Sensitivity analysis for nonlinear hyperbolic systems of conservation laws

March 6th, 2019, Roscoff

Camilla Fiorini

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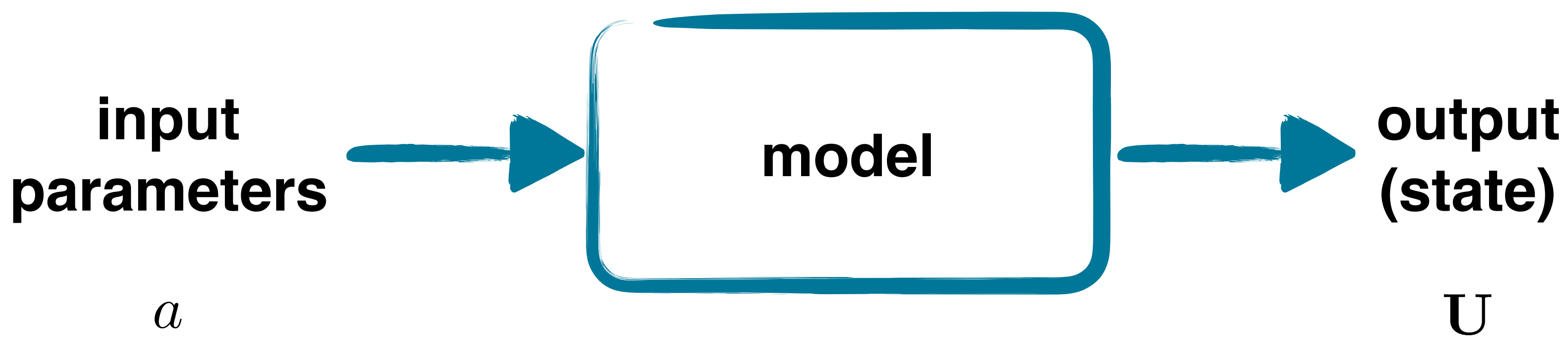
Sensitivity analysis: study of how changes in the **inputs** of a model affect the **outputs**



Sensitivity: $$\frac{\partial \mathbf{U}}{\partial a} = \mathbf{U}_a$$

Discretise then differentiate

analytical state model

↓ discretise

discrete state model

↓ differentiate

discrete sensitivity model

Differentiate then discretise

analytical state model

↓ differentiate

analytical sensitivity model

↓ discretise

discrete sensitivity model

👍 analytical sensitivity model

no discretisation of computational facilitators

👎 could lead to inconsistent gradients

Standard techniques of sensitivity analysis

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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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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Definition of the source term

In order to have a sensitivity system whose solution does not present Dirac delta functions, even 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:

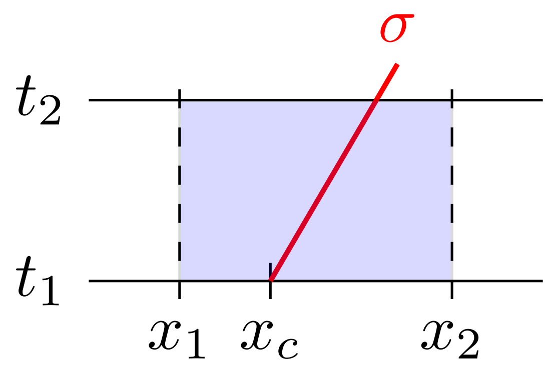
$$\mathbf{S} = \sum_{k=1}^{N_s} \boldsymbol{\rho}_k \delta(x - x_{k,s}(t)),$$

- N_s: number of discontinuities
- $x_{k,s}$: position of the k-th discontinuity
- $\boldsymbol{\rho}_k$: 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.

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



By integrating the sensitivity equations with the source term on the control volume, one has:

$$\boldsymbol{\rho}_k = (\mathbf{U}_a^- - \mathbf{U}_a^+)\sigma_k + \mathbf{F}_a^+ - \mathbf{F}_a^-$$

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

Differentiating them w.r.t. the parameter:

$$(\mathbf{U}_a^+ - \mathbf{U}_a^-)\sigma_k + (\mathbf{U}^+ - \mathbf{U}^-)\sigma_{k,a} + \sigma_k(\partial_x \mathbf{U}^+ - \partial_x \mathbf{U}^-)\partial_a x_{k,s}(t) =$$
$$= \mathbf{F}_a^+ - \mathbf{F}_a^- + \left(\frac{\partial \mathbf{F}(\mathbf{U}^+)}{\partial \mathbf{U}}\partial_x \mathbf{U}^+ - \frac{\partial \mathbf{F}(\mathbf{U}^-)}{\partial \mathbf{U}}\partial_x \mathbf{U}^-\right)\partial_a x_{k,s}(t).$$

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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The Riemann problem for the Euler equations

The Euler equations are:

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

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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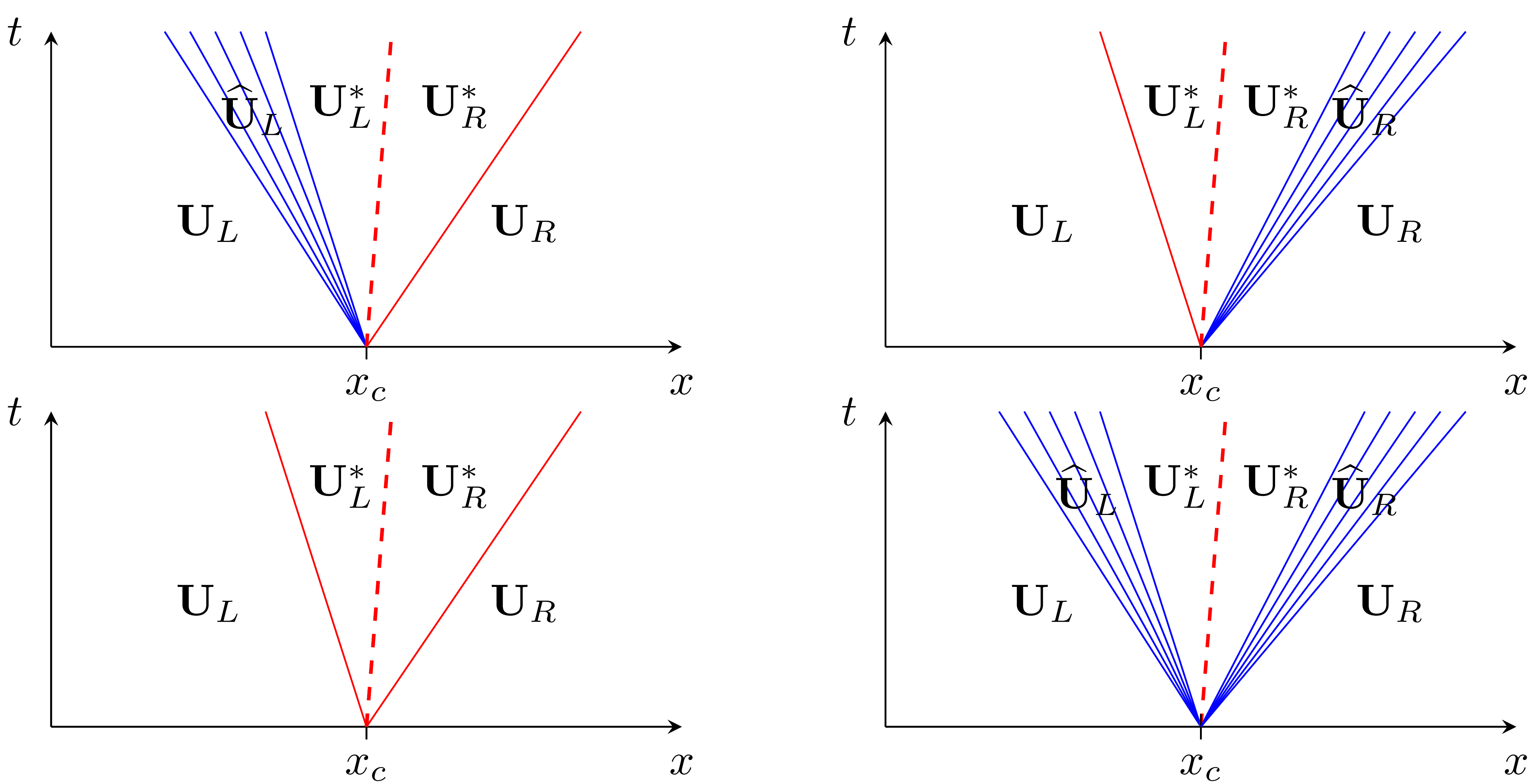


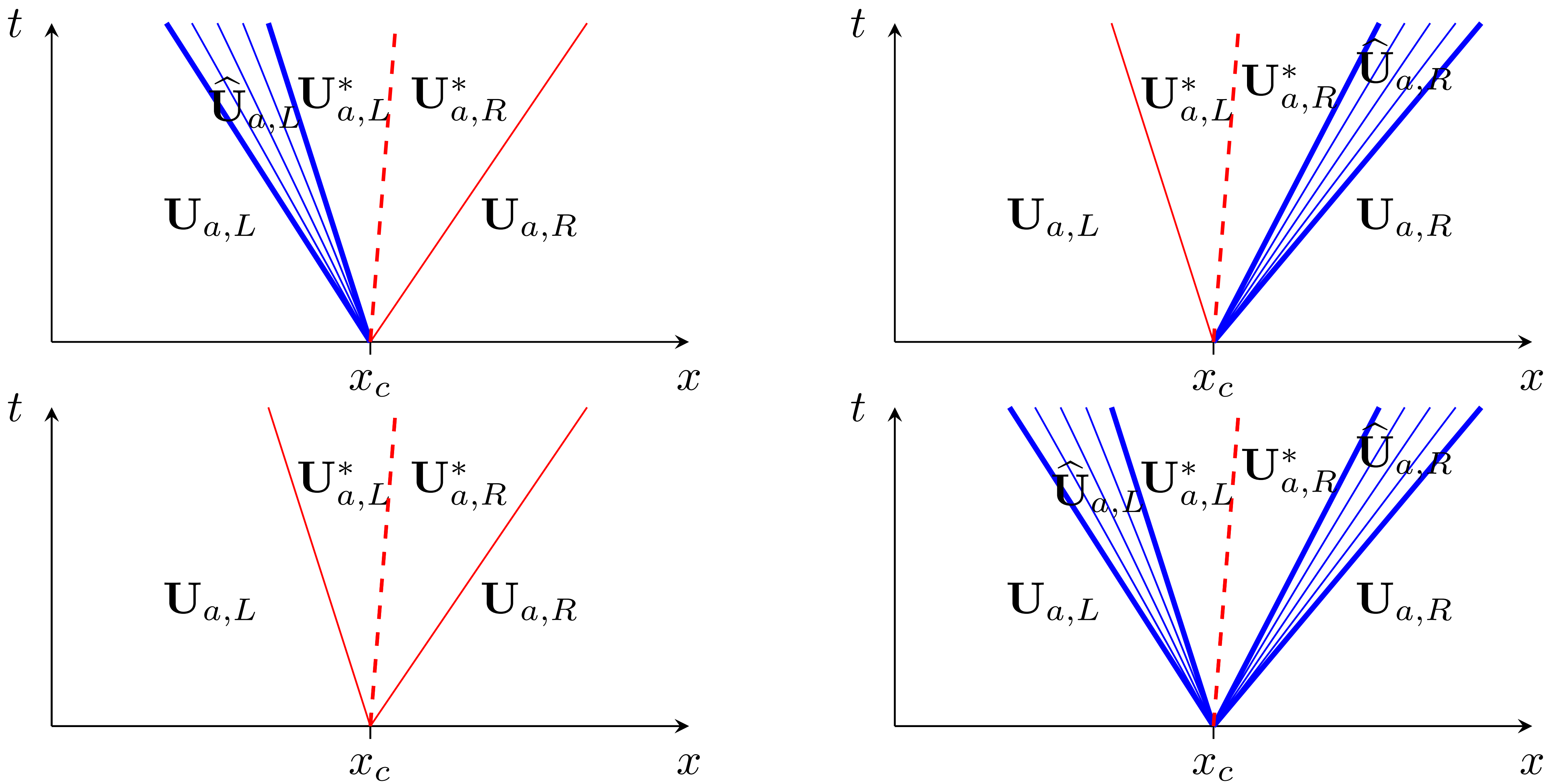
The Riemann problem for the sensitivity equations

