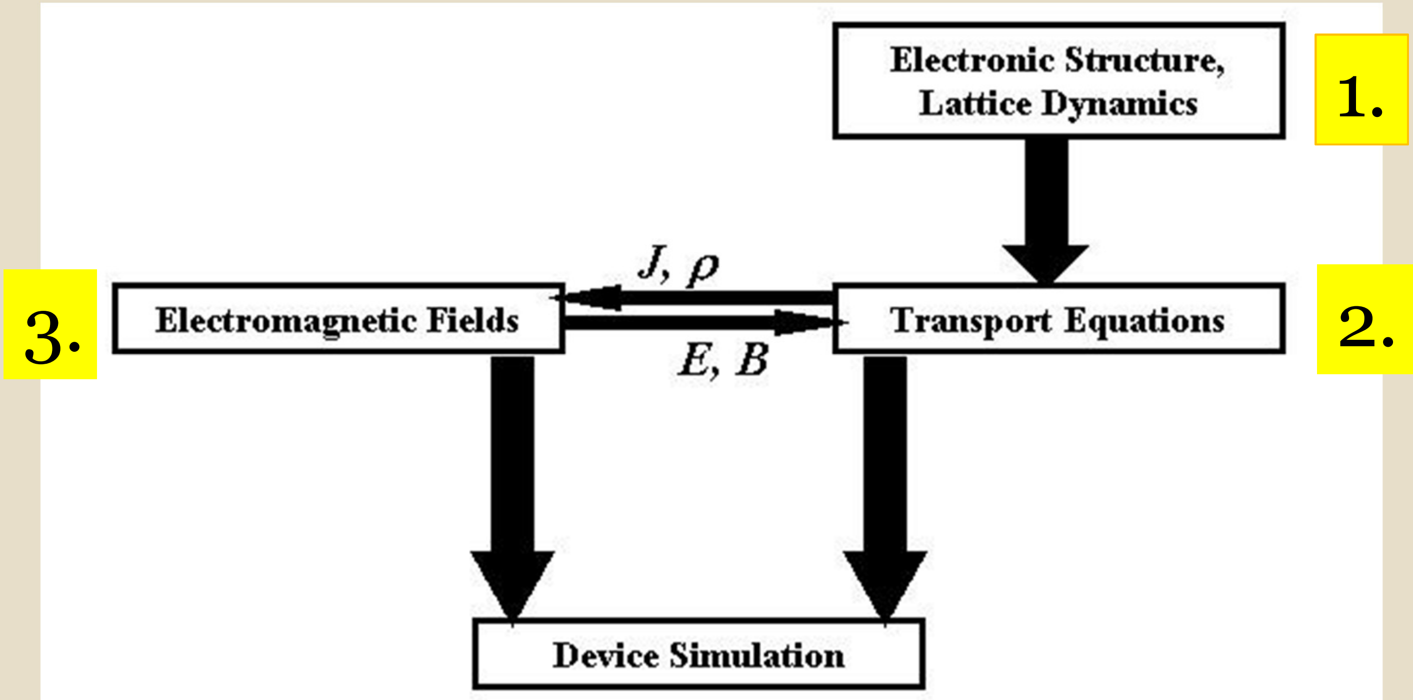
General Concepts of Modeling Semiconductor Devices

Bandstructure Effect

The Choice of the Transport Kernel

The Maxwell→Poisson Equations Solutions

General Device Simulator



D. Vasileska and S.M. Goodnick, *Computational Electronics*, published by Morgan & Claypool , 2006.
D. Vasileska, S. M. Goodnick and G. Klimeck, Computational Electronics: Semi-classical and Quantum Transport Modeling, Taylor & Francis, 2010.

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Electronic Structure

$$H=\sum_j \frac{p_j^2}{2m_j}+\frac{1}{2}\sum_{j,j'}\frac{e^2}{|\bar{r}_j-\bar{r}_{j'}|}+\sum_i \frac{P_i^2}{2M_i}+\frac{1}{2}\sum_{i,i'}\frac{e^2 Z_i Z_{i'}}{|\bar{R}_i-\bar{R}_{i'}|}-\sum_{i,j}\frac{e^2 Z_i}{|\bar{r}_j-\bar{R}_i|}$$

