Automatic Differentiation in Developing LES Models

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Collaborators

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- Jeff Borggaard, Traian Iliescu, and Grant Boquet
  - ICAM/Virginia Tech

Automatic Differentiation

Abstractly, computer programs can be regarded as

$$a \equiv (a_1, a_2, \ldots, a_m)$$

$$\downarrow$$

$$z \equiv (z_1, z_2, \ldots, z_p), \quad p >> m + n$$

$$\downarrow$$

$$u \equiv (u_1, u_2, \ldots, u_n)$$

where

$$z_k = f^k_{\text{elem}}(z_i), \qquad i < k,$$

(-, pow(·), sin(·), . . .),

Automatic Differentiation

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$$u \equiv (u_1, u_2, \ldots, u_n)$$

or

$$z_k = f^k_{\text{elem}}(z_i, z_j), \qquad i < k, \quad j < k,$$

(+, /, . . .).

Automatic Differentiation

- Forward (Direct) Mode:

$$\frac{dz_k}{da} = \frac{\partial f^k_{\text{elem}}}{\partial z_i}\frac{dz_i}{da} + \frac{\partial f^k_{\text{elem}}}{\partial z_j}\frac{dz_j}{da}.$$

(*computes* all of the $\frac{dz_k}{da}$ terms)

Automatic Differentiation

- Forward (Direct) Mode:

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(*computes* all of the $\frac{dz_k}{da}$ terms)

- Reverse (Adjoint) Mode:

$$\frac{du}{dz_i} = \frac{\partial f^k_{\text{elem}}}{\partial z_i}\frac{du}{dz_k} \quad \text{and} \quad \frac{du}{dz_j} = \frac{\partial f^k_{\text{elem}}}{\partial z_j}\frac{du}{dz_k}.$$

(requires that $\frac{\partial f^k_{\text{elem}}}{\partial z_j}$ be *stored*)

Automatic Differentiation

Example: $u = a_1 2 a_2 + \sin(a_2 a_3)$

$$
\begin{array}{lll l}
z_1 & \leftarrow & a_1 & \text{(input)} \\
z_2 & \leftarrow & a_2 & \text{(input)} \\
z_3 & \leftarrow & a_3 & \text{(input)} \\
z_4 & \leftarrow & \mathrm{pow}(z_1, 2) & (a_1 2) \\
z_5 & \leftarrow & z_4 * z_2 & (a_1 2 a_2) \\
z_6 & \leftarrow & z_2 * z_3 & (a_2 a_3) \\
z_7 & \leftarrow & \sin(z_6) & (\sin(a_2 a_3)) \\
z_8 & \leftarrow & z_5 + z_7 & (u)
\end{array}
$$

AD: Forward Mode

Forward Mode: (Find $\frac{\partial u}{\partial a_1}$, i.e. $a = a_1$)

$$\frac{\partial z_1}{\partial a} \leftarrow \frac{\partial a_1}{\partial a} \qquad \text{(input = 1)}$$

$$\frac{\partial z_2}{\partial a} \leftarrow \frac{\partial a_2}{\partial a} \qquad \text{(input = 0)}$$

$$\frac{\partial z_3}{\partial a} \leftarrow \frac{\partial a_3}{\partial a} \qquad \text{(input = 0)}$$

$$\frac{\partial z_4}{\partial a} \leftarrow 2z_1 \frac{\partial z_1}{\partial a} \qquad (2z_1)$$

$$\frac{\partial z_5}{\partial a} \leftarrow \frac{\partial z_4}{\partial a} z_2 + z_4 \frac{\partial z_2}{\partial a} \qquad (2z_1 z_2)$$

$$\frac{\partial z_6}{\partial a} \leftarrow \frac{\partial z_2}{\partial a} z_3 + z_2 \frac{\partial z_3}{\partial a} \qquad (0)$$

$$\frac{\partial z_7}{\partial a} \leftarrow \cos(z_6) \frac{\partial z_6}{\partial a} \qquad (0)$$

$$\frac{\partial z_8}{\partial a} \leftarrow \frac{\partial z_5}{\partial a} + \frac{\partial z_7}{\partial a} \qquad (2z_1 z_2)$$

AD: Forward Mode

Forward Mode

- Implemented by *operator overloading*

  z_2 (and $\frac{\partial z_2}{\partial a}$)

  z_3 (and $\frac{\partial z_3}{\partial a}$)

  $z_2 * z_3$ (and $\frac{\partial z_2}{\partial a} z_3 + z_2 \frac{\partial z_3}{\partial a}$)

- **ADMAT**:**A**utomatic **D**ifferentiation for MATLAB
  - Coleman and Verma
- Or implemented by *source transformation*

AD: Reverse Mode

Reverse Mode: (Find $\frac{\partial u}{\partial a}$, a is an arbitrary input)

$$
\begin{array}{ccccc}
\frac{\partial z_8}{\partial a} & \leftarrow & \frac{\partial z_8}{\partial z_5}\frac{\partial z_5}{\partial a} + \frac{\partial z_8}{\partial z_7}\frac{\partial z_7}{\partial a} & = & \underline{1}\,\frac{\partial z_5}{\partial a} + \underline{1}\,\frac{\partial z_7}{\partial a} \\
\frac{\partial z_7}{\partial a} & \leftarrow & \frac{\partial z_7}{\partial z_6}\frac{\partial z_6}{\partial a} & = & \underline{\cos(z_6)}\,\frac{\partial z_6}{\partial a} \\
\frac{\partial z_6}{\partial a} & \leftarrow & \frac{\partial z_6}{\partial z_2}\frac{\partial z_2}{\partial a} + \frac{\partial z_6}{\partial z_3}\frac{\partial z_3}{\partial a} & = & \underline{z_3}\,\frac{\partial z_2}{\partial a} + \underline{z_2}\,\frac{\partial z_3}{\partial a} \\
\frac{\partial z_5}{\partial a} & \leftarrow & \frac{\partial z_5}{\partial z_4}\frac{\partial z_4}{\partial a} + \frac{\partial z_5}{\partial z_2}\frac{\partial z_2}{\partial a} & = & \underline{z_2}\,\frac{\partial z_4}{\partial a} + \underline{z_4}\,\frac{\partial z_2}{\partial a} \\
\frac{\partial z_4}{\partial a} & \leftarrow & \frac{\partial z_4}{\partial z_1}\frac{\partial z_1}{\partial a} & = & \underline{2z_1}\,\frac{\partial z_1}{\partial a}
\end{array}
$$

With the stored values of $\frac{\partial z_8}{\partial z_5}$, $\frac{\partial z_8}{\partial z_7}$, etc. on the forward sweep, we can determine $\frac{\partial u}{\partial a_1}$ by prescribing

$$
\frac{\partial z_1}{\partial a} = 1 \qquad \frac{\partial z_2}{\partial a} = 0 \qquad \frac{\partial z_3}{\partial a} = 0.
$$

AD: Reverse Mode

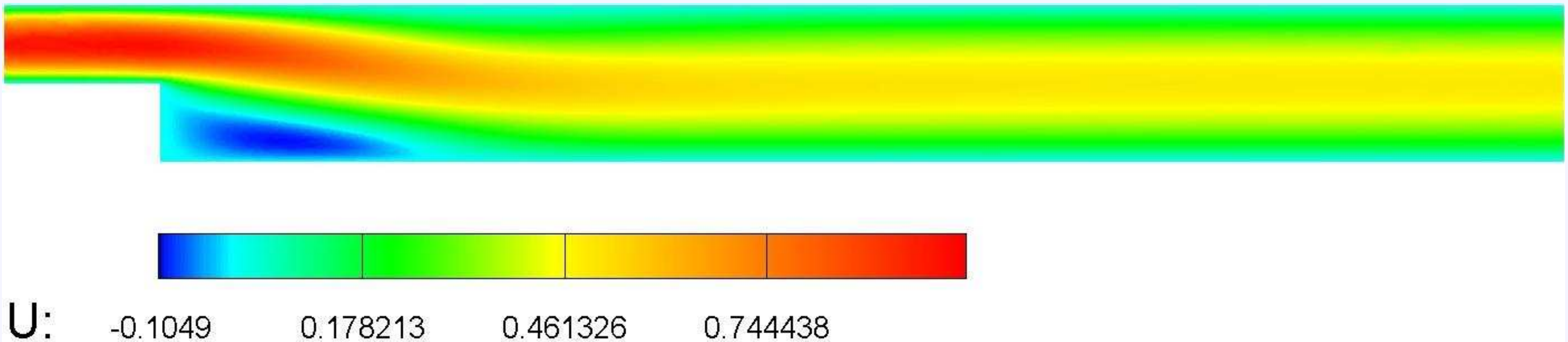
Reverse Mode

- Implemented by storing (underlined) variables on the “forward” solve.
- Preprocessing can be done to remove unneccessary storage.
- We can find $\frac{\partial u}{\partial a_1}$, $\frac{\partial u}{\partial a_2}$ and $\frac{\partial u}{\partial a_3}$ for the same work
- The *Cheap Gradient Theorem* states that we can find the gradient wrt an arbitrary number of inputs for $4\times$ function cost.
- These two modes can be combined.

