Sensitivity analysis for nonlinear hyperbolic systems of conservation laws



11 / 07 / 2018

PhD defence

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Under the supervision of

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Outline of the talk

- Sensitivity analysis
- Sensitivity analysis for hyperbolic equations
- Riemann problem for the Euler equations and their sensitivity
- Classical numerical schemes
- Anti-diffusive numerical schemes
- Applications

Sensitivity Analysis

Sensitivity Analysis

Sensitivity analysis: study of how changes in the **inputs** of a model affect the **outputs**



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Optimization [5]

Problem: $\min_{a \in A} J(\mathbf{U})$, where $J(\mathbf{U}) = \frac{1}{2}b(\mathbf{U}, \mathbf{U})$ and b is bilinear.

Classical optimization techniques call for the differentiation of the cost function:

$$a^{new} = a^{old} - \alpha \frac{\partial J(\mathbf{U})}{\partial a} \qquad \qquad \frac{\partial J(\mathbf{U})}{\partial a} = b(\mathbf{U}, \mathbf{U}_a)$$

[5] Borggaard, J., & Burns, J. (1997). A PDE sensitivity equation method for optimal aerodynamic design. *Journal of Computational Physics*, *136*(2), 366-384.

[6] Duvigneau, R., & Pelletier, D. (2006). A sensitivity equation method for fast evaluation of nearby flows and uncertainty analysis for shape parameters. *International Journal of Computational Fluid Dynamics*, *20*(7), 497-512.
[7] Delenne, C. (2014). Propagation de la sensibilité dans les modèles hydrodynamiques (HDR, Montpellier II).

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- Optimization [5]
- Quick evaluation of close solutions [6]

$$\mathbf{U}(a+\delta a) = \mathbf{U}(a) + \delta a \mathbf{U}_a(a) + o(\delta a^2)$$

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- Optimization [5]
- Quick evaluation of close solutions [6]
- Uncertainty quantification [7]

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Two approaches



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Standard techniques of sensitivity analysis call for the differentiation of the state system:

 $\begin{cases} \partial_t \mathbf{U} + \partial_x \mathbf{F}(\mathbf{U}) = 0 & \Omega \times (0, T), \\ \mathbf{U}(x, 0) = \mathbf{g}(x) & \Omega, \end{cases}$

[8] Bardos, C., & Pironneau, O. (2002). A formalism for the differentiation of conservation laws. *Comptes Rendus Mathematique*, *335*(10), 839-845.

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For the **Burgers' equation**: $\mathbf{F}(\mathbf{U}) = \frac{u^2}{2}$ $\mathbf{F}_a(\mathbf{U}, \mathbf{U}_a) = uu_a$

This can be done under hypotheses of regularity of the state U[8].

If these techniques are applied to hyperbolic equations, **Dirac delta functions** will appear in the sensitivity.

[8] Bardos, C., & Pironneau, O. (2002). A formalism for the differentiation of conservation laws. *Comptes Rendus Mathematique*, *335*(10), 839-845.

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From different point of view: the global system is weakly hyperbolic.

The Jacobian matrix of the global system has the following form:





therefore it has repeated eigenvalues.

We proved that in the general case it is not diagonalisable.

Sensitivity analysis for hyperbolic equations In order to have a sensitivity system which is valid also when the state is discontinuous, we add a correction term [9]:

 $\begin{cases} \partial_t \mathbf{U}_a + \partial_x \mathbf{F}_a(\mathbf{U}, \mathbf{U}_a) = \mathbf{S} & \Omega \times (0, T), \\ \mathbf{U}_a(x, 0) = \mathbf{g}_a(x) & \Omega, \end{cases}$

defined as follows:

 $\mathbf{S} = \sum \rho_k \delta(x - x_{k,s}(t)),$

number of discontinuities

position of the k-th discontinuity

amplitude of the k-th correction (to be computed)

Remark: a shock detector is necessary to discretise such source term.

[9] Guinot, V., Delenne, C., & Cappelaere, B. (2009). An approximate Riemann solver for sensitivity equations with discontinuous solutions. *Advances in Water Resources*, *32*(1), 61-77.

