



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

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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**)

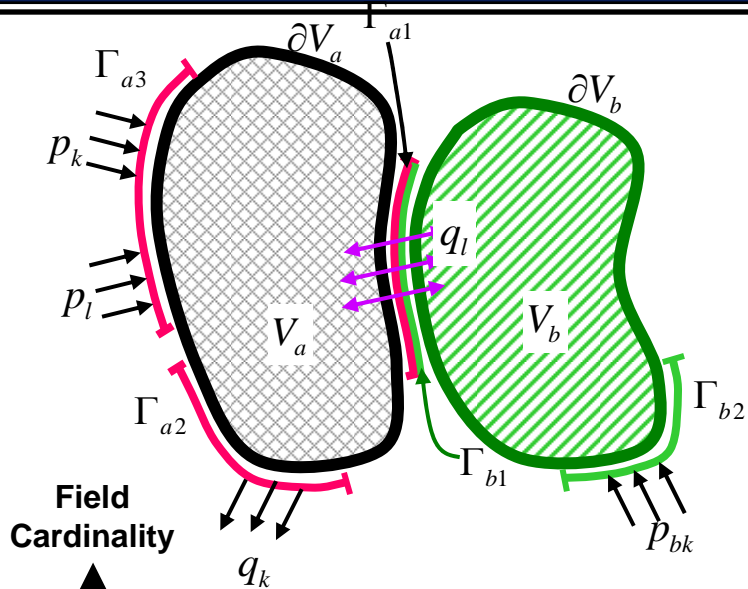


System-Model-Behavior

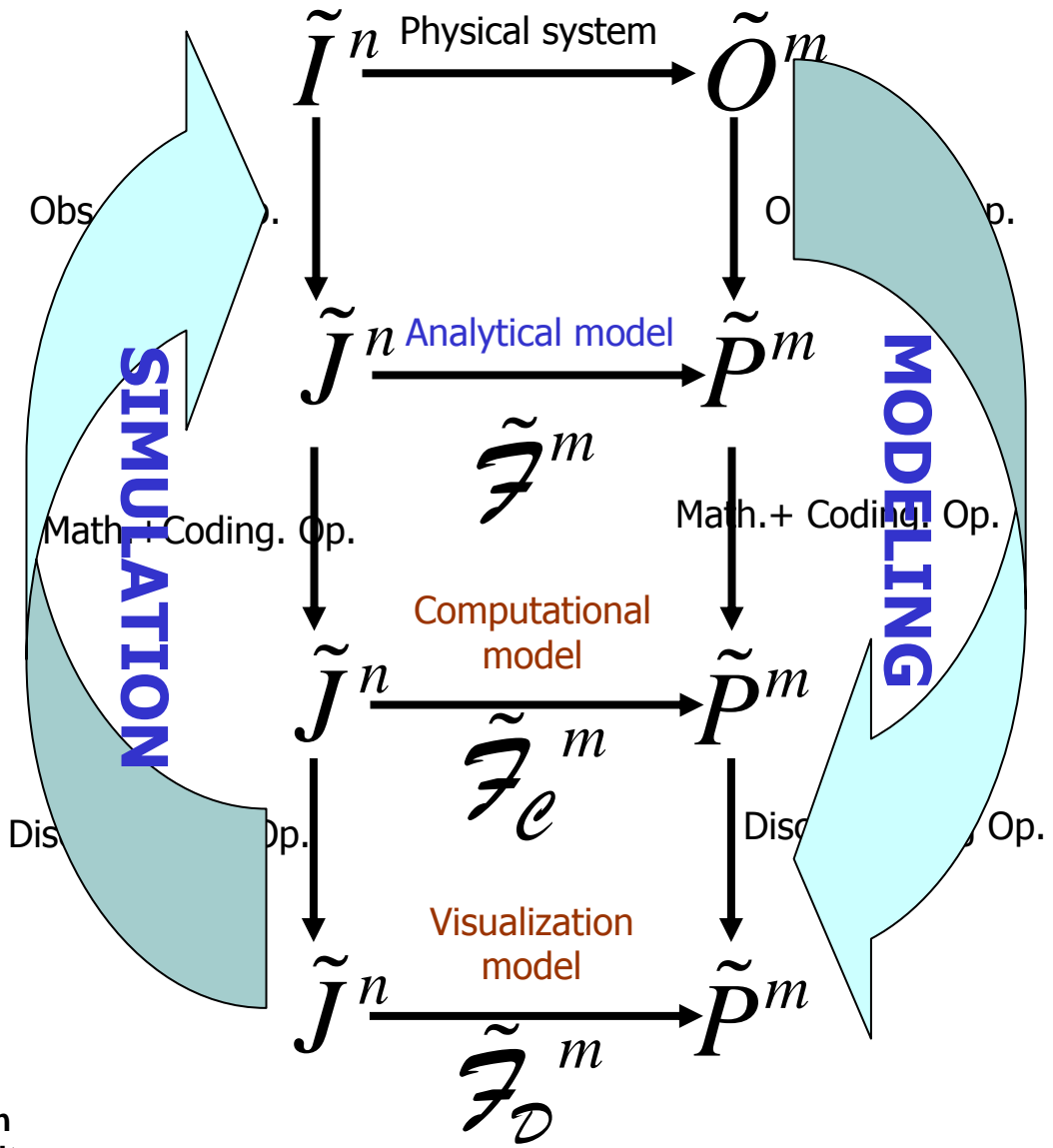
	System External Appearance	Internal Appearance	Behavior Appearance
Physical World	<p>Physical System P</p>		<p>Hybrid 10 Load versus Stroke Open Hole, Net Tension</p>
Conceptual World	<p>Modeled System</p>	$R(P, \delta) = 0$ $P(\delta)$ $\delta(P)$	<p>Hybrid 10 Load versus Stroke Open Hole, Net Tension</p>



MODELING A MULTIPHYSICS SYSTEM



	Field Cardinality	
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
	One Domain	Multiple Domains
	Domain Cardinality	

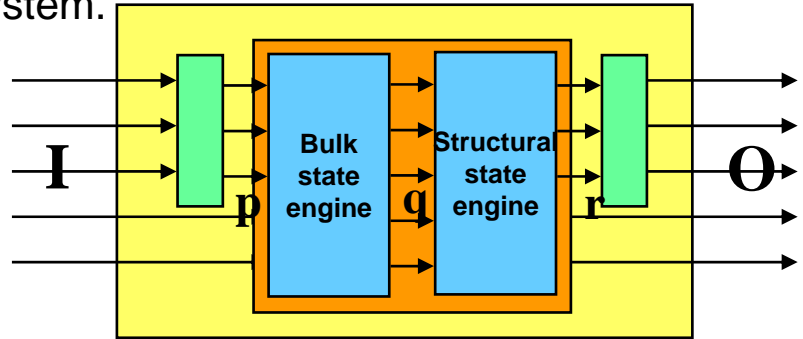




MODELING A MULTIPHYSICS SYSTEM

$\mathcal{U} : I_{in} \rightarrow O_{in}, I_{in} \subseteq \mathcal{W}_{in}, O_{in} \subseteq \mathcal{W}_{in}$ **Behavior Functional** relating the output to the inputs of the system.

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



$\mathcal{Q} = \mathcal{Q}(\xi, \zeta, b)$ **Bulk Constitutive Relations:** Functional dependence, of dependent variables on independent variables and parameters.

$\mathcal{R} = \mathcal{R}(\xi, \zeta, \xi) \cdot \xi$

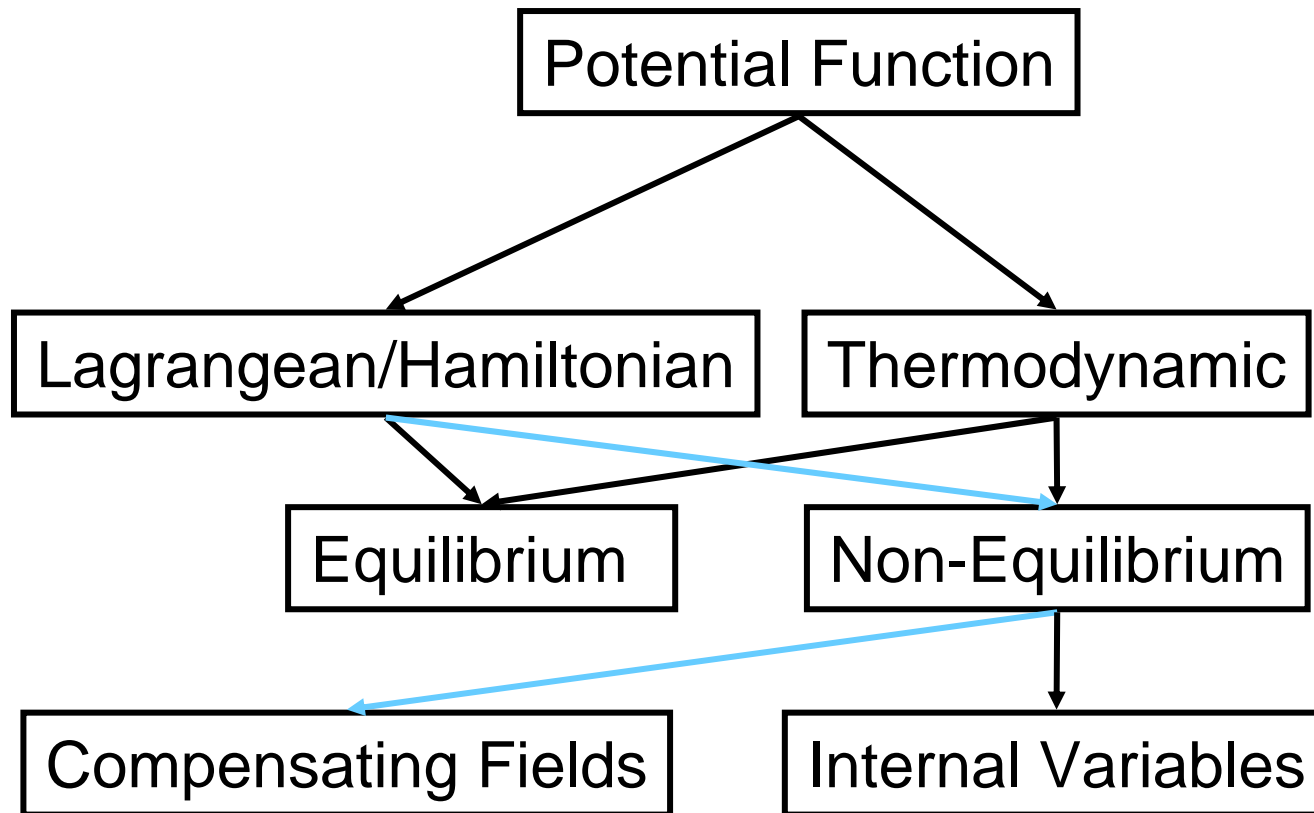
$\mathcal{N}^i(\Delta_{in} \xi, \frac{\partial f_{in}}{\partial \xi} \xi, \dots) = 0$ **Composition Behavior through Conservation Law Relations:** Dependence, of dependent variables on position in the structure, and time.

