Modeling and Simulation of SEERS

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Plasma Modeling and Simulation

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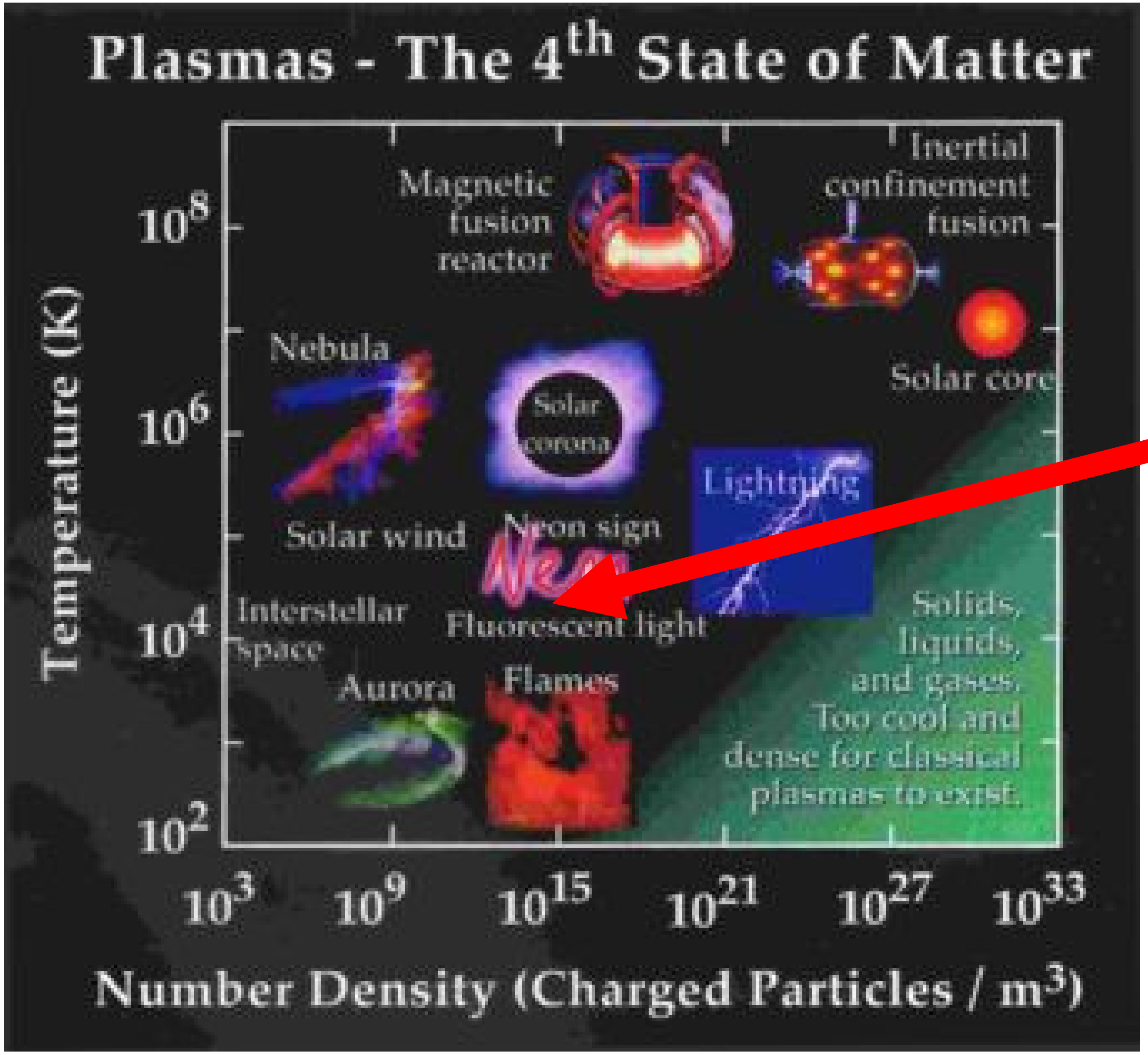
Plasma reactors

Typical regime:

- 1 kW RF power
- 1 Pa gas pressure
- 10^{-2} m^3 volume
- 10^{17} m^{-3} density

Source: Sentech

Plasma regimes



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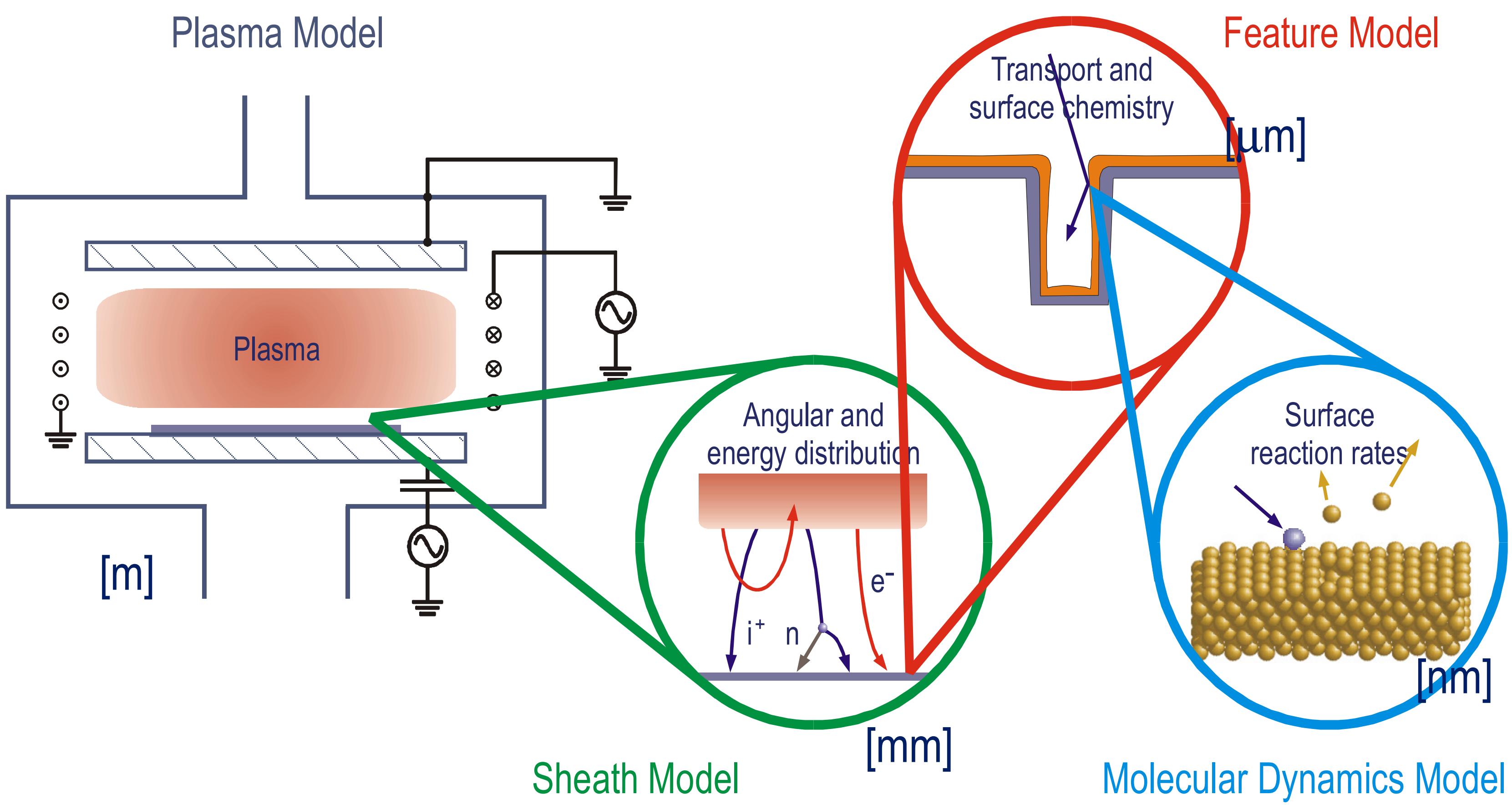
Plasma modeling



Plasma modeling: Multiple scales, multiple physics!!!

