h):  15462218.2  257703.64  4295.061
-
- For major independent code sections, cpu and wall times (sec),
- as well as % of the time and number of calls for node 0-
- routine            cpu      %      wall    %      number of calls
- projbd             827615.294 -48.2  827772.828  5.4      23130041
- nonlop(apply)     217497.194 -12.7  217439.177  1.4      10514623
- fourwf(G->r)      148115.972  -8.6  148126.459  1.0      6052608
- vtorho3:synchro   82511.500  -4.8  82511.430  0.5       5642
- vtowfk3(contrib)  77652.417  -4.5  77603.836  0.5       -1
- fourwf(pot)       -1680975.551 97.9  466640.132  3.0     12596223
- 64 others         102937.882  -6.0  102603.168  0.7
- subtotal          -224645.292 13.1 1922697.030 12.4
-
- For major independent code sections, cpu and wall times (sec),
- as well as % of the total time and number of calls
- routine            cpu      %      wall    %      number of calls
-                   (-1=no count)
- projbd             2211912.275 -128.86507499.675 42.1     185041859
- vtorho3:synchro   909145.486  -52.9  909151.773  5.9       45136
- cgwf3-0(npw)      409896.359  -23.9  409111.938  2.6        -8
- nonlop(forces)    183923.647 -10.7  184065.676  1.2     39063552
- getghc-other      91982.634  -5.4   91700.890  0.6        -8
- fourwf(pot)       -608397.671 35.43686861.315 23.8     100770282
- fourwf(G->r)      -979085.338 57.01168266.072  7.6     48420864
- vtowfk3(contrib) -1532198.912 89.2  615616.228  4.0        -8
- nonlop(apply)     -2610221.618 152.0  1684749.302 10.9     84117482
- 61 others         121000.601  -7.0  120970.585  0.8
- subtotal          -1802042.537 104.9***** 99.5
-----

```

### Što proučavamo? I kako?

- svojstva materijala  $\rightarrow$  elektroni
- kvantno-mehaničke jednačbe
- broj varijabli

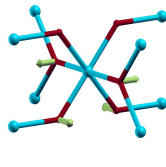
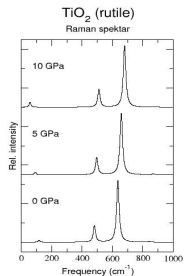
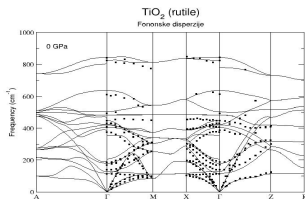
### Tipična kristalna ćelija (ZnS)



2 atoma  $\rightsquigarrow$  18  
valentnih  
elektrona

## Teme istraživanja i planovi

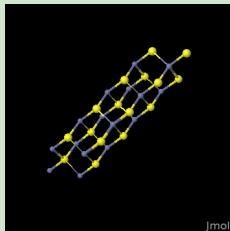
- strukturna svojstva
- dopiranje nano-materijala



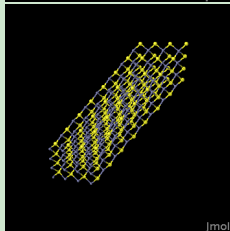
## Teme istraživanja i planovi

- strukturna svojstva
- dopiranje nano-materijala

## Dopirana ćelija nano-kristala (ZnS)



ZnS nanožica ~↔  
 32 atoma ~↔ 288  
 valentnih  
 elektrona



6.25% dopirana  
 ZnS nanožica ~↔  
 256 atoma ~↔  
 4608 valentnih  
 elektrona

# Sadržaj

- 1 Problematika
- 2 ABINIT na CRO-NGI**
- 3 Prednosti korištenja CRO-NGI

- mnogobrojni kodovi:
  - ABINIT - [www.abinit.org](http://www.abinit.org)
  - Quantum Espresso - [www.quantum-espresso.org](http://www.quantum-espresso.org)
  - Wien2k - [www.wien2k.at](http://www.wien2k.at)
  - CASTEP - [www.castep.org](http://www.castep.org)
  - SIESTA - [www.icmab.es/siesta-joomla](http://www.icmab.es/siesta-joomla)
  - VASP - [cms.mpi.univie.ac.at/vasp/](http://cms.mpi.univie.ac.at/vasp/)
  - ...
- baza - DFT (Teorija funkcionala gustoće)

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The ETSF offers its expertise to researchers, industry, and students in the form of collaborative projects, free scientific software and training. Proposals to benefit from these services can be submitted at any moment, and are evaluated twice a year by an external scientific panel.

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**News & Events**

 27 May 2012 **Young Researchers Meeting 2012**  
 4 Jan 2012 **6th School & Workshop on "Time-Dependent Density-Functional Theory: Prospects And Applications"**

The Young Researchers Meeting 2012 (YRM2012) will be held in Brussels, from 21st to 25th... [Read more.](#)

This School & Workshop is the fifth of a very successful series that started in 2004. The positive response... [Read more.](#)

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[www.etsf.eu](http://www.etsf.eu)

### Zahtjevi koda (verzija 5.x.x)

- programski prevoditelji
- MPI (Intel MPICH)
- vanjske knjižnice (bigdft, wannier90, netcdf, linalg, fftw, fox, xmlf90, etsf-io, etsf-xc)

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Problem s LAPACK knjižnicom?

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## Pristupanje kodu (verzija 5.x.x)

- 1 condor skripta
- 2 run skripta

## Zahtjevi koda (verzija 6.x.x)

### Problem s LAPACK knjižnicom?