The sensitivity system is:

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

Eigenvalues:

$$\lambda_1(\mathbf{U}) = u - c,$$
$$\lambda_2(\mathbf{U}) = u,$$
$$\lambda_3(\mathbf{U}) = u + c.$$



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Godunov-type schemes

approximate Riemann solvers are used

Step 0 : initial data discretisation

Step 1 : solution of a Riemann problem for each interface $x_{j-1/2}$ obtaining $\mathbf{v}(x, t^{n+1})$

Step 2 : average $\mathbf{V}_j^{n+1} = \frac{1}{\Delta x} \int_{x_{j-1/2}}^{x_{j+1/2}} \mathbf{v}(x, t^{n+1}) \mathrm{d}x$

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

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

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

$\lambda_1^{ROE} = \tilde{u} - \tilde{c} \qquad \lambda_2^{ROE} = \tilde{u} \qquad \lambda_3^{ROE} = \tilde{u} + \tilde{c}$ Roe-averaged eigenvalues

$\mathbf{U}_R - \mathbf{U}_L = \sum_{k=1}^{3} \alpha_i \tilde{\mathbf{r}}_i$ decomposition along Roe-averaged eigenvectors

$$\mathbf{U}_L^* = \mathbf{U}_L + \alpha_1 \tilde{\mathbf{r}}_1 \qquad \mathbf{U}_R^* = \mathbf{U}_R - \alpha_3 \tilde{\mathbf{r}}_3$$

Approximate Riemann solvers for the sensitivity

- HLL-type scheme: simpler structure than the state solver.

HLL consistency conditions yield:

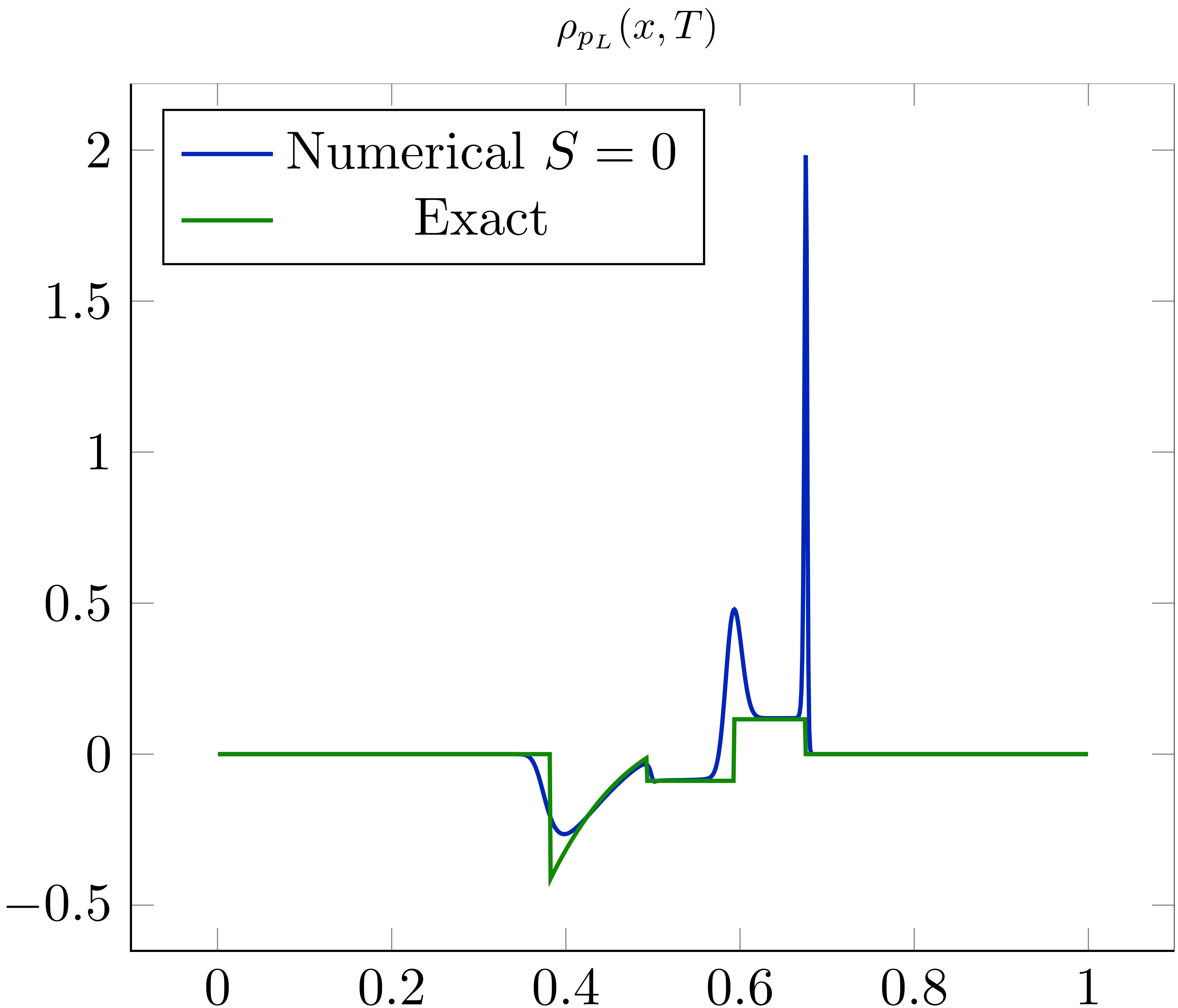
$$\mathbf{U}^*_{a,j-1/2} = \frac{1}{\lambda_3^{ROE} - \lambda_1^{ROE}} \Big(\lambda_3^{ROE} \mathbf{U}^n_{a,j} - \lambda_1^{ROE} \mathbf{U}^n_{a,j-1} - \mathbf{F}_a(\mathbf{U}_j, \mathbf{U}_{a,j}) + \mathbf{F}_a(\mathbf{U}_{j-1}, \mathbf{U}_{a,j-1}) + \mathbf{S}_{j-1/2} \Big)$$

$$\begin{aligned} \mathbf{S}_{j-1/2} =& \partial_a \lambda^{ROE}_{1,j-1/2} (\mathbf{U}^*_{L,j-1/2} - \mathbf{U}_{j-1}) d_{1,j-1/2} \\ &+ \partial_a \lambda^{ROE}_{2,j-1/2} (\mathbf{U}^*_{R,j-1/2} - \mathbf{U}^*_{L,j-1/2}) \\ &+ \partial_a \lambda^{ROE}_{3,j-1/2} (\mathbf{U}_j - \mathbf{U}^*_{R,j-1/2}) d_{3,j-1/2} \end{aligned}$$

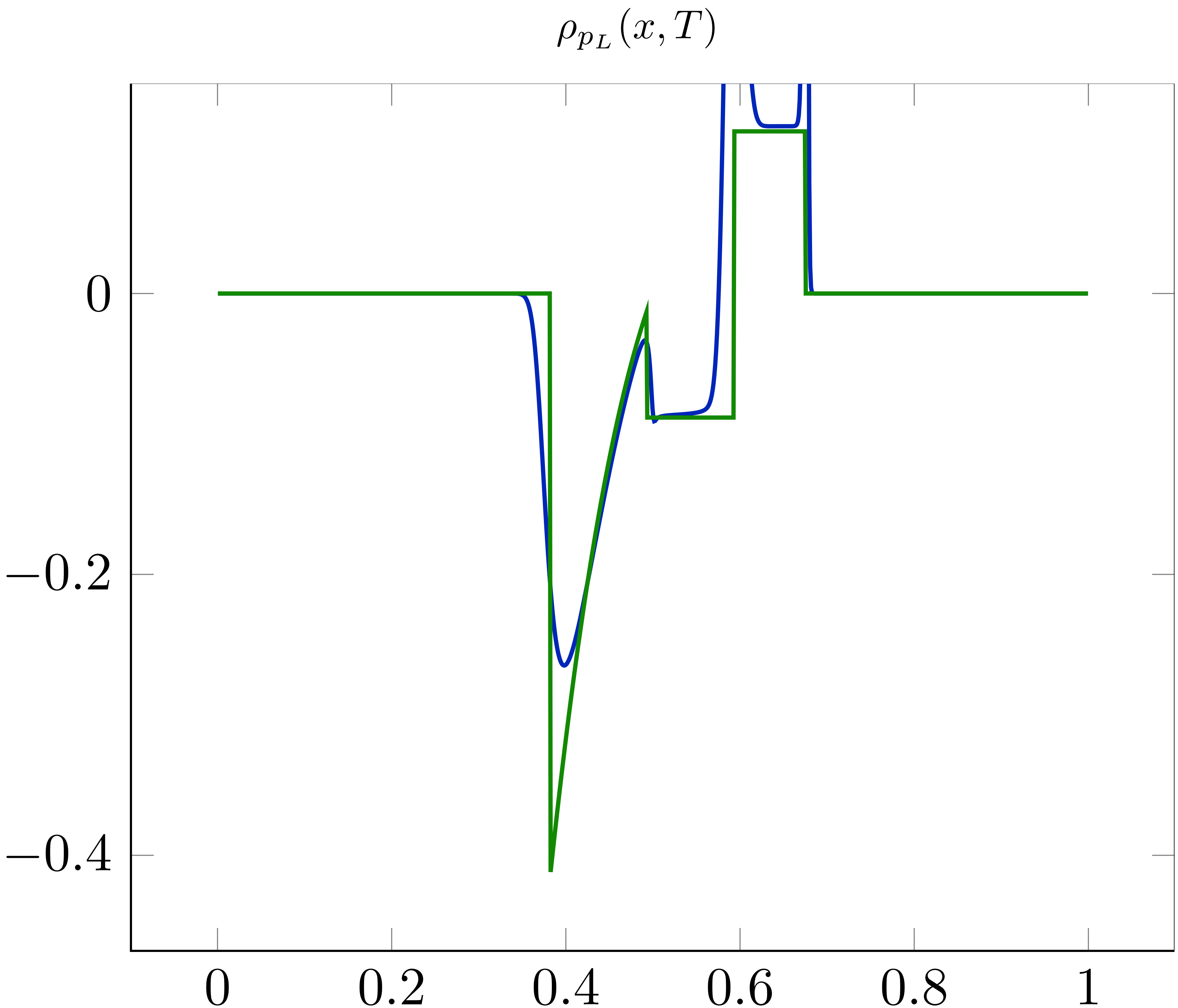
- HLLC-type scheme: same structure as the state.

