Numerical Semiconductor Device Modeling

EE614- Spring 08

Prof. Eric Polizzi

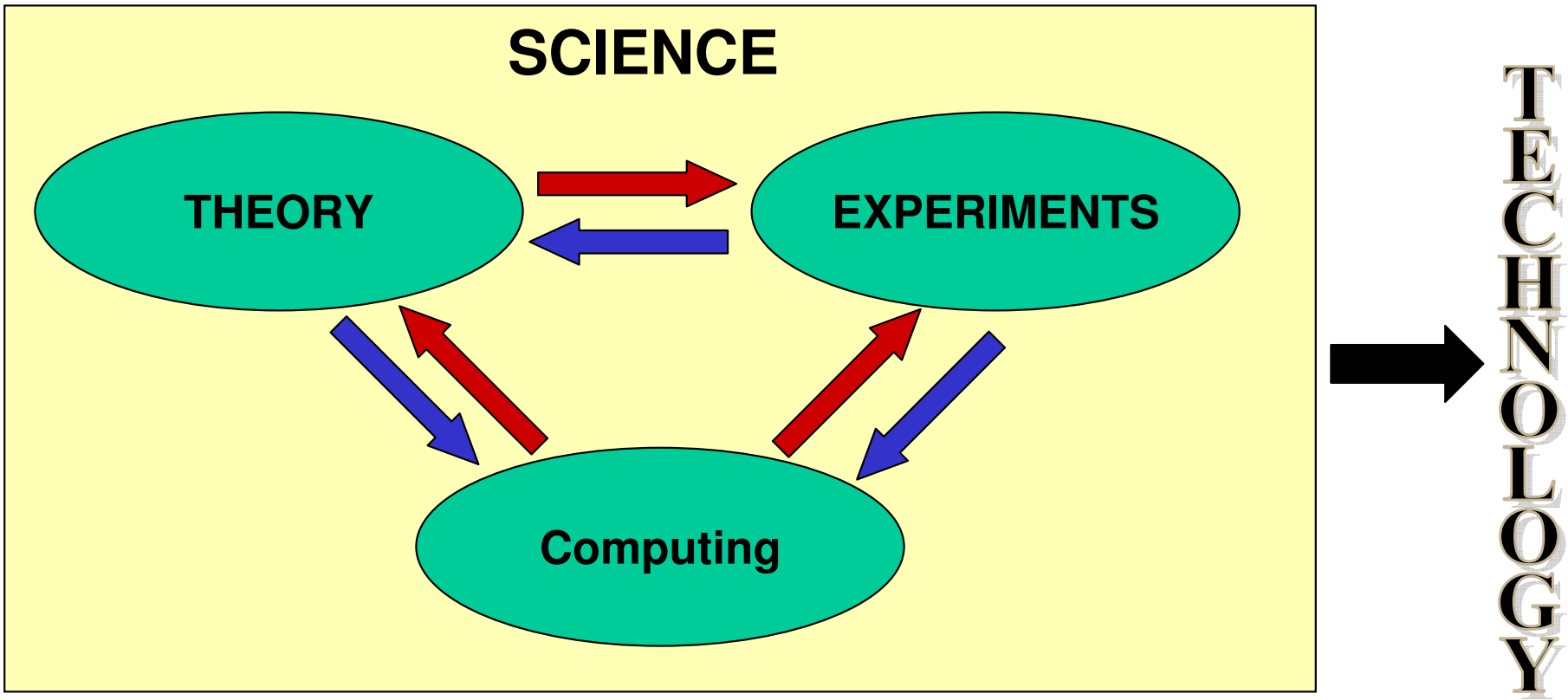
Department of Electrical and Computer Engineering, University of Massachusetts, Amherst, USA

Information

- **Instructor:** Prof. Eric Polizzi
- **Office:** Marcus 201C
- **Day and Time:** Tue-Thu 1:00-2:15
- **Place:** ELAB-325
- **Office Hours:** After class (up to 2:40pm), and Wed 11am-12
- **E-mail:** polizzi@ecs.umass.edu
- http://www.ecs.umass.edu/ece/polizzi
  - Go under Teaching and find also homework, and handouts.
- Homework (numerical) 40%, Final Project 40%, Final Report and Presentation 20%
- Account for Homework and Project:
  - **explorer.ecs.umass.edu** using your login id
  - ssh connection from linux/unix/windows/mac (free software)
  - Fortran 90/95, MPI, ...
- Prerequisite: 609 or equivalent

