SEMICONDUCTOR PROCESS MODELING

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Some historical dates:

- Bipolar transistor:	1947	- DTL - technology	1962
- Monocrystal germanium:	1950	- TTL - technology	1962
- First good BJT:	1951	- ECL - technology	1962
- Monocrystal silicon:	1951	- MOS integrated circuit	1962
- Oxide mask, Commercial silicon BJT:	1954	- CMOS	1963
- Transistor with diffused base:	1955	- Linear integrated circuit	1964
- Integrated circuit:	1958	- MSI circuits	1966
- Planar transistor:	1959	- MOS memories	1968
- Planar integrated circuit:	1959	- LSI circuits	1969
- Epitaxial transistor:	1960	- MOS processor	1970
- MOS FET:	1960	- Microprocessor	1971
- Schottky diode:	1960	- I^2L	1972
- Commercial integrated circuit (RTL):	1961	- VLSI circuits	1975
		- Computers using VLSI technology	1977
		- ...	

Why need semiconductor modeling?

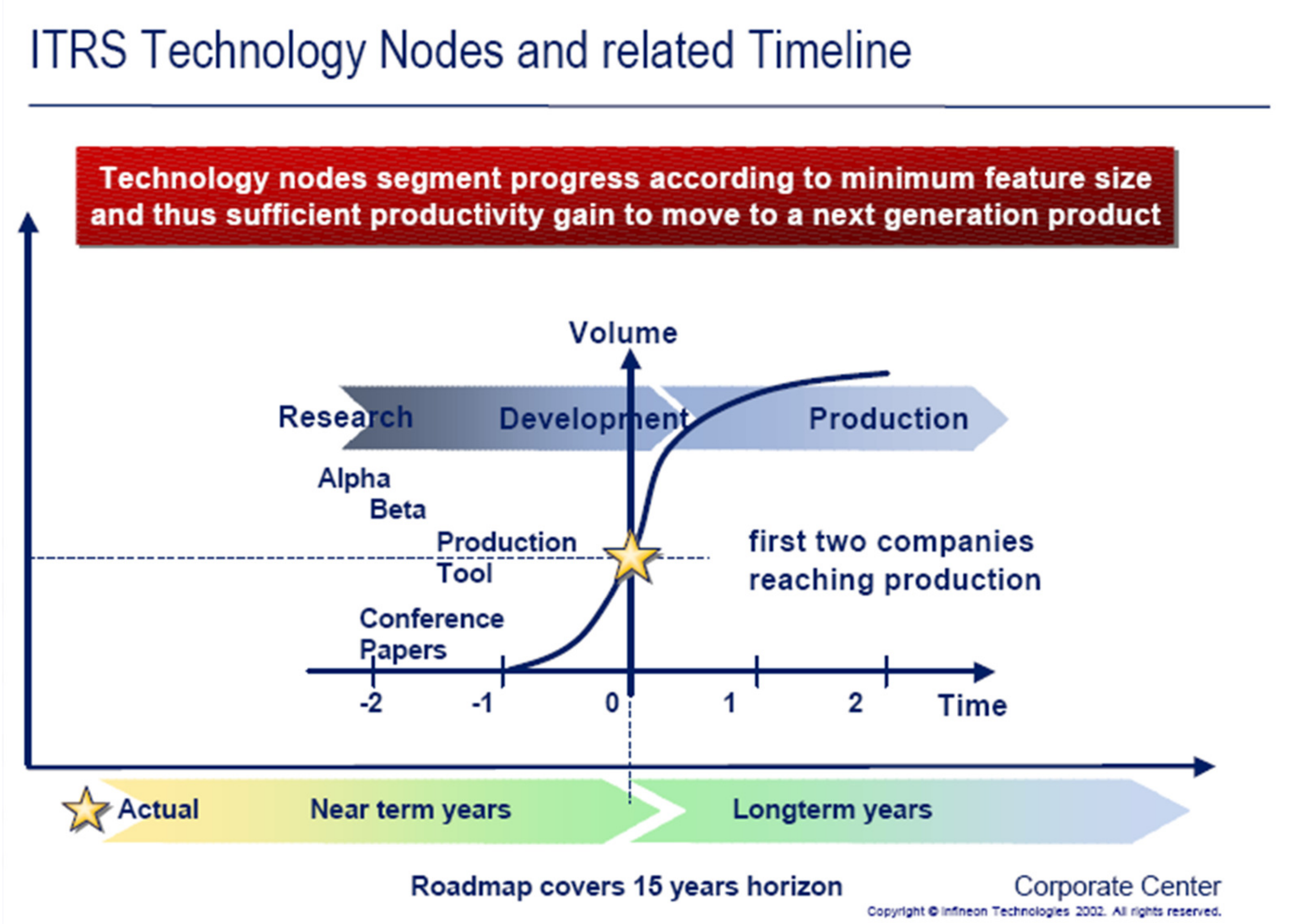
- It's a *computational modeling*.

