Model Order Reduction and Uncertainty Quantification for Complex Biomedical Systems

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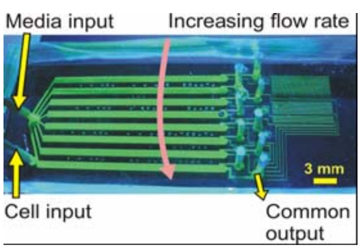
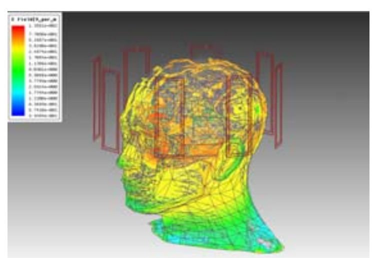
J. Villena


A. Polimeridis

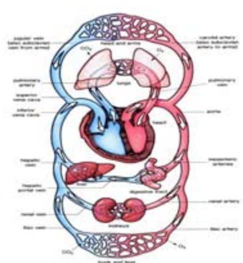
Main Trend: Interdisciplinary Analysis, Design, Diagnosis and Optimization of Complex Biomedical Systems



Nano-fluidic Channels
(Voldman, Han, MIT)



MRI scanners



Blood delivery network

Biomedical Implanted Lab-on-chip

e.g. for monitoring of glucose level in the blood

Body-Area Clothing Network
(Chandrakasan, MIT)

Trend: Typical Development/Analysis Flow for Complex Biomedical Systems is Hierarchical

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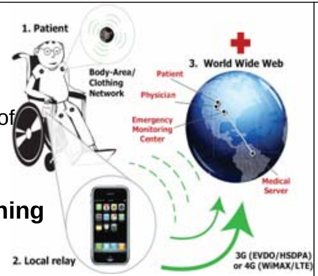
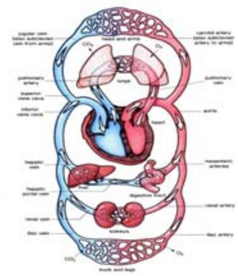
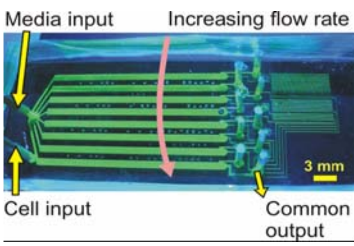
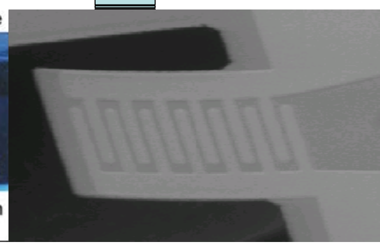




Entire Cardiovascular System

e.g. for non-invasive diagnoses, (Simakov Moscow State)





Nano-fluidic Channels
(Voldman, Han, MIT)

Energy Harvesting MEMs
(Kim, Lang MIT)

Arterial Bifurcation
(Vassilevski, INM; Olshanskii U. Houston)

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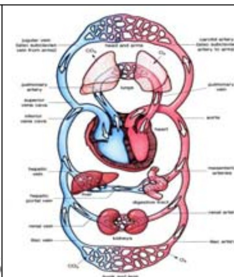

Entire Cardiovascular System

e.g. for non-invasive diagnoses, (Simakov, Moscow State)

$$\rho\left(u_t + (u \cdot \nabla)u\right) = -\nabla P + \mu \nabla^2 u + f$$

$$\rho A \frac{\partial^2 u}{\partial t^2} - bA \frac{\partial^3 u}{\partial t \partial x^2} - YA \frac{\partial^2 u}{\partial x^2} = \frac{\partial f}{\partial x}$$

Step 1: Develop efficient PDE solvers for emerging technologies

"Component" Designs

Nano-fluidic Channels
(Voldman, Han, MIT)

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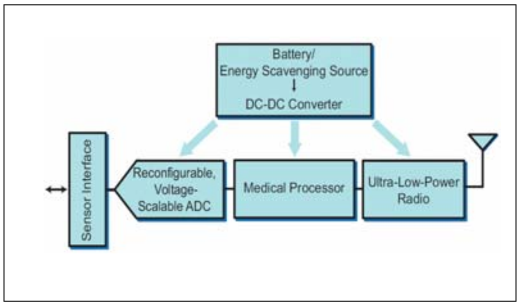

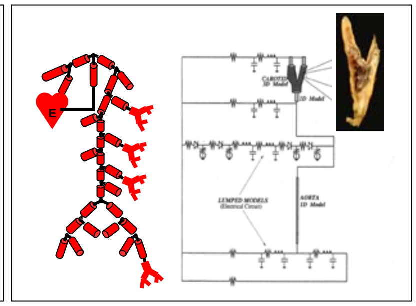

Step 2: Develop techniques that generate compact dynamical models automatically from PDE solvers and from component measurements

Step 1: Develop efficient PDE solvers for emerging technologies

"Component" Designs

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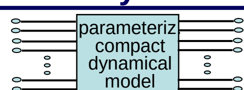
Trend: Typical Development/Analysis Flow for Complex Biomedical Systems is Hierarchical

- automatically
- with field solver accuracy
- small (only 10-15 Eqns.)
- geometrically parameterized

