Drift-diffusion Solver

Informative session

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November 2, 2025

Overview

- Introduction
- Configuring DD-solver Easy-to-use config files
- Available analyses

Small-signal analysis Mixed-mode analysis Electro-thermal simulations

Physics in DD solver

Contact boundary conditions Band structure models Mobility models Recombination models Dynamics of recombination centers (Traps)

6 Licenses



Introduction

Configuring DD-solver Easy-to-use config files

Available analyses

Small-signal analysis
Mixed-mode analysis
Flectro-thermal simulation

Physics in DD solver

Contact boundary conditions
Band structure models
Mobility models
Recombination models
Dynamics of recombination centers (Traps

6 Licenses



The drift-diffusion solver (DD-solver) simulates the electronic device by solving *Poisson*, and electron/hole *continuity* equations.

Salient features of the DD-solver are -

- Can perform a quasi-stationary DC ramp, small-signal analysis at a fixed DC bias, and a transient analysis.
- Coupled Poisson, electron, and hole continuity equations are solved in the DD-solver for the above mentioned analyses.
- Coupled electro-thermal simulations can also be performed in the DD solver by solving temperature equation coupled with the continuity and Poisson equation.
- The mixed-mode-system consisting of the semiconductor devices and the external components can be solved coupled with drift-diffusion equations.
- Physics-based models can be activated to model mobility, recombination phenomena, traps, etc. in semiconductors.
- The model parameters can be edited in the material config file, thus allowing the models to be calibrated to the
 experimental data.
- Convinient 'Python' interface for simulation setup and post-processing.



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DD-Solver

November 2, 2025 4

- Introduction
- 2 Configuring DD-solver Easy-to-use config files
- Available analyses
 Small signal analyses

Small-signal analysis
Mixed-mode analysis
Electro-thermal simulation

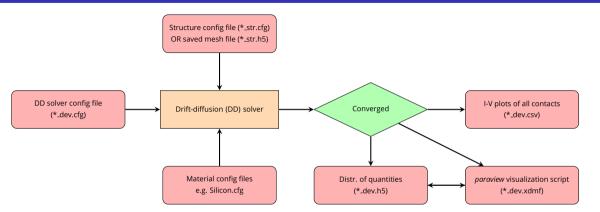
Physics in DD solver

Contact boundary conditions
Band structure models
Mobility models
Recombination models
Dynamics of recombination centers (Trans

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DD solver interface and config files



To run a DD solver simulation...

- Create and save solver config file, structure config or mesh file, material files (if modified), and other required files in the same folder.
- Run simulations using the following command >> ddsolver ddsolver diode_dev.cfg

```
File:
  Device = "FinFET str.cfg";
  Out = "FinFET";
Contacts: {
  gate: {Voltage = 0.0; WorkFunction = 4.8;
Type = ["Insulator"]; }
  source: {Voltage = 0.0; Type = ["Semiconductor"]; }
  drain: {Voltage = 0.0; Type = ["Semiconductor"]; }
Physics: {
  BandStructure: (
    CarrierDistribution: { ApproximateFermi: []; }
  Recombination:
    SRHRecombination = ["DopingDep"];
Physics*Region*RegSi:
  Mobility: {
    DopingDep: {
      Masetti: [];
    FieldDep: {
      Lombardi: []:
Plot:
  Ouantities = ["ElectronDensity", "AbsElectricField",
               "ElectrostaticPotential".
                "TotalRecombination",
               "AbsElectronCurrent"1;
```

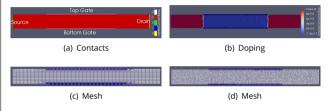


Figure: Device structure

- File: set Device structure with .cfg file or .h5 file.
- Contacts: Set properties of contacts defined in Device.
- Physics: Set *globally* active models.
- Physics*Region*RegSi: Set region-wise active models.
- Plot: Datasets to be stored at each specified bias point.