Perspectives on SEERS

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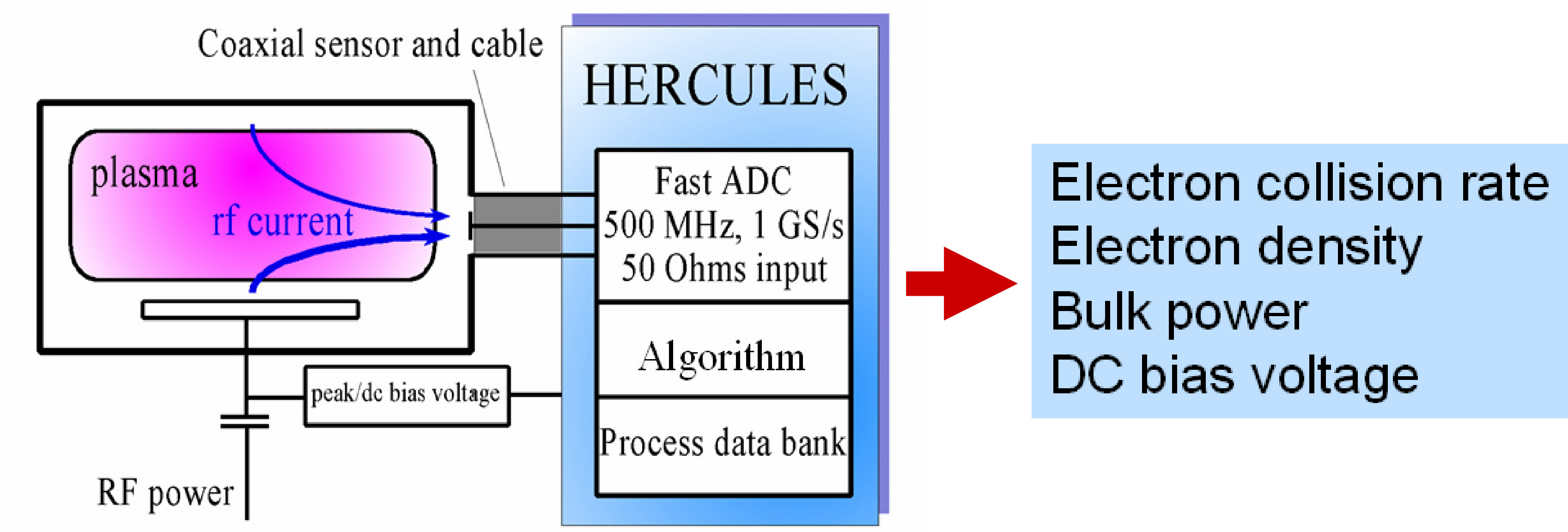
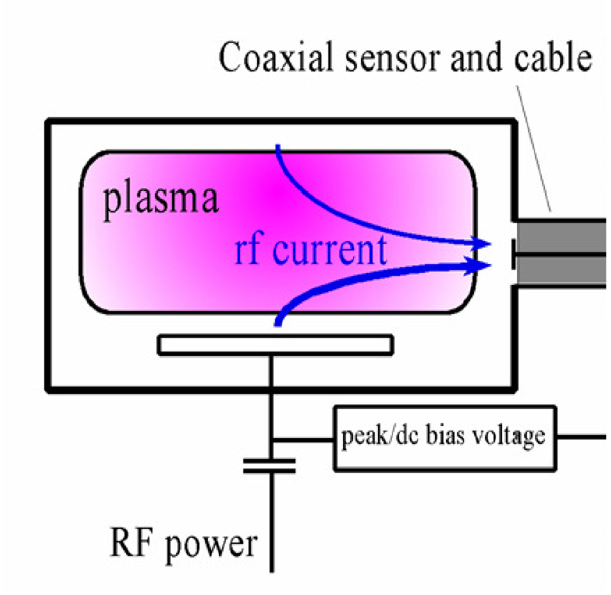
Practitioners view on SEERS

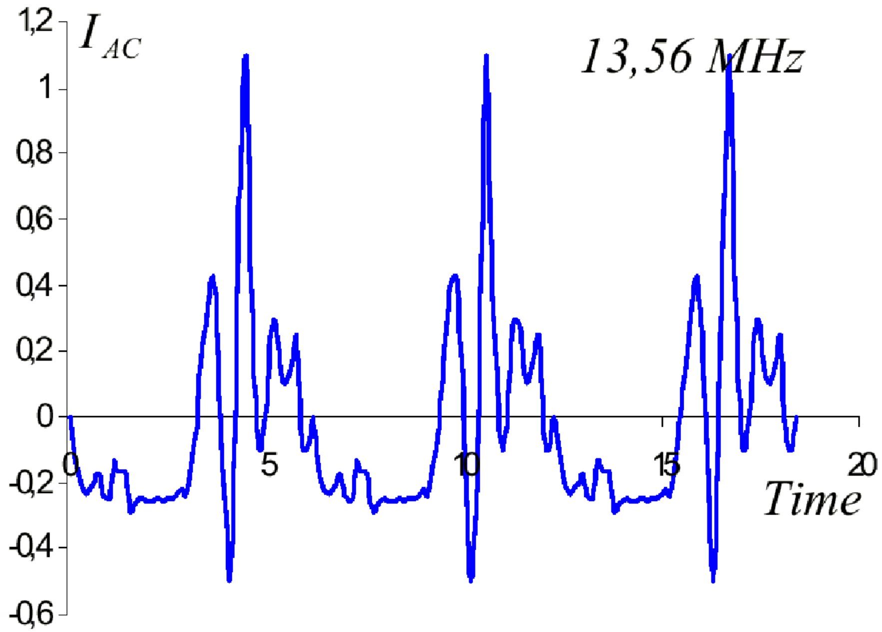


Typical points of investigation:

- How are the parameters related to the process result?
- Which of the parameters is the most sensitive?
- How does SEERS compare with other diagnostics?

Our view on SEERS

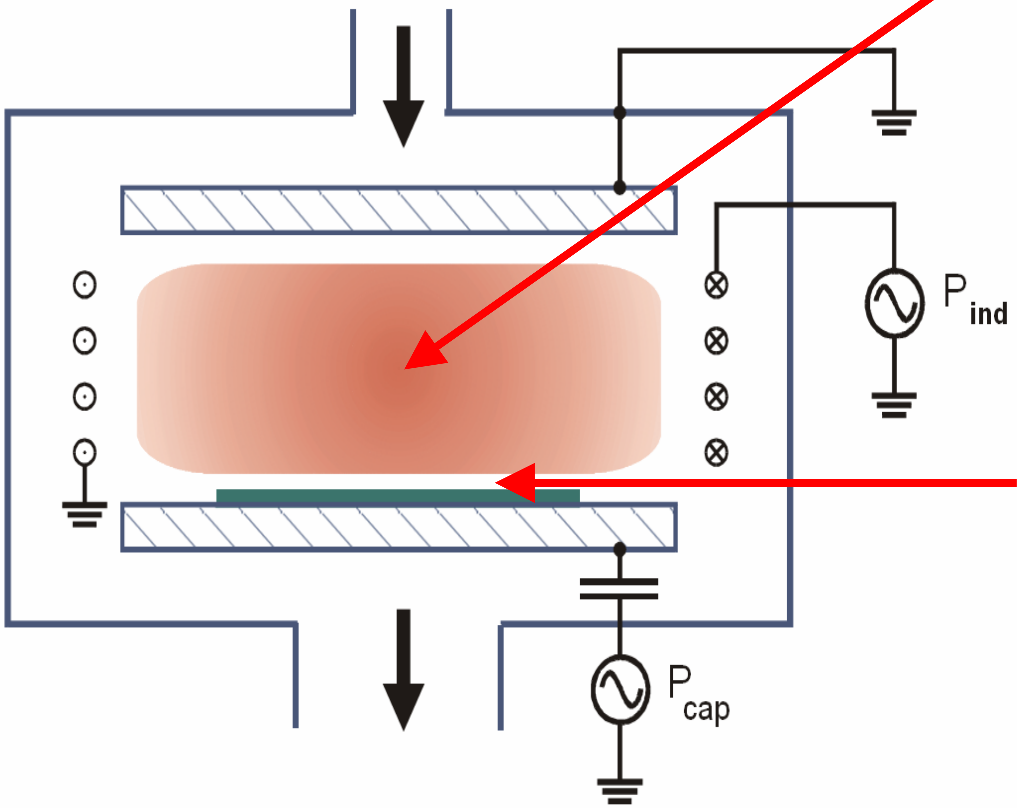




Our points of investigation:

- What is the physical background of the resonance?
- What exactly do the SEERS parameter mean?
- Is there more information in the SEERS signal?

Nature of the resonance



Bulk is "induktive":

$$m\frac{\partial v}{\partial t} = -eE - \nu_c v$$

$$\rightsquigarrow \frac{\partial j}{\partial t} = -\frac{e^2 n}{m_e}E - \nu_c j$$

