Scientific Computing

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CHT problems and computing coupled discrete adjoints using AD

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1 Introductory example

2 Computing accurate (discrete) adjoints in SU2

3 Coupled problems and validations

Conjugate heat transfer (CHT) problems

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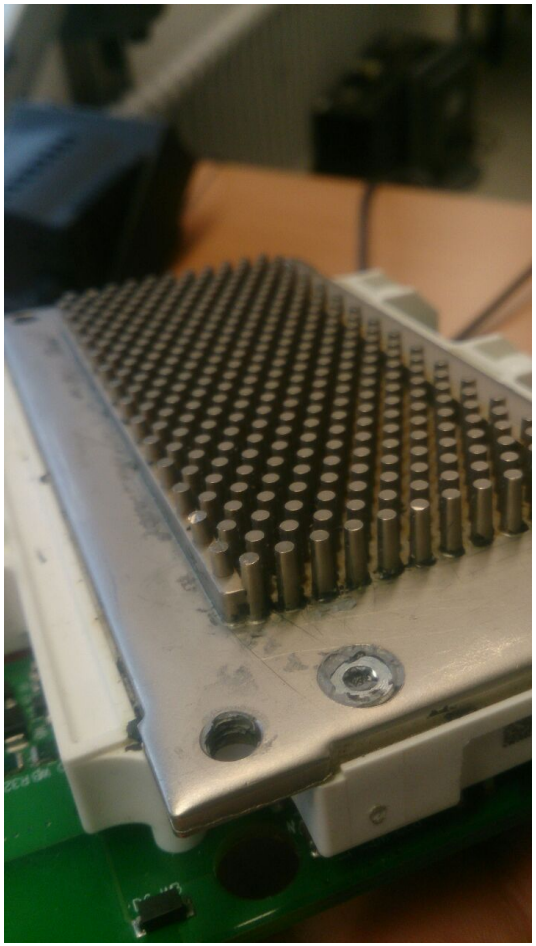
Problem characteristics:

- multiple physical zones that exchange heat at some interfaces
- different governing equation sytems, conductivities, timesteps, ...

Why to start developments in SU2?

- approach from a Bosch research department working on pin-fin cooler optimizations
- joint project with them since 2017

Can SU2 give accurate sensitivities?



Forward (primal) implementation

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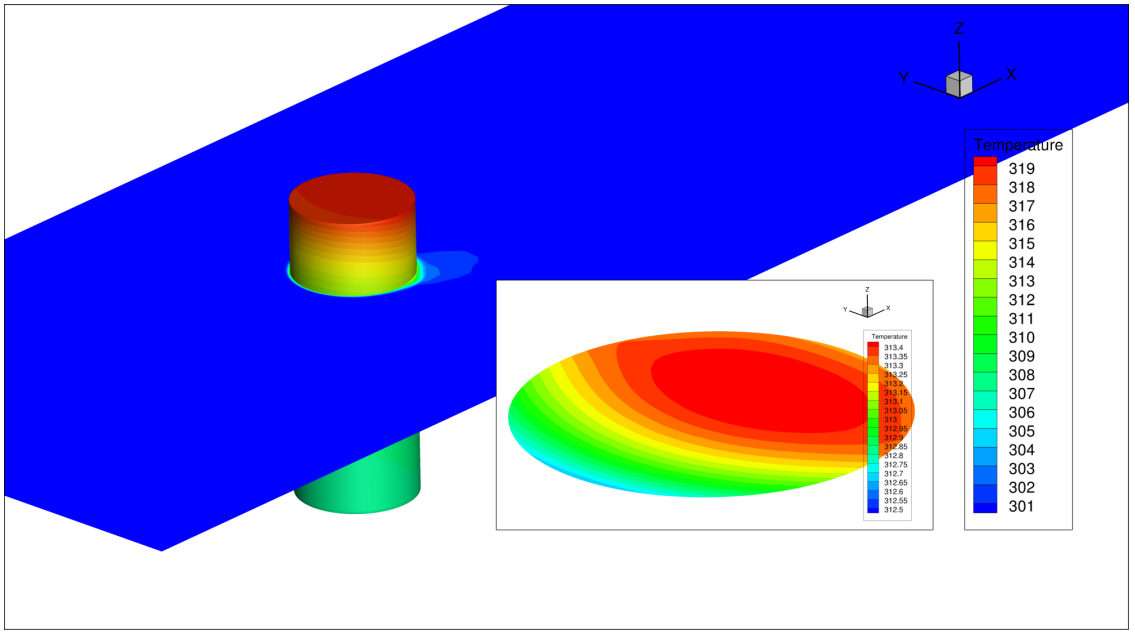
Required ...

