Fast, Physics-based Models for Real-time Process Control And Monitoring

Sarbajit Ghosal, Jon Ebert, Narasimha Acharya, Dick de Roover,
La Moyne Porter, Abbas Emami-Naeni

SC Solutions, Inc.
1261 Oakmead Pkwy, Sunnyvale, CA 94085
scsolutions.com/controls/

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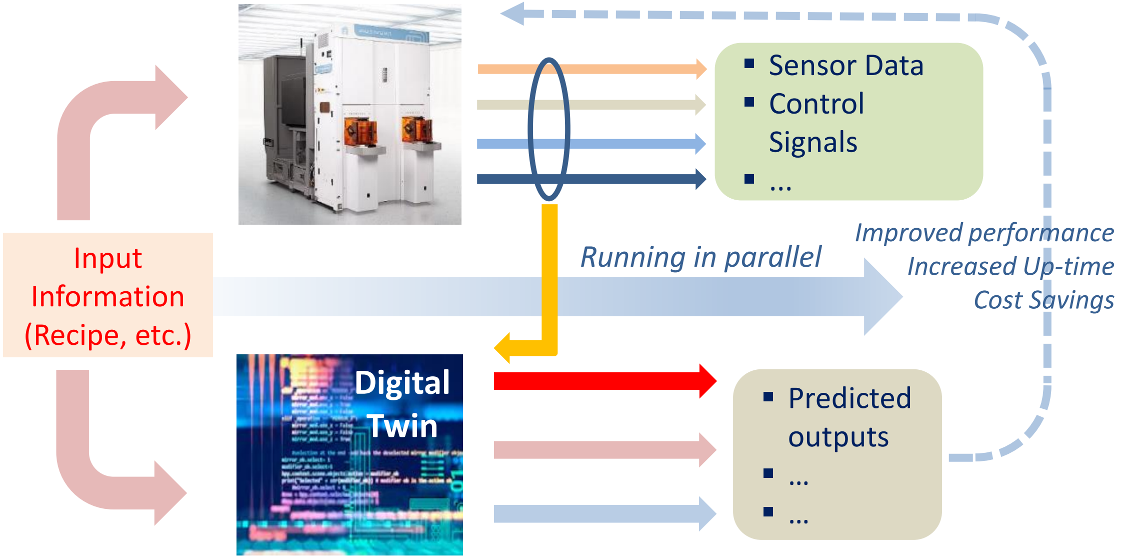
Overview

- **Models used for digital twins (DT).**
- **How we use fast, physics-based, models at SC.**
- **How SC's fast models may be used in DTs.**
- **Examples:**
  - RTP (generic model with animation of sim results).
  - Etch subsystem models intended for process monitoring.
- **Comments and questions.**

Digital Twin

- The standards document on digital twin framework for manufacturing (ISO 23247*) defines a digital twin (DT) as a “fit for purpose digital representation of an observable manufacturing element with synchronization between the element and its digital representation”.

- **For this talk, we define DT in simpler terms as a purpose-driven dynamic model of a wafer processing system with predictive capabilities:**
  - A DT simulation runs faster than real time and describes the system’s change in behavior with time with acceptable accuracy.
  - DT is dynamically updated with sensor data.
  - DT is not quite a digital replica of the system. Outputs are probabilistic, not deterministic.



** ISO 23247-1: Automation Systems and Integration - Digital Twin Framework for Manufacturing – Part 1: Overview and general principles. International Organization for Standardization, Geneva, Switzerland (2021).*

Applications in the Semiconductor Industry

Digital Twins find use in high-value or safety-critical applications.

Control & Diagnostics

- Process control.
- Process optimization.
- System (chamber) matching.
- Fault diagnostics.
- Virtual sensing.

Prognostic & Monitoring

- Predictive maintenance.
- Lifetime prediction.
- Performance assurance.
- Assembly verification.
- Supply chain monitoring through model linking.

Dynamic Process Models for DT

- **A key component of DT is dynamic process model that has predictive capability.**
- **Underlying physics governed by sets of coupled, nonlinear PDE’s.**
- **High-fidelity discretized physics-based model typically consist of hundreds of thousands or even millions of ODE’s:**
  - too computationally intensive to simulate in real time.
  - uncertain values of physical parameters.
- **DT’s need models that:**
  - Run faster than real time.
  - Predict key states with sufficient accuracy.
  - May have parameters that can be tuned continually based on sensor data.

Developing Fast, Low-Order Dynamic Models

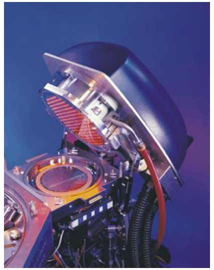
- **Reduced-order versions of first-principles, high-order models developed using various techniques:**
  - Galerkin.
  - Aggregation.
  - Balanced Realization.
  - Proper Orthogonal Decomposition (POD).
  - Krylov.
- **Combination of first-principles and phenomenological models:**
  - data-based models (grey box models)
  - machine learning, e.g., deep neural networks (DNN).

SC's Low-Order Model Development for Semiconductor Manufacturing

- **SC has developed a wide range of low-order models of subsystems and components of wafer processing equipment for over 25 years.**
  - "Control relevant" models that run sims faster than real time.
  - Physics-based and have adjustable parameters.
  - Implemented in ANSI C.
  - Successfully incorporated in our commercial software products.

- **SC uses these low order models for:**
  - Design of real-time feedback or feedforward control.
  - Offset tuning.
  - Evaluating closed-loop performance.
  - Developing virtual sensors.
  - Health monitoring.

