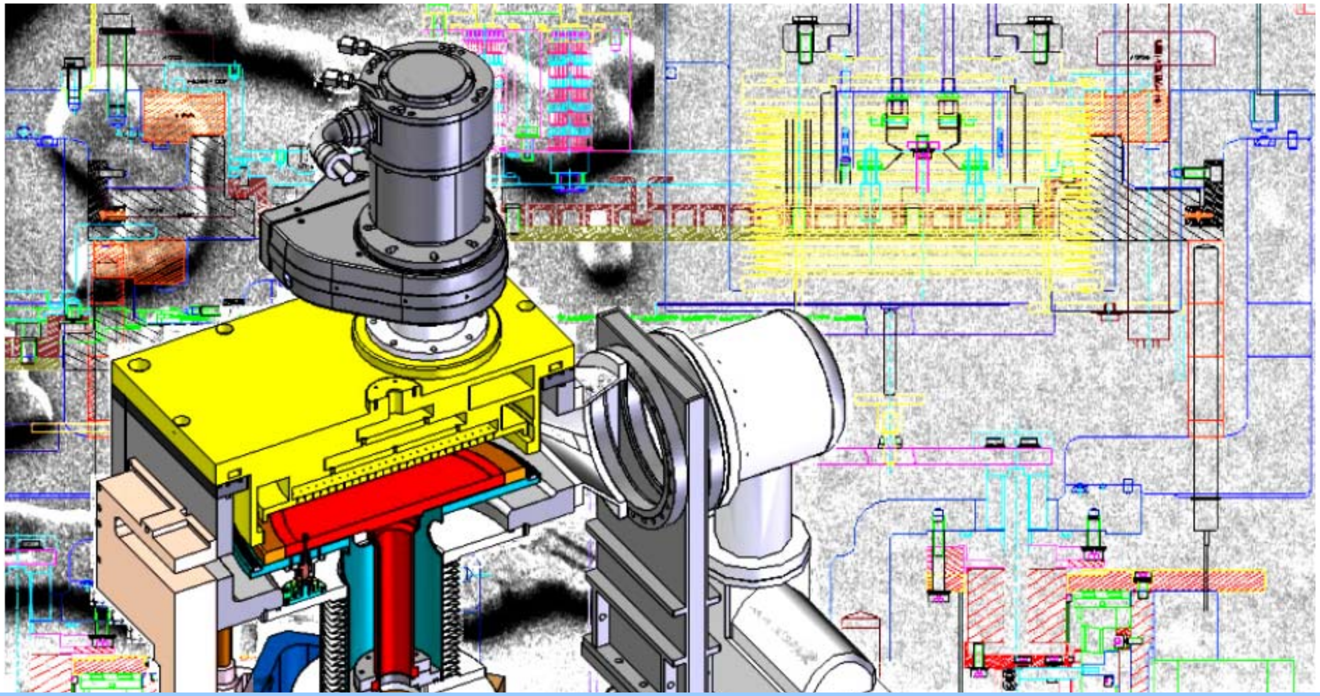

Stochastic Approach in Approximation of the Transient Plasma Sheath Behavior in FEM

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Abstract

Recently, the advanced plasma tools have been using very high frequency power sources (>100 MHz) and their combination to excite plasma utilized in semiconductor tech-nology. This approach is evoking the regimes that are less understood and currently a subject to many studies and experimental investigations. The paper describes quasi-stochastic approach applied for sheath properties and used in dual frequency (f1>>f2) capacitively coupled plasma transient simulations. The initial phase of these modeling activities and investigations shown a good numerical stability of a computational scheme. The validation of a proposed numerical model and its equivalence to full transient solution are discussed. .

Outline

- CCP model formulation and requirements
- Single frequency model
- Transient model DF
- Stochastic model DF
- Validation stochastic against transient model
- Conclusions

CCP etching

Motivation:

- **Attractive capacitively coupled plasma performance at increased excitation frequency ~ 100 MHz**
- **Enhancement and control by a dual frequency implementation ~ 2 MHz**

Hardware variation

Chemistry variation

Industrial level implementation

flexible, reliable, comprehensive means and approach to investigate

Computational characterization

of the plasma, reaction chemistry and etch performance

Business requirements

- **optimal solutions at increased complexity of the process and expectations towards the tool performance**
- **integration with CAD, engineering tools**
- **minimize interference from the 3rd party, operations, cost, ….**
- **quick turnaround & feedback**

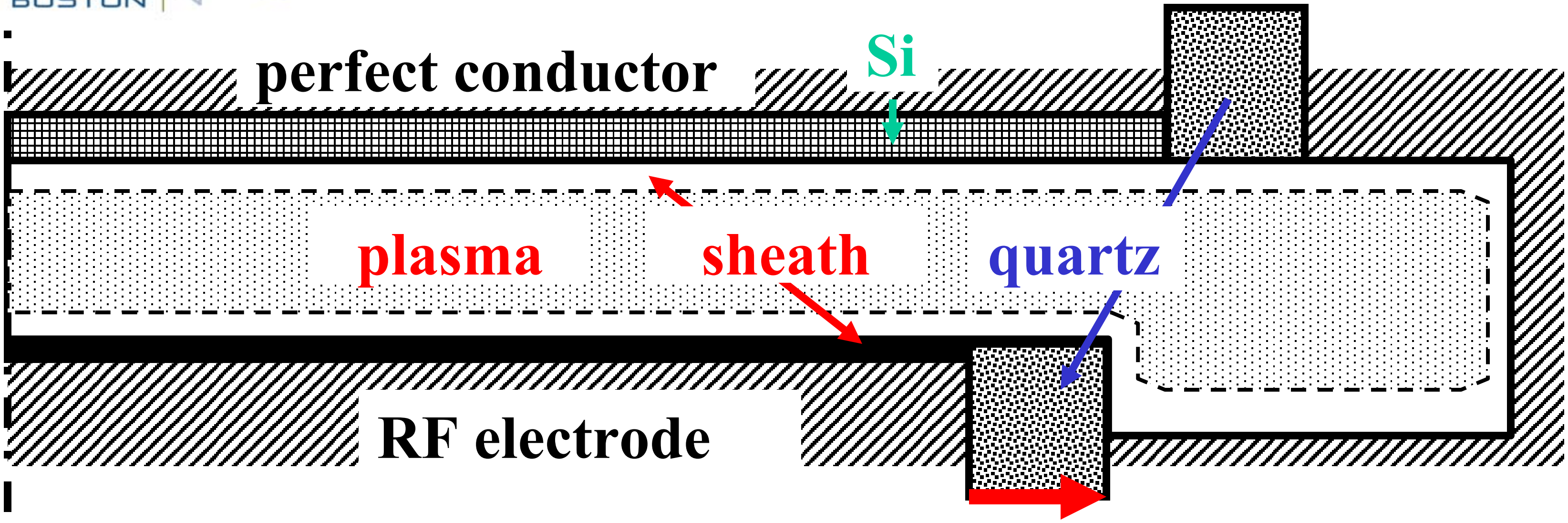
Physics & modeling requirements

- **provide mutual coupling between**
  - various model components & variables, physics & chemistry
  - … and still convergent
- **self-consistent approach**
- **additional capabilities … extension up to 3D**

In past experiencing with various codes & sw packages …

FEM approach

Plasma model features – 2D axial symmetry



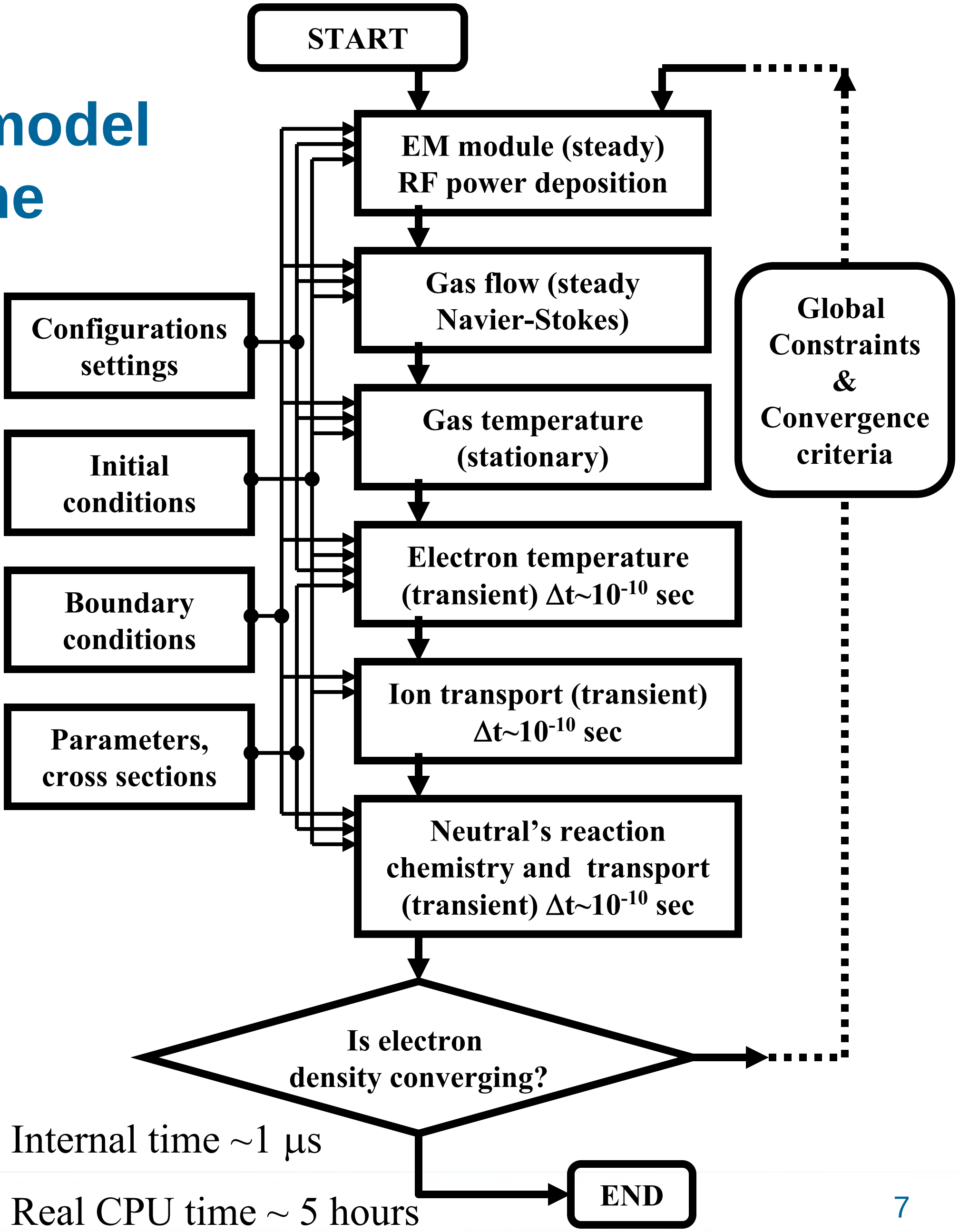
- **Formulated CCP Plasma Fluid Model**
  - plasma species transport by an ambipolar drift – diffusion interpretation[1)] superimposed over the actual gas flow
  - single frequency excitation – averaged power through one RF period (high frequency)
  - Bohm flux at plasma-sheath interface
  - sheath model in “LGL” interpretation[2)]

[1)] M. A. Lieberman, A.J. Lichtenberg, *Principles of plasma discharges and materials processing*, 129, 327-388. John Wiley & Sons, New York (1994)

[2)] Lee I., Graves D.B. and Lieberman M.A, Modeling electromagnetic effects in capacitive discharges, *Plasma Sources Sci. Technol.*, 17, 1-16 (2008)

Coupled model scheme

- Single frequency 100 MHz → RF period ~ 10 ns
- Solving transient sub-modules in this scheme starts from numerical time steps $\Delta t \sim 10^{-10}$ sec
- Convergence is occurring in internal times approximatelly t>1 μs up to t~100 μs
- In terms of the CPU real time this is accomplished in 4-6 hours



START

EM module (steady) RF power deposition

Gas flow (steady Navier-Stokes)

Gas temperature (stationary)

Electron temperature (transient) $\Delta t \sim 10^{-10}$ sec

Ion transport (transient) $\Delta t \sim 10^{-10}$ sec

Neutral's reaction chemistry and transport (transient) $\Delta t \sim 10^{-10}$ sec

Configurations settings

Initial conditions

Boundary conditions

Parameters, cross sections

Global Constraints & Convergence criteria

Is electron density converging?