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Definition of the source term

To compute the amplitude of the correction, we consider an infinitesimal control volume containing a single discontinuity: σ

By integrating the sensitivity equations with the source term on the control volume, one has: $\rho_k = (\mathbf{U}_a^- - \mathbf{U}_a^+)\sigma_k + \mathbf{F}_a^+ - \mathbf{F}_a^-$

Rankine-Hugoniot conditions for the state: $(\mathbf{U}^+ - \mathbf{U}^-)\sigma_k = \mathbf{F}^+ - \mathbf{F}^-$

Differentiating them w.r.t. the parameter:

$$\begin{aligned} (\mathbf{U}_{a}^{+} - \mathbf{U}_{a}^{-})\sigma_{k} + (\mathbf{U}^{+} - \mathbf{U}^{-})\sigma_{k,a} + \sigma_{k}(\partial_{x}\mathbf{U}^{+} - \partial_{x}\mathbf{U}^{-})\partial_{a}x_{k,s}(t) &= \\ &= \mathbf{F}_{a}^{+} - \mathbf{F}_{a}^{-} + \left(\frac{\partial\mathbf{F}(\mathbf{U}^{+})}{\partial\mathbf{U}}\partial_{x}\mathbf{U}^{+} - \frac{\partial\mathbf{F}(\mathbf{U}^{-})}{\partial\mathbf{U}}\partial_{x}\mathbf{U}^{-}\right)\partial_{a}x_{k,s}(t). \end{aligned}$$

Finally, we obtain the following amplitude:

$$\boldsymbol{\rho}_{k} = (\mathbf{U}^{+} - \mathbf{U}^{-})\sigma_{k,a} + \sigma_{k}(\partial_{x}\mathbf{U}^{+} - \partial_{x}\mathbf{U}^{-})\partial_{a}x_{k,s}(t) - \left(\frac{\partial\mathbf{F}(\mathbf{U}^{+})}{\partial\mathbf{U}}\partial_{x}\mathbf{U}^{+} - \frac{\partial\mathbf{F}(\mathbf{U}^{-})}{\partial\mathbf{U}}\partial_{x}\mathbf{U}^{-}\right)\partial_{a}x_{k,s}(t).$$

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Thesis synopsis

- Chapter 1: introduction
- Chapter 2: scalar case
- Chapter 3: the p-system [1,2]
- Chapter 4: the Euler system [3]
- Chapter 5: quasi 1D Euler system
- Chapter 6: conclusion and perspectives
- Appendix A: modelling of running strategies [4]

Chalons, C., Duvigneau, R., & Fiorini, C. (2017). Sensitivity analysis for the Euler equations in Lagrangian coordinates. In *International Conference on Finite Volumes for Complex Applications* (pp. 71-79). Springer, Cham.
 Chalons, C., Duvigneau, R. & Fiorini, C. (2017). Sensitivity analysis and numerical diffusion effects for hyperbolic PDE systems with discontinuous solutions. The case of barotropic Euler equations in Lagrangian coordinates. Submitted to *SJSC*.
 Fiorini, C., Chalons, C., Duvigneau, R (2018). Sensitivity equation method for Euler equations in presence of shocks applied to uncertainty quantification. Submitted to *JCP*.
 Fiorini, C. (2017). Optimization of Pupping Strategies According to the Physiological Parameters for a Two Pupper Model.

[4] Fiorini, C. (2017). Optimization of Running Strategies According to the Physiological Parameters for a Two-Runner Model. Bulletin of mathematical biology, 79(1), 143-162.

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Riemann problem for Euler equations and their sensitivity

The Riemann problem for Euler equations

The Euler equations write:

 $\begin{cases} \partial_t \rho + \partial_x (\rho u) = 0, \\ \partial_t (\rho u) + \partial_x (\rho u^2 + p) = 0, \\ \partial_t (\rho E) + \partial_x (u(\rho E + p)) = 0, \end{cases}$

Eigenvalues:	Eigenvectors:
$\lambda_1(\mathbf{U}) = u - c,$	$\mathbf{r}_1(\mathbf{U}) = (1, u - c, H - uc)^t,$
$\lambda_2(\mathbf{U}) = u,$	$\mathbf{r}_2(\mathbf{U}) = (1, u, \frac{u^2}{2})^t,$
$\lambda_3(\mathbf{U}) = u + c.$	$\mathbf{r}_3(\mathbf{U}) = (1, u + c, H + uc)^t.$

Genuinely nonlinear

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Linearly degenerate

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The Riemann problem for Euler equations



The Riemann problem for the sensitivity equations

The sensitivity system writes:

$$\begin{aligned} \partial_t \rho_a + \partial_x (\rho u)_a &= S_1, \\ \partial_t (\rho u)_a + \partial_x (\rho_a u^2 + 2\rho u u_a + p_a) &= S_2, \\ \partial_t (\rho E)_a + \partial_x (u_a (\rho E + p) + u((\rho E)_a + p_a)) &= S_3, \end{aligned}$$

Eigenvalues:

$$\lambda_1(\mathbf{U}) = u - c,$$

$$\lambda_2(\mathbf{U}) = u,$$

$$\lambda_3(\mathbf{U}) = u + c.$$



Classical Numerical Schemes



Remark: the state and the sensitivity systems are not solved as a global system.

