SCAPS 3.0
An introduction

Koen Decock & Marc Burgelman

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Overview

- Getting started
- General working principles
- Tips & Tricks
  - Numerical limitations
  - The numerical panel
  - A neutral defect
  - Curve Info: *Get informed!*
  - Preserve your work for the future: *saving and commenting*.
  - Speeding up: *Batch – Recorder – Script*
  - Grading
  - Zooming: *Get a closer look!*
  - The blue button

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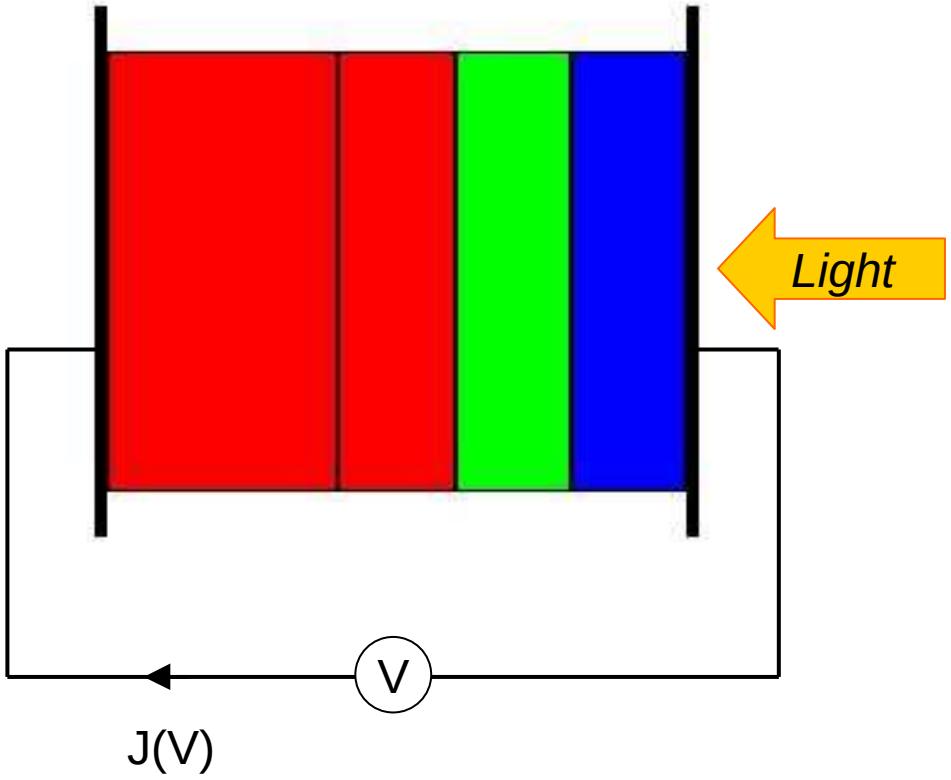
Getting Started…



- Opto-electrical simulation of 1-D structure of semiconductor layers
- Special attention for contacts and interfaces
- Variable bias voltage, temperature & illumination
- DC & AC calculations
- Designed for CdTe and CIGS Solar Cells, but also used in other material systems ☺

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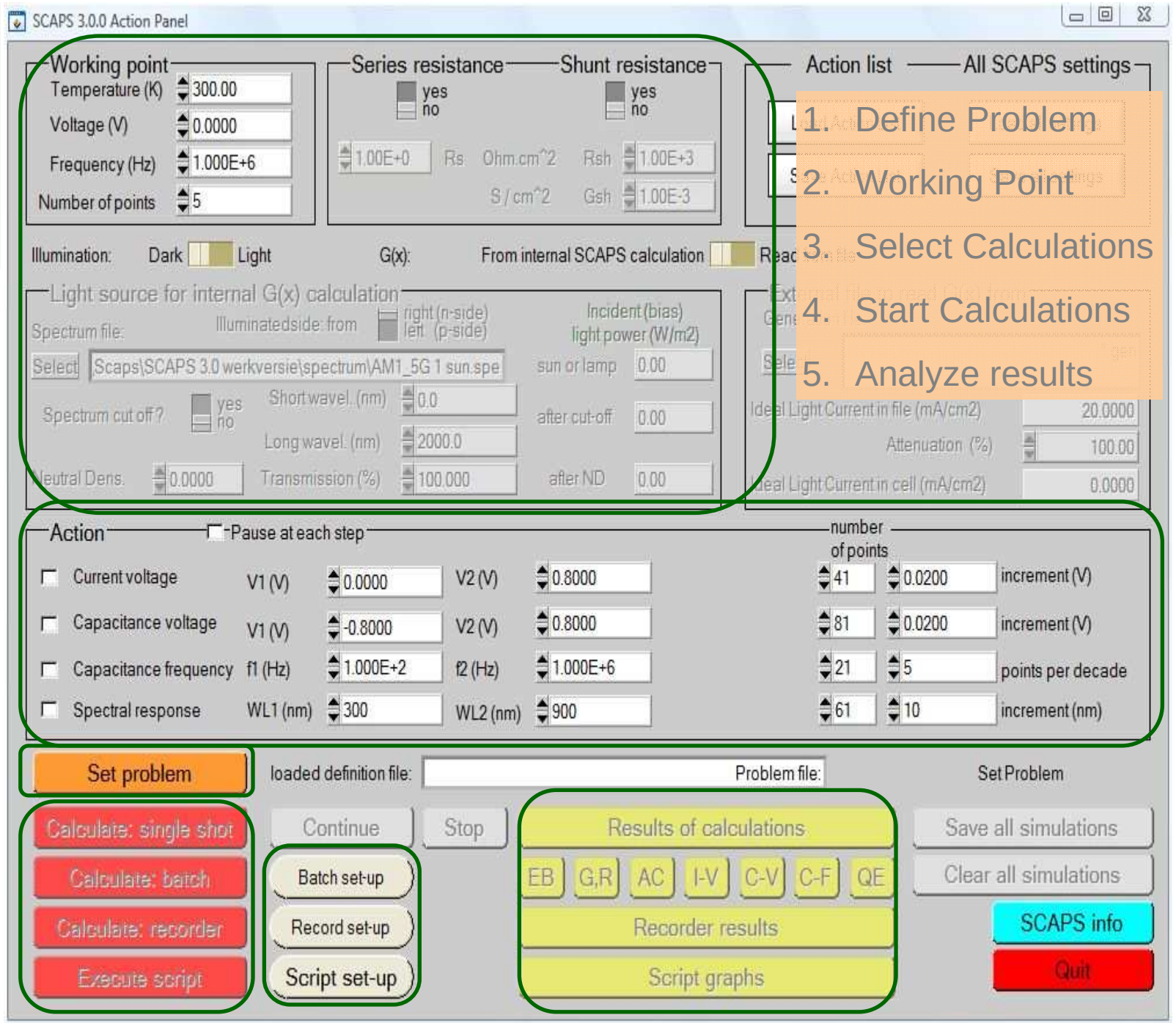
Getting Started