Outline

- Problem Description
- Software
  - ViTLES
  - ADIC
  - PETSc
- Numerical Experiments
- Future Work

Problem Description



- Navier-Stokes Equation
- LES Models
- Sensitivities

Problem Description

Navier-Stokes equation

$$
\begin{aligned}
\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} - \nabla \cdot \tau(\mathbf{u}) + \nabla p &= \mathbf{f} \\
\nabla \cdot \mathbf{u} &= \mathbf{0}
\end{aligned}
$$

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Let $\bar{\mathbf{u}}(t) := [\mathbf{g}_\delta * \mathbf{u}](\mathbf{t})$.

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$$

Let $\bar{\mathbf{u}}(t) := [\mathbf{g}_\delta * \mathbf{u}](\mathbf{t})$. Then filtered N.S.

$$
\begin{aligned}
\frac{\partial \bar{\mathbf{u}}}{\partial t} + \nabla\cdot(\overline{\mathbf{u}\mathbf{u}}) - \nabla\cdot\tau(\bar{\mathbf{u}}) + \nabla \bar{p} &= \bar{\mathbf{f}} \\
\nabla\cdot\bar{\mathbf{u}} &= \mathbf{0}
\end{aligned}
$$

Problem Description

Navier-Stokes equation

$$\begin{aligned} \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} - \nabla \cdot \tau(\mathbf{u}) + \nabla p &= \mathbf{f} \\ \nabla \cdot \mathbf{u} &= \mathbf{0} \end{aligned}$$

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$$\begin{aligned} \frac{\partial \bar{\mathbf{u}}}{\partial t} + \nabla \cdot (\overline{\mathbf{u}\mathbf{u}}) - \nabla \cdot \tau(\bar{\mathbf{u}}) + \nabla \bar{p} &= \bar{\mathbf{f}} \\ \nabla \cdot \bar{\mathbf{u}} &= \mathbf{0} \end{aligned}$$

To close the system we need to model the $\nabla \cdot (\overline{\mathbf{u}\mathbf{u}})$ term since $\overline{\mathbf{u}\mathbf{u}} \neq \bar{\mathbf{u}}\bar{\mathbf{u}}$.

Problem Description

- **Some LES Models**
  - Smagorinsky Model
  - Deconvolution Model

Problem Description

Smagorinsky Model

Approximate $\nabla \cdot (\overline{\mathbf{uu}})$ term by

$$\nabla \cdot (\overline{\mathbf{uu}}) \approx \nabla \cdot (\bar{\mathbf{u}}\bar{\mathbf{u}}) - \nabla \cdot \left[(C_s\delta)^2 \|\mathbf{D}(\bar{u})\|\mathbf{D}(\bar{u})\right]$$

where $\mathbf{D}(\bar{u}) := \frac{1}{2}\left(\nabla u + \nabla u^T\right)$

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where $\mathbf{D}(\bar{u}) := \frac{1}{2} \left(\nabla u + \nabla u^T \right)$

Deconvolution Model

$$\nabla \cdot (\overline{\mathbf{uu}}) \approx \nabla \cdot (\bar{\mathbf{u}}\bar{\mathbf{u}}) + \nabla \cdot \tilde{\tau}$$

where $\tilde{\tau} = (\tilde{\tau}_{ij})$ with $\tilde{\tau}_{ij}$ solving

$$(I - \delta^2 \Delta) \tilde{\tau}_{ij} = 2\delta^2 \nabla \bar{u}_i \nabla \bar{u}_j$$

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Sensitivities

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Problem: Determine sensitivity of turbulent flow to closure model parameters.

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Parameter:

A filter radius δ

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Smagorinsky and Deconvolution Model Sensitivities

Parameter:

A filter radius δ

Determine:

Sensitivities $\frac{\partial \bar{\mathbf{u}}(x,t)}{\partial \delta}$ and $\frac{\partial \bar{\mathbf{p}}(x,t)}{\partial \delta}$

Software

ViTLES (Virginia Tech Large Eddy Simulation)

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ViTLES (Virginia Tech Large Eddy Simulation)

- FEM (Finite Element Method)
- PETSc(Portable, Extensible Toolkit for Scientific Computation)
- ADIC(Automatic Differentiation of ANSI C)
- The Virginia Tech system X is used for computations

Software

Applying AD

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Let δ be a closure model parameter.

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One time step of discretized N.S. (Crank-Nicholson)

$$\mathbf{F}(\mathbf{x}(\delta), \tilde{x}(\delta), \delta) + \mathbf{G}(\mathbf{y}(\delta), \tilde{y}(\delta), \delta) = 0$$

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One time step of discretized N.S. (Crank-Nicholson)

$$\mathbf{F}(\mathbf{x}(\delta), \tilde{x}(\delta), \delta) + \mathbf{G}(\mathbf{y}(\delta), \tilde{y}(\delta), \delta) = 0$$

where

$\mathbf{x}$ and $\mathbf{y}$ are state vectors at $n+1$ and n time steps

$\tilde{x}$ and $\tilde{y}$ are vectors of D.B.C. at $n+1$ and n time steps

Applying AD

We look for a sensitivity $\frac{\partial \mathbf{x}}{\partial \delta}$.

$$\mathbf{F}_{\mathbf{x}}(\mathbf{x},\tilde{x},\delta)\frac{\partial \mathbf{x}}{\partial \delta} = -\left[\mathbf{F}_{\tilde{x}}(\mathbf{x},\tilde{x},\delta)\frac{\partial \tilde{x}}{\partial \delta} + \mathbf{F}_{\delta}(\mathbf{x},\tilde{x},\delta) + \mathbf{G}_{\mathbf{y}}(\mathbf{y},\tilde{y},\delta)\frac{\partial \mathbf{y}}{\partial \delta} + \mathbf{G}_{\tilde{y}}(\mathbf{y},\tilde{y},\delta)\frac{\partial \tilde{y}}{\partial \delta} + \mathbf{G}_{\delta}(\mathbf{y},\tilde{y},\delta)\right]$$

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$$\left. \mathbf{G}_{\mathbf{y}}(\mathbf{y}, \tilde{y}, \delta)\frac{\partial \mathbf{y}}{\partial \delta} + \mathbf{G}_{\tilde{y}}(\mathbf{y}, \tilde{y}, \delta)\frac{\partial \tilde{y}}{\partial \delta} + \mathbf{G}_{\delta}(\mathbf{y}, \tilde{y}, \delta)\right]$$

Set dependent variables and gradients and evaluate RHS by finding

$$\frac{\partial}{\partial \delta}\mathbf{F}(\mathbf{x}, \tilde{x}(\delta), \delta) = \mathbf{F}_{\tilde{x}}(\mathbf{x}, \tilde{x}, \delta)\frac{\partial \tilde{x}}{\partial \delta} + \mathbf{F}_{\delta}(\mathbf{x}, \tilde{x}, \delta)$$

$$\frac{\partial}{\partial \delta}\mathbf{G}(\mathbf{y}(\delta), \tilde{y}(\delta), \delta) = \mathbf{G}_{\mathbf{y}}(\mathbf{y}, \tilde{y}, \delta)\frac{\partial \mathbf{y}}{\partial \delta} + \mathbf{G}_{\tilde{y}}(\mathbf{y}, \tilde{y}, \delta)\frac{\partial \tilde{y}}{\partial \delta} + \mathbf{G}_{\delta}(\mathbf{y}, \tilde{y}, \delta)$$

Numerical Experiments

2D Smagorinsky Model

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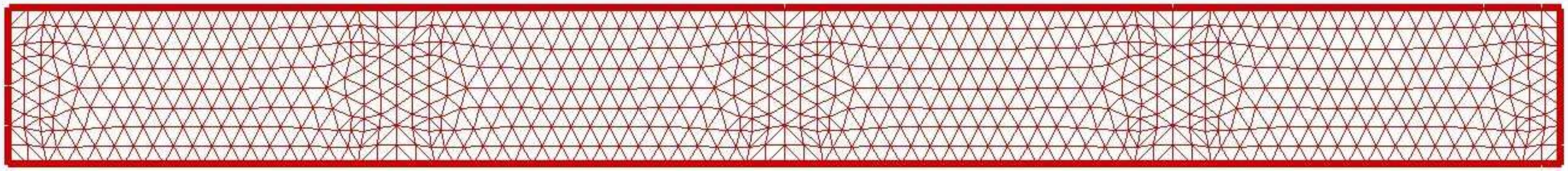
2D Smagorinsky Model