 $\begin{cases} \partial_t \mathbf{U} + \partial_x \mathbf{F}(\mathbf{U}) = 0\\ \partial_t \mathbf{U}_a + \partial_x \mathbf{F}_a(\mathbf{U}, \mathbf{U}_a) = \mathbf{S}(\mathbf{U}) \qquad \mathbf{S}(\mathbf{U}) = \sum_{k=1}^{N_s} \sigma_{a,k} (\mathbf{U}_k^+ - \mathbf{U}_k^-) \end{cases}$

Remark: HLL-type schemes cannot be used for the state, two intermediate star states are necessary to have a well-defined the source term for the sensitivity.

Approximate Riemann solver for the state

First order Roe-type scheme

$$\begin{split} \lambda_1^{ROE} &= \tilde{u} - \tilde{c}_3 \quad \lambda_2^{ROE} = \tilde{u} \quad \lambda_3^{ROE} = \tilde{u} + \tilde{c} \quad \text{Roe-averaged eigenvalues} \\ \mathbf{U}_R - \mathbf{U}_L &= \sum_{k=1}^3 \alpha_i \tilde{\mathbf{r}}_i \quad \text{decomposition along Roe-averaged eigenvectors} \\ \mathbf{U}_L^* &= \mathbf{U}_L + \alpha_1 \tilde{\mathbf{r}}_1 \quad \mathbf{U}_R^* = \mathbf{U}_R - \alpha_3 \tilde{\mathbf{r}}_3 \end{split}$$

[10] Bouchut, F. (2004). Nonlinear stability of finite Volume Methods for hyperbolic conservation laws: And Well-Balanced schemes for sources. Springer Science & Business Media.

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Approximate Riemann solver for the state

- First order Roe-type scheme
- Second order Roe-type scheme

Time discretisation: two-step Runge-Kutta method

Space discretisation: MUSCL-type scheme [10]



schemes for sources. Springer Science & Business Media.

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 $\begin{cases} \partial_t \mathbf{U} + \partial_x \mathbf{F}(\mathbf{U}) = 0\\ \partial_t \mathbf{U}_a + \partial_x \mathbf{F}_a(\mathbf{U}, \mathbf{U}_a) = \mathbf{S}(\mathbf{U}) \qquad \mathbf{S}(\mathbf{U}) = \sum_{k=1}^{N_s} \sigma_{a,k} (\mathbf{U}_k^+ - \mathbf{U}_k^-) \end{cases}$

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Sensitivity Analysis for nonlinear hyperbolic PDEs

 $x_{j+3/2}$

 \mathcal{X}

 $\begin{cases} \partial_t \mathbf{U} + \partial_x \mathbf{F}(\mathbf{U}) = 0\\ \partial_t \mathbf{U}_a + \partial_x \mathbf{F}_a(\mathbf{U}, \mathbf{U}_a) = \mathbf{S}(\mathbf{U}) \qquad \mathbf{S}(\mathbf{U}) = \sum_{k=1}^{N_s} \sigma_{a,k} (\mathbf{U}_k^+ - \mathbf{U}_k^-) \end{cases}$

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Approximate Riemann solvers for the sensitivity

HLL-type scheme: simpler structure that the state solver.
 HLL consistency conditions yield:

 $\begin{aligned} \mathbf{U}_{a,j-1/2}^{*} &= \frac{1}{\lambda_{3}^{ROE} - \lambda_{1}^{ROE}} \left(\lambda_{3}^{ROE} \mathbf{U}_{a,j}^{n} - \lambda_{1}^{ROE} \mathbf{U}_{a,j-1}^{n} - \mathbf{F}_{a}(\mathbf{U}_{j}, \mathbf{U}_{a,j}) + \mathbf{F}_{a}(\mathbf{U}_{j-1}, \mathbf{U}_{a,j-1}) + \mathbf{S}_{j-1/2} \right) \\ &\qquad \mathbf{S}_{j-1/2} = \partial_{a} \lambda_{1,j-1/2}^{ROE} (\mathbf{U}_{L,j-1/2}^{*} - \mathbf{U}_{j-1}) d_{1,j-1/2} \\ &\qquad + \partial_{a} \lambda_{2,j-1/2}^{ROE} (\mathbf{U}_{R,j-1/2}^{*} - \mathbf{U}_{L,j-1/2}^{*}) \\ &\qquad + \partial_{a} \lambda_{3,i-1/2}^{ROE} (\mathbf{U}_{j} - \mathbf{U}_{R,i-1/2}^{*}) d_{3,j-1/2} \end{aligned}$

▶ HLLC-type scheme: same structure as the state.