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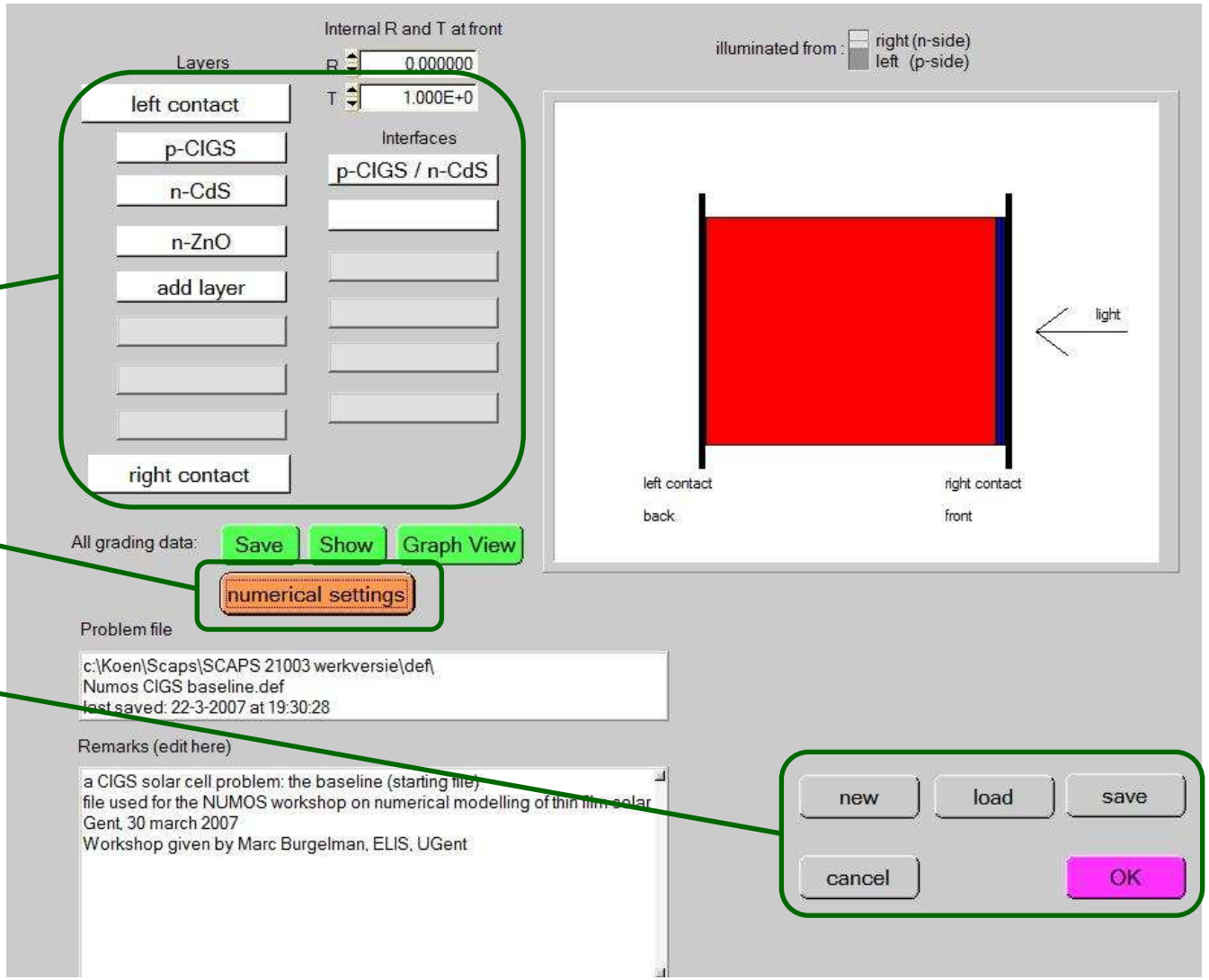
Getting Started: Define Problem

- Setting Layer, Interface & Contact properties
- Setting Numerical preferences
- Saving & Loading



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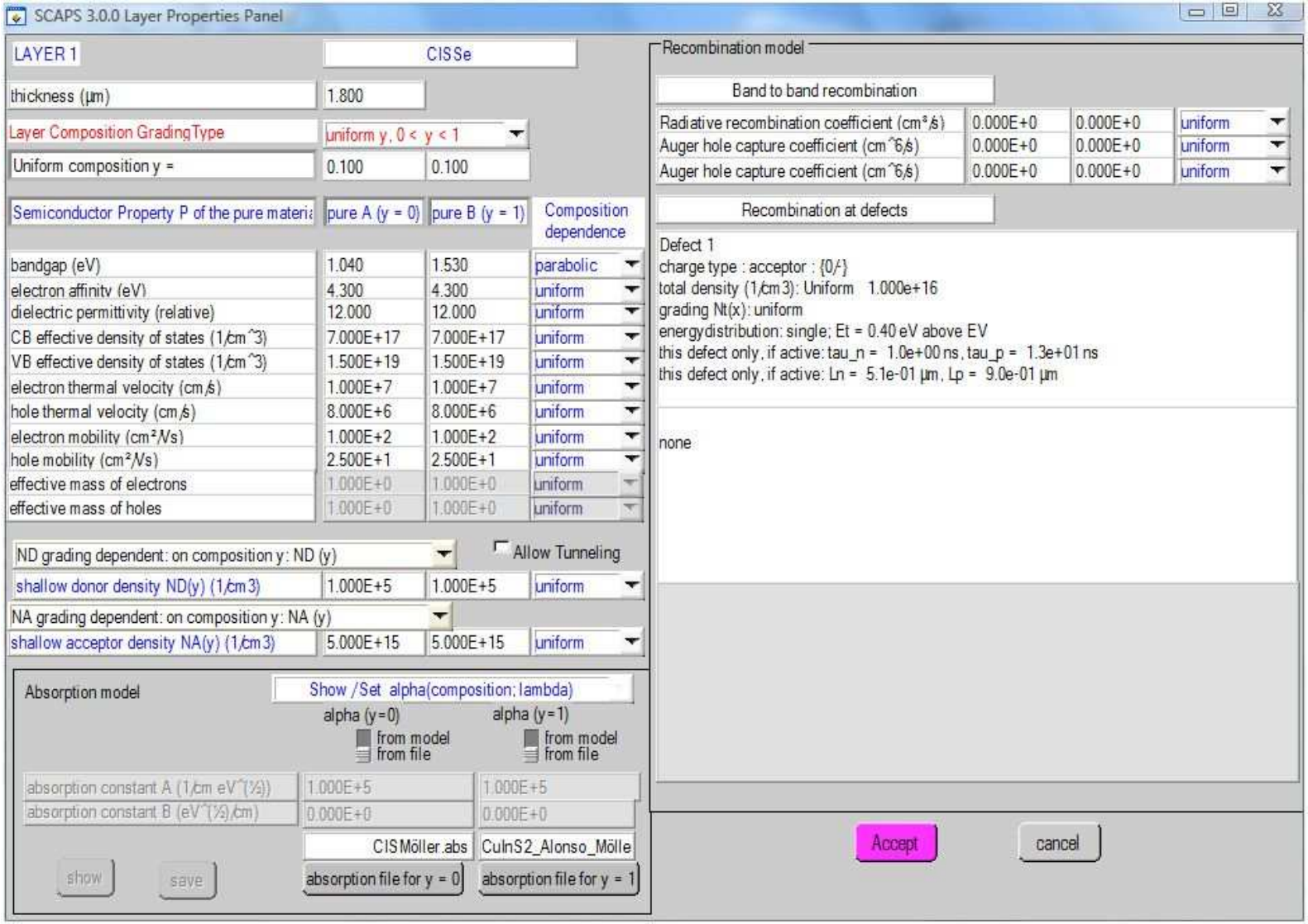