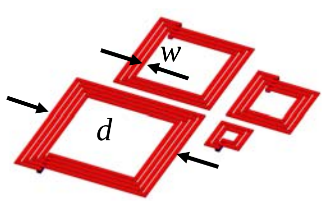


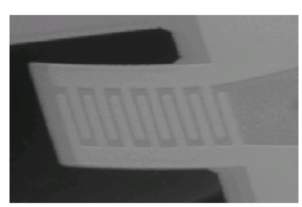
Step 2. Parameterized Model Order Reduction

$$\frac{dx}{dt} = \left[A(w,h,d) \right] \left[x(t) \right] + \left[B \right] u(t)$$

(1 Million Eqns)

Step 1. from Field Solvers "guts"





Background: the Standard Projection Framework (graphically)

$$\underbrace{V^T}_{qxn}\underbrace{V}_{nxq}\frac{d\hat{x}}{dt} = \underbrace{V^T}_{qxn}\underbrace{A}_{nxn}\underbrace{V}_{nxq}\hat{x}+V^T bu$$

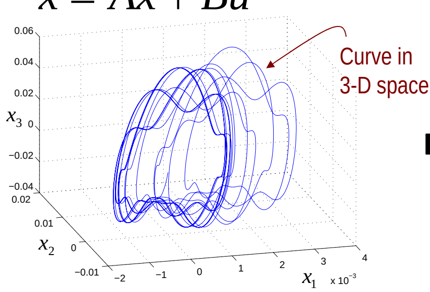
orthonormal projection

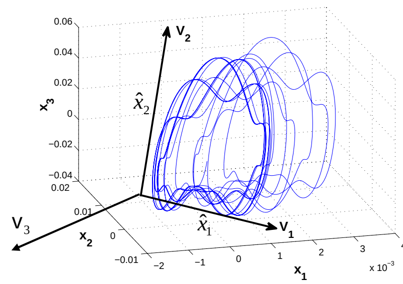
$$\frac{d\hat{x}}{dt} = \underbrace{\boxed{\hat{A}}}_{qxq}\hat{x}(t)+\hat{b}u(t)$$

Key Question: how do you choose V?

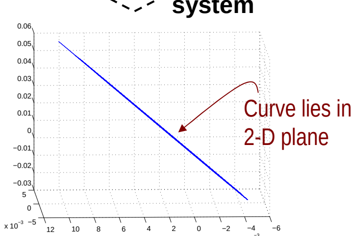
How to choose V?

$$\dot{x} = Ax + Bu$$





Rotate coordinate system



Projection: Rotation + Truncation

$$x \approx V \hat{x}$$

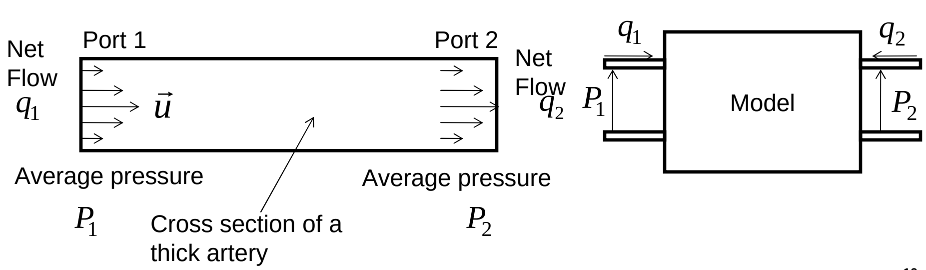
Step 2: Automated Compact Dynamical Modeling for LINEAR Systems

	Basic Technique	
TBR, Hankel	Moore 81 Glover 84	Control/Systems
POD, KL, PCA, SVD	Wilcox Peraire91, PMTBR04	Mechanical Aero/Astro Statistics, E.D.A.
Moment, Matching	AWE90, PVL Felmann94 Rutishauser55	E.D.A. Num Linear Algebra

All can be seen as a projection framework with different choices of V

Example : Cardiovascular Modeling

- **Model of Artery flow relates the average pressure and net flow at the ends of the section (ports).**

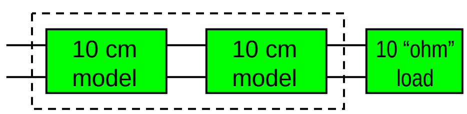


Step 2: Automated Compact Dynamical Modeling for LINEAR Systems

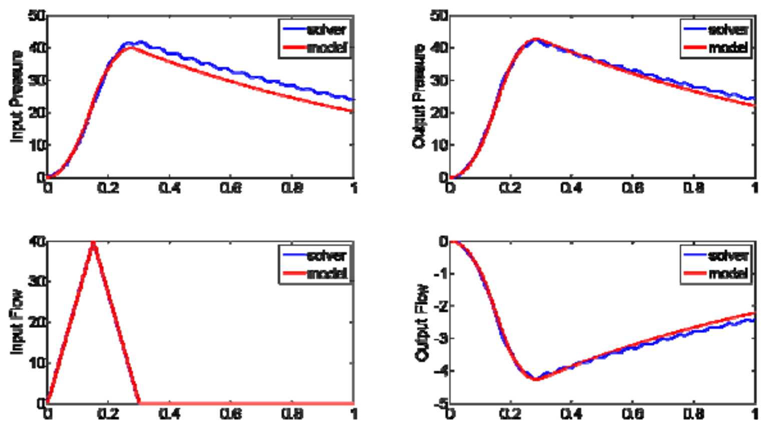
	Basic Technique	Stability/ Passivity
TBR, Hankel	Moore 81 Glover 84	Phillips Daniel02, Wong04
POD, KL, PCA, SVD	Wilcox Peraire91, PMTBR04	Bond Daniel ICCAD08 indefinite $E, A+A^T$
Moment, Matching	AWE90, PVL Felmann94 Rutishauser55	PRIMA97 only if $E>0$, $A+A^T<0$ Bond Daniel ICCAD08 indefinite $E, A+A^T$