```

Executable=run_local.sh
Log=condorG.log
Output=run.$(cluster).out
Error=run.$(cluster).err
transfer input files = /home/ilukacev/abinit-5.4.4p/tests/tutorial/Input/Work5/tll.in, /home/ilukacev/abinit-5.4.4p/tests/Psps_for_tests/22t1.pspnc, /home/ilukacev/abinit-5.4.4p/tests/Psps_for_tests/8o.pspnc, /home/ilukacev/abinit-5.4.4p/tests/Psps_for_tests/7n.pspnc, /home/ilukacev/abinit-5.4.4p/tests/tutorial/Input/Work5/tlx.err.files
transfer output files = tll.out, log
should transfer files = yes
WhenToTransferOutput = ON_EXIT
universe=grid
grid_resource = qt2.ce.srce.cro-ngi.hr/jobmanager-sge
Requirements = TARGET.MaxMatches >= 2
Rank = TARGET.ParallelOnly =?= 1
xS09userprop = /tmp/xS09up.us$1
environment = "PE_MODE=single"
globusrsl = (jobtype=single)(count=8)
notify_user = ilukacevic@fizika.unios.hr
notification = Always
queue
  
```

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Problem s LAPACK knjižnicom?

```
#!/bin/sh
currDir="pwd"
cp t11.in Z2t1.pspnc 8o.pspnc 7n.pspnc t1x.emir.files $TMPDIR/
cd $TMPDIR
sed -i s:t11.out:${currDir}/t11.out: t1x.emir.files
mpirun -np 8 -machinefile $TMPDIR/machines /usr/local/bin/abinip <t1x.emir.files> $s
currDir/log
ls
mv log $currDir/
```

# Sadržaj

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### Paralelni ABINIT kod

- po  $k$  točkama
- po stanjima elektrona
- po spinovima
- po smetnjama
- kombinirano stanja/FFT
- kombinirano stanja/FFT/ $k$  točke/spin

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Paralelizacija po  $k$  točkama

- $nkpt = n \cdot N_{CPU}$ ,  $n \in \mathbb{N}$
- $N_{CPU} > nkpt \Rightarrow$  saturacija  
 $N_{CPU} = n_{dblock} \cdot nkpt$

Broj  $k$  točaka u računima

	današnji računi	budući računi
# $k$ točaka	30	936

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 $N_{CPU} = n_{dblock} \cdot nkpt$

## Paralelizacija po stanjima

$$\langle \psi_n | \psi_m \rangle = 0 \Rightarrow N_{CPU} \leq 4$$

Broj  $k$  točaka u računima

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### Ograničenje

- ABINIT  $\rightarrow$  "shared memory"
- čvor srce  $\rightarrow N_{CPU} \leq 32$

## “Hardware”

- RAM
- diskovni prostor
- mreža
- broj procesora

DATASET 29 : space group Pb c n (# 60); Bravais oP (primitive ortho.)

=====

Values of the parameters that define the memory need for DATASET 29 (RF).

intxc =	0	iscf =	7	xclevel =	1	lmnmax =	4
lnmax =	4	mband =	50	mffmem =	1	mgfft =	80
P mkmem =	8	mkqmem =	8	mklmem =	8	mpssoang =	3
mpw =	23125	mqgrid =	3001	natom =	12	nfft =	414720
nkpt =	64	nloalg =	4	nspden =	1	nspinor =	1
nsppl =	1	nsym =	8	nlxccc =	0	ntypat =	2
occopt =	1						

=====

P This job should need less than

Rough estimation (10% accuracy) of disk space for files :

WF disk file : 1129.152 Mbytes

DEN or POT disk file : 3.166 Mbytes.

548.172 Mbytes of memory.

↓

disk

↓

RAM

## “Hardware”

- RAM
- diskovni prostor
- mreža
- broj procesora

## “Software”

- prevoditelji
- knjižnice

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### Sigurnost

- pouzdanost sustava
- zaštita

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- diskovni prostor
- mreža
- broj procesora

### "Software"

- prevoditelji
- knjižnice

### Sigurnost

- pouzdanost sustava
- zaštita

### Podrška

- pomoć pri problemima u radu
- pri registraciji i obnavljanju certifikata

## Što je problem bio prije...danas više nije(?)

- 1 dohvat međurezultata ~> *remote-scratch-get* skripta
  - što ako ne znam kako se datoteka zove?
- 2 koliki je postotak iskorištenosti grid-a?
- 3 raspodjela poslova po krosnicima
- 4 broj korisnika u regiji ~> isti
- 5 automatsko osvježavanje certifikata ~> *myproxy-manage* skripta

Hvala na pozornosti!