Development of discrete adjoint incompressible flow solvers using Automatic Differentiation

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Why bother with Ajoins?

Navier Stokes equations, fixed-point iteration to steady state:

\[ R(U(\alpha), \alpha) = 0 \]

Linearisation with respect to a design (control) variable \( \alpha \)

\[ \frac{\partial R}{\partial U} \frac{\partial U}{\partial \alpha} = - \frac{\partial R}{\partial \alpha}, \]

\[ Au = f. \]

Sensitivity of an objective function \( L \) with respect to \( \alpha \)

\[ \frac{dL}{d\alpha} = \frac{\partial L}{\partial \alpha} + \frac{\partial L}{\partial U} \frac{\partial U}{\partial \alpha} = \frac{\partial L}{\partial \alpha} + g^T u = \frac{\partial L}{\partial \alpha} + g^T A^{-1} f \]

\( \frac{\partial L}{\partial \alpha} \) is directly computable, \( g^T u \) requires an expensive solve for the perturbation flow field \( u \) for each \( \alpha_i \).
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\begin{align*}
\frac{\partial R}{\partial U} \frac{\partial U}{\partial \alpha} &= -\frac{\partial R}{\partial \alpha}, \\
A u &= f.
\end{align*}
\]

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The Adjoint Equations

Regroup the terms in the sensitivity computation:

\[
\frac{dL}{d\alpha} = \frac{\partial L}{\partial \alpha} + \frac{\partial L}{\partial \alpha} g^T A^{-1} f = \frac{\partial L}{\partial \alpha} + (A^{-T} g)^T f = \frac{\partial L}{\partial \alpha} + v^T f
\]

leads to the definition of the adjoint equation:

\[
A^Tv = g
\]

\[
\left(\frac{\partial R}{\partial U}\right)^T \frac{\partial L}{\partial R} = \left(\frac{\partial L}{\partial U}\right)^T .
\]

From this follows the Adjoint Equivalence

\[
g^T u = (A^Tv)^T u = v^T Au = v^T f
\]

Using \( v^T f \), needs a single solve of \( A^Tv = g \) and the evaluation of \( f_i \) for each \( \alpha_i \).
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Using \(v^T f\), needs a single solve of \(A^T v = g\) and the evaluation of \(f_i\) for each \(\alpha_i\).
Advantages of adjoint sensitivities

- Each design step requires a solve for \( \mathbf{R}(\mathbf{U}) = 0 \).
- Gradient-based optimisation requires a gradient for each design variable \( \alpha_i \).
- Using \( g^T u \), each \( \alpha_i \) needs a solve of \( A u = f \).
- Using \( v^T f \), needs a single solve of \( A^T v = g \) and the evaluation of \( f_i \) for each \( \alpha_i \).
- Roughly speaking, solving \( \mathbf{R}(\mathbf{U}) = 0, A u = f \) and \( A^T v = g \) incur a similar cost.
- Computing \( f \) is of the order of a single explicit sweep, simplified boundary formulations exist.
- Using the adjoint, the cost of gradient calculations for large design problems is essentially constant.
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- Computing $\mathbf{f}$ is of the order of a single explicit sweep, simplified boundary formulations exist.
- **Using the adjoint, the cost of gradient calculations for large design problems is essentially constant.**
Physical meaning of the adjoint solution: lifting aerofoil

NACA 0012, $Ma=0.4$, $\alpha = 2^\circ$
Sensitivity w.r.t. lift

mass flux

y-momentum
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Development of incompressible adjoint solvers

AD on industrial CFD codes

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Summary
Simple example of AD

Compute $\frac{\partial y}{\partial x_1}$ for

$$
\begin{bmatrix}
  y_1 \\
  y_2
\end{bmatrix} =
\begin{bmatrix}
  \pi \cos(3x_1 + 2x_2 + x_3) \cdot \pi \sin(3x_1 + 2x_2 + x_3) \\
  \pi \cdot \sin(3x_1 + 2x_2 + x_3)x_1
\end{bmatrix}
$$

$$
\begin{align*}
u &= 3x(1) + 2x(2) + x(3) \\
pi &= 3.14 \\
v &= \pi \cdot \cos(u) \\
w &= \pi \cdot \sin(u) \\
sum &= v + u \\
y(1) &= v \cdot w \\
y(2) &= w \cdot x(1)
\end{align*}
$$

$$
\begin{align*}
gx(1) &= 1 \\
gx(2) &= gx(3) = 0 \\
gu &= 3gx(1) + 2gx(2) + gx(3) \\
gv &= -gu \cdot \pi \cdot \sin(u) \\
gw &= gu \cdot \pi \cdot \cos(u) \\
gy(1) &= gv \cdot w + v \cdot gw \\
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The initial values in the chain rule need to be seeded, either set at the beginning of the computation, or computed in a preceding function call.
Simple example of AD