- What is *computational modeling*?

  - Evaluation and optimization of various design is possible, without resorting to costly and time-consuming trial fabrication and measurement steps.
  - Provides valuable insight into important physical quantities.
  - Shortened development cycles.
  - Reduced cost.
  - Increased quality and reliability of final products.

A important field of computational modeling related to semiconductor manufacturing belongs to *process modeling*.

SIA Challenges



Semiconductor Modeling

- ***Process Modeling***
  - In technology development phase
  - In technology characterization phase
- ***Device Modeling***
- ***Circuit Modeling***

Summary of Basic Semiconductor Equations

Electron and hole current densities in low electric field	$\mathbf{j}_n = q\left(n\mu_n\mathbf{F} + D_n\nabla n\right)$ $\mathbf{j}_p = q\left(p\mu_p\mathbf{F} - D_p\nabla p\right)$
Ohm's law	$\mathbf{j} = \sigma\mathbf{F} \qquad I = \frac{\sigma S}{L}FL = \frac{U}{R}$
Sample resistance	$R = L/\sigma S$
Electron and hole current densities in arbitrary electric field	$\mathbf{j}_n = q\left[-n\mathbf{v}_n(\mathbf{F}) + D_n(\mathbf{F})\nabla n\right]$ $\mathbf{j}_p = q\left[p\mathbf{v}_p(\mathbf{F}) - D_p(\mathbf{F})\nabla p\right]$
Poisson's equation	$\nabla\cdot\mathbf{F} = \rho/\varepsilon$
Continuity equations for electrons and holes	$\frac{\partial n}{\partial t} = \frac{1}{q}\nabla\cdot\mathbf{j}_n + G - R$ $\frac{\partial p}{\partial t} = -\frac{1}{q}\nabla\cdot\mathbf{j}_p + G - R$
Ambipolar diffusion coefficient and ambipolar mobility	$D_a = \frac{\mu_p p_n D_n + \mu_n n_n D_p}{\mu_n n_n + \mu_p p_n}$ $\mu_a = \frac{\mu_n\mu_p(n_n - p_n)}{\mu_n n_n + \mu_p p_n}$
Total current density (including displacement current)	$\mathbf{j}(t) = \mathbf{j}_n + \mathbf{j}_p + \varepsilon\frac{\partial}{\partial t}\mathbf{F}$