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



MODELING A MULTIPHYSICS SYSTEM

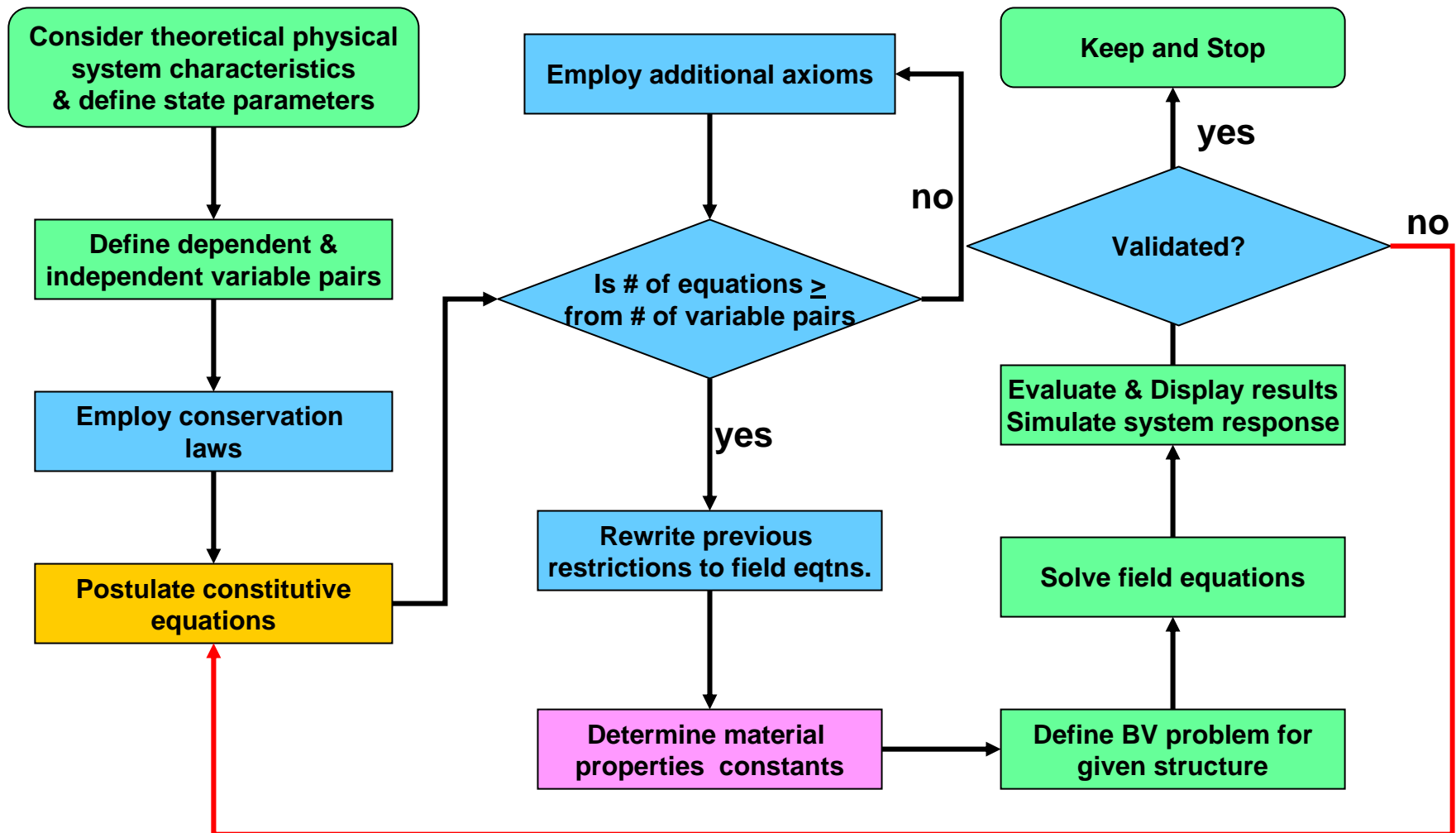
Methodologies for Developing Potential Functions





MODELING A MULTIPHYSICS SYSTEM

Model driven coupled field methodology





MODELING A MULTIPHYSICS SYSTEM

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 $\{X \rightarrow \underline{X}\}$ and "microscopic time reversal" as $\{t \rightarrow -t\}$ 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.



MODELING A MULTIPHYSICS SYSTEM

MAIN SCIENTIFIC CHALLENGES OF MODEL DRIVEN APPROACH

- Impossible Uncoupled Experiments for Coupling coefficients Determination?

EXAMPLE: Isotropic Nonlinear Electromagnetic Solids. Two of the 20 a priori 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

Ettinghausen's effect

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

Ohm's effect

Seebeck's effect

Anisotropic Seebeck's effect

Hall's effect

Nerst's effect

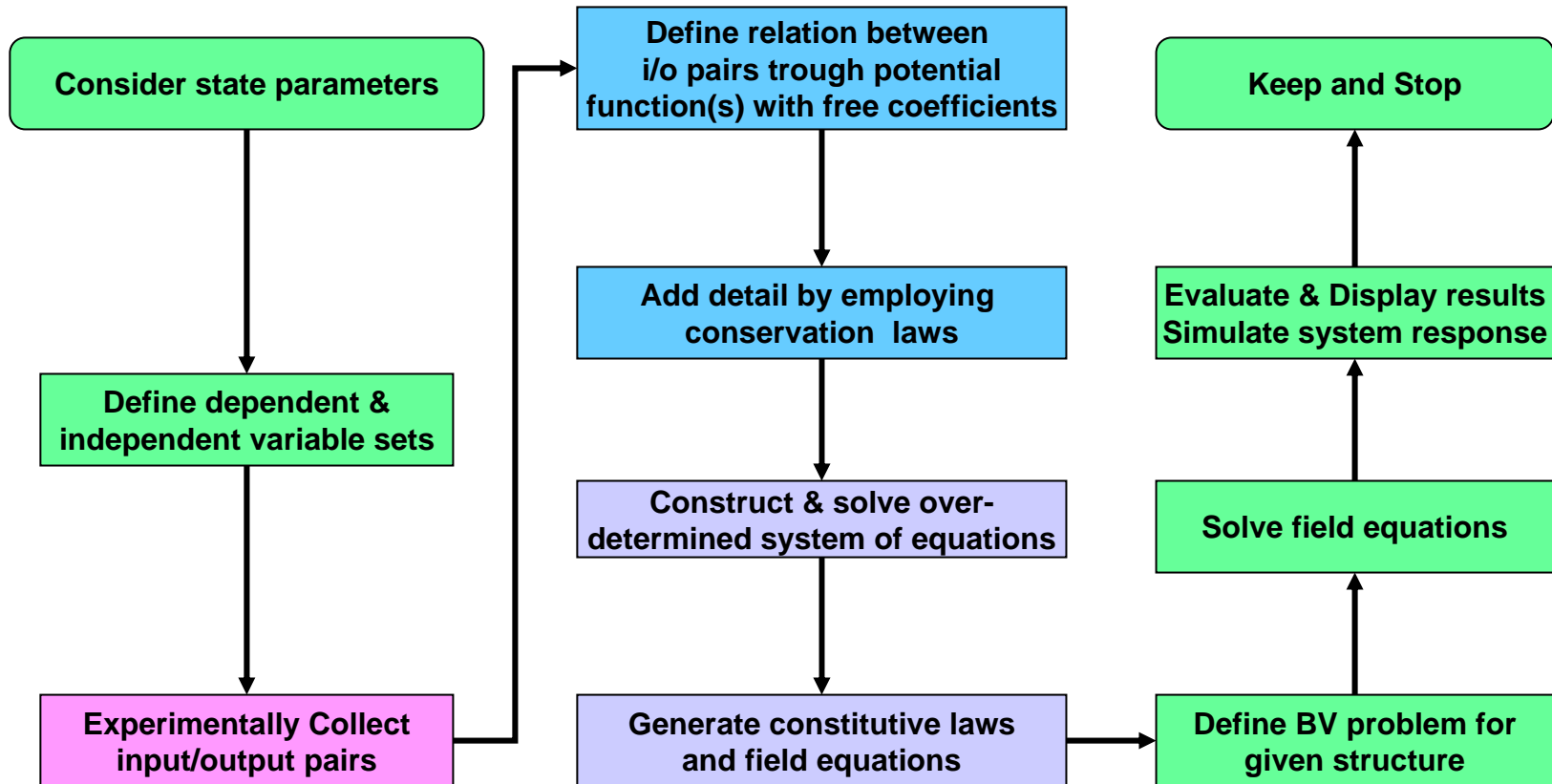
$$\begin{aligned}\tilde{J} = & \lambda_1 \tilde{E} + \lambda_2 \nabla T + \lambda_3 \tilde{e}^{-1} \tilde{E} + \lambda_4 \tilde{e}^{-1} \nabla T + \lambda_5 \tilde{E} \times \tilde{B} + \lambda_6 \nabla T \times \tilde{B} \\ & + \lambda_7 \tilde{e}^{-2} \tilde{E} + \lambda_8 \tilde{e}^{-2} \nabla T +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

- Potentially **NON TERMINATING**



MODELING A MULTIPHYSICS SYSTEM

Data driven Modeling methodology





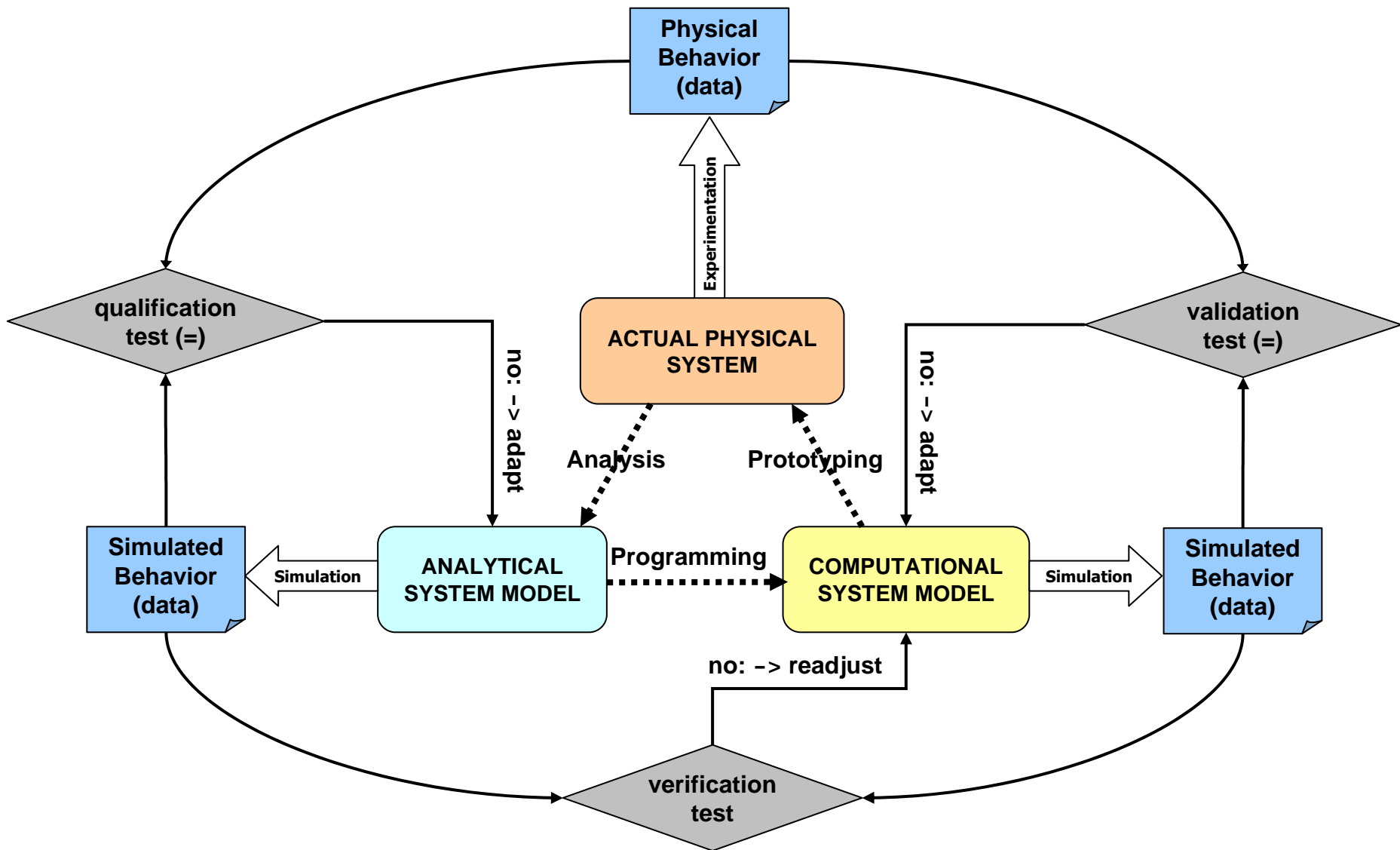
QV&V Definitions

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.