$$\rightsquigarrow U = L\frac{dI}{dt} + RI$$

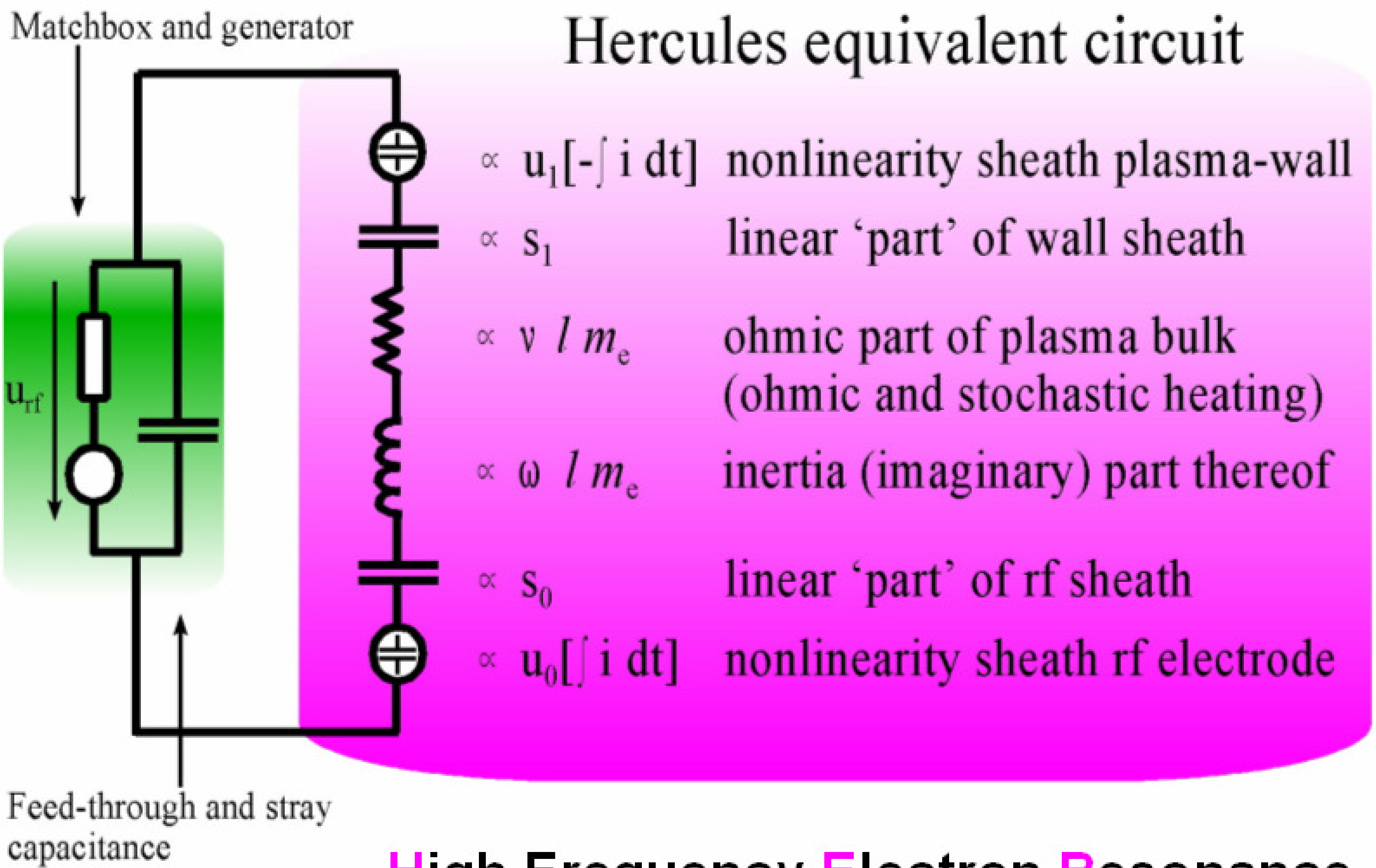
Sheath is capacitive

$$j = \epsilon_0 \frac{\partial E}{\partial t}$$

$$U = EH$$

$$\rightsquigarrow \frac{dU}{dt} = \frac{1}{C}I$$

Equivalent circuit



High Frequency **E**lectron **R**esonance
Current **L**ow Pressur**e** **S**pectroscopy

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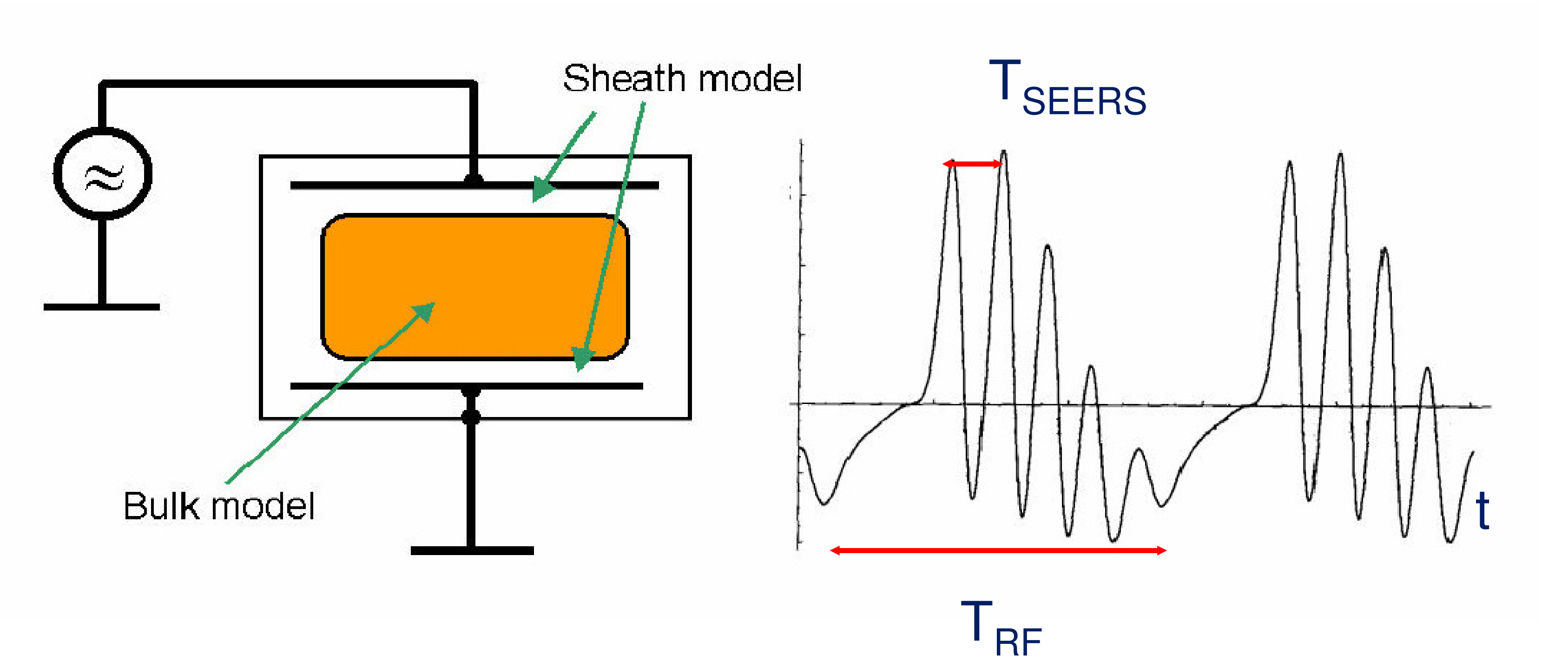
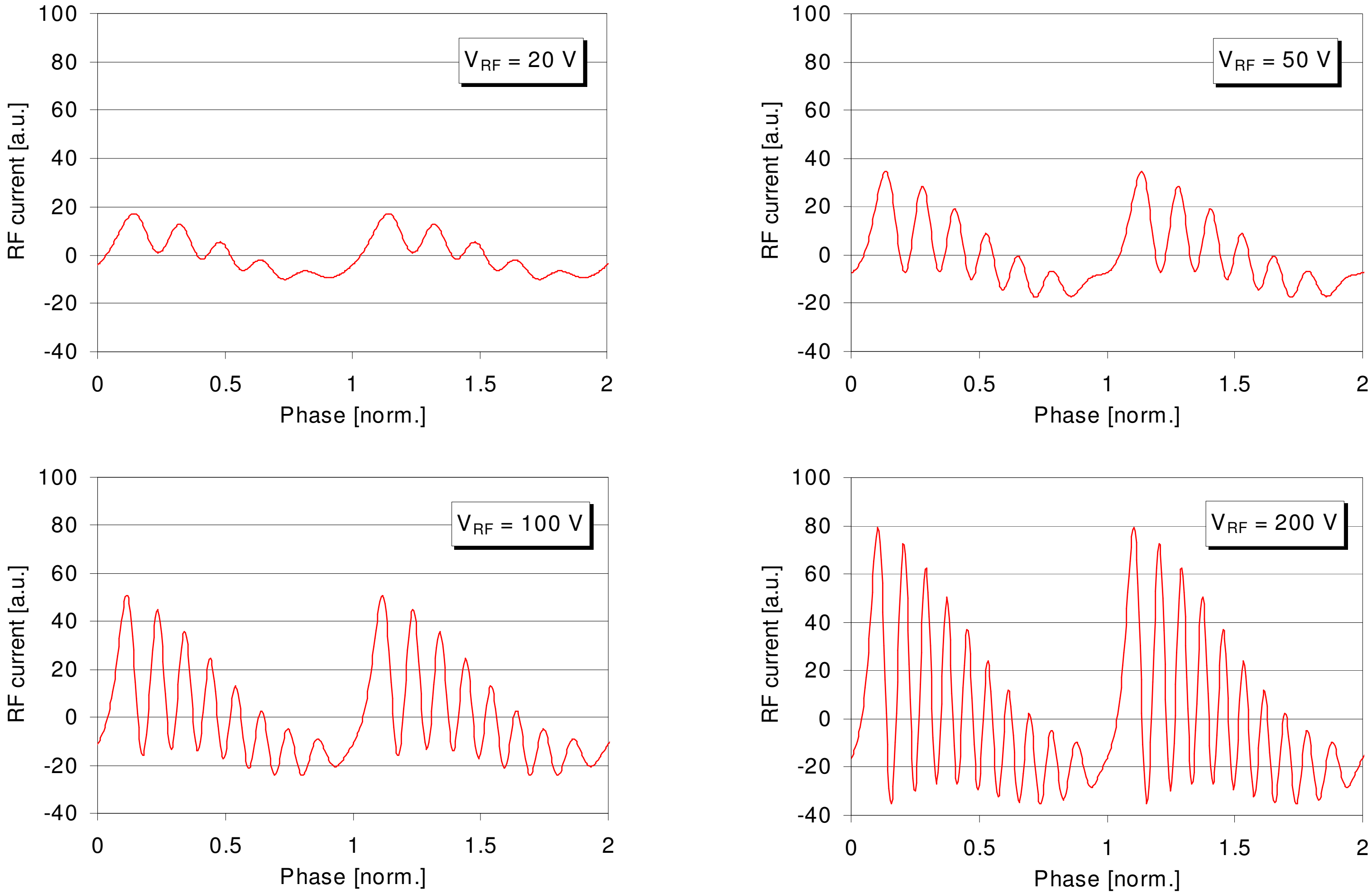
Lumped Circuit Models

Lumped circuit model



- Linear bulk model to represent effective impedance
- One or two instances of a non-linear sheath model
- Solved either analytically of numerically

Parameter study: RF-voltage



Amplitude of the oscillation increases with excitation.