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y(1) = v \ast w \quad gy(1) = gv*w + v*gw
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“Transposing” a statement in reverse-mode

Primal statement: \( y(1) = v*w \)

**forward-mode**

\[
\begin{bmatrix}
gv \\
gw \\
gy_1
\end{bmatrix}_7 =
\begin{bmatrix}
1 & 1 \\
0 & 1 \\
w & v & 0
\end{bmatrix}
\begin{bmatrix}
gv \\
gw \\
gy_1
\end{bmatrix}_6
\]

\[
\dot{z}_{n+1} = E_n \dot{z}_n
\]

**reverse-mode**

\[
\begin{bmatrix}
vb \\
wv \\
yb_1
\end{bmatrix}_6 =
\begin{bmatrix}
1 & 0 & w \\
0 & 1 & v \\
0 & 0 & 0
\end{bmatrix}
\begin{bmatrix}
vb \\
wv \\
yb_1
\end{bmatrix}_7
\]

\[
\bar{z}_n E_n = \bar{z}_{n-1}
\]

\[
(\bar{z}_n E_n)^T = E_n \bar{z}_n^T = \bar{z}_{n-1}^T
\]
“Transposing” a statement in reverse-mode

Primal statement: \( y(1) = v \cdot w \)

forward-mode

\( g_y(1) = g_v \cdot w + v \cdot g_w \)

\[
\begin{bmatrix}
g_v \\
g_w \\
g_y_1
\end{bmatrix}_7 = \begin{bmatrix} 1 & 1 \\ 0 & 1 \\ w & v & 0 \\
g_v & g_w & g_y_1
\end{bmatrix}_6
\]

reverse-mode

\( v_b = v_b + w \cdot y_b(1) \)
\( w_b = w_b + v \cdot y_b(1) \)

\[
\begin{bmatrix}
v_b \\
w_b \\
y_b_1
\end{bmatrix}_6 = \begin{bmatrix} 1 & 0 & w \\ 0 & 1 & v \\ 0 & 0 & 0 \\
v_b & w_b & y_b_1
\end{bmatrix}_7
\]

\( \dot{z}_{n+1} = E_n \dot{z}_n \)

\[
\begin{align*}
\bar{z}_n E_n &= \bar{z}_{n-1} \\
(\bar{z}_n E_n)^T &= E_n \bar{z}_n^T = \bar{z}_{n-1}^T
\end{align*}
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\[
\ddot{z}_{n+1} = E_n \ddot{z}_n
\]

\[
\ddot{z}_n E_n = \ddot{z}_{n-1}
\]

\[
(\ddot{z}_n E_n)^T = E_n^{T} \ddot{z}_n^{T} = \ddot{z}_{n-1}^{T}
\]
“Transposing” a statement in reverse-mode

Primal statement: \( y(1) = v \cdot w \)

forward-mode

\[
gy(1) = gv \cdot w + v \cdot gw
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\begin{bmatrix}
gv \\
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1 & 1 \\
0 & 1 \\
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\begin{bmatrix}
gv \\
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\]

\[\dot{z}_{n+1} = E_n \dot{z}_n\]

reverse-mode

\[
v_b = v_b + w \cdot y_b(1)
\]

\[
w_b = w_b + v \cdot y_b(1)
\]

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w_b \\
y_b_1
\end{bmatrix}_7
\]

\[
\ddot{z}_n E_n = \ddot{z}_{n-1}
\]

\[
(\ddot{z}_n E_n)^T = E_n^T \ddot{z}_n^T = \ddot{z}_{n-1}^T
\]
“Transposing” a statement in reverse-mode