Over all e's — Over all nuclei — e-nuclei

- **1st Approximation**: core vs. valence e's

Still Eq. Above Applies with:
Core e's + nucleus → ion core
e's → valence e's

- **2nd Approximation**: Adiabatic Approximation

IV Semiconductor

C $1s^2 2s^2 2p^2$

Si $1s^2 2s^2 2p^6 3s^2 3p^2$

Ge $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^2$

semicore

III-V Semiconductor

Ga $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^1$

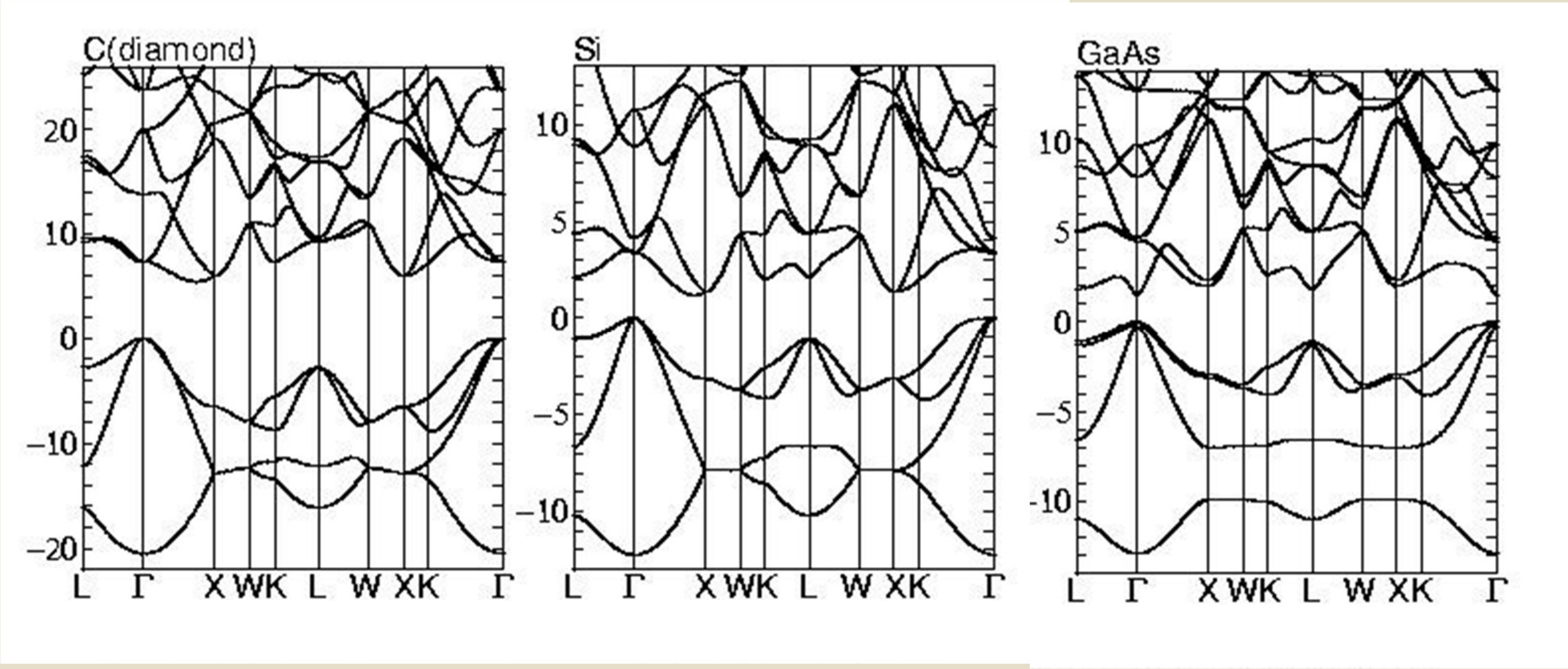
As $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^3$

Advantages of Particular Methods

- Semi-Empirical Methods
  - Empirical Pseudopotential Method
    - Predicts optical gaps
  - k.p Method
    - Predicts effective masses
  - Tight-Binding Method
    - Can include strain and disorder, can simulate finite structures (not just bulk or infinite 2D or 1D)
- *Ab Initio* Methods
  - GW Method
    - Predicts Energy gaps of Materials correctly

