Achievements and Challenges in Automated Parameter, Shape and Topology Optimization for Divertor Design

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Divertor design challenges

• Interpretation of experimental data
  o To improve models for design
  o “Control” variables: modeling parameters to be estimated: transport coefficients, boundary conditions at outermost flux surface, …

• Divertor shape design
  o “Control” variables: shape of targets, dome, baffles,…

• Design of divertor magnetic configuration
  o “Control” variables: currents through coils, location of coils,…

• Design of cooling
  o “Control” variables: topology, size, mass flow rates, …

Note: “Control variable” refers to terminology used in optimization

Divertor design challenges
A modeling perspective

Large number of design variables
(Parameterized) shape of divertor, currents through divertor coils,...

Complex physical model
Time consuming simulations
Fluid plasma model (e.g. B2) kinetic neutrals (e.g. EIRENE)

Physics, material and engineering constraints
E.g. core stability, peak heat flux limits, neutron shielding,...

http://www.iter.org
Design challenges in aerodynamics

Drag reduction at constant lift

Reduction of shock-blade interaction

Unoptimized

Optimized

32% drag reduction

Solved with adjoint based shape optimization

(Gauger, VKI LS on MDO, May 2010.)

(Shahpar, VKI LS on MDO, May 2010.)
Design challenges in structural mechanics

Design of light weight construction

First fluid engineering application
Lowest pressure drop for fluid volume
max. 1/3 of domain

Borrvall & Peterson (2003), Int. J. Num. Meth.Fluids

Solved with adjoint based topology optimization
Outline

• Introduction

• Edge plasma codes: from analysis to optimization tools?

• Achievements and challenges
Edge codes as *analysis* tools

Magnetic equilibrium

Vessel, divertor

Simulation (forward)

Parameters, BCs,...

Output

Design variables (currents, shape) and constraints (stability, shielding,...)
Profiles of plasma parameters

Edge codes as analysis tools

Magnetic equilibrium
Vessel, divertor

Parameters, BCs,...

Simulation (forward)

Fluxes to PFCs
Profiles of plasma parameters
...

Relatively large number of inputs, constraints,...

Relatively small number of outputs, well defined objectives

Required for model validation, simulation based design,...:
Edge codes as *optimization* tools

**Magnetic equilibrium**

**Vessel, divertor**

**Simulation (forward)**

**Analysis**

Adjoint simulation

Desired change

Experimental data

Simulation result

sensitivity information?

A way to compute sensitivities to all parameters at once

Adapt transport coefficients, model parameters

Experimental data

Simulation result

sensitivity information?
Outline

• Introduction

• Edge plasma codes: from analysis to optimization tools

• Achievements and challenges
  o Model parameter estimation from experimental data
  o Shape optimization in divertors
  o Magnetic optimization
  o Thermal-fluid optimization of heat sinks
Model parameter estimation

Status

• Proof of principle
• First results on real case¹
  M. Baelmans et al. (2014), PPCF 56(11), 114009

Challenges

• Introduce Bayesian/likelihood estimators to
  o Incorporate a priori knowledge
  o Achieve most reliable models corresponding to available data sets
• Global vs. local optima might require hybrid approach (GA/adjoint)
Shape optimization

Magnetic equilibrium

Vessel, divertor

Simulation (forward)

Analysis

Change in design

Adjoint simulation

Desired change

sensitivity information?
Radiation and adjoint radiation models

- Vessel, divertor
- Simulation (forward)
- Radiation simulation
- Analysis
- Change in design
- Adjoint simulation
- Adjoint radiation
- Desired change

Parameter: Q (MW m⁻²)

$r (m)$ axis:
- $Q_{in}$
- $Q_d$

$r (m)$ range:
- $-0.02$ to $0.04$
- $-40$ to $40$
Reactor shape optimization

- Thermal flow (PDE) and Radiation (MC)
Shape optimization

Status

• Proof of principle
• Results on real geometry\textsuperscript{1}
• Results on FV with MC radiation simulations\textsuperscript{2}
  o Need for additional filtering for smooth gradient
• Improved optimization procedures\textsuperscript{3}
  o Improvement achieved in approximately 15 equivalent forward simulations

Challenges

• Introduce more accurate neutral models (MC or hybrid MC/FV $\rightarrow$ ER)
• Improve speed and convergence issues in plasma edge models

\textsuperscript{1}W. Dekeyser et al. (2014), Nucl.Fus. 54
\textsuperscript{2}W. Dekeyser et al. (2015), J.Nucl.Mat. 463
\textsuperscript{3}W. Dekeyser et al. (2014), JCP 278
Magnetic field optimization

Magnetic equilibrium

Design update
Make step in coil currents

Grid

Sensitivity calculation
Finite differences + Adjoint

Simulation (forward)

Adjoint simulation

Analysis

sensitivity information?