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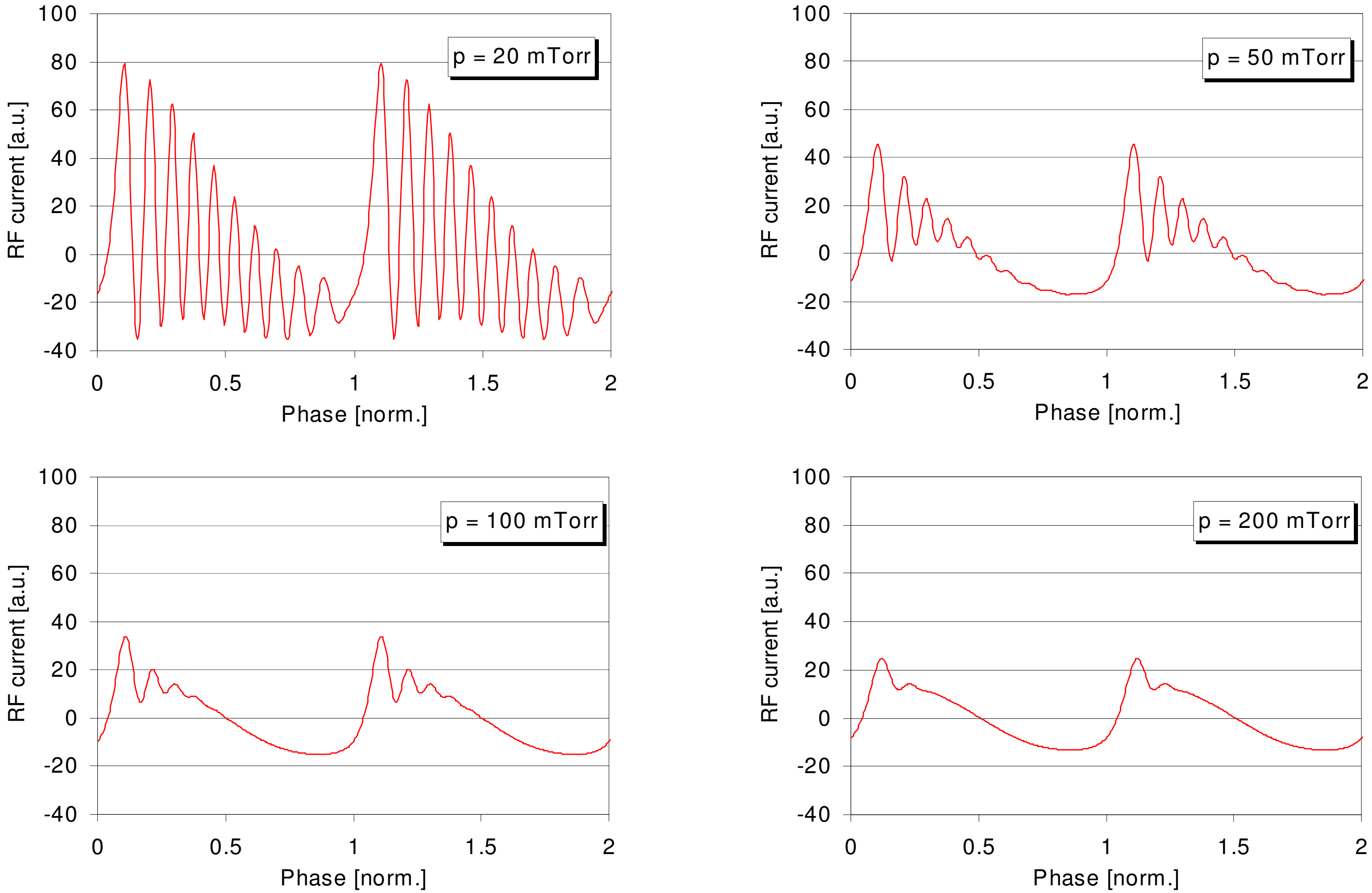
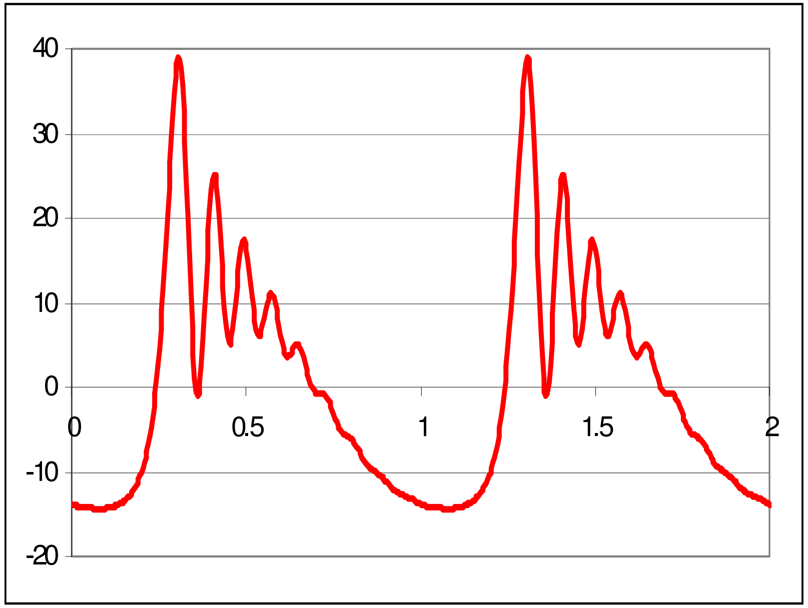
Parameter study: Pressure

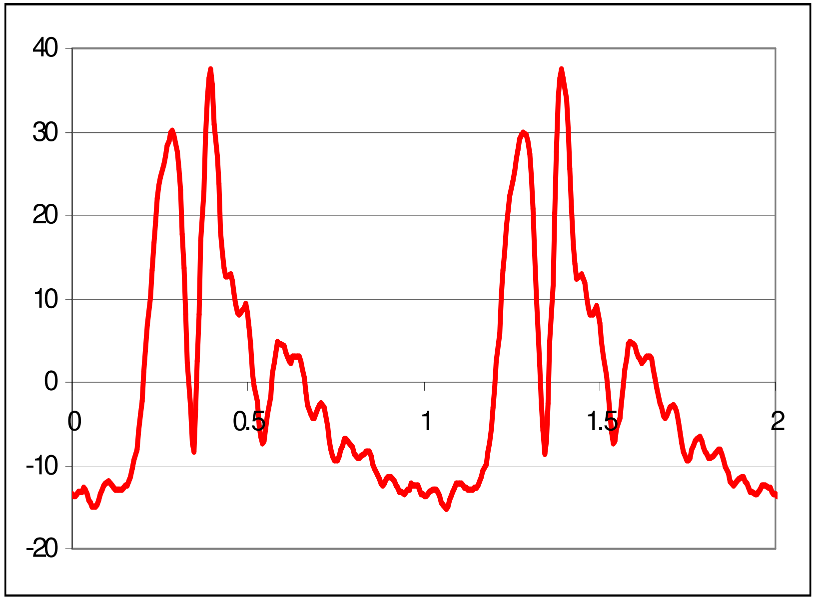


Damping increases with neutral gas pressure.

Comparing with reality



Simulation



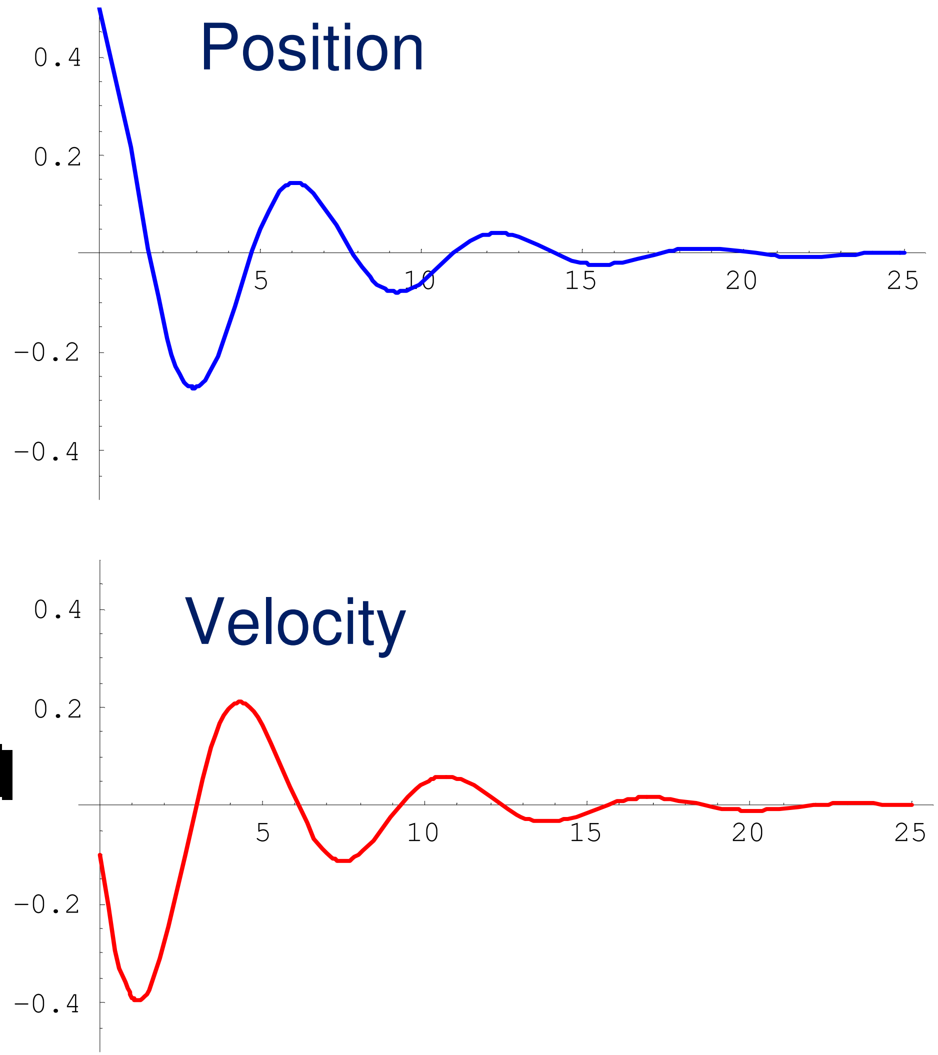
SEERS Sensor-Data

- Good "qualitative" correspondence (form, trends).
- No quantitative agreement, no "fine structures"

The real signal is obviously much more complex! WHY?