Primal statement: \( y(1) = v \cdot w \)

forward-mode

\[
\begin{bmatrix}
gv \\
gw \\
gy_1
\end{bmatrix}_7 = \begin{bmatrix} 1 & 1 \\ 0 & 1 \\ w & v & 0 \end{bmatrix} \begin{bmatrix}
gv \\
gw \\
gy_1
\end{bmatrix}_6
\]

\[
\dot{z}_{n+1} = E_n \dot{z}_n
\]

reverse-mode

\[
\begin{bmatrix}
v_b \\
w_b \\
y_b_1
\end{bmatrix}_6 = \begin{bmatrix} 1 & 0 & w \\ 0 & 1 & v \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix}
v_b \\
w_b \\
y_b_1
\end{bmatrix}_7
\]

\[
\bar{z}_{n} E_n = \bar{z}_{n-1}
\]

\[
(\bar{z}_n E_n)^T = E_n^T \bar{z}_n^T = \bar{z}_{n-1}^T
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"Transposing" a statement in reverse-mode

Primal statement: \( y(1) = v \cdot w \)

**forward-mode**

\[
\begin{bmatrix}
gv \\
gw \\
gy_1
\end{bmatrix}_7 = \begin{bmatrix}
1 & 1 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 \\
w & v & 0 & 0 & 0 & 0
\end{bmatrix}_6 \begin{bmatrix}
gv \\
gw \\
gy_1
\end{bmatrix}_6
\]

\[
\dot{z}_{n+1} = E_n \dot{z}_n
\]

**reverse-mode**

\[
\begin{bmatrix}
vb \\
wv \\
yb_1
\end{bmatrix}_7 = \begin{bmatrix}
1 & 0 & w & 0 & 0 & 0 \\
0 & 1 & v & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}_6 \begin{bmatrix}
vb \\
wv \\
yb_1
\end{bmatrix}_6
\]

\[
\bar{z}_n E_n = \bar{z}_{n-1}
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(\bar{z}_n E_n)^T = E_n^T \bar{z}_n^T = \bar{z}_{n-1}^T
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“Transposing” a statement in reverse-mode

Primal statement: \( y(1) = v \cdot w \)

**forward-mode**
\[
\begin{align*}
gy(1) &= gv \cdot w + v \cdot gw \\
\begin{bmatrix}
   gv \\
gw \\
gy_1
\end{bmatrix}_7 &= 
\begin{bmatrix}
   1 & 0 & 1 \\
   0 & w & v \\
w & v & 0
\end{bmatrix}_6
\begin{bmatrix}
   gv \\
gw \\
gy_1
\end{bmatrix}_6
\end{align*}
\]

**reverse-mode**
\[
\begin{align*}
v_b &= v_b + w \cdot y_b(1) \\
w_b &= w_b + v \cdot y_b(1) \\
\begin{bmatrix}
v_b \\
w_b \\
y_b
\end{bmatrix}_7 &= 
\begin{bmatrix}
   1 & 0 & w \\
   0 & 1 & v \\
0 & 0 & 0
\end{bmatrix}_7
\begin{bmatrix}
v_b \\
w_b \\
y_b
\end{bmatrix}_7
\end{align*}
\]

\( \dot{z}_{n+1} = E_n \dot{z}_n \)

\[
\begin{align*}
\bar{z}_n E_n &= \bar{z}_{n-1} \\
(\bar{z}_n E_n)^T &= E_n^T \bar{z}_n^T = \bar{z}_n^{T-1}
\end{align*}
\]
Example of reverse-mode AD

\[ y = \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} \pi \cos(3x_1 + 2x_2 + x_3) \cdot \pi \sin(3x_1 + 2x_2 + x_3) \\ \pi \cdot \sin(3x_1 + 2x_2 + x_3)x_1 \end{bmatrix} \]

\[
gx(1) = 1 \\
gx(2) = gx(3) = 0 \\
gu = 3*gx(1)+2*gx(2)+gx(3) \\
u = 3*x(1)+2*x(2)+x(3) \\
pi = 3.14 \\
gv = -gu*\pi*\sin(u) \\
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gy(1) = gv*w + v*gw \\
y(1) = v \cdot w \\
gy(2) = gw*x(1) + gx(1)*w \\
y(2) = w*x(1) \\
yb(1) = 1., yb(0) = 0. \\
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\[ \mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} \pi \cos(3x_1 + 2x_2 + x_3) \cdot \pi \sin(3x_1 + 2x_2 + x_3) \\ \pi \cdot \sin(3x_1 + 2x_2 + x_3)x_1 \end{bmatrix} \]