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

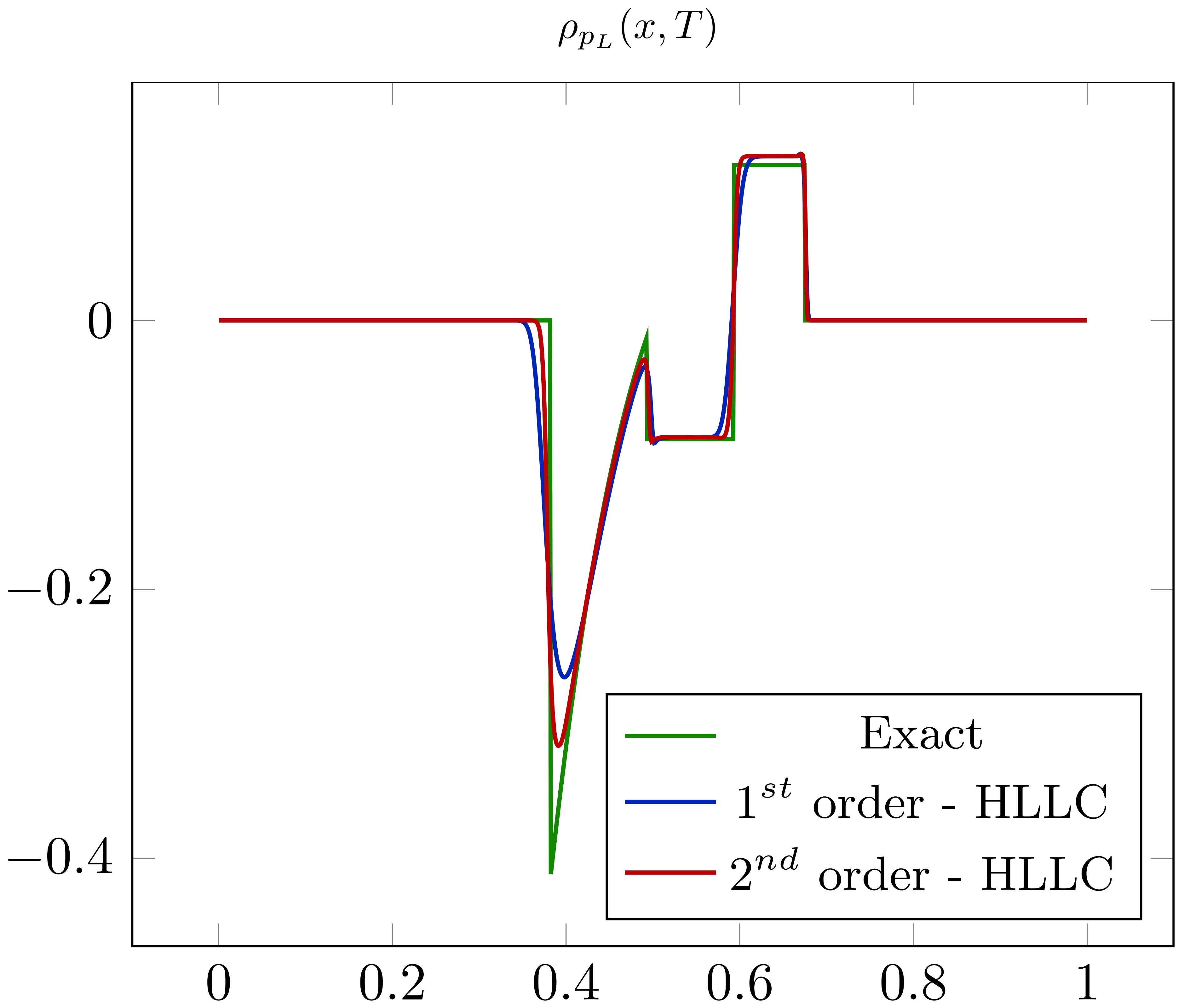
$$\mathbf{U}^*_{a,L} = \mathbf{U}_{a,L} + \alpha_{1,a} \tilde{\mathbf{r}}_1 + \alpha_1 \tilde{\mathbf{r}}_{1,a} \qquad \mathbf{U}^*_{a,R} = \mathbf{U}_{a,R} - \alpha_{3,a} \tilde{\mathbf{r}}_3 - \alpha_3 \tilde{\mathbf{r}}_{3,a}$$


$\rho_{p_L}(x,T)$
Numerical $S = 0$
Exact
2
1.5
1
0.5
0
−0.5
0
0.2
0.4
0.6
0.8
1

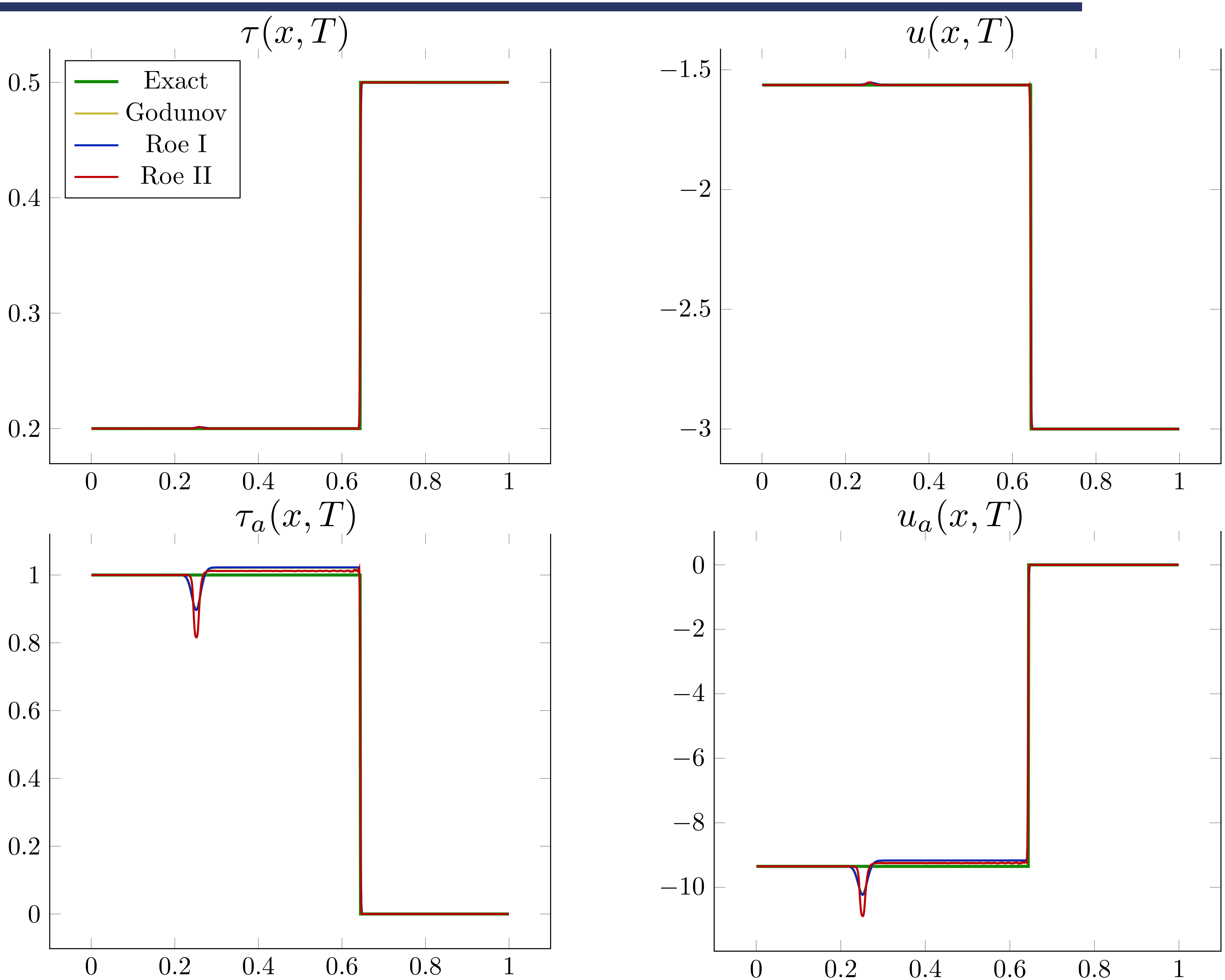
Classical numerical schemes



Classical numerical schemes



Isolated shock for the p-system



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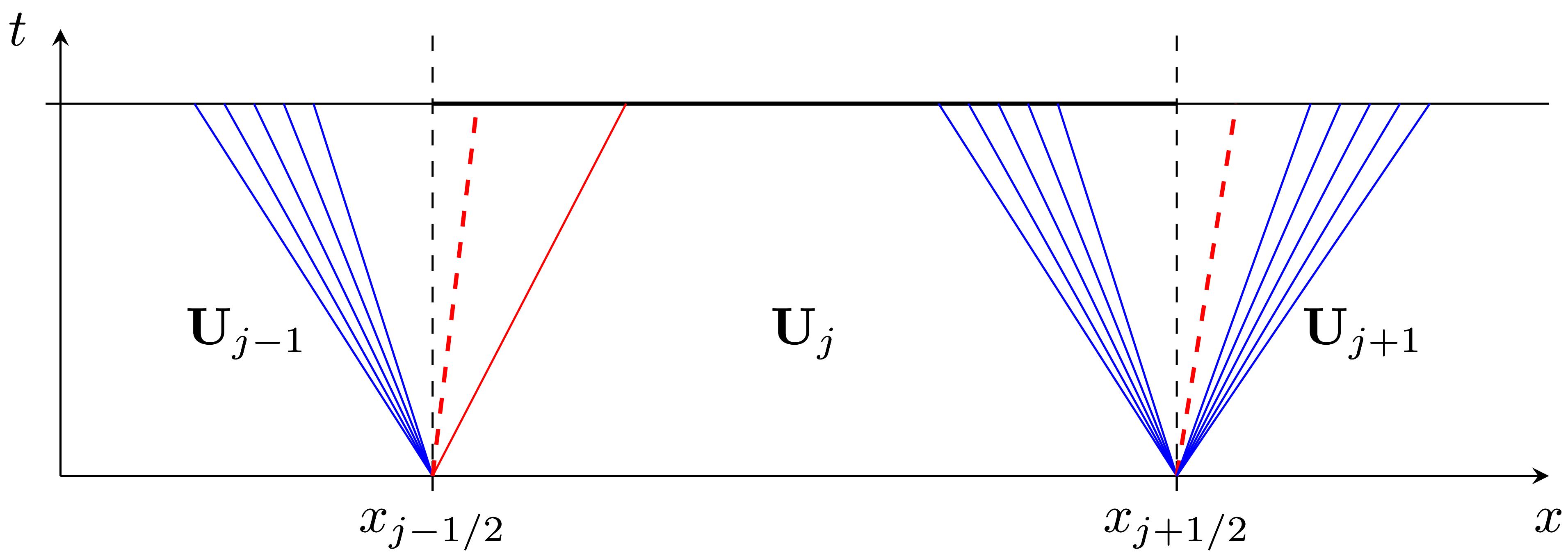
Scheme without numerical diffusion

