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Sensitivity Analysis and Error Propagation for Plasma Edge Codes

Status and Challenges

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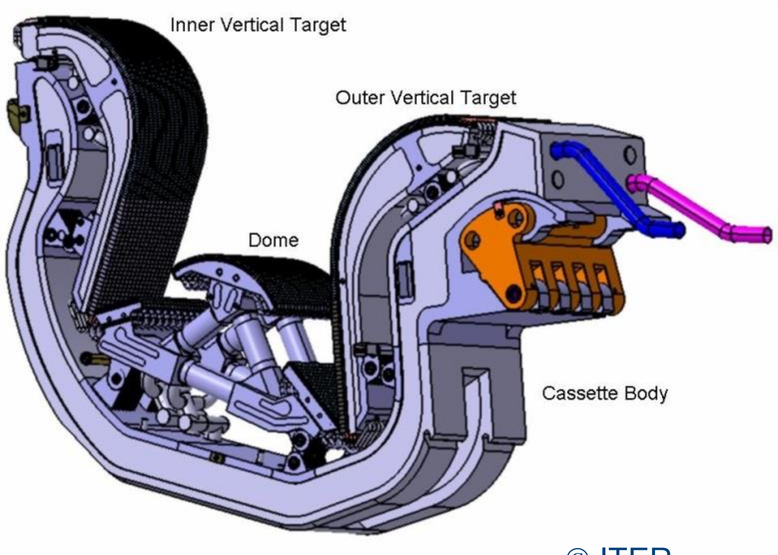
Role of plasma edge modeling

- Design of divertors and power exhaust scenarios for next generation machines still an open question
  - Limit power load to PFCs to acceptable levels
  - Manage particle exhaust
  - Ensure compatibility with burning plasma conditions in the core
- Numerical codes (e.g. SOLPS-ITER) essential to consistently model the complex plasma edge
  - (Multi-)fluid plasma – kinetic neutral models
  - Highly nonlinear, anisotropic, strongly coupled PDEs
  - Coupling with PWI models, MHD equilibrium,…
  - Coupled Finite Volume / Monte Carlo codes



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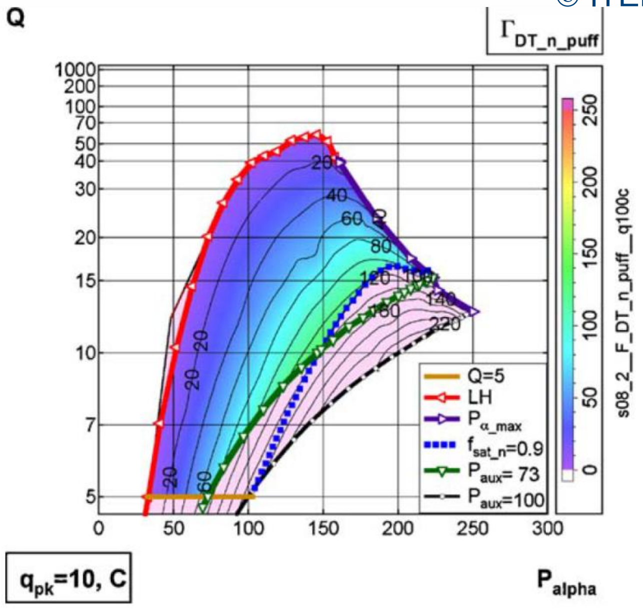

[A.S. Kukushkin et al., Fusion Eng. Des. **96** (2011) 2865.]

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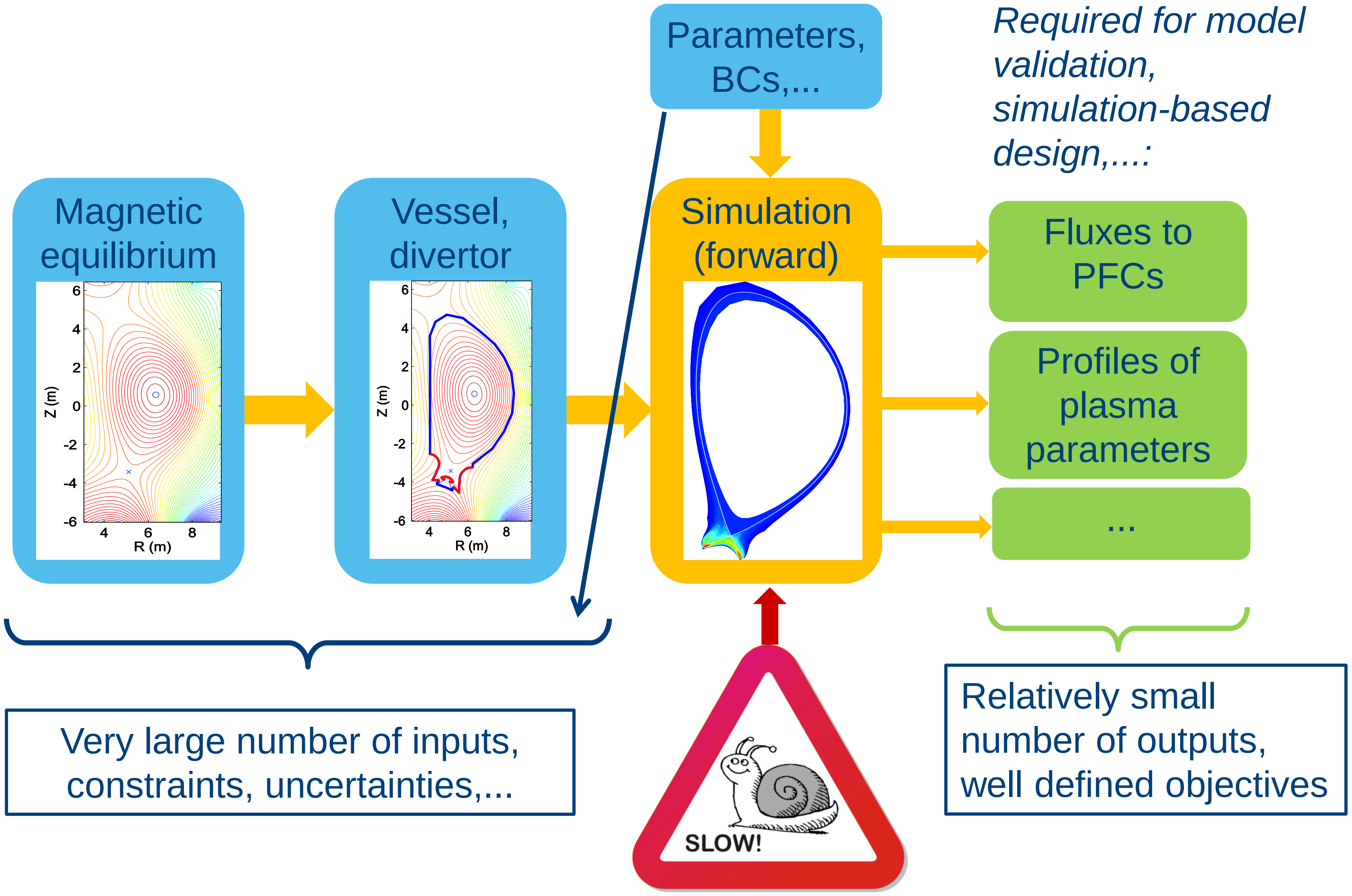
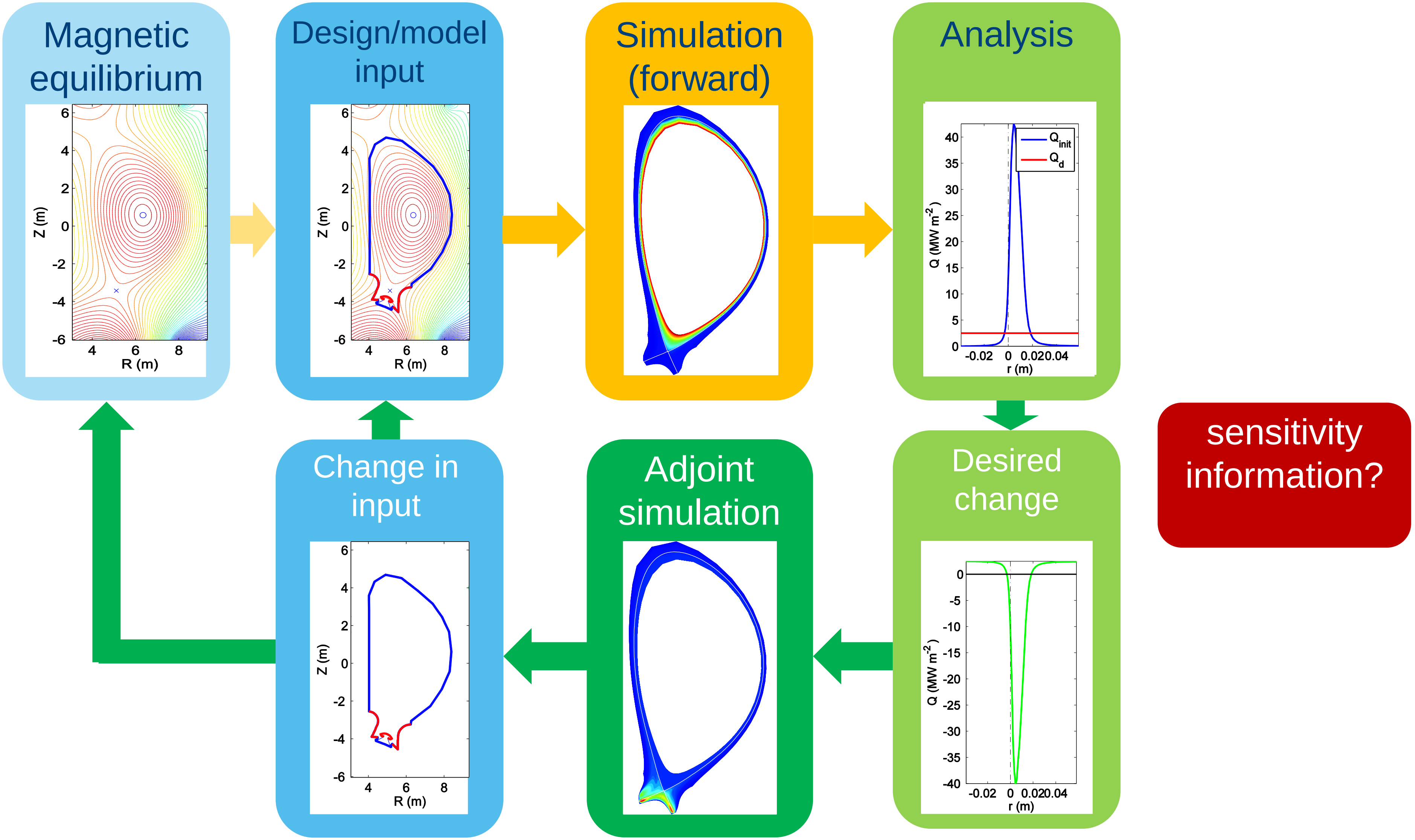
Plasma edge codes as *analysis* tools