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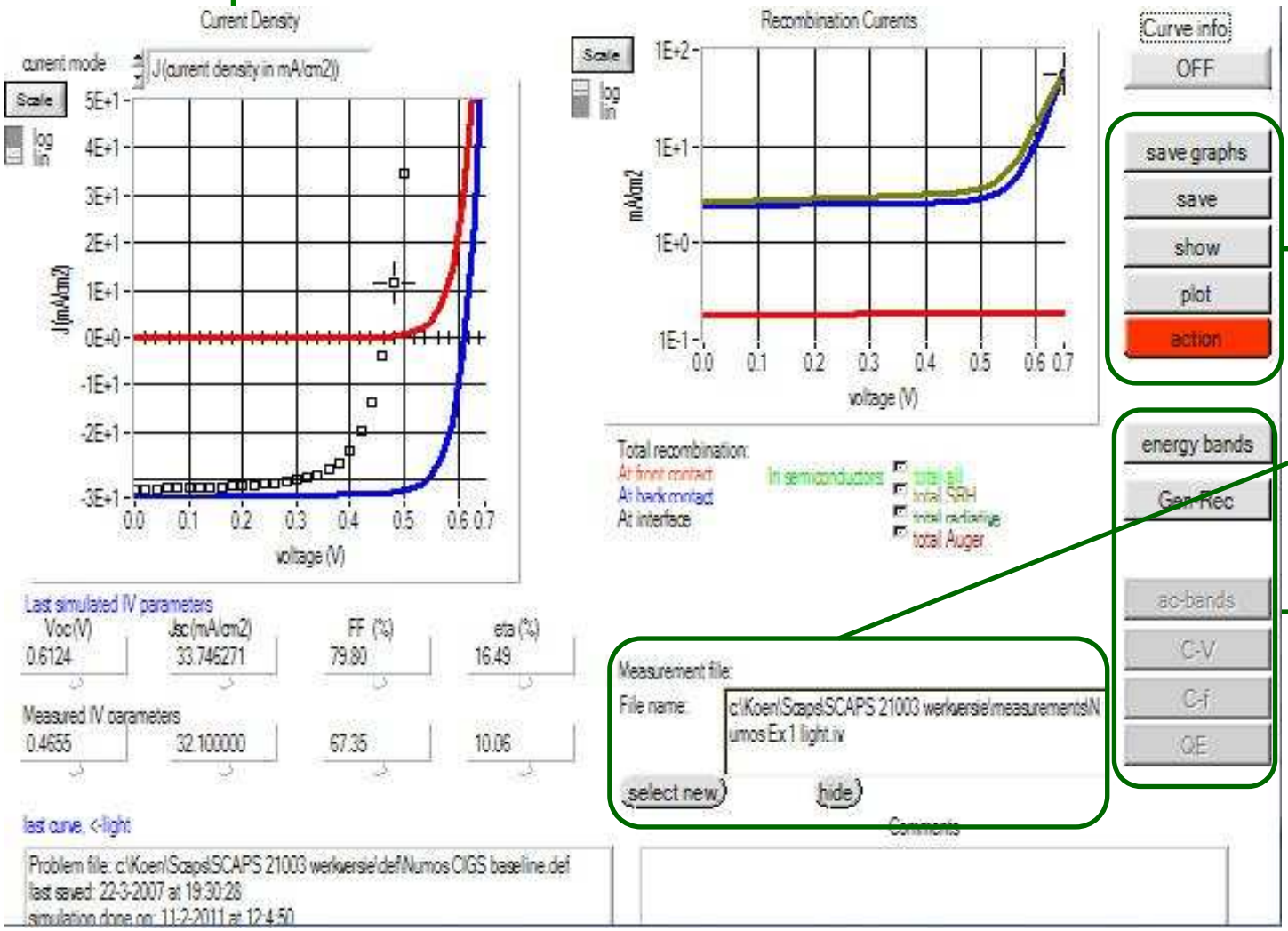
Getting Started: Analyze results



- Display results
- Export results
- Compare with measured data
- Navigate to other panels

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General working principles:

Semiconductor equations

$$\begin{cases} \dfrac{\partial}{\partial x}\left(\varepsilon \dfrac{\partial \psi}{\partial x}\right) = -\dfrac{q}{\varepsilon_0}\left[-n + p - N_A^- + N_D^+ + \dfrac{1}{q}\rho_{defect}(n,p)\right] \\ -\dfrac{\partial j_n}{\partial x} + G - U_n(n,p) = \dfrac{\partial n}{\partial t} \\ -\dfrac{\partial j_p}{\partial x} + G - U_p(n,p) = \dfrac{\partial p}{\partial t} \end{cases}$$

Poisson

Continuity relations

Constitutive relations

$$\begin{cases} j_n = -\dfrac{\mu_n}{q} n \dfrac{\partial E_{Fn}}{\partial x} \\ j_p = \dfrac{\mu_p}{q} p \dfrac{\partial E_{Fp}}{\partial x} \end{cases}$$

- Boundary conditions at interfaces and contacts
- RESULT: system of coupled differential equations in {ψ, *n*, *p*} or {ψ, E_{Fn}, E_{Fp}}
- Solved numerically

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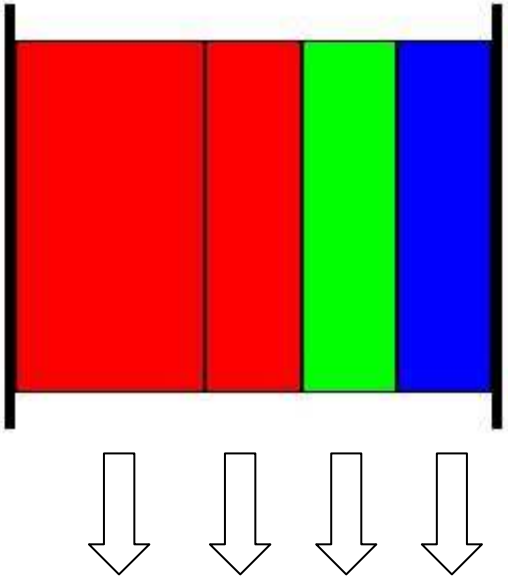
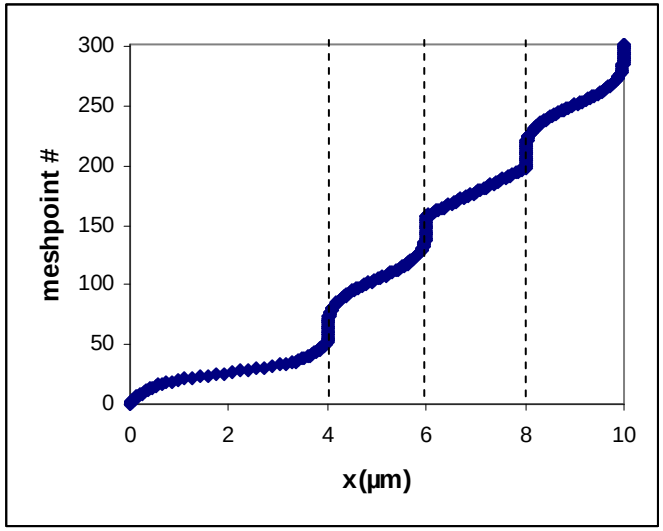
General working principles:

Discretization

- Equations solved using finite differences
- Structure discretized => MESH
  - Coarse meshing in the middle of a layer
  - Finer mesh near the interfaces & contacts
  - Two discretization points for each interface
  - Meshing can be updated during simulation process (numerical panel)





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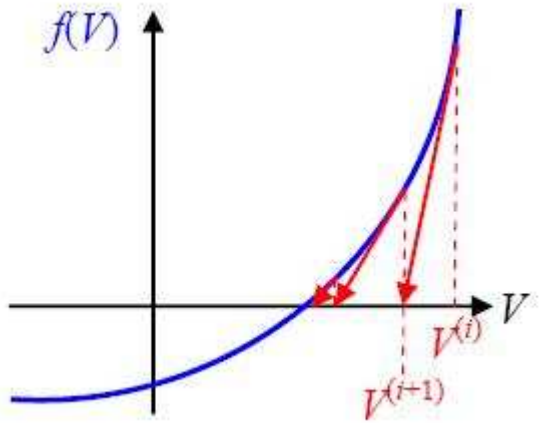
General working principles:

The pathway to a solution[1]

¿Gummel scheme with Newton Raphson substeps?