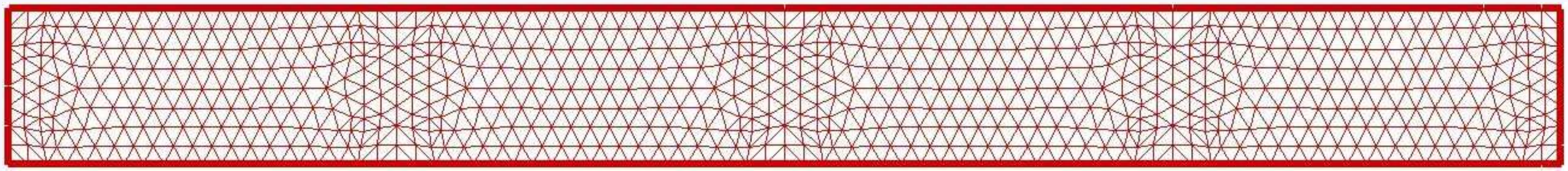
- Channel



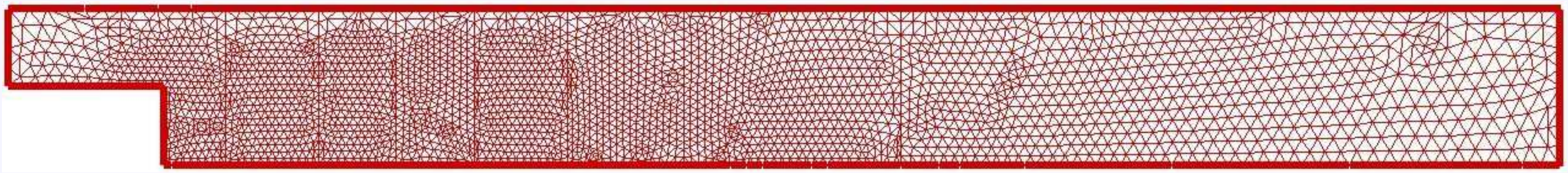
Numerical Experiments

2D Smagorinsky Model

- Channel



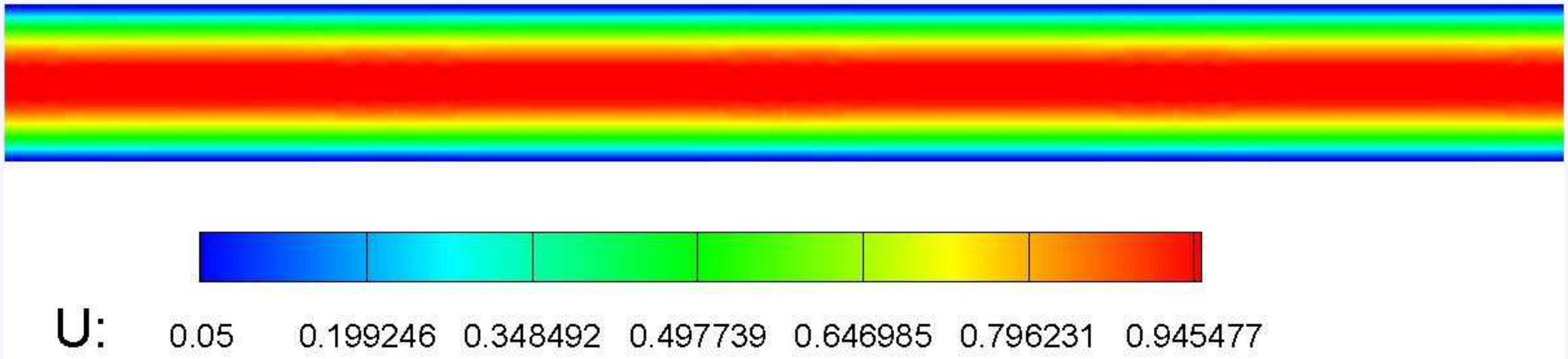
- Backward Facing Step



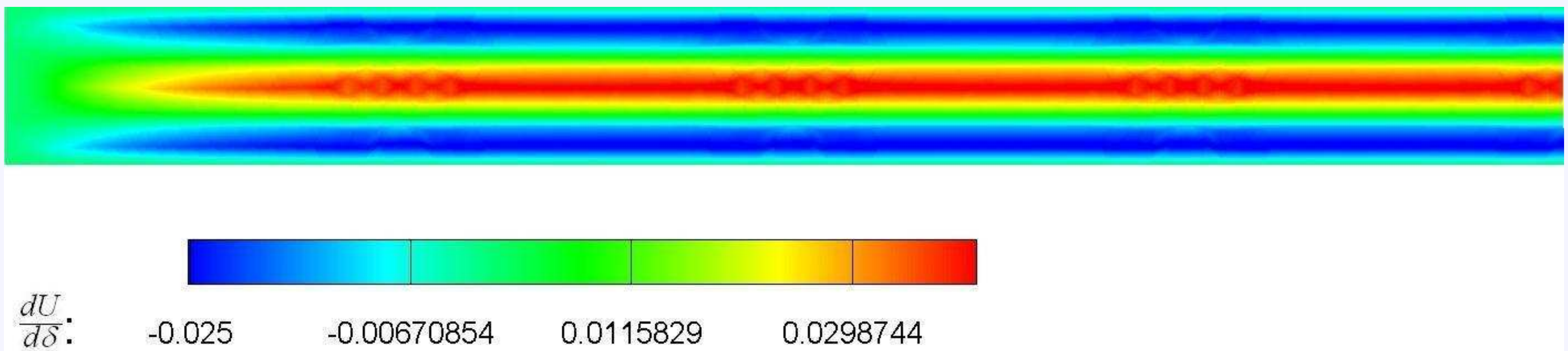
Numerical Experiments

Channel

1st velocity component



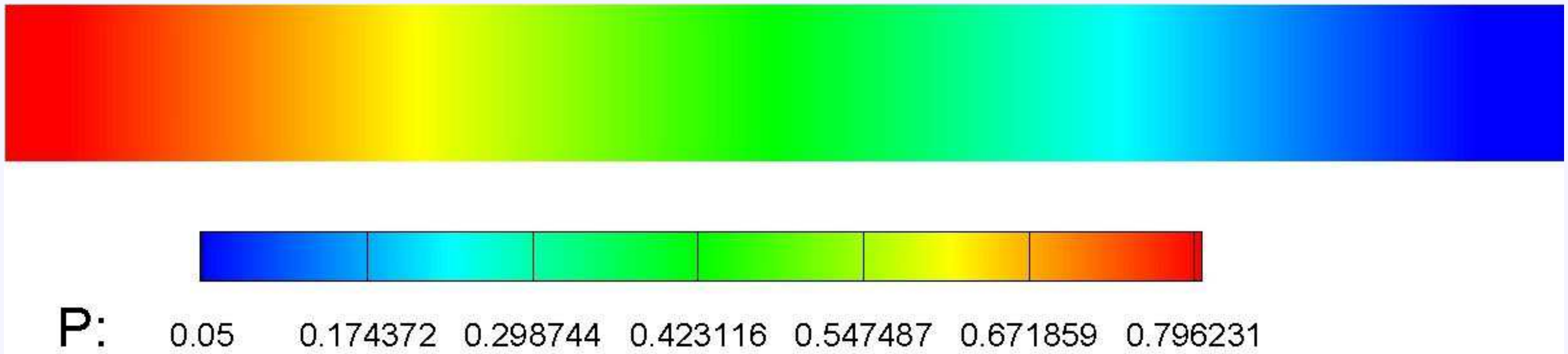
1st velocity component sensitivity



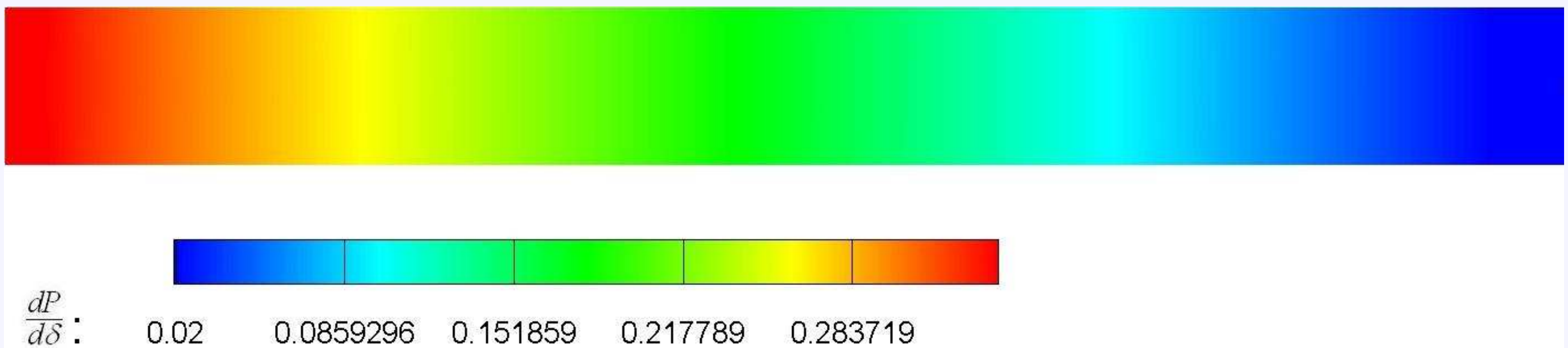
Numerical Experiments