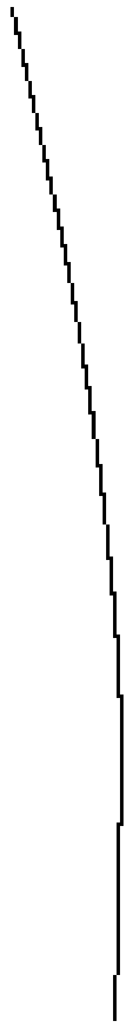
A General Mathematical Model

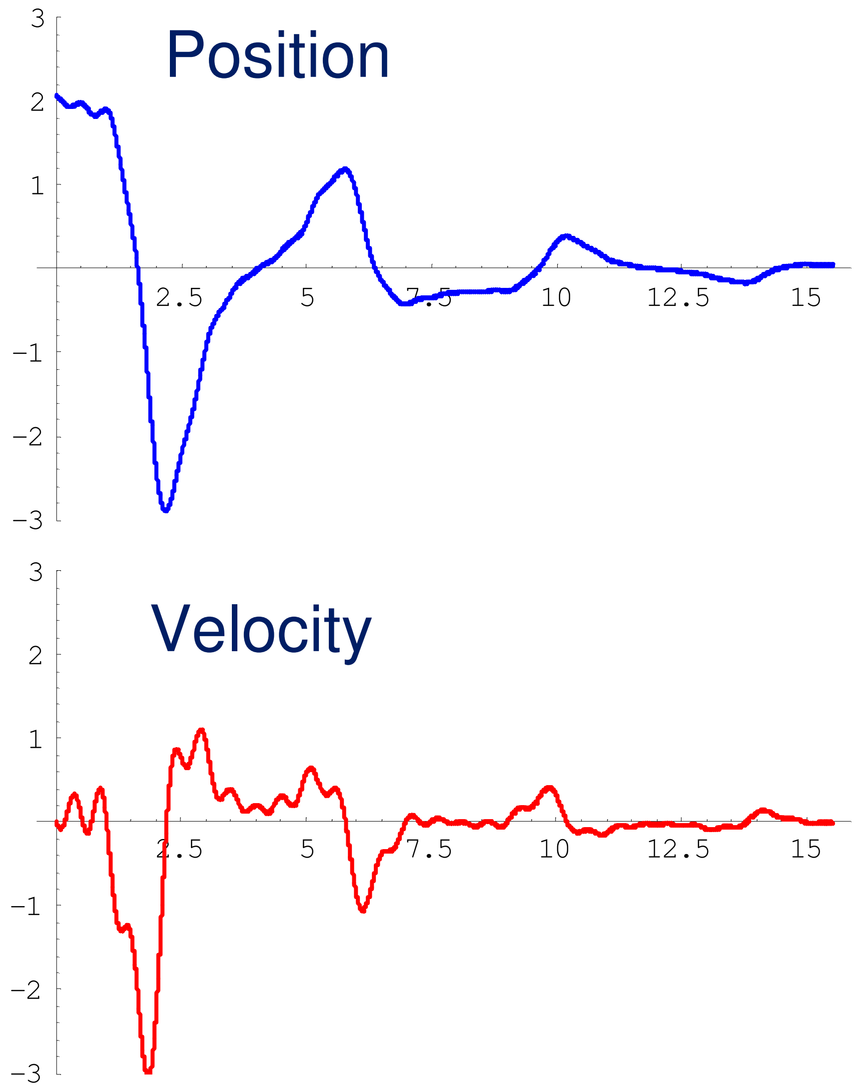
Analogy: Pendulum



Lumped model: Only a simple oscillation pattern possible

Analogy: Chain



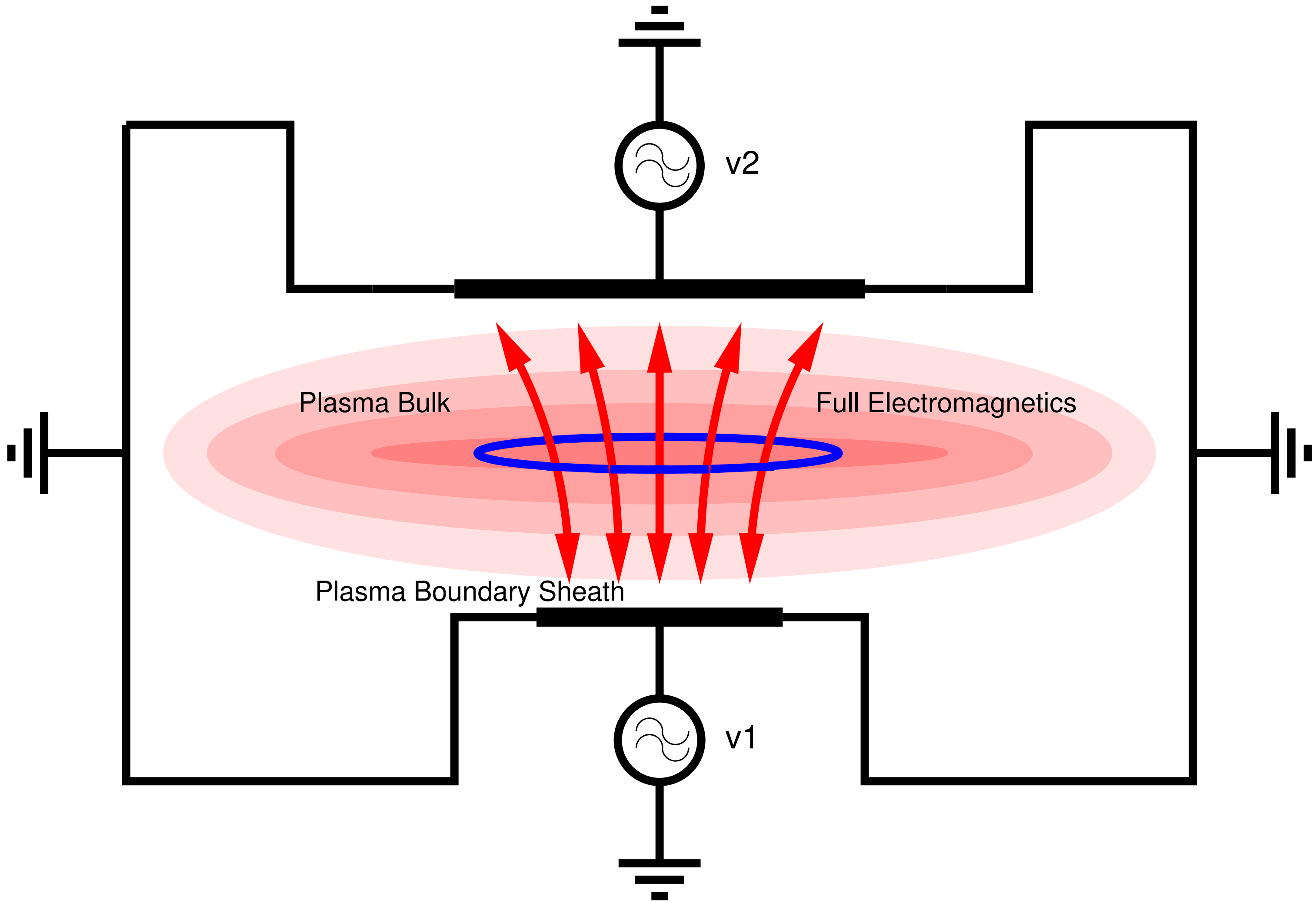


Distributed model: Complex oscillation patterns possible

Analogy: Chain

Eigenmode analysis: Superposition of oscillation modes

General reactor model



Arbitrary geometry, arbitrary number of applied voltages ...

