On the Fundamental Tautology of Validating Data-Driven Models and Simulations

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International Conference on Computational Sciences 2005
Atlanta, GA USA,, 22-25 May 2005

This material is based upon work supported by the National Science Foundation under Grant No. ITR-0205663

OUTLINE

- Motivational Aspects
- Qualification Verification Validation In general
- “Embedded Validation”
- Epistemological Aspects
- Example
- Conclusions

Motivational Aspects

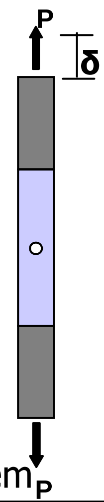
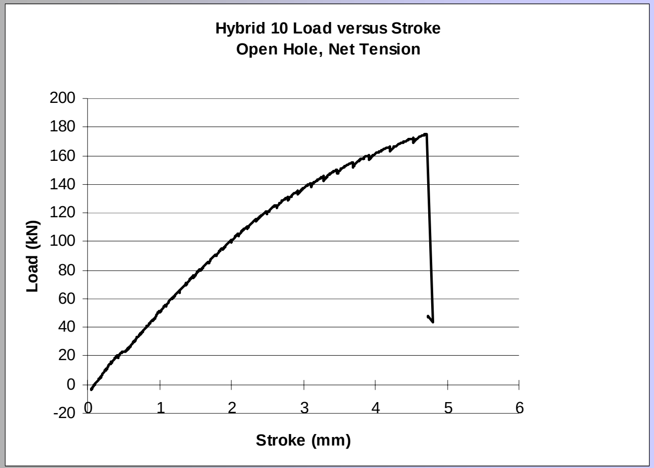
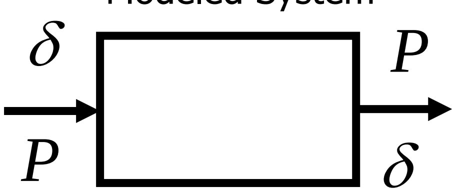
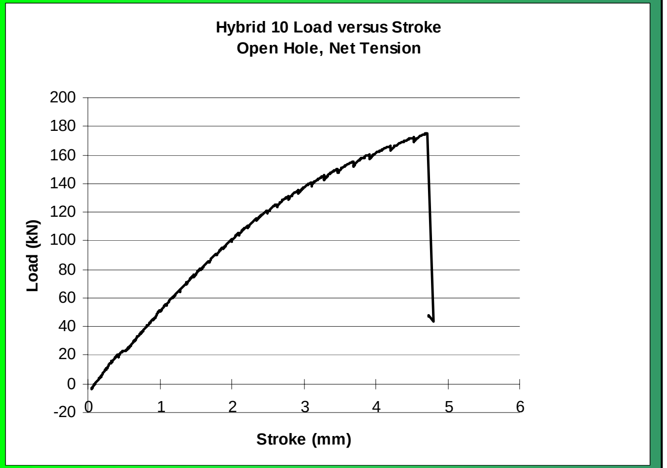
Answer Some Questions for systems where BOTH input and output are measurable:

- Are data-driven modeling and simulation practices equivalent to the non data-driven (or model driven) practices the same from the QV&V perspective?
- Do data-driven models require validation in the model-driven modeling sense?

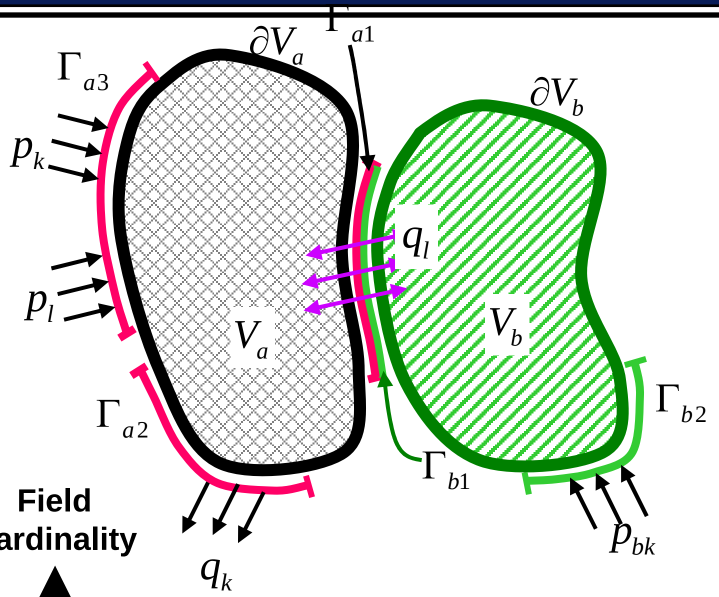
Term Definitions

- ***Modeling:*** Establishing, a conceptual (analytical, mathematical) and computational (discretization, algorithmic, programmatic, visualization) representation of the system such that its behavior is the same with that of the actual physical system.
- ***Simulation:*** Generating predictive behavior of the system through exercising the a previously established model of the system.
- ***Model-Driven:*** Modeling uses some a priori concept of how the system works from an inside-out perspective (Bottom-Up)
- ***Data-Driven:*** Modeling uses only behavioral data and ignores internal composition (Top-Down)

System-Model-Behavior

	System External Appearance	Internal Appearance	Behavior Appearance
Physical World	 Physical System		
Conceptual World	Modeled System 	$R(P,\delta)=0$ $P(\delta)$ $\delta(P)$	

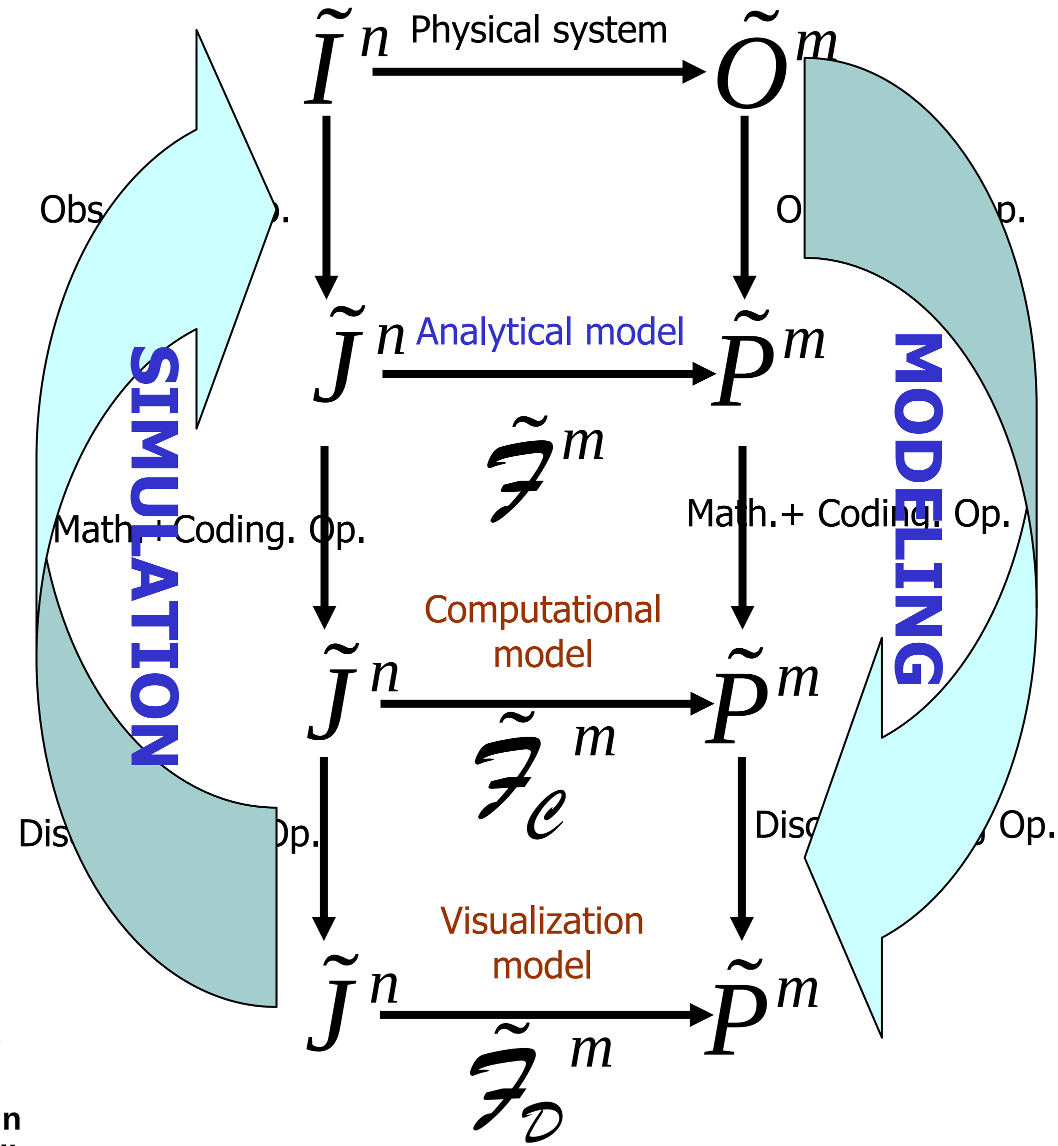
MODELING A MULTIPHYSICS SYSTEM



Field Cardinality

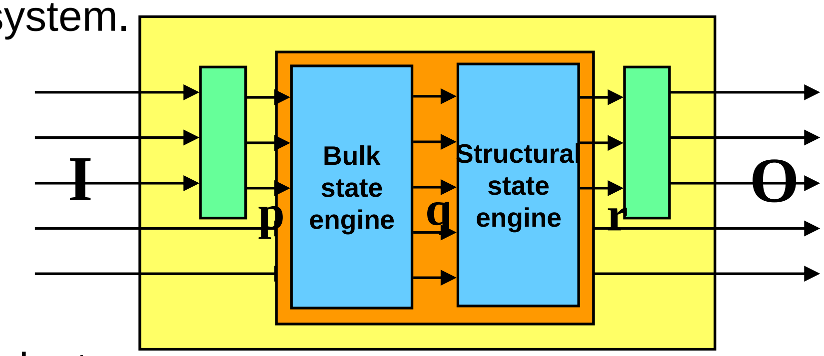
	One Domain	Multiple Domains
Multiple Fields	**Homogeneous System Multiple Fields i.e. Electro-Thermo-elastic Media**	**Multiple System Multiple Fields i.e. Thermoelastic media In Fluids**
One Field	**Homogeneous System Homogeneous Fields i.e. Deformable Media**	**Multiple System Homogeneous Fields i.e. Deformable Media In contact**

Domain Cardinality



MODELING A MULTIPHYSICS SYSTEM

$\mathcal{B} : I_n \rightarrow O_m, I_n \subset \Re_n, O_m \subset \Re_m$ ***Behavior Functional*** relating the output to the inputs of the system.



$\mathcal{R}(d, \xi, p) = 0$ ***Relational restriction*** over dependent, independent, parameter variables.

$d = \mathcal{G}(\xi, p)$

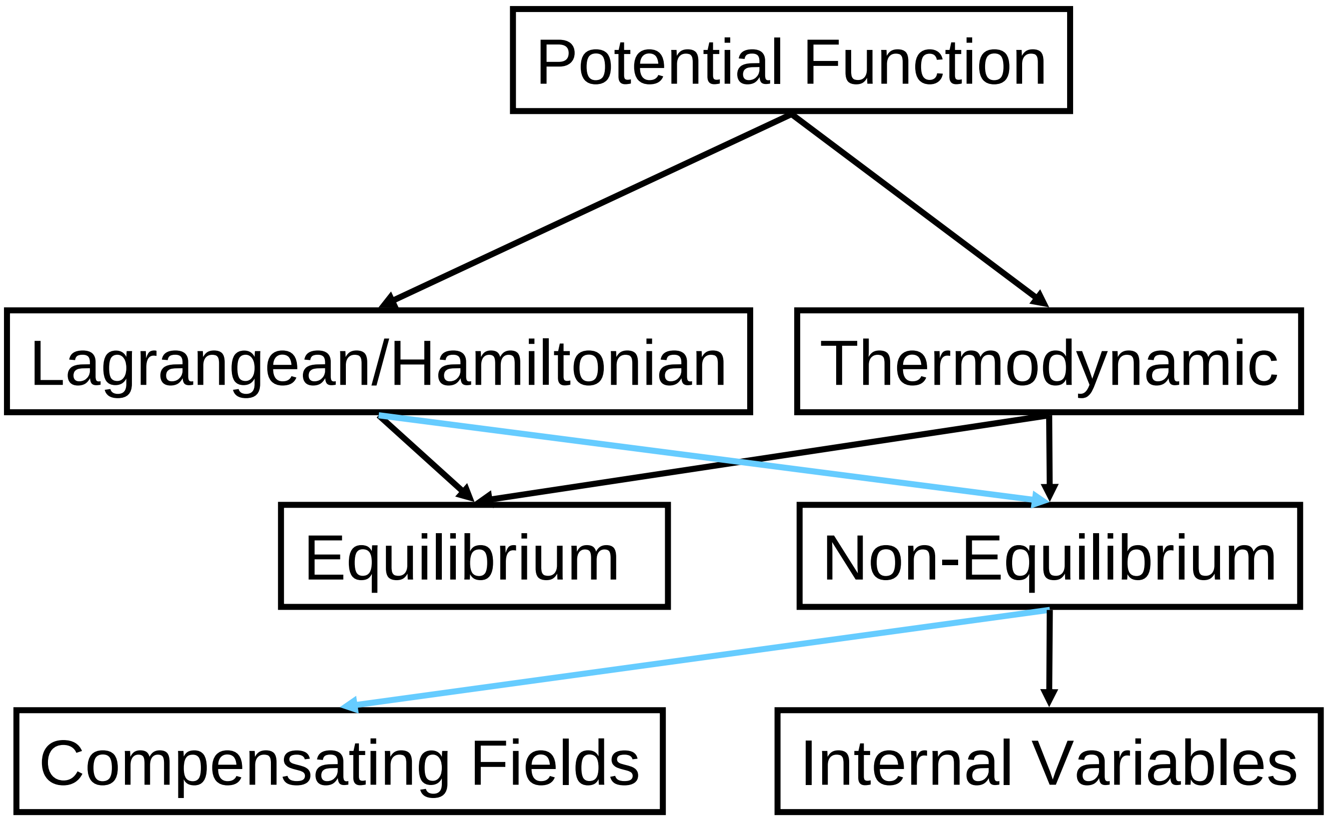
$\rho = \mathcal{G}(\xi, \varepsilon) \cdot \varepsilon$

Bulk Constitutive Relations: Functional dependence, of dependent variables on independent variables and parameters.

$\mathcal{K}^{i}(\nabla_n d, \frac{\partial t_m}{\partial_m} d, \cdots) = 0$ ***Composition Behavior through Conservation Law Relations***: Dependence, of dependent variables on position in the structure, and time.

