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Progress towards robust divertor and exhaust scenario optimization with SOLPS-ITER

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EUROfusion

This work has been carried out within the framework of the EUROfusion Consortium, funded by the European Union via the Euratom Research and Training Programme (Grant Agreement No 101052200 — EUROfusion). Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the European Commission. Neither the European Union nor the European Commission can be held responsible for them.

Role of edge codes in divertor design challenge

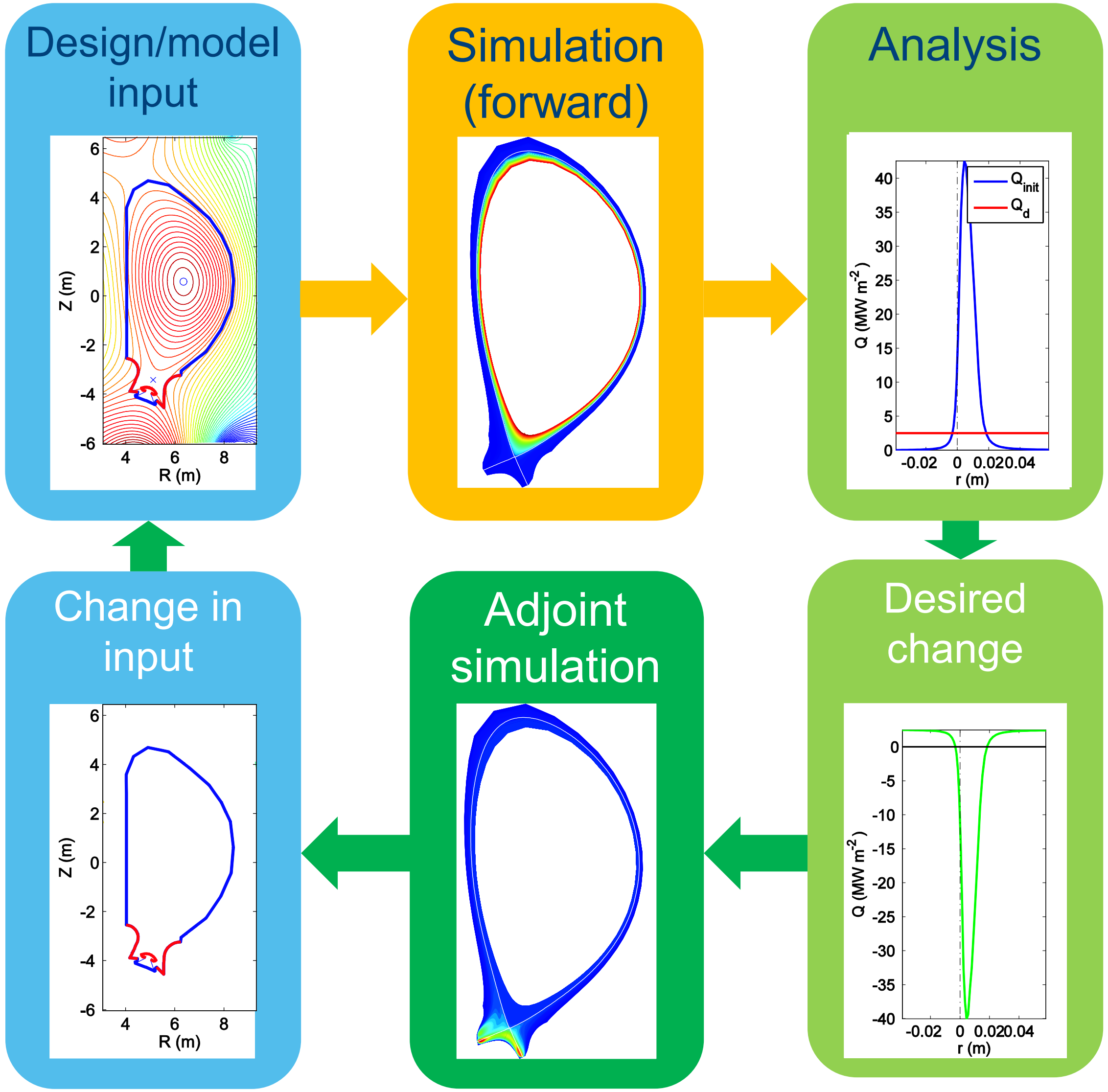
Large number of design variables *(divertor shape, coil currents,…)*

Complex, time-consuming models; uncertain parameters

Physics, material, and engineering constraints

How can we most efficiently exploit the knowledge in the edge codes, and find the 'best', 'robust' designs?

Plasma edge codes as *optimization* tools



- **Objective functional** to be minimized:

$$J(\phi, \mathbf{q}) = \frac{1}{2}\int_{t} (Q_o - Q_d)^2 \, d\sigma$$

ϕ : control variable (shape, coil currents,…)
$\mathbf{q}$: ‘state’ variables (density, temperature,...)

+ constraint: model eqs. must be satisfied
+ possibly additional constraints

- Solve with **gradient-based** approach
  - *Adjoint sensitivities*: cost independent of number of design variables
  - *One-shot* optimization: solve design problem during convergence of the state problem

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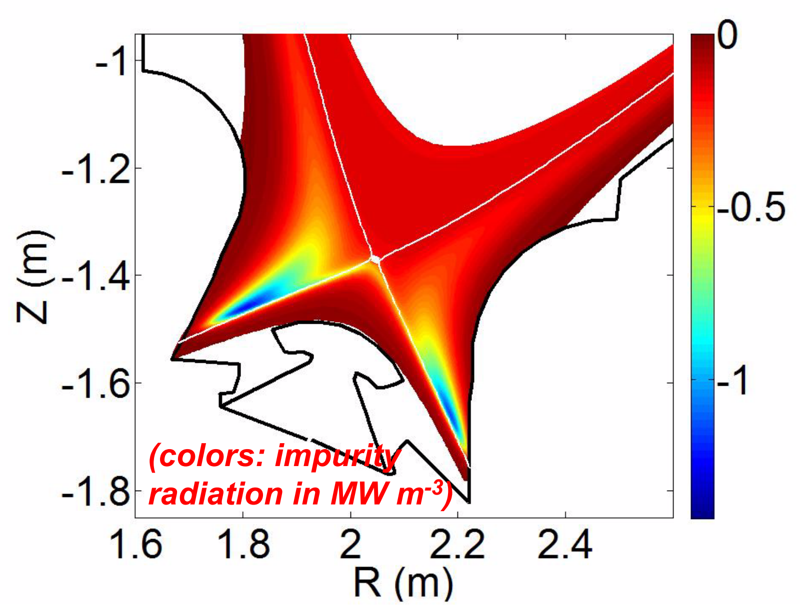
Divertor shape optimization for downsized ITER

[W. Dekeyser et al., Nucl. Fusion **54** (2014) 073022.]