- A heat solver (cf. `CHeatSolverFVM`) that can be run in solid zones and coupled to `CIncNSSolver`
- Transfer routines to communicate energies (cf. `CTransfer_ConjugateHeatVars`-class)
- A new driver to iterate the solvers with this kind of coupling (ended up in a much more general approach to handle arbitrary ones, cf. `CMultiphysicsZonalDriver`)

3D test case

Heated aluminium cylinder in (coolant) water flow (at $0,25\frac{m}{s}$, 300K at inlet, 4W heat load at pin's top).



Pin's height/diameter: 5mm/2mm. **Reaches 319K** in average at its top in good agreement to FLUENT.

Optimization with shape gradients

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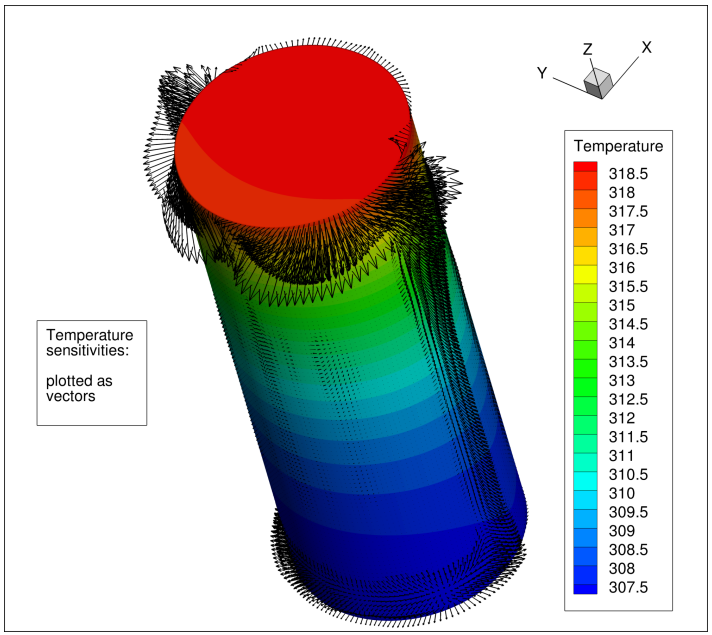
Define

- X be the vector of mesh node *coordinates* determining the pin's surface
- an objective function $J(X)$, e.g. the average temperature at a pin's tip



$\nabla J(X^*)$ suggests the geometry update for minimization of J. It should be passed

- to an appropriate shape update function (FFD, filtering, ...)
- and an optimizer.

How to obtain such sensitivities?

$J(X)$ depends – more precisely – on a state vector U holding pressure, momentum and temperature solutions at each node,

$$J(X) = \tilde{J}(X, U(X)).$$

Denote by $\mathcal{G}$ a CFD solver iterating the vectors U_k, that is

$$U_{k+1} = \mathcal{G}_{(X)}(U_k).$$

The solution $U(X)$ is given by the first iterate solution fulfilling

$$\|\mathcal{G}_{(X)}(U) - U\| < \varepsilon.$$

The computation cost of $\nabla J(X)$ crucially depends on the complexity of $\mathcal{G}$.

Rewriting $J(X)$ as a Lagrangian

Regard J and $\mathcal{G}$ as functions of *two* vectors X, U and set up the **Lagrangian**

$$L(X, U) = \tilde{J}(X, U) + (\tilde{\mathcal{G}}(X, U) - U)^T \cdot \lambda.$$

Along actual flow solutions, L equals $\tilde{J}$, independent of the choice of λ.

By λ we denote the factor („Lagrange multiplier“) such that

$$\nabla_U \tilde{J}(X, U) = (D_U \tilde{\mathcal{G}}^T(X, U) - \mathrm{Id}) \cdot \lambda.$$

This condition ensures that at flow solutions we have

$$\nabla J(X) = \nabla_X L(X, U)$$

which is cheap to compute as it **does not involve the flow solver anymore**.

Method in SU2: fixed point iteration for λ

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To obtain λ, we carry out the fixed point iteration

$$\lambda \stackrel{!}{=} \nabla_U \tilde{J}(X, U) + D_U \tilde{\mathcal{G}}^T(X, U) \cdot \lambda$$

Note that so far we didn't make any assumptions on $\mathcal{G}$ except for being able to carry out the derivative

$$D_U \tilde{\mathcal{G}}^T(X, U) \cdot \lambda$$

subject to an arbitrary vector λ to compute $\nabla J(X)$.