Examples (11): Cardiovascular Modeling (4)

- **Generate linear model for straight segment of length 10cm.**



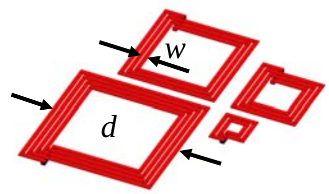
- **Compare against solver results for a 20cm segment**



Results joint with Tarek El Moselhy, MIT

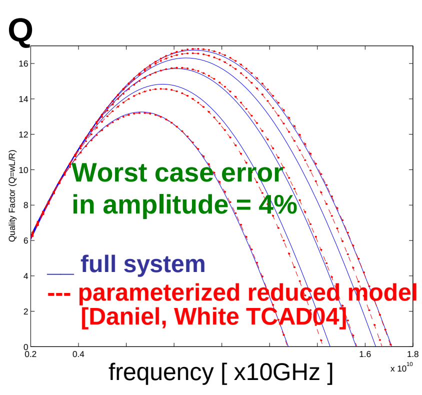
Step 2: Automated Compact Dynamical Modeling for LINEAR Systems

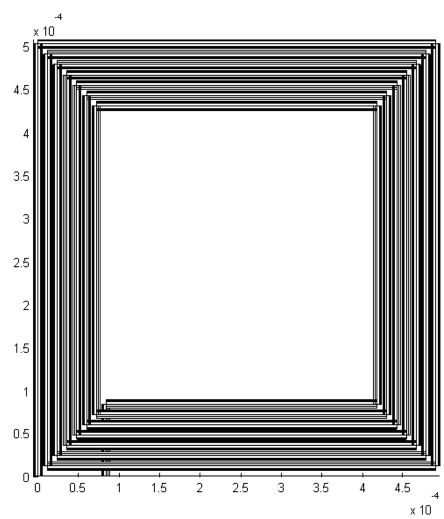
	Basic Technique	Stability/ Passivity	Parameters/ Variations
TBR, Hankel	Moore 81 Glover 84	Phillips Daniel02, Wong04	Heydari01
POD, KL, PCA, SVD	Wilcox Peraire91, PMTBR04	Bond Daniel ICCAD08 indefinite $E, A+A^T$	Phillips04
Moment, Matching	AWE90, PVL Felmann94 Rutishauser55	PRIMA97 only if $E>0$, $A+A^T<0$ Bond Daniel ICCAD08 indefinite $E, A+A^T$	one-param, Weile99 Multi-param Daniel04, Statistical Moselhy Daniel10



Example of Parameterized Model Order Reduction for an RF inductor

Wire separation = 1,2,3,4,5um





Ref: Daniel, Ong, Low, Lee, White, "A Multiparameter Moment Matching Model Reduction Approach for Generating Geometrically Parameterized Interconnect Performance Models", IEEE Trans on CAD, May 2004.

Step 2: Automated Compact Dynamical Modeling for NON-LINEAR Systems

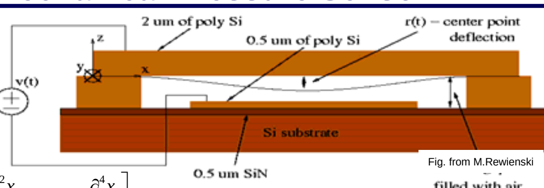
				Non-Linear Systems		
	Basic Technique	Stability/ Passivity	Parameters/ Variations	Basic Technique	Stability/ Passivity	Parameter/ Variations
TBR, Hankel	Moore 81 Glover 84	Phillips Daniel02, Wong04	Heydari01	TBR-TPWL Vasilyev03		
POD, KL, PCA, SVD	Wilcox Peraire91, PMTBR04	Bond Daniel ICCAD08 indefinite $E, A+A^T$	Phillips04	Wilcox Peraire99	Stable-TPWL Bond Daniel ICCAD07, TCAD09	Parameter-TPWL Bond Daniel ICCAD05, TCAD07
Moment, Matching	AWE90, PVL Felmann94 Rutishauser55	PRIMA97 only if $E>0$, $A+A^T<0$ Bond Daniel ICCAD08 indefinite $E, A+A^T$	one-param, Weile99 Multi-param Daniel04, Statistical Moselhy Daniel10	Quadratic Chen00, TPWL01, PWP03, NORM03		

Example of PMOR of a Nonlinear System: Micro-Electro-Mechanical Pressure Sensor

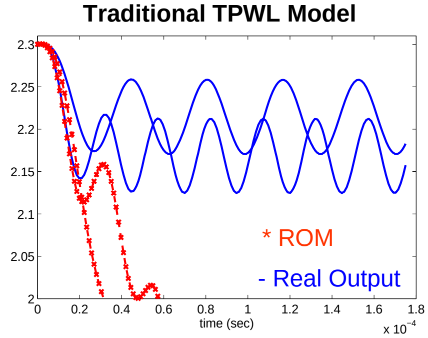
$$\frac{dx_1}{dt} = \frac{x_2}{3x_1^3}$$

$$\frac{dx_3}{dt} = -\frac{x_2 x_3}{3x_1^3} + \frac{1}{12\mu x_1}\nabla\left[\left(1+6\frac{\lambda}{x_1}\right)x_1^3 x_3 \nabla x_3\right]$$