- Downsized ITER F57 (40%)
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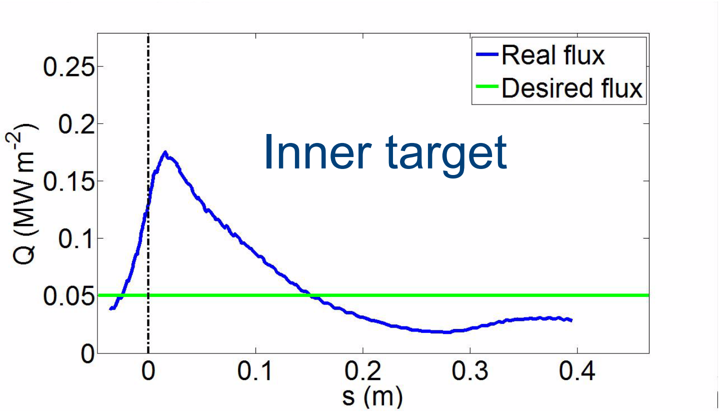
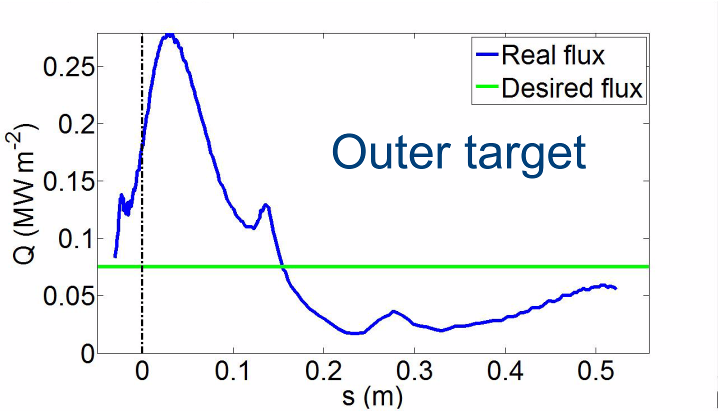
- Q = 3 MW
- Pumping speed 130 m^3 s^{-1}





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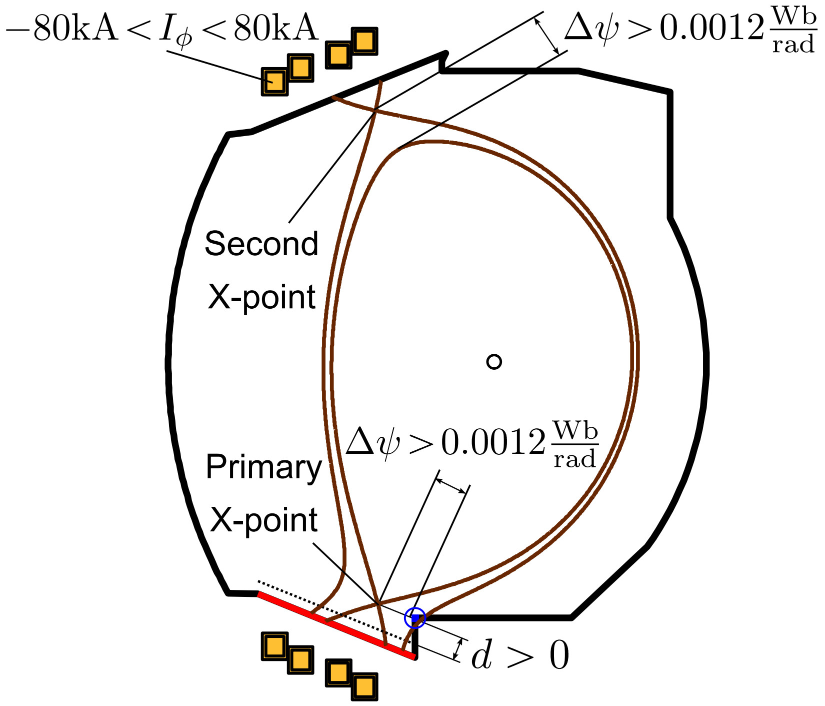
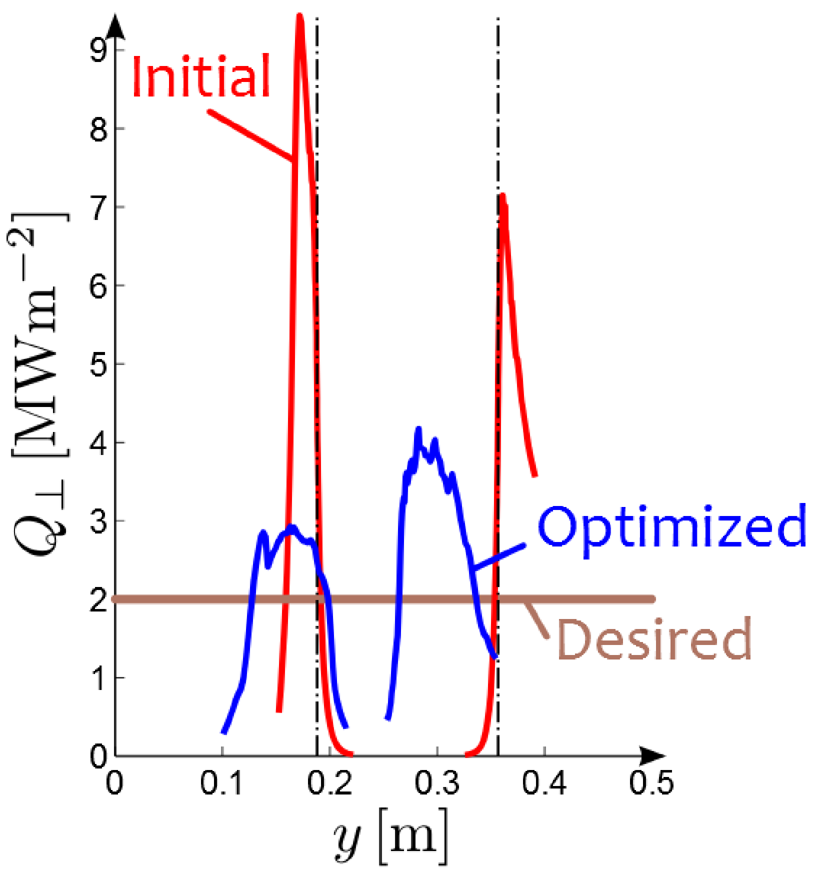
Magnetic field optimization for WEST

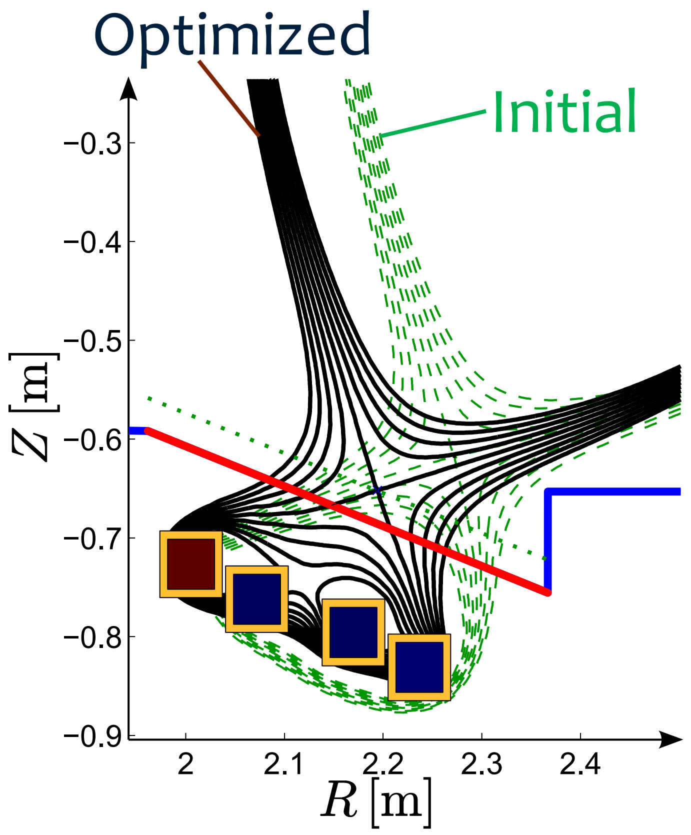
[M. Blommaert et al., J. Nucl. Mater. **463** (2015) 1220.]