Plasma edge codes as *optimization* tools



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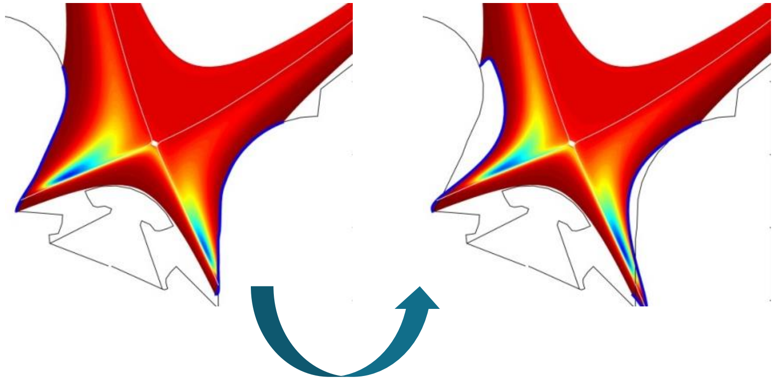
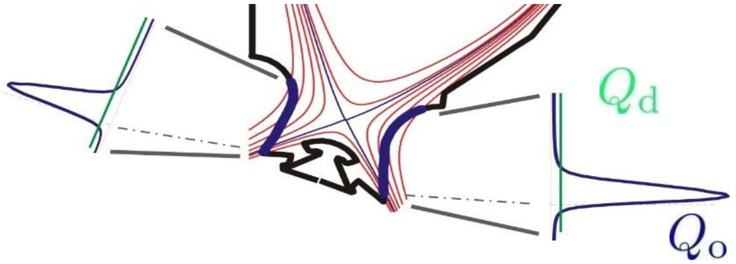
Applications of *optimization* tools

[W. Dekeyser et al., Nucl. Fusion ***54*** *(2014) 073022, and M. Blommaert et al., Nucl. Fusion* ***55*** *(2015) 013001.]*

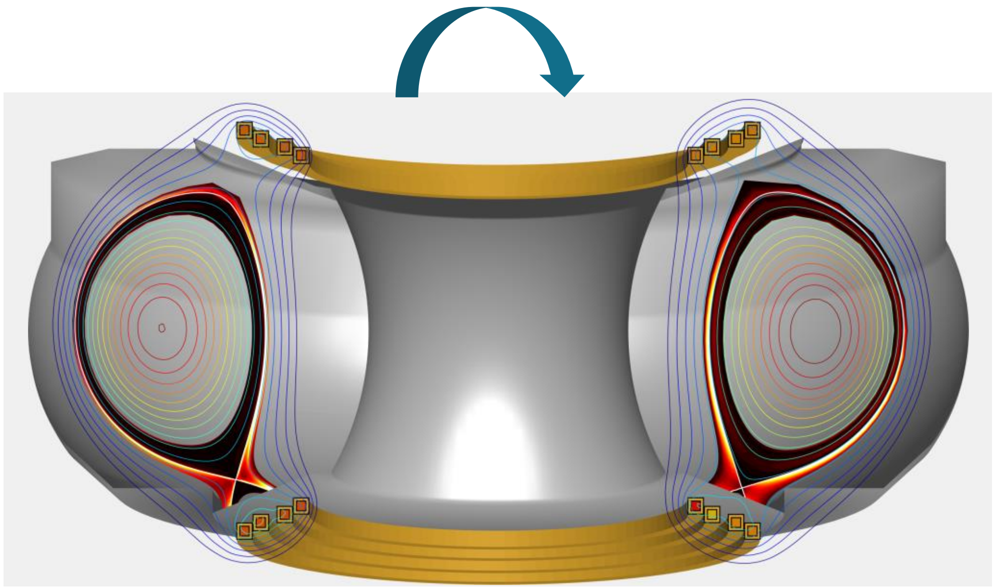


Divertor Shape optimization



$$J(\Omega, \mathbf{q}) = \frac{1}{2}\int_{\mathrm{t}} (Q_\mathrm{o} - Q_\mathrm{d})^2 \,\mathrm{d}\sigma$$

Magnetic divertor optimization



Using adjoint techniques, entire optimization problem solved at a cost of only a few forward simulations!

Model calibration through optimization

*[M. Baelmans et al., PPCF **56** (2014) 114009.]*

- **Cost function: match to "experimental data"**

$$\min_{\phi,\mathbf{q}} \quad J(\phi,\mathbf{q}) = \sum_{l=\mathrm{OM},\ldots} \frac{1}{\Omega_l}\int_{\Omega_l}\left(\frac{\alpha_{l,n}}{2}\frac{(n-n^{\exp})^2}{n_l^2}+\frac{\alpha_{l,T}}{2}\frac{(T-T^{\exp})^2}{T_l^2}\right)\mathrm{d}\Omega$$

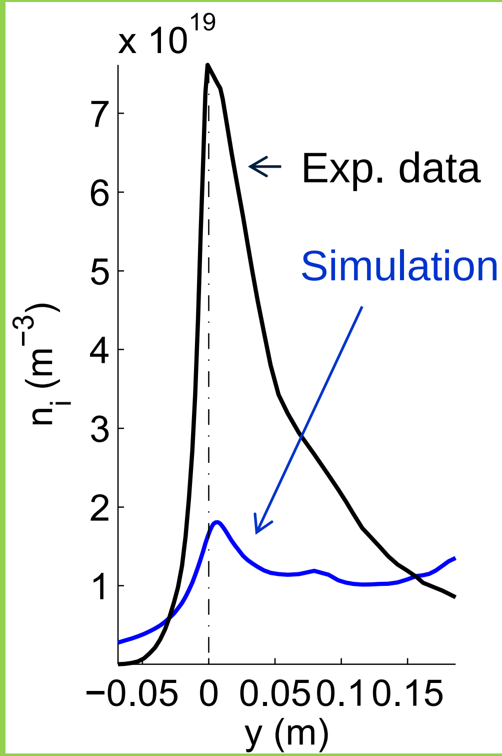
$$\text{s.t.} \quad \boldsymbol{\mathcal{B}}(\phi,\mathbf{q}) = 0$$

ϕ transport coefficients and plasma edge model constants (the *control* variables)

$\mathbf{q}$ state variables: plasma density, temperature,…

$\boldsymbol{\mathcal{B}}(\phi,\mathbf{q})$ plasma edge model: set of PDEs and boundary conditions

- **Efficient solution through adjoint sensitivity analysis**
- **Challenges:** accounting for multiple diagnostics? Prior information about uncertainties (Bayesian setting)? …



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Potential of sensitivity analysis for edge plasma model validation

- Efficient solution of UQ problems through optimization

- Identification of dominant uncertainties, guide for parameter space reduction

- Efficient parametrization of input and output PDFs, efficient propagation of uncertainty though the codes

- Construction of surrogate models

…but: several challenges to be addressed to enable application to realistic problems!