KU LEUVEN
Magnetic field optimization

- Heat load optimization for WEST

Peak heat load decreases with more than 50%
Magnetic field optimization

Status

• Proof of principle
• Results on real geometry (JET\(^1\), WEST\(^2\))
• Results including free boundary equilibrium FEM code\(^3\)
  o In parts adjoint procedure
• Improved grid generation procedure
  o 50% reduction in cost function after 10 equivalents forward simulations

Challenges

• Increase flexibility in magnetic configurations
• Further acceleration by one-shot procedure
• Integrated magnetic field and plasma simulations (incl. core model)

\(^1\)M. Blommaert et al. (2015), Nucl.Fus. 55
\(^2\)M. Blommaert et al. (2015), J.Nucl.Mat. 463
\(^3\)M. Blommaert et al. (2015), PET-2015

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Topology optimization for cooling

**Electronics cooling**
- Silicon micro heat sink: 1cm x 1cm x 500µm
- Fixed pressure drop: 10 kPa
- Heat source 40 K above coolant inlet

Heat sink for **constant temperature** heat source:

**Objective:**
Maximal heat removal from the heat source

Heat sink for **constant heat flux** source:

**Objective:**
Minimal deviation from desired temperature

Easily extended to given heat flux profile and desired temperature
Topology optimization for cooling

1. Build a grid fulfilling constraints
2. Compute pressure and velocity field
3. Compute temperature field
4. Solve energy equation
5. Solve adjoint flow field
6. Solve adjoint thermal field
7. Compute sensitivities
8. Compute adj. temperature
9. Desired change
10. Lower Thermal resistance or hotspot temperature

Design variables grey-values
Heat sink topology optimization

- Start with grey; evolve to b/w
- Total heat removed: 794 W ($\approx$8MW/m²)
- 30x better than empty cooler
Topology optimization

Status
• Only recently developed for heat transfer applications
• Limited to low Re-flows
• First use in micro-electronics cooling applications
• Account for production limits is possible

Challenges
• Improve modeling assumptions
• Expand to other applications
• Flexible introduction of production limits

Conclusions

Adjoint methods provide sensitivities

Optimization methodology from aerodynamics is extended for use in fusion research:
• Model parameter estimation from experimental data
• Shape optimization in divertors
• Magnetic optimization

Optimization methodology from structural mechanics is interesting for innovative cooling concepts
• Thermal-fluid optimization of heat sinks
• First results in micro-electronics cooling applications reaching 8 MW/m² with water cooling
Questions & comments

Thank you for your attention
Extra slides
What can the adjoint approach do?

- Efficient computation of sensitivities w.r.t. all input parameters (cost of 1 flow simulation per output variable)
  - Design variables: divertor shape, magnetic field, …
  - (Uncertain) model parameters: anomalous transport coefficients, boundary conditions,…
  - Operational window

- Automated simulation procedure
  - Automated design
    - Divertor shape (W. Dekeyser)
    - Magnetic field (M. Blommaert)
    - Topology of coolers (T. Van Oevelen)
  - Automated Uncertainty Quantification (several MSc students)
    - ‘Forward’: determine uncertainty on output due to uncertain inputs
    - ‘Backward’: parameter estimation
  - Robust design (i.e. a combination of these two…)

- Natural framework to include various (design) constraints
- Optimal numerical procedures (grids, iterative procedures)
Adjoint formalism for PDEs

Cost function: match to “experimental data”

\[
J(q(\Phi), \Phi) = \int_{T_{l,OM}} \frac{1}{L_0} \left( \frac{1}{n_0^2} \frac{(n - n^{exp})^2}{2} + \frac{1}{T_0^2} \frac{(T - T^{exp})^2}{2} \right) h_r dr
\]

s.t.

\[
\begin{align*}
B(q, \Phi) &= 0 \\
B_S(q, \Phi) &= 0
\end{align*}
\]

\(\Phi\): transport coefficients and plasma edge model constants

\(B\): plasma edge model with \(B_S\) related boundary conditions

Control variables: unknown parameters \(\Phi\) to match

Volume averaged quantities in cases presented
Adjoint formalism for PDEs

Simple plasma edge model

\[ B(q, \Phi) = \frac{1}{\sqrt{g}} \frac{\partial}{\partial \theta} \left( \sqrt{\frac{g}{h_\theta}} C(q) - \sqrt{\frac{g}{h_\theta^2}} D^\theta(q) \frac{\partial q}{\partial \theta} \right) - \frac{1}{\sqrt{g}} \frac{\partial}{\partial r} \left( \sqrt{\frac{g}{h_r^2}} D^r(q) \frac{\partial q}{\partial r} \right) - S(q) = 0 \]

\[ q = \begin{bmatrix} n_i \\ p_n \\ u_{\parallel} \\ T \end{bmatrix} \quad C^\theta(q) = \begin{bmatrix} n_i u_{\parallel} \\ 0 \\ \frac{m n_i u_{\parallel} u_{\parallel}}{2 (1 + Z_i) n_i u_{\parallel} T} \end{bmatrix} \quad D^\theta(q) = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & D_p^n & 0 & 0 \\ 0 & 0 & \eta_i & 0 \end{bmatrix} \quad D^r(q) = \begin{bmatrix} D_i & 0 & 0 & 0 \\ 0 & m u_{\parallel} D_i & 0 & 0 \\ 0 & 0 & \eta_i & 0 \end{bmatrix} \]