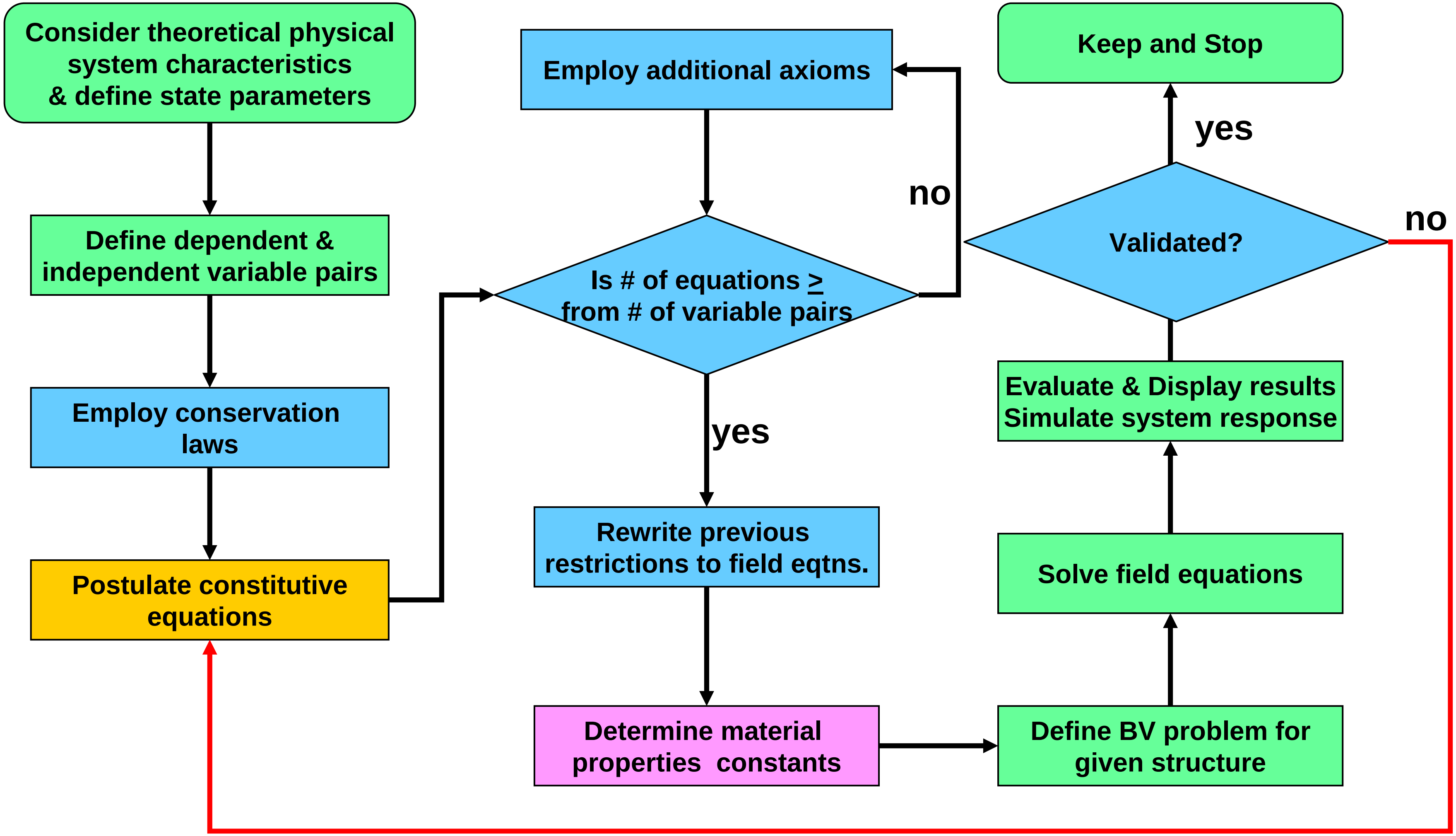
$d = \nabla^{p} \Xi(\xi, p)$ ***Vector Function Storage Mechanism:*** Potential or Energy Density function.

Methodologies for Developing Potential Functions



MODELING A MULTIPHYSICS SYSTEM

Model driven coupled field methodology



AXIOMS OF CONSTITUTIVE BEHAVIOR DERIVATION PROCESS

Axiom (I) *Causality:* The motion, temperature, electric field, and magnetic induction of the material points of a body are self-evident and observable in any thermoelectromechanical behavior of a body. The remaining quantities (other than those derivable from the motion, temperature, electric field, and magnetic induction) excluding the body force, energy supply, and free charge density that enter the balance laws and the entropy inequality, are the dependent variables.

Axiom (II) *Determinism:* The value of any dependent variable, at material point ***X*** of the body B at time t, is determined by the history of all material points of B.

Axiom (III) *Equipresence:* At the outset, all constitutive response functionals are to be considered to depend on the same list of constitutive variables, until the contrary is deduced.

Axiom (IV) *Objectivity:* The constitutive response functionals are form-invariant under arbitrary rigid motions of the spatial frame of reference and a constant shift of the origin of time.

Axiom (V) *Time Reversal:* The entropy production must be nonnegative under time reversal.

Axiom (VI) *Material Invariance:* The constitutive response functionals must be form-invariant with respect to a group of transformations of the material frame of reference {***X*** ---> ***X̲*** } and "microscopic time reversal" as {*t* ---> -*t* } representing the material symmetry conditions. These transformations must leave the density and charge at { ***X***, t } unchanged.

Axiom (VII) *Neighborhood:* The values of the response functionals at ***X*** are not affected appreciably by the values of the independent constitutive variables at distant points from ***X***.

Axiom (VIII) *Memory:* The values of the constitutive variables, at a distant past from the present, do not affect appreciably the values of the constitutive response functionals at present.

Axiom (IX) *Admissibility:* Constitutive equations must be consistent with the balance laws and the entropy inequality.

MAIN SCIENTIFIC CHALLENGES OF MODEL DRIVEN APPROACH

- Impossible Uncoupled Experiments for Coupling coefficients Determination?

  EXAMPLE: Isotropic Nonlinear Electromagnetic Solids. Two of the 20 apriori derived constitutive relations for the spatial vectors for heat and current define some of the known “effects”:

Thermal conductivity | **Peltier’s effect** | **Anisotropic Peltier’s effect** | **Righi-Leduc’s effect** | **Ettinghaussen’s effect**

$$\tilde{q} = \boxed{\kappa_1 \nabla T} + \boxed{\kappa_2 \tilde{E}} + \kappa_3 \tilde{e}^{-1} \nabla T + \boxed{\kappa_4 \tilde{e}^{-1} \tilde{E}} + \boxed{\kappa_5 \nabla T \times \tilde{B}} + \boxed{\kappa_6 \tilde{E} \times \tilde{B}}$$
$$+ \kappa_7 \tilde{e}^{-2} \nabla T + \kappa_8 \tilde{e}^{-2} \tilde{E} + \kappa_9 (\tilde{B} \cdot \nabla T) \tilde{B} + \kappa_{10} (\tilde{B} \cdot \tilde{E}) \tilde{B}$$
$$+ \kappa_{11} [\tilde{e}^{-1} (\nabla T \times \tilde{B}) - (\tilde{e}^{-1} \nabla T) \times \tilde{B}] + \kappa_{12} [\tilde{e}^{-1} (\tilde{E} \times \tilde{B}) - (\tilde{e}^{-1} \tilde{E}) \times \tilde{B}]$$

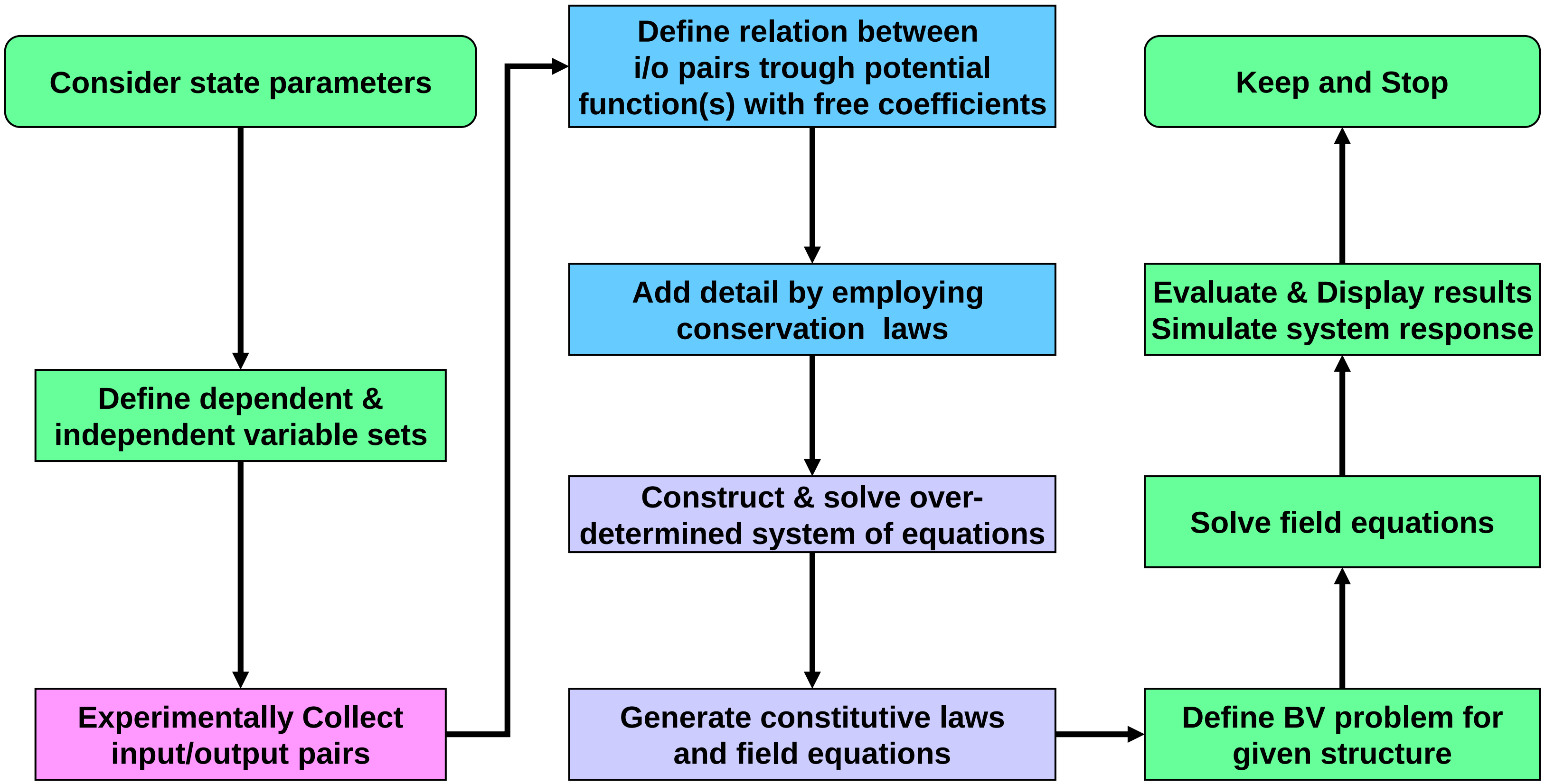
Ohm’s effect | **Seebeck’s effect** | **Anisotropic Seebeck’s effect** | **Hall’s effect** | **Nerst’s effect**

$$\tilde{J} = \boxed{\lambda_1 \tilde{E}} + \boxed{\lambda_2 \nabla T} + \lambda_3 \tilde{e}^{-1} \tilde{E} + \boxed{\lambda_4 \tilde{e}^{-1} \nabla T} + \boxed{\lambda_5 \tilde{E} \times \tilde{B}} + \boxed{\lambda_6 \nabla T \times \tilde{B}}$$
$$+ \lambda_7 \tilde{e}^{-2} \tilde{E} + \lambda_8 \tilde{e}^{-2} \nabla T + \lambda_9 (\tilde{B} \cdot \tilde{E}) \tilde{B} + \lambda_{10} (\tilde{B} \cdot \nabla T) \tilde{B}$$
$$+ \lambda_{11} [\tilde{e}^{-1} (\tilde{E} \times \tilde{B}) - (\tilde{e}^{-1} \tilde{E}) \times \tilde{B}] + \lambda_{12} [\tilde{e}^{-1} (\nabla T \times \tilde{B}) - (\tilde{e}^{-1} \nabla T) \times \tilde{B}]$$

- Potentially NON TERMINATING

MODELING A MULTIPHYSICS SYSTEM

Data driven Modeling methodology



QV&V Definitions

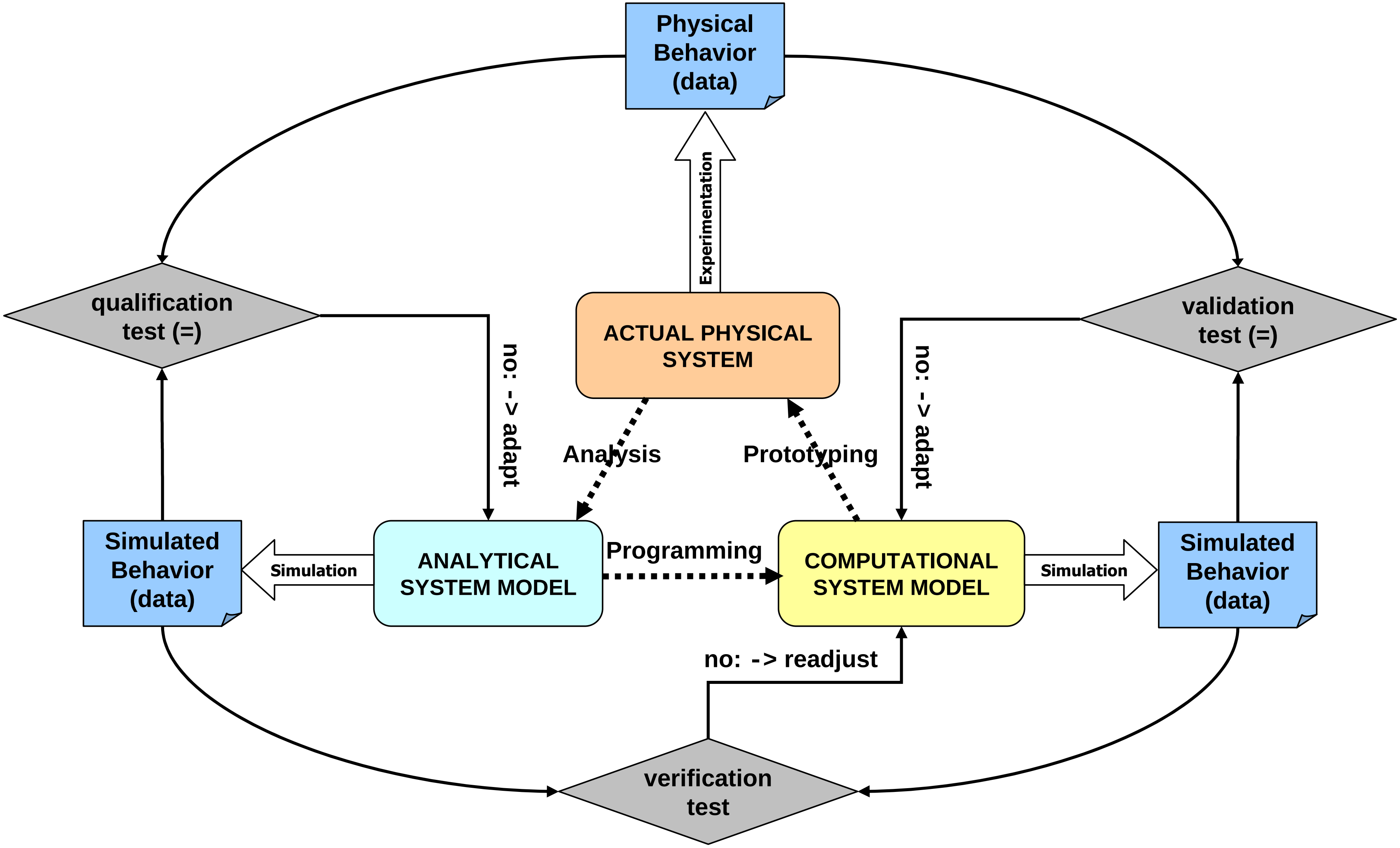
Intersecting definitions according to AIAA, DMSO, ASME, DOE/DP-ASCI

- ***Qualification:*** determination that a conceptual model implementation represents correctly a real physical system.