Channel

pressure

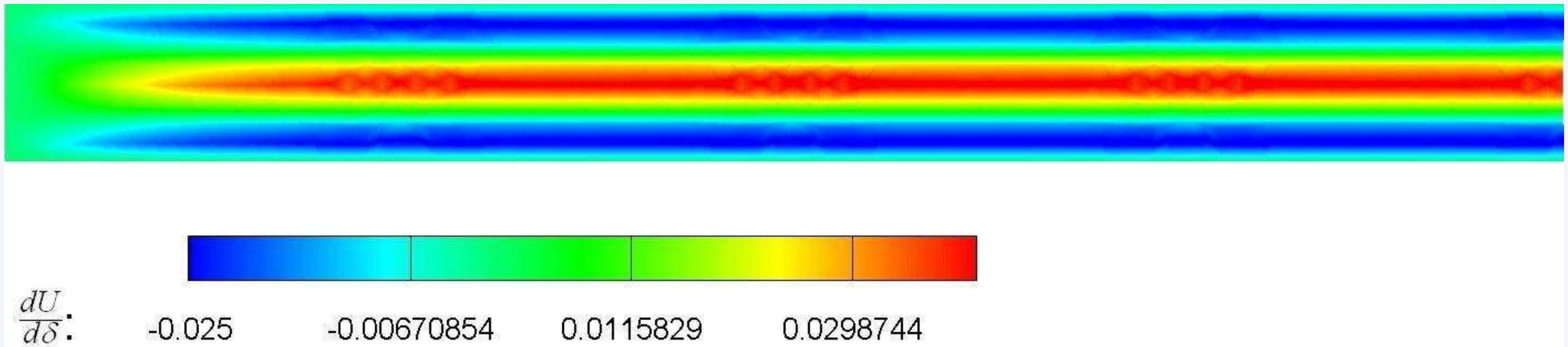


pressure sensitivity

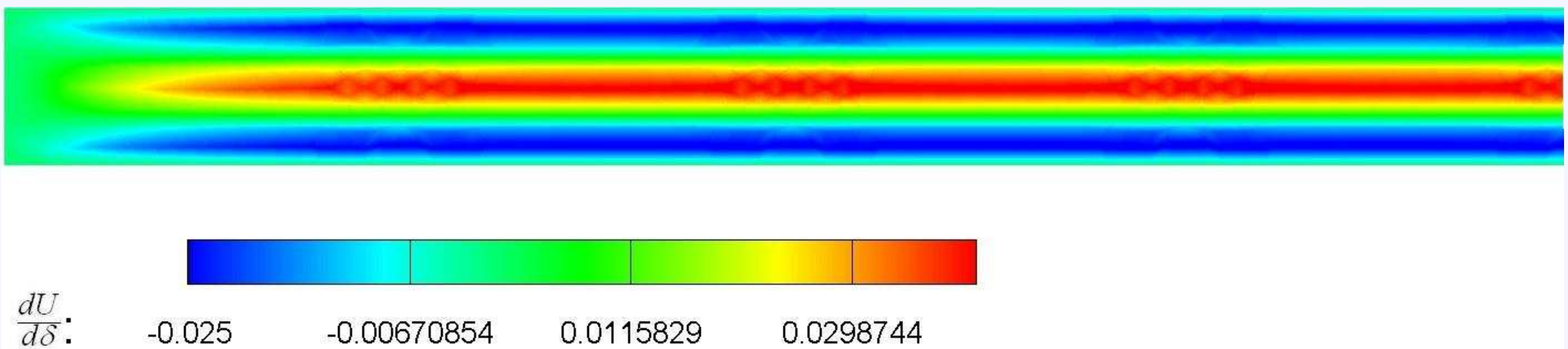


Channel: Finite Difference Test (Velocity U Sensitivity)

automatic differentiation



finite difference



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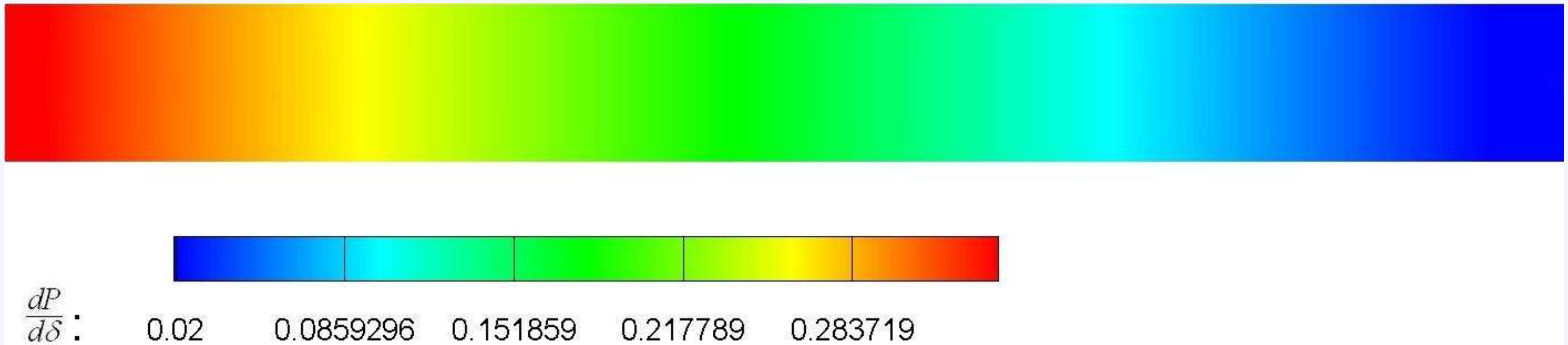

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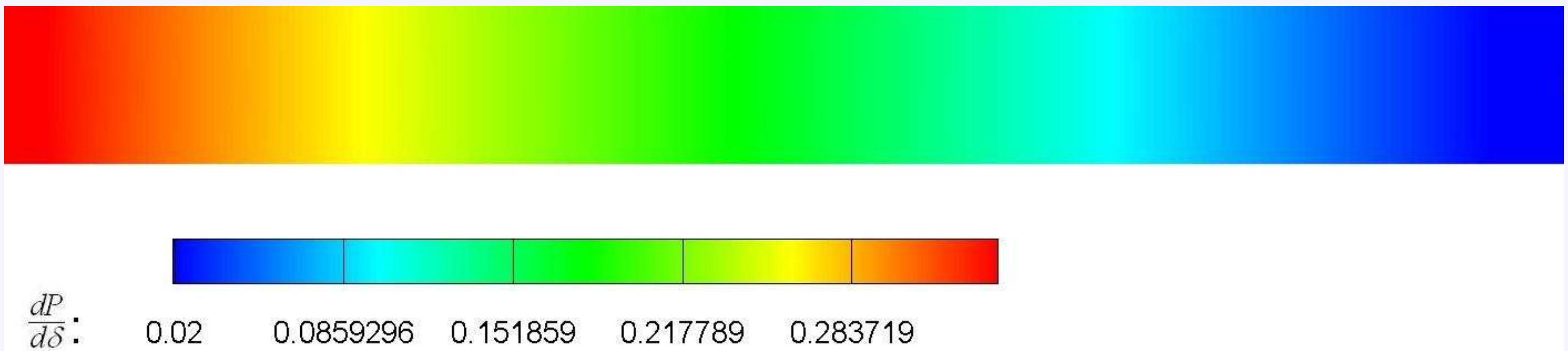
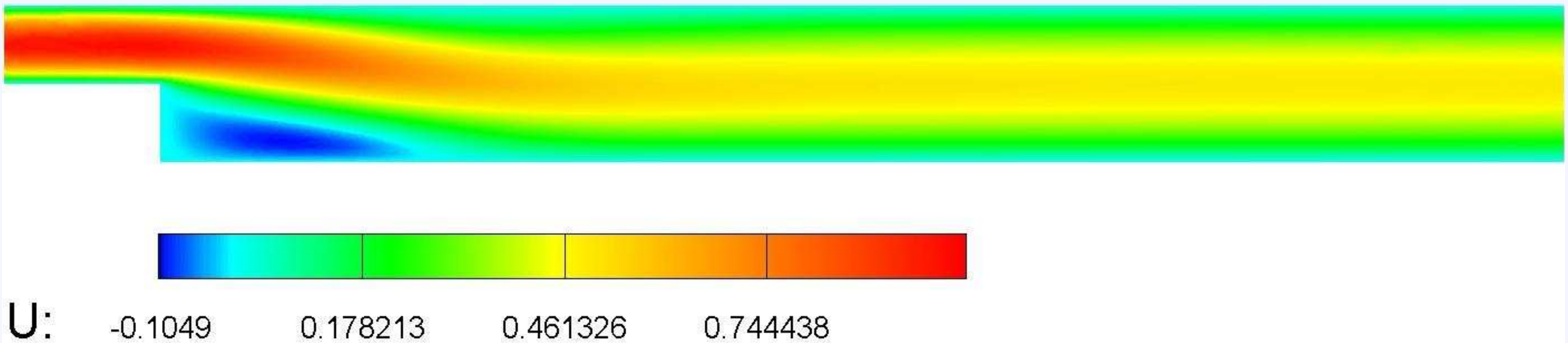