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Outline

- Motivation
- Sensitivities in the presence of MC noise
- Partially adjoint techniques for simulation chains
- Practical implementation in *big* codes
- Summary and outlook

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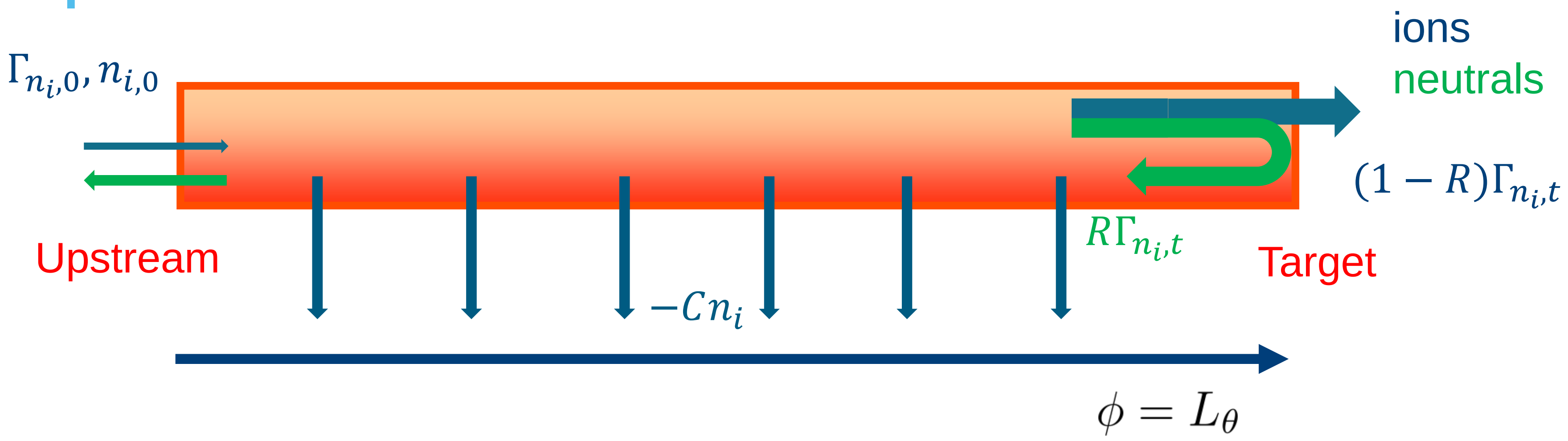
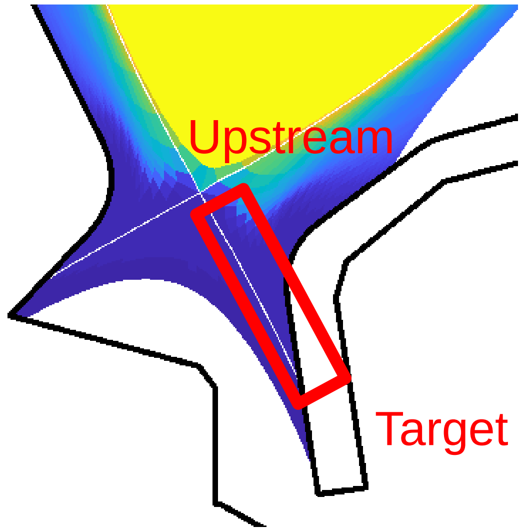
Optimization for fluid-kinetic models





- Sources from kinetic neutrals, but 'only flying left and right'
  $\rightarrow$ Can be solved with Monte Carlo or finite volume method
- Some essential features of SOL models are present
  - Fluid-kinetic coupling, Monte Carlo noise, nonlinear source terms, …

- **Optimization of "divertor fluxes":**

$$\min_{\phi,\mathbf{q}} \quad J(\phi,\mathbf{q}) = \frac{\lambda}{2}(\Gamma - \Gamma_{\mathrm{d}})^2|_{\mathrm{t}} + \frac{\lambda_0}{2}(\phi - L_0)^2$$

$$\text{s.t.} \quad \boldsymbol{\mathcal{B}}(\phi,\mathbf{q}) = S - A(\phi,\mathbf{q}) = 0$$

plasma continuity and parallel momentum,
state variables $\mathbf{q} = \{n_{\mathrm{i}}, u_{||}\}^T$

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Finite Difference (FD) sensitivities

- Reduced cost function/state solver as 'black box'

$$\min_{\phi} \hat{J}(\phi) \equiv J(\phi, \mathbf{q}(\phi))$$

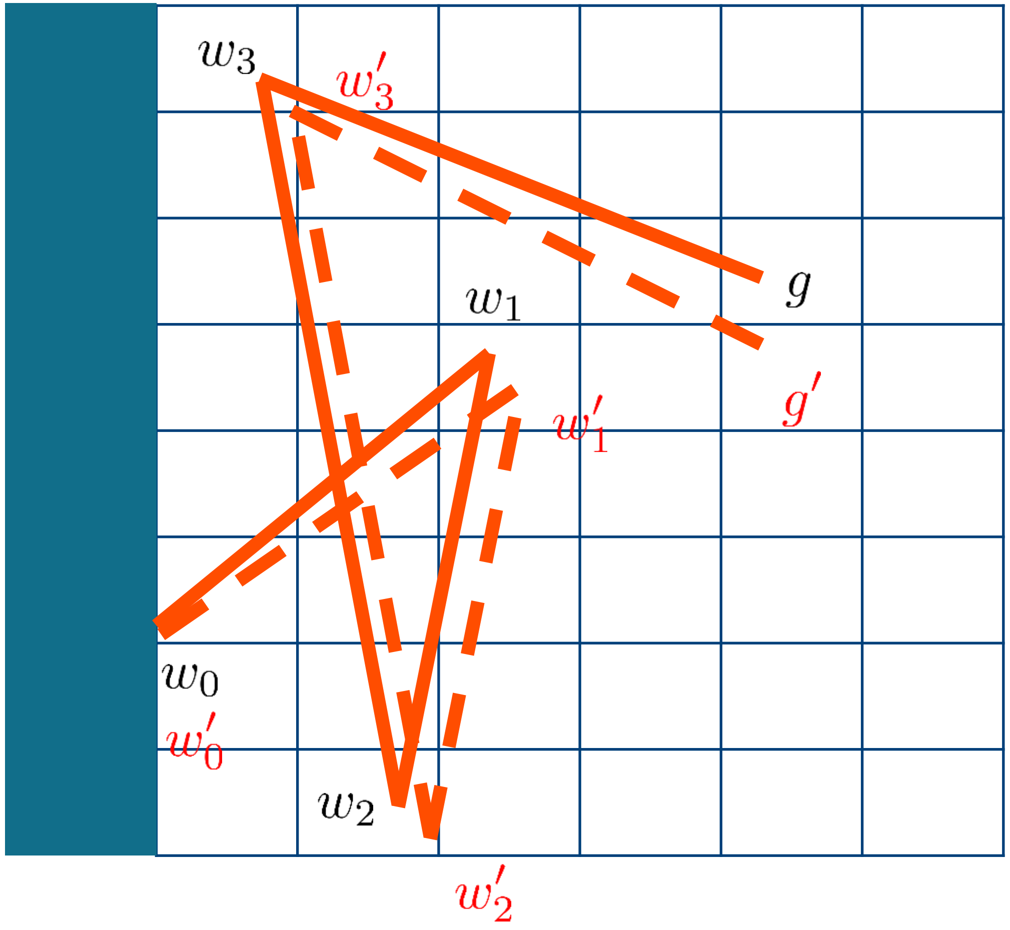
- Sensitivity

$$\frac{\mathrm{d}\hat{J}}{\mathrm{d}\phi}\delta\phi \approx \frac{J(\phi+\delta\phi, \mathbf{q}(\phi+\delta\phi)) - J(\phi-\delta\phi, \mathbf{q}(\phi-\delta\phi))}{2}$$

  - **Cost** scales with number of design variables
  - **Correlated random numbers** to reduce variance

    $$\mathrm{Var}(X_1 - X_2) = \mathrm{Var}(X_1) + \mathrm{Var}(X_2) - 2\mathrm{Cov}(X_1, X_2)$$

  - Some decorrelation hard/impossible to avoid in practice



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The adjoint approach to sensitivity calculation