- Solve (1) for ψ with given E_{Fn} & E_{Fp}
- Solve (2) for E_{Fn} with given ψ & E_{Fp}
- Solve (3) for E_{Fp} with given ψ & E_{Fn}

$$\begin{cases} (1): \dfrac{\partial}{\partial x}\left(\varepsilon \dfrac{\partial \psi}{\partial x}\right) = -\dfrac{q}{\varepsilon_0}\left[-n + p - N_A^- + N_D^+ + \rho_{defect}(n,p)\right] \\ (2): -\dfrac{\partial j_n}{\partial x} + G - U_n(n,p) = \dfrac{\partial n}{\partial t} \\ (3): -\dfrac{\partial j_p}{\partial x} + G - U_p(n,p) = \dfrac{\partial p}{\partial t} \end{cases}$$



- Make first guess of solution
- Improve guess with tangent lines
- Works well if first guess was not too bad

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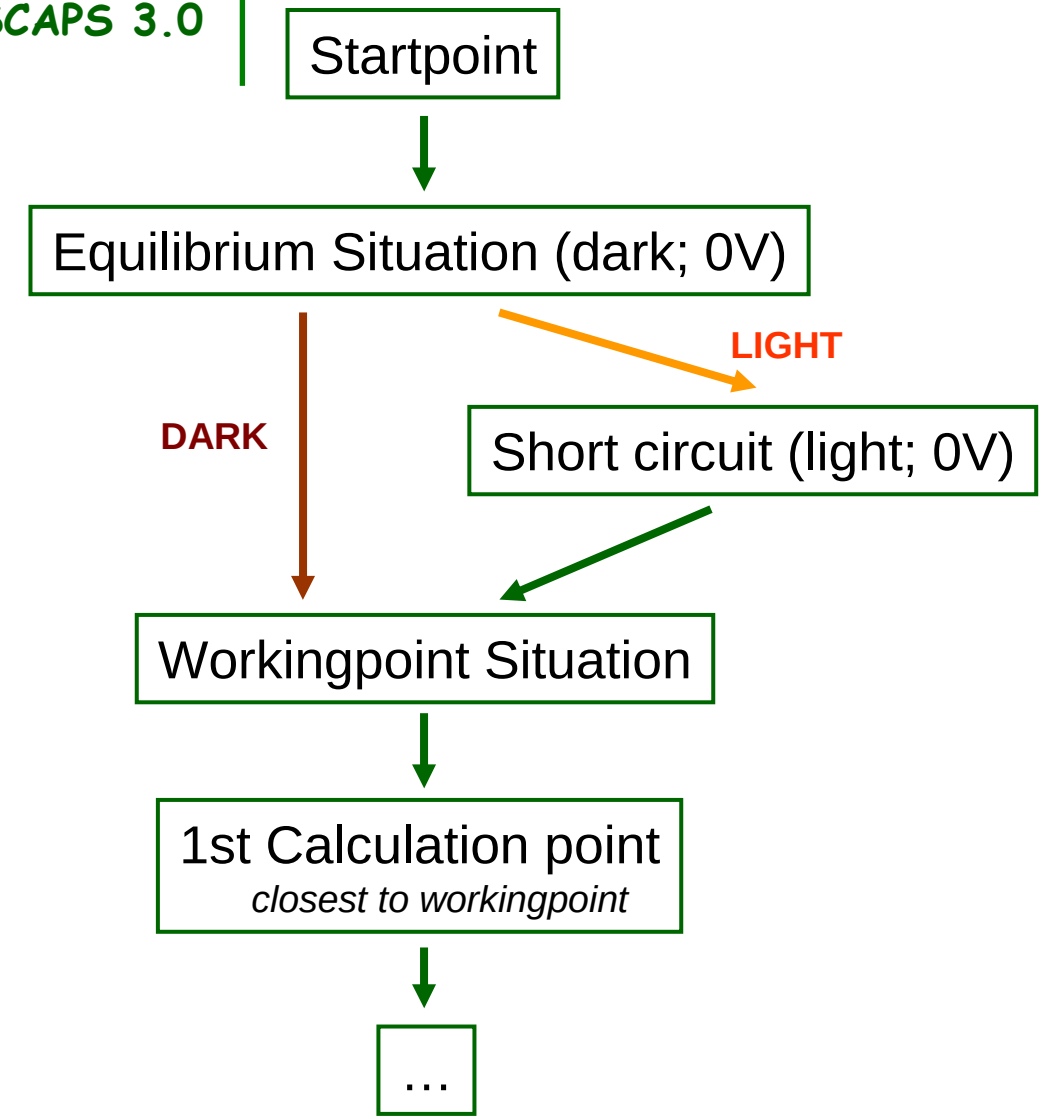
General working principles:

The pathway to a solution[2]



- Difference between several steps should not be too large
- Number of intermediate steps to get to the workingpoint can be set
- Every batch step starts at the startpoint

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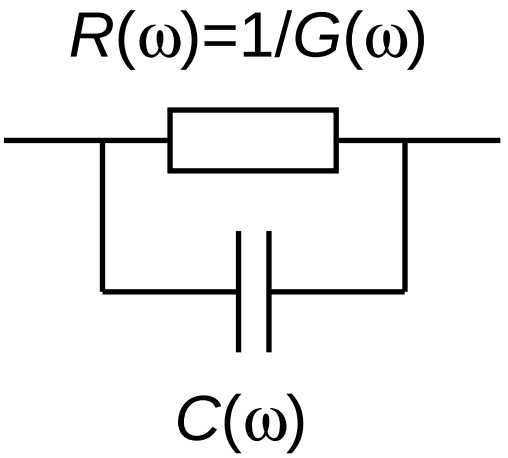
General working principles:

AC-analysis

- Small signal analysis: $\tilde{V} \to 0$
- Small signal values are complex numbers!!!
- Small signal currents, potential (ψ) and Fermi levels displayed on ac-panel
- Admittance interpreted as capacitance-conductance circuit

$$\begin{cases} V = V_{DC} + \tilde{V}e^{j\omega t} \\ \psi = \psi_{DC} + \tilde{\psi}e^{j\omega t} \\ E_{Fn} = E_{Fn,DC} + \tilde{E}_{Fn}e^{j\omega t} \\ j_n = j_{n,DC} + \tilde{j}_n e^{j\omega t} \end{cases}$$



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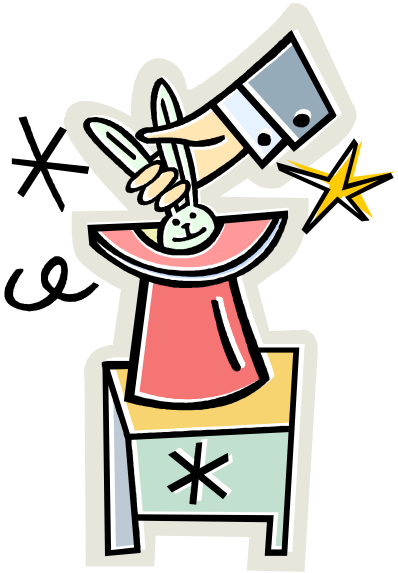