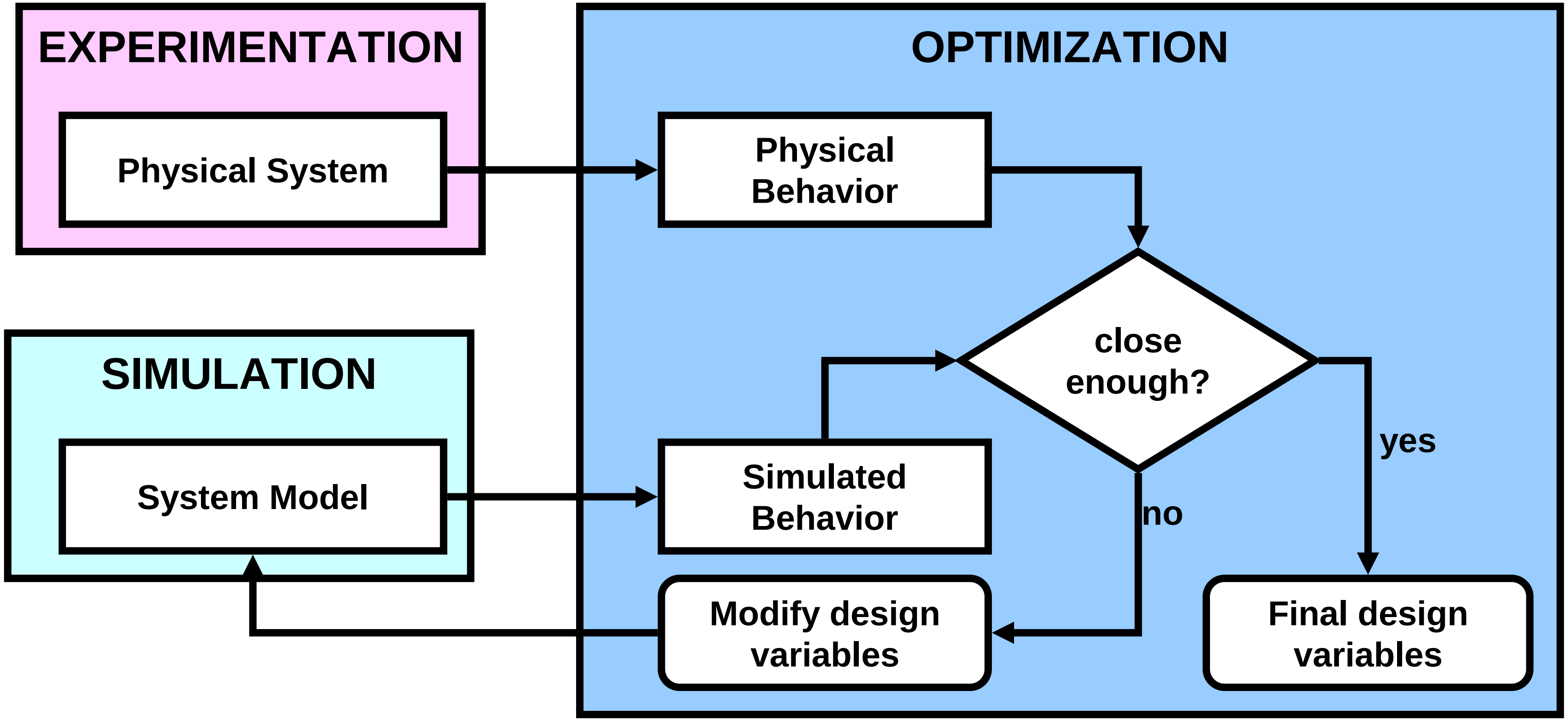
- ***Verification:*** determination that a computational model implementation represents correctly a conceptual model of the physical system.

- ***Validation:*** determination of the degree to which a computer model is an accurate representation of the real physical system from the perspective of the intended uses of the model.

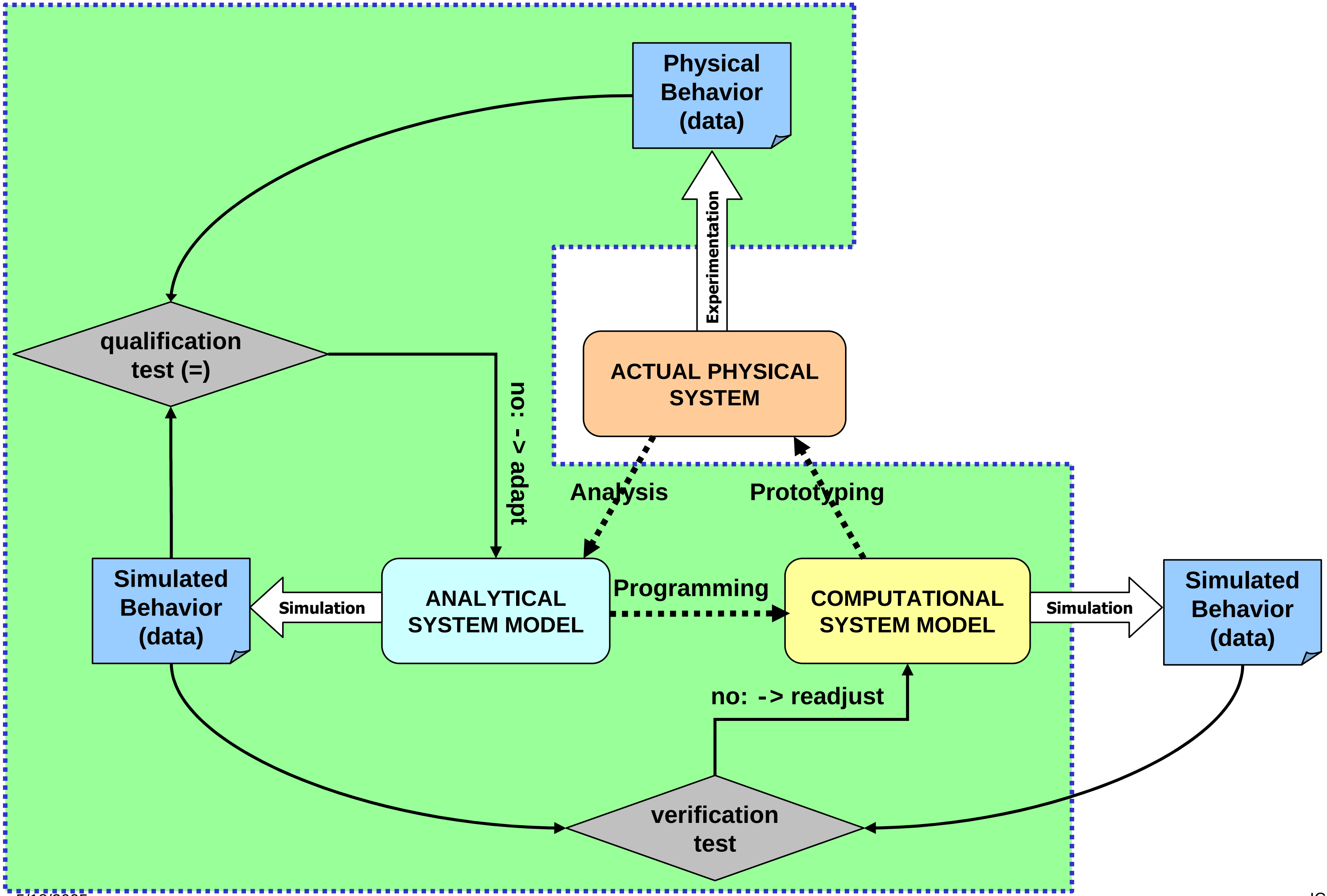
Model-Driven Approach for Q&VV



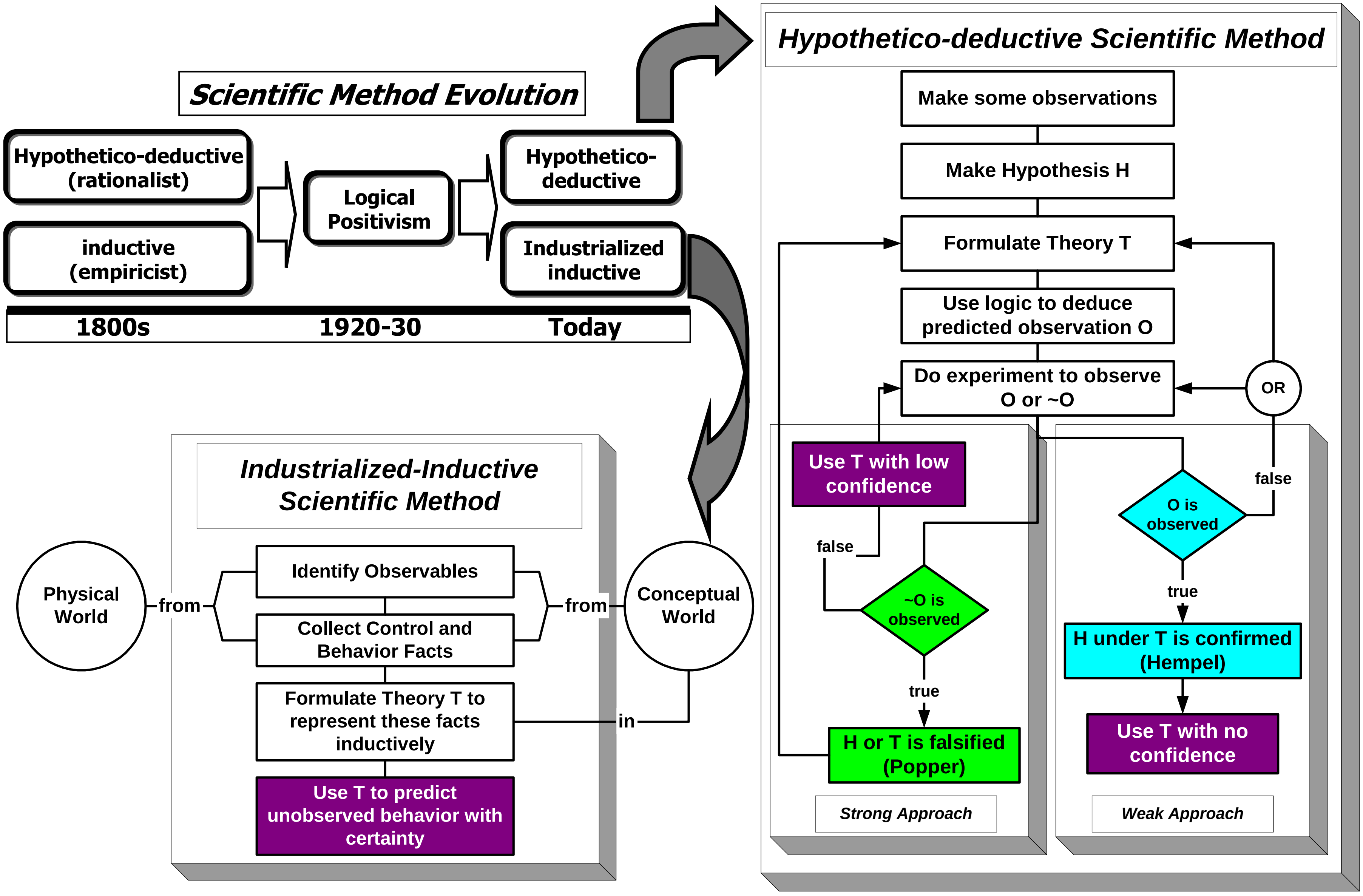
General Optimization Approach



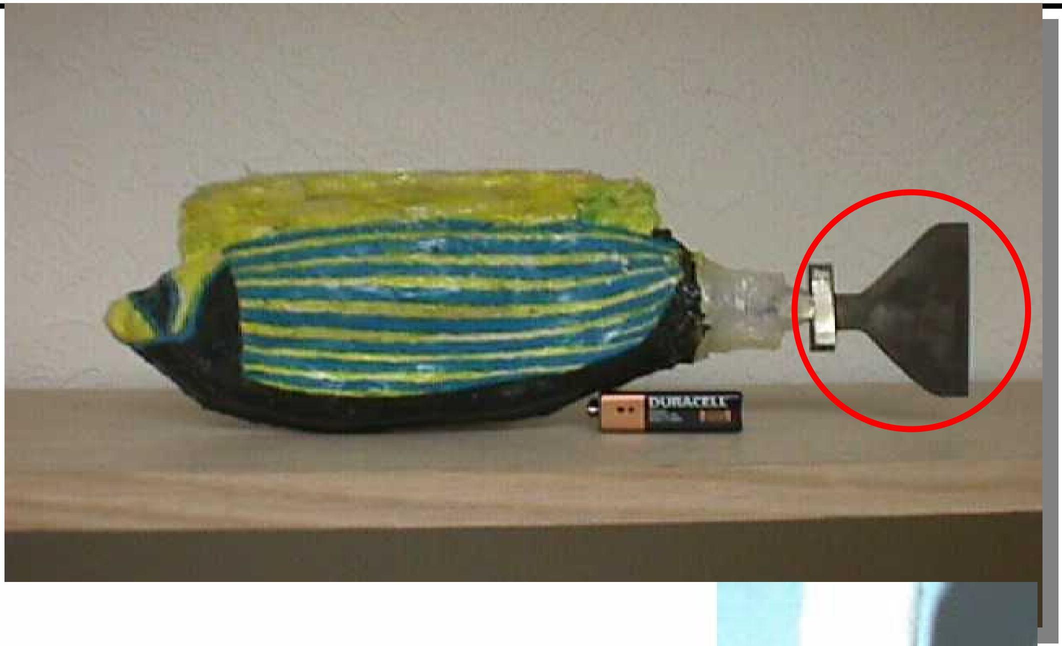
Data-Driven Approach for Q&VV

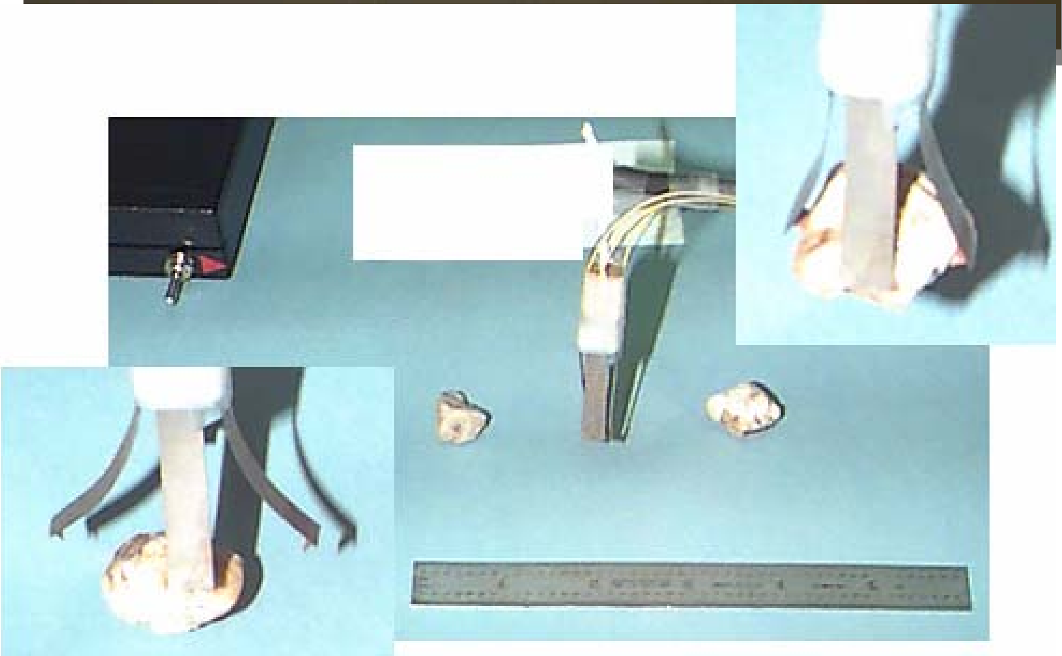


EPISTEMOLOGICAL BACKGROUND



EXAMPLE: IONIC POLYMER COMPOSITE ARTIFICIAL MUSCLES





For Electric and Mechanical activation only without mass transport:

$$\nabla^2\nabla^2 w-(1+\nu)p_k\nabla^2 E_k=\frac{h}{N}\left(\frac{q}{h}+F_{,22}w_{,11}-2F_{,12}w_{,12}+F_{,11}w_{,22}\right),$$

$$\nabla^2\nabla^2 F-Ep_k\nabla^2 E_k=E[(w_{,12})^2-w_{,11}w_{,22}]$$

$$\varepsilon_0\nabla^2 V+p_i\left\{\frac{1-2\nu}{Eh}\nabla^2 F-p_kE_k\right\}=\rho_c$$

or equivalently:

$$\nabla^2\nabla^2 w-c_1\nabla^2 V=\frac{h}{N}\left(\frac{q}{h}+F_{,22}w_{,11}-2F_{,12}w_{,12}+F_{,11}w_{,22}\right),$$

$$\nabla^2\nabla^2 F-c_2\nabla^2 V=E[(w_{,12})^2-w_{,11}w_{,22}]$$

$$\nabla^2 V+c_3\nabla^2\nabla^2 F+c_4V+c_5=0$$

Multi-Objective Function Optimization

$$\min f^{o}(c_j) = \min\{\sum_{i=1}^{n}[w_i^s(c_j) - w_i^e]^2 + \sum_{i=1}^{n}[F_i^s(c_j) - F_i^e]^2 + \sum_{i=1}^{n}[V_i^s(c_j) - V_i^e]^2\}$$

subject to constrains: $t_j^u \geq c_j \geq t_j^l$

where: w_i^e, F_i^e, V_i^e are the experimentally observed state variables at each point i

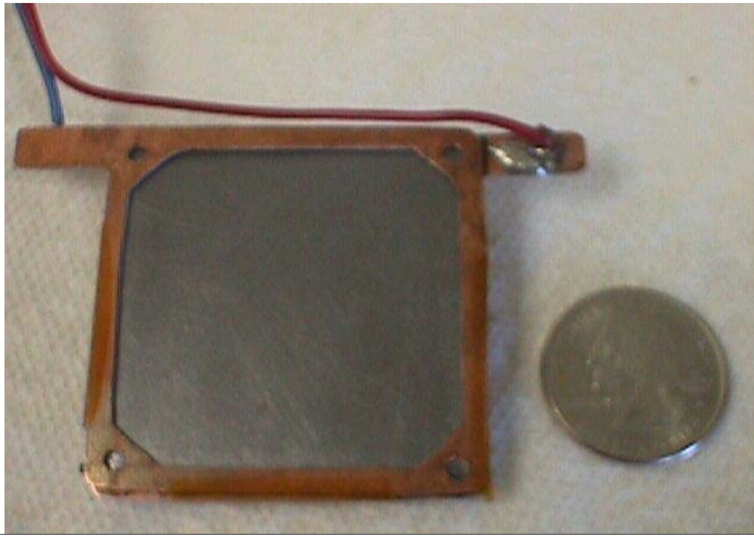
$w_i^s(c_j), F_i^s(c_j), V_i^s(c_j)$ are the simulated state variables at each point i

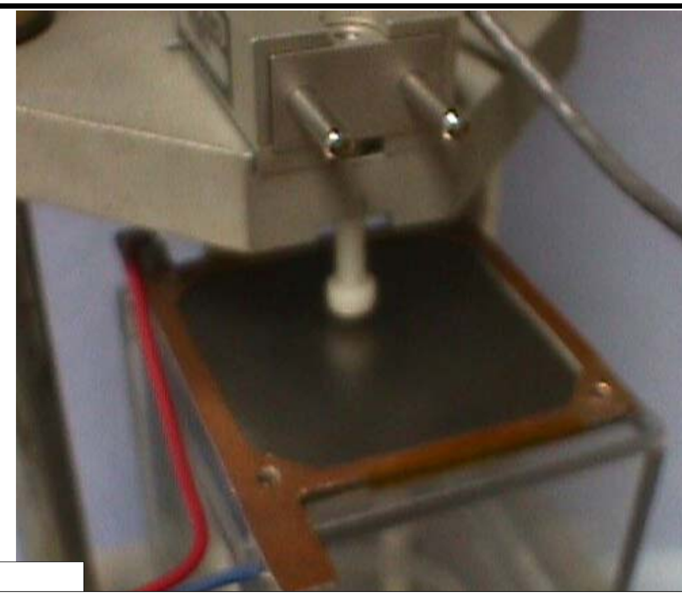
c_j are the uknown constants to be identified

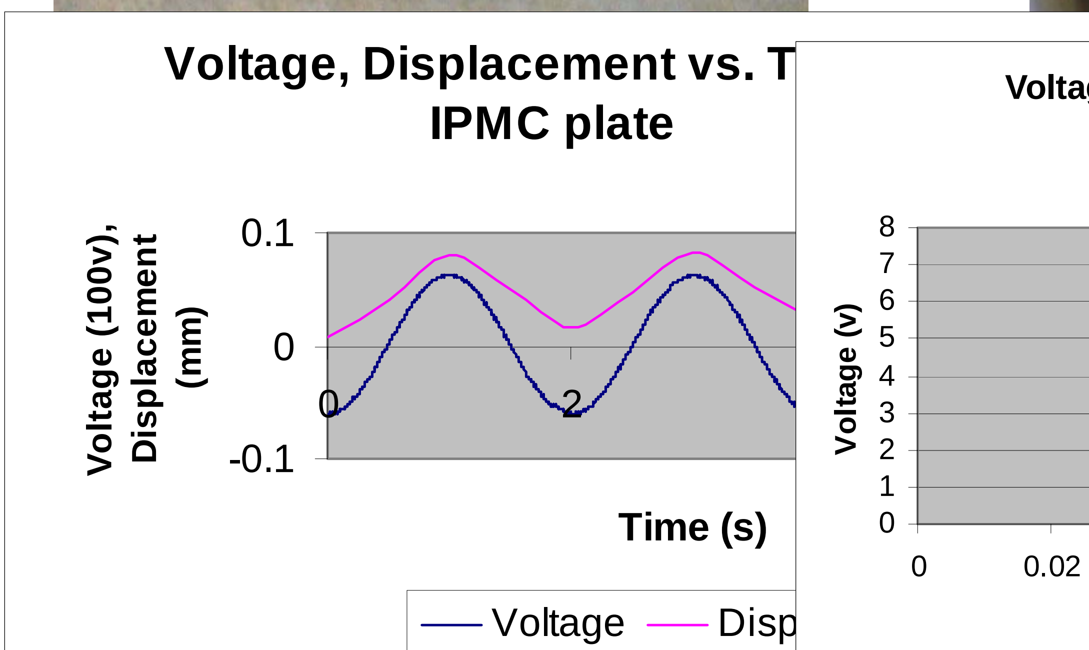
t_j^u, t_j^l are the upper and lower limits constraining each uknown j

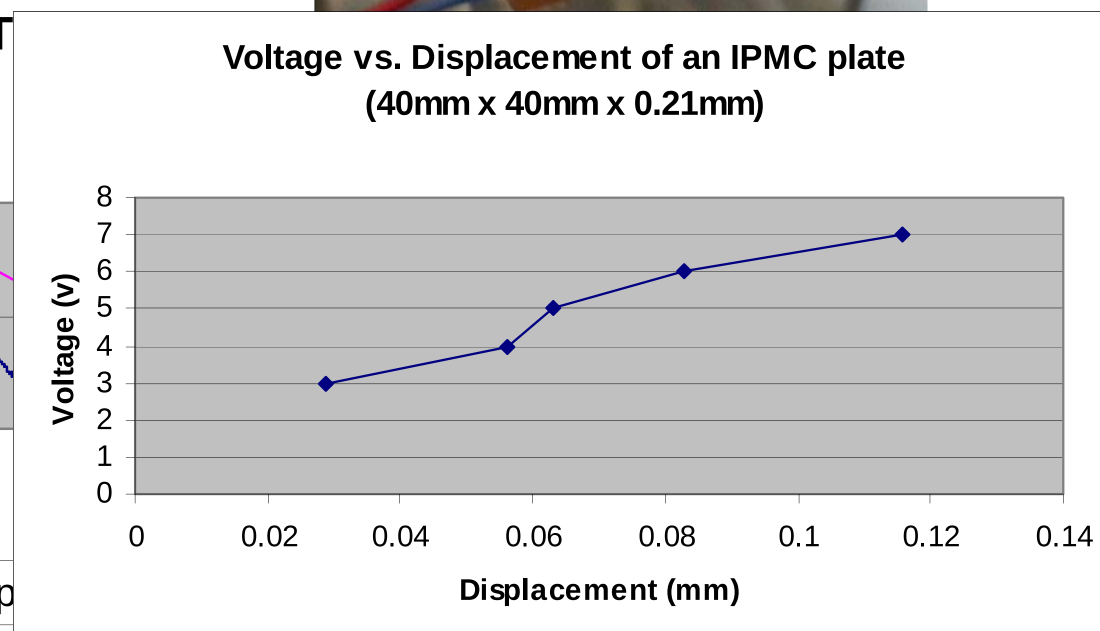
To fully characterize c_i we need a family of experiments that sweeps across boundary values of w, F, V and measures them on a grid superimposed on the domain of the plate

IPMC Large Deflection Plates: Experimental Results
(M. Shahinpoor UNM)









IPMC Large Deflection Plates: Biharmonic Single-Field Bases

$$w^{s1}(x,y)=\frac{16q}{\pi^6 D}\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}\frac{a^4b^4}{mn(b^2m^2+a^2n^2)^2}\sin\frac{m\pi(2x+a)}{2a}\sin\frac{m\pi(2y+b)}{2b}$$

$$w^{s2}(x,y)=\frac{4qa^4}{\pi^5 D}\sum_{m=1,3,5,\ldots}^{\infty}\frac{(-1)^{(m-1)/2}}{m^5}\cos\frac{m\pi x}{a}(1-\frac{\alpha_m\tanh\alpha_m+2}{2\cosh\alpha_m}\cosh\frac{m\pi y}{a}+$$

$$+\frac{1}{2\cosh\alpha_m}\frac{m\pi y}{a}\sinh\frac{m\pi y}{a})$$

$$\alpha_m=\frac{m\pi b}{2a}$$

where: $w^{s(1,2)}(x,y)$ single-field plate deflection at point (x,y)

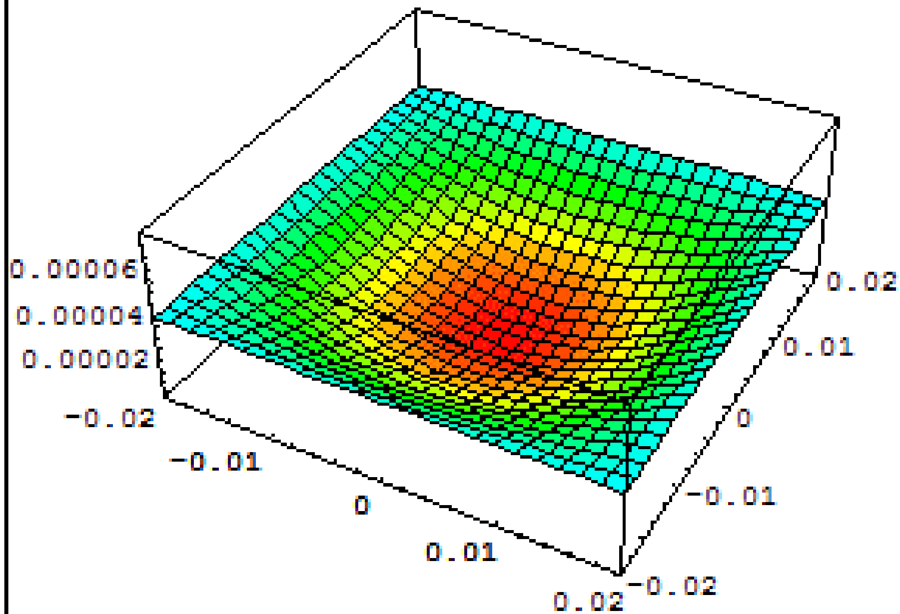
$q=q(x,y)$ mechanical load distribution on the plate

$D=$ Flexural rigility of the plate

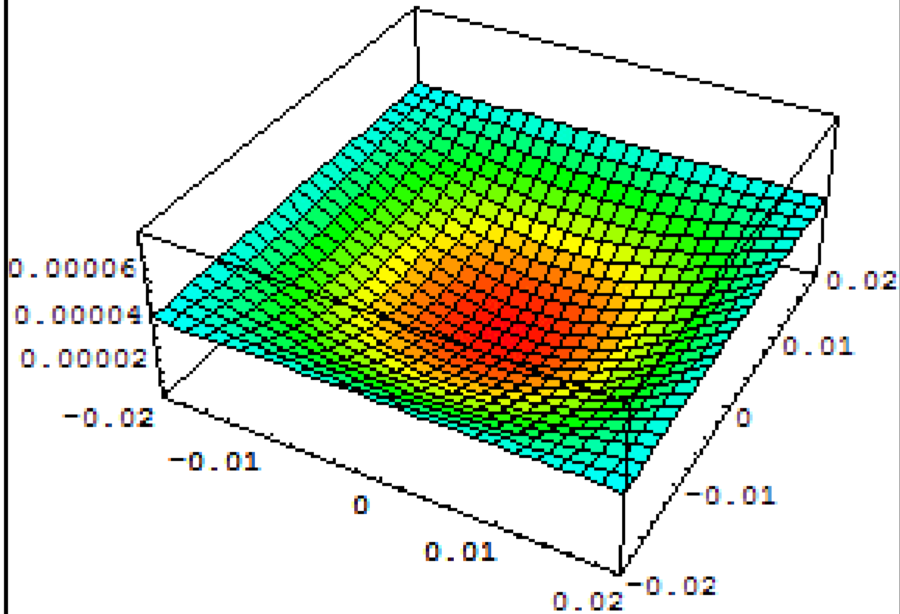
a,b length and width of the plate along x and y axes