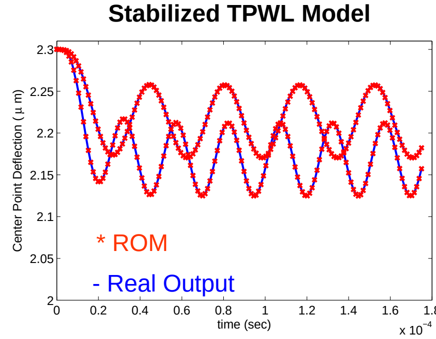
$$\frac{dx_2}{dt} = \frac{2x_2^2}{3x_1^3} - \frac{3\varepsilon_0}{2\rho_0 h}v^2 + \frac{3x_1^3}{\rho_0 h w}\left[\int_0^w (x_3 - p_a)dy + S_0 h w\frac{\partial^2 x_1}{\partial x^2} - E I_0 h^3 w \frac{\partial^4 x_1}{\partial x^4}\right]$$



Traditional TPWL Model

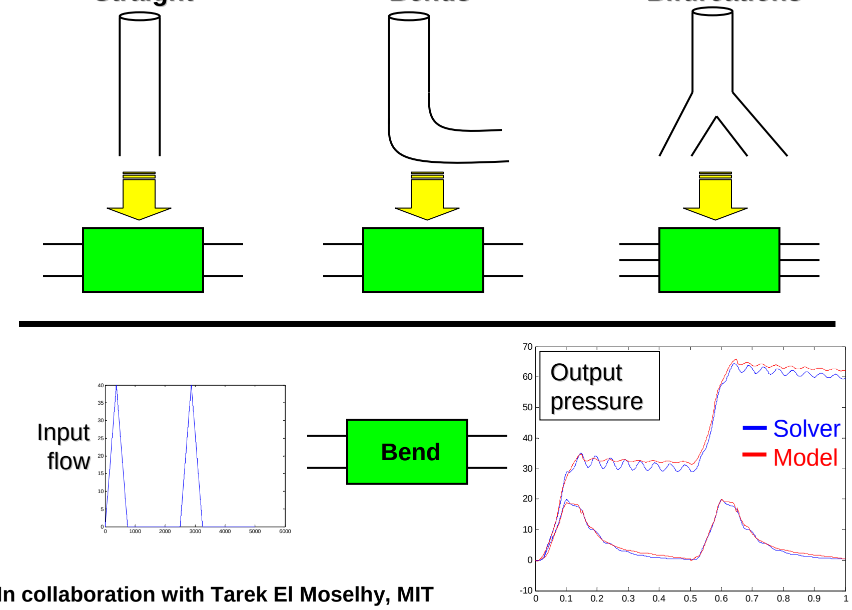


Stabilized TPWL Model



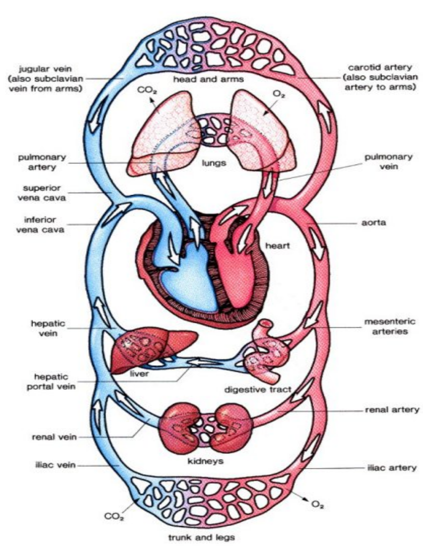
Reference: Bond, Daniel, "Stable Macromodels for Nonlinear Descriptor Systems through Piecewise-Linear Approximation and Projection", IEEE Trans on CAD, Oct 2009.

Examples (9): Cardiovascular Modeling (2)

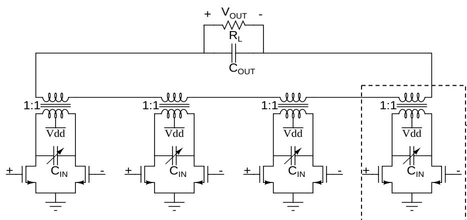


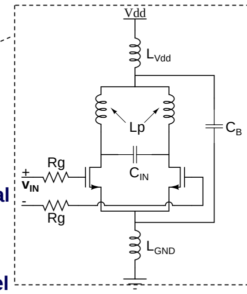
In collaboration with Tarek El Moselhy, MIT

Example of Cardiovascular system



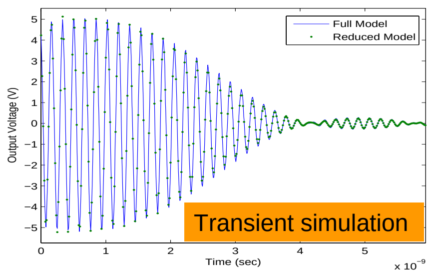
Example of analysis of Electronic Complex System with PMOR: e.g. RF or mm-wave distributed amplifier [Bond, Mahmood, Daniel 10]

