Output-Based Error Estimation and Adaptation for Uncertainty Quantification

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Outline

1. Introduction
2. Discretizations
3. Error Estimation
4. Results
5. More Stochastic Dimensions
6. Conclusions and Future Work

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Introduction

Uncertainty Quantification for Computer Simulations

- Needed when PDE-governed system has uncertainty due to random inputs
- Includes propagating uncertainty to outputs efficiently
- Used for design, optimization, and characterization

Output-based adaptive methods

- Provide accurate outputs with efficient use of computing resources
- Return estimates of error in output calculation

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Goal and Approach of this Work

Goal

To develop a nonintrusive method for output-based error estimation and adaptation in both deterministic and stochastic spaces

Approach

- Choose simulations to refine and new $\vec{\alpha}$'s to simulate
- Consider exact solution in deterministic ($\vec{x}$) and stochastic ($\vec{\alpha}$) spaces: $u(\vec{x}, \vec{\alpha})$
- Define statistical output $J(u(\vec{x}, \vec{\alpha}), \vec{x}, \vec{\alpha})$ (may include priors)
- Use deterministic adjoint and residual information for adaptation
- Restrict present study to one dimension in x and α and

$$J(y) \equiv \int f(y(u(x, \alpha)))d\alpha$$

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Deterministic Space

1D model problem

$$-\alpha \frac{\partial^2 u}{\partial x^2} + c\frac{\partial u}{\partial x} = S(x, \alpha)$$

- Solve via LDG method
  - $C_{11} = (p_x + 1)^2/h$
- DG test functions $\phi_H^i(x) \in \mathcal{P}^{p_x}$
- Solution $u_H(x) \in \mathcal{P}^{p_x}$ s.t. $R_H^x(u_H, \phi_H^i) = 0, \quad \forall i$

Dual problem

- Define output $y(u(x))$
- Adjoint equation

$$\frac{\partial R_H^x}{\partial u_H}^T \psi_H = \frac{\partial y_H}{\partial u_H}^T$$

- Solved by inverting the Jacobian-transpose
- LDG is dual-consistent

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Deterministic Space

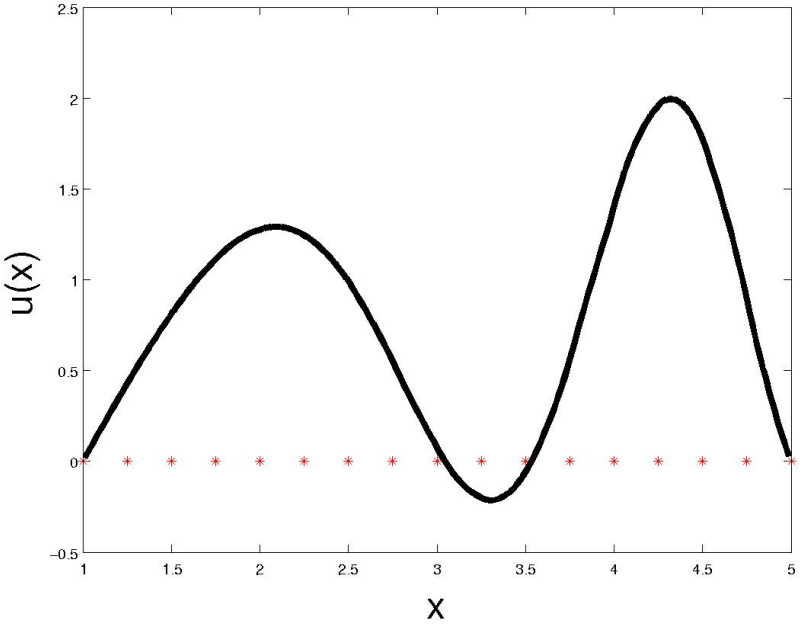
$$c = 5, \alpha = 2.11$$

$$S = \frac{4}{25}\alpha^3 x^2 \sin(\alpha x^2/5) - \frac{2}{5}\alpha^2 \cos(\alpha x^2/5) + \frac{\alpha}{x^2} + \frac{2}{5}\alpha c x \cos(\alpha x^2/5) + \frac{c}{x}$$

