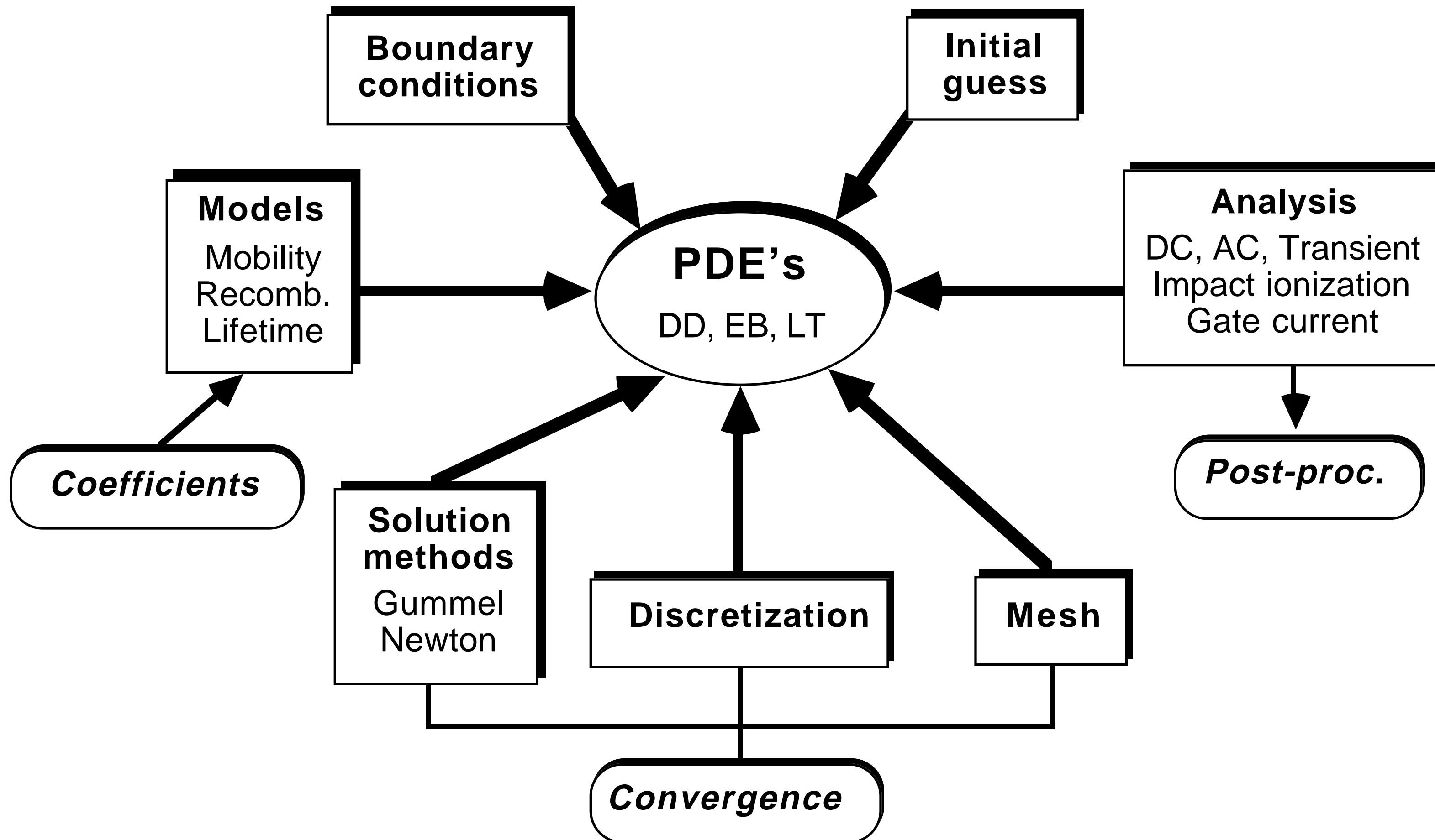
Basic Ingradients in Device Simulation



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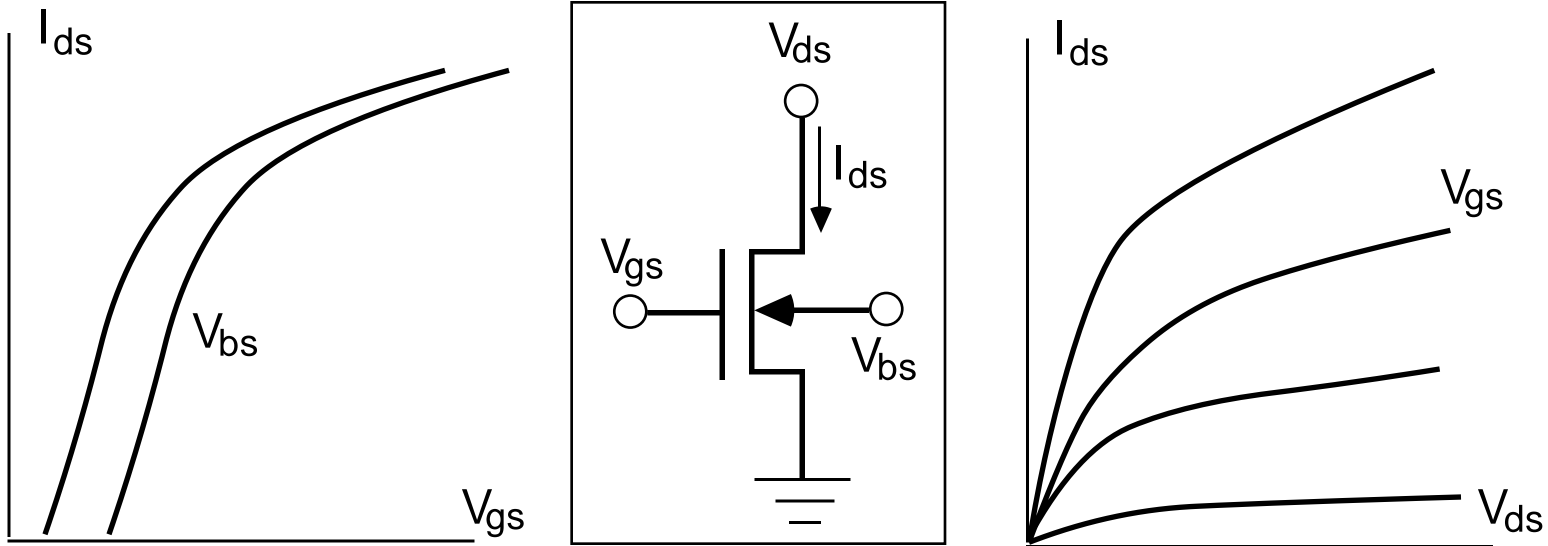
Device Characterization



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Basic Semiconductor Equations

❑ Poisson's equation

$$\varepsilon\nabla^2\psi = -q(p - n + N_D^+ - N_A^-) - \rho_s$$

❑ Continuity equations

$$\frac{\partial n}{\partial t} = \frac{1}{q}\nabla\bullet\boldsymbol{J}_n - U_n = F_n(\psi,n,p)$$

$$\frac{\partial p}{\partial t} = \frac{1}{q}\nabla\bullet\boldsymbol{J}_p - U_p = F_p(\psi,n,p)$$

❑ Drift-diffusion equations

$$\boldsymbol{J}_n = q\mu_n n\mathcal{E}_n + qD_n\nabla n$$

$$\boldsymbol{J}_p = q\mu_p p\mathcal{E}_p - qD_p\nabla p$$

Macroscopic

- $\boldsymbol{J}_n = qn\boldsymbol{v}$, $\boldsymbol{v} = \mu\mathcal{E}$
- $D = (kT/q)\mu$

Microscopic

- $\mu = q\langle\tau\rangle/m_c^*$
- $1/\mu = \sum(1/\mu_i)$

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Grid in MEDICI

❑ Importance

- The correct grid allocation in device simulation has a direct influence on the simulation accuracy and time
- Accurate representation of small device geometries and non-planar devices

