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## Simulating experimental techniques: Kelvin Probe Force Microscopy NanoTechnology-NN22

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Horizon 2020

*NanoTechnology-NN22*



# Simulating experimental techniques : Kelvin Probe Force Microscopy

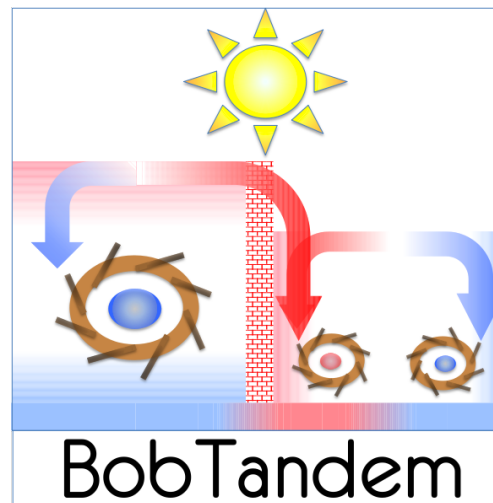
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<sup>4</sup> Silvaco Europe, Cambridge, UK



## *Summary*

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- Kelvin probe force microscopy : an introduction
- Analytical and numerical methods
- Simulating the experiment

# *Kelvin probe force microscopy*

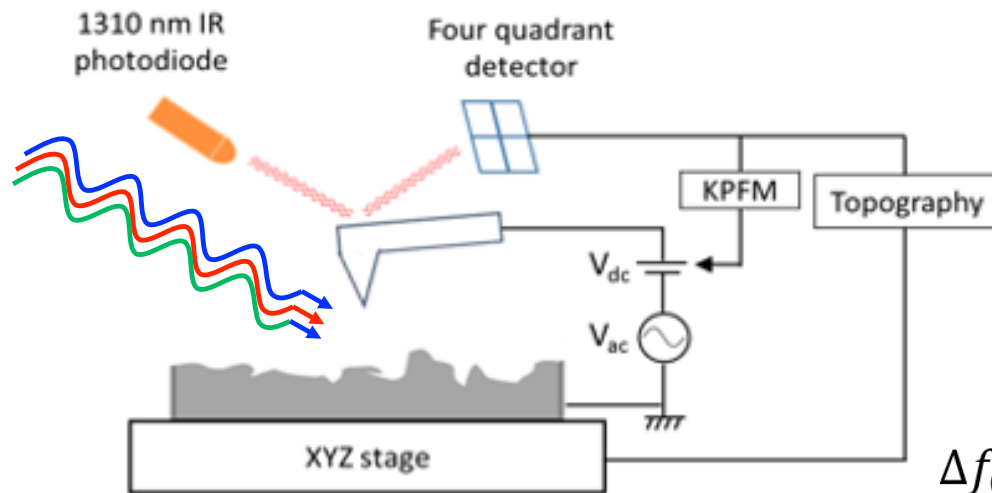
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- Measurement of **surface voltage** versus **incident photon energy**
- **Surface Photovoltage embodiment** : Light signal minus dark as a function of photon energy
- Semiconductor materials (surfaces, interfaces, and bulk) and optoelectronic devices
- Contactless technique and non destructive
- No need sample preparation or junction fabrication
- Information extracted : semiconductor type (n or p), electronic transitions (band-to-band, defect-band), **diffusion length**, **minority carrier-lifetime**, open-circuit voltage...
- Challenge : Analysis of surface techniques dominated by surface defects

=> Solution : Modelling



# Kelvin probe force microscopy : The technique



Two-pass mode scanning :

- 1<sup>st</sup> topography
- 2<sup>nd</sup> KPFM

## Amplitude Modulation

$$F_{\omega} = \frac{\partial C}{\partial z} (V_{DC} - CPD) V_{AC} \cos(\omega t)$$

## Frequency Modulation

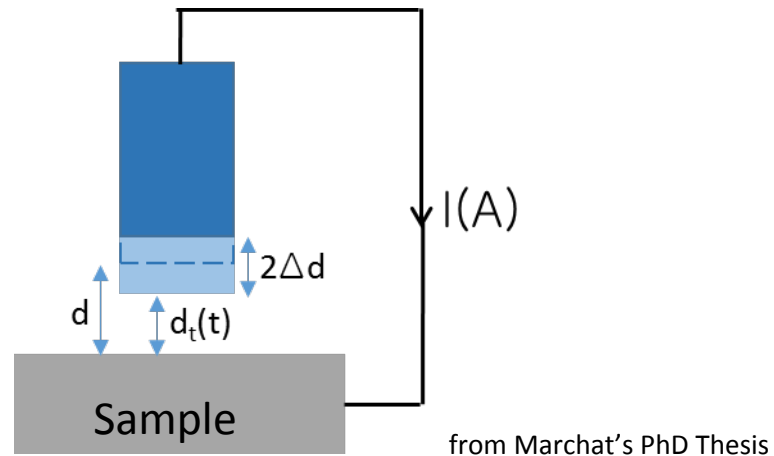
$$\Delta f_0(\omega) \propto \frac{\partial F_{\omega}}{\partial z} = \frac{\partial^2 C}{\partial z^2} (V_{DC} - CPD) V_{AC} \sin(\omega t)$$

$$CPD_{KPFM} = \frac{(W_{sonde} - W_{surf})}{q}$$

# *Kelvin probe force microscopy : basic principle*

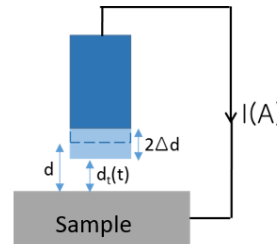
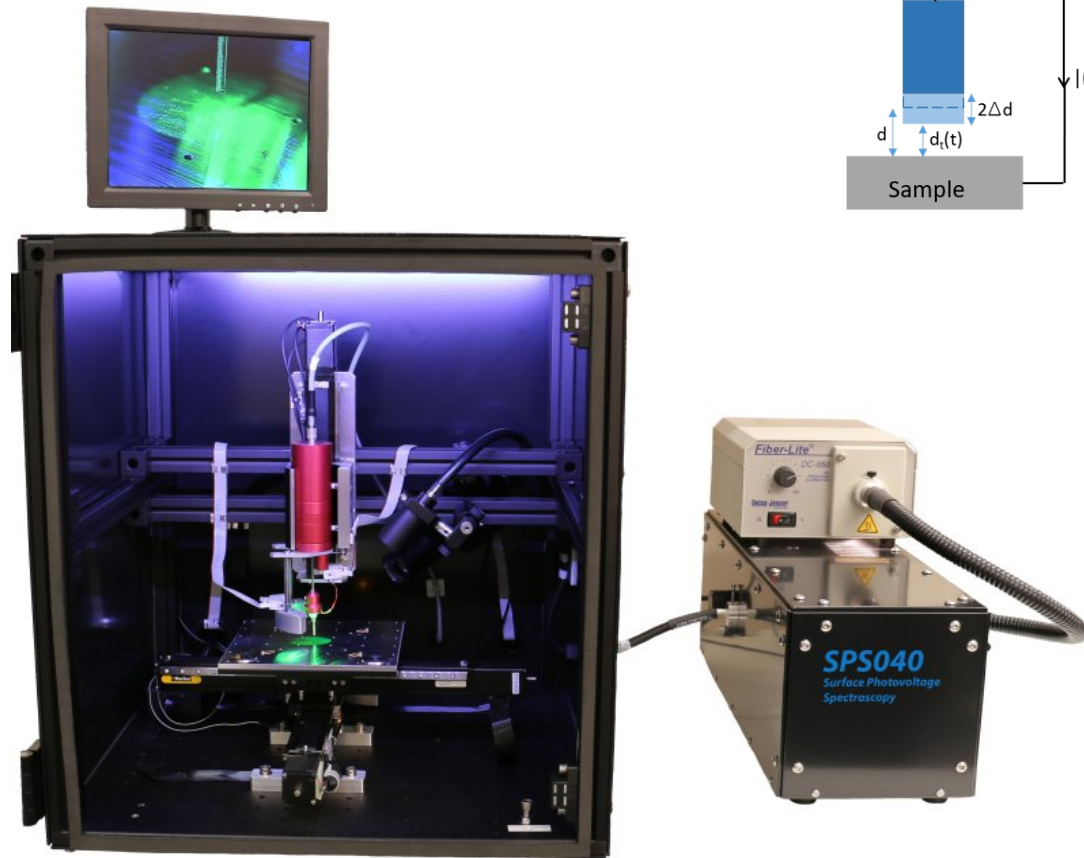
---

**DC light**



Vibrating probe/capacitor :  
**Kelvin probe**

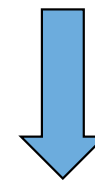
# Kelvin probe force microscopy : CPD and SPV



Surface Voltage or Contact  
Potential Difference (CPD)  
=> Work Function ( $W_F$ )

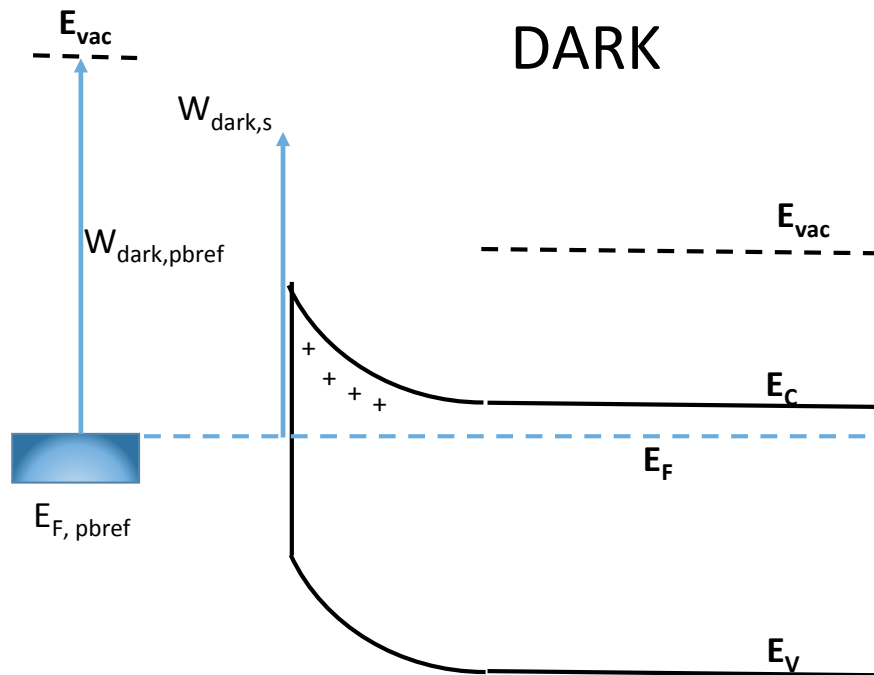


Lamp and Monochromator

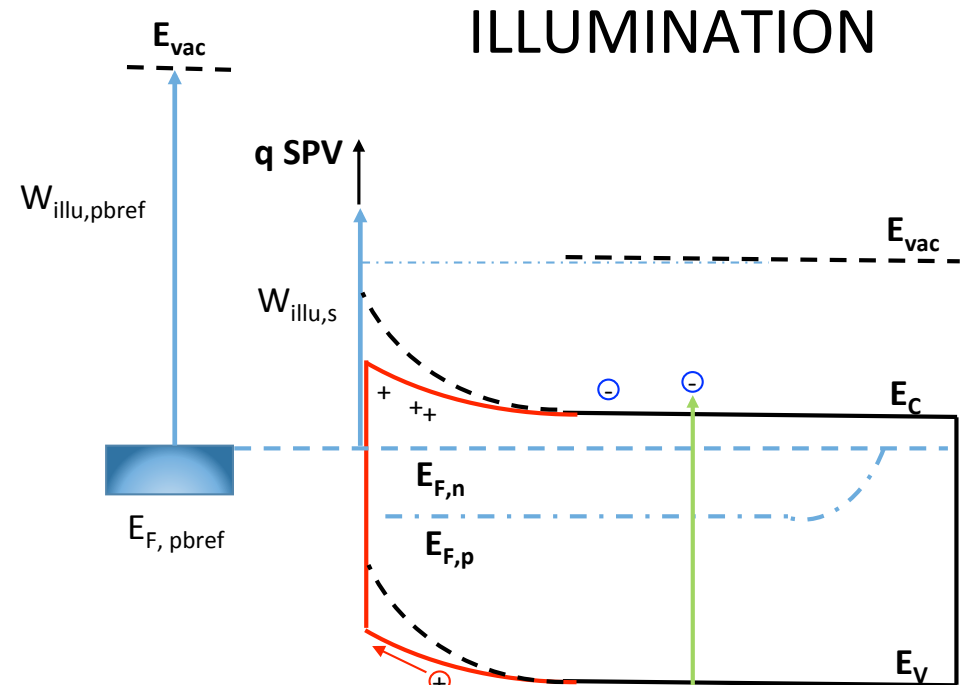


SPV-Spectroscopy

# Kelvin probe force microscopy : Surfaces



$$q \text{ CPD}_{\text{dark}} = W_{\text{dark, pbref}} - W_{\text{dark, s}}$$



$$q \text{ CPD}_{\text{illu}} = W_{\text{illu, pbref}} - W_{\text{illu, s}}$$

$$\text{SPV} = (\text{CPD}_{\text{illu}} - \text{CPD}_{\text{dark}}) = - (W_{\text{illu, s}} - W_{\text{dark, s}}) / q = (E_{F, p} - E_{F, n}) / q$$

**Dark :** Work function affected by surface states / charges  
**Light :** Signal modified by QFL splitting

## *Analytical / numerical models sketch:*

---

### *Analytical model :*

- Charge :  $q(p-n+N_d-N_a)$  – electrons, holes, donors, acceptors
- Solve Poisson equation ([Matlab](#))

=> Surface field as a function of acceptor and donor defects

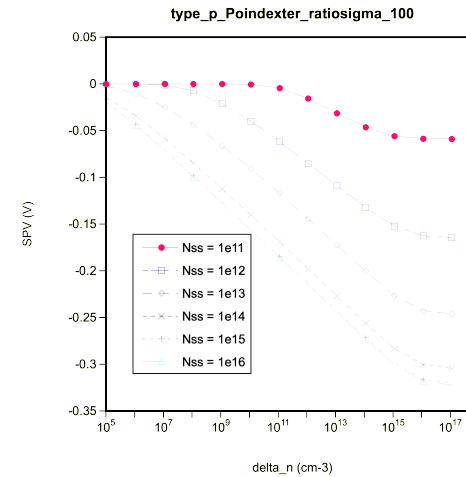
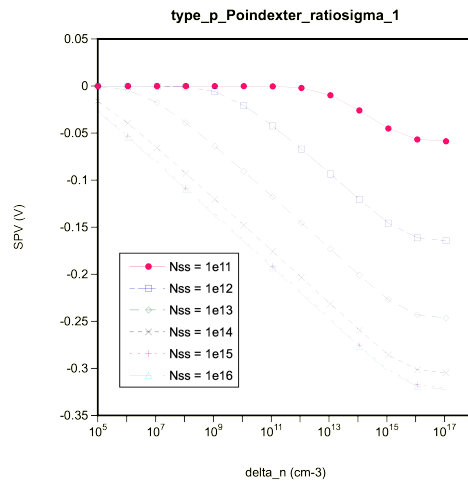
### *Numerical model :*

- Solve current and continuity numerically ([Silvaco](#))
- Arbitrary (within reason) defect distributions