- Constrained optimization problem

$$\min_{\phi \in \phi_{\mathrm{ad}}, \mathbf{q}} J(\phi, \mathbf{q}) \quad \text{subject to} \quad \boldsymbol{\mathcal{B}}(\phi, \mathbf{q}) = 0 \quad (= S - A(\phi, \mathbf{q}))$$

- *Reduced* cost functional

$$\min_{\phi \in \phi_{\mathrm{ad}}} \hat{J}(\phi) \equiv J(\phi, \mathbf{q}(\phi))$$

- Chain rule for sensitivity computation

$$\begin{aligned} \hat{J}_\phi \delta\phi &= J_\phi \delta\phi + J_{\mathbf{q}} \delta\mathbf{q} \\ &= J_\phi \delta\phi - J_{\mathbf{q}} \boldsymbol{\mathcal{B}}_{\mathbf{q}}^{-1} \boldsymbol{\mathcal{B}}_\phi \delta\phi \\ &= J_\phi \delta\phi - (\boldsymbol{\mathcal{B}}_{\mathbf{q}}^{-T} J_{\mathbf{q}}^T)^T \boldsymbol{\mathcal{B}}_\phi \delta\phi \\ &= J_\phi \delta\phi + (\mathbf{q}^*)^T \boldsymbol{\mathcal{B}}_\phi \delta\phi \end{aligned}$$

$$\boldsymbol{\mathcal{B}}_\phi \delta\phi + \boldsymbol{\mathcal{B}}_{\mathbf{q}} \delta\mathbf{q} = 0$$

$$\boldsymbol{\mathcal{B}}_{\mathbf{q}}^T \mathbf{q}^* = -J_{\mathbf{q}}^T$$

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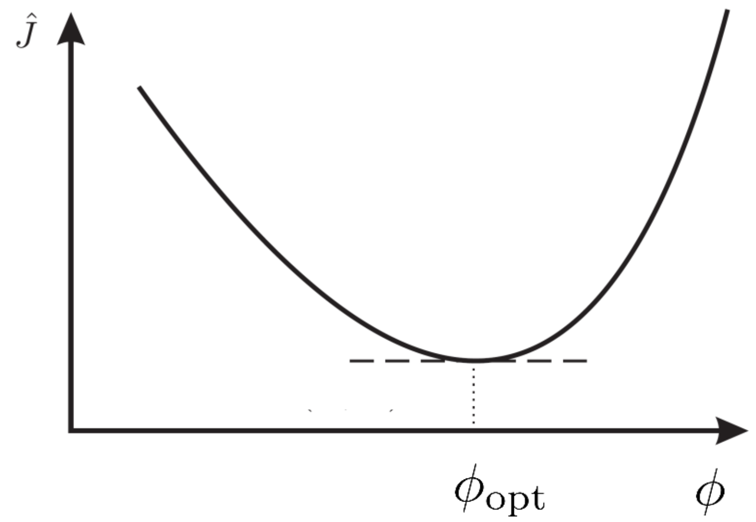
Optimality conditions

- Lagrangian

$$L(\phi, \mathbf{q}, \mathbf{q}^*) = J(\phi, \mathbf{q}) + \langle \mathbf{q}^*, \boldsymbol{\mathcal{B}}(\phi, \mathbf{q}) \rangle$$



- First order optimality conditions:

$$\begin{aligned} 0 &= \nabla_{\mathbf{q}^*} L &= \boldsymbol{\mathcal{B}}(\phi, \mathbf{q}) \\ 0 &= \nabla_{\mathbf{q}} L &= \nabla_{\mathbf{q}} J + \boldsymbol{\mathcal{B}}_{\mathbf{q}}^* \mathbf{q}^* \\ 0 &= \nabla_{\phi} L &= \nabla_{\phi} J + \boldsymbol{\mathcal{B}}_{\phi}^* \mathbf{q}^* \end{aligned}$$

State equations
Adjoint equations
Design equations

$\rightarrow$ Again a **coupled FV-MC system**!
$\rightarrow$ How can we achieve low variance on the sensitivities?

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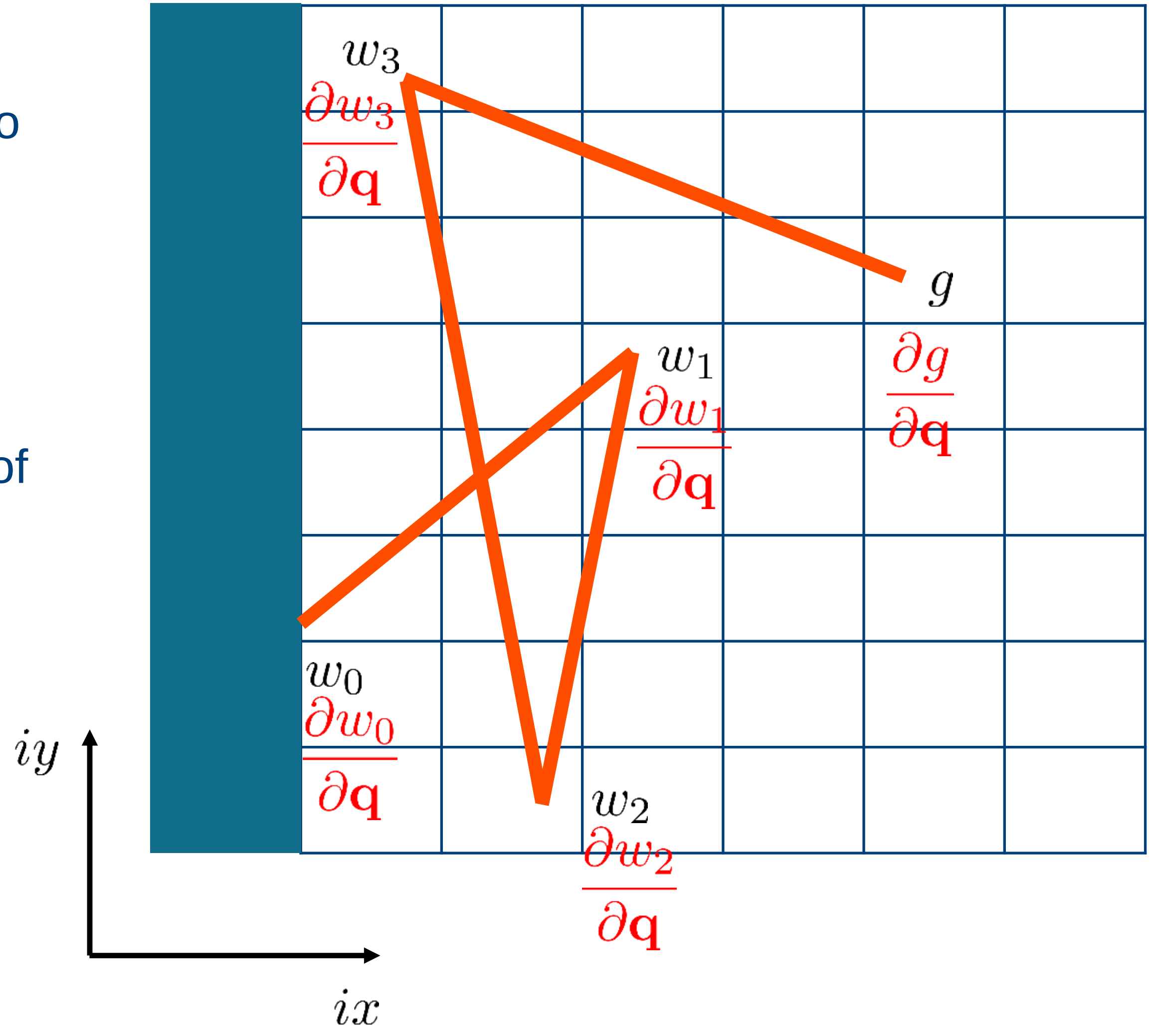
The discrete adjoint approach

Forward simulation

Contribution of particle to source in cell ix, iy

$$S_{ix,iy} = g_{ix,iy}\Pi_{i=0}^{3} w_i$$

Accumulated weight factor will be a function of plasma properties in *all* the cells crossed by the particle



Adjoint simulation

Contribution of particle to source in cell ix, iy

$$\left(\frac{\partial S_{ix,iy}}{\partial \mathbf{q}}\right)^T q^*_{ix,iy}$$

$$= q^*_{ix,iy}\left(\frac{\partial g_{ix,iy}}{\partial \mathbf{q}}\right)^T \Pi_{i=0}^{3} w_i$$

$$+ q^*_{ix,iy} g_{ix,iy} \Pi_{i=0}^{3} w_i \sum \frac{\left(\frac{\partial w_i}{\partial \mathbf{q}}\right)^T}{w_i}$$

Adjoint particle contributes to source in *all* of the cells it crossed

$\rightarrow$ more ***complex*** simulation

$\rightarrow$ but ***exact*** correlation!