A Digital Twin for Rapid Thermal Processing (RTP)

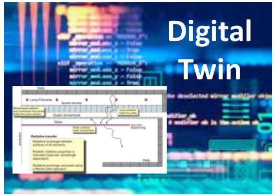


Input Information (Recipe, etc.)

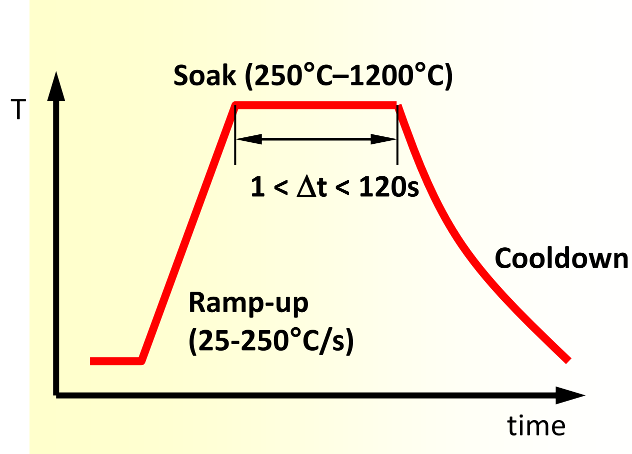
- Pyrometer Data
- Lamp commands
- …

Real time

Running in parallel

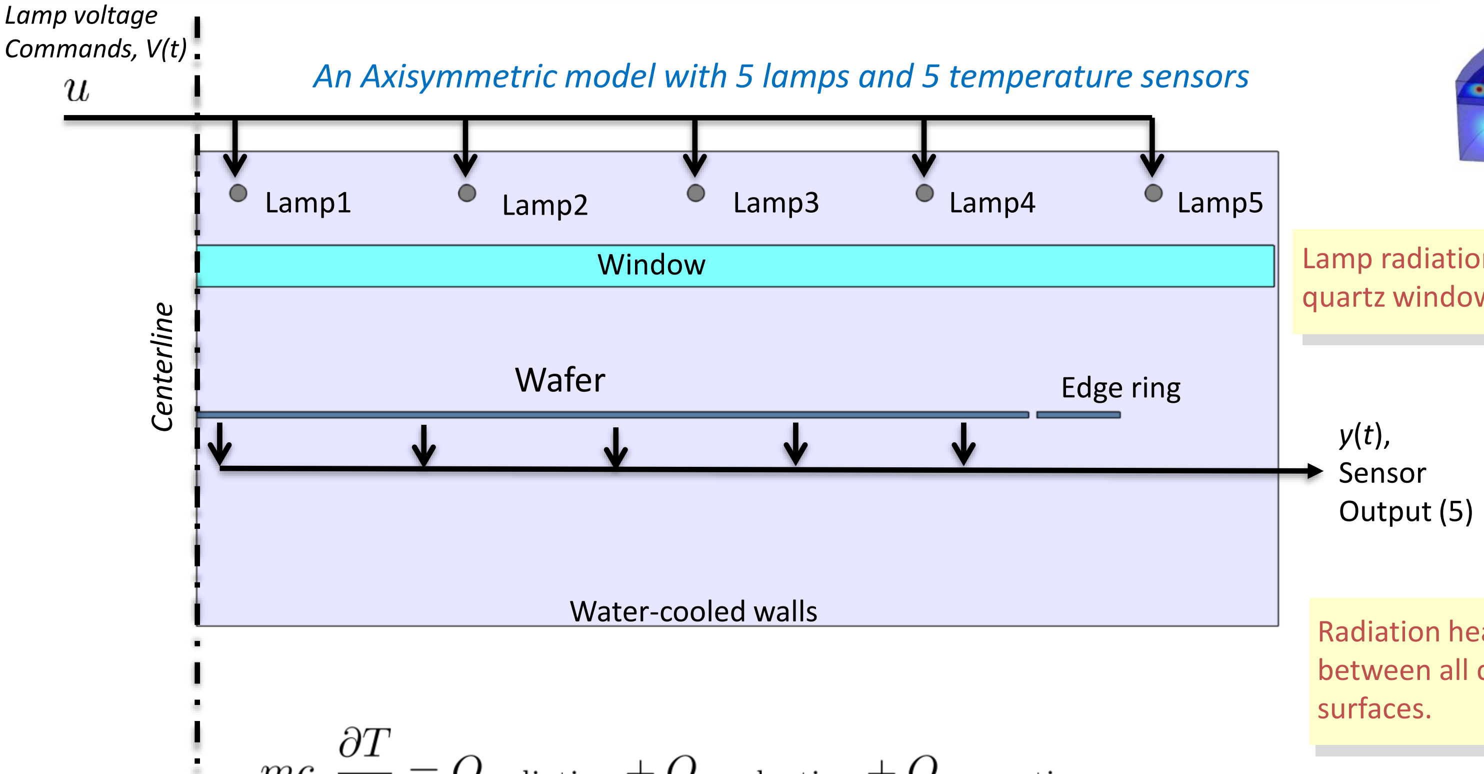


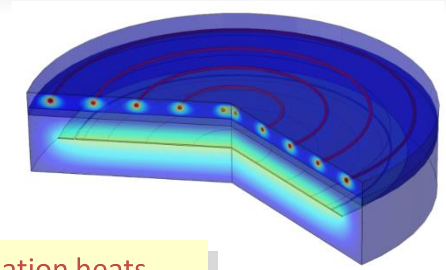
- Optimize film Quality
- Lamp failure detection
- Predictive maintenance
- Optimize control based on emissivity, pattern detection