❑ Capabilities

- Supports general irregular grid structure for arbitrarily shaped devices
- Allows the refinement of particular regions with minimum impact on others
- Choice of Cartesian or cylindrical coordinate system
- Maximum number of nodes and virtual memory requirement

PROGRAM version	3200	10,000	20,000
Max. nodes available for mesh	3200	10,000	20,000
Max. nodes for 0- or 1-carrier, reduced or all couplings	3200	10,000	20,000
Max. nodes for 2-carrier, reduced couplings	3200	10,000	20,000
Max. nodes for 2-carrier, all couplings	3200	10,000	20,000
Max. nodes for 2-carrier, fully coupled with energy balance	1842	5,736	11,464
Max. nodes for 2-carrier, fully coupled with heat equation	1842	5,736	11,464
Approximate virtual memory required (Mbytes)	22.3	76.2	202

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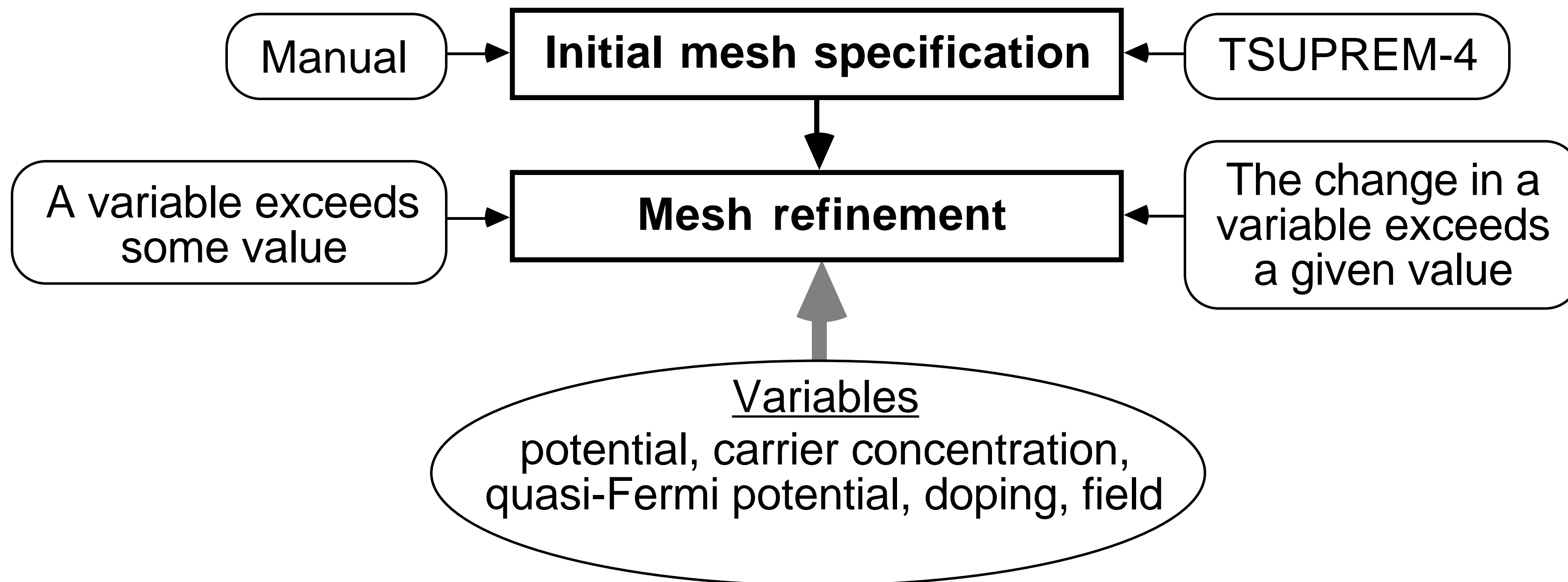
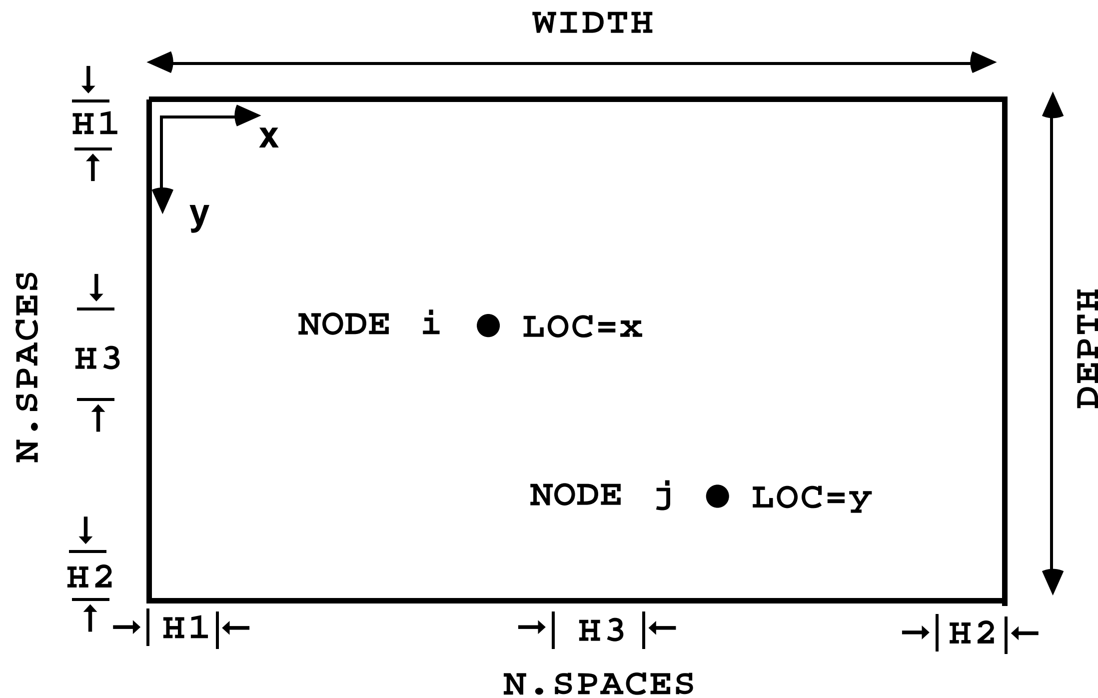
Grid Specification