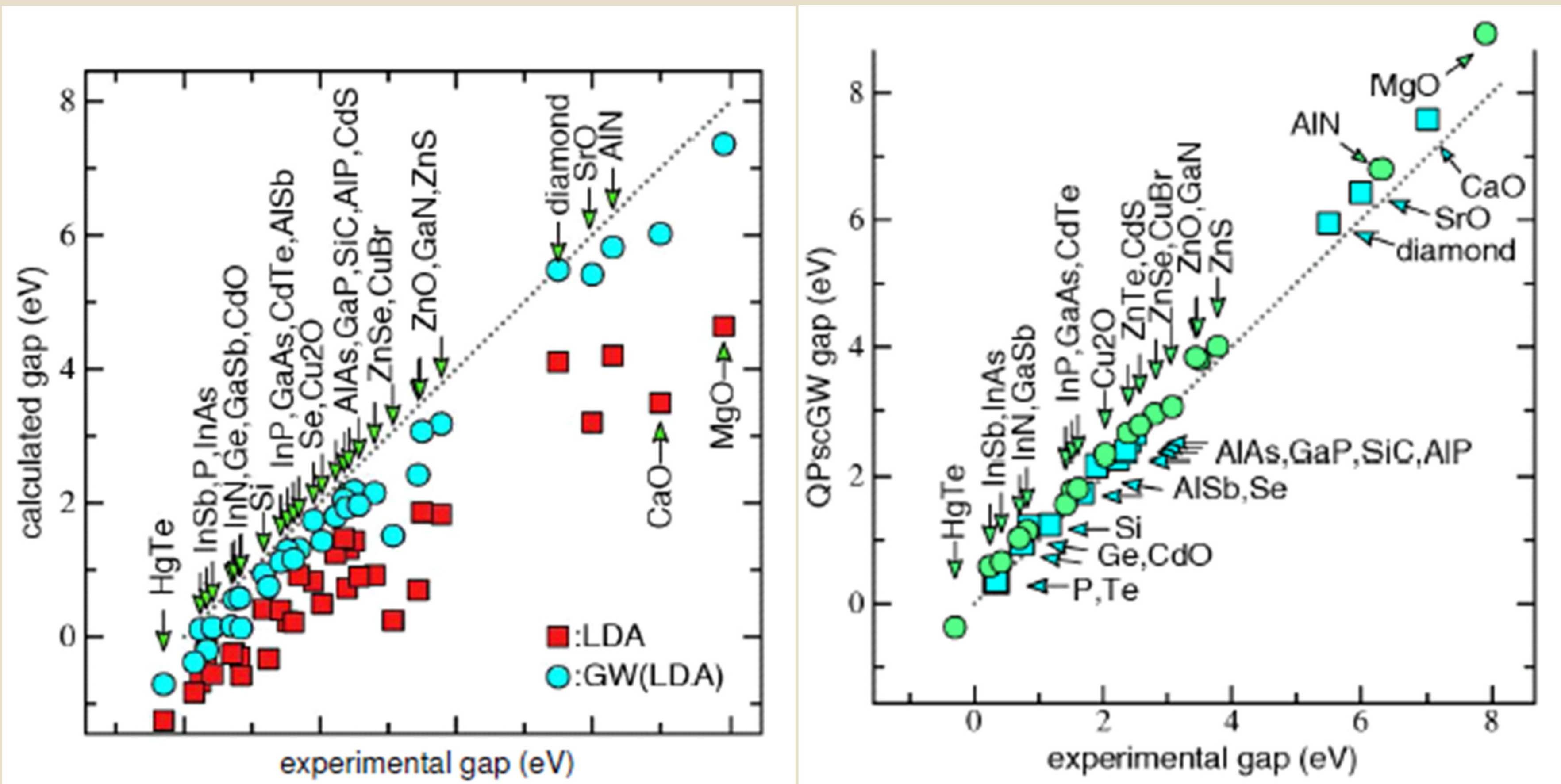
The sp³d⁵s* Tight-Binding Hamiltonian
- [Jancu et al. PRB 57 (1998)] -

Many parameters, but works quite well !



QPscGW *Ab Initio* Results

- Mark van Schilfgaarde -



M. van Schilfgaarde, Takao Kotani, S. V. Faleev, *Quasiparticle self-consistent GW theory*, Phys. Rev. Lett. 96, 226402 (2006)