Numerical Experiments

Backward Facing Step

1st velocity component



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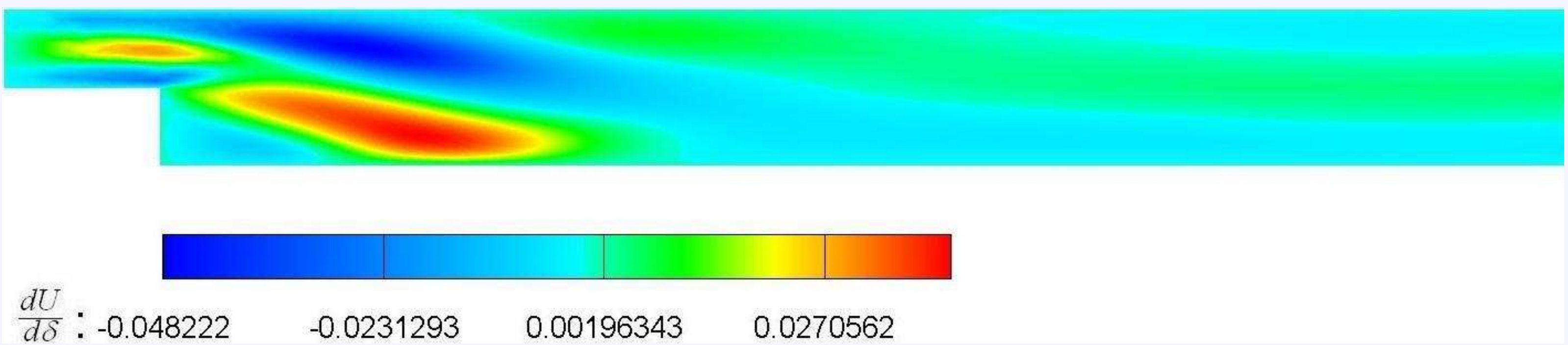
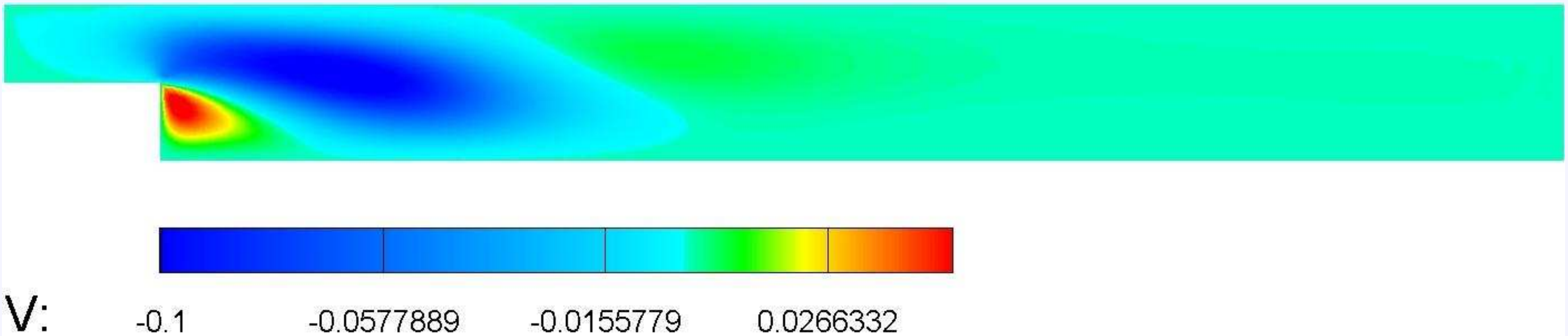