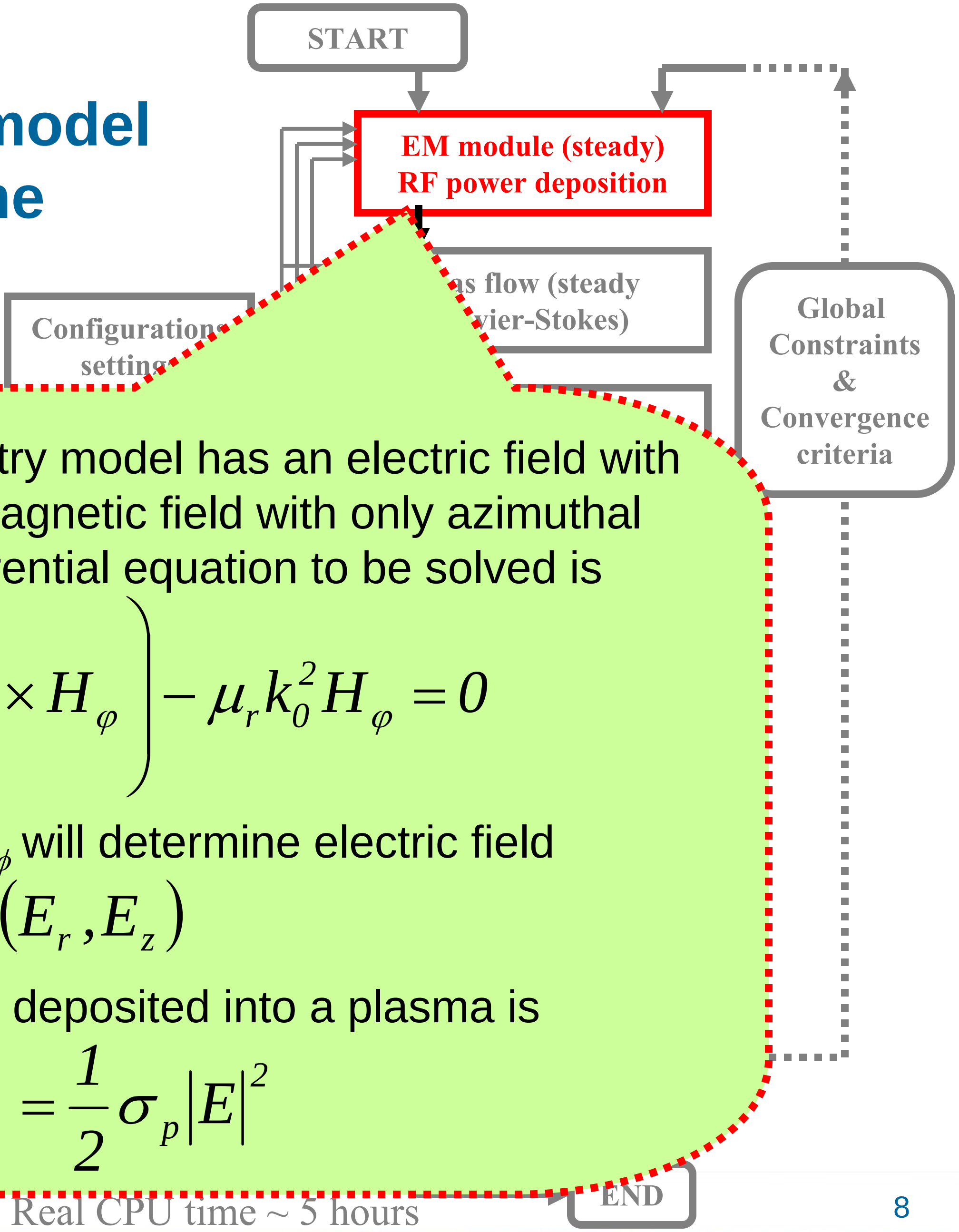
END

Internal time ~1 μs

Real CPU time ~ 5 hours

Coupled model scheme

- **Equations**



The TM wave in 2D axial symmetry model has an electric field with components in *r-z* plane and magnetic field with only azimuthal component, thus partial differential equation to be solved is

$$\nabla\times\left(\left(\varepsilon_r - j\frac{\sigma}{\omega\varepsilon_0}\right)^{-1}\nabla\times H_\varphi\right) - \mu_r k_0^2 H_\varphi = 0$$

Solving this equation for H_ϕ will determine electric field

$$H_\varphi \Rightarrow \left(E_r , E_z\right)$$

Thus , formally, the power deposited into a plasma is

$$Q_{abs} = \frac{1}{2}\sigma_p\left|E\right|^2$$

Gas flow assuming low Reynolds number and laminar flow in 2D axial symmetry geometry

$$\rho\frac{\partial\vec{u}}{\partial t}-\nabla\cdot\left[-p\vec{I}+\eta\left(\nabla\vec{u}+(\nabla\vec{u})^{T}\right)\right]+\rho(\vec{u}\cdot\nabla)\vec{u}=\vec{F}$$

the mass continuity equation under incompressible gas assumption

$$\nabla\cdot\vec{u}=0$$

Energy conservation, Te

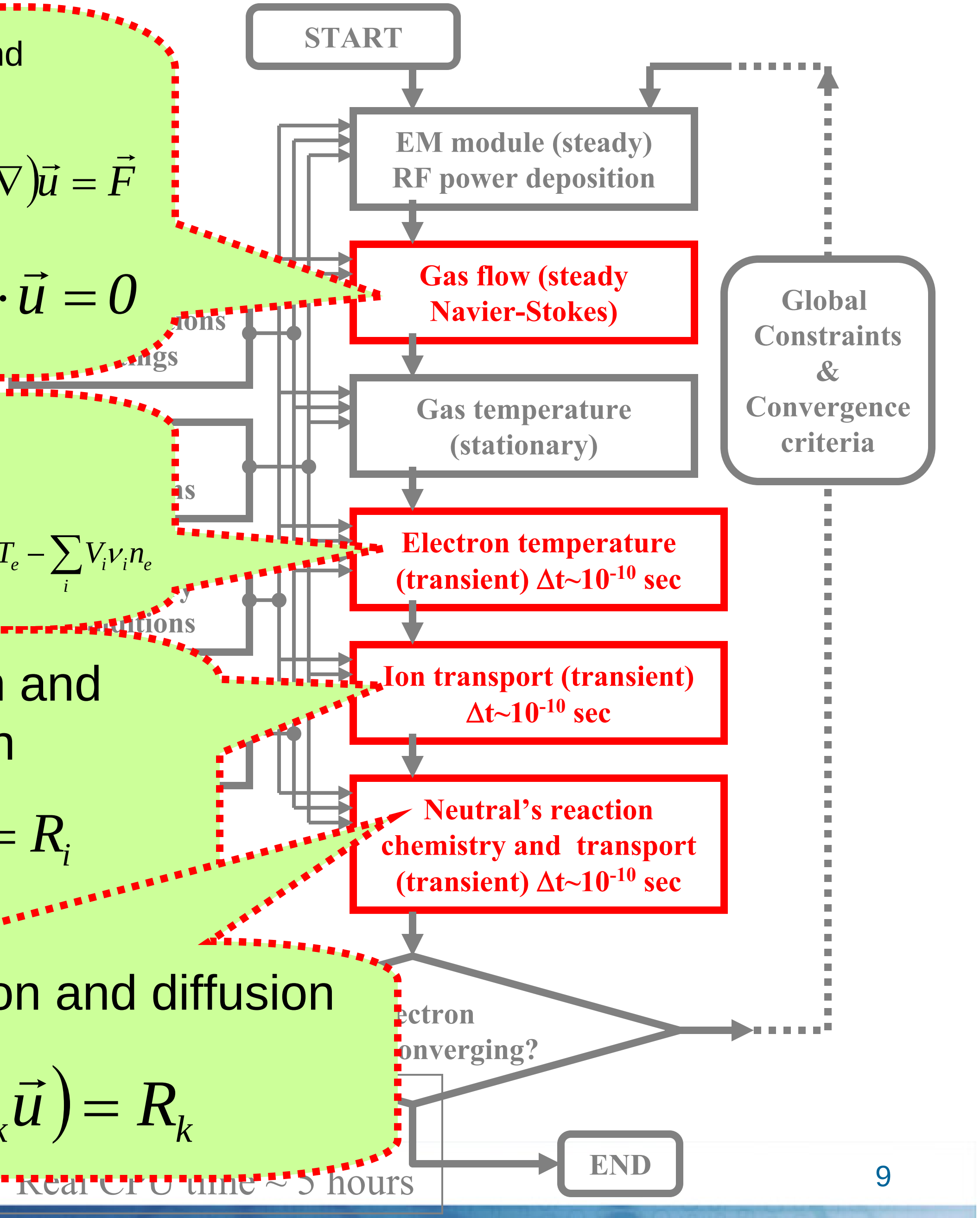
$$\frac{\partial}{\partial t}\left(\frac{3}{2}n_eT_e\right)+\nabla\left(\frac{5}{2}T_e\Gamma_e-k\nabla T_e\right)=Q_{abs}-e\Gamma_eE_a-\frac{3m}{M}\nu_m n_e T_e-\sum_i V_i\nu_i n_e$$

Ions transport by convection and ambipolar drift - diffusion

$$\frac{\partial n_i}{\partial t}+\nabla\left(-D_a\nabla n_i+n_i\vec{u}\right)=R_i$$

Neutrals transport by convection and diffusion

$$\nabla\left(-D_k\nabla n_k+n_k\vec{u}\right)=R_k$$



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Neutral's reaction chemistry and transport (transient) $\Delta t\sim10^{-10}$ sec

ectron onverging?