General model: Equations

Definition of a state space:

$$Z = \left\{ |z\rangle = (\boldsymbol{j}, \boldsymbol{B}, Q) \,\middle|\, \nabla\cdot\boldsymbol{B} = 0, \frac{1}{\mu_0}\nabla\times\boldsymbol{B} = \boldsymbol{j}, \boldsymbol{B}\cdot\boldsymbol{n}\big|_{\partial V} = 0 \right\}$$

Dynamical equations:

$$\frac{\partial \boldsymbol{j}}{\partial t} = \frac{e^2 n_e}{m_e}\boldsymbol{E} - \nu_c \boldsymbol{j}$$

Electron equation of motion

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

Magnetic induction law

$$\frac{\partial Q}{\partial t} = \boldsymbol{n}\cdot\boldsymbol{j}\big|_{\partial V}$$

Sheath charging

Boundary conditions:

$$\boldsymbol{n}\times\boldsymbol{E}\big|_{\partial V} = -\boldsymbol{n}\times\boldsymbol{\nabla}(V_S(Q) + \Phi_{RF})\big|_{\partial V}$$

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General model: Analysis

The state space Z can be interpreted as a Hilbert space, with an inner product motivated by an energy functional

- The concept of orthogonality applies
- The tools of functional analysis can be used

Abstract formulation of the dynamics:

$$\frac{\partial \left|z\right\rangle}{\partial t} = \mathsf{T}_C \left|z\right\rangle + \mathsf{T}_D \left|z\right\rangle + \mathsf{T}_{NL} \left|z\right\rangle\left|z\right\rangle + u\cos(\omega t) \left|e\right\rangle$$

T_C	Conservative part: pure oscillation
T_D	Dissipative part: damping
T_{NL}	Nonlinear harmonics generation
$u\cos(\omega t) \left\|e\right\rangle$	External excitation

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General model: Solution

The equation can be solved by a triple series expansion (power series, Fourier series, eigenmode expansion)

$$|z\rangle = \sum_{n=1}^{\infty} \sum_{k=-n}^{n} \sum_{l=1}^{\infty} z_{kl}^{(n)} u^n e^{ik\omega t} |r_l\rangle$$

The series coefficients can be found by recursion:

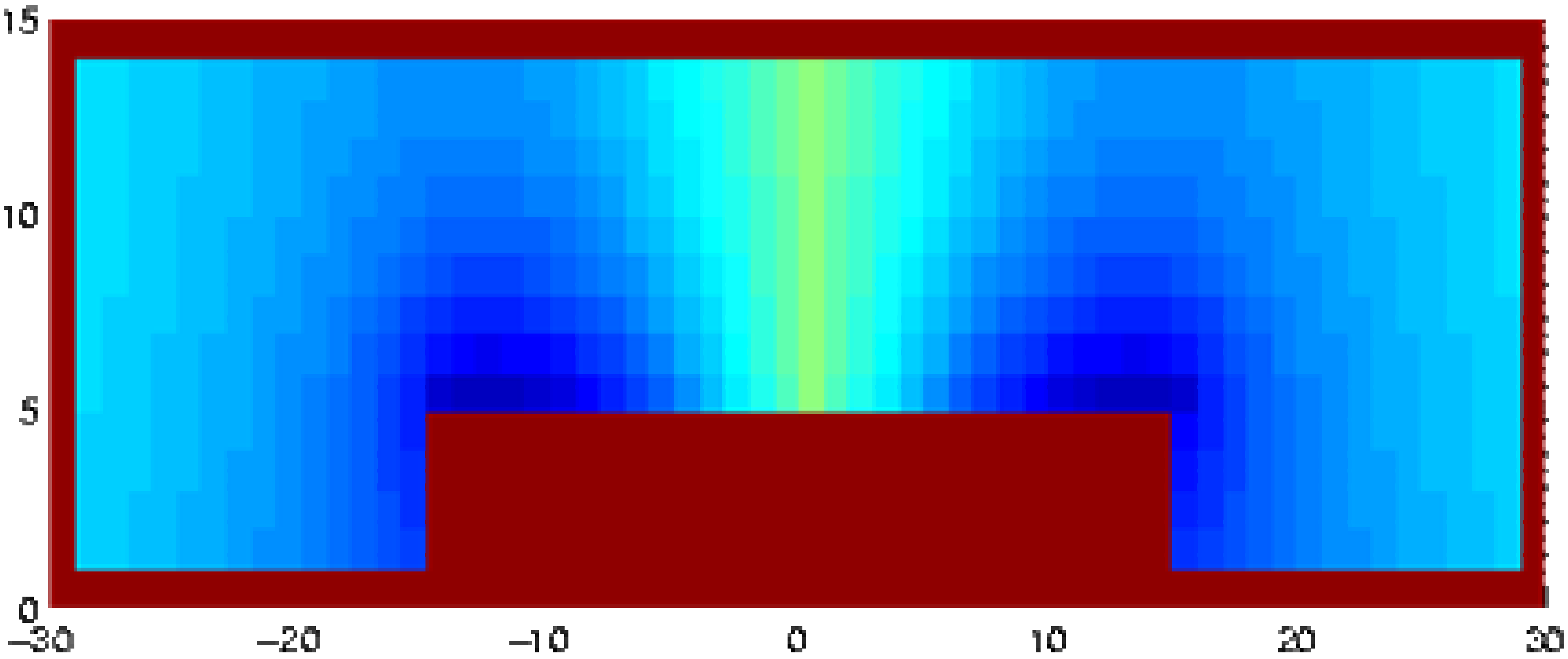
$$z_{kl}^{(1)} = \frac{1}{2(il\omega - p_k)} \langle l_k \,|\, e \rangle$$

$$z_{kl}^{(n)} = \frac{1}{il\omega - p_k} \sum_{s=1}^{n-1} \sum_{\bar{k}=1}^{\infty} \sum_{\tilde{k}=1}^{\infty} \sum_{|\bar{l}| \le s,\, |\tilde{l}| \le n-s,\, \bar{l}+\tilde{l}=l} \langle l_k | \, T_{NL} \, | r_{\bar{k}} \rangle \, | r_{\tilde{k}} \rangle \, z_{\bar{k}\bar{l}}^{(s)} \, z_{\tilde{k}\tilde{l}}^{(n-s)}$$

Algebra in the solution space of the linear problem:

➔ Numerically tractable even for complicated situations

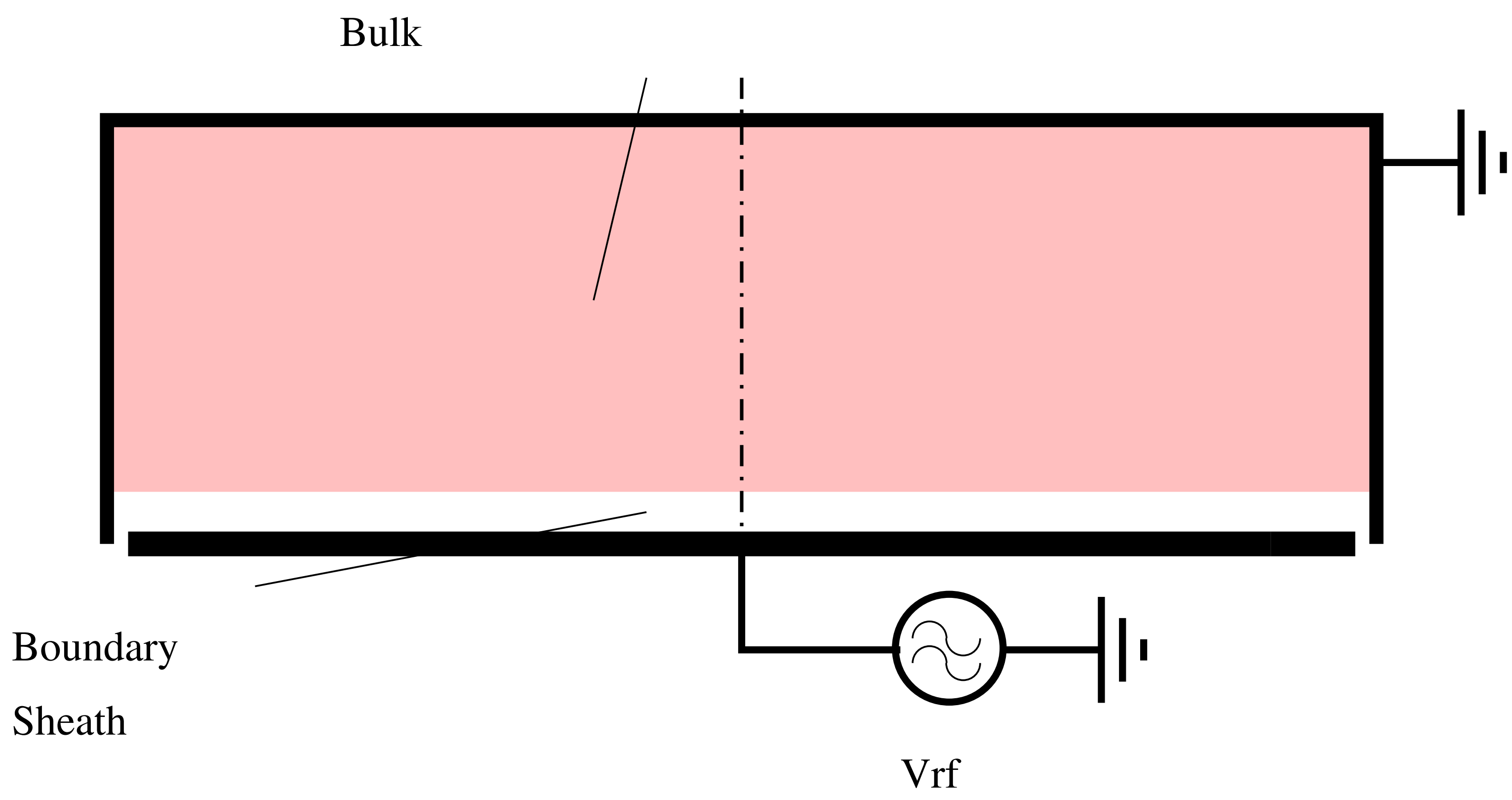
General model: Example



- Numerical scheme with consistent discretization
- Any 2D-geometry, any electron density distribution
- Tested with analytical solutions for special cases