Deflection Time Histories in 3D carpet plots

EXPERIMENT

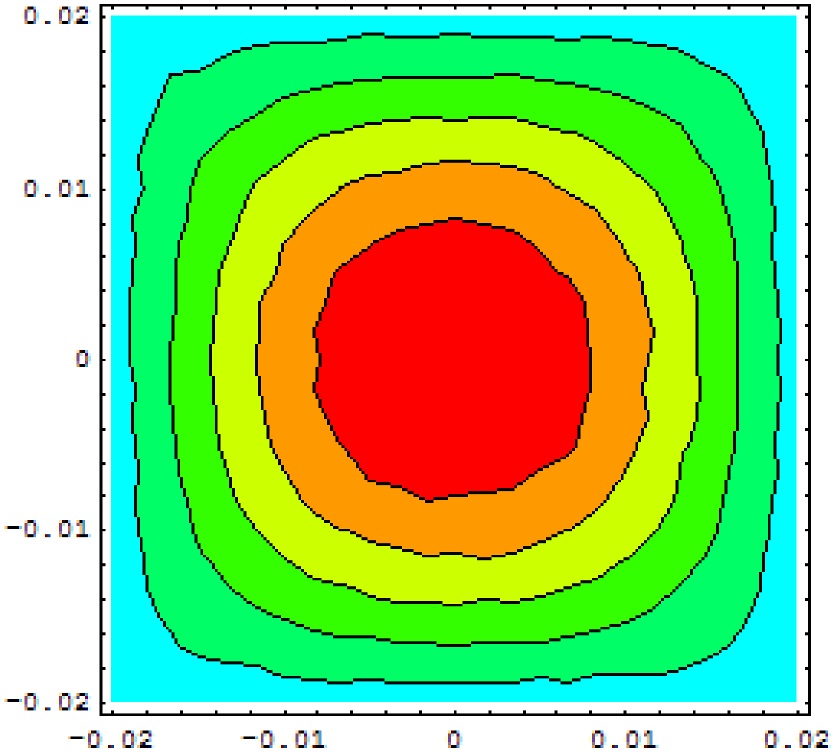


COMPUTED



Deflection Time Histories in Contour plots

EXPERIMENT



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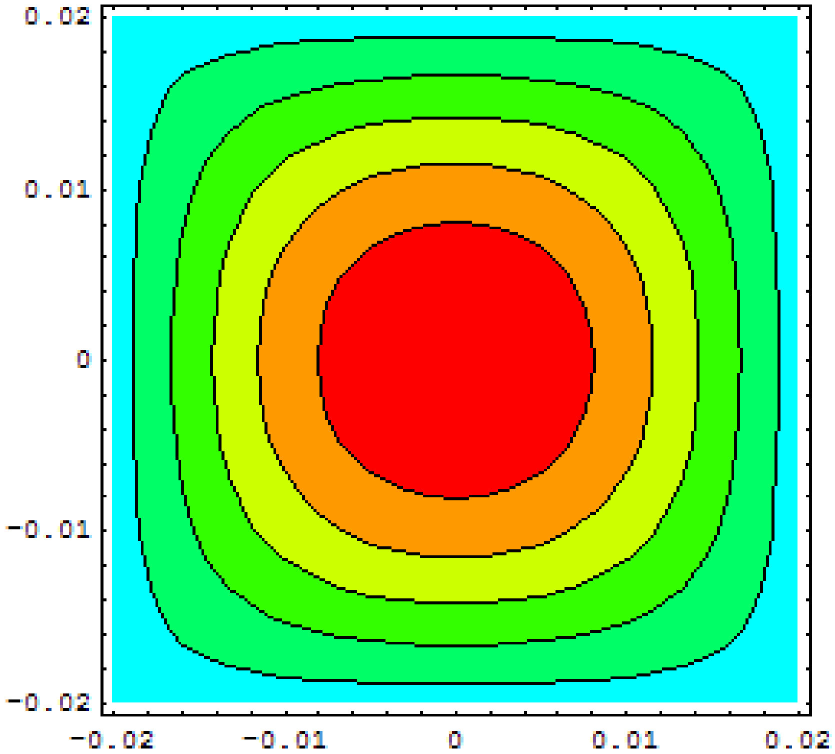


Conclusions

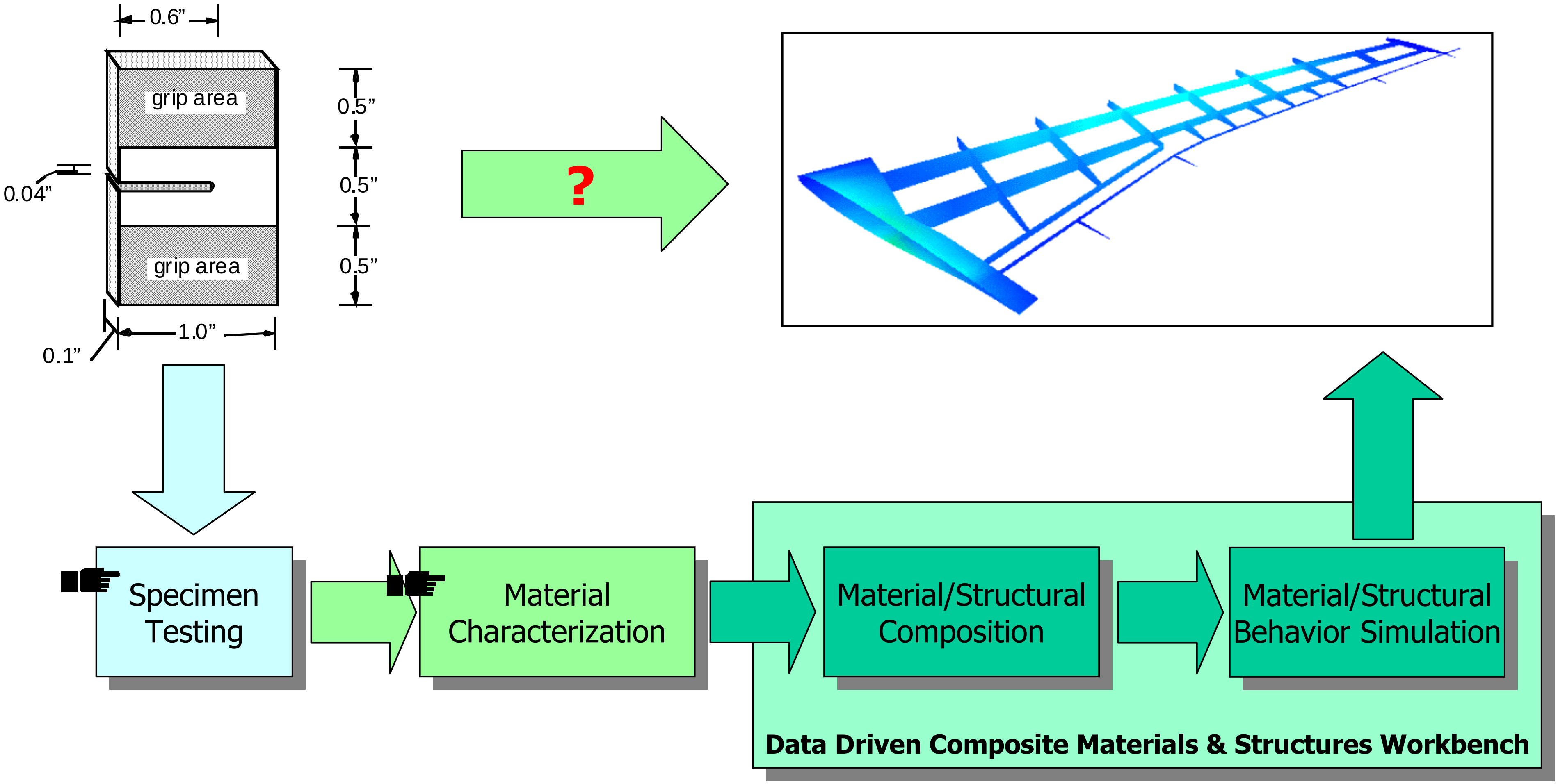
- Data driven models and simulations contain validation
- Model-driven models have epistemologic origins
- When data exist “data-driven” is preferable

THANK YOU FOR YOUR ATTENTION

QUESTIONS?

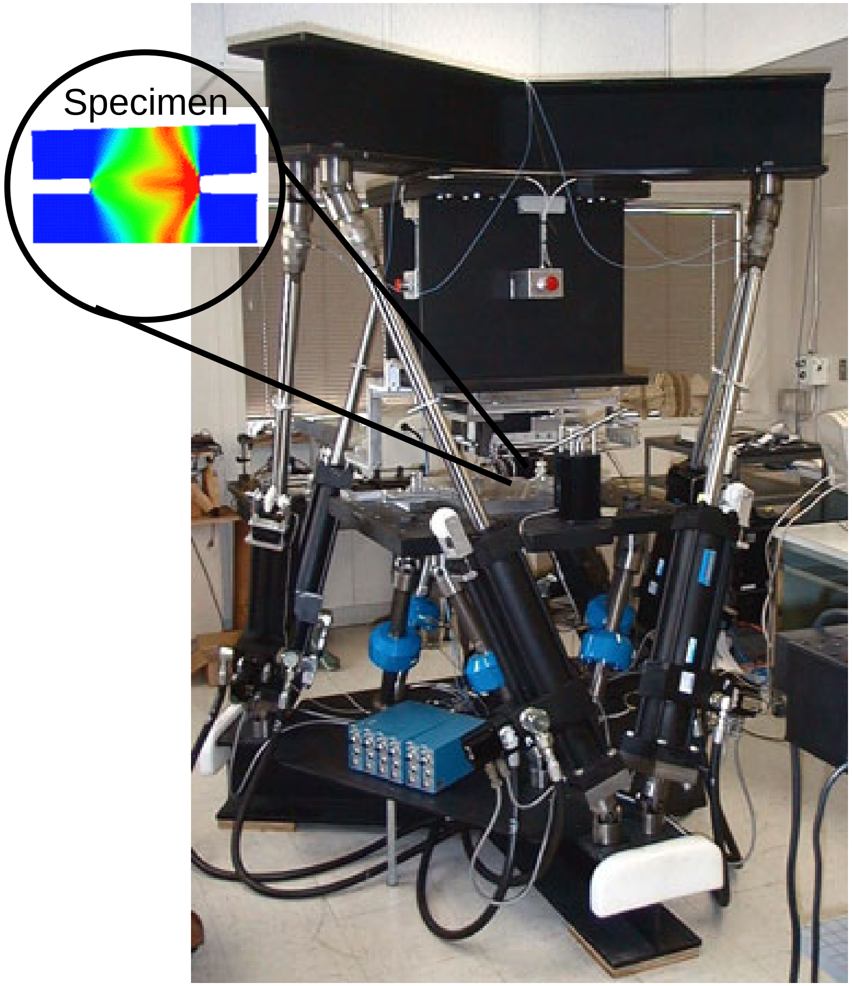
Data-Driven Approach: Example

Identify material from small specimens to predict behavior of large system



General Case:

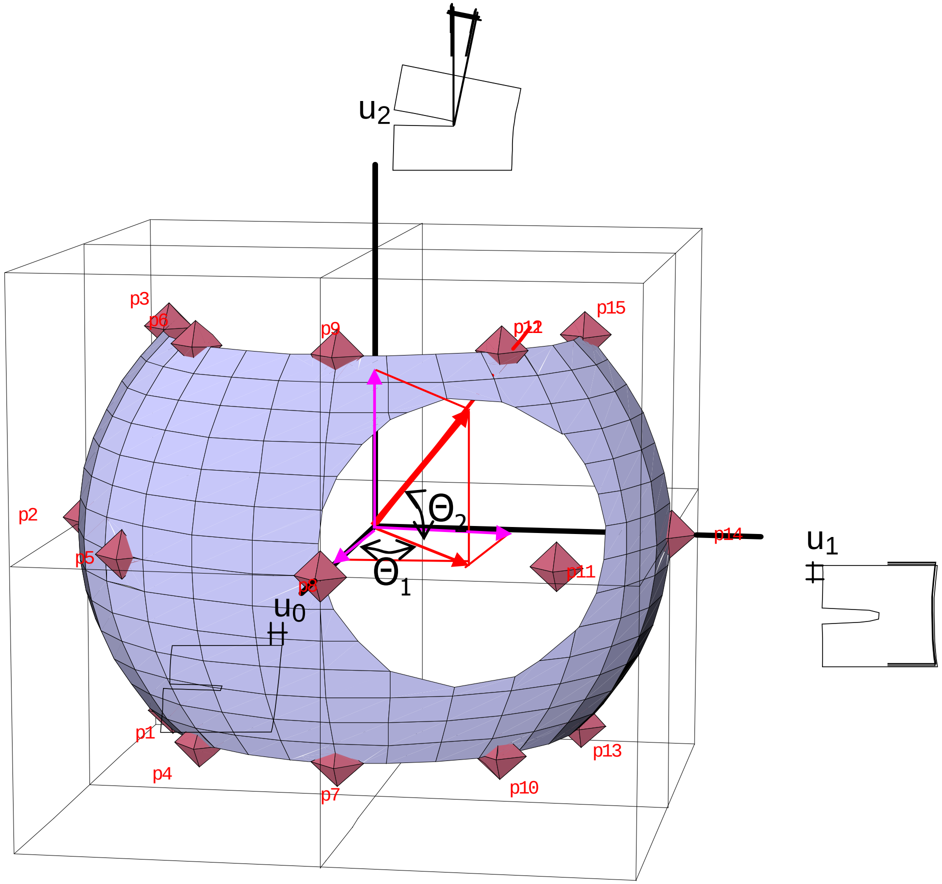
3 displacements + 3 rotations + 3 forces + 3 moments + Np x 3 strains + Np x Nf = 12+ (3+Nf)xNp Datastreams



