Complexity Reduction in Multiphysics Modeling

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Outline

- Introduction
- Modeling procedure
- Multiphysics basics
- Coupled problems
- Complexity reduction
- Conclusions

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- **Multiphysics basics**
- **Coupled problems**
- **Modeling procedure**
- **Complexity reduction**
- **Conclusions**

Modeling Multiphysics Systems and their Complexity Reduction

- It is presented my experience within this course at doctoral level
- coordinated by invited professor Daniel IOAN (daniel@lmn.pub.ro)
- organized in Jan-Feb 2015 by
- the Institute of Mathematical Modelling, Analysis and Computational Mathematics (IMACM)
- Bergische Universität Wuppertal (BUW)

Course objectives

- To provide the participants the state of the art knowledge in the field **of Modeling and Simulation of Multiphysics Systems**.
- The main goal of the course is to give to the participants the understanding of **the bridges between the three pillars of the computer modeling: mathematics, physics and computing,**
- and how their principles are **integrated into design flows**, as a new knowledge fitting the designer's requirements for **efficiency, reduced complexity and accuracy**. Beside MOR standard techniques, other approaches to reduce the complexity of the extracted models will be presented.
- The course is not a substitute of the disciplines that constitute the pillars above, but it is focused on **the interdisciplinary aspect** and how several particular mathematical, physical and algorithmic aspects influence the global modeling efficiency.
- After the course, the student should be able to recognize **multiphysics coupling** in complex problems and to distinguish between different types of coupling
- to describe the **methodology applied to extract reduced models of coupled systems**
- and to use an **appropriate software environment** for modeling and simulation of coupled problems, e.g. COMSOL MultiPhysics.

The course content

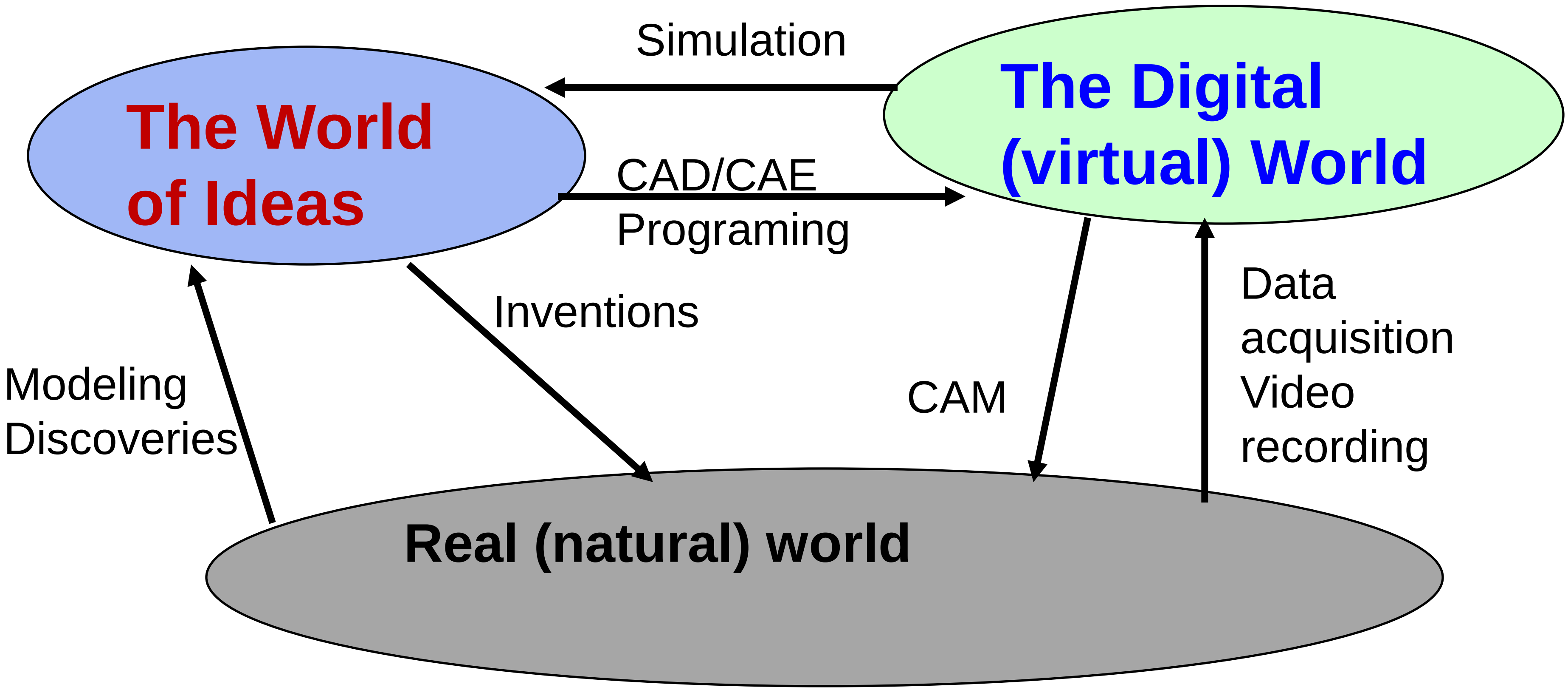
- **Introduction:** context and objectives
- **First part: overview on single and multi-physic theoretic background**
  - Electromagnetic fields
  - Electrical circuits
  - Heat transfer (by analogy)
  - Linear elasticity (by analogy)
  - Fluid dynamics (by analogy)
  - Multiscale (MS) and Multirate (MR) modeling
  - Multi-physics couplings
- **Second part: the steps of the modeling procedure**
  - Conceptual modeling
  - Mathematical modeling
  - Analytic modeling (optional)
  - Numerical modeling. Space discretization (optional: FIT, FEM, BEM).
  - Computational modeling. Software implementation. Meshing. Solving linear and non-linear systems of equations generated by discretization. Time integration. Simulations. Solution visualization. Parallelization.
  - Model extraction and order reduction.
  - Verification and validation.
- **Third part: applications, study cases and demonstrations (optional)**

Similar courses over the world

- Introduction to Modelling of Multiphysics Problems by Tomasz G. Zieliński (PL)
- Modelling of Multiphysics Systems by Prof Piero Triverio (USA)
- 8 hours course: Multi-Domain Simulations in Power Electronics: Combining Circuit Simulation, Electromagnetic and Heat Transfer by Andreas Müsing and Marcelo Lobo Heldwein (CH)
- Method Course: Finite element modeling of multiphysics phenomena by Markus Sause, Peter Zelenyak (DE)
- Multiphysics Modelling using COMSOL by J.J.L. Neve (NL)
- Multiscale and Multiphysics Modeling Courses by Zhenhai Xia (USA)
- Numerical Multiphysics Modelling in Biology and Physiology Jonathan Whiteley (UK)
- COMSOL Multiphysics Intensive Trening (SWE)
- CST STUDIO SUITE® Multiphysics Trening (DE)
- Heat Transfer Modeling Using ANSYS FLUENT (USA)

The context

After 3 Revolutions: Renaissance, Industrial, and Digital we live now in three words:



The evolution the sizes of these worlds

Human Population Explosion

- Around 8000 BCE the population of the world was approximately 5 million
- It has been growing continuously since the end of the Black Death (year1350): 375 million by 1400
- 2015 the world's human population is estimated to be 7.219 billion

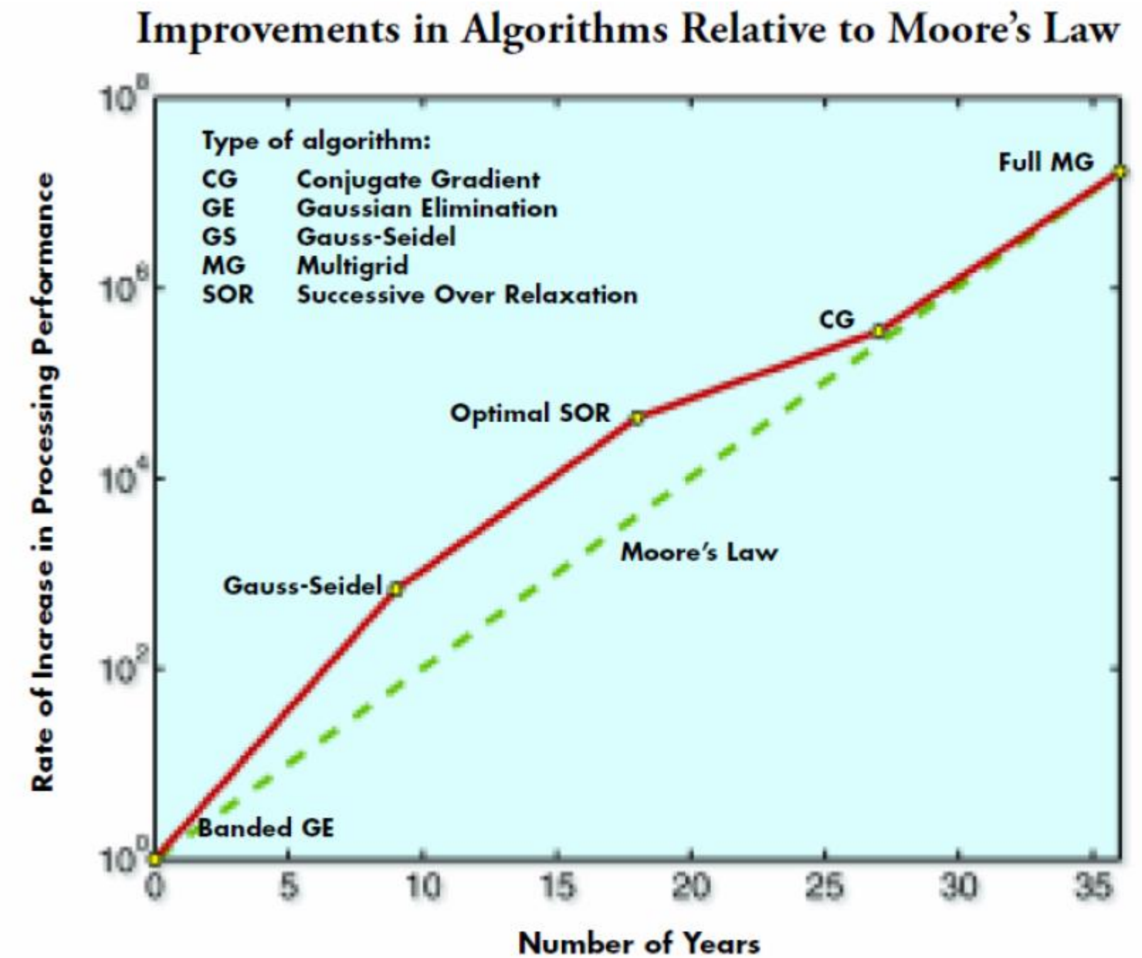
Moore law: in the integrated circuits, the transistor densities are double every three years

- Although this trend has continued for more than half a century, "Moore's law" should be considered an observation or conjecture and not a physical or natural law.
- Consequences:
  - More memory, more functions
  - Faster and cheaper devices

Moore law for numerical methods… and for scientific production.

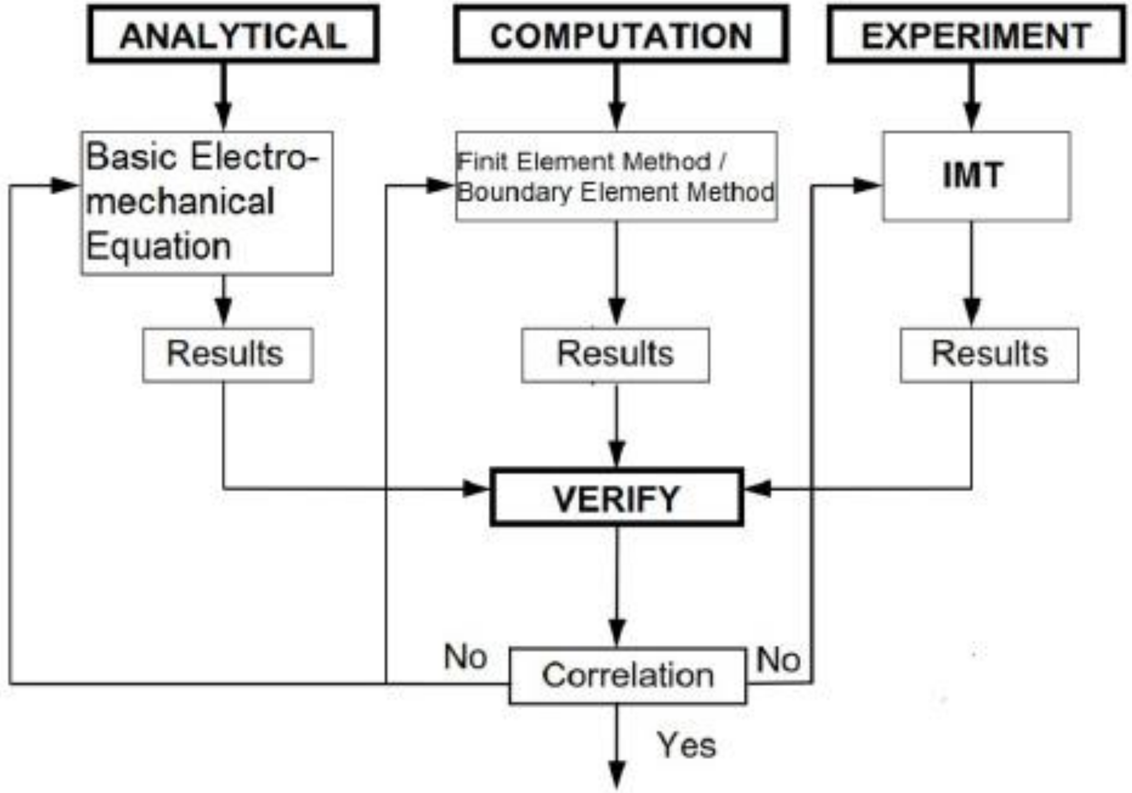
Numerical version of Moore's law

- Schilders, Wilhelmus HA, Henk A. Van der Vorst, and Joost Rommes. Model order reduction: theory, research aspects and applications. Vol. 13. Berlin, Germany:: Springer, 2008.



Research methodology

- **ACES:** Analytical, Computational and Experimental solutions methodology



- **TES Triangle:** Theory-Experiment-Simulation

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Modeling procedure steps

1. Conceptual modeling
2. Mathematical modeling
3. Analytic (approximate) modeling
4. Numerical modeling. Space and time discretization
5. Computer models. Software implementation.
6. Model extraction and order reduction.
7. Verification and validation

Conceptual modeling

- **Geometric (spatial) approximations:**
  - 0D – no spatial variables
  - 1D – only one spatial variables 1.5D?
  - 2D - two spatial variables (Cartezian or polar) 2.5D?
  - 3D – all three spatial variables (Cartezian or others)

  Perfect shapes/domains/surfaces/interfaces!
- **Temporal approximations:**
  - Static problems
  - Harmonic problems
  - Periodic problems
  - Transient (arbitrary dynamic) problems
- **Physical approximations:**
  - Only relevant phenomena are kept, others are neglected

As a result: a list of **simplified hypothesis and the field regime** is determined

Mathematical modeling

A field problem is defined by:

Input data

- **computational domain:** shape and size
- **material characteristics** (constitutive relations – operators, functions or parameters)
- **internal** (field) sources
- **external sources** (boundary conditions values) and/or
- **anterior sources** (initial conditions)

→ **Equations and boundary conditions** →

Solution (Unknowns)

- **local and**
- **global variables**

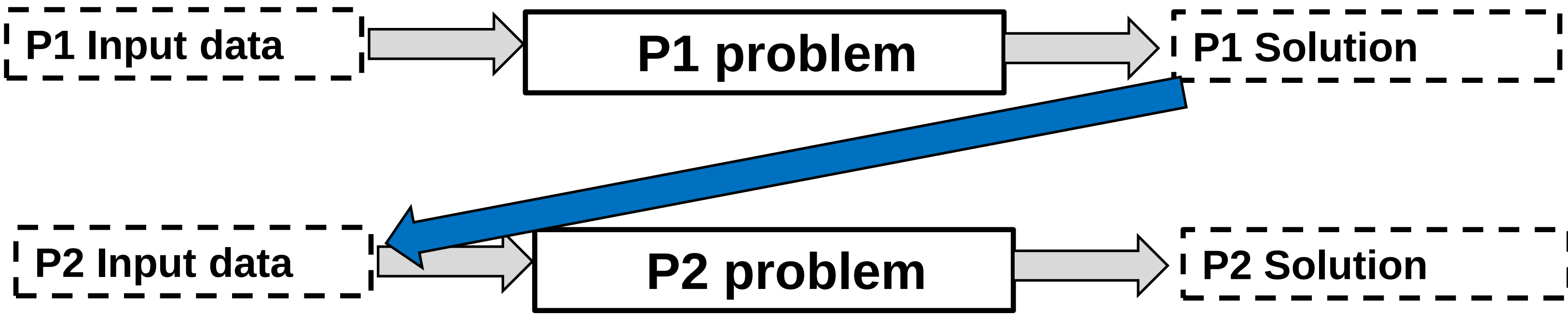
Correct formulation of the problem (well posed in the sense of Hadamard, exclusively in mathematical terms):

- Solution **existence**
- Solution **uniqueness** (the most important!!)
- Solution **continuity** – well conditioning of the problem

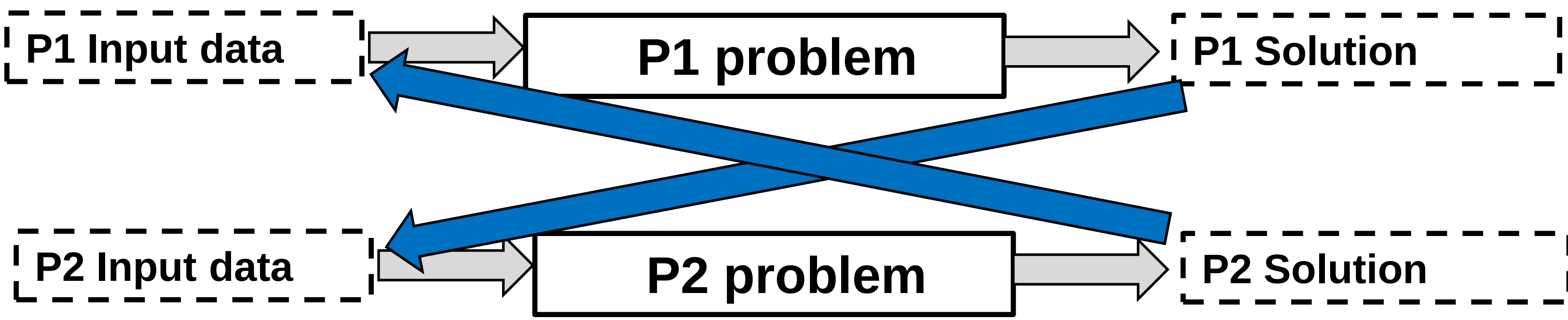
The set-up of the functional framework is a must.
Problem is re-formulated as PDE (SF): DF ↔ WF ↔ IE (acc. to next step).