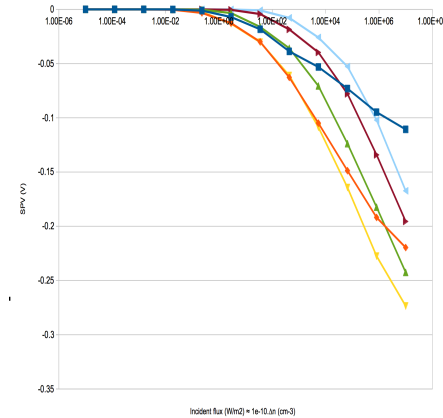
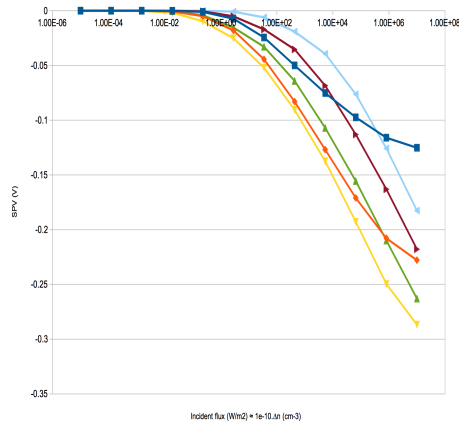
### *The object :*

- Bulk silicon
- 2D surface acceptor and donor defect states (analytical)
- 3D surface acceptor and donor defect states (numerical)

# Analytical : equal trap capture cross section



# Numerical : equal trap capture cross section

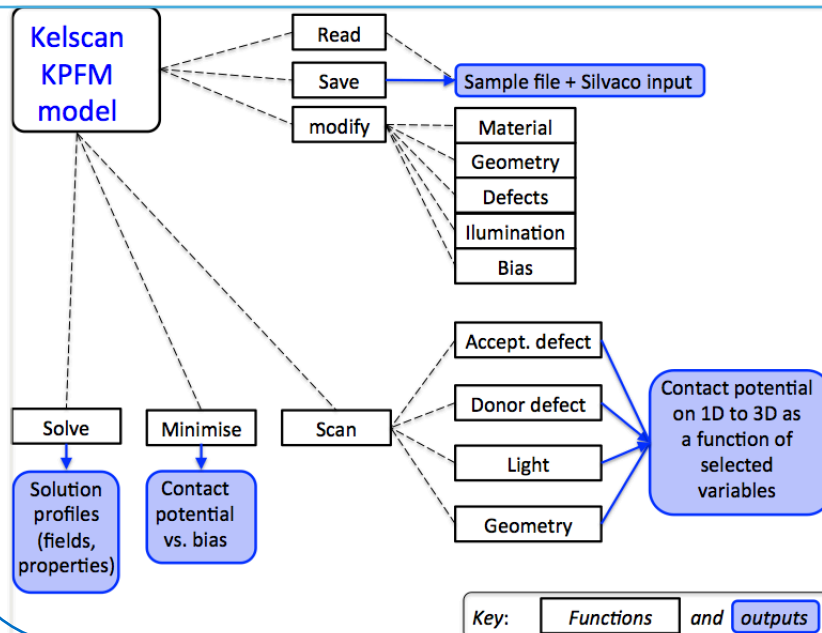


=> qualitative agreement in trends – future work.

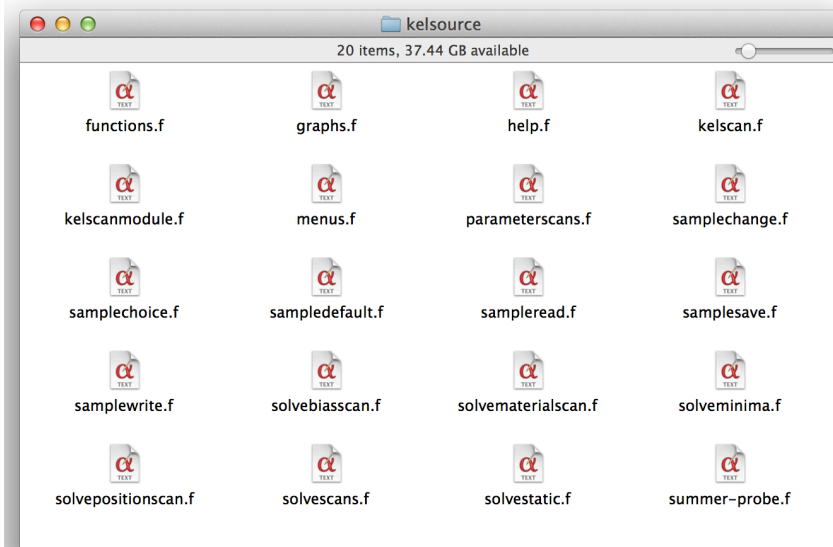
# Scanning KPFM modelling:

- Dynamic simulation :                      Computationally intensive  
   Requires software development
- Static simulation :                              Solve work function statically  
   Sequentially move the probe
- Method :    Call numerical software as computational engine  
   Develop driver software "**KELSCAN**"

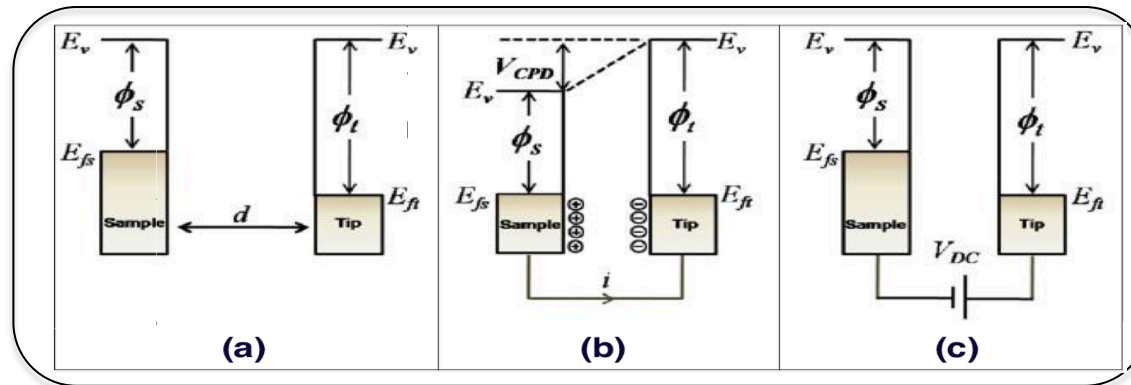
Flowchart:



Files ( $\approx$  5000 lines):



# Reminder : Kelvin Probe Force Microscopy KPFM



Kelvin probe force microscopy: work function measurement.

(a) Sample and tip far apart.

(b) Sample and tip in contact: Fermi levels align, current flows. The vacuum level step:  $V_{CPD}$

(c) External applied bias equal to  $V_{CPD}$  equilibrates vacuum levels.

=> Known KPFM tip vacuum and  $V_{CPD}$  levels gives sample work function.

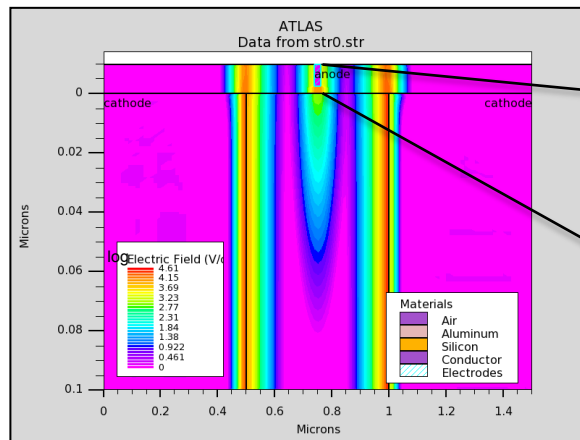


Fig. 2

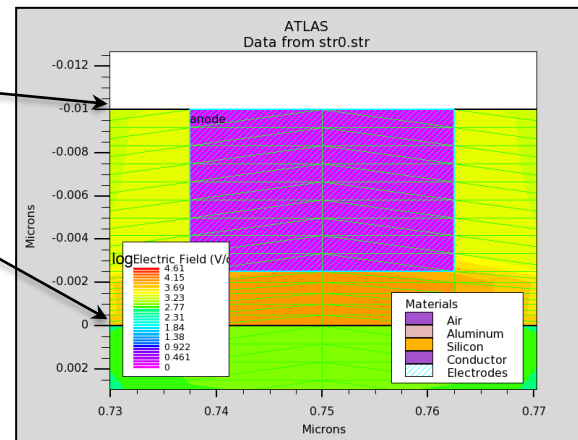
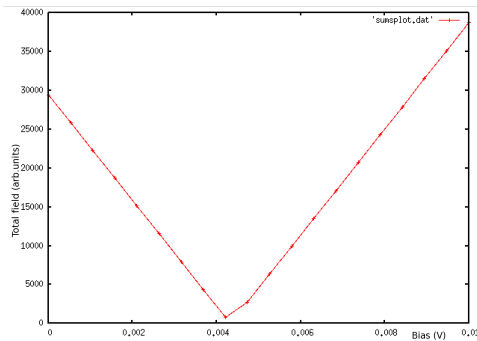


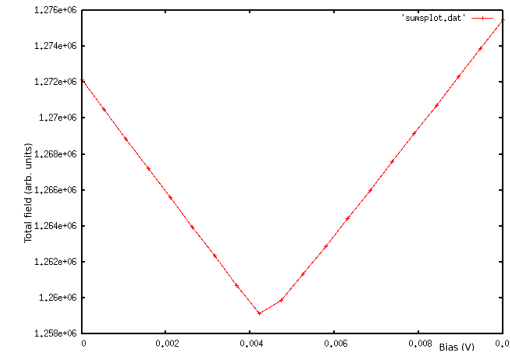
Fig. 3



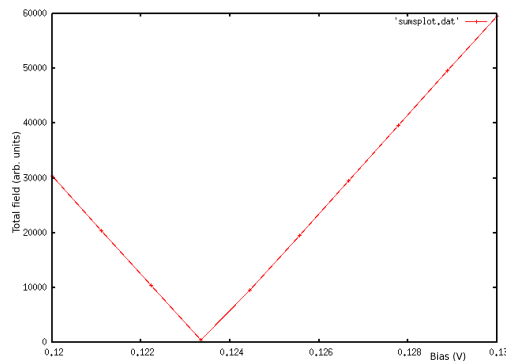
# Solution method : minimum tip / probe field



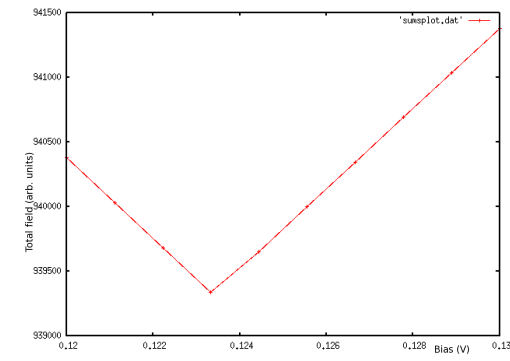
No defects: "Gap" field as a function of applied bias:  
Minimum  $\approx 4\text{meV}$



"No defects: Bulk" field as a function of applied bias:  
Minimum  $\approx 4\text{meV}$



"Gap" field as a function of applied bias: Minimum  $\approx 50\text{meV}$



"Bulk" field as a function of applied bias: Minimum  $\approx 50\text{meV}$

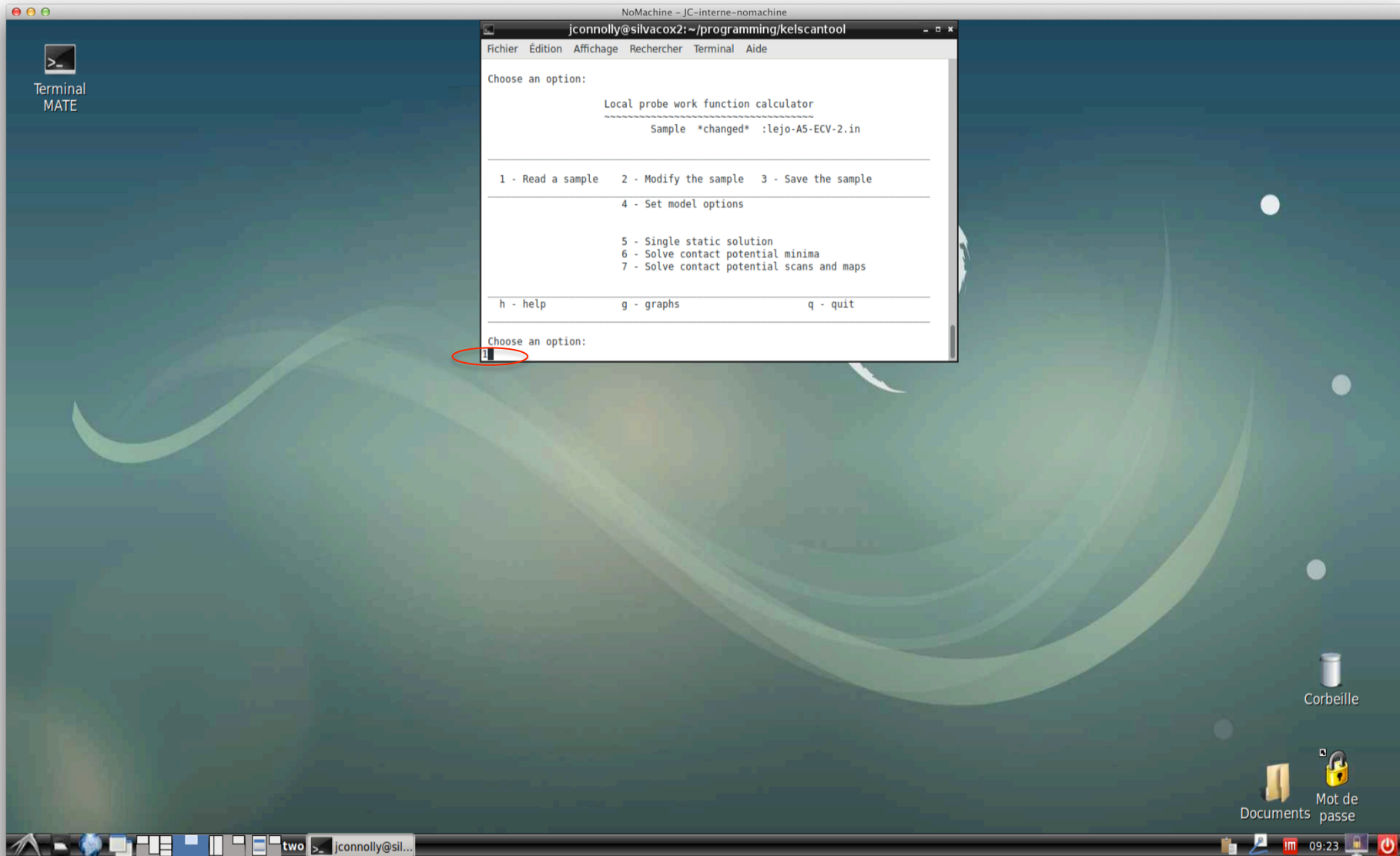
"Gap" / "Bulk" methods for Vcpd comparison :

