INRIA work in Task 3.1

INRIA contributions is focused on the application of Automatic Differentiation tool ODYSSEE to the assembly of adjoints.

- **Proposition of a strategy for assembling an adjoint with ODYSSEE.**

- **Technical support to partners :**

Dassault, Alenia, HCSA, ...

- **Demonstration on a example.**

1. MAKING AVAILABLE AN A.D. TOOL

ODYSSEE is a software that produces, from a FORTRAN program, a FORTRAN program that computes the derivetive of the first one.

ODYSSEE is available on `ftp://ftp-sop.inria.fr/tropics/`.

1. USING AN A.D. TOOL FOR ADJOINT ASSEMBLY

Given a subroutine

```
FLUX(in:XMESH(1:M), in:WFLO(1:N), out:PSIFLU(1:N))
```

computing the flow equation residual

$$X_M, W_N \mapsto \Psi(X, W)_N$$

1. USING AN A.D. TOOL FOR ADJOINT ASSEMBLY

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`FLUX(in:XMESH(1:M), in:WFLO(1:N), out:PSIFLU(1:N))`

computing the flow equation residual

$$X_M, W_N \mapsto \Psi(X,W)_N$$

the subroutine(s) computing the main part of adjoint residual

$$\Pi_N \mapsto (\frac{\partial \Psi}{\partial W}(X,W))^*_{N\times N} \cdot \Pi_N$$

can be obtained by A.D. using the so-called reverse mode:

```
diff -cl -h flux -vars wflo
```

Strategy for adjoint assembly

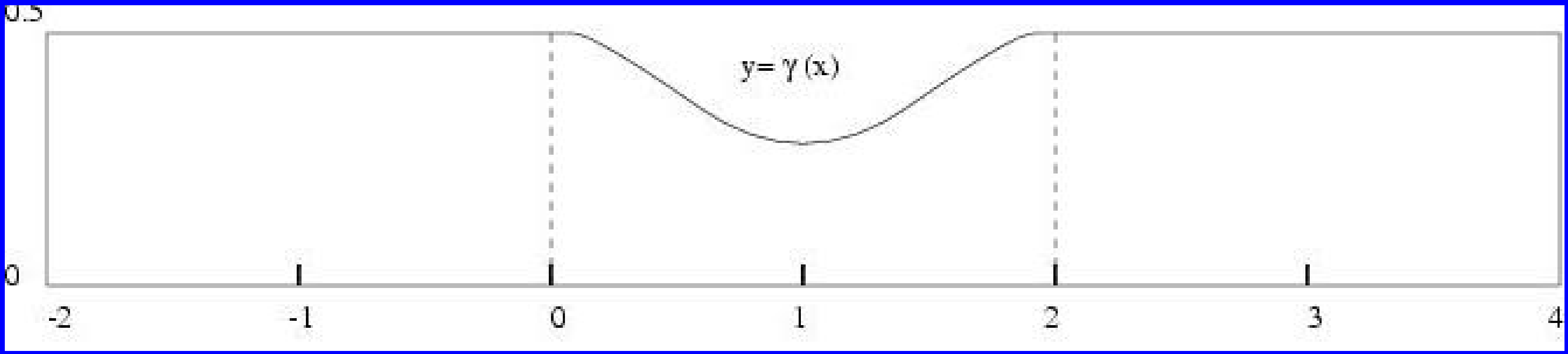
A strategy for adjoint assembly has been built and described in details in the last january meeting, and in the diffeernt version of tthe 3.18 report (first version were available in january).