Step 0 : initial data discretisation

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

Step 2 : ~~average~~

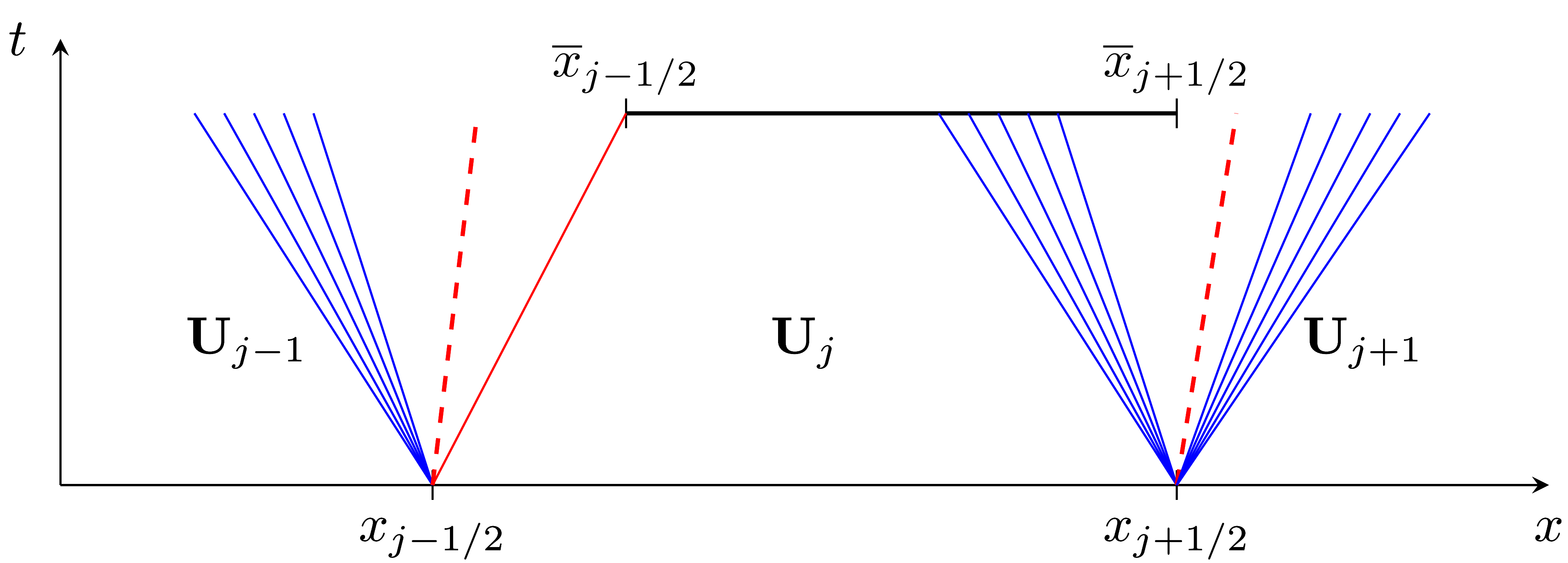


Scheme without numerical diffusion

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]



$$\overline{x}_{j-1/2} = x_{j-1/2} + \sigma_{j-1/2}\Delta t$$

[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.

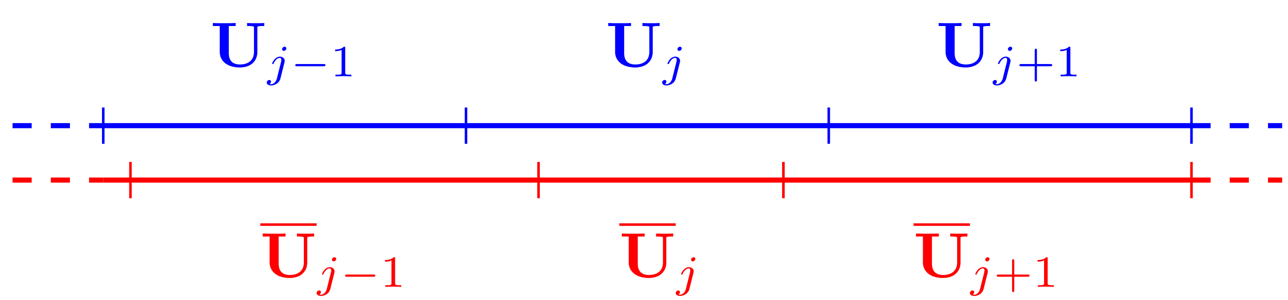
Scheme without numerical diffusion

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]

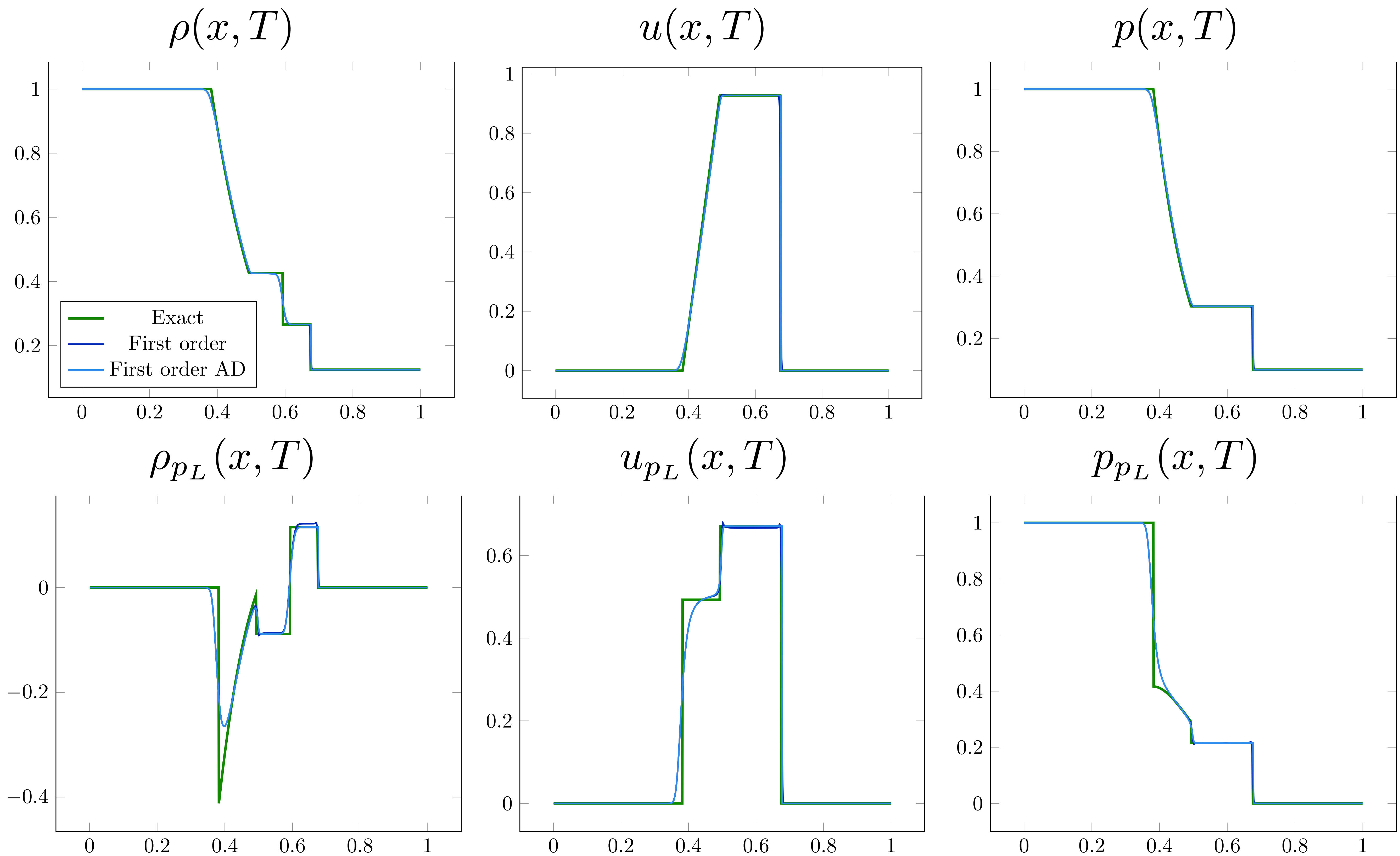


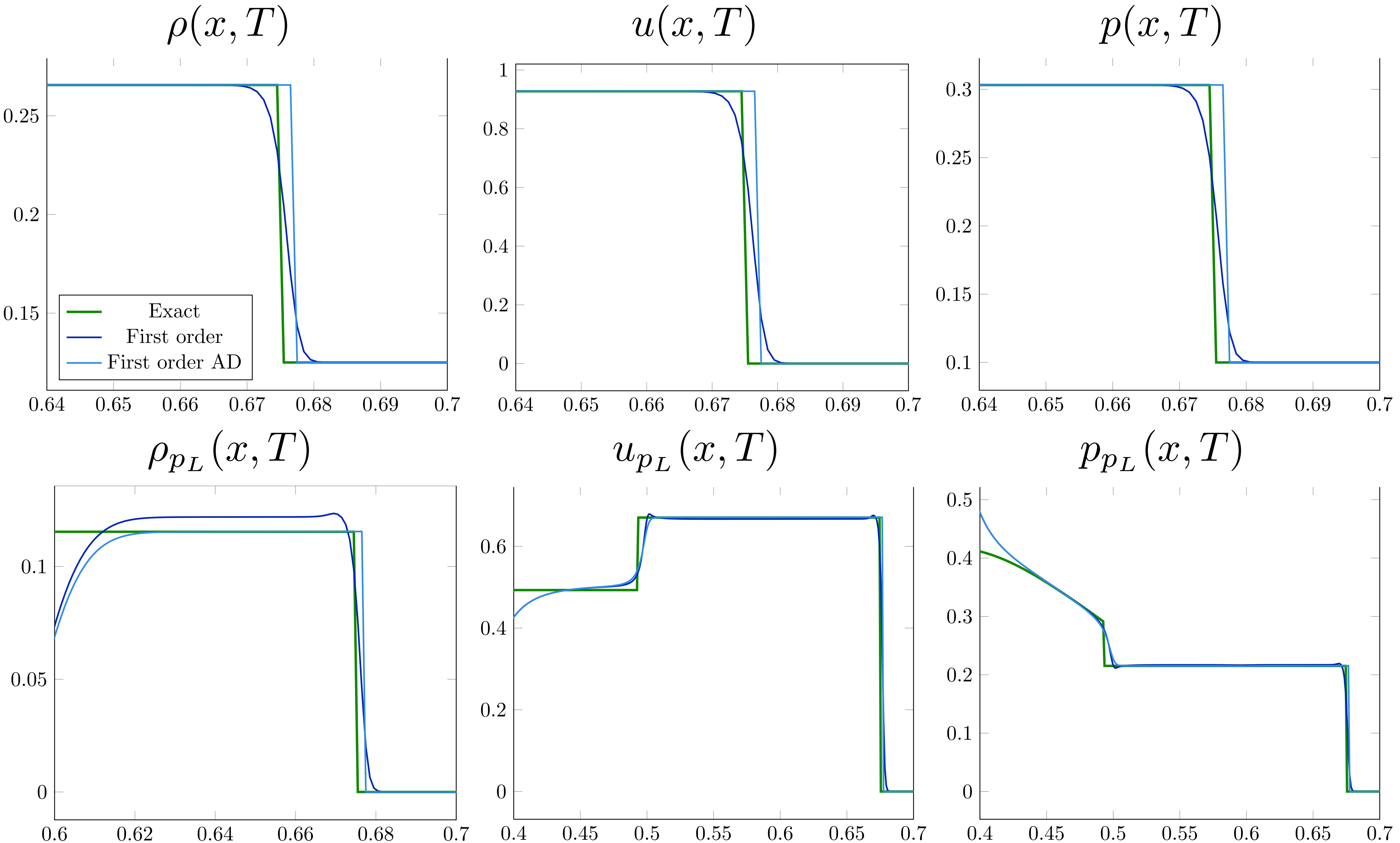
$$\mathbf{U}_j = \begin{cases} \overline{\mathbf{U}}_{j-1} & \text{if } \alpha \in \left(0, \frac{\Delta t}{\Delta x} \max(\sigma_{j-1/2}, 0)\right), \\ \overline{\mathbf{U}}_j & \text{if } \alpha \in \left[\frac{\Delta t}{\Delta x} \max(\sigma_{j-1/2}, 0), 1 + \frac{\Delta t}{\Delta x} \min(\sigma_{j+1/2},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