Problem couplings

Unidirectional coupling



Bidirectional coupling



Multidirectional coupling: P1, P2,…Pn **Unidirectional multicoupled?**

Multiphysic coupling: P1 and P2 belong to different disciplines (theories).

Numerical modeling

Space and time (semi)discretization (by FEM, FIT or BEM)

Method	FDM/FIT	FEM	BEM
Mesh	Regular (Cartesian)	Unstructured	On interface
Discretized equations	Differential Eq/Form (PDE SF)/Global (DF)	Weak form (WF)	Integral Equation (IE)
DoF	Nodal/edge-face	Nodal, edge	Nodal on interface
Matrix	Sparse non-symmetric	Sparse symmetric	Full non-symmetric

- Static problems (elliptic PDE) are approximated by linear/nonlinear system of algebraic equations
- Dynamic problem (parabolic and hyperbolic PDE) are approximated by systems of ODE/DAE (solved by time integration) or
- in the linear case they are solved in the frequency domain, as complex static problems, by Fourier/Laplace transform

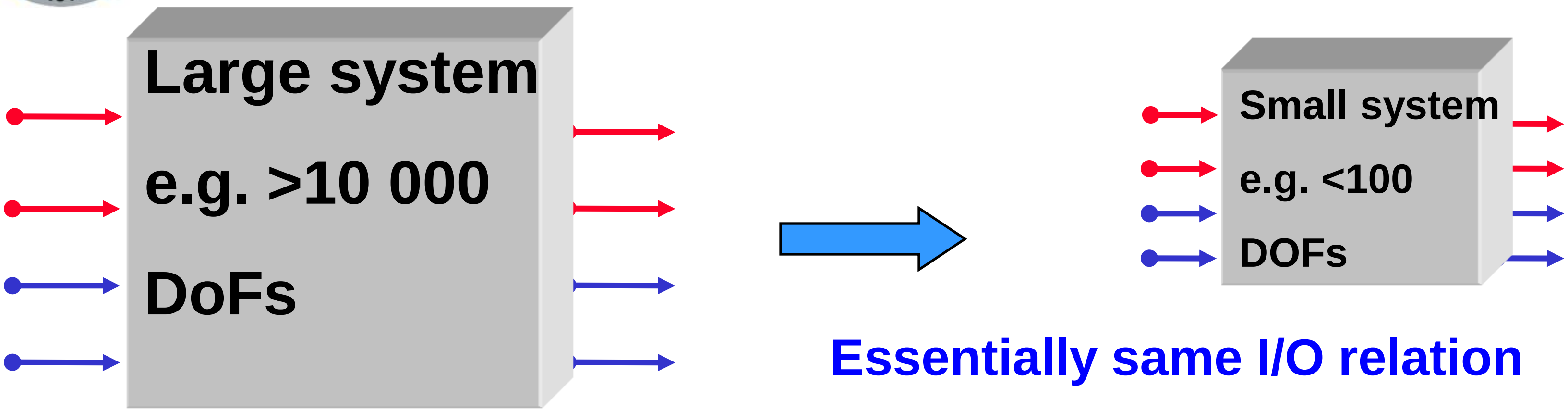
Software implementation

- **Structure of a CAD software package**: (automatic) problem description (by GUI or TUI in an suitable language - appropriate for parametrization), preprocessing (meshing, eq. discretization), solving, post processing.
- **Meshing:** Regular mesh, Unstructured mesh (triangular, tetrahedral, hexahedral), Automatic meshing, adaptive meshing, based on h, p, h-p FEM refining.
- **Solving linear systems** of equations generated by discretization (direct methods, iterative preconditioned methods, KSM Krylov subspace).
- Solving **non-linear systems** (Picard-Banach, Newton-Raphson, JFNK – Jacobian-free Newton-Krylov method)
- **Time integration** (implicit, explicit, Runge-Kutta).
- **Simulations**. Benchmarks - study cases.
- **Solution visualization.**
- **Parallelization** (on distributed computer systems – cluster, multi core/CPU systems or Massive parallel architectures – GPU, grid/cloud).

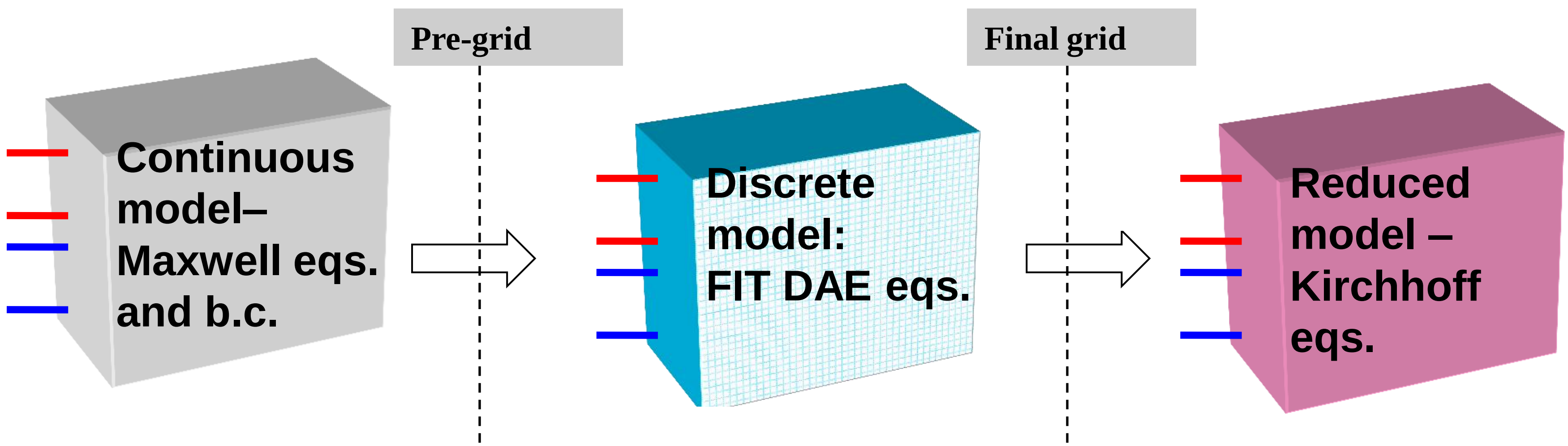
Model extraction and order reduction

- **Simulation**: compute the solution for a given excitation
- **Modeling**: extract from reality the dependence between excitation and system response, described by equations, data-bases or circuits.
- **Model reduction**: find an approximate, simplified model of the relation between excitation and response, which have an acceptable accuracy and preserves essential characteristics of the original model (e.g. passivity)
- **Model order** (complexity measure): number of the state variables (size of the state space)
- After **Model Order Reduction** (MOR) the simulation is done with low computational cost, in the standard design environment, for different excitations and couplings
- The **designers** are not interested in field solution, but in an enough accurate input-output system model, with lowest complexity, extracted in an automatic manner. It should preserve the characteristics of the original model (e.g. its passivity, stability). Parametric models are desired.

MOR - What is Order/Complxeity Reduction



Essentially same I/O relation



Apriori ROM (discretization)

Reduction on the fly

Aposteriori ROM and model realization

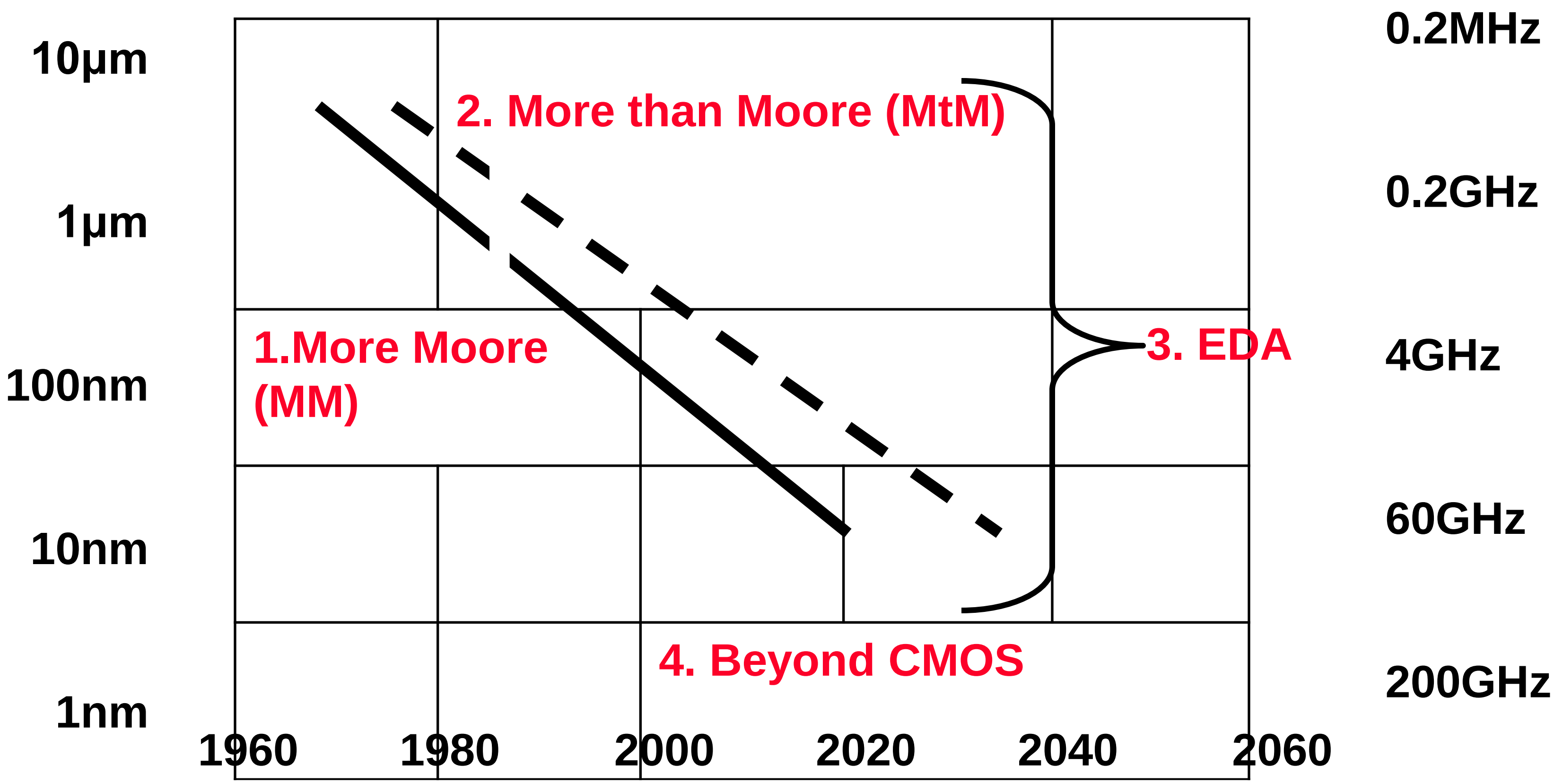
Verification and validation

- Model **verification**: “ensuring that the computer program of the computerized model and its implementation are correct”
- Model **validation**: “substantiation that a computerized model within its domain of applicability possesses a satisfactory range of accuracy consistent with the intended application of the model”
- A model may be valid for one set of experimental conditions and invalid in another.
- A model is considered valid for a set of experimental conditions if the model’s accuracy is within its acceptable range, which is the amount of **accuracy required for the model’s intended purpose**.

- **Verification checks if the problem is correct solved and**
- **validations checks if the problem is correct formulated**!