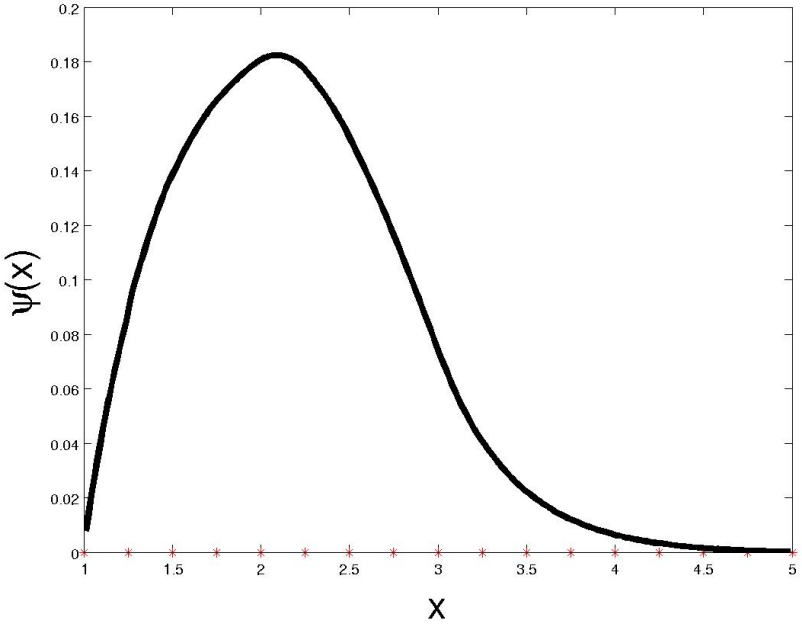
For $x \in [1, 5]$, BC: $u(1, \alpha) = u(5, \alpha) = 0$, with $N_x = 16$ elements, $p_x = 2$

$$y = \int_2^3 u(x)dx = 0.874$$

Example solution



Example dual solution



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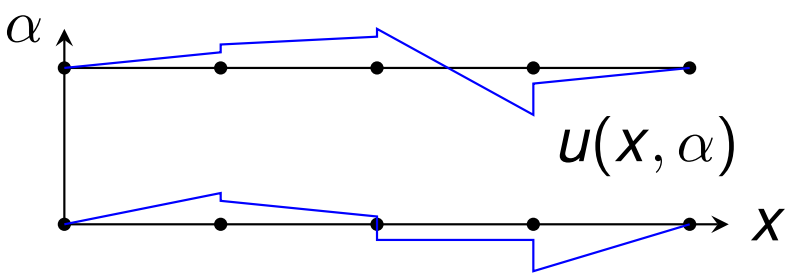
Stochastic Space

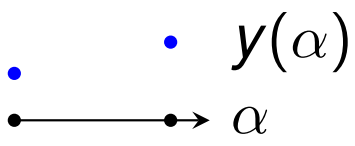
Parameters

- Consider parameters of PDE, e.g. μ, c
- Each parameter yields another dimension of $u(\vec{x}, \vec{\alpha})$
- Collocation in $\vec{\alpha}$: nonintrusive, but sabotages dual-basis

Solution and Output

- Interpolate $u(\vec{x})$ in $\vec{\alpha}$-space in tensor-product fashion
- Statistical output $J(y(\vec{\alpha}))$ defined over entire parameter space
  - e.g. std. dev. of performance, probability of failure