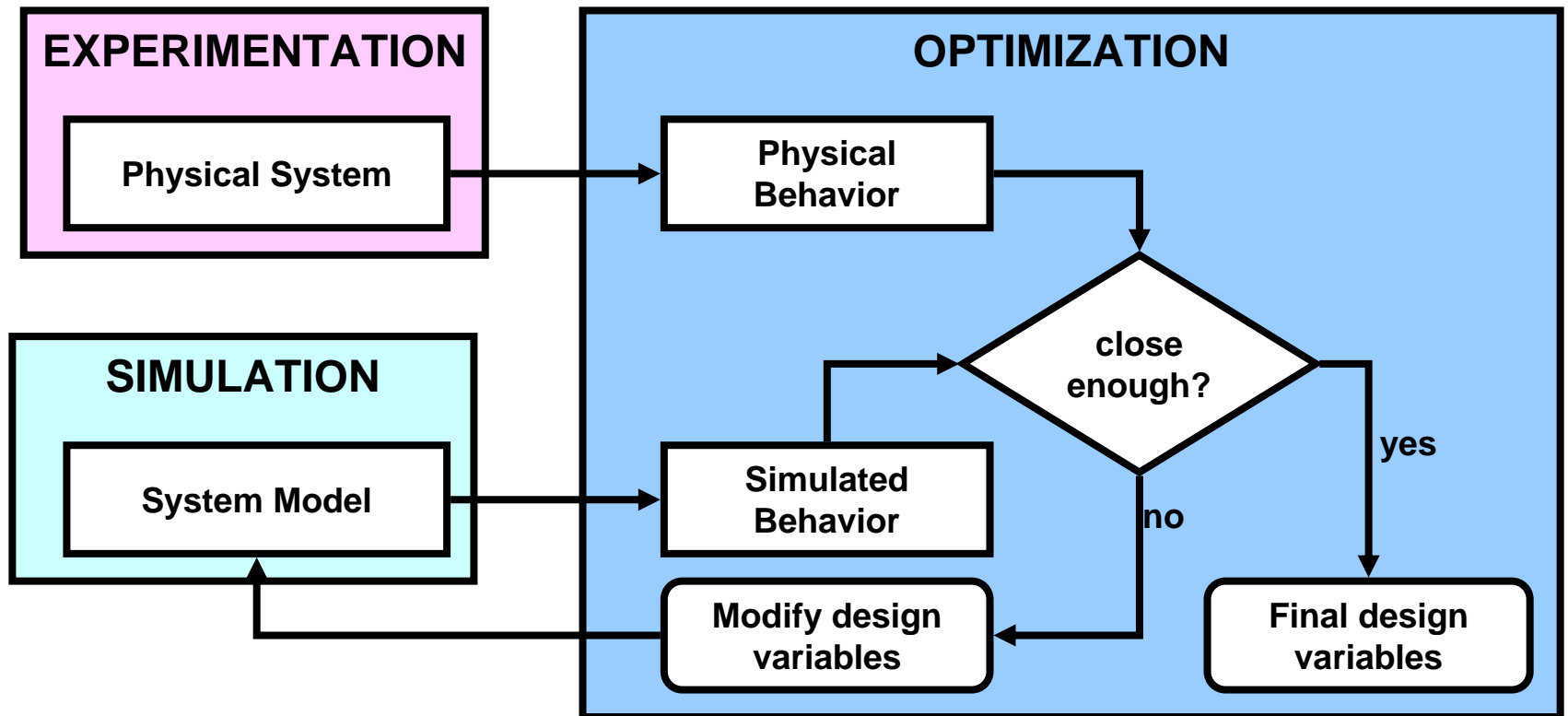


Model-Driven Approach for Q&VV



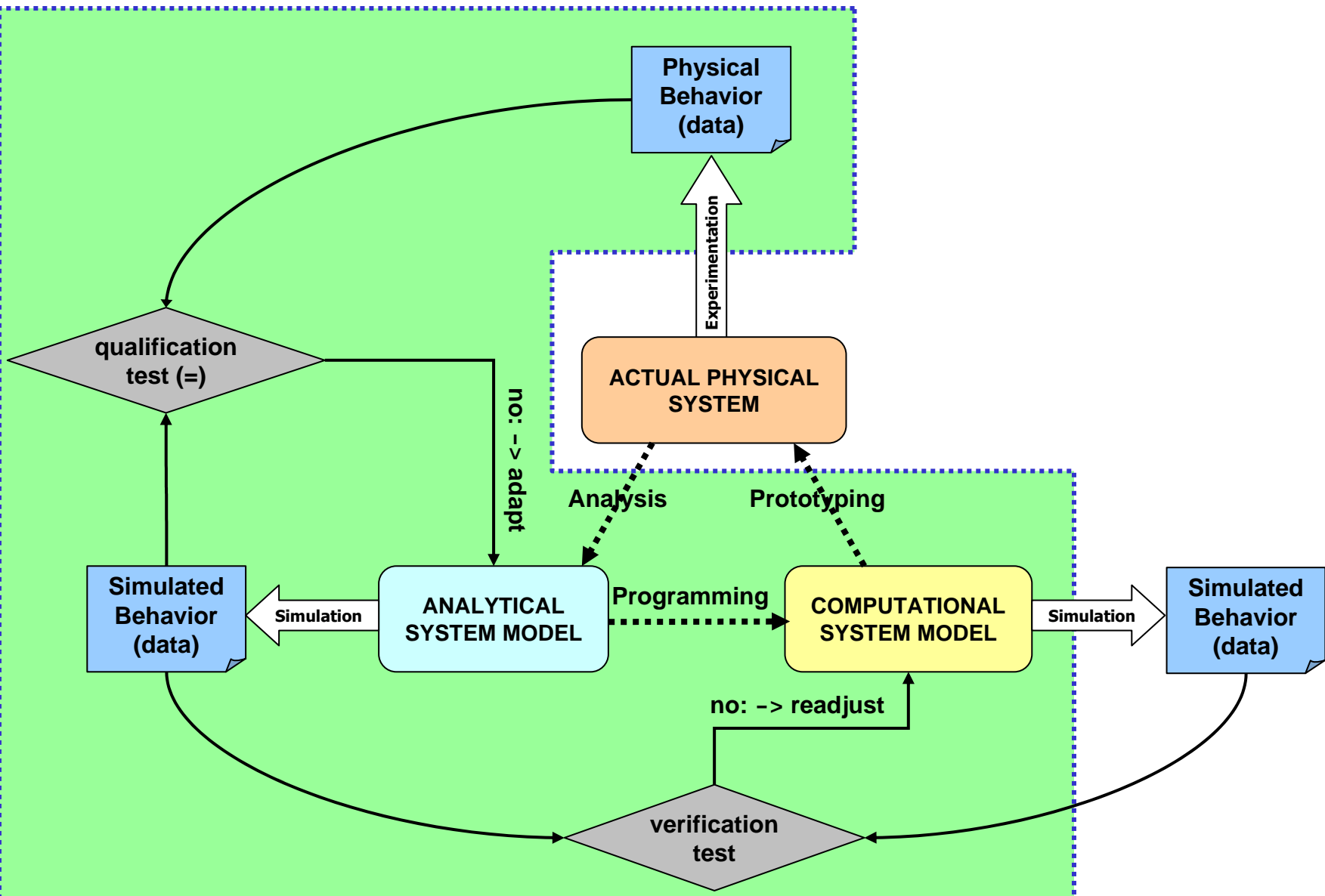


General Optimization Approach





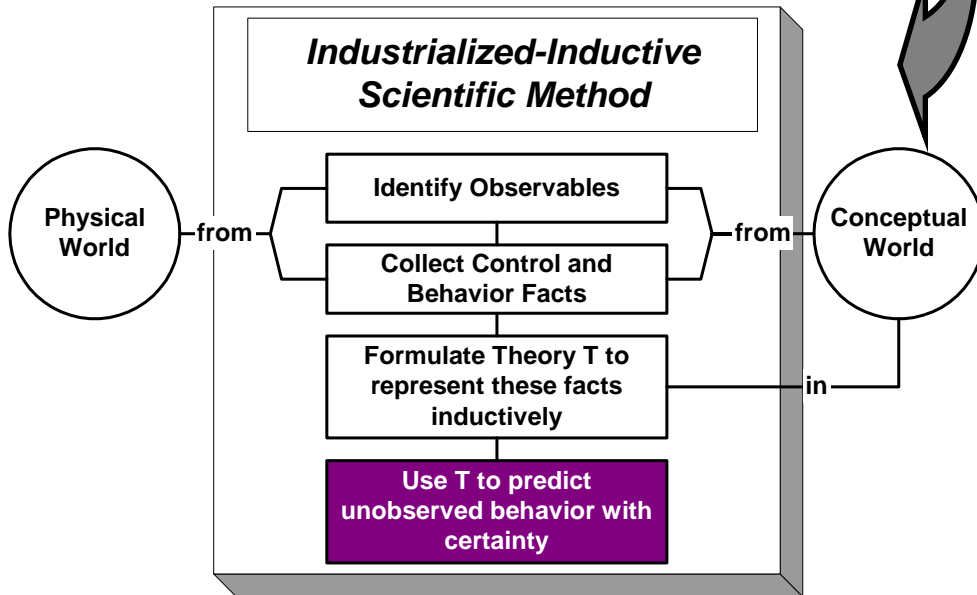
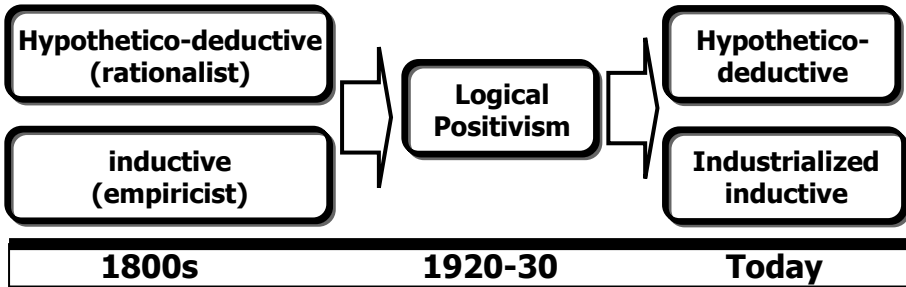
Data-Driven Approach for Q&VV



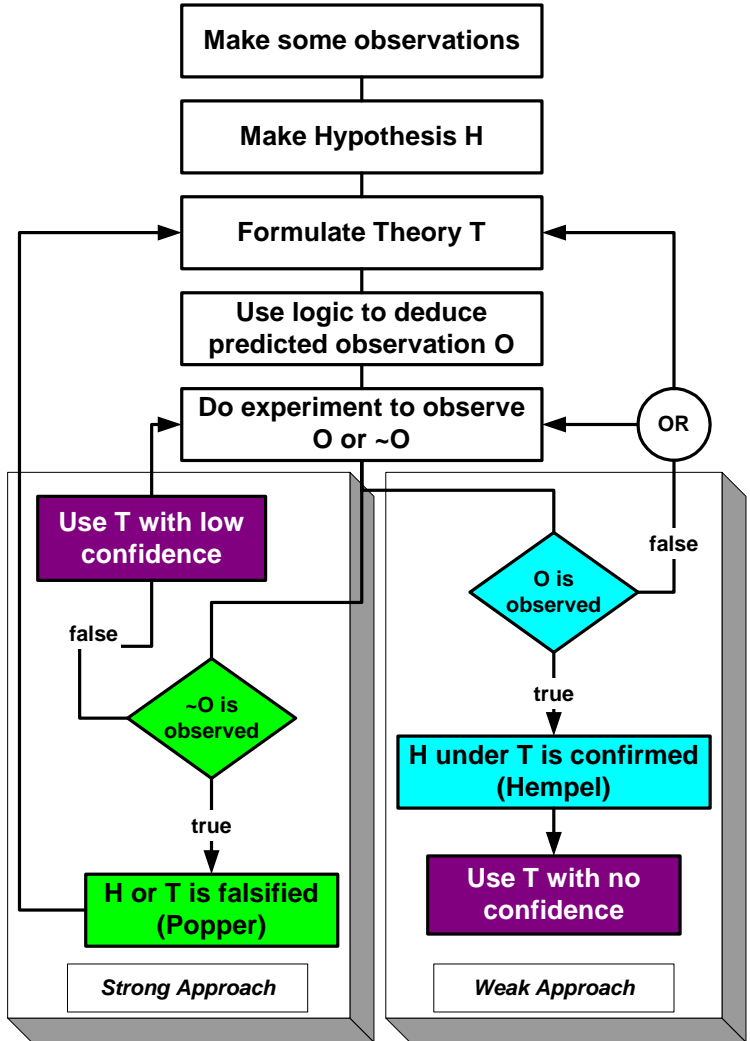


EPISTEMOLOGICAL BACKGROUND

Scientific Method Evolution

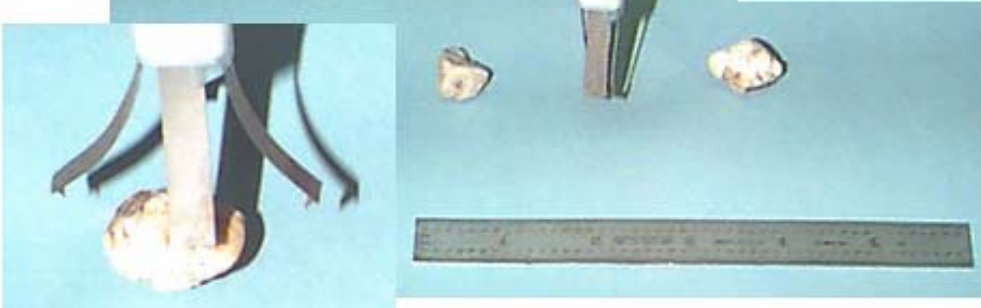


Hypothetico-deductive Scientific Method





EXAMPLE: IONIC POLYMER COMPOSITE ARTIFICIAL MUSCLES





Ionic Polymer Metal Composite (IPMC) Large Deflection Plates

Non-linear electro-elasto-dynamic field PDEs:

For Electric and Mechanical activation only
without mass transport:

$$\begin{aligned}\nabla^2 \nabla^2 w - (1 + \nu) p_k \nabla^2 E_k &= \frac{h}{N} \left(\frac{q}{h} + F_{,22} w_{,11} - 2F_{,12} w_{,12} + F_{,11} w_{,22} \right), \\ \nabla^2 \nabla^2 F - E p_k \nabla^2 E_k &= E [(w_{,12})^2 - w_{,11} w_{,22}] \\ \varepsilon_0 \nabla^2 V + p_i \left\{ \frac{1 - 2\nu}{Eh} \nabla^2 F - p_k E_k \right\} &= \rho_c\end{aligned}$$

or equivalently:

$$\begin{aligned}\nabla^2 \nabla^2 w - c_1 \nabla^2 V &= \frac{h}{N} \left(\frac{q}{h} + F_{,22} w_{,11} - 2F_{,12} w_{,12} + F_{,11} w_{,22} \right), \\ \nabla^2 \nabla^2 F - c_2 \nabla^2 V &= E [(w_{,12})^2 - w_{,11} w_{,22}] \\ \nabla^2 V + c_3 \nabla^2 \nabla^2 F + c_4 V + c_5 &= 0\end{aligned}$$



Multi-Objective Function Optimization

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

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 unknown constants to be identified

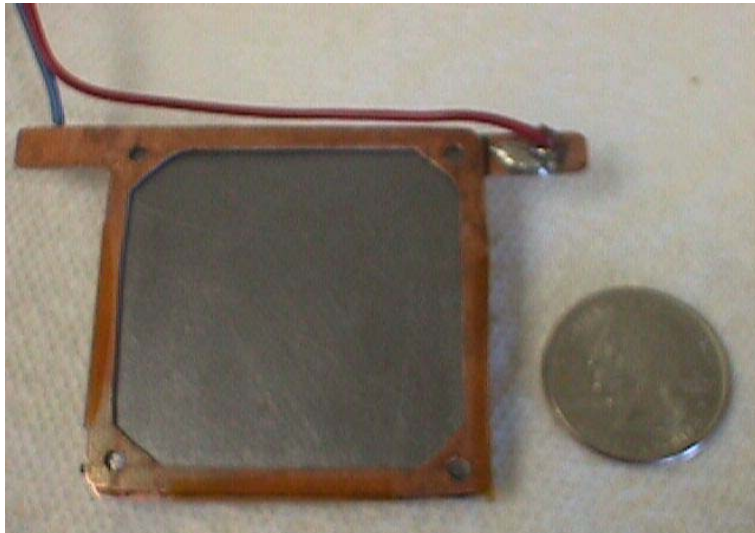
t_j^u, t_j^l are the upper and lower limits constraining each unknown j

To fully characterize c_j 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

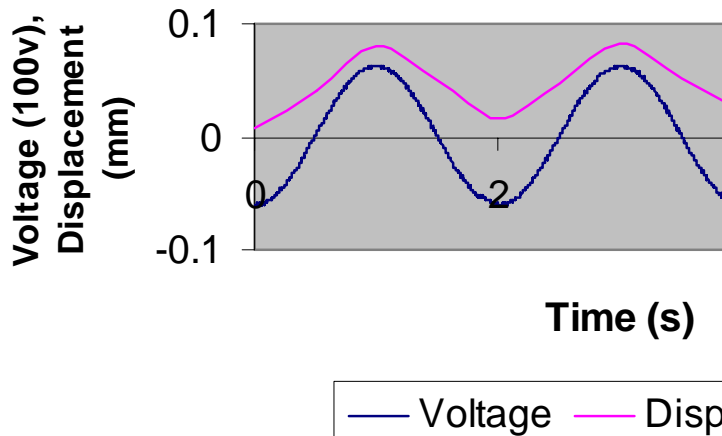


IPMC Large Deflection Plates: Experimental Results

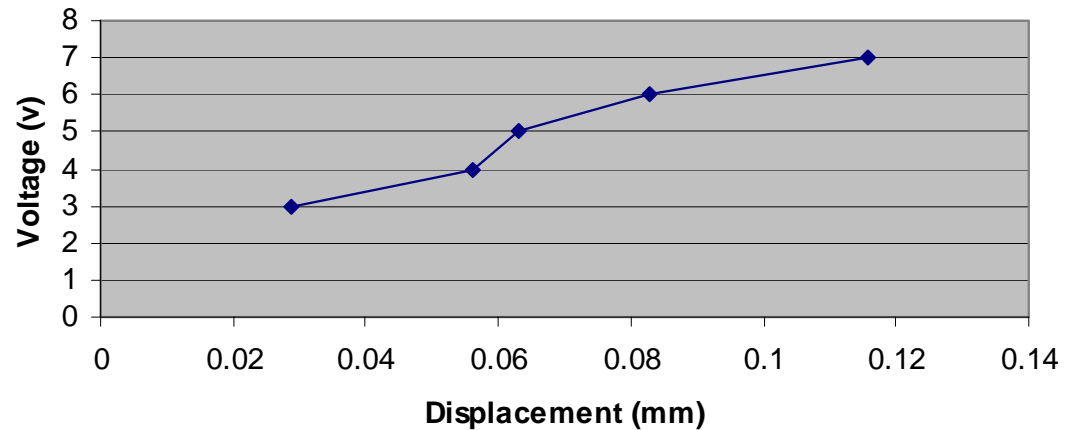
(M. Shahinpoor UNM)



Voltage, Displacement vs. Time of an IPMC plate



Voltage vs. Displacement of an IPMC plate (40mm x 40mm x 0.21mm)