Use of AD (in reverse mode)

For an arbitrary implementation of a function $f : \mathbb{R}^n \to \mathbb{R}^n$ and an arbitrary vector $y \in \mathbb{R}^n$, automatic differentiation in reverse mode computes

$$Df^T(\tilde{x}) \cdot \lambda$$

by the following steps:

- registering the input variables x of the computer program f
- recording a tape while running f at a given point $\tilde{x}$, that is storing $Df(\tilde{x})$
- setting the values λ
- evaluating $Df^T(\tilde{x}) \cdot \lambda$

How to use this generality for multiphysics?

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Let our iterator $\mathcal{G}$ actually consist of two **coupled iterators**, $\begin{pmatrix}\mathcal{G}^A\\ \mathcal{G}^B\end{pmatrix}$, with two sets of meshes X, Y and variables U^A, U^B being iterated like

$$U_k^A \mapsto \mathcal{G}^A(X, U_k^B, U_k^A) = U_{k+1}^A$$
$$U_k^B \mapsto \mathcal{G}^B(Y, U_k^A, U_k^B) = U_{k+1}^B.$$

We then compute $\nabla J(X, Y)$ by simply computing both λ^A and λ^B in the corresponding Lagrangian

$$\tilde{J}(X, Y, U^A, U^B) + \begin{pmatrix}\mathcal{G}^A(X, U^B, U^A) - U^A\\ \mathcal{G}^B(Y, U^A, U^B) - U^B\end{pmatrix} \cdot \begin{pmatrix}\lambda^A\\ \lambda^B\end{pmatrix}.$$

Taking care of the cross terms

The fixed point interation for obtaining $\begin{pmatrix} \lambda^A \\ \lambda^B \end{pmatrix}$ now contains cross derivatives:

$$\begin{pmatrix} \lambda^A_{k+1} \\ \lambda^B_{k+1} \end{pmatrix} = \begin{pmatrix} \frac{\partial}{\partial U^A}\mathcal{G}^A & \frac{\partial}{\partial U^A}\mathcal{G}^B \\ \frac{\partial}{\partial U^B}\mathcal{G}^A & \frac{\partial}{\partial U^B}\mathcal{G}^B \end{pmatrix} \cdot \begin{pmatrix} \lambda^A_k \\ \lambda^B_k \end{pmatrix}$$

To keep the multizone discrete adjoint driver as **modular** as possible, the implementation allows for:

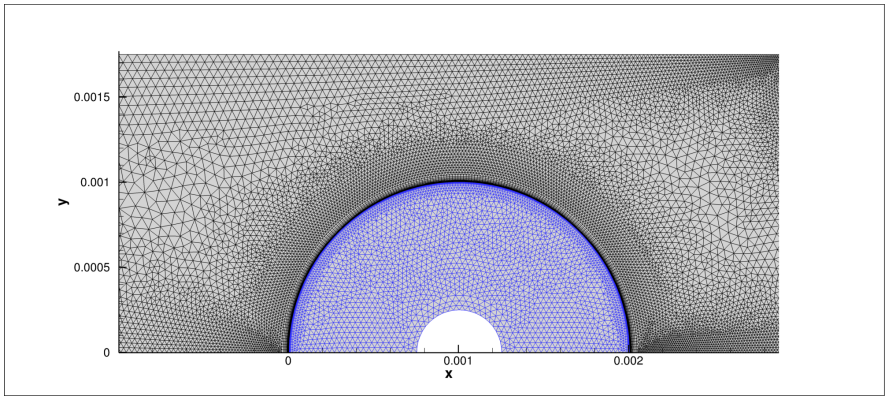
- initialising only parts of the right hand side adjoint vector
- evaluating with respect to arbitrary variable vectors
- restricting the evaluation to parts of the computational graph.

This provides a fair functionality for further **stable and efficient** developments.

Cylinder test case

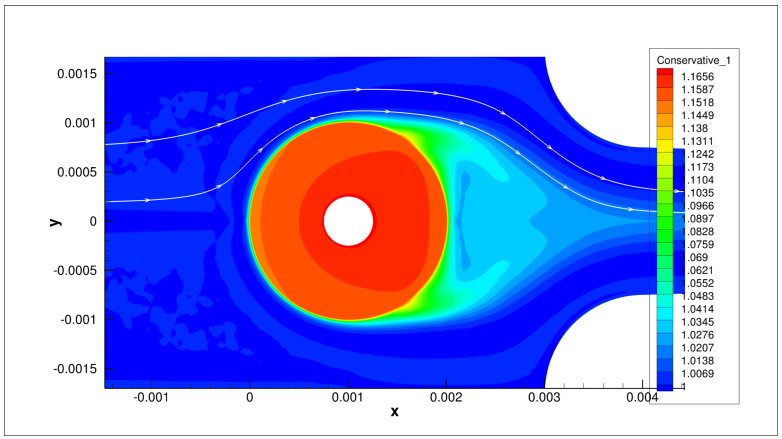
Let $\mathcal{G}^A$ be a **RANS solver** (with coupled heat equation) and $\mathcal{G}^B$ a **heat solver**, both coupled by transferring temperature and heat flux data.