- Introduction
- Configuring DD-solver Easy-to-use config files
- Available analyses

Small-signal analysis
Mixed-mode analysis
Electro-thermal simulations

Physics in DD solver

Contact boundary conditions
Band structure models
Mobility models
Recombination models
Dynamics of recombination centers (Traps

6 Licenses



Quasi-stationary Analysis

```
Math:
  IterationsFC = 40:
  InnerIterationsFC = 10;
  FCSolverTolerance = 1.:
  SolverSettings = [
            "InterpolateElecPotential",
            "InterpolateElecFermi"
            ."InterpolateHoleFermi"
Solve:
  Static*Poisson: {
   Coupled: ["Poisson"];
  Quasistationary*Drain: {
    initstep = 1E-3; minstep = 1E-5;
   maxstep = 0.1; incr = 1.35; decr = 2;
    Ramp:
      Voltage*drain = 1.:
   Coupled: ["Poisson", "Electron"]
   PlotTime = [0., 0.5, 1.0];
   Math: {
      IterationsFC = 40:
```

- Math: Specify various numeric parameters and solver settings.
- Solve: Provide information on solve steps to perform consecutively.

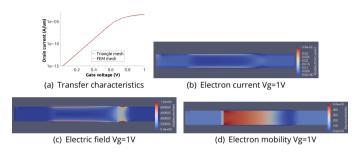


Figure: Simulated device transfer characteristics and spatial distributions.

- Quasistationary, Static, and Transient ramps can be initialized.
- \bullet In <code>Quasistationary</code> ramp, a fictitious time variable is ramped from 0 to 1.
- Voltage*drain: Voltage of drain contact is ramped to the specified value.
- Coupled: Which equations to solved in the coupled solver. Alternately SelfConsistent solving is possible.
- Plot: Spatial distribution of Quantities is stored in an hdf file at each time-point Time

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Small-signal analysis

```
Plot:
 ACQuantities = ["ElectronDensity",
    "AbsElectricField".
    "ElectrostaticPotential"]:
Solve:
  Static*Poisson: {
   Coupled: ["Poisson"]:
  Quasistationary*Drain:
   initstep = 1E-3; minstep = 1E-5;
   maxstep = 0.1; incr = 1.35; decr = 2;
    Ramp: {
      Voltage*drain = 1.:
   Coupled: ["Poisson", "Electron"]
  Ouasistationarv*Gate:
    initstep = 1E-3; minstep = 1E-5;
   maxstep = 0.1; incr = 1.35; decr = 2;
   Ramp: 8
     Voltage*gate = 1.0;
   Coupled: ["Poisson", "Electron"]
   Plot: { Time = [0., 0.05, 0.5, 1.0]; }
   ACAnalysis: {
      Nodes = ["gate", "source", "drain"];
     Time = [0.99]; PointsPerDecade = 3;
     MinFrequency = 1E2: MaxFrequency = 1E6:
      PlotFrequency = [1E3, 1E6];
```





(a) Effect of small-signal voltage at drain

(b) Effect of small-signal voltage at gate



(c) Effect of small-signal voltage at source

Figure: FinFET: Spatial small-signal variation of electron density because of application of small-signal voltage at (a) drain, (b) gate, and (c) source.

- ACAnalysis specifies DC bias point(s) with Time at which analysis is done.
- Nodes: Contacts which will be included in the AC analysis.
- ACQuantities in Plot section list the quantities to be stored in AC analysis.
- \bullet $\,$ PlotFrequency: at these frequencies the AC quantities are stored.



Mixed-mode analysis

```
Device*MOS1: {
 File: { ... }
  Contacts: { ... }
  Physics: { ... }
Math:
System: {
  //SpiceCircuitFiles = [ "SpCkt1.cir"];
  SpiceCircuit:
    ".subckt Amplifier Vc Vg Vout
    R1 Vc Vout 1K.
   R2 Vs 0
              10.
             100.
   R3 Va 0
   R4 Vc Va 4K.
   W1 Vout Vg Vs MOS1
    ende
   Vsupply Vc 0 DC 0.0
   X1 Vout1 Vin Vc Amplifier
    end"
Solve:
  Static*Poisson:
   Coupled: ["Poisson", "Electron", "Circuit"]:
   Plot: { Time = [0.]; }
```

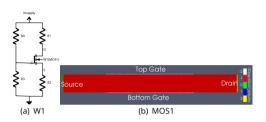


Figure: MOSFET system shown in the System section on the LHS.