- Little difference for these doping levels
- Differences nevertheless expected

**$\Rightarrow$  Rapid "gap" or spot method preferred**

# Kelscan demonstration

Splash screen choice "1" – choose sample



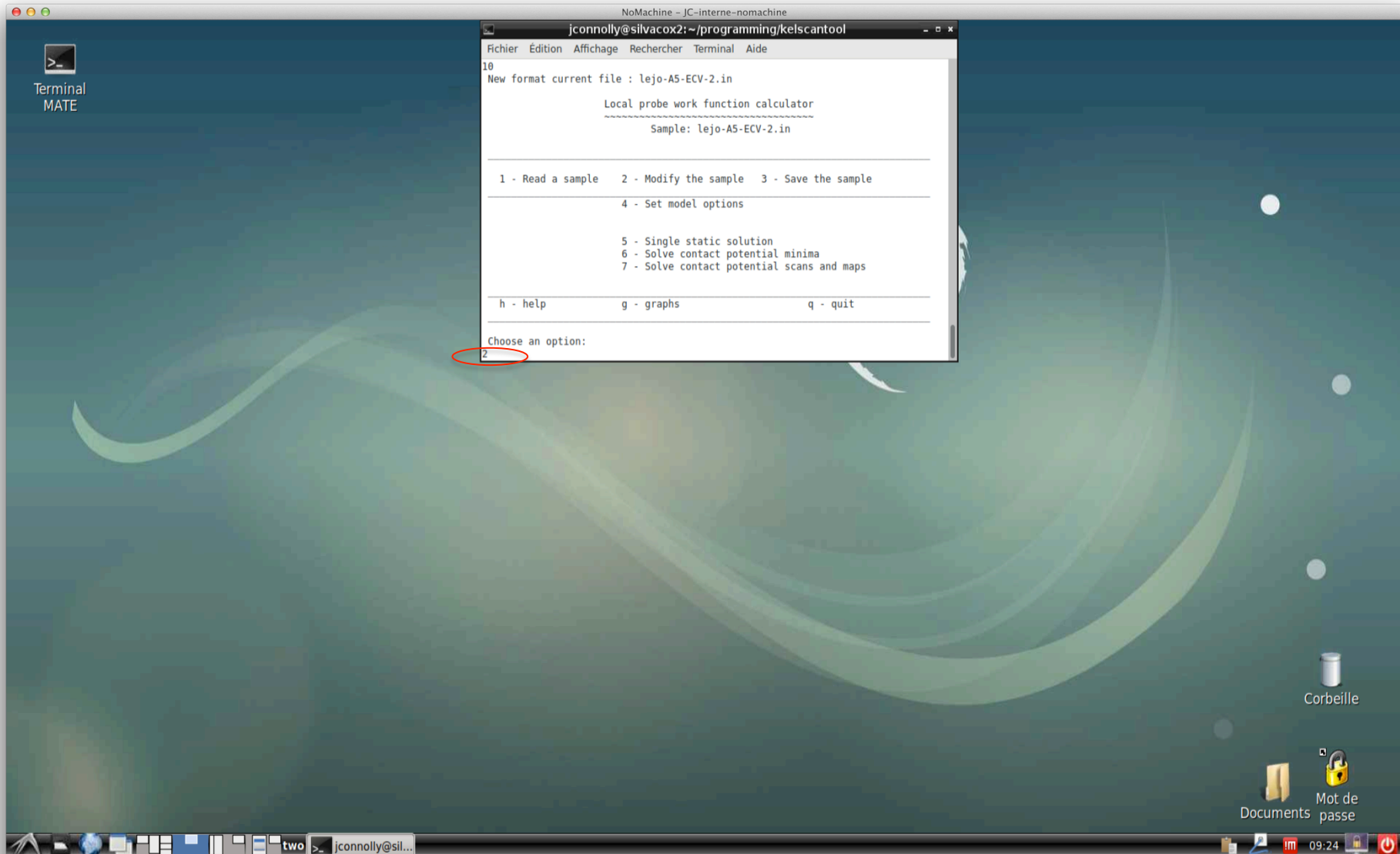
# Kelscan demonstration

## Sample choice



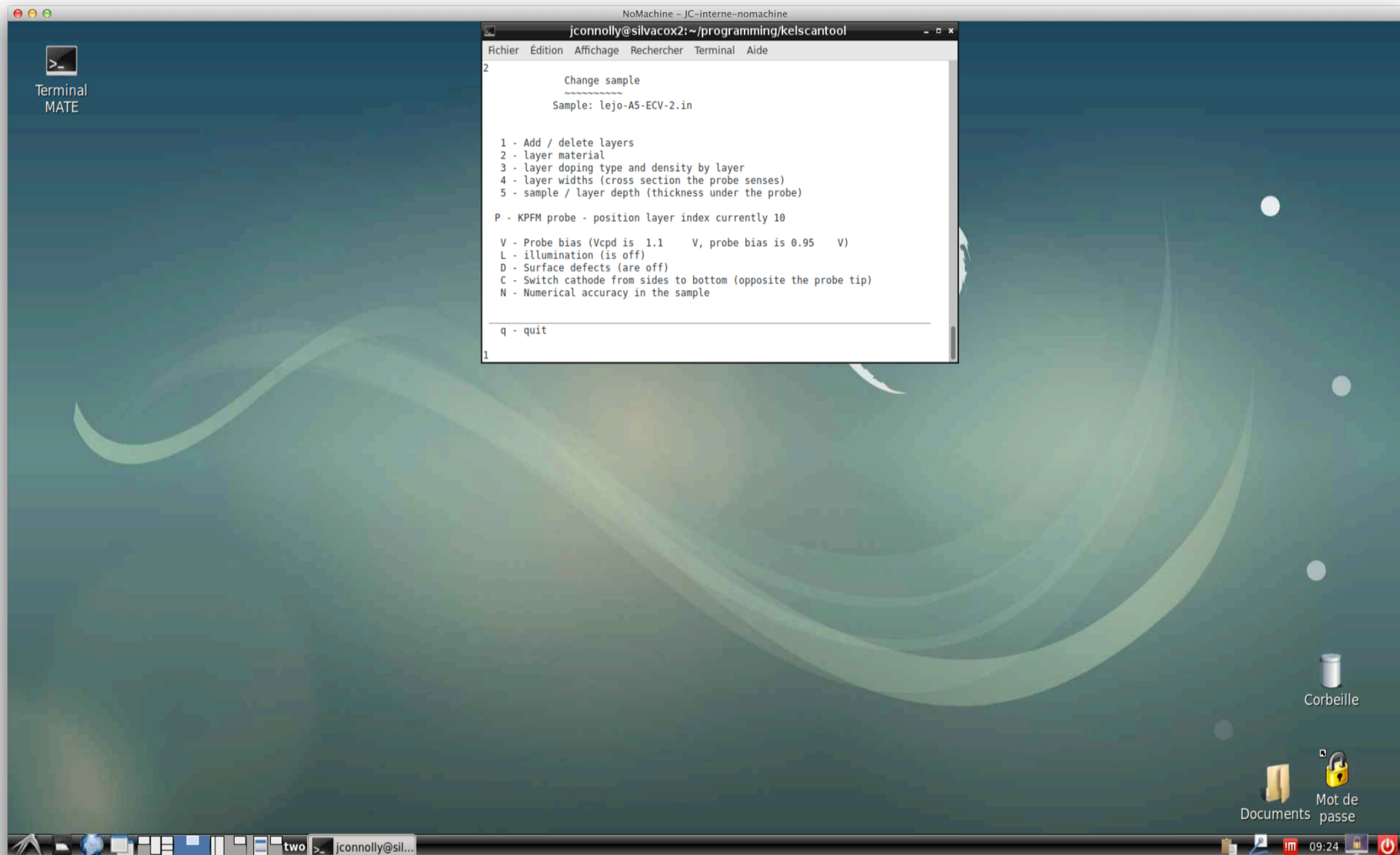
# Kelscan demonstration

## Sample modification menu



# Kelscan demonstration

The **sample file format**: Saves all simulation parameters shown here.  
Silvaco compatible : can be directly run by Silvaco Deckbuild



The screenshot shows a Linux desktop environment with a terminal window open. The terminal window title is "jconnolly@silvaco2: ~/programming/kelscantool". The terminal content displays the Kelscan tool interface, which includes a menu bar (Fichier, Edition, Affichage, Rechercher, Terminal, Aide), a prompt "2", and a list of commands and options. The commands listed are: 1 - Add / delete layers, 2 - layer material, 3 - layer doping type and density by layer, 4 - layer widths (cross section the probe senses), 5 - sample / layer depth (thickness under the probe). The options listed are: P - KPFM probe - position layer index currently 10, V - Probe bias (Vcpd is 1.1 V, probe bias is 0.95 V), L - illumination (is off), D - Surface defects (are off), C - Switch cathode from sides to bottom (opposite the probe tip), N - Numerical accuracy in the sample, and q - quit. The terminal also shows a prompt "1" at the bottom left.

```

NoMachine - JC-interne-nomachine
jconnolly@silvaco2: ~/programming/kelscantool
Fichier Edition Affichage Rechercher Terminal Aide
2
  Change sample
  -----
  Sample: lejo-A5-ECV-2.in

1 - Add / delete layers
2 - layer material
3 - layer doping type and density by layer
4 - layer widths (cross section the probe senses)
5 - sample / layer depth (thickness under the probe)

P - KPFM probe - position layer index currently 10

V - Probe bias (Vcpd is 1.1 V, probe bias is 0.95 V)
L - illumination (is off)
D - Surface defects (are off)
C - Switch cathode from sides to bottom (opposite the probe tip)
N - Numerical accuracy in the sample

-----
q - quit
1
```

# Kelscan demonstration

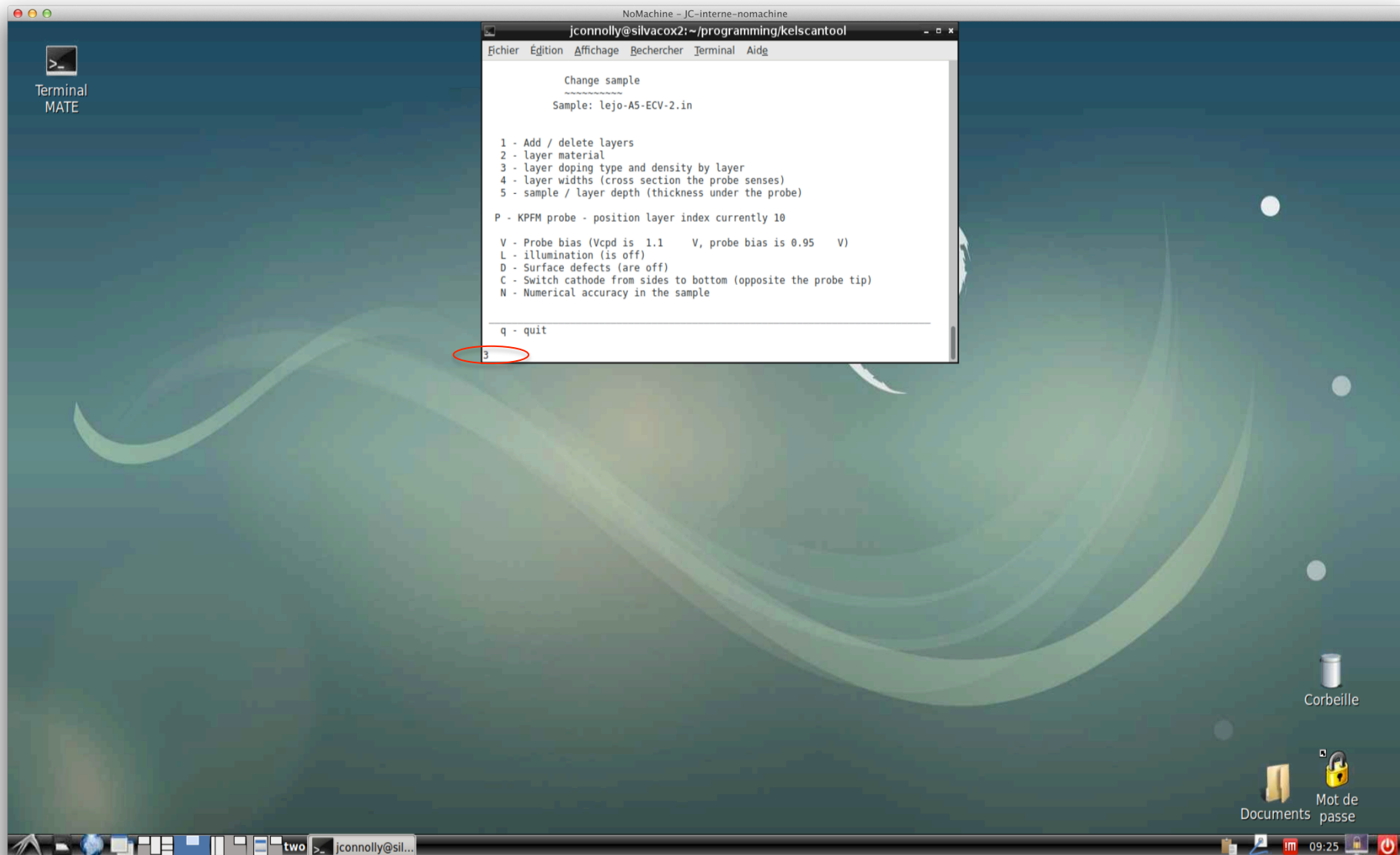
Sample properties of multi-layer sample simulating Lejo Joseph doping profile measurement

Index	Width (um)	Doping (/cm3)	Type (p or n)	Material (name)
1)	0.750E-01	0.280E+20	p	silicon
2)	0.750E-01	0.330E+20	p	silicon
3)	0.750E-01	0.313E+20	p	silicon
4)	0.750E-01	0.295E+20	p	silicon
5)	0.750E-01	0.249E+20	p	silicon
6)	0.750E-01	0.184E+20	p	silicon
7)	0.750E-01	0.133E+20	p	silicon
8)	0.750E-01	0.723E+19	p	silicon
9)	0.750E-01	0.173E+19	p	silicon
10)	0.750E-01	0.261E+18	p	silicon
11)	0.750E-01	0.108E+18	n	silicon
12)	0.750E-01	0.178E+18	n	silicon
13)	0.750E-01	0.180E+18	n	silicon
14)	0.750E-01	0.150E+18	n	silicon
15)	0.750E-01	0.122E+18	n	silicon
16)	0.750E-01	0.214E+18	n	silicon
17)	0.750E-01	0.372E+16	n	silicon
18)	0.750E-01	0.512E+16	n	silicon
19)	0.750E-01	0.645E+16	n	silicon
20)	0.750E-01	0.117E+18	n	silicon

Add or delete (existing layers will be copied) ? (a/d or quit)

# Kelscan demonstration

## Doping levels



```

NoMachine - JC-interne-nomachine
jconnolly@silvacox2: ~/programming/kelscantool
Fichier Edition Affichage Rechercher Terminal Aide

Change sample
-----
Sample: lejo-A5-ECV-2.in

1 - Add / delete layers
2 - layer material
3 - layer doping type and density by layer
4 - layer widths (cross section the probe senses)
5 - sample / layer depth (thickness under the probe)

P - KPFM probe - position layer index currently 10

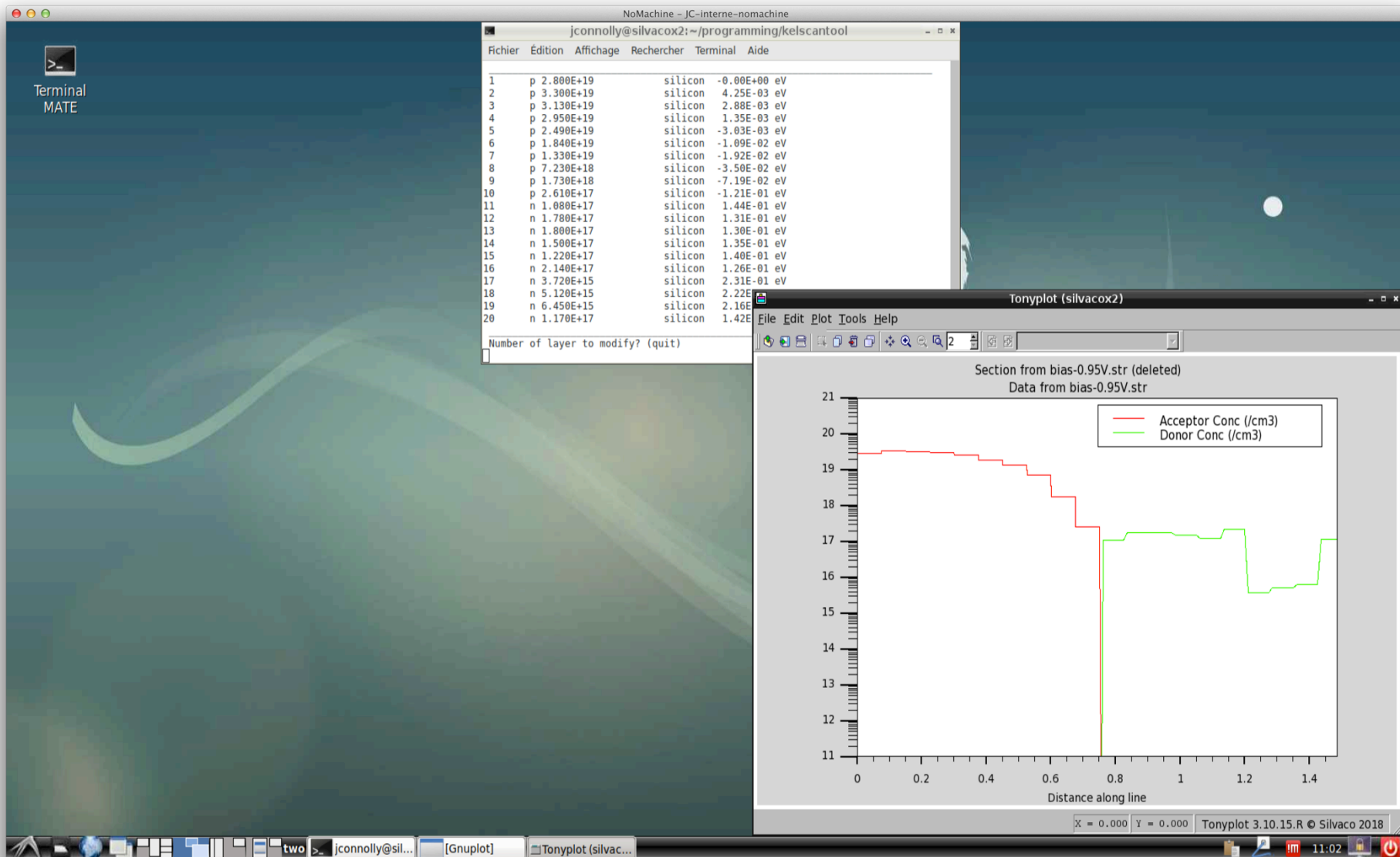
V - Probe bias (Vcpd is 1.1 V, probe bias is 0.95 V)
L - illumination (is off)
D - Surface defects (are off)
C - Switch cathode from sides to bottom (opposite the probe tip)
N - Numerical accuracy in the sample

q - quit
3