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

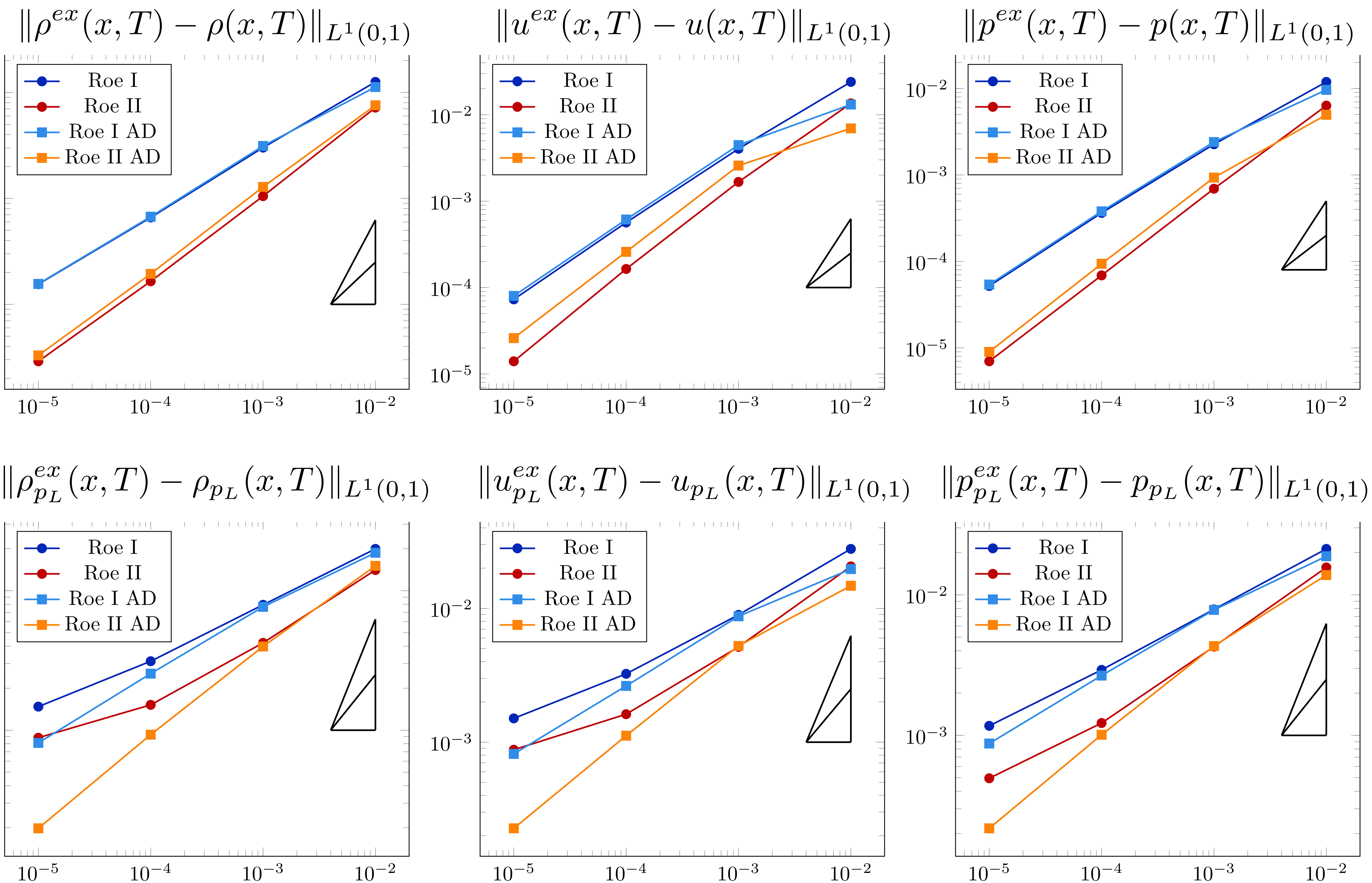
[12] Glimm, J. (1965). Solutions in the large for nonlinear hyperbolic systems of equations. *Communications on pure and applied mathematics*, *18*(4), 697-715.

Numerical results




$\rho(x,T)$
$u(x,T)$
$p(x,T)$
Exact
First order
First order AD
$\rho_{p_L}(x,T)$
$u_{p_L}(x,T)$
$p_{p_L}(x,T)$

Convergence



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

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

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

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

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

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

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:

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

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

Therefore, we have the following first order estimates:

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

Test case:

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

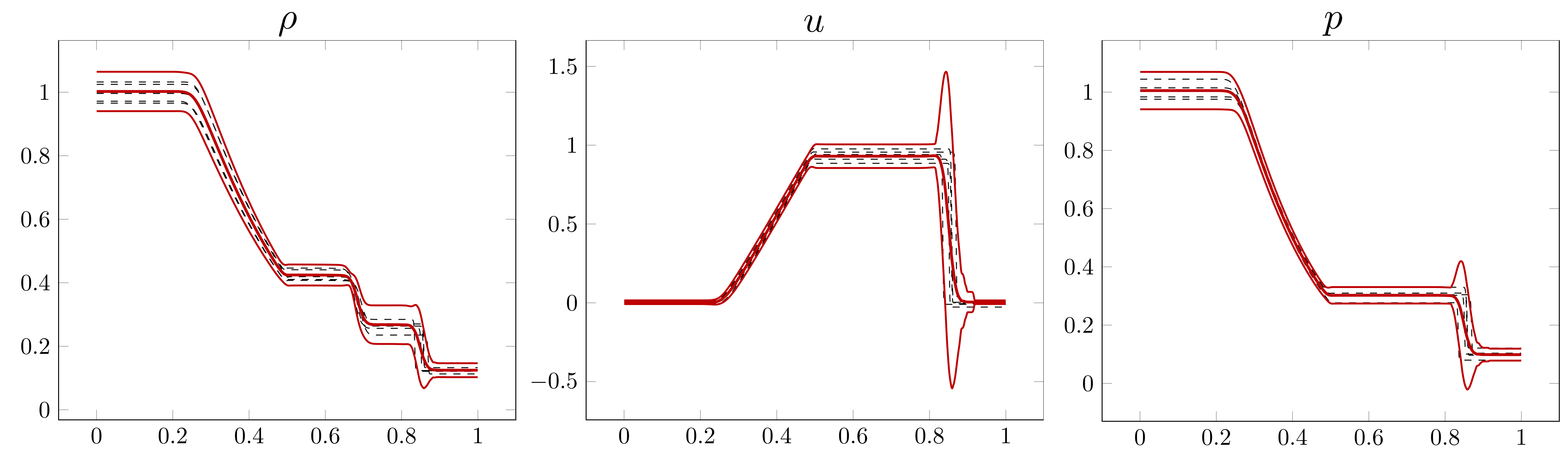
with the following average and covariance matrix:

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

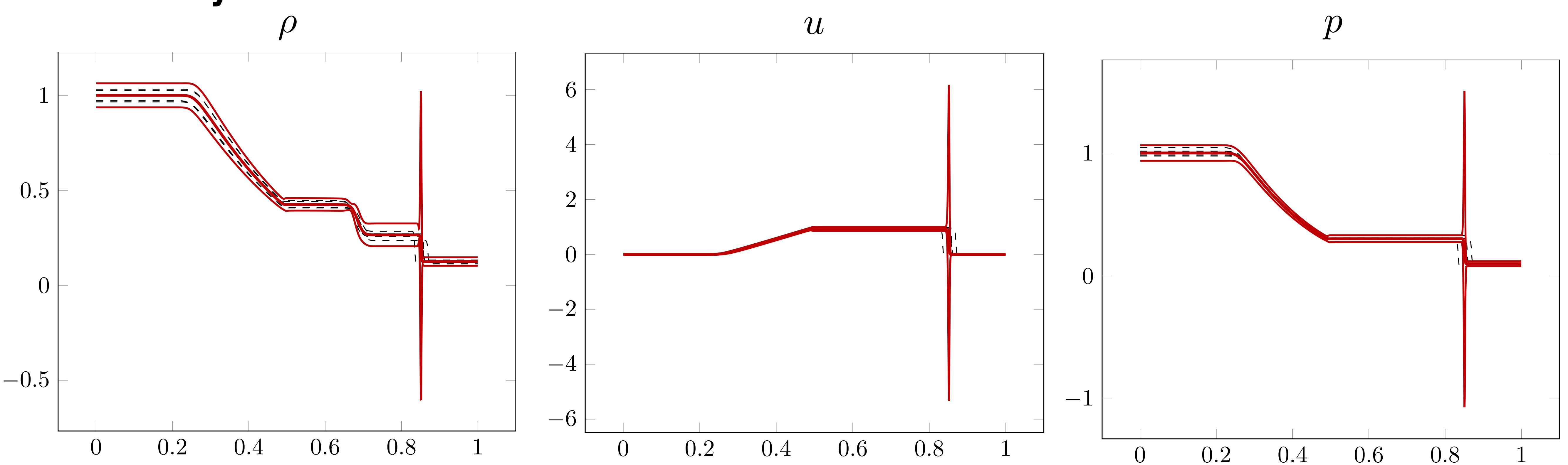
Since the covariance matrix is diagonal, the previous estimate is simplified:

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

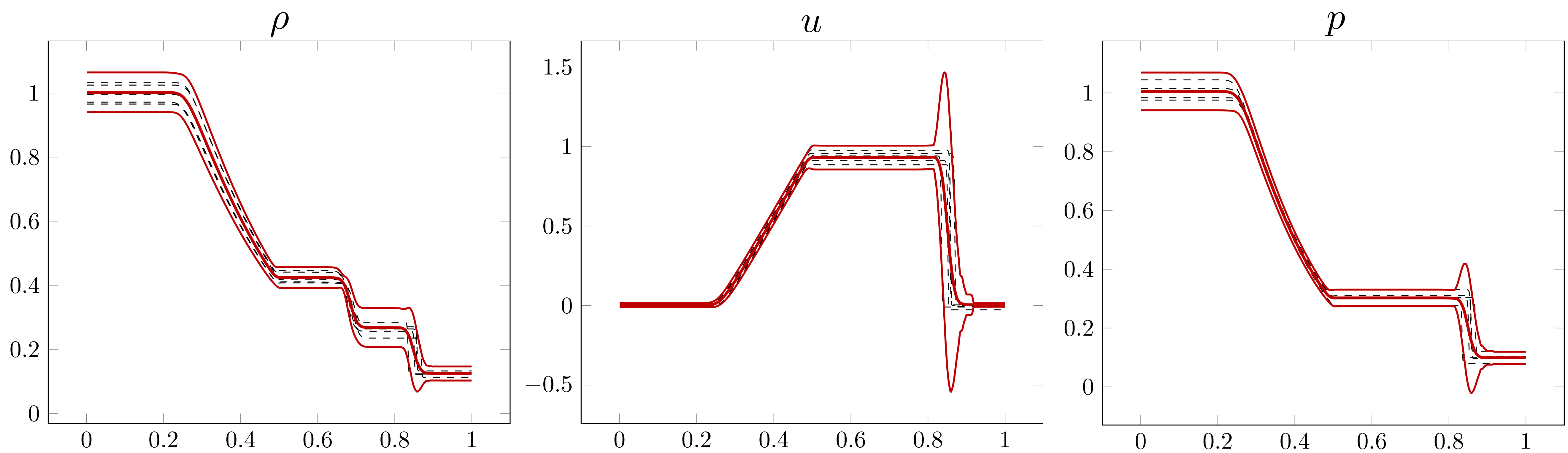
Monte Carlo method:



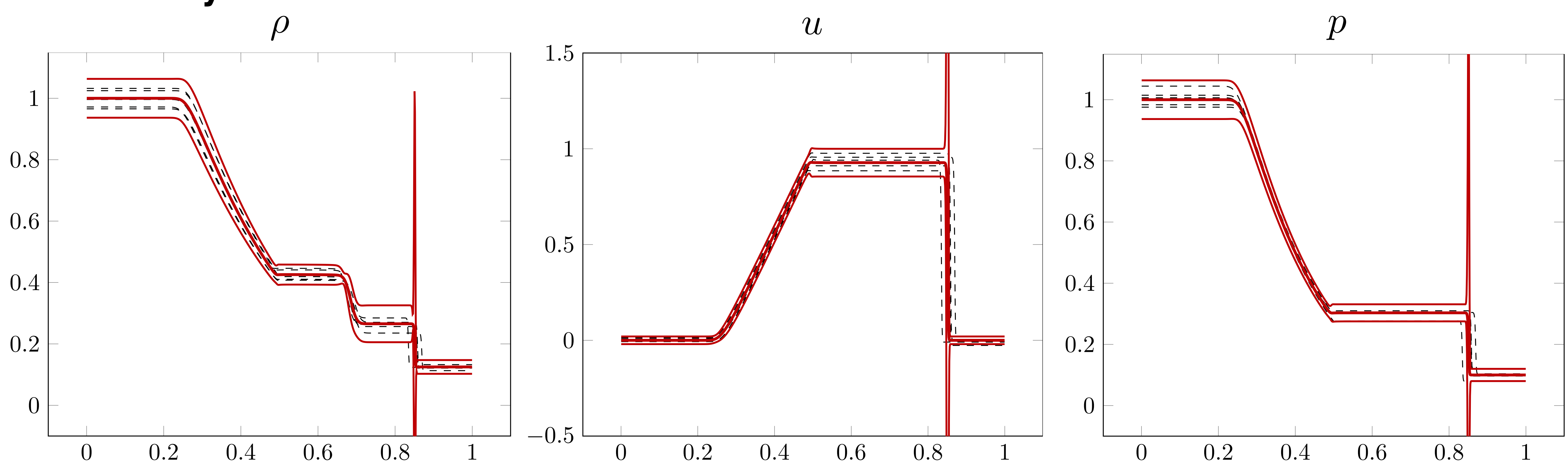
Sensitivity method without correction:



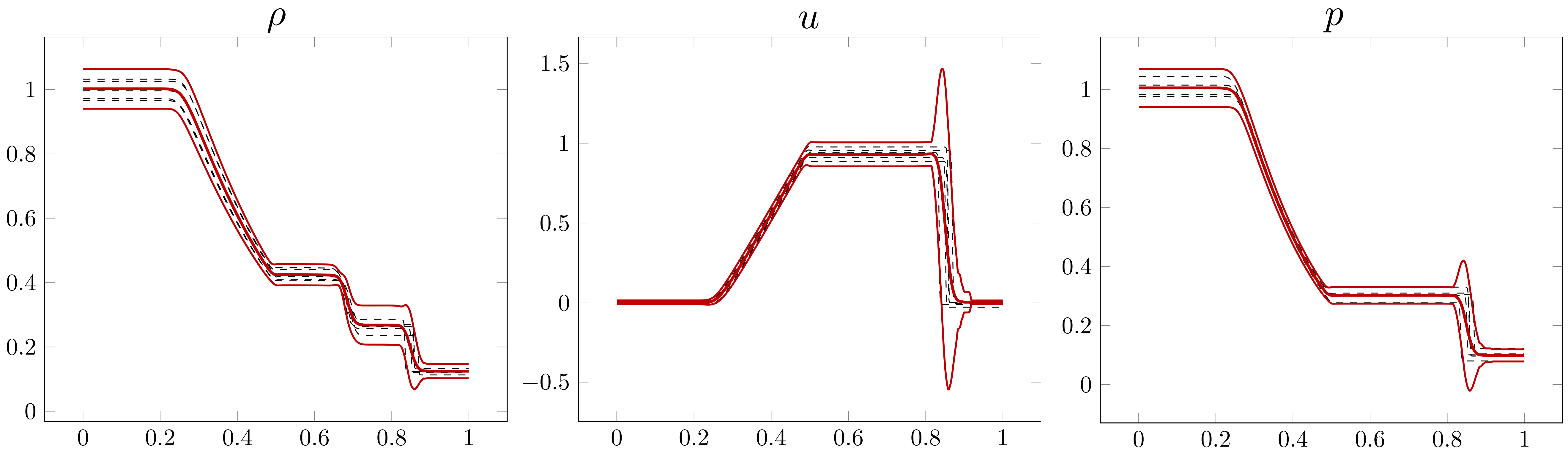
Monte Carlo method:



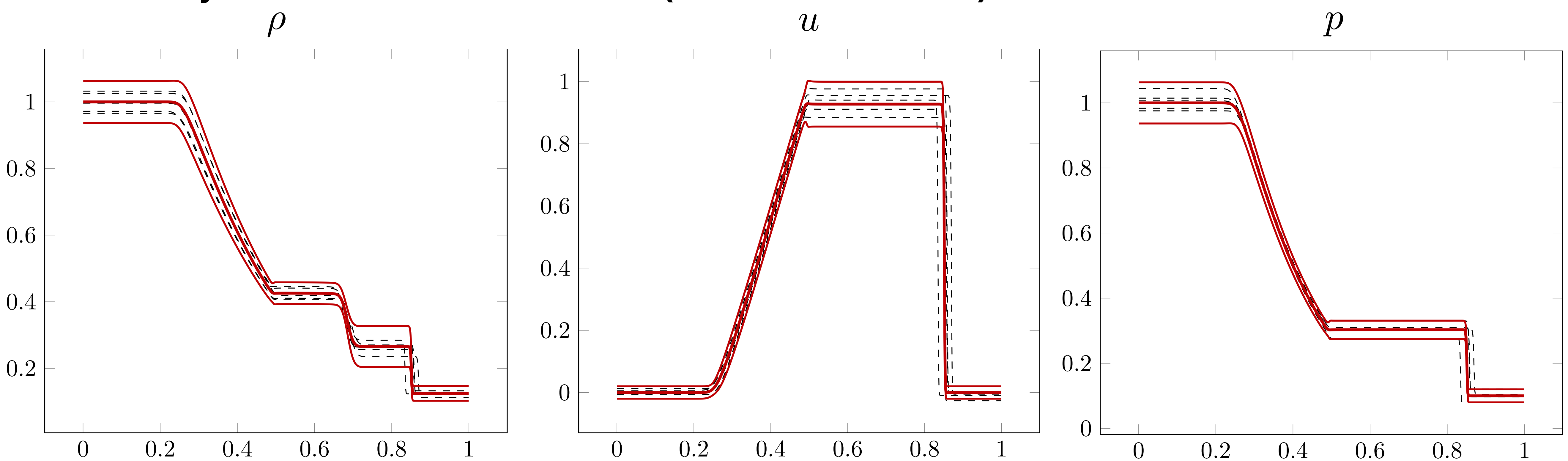
Sensitivity method without correction:



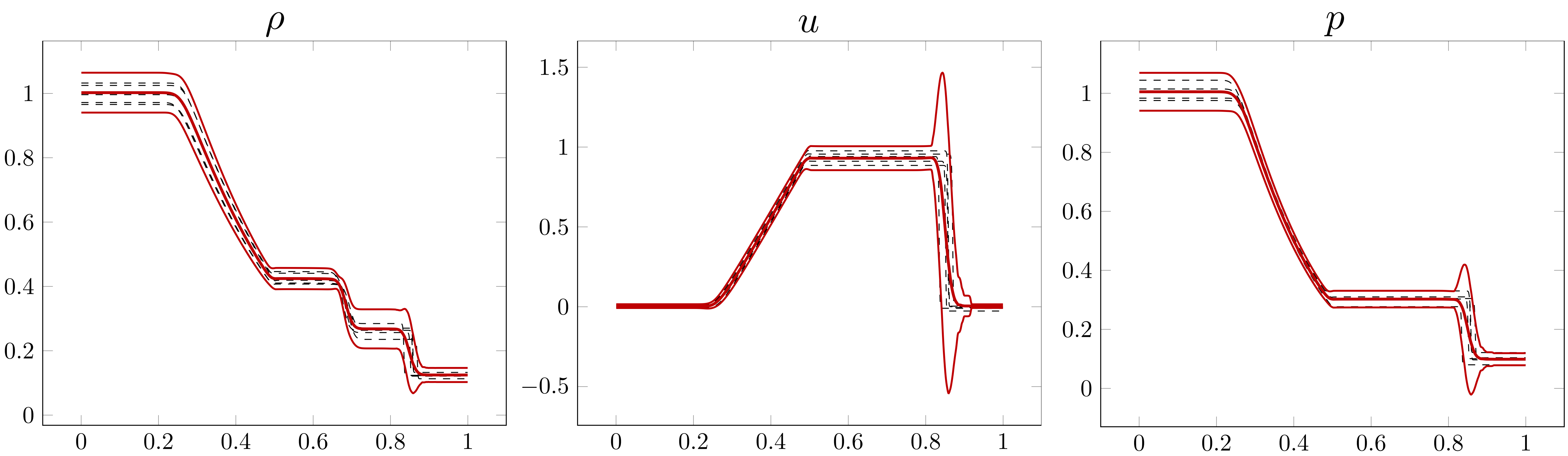
Monte Carlo method:



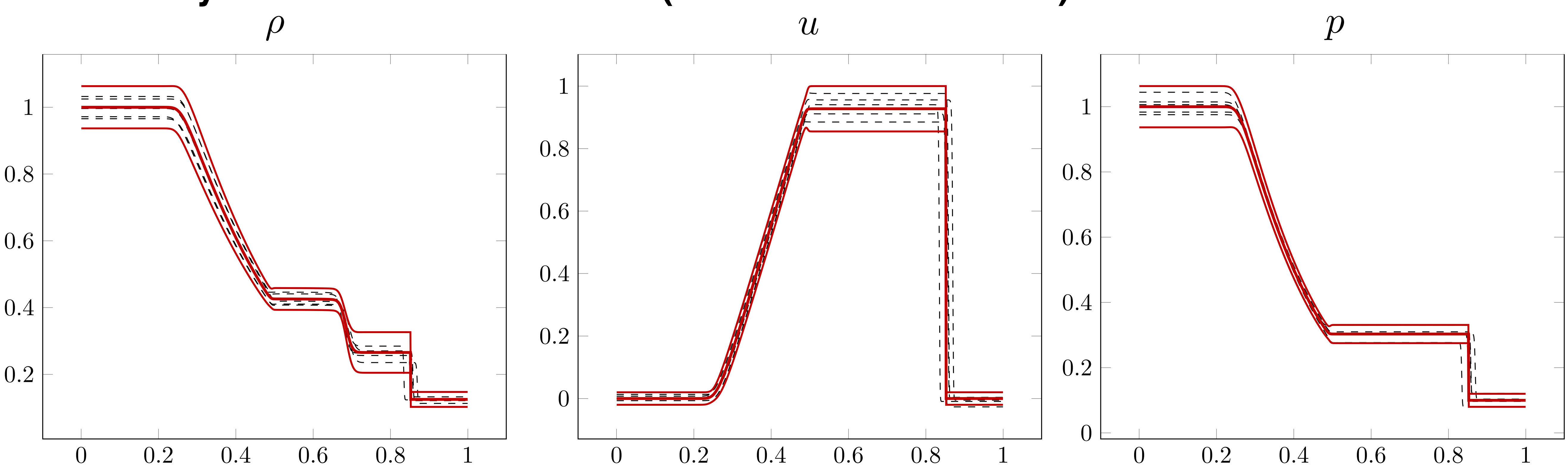
Sensitivity method with correction (diffusive method):



Monte Carlo method:



Sensitivity method with correction (anti-diffusive method):