- **An initial coarse rectangular mesh is generated by the user using input statements or from TSUPREM-4 result**
- **MEDICI provides a regridding mechanism which automatically refines an initial grid wherever key variables vary rapidly**

Three Ways of Initial Mesh Generation

- **Method 1:** **NODE**, **LOCATION**, and **RATIO**
- **Method 2:** **LOCATION** and **SPACING** (TSUPREM-4 method)
- **Method 3:** {**WIDTH**|**DEPTH**}, **N.SPACES**, **H1**, **H2**, **H3**, and **RATIO**



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Major Physical Models

- **Basic semiconductor equation**
  - Poisson’s equation
  - Continuity equations
  - Drift-diffusion equations
- **Recombination models**
  - SRH, Auger, direct, and surface recombinations
  - Concentration-dependent lifetimes
- **Semiconductor statistics**
  - Boltzmann and Fermi–Dirac statistics
  - Incomplete ionization of impurities
- **Mobility models**
  - Low-field and high-field mobilities
  - Surface scattering and electron–hole scattering

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Mobility Models

❑ Low-field mobilities

- Constant mobility
- Concentration dependent mobility (**`CONMOB`**)
- Analytic mobility (**`ANALYTIC`**)
- Arora mobility (**`ARORA`**)
- Carrier–carrier scattering mobility (**`CCSMOB`**)
- Philips unified mobility (**`PHUMOB`**)

❑ High-field mobilities

- Parallel field-dependent mobility (**`FLDMOB`**)
- Caughey–Thomas mobility (**`FLDMOB=`**1)
- Gallium Arsenide-like mobility (**`FLDMOB=`**2)
- Hewlett-Parkard mobility (**`HPMOB`**)