$$\hat{J} = \frac{1}{2}\lambda_Q \int_{\text{t}} (Q_{\text{o}} - Q_{\text{d}})^2 \, \mathrm{d}\sigma + \frac{1}{2}\lambda_\phi \sum_i \phi_i^2$$

heat loading — Joule loss





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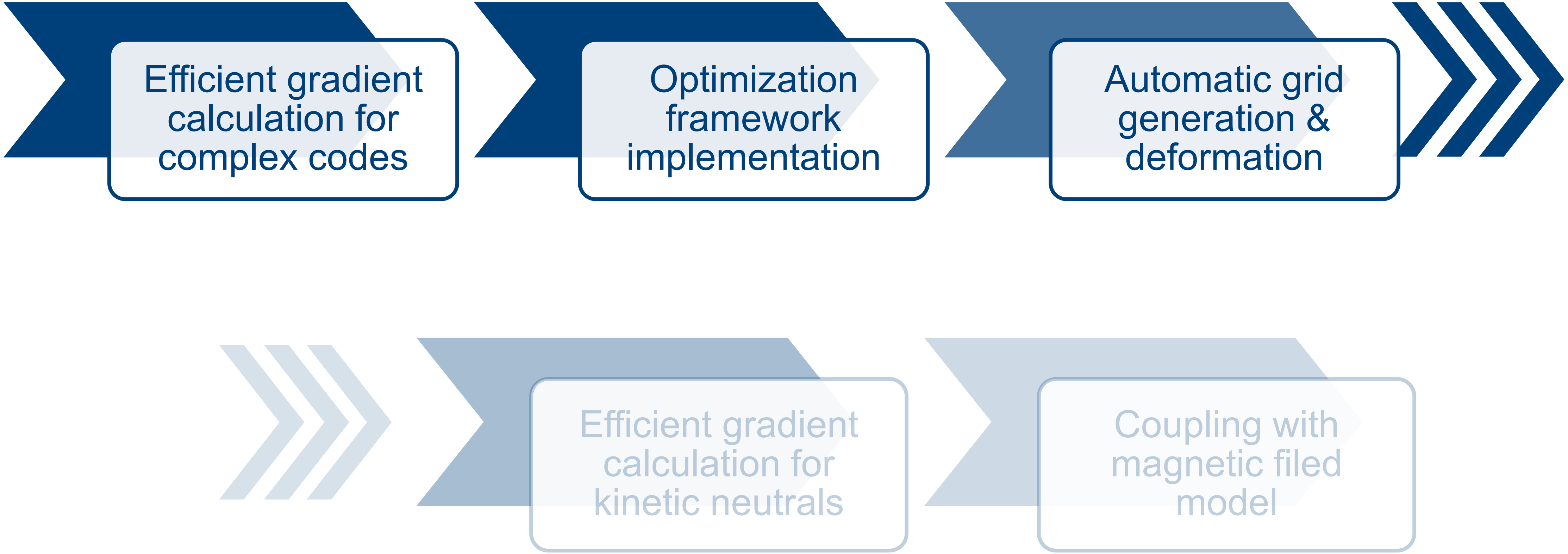
Towards optimal divertor design with SOLPS-ITER



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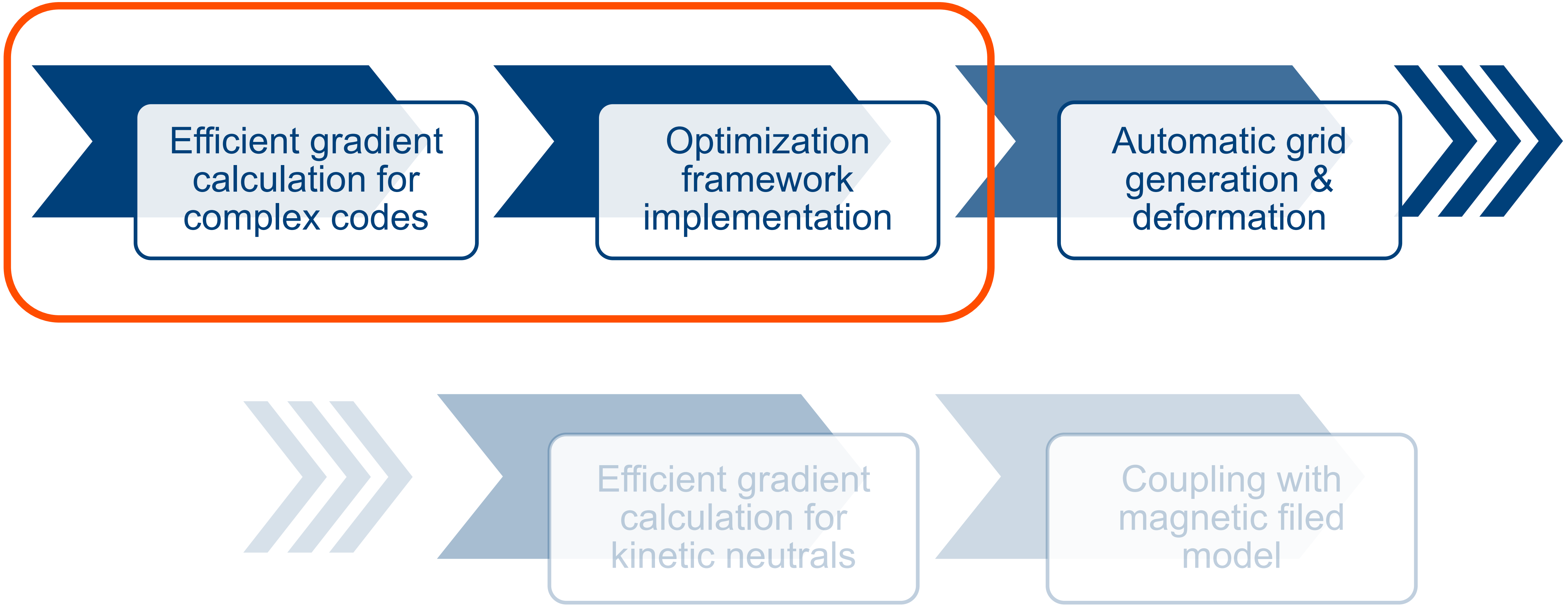

Efficient gradient calculation

- Finite differences (FD):
  - cost proportional to number of inputs
  - truncation error; step size?

- Adjoint equations:
  - cost independent of number of inputs
  - implementation in continuously developing code?

→ Algorithmic (a.k.a. Automatic) Differentiation (AD)
  - Exact to floating point
  - Cost independent of number of inputs

AD workflow and advantages

[S. Carli, EUROfusion ERG & FWO - Flanders.]

SOLPS-ITER = a code to evaluate $\boldsymbol{J} = \boldsymbol{y}(\boldsymbol{x})$, m outputs, n inputs

AD tool (TAPENADE – INRIA) will

1. Analyze code
2. Identify elementary operations
3. Writes *new code* with derivative of elementary operations (chain rule)

Two AD modes:

Tangent AD

- Repeat for each input
- Verified in SOLPS-ITER
  [Carli *et al* 2019 *NME* **18**]

$$\begin{pmatrix} \frac{\partial y_1}{\partial x_1} & \frac{\partial y_1}{\partial x_2} & \cdots & \frac{\partial y_1}{\partial x_n} \\ \frac{\partial y_2}{\partial x_1} & \frac{\partial y_2}{\partial x_2} & \cdots & \frac{\partial y_2}{\partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial y_m}{\partial x_1} & \frac{\partial y_m}{\partial x_2} & \cdots & \frac{\partial y_m}{\partial x_n} \end{pmatrix}$$

Adjoint AD

- Independent of input dimension
- Recompute vs store issue
- Verified in SOLPS-ITER