 ${\tt System}$ command solves the mixed-mode system containing electronic device which is connected to the external components.

```
Note: Use the following for mixed-mode simulations.
>> DDSolver systemsolver FinFETSys_dev.cfg
```

- System section defines external circuit and links the Device named MOS1 to it as follows - W1 Vout Vg Vs MOS1
- Solve coupled circuit, Poisson, continuity equations using Coupled: ["Poisson", "Electron", "Circuit"];

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Electro-thermal simulations

```
Contacts:
  Anode: {Voltage = 0.0; Type = ["Semiconductor"];
          Temperature=300.1
 Cathode: {Voltage = 0.0; Type = ["Semiconductor"];
           Temperature=310.}
ThermalContacts: { ... }
Physics: {
  ThermalProperties: {
    HeatCapacity: ["TempDep"];
    HeatConductivity: ["TempDep"];
Plot: 4
  Ouantities = ["eJouleHeat".
              "hJouleHeat".
              "HeatGeneration".
              "Temperature"1:
Solve: {
 Static*PoiTemp: {
    Coupled: [ "Poisson", "Temperature"];
   Plot: { Time = [0.0]: }
  Static*Poisson:
    Coupled: ["Poisson", "Electron", "Hole",
              "Temperature"];
    Plot: { Time = [0.]; }
```

Electro-thermal simulations solve Poisson and/or continuity equations with heat transport equation.





(a) Temperature distr. in Copper plate at 1V

(b) Copper plate conductivity at 1V

Figure: Heat generation in a 2D copper plate

- Contacts: Each electrical contact acts as a heat-sink if Temperature is specified.
- If ThermalContacts are defined in structure config file, then list them in ThermalContacts: { ... }.
- In Physics Section, ThermalProperties list which thermal models are active.
- In Coupled command, add Temperature for adding heat equation to the coupled solver.

- Introduction
- Configuring DD-solver Easy-to-use config files
- Available analyses
 Small-signal analysis
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 Band structure models
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Solver equations

- The solver supports solving Poisson, electron/hole continuity, circuit, and heat-flow equations.
- Poisson equation is given by –

$$-\nabla^2 \Psi(\vec{r}) = \rho_C(\vec{r}) + n(\Psi(\vec{r})) - p(\Psi(\vec{r})) \tag{1}$$

Here, $\rho_{C}(\vec{r})$ includes dopants, bulk, and interface charges, and charged traps.

• Electron/hole continuity equations are given by -

$$\frac{\partial n}{\partial t} = \nabla \cdot \vec{J}_n/q - (R_n - G_n) \text{ and } \frac{\partial p}{\partial t} = -\nabla \cdot \vec{J}_p/q - (R_p - G_p)$$
 (2)

Here, $R_{n/p} - G_{n/p}$ term include all the recombination mechanisms, e.g. SRH, Band-to-band, impact ionization, recombination at bulk/interface defects.

Heat-flow equation is given by –

$$c \cdot \frac{\partial T}{\partial t} - \nabla \cdot (\kappa \nabla T) = G_{\text{Heat}}$$
 (3)

Here, $G_{\rm Heat}$ includes heat generation in semiconductors as well as metals.

Circuit equation is solved by modified nodal analysis.

Nonlinear solver: The DD solver uses a damped Newton's solver reported in Bank et al.

$$\mathbf{g}'(\vec{x}_i) \cdot d\vec{x}_i = -g(\vec{x}_i) \tag{4}$$

$$\vec{x}_{i+1} = \vec{x}_i + \gamma \vec{dx}_i \tag{5}$$

Damping parameter (γ) calculated such that $\frac{\|g(\vec{x}_{j+1})\|}{\|g(\vec{x}_i)\|} < 1$ and $\frac{\|g(\vec{x}_{j+1})\|}{\|g(\vec{x}_i)\|} \to 1$.

Coupled solver: All equations are coupled to calculate the Jacobian ($\mathbf{g}'(\vec{x})$).

$$\mathbf{g}'(\vec{x}) = \begin{bmatrix} \frac{\partial P}{\partial \psi} & \frac{\partial P}{\partial n} & \frac{\partial P}{\partial p} \\ \frac{\partial J_n}{\partial \psi} & \frac{\partial J_n}{\partial n} & \frac{\partial J_n}{\partial p} \\ \frac{\partial J_p}{\partial \psi} & \frac{\partial J_p}{\partial n} & \frac{\partial J_p}{\partial n} \end{bmatrix}$$
(6)

Self-consistent solver: Equations solved one after the other until convergence is reached.

$$\mathbf{g}'(\vec{x}) = \frac{\partial P}{\partial \psi}$$
 then $\mathbf{g}'(\vec{x}) = \frac{\partial J_n}{\partial n}$ then $\mathbf{g}'(\vec{x}) = \frac{\partial J_p}{\partial p}$