The Role of Computing in Science and Engineering

- **Goal:** Modeling and simulation (i.e. Computing) as the third component of science



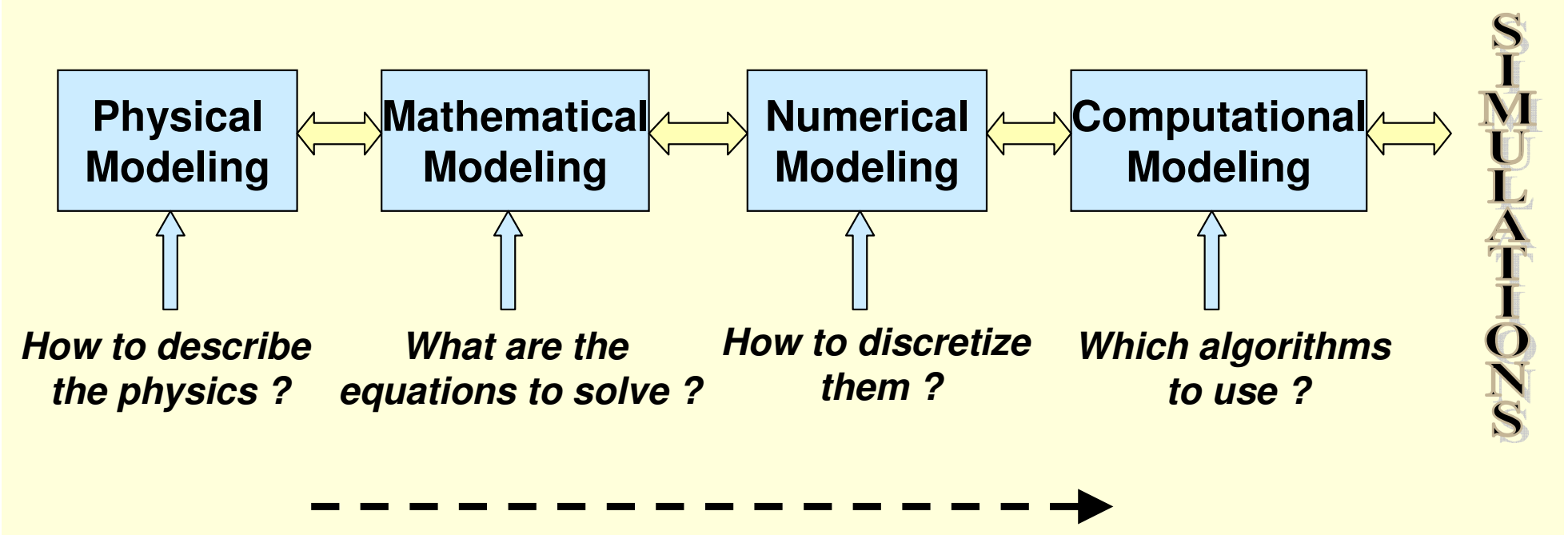
EE614- Overview/Objectives

Objectives of numerical device engineering (Computational Electronics)

- **Supplement the past/current device R&D experimental cycle**
- **Is used to push the scaling limit of the MOS technology (investigates/predicts the ultimate size of MOS devices towards quantum effects and physical limitations)**
- **Is expected to lead the exploration of new class of devices that relies on quantum effects (nanoelectronics- high speed/Terahertz and high functionality devices)**

EE614 – Overview/Approach

Our modeling & simulation framework is a process involving different steps.