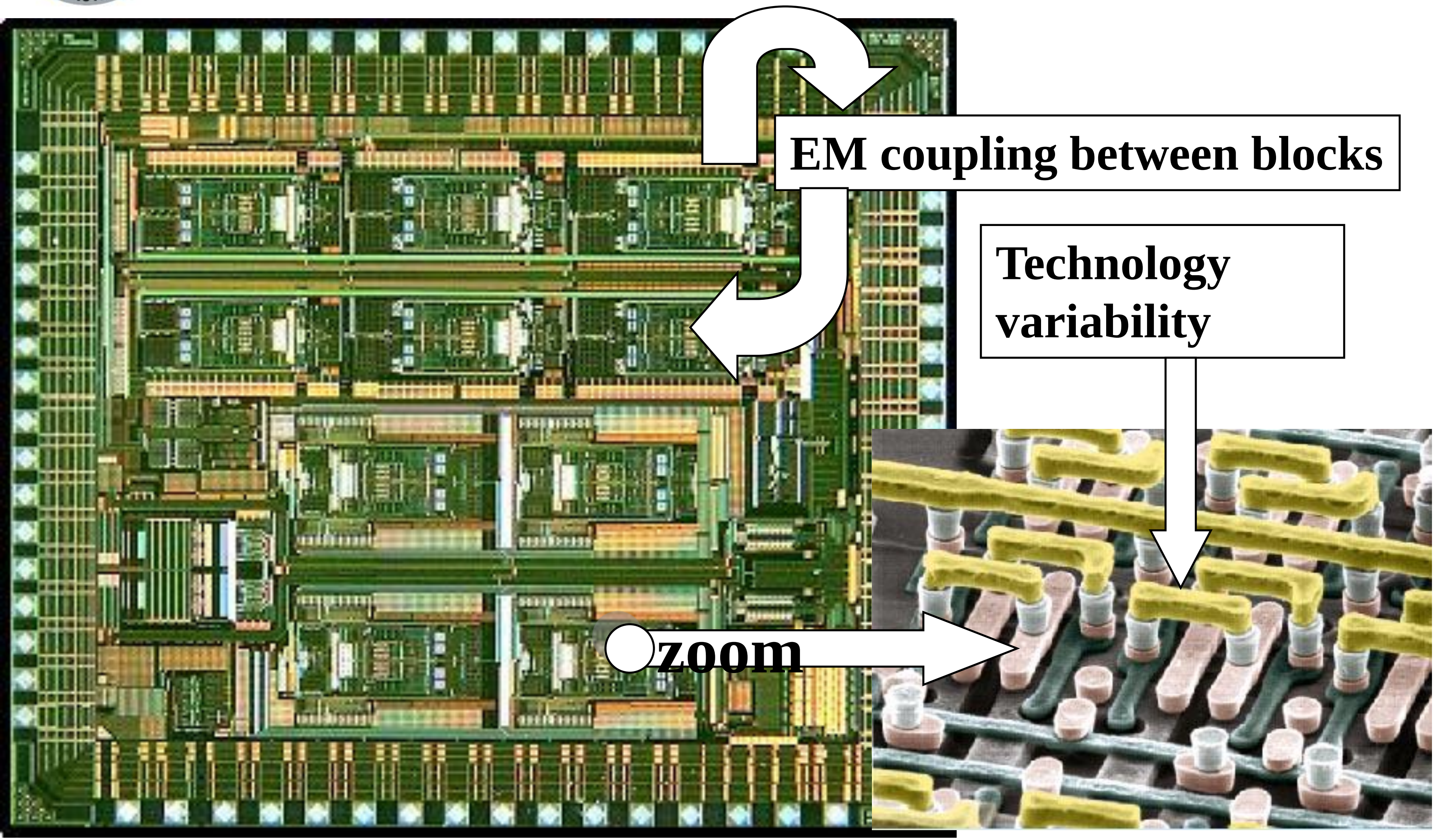
EU nano-electronic Technology Platform

Strategic Research Agenda

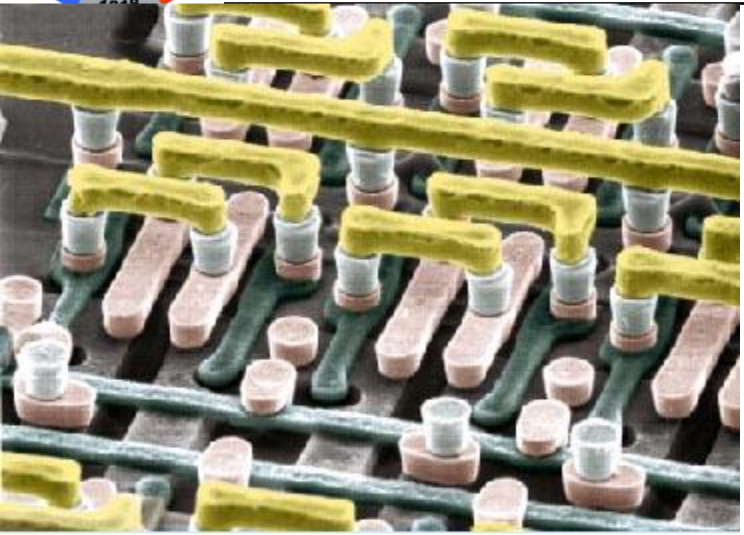


See www.eniac.eu for more details

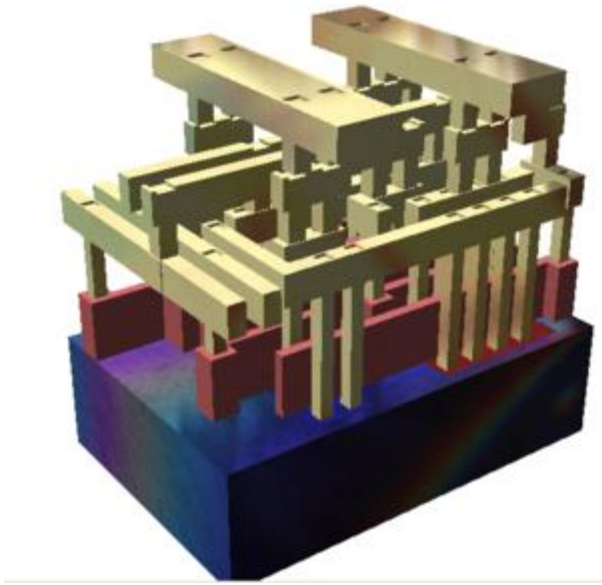
Real life complexity

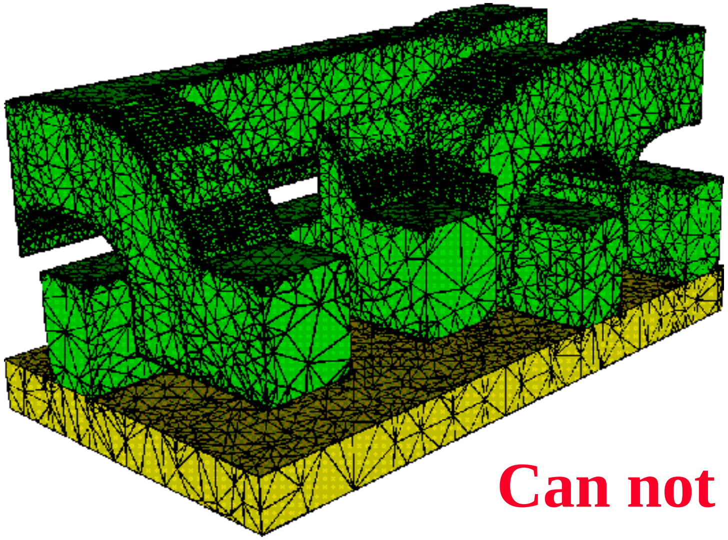


Classic numeric approaches used to compute EM field

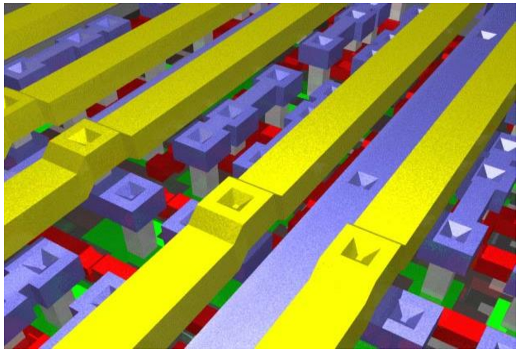


Idealized geometry models





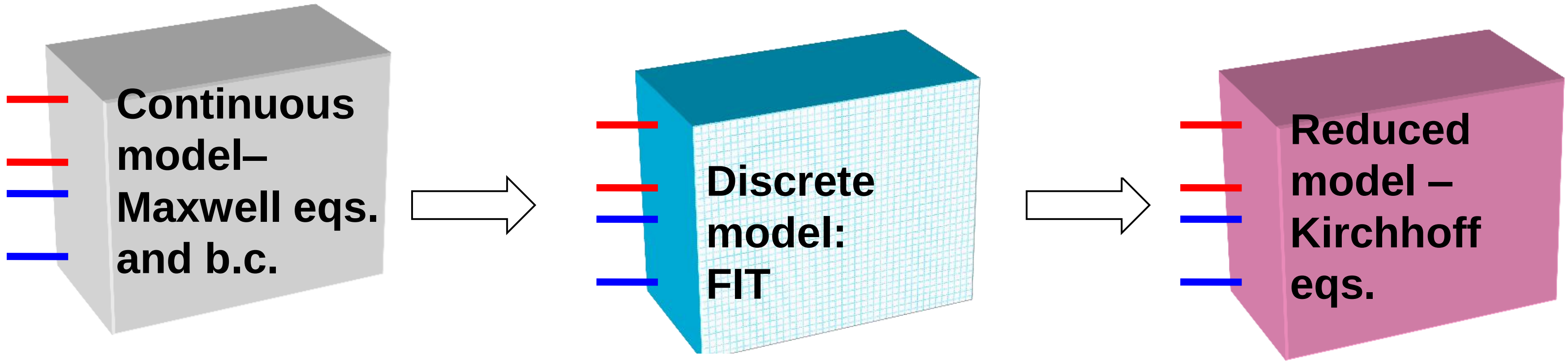
BEM or FEM mesh



Can not handle the complexity of real designs !

An alternative approach based on Model Reduction at every step

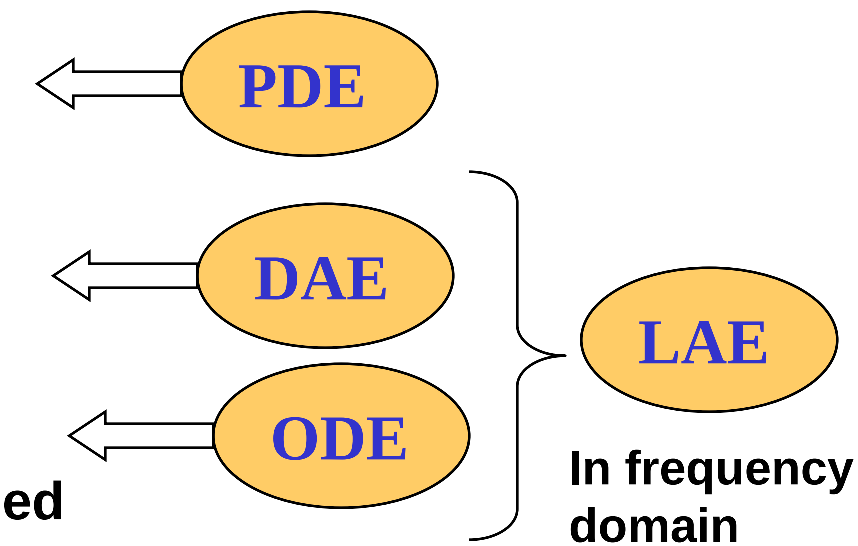
Model extraction: from Maxwell to Kirchhoff



- EM field problem for passive components after Domain Partitioning:
  - Maxwell equations with
  - appropriate boundary conditions
    for EM coupling modeling

- After discretization (not solving!)
  non-compact model is generated

- After reduction by MOR an equivalent
  parametric reduced circuit is synthesized



In frequency domain

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Usual Multiphysics domains

Discipline	Field PDE equations: field quantities	Circuit/network ODE/DAE equations
Electric/magnetic	Maxwell: **A**, V (magnetic vecotr potential and electric scalar potential)	Kirchhoff – El/Mg circuits Electric currents Magneici fluxes and El/Mg voltages
Thermal	Fourier: T (temperature)	Thermal networks (temperature, heat flow)
Structural	Navier: **u (**displacement)	Truss (displacement, force)
Fluidic	Navier-Stokes: **v** (fluid velocity)	Pipes networks (pressure and flow rate)

Diagram of fundamental EM phenomena (causal relations)

$$1.\ \nabla \cdot \boldsymbol{D} = \rho$$

$$2.\ \nabla \cdot \boldsymbol{B} = 0$$

$$3.\ \nabla \times \boldsymbol{E} = -\frac{\partial \boldsymbol{B}}{\partial t}$$

$$4.\ \nabla \times \boldsymbol{H} = \boldsymbol{J} + \frac{\partial \boldsymbol{D}}{\partial t}$$

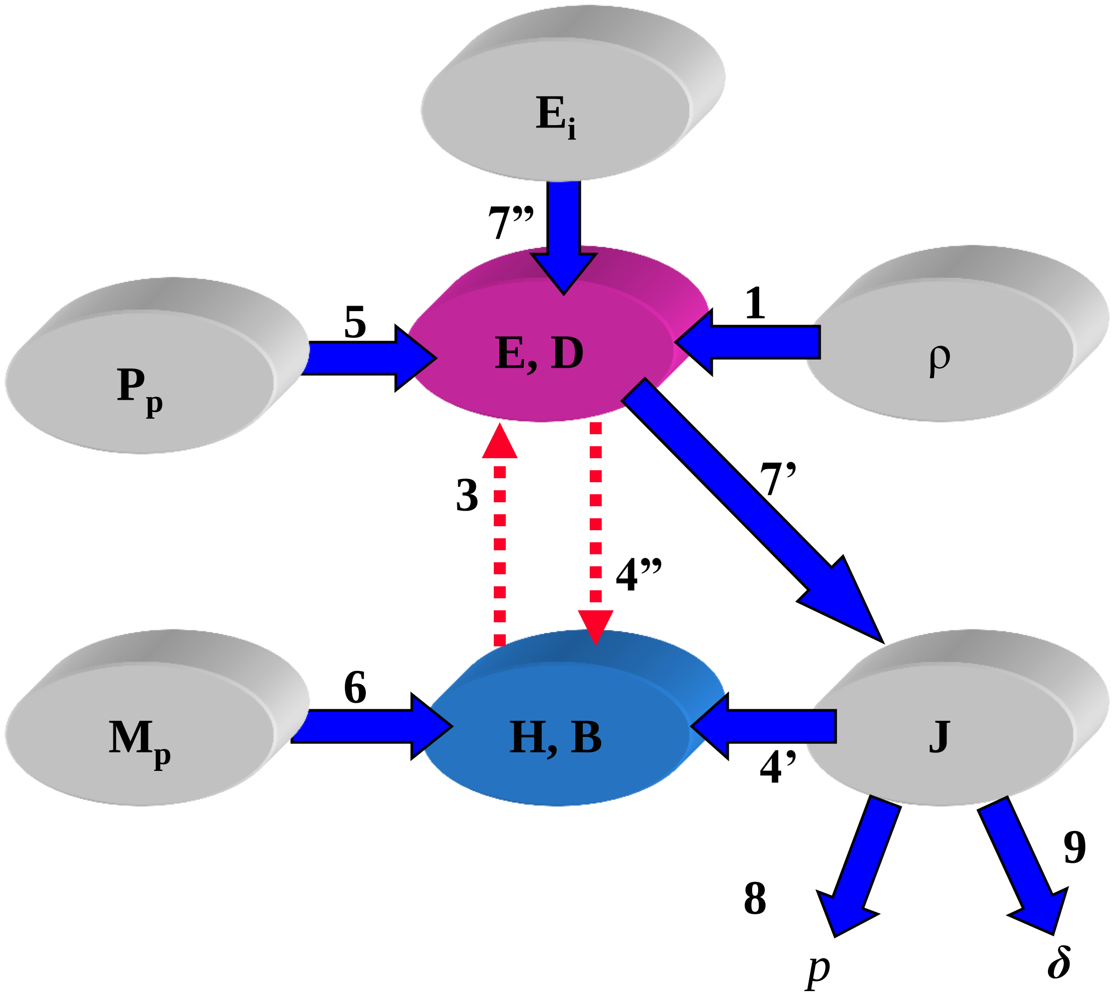
$$5.\ \boldsymbol{D} = \varepsilon\ \boldsymbol{E} + \boldsymbol{P}_p(\boldsymbol{E})$$

$$6.\ \boldsymbol{B} = \mu\ (\boldsymbol{H} + \boldsymbol{M}_p(\boldsymbol{H}))$$

$$7.\ \boldsymbol{J} = \sigma(\boldsymbol{E} + \boldsymbol{E}_i(\boldsymbol{E}))$$

$$8.\ p = \boldsymbol{J} \cdot \boldsymbol{E}$$

$$9.\ \boldsymbol{\delta} = k\boldsymbol{J}$$



Tonti's diagram (Maxwell house)
Functional framework of EM field

In several regimes, it is reduced to:

ES: front wall (V,E,D,ρ)

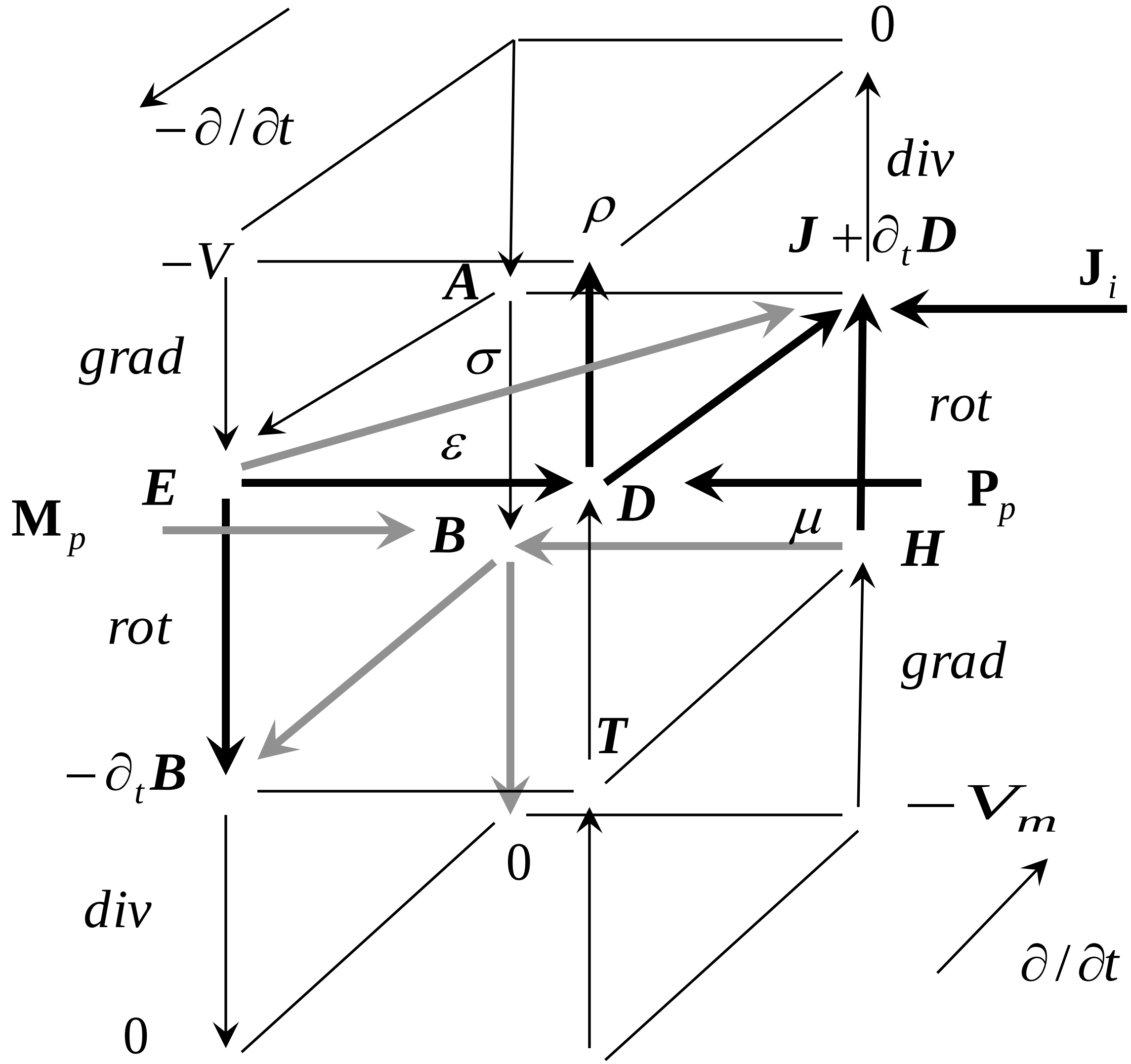
MS: back wall (Vm,H,B,0)

EC: V,E,J,0

MG: back wall

MQS: E,J, H, B (no D)

EQS: E,J,D (noB)



Summary of the Circuit Theory Foundation

- **Definition: electric circuit** is a set of ideal elements with interconnected terminals, described by its graph G
- **Primitive quantities:** current $i = f(t)\ [A]\ f:(t_{\min}, t_{\min}) \to \mathbb{R}$

  voltage $u = f(t)\ [V]\ f:(t_{\min}, t_{\min}) \to \mathbb{R}$
- **Derived quantities:** currents vector $\mathbf{i}$ on G_i graph and voltages vector $\mathbf{v}$ on G_u
- **Laws:** Current Kirchhoff's law $\boxed{\sum_{k\in(n)}{}^{A} i_k = 0}$

  Voltage Kirchhoff's law $\boxed{\sum_{k\in[b]}{}^{A} u_k = 0}$

  Law of transferred power $\boxed{p = \sum_{k=1}^{m-1} v_k i_k} = \mathbf{v}_m{}^T \mathbf{i}_m = \mathbf{i}_m{}^T \mathbf{v}_m$
- **Constitutive equations of ideal**

primitive elements: Resistor (R): $u = R\,i$; Voltage source (E): $u = e$,

Capacitor (C): $i = C\,du/dt$, Perfect diode (PD): $u<0 \Rightarrow i=0,\ u=0 \Rightarrow i>0$

