Improvements in heat flux calculations for water-cooled plasma-facing components in W7-X Progress report

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23.06.2023

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Outline

Motivation

- New divertor structure
- Simulation with THEODOR
- Improvement potential

2 LayerTHEODOR

- 2D divertor model
- Heat diffusion equation
- Code structure

3 Preliminary results

• 1D semi-infinite solid model

Summary

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Motivation - New divertor structure

OP 2.1 divertor overview



Figure: 3D model of the divertors. For the red regions there are thermocouples measuring the cooling water temperature [1].

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Sebastian Thiede	Improvements in heat flux calculations			23.	06.2	2023			3/19

Motivation - New divertor structure



Figure: 3D model of a divertor finger. CFC (Carbon Fiber Composite) is facing the plasma

*AMC = Active Metal Casting, a bonding technique [2]

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Motivation - New divertor structure

middle divertor structure



Figure: middle divertor - low heat flux region. (Sigraflex is a carbon based material) [3]

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- \bullet OP 2 specification: max. 10 MW m $^{-2}$ on HHF (high heat flux) divertors, max. 1 MW m $^{-2}$ on middle divertors
- $\bullet\,$ measurement of top surface temperature with IR thermography $\Rightarrow\,$ no issue with plasma facing layers
- material limitations: T ≤ 550 °C for the Cu interlayer, T ≤ 450 °C for the CuCrZr heat sink
 how to get the maximum temperature in those layers?
 Thermocouples are very sparsely distributed → not enough information.
- accurate knowledge of heat flux from plasma is needed (to know the deposited power, further physics studies)

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Motivation - Simulation with THEODOR

Insufficiencies of THEODOR - comparison with ANSYS simulation [1]



Reasons for this mismatch:

- watercooled divertor layers have different material properties, but THEODOR can only model one
- the bottom heat transfer coefficient was adjusted "by hand" ⇒ doesn't model the actual divertor well

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Possible improvements:

- multiple layers
- use the experimental data of thermocouples at the heatsink (model water cooling pipes as boundary conditions)
- THEODOR only allows one predefined expression for the material properties as functions of temperature \rightarrow allow lookup tables and other functions
- \bullet better execution times \rightarrow full C++ implementation
- provide documentation on how to use the software and how it works

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LayerTHEODOR - 2D divertor model

Defining a goal:



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Heat diffusion equation for temperature dependent material properties:

$$c_{p}(T)\rho(T)\frac{\partial T}{\partial t} = \vec{\nabla}\cdot(\underbrace{\kappa(T)\vec{\nabla}T}_{=\vec{\phi}}) + \dot{q}$$
(1)

where

- T ... temperature
- $c_p(T)$... specific heat capacity
- $\rho(T)$... mass density
- $\kappa(T)$... (anisotropic) heat conductivity
- $\vec{\phi}$... heat flux
- q ... additional volumetric energy sources

here, κ can only be of the form (2D !):

$$oldsymbol{\kappa}(T) = egin{pmatrix} \kappa_x(T) & 0 \ 0 & \kappa_y(T) \end{pmatrix}$$

 \longrightarrow no hope for analytical solution

(2)

numerical solution required \Rightarrow (e.g.) finite difference method (FDM) meaning:

$$\begin{aligned} x &= i \cdot \Delta x \text{ for } i \in \{0, ..., N_x\} \subseteq \mathbb{N} \\ y &= j \cdot \Delta y \text{ for } j \in \{0, ..., N_y\} \subseteq \mathbb{N} \\ t &= n \cdot \Delta t \text{ for } n \in \{0, ..., N_t\} \subseteq \mathbb{N} \\ T(x, y, t) \Rightarrow T_{i,j}^n \\ \frac{\partial T(x, y, t)}{\partial x} \Rightarrow \frac{T_{i+1,j}^n - T_{i,j}^n}{\Delta x} \text{ (analogous for y)} \\ \frac{\partial T(x, y, t)}{\partial t} \Rightarrow \frac{T_{i,j}^{n+1} - T_{i,j}^n}{\Delta t} \end{aligned}$$

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(3)