❑ Surface scattering

- Surface mobility (**`SRFMOB`**)
- Enhanced surface mobility (**`SRFMOB2`**)
- Perpendicular field-dependent mobility (**`PRPMOB`**)
- Lombardi surface mobility (**`LSMMOB`**)

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Choice of Mobility Models

<table>
<tr><th>Low Field</th><th>Transverse Field</th><th>Parallel Field</th></tr>
<tr><td>CCSMOB</td><td colspan="2">HPMOB</td></tr>
<tr><td colspan="2">LSMMOB</td><td>FLDMOB</td></tr>
<tr><td>ANALYTIC</td><td>PRPMOB</td><td>TMPMOB</td></tr>
<tr><td>ARORA</td><td>SRFMOB</td><td></td></tr>
<tr><td>CONMOB</td><td>SRFMOB2</td><td></td></tr>
<tr><td>PHUMOB</td><td></td><td></td></tr>
</table>

Example

- ***Valid***:

```
MODEL  CONMOB  PRPMOB  +
  FLDMOB
MODEL  PHUMOB  PRPMOB2
```

- ***Invalid***:

```
MODEL  LSMMOB  HPMOB
MODEL  HPMOB  PRPMOB
```

- **Must not be selected with overlap of different columns**

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Boundary Conditions

- **Ohmic contacts** (Dirichlet B.C.'s) — (ψ_s, n_s, p_s) fixed, $\phi_n = \phi_p = V_{applied}$
  - $\psi_s = \phi_n + \frac{kT}{q}\ln\left(\frac{n_s}{n_{ie}}\right) = \phi_p - \frac{kT}{q}\ln\left(\frac{p_s}{n_{ie}}\right)$
- **Schottky contacts** — finite surface recombination velocity
  - $\psi_s = \chi_{semi} + \frac{Eg}{2q} + \frac{kT}{2q}\ln\left(\frac{N_C}{N_V}\right) - \mathbf{WORKFUNC} + V_{applied}$
  - $J_{sn} = qv_{sn}(n_s - n_{eq})$ $\quad J_{sp} = qv_{sp}(p_s - p_{eq})$
  - $v_{sn} = \mathbf{ARICHN}\ T^2/qN_C$ $\quad v_{sp} = \mathbf{ARICHP}\ T^2/qN_V$
  - Field-dependent barrier lowering: $\Delta\phi_b = \left[\frac{q}{4\pi\varepsilon_{semi}}\right]^{1/2} \mathcal{E}^{1/2} + \mathbf{ALPHA}\ \mathcal{E}$
- **Insulator contacts** — $n_s = p_s = 0$
- **Neumann boundaries** — homogeneous (reflecting) B.C.'s
  - $\hat{\boldsymbol{n}}_1 \bullet \varepsilon_1 \nabla \psi_1 - \hat{\boldsymbol{n}}_2 \bullet \varepsilon_2 \nabla \psi_2 = \sigma_s = \sigma_f + \sigma_{a,p} + \sigma_{a,n} + \sigma_{d,p} + \sigma_{d,n}$

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Solution Specification

❑ Numerical methods

- Discretization
- Gummel's method (decoupled)
- Newton's method (coupled)
- Continuation method

❑ Electrical analyses

- DC analysis
- Transient analysis
- Small-signal analysis
- Impact ionization analysis
- Gate current analysis

❑ Choice of methods

- No single method is optimal in all cases, use the "numerical engine" *efficiently*
- At zero bias, a Poisson solution alone is sufficient (zero carrier)
- For MOSFETs, only one carrier need be solved for (unless for breakdown)
- In bipolar devices, both carriers are needed, and depends on the operating conditions
- Trade-off between stability and speed of the method