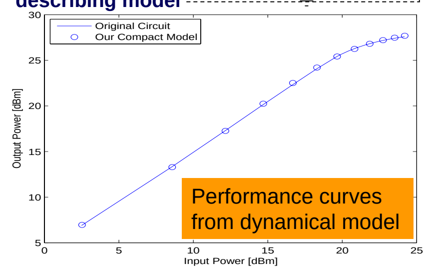




$$y_t = \frac{p_3(y_{t-1}, w_t, w_{t-1}, u_t, u_{t-1})}{q_4(y_{t-1}, w_t, w_{t-1}, u_t, u_{t-1})}$$

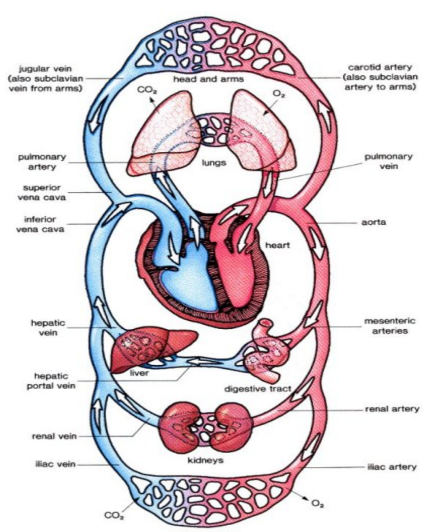
- **Identified rational model with feedback**
- **106 coefficients describing model**





Reference: Bond, Mahmood, Sredojevic, Li, Megretski, Stojanovic, Avniel, Daniel, "Compact Stable Modeling of Nonlinear Analog Circuits using System Identification via Semi-Definite Programming and Robustness Certification," IEEE Trans. on CAD, Sep. 2010

Need Uncertainty Quantification Tools (i.e. Stochastic Field Solvers) for Complex Systems in Bio-Medical Engineering



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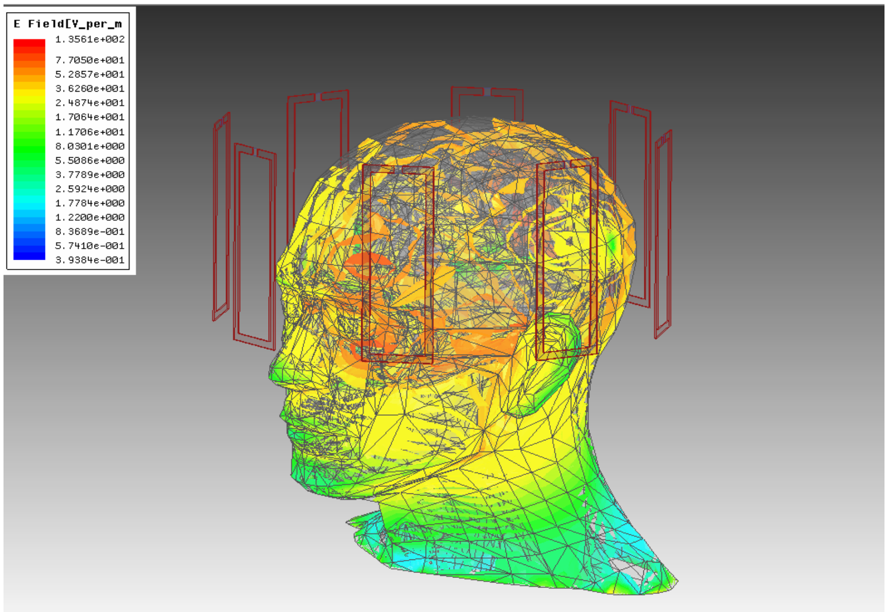


General Background for all Field Solvers

All Field solvers transform some form of the PDE into a parameterized linear system

PDE form

OR

Integral form

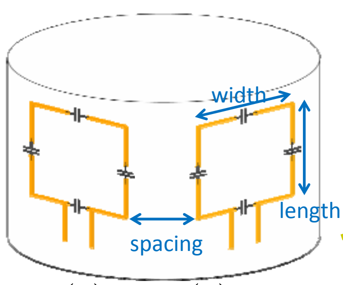
FD or FEM

BEM

$$\mathbf{A}(\mathbf{p})\mathbf{x}(\mathbf{p}) = \mathbf{b}$$

vector of parameters
- *e.g. width, length, spacing,*
- *e.g. correlation length of roughness*

X *vector of unknowns:*
- *e.g. Coil current distribution*
- *e.g. Fluid flow*
- *e.g. Surface Fields*