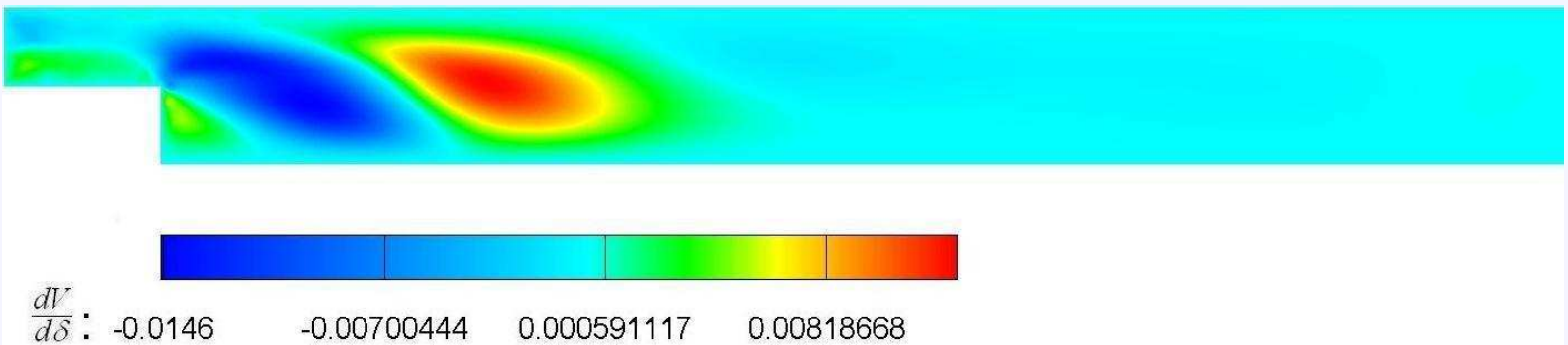
Numerical Experiments

Backward Facing Step

2nd velocity component



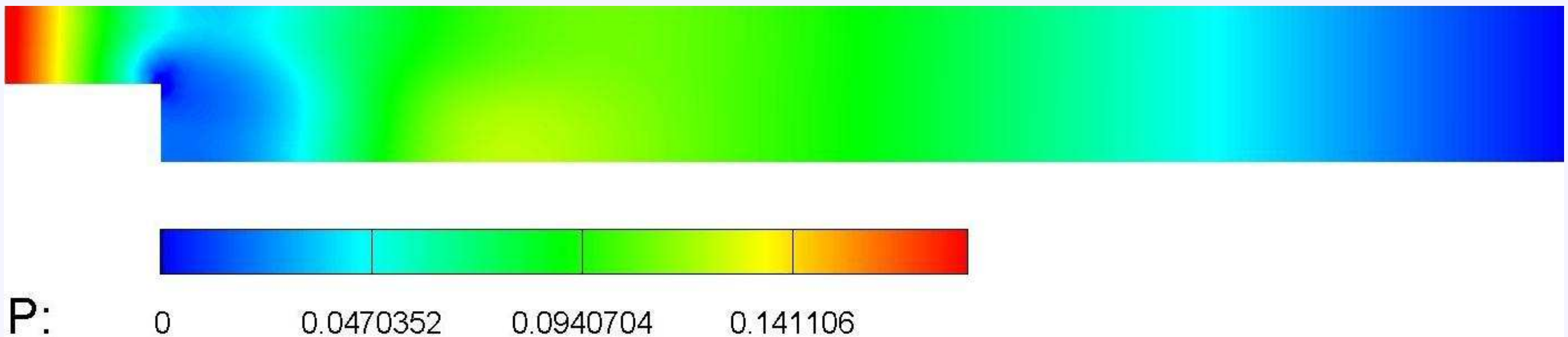
2nd velocity component sensitivity



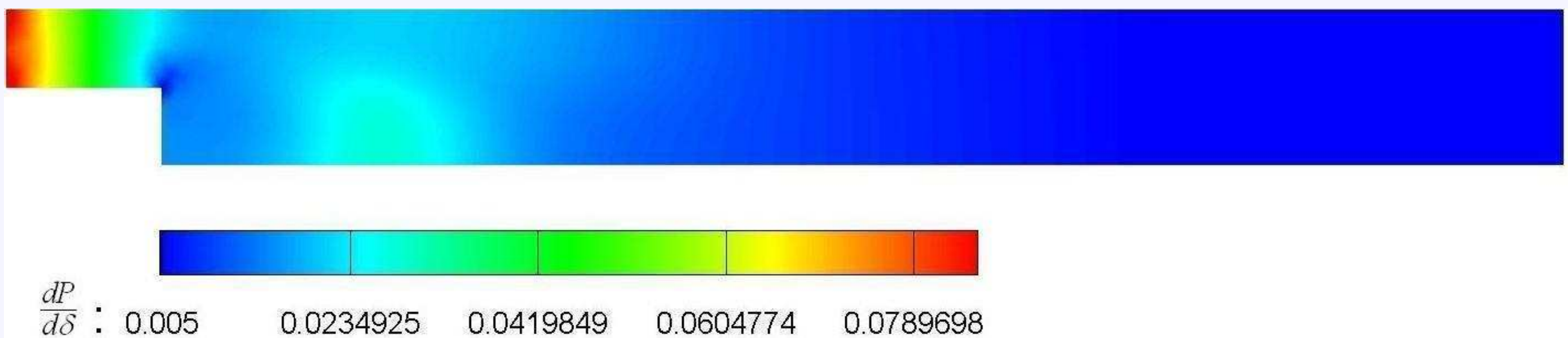
Numerical Experiments

Backward Facing Step

pressure

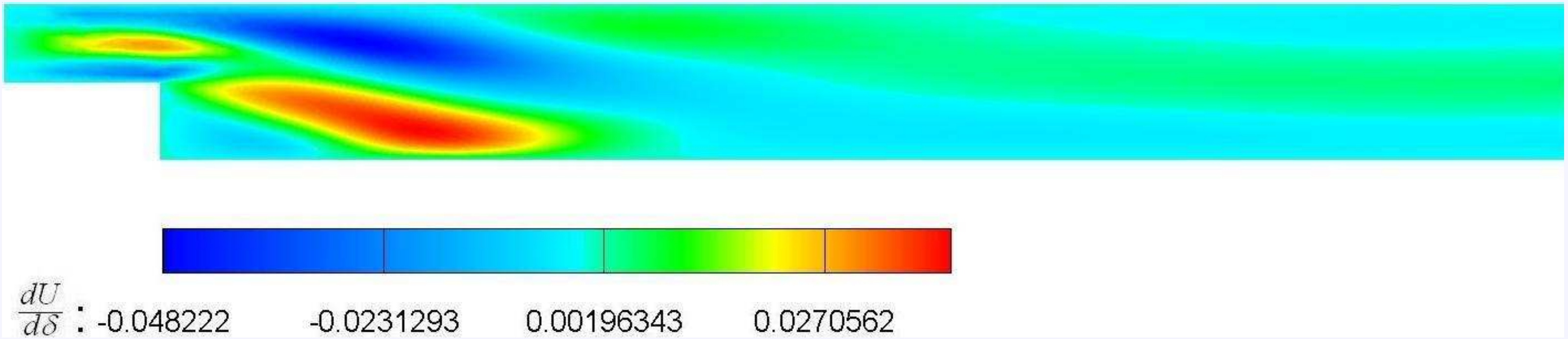


pressure sensitivity

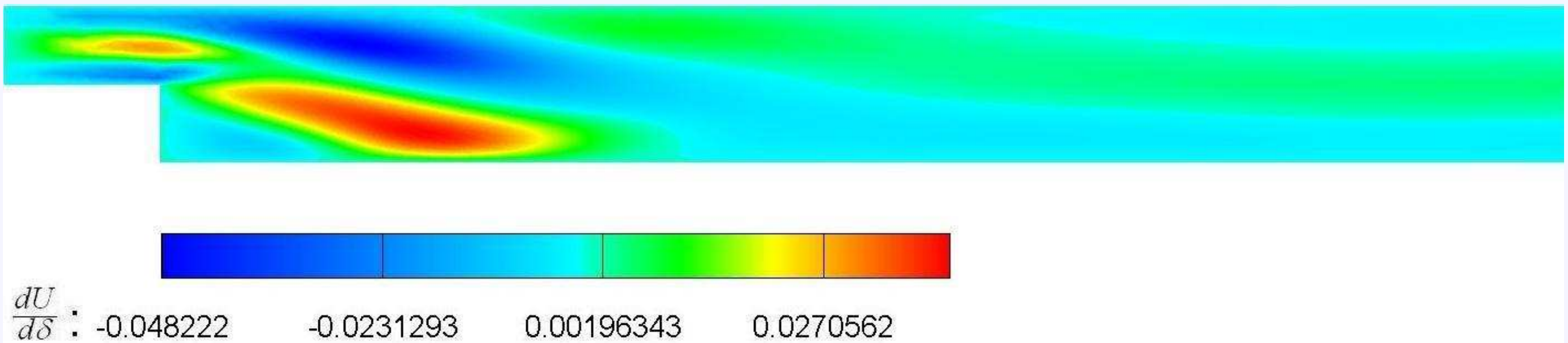


BFS: Finite Difference Test (Velocity U Sensitivity)

automatic differentiation



finite difference



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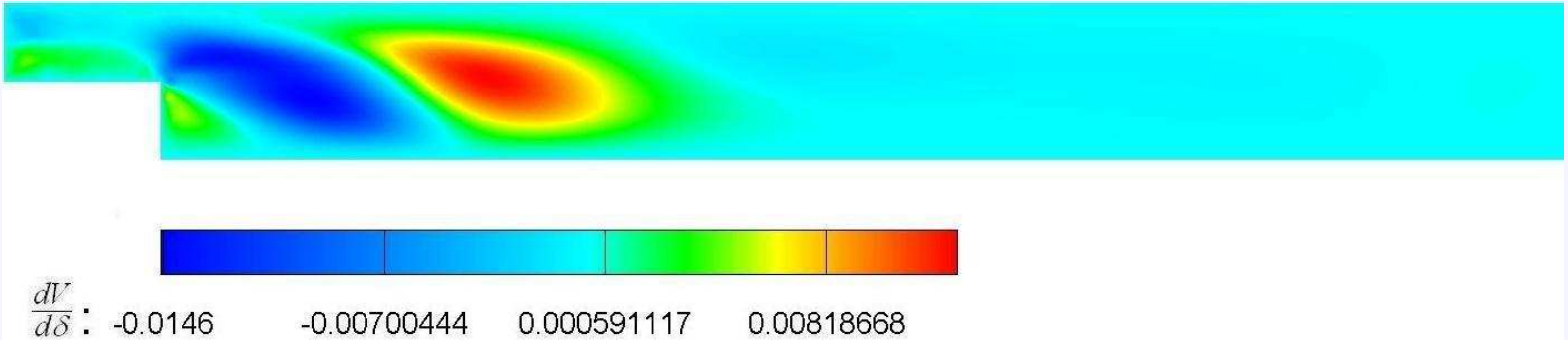
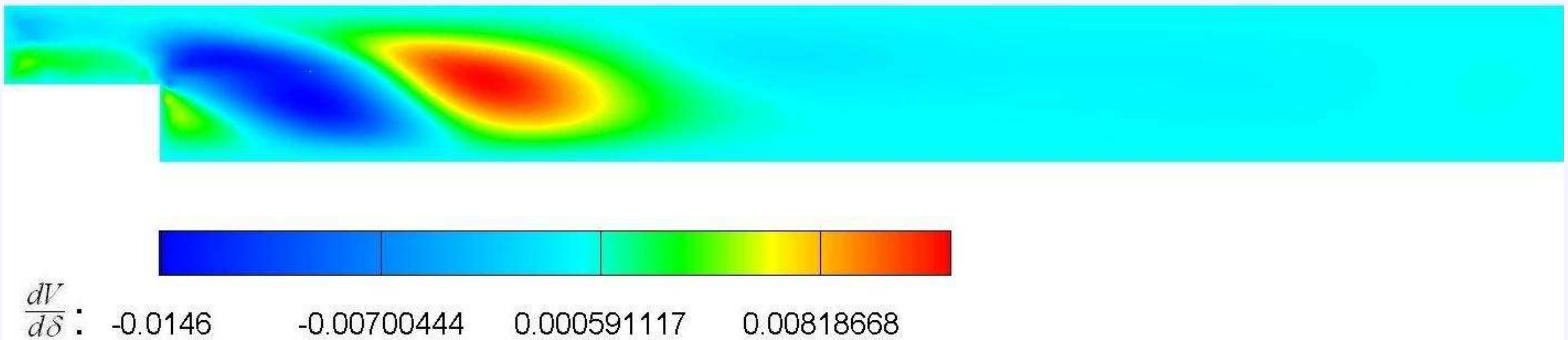


finite difference



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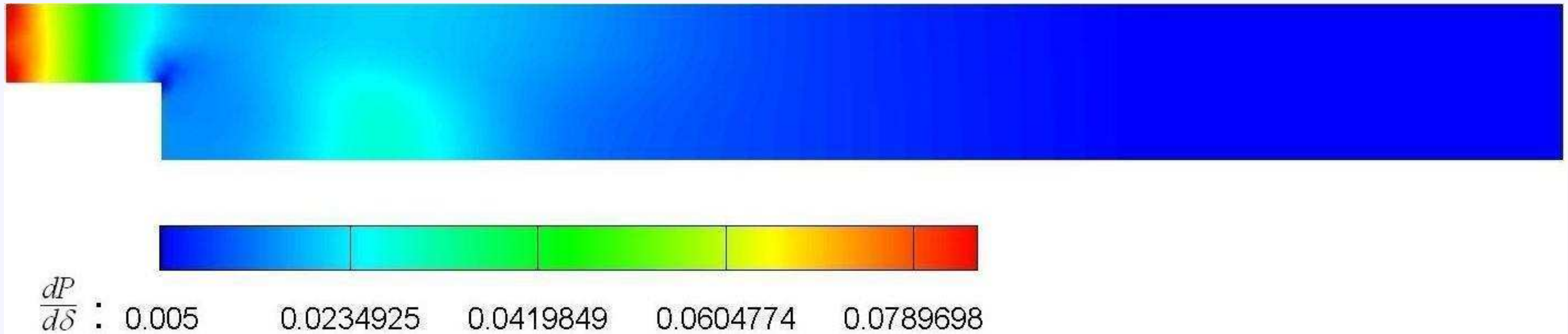