And

\[ D_n^p = \frac{C_1}{T} + \frac{C_2}{m (n_i K_{CX} + n_e K_i)} \]

With sources for ionization, recombination and charge exchange

\[ S(q, \nabla_\theta q, \nabla_r q) = S_n(q, \nabla_\theta q, \nabla_r q) + S_z(q, \nabla_\theta q, \nabla_r q) + S_p(q, \nabla_\theta q, \nabla_r q) \]

\[ S_n = \begin{bmatrix} n_e n_n K_i - n_i n_e K_r \\ -n_e n_n K_i + n_i n_e K_r \\ -m n_i n_n K_{CX} u_{\parallel} \\ -E_n n_i n_n K_i \end{bmatrix} \quad S_z = \begin{bmatrix} 0 \\ 0 \\ 0 \\ -c_z n_i n_e L_z \end{bmatrix} \quad S_p = \begin{bmatrix} 0 \\ 0 \\ \frac{b_p \nabla p}{b_\theta \nabla \theta} \\ 0 \end{bmatrix} \]
Adjoint formalism for PDEs

The adjoint approach to compute sensitivities

Langrangian approach

\[
L(q, \Phi, q^*, q_S^*) = J(q, \Phi) - \int_V (q^*)^T B(q, \Phi) d\Omega - \int_S (q_S^*)^T B_S(q, \Phi) d\sigma
\]

\[
\begin{cases}
\nabla_{q^*}L(q, \Phi, q^*, q_S^*) = 0 & \text{state equations} \\
\nabla_{q_S^*}L(q, \Phi, q^*, q_S^*) = 0 & \text{boundary conditions} \\
\nabla_qL(q, \Phi, q^*, q_S^*) = 0 & \text{adjoint equations} \\
\nabla_\Phi L(q, \Phi, q^*, q_S^*) \geq 0 & \text{design equation}
\end{cases}
\]

And gradient computation

\[
\frac{dL}{d\Phi'} = \frac{dJ_q}{d\Phi'} + \frac{dJ_\Phi}{d\Phi'} - \int_V (q^*)^T (B_{q,q} \Phi' + B_{q,\Phi} \Phi') d\Omega - \int_S (q_S^*)^T (B_{S,q} q^* \Phi' + B_{S,\Phi} \Phi') d\sigma
\]

\[
= J_\Phi \Phi' - \int_V (q^*)^T B_{\Phi} \Phi' d\Omega - \int_S (q_S^*)^T (B_{S,\Phi} \Phi') d\sigma
\]
Adjoint formalism for PDEs

The resulting adjoint equations, e.g. continuity equation

\[
\frac{\partial n_i}{\partial t} + \frac{1}{\sqrt{g}} \frac{\partial}{\partial \theta} \left( \frac{\sqrt{g}}{h_\theta} n_i u_\theta \right) - \frac{1}{\sqrt{g}} \frac{\partial}{\partial r} \left( \frac{\sqrt{g}}{h_r^2} D_i \frac{\partial n_i}{\partial r} \right) = S_{n_i}
\]

is given by

\[
-\frac{\partial n_i^*}{\partial \theta} - \frac{1}{\sqrt{g}} \frac{\partial}{\partial \theta} \left( \frac{\sqrt{g}}{h_\theta} n_i^* u_\theta \right) - \frac{1}{\sqrt{g}} \frac{\partial}{\partial r} \left( \frac{\sqrt{g}}{h_r^2} D_i \frac{\partial n_i^*}{\partial r} \right) = \frac{\partial S_{n_i}}{\partial n_i} n_i^* + f \left( u_\parallel^*, \nabla u_\parallel^* T_\parallel^*, \nabla T_\parallel^*, p_\parallel^*, \nabla p_\parallel^* \right) - \frac{\partial J}{\partial n_i}
\]

- Adjoint equations trace back the influence of cost function by “back flow in time”
- Continuous adjoint approach provides a hard test on numerical implementation and accuracy (5-point stencils vs. 9-point, discretization errors)
Adjoint formalism for PDEs

Computing the gradient

\[
\frac{dJ}{d\Phi} \Phi' = \frac{dL}{d\Phi} \Phi' = J_\Phi \Phi' - \int_V (q^*)^T B_\Phi \Phi' d\Omega - \int_S (q_s^*)^T (B_{s,\Phi} \Phi') d\sigma
\]

Use this information to optimize \( \Phi \), i.e.

- change unknown transport coefficients using BFGS (Quasi-Newton) with strong Wolfe conditions
- Solution as close as possible to measured data

**Note:** \( \frac{dJ}{d\Phi} \) gives also sensitivity w.r.t. uncertain transport coefficients \( \Rightarrow \) uncertainty quantification
Can/should we learn from this?

**Computational Divertor Design - Design-by-Analysis**

- Large number of design variables
- Complex plasma-neutral flows
- Physics, engineering, material constraints

**Aerodynamics, Fluid Mechanics,... Design-by-Optimization**

- Adjoint sensitivity computation
- Efficient optimization algorithms
- Natural framework for constraints

In recent years we tried to answer the question,
Let’s have a look at the outcome