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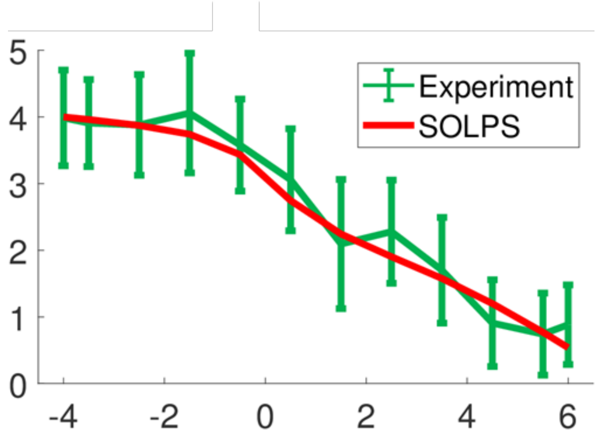
Parameter estimation through optimization with SOLPS-ITER

- Control variables: unknown/uncertain input parameters
  - E.g. anomalous transport coefficients or RANS model parameters



- Introduce cost function as indicator of goodness-of-fit
  - Nonlinear regression [Coster et al. CTPP 40 (2000)]

$$J(\phi, q) = \frac{1}{\Omega}\int_{\Omega} \omega_q \left(\frac{1}{\overline{\mathcal{D}}^2}(q - \mathcal{D})^2\right) d\Omega$$

  - Robust Bayesian MAP estimation

$$\min_{\phi} -\mathcal{L}(\mathcal{D}|\phi)\pi(\phi)\ , \qquad \mathcal{L}(\mathcal{D}|\phi) = \prod_{i=1}^{N_{\mathcal{D}}} \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{1}{2}\frac{\epsilon_i^2}{\sigma^2}\right)$$

  - Consistent integration of data from various diagnostics!

- Minimize cost function with gradient-based optimization
  - Coupling to external optimization libraries (PETSC/TAO, IPOPT)

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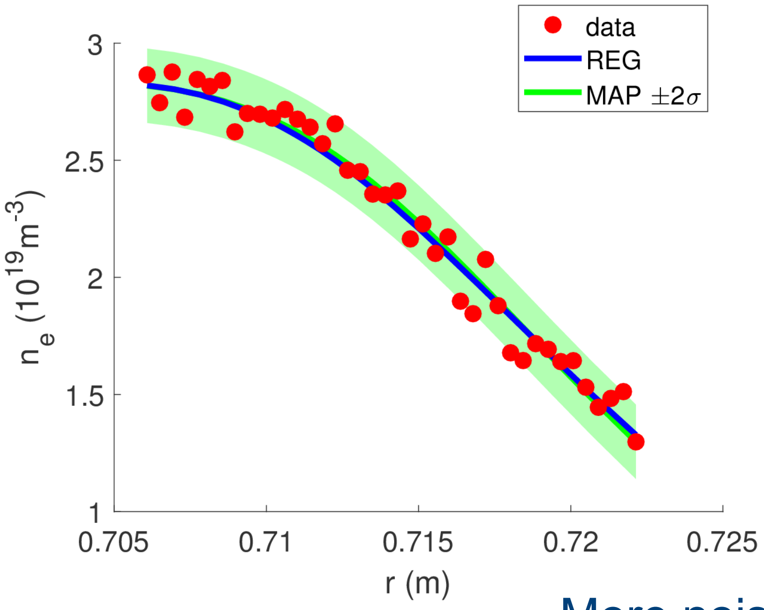
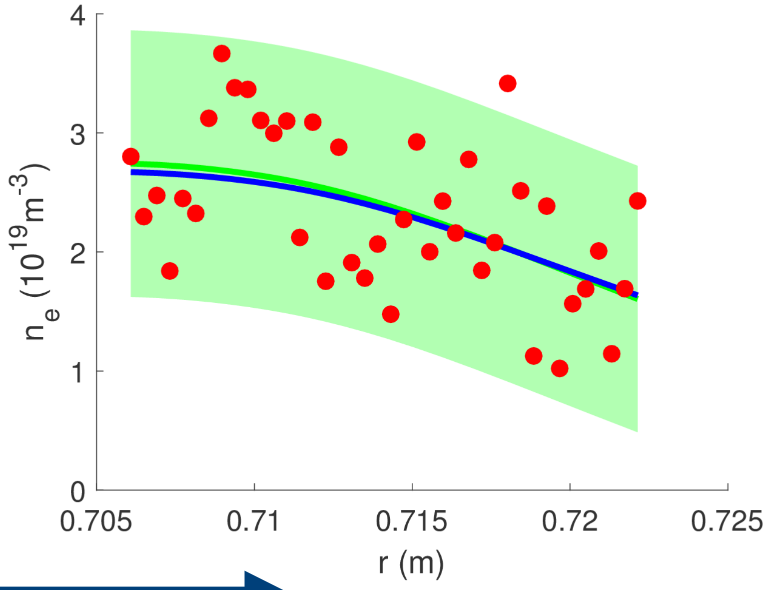
Bayesian MAP verification

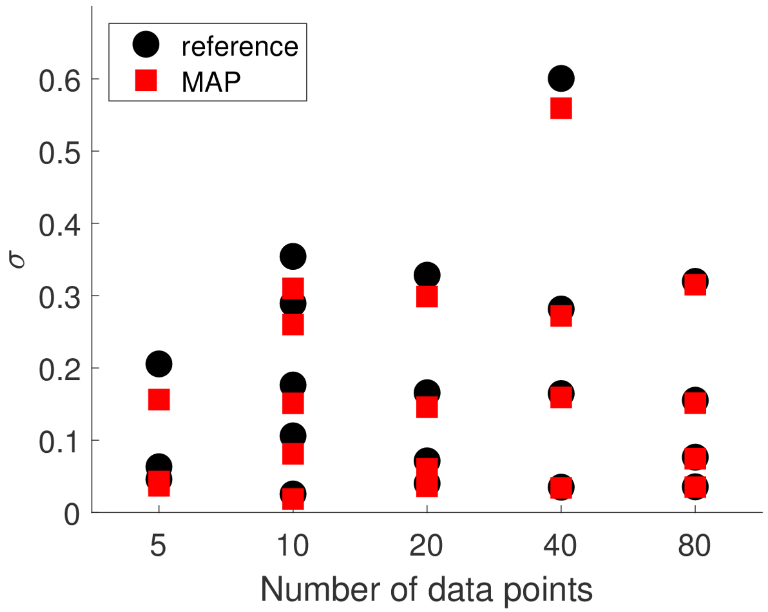
[S. Carli et al., CPP 62 (2021) e202100184.]

- Fictitious experimental data from known SOLPS solution
- Can we reproduce density profile and estimate uncertainty?