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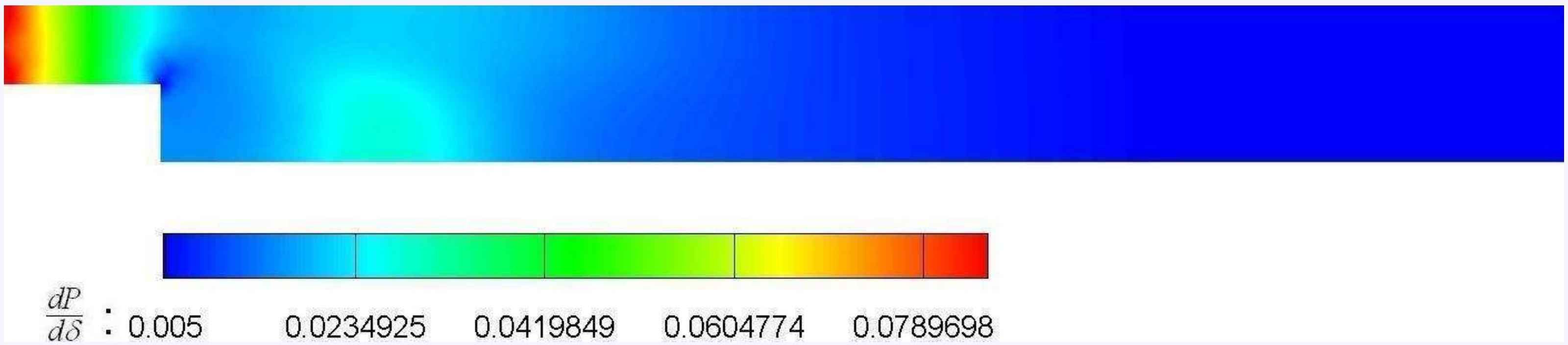
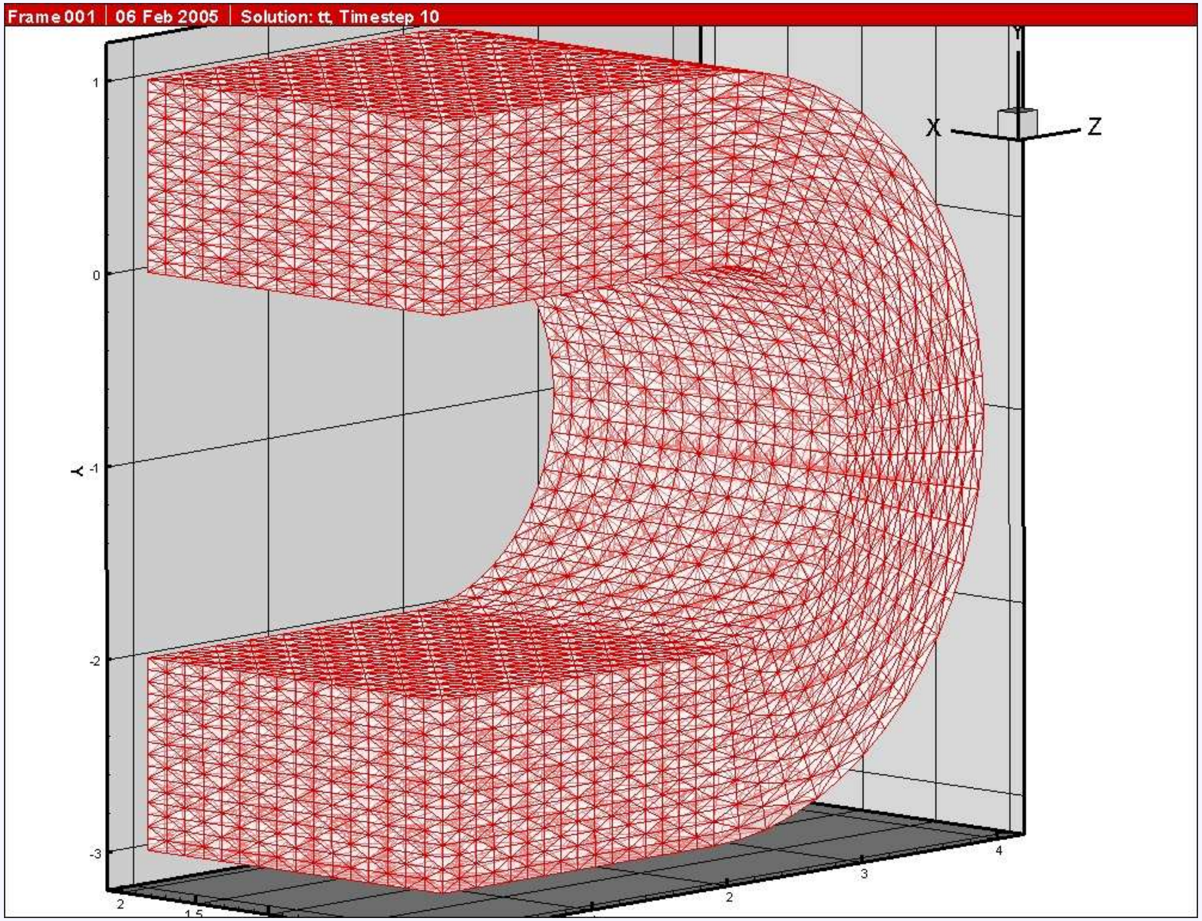


Future Work

3D Navier-Stokes and Sensitivity Computations

mesh



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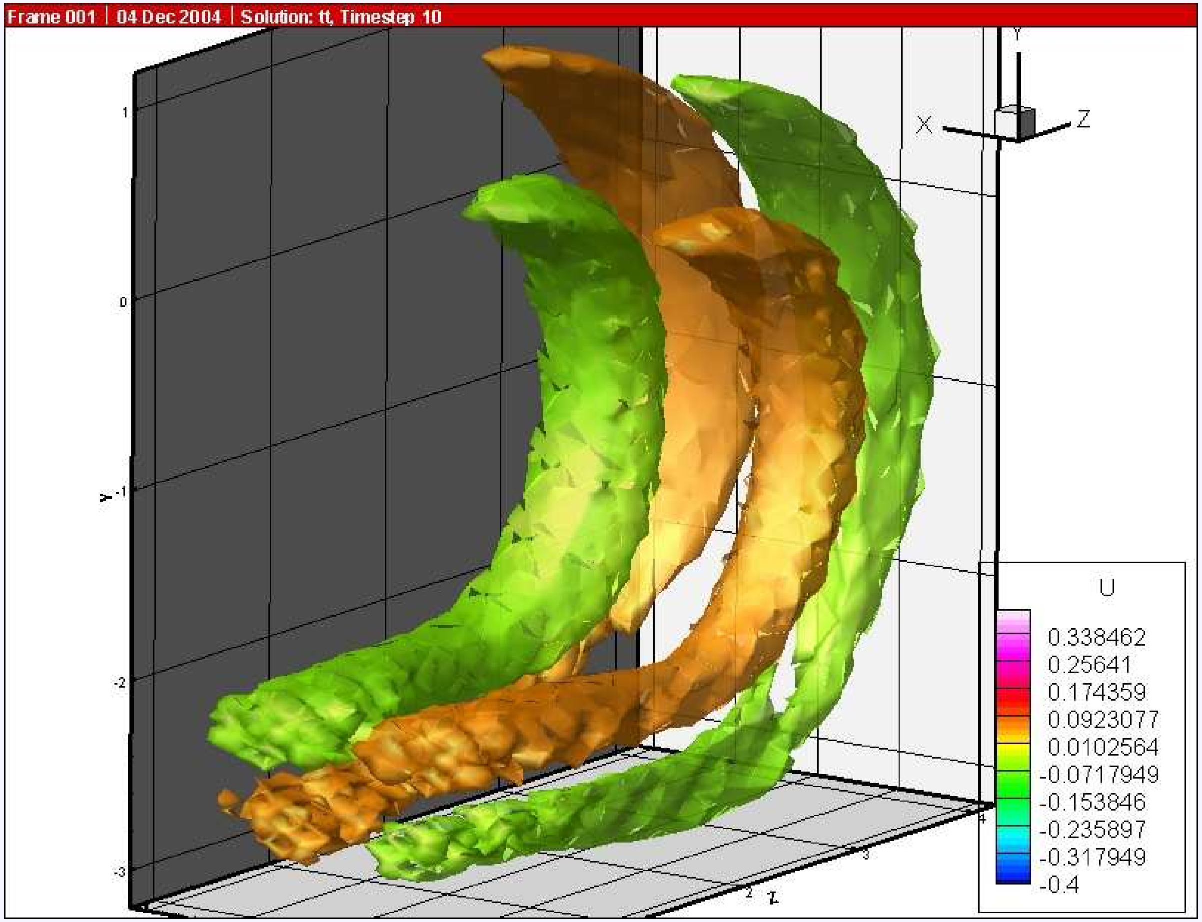
3D Navier-Stokes and Sensitivity Computations