Tips and Tricks

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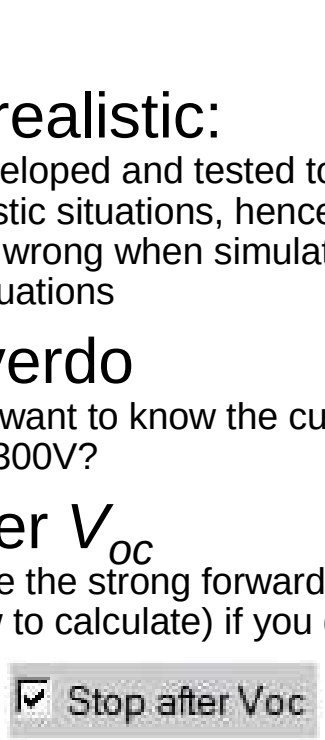
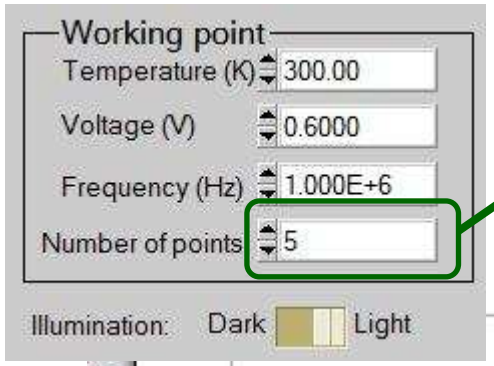
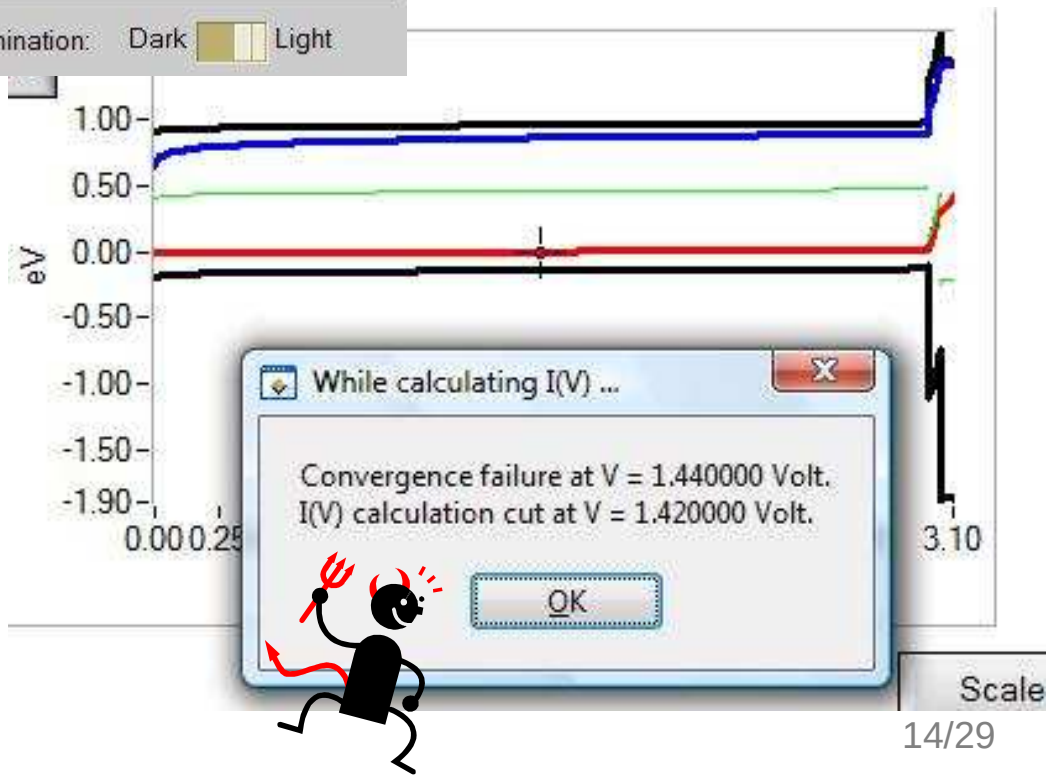
Numerical limitations

- Keep the variation between different calculation steps limited.
- Keep it realistic:
  SCAPS is developed and tested to simulate realistic situations, hence things can go wrong when simulating unphysical situations
- Don't overdo
  Do you really want to know the current at T=20K, V=300V?
- Stop after V_{oc}
  Don't calculate the strong forward currents (slow to calculate) if you don't need them.



Large number of points:
→Slower calculation
→ Less chance of convergence failure





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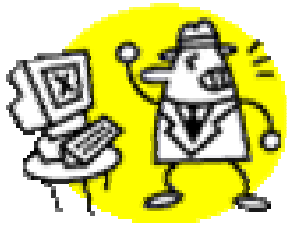
Numerical limitations

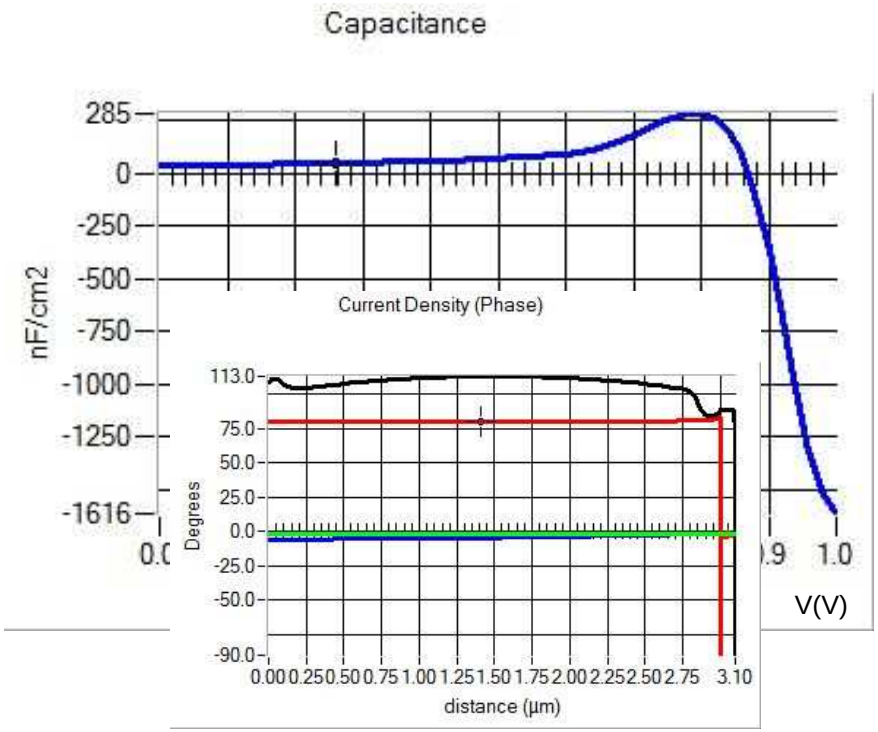


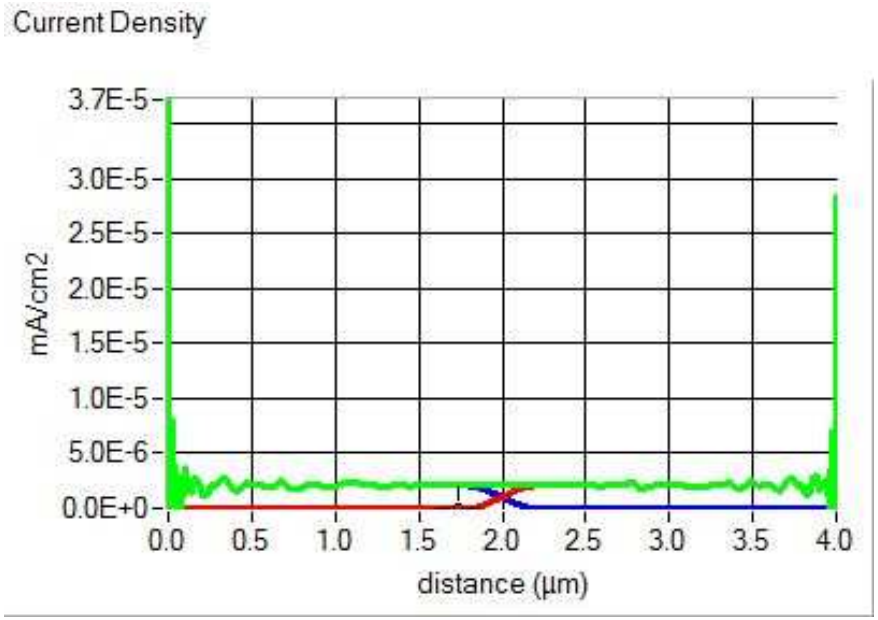
$$1.000 - 10^{-15} \neq 1.000$$

AC-calculation when Re(J) » Im(J)