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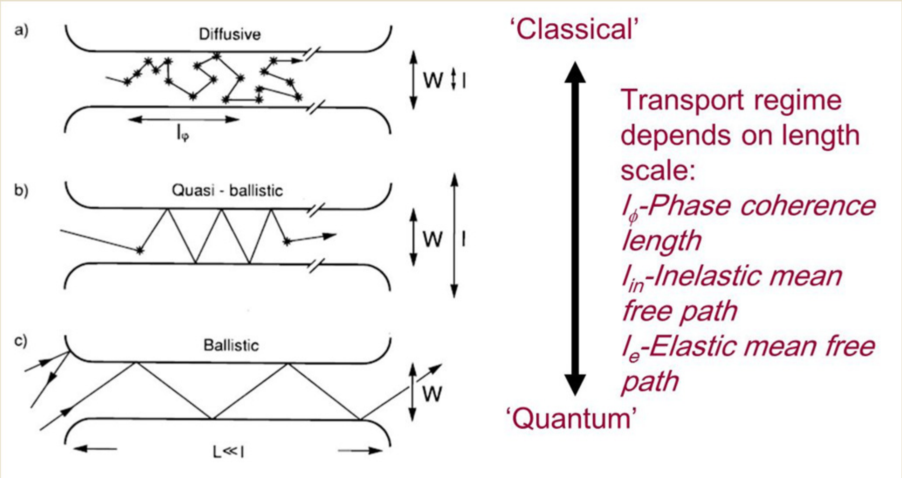
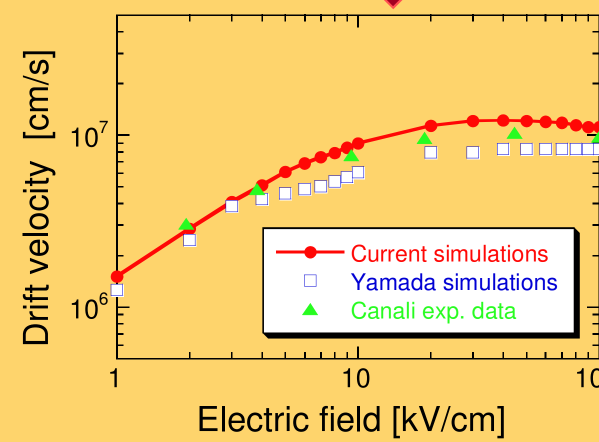


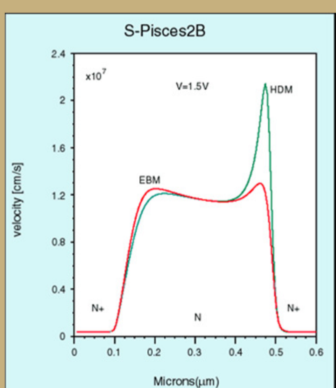
What Transport Models exist?

- Semiclassical **FLUID** models (ATLAS, Sentaurus, Padre)
  - Drift – Diffusion
  - Hydrodynamics

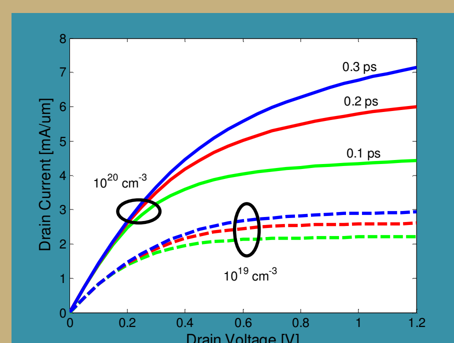
1. **PARTICLE DENSITY**
2. velocity saturation effect
3. mobility modeling crucial



1. Particle density
2. **DRIFT VELOCITY, ENERGY DENSITY**
3. velocity overshoot effect



problems



What Transport Models Exist?

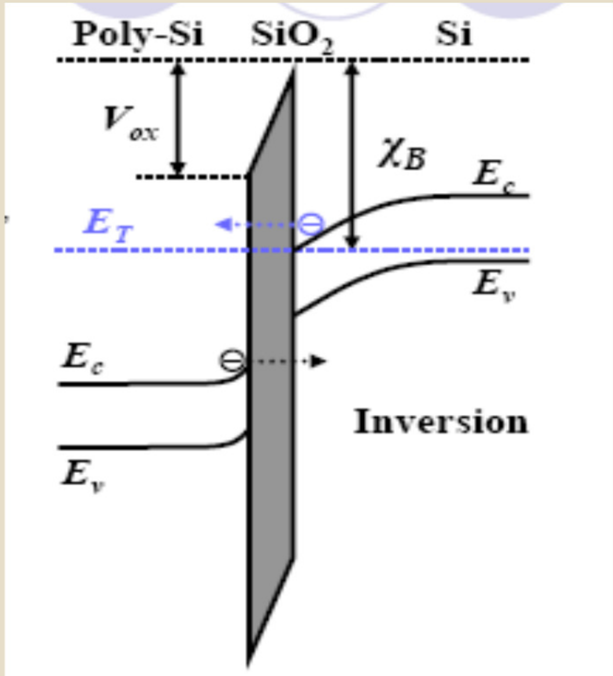
Semiclassical **PARTICLE-BASED** Models:

- Direct solution of the BTE Using Monte Carlo method

  - Eliminates the problem of Energy Relaxation Time Choice
  - Accurate up to semi-classical limits
  - One can describe scattering very well
  - Can treat ballistic transport in devices

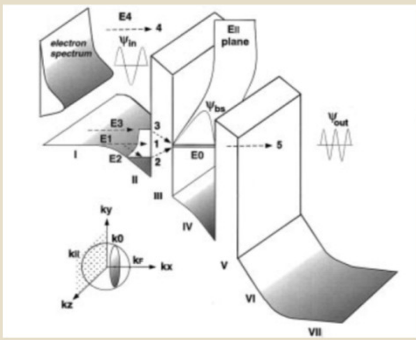
Why Quantum Transport?