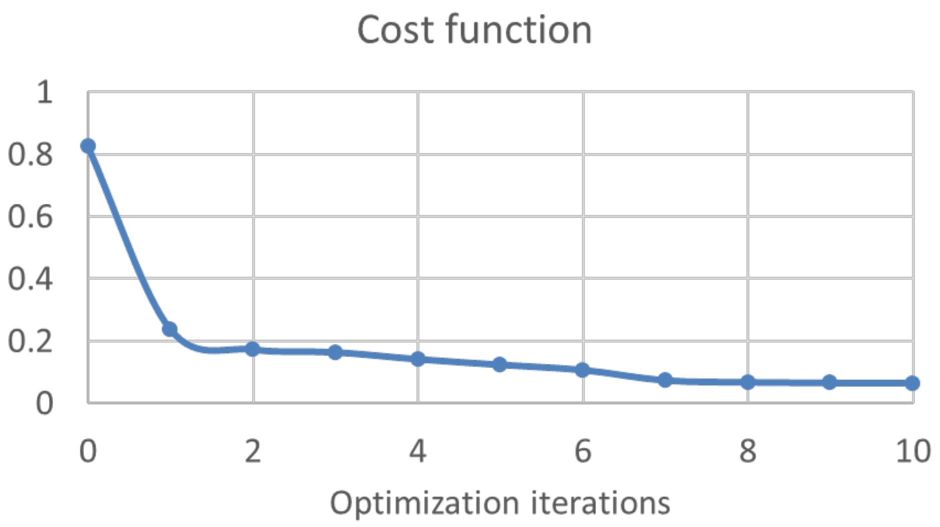
More noise

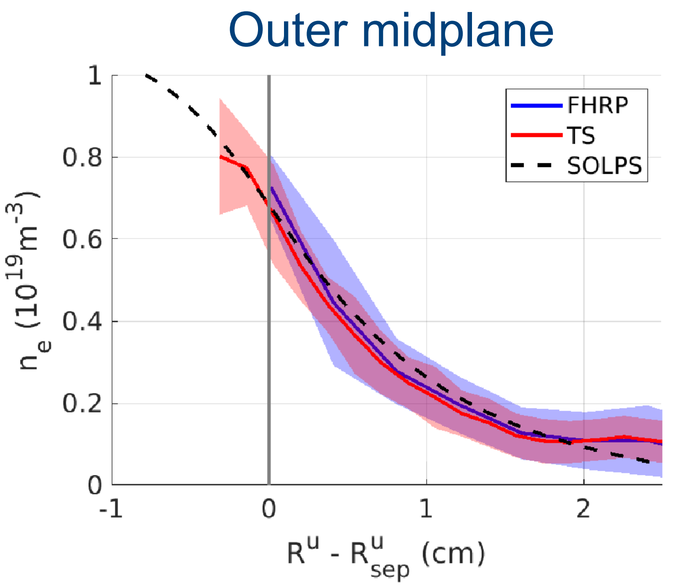


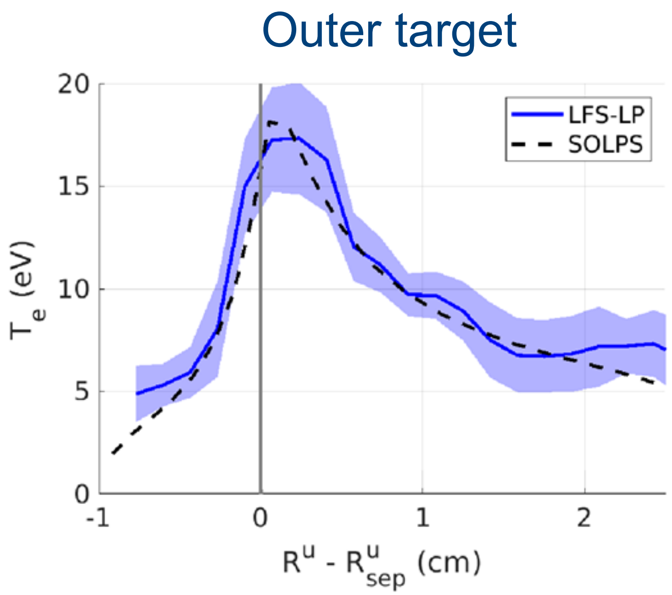


Application to real TCV case

- Advanced fluid neutrals, pure D
- Optimized constant anomalous transport and core density BC







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Towards optimal divertor design with SOLPS-ITER

- Efficient gradient calculation for complex codes
- Optimization framework implementation
- Automatic grid generation & deformation
- Efficient gradient calculation for kinetic neutrals
- Coupling with magnetic filed model

Grid deformation

[S. Van den Kerkhof, EUROfusion EEG.]

- **Optimize the vertex coordinates** (x, y) by solving an optimization problem
- **Cost function based on the desired grid metrics:** no manual tuning required!
- Good for simulation: better grid → more accurate results & faster convergence
- Needed for optimization: automated, robust, and fast adaptation of the grids to the changing design!

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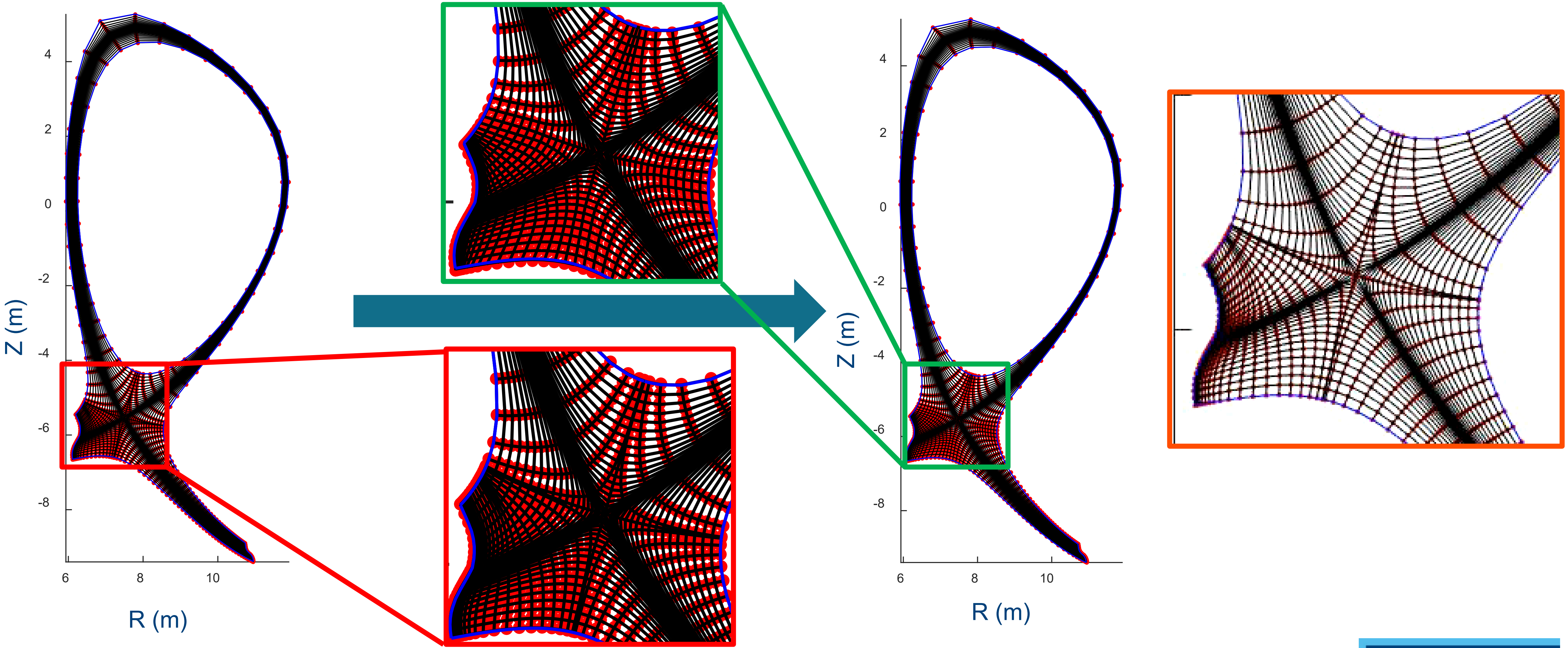
Preliminary results – ADC SX



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Derivates in presence of statistical noise?