Perfect Operational Amplifier (POA): $u_i = 0;\ i_i = 0.$

Real elements modeling: extraction of the equivalent circuit with ideal elements

Ideal and primitive circuit elements

Primitive ideal elements

Element	Category	Equation
1. Resistor	**Resistive** dipolar linear	u = R I
2. IVS	**Active** dipolar nonlinear	u = e
3. Capcitor	**Reactive** linear dipolar	i = C du/dt
4. Perfect diode	N**onlinear** dipolar resistive	u<0=>i=0, u=0=> i>0
5. POA	**Nonreciprocical,** multipolar, linear	ui=0; ii=0

Frequently used ideal elements:

- Dipolar linear: R, L, C, perfect insulator/conducotr
- Parametric ideal: K (comutatorul)
- Resistive nonlinear: e, j, dioda
- Multipolar linear: CCCS, VCVS. CCVS, VCCS, POA, M
- Multipolar nonlinear: nPOA

Nodal equations of voltage controlled circuits:

$$\mathbf{A}\,\mathcal{Y}\mathbf{A}^T\mathbf{v} = -\mathbf{A}\mathbf{j}$$

MNA: Modified Nodal:

$$\begin{bmatrix} \mathcal{Y}_n & \mathcal{B}_m \\ \mathcal{A}_m & \mathcal{Z}_m \end{bmatrix}\begin{bmatrix} \mathbf{v} \\ \mathbf{i}_m \end{bmatrix} = \begin{bmatrix} \mathbf{j}_n \\ \mathbf{e}_m \end{bmatrix}$$

Circuit model extraction is a EM field problem not one in Circuit theory

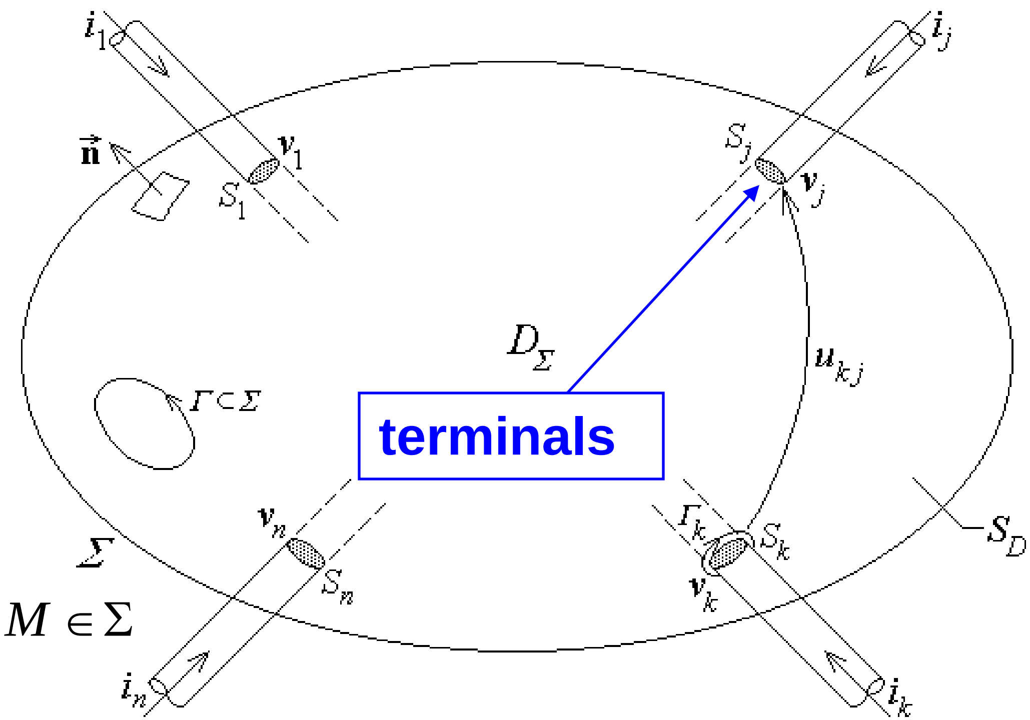
Electric Circuit Element with multiple terminals and distributed parameters

It is defined as a simply connected domain with terminals and b. conditions:

A: no magnetic coupling

B: electric coupling only through terminals

C: eqi-potential terminals



A: $\boldsymbol{n}\cdot\dfrac{\partial \boldsymbol{B}(M,t)}{\partial t}=0 \Leftrightarrow \boldsymbol{n}\cdot\nabla\times\boldsymbol{E}=0;\; M\in\Sigma$

B: $\boldsymbol{n}\cdot\nabla\times\boldsymbol{H}=0 \quad , \quad M\in S_D=\Sigma\setminus\bigcup_{k=1}^{k=n}S_k$

$$i_k=-\int_{S_k}\left(\boldsymbol{J}+\frac{\partial \boldsymbol{D}}{\partial t}\right)\cdot\boldsymbol{n}dS$$

$$u_{kj}(t)=\int_{C_{kj}\in\Sigma}\boldsymbol{E}\cdot d\boldsymbol{r}$$

C: $\boldsymbol{n}\times\mathrm{E}(M,t)=0 \quad , \quad M\in S_k \quad , \quad k=1,2,\ldots,n$

Circuit's fundamental relations

On the boundary surface:

- **total current conservation**

$$\oint_{\Sigma}\left(\mathrm{J}+\frac{\partial \mathrm{D}}{\partial t}\right)\cdot \mathbf{n}\, dS=\oint_{\Sigma}(\mathbf{rot}\,\mathrm{H})\cdot \mathbf{n}\, dS=\int_{D_{\Sigma}}[\mathrm{div}(\mathbf{rot}\,\mathrm{H})]\cdot \mathbf{n}\, dS=0$$

- **zero e.m.f. (A: ➔)**

$$\oint_{\Gamma\subset\Sigma}\mathrm{E}\cdot d\mathbf{r}=\int_{S_{\Gamma}}(\mathbf{rot}\,\mathrm{E})\cdot \mathbf{n}\, dS=-\int_{S_{\Gamma}}\frac{\partial \mathbf{B}}{\partial t}\cdot \mathbf{n}\, dS=0$$

Global characteristic quantities:

- **Terminal current:**

$$i_k=_{def}\oint_{\Gamma_k}\mathrm{H}\cdot d\mathbf{r}=-\int_{S_k}(\mathbf{rot}\,\mathrm{H})\cdot \mathbf{n}dS=-\int_{S_k}\left(\mathbf{J}+\frac{\partial \mathbf{D}}{\partial t}\right)\cdot \mathbf{n}dS$$

- **Terminal voltage:**

$$u_{kj}(t)=_{def}\int_{C_{kj}\in\Sigma}\mathrm{E}\cdot d\mathbf{r}=\int_{C_{kj}\in\Sigma}\mathrm{E}_t\cdot d\mathbf{r}=v_k(t)-v_j(t)$$

C: ➔

$$\int_{MN\subset S_k}\mathrm{E}\cdot d\mathbf{r}=\int_{MN\subset S_k}\mathrm{E}_t\cdot d\mathbf{r}=v(M,t)-v(N,t)=0$$

Kirchhoff Laws:

KCL (B:➔)

$$0=\int_{S_D}\left(\mathrm{J}+\frac{\partial \mathrm{D}}{\partial t}\right)\cdot \mathbf{n}\, dS=\int_{S_D}(\mathbf{rot}\,\mathrm{H})\cdot \mathbf{n}\, dS+\sum_{k=1}^{n}\int_{S_k}(\mathbf{rot}\,\mathrm{H})\cdot \mathbf{n}dS=0+\sum_{k=1}^{n}(-i_k)\Rightarrow \boxed{\sum_{b\in\Sigma} i_b=0}$$

KVL (A:➔)

$$\oint_{\Gamma\subset\Sigma}\mathrm{E}\cdot d\mathbf{r}=0\Rightarrow \boxed{\sum_{b\in\Gamma}u_b=0}$$

Expression of the electric power transferred by a multi-polar element

$$\int_{C_{AB}\subset\Sigma} \boldsymbol{E}\cdot d\boldsymbol{r} = \int_{C_{AB}\subset\Sigma} \boldsymbol{E}_t \cdot d\boldsymbol{r} = v(A,t) - v(B,t) \quad \text{independent } of \ \mathrm{C}_{AB}\subset\Sigma \Rightarrow$$

$$(\exists)v:\Sigma\rightarrow\mathbf{R},\ \text{s.t.}\mathbf{E}_t = -\mathbf{grad}\, v \qquad \mathbf{rot}\,(v\mathbf{H}) = (\mathbf{grad}\, v)\times\mathbf{H} + v(\mathbf{rot}\,\mathbf{H})$$

$$P_\Sigma = \oint_\Sigma (\mathbf{E}\times\mathbf{H})\cdot(-\mathbf{n})dS = -\oint_\Sigma [(-\mathbf{grad}\, v)\times\mathbf{H}]\cdot(-\mathbf{n})dS =$$

$$\oint_\Sigma [\mathbf{rot}\,(v\mathbf{H})]\cdot\mathbf{n}\, dS - \oint_\Sigma [v(\mathbf{rot}\,\mathbf{H})]\cdot\mathbf{n}\, dS =$$

$$0 + \sum_{k=1}^{n}\int_{S_k} [v(\mathbf{rot}\,\mathbf{H})]\cdot\mathbf{n}\, dS = \sum_{k=1}^{n} v_k \int_{S_k} (\mathbf{rot}\,\mathbf{H})\cdot\mathbf{n}\, dS =$$

$$\sum_{k=1}^{n} v_k \int_{S_k} (\mathbf{rot}\,\mathbf{H})\cdot\mathbf{n}\, dS = \sum_{k=1}^{n} v_k i_k \Rightarrow \boxed{P_\Sigma = \sum_{k=1}^{k=n} v_k\, i_k}$$

P has the conventional sense of i

Uniqueness and the constitutive relation of the multi-polar circuit element

The case of voltage excitation

Excitations (input signals): $\int_{C_{kn}\in\Sigma} \boldsymbol{E}_t \cdot d\boldsymbol{r} = v_k(t)$ Known for $\mathrm{k} = 1,2, \ldots, \mathrm{n\text{-}1}$

Responses (output signals): $i_k = \oint_{\Gamma_k} \boldsymbol{H} \cdot d\boldsymbol{r}$ Computed from the field solution, for $\mathrm{k} = 1,2, \ldots, \mathrm{n}$

Let consider D a linear domain without permanent sources (D=εE, B=μH, J=σE) with zero initial field and boundary conditions given by A, B, C and excitations.

The fundamental problem may be simplified: input signals: **v** = [v1, v2, .., vn-1], response – output signals: **i** = [i1, i2, …, in-1].

The input-output relation **i = Y v** is described by the admittance **Y**. It is a linear, well defined operator due to the solution uniqueness and superposition. These theorems are based on the lemma of the trivial solution for a circuit element: zero excitations produce zero responses. **v** = 0 ➔ **i** = 0:

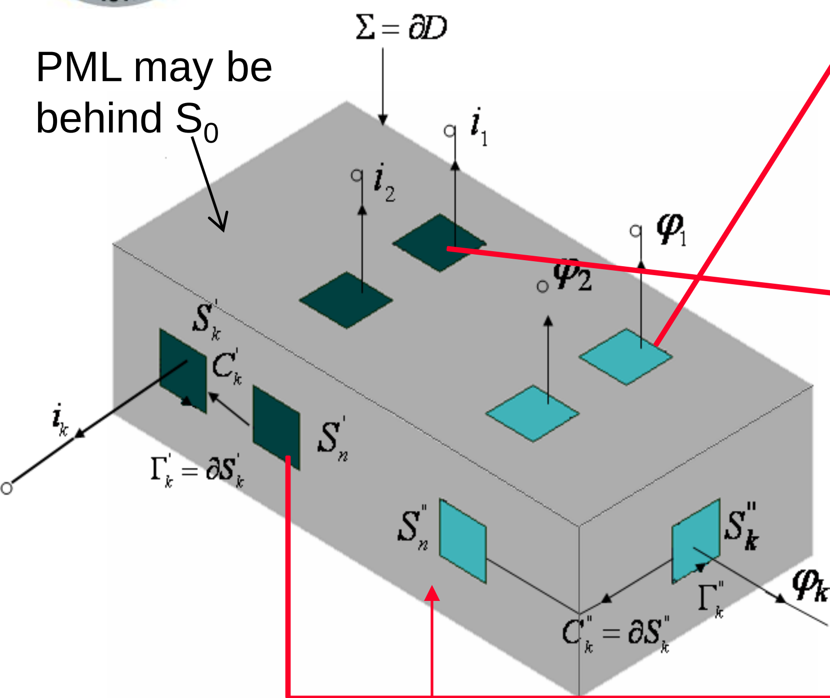
$$\int_D \sigma \mathrm{E}^2 dV + \frac{1}{2}\frac{\partial}{\partial t}\int_{D_\Sigma} \left(\mu \mathrm{H}^2 + \varepsilon \mathrm{E}^2\right) dV = \oint_\Sigma \left(\mathrm{E}\times\mathrm{H}\right)\cdot\left(-\mathbf{n}\right) dS = \sum_{k=1}^{n} v_k i_k 0 \Rightarrow$$

$$0 \le \int_{D_\Sigma} \left(\mu \mathrm{H}^2 + \varepsilon \mathrm{E}^2\right) dV = -2\int_0^t \int_D \sigma \mathrm{E}^2 dV \le 0 \Rightarrow \mathrm{H} = 0 \Rightarrow i_k = 0$$

The dual case of current excitation: **v =Z i**

EMCE Boundary conditions

PML may be behind S_0



- Magnetic flux only through magnetic connectors:

$$\mathbf{n}\, curl\, \mathbf{E}(P,t) = 0 \qquad \forall P \in S_0$$

- Electric current only through electric terminals/ connectors:

$$\mathbf{n}\, curl\, \mathbf{H}(P,t) = 0 \qquad \forall P \in S_0$$

- Electric scalar potential is constant over each electric terminal/connector

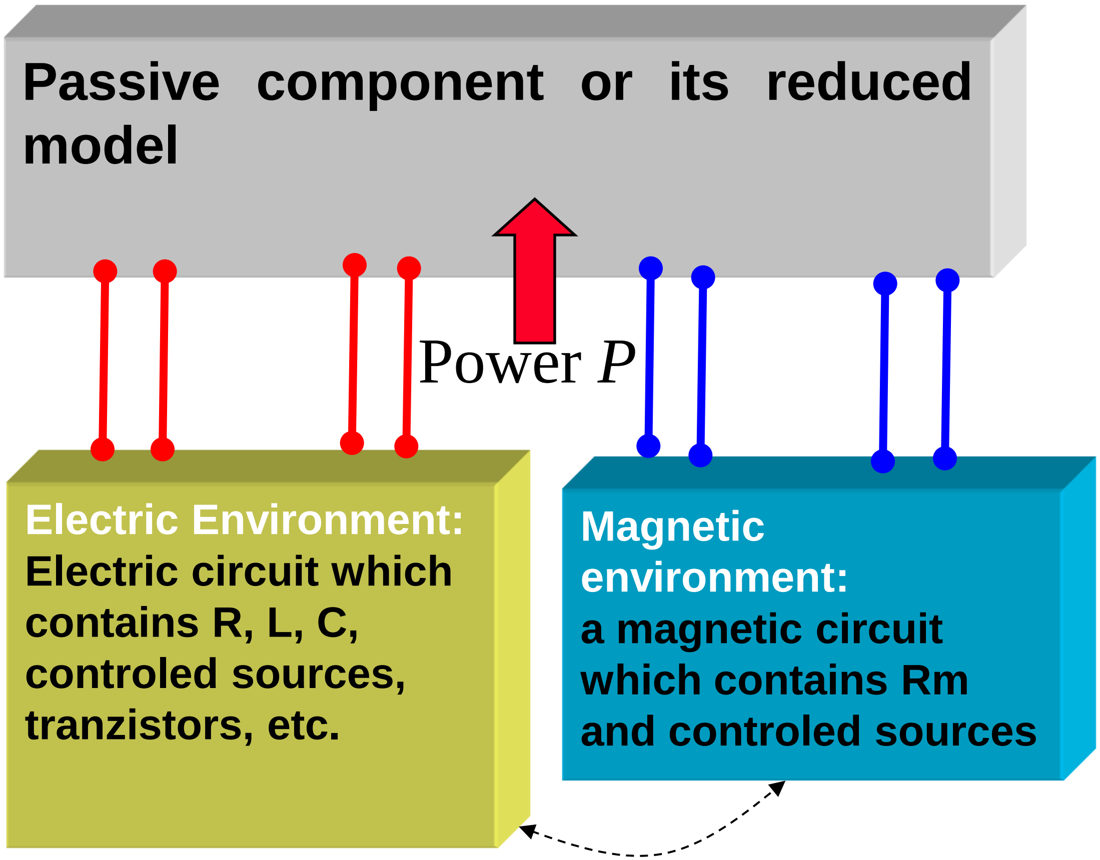
$$\mathbf{n} \times \mathbf{E}(P,t) = \mathbf{0} \qquad \forall P \in \bigcup S_k^{'}$$

- Magnetic scalar potential is constant over each magnetic connector

$$\mathbf{n} \times \mathbf{H}(P,t) = \mathbf{0} \qquad \forall P \in \bigcup S_k^{''}$$

They assure uniqueness for the solution of Maxwell equations and allow the compatibility and interconnection with external circuits.