END

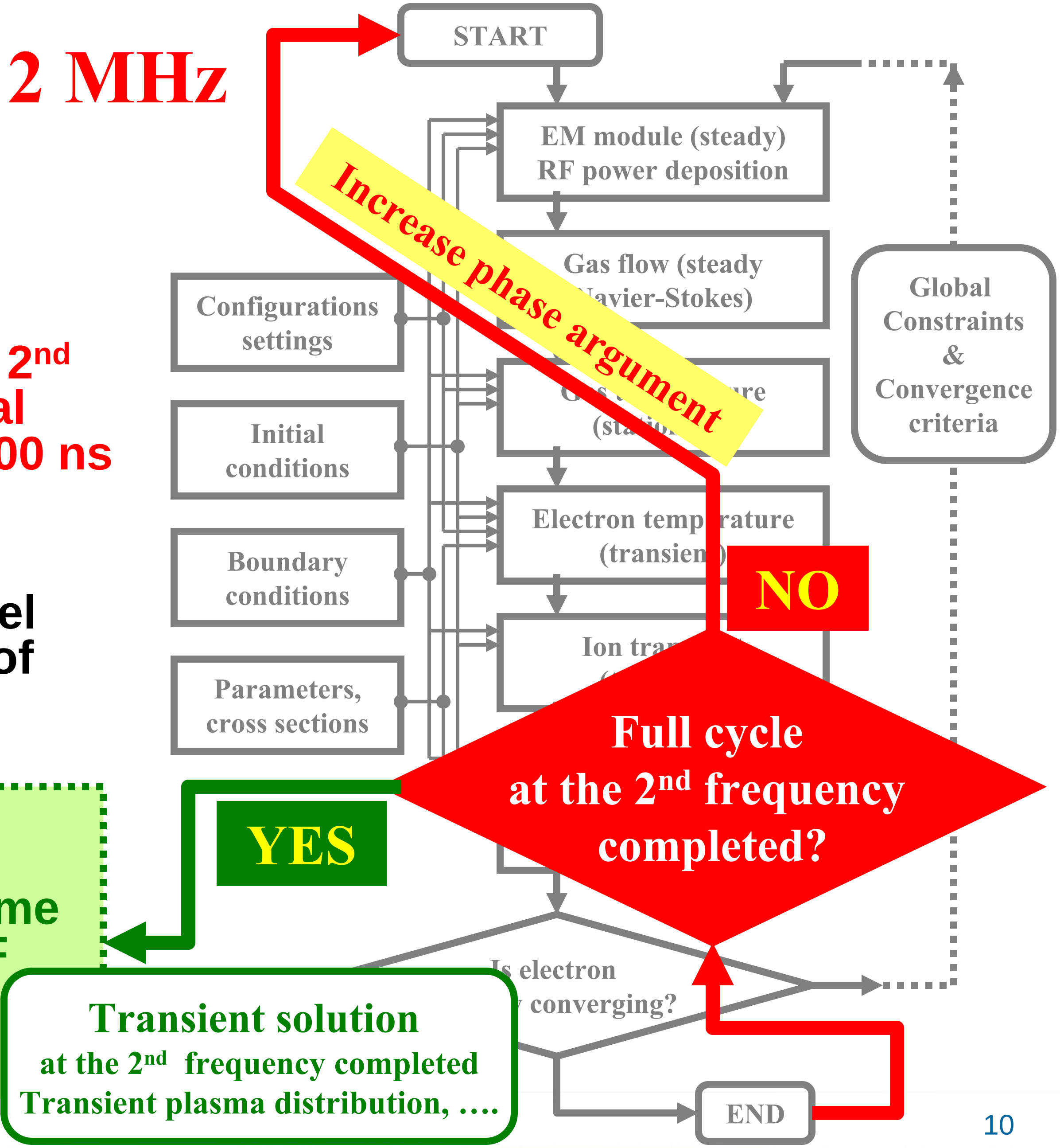
Global Constraints & Convergence criteria

Real CPU time ~ 5 hours

Coupled model transient scheme

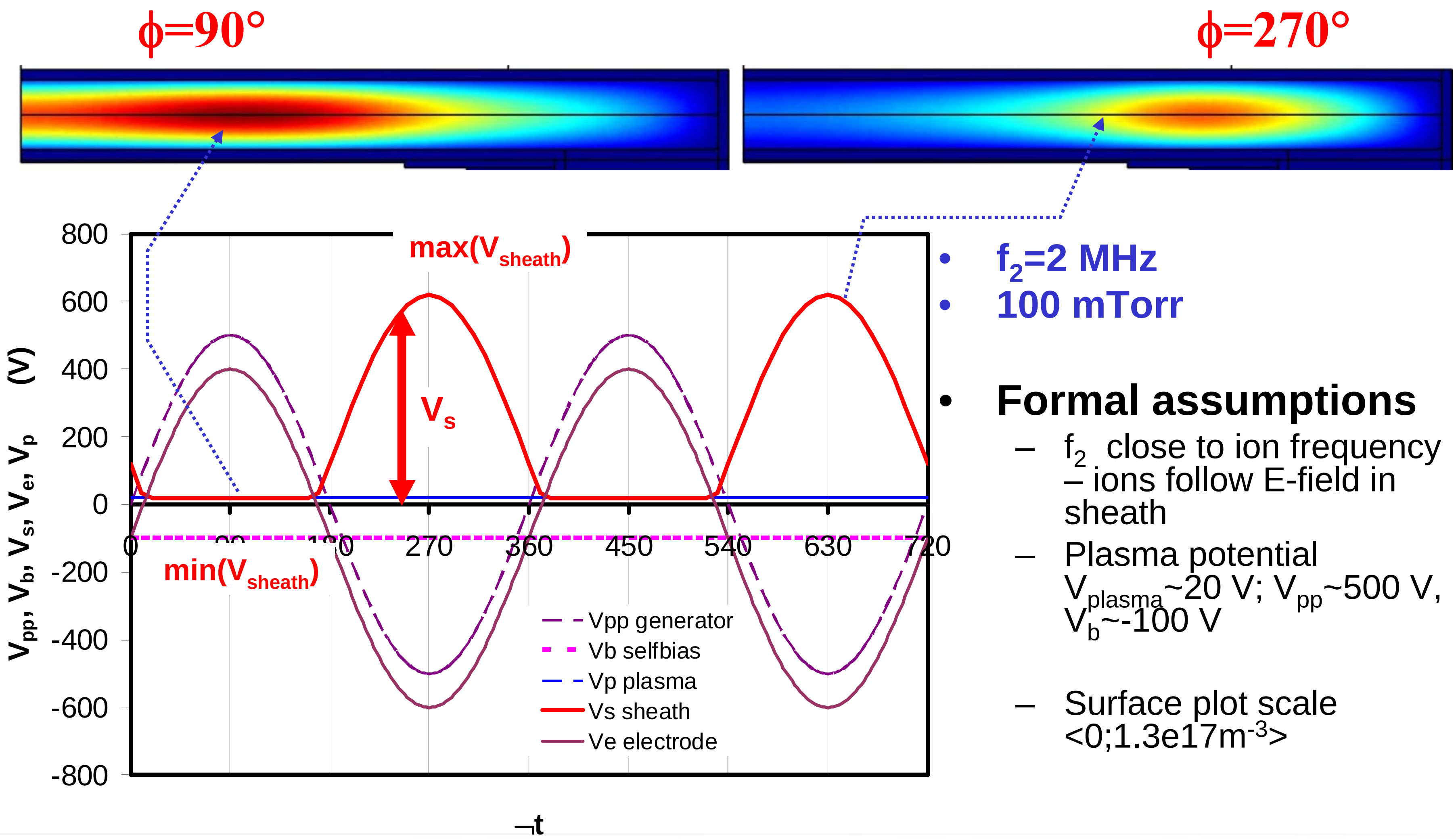
2 MHz

- Implementation of the 2nd frequency → additional loop at time scale ~ 500 ns (one period at 2 MHz)
- Single frequency model scheme → sub-block of the transient dual frequency scheme
- After straightforward implementation and time step ~5% (25 ns) of RF cycle it can be solved within ~ 100 hours



Transient solution
at the 2nd frequency completed
Transient plasma distribution, ….

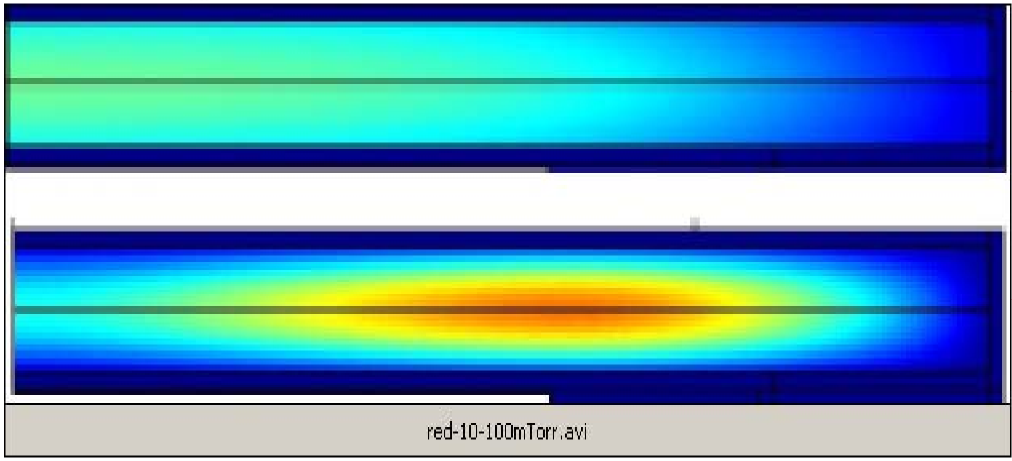
Sheath voltage & electron density



- **f_2=2 MHz**
- **100 mTorr**

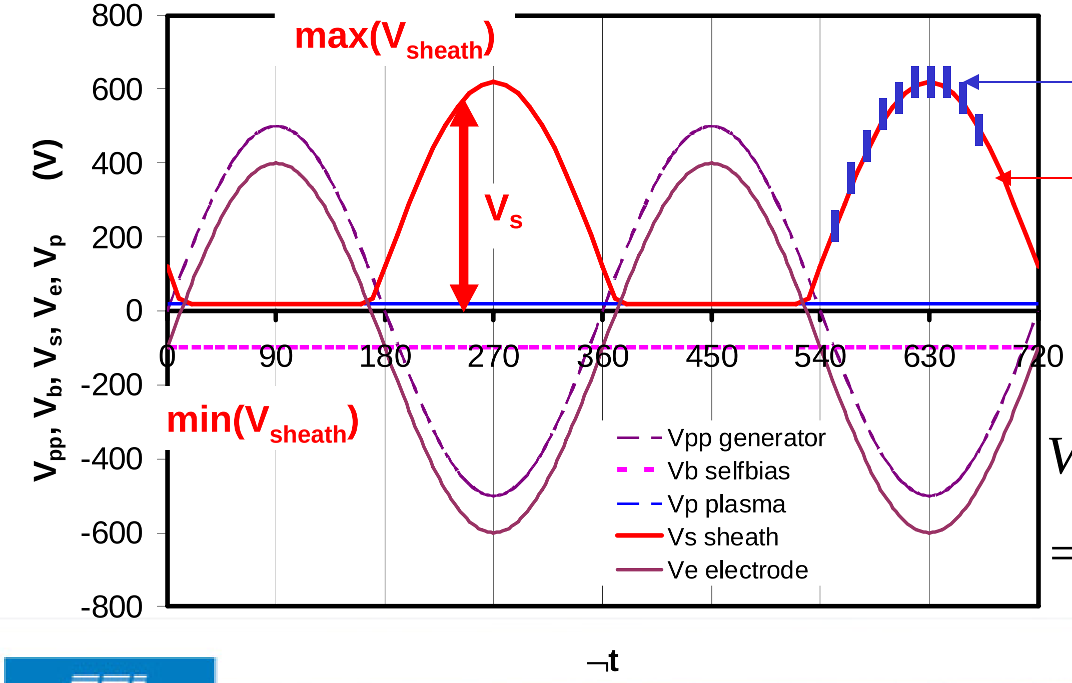
- **Formal assumptions**
  - f_2 close to ion frequency – ions follow E-field in sheath
  - Plasma potential V_{plasma}~20 V; V_{pp}~500 V, V_b~-100 V
  - Surface plot scale <0;1.3e17m^{-3}>