The test geometry (denoted by X^*) is a cylinder, heated from the inside and surrounded by a fluid flow:



- Water, $300K$ / $0,25\frac{m}{s}$ at inlet
- Fixed conductivity ($\mathrm{Pr} = 7$)
- Aluminium
- Heat load at inner wall: $4\frac{kW}{m}$

Primal solve and objective function



- Obtained flow solution U^*
- Using averaged temperature at interface as objective function
- $\tilde{J}(X^*, U^*) = 415K$

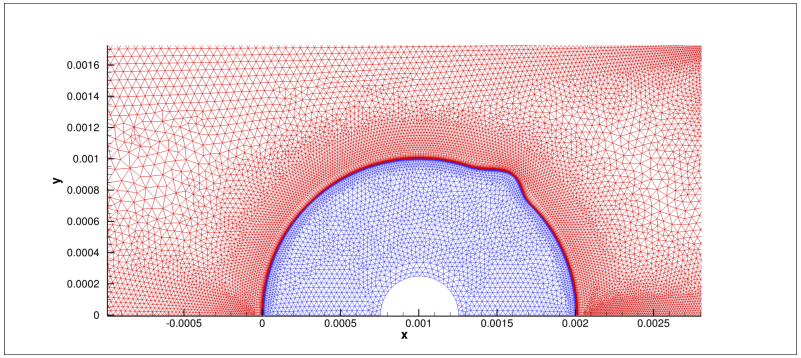
We easily compute the value

$$\nabla J(X) = \nabla_X \tilde{J}(X^*, U^*) + D_X \mathcal{G}^T(X^*, U^*) \cdot \lambda.$$

with the help of λ. **To validate ...**

Geometry change to validate $\nabla J(X)$

- we suggest a new geometry $Y_h = X + h\delta$
- $J(Y) \approx J(X) + h\nabla J(X) \cdot \delta$
- check $\lim_{h \to 0} \frac{J(Y_h) - J(X)}{h} \stackrel{?}{=} \nabla J(X) \cdot \delta$



Changing the value of h, we obtain the following data:

h (in mm)	$J(Y)$ (in K)	$\frac{J(Y)-J(X)}{h}$ (in $\frac{K}{m}$)	rel. error to $\nabla J(X) \cdot \delta$
$1.0e^{-1}$	$417,873795$	$-65,89$	$8,68\%$
$5.0e^{-2}$	$417,877298$	$-61,74$	$1,83\%$
$1.0e^{-3}$	$417,879767$	$-60,7$	$1,15\%$
$5.0e^{-3}$	$417,880081$	$-60,6$	$0,05\%$

Feature work

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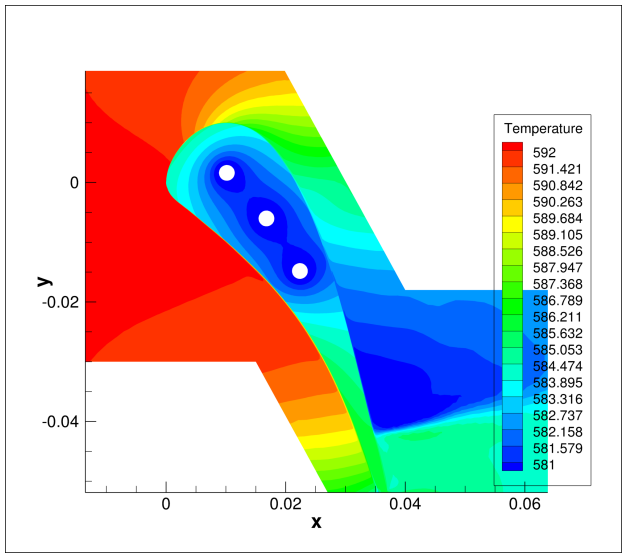
- Uniting the CHT and turbomachinery functionalities for cooled turbine blade optimizations



- Speed up existing coupled simulations
- Trying out vertex-morphing optimizers, especially for internal flow applications