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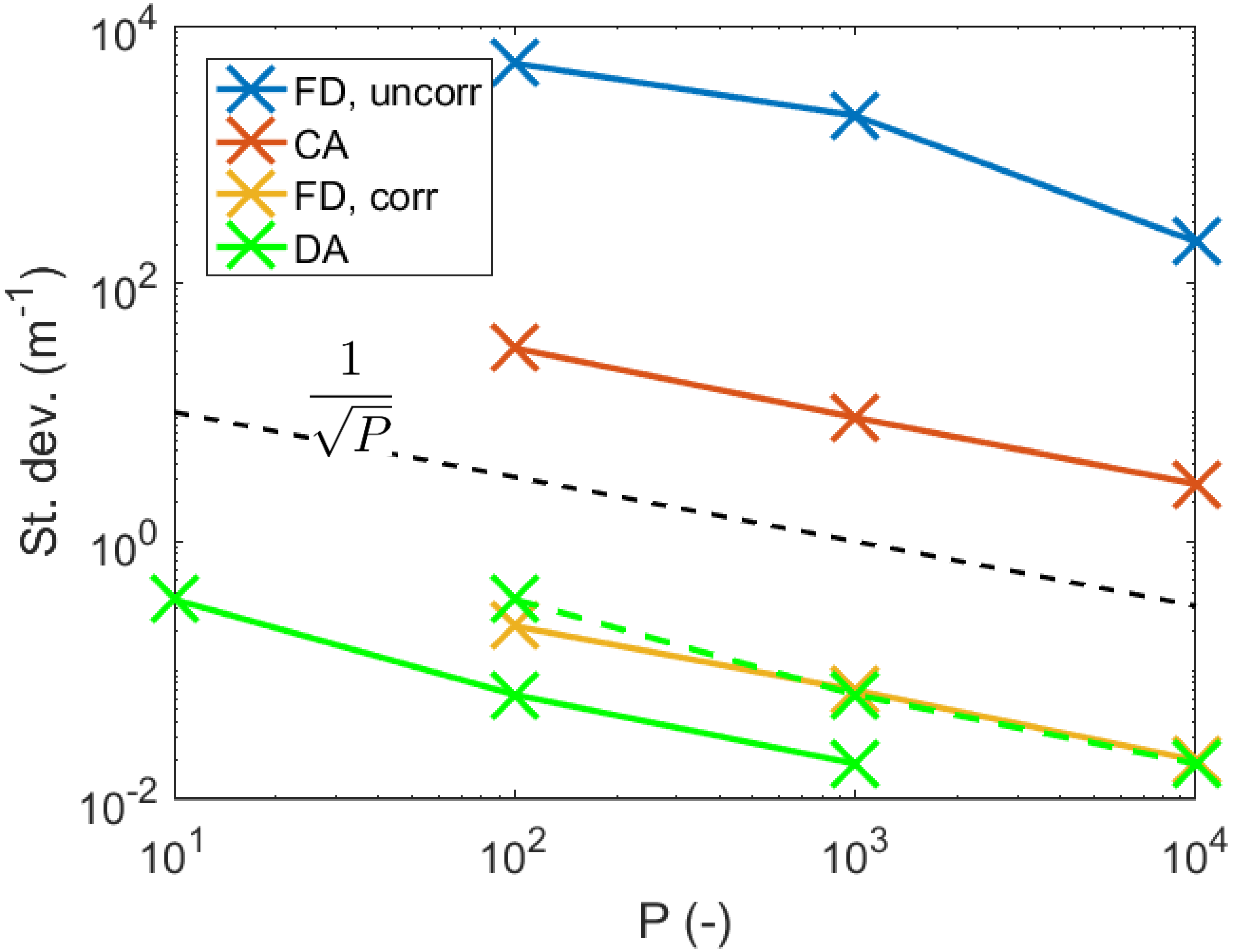
(Relative) standard deviation on sensitivity

[W. Dekeyser et al., Contrib. Plasma Phys. ***58*** *(2018) 718.]*



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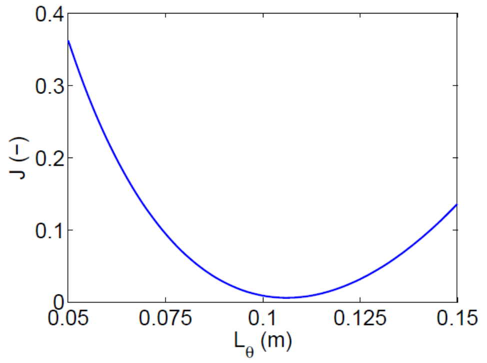
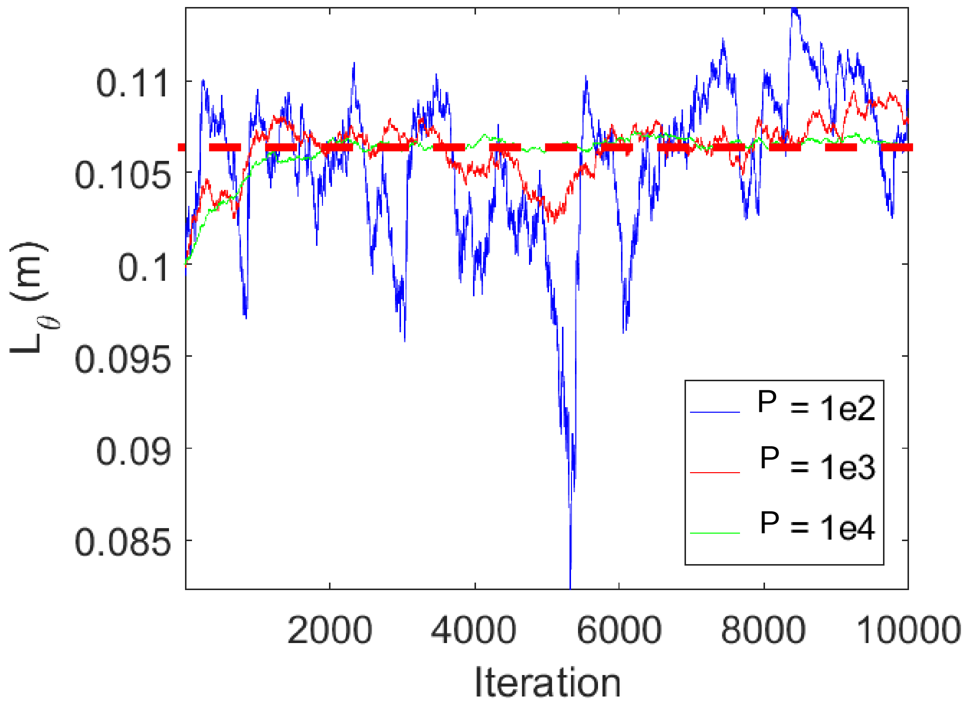
Performance of the optimization algorithm



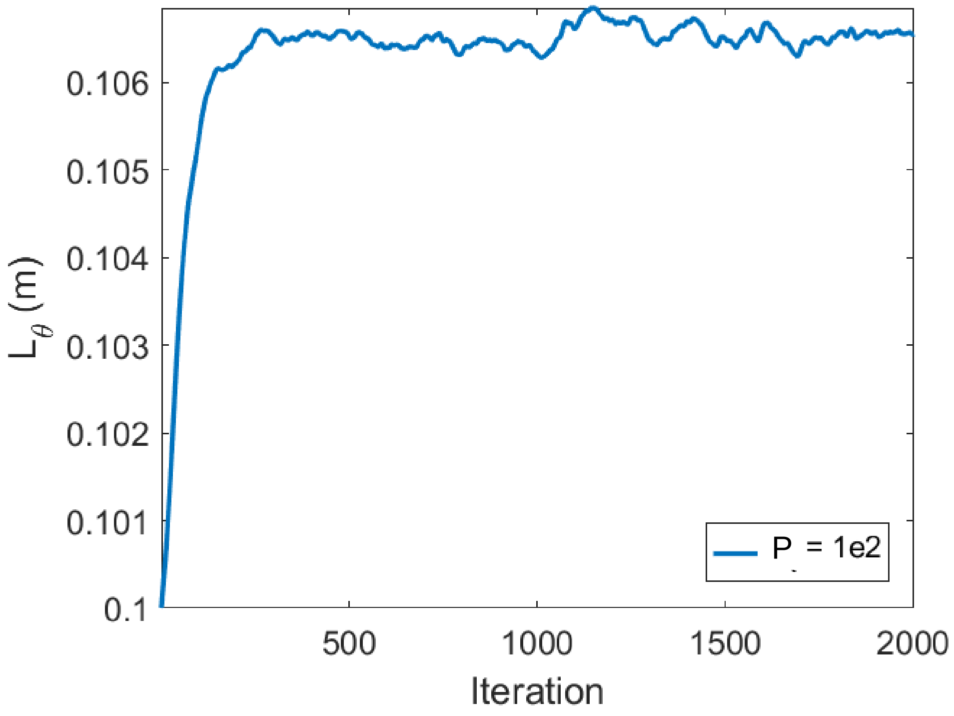
Continuous adjoint



Convergence 'on average'; reliable?