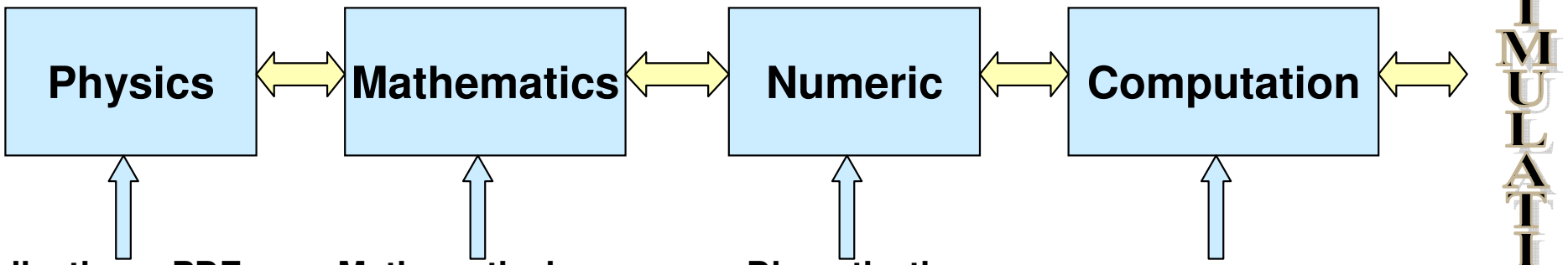


Two difficulties:

(i) answering the questions above, multidisciplinary approach

(ii) making links between communities, interdisciplinary activity

EE614 - Syllabus



Applications: PDE Representation (Deterministic)
- Electronic Structure (from atoms to devices)
- Molecular/Lattice Dynamic
- Transport Equations
- Device Physics (Input Parameters, Output characteristics)

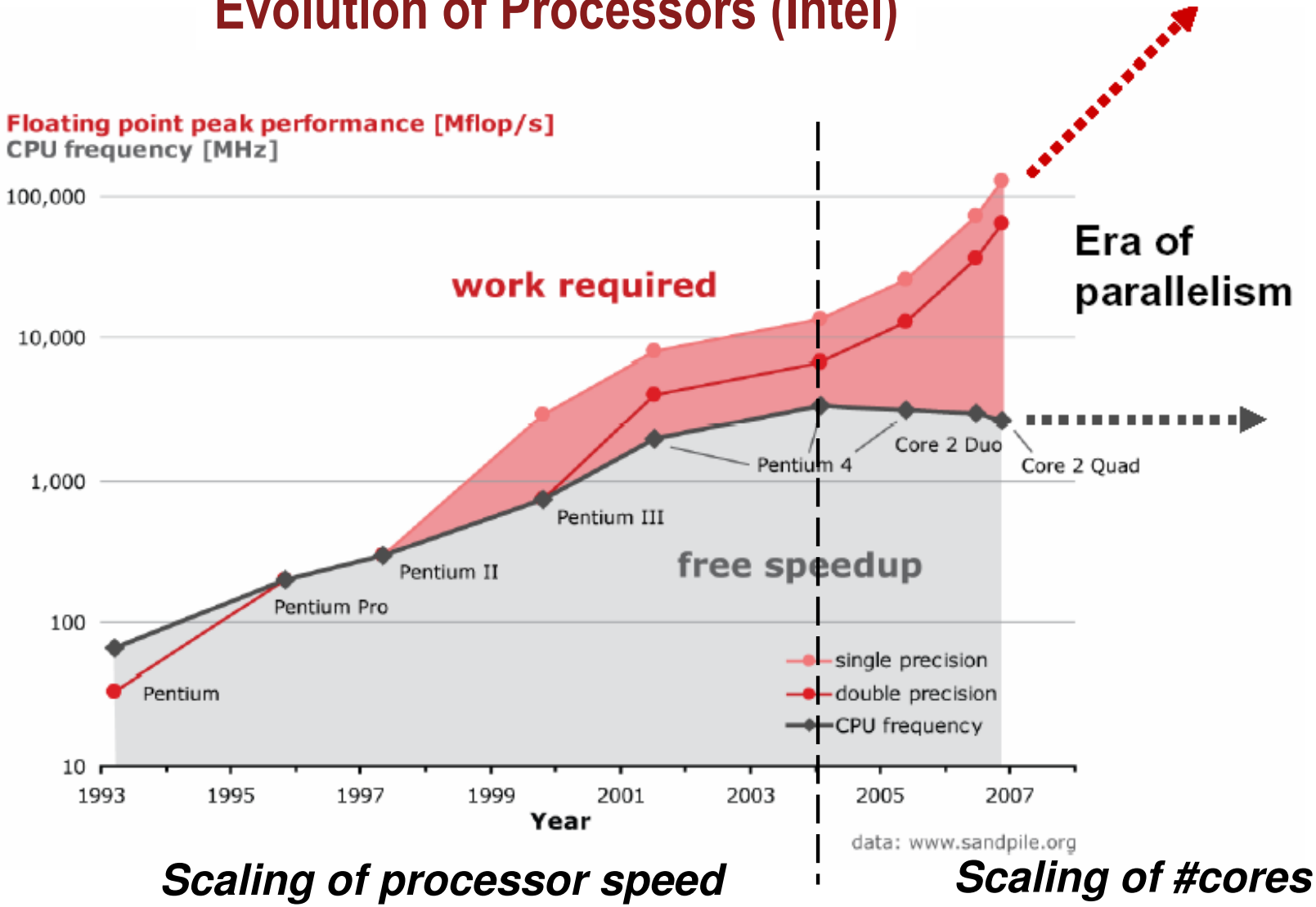
Mathematical Representation/ Treatment
- Computational domain, Boundary Conditions
- Variational techniques
- Integral equation (Green's function)
- Theorem of existence /uniqueness of solutions
- Non-linear equations and techniques
- Decomposition techniques
- Multiscale techniques