HLL consistency conditions + Rankine-Hugoniot conditions. Equivalent to:

$$\mathbf{U}_{a,L}^* = \mathbf{U}_{a,L} + \alpha_{1,a}\tilde{\mathbf{r}}_1 + \alpha_1\tilde{\mathbf{r}}_{1,a} \qquad \mathbf{U}_{a,R}^* = \mathbf{U}_{a,R} - \alpha_{3,a}\tilde{\mathbf{r}}_3 - \alpha_3\tilde{\mathbf{r}}_{3,a}$$

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Isolated shock for the *p*-system



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Sensitivity Analysis for nonlinear hyperbolic PDEs

Numerical Scheme without diffusion



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Step 0 : initial data discretisation

Step 1 : solution of the Riemann problems, one for each interface



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Step 0 : initial data discretisation

Step 1 : solution of the Riemann problems, one for each interface

Step 2 : average



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Step 0 : initial data discretisation

Step 1 : solution of the Riemann problems, one for each interface



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Step 0 : initial data discretisation

Step 1 : solution of the Riemann problems, one for each interface

Step 2 : definition of a staggered mesh on which the average is performed [11]



[11] Chalons, C., & Goatin, P. (2008). Godunov scheme and sampling technique for computing phase transitions in traffic flow modeling. *Interfaces and Free Boundaries*, *10*(2), 197-221.

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Step 0 : initial data discretisation

Step 1 : solution of the Riemann problems, one for each interface

Step 2 : definition of a staggered mesh on which the average is performed

Step 3 : projection on the initial mesh [12]

$$\overline{\mathbf{U}_{j-1}} \qquad \overline{\mathbf{U}_{j}} \qquad \overline{\mathbf{U}_{j+1}}$$

$$\overline{\mathbf{U}_{j-1}} \qquad \overline{\mathbf{U}_{j}} \qquad \overline{\mathbf{U}_{j+1}}$$

$$\mathbf{U}_{j} = \begin{cases} \overline{\mathbf{U}}_{j-1} & \text{if } \alpha \in \left(0, \frac{\Delta t}{\Delta x} \max(\sigma_{j-1/2}, 0)\right), \\ \overline{\mathbf{U}}_{j} & \text{if } \alpha \in \left[\frac{\Delta t}{\Delta x} \max(\sigma_{j-1/2}, 0), 1 + \frac{\Delta t}{\Delta x} \min(\sigma_{j+1/2}, 0)\right), \\ \overline{\mathbf{U}}_{j+1} & \text{if } \alpha \in \left[1 + \frac{\Delta t}{\Delta x} \min(\sigma_{j+1/2}, 0), 1\right). \end{cases}$$

 $\alpha \sim \mathcal{U}([0,1])$

[12] Glimm, J. (1965). Solutions in the large for nonlinear hyperbolic systems of equations. *Communications on pure and applied mathematics*, *18*(4), 697-715.

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Convergence



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Sensitivity Analysis for nonlinear hyperbolic PDEs

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Let **a** be a random vector, with the following average and variance:

$$\mu_{\mathbf{a}} = \begin{bmatrix} \mu_{a_1} \\ \vdots \\ \mu_{a_M} \end{bmatrix}, \quad \sigma_{\mathbf{a}} = \begin{bmatrix} \sigma_{a_1}^2 & \operatorname{cov}(a_1, a_2) & \dots & \operatorname{cov}(a_1, a_M) \\ \operatorname{cov}(a_1, a_2) & \sigma_{a_2}^2 & \dots & \operatorname{cov}(a_2, a_M) \\ \vdots & & \ddots & \vdots \\ \operatorname{cov}(a_1, a_M) & \dots & \sigma_{a_M}^2 \end{bmatrix}$$

Aim: determine a **confidence interval** $CI_X = [\mu_X - \kappa \sigma_X, \mu_X + \kappa \sigma_X]$