Contact boundary conditions

Contact properties are assigned in the *Device* config file (e.g. diode_dev.cfg) –

```
Contacts: {
    Anode: {
        Voltage = 0.0; Type = ["Semiconductor"];
        SchottkyBarrier = 0.5; Resistance=lE1;
    }
    Cathode: {
        Voltage = 0.0; Type = ["Semiconductor"];
        Resistance=lE1;
    }
}
```



(a) Electrostatic potential under reverse bias



(b) I-V plot of the Schottky diode

Default boundary conditions for the drift-diffusion equations -

- Electric field normal to the device-domain boundary is zero $\nabla \psi \cdot \hat{n}$ = 0.
- Electron current (J_n) and Hole current (J_p) at the semiconductor-insulator/gas boundary is zero, $J_n \cdot \hat{n} = J_p \cdot \hat{n} = 0$.
- Note: The above equations impose reflective BCs at the domain boundaries.

Semiconductor contact boundary conditions -

- Two types of semiconductor contacts *Ohmic* and *Schottky* contacts.
- Semiconductor contacts are, by default, *Ohmic* contacts.
- Schottky contact is set by adding an argument SchottkyBarrier=0.5 in the contact definition. Here 0.5eV is a Schottky barrier. The barrier enters the electrostatics as follows.
- A resistive contact is set by adding an argument Resistance=0.1. in the contact definition. Here, 0.1 Ω is the contact resistance.

Insulator contact boundary conditions -

 Contacts at the insulator boundary are used to specify metal/insulator interface of the gate.

```
Contacts: {
gate: (Voltage = 0.0; WorkFunction = 4.8; Type = ["Insulator"]; 2V
```

Physical models are activated in the *Device* config file (e.g. diode_dev.cfg) –

```
Physics: {
  BandStructure: {
    CarrierDistribution: { ApproximateFermi: []; }
    BandGapNarrowing: { Slotboom: []; }
}
```

Physical model parameters are set in *Material* parameter file (e.g. Silicon.cfg) –

• Temperature dependence of the band gap is modeled by Varshneys law.

$$E_g(T) = E_g(T_0) + \frac{\alpha T_0^2}{T_0 + \beta} - \frac{\alpha T^2}{T + \beta} - E_{bgn}$$
 (7)

- Band-gap narrowing (E_{bgn}) caused by high dopant conc. can be modeled by one of the following models - DelAlamo, Slotboom, or BennetWilson models.
- Relation between Fermi energy and carrier density is given by Fermi-Dirac integral.

$$n(\vec{r}) = N_C \mathcal{F}_{1/2} \left(\frac{q(\phi_n - E_C)}{kT} \right) \text{where} \mathcal{F}_{1/2}(\eta) = \int_{\epsilon=0}^{\infty} \frac{\epsilon^{1/2}}{1 + \exp{(\epsilon - \eta)}} d\epsilon$$
(8)

Analytic approximation of Fermi integral is modeled by -

- $\mathcal{F}_{1/2}(\eta) = \exp(\eta) \cdots$ as in Boltzmann model.
- $\mathcal{F}_{1/2}(\eta) = \frac{1}{\exp{(-\eta)} + 0.27} \cdots$ as in ApproximateFermi model.

Note: The latter model is valid over a slightly wider range of η .

 DOS in Eq. 8 can be set from niFixed (user-defined intrinsic carrier density) or by specifying Nc300, Nv300 or from me, nv.

Defining material grading

Physical models are activated in the *Device* config file (e.g. diode_dev.cfg) –

```
Physics*Region*Reg1: {
    MoleFraction: {
        MoleFraction: {
            Direction = [0.1, 0., 0.];
            Position = [0., 0., 0.];
            Position = [0., 0., 0.];
            EndVal = 0.;
            Distance = 0.1;
            Shape = "Quadratic";
            Bow = 0.01;
        }
}
```

Composition dependent parameters are set in *Material* parameter file (e.g. AlGaAs.cfg) –

Band-diagram at the interface (a) without grading SY 60 SY 80 SY

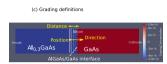


Figure: Grading at the hetero-interface

- Material mole fraction (x) in a region is set in MoleFraction.
- In the bulk of the region, x set by BulkXFraction.
- x changes from its bulk value to the EndVal starting from Position in the Direction. x takes a constant value at a plane normal to Direction.
- Shape of the 1D profile is given by <code>Shape.</code> σ of exponential and Gaussian shapes is given by <code>Distance.</code>

Mole-fraction (x) dependence of a parameter in a material config file.