- negative capacitances
- *C* increases with frequency

pn ↔ *np*-structure





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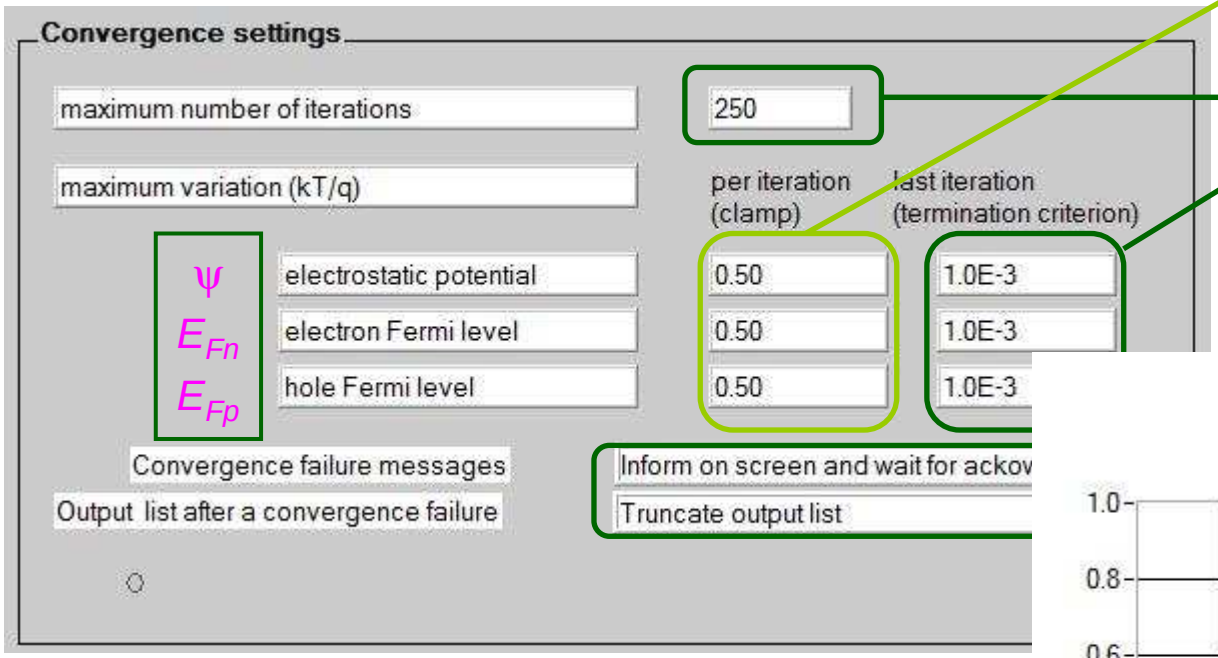
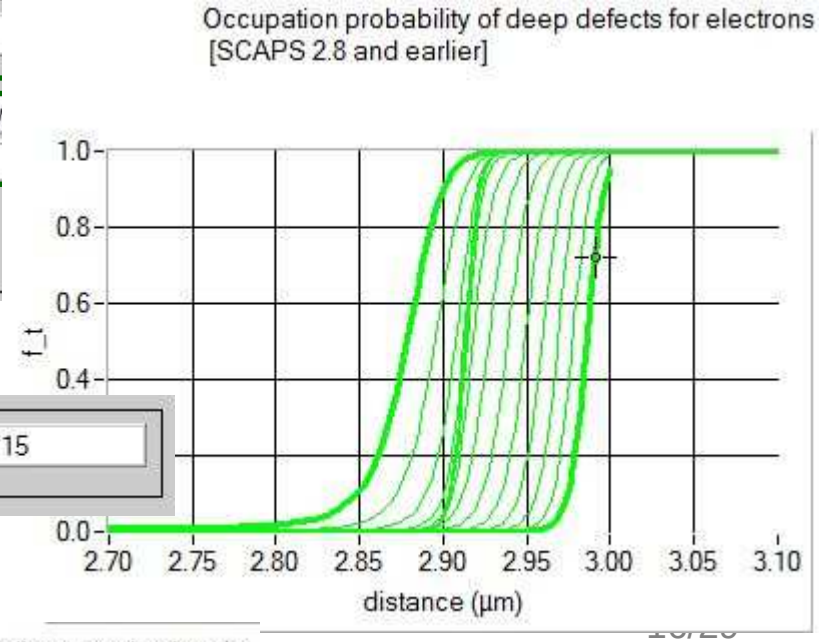
The numerical panel[1]

Avoid too big variations between iterations

Terminations criteria Newton-Raphson





Plot all occupation levels

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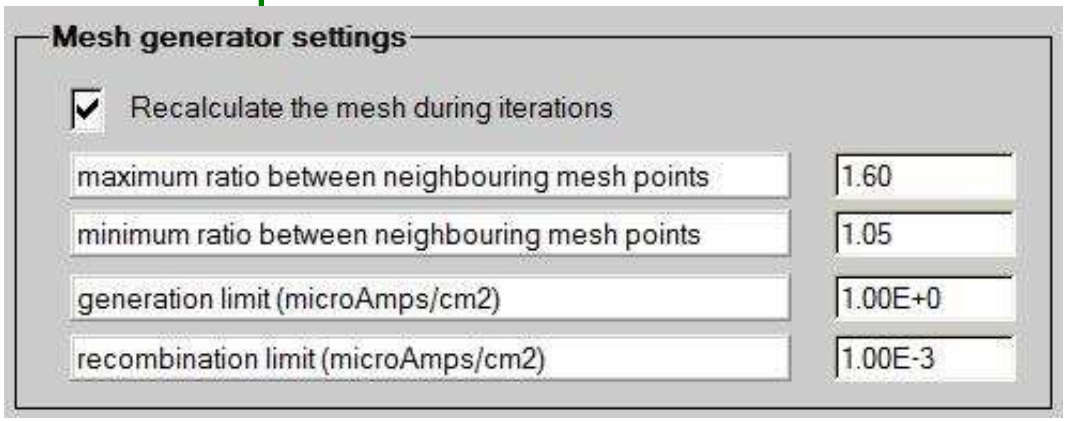
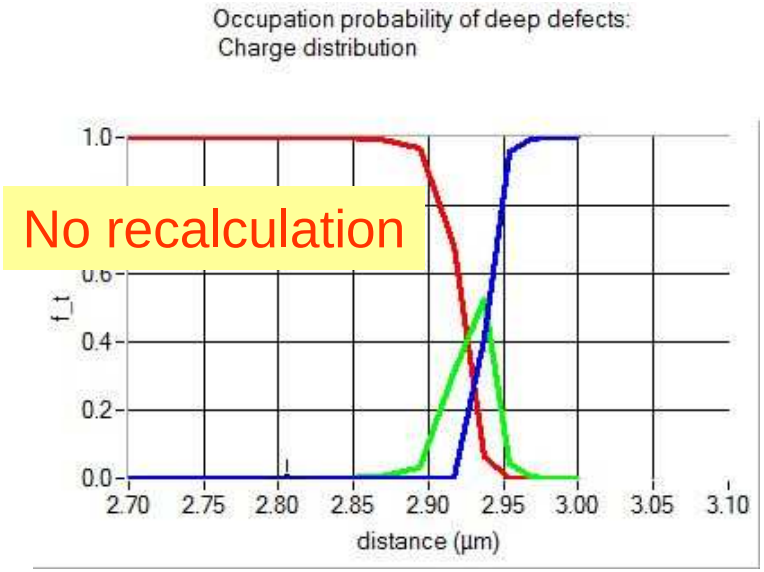
The numerical panel[2]

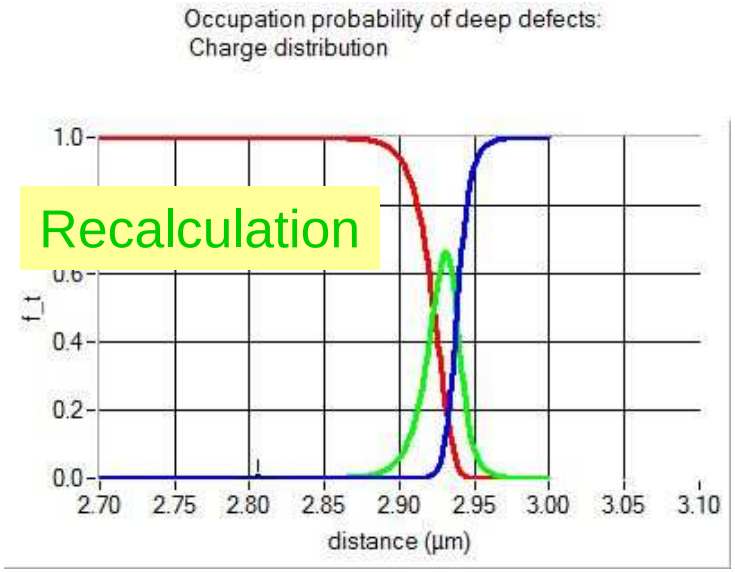


Remove/add mesh points:

based on:

- ψ, E_{Fn} and E_{Fp}
- Generation
- Recombination





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A Neutral Defect

- Recombination present $\leftrightarrow$ No influence on charges
  - Separation of direct and charge related effects of defects
- Does not exist in real materials
- Handy in simulation
  - Whilst building model
  - For unimportant layers
- Neutral defect + shallow doping ~ charged defect

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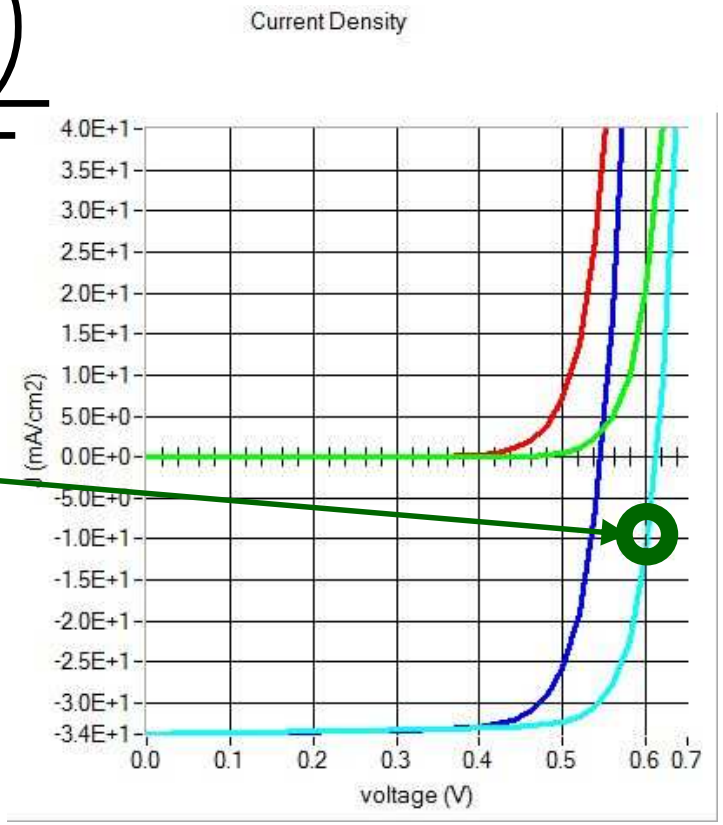
Curve Info

graph: J-V curve: J(V)
(lin-lin plot)

curve: Batch simulation 1: 2 param., step 4/4
temperature [K]: 3.000e+02
illumination>>dark ?: 0.000e+00
---

point: point # 30
6.0000e-01 voltage (V)
-1.1543e+01 J (mA/cm2)



- Information about Graph/Curve/Point when clicking on a plot:
- Point/Curve nearest to mouse-click selected.
- ¿Which curve corresponds to which simulation?

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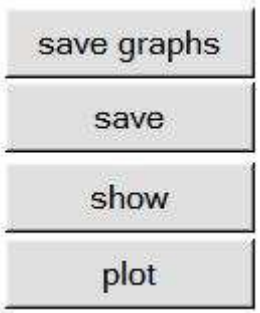
Save your work and settings

- Save settings:
  - Cell structure (.def)
    [some of the numerical settings are included here]
  - Batch (.sbf & .bdf)
  - Recorder (.srf)
  - Action panel (.act)

All together (.scaps)

- Save results:



- To figure format (.png/.jpg/.bmp)
- To text file (or .xls-file)
- To screen
- To printer (or pdf-printer)

All files can be read with a text editor

- ADDING COMMENT STRONGLY RECOMMENDED!

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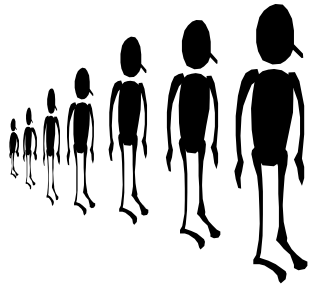
Speeding up:

Batch



Parameters varied simultaneously

Vary entire definition files

- Linear variation
- Logarithmic variation
- Custom defined variation

Simultaneous

Vary definition files

					From	To	Steps	Custom list	
Remove	p-CIGS (L1)	defect 1	total defect de	left side	1.000E+15	1.000E+16	7	Lin Log	☐
Remove	☐ n-CdS (L2)	thickness[µm]			0.100	0.150	2	Lin Log	☐
Remove	■ n-ZnO (L3)	thickness[µm]			0.250	0.150	2	Lin Log	☐
Remove	☐ T [K]								☑
Remove	☐ illumination...	Spectrum file							☑

Add

Set custom values

Set

Set

3 values saved in three temperatures.bdf

unsaved list of 2 spectrum files

file as parameter!

Up to 9 parameters

Keep SHIFT pressed to interrupt a batch calculation

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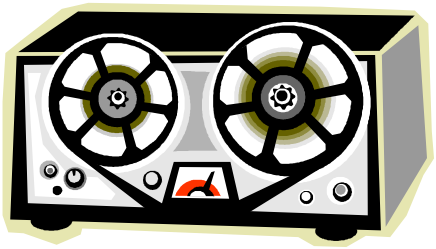
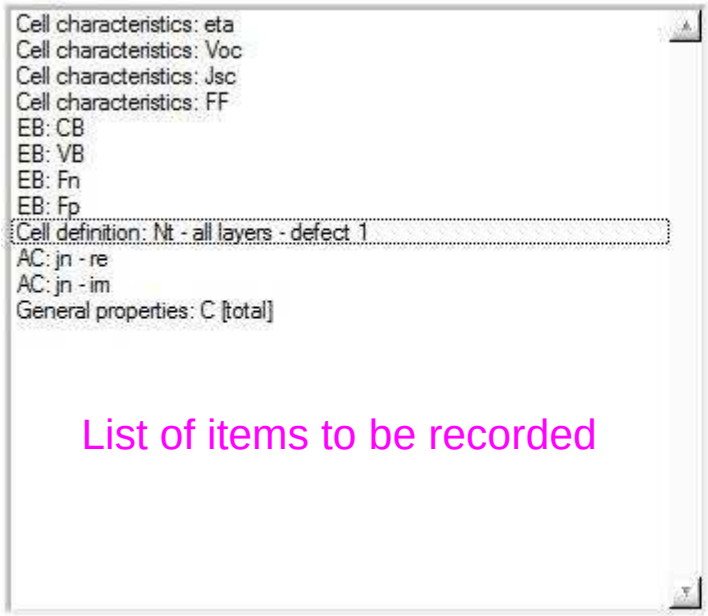
Speeding up:

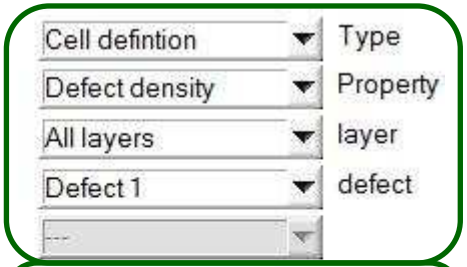
Recorder[1]



Properties to be recorded



List of items to be recorded



1. Select item to be recorded

2. Press to add to the list

- The recorder overrules all calculations set at the action panel
  - Items recorded at workingpoint conditions
  - Only simulations to get to the asked properties are performed

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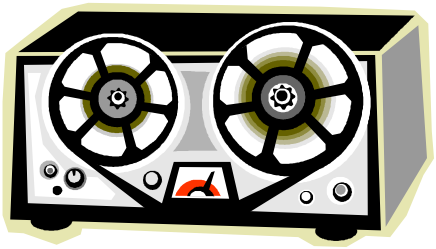
Speeding up:

Recorder²



Recorded items shown as function of:

- Batch parameters (cell characteristics – general properties – interface properties)
- Mesh (other properties)

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Speeding up:

Script

- Run *SCAPS* from command-line or external program
- Automatize user-interface operations
- Analyze results in a non standard way
  - Make your own extension to *SCAPS*: `SCAPSUserFunction.dll`
  - Root/extrema finding available
  - Access all recordable variables: `singleshotbatch`