IPMC Large Deflection Plates: Biharmonic Single-Field Bases

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

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

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

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

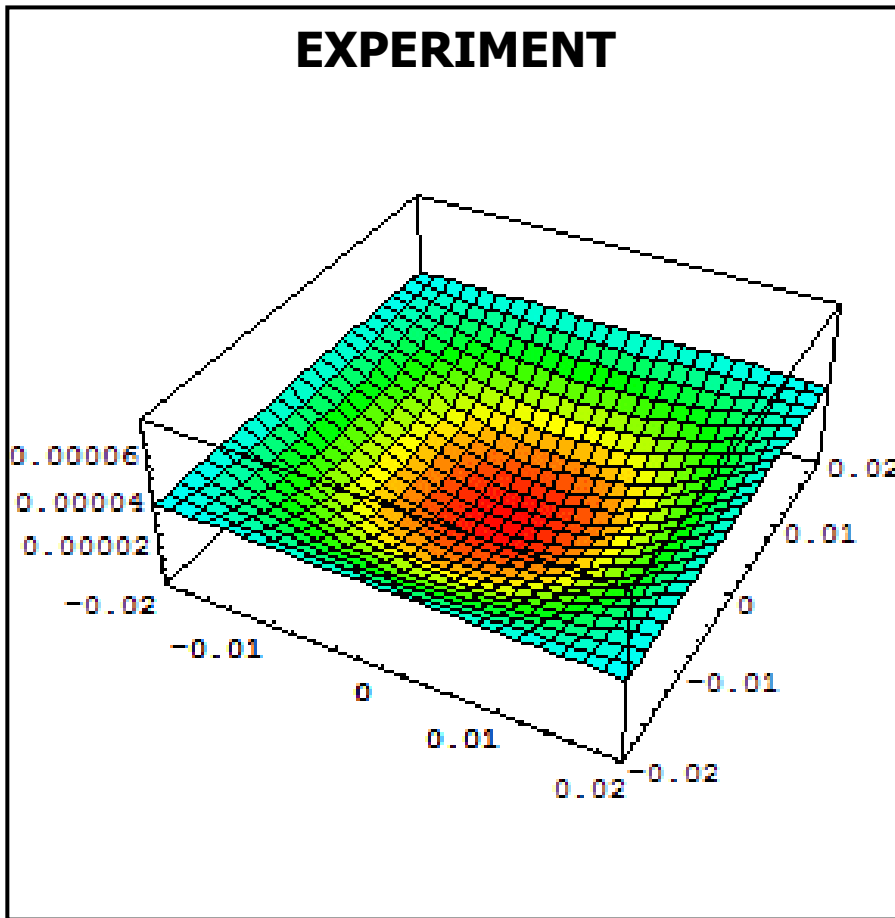
$D =$ Flexural rigidity of the plate

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

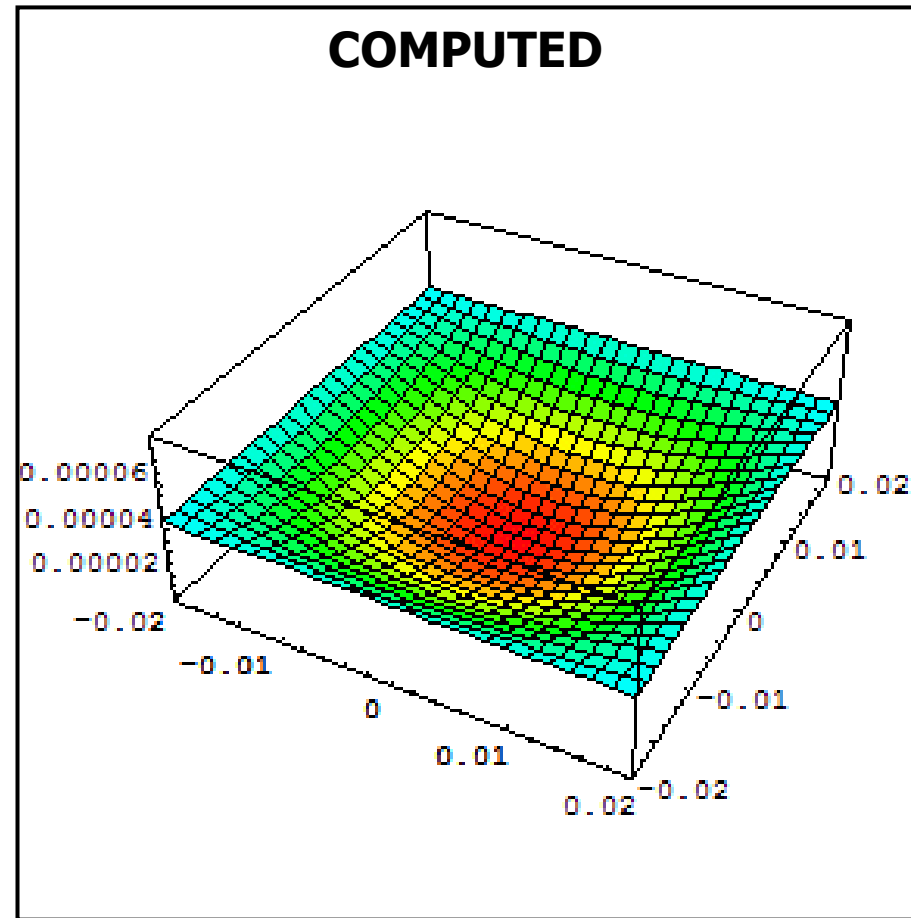


Deflection Time Histories in 3D carpet plots

EXPERIMENT



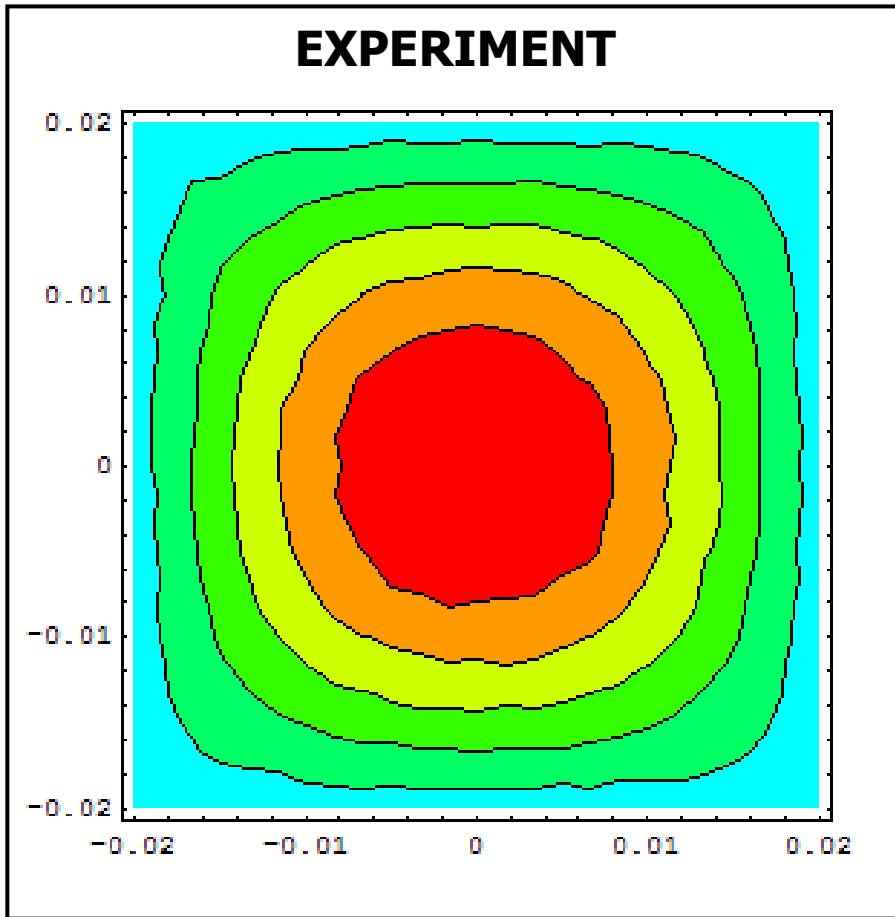
COMPUTED



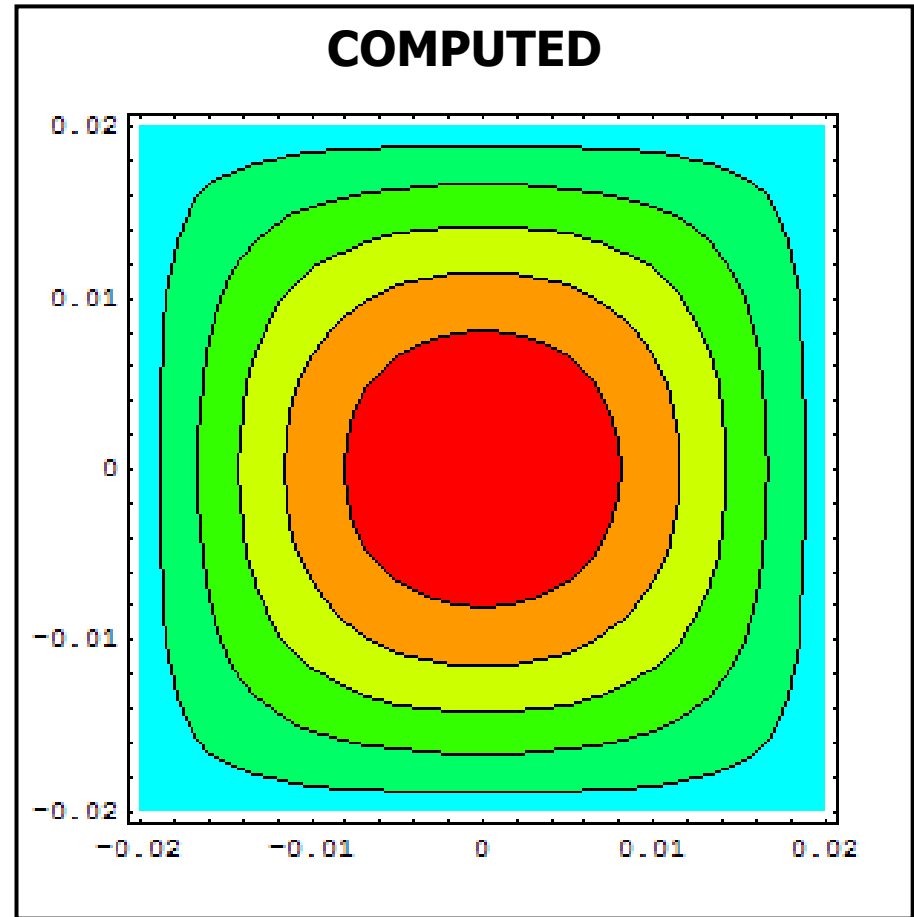


Deflection Time Histories in Contour plots

EXPERIMENT



COMPUTED





Conclusions

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

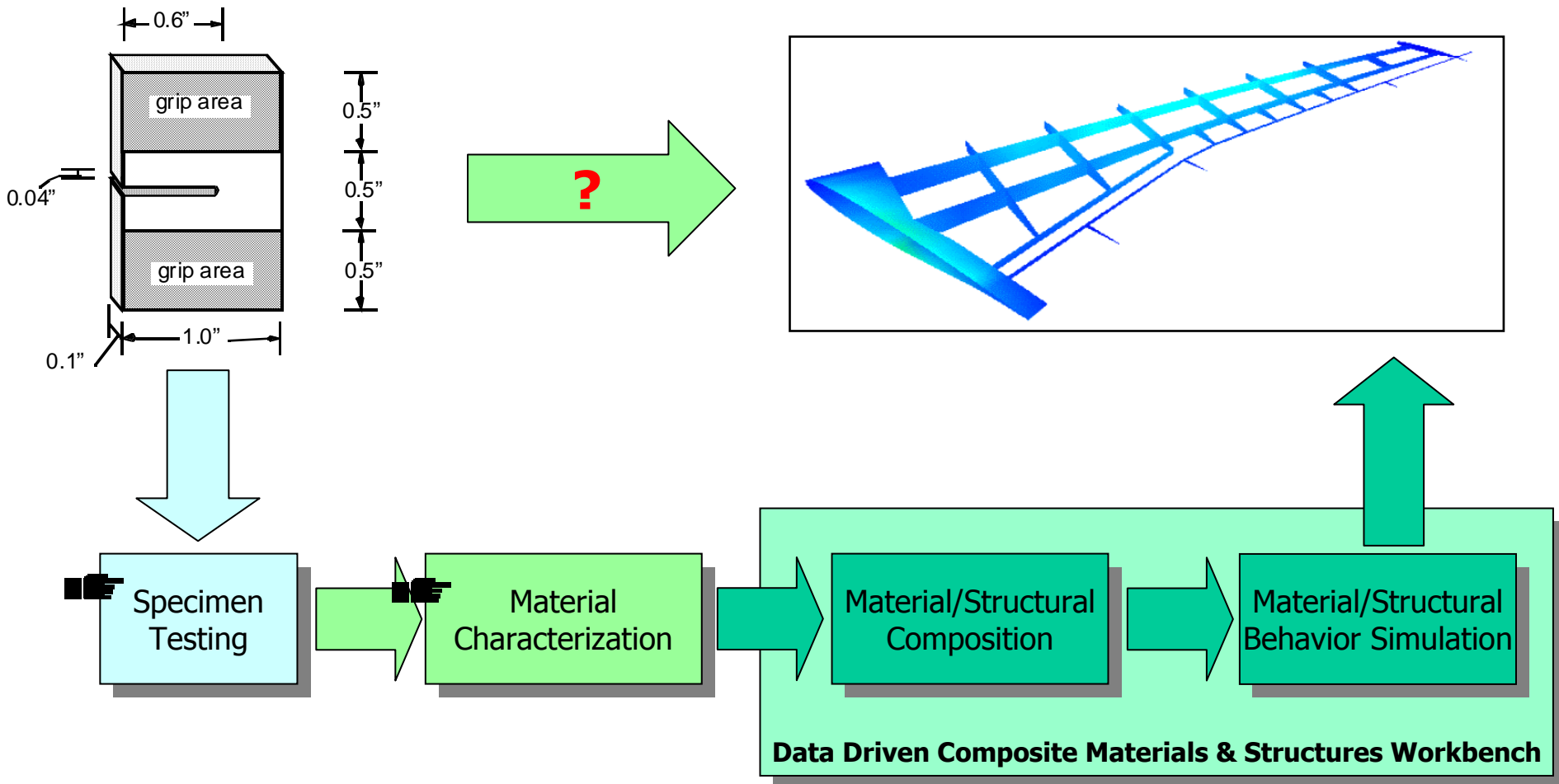


**THANK YOU FOR YOUR ATTENTION
QUESTIONS?**



Data-Driven Approach: Example

Identify material from small specimens to predict behavior of large system

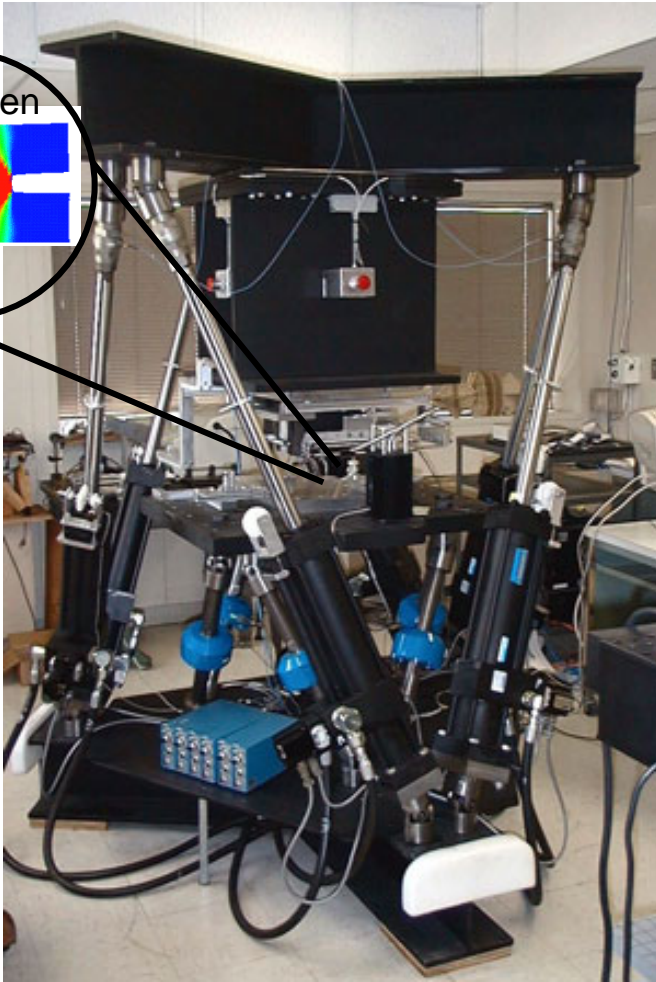




MECHATRONICALLY AUTOMATED APPROACH: Overview

General Case:

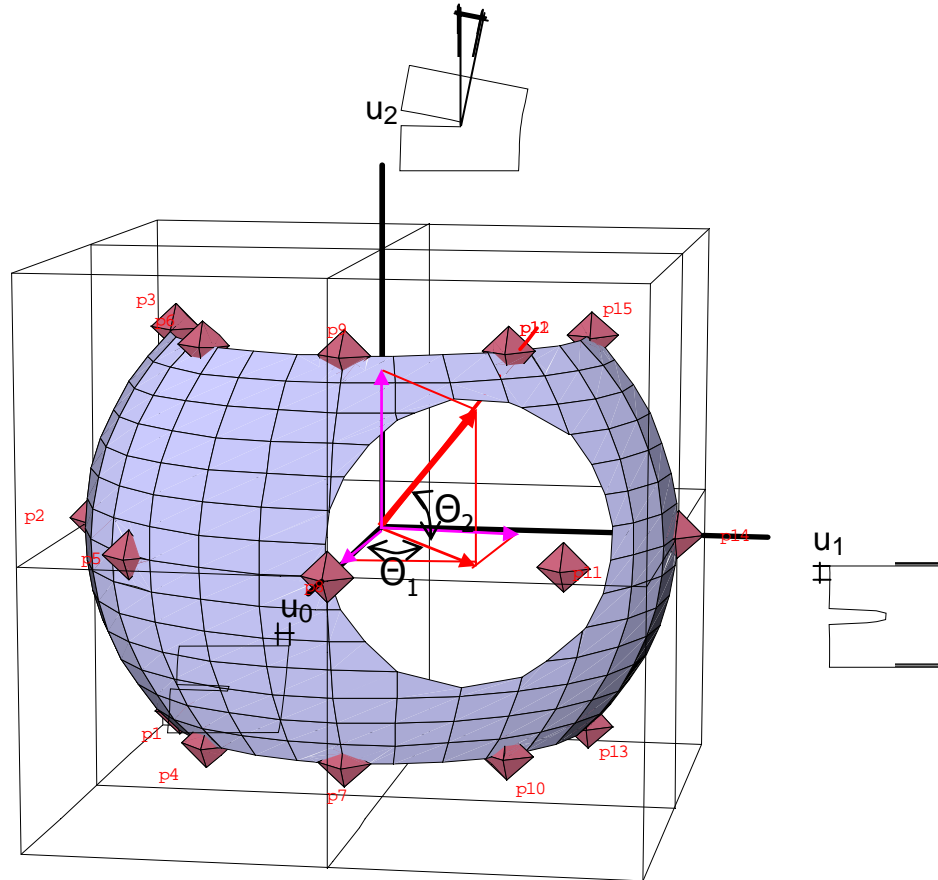
3 displacements + 3 rotations + 3 forces + 3 moments + $N_p \times 3$ strains + $N_p \times N_f = 12 + (3 + N_f) \times N_p$ Datastreams