Field-circuit coupling



For electric terminals:

$$i_k(t) = \int_{\Gamma_k} \mathbf{H} d\mathbf{r}$$

$$v_k(t) = \int_{\mathbf{C_k}} \mathbf{E} d\mathbf{r}$$

For magnetic terminals:

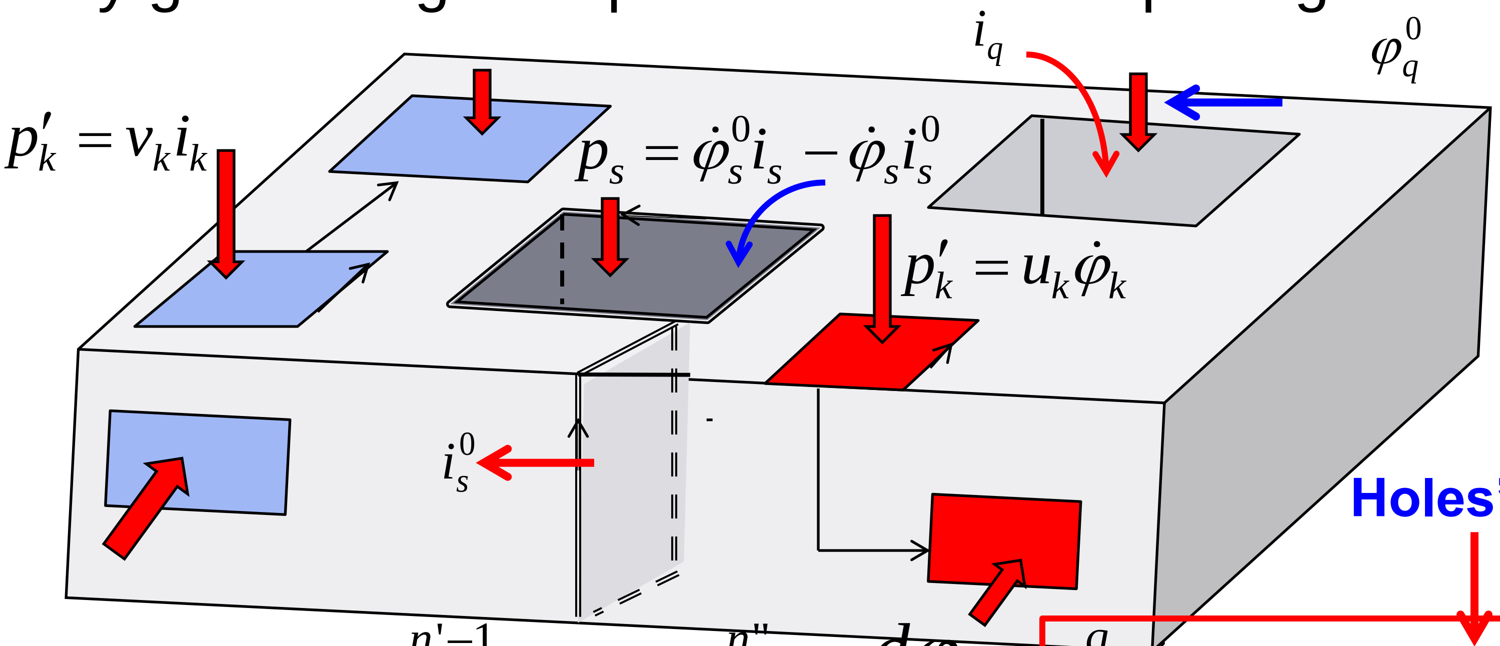
$$\dot{\varphi}_k(t) = \int_{\Gamma_k} \mathbf{E} d\mathbf{r}$$

$$u_k(t) = \int_{C_k} \mathbf{H} d\mathbf{r}$$

$$P = -\oint_{\Sigma} (\mathbf{E} \times \mathbf{H}) d\mathbf{A} = \sum_{k=1}^{n'-1} (v_k i_k) + \sum_{k=1}^{n''} u_k \frac{d\varphi_k}{dt}$$

Boundary conditions of multiple connected EMCE

Power is transfered by magn. and el. terminals and by holes.
Each entity generating an input and and an output signal.



$$P_\Sigma = -\oint_\Sigma (\mathbf{E}\times\mathbf{H})d\mathbf{A} = \sum_{k=1}^{n'-1} v_k \cdot i_k + \sum_{j=1}^{n''} u_j \frac{d\varphi_j}{dt} + \boxed{\sum_{s=1}^{q}\left(e_s \cdot f_s^{\,0} - e_s^0 \cdot f_s\right)}$$

$$e_s = \oint_{\Gamma_s} \mathbf{E}\cdot d\mathbf{r} = -\frac{d\varphi_{S_q}}{dt};\ f_s = \oint_{\Gamma_s} \mathbf{H}\cdot d\mathbf{r} = i_{S_q};\ e_s^0 = \oint_{\Gamma_s^0} \mathbf{E}\cdot d\mathbf{r} = -\frac{d\varphi_{S_q^0}}{dt};\ f_s^{\,0} = \oint_{\Gamma_s^0} \mathbf{H}\cdot d\mathbf{r} = i_{S_q^0}$$

Multiphysics circuits analogies

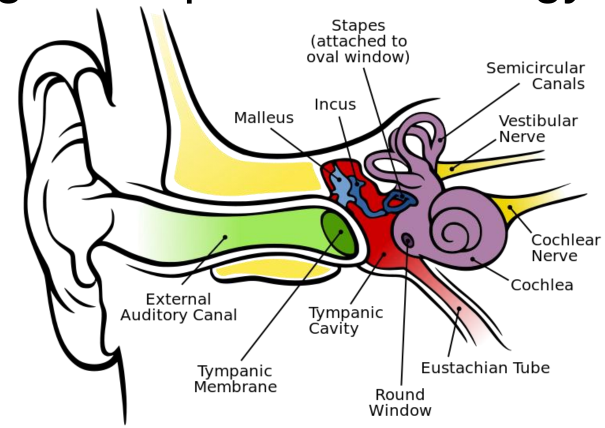
General	Electrical	Mechanical	Fluidic	Thermal
Effort (e)	Voltage, V	Force, F	Pressure, P	Temp. diff., ΔT
Flow (f)	Current, I	Velocity, v	Vol. flow rate, Q	Heat flow
Displacement (q)	Charge, Q	Displacement, x	Volume, V	Heat, Q
Momentum (p)	-	Momentum, p	Pressure Momentum, Γ	-
Resistance	Resistor, R	Damper, b	Fluidic resistance, R	Thermal resistance, R
Capacitance	Capacitor, C	Spring, k	Fluid capacitance, C	Heat capacity, mcp
Inertance	Inductor, L	Mass, m	Inertance, M	-
Node law	KCL	Continuity of space	Mass conservation	Heat energy conservation
Mesh law	KVL	Newton's 2nd law	Pressure is relative	Temperature is relative

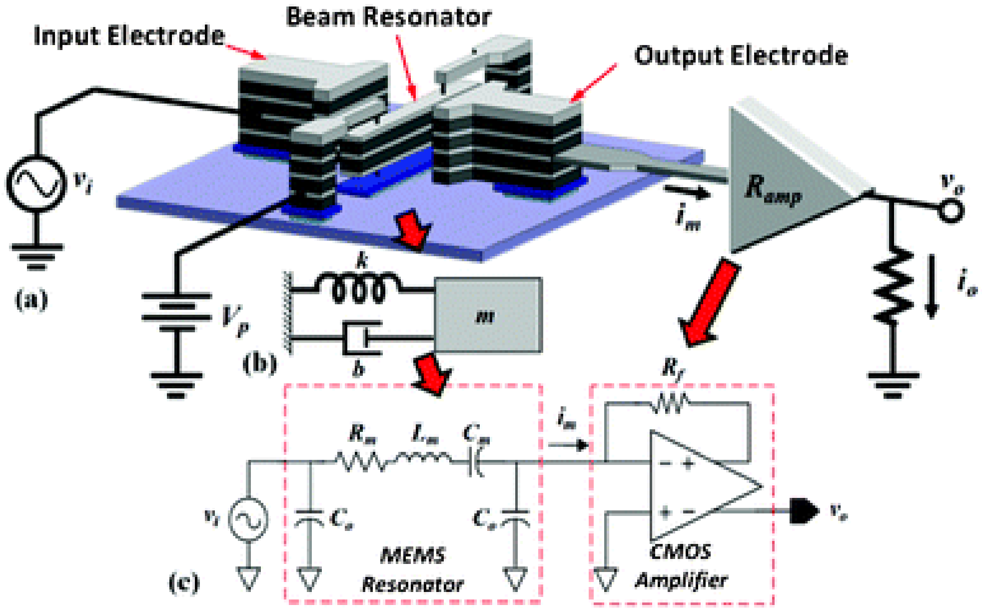
Cite as: Joel Voldman, course materials for 6.777J / 2.372J Design and Fabrication of Microelectromechanical Devices, Spring 2007. MIT OpenCourseWare (http://ocw.mit.edu/), Massachusetts Institute of Technology. Downloaded on [DD Month YYYY].

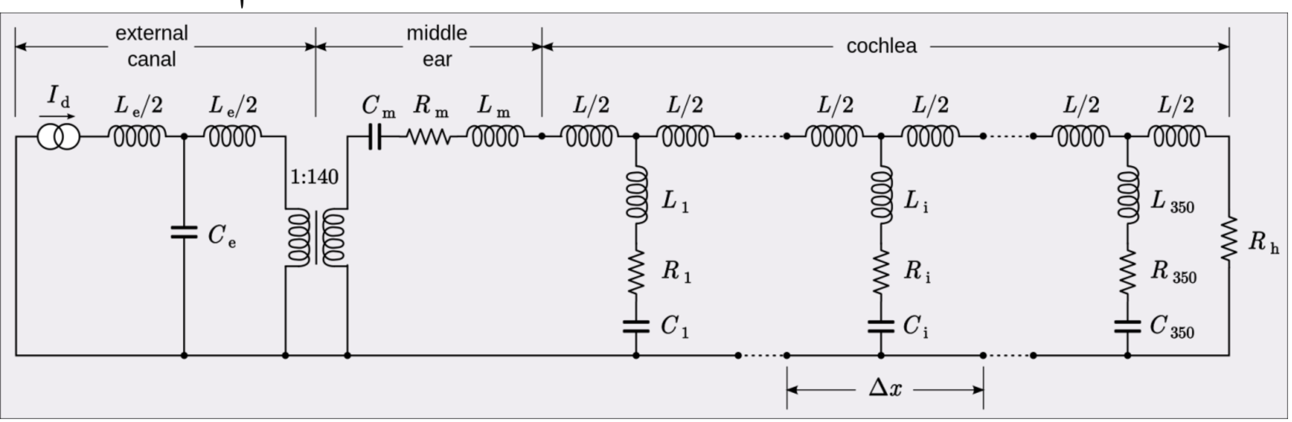
JV: 6.777J/2.372J Spring 2007, Lecture 8 - 24

Applications. Model reduction by field to circuit representation

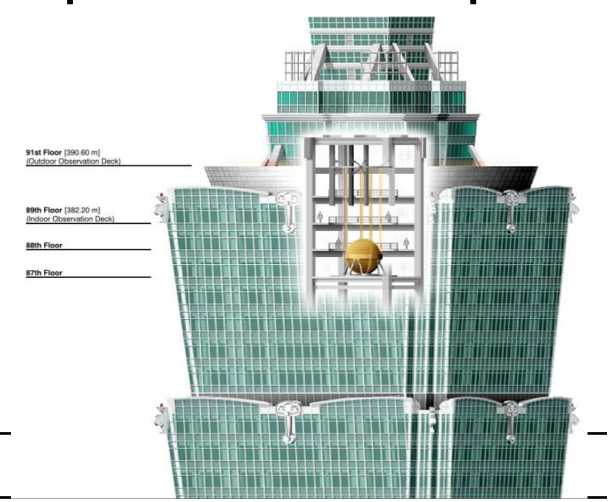
- **MEMS modeling**
- Equivalent circuit of the **human ear** using the impedance analogy







Taipei 101 – mass dumper



What is Multiphysics? Attributes of Multiphysics problems

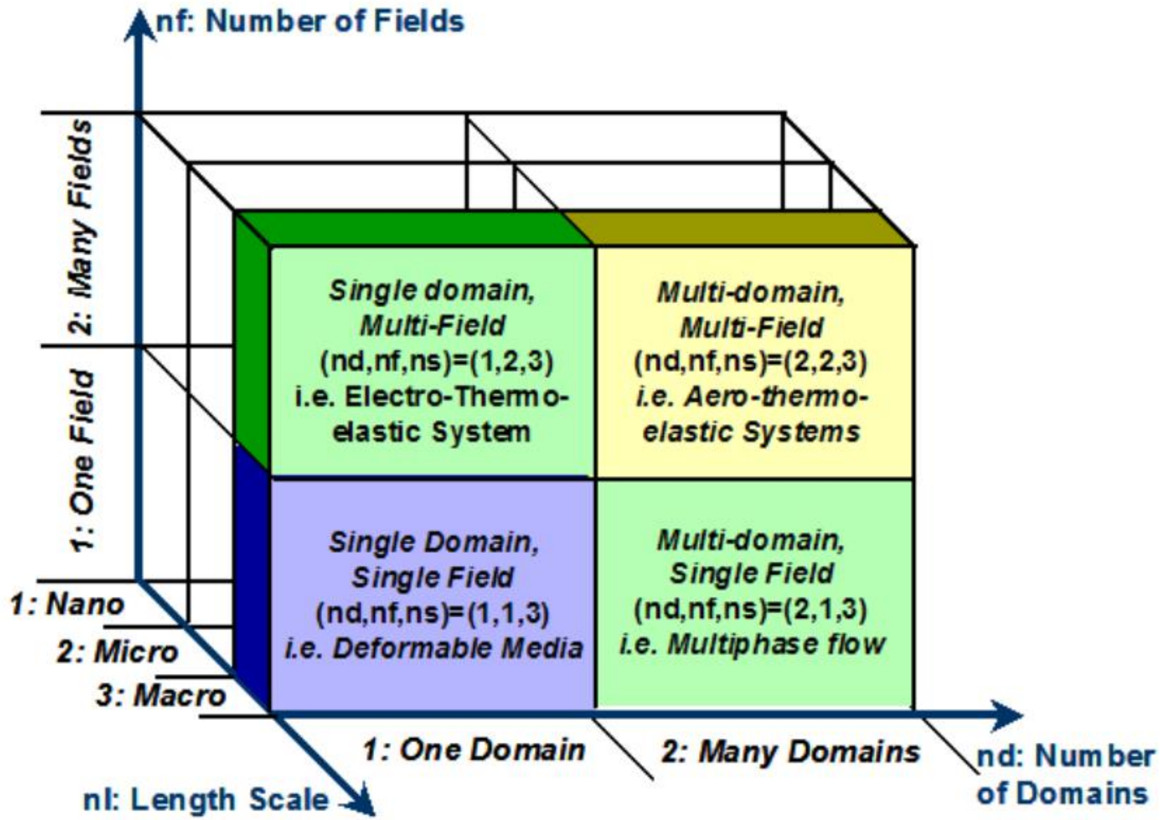
Multiphysics attribute space:

- Fields: electric, thermal, etc
- Domains: 1,2, ..
- Scales: nano, micro, macro

Multiphysics definition:

(nd,nf,ns) ≠ (1,1,1)

The physical difference between coupled problems is not so relevant, but the coupling is relevant.



May be coupled ES and EQS fields or EQS field with RC Circuits or other fields, scales or domains.

A multiphisycs problem may be multifield, multidomain and/or multiscale.

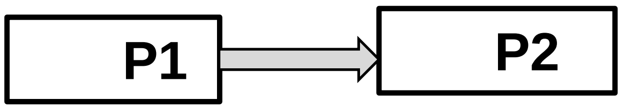
http://citeseerx.ist.psu.edu/viewdoc/download?doi=10.1.1.88.3093&rep=rep1&type=pdf

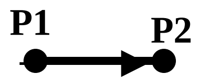
Outline

- Introduction
- Modeling procedure
- Multiphysics basics
- **Coupled problems**
- Complexity reduction
- Conclusions

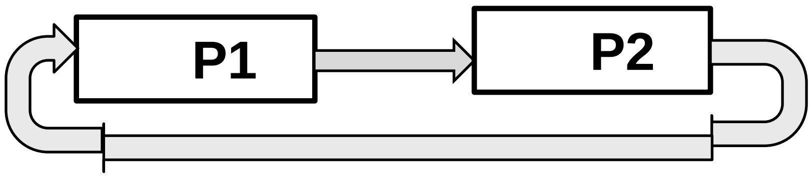
Coupled problems

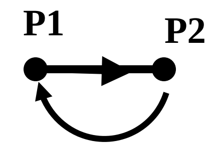
Unidirectional coupling



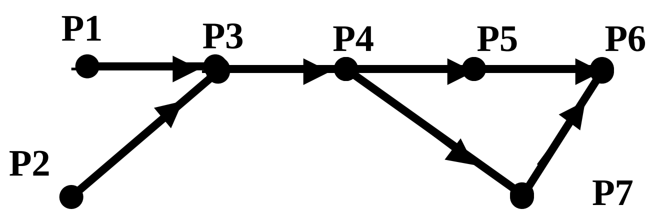


Bidirectional coupling

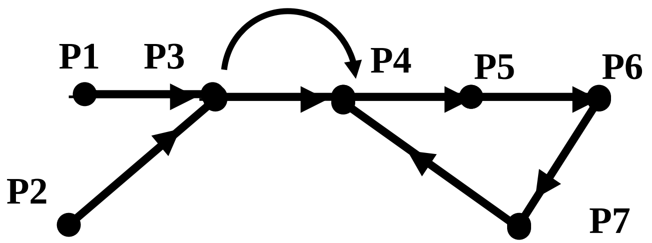




Multiple unidirectional (acyclic) couplings



Multiple bidirectional (cyclic) couplings



Prototype Algebraic Forms. Solving techniques

- Let consider a system of two coupled problems, described at equilibrium by

$$\begin{cases} F_1(u_1,u_2)=0 \\ F_2(u_1,u_2)=0 \end{cases} \qquad (1)$$

- And two evolution problems, described by

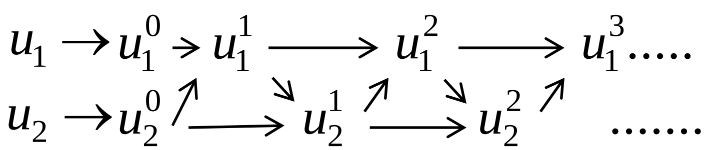
$$\begin{cases} \dfrac{\partial u_1}{\partial t} = f_1(u_1,u_2) \\ \dfrac{\partial u_2}{\partial t} = f_2(u_1,u_2) \end{cases} \qquad (2)$$

- When (2) is semi-discretized in time it takes form (1) and it is solved sequentially to compute u(t) at discrete time values. The solution of multiphysics problems may have many components: $u=(u_1,u_2, ,,,,,un)$, but for presentation simplicity was taken n = 2.
- We assume that dF_1/du_1 and dF_2/du_2 are nonsingular, the coupled problem is formed by two well-posed individually systems.
- Many times, the splitting it is done in practice based on existence of software able to solve individual problems, but this may be a wrong decision, for example, if the two problems are strongly coupled.