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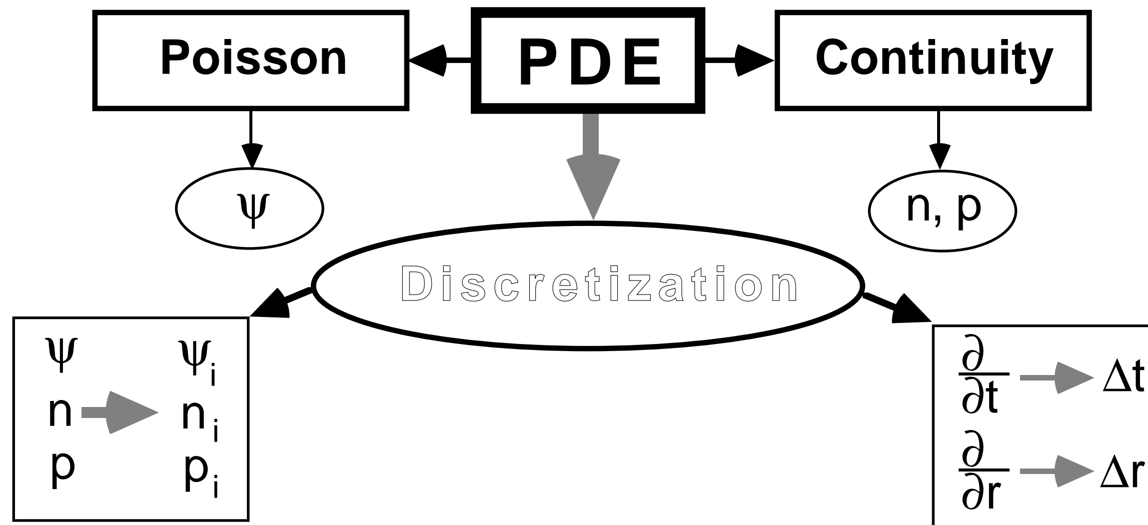
Discretization



- **The PDE's describes the bulk behavior of semiconductor devices**
- **The continuous functions (ψ,*n*,*p*) are represented by vectors of function values at the nodes**
- **The differential operators are replaced by suitable difference operators**
- **Solving 3 unknown functions becomes solving for 3*N* unknown real numbers**

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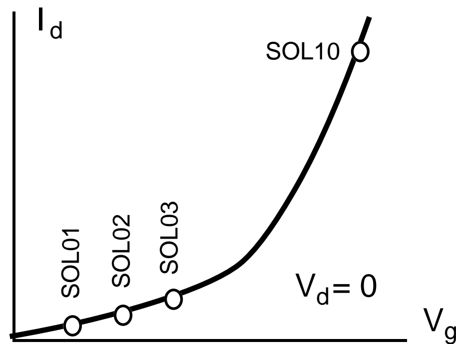
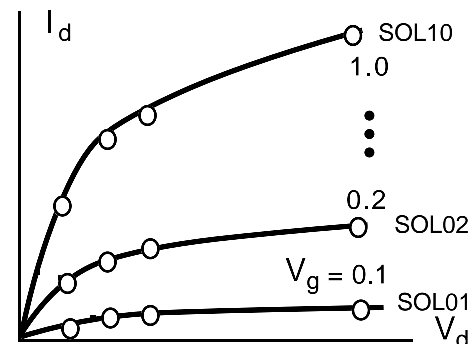
DC Analysis

- **SOLVE ELECTROD {VSTEP|ISTEP} NSTEPS SAVE.BIA …**

❑ **Example**

```
SOLVE V(gate)=0 V(source)=0 V(drain)=0
$ Bias up the gate
SOLVE ELECTROD=gate VSTEP=0.1 NSTEP=10 OUT.FILE=SOL01
$ Drain curves
LOOP STEPS=10
   ASSIGN NAME=SFX C.VAL=01 DELTA=1
   LOAD   IN.FILE="SOL"@SFX
   SOLVE  ELECTROD=drain VSTEP=0.5 NSTEP=20
L.END
```





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Parameter Extraction

- **EXTRACT** — extracts selected data for the solution over a specified cross section of the device