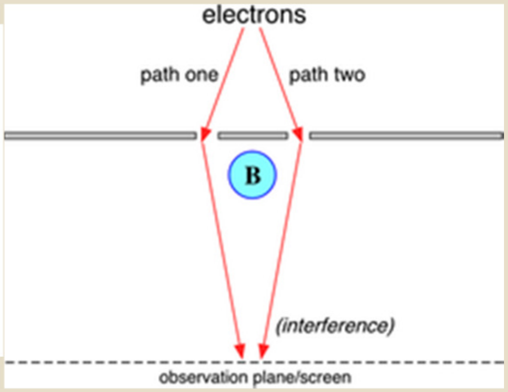
1. Quantum Mechanical TUNNELING



2. SIZE-QUANTIZATION EFFECT

3. QUANTUM INTERFERNCE EFFECT



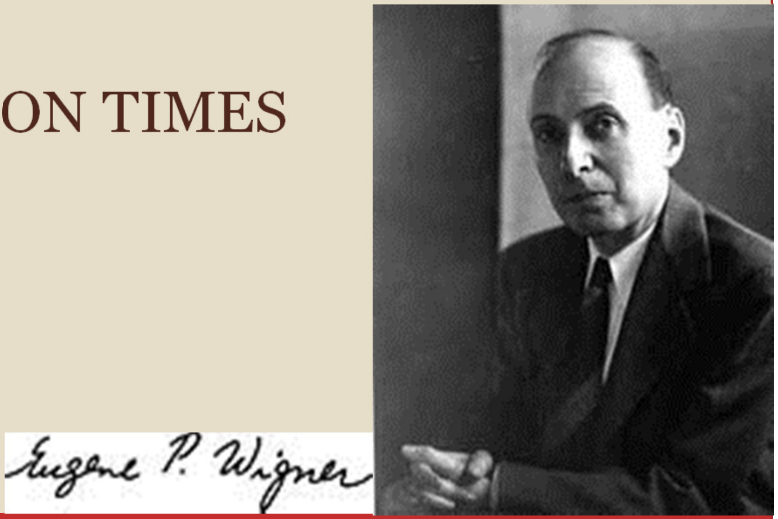


What Transport Models Exist?

- Quantum-Mechanical **WIGNER** Function and **DENSITY** Matrix Methods:
  - Can deal with correlations in space BUT NOT WITH CORRELATIONS IN TIME

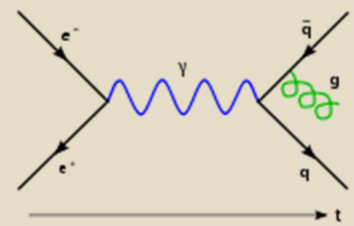
  Advantages: Can treat SCATTERING rather accurately

  Disadvantages: LONG SIMULATION TIMES



What Transport Models Exist?

- **Non-Equilibrium Green's Functions approach** is MOST accurate but also MOST difficult quantum approach
- FORMULATION OF SCATTERING rather straightforward, IMPLEMENTATION OF SCATTERING rather difficult
- Computationally INTENSIVE



Approximate ↑ — *Exact* ↓ (Semi-classical approaches; Quantum approaches)

Easy, fast ↑ — *Difficult* ↓

	Model	Improvements
Semi-classical approaches	Compact models	Appropriate for Circuit Design
Semi-classical approaches	Drift-Diffusion equations	Good for devices down to 0.5 μm, include μ(**E**)
Semi-classical approaches	Hydrodynamic Equations	Velocity overshoot effect can be treated properly
Semi-classical approaches	Boltzmann Transport Equation Monte Carlo/CA methods	Accurate up to the classical limits
Quantum approaches	Quantum Hydrodynamics	Keep all classical hydrodynamic features + quantum corrections
Quantum approaches	Quantum Monte Carlo/CA methods	Keep all classical features + quantum corrections
Quantum approaches	Quantum-Kinetic Equation (Liouville, Wigner-Boltzmann)	Accurate up to single particle description
Quantum approaches	Green's Functions method	Includes correlations in both space and time domain
Quantum approaches	Direct solution of the *n*-body Schrödinger equation	Can be solved only for small number of particles

D. Vasileska, PhD Thesis, Arizona State University, December 1995.

Range of Validity of Different Methods

	$L << l_{e-ph}$			$L \sim l_{e-ph}$	$L >> l_{e-ph}$
	$L < \lambda$	$L < l_{e-e}$	$L >> l_{e-e}$		
Transport Regime	Quantum	Ballistic	Fluid	Fluid	Diffusive
Scattering	Rare	Rare	e-e (Many), e-ph (Few)		Many
Model:					
Drift-Diffusion					
Hydrodynamic	Quantum Hydrodynamic				
Monte Carlo					
Schrodinger/Green's Functions	Wave				
Applications	Nanowires, Superlattices	Ballistic Transistor	Current IC's	Current IC's	Older IC's