- Band-gap dependent material parameters (e.g. Eg0) are listed as a pair of mole-fraction and value in brackets (...) instead of a single value
- Band-gap dependent parameters of electrons and holes (e.g. taumax) are listed as triplets of mole-fraction, vale, and val_h in brackets (...).



Physical models are activated in the *Device* config file (e.g. diode_dev.cfg) –

```
Physics: {
  Mobility: {
    DopingDep: { Masetti: []; }
    FieldDep: { Lombardi: []; }
    HighFieldSat: { Canali = []; }
  }
  ...
}
```

Physical model parameters are set in *Material* parameter file (e.g. Silicon.cfg) –

```
Mobility: {
    ConstantMob: {
        mu0 = [1450.0, 450.0];
        alpha = [1.4, 1.4];
    }

Masetti: {
        mumin1 = [52.2, 44.9];
        mu1 = [43.4, 29.];
    }

Canali: {
        vsat0 = [1.07E7, 8.37E6];
        vsatexp = [0.87, 0.52];
    }

Lombardi: {
        B = [4.75e7, 9.925e6];
        C = [5.8e2, 2.947e3];
    }
}
```

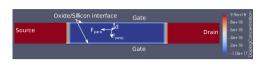


Figure: Mobility degradation at oxide/Si interface

- ConstantMob model for e/h mobility in low-doped Semiconductors.
 It is always active.
- Masetti model for Doping dependent e/h mobility $\mu_b(N_D)$. It depends on N_D the net doping at the given location.
- Lombardi model describes mobility degradation in the MOS channel due to phonon scattering (μ_{ac}) and surface-roughness scattering (μ_{sr}). Both depend on F_{\perp} electric field perpendicular to oxide-Silicon interface.
- Canali model mobility saturation due to high electric field along the transport direction.
- Mattheisen's rule: Low field mobility models are combined using Mattheisen's rule as follows.

$$\frac{1}{\mu_{\text{low}}} = \frac{1}{\mu_0} + \frac{1}{\mu_b} + \exp\left(-\frac{d}{l_{\text{crit}}}\right) \left(\frac{1}{\mu_{\text{ac}}} + \frac{1}{\mu_{\text{sr}}}\right)$$



Physical models are activated in the *Device* config file (e.g. diode_dev.cfg) –

```
Physics: {
  Recombination: {
    SRRRecombination = ["DopingDep"];
    BandZBandGen = [];
    AvalancheGen = ["vanOverstraeten"];
  }
  ...
}
```

Physical model parameters are set in *Material* parameter file (e.g. Silicon.cfg) –

```
Recombination: {
    SRHRecombination: {
        taumax = [1E-6, 1E-6];
        taumin = [1E-9, 1E-9];
}

BandToBandGen: {
    Alp5 = 3.4E21;
    B = 21.9E6;
}

VanOverstraeten: {
    a1 = [7.03E5, 1.582E6];
    b1 = [1.231E6, 2.036E6];
}
}
```

The following models describe non-radiative G-R phenomena in Semiconductors.

- SRHRecombination models G-R rate arising mainly from deep energy traps. Doping-dependence of carrier life-times is activated by DopingDep keyword and are calculated by Scharfetter model.
- Band2BandGen model accounts for generation of carrier by band-to-band tunneling in high electric field regions. It calculates generation rate by the following expression-

$$G_{\text{btb}} = A_{p} \cdot |F|^{p} \cdot \exp\left(-\frac{B}{|F|}\right)$$
 (10)

Here, p = 1., 1.5, 2.0.

 AvalancheGen model accounts for generation of carriers by impact-ionization process which takes place when the semiconductor is subject to very high electric field. The generation rate is given by,

$$G_{II} = \alpha_n \left| \vec{J}_n \right| + \alpha_p \left| \vec{J}_p \right| \tag{11}$$

The multiplication factors $\alpha_{n/p}$ are modeled by <code>vanOverstraeten</code> model as follows.

$$\alpha_{n/p}(F_{\text{ava},n/p}) = \gamma \cdot a_{n/p} \cdot \exp\left(-\frac{\gamma b_{n/p}}{F_{\text{ava},n/p}}\right) \tag{12}$$