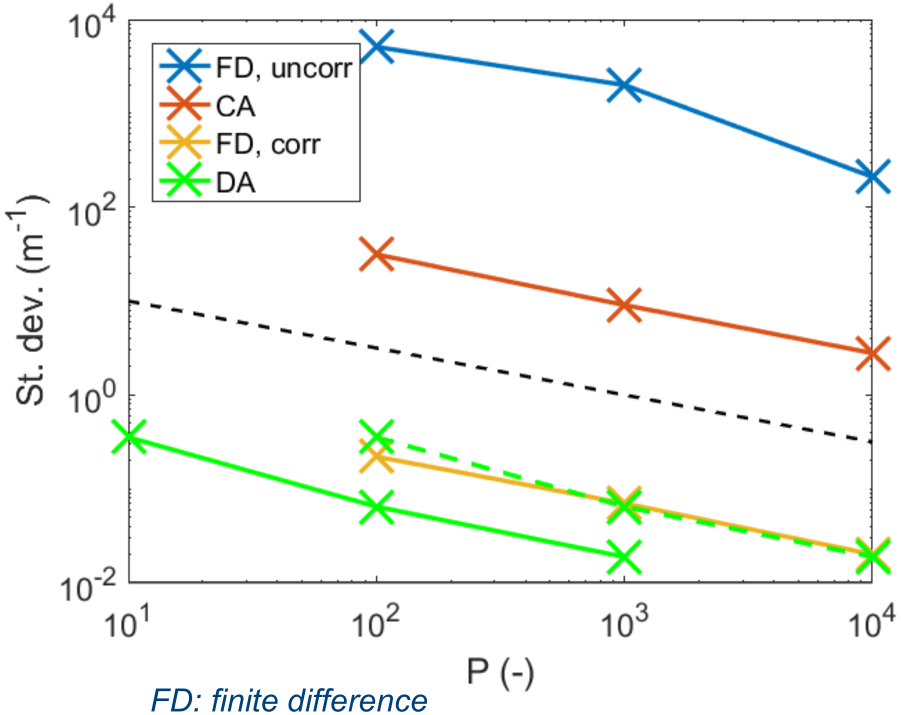
- Finite difference sensitivities
  - **Cost** scales with number of design variables
  - **Correlated random numbers** to reduce variance

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

  - Some decorrelation hard/impossible to avoid in practice

- Discontinuous adjoint ≈ backwards Algorithmic Differentiation
  - Cost **independent** of number of design variables
  - **Exact correlation** with forward simulation
  - Full forward neutral distribution not needed

(Rel.) st. dev. on sensitivity



FD: finite difference
CA: continuous adjoint
DA: discrete adjoint

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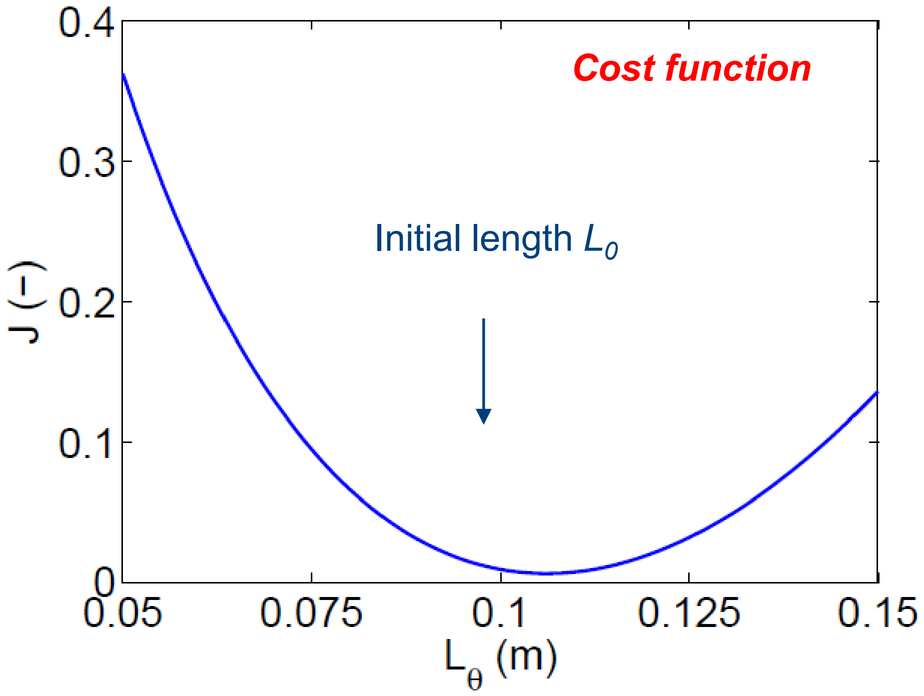
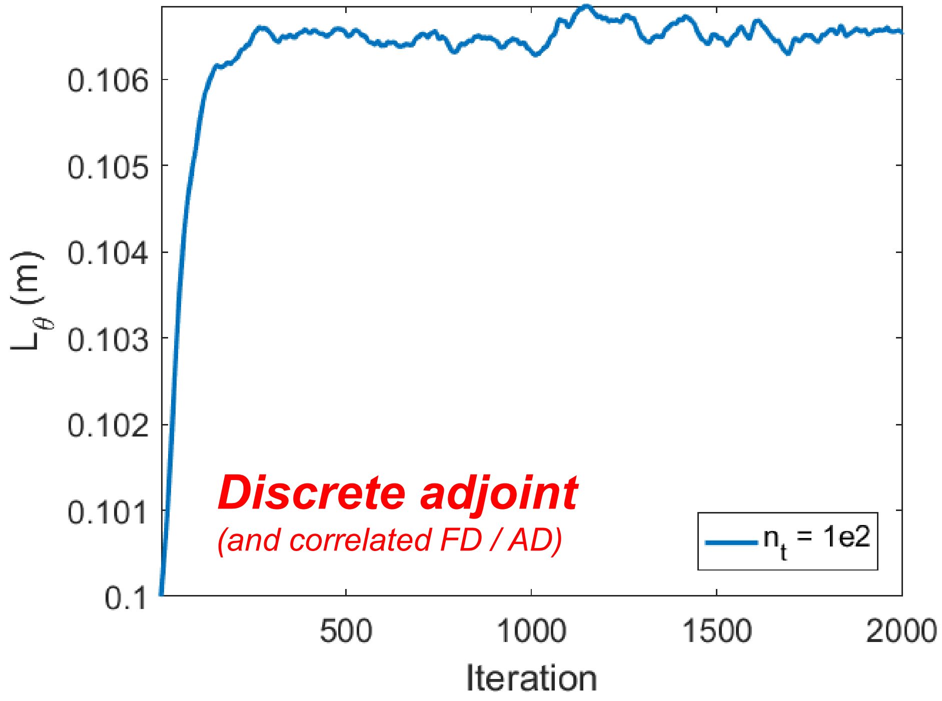
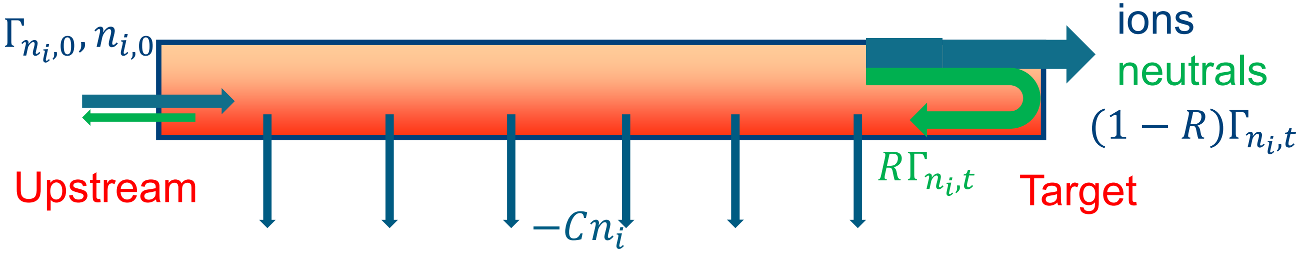
Optimization in presence of statistical noise

[Dekeyser et al., Contrib. Plasma Phys. **58** (2018) 643–651.]