```

# Kelscan demonstration

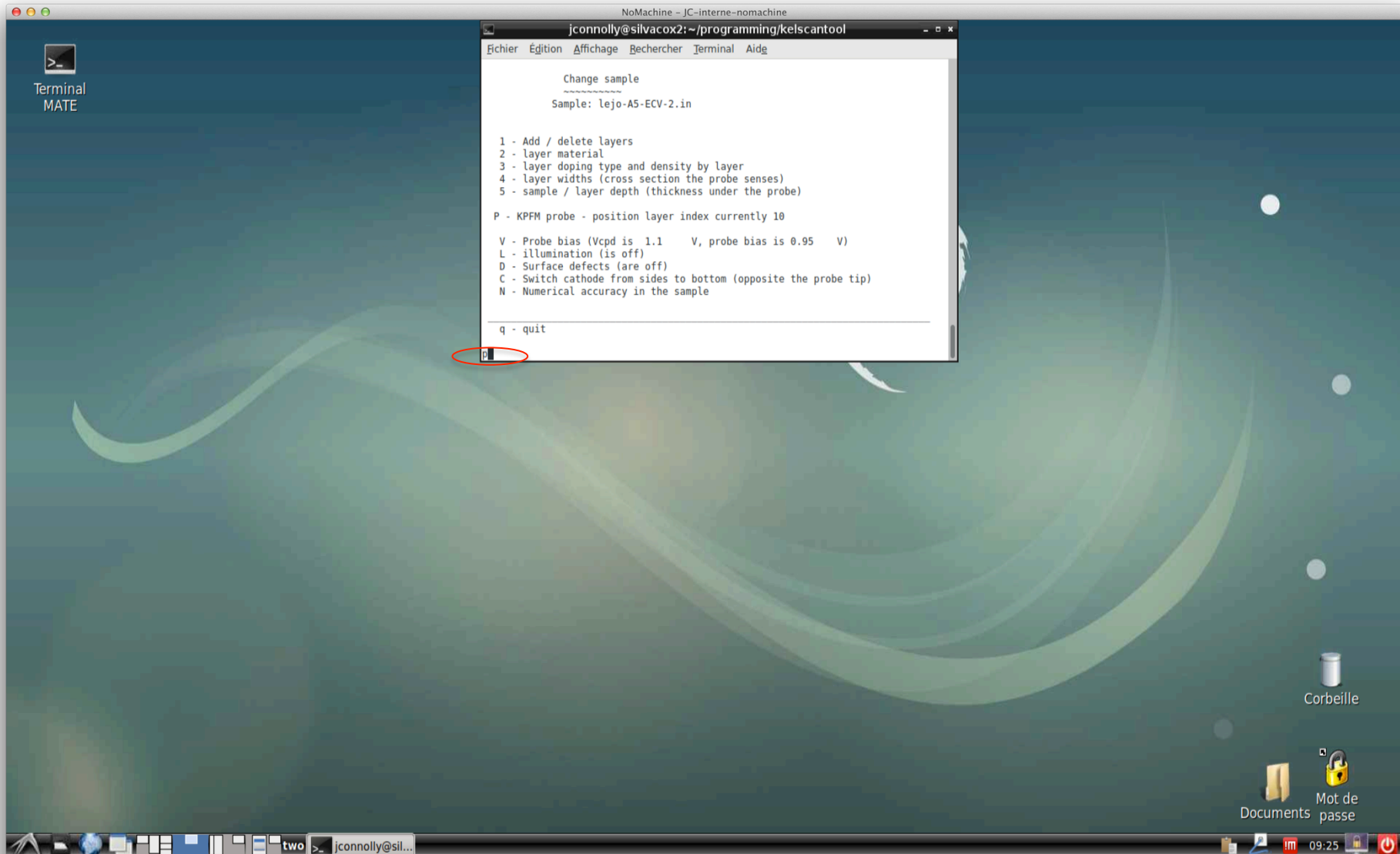
## Doping levels and tonyplot doping graph





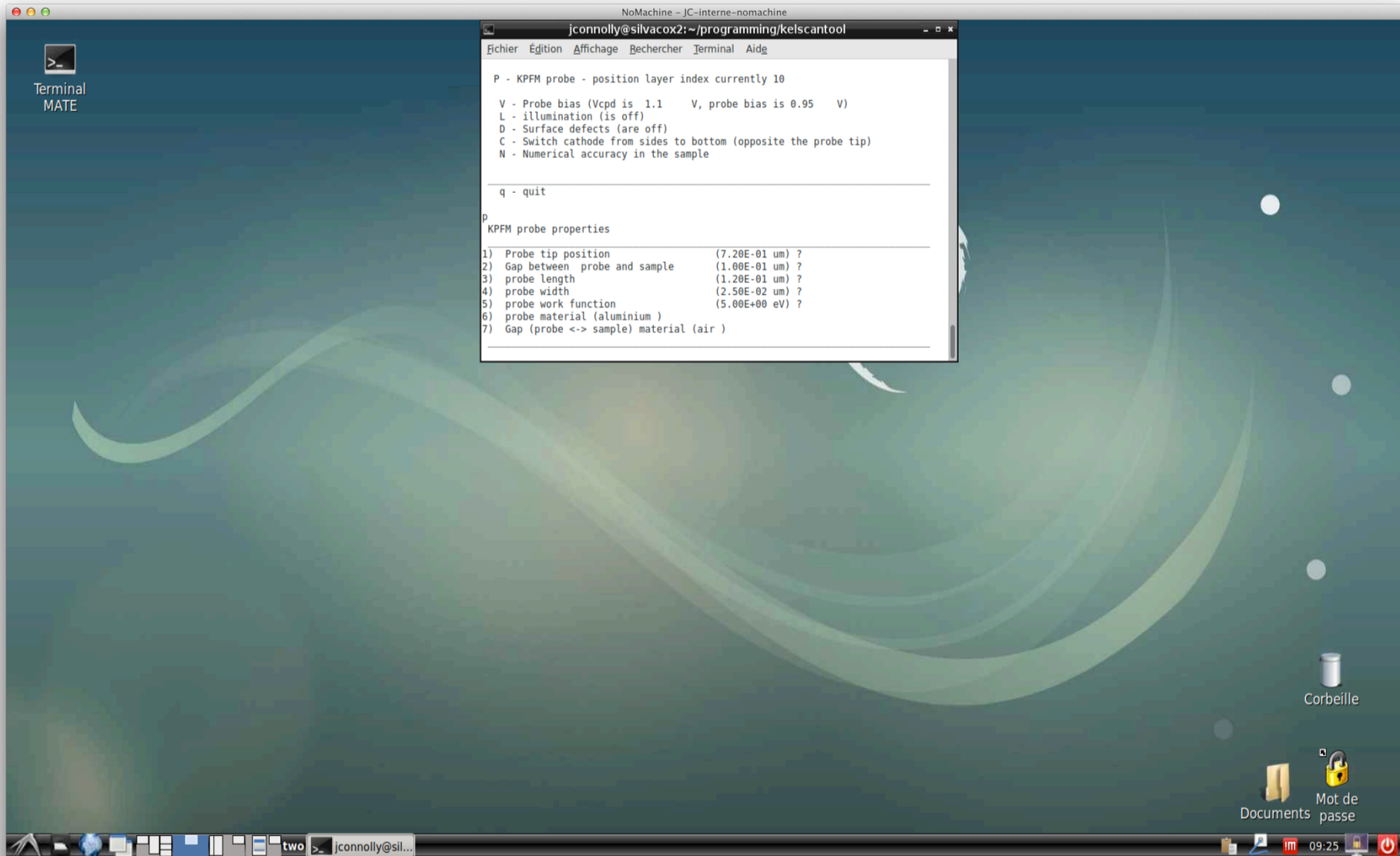
# Kelscan demonstration

## Sample modify – KPFM probe



# Kelscan demonstration

## Sample modify – KPFM probe properties



The screenshot shows a terminal window titled "jconnolly@silvacox2:~/programming/kelscantool". The terminal displays the following text:

```
Fichier Edition Affichage Rechercher Terminal Aide

P - KPFM probe - position layer index currently 10

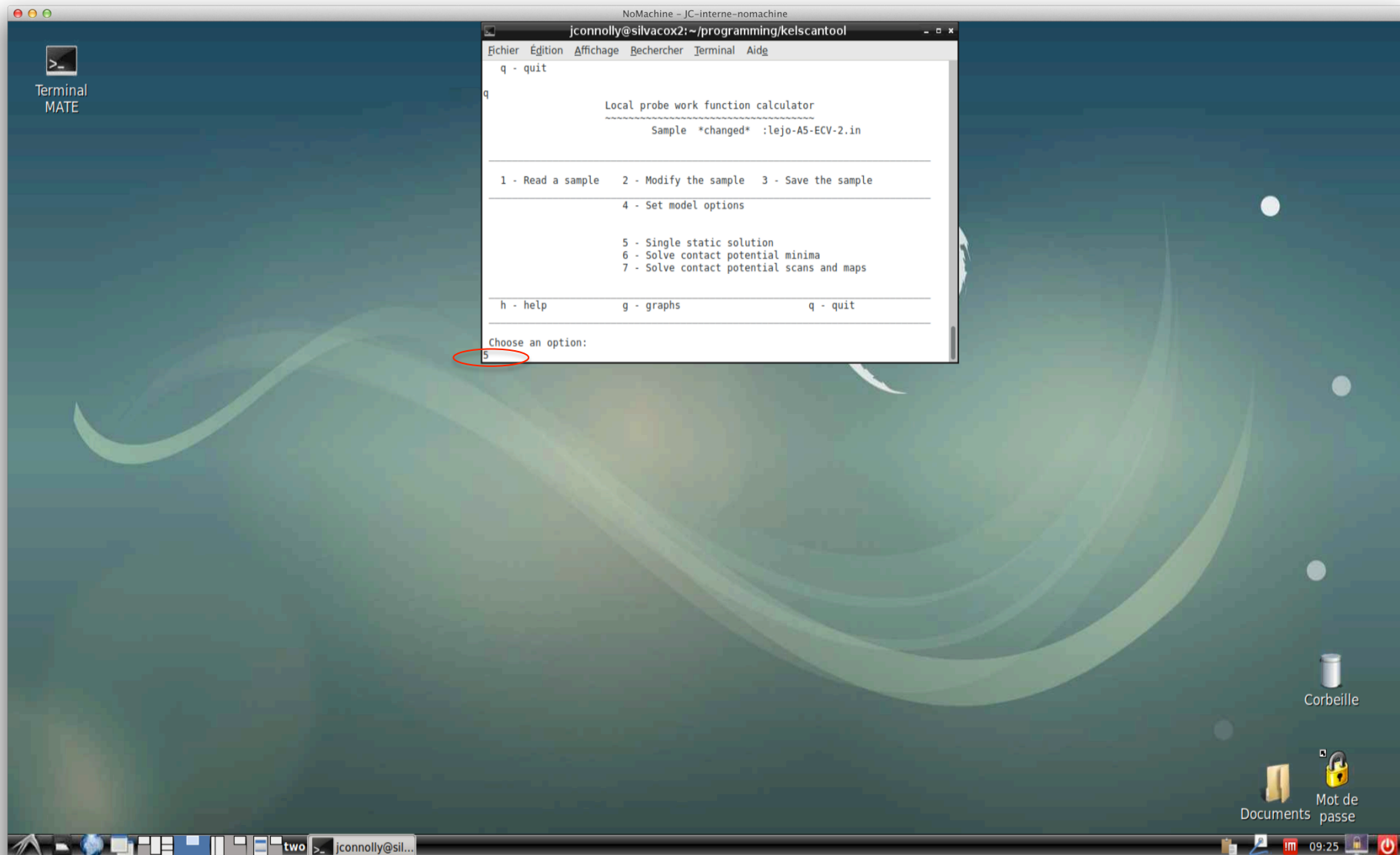
V - Probe bias (Vcpd is 1.1 V, probe bias is 0.95 V)
L - illumination (is off)
D - Surface defects (are off)
C - Switch cathode from sides to bottom (opposite the probe tip)
N - Numerical accuracy in the sample

q - quit

P
KPFM probe properties
-----
1) Probe tip position (7.20E-01 um) ?
2) Gap between probe and sample (1.00E-01 um) ?
3) probe length (1.20E-01 um) ?
4) probe width (2.50E-02 um) ?
5) probe work function (5.00E+00 eV) ?
6) probe material (aluminium)
7) Gap (probe <-> sample) material (air)
```