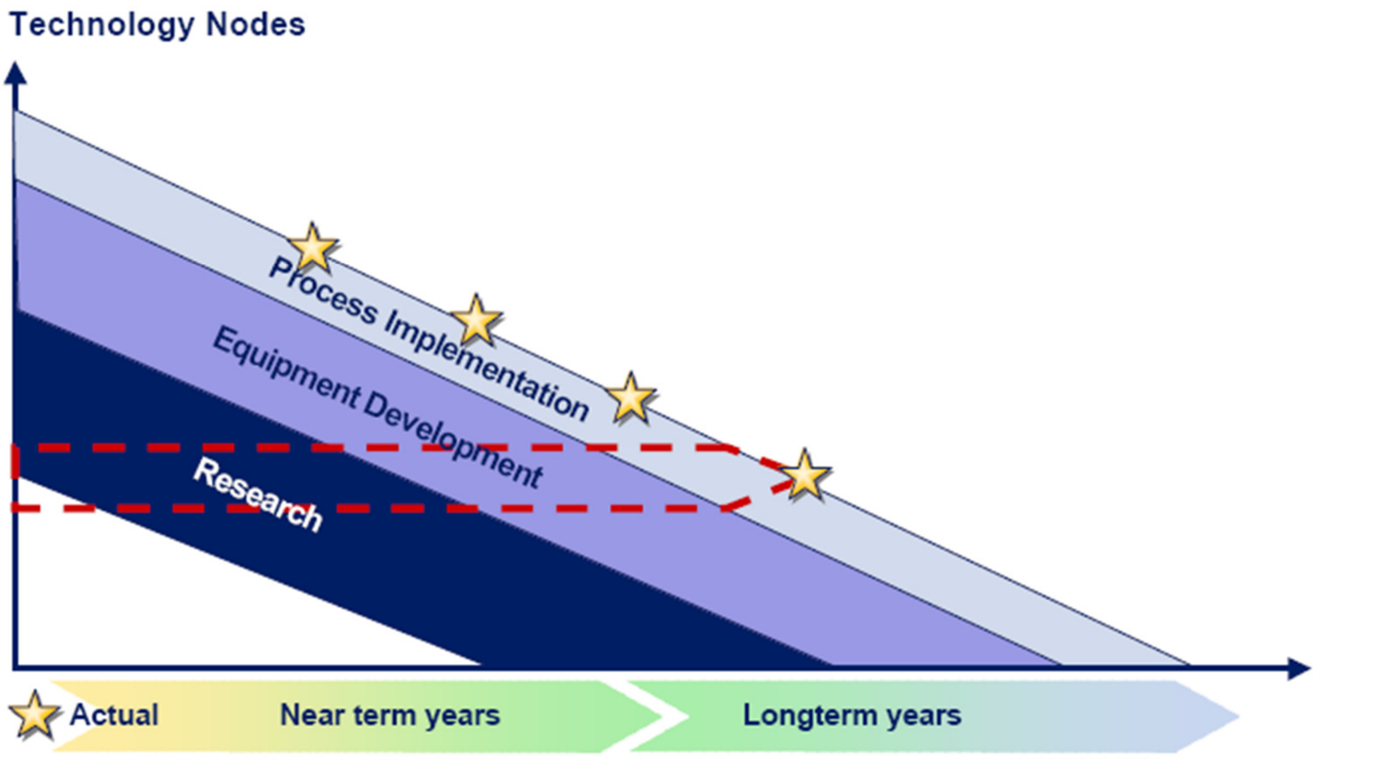
Semiconductor Process Modeling

The ***aim*** of process modeling:

Predict geometries and material properties of the wafer structures and semiconductor devices as they result from the manufacturing process.