Iterative solving

Traditionally algorithms preserve the integrity of the two coupled problems, that means they are solved iteratively. There are two kinds of approaches:

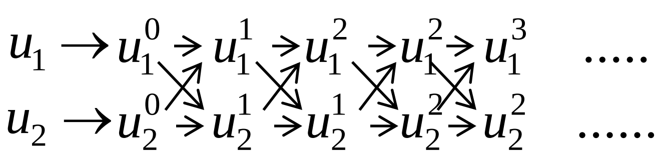
- **GS: Gauss-Seidel manner**



Algorithm 1 Gauss-Seidel Multiphysics Coupling

> Given initial iterate $\{u_1^0, u_2^0\}$
> **for** $k = 1, 2, \ldots,$ (until convergence) **do**
>   Solve for v in $F_1(v, u_2^{k-1}) = 0$; set $u_1^k = v$
>   Solve for w in $F_2(u_1^k, w) = 0$; set $u_2^k = w$
> **end for**

- **J: Jacobi manner**



Algorithm 2 Multiphysics Operator Splitting

> Given initial values $\{u_1(t_0), u_2(t_0)\}$
> **for** $n = 1, 2, \ldots, N$ **do**
>   Evolve one timestep in $\partial_t u_1 + f_1(u_1, u_2(t_{n-1})) = 0$ to obtain $u_1(t_n)$
>   Evolve one timestep in $\partial_t u_2 + f_2(u_1(t_n), u_2) = 0$ to obtain $u_2(t_n)$
> **end for**

- GS is expected to be faster than J, but in J solutions may be find in parallel
- J implements a "**loosely coupled**" systems, that means each of components has as little possible knowledge of other separate components.
- An alternative is to implement a "**tightly coupled**" systems such in Newton method used to solve the nonlinear systems

Strong, weak, tight and loose couplings

- **N: Newton manner**

$$\begin{matrix} u_1 \to \\ u_2 \to \end{matrix} \begin{pmatrix} u_1^0 \\ u_2^0 \end{pmatrix} \to \begin{pmatrix} u_1^1 \\ u_2^1 \end{pmatrix} \to \begin{pmatrix} u_1^2 \\ u_2^2 \end{pmatrix} \to \dots$$

Algorithm 3 Newton's method

Given initial iterate u^0
for $k = 1, 2, \dots,$ (until convergence) **do**
  Solve $J(u^{k-1})\,\delta u = -F(u^{k-1})$
  Update $u^k = u^{k-1} + \delta u$
end for

The nonlinear problem uses at each iteration the Jacobian matrix with nonzero off-diagonal blocks:

$$F(u) \equiv \left(\begin{array}{c} F_1(u_1, u_2) \\ F_2(u_1, u_2) \end{array} \right) = 0, \quad \Rightarrow \quad J = \left[\begin{array}{cc} \frac{\partial F_1}{\partial u_1} & \frac{\partial F_1}{\partial u_2} \\ \frac{\partial F_2}{\partial u_1} & \frac{\partial F_2}{\partial u_2} \end{array} \right]$$

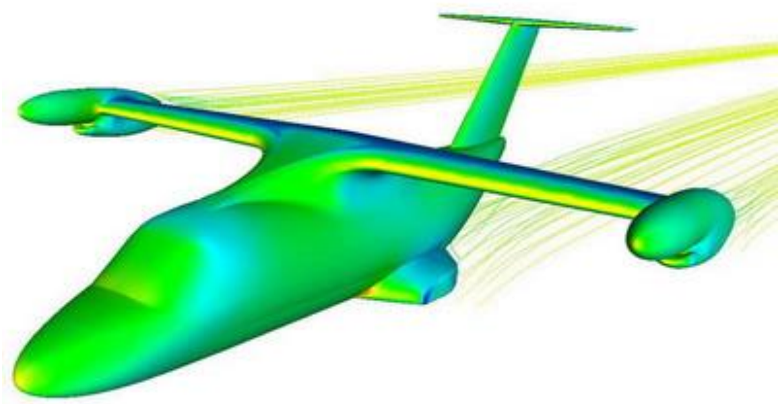
- The approaches describing here by three algebraic prototypes are relevant to many divide-and-conquer strategies, wither the coupled sub-problems have different position in the multiphysics attribute space.
- **Strong vs weak coupling** of physical models: intrinsic interaction between natural processes. The off-diagonal blocks in Jacobian are full and/or large.
- **Tight versus loose coupling** of numerical models: how the state variables of several computer/algorithmic models are synchronized. In tight coupling, they are as synchronized as possible across different models at all times.
- Any of four combination (ST, RL, WT, WL) may be encountered.

Examples of coupled problems

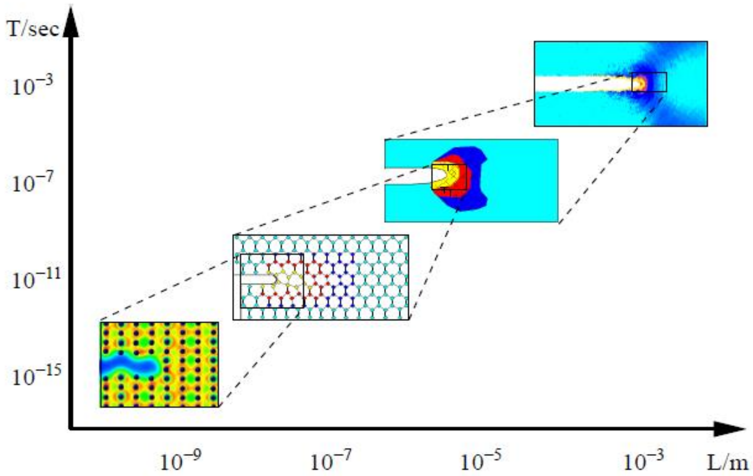
- **FSI – Fluid-Structure Interaction** the multiphysic coupling of Structural mechanics with Fluid Dynamics encountered mainly in transport (aerospace, cars, vesels). It was solved by using all three approaches: GS, J and N. For details see http://www.global-sci.com/openaccess/v12_337.pdf

- **Multiscale methods in crack propagation**

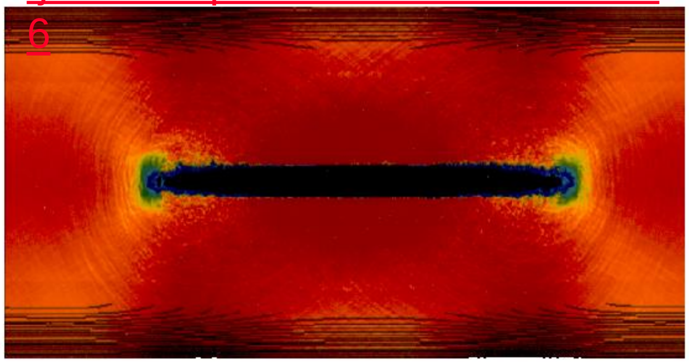
The silicon slab was decomposed into the five different dynamic regions of the simulation: the continuum finite-element (FE) region; the atomistic molecular-dynamics (MD) region;
the quantum tight-binding (TB) region; the FE-MD "handshaking" region; and the MD-TB "handshaking" region. Details in Abraham, Farid F., et al. "Spanning the length scales in dynamic simulation."*Computers in Physics* 12.6 (1998): 538-546.



http://www.cenaero.be/Page.asp?docid=15334&langue=EN



http://scitation.aip.org/content/aip/journal/cip/12/6/10.1063/1.168756



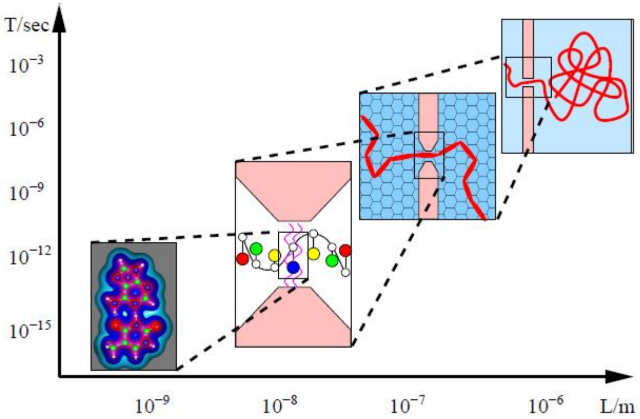
Examples of coupled problems

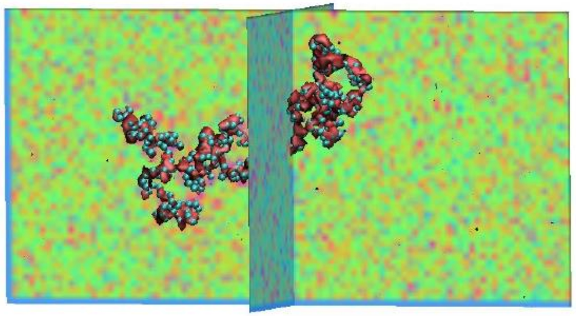
- **Multiscale methods in ultra fast DNS sequencing**

Electronic signals generated by DNE during translocation through nanopores.

See http://www.mcs.anl.gov/uploads/cels/papers/ANL_MCS-TM-321.pdf

Fluid, electric, molecular and atomic levels:





- **Particle accelerators design**

http://slac.stanford.edu/pubs/slacpubs/13250/slac-pub-13280.pdf

EM, Thermal and Structural analysis

Multiphisycs solving strategies. Types of couplings

Basically there are there types of coupled systems (see figures): a) systems within a shared spatial domain; b) interfacially coupled systems and c)Network systems. A system P2 is coupled (controlled) if it has the input data of its fundamental problem of field analysis dependent by the output results of other (control) problem P1. So the couplings may be realized by:

1.Domain shape and size (P1 may change the domain of P2);

2.Material parameters (of P2 are influenced by P1 solution), it is of type a);

3.Internal field sources (P1 domain is includes strict or not in the domain of P2, and the solution of P1 describes the sources of field in P2), type a);

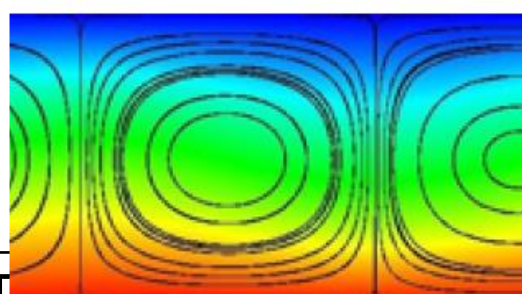
4.External field sources, boundary conditions (the coupled problems share a part of their boundaries, there is an unidirectional or bidirectional influence between the b.c of P1 and P2), including type c) couplings, e.g. ECE;

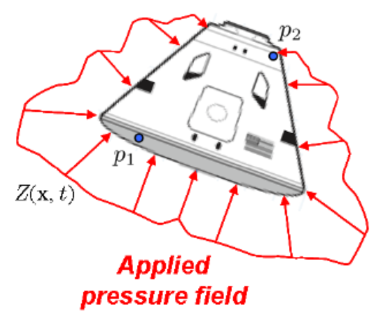
5.Initial conditions (solution of P1 influence the initial values of P2), it is of type a);

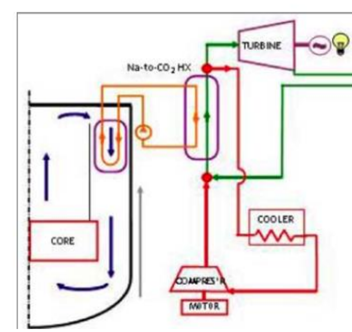
Example of type 1:

MEMS, P1=elastic

P2=electrostatic.







Multiphisycs solving strategies. Multi-fields couplings

- Let consider for simplicity only two fields, and their fundamental problems of field analysis: P1 and P2.

P1	P2
1.1. Spatial domain D1	2.1. Spatial domain D2
1.2. Material parameters M1	2.2. Material parameters M2
1.3. Internal field causes C1	2.3. Internal field causes C2
1.4. Boundary conditions B1	2.4. Boundary conditions B2
1.5. Initial conditions I1	2.5. Initial conditions I2

We can imagine 5 uni- and 10 bi-directional simple couplings. Each table entry may be influenced by the solution of the other problem. In the real systems they may be combined. Solutions of two problems are

S1(D1,M1,C1,B1,I1); S2(D2,M2,C2,B2,I2)

They are coupled if there is at least one nontrivial interdependence:

S1(D1(S2),M1(S2),C1(S2),B1(S2),I1(S2));
S2(D2(S1),M2 (S1),C2 (S1),B2(S1),I2 (S1)).

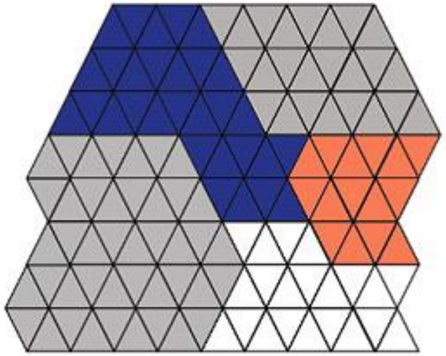
Multiphisycs solving strategies. Multi-domain couplings

Multidomain coupling means we have at least two different domains which interact through their common interface. I the general case we have n non-overlapped sub-domains which have common parts of boundaries. It is the case of computational domain partition, encountered in **the DD (Domain Decomposition) Method.** A more general case is that of sub-domain overlapping.

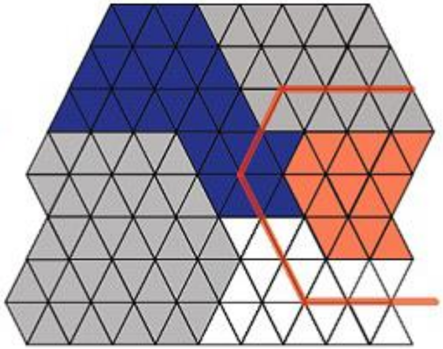
A fundamental step is the partitioning of computational domain, so that:

- sub-domains to be well balanced and
- their interface to be as small as possible.

These conditions facilitate the computations **parallelization**, when sub-domains are allocated to several CPUs.



non-overlapped sub-domains



overlapped sub-domains

The procedure is called graph partitioning, such as METIS and SCOTCH . For details see:

https://hal.archives-ouvertes.fr/cel-01100932v2/document

http://en.wikipedia.org/wiki/Graph_partition

http://glaros.dtc.umn.edu/gkhome/views/metis

http://people.sc.fsu.edu/~jburkardt/c_src/metis/metis.html

http://www.labri.fr/perso/pelegrin/scotch

Multiphisycs solving strategies.
Field-circuits coupling

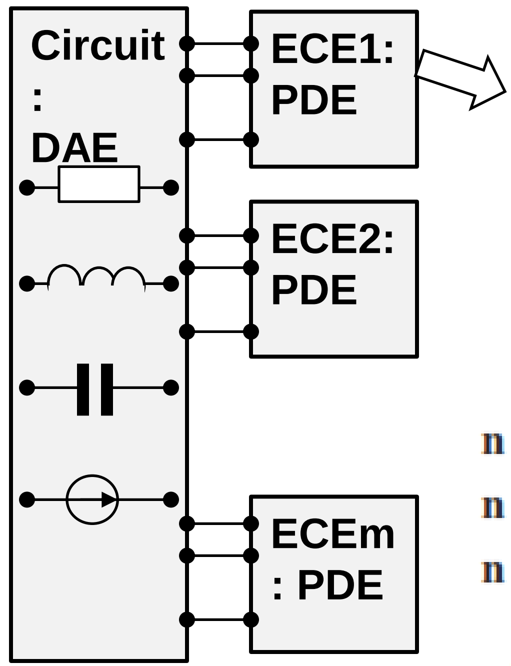
The modeled system is structured in:

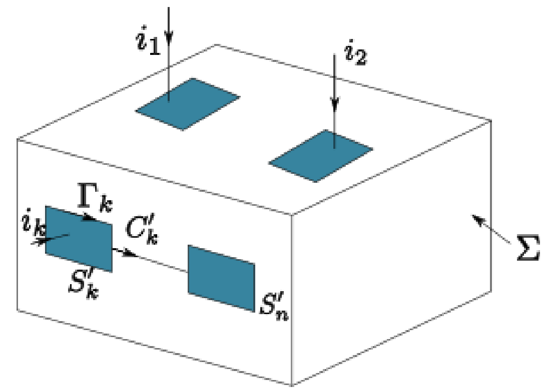
- Lumped circuit (R, L, C, M, e, j,, c.s.), described by Kirchhoff (algebraic) and constitutive (differential or algebraic) equations: DAE
- Elements with distributed parameter, described by Maxwell's equations: PDE with ECE boundary conditions, compatible with circuits eqs:

The interaction is done through the field domains boundaries.