A Generic RTP System

An Axisymmetric model with 5 lamps and 5 temperature sensors





Lamp radiation heats quartz window and wafer

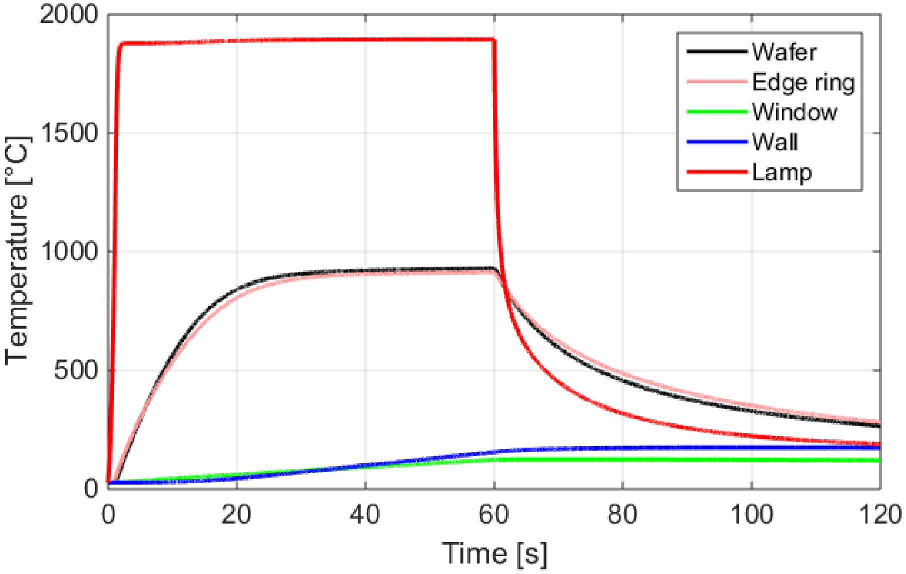
Radiation heat exchange between all component surfaces.

$$mc_p \frac{\partial T}{\partial t} = Q_{\text{radiation}} + Q_{\text{conduction}} + Q_{\text{convection}}$$

Dominant *Important* *Minor*

Heat Transfer Model for RTP

- Since radiative transfer is dominant, it is important to model radiative properties with sufficient accuracy: wavelength-dependence, specular/diffuse.
- Radiative exchange factors computed using Monte-Carlo method.
- Conduction is important – temperature-dependent thermal properties needed.
- Convection is least important -- incorporated using heat transfer coefficients.



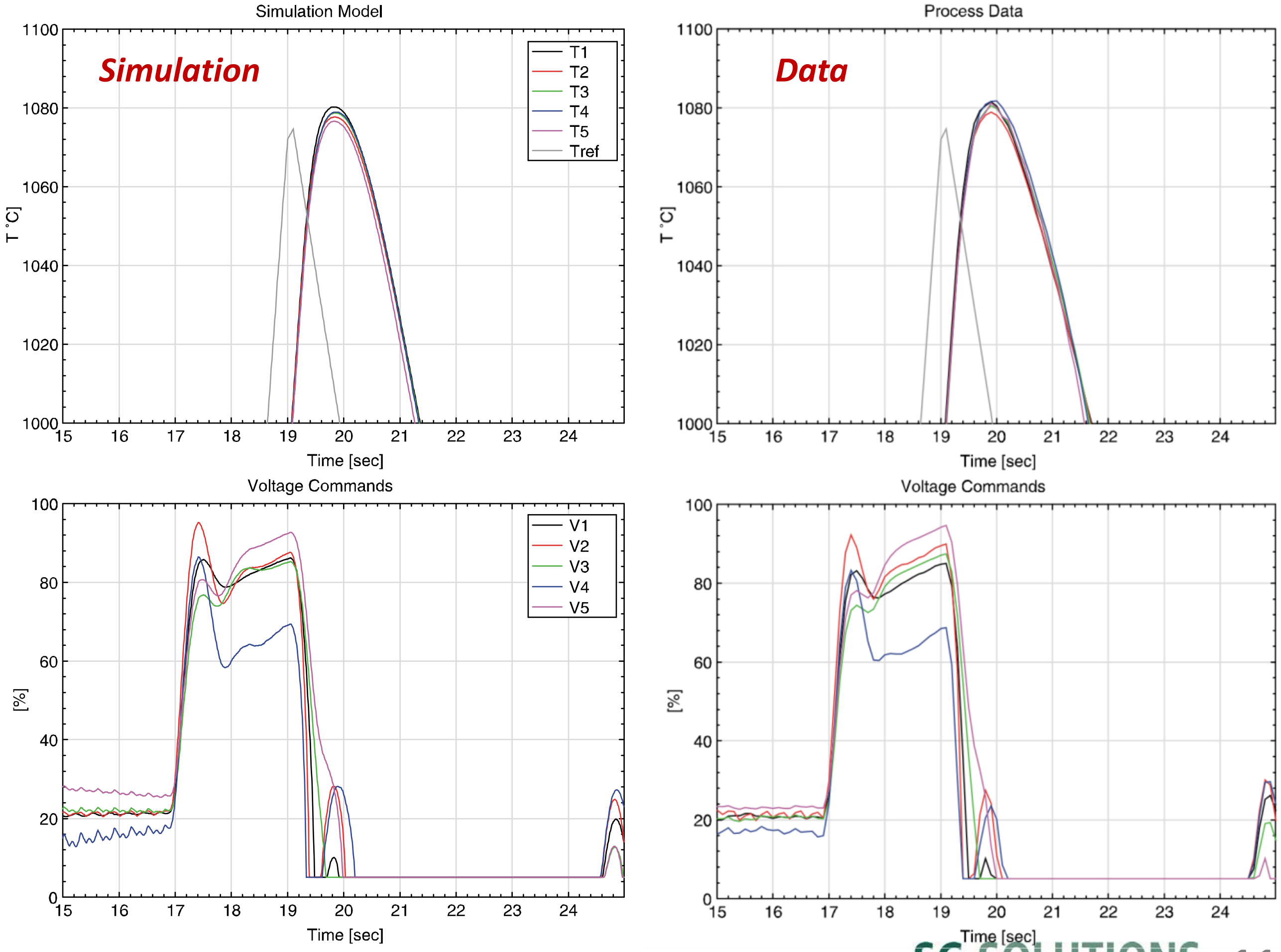
91-state model runs 120-second simulation in about a second.