NRL's Automated 6-D Loader

Special Case:

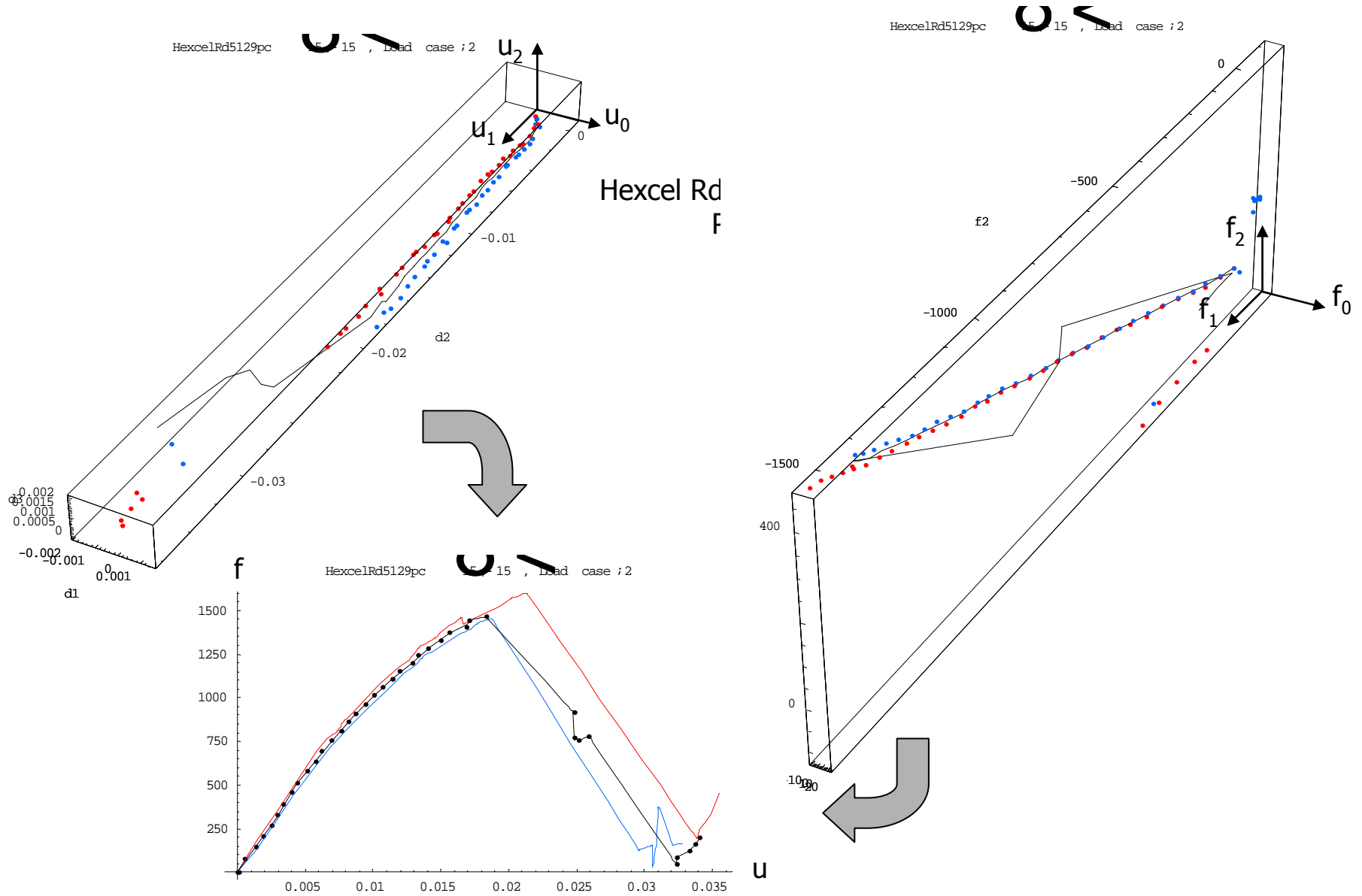
2 displacements + 1 rotation = 3DOFs = 6 Datastreams





Approach

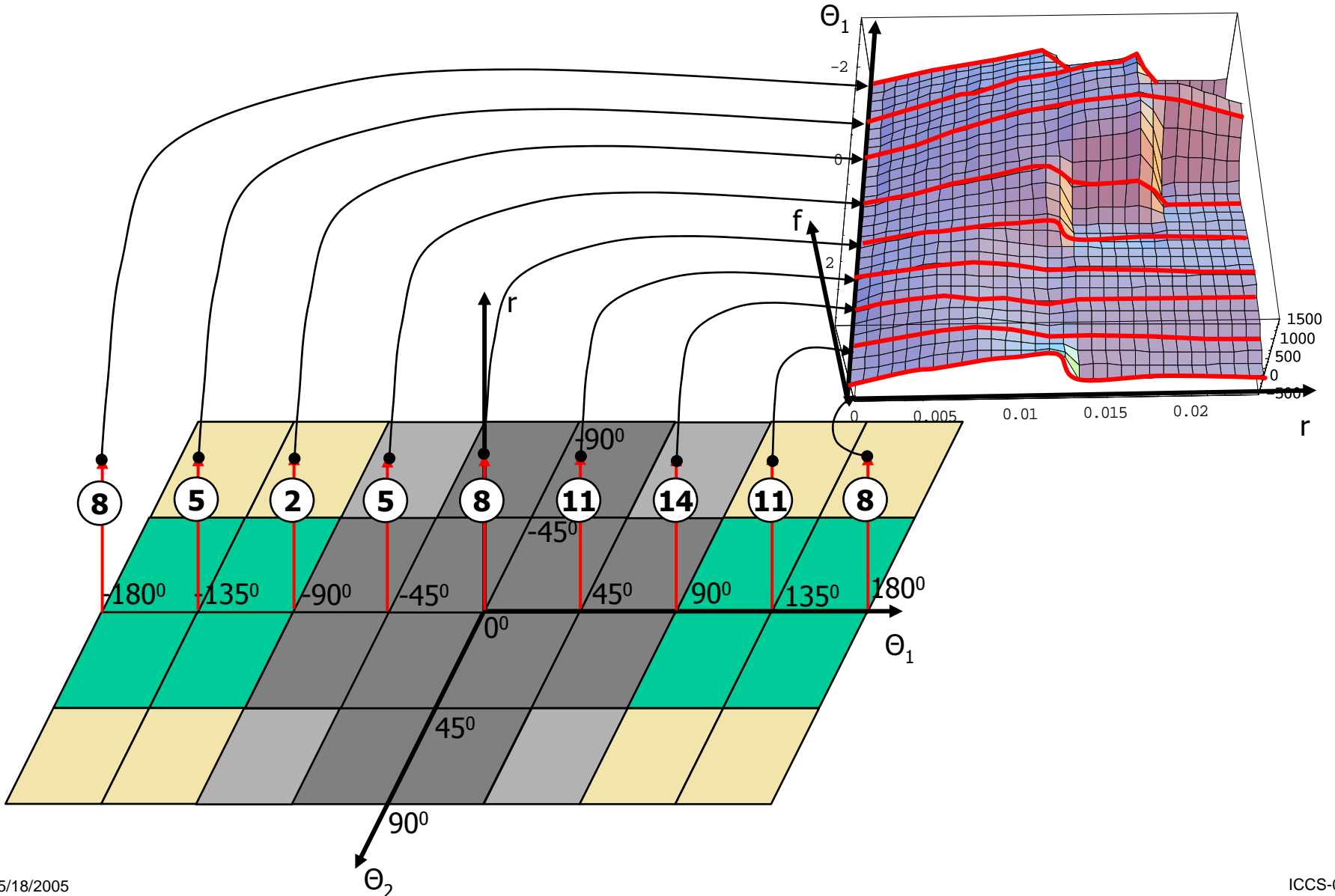
Data driven methodology for PMCs: Data Collection





Approach

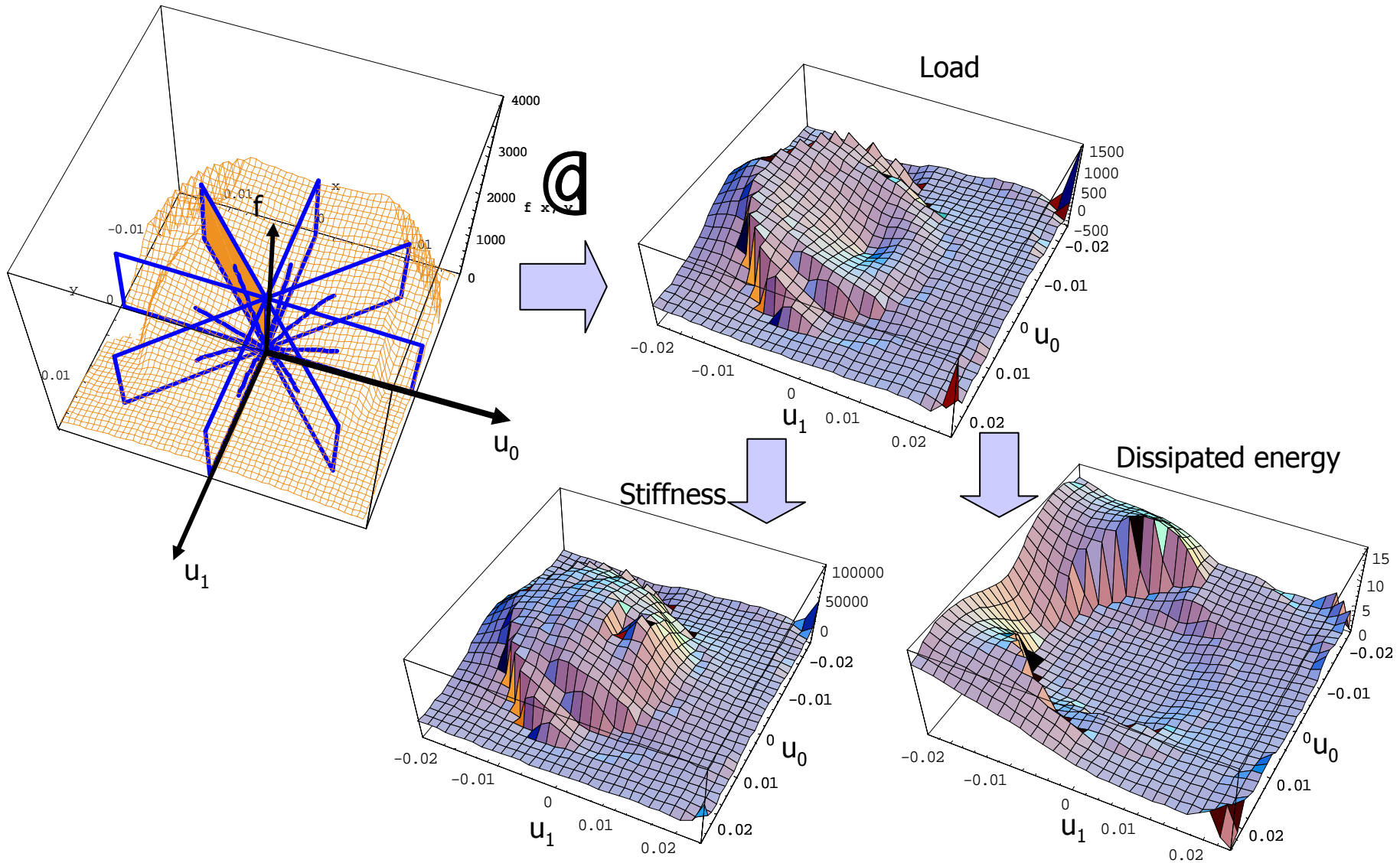
Data driven methodology for PMCs: Data Reduction