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y(2) &= w*x(1)
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\end{align*}
Example of reverse-mode AD

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Example of reverse-mode AD

\[ y = \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} \pi \cos(3x_1 + 2x_2 + x_3) \cdot \pi \sin(3x_1 + 2x_2 + x_3) \\ \pi \cdot \sin(3x_1 + 2x_2 + x_3) x_1 \end{bmatrix} \]

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y_2
\end{bmatrix} = \begin{bmatrix}
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xb( :) &= 0. \\
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Example of reverse-mode AD

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gy(2) = gw*x(1) + gx(1)*w

y(2) = w*x(1)

yb(1) = 1., yb(0) = 0.

u = 3*x(1) + 2*x(2) + x(3)

pi = 3.14

v = pi*cos(u)

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xb(:) = 0.

wb = x(1)*yb(2)

xb(1) = xb(1) + w*yb(2)

vb = w*yb(1)

wb = wb + v*yb(1)

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\[ y_b(1) = 1., y_b(0) = 0. \]
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Implementation the reverse-mode AD

- For each cost-function we need to seed with $\bar{y_i} = 1$.
- We obtain all the derivatives of $y_i$ w.r.t. all $x$ in one invocation.
- The logic is followed in reverse, hence we need to store or recompute all the intermediate values needed to compute the derivatives.
Contents

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Summary
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- Fortran 90/95, using its more modern programming features.
- The algorithm computes laminar/turbulent flow through complex 2/3D geometries.
- Code design mimicks typical CFD code setup and algorithms, exploiting support by Automatic differentiation tools to the maximum.
- Via the makefile, either the primal, primal with tangent or with adjoint can be built automatically.
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Validation case: VW S-Bend

- Simplified vehicle climatisation duct.
- Uniform flow at inlet, shape modifications only in the bend.
- Objective: total pressure loss. Sensitivities are computed w.r.t. vertex coordinates.
- Turbulent viscosity is approximated using the Spalart-Allmaras model. For $y^+ > 11.225$ the standard wall function approximates the near-wall turbulent viscosity.
Duct flow case with turb. model, $Re_H = 60$

(a) Convergence of primal and adjoint

(b) Fluid speed
Duct flow case with turb. model, $Re_H = 60$

(c) Bottom view

(d) Top view
Duct flow case with turb. model, $Re_H = 600$

(e) Convergence of primal and adjoint

(f) Fluid speed
Duct flow case with turb. model, $Re_H = 600$

(g) Bottom view
(h) Top view
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AD on industrial CFD codes

- A number of industrial CFD packages are intending to have (Star-CCM+) or already have (Fluent 13, OpenFOAM 2.0) adjoint versions.
- So far, none of the current sensitivity implementations use automatic differentiation (AD) to generate the sensitivity algorithm.
- Here we apply AD to incompressible commercial flow solver, ESI’s ACE+.
  - Original / Full Source Code Size: 3000 files, 1.1M lines / 40MB of source code.
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- To aid the construction of the sensitivity algorithm, source code pre- and post-processing is performed either side of differentiation.

- Pre- and post-processing involve
  1. remove dead code in the original source code via C preprocessor pragmas
  2. reorganise modules, types and procedures in the generated source code in addition to optimising fixed-point iterators and introducing library functions where appropriate (such as the sparse linear solver).

- Source code processing is where the bulk of the work lies in order to successfully generate adjoint algorithms using AD, but the tools are very difficult to implement.
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AD on industrial CFD codes: flow-graph

Original source code

Pre-process source code (strip out non-algorithmic code)

Generate source code which computes the sensitivity algorithm

Post-process generated source code (purge, rename, optimize)

Build complete program

Sensitivity source code
Pre-processing

- This task identifies and extracts the relevant source code which needs to be differentiated from the entire program source code.
- For large programs (100,000+ lines) this becomes tedious and error-prone to perform manually.
- By making use of the call-graph generated by AD tool Tapenade, the tedium of tracing dependencies is removed.
- Knowledge is still required to know which dependent routines are non-essential so can be ignored.
Pre-processing: example of call tree to be pruned
Pre-processing: pruning algorithm