Radiative Properties

Band 1 (λ<3.705μm)				Band 2 (λ>3.705μm)			
Component	ε_{eff}	n	k	*Component*	ε_{eff}	n	k
Lamp	0.3			Lamp	0.1		
Window	0	1.5	0	Window	0.19	2.55	0.01
Wafer	0.7	3.5	0.01	Wafer	0.7	3.5	0.01
Guard Ring	0.7	3.5	0.01	Guard Ring	0.7	3.5	0.01
Walls	0.3	diffuse		Walls	0.3	diffuse	

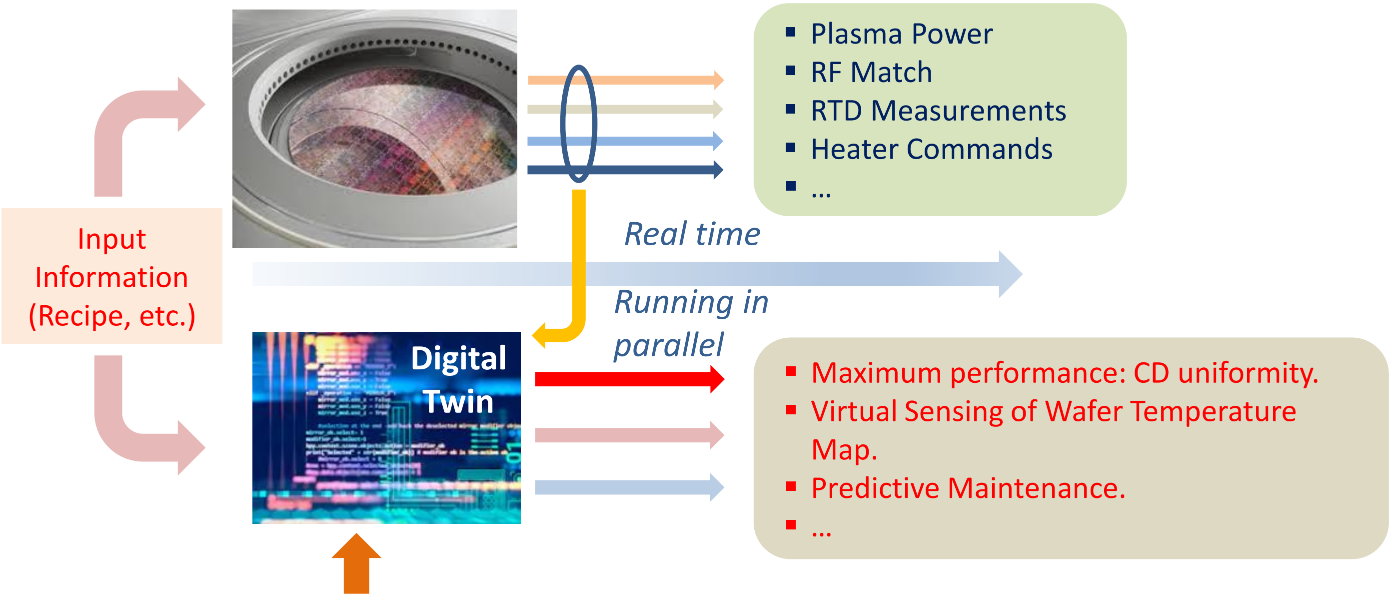
Closed-Loop RTP Response

Comparison of closed-loop simulation results with data from a commercial RTP system.*



** A. Emami-Naeini, et al., 'Modeling and Control of Distributed Thermal Systems', IEEE Trans. Control Technology, Vol. 11, No. 5, pp. 668-683, 2003.*

Components of a Digital Twin for Plasma Etch System

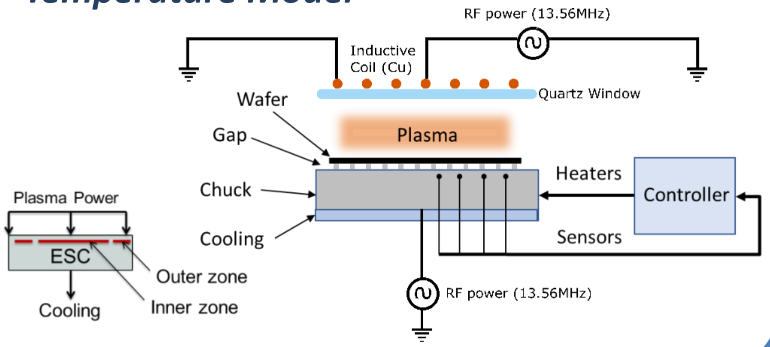


Subsystem models that may be used in a DT for etch systems:

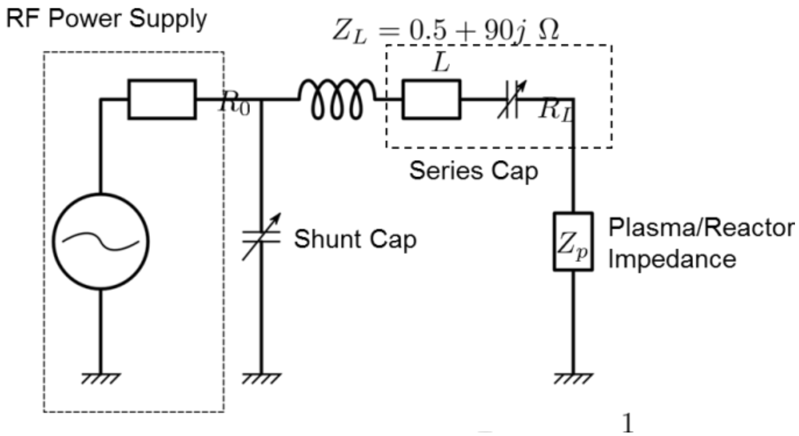
- Plasma model.
- Chamber Pressure Model.
- ESC Temperature Model.
- RF Impedance Model.

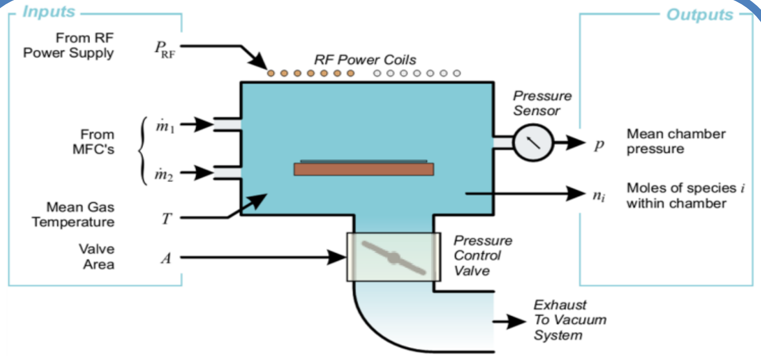
Fast Subsystem Models for Plasma Etch Chamber