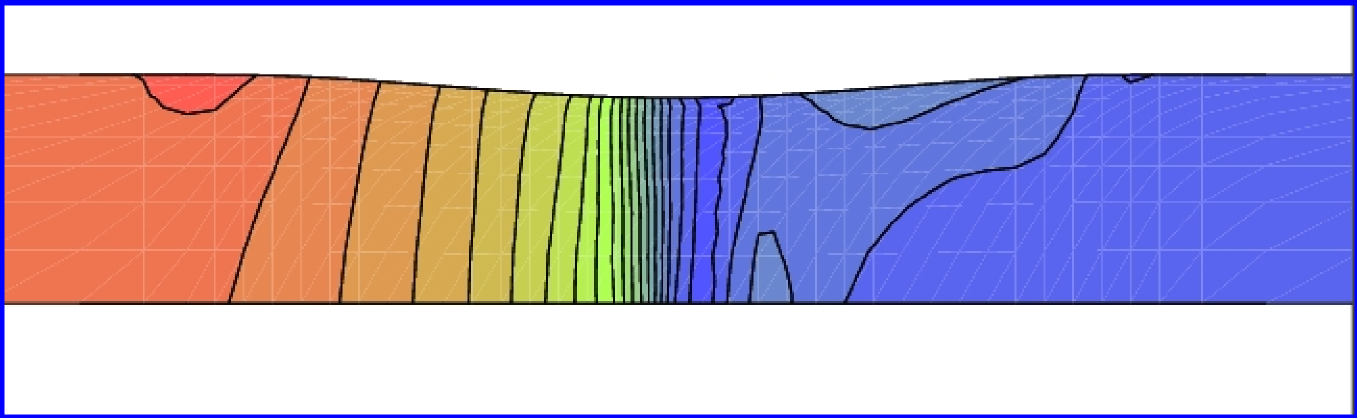
Technical support to partners:

Dassault (one travel to Paris in 2001), Alenia (Visit by V. Selmin ; the new version of ODYSSEE has been ported on IRIX), HCSA (visit by D. Petropoulou), visit by T. Evans (BAE) overseen in near future.
Partners come with their software and work with us, learning ODYSSEE, applying it to their software.

Demonstration test case:

- Euler flow in a nozzle.





Work achieved today by INRIA in 3.1

- The method is specified, described in details and applied in D3.18

- Its application to a in-house CFD software for the Euler model, first-order accurate and second-order accurate.

- Results are validated with respect to divided differences.

- Consolidated Memory measures

- Consolidated CPU measures

- "Second-order" adjoint resolution by a fixed point algorithm with first-order preconditioning ("Defect Correction"). Comparaison of different options.

- Complete gradient assembly and validation.

Future work

- The prototype obtained will be used for the Task.3.4 investigations and developments validation.

- Extension to Navier-Stokes.

- Feedback from partners experiments contribute to the specification of the new version of ODYSSEE under development (not funded by AEROSHAPE).

TASK 3.4 : OPTIMISATION ALGORITHMS

PURPOSE OF THE TASK

Partners SYNAPS, HCSA, and INRIA concentrate on the necessary evolution of optimization algorithms methodology and practise for the new industrial optimization problems.

Innovations are needed by the many unconvex problems that are now addressed.

The use of adjoint-based sensitivities is also a motivation for re-visiting the gradient-based optimization loop.

TASK 3.4 : OPTIMISATION ALGORITHMS

PARTNERS WORK IN TASK 3.4

- HCSA: HCSA has concentrated its contribution on the adjoint asssembly by applying ODYSSEE. Report D3.18 delivered.

- SYNAPS: prototype development and series of experiments for the research of global minima (1) with fuzzy logics and (2) with neuronal networks. Report D3.18 delivered.

- INRIA: contribution to advanced SQP-based gradient-like optimization loop. Preliminary phase. Report D3.18 delivered.

TASK 3.4 : INRIA CONTRIBUTION

INRIA contribution relies on expertise concerning Convex Optimization. "INRIA will work on the application of Convex Optimization algorithme to the specific case of Optimal Design with adjoint state calculation, with and without constraints (other than the state equation)".

Unconstrained case:

The state equation is considered as a constraint.

(i) In deliverable D3-18, INRIA proposes a panorama of recent SQP methods and explains how they apply to Optimum Design.

(ii) A particular SQP technique, the trust region method is reformulated in order to propose a robust one-shot SQP-like algorithm (preliminary work in validation phase).

Constrained case:

Investigation of methods taking into account the important cost of each extra adjoint state (for each constraint). Application of Interior Point approaches.