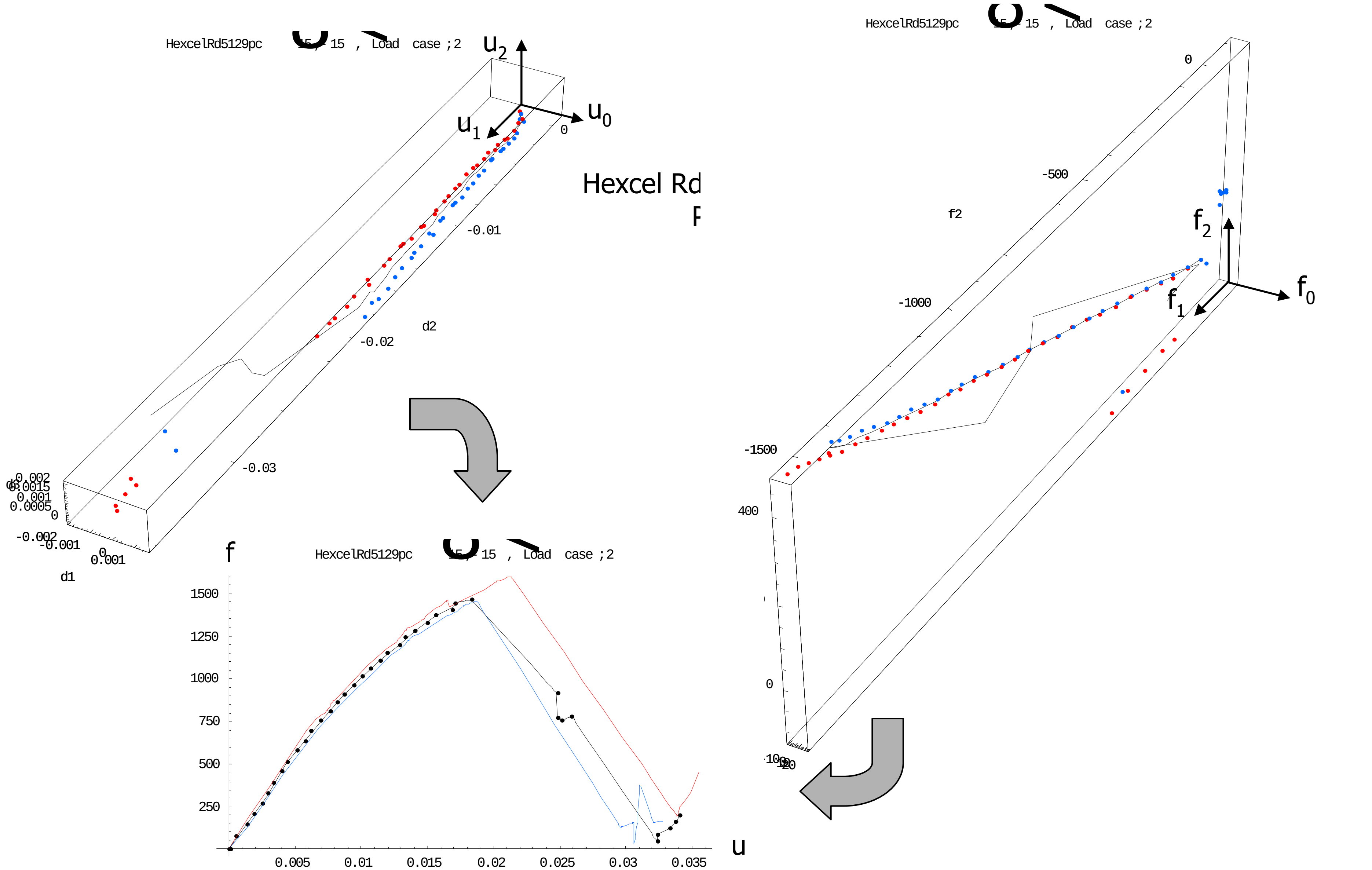
NRL's Automated 6-D Loader

Special Case:

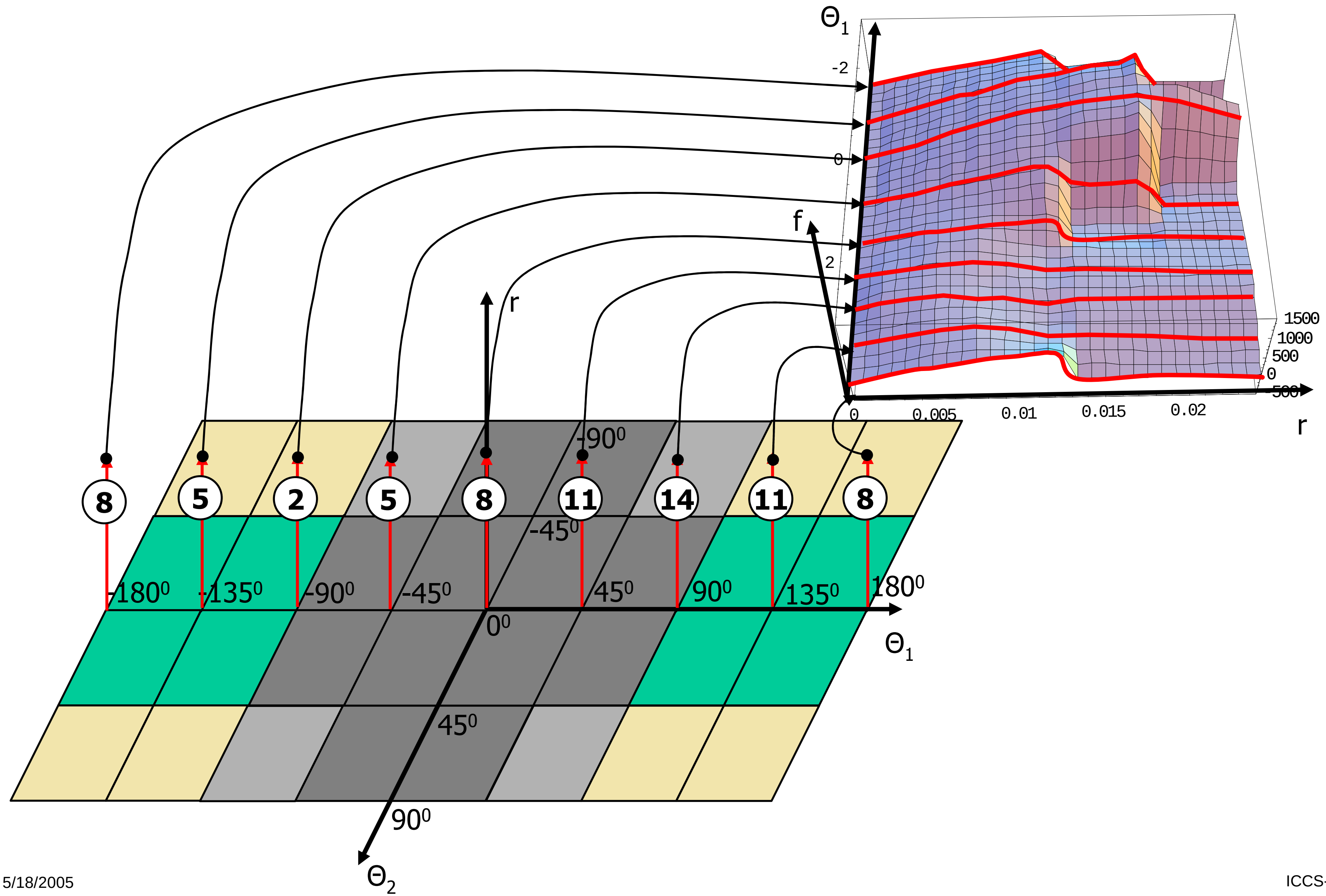
2 displacements + 1 rotation=3DOFs=6Datastreams



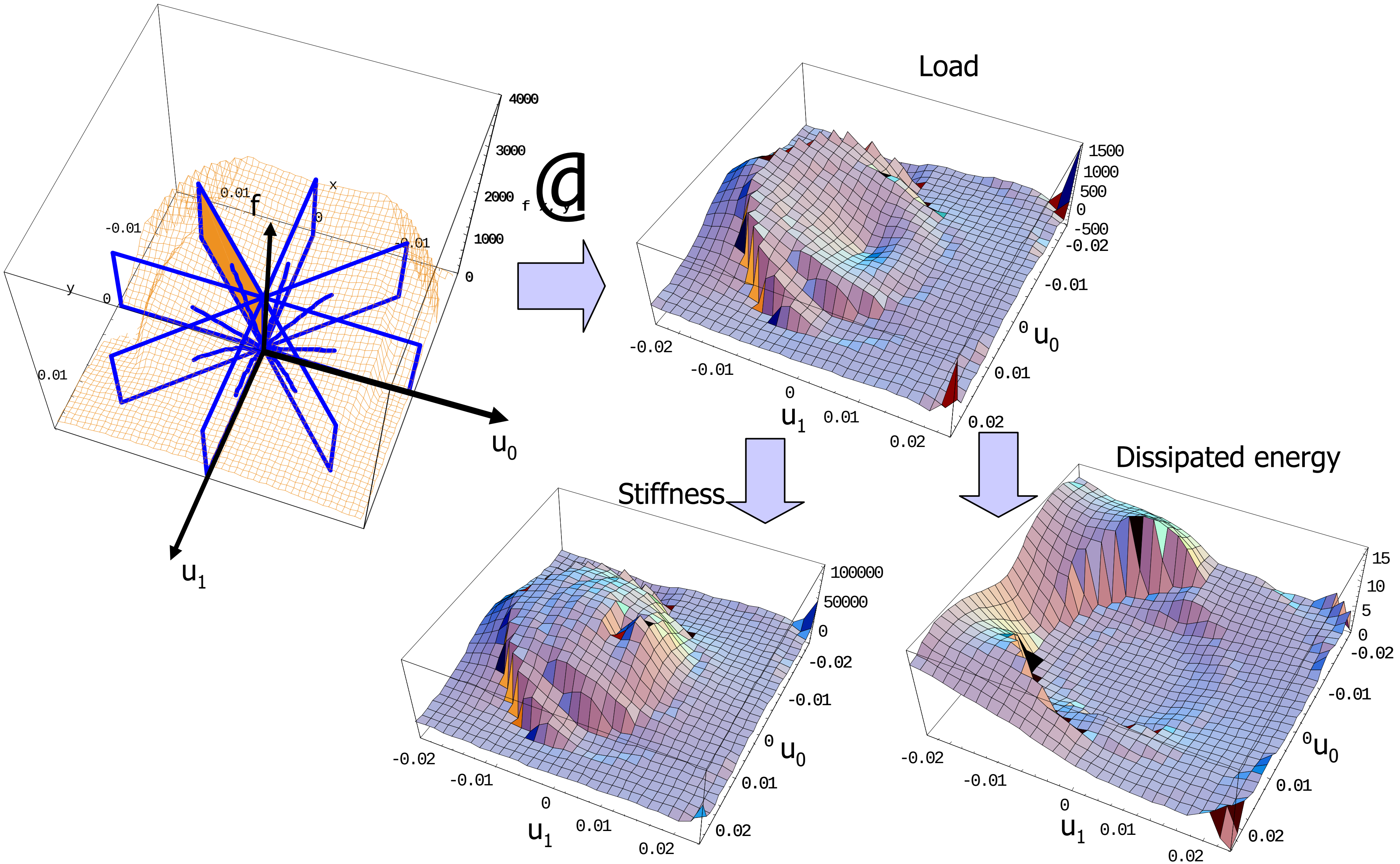
Data driven methodology for PMCs: Data Collection



Data driven methodology for PMCs: Data Reduction



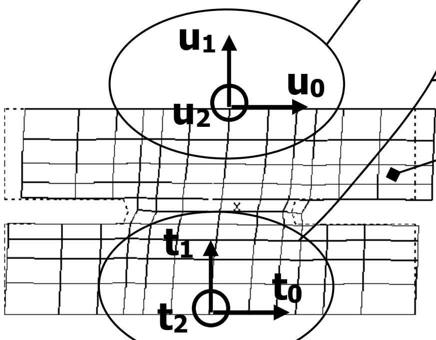
Data driven methodology for PMCs: Data Reduction



MECHATRONICALLY AUTOMATED APPROACH: Inverse Model

General Problem: Build a function out of knowing some of its values trough a collocation method

Energy Balance: $$\int_0^{u_r} t_u q_v dq^v - \frac{1}{2} t_s u_t u^v = \int_{\partial V} \phi(\varepsilon_i(x_j))dx_j$$

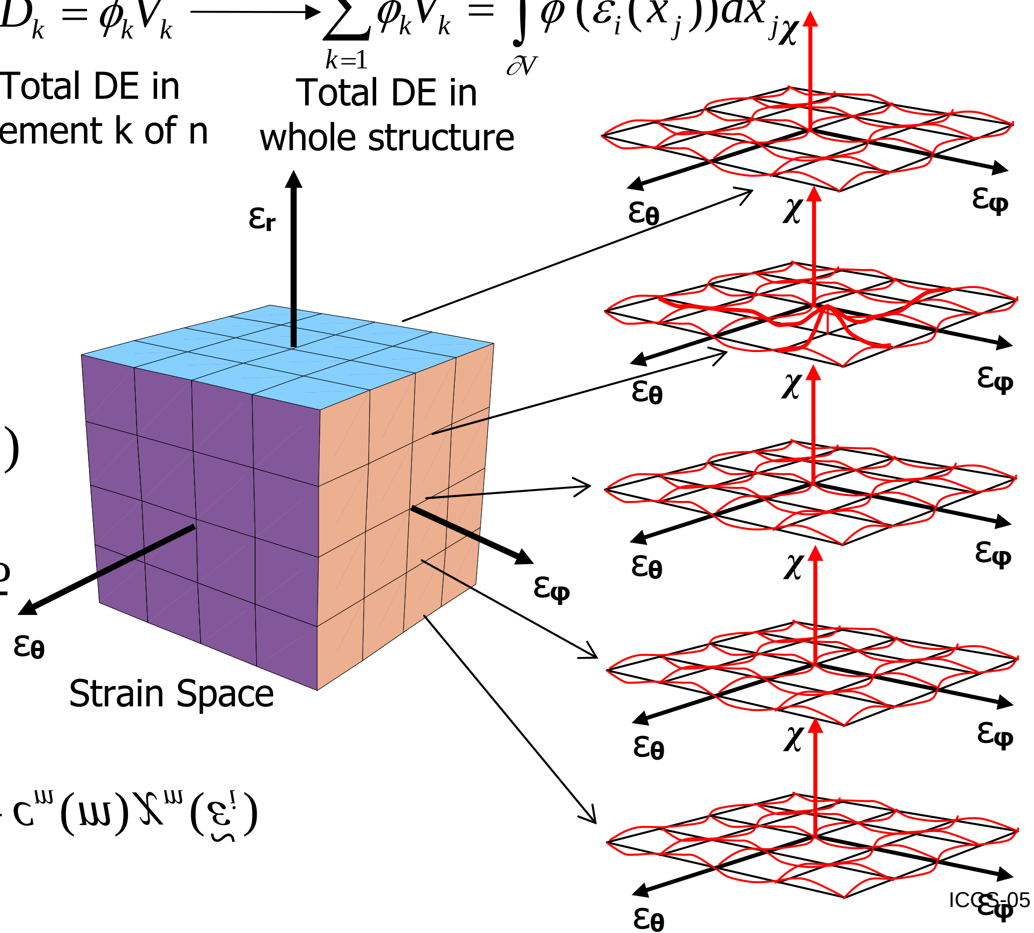


n discrete elements

$$D_k = \phi_k V_k \longrightarrow \sum_{k=1}^{n} \phi_k V_k = \int_{\partial V} \phi(\varepsilon_i(x_j))dx_j$$

Total DE in element k of n

Total DE in whole structure



Strain Space

$$\phi(\underset{\sim}{c},\underset{\sim}{\varepsilon}) = \underset{\sim}{c}\cdot\underset{\sim}{X}(\underset{\sim}{\varepsilon}(\underset{\sim}{x})) = c_i(m)X_i(\underset{\sim}{\varepsilon})$$

$$X_i(\underset{\sim}{\varepsilon}_j) = \begin{cases} 0, & i \neq j \\ 1, & i = j \end{cases} \text{ for } i, j = 1, 2, \ldots, 125$$

$$\phi(\underset{\sim}{\varepsilon}_j) = 0 + \cdots + c_j(m) + \cdots + 0 = c_j(m)$$

$$\phi(\underset{\sim}{\varepsilon}_j) = c_1(m)X_1(\underset{\sim}{\varepsilon}_j) + \cdots + c_j(m)1 + \cdots + c_m(m)X_m(\underset{\sim}{\varepsilon}_j)$$

MECHATRONICALLY AUTOMATED APPROACH:Optimization

$$\int_0^{u_r} t_u q_v dq^v - \frac{1}{2} t_s u_t u^v = \int_{\partial V} \phi(\varepsilon_i(x_j)) dx_j$$