$$\mathbf{y}(\mathbf{p}) = \mathbf{c}^T\mathbf{x}(\mathbf{p})$$

- *e.g. arm blood pressure*
- *e.g. MRI deposited heat*

State of the Art of Sampling-Based Stochastic Solvers

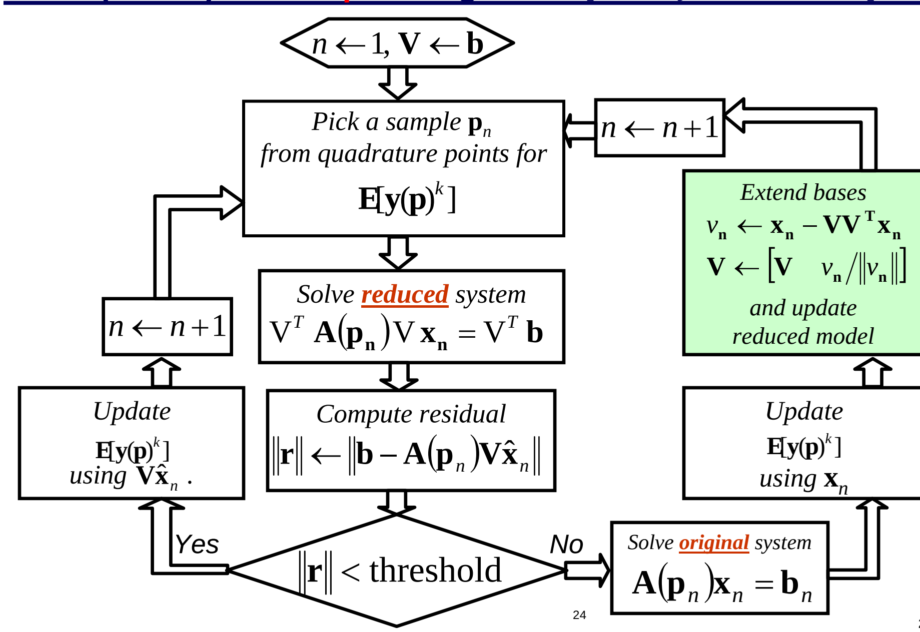
$$\mathbf{A}(\mathbf{p}_i)\mathbf{x}(\mathbf{p}_i) = \mathbf{b}$$

solve at different values in parameter space

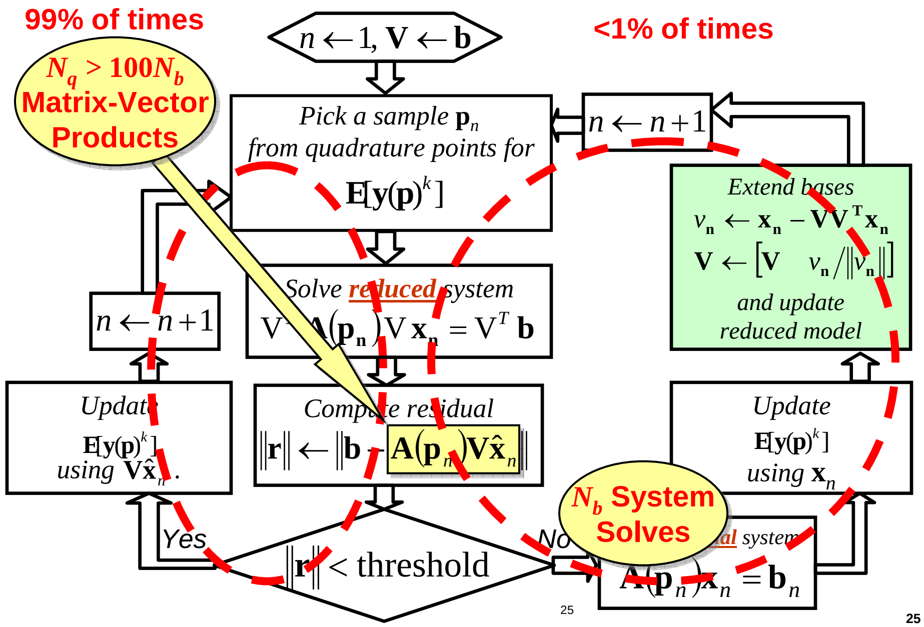
⟹ ***Challenge: very large number of system solves***

- Strategies **to sample the parameter space** effectively:
  - **Monte Carlo Method**, quite effective for more than 100 parameters
  - **Sparse Grid Stochastic Collocation Method (SCM)** [Mathelin03, H. Zhu07], speedups around 25x for small number of parameters. Not effective for more than 100 parameters (after de-correlation)
  - **Greedy Adaptive Sampling** [Prod'homme02, Veroy03, Bui-Thanh08, Villena09, Boyayal10, Moselhy Daniel10] select points of maximum residua (= proximity measure)
- Strategies **to solve the many SIMILAR systems** effectively:
  - **Parallelize**
  - **Krylov subspace recycling** [Telichevescky96, Parks SIAM J.Sci.Comput.04, Ye TCAD09], speedup less than 5x
  - **Parameterized model order reduction** (PMOR) [Variational PMTBR Phillips04, Bui-Thanh08, Villena 09, Boyayal10, Moselhy Daniel10]

Stochastic Solver via Parameterized Model Order Reduction (SMOR): an Adaptive Algorithm [Moselhy Daniel DATE10]



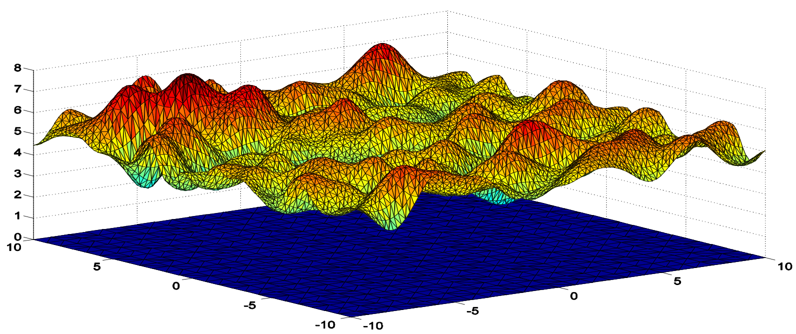
Stochastic Solver via Parameterized Model Order Reduction (SMOR): an Adaptive Algorithm [Moselhy Daniel DATE10]



Very Large 3D Example: Surface Roughness on I/O Pad

Example description:

- large square parallel place capacitor (N=21,000 discretization elements)
- with surface roughness (Gaussian, size=20x20 correlation lengths),



Ref: T. Moselhy, L. Daniel, “Variation-Aware Interconnect Extraction using Statistical Moment Preserving Model Order Reduction,” Design Automation and Test in Europe (DATE), 2010.