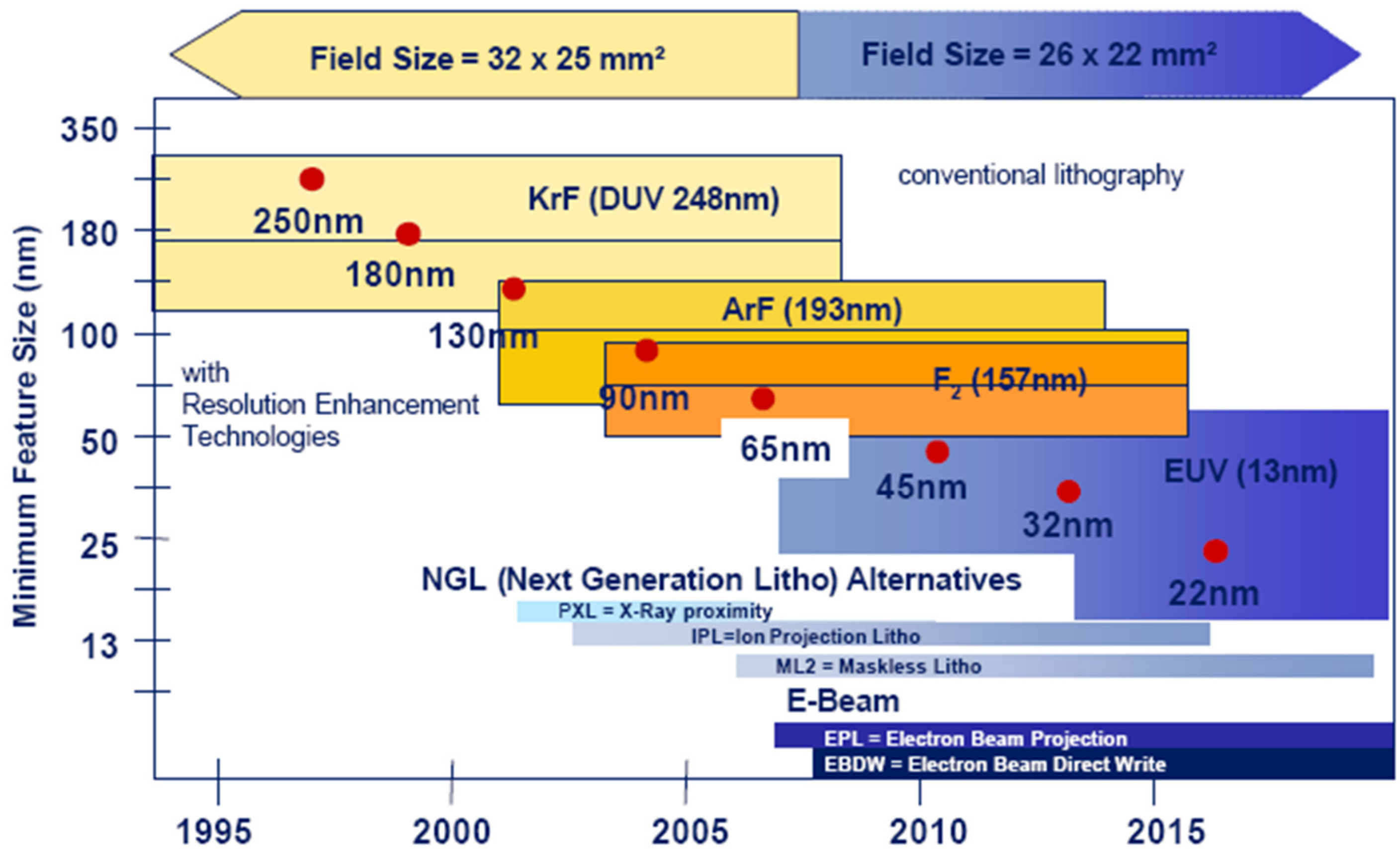
SIA Challenges

Technology Node Introduction requires Research and Equipment as well as Process Development in Advance



SIA Challenges

Technology Nodes below 100nm strongly depend on availability of extended 193nm and 157nm Litho or NGL



State of technology

- Role: Semiconductor process modeling has become an essential technology in semiconductor industry.

- Impressive progress in process modeling has been achieved, but there is still much more potential to be exploited.

State of technology

- Lack of predictive capabilities.
- The improved models, required for a new technology, usually are not available before the technology itself.
- The process modeling is required to accelerate so that the application is more effective than at present .