For a loading point p: $$\sum_{110}^{I=6} c_i(m) X_i(\underset{\sim}{\varepsilon}_p{}^e) V_p{}^e + e_p = D_p$$

For all selected loading points: $$[X]\underset{\sim}{c} + \underset{\sim}{e} = \underset{\sim}{d}$$

Using 17 points per loading path generates 255 loading points leading to 255 equations for 125 unknowns

DED monotonicity: $$[M]\underset{\sim}{c} \geq 0$$

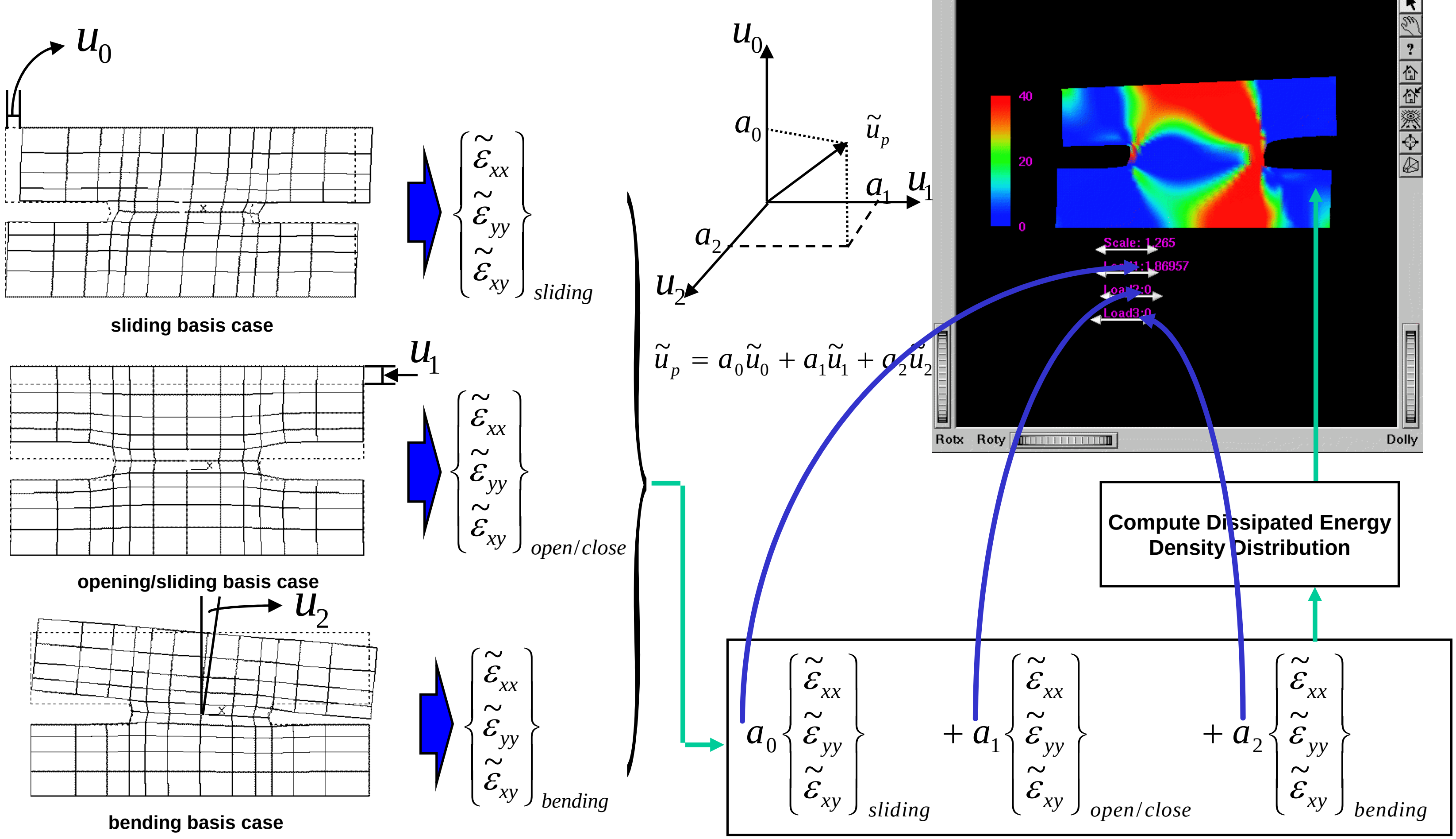
100 additional constrains

Final Problem: Minimize $\left\|\underset{\sim}{e}\right\|$ subject to $[M]\underset{\sim}{c} \geq 0$

Solution Method: Least Squares with Linear Constrains

MECHATRONICALLY AUTOMATED APPROACH:Simulation Synthesis

UTILIZATION OF BASIS LOADING CASES RESPONSE THROUGH LINEAR COMBINATION OF RESULTING STRAIN FIELDS



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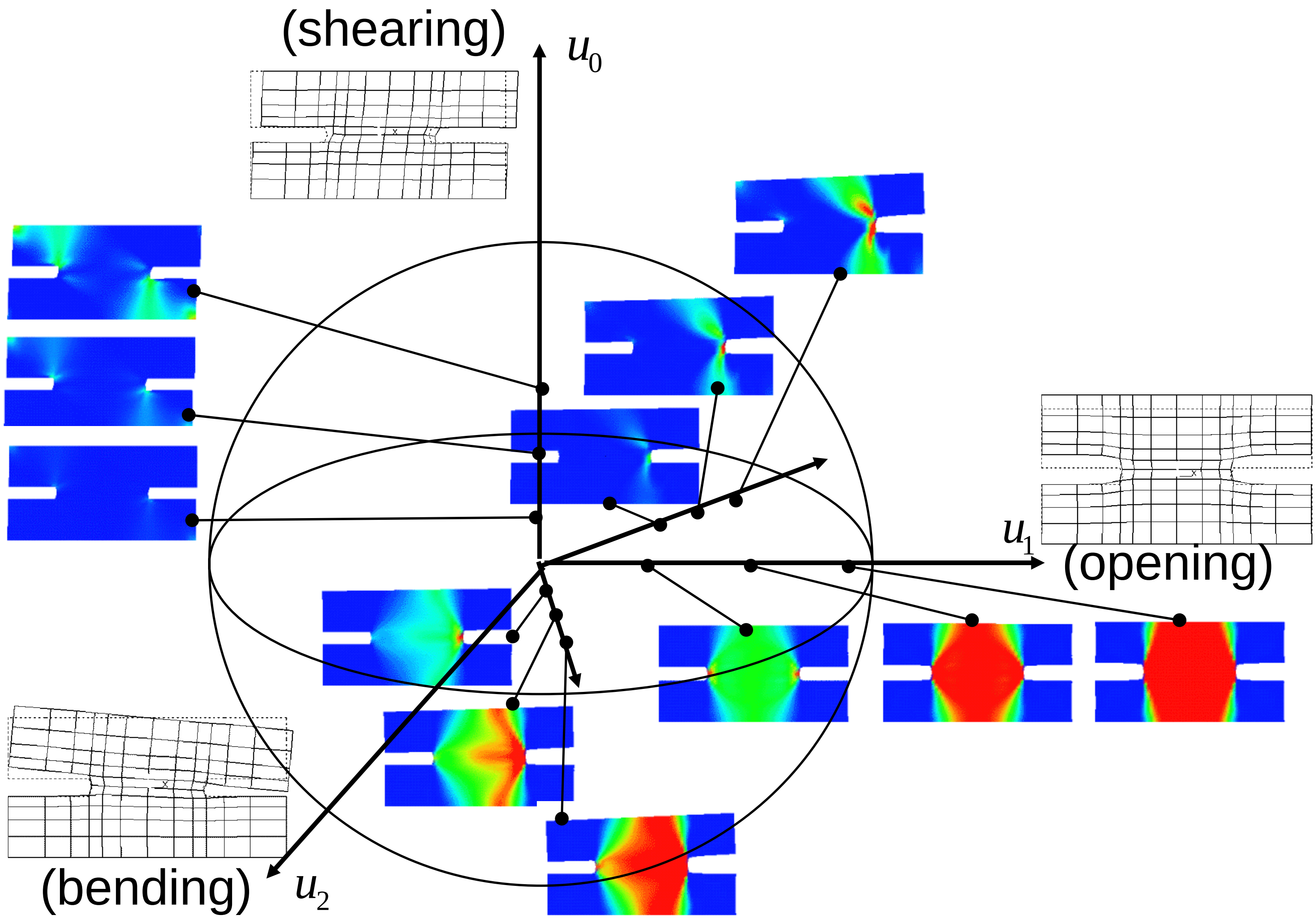
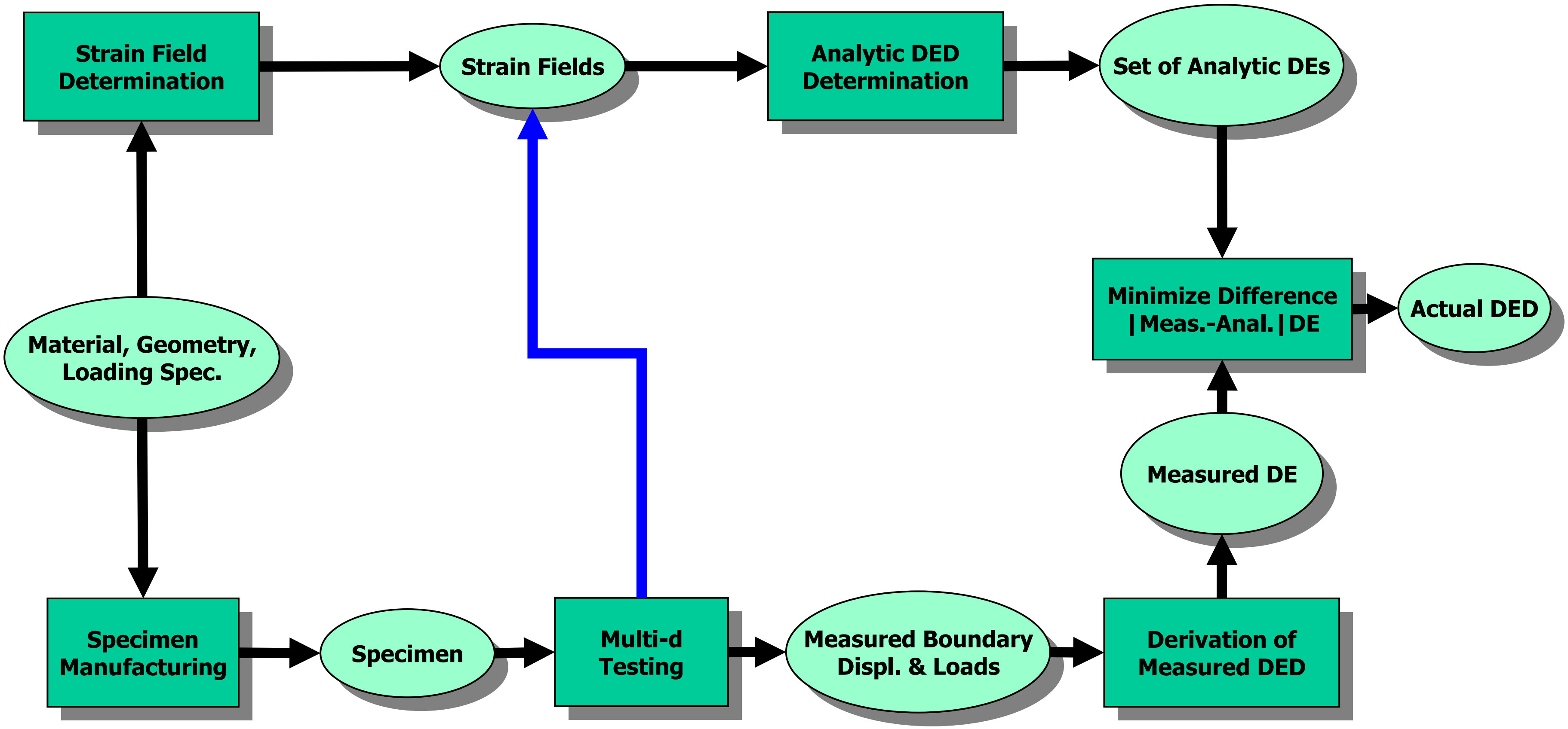
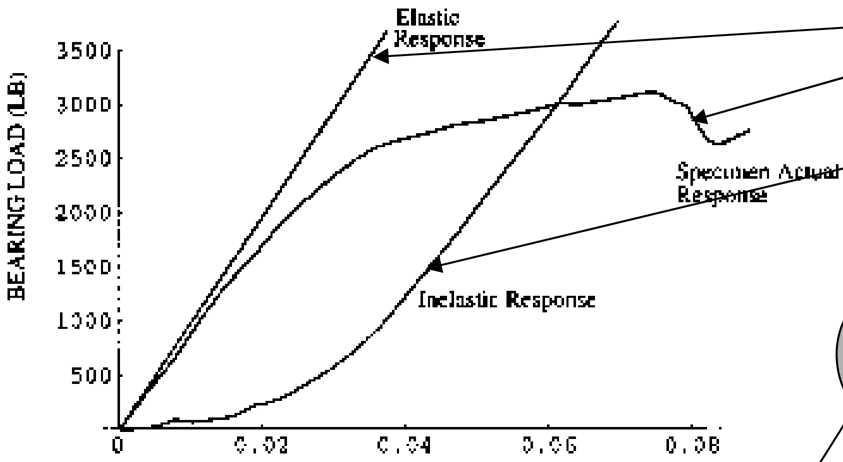
MECHATRONICALLY AUTOMATED APPROACH:Simulation Synthesis