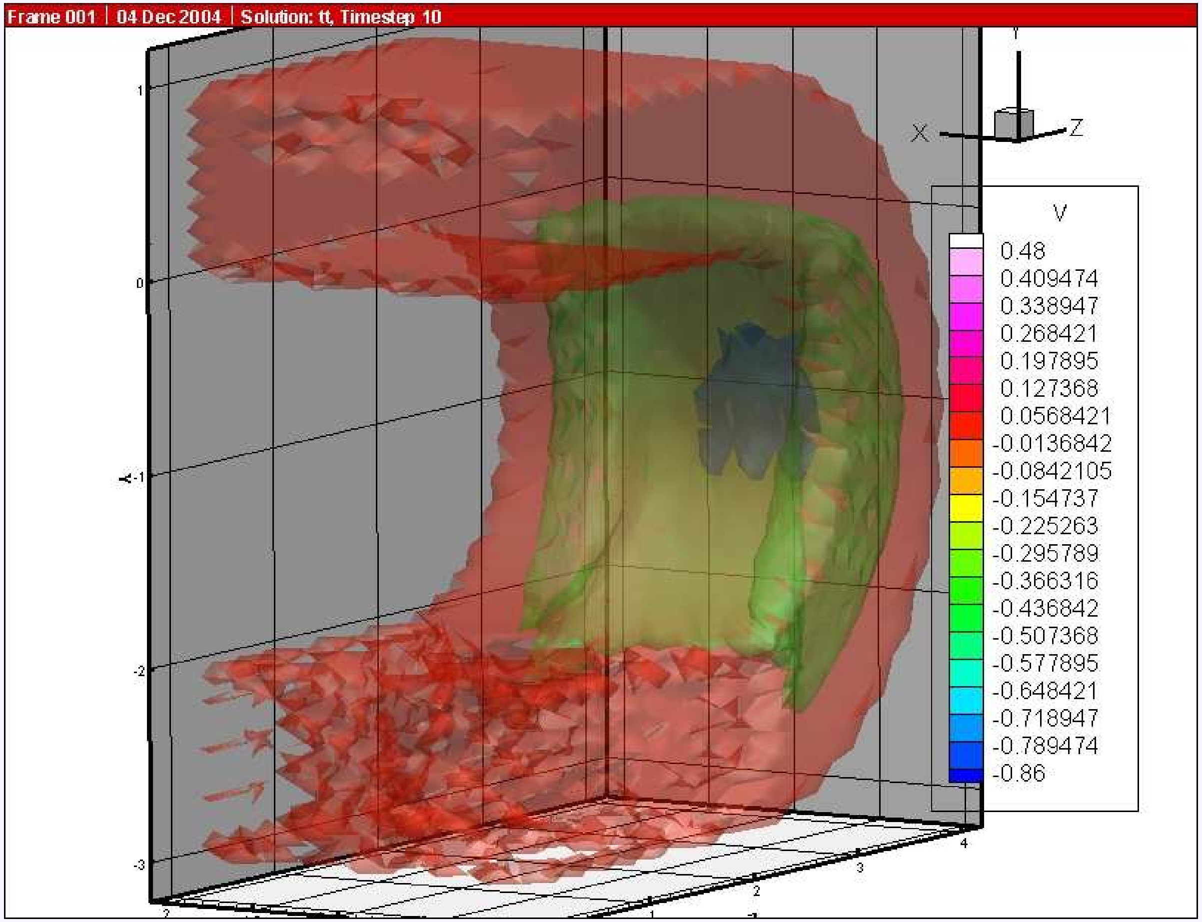
1st velocity component iso-surfaces



Future Work

3D Navier-Stokes and Sensitivity Computations

2nd velocity component iso-surfaces



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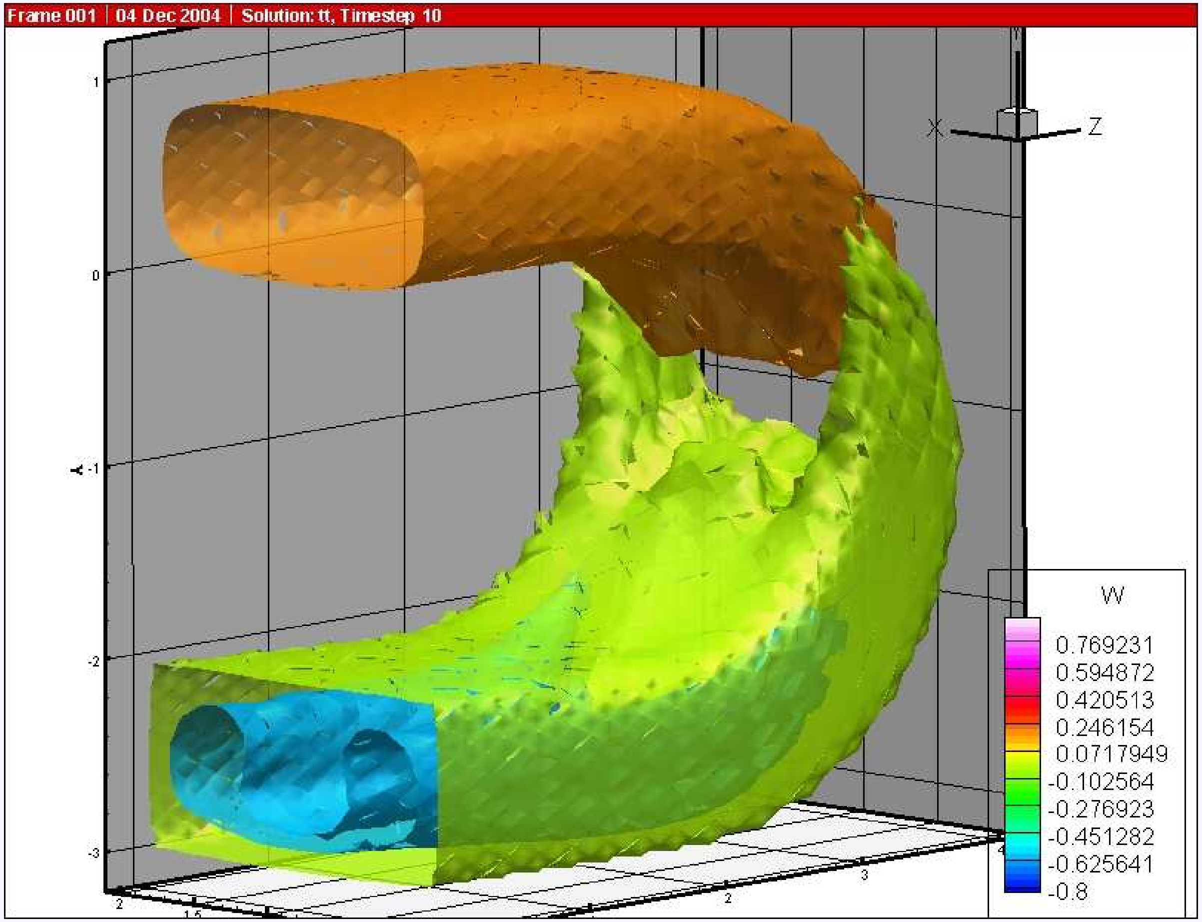
3D Navier-Stokes and Sensitivity Computations

3rd velocity component iso-surfaces



Future Work

Sensitivity Computation for Deconvolution Model

We approximate $\nabla \cdot (\overline{\mathbf{u}\mathbf{u}})$ term by

$$\nabla \cdot (\overline{\mathbf{u}\mathbf{u}}) \approx \nabla \cdot (\bar{\mathbf{u}}\bar{\mathbf{u}}) + \nabla \cdot \tilde{\tau}$$

where $\tilde{\tau} = (\tilde{\tau}_{ij})$ with $\tilde{\tau}_{ij}$ solving

$$(I - \delta^2 \Delta)\tilde{\tau}_{ij} = 2\delta^2 \nabla \cdot \bar{u}_i \nabla \bar{u}_j$$

Future Work

Sensitivity Computation for Deconvolution Model

Let $s_i = \frac{\partial \bar{\mathbf{u}}}{\partial \delta}$. Then at n-th time step solve for $\frac{\partial \tilde{\tau}_{ij}}{\partial \delta}$

$$-2\delta\Delta\tilde{\tau}_{ij} + (I - \delta^2\Delta)\frac{\partial \tilde{\tau}_{ij}}{\partial \delta} = 2\delta\nabla\bar{u}_i\nabla\bar{u}_j + \delta^2(\nabla s_i\nabla\bar{u}_j + \nabla\bar{u}_i\nabla s_j)$$

Future Work

Sensitivity Computation for Deconvolution Model

Let $s_i = \frac{\partial \bar{\mathbf{u}}}{\partial \delta}$. Then at n-th time step solve for $\frac{\partial \tilde{\tau}_{ij}}{\partial \delta}$

$$-2\delta\Delta\tilde{\tau}_{ij} + (I - \delta^2\Delta)\frac{\partial \tilde{\tau}_{ij}}{\partial \delta} = 2\delta\nabla\bar{u}_i\nabla\bar{u}_j + \delta^2(\nabla s_i\nabla\bar{u}_j + \nabla\bar{u}_i\nabla s_j)$$

Let $\tilde{T}$ denote a discretized version of $\tilde{\tau}_{ij}$ computed at n-th time step.

One time step of discretized N.S. (Crank-Nicholson)

$$\mathbf{F}(\mathbf{x}(\delta), \tilde{x}(\delta), \delta) + \mathbf{G}(\mathbf{y}(\delta), \tilde{y}(\delta), \tilde{T}(\delta), \delta) = 0$$

Future Work

Sensitivity Computation for Deconvolution Model

Using data $\tilde{T}_{ij}$ and $\frac{\partial \tilde{T}_{ij}}{\partial \delta}$ we set dependent variables and gradients.

Then solve for a $\frac{\partial \mathbf{x}}{\partial \delta}$

$$\begin{aligned}\mathbf{F}_{\mathbf{x}}(\mathbf{x},\tilde{x},\delta)\frac{\partial \mathbf{x}}{\partial \delta} = -\Bigg[&\mathbf{F}_{\tilde{x}}(\mathbf{x},\tilde{x},\delta)\frac{\partial \tilde{x}}{\partial \delta} + \mathbf{F}_{\delta}(\mathbf{x},\tilde{x},\delta) + \\ &\mathbf{G}_{\mathbf{y}}(\mathbf{y},\tilde{y},\tilde{T},\delta)\frac{\partial \mathbf{y}}{\partial \delta} + \mathbf{G}_{\tilde{y}}(\mathbf{y},\tilde{y},\tilde{T},\delta)\frac{\partial \tilde{y}}{\partial \delta} \\ &+\mathbf{G}_{\delta}(\mathbf{y},\tilde{y},\tilde{T},\delta) + \mathbf{G}_{\tilde{T}}(\mathbf{y},\tilde{y},\tilde{T},\delta)\frac{\partial \tilde{T}}{\partial \delta}\Bigg]\end{aligned}$$