Discrete adjoint

(and correlated FD)



Low noise, smooth convergence!

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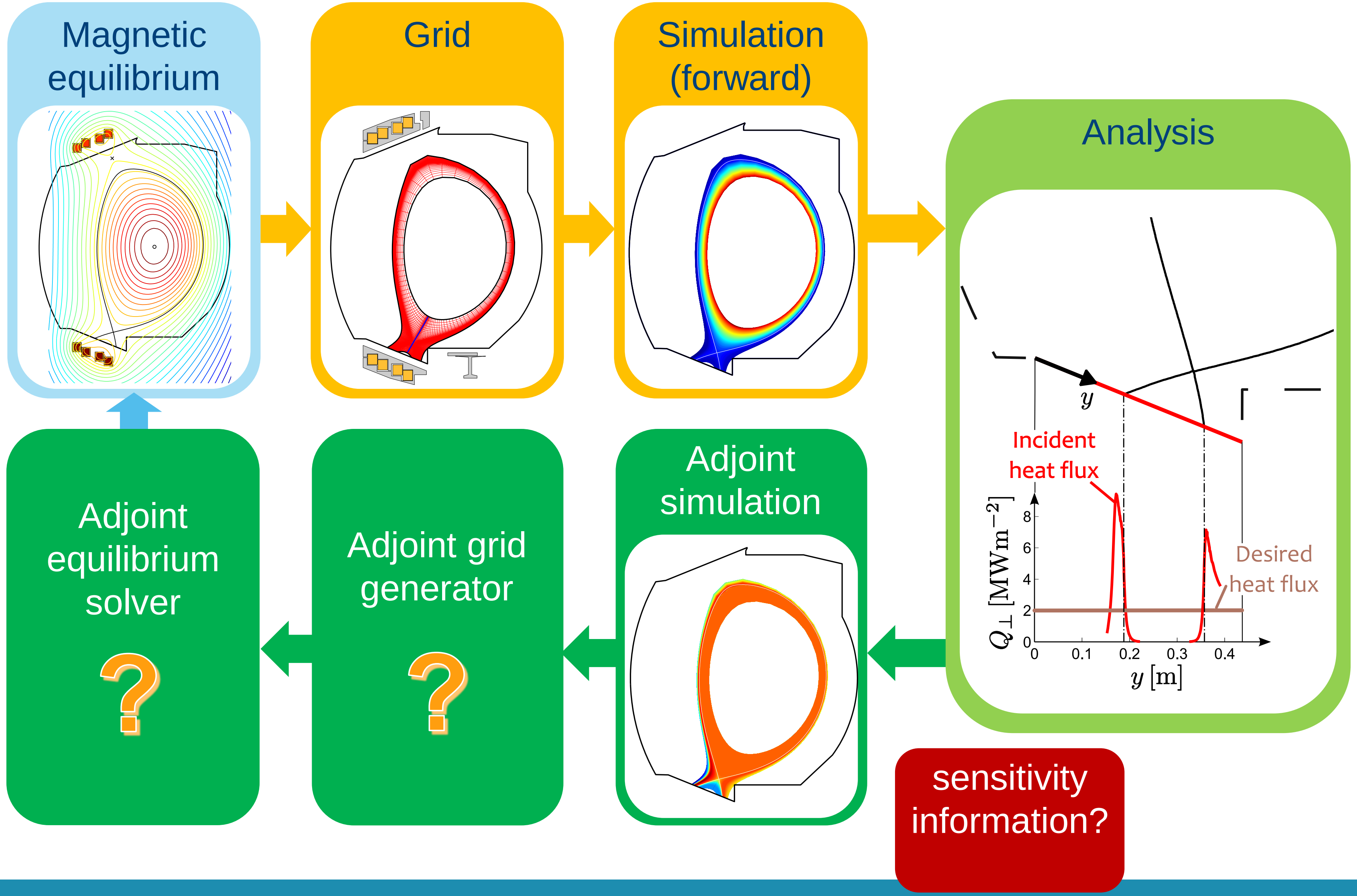
Propagating sensitivities through simulation chains



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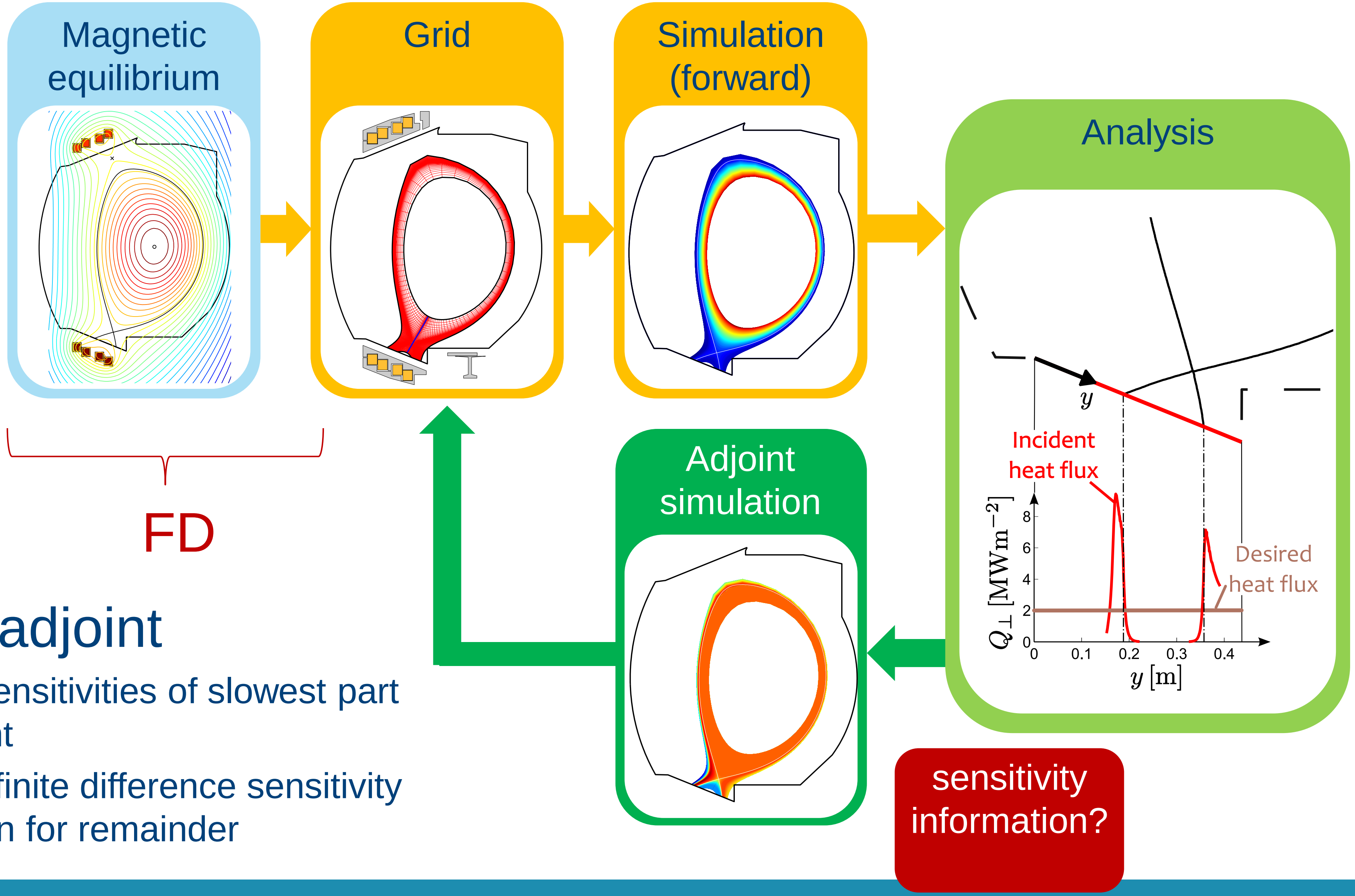
Propagating sensitivities through simulation chains