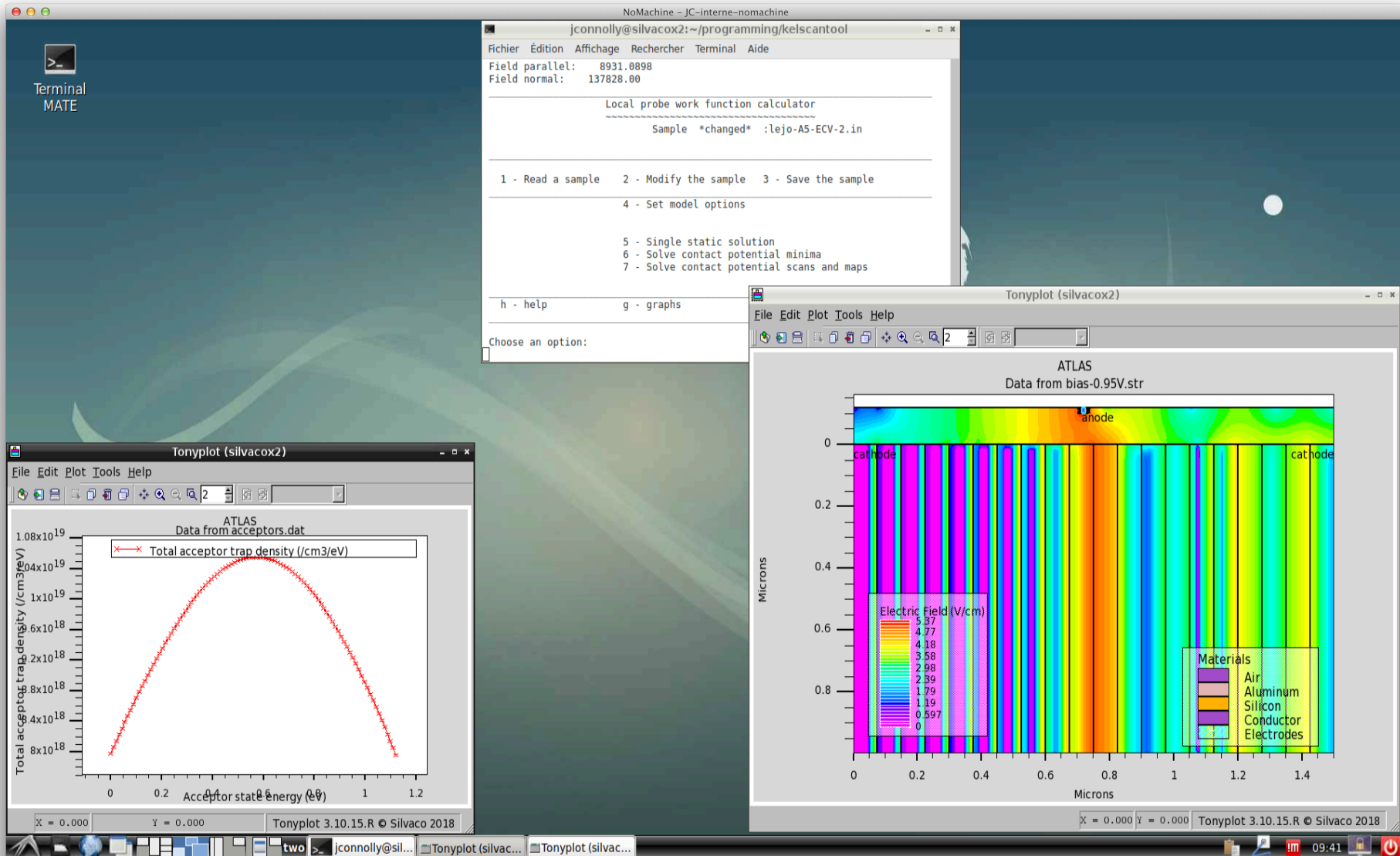
# Kelscan demonstration

Single solution of structure for specified structure including probe position, defects, and illumination



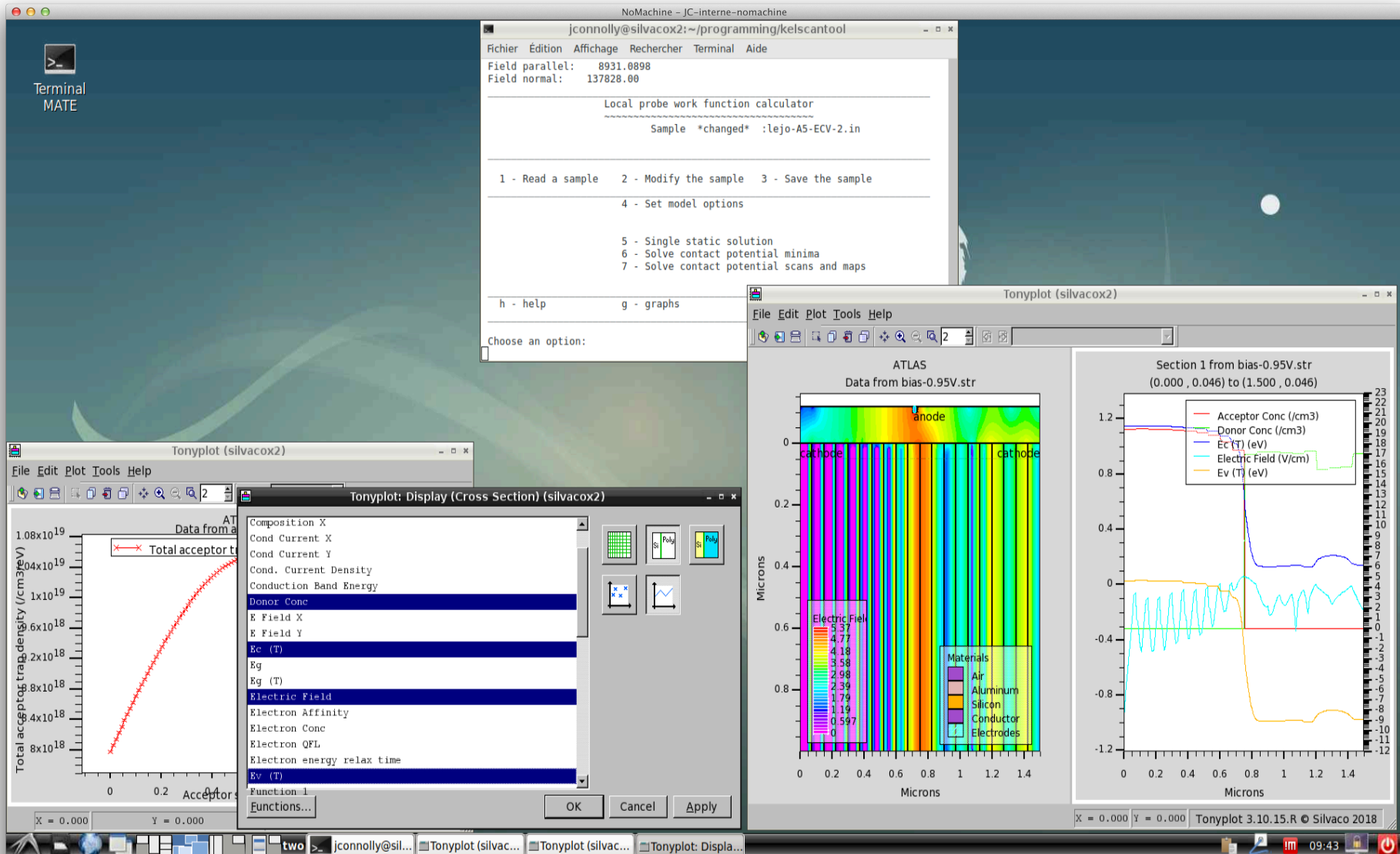
# Kelscan demonstration

Single solution showing acceptor type defects and fields in a multilayer structure



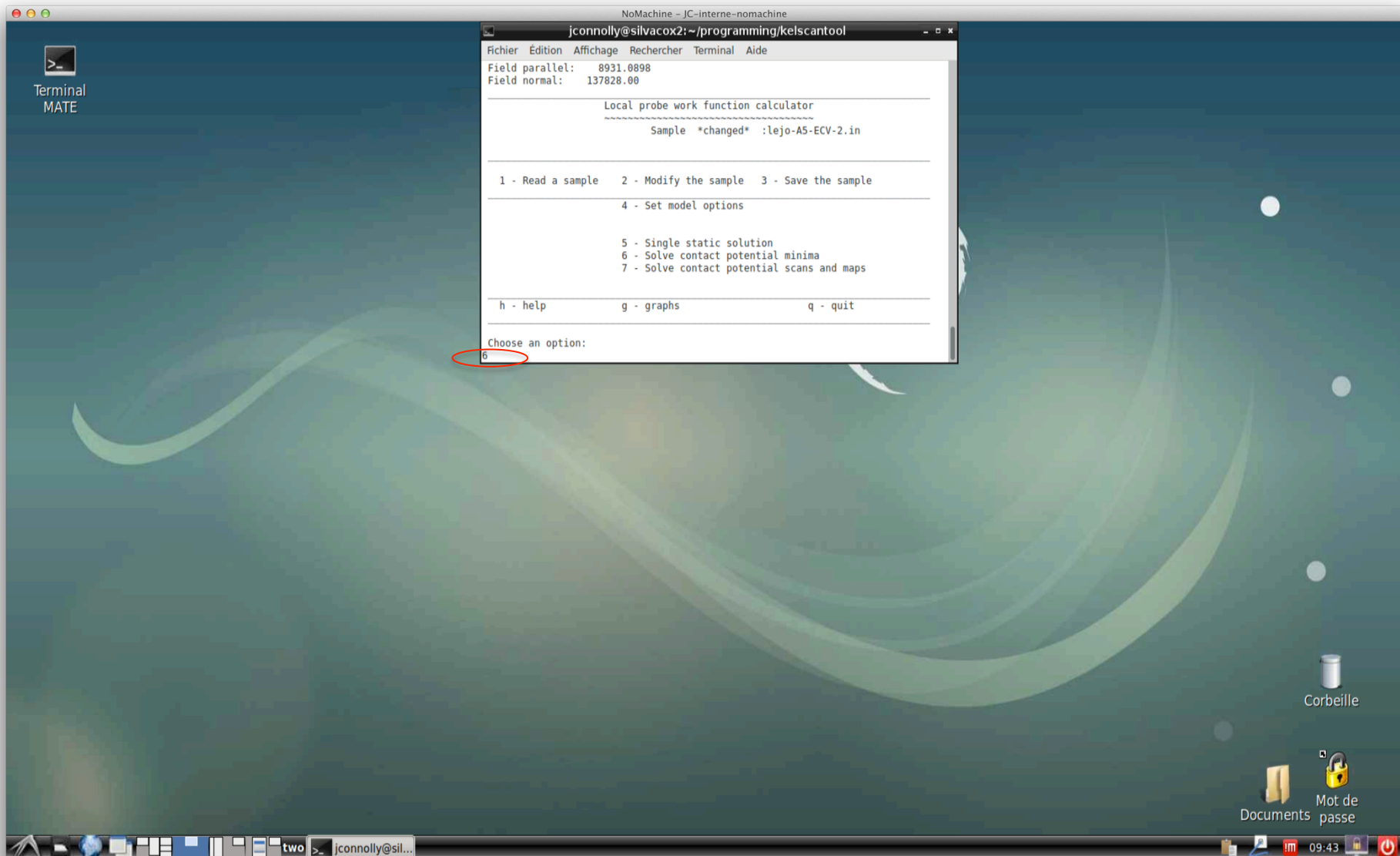
# Kelscan demonstration

Single solution Tonyplot parameter lists – here band structure and field



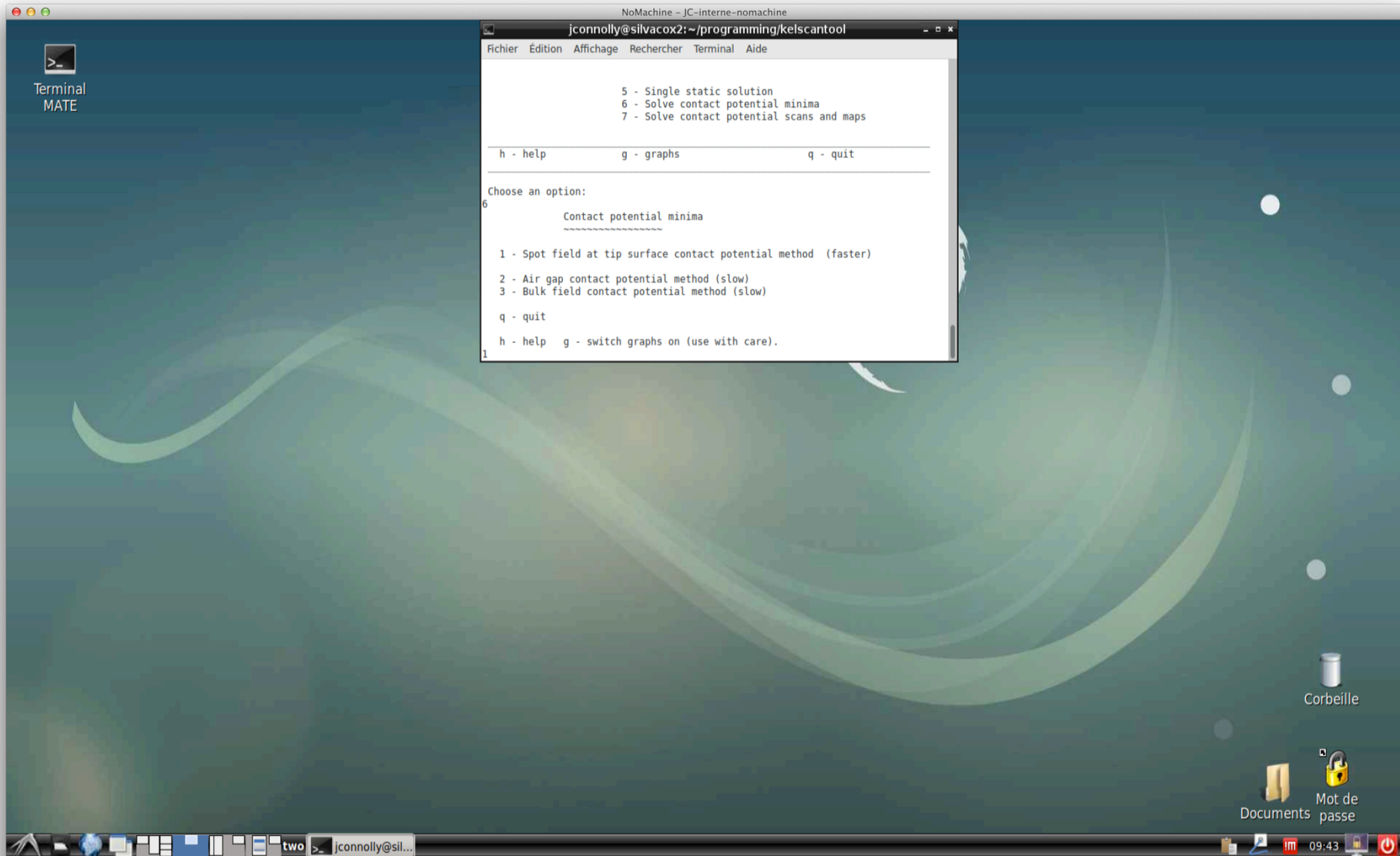
# Kelscan demonstration

The prime function : the contact potential solution



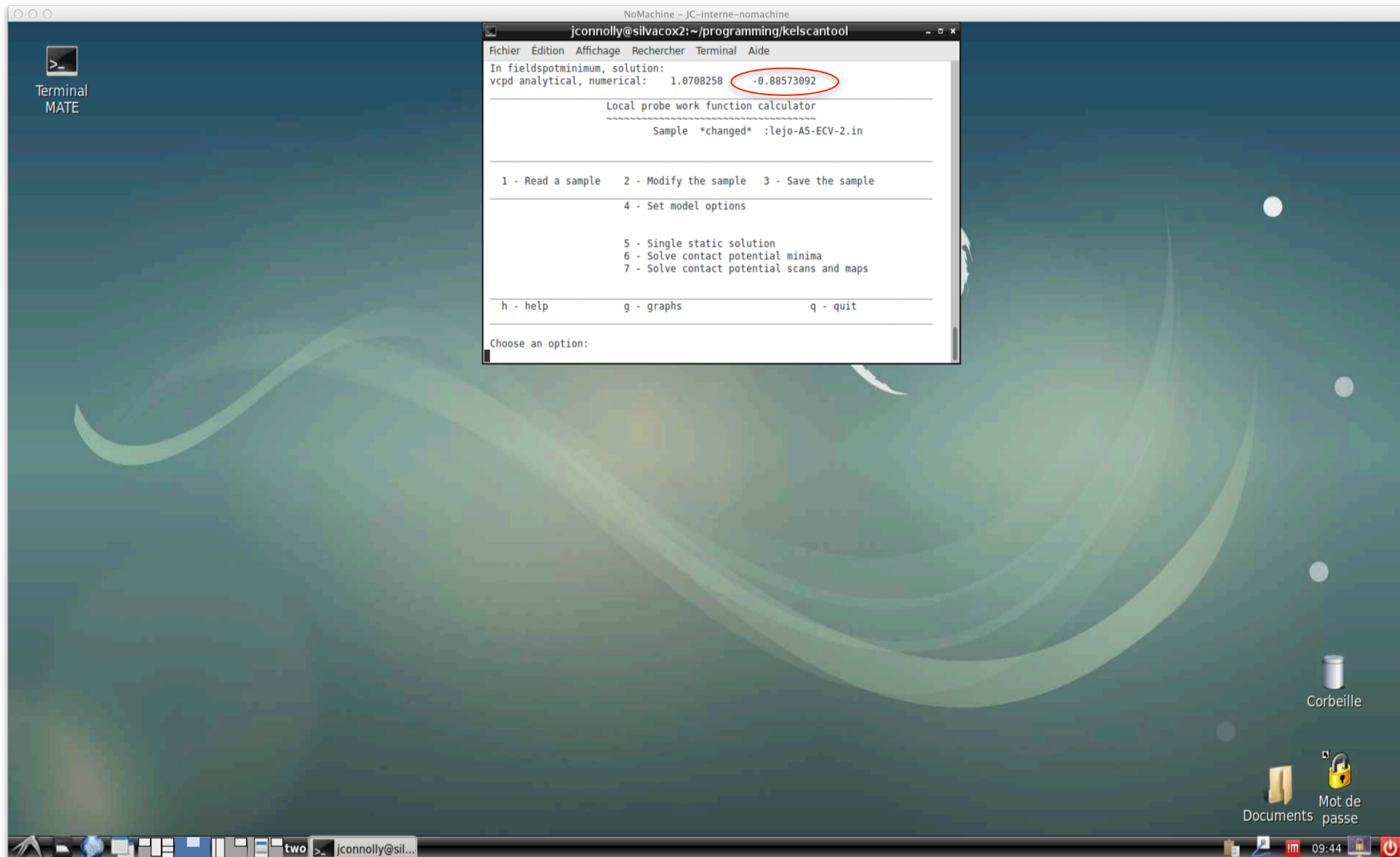
# Kelscan demonstration

A range of methods for flexibility: Spot method preferred (Speed).