LayerTHEODOR approach: heat flux matricies per layer of the divertor



$$\phi_{(i,j)\to(k,l)} = -\phi_{(k,l)\to(i,j)}$$

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Improvements in heat flux calculations

heat flux:

$$\phi_{(i,j)\to(k,l)}^{n} = \kappa_{x/y} \left(\frac{T_{i,j}^{n} + T_{k,l}^{n}}{2} \right) \cdot \underbrace{\frac{T_{i,j}^{n} - T_{k,l}^{n}}{\bigtriangleup x/\bigtriangleup y}}_{\text{discrete T derivative}}$$
(4)

(discretized Fourier's law, $(k = i \pm 1)\dot{\vee}(l = j \pm 1)$, x or y chosen accordingly) used in heat flux equation:

$$c_{\rho}(T_{i,j}^{n})\rho(T_{i,j}^{n})\frac{T_{i,j}^{n+1}-T_{i,j}^{n}}{\triangle t} = \frac{\phi_{(i-1,j)\to(i,j)}^{n}-\phi_{(i,j)\to(i+1,j)}^{n}}{\triangle x} + \frac{\phi_{(i,j-1)\to(i,j)}^{n}-\phi_{(i,j)\to(i,j+1)}^{n}}{\triangle y} + \dot{q}$$
(5)

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- FDM are not unconditionally stable
- important quantity: thermal diffusivity $D_{x/y} = \frac{\kappa_{x/y}}{\rho c_p}$
- Stability criterion:

$$\frac{\max\left(D_x, D_y\right) \cdot \bigtriangleup t}{\min\left(\bigtriangleup x^2, \bigtriangleup y^2\right)} \le \frac{1}{2} \tag{6}$$

• choosing smaller timestep might require finer spatial resolution and vice-versa

LayerTHEODOR - Code structure

Model framework:



Used external C++ libraries:



(a) Eigen [4] for parallelized matrix operations

pybind11

(b) pybind11 [5] to create a Python interface

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Improvements in heat flux calculations

23.06.2023

15 / 19

Preliminary results - 1D semi-infinite solid model

 $\bullet \ \phi^{\rm top} = {\rm const.}$

• solve heat diffusion equation on $y \ge 0$

$$c_p \rho \frac{\partial T}{\partial t} = \kappa \frac{\partial^2 T}{\partial y^2}$$

for κ, ρ, c_p constant and isotropic, $T(y, t = 0) = T_0$ • Solution:

$$T(y \ge 0, t) = T_0 + 2\phi^{\text{top}} \sqrt{\frac{t}{\pi\kappa\rho c_p}} \exp\left(\frac{-y^2\rho c_p}{4\kappa t}\right) \\ -\frac{\phi^{\text{top}}}{\kappa} \operatorname{erfc}\left(\frac{y}{2}\sqrt{\frac{\rho c_p}{\kappa t}}\right)$$

• input for THEODOR and LayerTHEODOR:

$$T(y=0,t)=T_0+2\,\phi^{
m top}\,\sqrt{rac{t}{\pi\kappa
ho c_{
m p}}}$$

T(y=0)

T

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Preliminary results - 1D semi-infinite solid model

Comparison THEODOR and LayerTHEODOR

input data each 10 ms



Preliminary results - 1D semi-infinite solid model

THEODOR and LayerTHEODOR have vastly different accuracy and runtime \rightarrow we don't know yet why THEODOR is less accurate. Possible reasons:

- artifact of interpolating the inputted temperature data (figure below)
- THEODOR uses the so-called heat flux potential, while LayerTHEODOR operates on temperatures directly (different discretized equations)
- fixing error in how output flux is calculated removes most of the error for LayerTHEODOR (red line, averaging over the "microsteps" between new data input instead of just outputting the last)
- In any case choosing smaller timesteps decreases error.
- Why is it also faster? (for small timesteps \sim 2.8 times)
 - \bullet internally 100% C++ code, less passing data Python \leftrightarrow C(++)
 - "Eigen" library parallelization \rightarrow speed improvement is heavily dependent on architecture



- THEODOR was improved to handle multiple layers of the divertor
- the accuracy and runtime was also improved
- first tests suggest that it works correctly for simple materials next steps:
 - find out why it is more accurate than THEODOR
 - check if anisotropic materials are handeled correctly
 - \bullet test with ANSYS (heat flux \rightarrow temperature) simulation
 - check against experimental data

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