Discretization Representation/ Treatment
- *Mesh, Grid*
- *FDM*
- *FEM*
- *Integration techniques, …*

Matrix Representation/ Treatment
- *Eigenvalue Problems*
- *Linear Systems Solvers*
- *Matrix Storage*
- *Direct/Iterative methods*
- *Sequential/ Parallel algorithms*
- *Coding (language and techniques, libraries)*

- **Suggested Reading:**
  - *Prof. T-W Tang notes, other courses on line (see website links)*
  - *Brigitte Lucquin and Olivier Pironneau, 1998, Introduction to Scientific Computing, Wiley, 1998*
  - *D. Vasileka, S. Goodnick, Computational Electronics, Morgan&Claypool publishers*

Evolution of Processors (Intel)



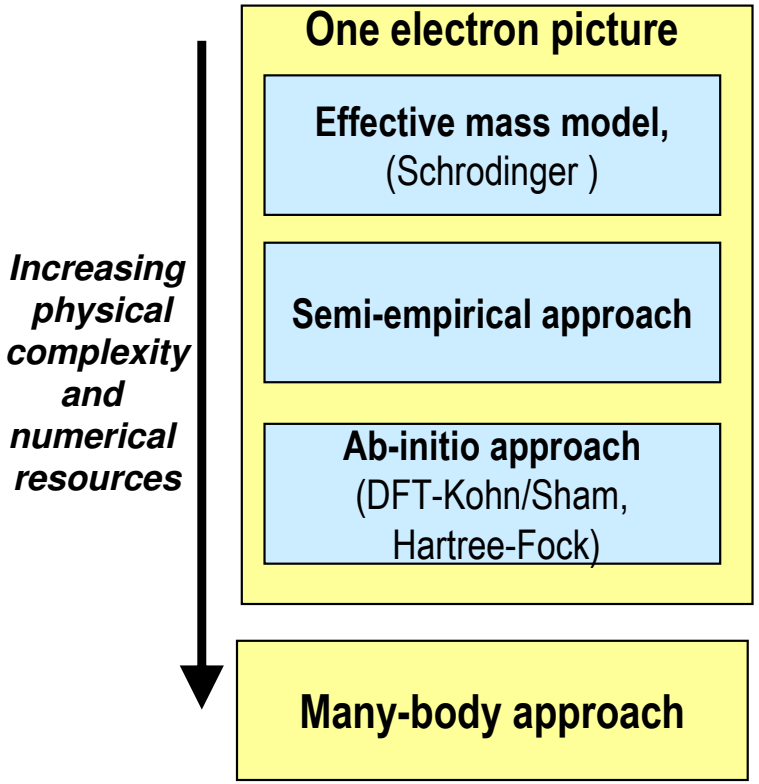
Scaling of processor speed ***Scaling of #cores***