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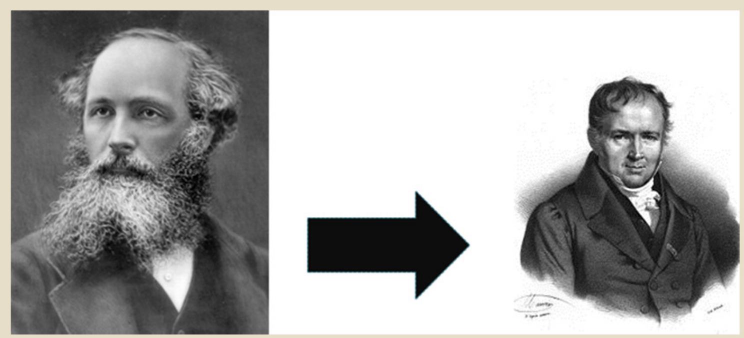
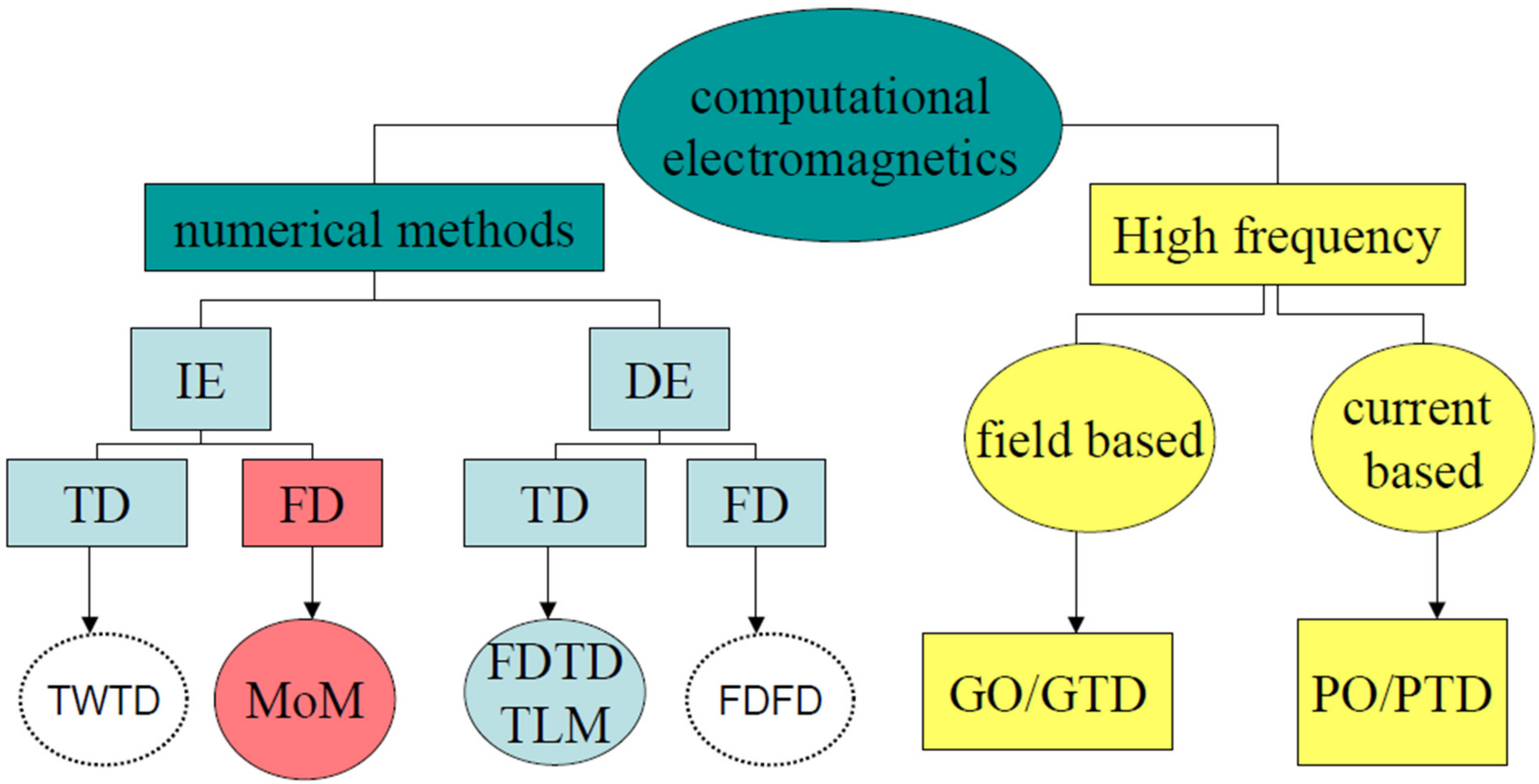
Maxwell→Poisson Equation Solvers