"Optimization of divertor fluxes" in 1D:

$$\min_{L_\theta,\mathbf{q}} \quad J(L_\theta,\mathbf{q}) = \frac{\lambda}{2}(\Gamma-\Gamma_\mathrm{d})^2|_\mathrm{t} + \frac{\lambda_0}{2}(L_\theta - L_0)^2$$
$$\text{s.t.} \quad A(L_\theta,\mathbf{q}) = S$$

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Summary and challenges

- Optimization-based design has the potential to find the ‘best’ solutions in complex applications
  - ‘Best’ as defined by a metric, i.e. the cost function
  - Exceeding what can be achieved through ‘engineering best practice’?

- Algorithmic Differentiation provides an answer to sensitivity computation in large edge codes, and is robust w.r.t. statistical noise

- Strategies to integrate this optimization into complex workflows exist, but remain to be fully developed for the divertor design case

- Towards robust design: robust cost functional formulations to include parametric uncertainty directly in the design stage

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Questions towards DEMO

- What are the most critical design criteria (i.e. *cost functionals*)?
  - Power?
  - Steady state or transient?
  - Operational scenario?

- What are the dominant constraints?

- Can we quantify the model uncertainty? Robust design?

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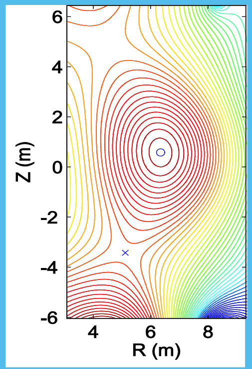
Thank you! Questions?

Plasma edge codes as *analysis* tools

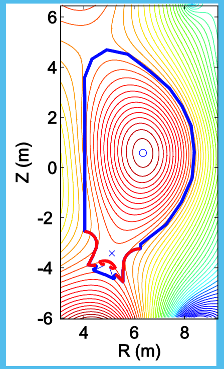
Parameters, BCs,...

Required for model validation, simulation-based design,...:

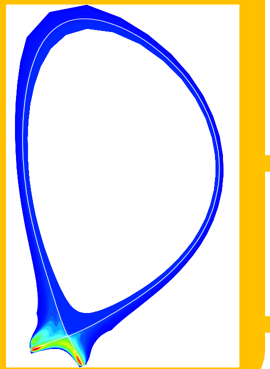
Magnetic equilibrium



Vessel, divertor



Simulation (forward)



Fluxes to PFCs

Profiles of plasma parameters

...

Relatively large number of inputs, constraints,...

Relatively small number of outputs, well defined objectives

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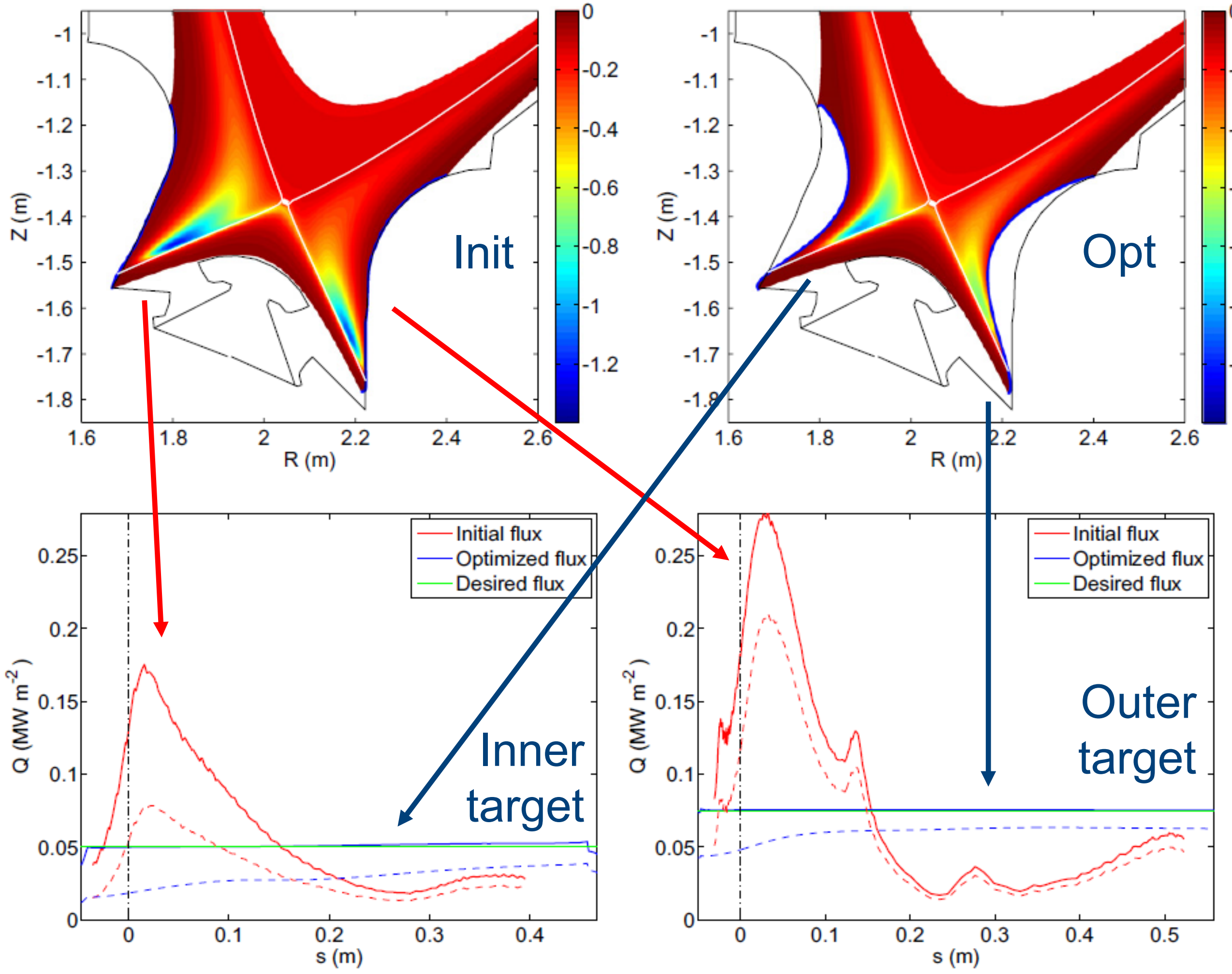

- Downsized ITER F57 (40%)
- $n_c = 3{\cdot}10^{19}\ m^{-3}$
- Q = 3 MW
- Pumping speed 130 $m^3\ s^{-1}$

(colors: impurity radiation in MW m^{-3})

solid lines: total load, conv. + cond. + surf. recomb.
dashed lines: conv. + cond.