Sheath voltage & electron density



10 mTorr

100 mTorr



- **f_1=100 MHz**
- **f_2=2 MHz**

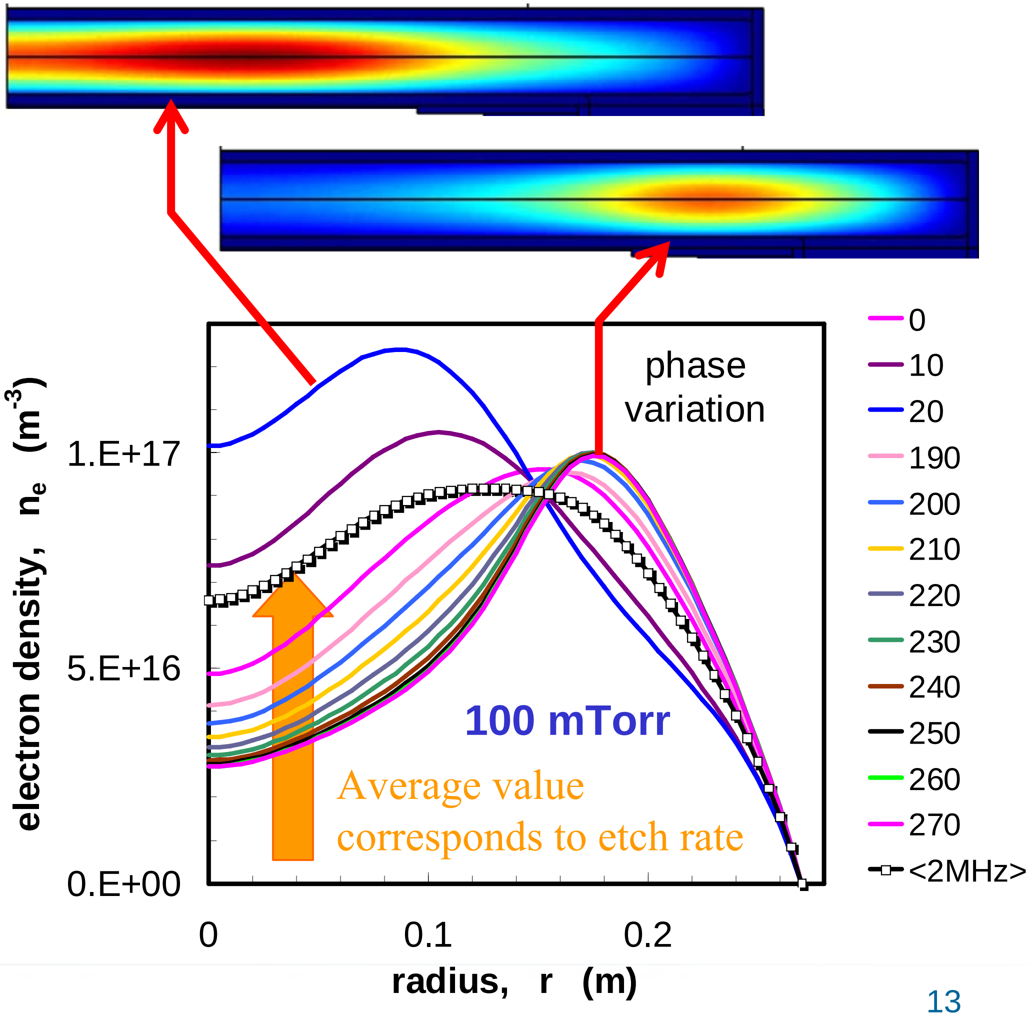
$$V_s = V_p - V_{el} = $$
$$= \max\{V_p, V_p - [V_{RF}\sin(\omega_2 t) - |U_b|]\}$$

Capacitively coupled plasma dual frequency reactor - 2D transient model

- **Simulation results on the dual frequency CCP can be achieved**
  - Plasma distribution is changing over the 2nd frequency cycle

- **BUT! transient case requires significant computational time resources**

- **Flexibility of a modular system is allowing to generate specific approach and algorithms to speed up computation**



Average value corresponds to etch rate

Problem to solve …

- **Computational time - major driving force for a new concepts**

- **Transient solution at the 2nd frequency**
  - Possible, but large time scale range → long real CPU time
  - Impractical / difficult to merge and accelerate development

- **Is there fast & accurate enough approach to be integrated into cost efficient workflow?**

Novel idea to create fast computation model

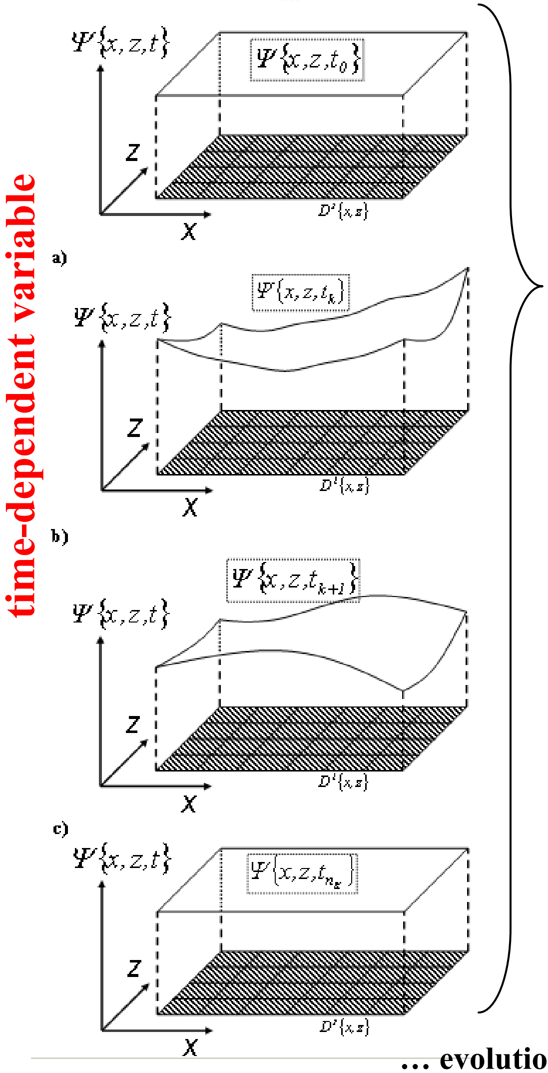
- **Instead of the transient variable characteristics, that is "time-fingerprint" in the model, let us consider spatial resolution of the variable (or parameter) – "spatial fingerprint" to achieve time-averaged plasma distribution within a significantly shorter computational times**

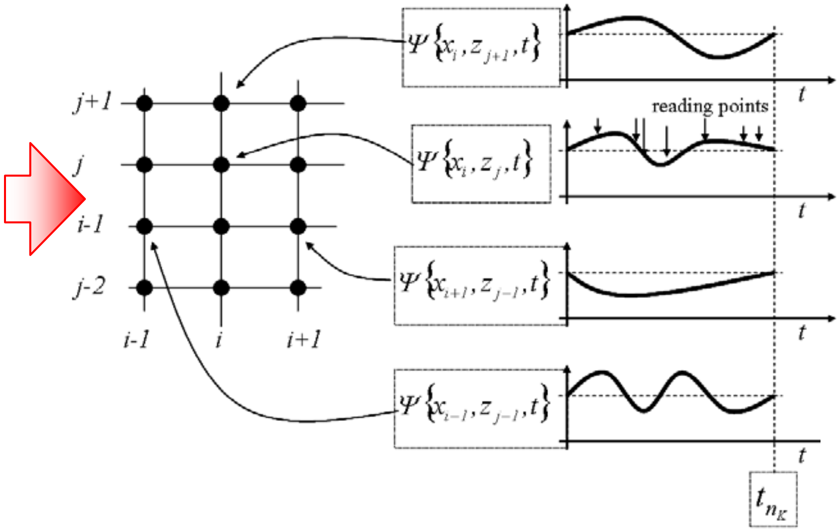
Stochastic Equivalence Approach

SEA

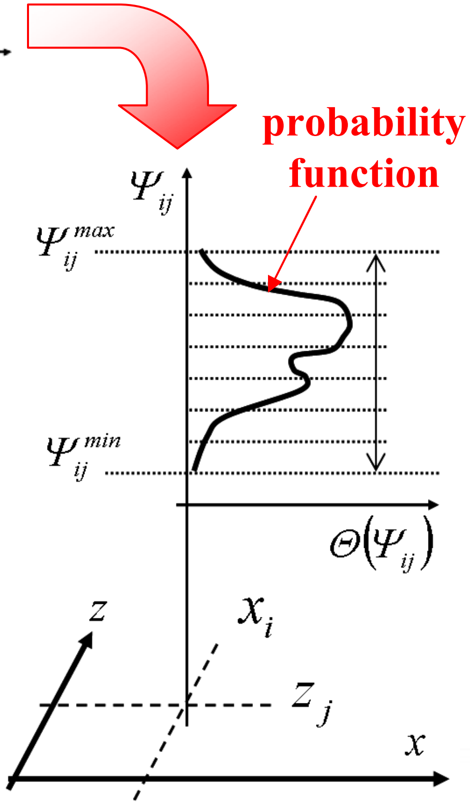
“time–to-space” conversion of arbitrary variable

$$\Psi(x,z,t)$$





… the regular grid in numerical domain with nodal points, and corresponding transient dependencies of the time-dependent variable in each individual node …



- **Different parameters can be represented as “t-s” variable, for example**
  - the sheath voltage
  - the source of contamination
  - internal surface properties
  - etc.,……

… evolution of time-dependent variable in computational domain through the sequence a) , … b) , c) , …, and d) …