- Keep the script manual close at hand
- Freedom has its price! While scripting you have more power to let things go wrong

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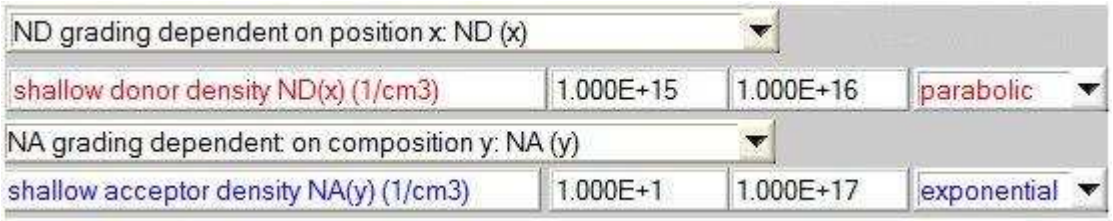
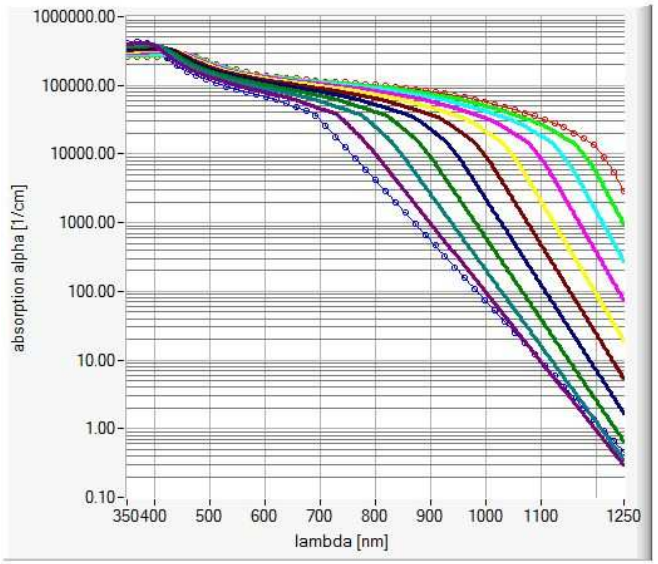
Grading



- Material driven approach
- N_A, N_D, N_T → Grading along composition or position
- What is UNIFORM?
  - Uniform A / Uniform B: Only one material present (nothing else can/should be graded)
  - Uniform Y: Uniform material is a mixture of two materials (other parameters can be graded)
- Special absorption interpolation

Graded variables available on the cell definition panel after calculation



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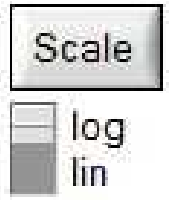
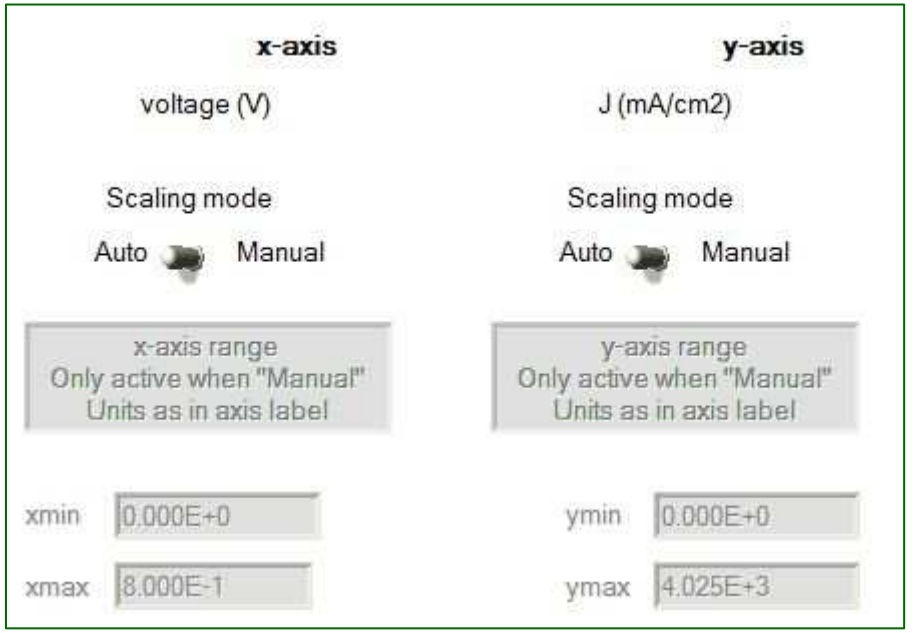
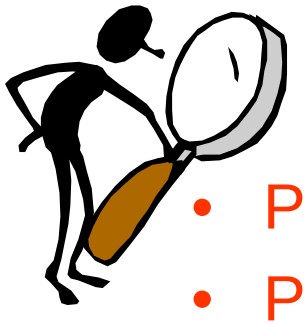
Zooming and Scaling

- Set scaling on the scaling panel
- Switch between Linear & Logarithmic







- Press CTRL and draw a rectangle in a graph to zoom in
- Press CTRL and right mouse button to zoom out.

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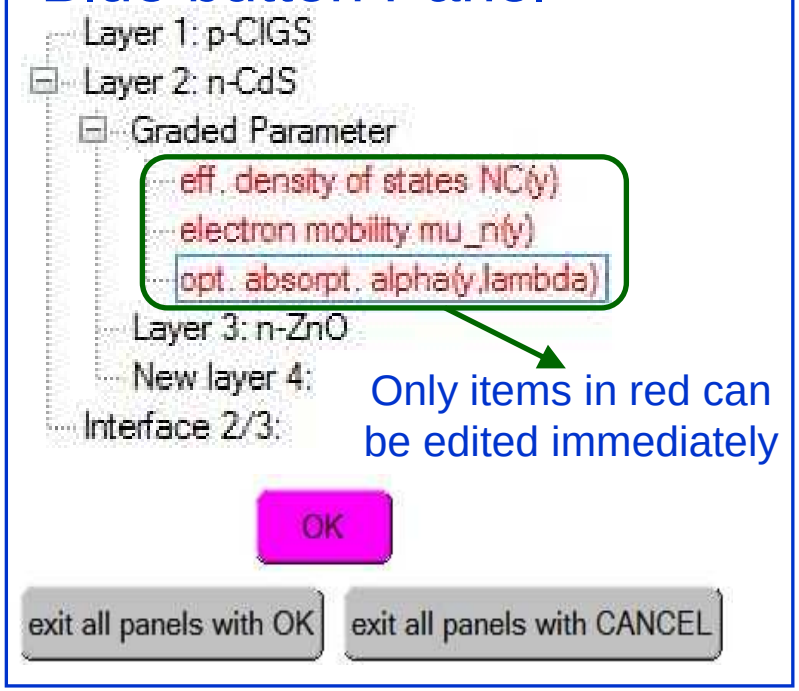
The blue button

Other panels need input first!

- Allows browsing of the cell definition
- Makes sure you find minimized panels back
- Uneditable panels are dimmed

Blue button Panel



EMERGENCY BUTTONS

- Press F1 to get to cell definition panel (where you can access the blue button)
- Press F2 to see the layer/interface panel

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Enjoy SCAPS

- SCAPS is freeware:
  - Register when using: Marc.Burgelman@Elis.Ugent.be
    Koen.Decock@Elis.Ugent.be
  - Cite when publishing:
    - M. Burgelman et al., *Thin Solid Films*, **361-362**, 527-532 (2000)
    - Other more specialized articles
- More Details:
  - Collection of (Add-on) user manuals
  - Contributions in literature

SCAPS info

More Questions?

- Raise your hand and ask!
- ✍ Marc.Burgelman@Elis.Ugent.be
  Koen.Decock@Elis.Ugent.be

☝ Please explain your problem, what you did and what you expected!

☝Please add .def- or .scaps- file with sufficient comments & results.