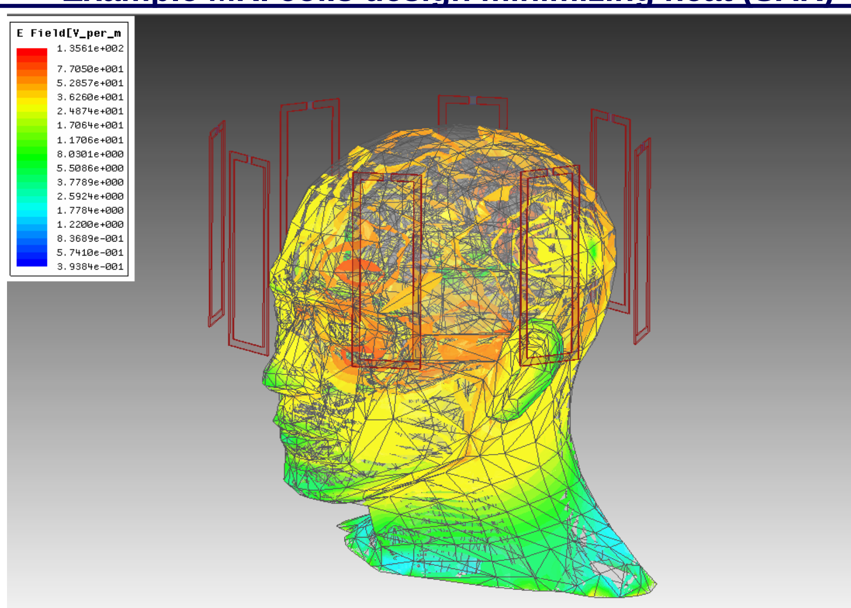
Very Large 3D Example: Surface Roughness on I/O Pad
Time & Memory Results

- MonteCarlo or Stochastic Collocation can only be estimated, since example is too large (323 uncorrelated parameters)
- All comparisons are for the same estimated 5% accuracy

Method	Time	Memory	Comments
Stochastic Collocation	(2000 hours)	5 GB	209,628 solves for 2nd order quadr.
Monte-Carlo	(150 hours)	5 GB	15,000 solves
SMOR [Moselhy Daniel10]	10 hours speedup 15x	5 GB	size reduced model: 997

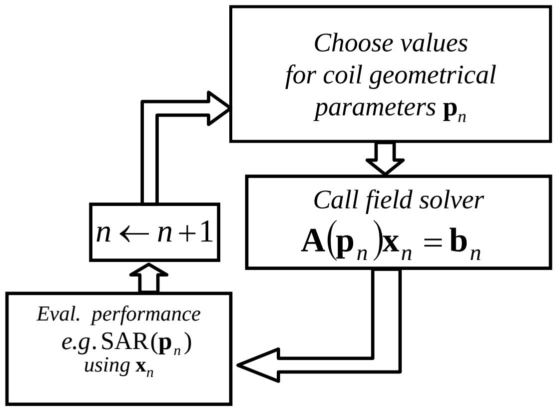
Ref: T. Moselhy, L. Daniel, "Variation-Aware Interconnect Extraction using Statistical Moment Preserving Model Order Reduction," Design Automation and Test in Europe (DATE), 2010.

Efficient Design Optimization of Complex Systems
Example MRI coils design minimizing heat (SAR)



Efficient Design Optimization of Complex Systems
Example MRI coils design minimizing heat (SAR)

Standard Optimization Loop e.g. for $\min_{p_n} \mathrm{SAR}(p_n)$



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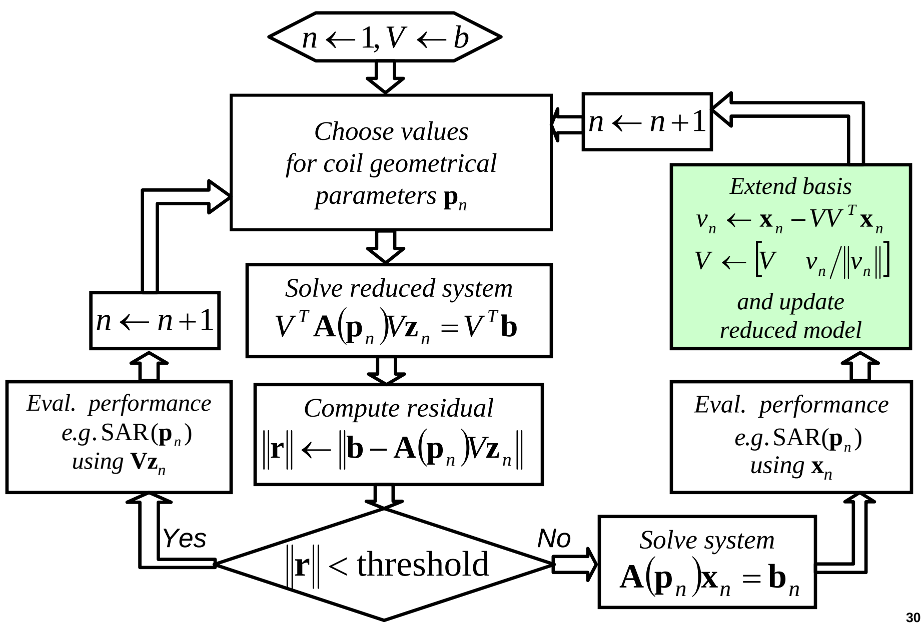