… geometrical relation of the probability function in respect to nodal point …

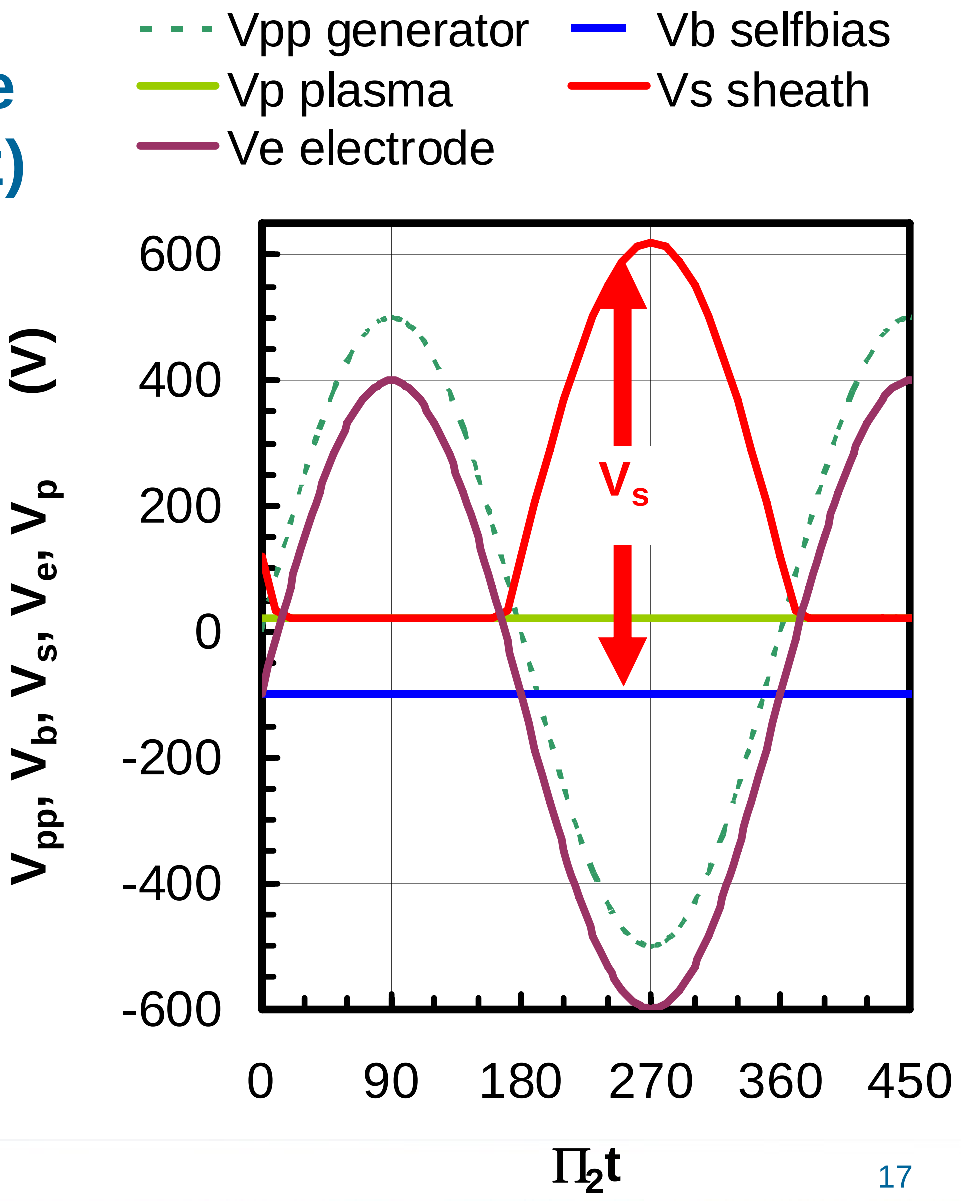
Sheath voltage

$V_{sh}(t) \rightarrow V_{sh}(x,z)$

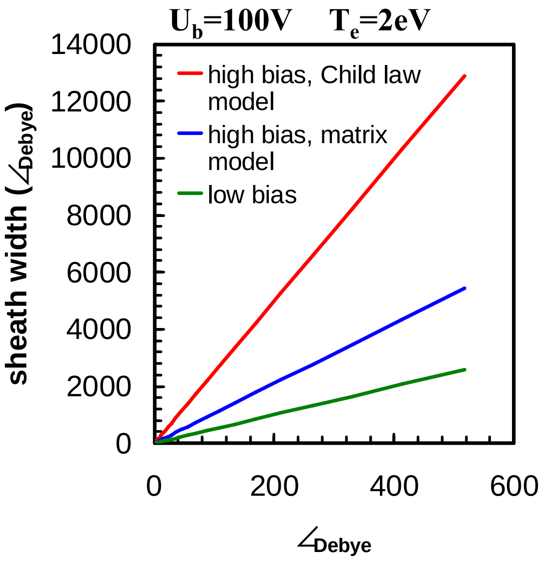
- **Transient-to-spatial conversion is applied to sheath properties – *$V_{sh}(t)$***
  - Generation of the probability function

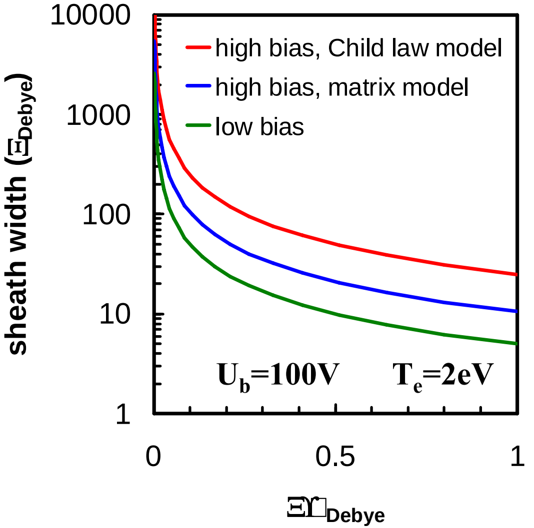
$$V_s = \left[V_p - V_{el}\right]_{\omega_2<\omega_i} = \\ = max\left\{V_p, V_p - \left[V_{RF}\ sin(\omega_2 t) - |U_b|\right]\right\}$$

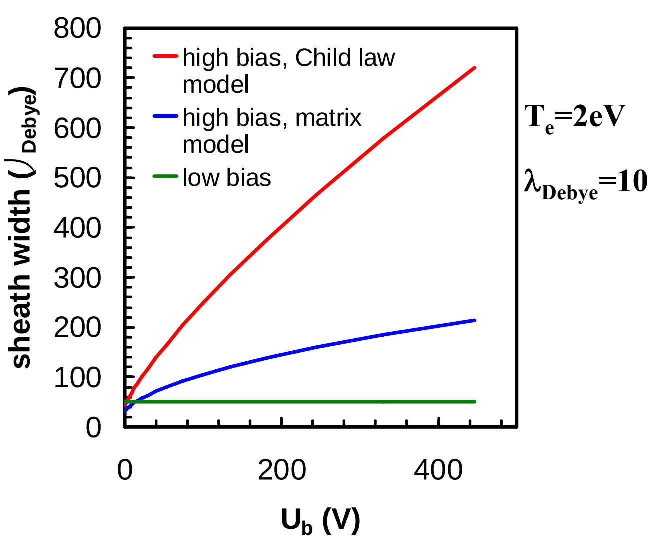
- **Randomize the effect: "*infinitively small*" spatial periods (about 0.1mm << grid dimensions << sheath or plasma dimensions)**
- **Formally – equivalent to probing "plasma-sheath interface" properties randomly in time and space >> T^{2MHz}**



Coupling with sheath & plasma parameters according various sheath models …

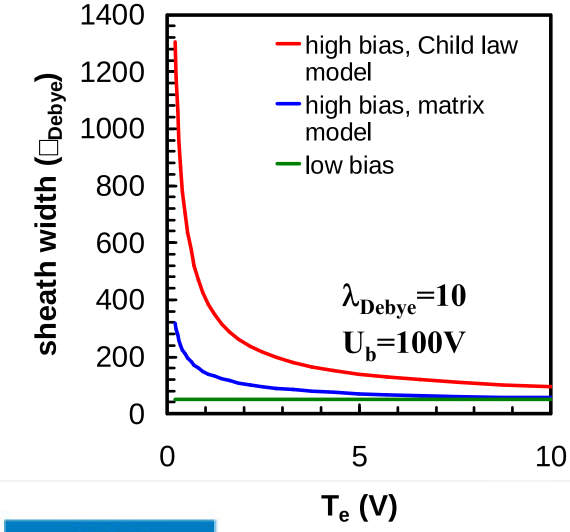






Pressure increase

BIAS increase



- **Sheath properties coupled to many plasma parameters**
- **Behaviour of plasma sheath – sheath voltage, current, etc are described by various models (colisional vs non-colisional, …)**

$$x_s = \gamma_s \lambda_{De}$$

Floating wall

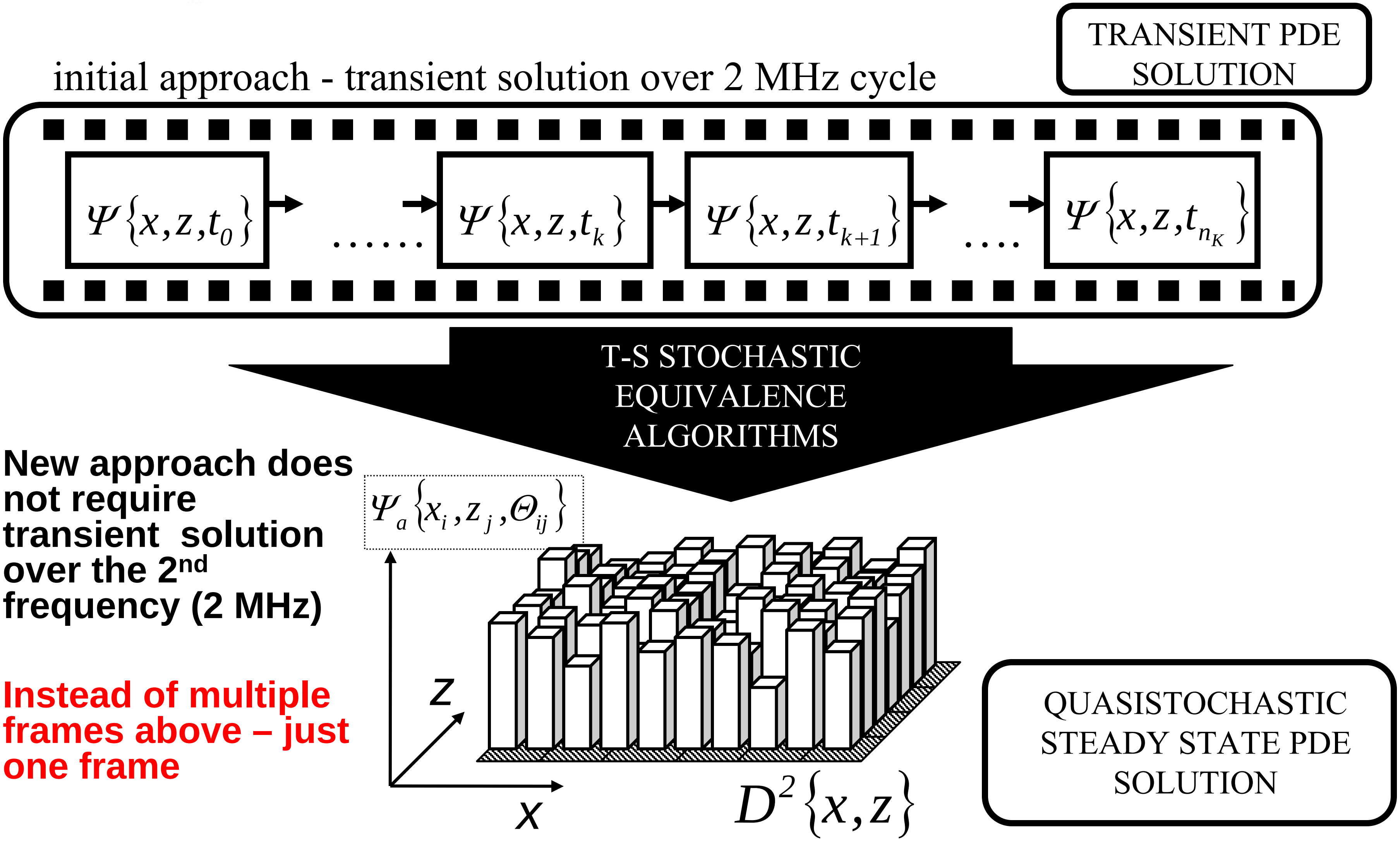
$$x_s = 1.41\left[\gamma_s + \frac{e|U_b|}{k_B T_e}\right]^{1/2} \lambda_{De}$$

Matrix model

$$x_s = 1.225\left(\gamma_s + \frac{e|U_b|}{k_B T_e}\right)^{3/4} \lambda_{De}$$

Child law sheath

Advantage of the proposed method



TRANSIENT PDE SOLUTION

initial approach - transient solution over 2 MHz cycle

$\Psi\{x,z,t_0\} \rightarrow \ldots\ldots \rightarrow \Psi\{x,z,t_k\} \rightarrow \Psi\{x,z,t_{k+1}\} \rightarrow \ldots\ldots \rightarrow \Psi\{x,z,t_{n_K}\}$