# Kelscan demonstration

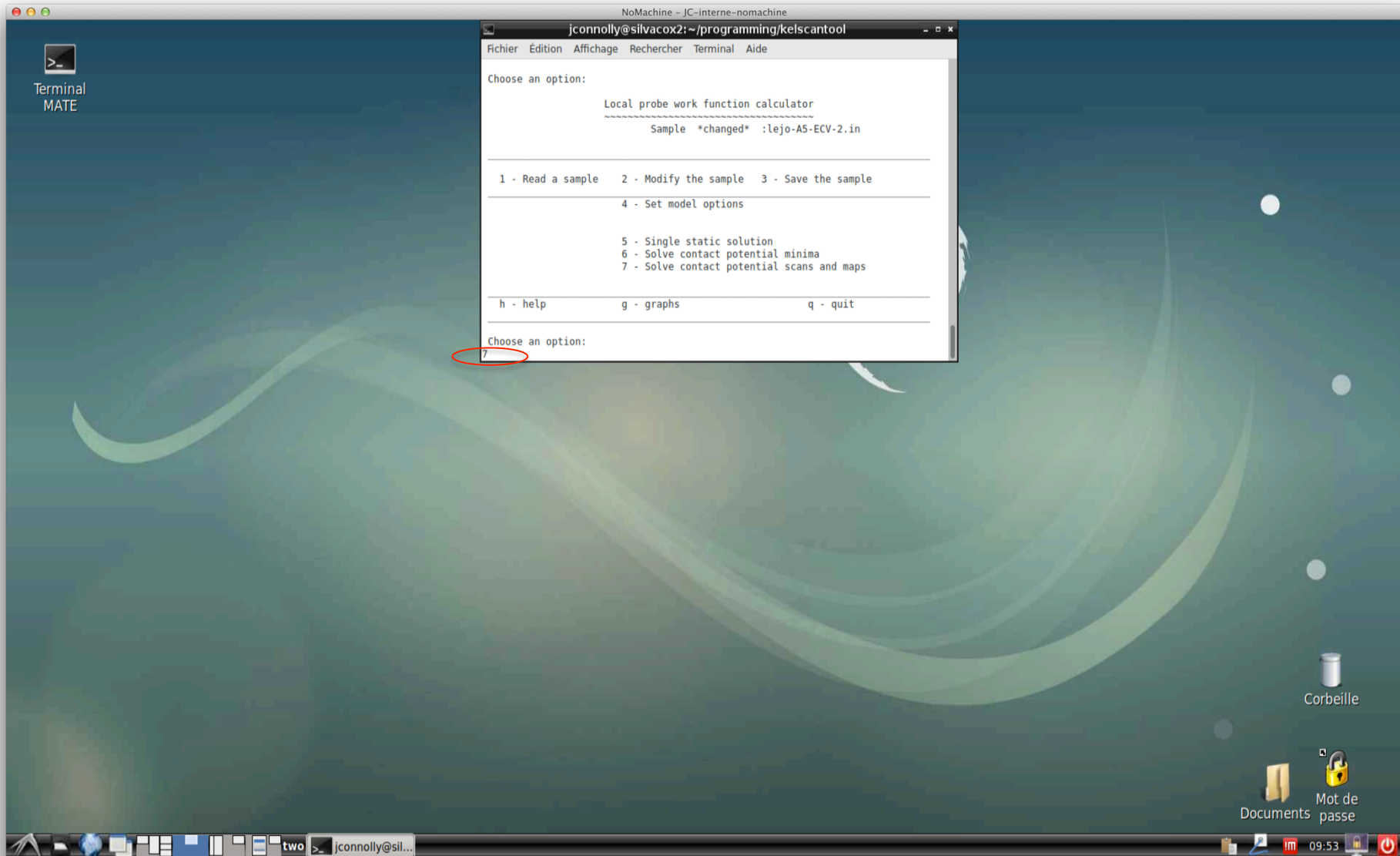
Contact potential evaluated from two points (assumes linearity)





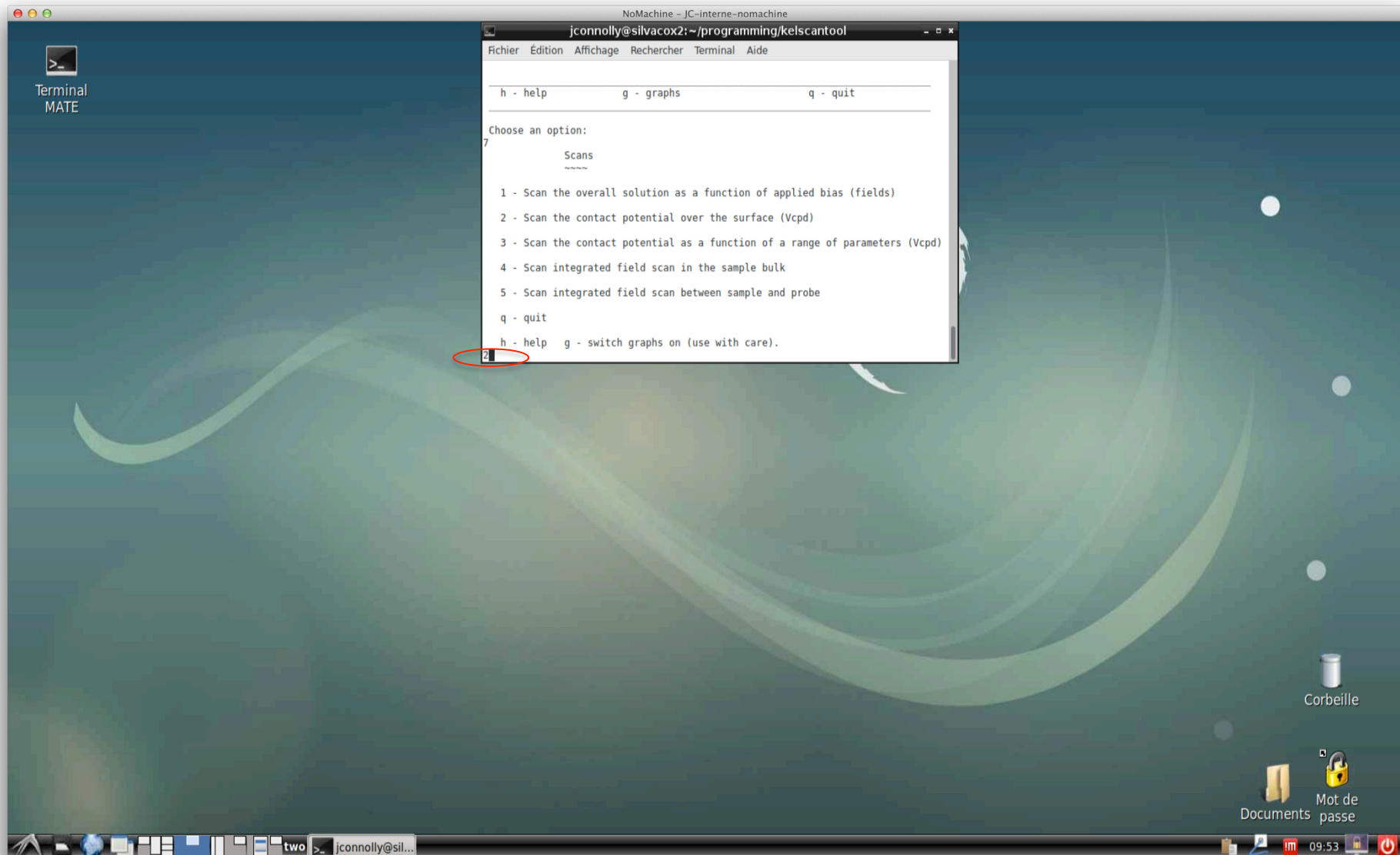
# Kelscan demonstration

## Contact potential scans



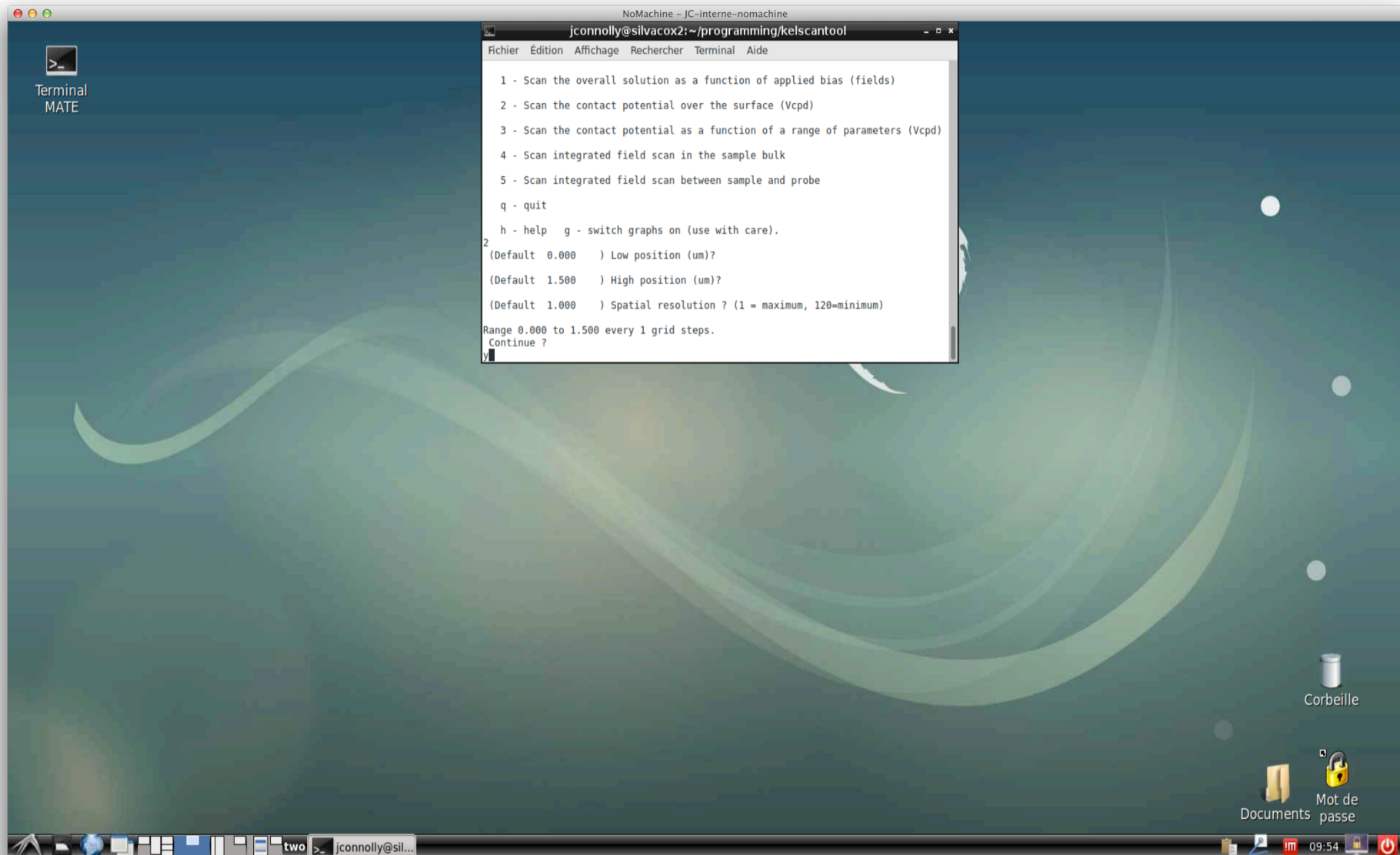
# Kelscan demonstration

## Contact potential scan over the surface



# Kelscan demonstration

Contact potential scan over the surface : range and resolution (integer grid spacing)



```

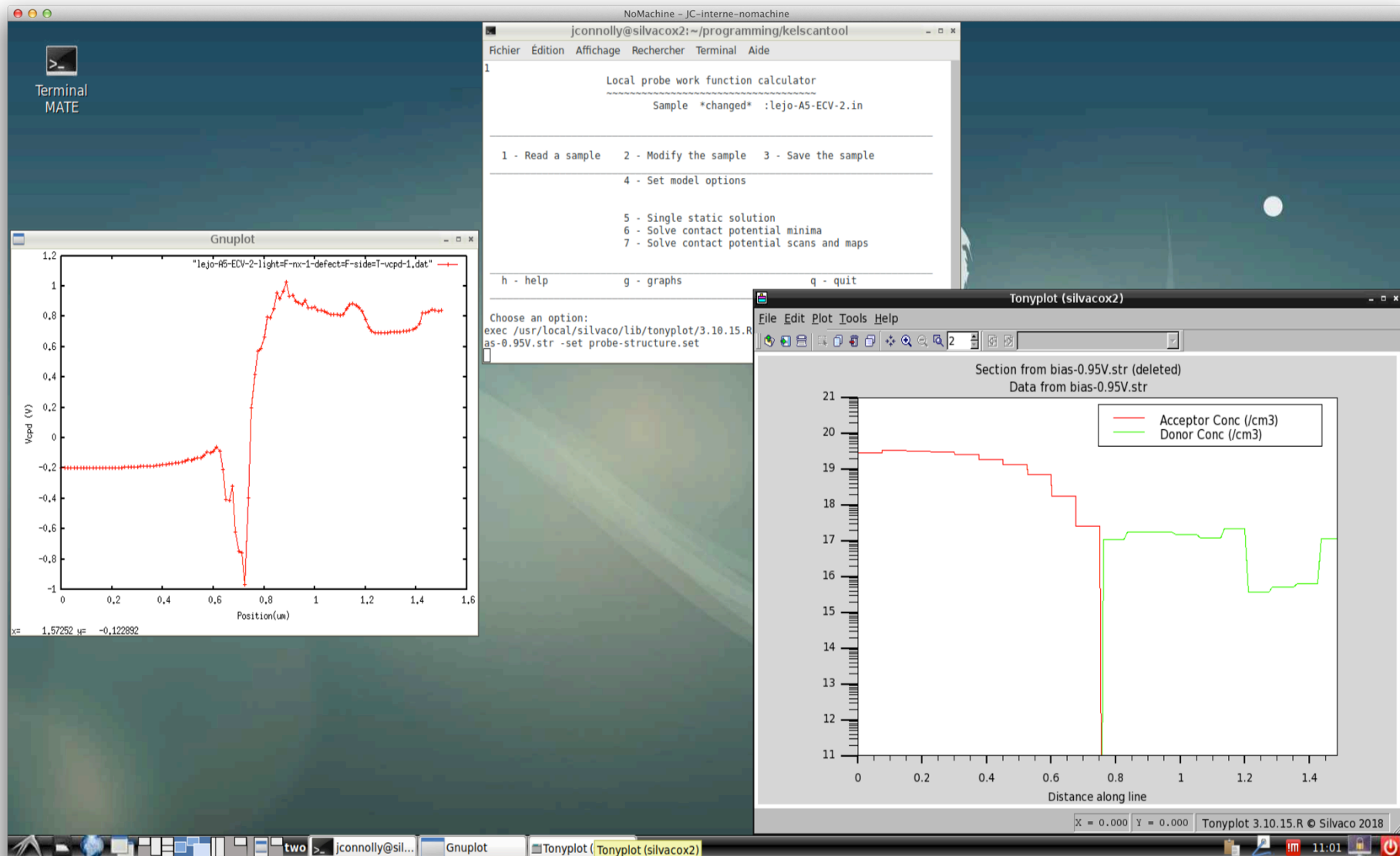
NoMachine - JC-interne-nomachine
jconnolly@silvacox2:~/programming/kelscantool
Fichier Edition Affichage Rechercher Terminal Aide

1 - Scan the overall solution as a function of applied bias (fields)
2 - Scan the contact potential over the surface (Vcpd)
3 - Scan the contact potential as a function of a range of parameters (Vcpd)
4 - Scan integrated field scan in the sample bulk
5 - Scan integrated field scan between sample and probe
q - quit
h - help g - switch graphs on (use with care).
2
(Default 0.000 ) Low position (um)?
(Default 1.500 ) High position (um)?
(Default 1.000 ) Spatial resolution ? (1 = maximum, 120=minimum)
Range 0.000 to 1.500 every 1 grid steps.
Continue ?
y