A Simplified Toy Model

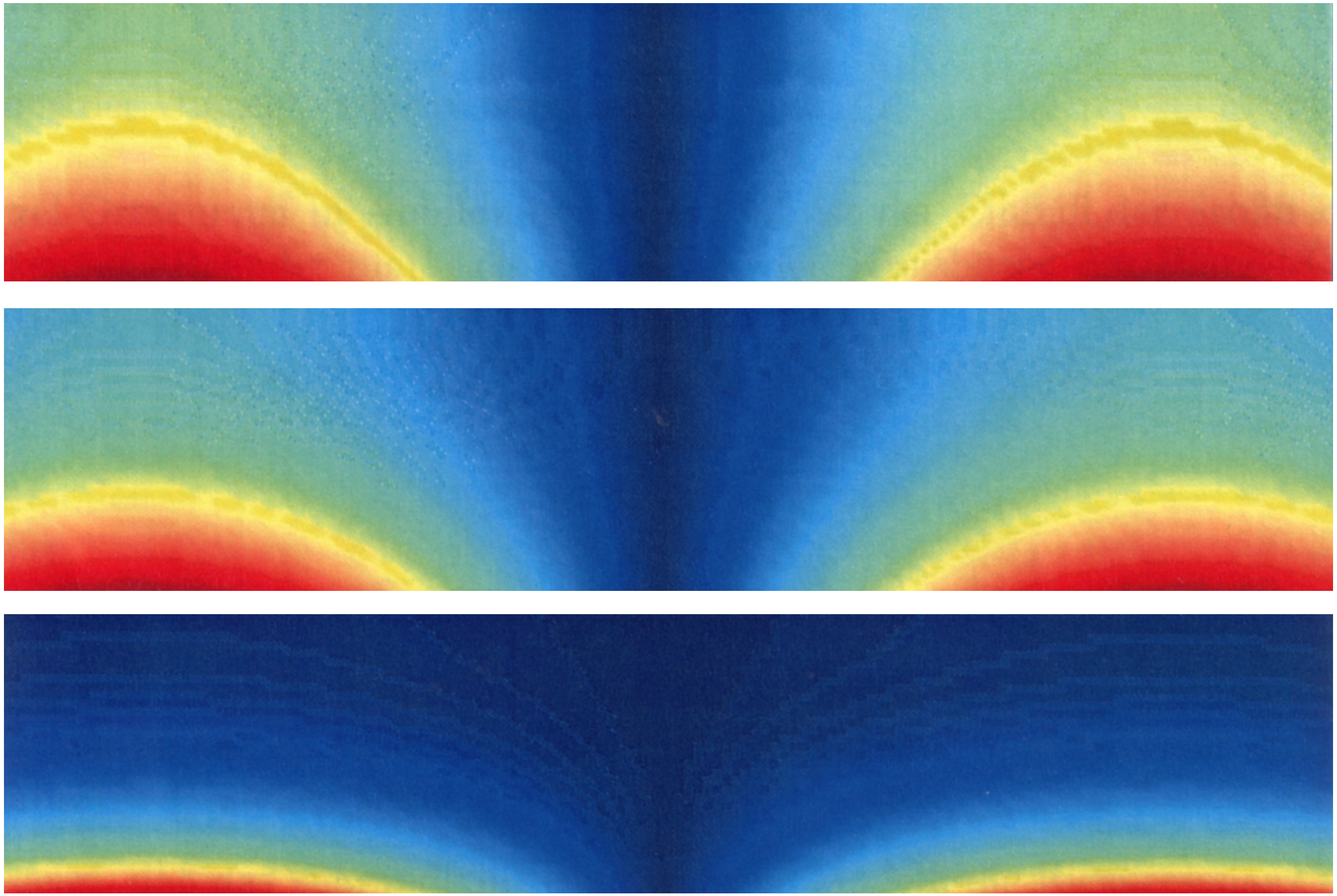
Toy model: Set-Up



Simplifications to facilitate an analytical treatment:

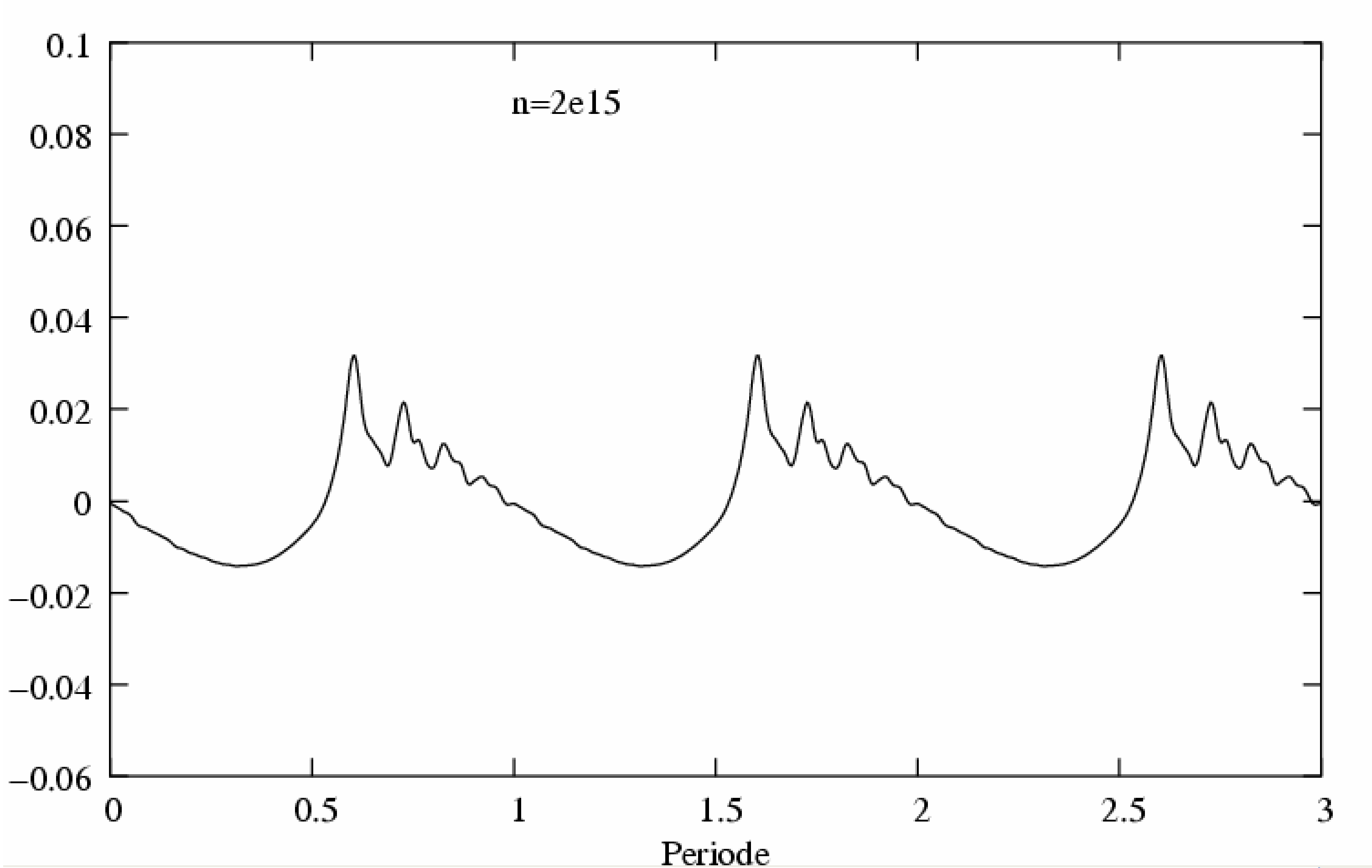
- Simple axi-symmetric cylinder geometry
- Constant bulk and sheath parameters

First eigenmode



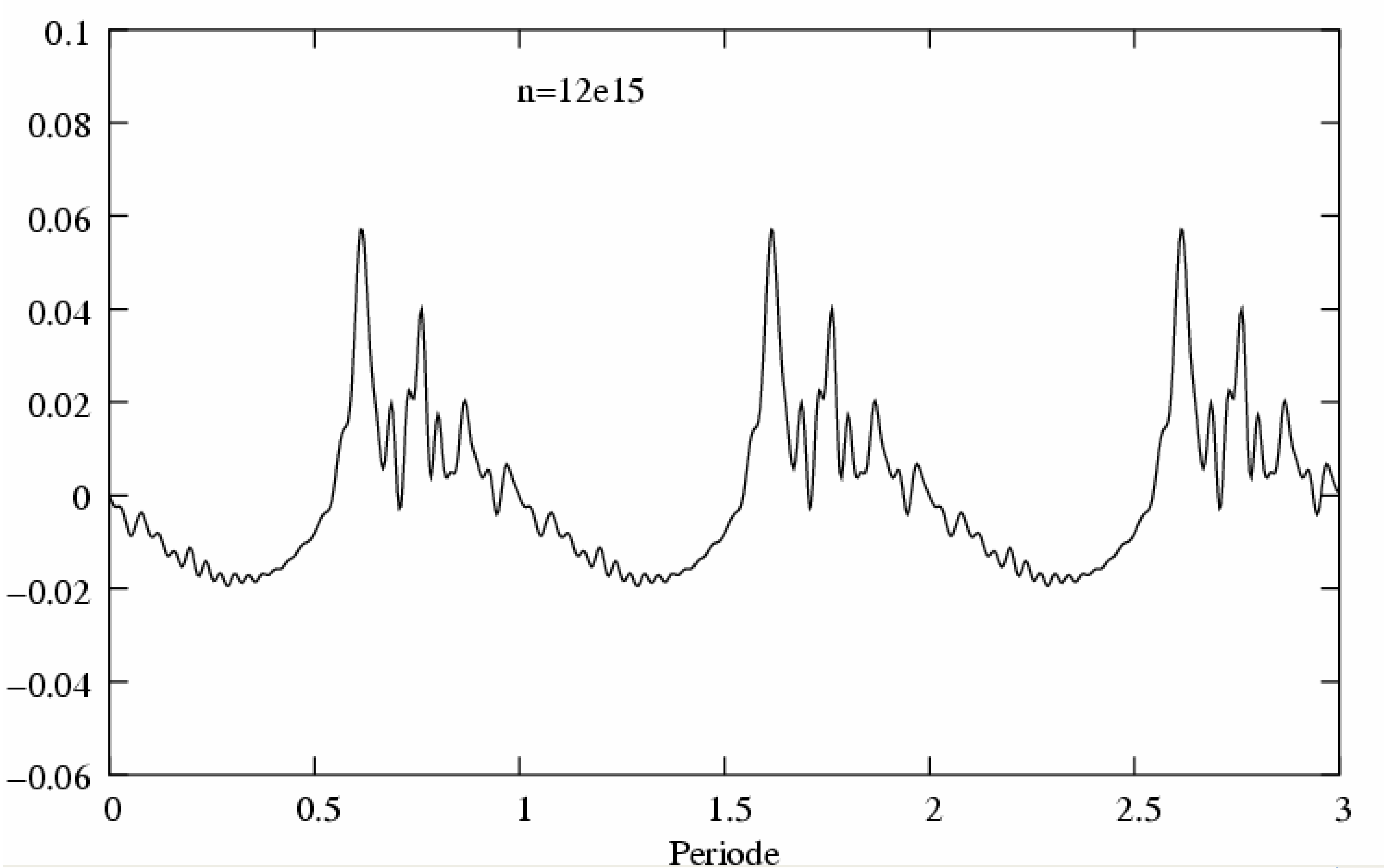
The eigenmode shape depends on the plasma density