State of technology and future trends

- Process modeling has to provide general concepts, guidance,and insights at a very early stage of process or technology development for the engineers.
- The most important needs for future processing modeling is the Semiconductor Industry Association Roadmap.

Semiconducter Industry Assosiation Roadmap

- The Semiconductor Industry Association Roadmap's priorities are:
  - automatic grid-generation and adaptation algorithms.
  - Defect-mediated dopant profile evolution.
  - combined equipment and feature scale topography models
  - 2D and 3D doping profile measurement tools.
  - etch model predict ability.
  - Silicidation models.

Great effect is directed towards 3D process simulation tools.

Monte Carlo simulation algorithms

- Defect-based dopant models for implantation, diffusion,and activation must start with underlying first-principle calculation and characterization methods.
- Monte Carlo simulation algorithms will become increasingly important because Monte Carlo method are inherently three-dimensional.

Interconnections

- For the determination of the overall chip performance, interconnections have become as important as the active semiconductor devices.
- Interconnection technology includes dielectric and metal-film formation as well as the etch process.

Interconnections

The accurate evaluation of

- the process variation,
- their effects on the performance,
- their effects on the reliability of interconnection.

Depends on :

the integration of equipment, feature-scale topography modeling of deposition, lithography, and etching.

Interconnections

- This includes a critical need for improved physical modeling of topography processes.
- The formulation of predictive models for deposition and etching is essential for the interconnect modeling
- These models are expected to have more improved statistical analysis methods and tools.

The lack of accurate experimental verification

- The lack of accurate experimental verification is a important obstacle for process model development and model calibration that should be overcome in the future.
- The problem is even more emphasized with damage distribution that are induced by implantation and their evolution during subsequent annealing processes.

(this phenomenon can’t be measured directly and is only verified indirectly by its effect on dopant distribution.)

The lack of accurate experimental verification

- A better understanding of the physics of buck particle transport increasingly demands further improvements in metrology.
- The limitation in measurement technology severely hampers the development of accurate multi-*domain* process modeling tools.