If PDE are linear, an equivalent linear circuit may be extracted by several procedures for complexity reduction:

- PDE are discretized
- The obtained DAE are reduced to smaller size ODE
- Equivalent circuit is synthetized





$$\mathbf{n}\cdot\mathrm{curl}\mathbf{E} = 0 \quad \text{on} \quad \partial\Omega,$$
$$\mathbf{n}\cdot\mathrm{curl}\mathbf{H} = 0 \quad \text{on} \quad \partial\Omega \setminus \cup_{k=1}^{n} S'_k$$
$$\mathbf{n}\times\mathbf{E} = \mathbf{0} \quad \text{on} \quad \cup_{k=1}^{n} S'_k$$

$$u_k = \int_{C_k \subset \partial\Omega} \mathbf{E}\cdot d\mathbf{r}, \quad i_k = \int_{\partial S'_k} \mathbf{H}\cdot d\mathbf{r},$$

Multiphisycs solving strategies. Multi-scale couplings

- The algebraic prototype of using multiple spatial scales is Multigrid technique in which are defined two inter-grid transfer operators: restrict ion and interpolation (http://en.wikipedia.org/wiki/Multigrid_method) http://ocw.mit.edu/courses/mathematics/18-086-mathematical-methods-for-engineers-ii-spring-2006/readings/am63.pdf
- Hierarchical Adapted data structures as they are used in Fast Multipole Method (FMM) and in Adaptive Mesh Refinement (AMR) are also models

http://math.nyu.edu/faculty/greengar/shortcourse_fmm.pdf

http://www.mpa-garching.mpg.de/lectures/ADSEM/SS05_Homann.pdf
http://www.fastfieldsolvers.com/ http://www.rle.mit.edu/cpg/research_codes.htm

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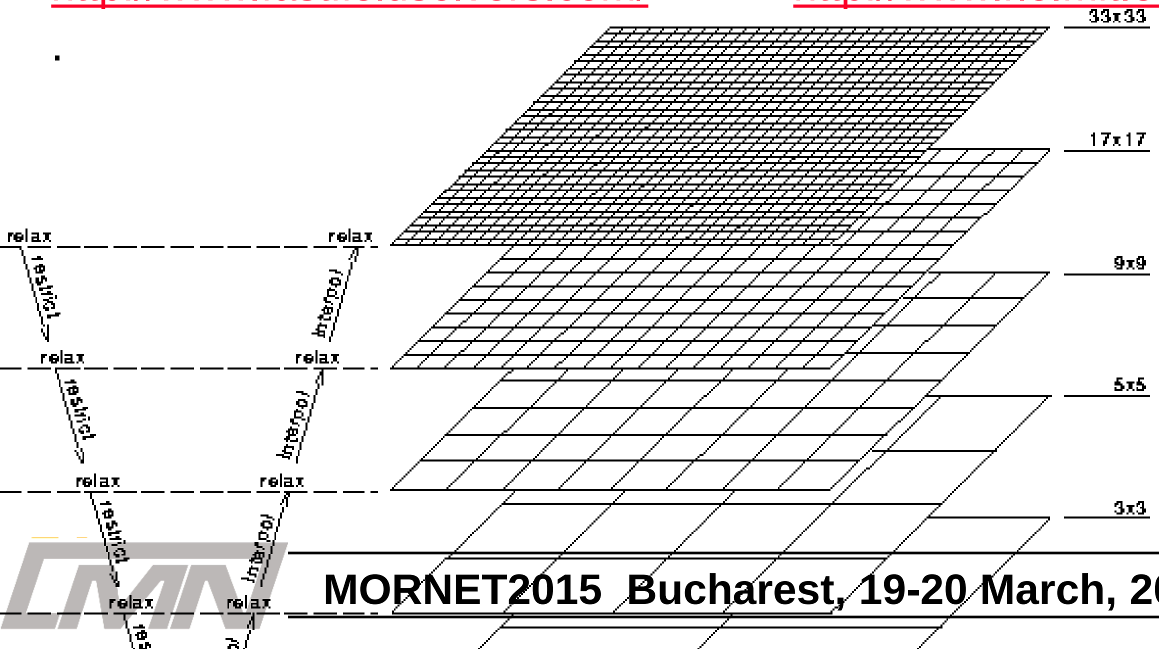
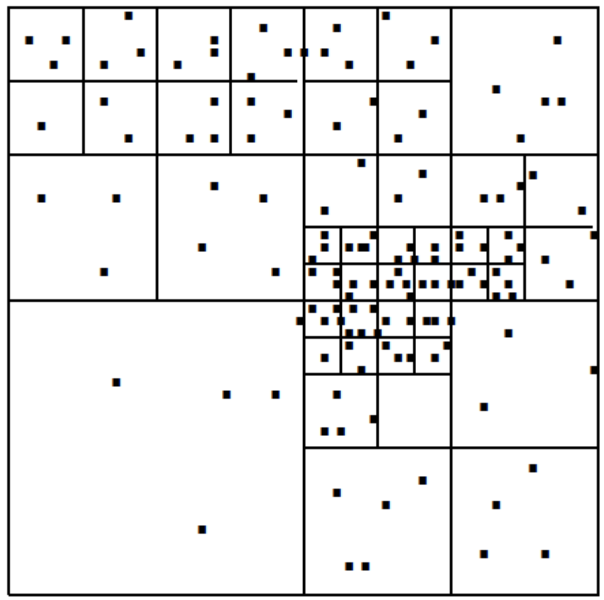




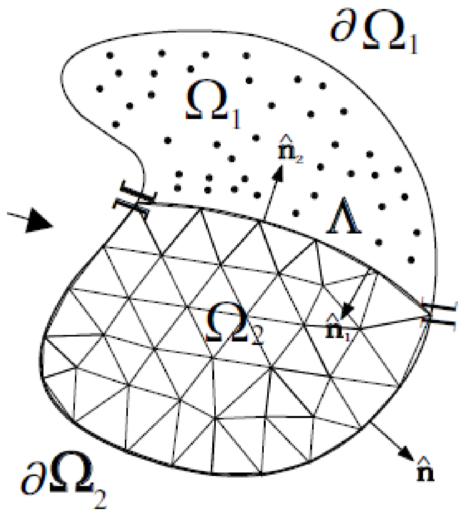
Multiphisycs solving strategies.
Multi-scale couplings

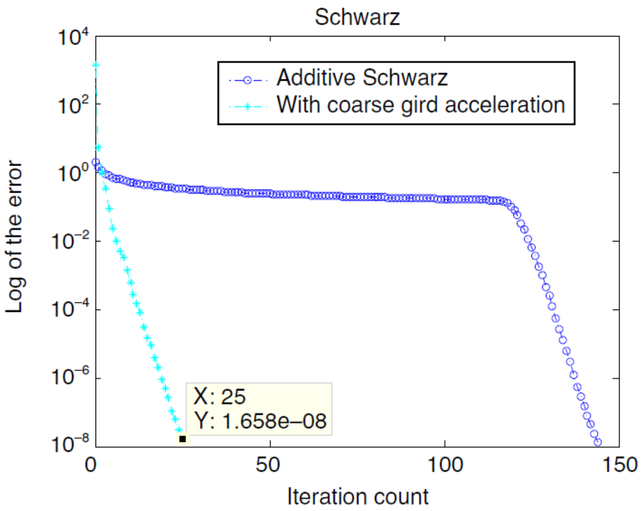
- Another prototype is the Two-Level Domain Decomposition Method
  http://ogst.ifpenergiesnouvelles.fr/articles/ogst/abs/2014/04/ogst130025/ogst130025.html

Use of an additional coarse grid accelerate very much the iterative process.

- In the multi-level multifield approach, the coupling between continuum (macroscopic) models and discrete (atomistic) models and Multiscale Modeling of Materials are the most important difficulties.
  http://www.engin.brown.edu/facilities/gm_crl/publications/tello_curtin.pdf

http://people.ds.cam.ac.uk/jae1001/CUS/research/Elliott_IMR_2011_corrected_proof.pdf





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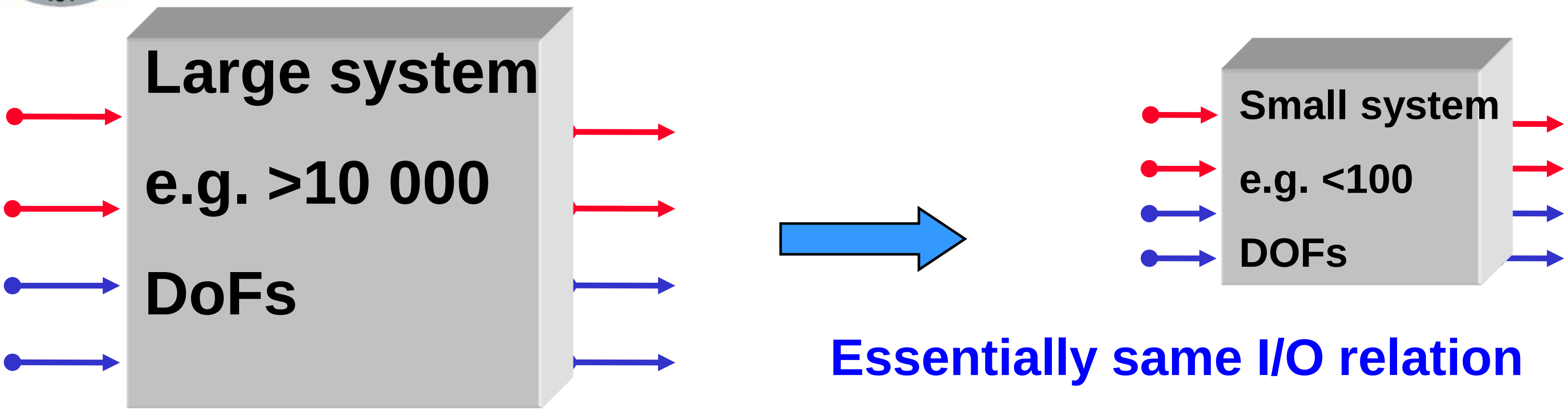
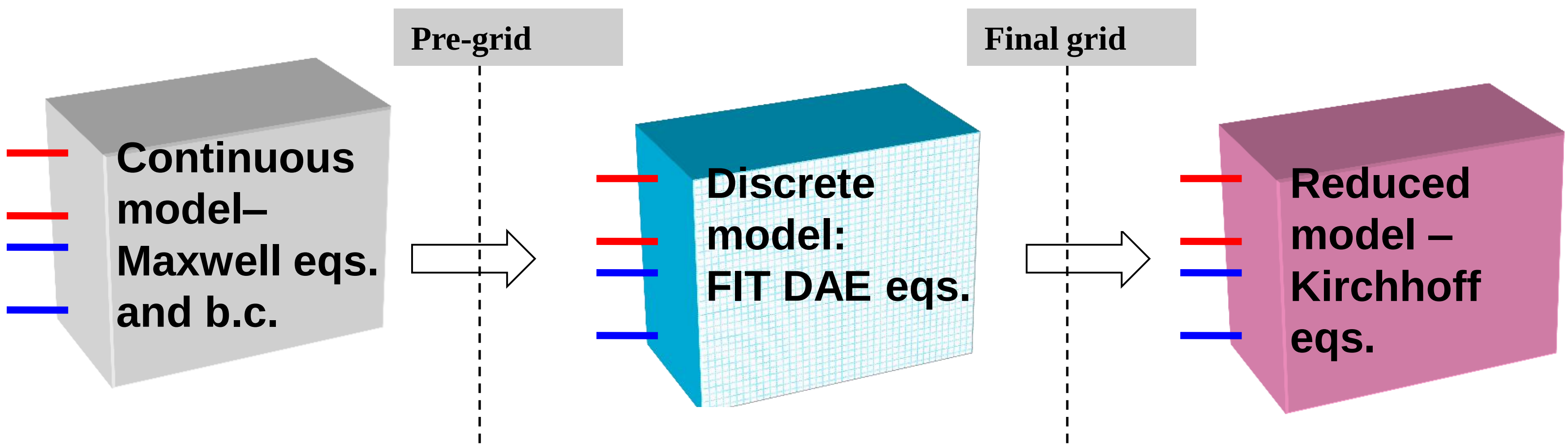
MOR - What is Complexity/Oder Reduction



Essentially same I/O relation



Apriori ROM (discretization)

Reduction on the fly

Aposteriori ROM and model realization

Aproiri Complexity Reduction Methods

Any pre-processing for an effective discretization:

- **Geometric approximations of the model domain** → **Optimal truncation of model domain (see ALROM)**
- **Simplification of material behaviour** → **Cell homogenization - CellHo**
- **Appropriate equations (field regime) in each sub-domain** → **EQS+MS in Si, (LL)FW in SiO2, MQS in metal, ES+MS in air**
- **Field problem (re)formulation: equations, quantities** → **Local-integral equations for field vectors, Fourier transform, TL**
- **Boundary and interface condition** → **EMCE boundary conditions, DD with EM hooks**

Examples of apriori order reduction techniques:

Reduction on the fly

Any technique to generate a discrete model with reduce number of DoFs:

Examples of such techniques:

- Domain Decomposition → Hierarchical structuring
- Numeric method for discretization → FIT, dFIT, dELOB
- Appropriate grid or mesh → Yee type for Manhattan geometries, local adapted grids
- Macro(cells)-models → Frequency dependent Hodge operators, FredHo for skin effect
- Equation sparsification → Algebraic Sparsified (ASPEEC), Hierarchical Substrate Struct. (HSS)
- Terminals reduction → Identification of optimal hooks

Aposteriori Reduction Order Methods and model realization

Any post-processing to generate a reduced circuit model:

Examples of aposteriori order reduction techniques:

- **State space projection methods** → **Krylov type, e.g. PvL, PRIMA, Proper Orthogonal Decomposition POD - SVD**
- **Truncate SS systems realizations** → **Hankel norm - Truncate balance realizations (TBR)**
- **Branches/nodes removing** → **Graph-based reduction (e.g. TICER)**
- **Interpolation or fitting in the frequency domain, rational approxomations** → **Vector Fitting (VF)**
- **Spice circuit synthesis** → **Differential Equation Macromodel (DEM) in time domain and Direct Stamping Macromodel (DSM) in frequency domain**
- **Parametric Model Order Reduction** → **Parametric pmTBA**

All Levels Reduced Order Modeling

Principle: reduction have to be applied as early as possible !
Steps of the Algorithm:

- Domain decomposition
  - 3D Grid (mesh) calibration with dFIT
  - Virtual Boundary Calibration with dELOB
  - 3D Frequency Analysis by AFS
  - Extr. of par. red. model by VF

Model extraction

Apriori order reduction

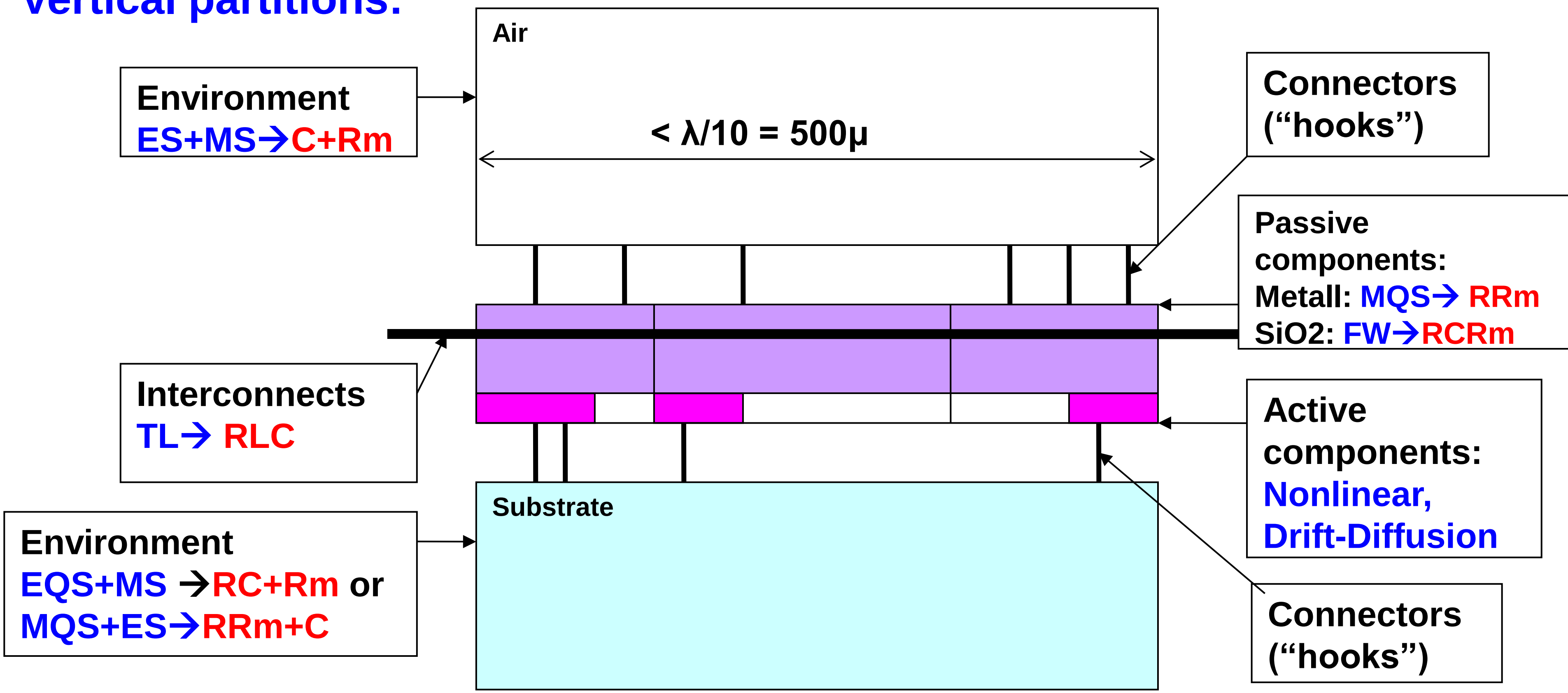
On the fly order reduction

Aposteriori order reduction

- Integration of compact parasitic extracted model into design and standard/variability (e.g. Monte Carlo) SPICE simulation

Multiphysics MOR by Domain Partitioning (DP) with several EM field regimes of ICs

Vertical partitions:



Horizontal partitions: 2D sub-domains – circuit components, according to the design schematic.

