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Computation of accurate adjoint-based gradients for optimization in conjugate heat transfer problems

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In computational fluid mechanics, so called CHT-simulations (conjugate heat transfer) become necessary when heating or cooling effects at the fluid domain's boundaries can't be neglected and the boundary conditions are therefore unknown.
Thus, further physical zones have to be added to the problem and coupled by common interfaces that replace the respective boundaries.
In the most common case, these additional zones are solids subjected to a (hot or cold) surrounding fluid flow. Think, for example, of turbine blades in a high-temperature airflow or hot metal parts in a coolant fluid.

By having added a (possibly convection-dependent) heat equation solver to SU2, we set up a sequential coupling method that naturally fits into the general pseudo-time iteration technique, but also allows for storing a computational graph of one iteration over all physical zones that fully captures the coupling influence.

The (discrete) adjoint solutions with respect to a heatflux- or temperature-related objective function J are then performed by a *duality-preserving iteration*.
Let $\mathcal{G}_\mathrm{F}$ and $\mathcal{G}_\mathrm{S}$ be the fluid and solid zone iterators mapping the current vectors of conservatives $(U_\mathrm{F}^i, U_\mathrm{S}^i)$ to $\left(U_\mathrm{F}^{i+1}, U_\mathrm{S}^{i+1}\right)$ in order to obtain a steady-state solution.
The fixed point iteration to obtain the adjoint solutions λ_F and λ_S at solution $(U_\mathrm{F}^*, U_\mathrm{S}^*)$ then takes the form

$$\left(\lambda_\mathrm{F}^{i+1}, \lambda_\mathrm{S}^{i+1}\right) = \frac{\partial}{\partial U} J(U_\mathrm{F}^*, U_\mathrm{S}^*) + \frac{\partial}{\partial U} \mathcal{G}_\mathrm{F}^\top(U_\mathrm{F}^*, U_\mathrm{S}^*) \cdot \lambda_\mathrm{F}^i + \frac{\partial}{\partial U} \mathcal{G}_\mathrm{S}^\top(U_\mathrm{F}^*, U_\mathrm{S}^*) \cdot \lambda_\mathrm{S}^i,$$

where all terms are evaluated by algorithmic differentiation (AD) in reverse mode (see [1] for further information).

Note that we incorporate the dependence of $\mathcal{G}_\mathrm{F}$ on U_S (and vice versa) by its interface coupling with the corresponding cross terms $\frac{\partial}{\partial U_\mathrm{S}} \mathcal{G}_\mathrm{F} \cdot \lambda_\mathrm{F}^i$.
This way, (shape) gradients calculated from the adjoints are accurate – even if turbulence models are involved in $\mathcal{G}_\mathrm{F}$ – as we show it by comparison with forward mode AD or in terms of finite differences.

REFERENCES

[1] T. Albring, M. Sagebaum and N.R. Gauger, Development of a Consistent Discrete Adjoint Solver in an Evolving Aerodynamic Design Framework. *AIAA Paper 2015-3240*, 2015.