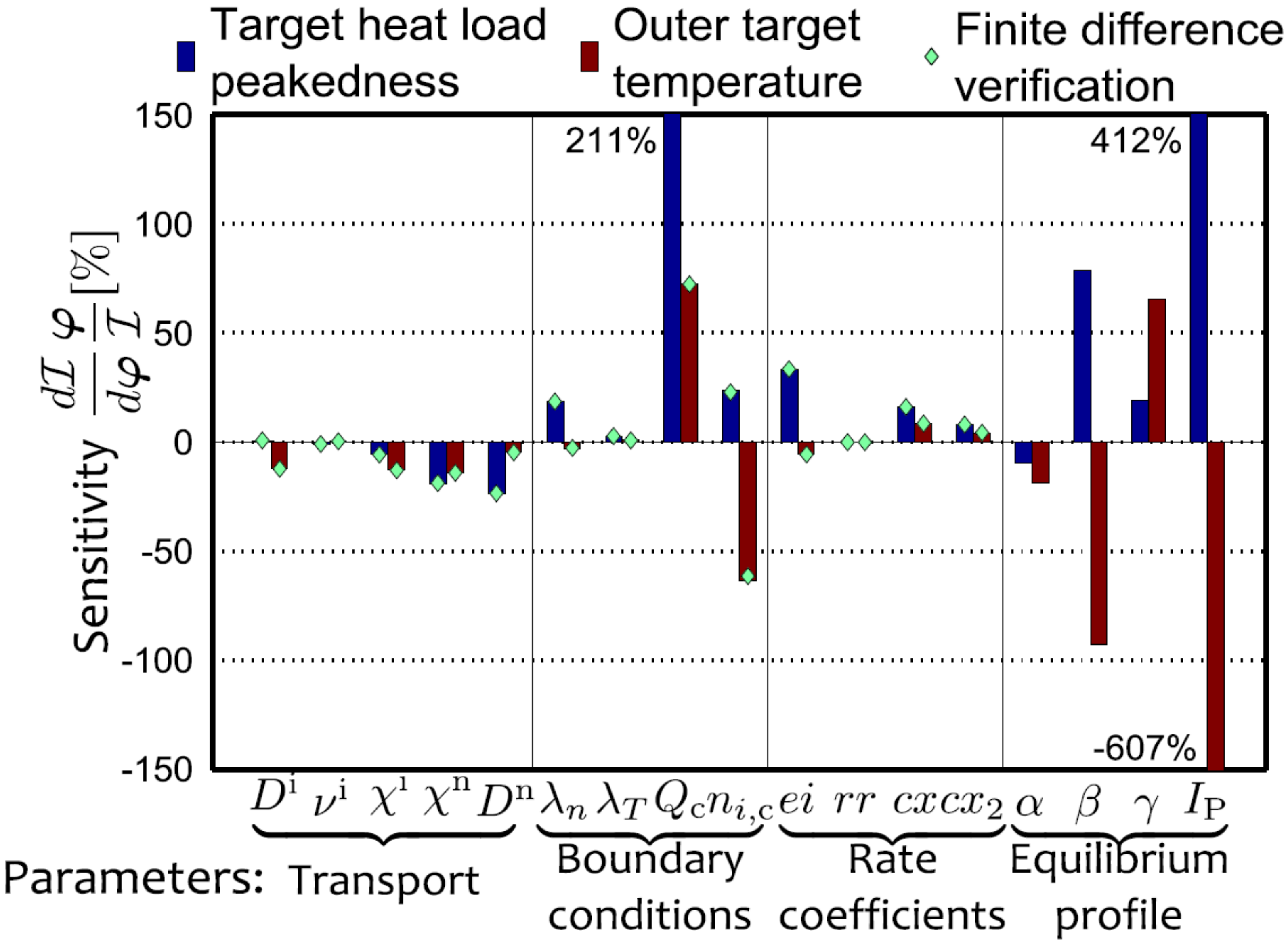


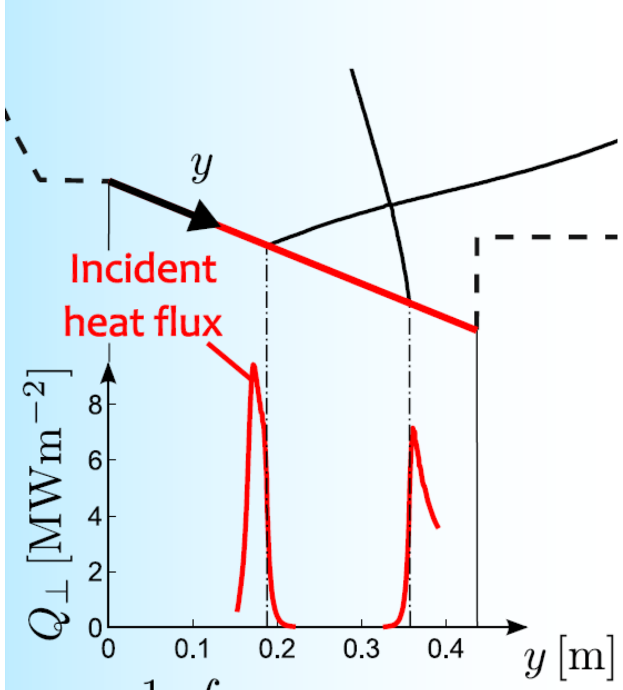
In-parts adjoint

- Fast as sensitivities of slowest part are adjoint
- Practical finite difference sensitivity calculation for remainder

Sensitivities w.r.t. edge plasma model parameters

*[M. Blommaert et al., NME **12** (2017) 1049.]*





- $\mathcal{I}_1 = \frac{1}{2}\int_{S_t} (Q_\perp - Q_d)^2 \, d\boldsymbol{\sigma}$

  $\approx$ Heat load peakedness

- $\mathcal{I}_2 =$ Outer separatrix T

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Implementation in full edge codes

- Challenges
  - Dealing with “legacy code”
  - Developer and user friendliness
  - Maintainability

- Current research tracks for SOLPS-ITER
  - Use of AD tools (“Automatic/Algorithmic Differentiation”): *TAPENADE (INRIA)*
    - Link to discrete adjoint approach, very robust w.r.t. statistical noise
  - Practical combination of adjoint and finite differences (*in-parts adjoint* technique)

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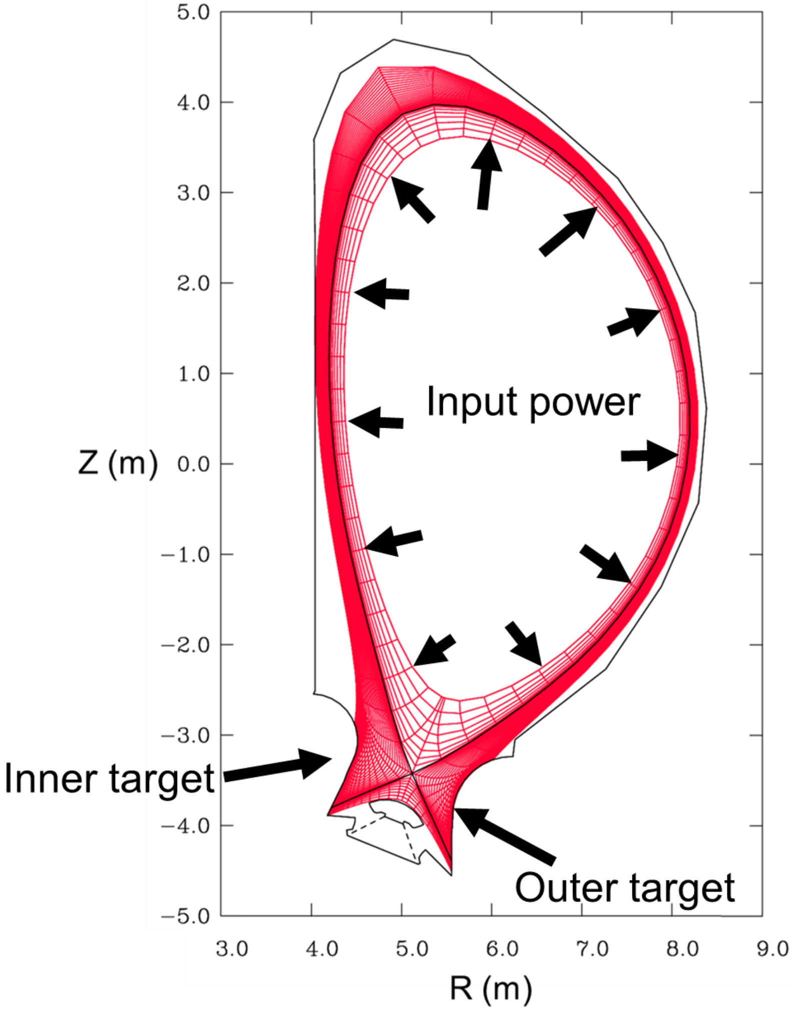
Proof-of-principle: forward AD in B2.5