T-S STOCHASTIC EQUIVALENCE ALGORITHMS

$\Psi_a\{x_i, z_j, \Theta_{ij}\}$

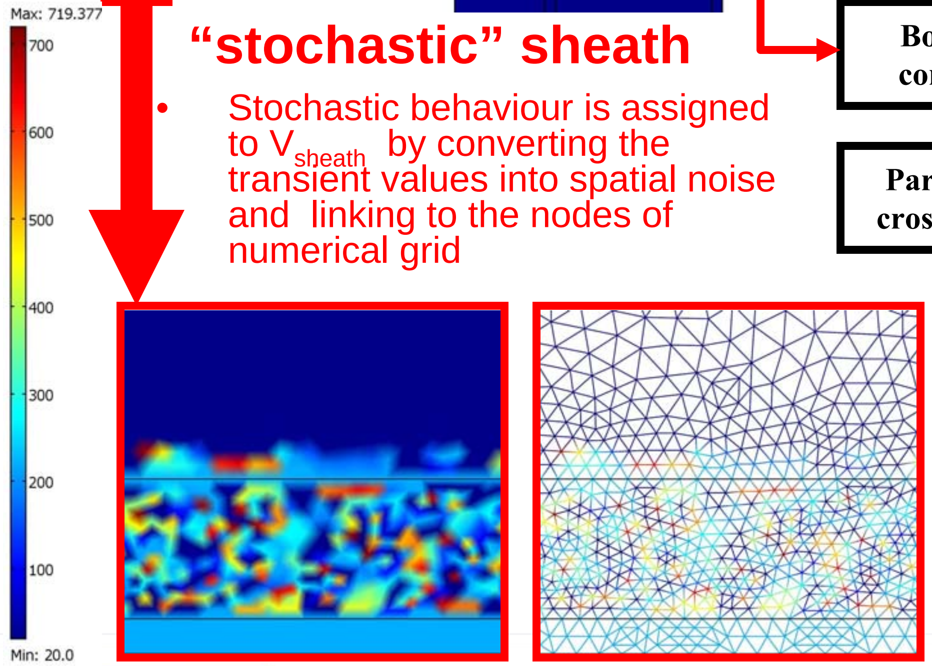
$D^2\{x,z\}$

QUASISTOCHASTIC STEADY STATE PDE SOLUTION

- **New approach does not require transient solution over the 2nd frequency (2 MHz)**
- **Instead of multiple frames above – just one frame**

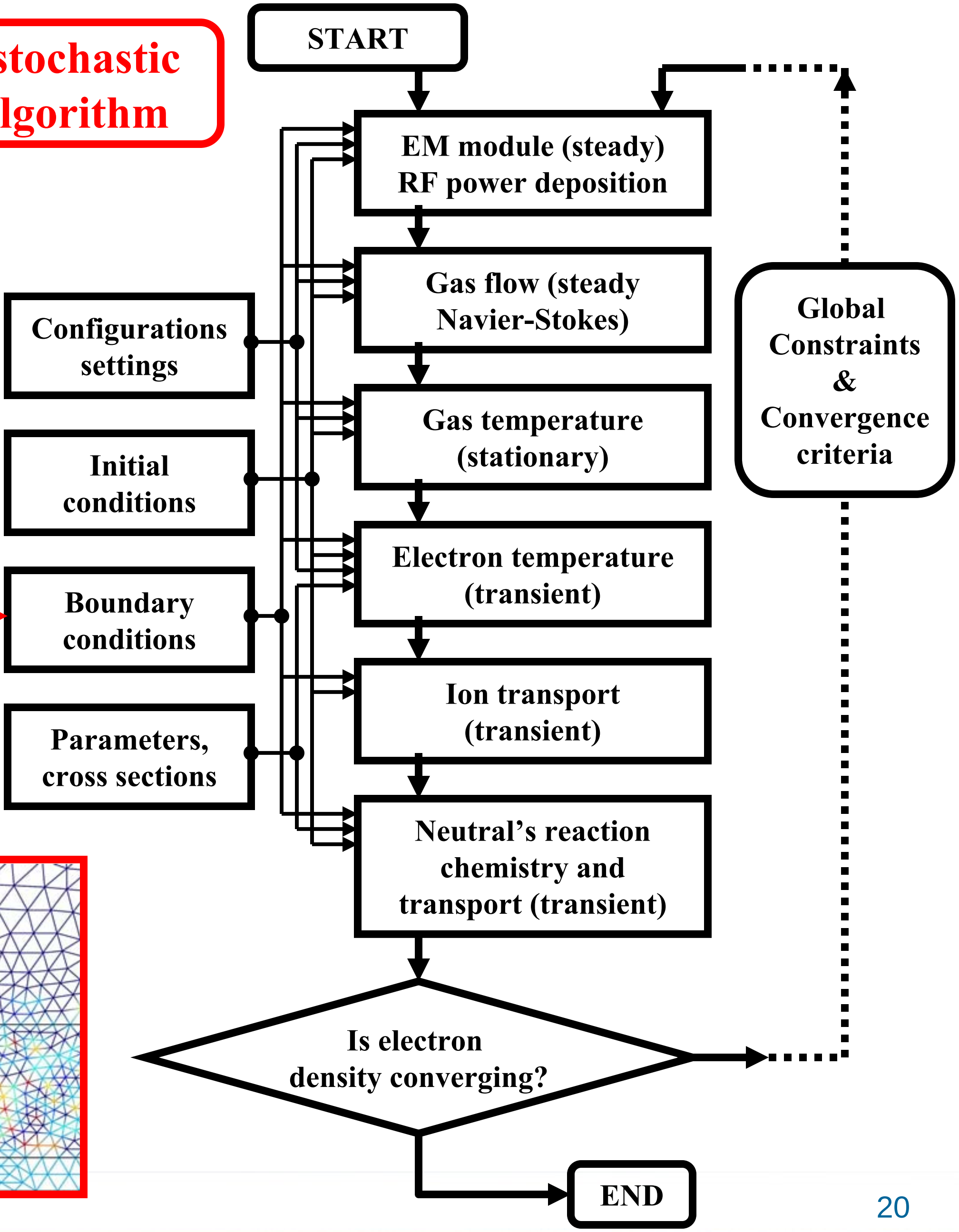
Coupled model fast scheme numerical implementation

Transient-to-stochastic conversion algorithm



“stochastic” sheath

- Stochastic behaviour is assigned to V_{sheath} by converting the transient values into spatial noise and linking to the nodes of numerical grid



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Electron temperature (transient)

Ion transport (transient)

Neutral’s reaction chemistry and transport (transient)

Is electron density converging?

END

Configurations settings

Initial conditions

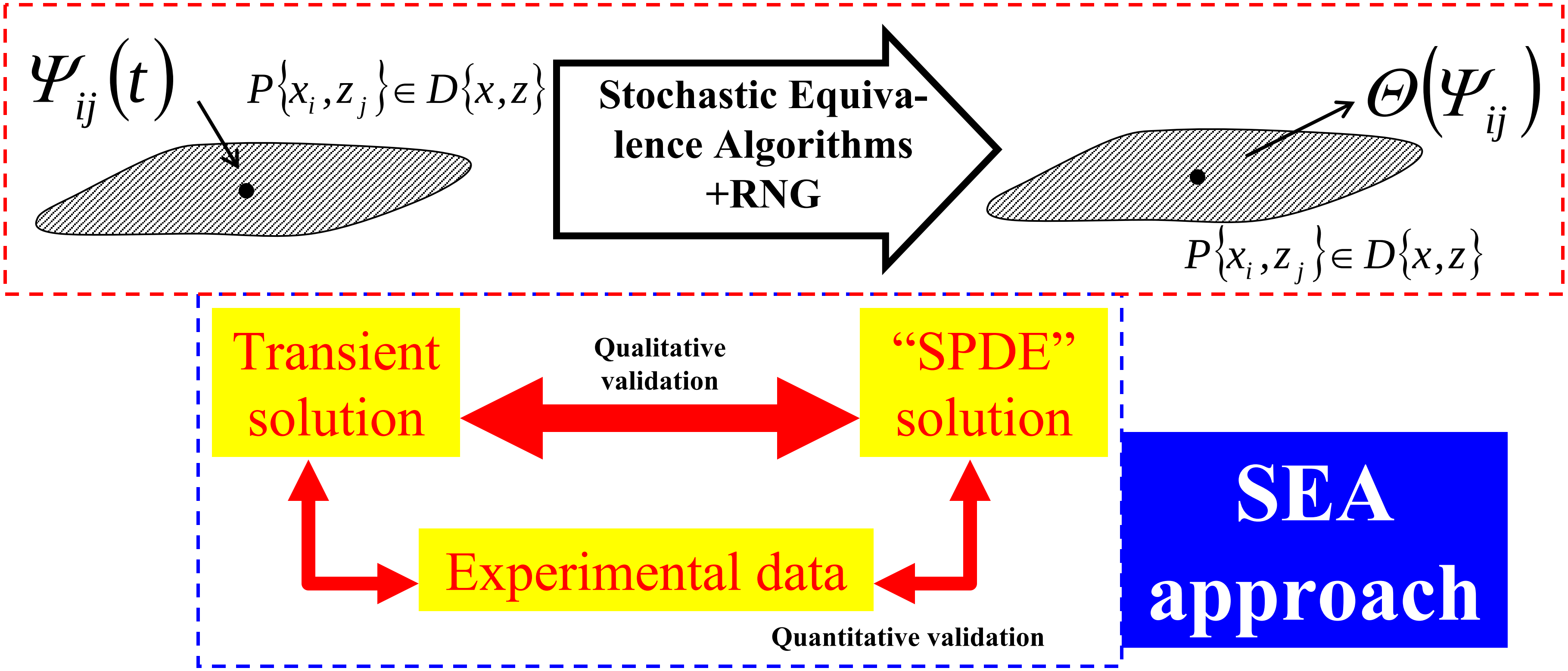
Boundary conditions

Parameters, cross sections

Global Constraints & Convergence criteria

implementation of the proposed method

- **New method should generate solution that is equivalent to the transient solution …**