```

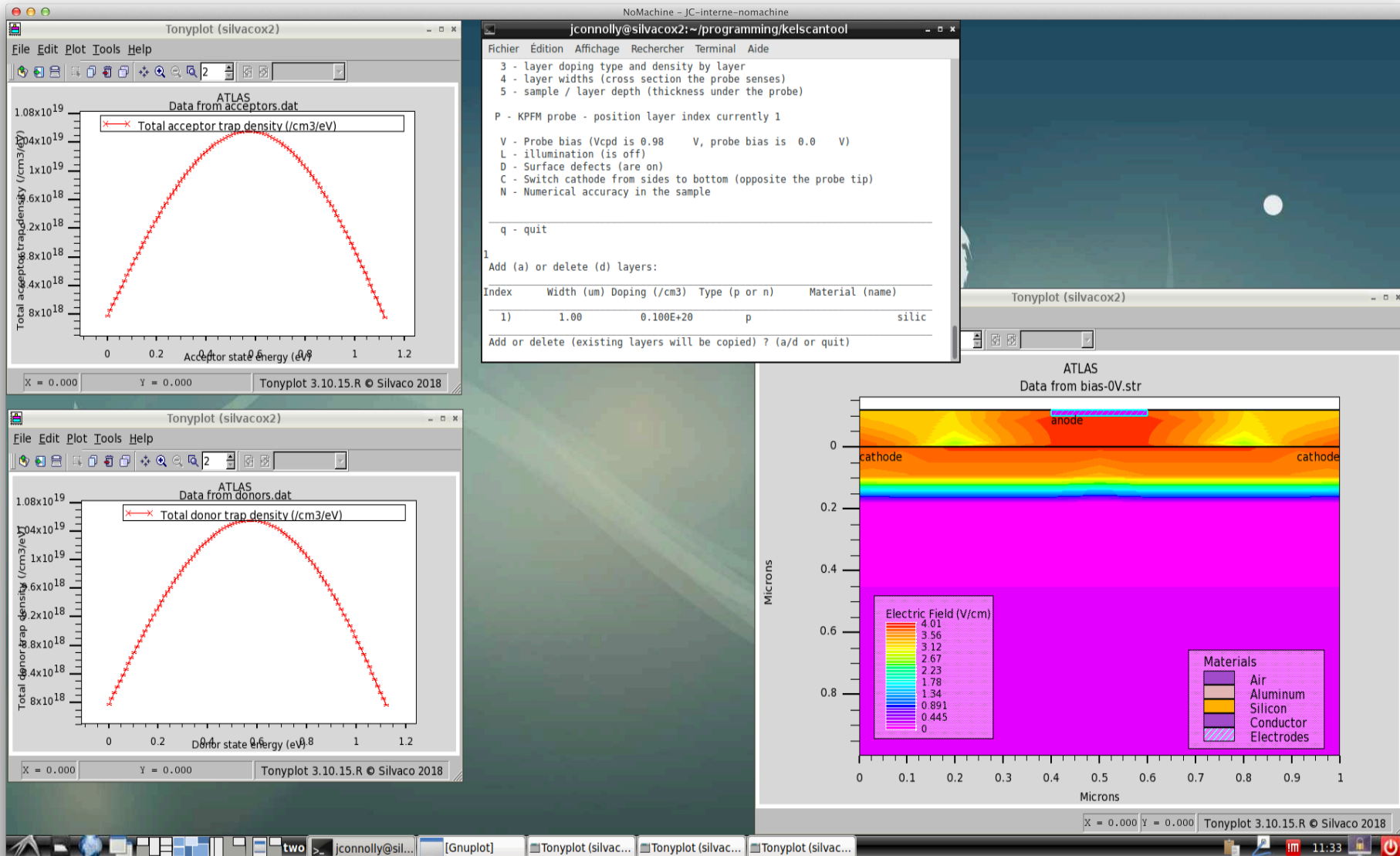
# Kelscan demonstration

## Contact potential scan : comparison with doping



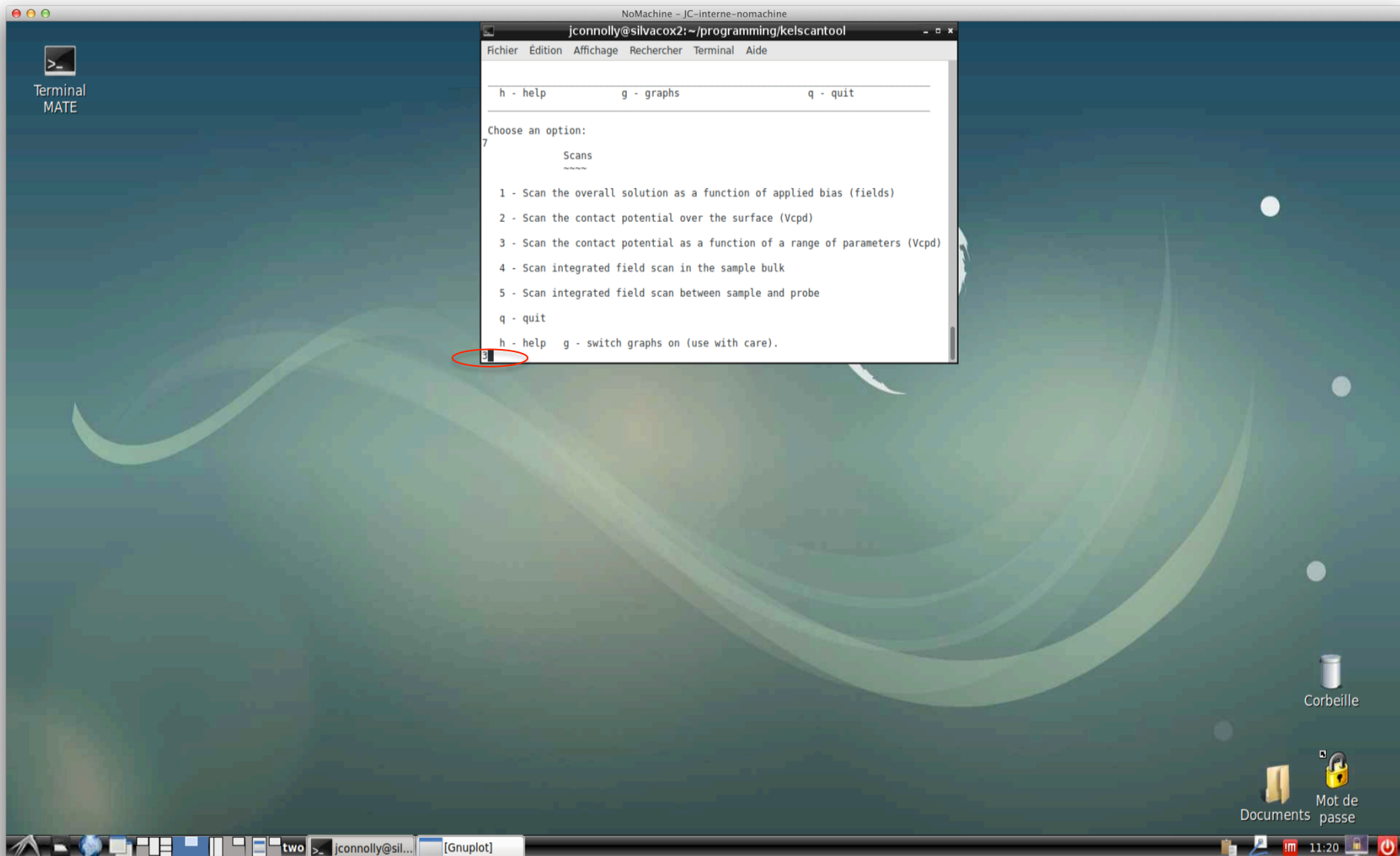
# Kelscan demonstration

Parameter scans : simple single layer homogeneous p-type Si



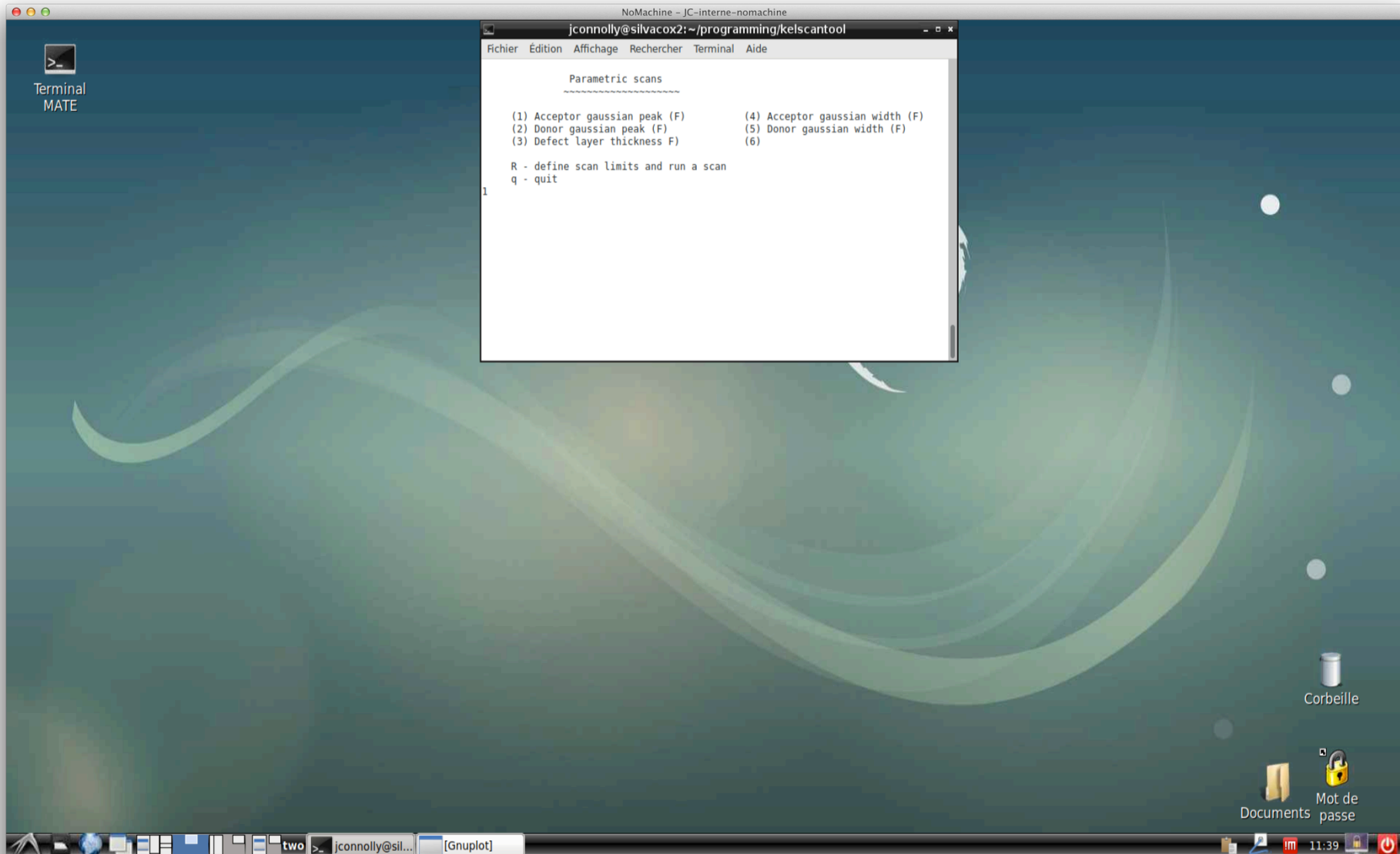
# Kelscan demonstration

## Scanning option 3 : Vcpd scans for a range of parameters



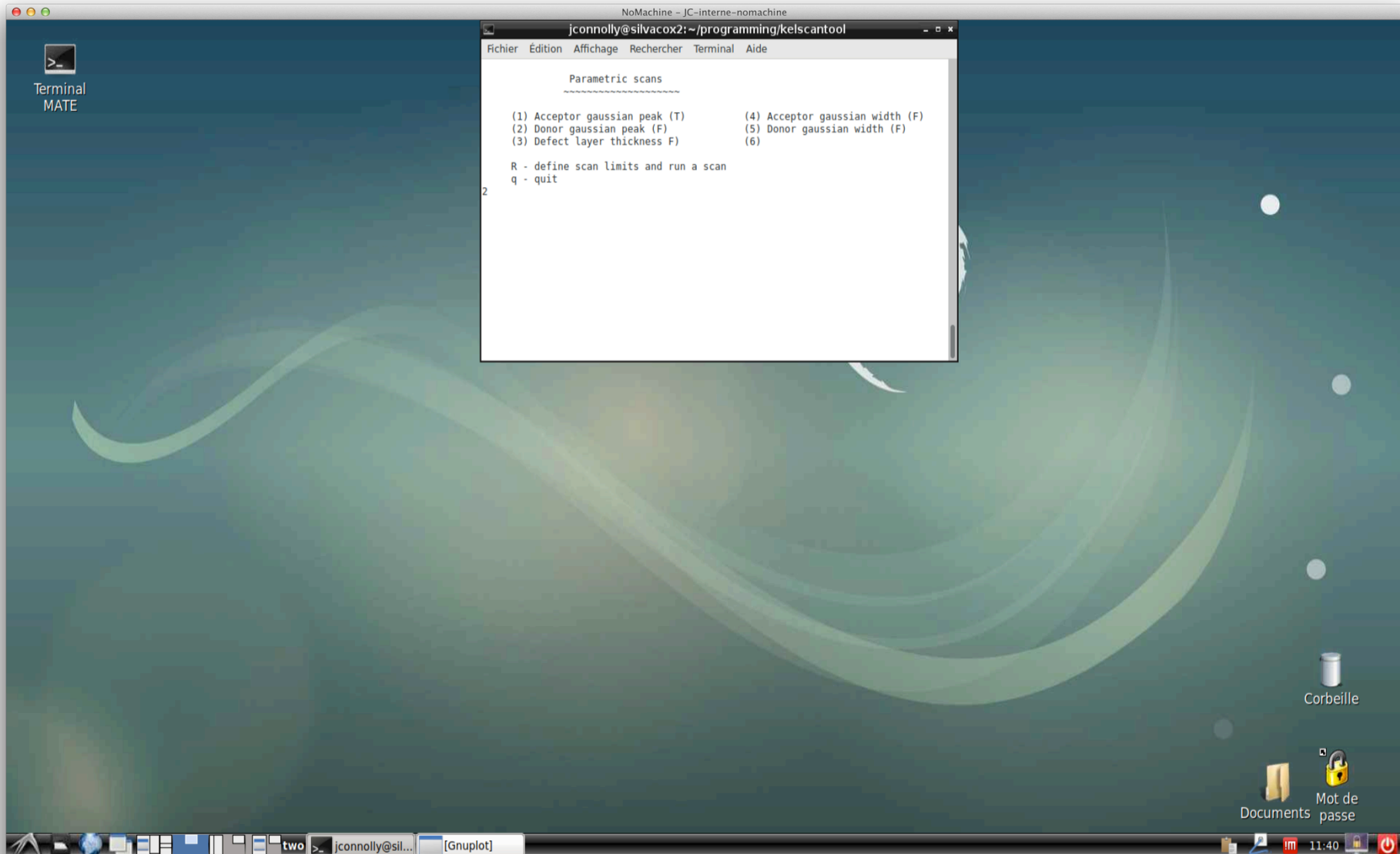
# Kelscan demonstration

2D scan example : First variable, acceptor defect peak density scan



# Kelscan demonstration

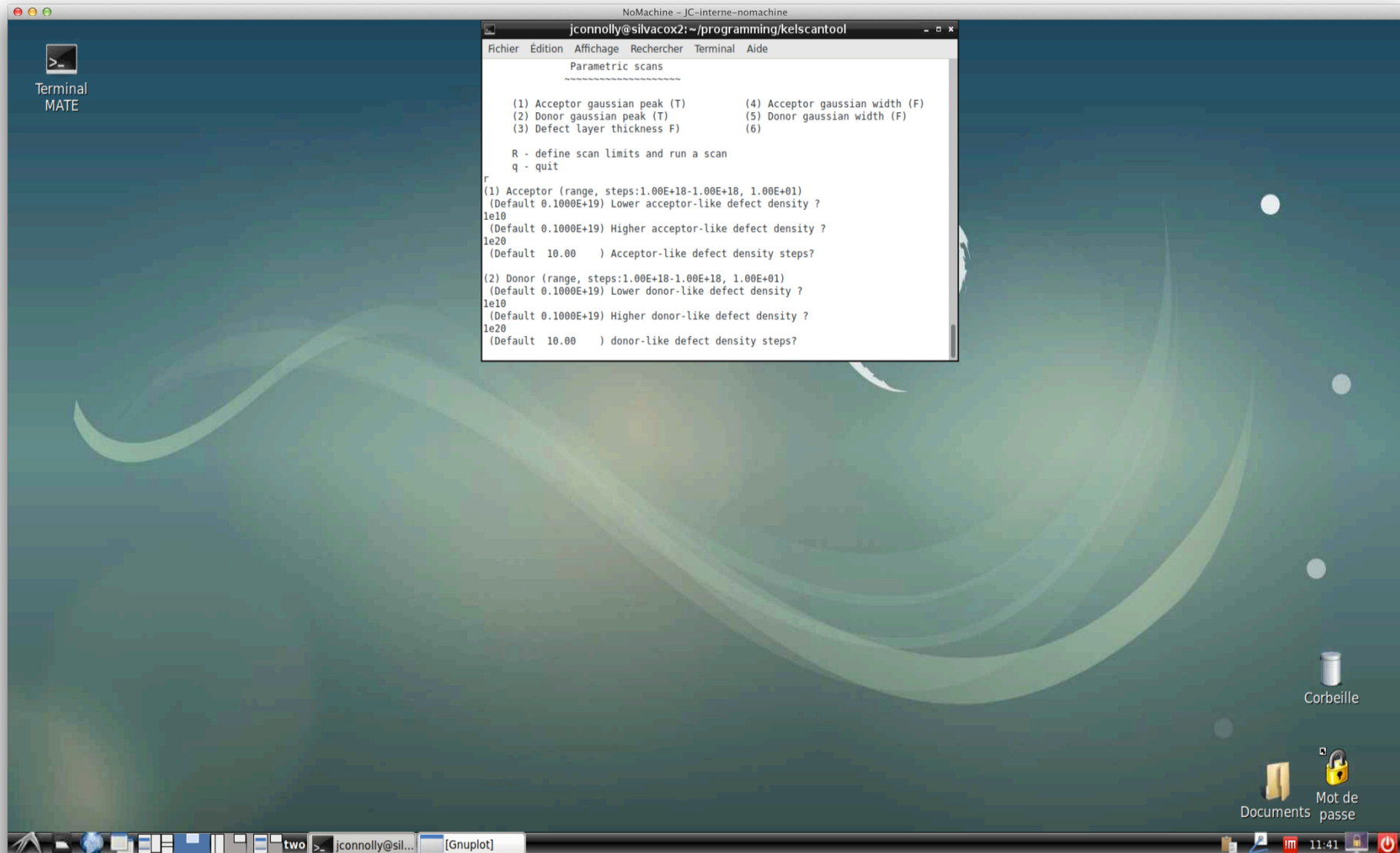
2D scan example : Second variable, donor defect peak density scan





# Kelscan demonstration

## Run 2D profile



```

NoMachine - JC-interne-nomachine
jconnolly@silvacox2: ~/programming/kelscantool
Fichier  Edition  Affichage  Rechercher  Terminal  Aide
-----
Parametric scans
-----
(1) Acceptor gaussian peak (T)      (4) Acceptor gaussian width (F)
(2) Donor gaussian peak (T)        (5) Donor gaussian width (F)
(3) Defect layer thickness (F)     (6)

R - define scan limits and run a scan
q - quit

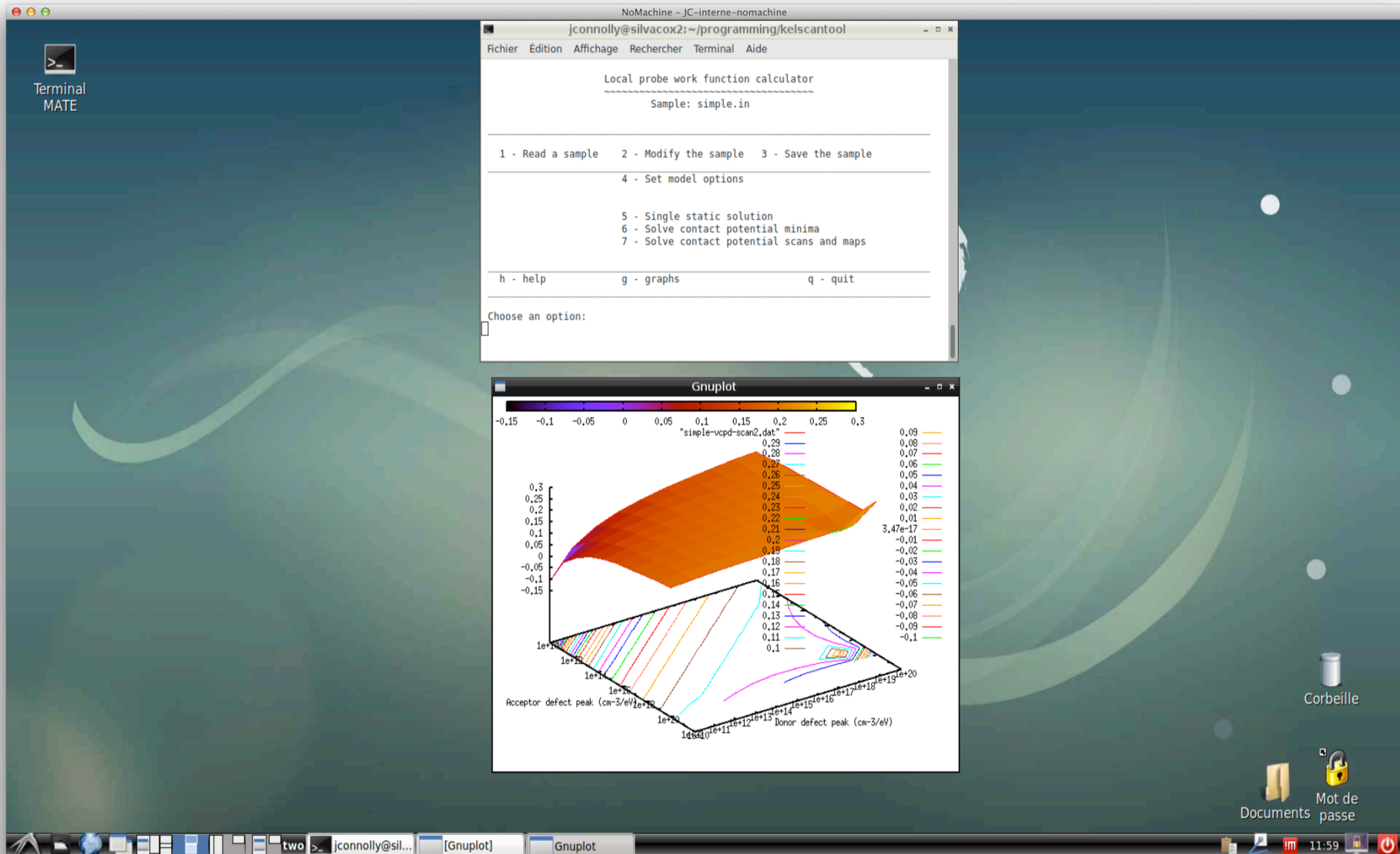
r
(1) Acceptor (range, steps:1.00E+18-1.00E+18, 1.00E+01)
(Default 0.1000E+19) Lower acceptor-like defect density ?
1e10
(Default 0.1000E+19) Higher acceptor-like defect density ?
1e20
(Default 10.00 ) Acceptor-like defect density steps?

(2) Donor (range, steps:1.00E+18-1.00E+18, 1.00E+01)
(Default 0.1000E+19) Lower donor-like defect density ?
1e10
(Default 0.1000E+19) Higher donor-like defect density ?
1e20
(Default 10.00 ) donor-like defect density steps?

```

# Kelscan demonstration

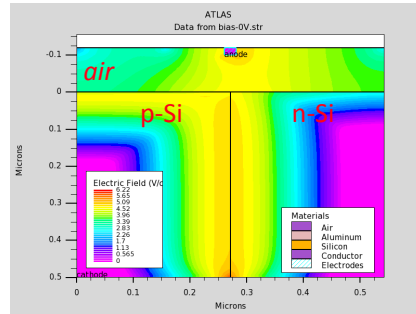
Resulting contact potential map : Data fitting identifies zone consistent with experiment



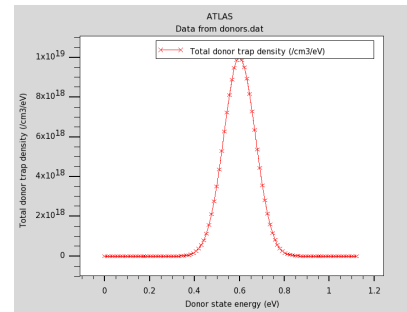
# Surface photovoltage simulations

## Definitions :

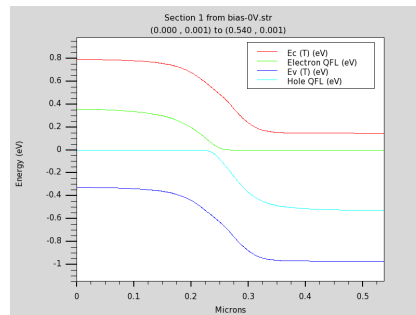