Data driven methodology for PMCs: Material Characterization





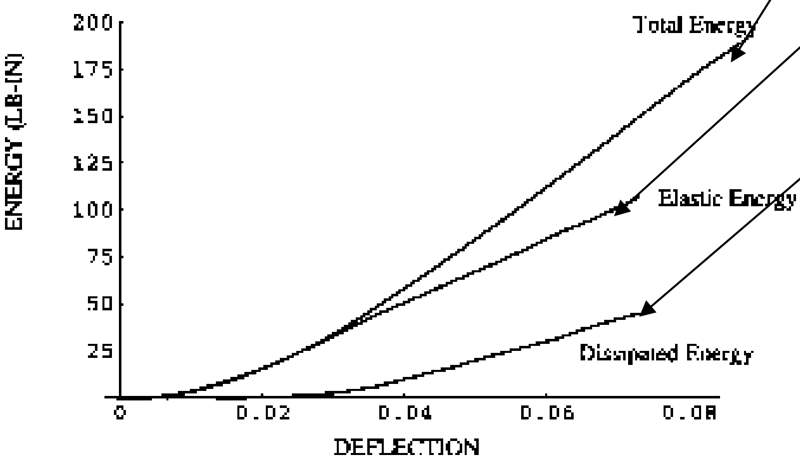
1-D Load Space Partitioned Model of Behavior

$$P = P(\delta) = P_{rec.}(\delta) + P_{irec.}(\delta) = m\delta + \psi(\delta)$$

$$W_{total}(\delta) = W_{rec.}(\delta) + W_{irec.}(\delta)$$

$$\int_0^{\delta} P(u)du = \frac{1}{2}(m\delta)\delta + \int_0^{\delta} \psi(u)du$$

$$\frac{d}{d\delta}W_{total}(\delta) = \frac{d}{d\delta}W_{rec.}(\delta) + \frac{d}{d\delta}W_{irec.}(\delta)$$



n-D Load Space Partitioned Model of Behavior

$$\int_0^{\delta_i} P_i(u_i)du_i = \frac{1}{2}(m_{jk}\delta_j)\delta_k + \oint_{\partial V} \psi(\tilde{u})d\tilde{u}$$

$$\psi(\tilde{u}) = \tilde{c} \cdot \tilde{\chi}(\tilde{u})$$

$$\int_0^{\delta_i} P_i(u_i)du_i = \frac{1}{2}(m_{jk}\delta_j)\delta_k + \oint_{\partial V} \tilde{c} \cdot \chi(\tilde{u})d\tilde{u}$$

$$A_{ij}c_i = b_i$$

How - Approach:
GENERAL CONTINUOUM SYSTEMS MODELING

Data driven methodology for PMCs

AXIOMS OF ENRICHMENT

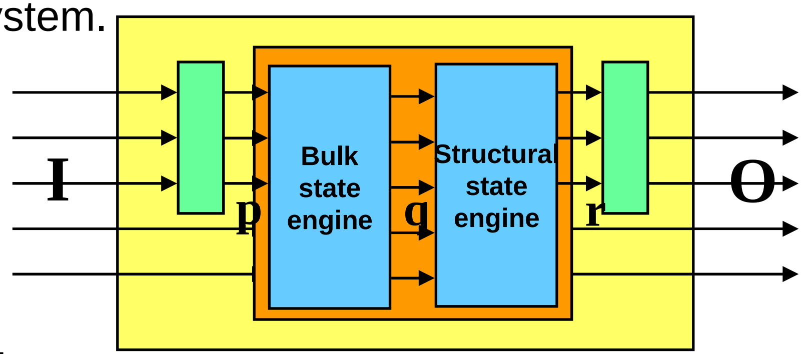
- All state variables are varying in a locally flat fashion both in space and time (continuity)
- The behavior of the whole structure is equivalent to the composition of the behaviors of structural discretization units (composition behavior)
- The observed behavior is repeatable when observed under identical conditions in various times (first order of reality)

ASSUMPTIONS

- Loading is either static or slowly varying
- The material behavior will be non-viscous, and independent of rate and load history
- The constitutive relation is continuous both in input and output variables
- Deformations are sufficiently small so that the infinitesimal stress and strain tensors may be employed

MODELING A MULTIPHYSICS SYSTEM

$\mathcal{B} : I_u \to O_w, I_u \subset \mathfrak{R}_u, O_w \subset \mathfrak{R}_w$ ***Behavior Functional*** relating the output to the inputs of the system.



$\mathcal{S}(d, \xi, b) = 0$ ***Relational restriction*** over dependent, independent, parameter variables.

$d = \mathcal{G}(\xi, b)$

$\rho = \mathcal{G}(\xi, \varepsilon) \cdot \varepsilon$

Bulk Constitutive Relations: Functional dependence, of dependent variables on independent variables and parameters.

$\mathcal{K}^{i}(\Delta_u d, \frac{\partial f_w}{\partial w} d, \cdots) = 0$ ***Composition Behavior through Conservation Law Relations***: Dependence, of dependent variables on position in the structure, and time.

$d = \Delta^{b} \Xi(\xi, b)$ ***Vector Function Storage Mechanism:*** Potential or Energy Density function.

MODELING A MULTIPHYSICS SYSTEM

Data driven Modeling methodology

$$\underset{\sim}{d} = \Delta^{\underset{\sim}{b}}\, \Xi(\underset{\sim}{\xi}, \underset{\sim}{b})$$

Vector Function Storage Mechanism:
Potential or Energy Density function.

$$\Xi(\underset{\sim}{\xi}, \underset{\sim}{b}) = \Phi(\underset{\sim}{\xi}, \underset{\sim}{b}) + \phi\,(\underset{\sim}{\xi}, \underset{\sim}{b})$$

Additivity of recoverable and non-recoverable components.

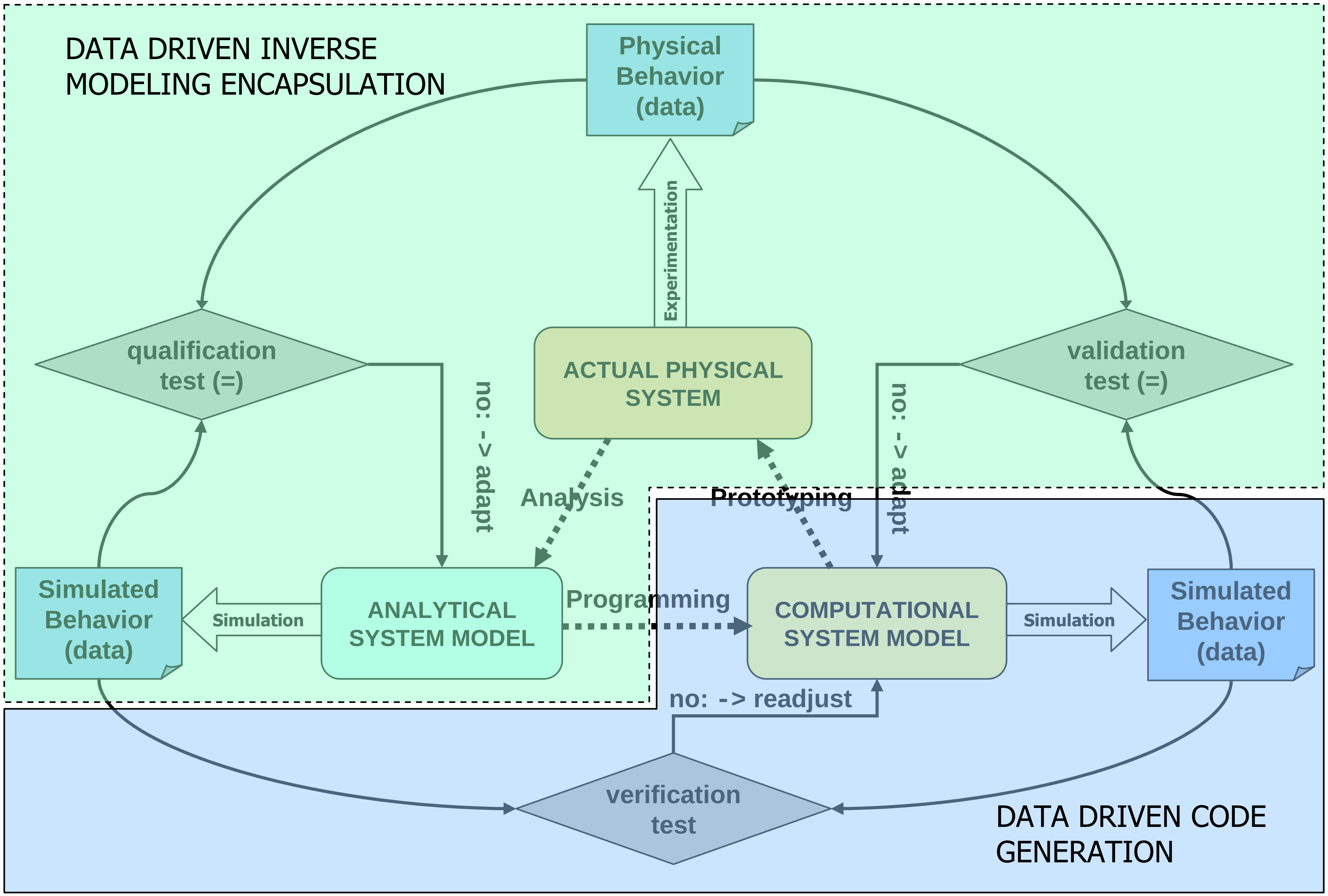
$$\Phi(\underset{\sim}{\xi}, \underset{\sim}{b}) = \frac{S}{J}\underset{\sim}{d}(\underset{\sim}{b}) \cdot \underset{\sim}{b}$$

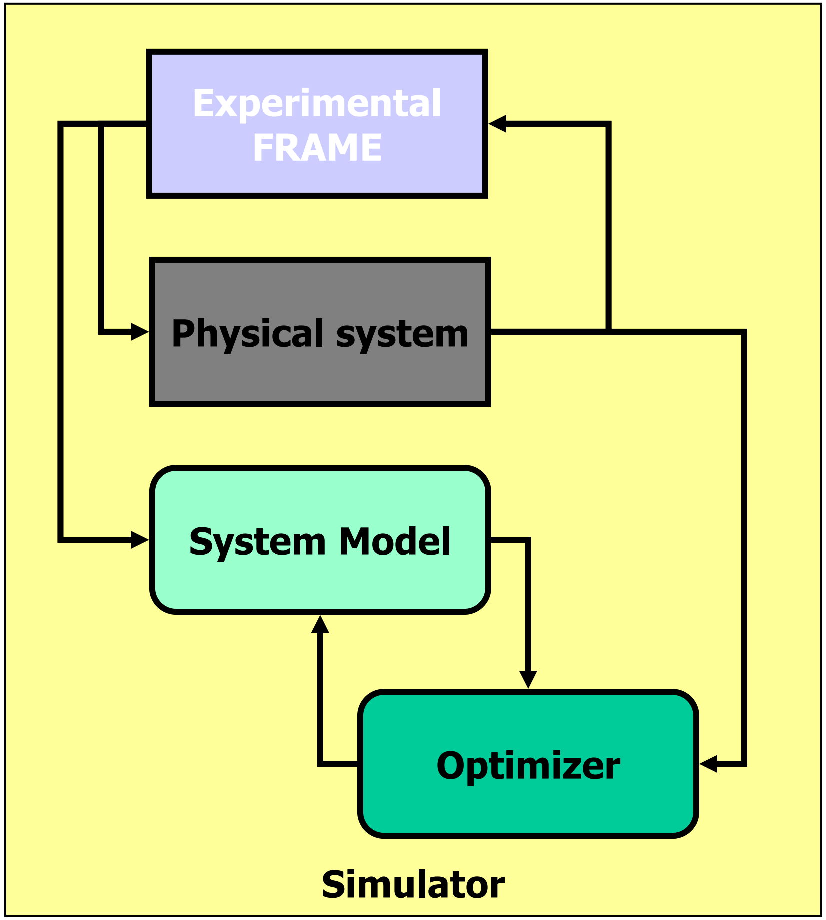
Recoverable energy definition.

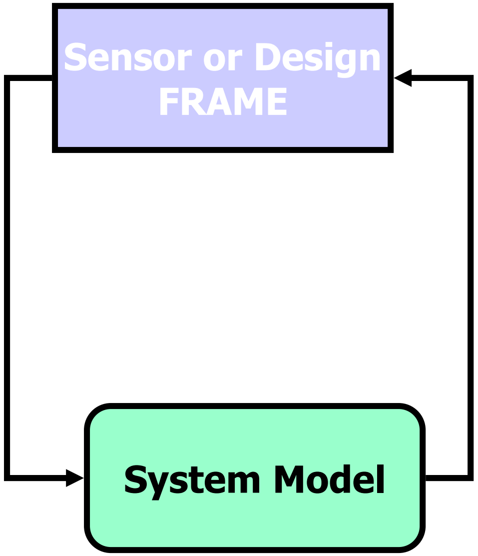
$$\phi\,(\underset{\sim}{\xi}, \underset{\sim}{b}) = \underset{\sim}{c} \cdot \underset{\sim}{X}\,(\underset{\sim}{\xi}, \underset{\sim}{b}(\underset{\sim}{x}))$$

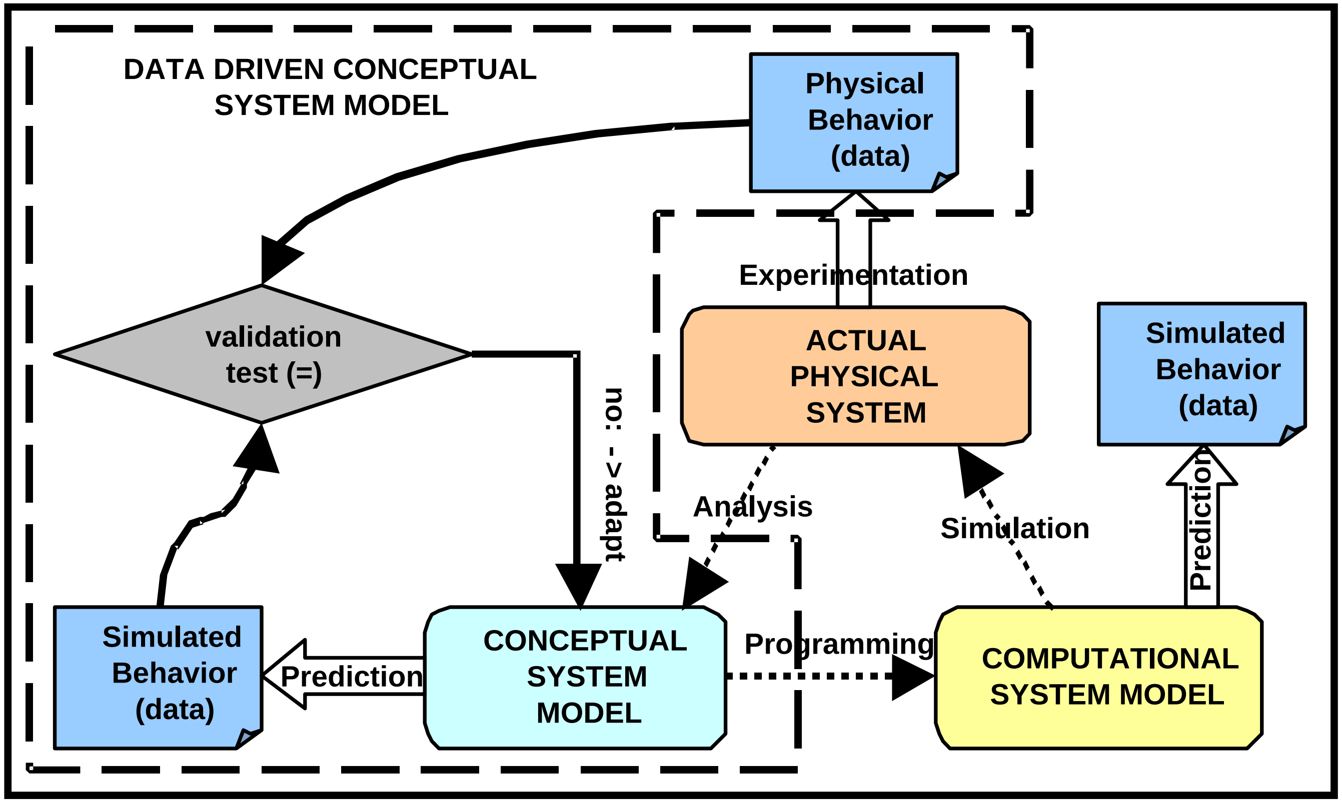
Non-recoverable energy definition.

Traditional vs. Data-Driven Approach of Q&VV




Experimental
FRAME
Physical system
System Model
Optimizer
Simulator


Sensor or Design
FRAME
System Model


DATA DRIVEN CONCEPTUAL SYSTEM MODEL
Physical Behavior (data)
Experimentation
validation test (=)
no: ->adapt
ACTUAL PHYSICAL SYSTEM
Simulated Behavior (data)
Analysis
Simulation
Prediction
Simulated Behavior (data)
Prediction
CONCEPTUAL SYSTEM MODEL
Programming
COMPUTATIONAL SYSTEM MODEL