Semiconductor Process Modeling …

Two traditional branches

- ***Wafer topography modeling***
- ***Bulk process modeling***

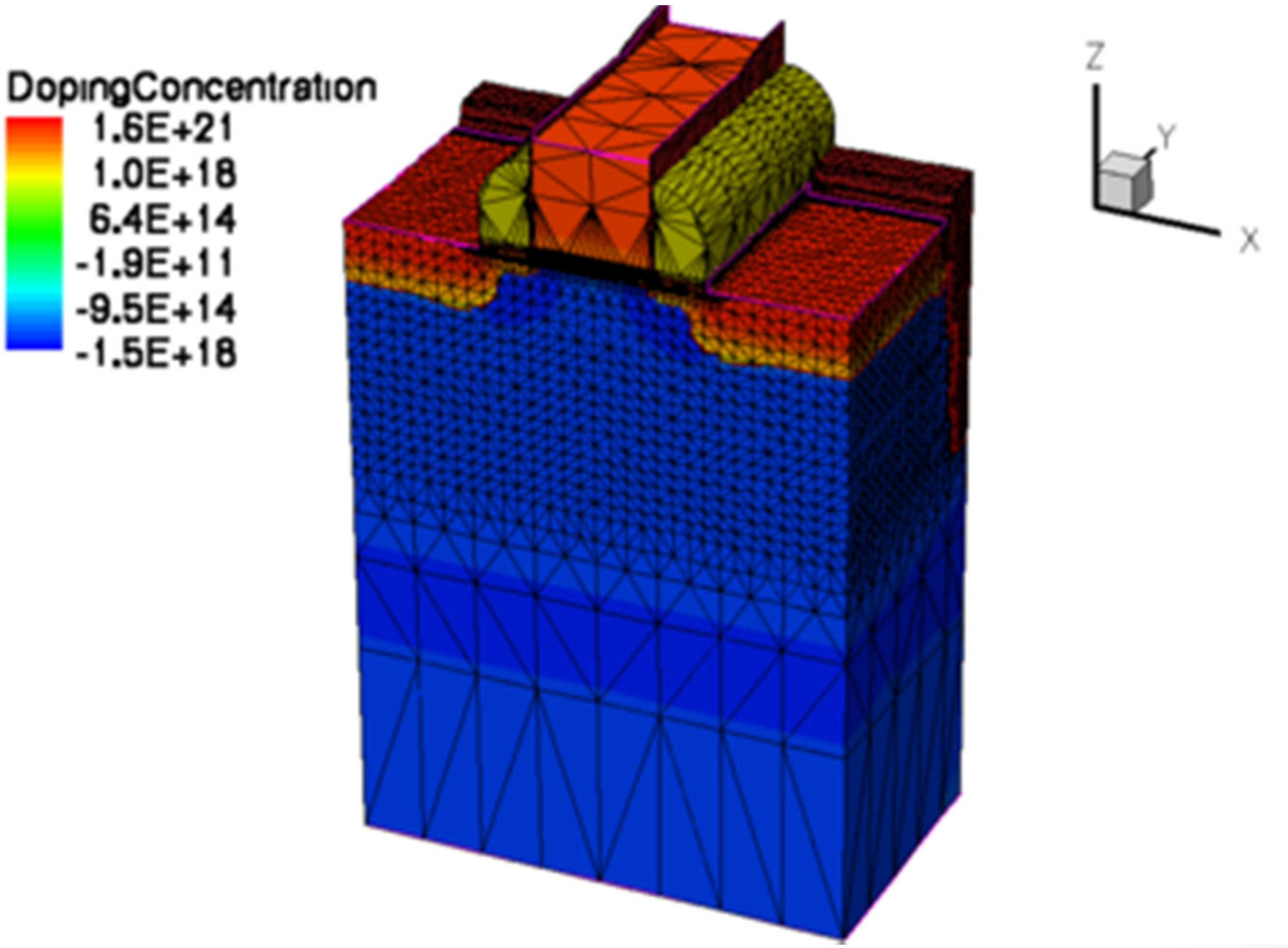
Semiconductor Process Modeling …

Two steps

- ***Physical Modeling***

- ***Discrete Modeling***

Physical Modeling



Physical Modeling

- What is the *physical modeling*?
- A hierarchy of physical model
  - *Bottom*: derived from principles using mechanisms of atomic level or fundamental laws
  - *Top*: simple analytical models
  - *Middle*: allow a trade-off of model generality for their simplicity
- Mathematical form: systems of non-linear PDEs or by algorithms

Sub-models of Physical Model

- Photolithography
- Etching and Deposition
- Ion Implantation
- Bulk Particle Transport
- Mechanical Deformation

Photolithography

- Lithography process
- Photolithography technology
- Factors that the model must account for light intensity distribution in the photoresist film
  - chemical reaction that changes photoresist etching properties
  - resulting photoresist profile after development

Etching and Deposition

- The formation of multilayer wafer structure
- The role of physical model in this process is to relate the propagation velocity of the surface *to* material properties and processing conditions.
- Process techniques used for Etching and Deposition range from *isotropic chemical* process to *directional physical* process.
- Most important model parameters

Ion Implantation

- The Ion Implantation process
- The process model concerns the distributions of stopped particles, the produced damage, and the energy
- The produced damage occurs when ions collide with a lattice atom and when they cause it to leave its original site in the lattice.

Bulk Particle Transport

- One of the most important group of physical models is related to the transport of particles within the bulk region.
- The principal physical mechanism for particle transport is *diffusion*. But the governing equations for particle transport should also account for advection due to electric field and various chemical reactions among particles.
- Hierarchically organization: range from single species diffusion equations to complex coupled systems of diffusion-drift-reaction PDEs.