(iii) A SQP barrier function algorithm is proposed in deliverable D3-18 for the treatment of multiple state constraints without solving several adjoint systemes at each iteration.

Trust region for one-shot SQP (1): restoration phases

For k=0,...
If $\|g_k - A_k\Pi_k\|_\infty < \varepsilon$ **et** $\|\Psi_k\|_\infty < \varepsilon$ **then stop.**

State restoration phase.

For Min$\frac{1}{2}\|\Psi(x)\|^2$. Consider Min$\frac{1}{2}\|\frac{\partial\Psi}{\partial W}v + \Psi(x_k)\|^2$.

Adjoint restoration phase.

For Min$\frac{1}{2}\|R\|^2 = \frac{1}{2}\|\left(\frac{\partial\Psi}{\partial W}\right)^T\Pi - \frac{\partial J}{\partial W}\|^2$ with respect to Π.Consider Min$\frac{1}{2}\|\left(\frac{\partial\Psi}{\partial W}\right)^T p + R_k\|^2$.

Trust region for one-shot SQP (2): minimisation phase.

Compute $\tilde{W}_k$ with an l-BFGS

approximation.

Compute Cauchy step $u_k^c = -\beta^c \tilde{g} = -\beta^c \left(- \left(\frac{\partial \Psi}{\partial \gamma} \right)^T \Pi_k + \frac{\partial J}{\partial \gamma} \right)$.

Compute pseudo Newton step u_k^n.

Compute horizontal step u_k.

Let $d_k = v_k + Z_k^- u_k$.

Trust region for one-shot SQP (3): validation phase

Updating the trust region size. Han merit function:

$$\Phi(x,\Pi) = J(x) + \tfrac{\mu}{2}\left(\|\Psi(x)\| + \| \left(\frac{\partial \Psi}{\partial W}\right)^T (x)\Pi - \frac{\partial J}{\partial W}\| \right).$$

Compute actual reduction $a - red = \Phi(x_k,\Pi_k) - \Phi(x_k + d_k,\Pi_k + p_k)$.

Compute predicted reduction $p - red = m_k(0,0) - m_k(d_k,p_k)$.

Enlarge or reduce the trust region.

End of validation phase.

End of loop: next k.

"One-adjoint" SQP for multiple state constraints

$$\begin{aligned} \text{min} \quad & \phi(z) \\ \text{subject to} \quad & c_E(z) = 0 \\ & c_I(z) \le 0. \end{aligned}$$

By introducing *slack variables* we obtain a problem in the variables z and σ,

$$\begin{aligned} \text{min} \quad & \phi(z) \\ \text{subject to} \quad & c_E(z) = 0 \\ & c_I(z) + \sigma = 0 \\ & \sigma \ge 0 \end{aligned}$$

One-adjoint SQP for multiple state constraints (end)

A *barrier function* approach:

$$\begin{aligned} \text{min} \qquad & \phi(z) - \mu \sum_{i=1}^{m_1} ln\sigma^{(i)} \\ \text{subject to} \qquad & c_E(z) = 0 \\ & c_I(z) + \sigma = 0 \end{aligned}$$

μ is a penalty parameter; $\sigma > 0$.

$$\begin{pmatrix} \nabla^2_{xx}L & 0 & A_E & A_I \\ 0 & \mu S^{-2} & 0 & I \\ A_E^T & 0 & 0 & 0 \\ A_I^T & I & 0 & 0 \end{pmatrix} \begin{pmatrix} d_x \\ d_\sigma \\ d_{\lambda_E} \\ d_{\lambda_I} \end{pmatrix} = \begin{pmatrix} \nabla\phi + A_E\lambda_E + A_I\lambda_I \\ -\mu S^{-1}e + \lambda_I \\ c_E(z) \\ c_I(z) + \sigma \end{pmatrix}$$

TASK 3.4 : INRIA CONTRIBUTION : NEXT STEPS

Next steps will show how the proposed algorithms:

- Reduced-Hessian SQP with trust region,

- One-shot reduced-Hessian SQP with trust region,

- A SQP barrier function for multiple state constraints,

apply to the model problem built by INRIA in Task 3.1.