Temperature Model



RF Impedance Model

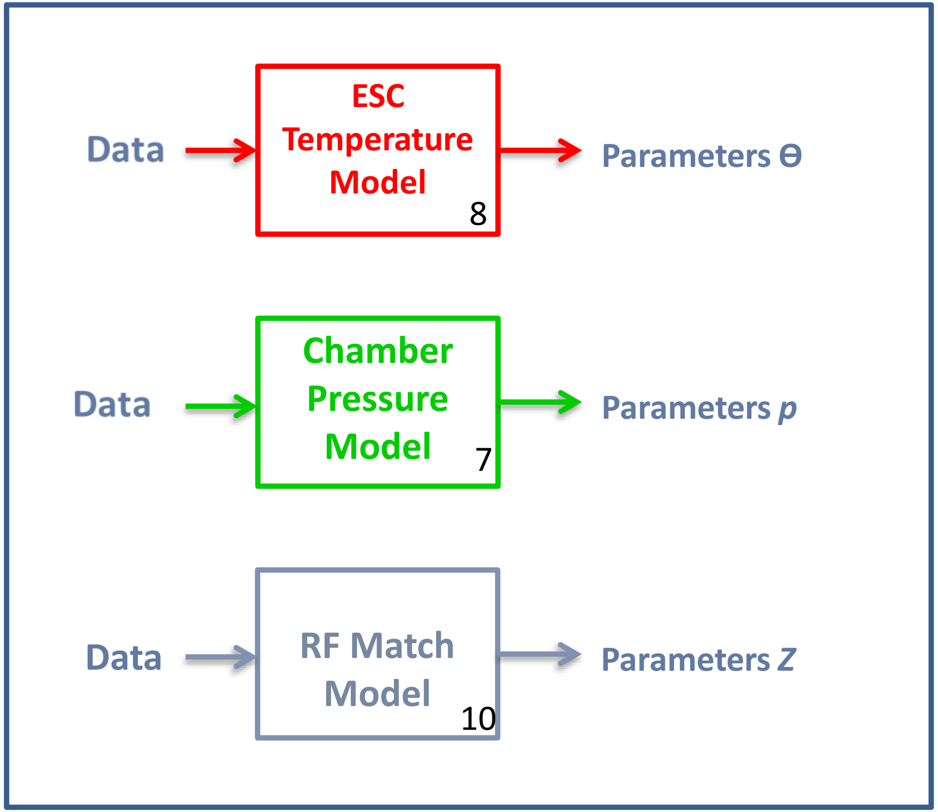




Chamber Pressure Model

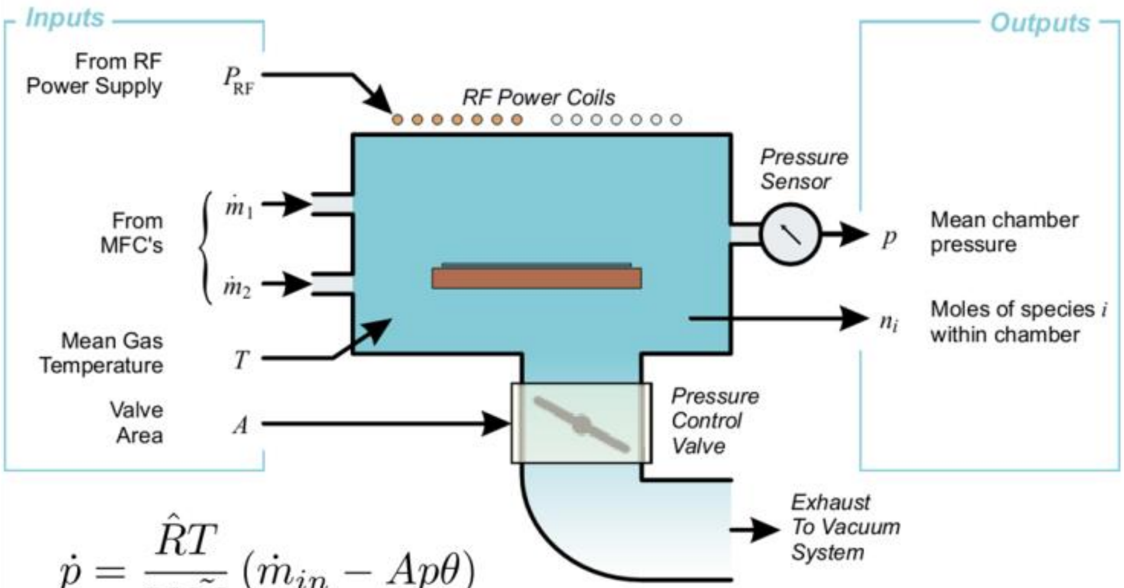
- Developed physics-based low-order models of etch chamber subsystems (less than 10 states/parameters each).
- Models calibrated with process data.

Updating Component Models with Data



- Model parameters values restricted to a pre-determined range in a properly operating system.
- It is possible to compress several process variables into relatively few model parameters in a physics-based model.
- A reduced range of variation of parameter values indicates an improved physics-based model.

Chamber Pressure Model



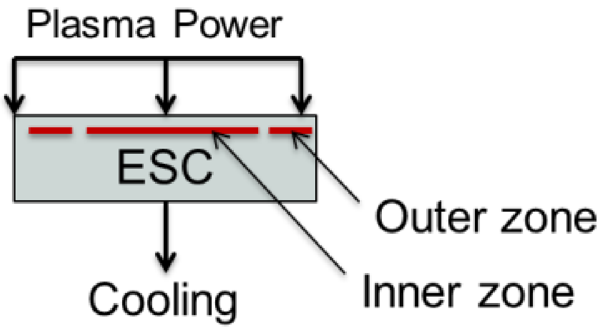
$$\dot{p} = \frac{\hat{R}T}{V\tilde{M}}\left(\dot{m}_{in} - Ap\theta\right)$$

Valve position command

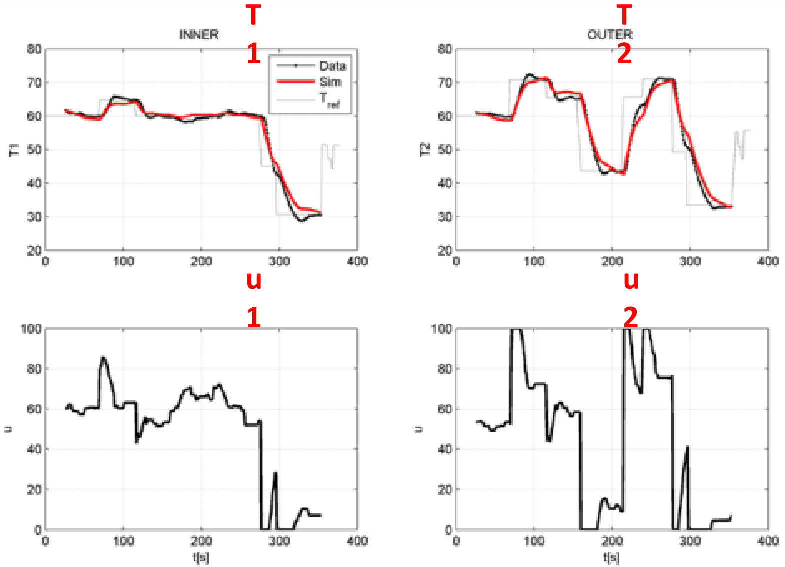
Mean molecular weight
(can change with RF power)

Assume that this MFC command is constant
during a given process step.

ESC Temperature Model



$$y = T - T_\infty$$
$$\dot{y}_1 = -\theta_{1,1} y_1 + \theta_{2,1} u_1 + \theta_{3,1}(y_2 - y_1) + \theta_{4,1} q_{RF}$$
$$\dot{y}_2 = -\theta_{1,2} y_2 + \theta_{2,2} u_2 + \theta_{3,2}(y_1 - y_2) + \theta_{4,2} q_{RF}$$