Name	Partial differential form	Integral form
Gauss's law:	$\nabla \cdot \mathbf{D} = \rho$	$\oint_A \mathbf{D} \cdot d\mathbf{A} = Q_{encl}$
Gauss's law for magnetism:	$\nabla \cdot \mathbf{B} = 0$	$\oint_A \mathbf{B} \cdot d\mathbf{A} = 0$
Faraday's law of induction:	$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$	$\oint_S \mathbf{E} \cdot ds = -\frac{d\Phi_B}{dt}$
Ampere's law + Maxwell's extension:	$\nabla \times \mathbf{H} = \mathbf{J} + \frac{\partial \mathbf{D}}{\partial t}$	$\oint_S \mathbf{H} \cdot ds = I_{enc} + \frac{d\Phi_\mathbf{D}}{dt}$

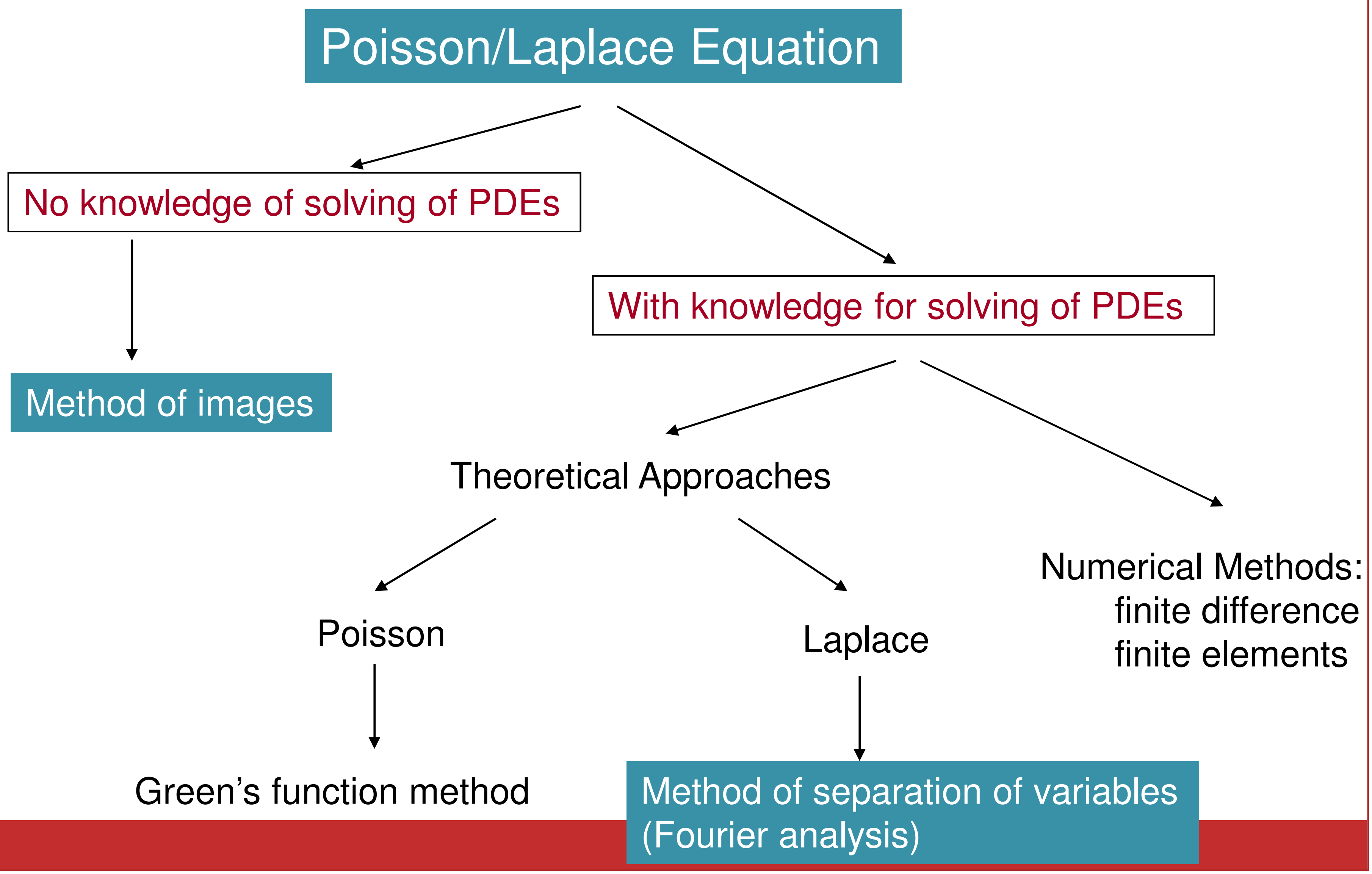
FDTD – Finite Difference Time Domain
Fourier Methods