Approach

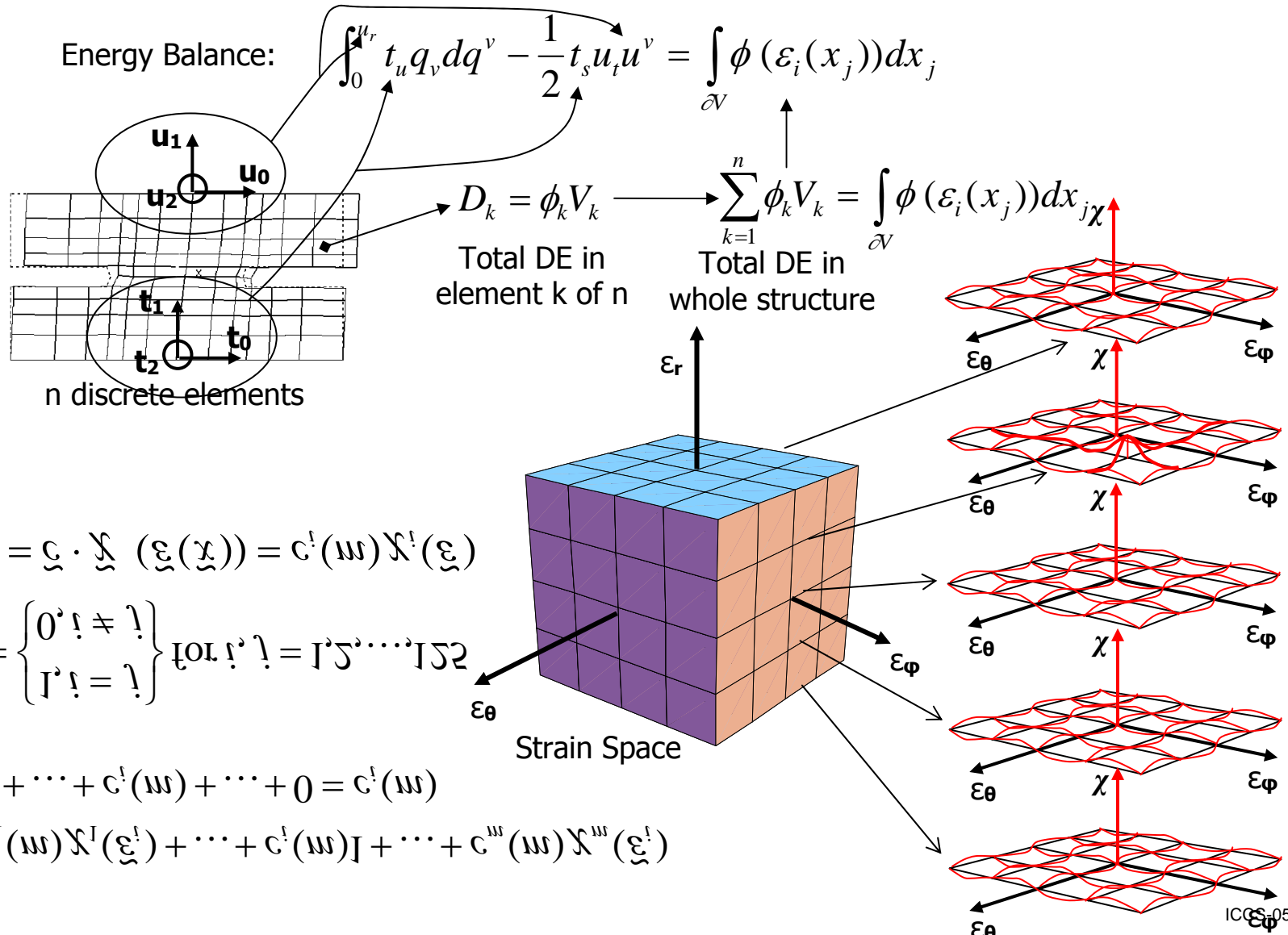
Data driven methodology for PMCs: Data Reduction





MECHATRONICALLY AUTOMATED APPROACH: Inverse Model

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





MECHATRONICALLY AUTOMATED APPROACH: Optimization

For a loading point p:

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

$$\sum_{\Gamma=1}^{\Gamma} c^{\Gamma}(W) X^{\Gamma}(\xi_b^{\Gamma}) \Lambda_b^{\Gamma} + \epsilon_b = D_b$$

For all selected loading points:

$$[X] \xi + \epsilon = q$$

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

DED monotonicity:

$$[W] \xi \geq 0$$

100 additional constrains

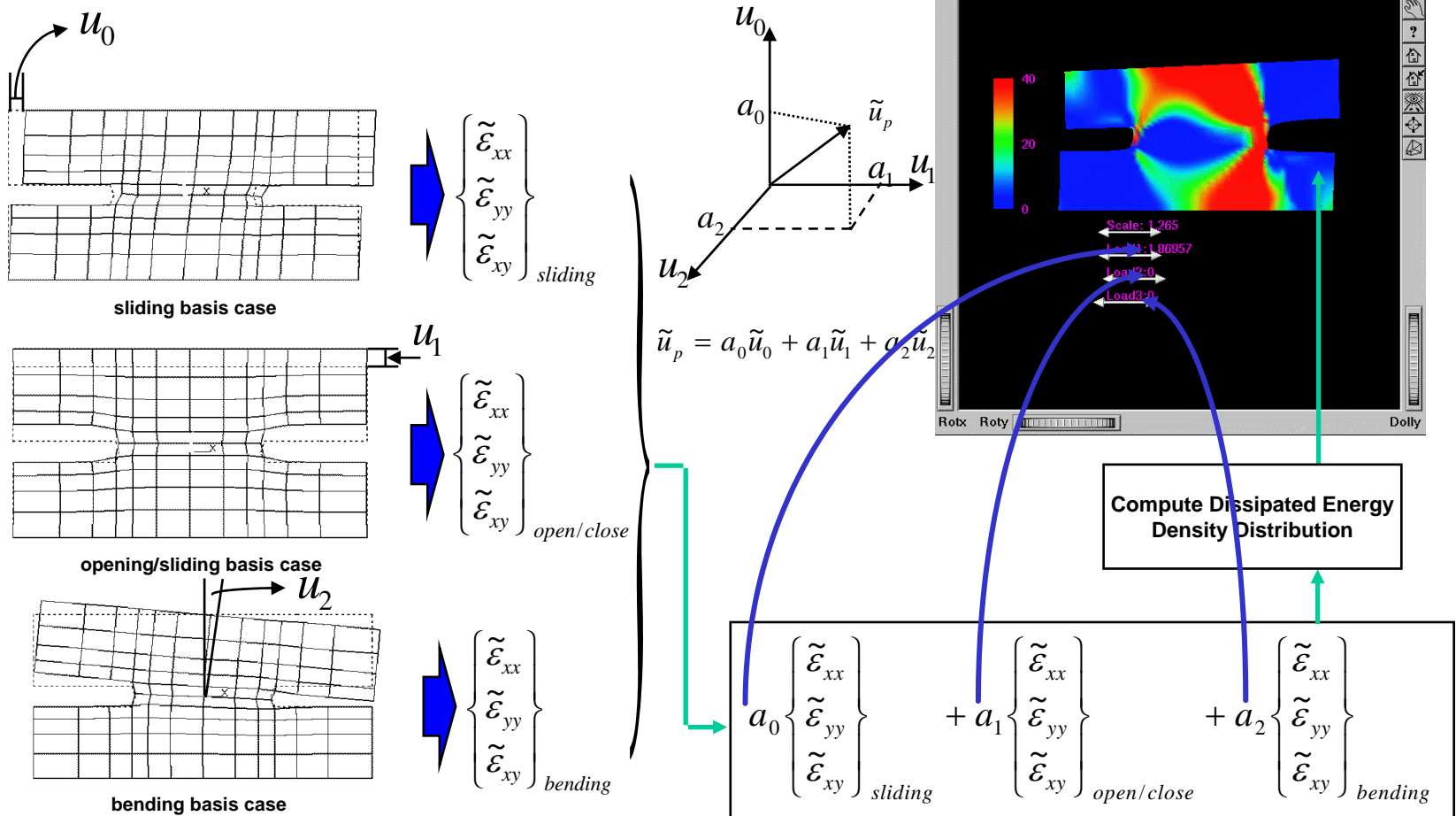
Final Problem: Minimize $\|\xi\|$ subject to $[W] \xi \geq 0$