- **Extraction using names and expressions**
  - **EXTRACT EXPRESSI NAME UNITS CONDITIO INITAL.V …**
- **Optimization using targets and expressions**
  - **EXTRACT TARGET WEIGHT MIN.REL MIN.ABS …**
- **Extract physical quantities from solution**
  - **EXTRACT {NET.CHAR|NET.CARR|ELECTRON|HOLE|RECOMBIN| + IONIZATI|RESISTAN|N.RESIST|P.RESIST|METAL.CH| + N.CURREN|P.CURREN|II.GENER|SHEET.RE}**
- **Extract MOS device parameters**
  - **EXTRACT MOS.PARA DRAIN GATE IN.FILE I.DRAIN**

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Data Post-Processing

❑ **Print**

- **PRINT** — prints specific quantities at points within a defined area

❑ **Plot**

- **PLOT.1D** — plots a specific quantity along a line segment through the device
- **PLOT.2D** — plots 2D characteristics, boundaries, junctions, depletion edges
- **PLOT.3D** — plots 3D physical quantities
- **3D.SURFACE** — plots the projection of a 3D view of the specified data
- **CONTOUR** — plots contours of a physical quantity on a 2D area
- **VECTOR** — plots vector quantities over an area
- **E.LINE** — plots potential gradient paths and calculates ionization integrals

❑ **Others**

- **FILL** — fills material regions with specified colors
- **LABEL** — plots character strings, symbols, and lines as part of a 1D/2D plot

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Input and Output

- **Saving I–V and AC terminal data**

  LOG OUT.FILE TIF AURORA ICCAP …

- **Saving solutions, structure, model and coefficients**

  SAVE OUT.FILE SOLUTION MESH W.MODELS TIF ALL …

- **Loading/saving solutions for continued simulations or post processing**

  LOAD IN.FILE IN.PREV ASCII.IN OUT.FILE …

- **Data stored in a solution file**
  - Potential and carrier concentrations at each node
  - Information describing the setup used to obtain the solution (e.g., physical parameters, boundary conditions, physical model selection)

- **When a solution is LOADed, the setup information will be used by default for all subsequent solutions unless modified**

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Documentation and Control

- **Assigned variable**

  ASSIGN NAME {N.VAL DELTA|C.VAL DELTA|L.VAL}

- **Looping**

  LOOP STEPS {OPTIMIZE|SENSITIV}

  L.MODIFY LEVEL STEPS {NEXT|BREAK}

  L.END BREAK ALL

- **Conditional**

  IF COND=*expression*

  ELSE COND=*expression*

  IF.END

- **Statement inclusion**

  CALL FILE=*fname*

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Interfacing with TSUPREM-4

❑ Significance

- Meaningful device design and optimization based on real fabrication process
- Realistic device structure and impurity profiles

❑ Key steps

- Use mask information from TMA LAYOUT
- Use the adaptive gridding in TSUPREM-4 (automatic)
- Use the regrid facility in MEDICI
- Require well calibrated process models and parameters
- Calibrate independently key device model parameters in MEDICI

❑ Interface

- In TSUPREM-4: **`SAVEFILE MEDICI OUT.FILE=mesh.ts4`**
  In MEDICI: **`MESH TSUPREM4 IN.FILE=mesh.ts4`**

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Discrepancies Between Simulation and Measurement

- **Simulation may be right, measurement may be "wrong"**
- **Device simulator unlikely produces incorrect results on correct structure**
- **First thing to check**
  - *Accuracy of the doping profile*: junction depths, peak concentrations, etc.
  - *Accuracy of the structure*: gate oxide thickness, etc.
- **Other possibilities**
  - Inadequate grid (need to have vertical grid spacing in the channel of 15–25Å)
  - Incorrect or incomplete specification of mobility and other physical models
  - Incorrect workfunction (recommended value of 4.35 eV for n^+ poly gates)
  - Forgetting to specify fixed oxide charge (use values extracted from C–V)
  - Forgetting to specify accurate lifetimes (use values measured on wafers)
  - Is lattice heating important? (use LT-AAM) Does traps exist? (use TC-AAM)
  - Is your measured device typical when compared to others on the same lot

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