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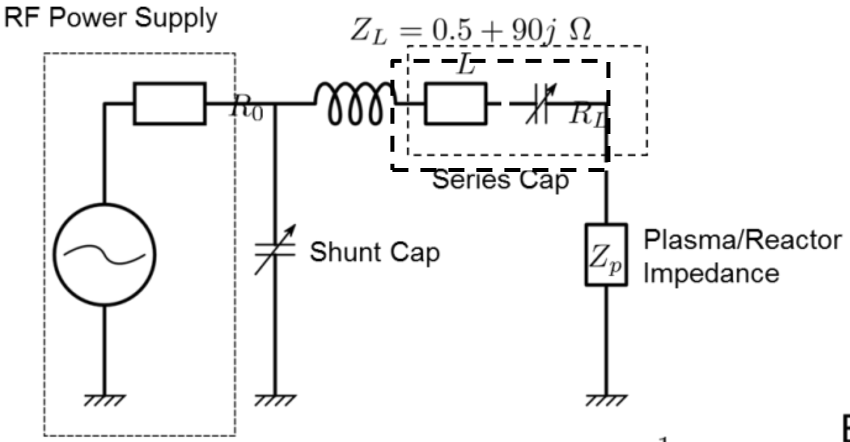
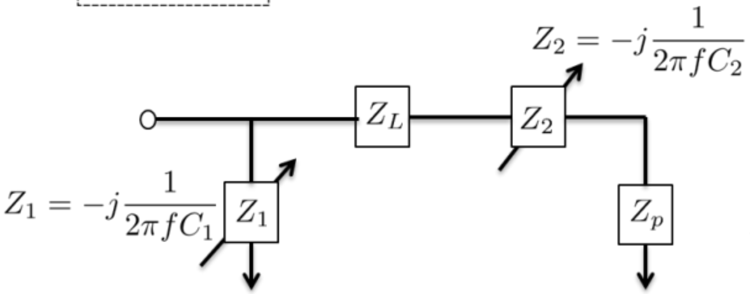
RF Impedance Model





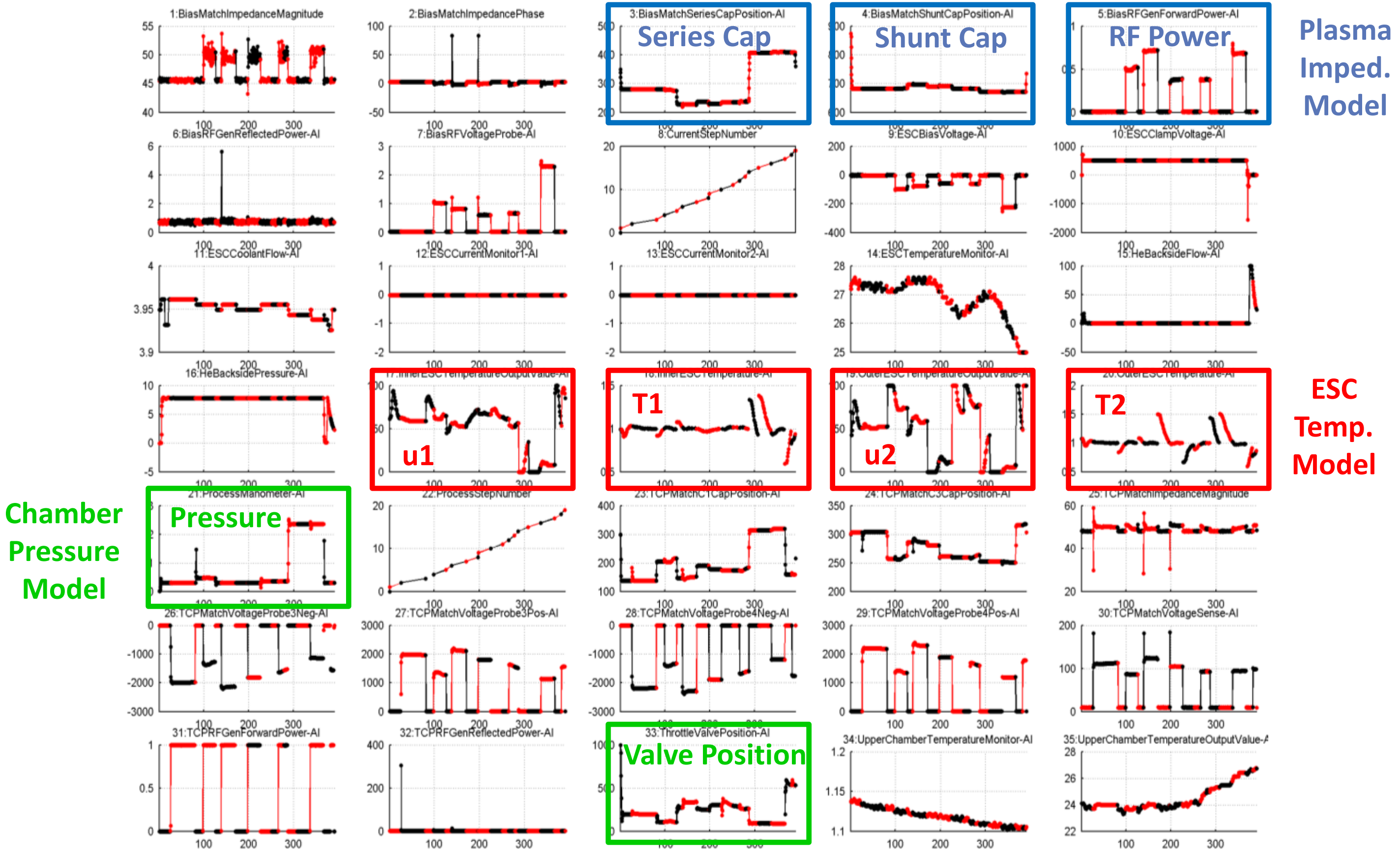
Equivalent Impedance

$$Z = \frac{Z_1(Z_2 + Z_L + Z_p)}{Z_1 + Z_2 + Z_L + Z_p}$$

"Plasma" Impedance

$$Z_p = \frac{Z_1(Z_2 + Z_L) - Z(Z_1 + Z_2 + Z_L)}{Z - Z_1}$$

Example Datalog Variables (model same for all power steps)



Combining Physics-based Models with Data-based Models

Physics-based Models

- **Pros:**
  Provides insights into the systems' behavior.
- **Cons:**
  Predictive capability is limited by unknown or unmodeled physics.