- Case setup
  - D only, fluid neutrals
  - Input power P_{SOL} = 31 MW, split equally between ions and electrons
  - Low recycling conditions, χ_e, χ_i = 6.0 $m^2 s^{-1}$

- Quantities of interest (@ targets):
  - Max. electron temperature $T_{e,max}$
  - Max. heat load q''_{max}

- Varied model parameters:
  - Input power (P_e, P_i)
  - Radial heat diffusion coefficients (χ_e, χ_i)



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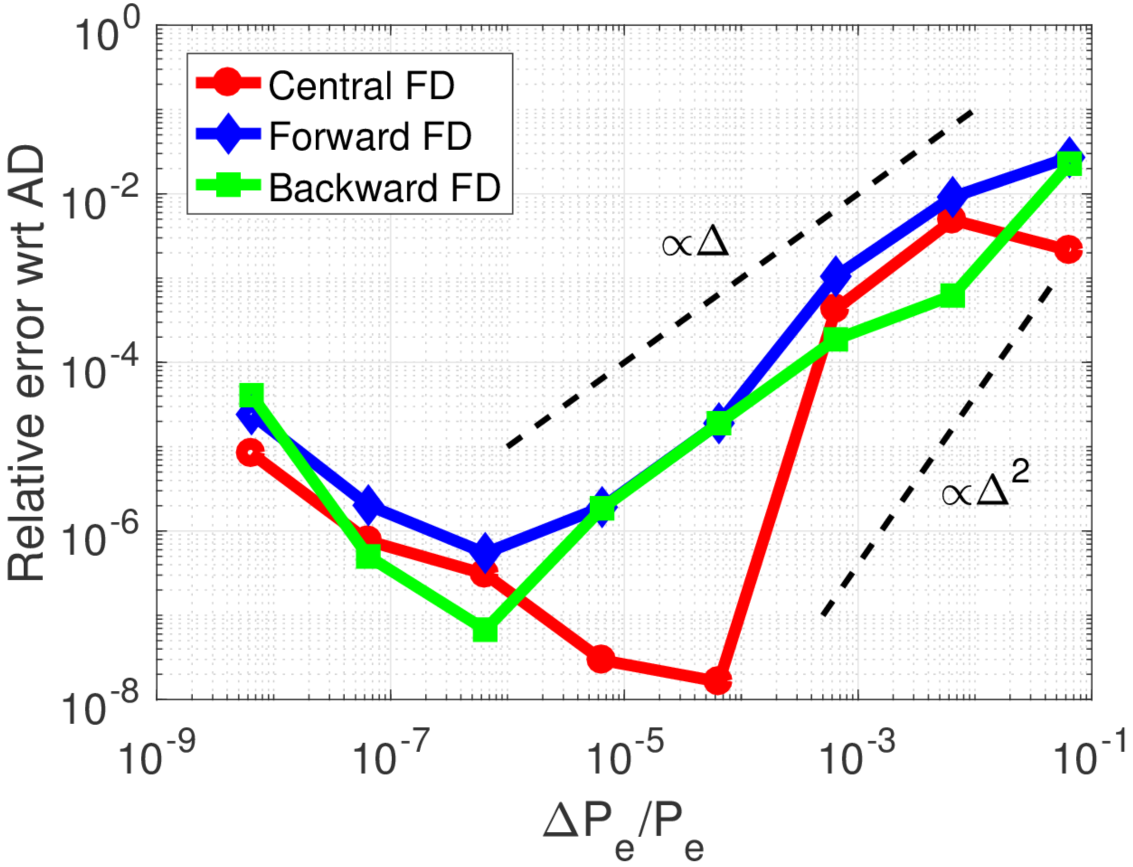
Verification of AD sensitivities



Relative error AD-central FD		
	$T_{e,max}$	q''_{max}
P_e	$\sim10^{-8}$	$\sim10^{-7}$
P_i	$\sim10^{-7}$	$\sim10^{-7}$
χ_e	$\sim10^{-9}$	$\sim10^{-6}$
χ_i	$\sim10^{-9}$	$\sim10^{-6}$

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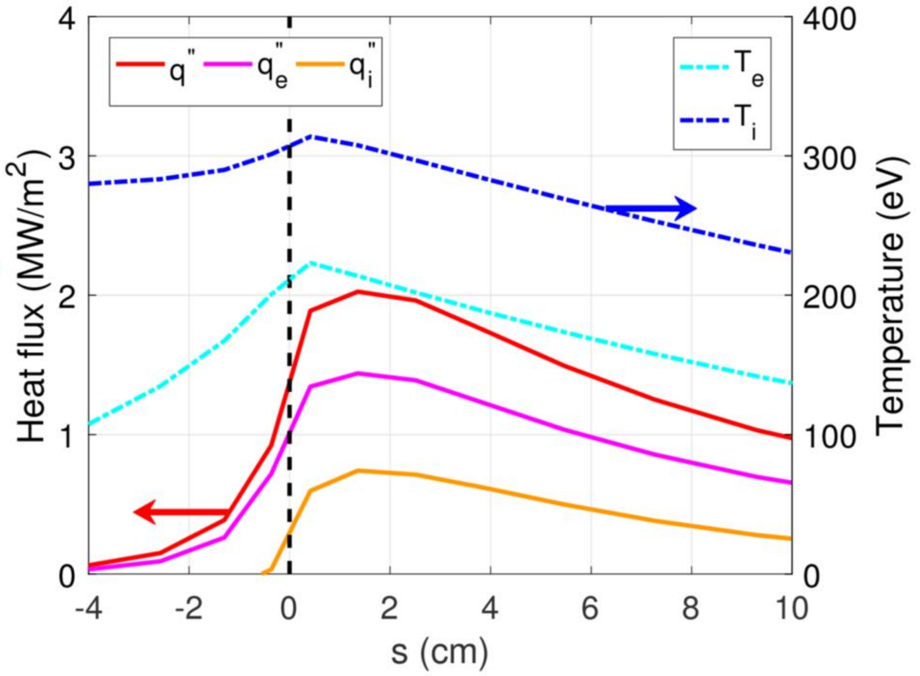
Sensitivity of target profiles

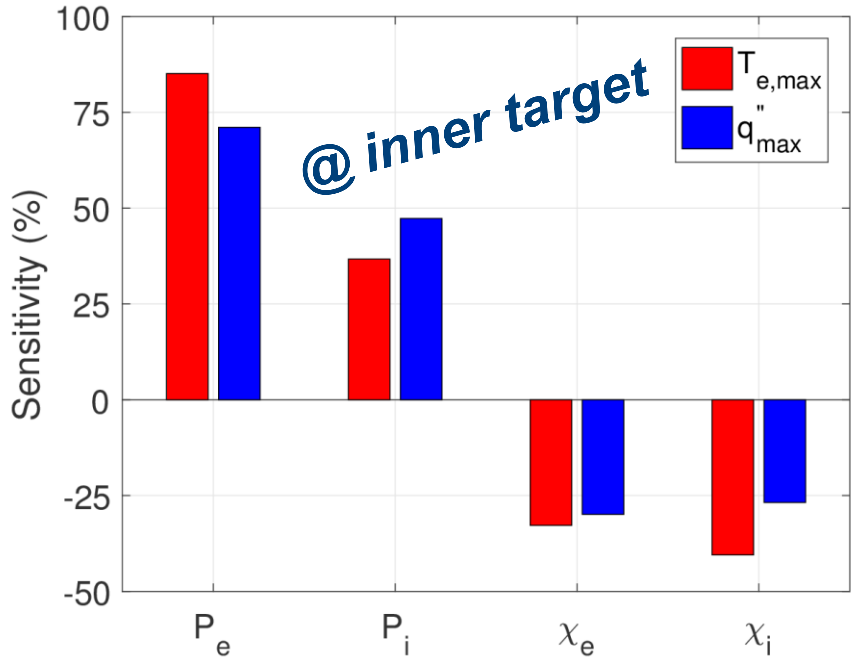
[S. Carli et al., NME **18** (2019) 6.]

- P_e strongly linked to T_e, ions need collisions
- *q”* mainly driven by e^- contribution
- χ → spreading of plasma power

Normalized sensitivities

e.g. $S = \left.\frac{\partial T_{e,max}}{\partial P_e}\right|_{OP} \cdot \frac{P_e}{T_{e,max}}$





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Summary and outlook

- Several challenges to compute accurate sensitivities of plasma edge code have been addressed:
  - Handling of statistical noise
  - Complex simulation chains
  - Dealing with *big* codes

- Sensitivities may be essential to enable UQ studies for plasma edge models
  - Solving UQ problems through optimization
  - Identifying dominant uncertainties over a parameter range (parameter space reduction)
  - Efficient parametrization of input and output PDFs
  - Construction of surrogate models
  - …

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Thank you for your attention!

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