1. Identify the routine (and its file) to be differentiated
2. Augment file name(s) with an underscore (add file to active group)
3. Process the source code using `tapenade -html -process <files>` to generate the dependency graph and write it to an html file
4. Parse the dependency graph file extracting the names of modules and procedures and find the files which contain their implementations
5. Insert pragmas to strip out redundant source code sections then preprocess (cpp)
6. Insert pragmas to strip out redundant source code sections then preprocess (cpp)
7. Empty file list?
   - No
     - Start
   - Yes
     - Stop

Automated task
Manual task
Pre-processing: primal source equipped with pragmas

```fortran
module matrix_utils_m
contains

#ifndef STRIP_AD
  !! passive
  subroutine print_matrix(mat)
    ...
  end subroutine
#endif

!! active non-differentiable
function coo_to_csr(i,j,ja,ia) result(kij)
#ifndef STRIP_AD
  ...
#elif
  kij = 0 ! retain a trivial dependency
#endif
end function

!! active differentiable
subroutine matrix_setup(a_ij,phi,ja,ia,res)
  ...
#ifndef STRIP
  if(use_advanced_feature) call adv_feature()
#endif
end subroutine
end module
```
Differentiation problems

- We use the source-transformation tool Tapenade that can handle F90.
- There has been significant progress with Tapenade, but the user cannot expect the AD tool to run as robustly as the compiler.
- In the current version 3.6 we need to work around the following issues:
  1. Using `save` as an attribute of a module scope causes incomplete differentiation,
  2. The case `default` must be the last case,
  3. The differentiation of statements involving pointers is under development.
  4. Differentiation of modules creates a complete copy, which causes problems with `use:only` statements.
Post-processing of AD’ed code

1. inherit original modules into their generated derivative modules,
2. purge generated code of all definitions of primal equivalent routines and data (except private data),
3. ensure that all references to primal routines and data refer to original code and not to equivalent generated code,
4. identify and remove generated derivative type definitions and replace associated declarations using that type with the original type,
5. for the adjoint of linear system solvers, use the hand coded alternative (this must be properly converged at each invocation),
6. in adjoint code, identify fixed-point iterations, reconfigure it to record once and restore once active primal variables,
7. in adjoint code, identify active quantities which can be assumed to behave like constants and remove their associated adjoint computation.
### Original code

```fortran
module pdes
use base
character (3) , private :: fmt = "csr"
type :: pde
  real , dimension (:) , &
  allocatable :: phi , rhs
  real :: reduc
  integer :: max_iter
end type

type(pde) :: pres , vel
contains
subroutine navier_stokes()
  ! A.x = b: not necessary since a fixed point is assumed to have been reached
  ! A adjoint of A.x = b: manual implementation
  call solve_c.b()
call setup_c.b() call gradient_c.b()
call solve_c.b()
call setup_c.b() call gradient_c.b()
end subroutine
end module
```

### Generated code (Tapenade)

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call setup_c.b() call gradient_c.b()
end subroutine
end module
```

### Modified (in-place) generated code

```fortran
module pdes
use pdes ! import original
use base
character (3) , private :: fmt = "csr"
type(pde) :: pres , vel
contains
subroutine navier_stokes()
  ! A.x = b: not necessary since a fixed point is assumed to have been reached
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  call solve_c.b()
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call solve_c.b()
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end subroutine
end module
```
ACE+ differentiation

- Using tapenade Version 3.6 (September 2011).
- Memory: 500-900MB RAM, 2.0-2.5GB VM.
- CPU Time: 10 minutes on Intel i5 Equivalent.
tangent-linear ACE+, laminar channel

Rectangular channel, with aspect ratio of 20, and with 10m/s inlet on the left, fixed-pressure outlet on the right, and no-slip walls on the top and bottom. Sensitivity of velocity integral wrt perturbation in uniform inlet velocity.

u-velocities, domain scaled by 1/10 in the x-direction
tangent-linear ACE+, laminar channel

pressure field
tangent-linear ACE+, laminar channel results

pressure sensitivity to inlet velocity perturbation
tangent-linear ACE+, laminar channel results

Residual Plot

- X-Direction Velocity
- Y-Direction Velocity
- Static Pressure
- Gradient

Residuals vs. Iterations

Pressure field
tangent-linear ACE+, S-Bend testcase

S-Bend testcase, tangent-linear discrete solution, pressure
tangent-linear $ACE^+$, S-Bend testcase

Pressure sensitivity to inlet variation
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Acknowledgements

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