Computational Hierarchy for Maxwell Solvers



Poisson/Laplace Equation Solution



Numerical Solution Details

Governing Equations ICS/BCS → Discretization → System of Algebraic Equations → Equation (Matrix) Solver → Approximate Solution

Governing Equations ICS/BCS	Discretization	System of Algebraic Equations	Equation (Matrix) Solver	Approximate Solution
Continuous Solutions	**Finite-Difference**	**Discrete Nodal Values**	**Tridiagonal**	$\varphi_i\,(x,y,z,t)$
	Finite-Volume		**SOR**	$p\;(x,y,z,t)$
	Finite-Element		**Gauss-Seidel**	$n\;(x,y,z,t)$
	Spectral		**Krylov**	
	Boundary Element		**Multigrid**	
	Hybrid			

Complexity of Linear Solvers

Algorithm	Type	Serial Time	PRAM Time	Storage	#Procs
Dense LU	D	N^3	N	N^2	N^2
Band LU	D	N^2	N	N^(3/2)	N
Inv(P)*bhat	D	N^2	log N	N^2	N^2
Jacobi	I	N^2	N	N	N
Sparse LU	D	N^(3/2)	N^(1/2)	N*log N	N
CG	I	N^(3/2)	N^(1/2)*log N	N	N
SOR	I	N^(3/2)	N^(1/2)	N	N
FFT	D	N*log N	log N	N	N
Multigrid	I	N	(log N)^2	N	N

```
Dense LU    : Gaussian elimination, treating P as dense
Band LU     : Gaussian elimination, treating P as zero
              outside a band of half-width n-1 near diagonal
Sparse LU   : Gaussian elimination, exploiting entire
              zero-structure of P
Inv(P)*bhat : precompute and store inverse of P,
              multiply it by right-hand-side bhat
CG          : Conjugate Gradient method
SOR         : Successive Overrelaxation
FFT         : Fast Fourier Transform based method
```

Complexity of Linear Solvers

Algorithm	Type	Serial Time	PRAM	Storage	#Procs
---------	----	------			
Dense LU	D	N^3			
Band LU	D	N^2			
Inv(P)*bhat	D	N^2			
Jacobi	I	N^2			
Sparse LU	D	N^(3/2)			
CG	I	N^(3/2)			
SOR	I	N^(3/2)			
FFT	D	N*log N			
Multigrid	I	N			

```
Dense LU     : Gaussian elimina
Band LU      : Gaussian elimina
               outside a band c
Sparse LU    : Gaussian elimina
               zero-structure c
Inv(P)*bhat  : precompute and s
               multiply it by r
CG           : Conjugate Gradie
SOR          : Successive Overr
FFT          : Fast Fourier Tra
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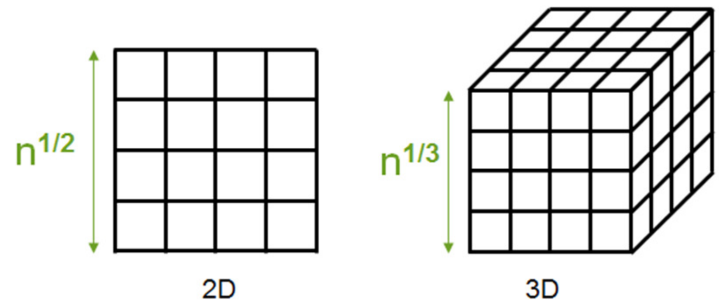
Complexity of linear solvers

Time to solve model problem (Poisson's equation) on regular mesh



	2D	3D
Sparse Cholesky:	$O(n^{1.5})$	$O(n^2)$
CG, exact arithmetic:	$O(n^2)$	$O(n^2)$
CG, no precond:	$O(n^{1.5})$	$O(n^{1.33})$
CG, modified IC:	$O(n^{1.25})$	$O(n^{1.17})$
CG, support trees:	$O(n^{1.20}) \rightarrow O(n^{1+})$	$O(n^{1.75}) \rightarrow O(n^{1.31})$
Multigrid:	$O(n)$	$O(n)$