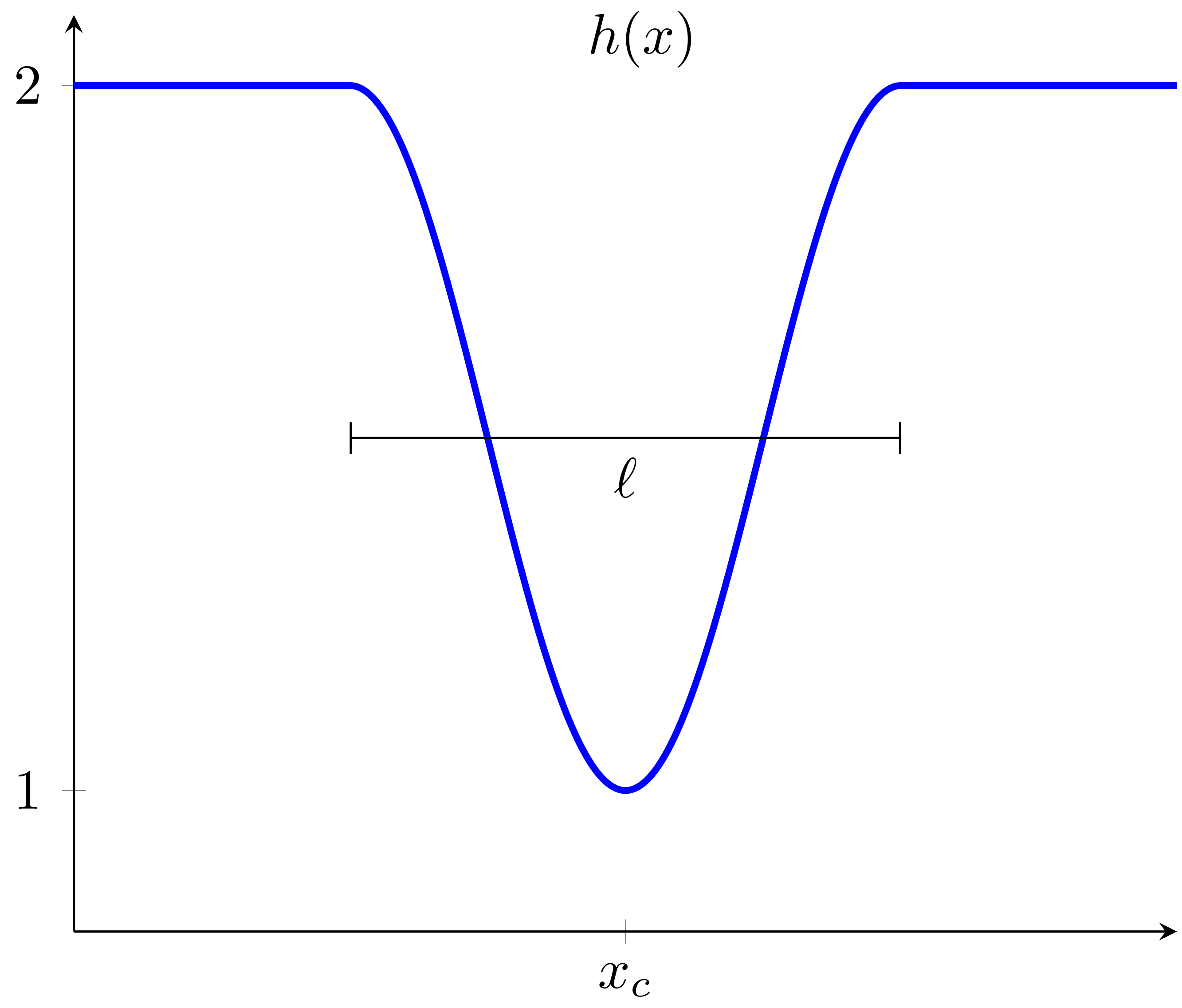


Optimization

The quasi-1D Euler equations are:

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

+b.c.



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

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

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

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

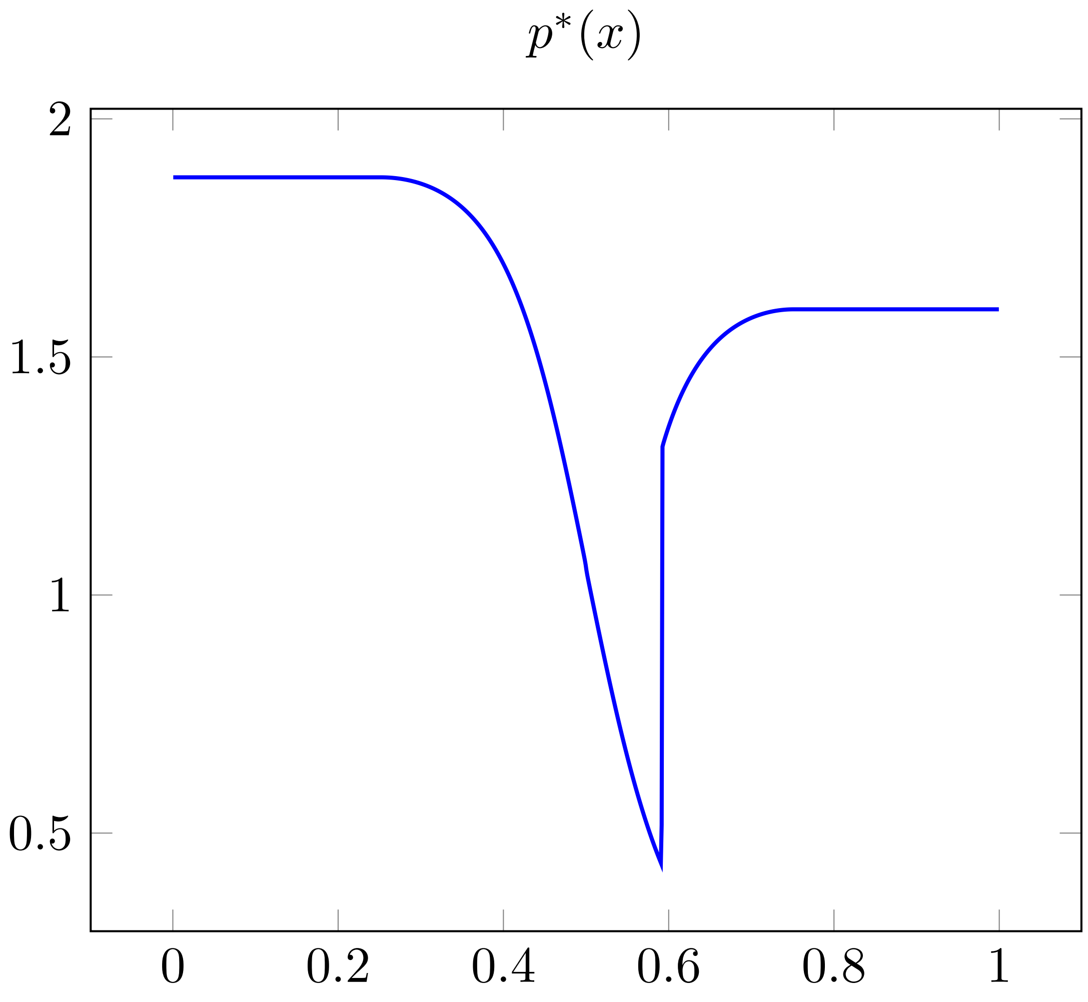
Optimization problem: $\min_{\mathbf{a}\in\mathcal{A}} J(\mathbf{U})$ subject to (1).

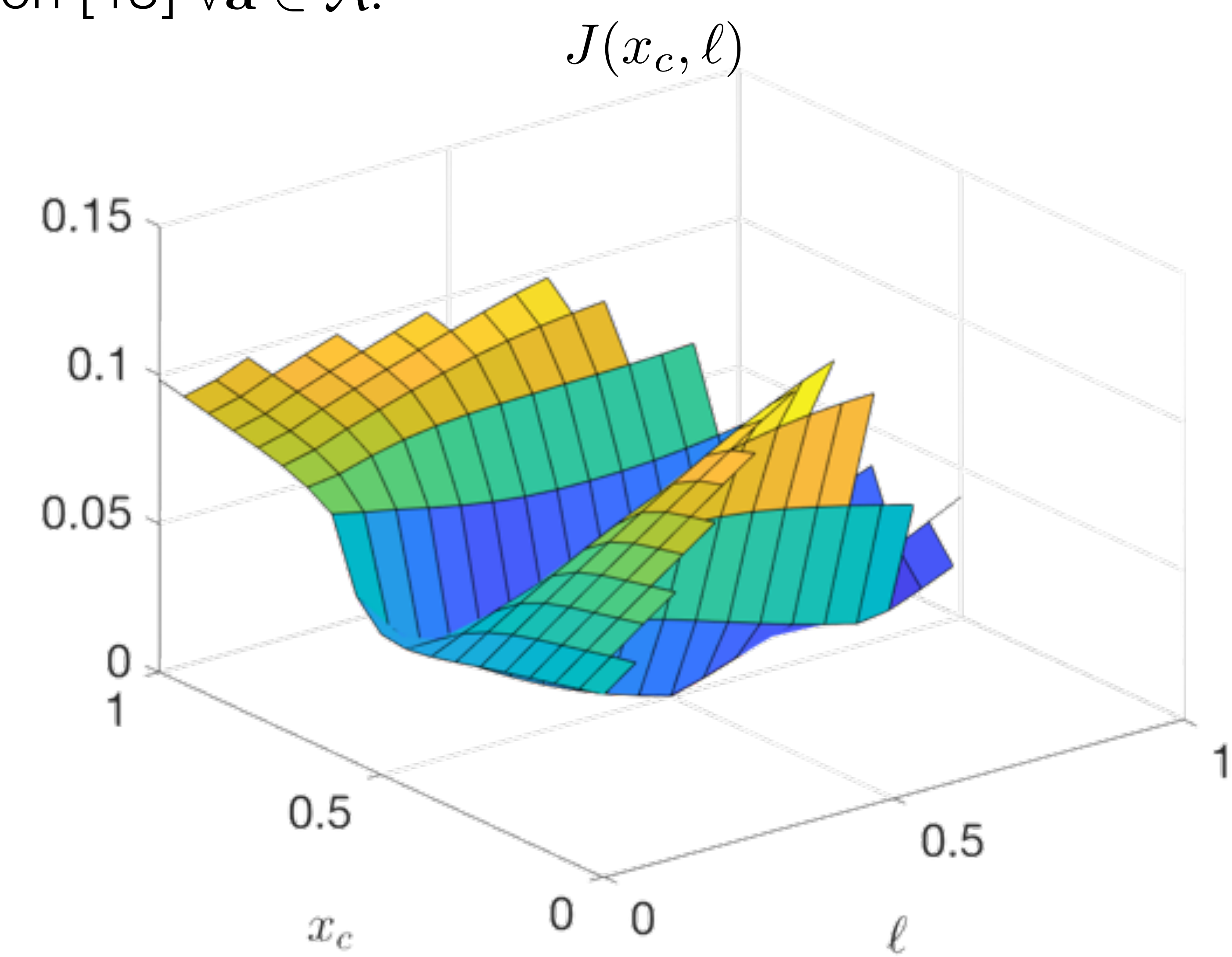
Boundary conditions:

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

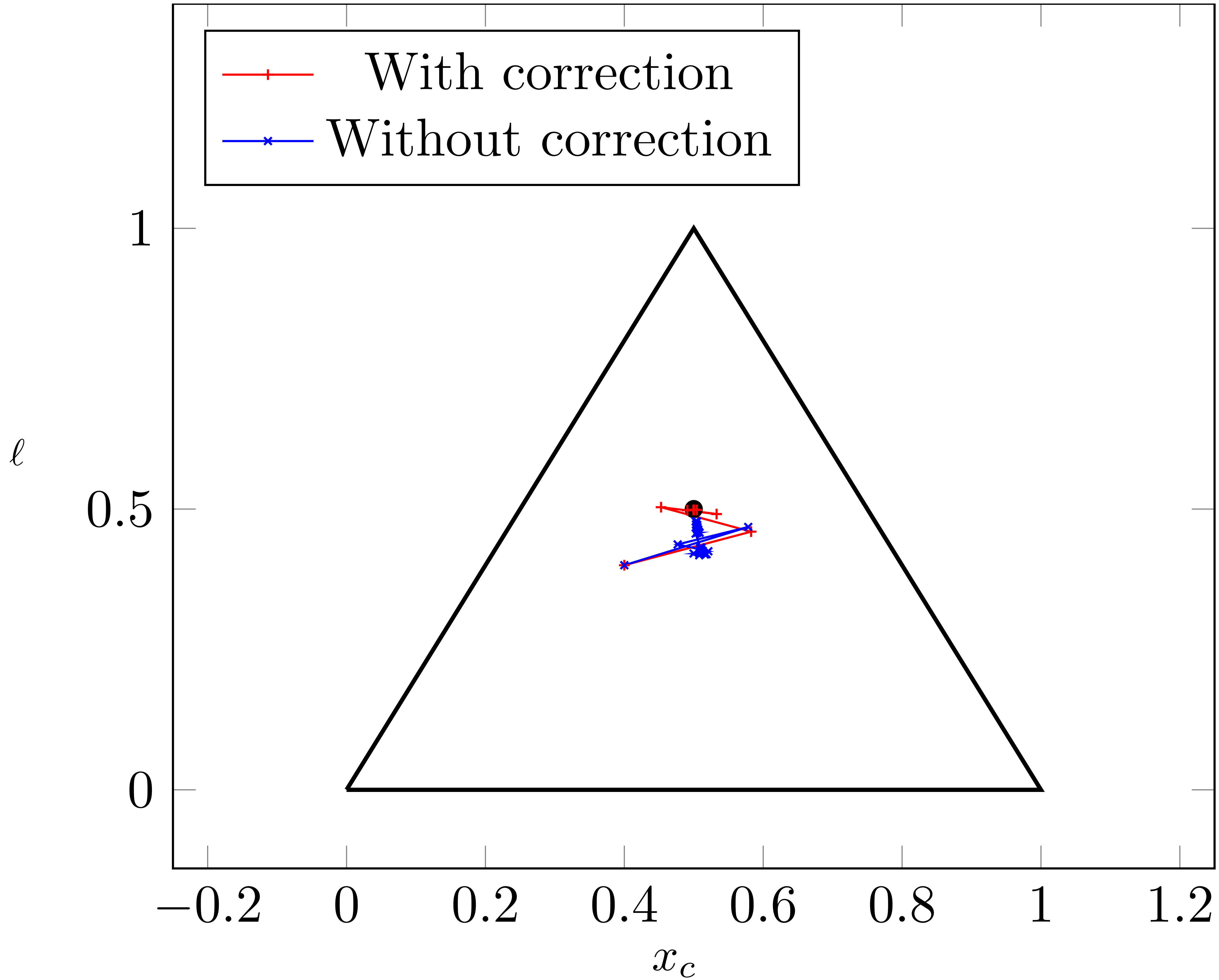
$$\begin{cases} H &= E + \dfrac{p}{\rho}, \\ p &= (\gamma - 1)\left(\rho E - \dfrac{1}{2}\rho u^2\right), \\ p_{tot} &= p + \dfrac{1}{2}\rho u^2. \end{cases}$$

These b.c. provide a discontinuous solution [13] $\forall \mathbf{a} \in \mathcal{A}$.

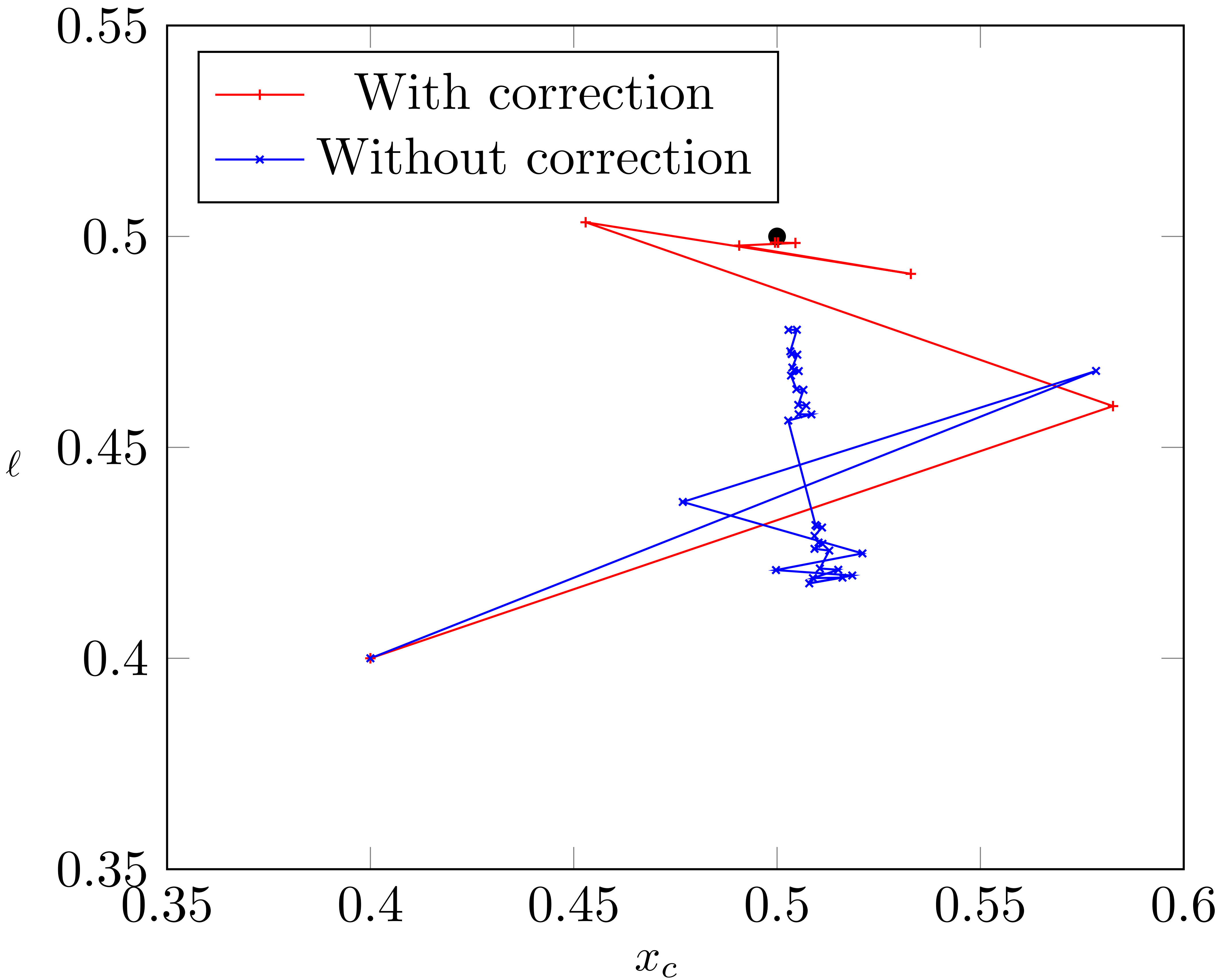


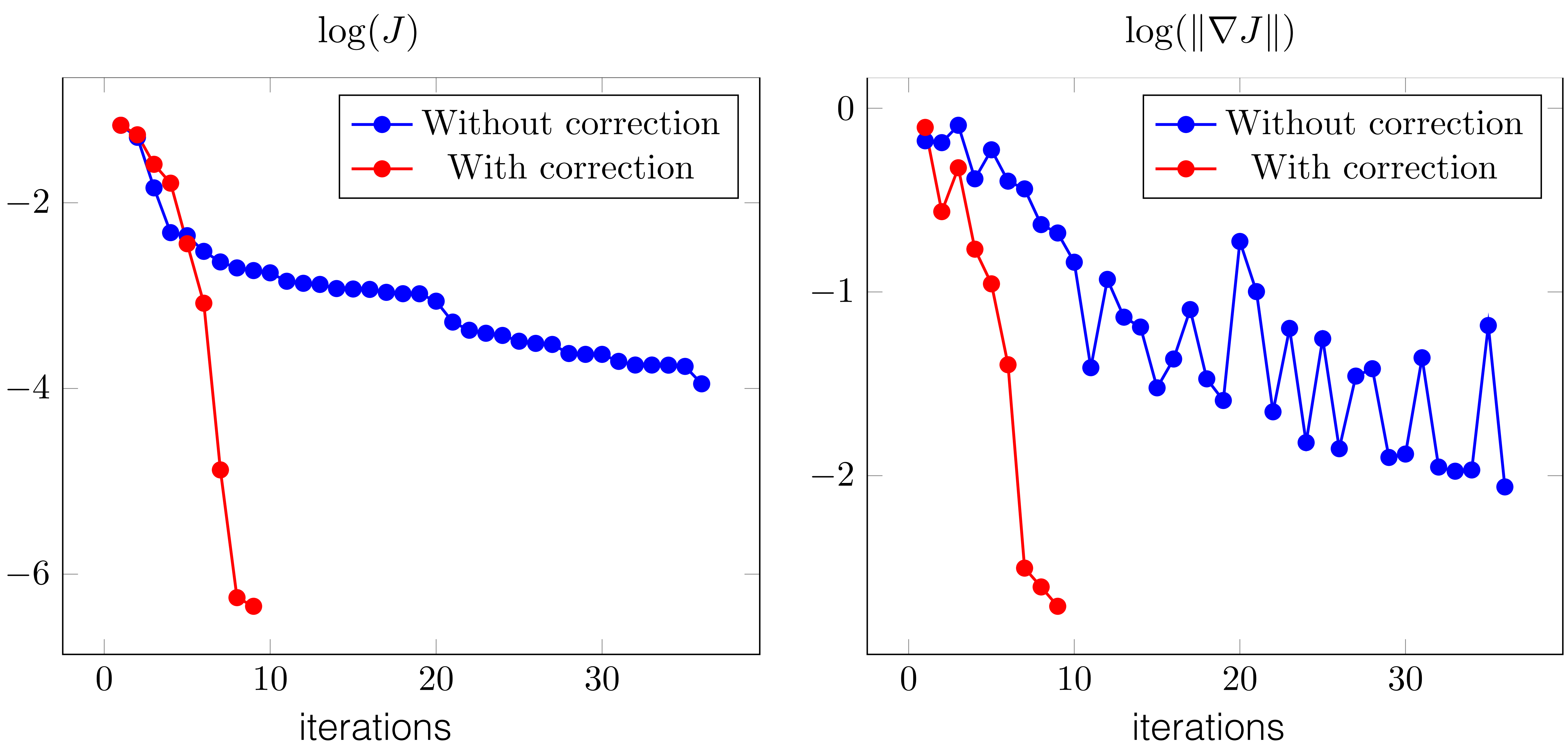


[13] Giles, M. B., & Pierce, N. A. (2001). Analytic adjoint solutions for the quasi-one-dimensional Euler equations. *Journal of Fluid Mechanics*, *426*, 327-345.


With correction
Without correction
1
0.5
0
−0.2
0
0.2
0.4
0.6
0.8
1
1.2
ℓ
x_c

Optimization





$\log(J)$
Without correction
With correction
−2
−4
−6
0
10
20
30
iterations
$\log(\|\nabla J\|)$
Without correction
With correction
0
−1
−2
0
10
20
30
iterations

Conclusion and perspective

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:

- Estimate of the variance of the shock position
- Effects of the numerical diffusion for the applications
- Extension to 2D
- Extension to different PDEs systems

Thank you

for your attention!