Monte Carlo approach: *N* samples of the state X_k

$$\mu_X = \frac{1}{N} \sum_{k=1}^N X_k \qquad \sigma_X^2 = \frac{1}{N-1} \sum_{k=1}^N |\mu_X - X_k|^2$$

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Sensitivity approach: let us consider the following first order Taylor expansion

$$X(\mathbf{a}) = X(\mu_{\mathbf{a}}) + \sum_{i=1}^{M} (a_i - \mu_{a_i}) X_{a_i}(\mu_{\mathbf{a}}) + o(\|\mathbf{a}\|^2).$$

Then, computing, the average one has:

$$\mu_X = E[X(\mathbf{a})] = X(\mu_{\mathbf{a}}) + \sum_{i=1}^M X_{a_i}(\mu_{\mathbf{a}})E[a_i - \mu_{a_i}] = X(\mu_{\mathbf{a}}),$$

And for the variance:

$$\sigma_X^2 = E[(X(\mathbf{a}) - \mu_X)^2] = E\left[\left(\sum_{i=1}^M X_{a_i}(\mu_{\mathbf{a}})(a_i - \mu_{a_i})\right)^2\right] = E\left[\left(\sum_{i=1}^M X_{a_i}(\mu_{\mathbf{a}})(a_i - \mu_{a_i})\right)^2\right]$$

$$= \sum_{i=1}^{M} X_{a_i}^2(\mu_{\mathbf{a}}) E[(a_i - \mu_{a_i})^2] + \sum_{\substack{i,j=1\\i \neq j}}^{M} X_{a_i}(\mu_{\mathbf{a}}) X_{a_j}(\mu_{\mathbf{a}}) E[(a_i - \mu_{a_i})(a_j - \mu_{a_j})].$$

Therefore, we have the following first order estimates:

$$\mu_X = X(\mu_{\mathbf{a}}), \quad \sigma_X^2 = \sum_{i=1}^M X_{a_i}^2 \sigma_{a_i}^2 + \sum_{\substack{i,j=1\\i\neq j}}^M X_{a_i} X_{a_j} \operatorname{cov}(a_i, a_j).$$

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Test case:

Riemann problem with uncertain parameters: $\mathbf{a} = (\rho_L, \rho_R, u_L, u_R, p_L, p_R)^t$

with the following average and covariance matrix:

 $\mu_{\mathbf{a}} = (1, 0.125, 0, 0, 1, 0.1)^t, \quad \sigma_{\mathbf{a}} = \text{diag}(0.001, 0.000125, 0.0001, 0.0001, 0.001, 0.0001).$

Since the covariance matrix is diagonal, the previous estimate is simplified:

$$\sigma_X^2 = \sum_{i=1}^6 X_{a_i}^2 \sigma_{a_i}^2$$

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2

h(x)

 x_c

The quasi-1D Euler equations are:

(1) $\begin{cases} \partial_t(h\rho) + \partial_x(h\rho u) = 0, \\ \partial_t(h\rho u) + \partial_x(h\rho u^2 + p) = p\partial_x h, \\ \partial_t(h\rho E) + \partial_x(hu(\rho E + p)) = 0, \\ + \text{b.c.} \end{cases}$

Cost functional:
$$J(\mathbf{U}) = \frac{1}{2} ||p - p^*||_{L^2}^2$$

Parameters: $\mathbf{a} = (x_c, \ell)^t$

Target pressure: $p^* = p(x_c = 0.5, \ell = 0.5)$

Gradient:
$$abla_{\mathbf{a}} J(\mathbf{U}) = \begin{bmatrix} (p - p^*, p_{x_c})_{L^2} \\ (p - p^*, p_\ell)_{L^2} \end{bmatrix}$$

Optimization problem:

 $\min_{\mathbf{a} \in \mathcal{A}} J(\mathbf{U}) \quad \text{subject to (1).}$



Boundary conditions:

- inlet: enthalpy H_L and total pressure $p_{tot,L}$
- outlet: pressure p_R



[13] Giles, M. B., & Pierce, N. A. (2001). Analytic adjoint solutions for the quasi-one-dimensional Euler equations. Journal of Fluid Mechanics, 426, 327-345.

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Conclusion and perspectives

Conclusion:

- We defined a sensitivity system valid in case of discontinuous state
- The correction term is well defined
- The correction term is important in applications

Future development:

- Extension to non-classical shocks
- Effects of the numerical diffusion for the applications
- Extension to 2D

Thank you for your attention!