Data-driven Models (e.g., DNNs)

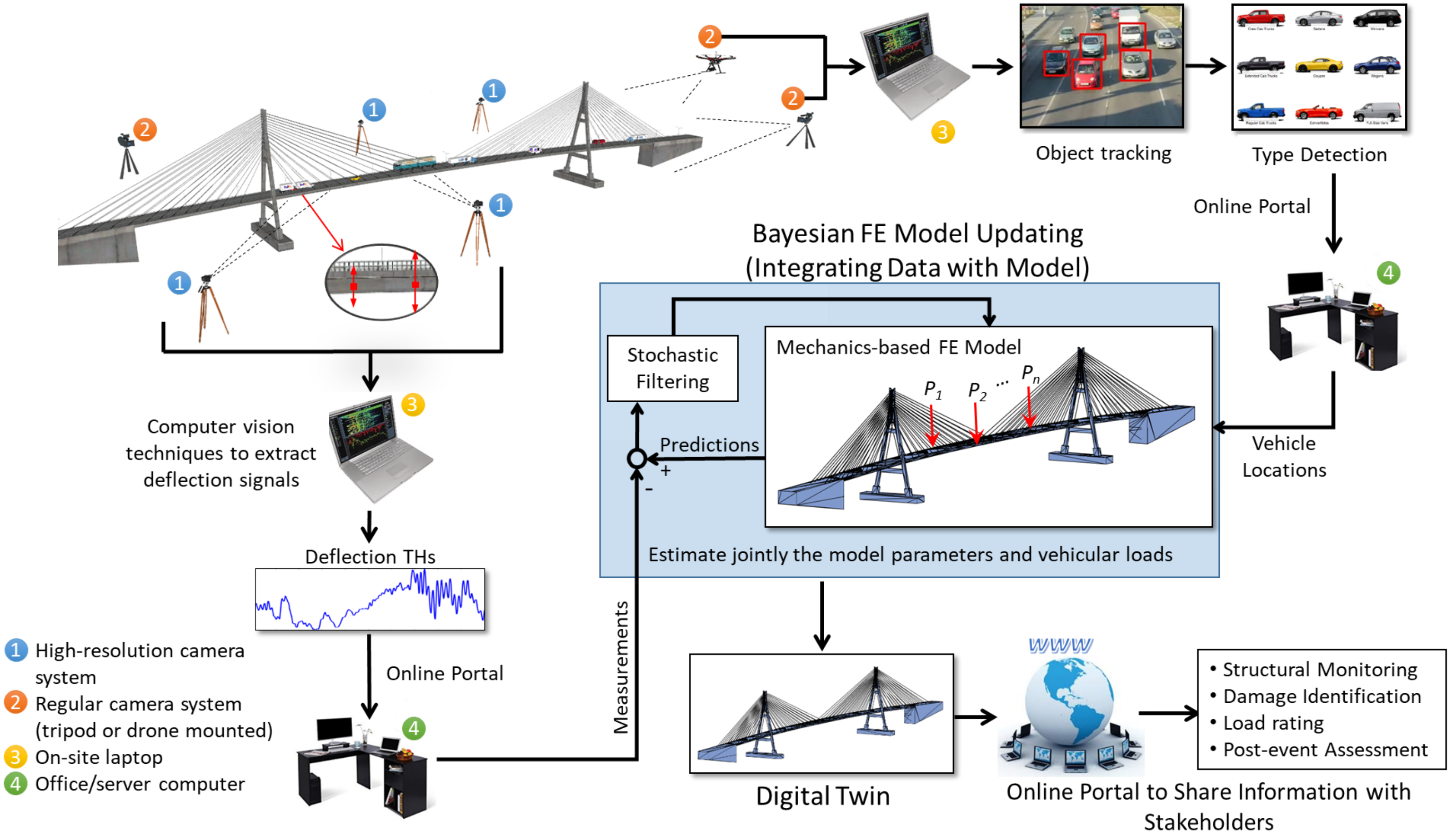
- **Pros:**
  Suitable for discovering representation of complex functions without a priori knowledge.
- **Cons:**
  - Lack of interpretability, output reliability.
  - Requires huge amount of training dataset.

*PAI Approach (Physics + AI)**

- Deep neural networks (DNNs) are trained with dataset generated from physics-based models with structured uncertainty model sets. The DNNs estimate both model and physical variables.
- Dynamic feedback loop with robust control uses the DNNs outputs to optimize system performance. If the level of model uncertainties exceeds a certain bound, the DNNs must be retrained.

** D. De Bruyker, R. L. Kosut, R. Valdez, S. Haymes, L. Schoeling, M. Petro, D. Weiner, A. Joseph, J. K. Lee, A. Emami-Naeini, J. L. Ebert, and S. Ghosal, Improving Recovery in the Yates Field Using Dynamic Feedback Loop based on Physics-Informed Artificial Intelligence, Proceedings of SPE Improved Oil Recovery Conference, Society of Petroleum Engineers, August 2020.*

Digital Twin for Bridge Health Monitoring (DoT-funded Program)



Summary

- Key to implementing DT technology: fast yet accurate dynamic models.
- Fast models are often based on low-order versions of high-fidelity physics-based models.
- Fast, physics-based model may need to be supplemented with other types of models: gray-box, machine learning.
- These fast models that may currently have different uses but can be brought together for successful implementation of DT's.

Thank You

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Value Through Innovation