Figure from: Markus Püschel, CMU

Overview of Electronic Structure Calculations

$$(E - H(V))\,\Psi_E = 0; \quad + \quad \text{B.C. (Boundary Conditions)}$$

Electronic structure



Nature of the problem

- **Dirichlet or Neumann B.C.**
  - *Isolated system*
  - *Energy levels are discretized*
- **Periodic B.C.**
  - *Infinite system*
  - *Bandstructure calculations (via Bloch states)*

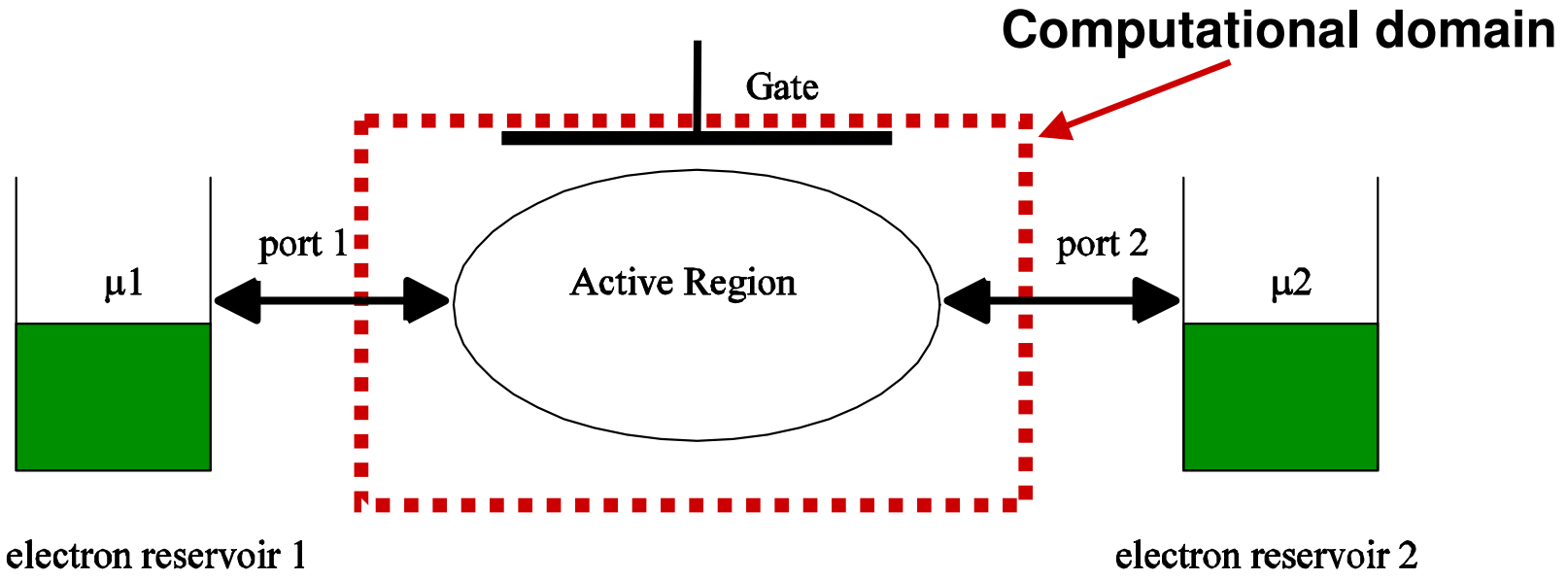
Eigenvalue problems

- **Mixed B.C. (Energy dependent)**
  - *Open system- Ballistic transport*
  - *Energy levels form a continuum (Broadening)*

Linear systems

$$\Psi_j = \Psi_j^{in} + \Psi_j^{out} \qquad \left(\frac{\partial}{\partial \eta_j} - K_j(E)\right)\Psi_j^{out} = 0$$

Overview of Device Modeling



Current-Voltage Characteristics obtained by **self-consistent simulations**: **Transport-Electrostatics**