Toy model: Results I



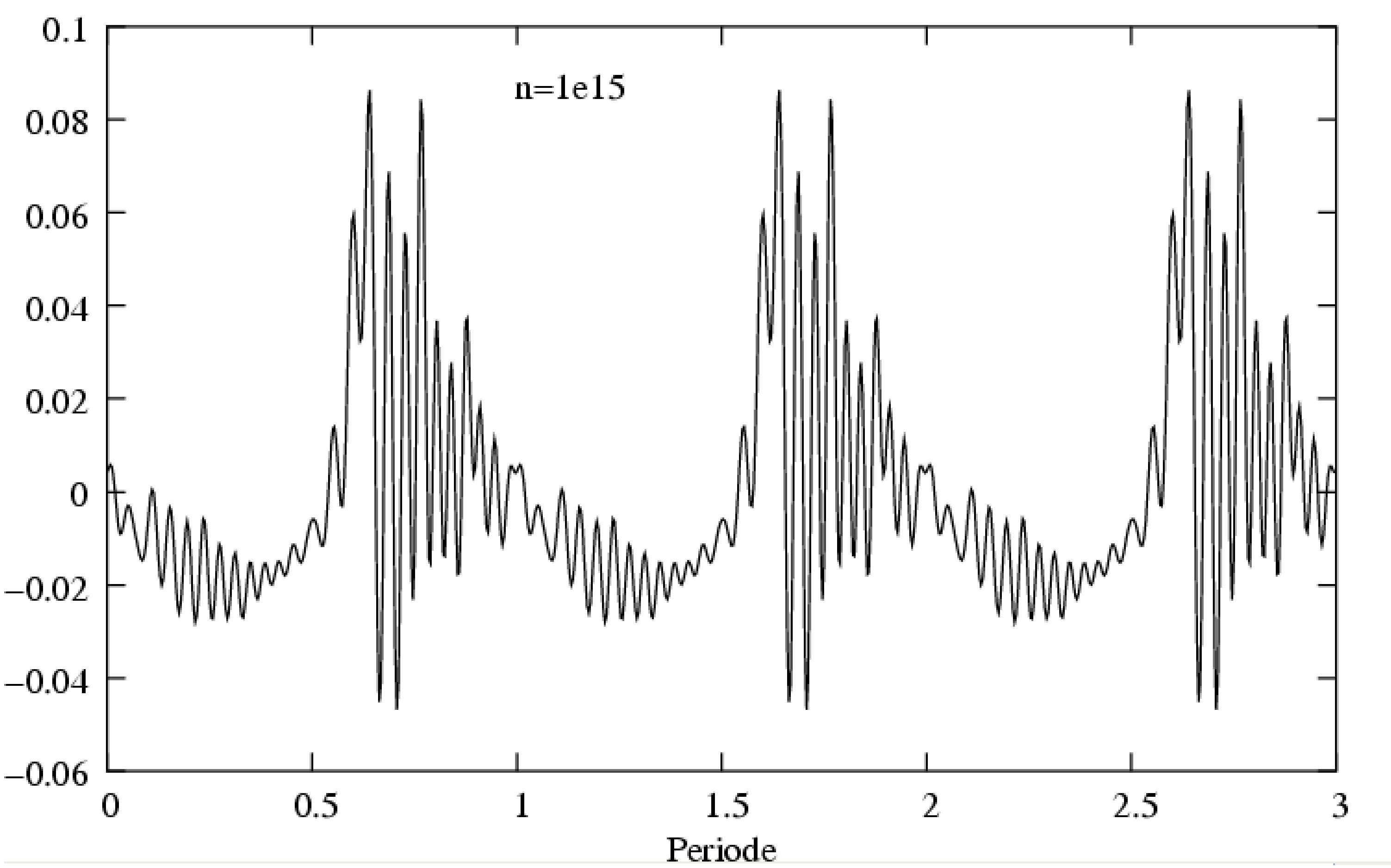
SEERS signal for a small amplitude of the RF excitation

Toy model: Results II



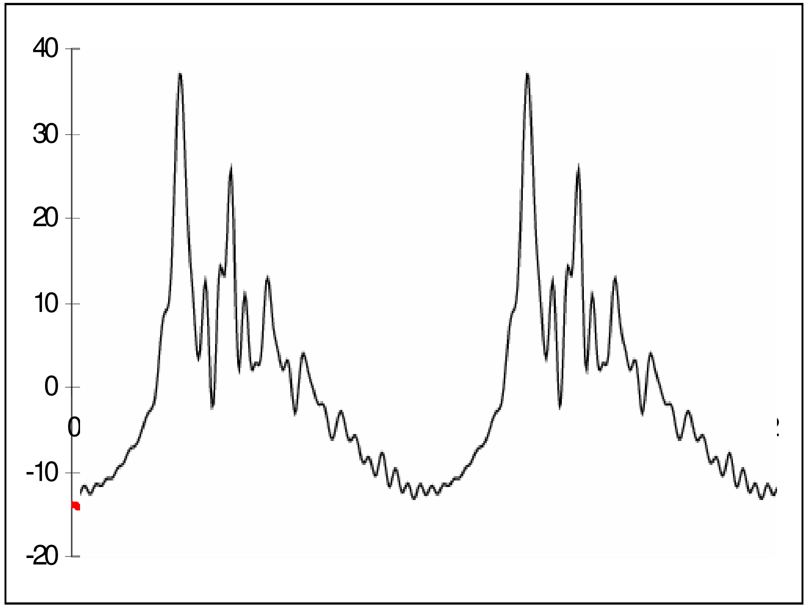
SEERS signal for a medium amplitude of the RF excitation

Toy model: Results III

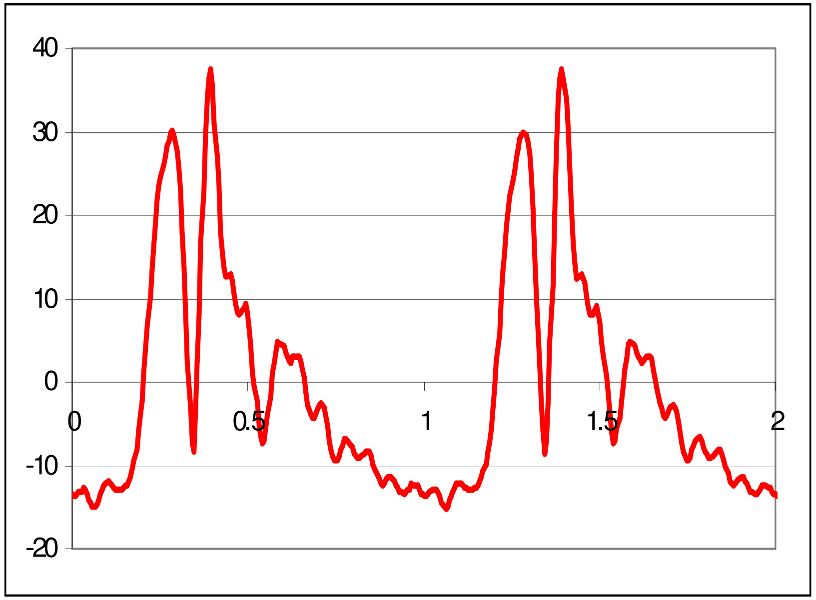


SEERS signal for a large amplitude of the RF excitation

Toy model: Comparing with reality



Simulation



SEERS Sensor-Data

- Good “qualitative” correspondence (form, trends).
- No quantitative agreement yet, but “fine structures”

For a quantitative agreement: Go beyond the toy model!

Perspective

Perspective

What have we learned?

- Consistent framework for modeling of the SEERS effect, without any restriction on geometry or homogenity.
- The nonlinear problem can be solved by “doing algebra” with the linear solutions. (In practice, few modes suffice).

Work in progress towards a full implementation:

- Essential elements already in place (nonlinear boundary sheath model, consistent numerical discretization ...).
- Current projects aim to include more physical effects (static magnetic fields, stochastic dissipation ...).
- Implementation into a full reactor simulator planned.
- Comparison with careful experiments is underway.

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Thank you!