Each subdomain has its own EM field regime and a reduced MEEC

Domain Decomposition versus Partitioning (DD vs DP)

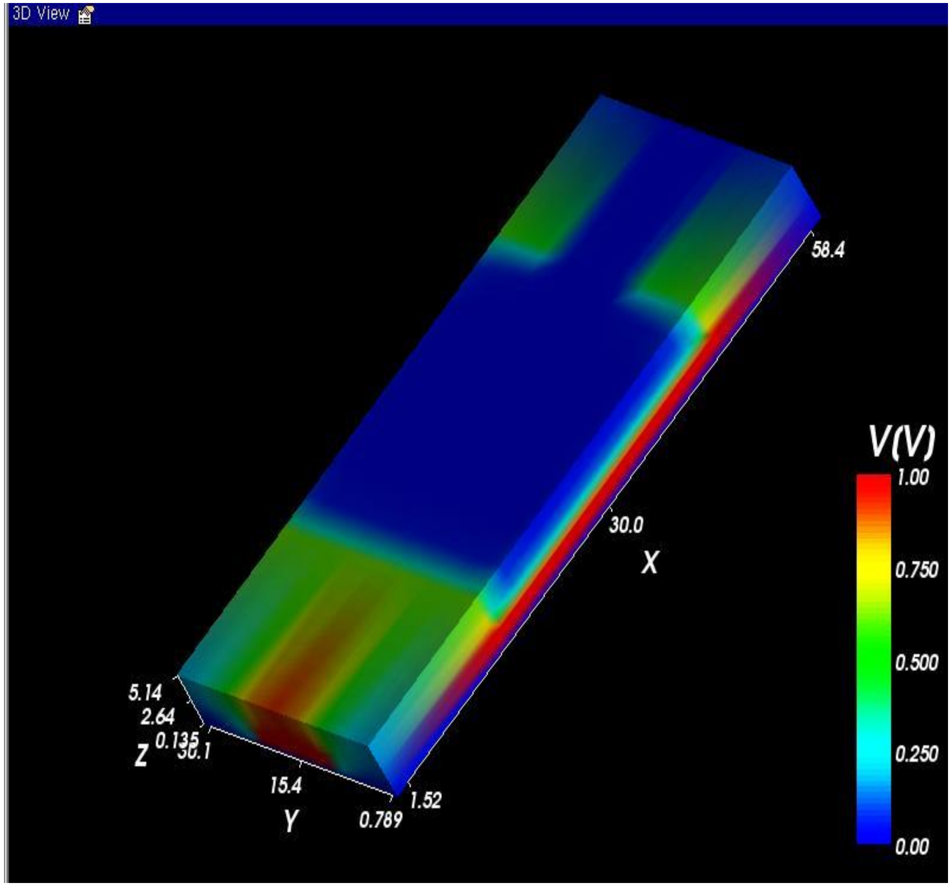
• The hooks technique has practical importance when their number is low (e.g. <10-100)

• In this case the extracted models are reduced (by using: frequency dependent circuit functions Y, state matrices ABCD, or reduced order Spice circuits) and then interconnected in the global model of IC. Thus the hierarchical structure is preserved

• Unlike DD, which is basically an iterative process, the proposed approach we call Domain Partitioning (DP) is a “direct” one

• The challenge to reduce the number of hooks has to be accepted, otherwise, the EM field modeling in nowadays RF-ICs is insolvable

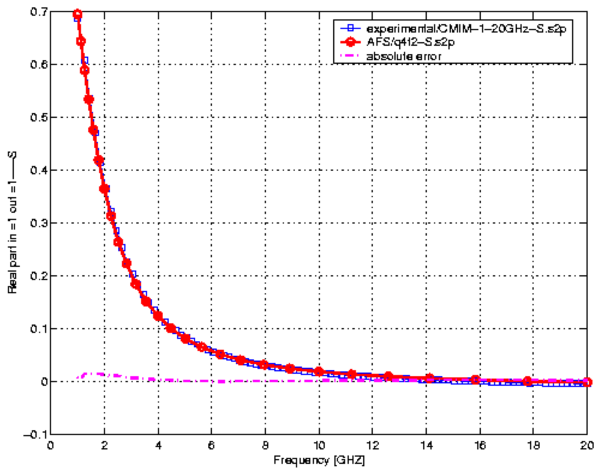
Example of reduction: CMIM - Benchmark

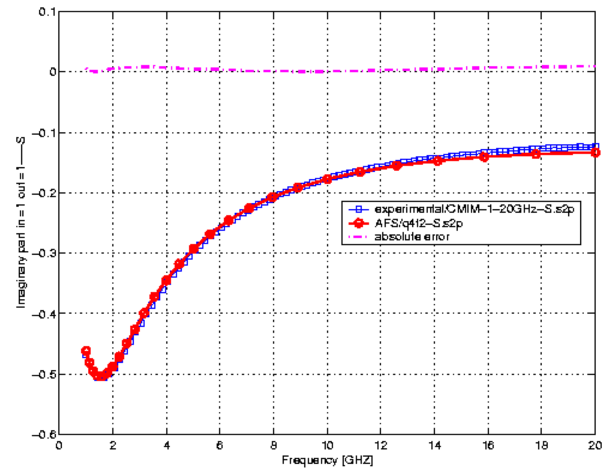


Voltage distribution over insulator

- Nodes of initial mesh = 833,280
- Initial no. of DOFs = 4,999,680
- Macromodel order n = 29,925
- ROM order q = 4
- Stable model
- ROM CPU Time = 0.1 s
- RMS $||S_s\text{-}S_R||_F$ = 0.2 %
- for 1-20 GHz

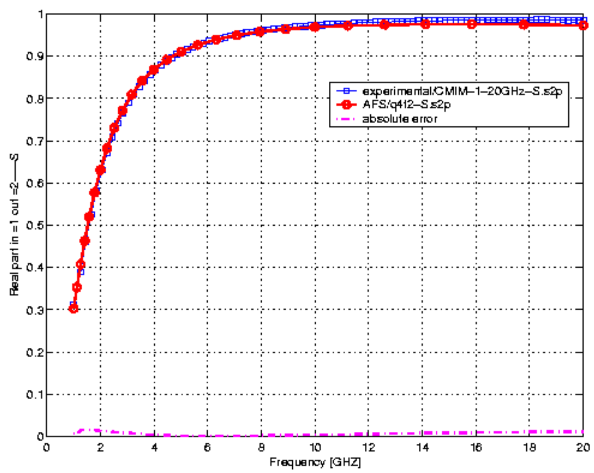
CMIM - measurement vs. reduced

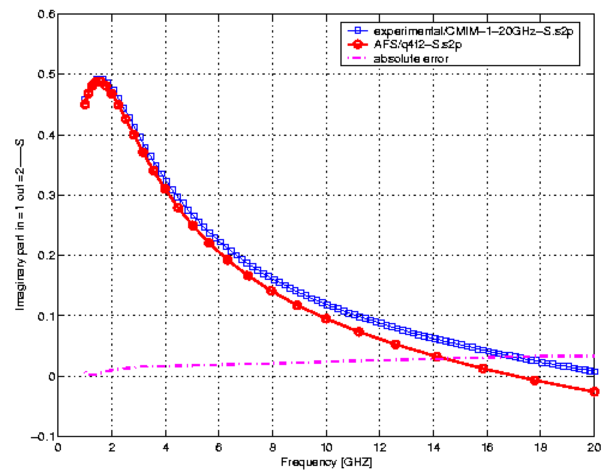




* **Rel.err (sim,red) =**

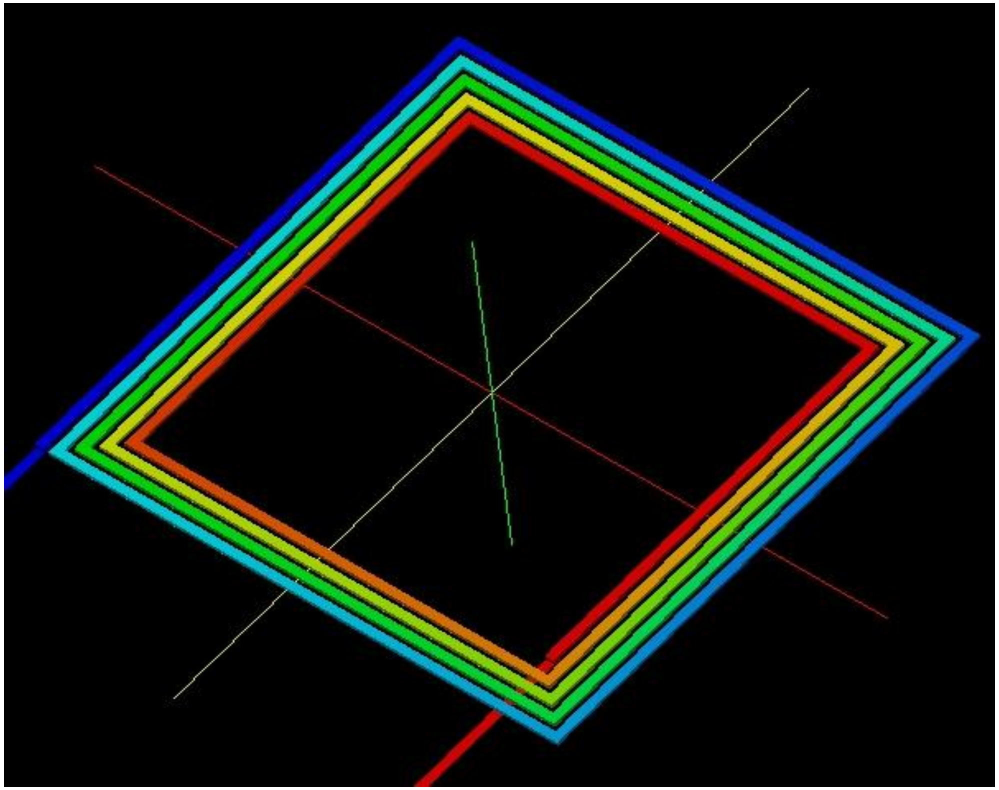
0.2 %





* **Rel.err (mas,red) = 3.75 %**

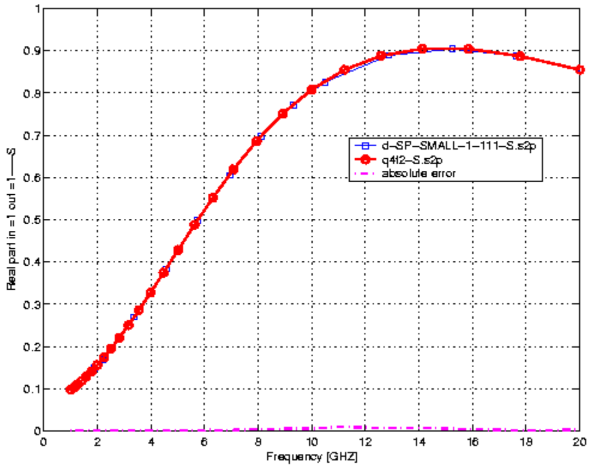
Example of reduction: SP_SMALL - benchmark

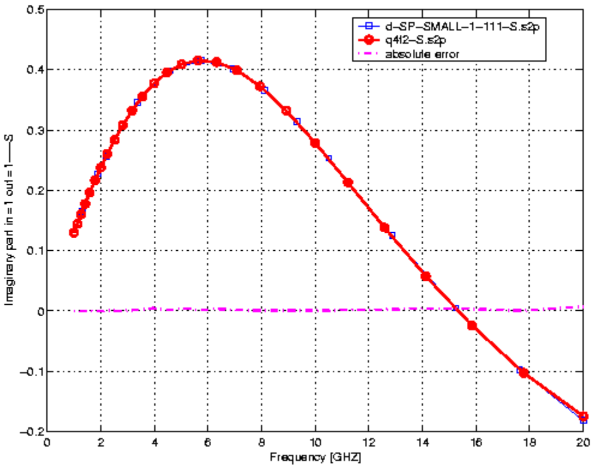


Static voltage

- Nodes of initial mesh = 596,068
- Initial no. of DOFs = 14,850,240
- Macromodel order n = 9,614
- ROM order q = 4
- Stable model
- ROM CPU Time = 0.1 s
- RMS $||S_s\text{-}S_R||_F$ = 0.5 %
- for 1-20 GHz

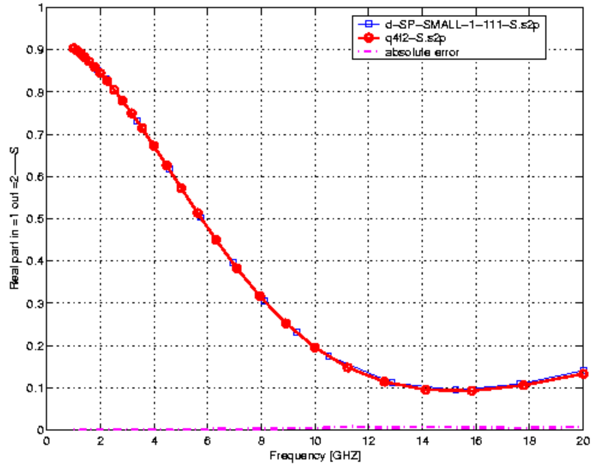
SP_SMALL - reduced model, order q = 4

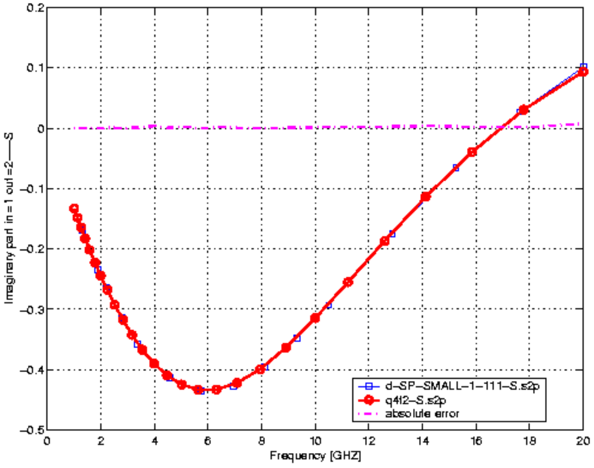




* Rel.err (sim,red) =

0.5 %





Outline

- Introduction
- Modeling procedure
- Multiphysics basics
- Coupled problems
- Complexity reduction
- **Conclusions**

Conclusions 1

- **ACES** (Analytic-Computational-Experimental solutions) is a research methodology based on **TES** (Theory-Experiment-Simulation) triangle, which have their vertices placed in the three worlds: real, ideas and virtual.
- **Scientific Modeling** is a seven step procedure. In each step is generated sequentially a special kind of model: conceptual, mathematical, analytical, numerical, computational, reduced and experimental model.
- **Multiphysics** means a coupled problem with different fields (equations, disciplines), scales and/or domains. **The attributes** of a multiphysics problem are: number of physical fields, number of scales and number of domains.
- The "**coupling**" is a more relevant term than "**multiphysics**". It is defined by the coupling graphs. The solution of the source problem is post-processed to obtain the output data in a format compatible with the input data of the destination problem: shape and/or size of the computational domain, material characteristics, input and output sources (boundary conditions), initial condition.

Conclusions 2

- ‘Gauss-Seidel, Jacobi and Newton are the possible **algebraic prototypes** of coupled problem solving. According to the problem type, the basic multiphysics **solving strategies** are: Multi-field, Multi-domain, Field-circuits and Multi-scale couplings. They have several prototype algorithms, such as: Domain Decomposition (DD), Multigrid (MG), Fast Multipole Method (FMM), Adaptive Mesh Refinement (AMR) and many others.
- Multiphysics is related to large, complex problems. Their solving requires use of **HPC techniques** (such as NKS: Newton–Krylov–Schwarz).
- **Strong - weak** is about intrinsic coupling of physical models. **Tight - loose** coupling is related to the synchronization of computational models in their parallel storage.
- **Model reduction** means reduction of the model **complexity** (e.g. by discretization, PDE are transformed in DAE or ODE or extraction of a circuit model) and in particular **MOR**. meaning the reduction of the size of state space. It can be done apriori, on the fly and aposteriori, based on physical and/or mathematical considerations.
- In the modeling procedure, **any reduction technique is recommended to be applied as early as possible**.

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