- SPV : The difference in light and dark work functions :  $SPV = \phi(Light) - \phi(Dark)$  independent of tip reference.
- Structure : Symmetric c-Si pn junctions (p-doped layer  $1E17cm^{-3}$   $0.3\mu m$  ; n-doped layer :  $1E17cm^{-3}$   $0.3\mu m$ )



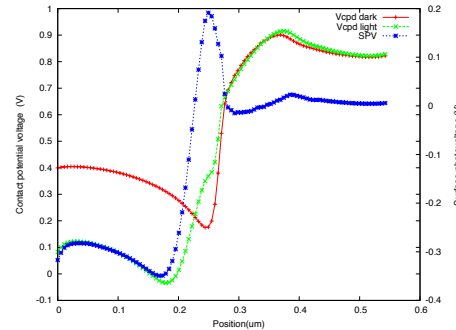
1) pn – surface donor defects  $1e19cm/2$



2) Surface defect donors



3) Surface transverse cut: Bands and populations (light)



4) Surface photovoltage – p side

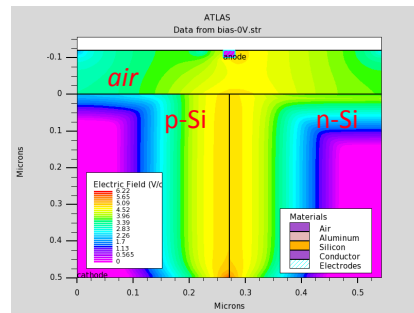
Surface donor defects : • p-side surface depletion and band bending.  
 • n-side close to charge neutral

=> SPV signal on p-side

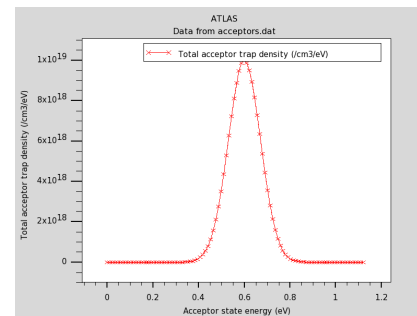
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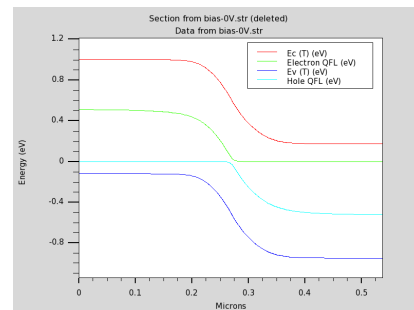
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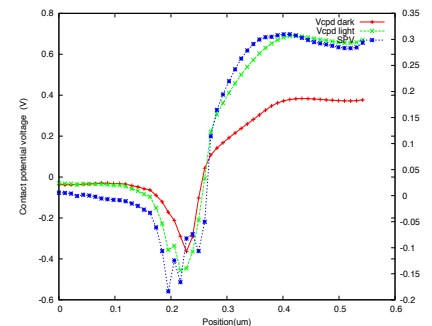
5) pn – surface acceptor defects  $1e19/cm^3$



6) Surface acceptor distribution



7) Surface transverse cut: Bands and populations (light)



8) Surface photovoltage – n side

- Surface acceptor defects :
- p-side surface depletion and band bending.
  - n-side close to charge neutral

=> SPV signal on p-side

## Concluding remarks

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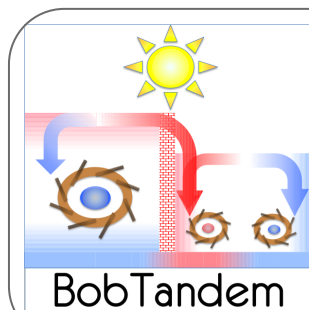
### 1) *Focus of this presentation*

- *Introduction to advanced KPFM techniques*
- *Presentation of user friendly numerical modelling*

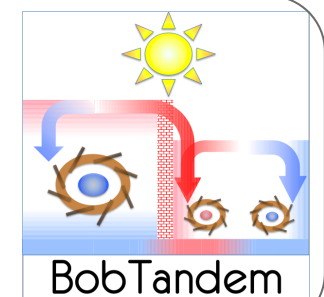
### 2) *Next steps :*

- *Refine description (KPFM tip size for example)*
- *Analyse real materials*

*=> Publication : NanoTexology partner EPJPV*



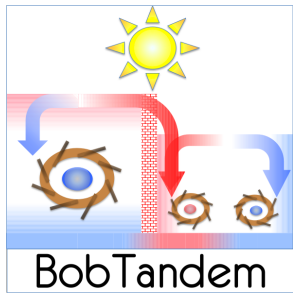
*Support for this work : H2020 - SolarEranet  
Project **BOBTandem** - 2019-2022  
<https://bobtandem.wordpress.com>*





Horizon 2020

*NanoTechnology-NN22*



*Thank you for your attention*