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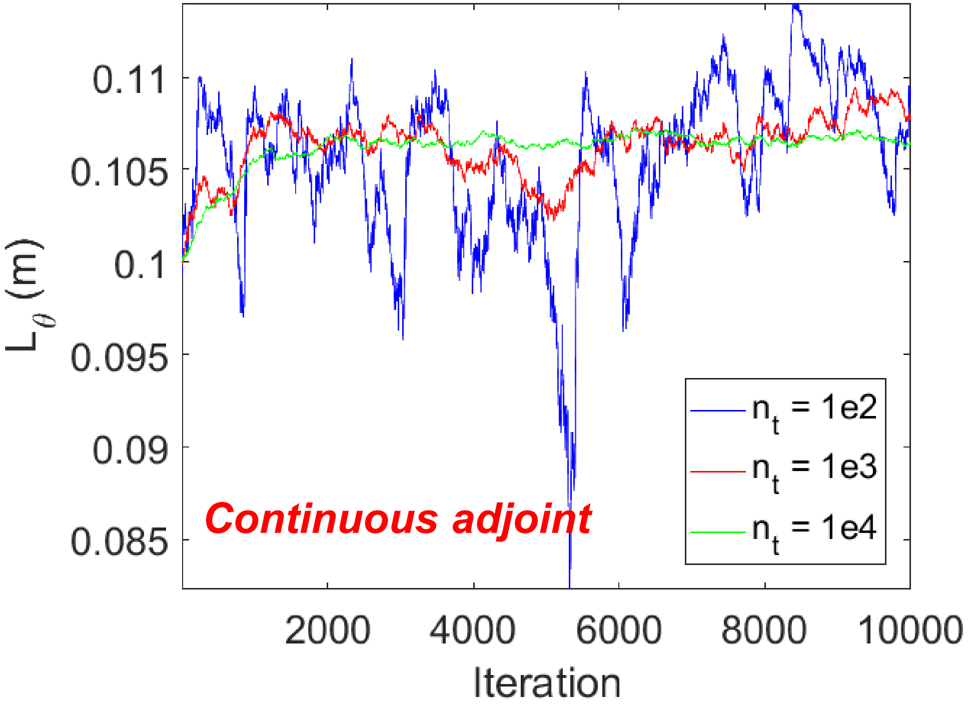

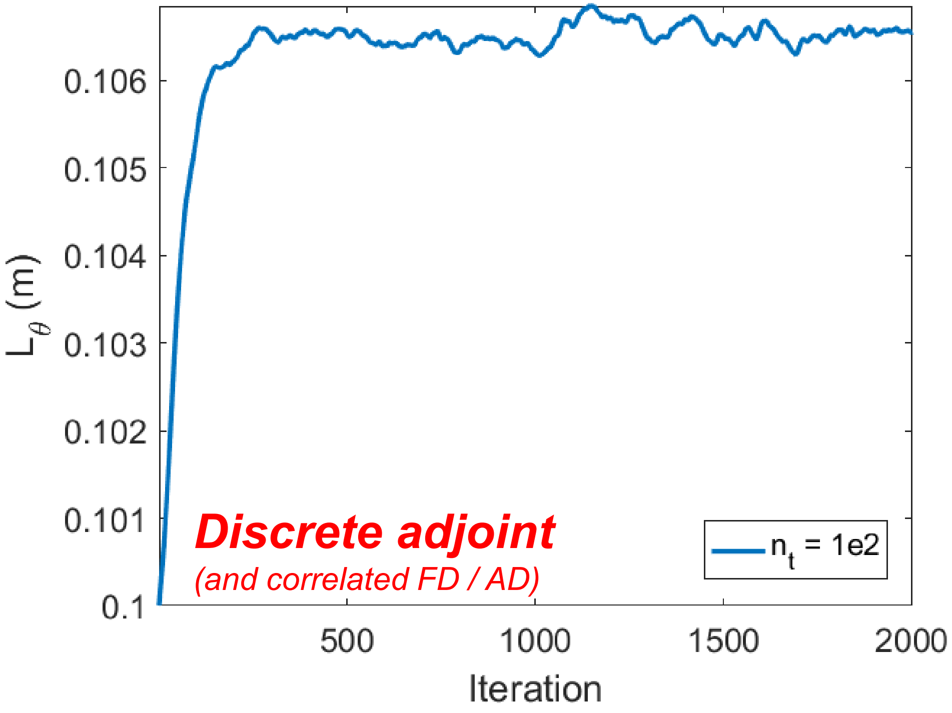

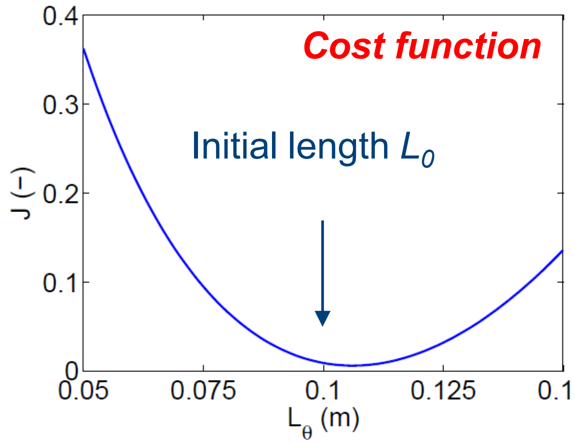

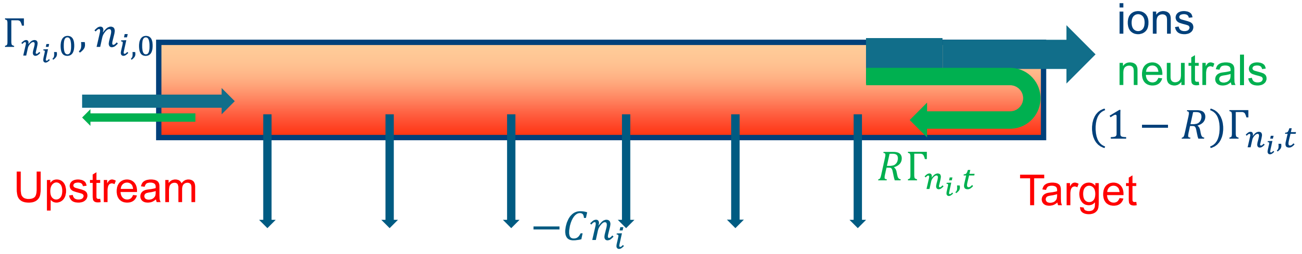

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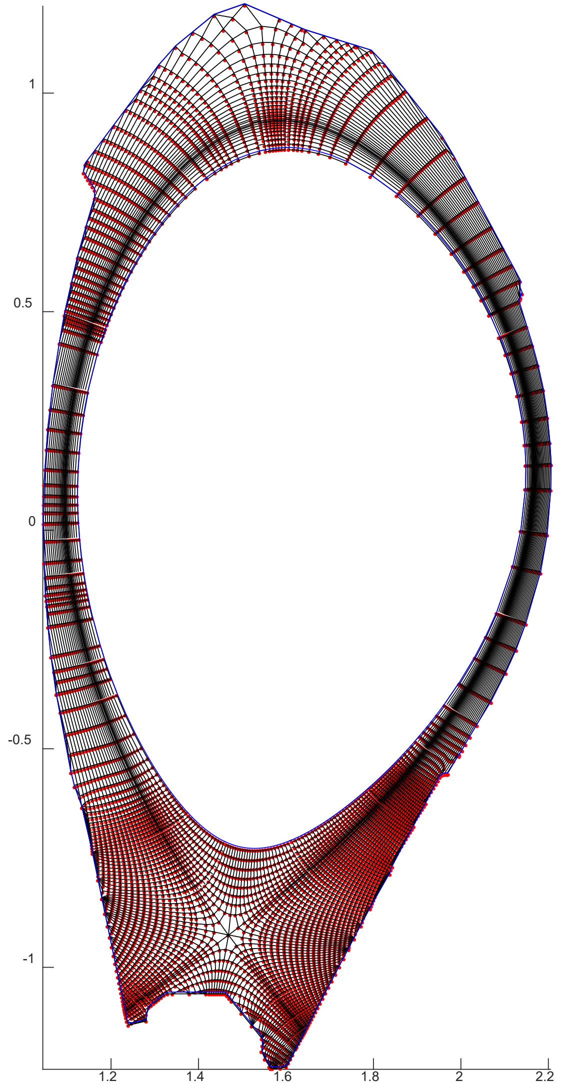

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