$\Psi_{ij}(t)$ $P\{x_i, z_j\} \in D\{x,z\}$

Stochastic Equivalence Algorithms +RNG

$\Theta(\Psi_{ij})$ $P\{x_i, z_j\} \in D\{x,z\}$

Transient solution

Qualitative validation

"SPDE" solution

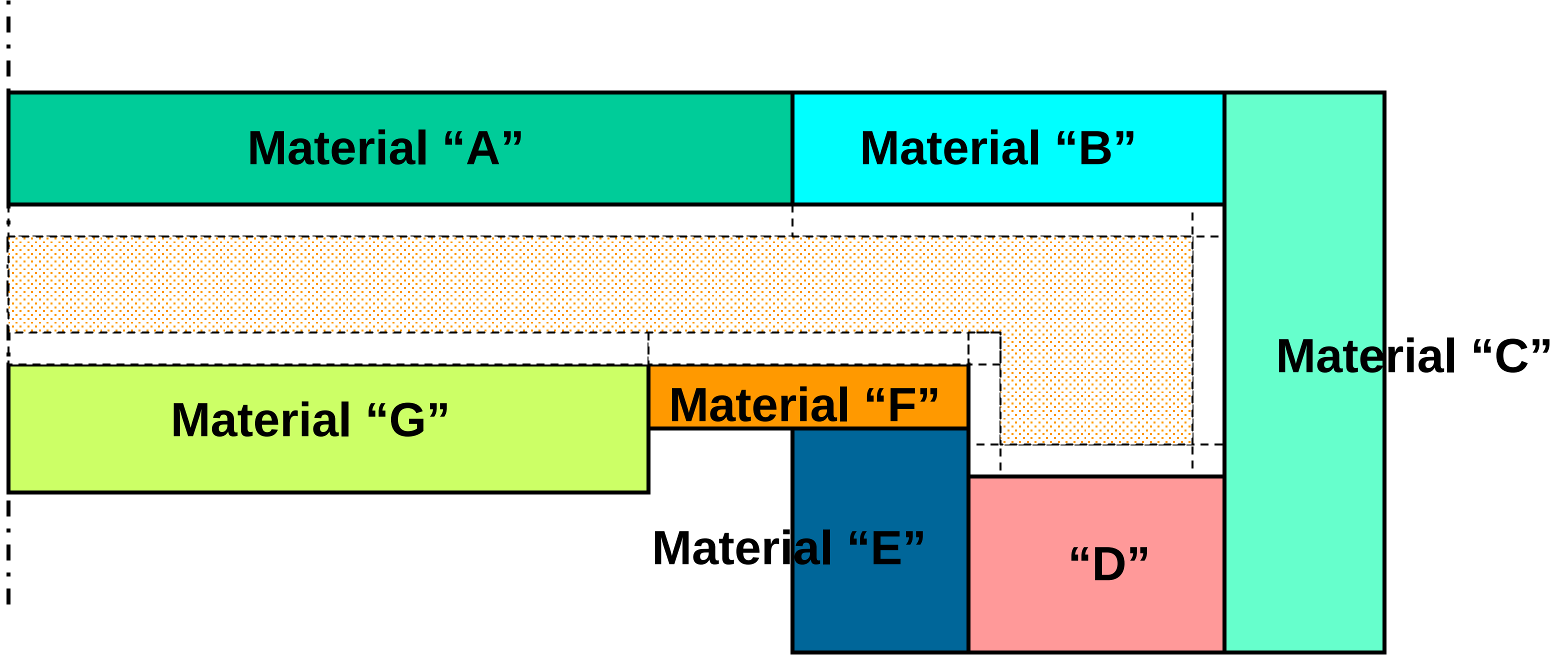
Experimental data

Quantitative validation

SEA approach

- **Implementation will require to validate SPDE model *vs.* Transient Solution (TS) and vs experimental results**

Impact on sheath domain assignments (generic chamber)



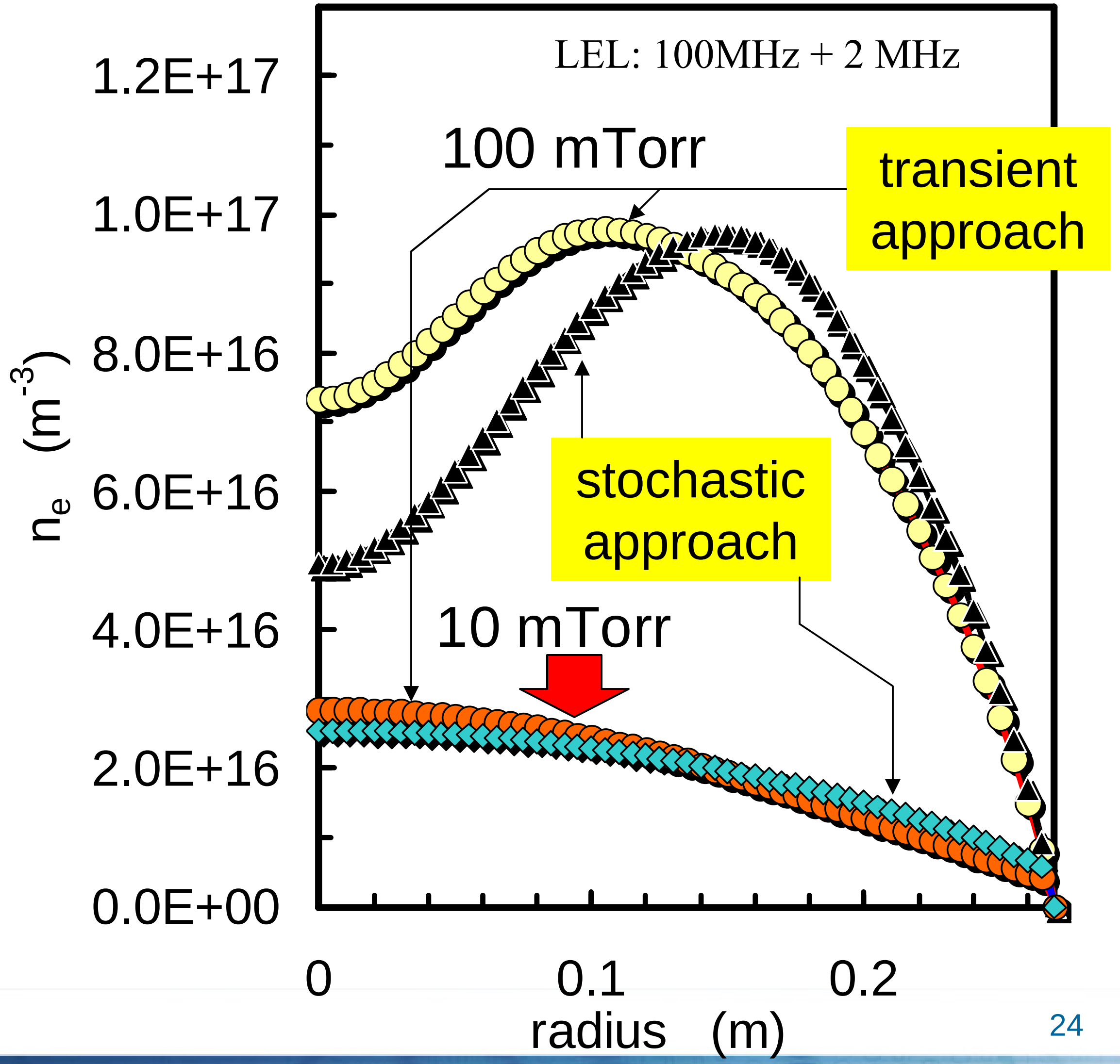
- **Geometry condition for selfbias determination and sheath formulation:**
  - Each material with surface exposed to plasma has assigned geometrically congruent sheath

Status of Computation with Proposed Method

- **Implemented simple version of stochastic sheath-plasma interface behaviour**
  - Model is numerically stable and convergent
  - It is by order faster to calculate dual frequency system than equivalent transient simulations
  - Provides an ability to execute many DOE series to investigate DF CCP performance at high savings on the time resources: EXAMPLES FOLLOW ON NEXT SLIDES

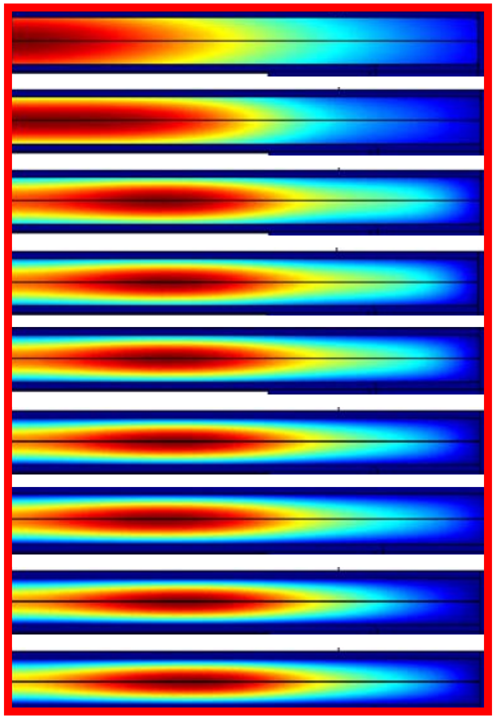
Validation transient & stochastic methods

- **Plasma distributions at various pressures by both methods:**
  - 10 mTorr
  - 100 mTorr
- **low pressure exhibited very good correlation**
- **Increased pressure – qualitative trends are well observed**
- **Computational time resources – great advantage for stochastic method**

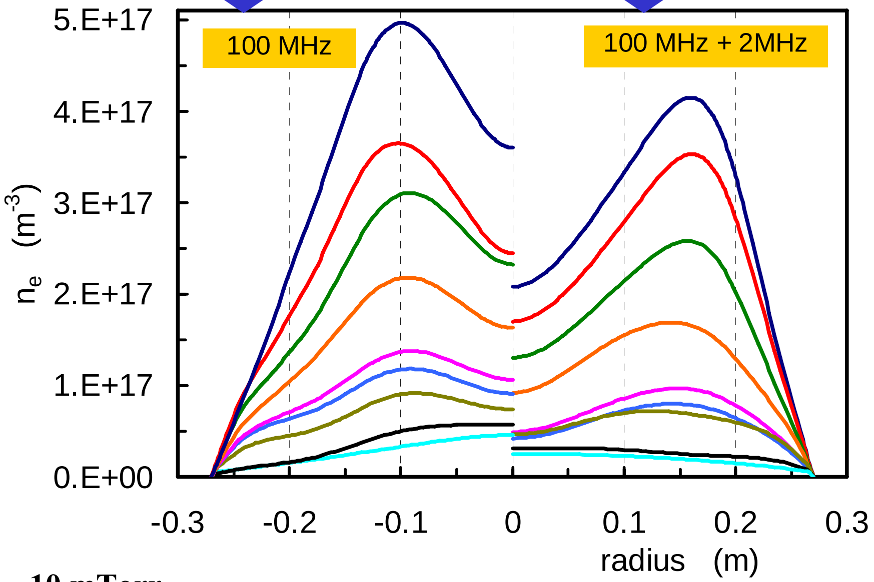


Dual frequency model: electron density vs pressure

@ 100 MHz (single frequency)

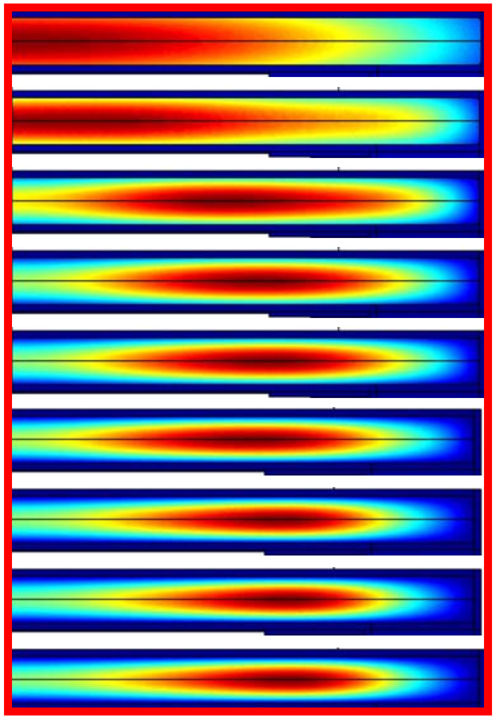


0-max(n_e) scale



10 mTorr
25 mTorr
50 mTorr
75 mTorr
100 mTorr
200 mTorr
300 mTorr
400 mTorr
500 mTorr

@ 100 MHz + 2 MHz (dual frequency)