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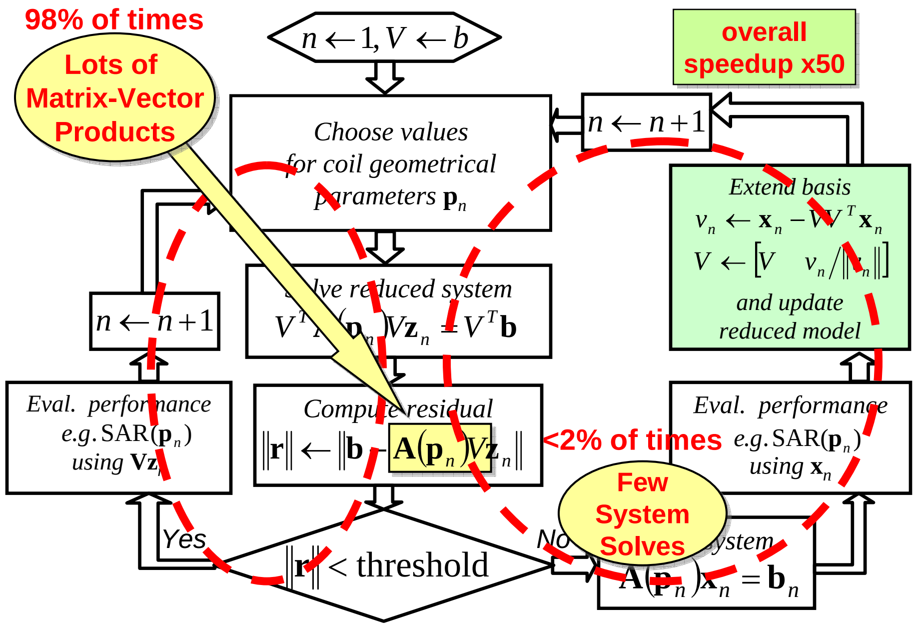


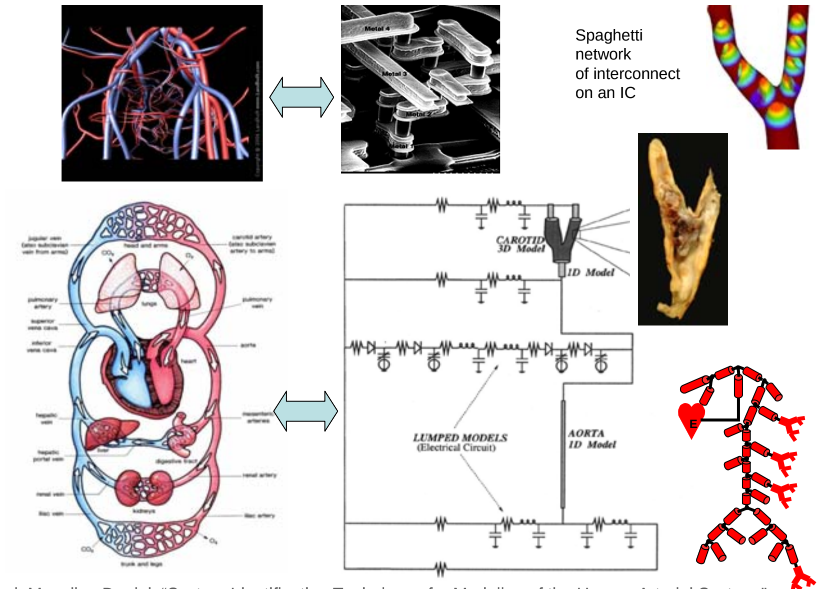
Efficient Design Optimization of Complex Systems
Example MRI coils design minimizing heat (SAR)

	SAR computation	coil optimization
SemCad (time domain approach)	**15h, 0.5GG**	**not feasible...**
HFSS (FEM frequency domain)	**12h, 250GB for S-matrix**	**not feasible...**
Developing new Field Solvers [Polimeridis, Villena, Hochman, White, Daniel12]	35h 8cores offline +15sec 9GB +800GB	**~ 4 conf/min**
Combined optimization loop with "on-demand construction" of Parameterized Reduced Model [Mahmood, Villena, Daniel expected 2014]		**~ 200 conf/min**

Efficient Characterization of Complex Systems
E.g.: Diagnosis of Cardiovascular Diseases

Spaghetti network of arteries and veins

Spaghetti network of interconnect on an IC



Reference: Bond, Moselhy, Daniel, "System Identification Techniques for Modeling of the Human Arterial System," SIAM Conference on the Life Sciences, Pittsburgh, PA, July 2010. (Invited Paper)

Conclusions
State of the Art and Trends in Complex Systems

- **Main Trend: be able to "handle" complex systems**
  - i.e. biomedical systems of interconnected dynamical components
  - hierarchical design/analysis flow.
- **Step1: Need effective PDE solvers to help "component" Engineers**
  - must handle uncertainty quantification
  - Result: Parameterized Model Order Reduction can accelerate any available sampling-based stochastic solver (15x-90x speedups)
- **Step2: Need Model Order Reduction to help "system" Engineers**
  - generate models automatically
  - preserve physical properties (stability, dissipativity)
  - Models can be instantiated for different values of parameters
  - Result: parameterized model order reduction can accelerate "inverse problems" on complex systems (speedups 50x)