19/25

Modify the Device config file (e.g. diode_dev.cfg)

```
File:
  OpticalGenerationFile1 =
          "fdtdFinFET TimeAvg AvgMid fdtd.h5";
  OpticalGenerationField = "AbsElectricField";
Physics:
  Recombination:
    GenerationFromFile = ["FileIds = 1",
             "Scaling = 0", "TimeRamp"];
    ApproxRadiativeRec = [ ];
    ConstantGeneration = ["Rate = 1E10".
             "TimeRamp"]:
Solve:
  Ouasistationarv*1: {
    Ramp: {
      Voltage*gate = 1.0;
      ConstantGeneration*Rate = 1E15:
      GenerationFromFile * Scaling = 1;
```

And, the Material parameter file -

```
Recombination: {
  RadiativeRec: {
    C = 1E18; // units of cm^3/sec
    A0Stim = 1E18; // units of cm^3/sec
    A1Stim = 1E18; // units of cm^3/sec
    N0Stim = 1E10; // units of 1/cm^3
  }
}
```

ApproxRadiativeRec analytically models G-R rate in the LEDs or LASERs.
 Recombination rate –

$$R = C \cdot n \cdot p \cdot \left(\frac{T}{T_{\text{par}}}\right)^{\alpha} \tag{13}$$

- ConstantGeneration model adds a constant generation rate in the regions where it is active.
- GenerationFromFile model adds a spatially varying generation rate (typically taken from optical simulations) to the regions where it is active. It is scaled by the Scaling factor before adding. Add the following arguments to the File section.
 - OpticalGenerationFile1: Specify the hdf5 file generated by the FDTD/BPM/Mode solvers. 20 such files can be specified.
 - OpticalGenerationField: Specify the optical field name to be added from the file.
- In last two models, generation rate can be ramped up in Quasistationary transient ramps to achieve convergence. Modify Solve command as shown in the file.



Dynamics of recombination centers (Traps)

Modify the *Device* config file (e.g. diode_dev.cfg)

And, the Material parameter file -

```
Recombination: {
    Traps: {
        vth0 = [2.3E6, 1.7E6];
        Jfactor = [0, 0];
        Gfactor = [2, 2];
        Xsection = [1E-15, 1E-15];
        ConstEmissionRate = [0, 0];
    }
}
```

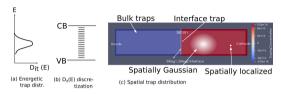


Figure: Trap definitions

- Bulk traps are instantiated in Traps subsection of region Physics, whereas interface traps in Traps subsection of region-interface Physics section.
- Trap types (e.g. Donor), concentration, and distribution (e.g. Gaussian, FromValenceBand) are specified in the trap instantiating groups.
- (De-)trapping rates are calculated by V-section or J-section models.

$$c_C^n = \sigma_n \left((1 - g_n^J) \cdot v_{\text{th}}^n \cdot n + g_n^J \cdot \frac{|\vec{J}_n|}{q} \right) \text{ and } e_C^n = \sigma_n \cdot v_{\text{th}}^n \cdot n 1 / g_n + e_C 0^n$$
(14)

- Trapping parameters σ_n , v_{th} , g^J , g_n , etc. are set in the material config file.
- Trap occupancy set by the *principle of detailed balance*, $f^n = \frac{c^n_C + e^n_V}{c^n_L + c^n_V + e^n_A + e^n_V} = \frac{V}{c^n_L + c^n_V + e^n_A + e^n_V}$

Conclusions

- Drift-diffusion solver supports,
 - quasistationary and transient simulations
 - small-signal analysis,
 - system analysis,
 - electro-thermal analysis.
- Various physical models necessary for semiconductor device modeling are implemented.
- Development of new physical models continues...
- Open to collaborations with our customers / partners.

- Introduction
- Configuring DD-solver Easy-to-use config files
- Available analyses
 Small-signal analysis
 Mixed-mode analysis
 Electro-thermal simulations
- Physics in DD solver
 Contact boundary conditions
 Band structure models
 Mobility models
 Recombination models
- 6 Licenses



Easy-to-install licenses

For ordering a license, along with the name and the organization details, please also provide -

- For the node-locked licenses: Ethernet mac address of the client machine on which the software will run.
 OR
- For the server licenses: Ethernet mac address of the server machine at the client organization.

If you purchased one or more node-locked licenses, you will receive the following license file by secured email.

• NodeLockedLicense.<id>.<Info>.lic, where <id> stands for license id and <Info> stands for customer identification in short.

Copy the license file to /var/local/oesoft/licenses/ on the machine whose mac-address has been provided and change its access rights to 777.

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The End

Questions? Comments?