Mechanical Deformation

- The models for mechanical deformation follows the evolution of the stress field in different material layers during manufacturing.
- Generally, the cumulative mechanical stress represents an important factor that could affect the reliability of semiconductor devices and the interconnection system.

Discrete Modeling

Discrete Modeling

- *Principal task*: generation and control of appropriate grid structures for arbitrarily shaped multilayer material domains and the derivation of the discrete analog of the governing mathematical description.

- The practical application of process modeling is enabled by simulation tools that integrate various physical and discrete models.

Issues in Discrete Modeling

- Subdivision of the complete physical domain into small subdomains (cells).

- Two phases: discretization and solution of algebraic problem.

Choosing Cells

Methods of choosing structured and unstructured meshes

- Finite-Difference Method (FD)
- Finite-Volume Discretization (FV)
- Finite-Element Method (FE)

How to select discretization method

The final selection of the *grid* and the *discretization* method should depend on:

- Geometry of the domain
- The PDE (including boundary conditions) to be solved
- The coordinate system used to describe the continuous problem

The trends towards 3D

- The trends towards 3D with more complex models leads to :

  - larger systems of coupled PDEs,

  - to more complex topologies,

  - to multilayer structures.
- This requires computing power provided in a ideal way by scalable parallel architecture.

The trends towards 3D

- Parallelization is innovative technique, it can be used for new algorithmic developments.
- A straightforward loop parallelization of initially sequential programs will be made on shared-memory machines.
- Grid partitioning is a typical approach to parallelize grid oriented PDE application.
- This technique is independent of the particular partial differential equation or system to be solved.

The trends towards 3D

- Load balancing and locality should be taken into account for an efficient parallelization.
- All processors are responsible for approximately the same number of discrete equations and variables.
- The data structure should be more regular.
- For low communication cost the algorithm should offer a large amount of locality.

The next-generation process simulation software

- Due to below become more complex:
  - model development,
  - automatic grid generations,
  - adaptive meshing,
  - regridding of time-dependent domain,
  - search for optimal solvers,
  - parallel programming,
  - pre and post processing of single simulation step
  - approximately complete simulation of processing step.

- These poses new challenges to the developers of software tools

The next-generation process simulation software

- Apart from the need of portability with respect to parallel programming,It also needs:
  - separate modeling,
  - discrete description,
  - solving from one another.
- A parallel programming environment keeps the formulation of the application, and away from particular solver.
- This idea represents the approach of the future.

Historical Perspective on Process Simulation Tools

The history of commercial process simulators began with the development of the Stanford University Process Modeling (SUPREM) program .

Building upon this beginning with improved models SUPREM II and SUPREM III were developed.

Technology Modeling Associates, Inc. (TMA) which was formed in 1979 was the first company to commercialize SUPREM III.

Later Silvaco also commercialized SUPREM and named the product ATHENA.

TMA commercialized SUPREM-IV (2D version) and called it TSUPREM4.

In 1992, Integrated Systems Engineering (ISE) came out with the 1D process simulator TESIM and the 2D process simulator DIOS.

At about the same time development of a new 3D process and device simulator began at TMA and after TMA was acquired by Avant!, the product was released in 1998 as Taurus.

Around 1994 a first version of the Florida Object Oriented Process Simulator (FLOOPS) was completed.

FLOOPS was later commercialized by ISE in 2002.

One other process simulator PROPHET was created around 1994 at Bell labs which later became Agere, but has not been sold commercially.

In 2002 Synopsys acquired Avant!, corp. and in 2004 Synopsys acquired ISE.

Synopsys has announced that a new process simulator will be released in mid 2005 combining the best features of Taurus, TSUPREM4, into the FLOOPS platform and will be called Sentaurus Process.

Besides these simulators, there are numerous other university and commercial simulators such as PROMIS, PREDICT, PROSIM, ICECREAM, DADOS, TITAN, MicroTec, DOPDEES, ALAMODE.