Solution Method: Least Squares with Linear Constrains



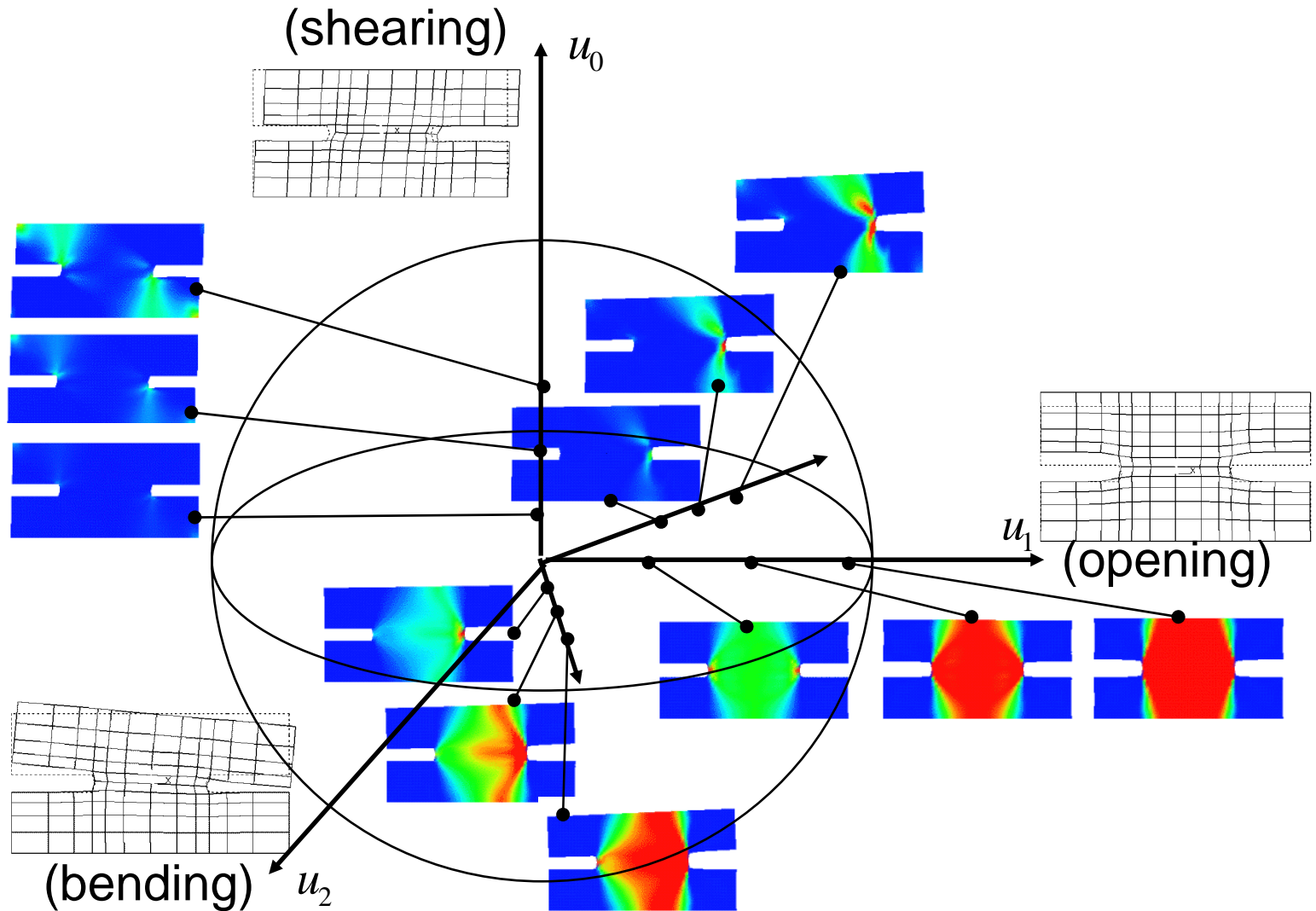


UTILIZATION OF BASIS LOADING CASES RESPONSE THROUGH LINEAR COMBINATION OF RESULTING STRAIN FIELDS





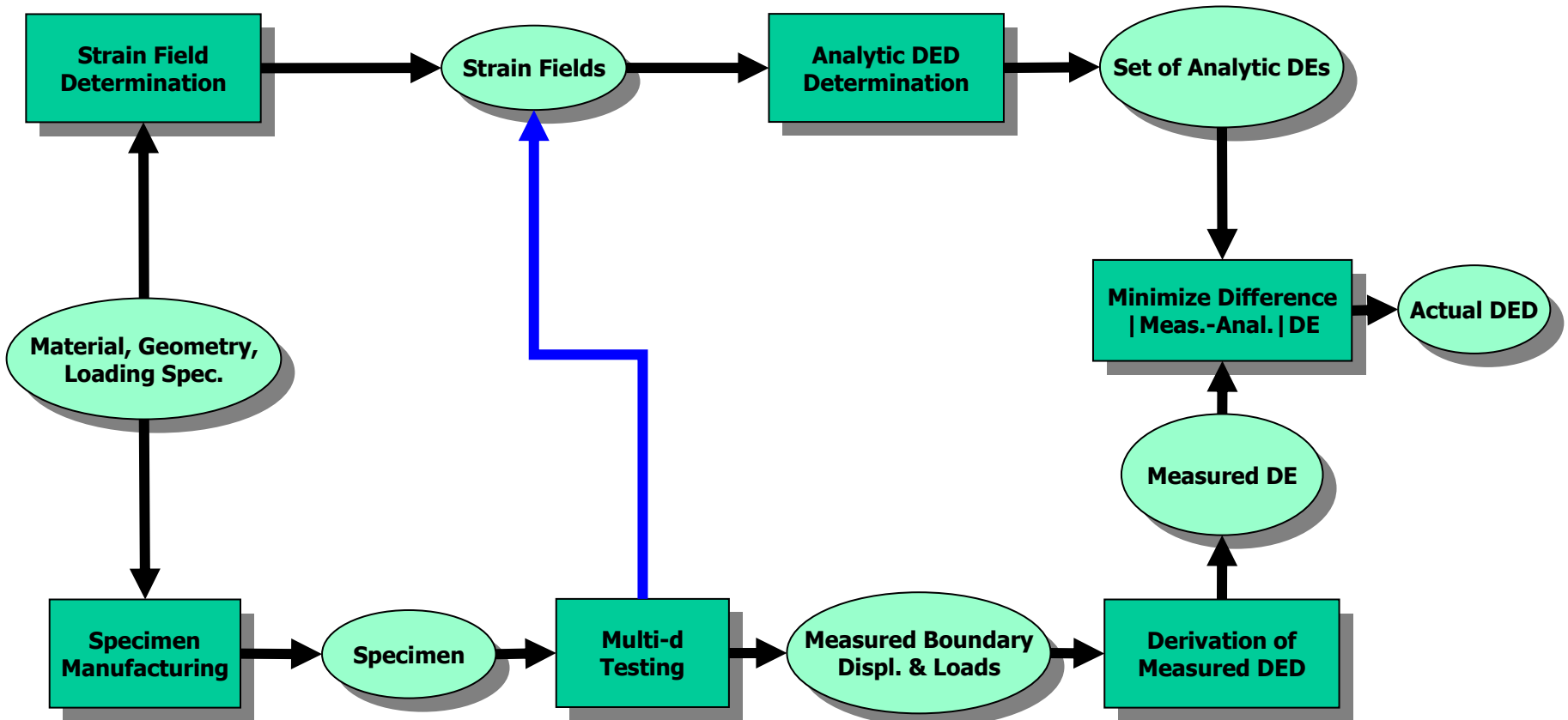
MECHATRONICALLY AUTOMATED APPROACH: Simulation Synthesis





Approach

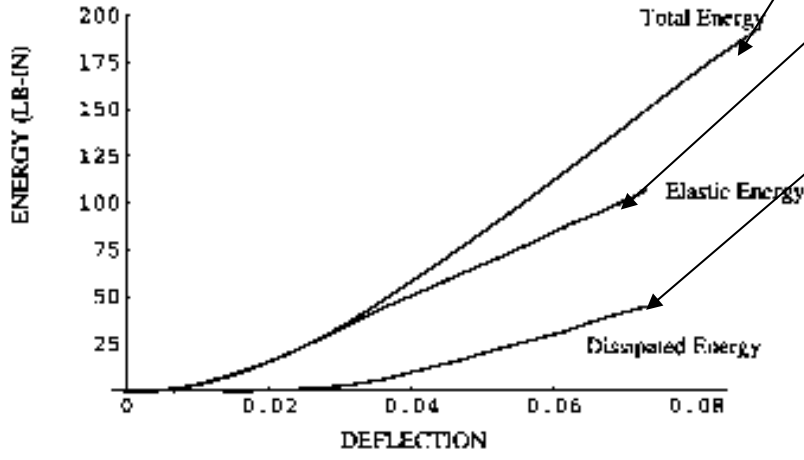
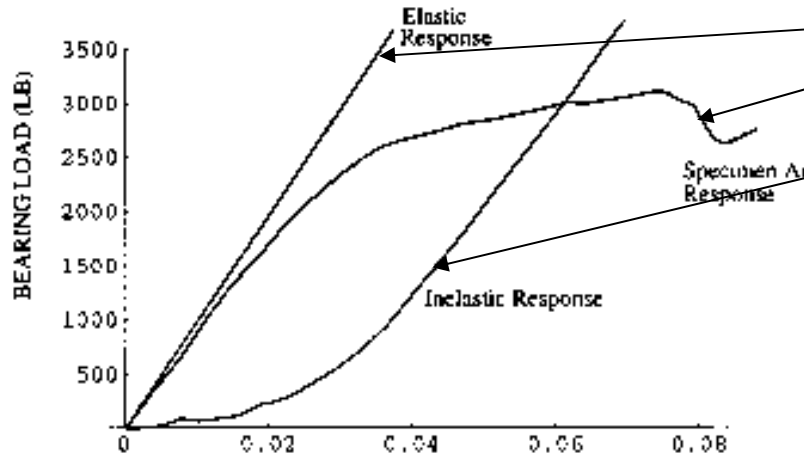
Data driven methodology for PMCs: Material Characterization





How - Approach

STRUCTURAL SYSTEM IDENTIFICATION-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

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

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

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

$$A_{ij}c_i = b_j$$



How - Approach: GENERAL CONTINUOUS 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

$\mathcal{W} : I_{in} \rightarrow O_{in}, I_{in} \subseteq \mathcal{W}, O_{in} \subseteq \mathcal{W}$ **Behavior Functional** relating the output to the inputs of the system.

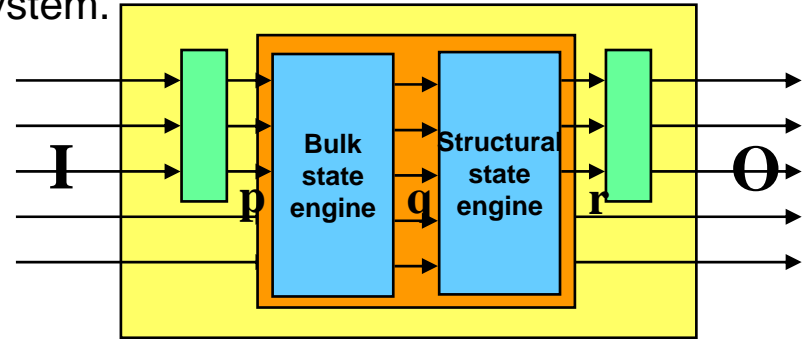
$\mathcal{K}(\xi, \zeta, b) = 0$ **Relational restriction** over dependent, independent, parameter variables.

$d = \mathcal{Q}(\zeta, b)$ **Bulk Constitutive Relations:** Functional dependence, of dependent variables on independent variables and parameters.

$\xi = \mathcal{Q}(\zeta, \xi) \cdot \xi$

$\mathcal{N}(\Delta, d, \frac{\partial f_{in}}{\partial d}, \dots) = 0$ **Composition Behavior through Conservation Law Relations:** Dependence, of dependent variables on position in the structure, and time.

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





MODELING A MULTIPHYSICS SYSTEM

Data driven Modeling methodology

$$\underline{d} = \Delta^{\underline{b}} \Xi(\underline{\zeta}, \underline{b}) \quad \text{Vector Function Storage Mechanism:}$$

Potential or Energy Density function.

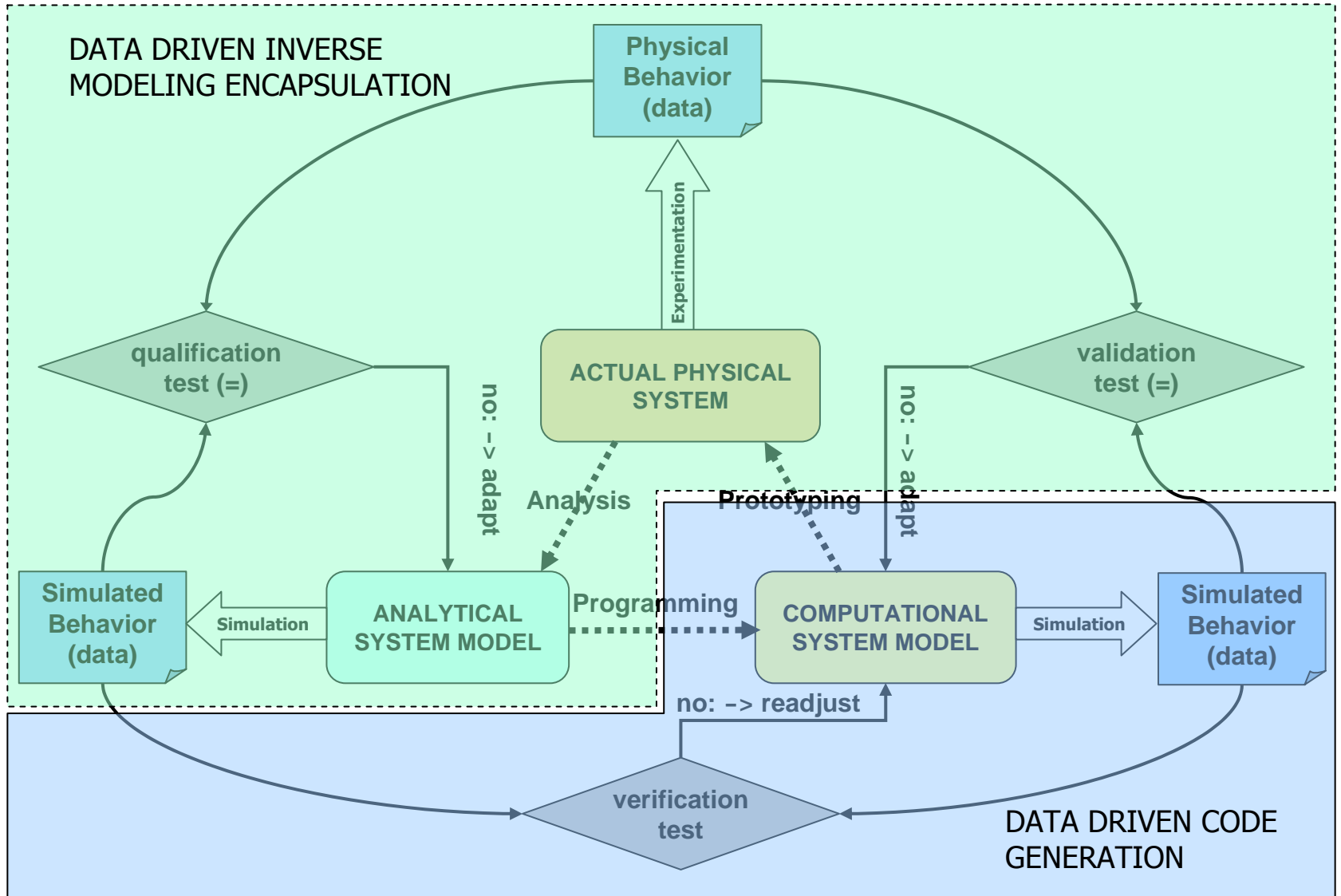
$$\Xi(\underline{\zeta}, \underline{b}) = \Phi(\underline{\zeta}, \underline{b}) + \phi(\underline{\zeta}, \underline{b}) \quad \text{Additivity of recoverable and non-recoverable components.}$$

$$\Phi(\underline{\zeta}, \underline{b}) = \int \underline{d}(\underline{b}) \cdot \underline{b} \quad \text{Recoverable energy definition.}$$

$$\phi(\underline{\zeta}, \underline{b}) = \underline{c} \cdot \underline{f}(\underline{\zeta}, \underline{b}(\underline{x})) \quad \text{Non-recoverable energy definition.}$$



Traditional vs. Data-Driven Approach of Q&VV





Data-Driven System Identification and Simulation