0-max(n_e) scale

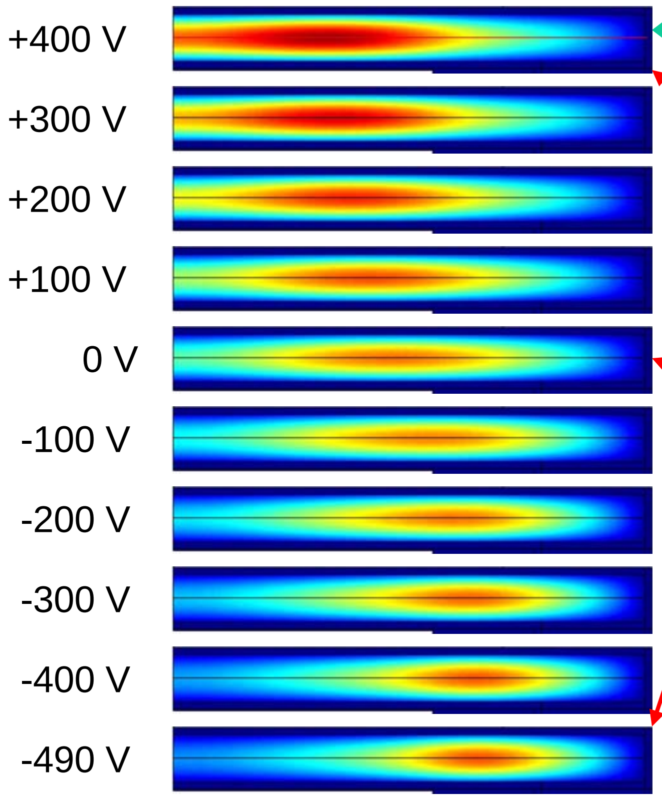
- **Single frequency : 100 MHz – trend is confirmed by experimental data**
- **DF : 100 MHz + 2 MHz - Computed by stochastic method applied to sheath voltage indicates is more off-center distribution – impact on nonuniformity**

Stochastic method

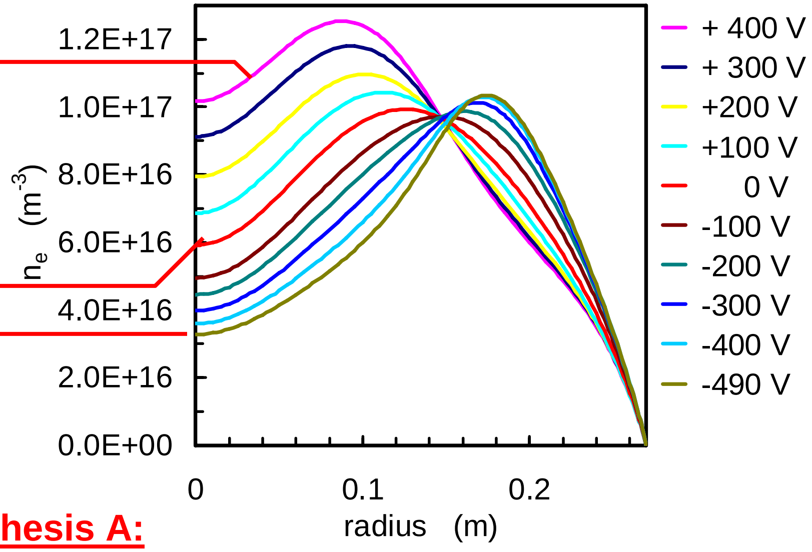
Plasma density distribution in dual frequency CCP: Stochastic method

Impact of selfbias Vb (f_1=100 MHz, f_2=2 MHz)

- only selfbias change V_b from -500 V to +500 V;
- Other parameters are kept constant (V_{pp} = 500 V, p = 100 mTorr)

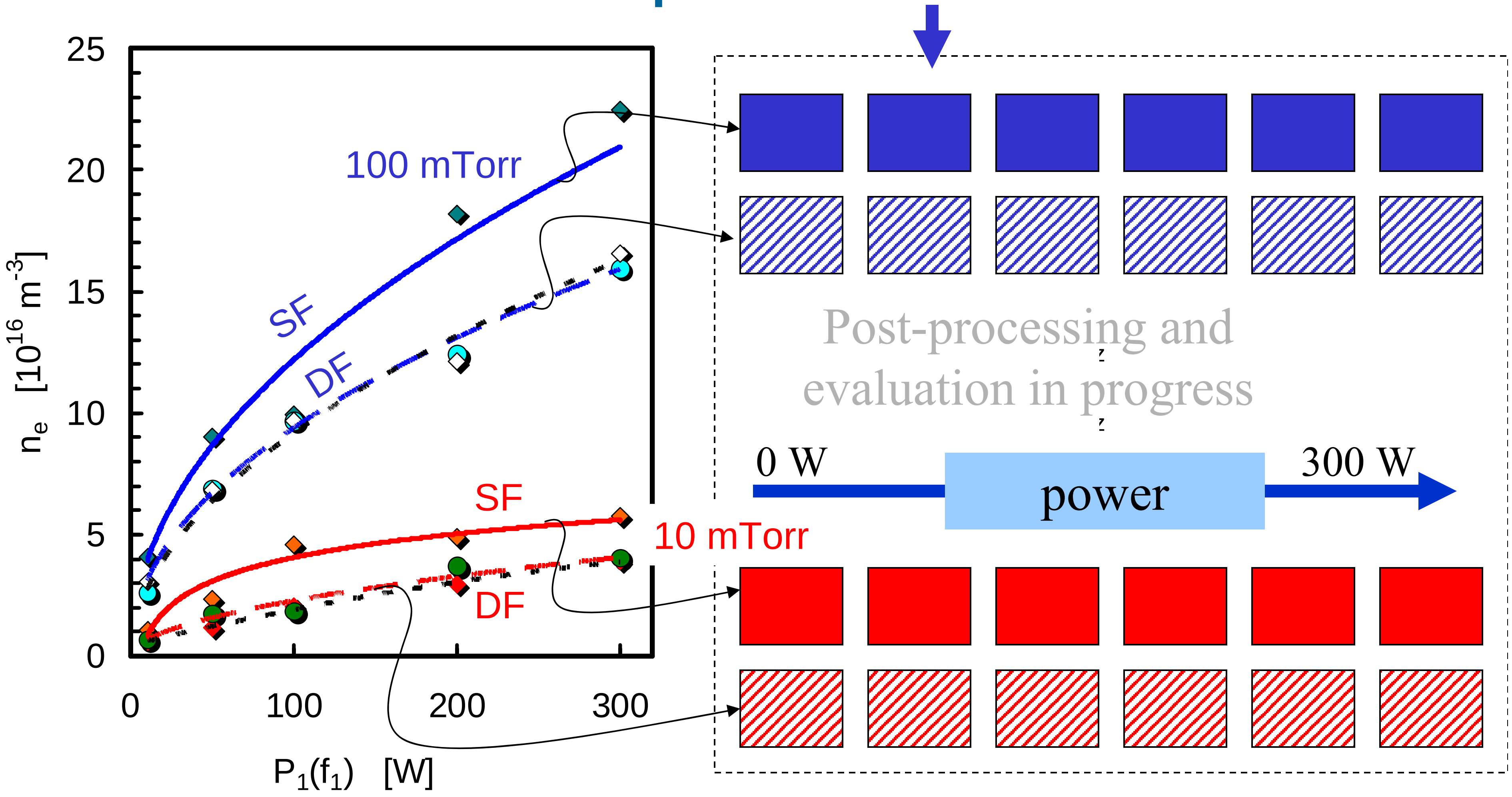


- **Selfbias & the 2nd frequency excitation have combined impact on $n_e(r)$**



- **Hypothesis A:**
  - High negative bias is repealing electrons from central area (more off center distribution), and increased sheath voltage is driving larger ion current from plasma
- **Hypothesis B:**
  - Forced positive bias $V_b \Rightarrow$ more centered distribution but lower sheath voltage is produced (driving less current out of plasma)

Dual frequency vs power (P_1) analysis plasma distribution

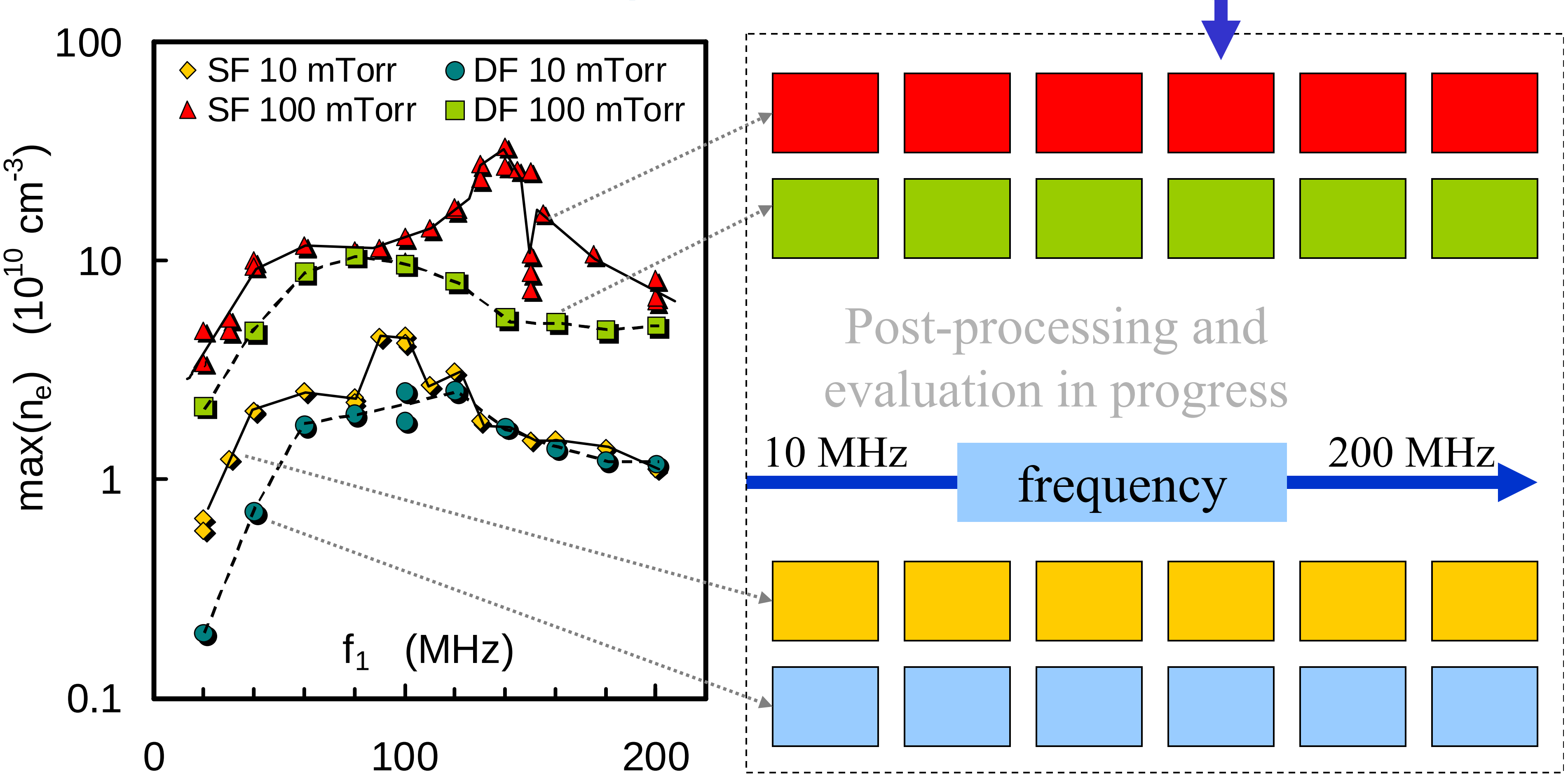


Post-processing and evaluation in progress

- **Valuable predictive information**

Single & dual frequency models investigations *vs* f_1

plasma distribution – radial profiles



Post-processing and evaluation in progress

- **Valuable insight & predictive inputs**

Conclusions

- Proposed and implemented fast approach in dual frequency CCP modeling
- Algorithm was validated against transient solution and has been confirmed with experimental data

- Predictions in a quite reasonable turn-around time
- Transient-to-stochastic FEM method has enhanced computation efficiency and may constitute an useful approach in technological development and optimization

- Possibility of the computational design of the experiment – generating virtual process results

Better understanding of physics and technological aspects

Acknowledgement

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Also thanks to TEL ESBU process team for an opportunity to validate simulation against the experimental data.