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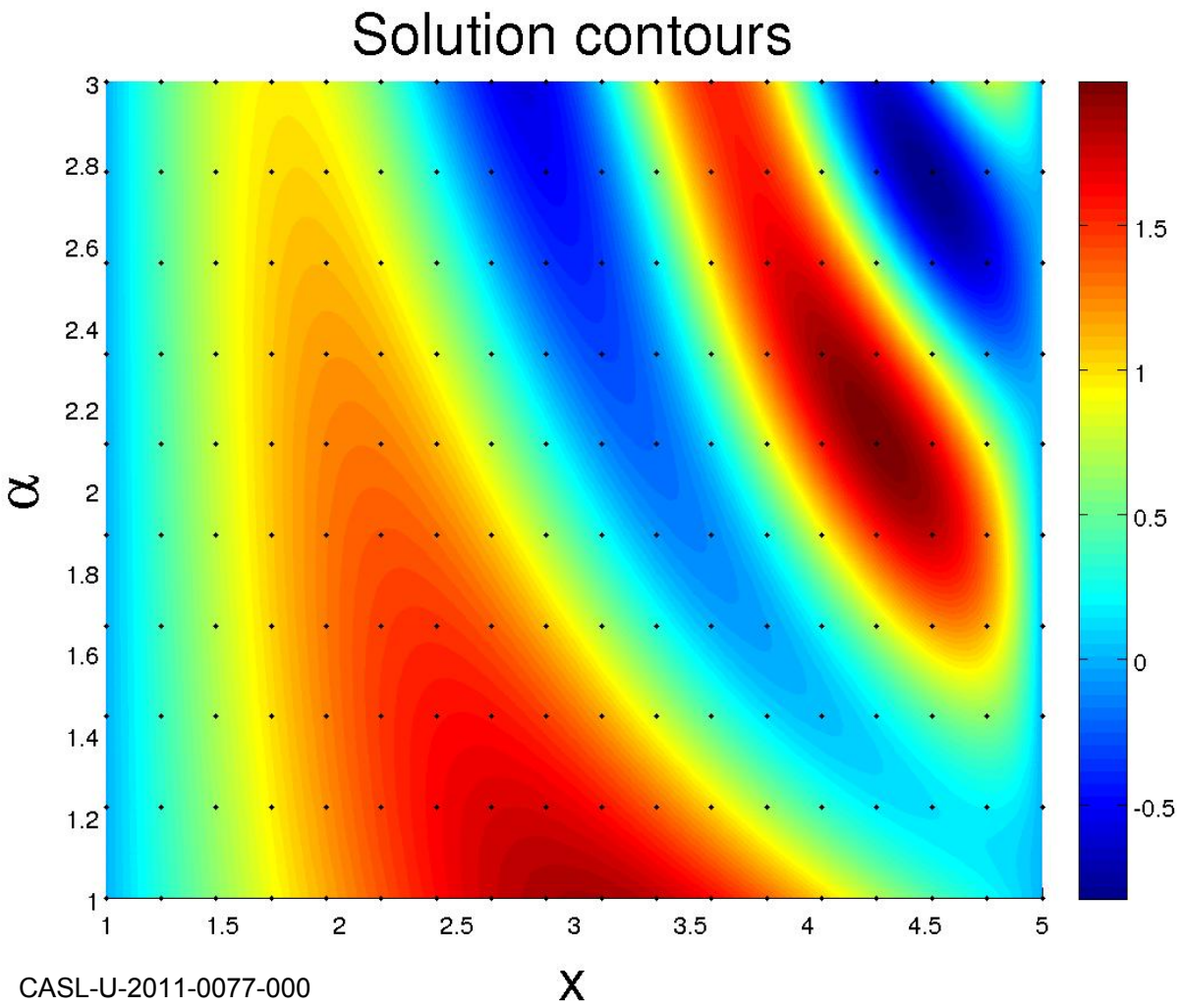
Stochastic Space

$$J = \int_1^3 y(\alpha) d\alpha = 1.8462$$



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Discrete DWR

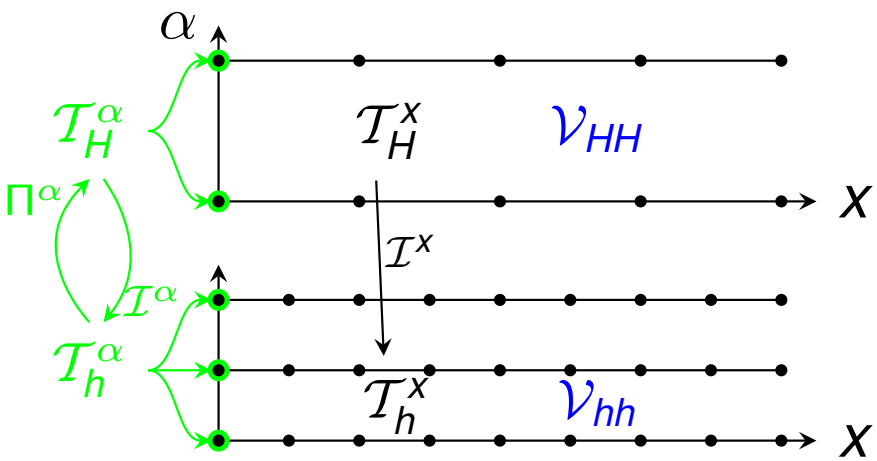
Output, correction, and error estimate

$$J = \sum_i w_i \, f(y(\alpha_i)), \quad \alpha_i \in \mathcal{T}_H^\alpha$$

$$\Delta J = \sum_i w_i \, \frac{\partial f_h}{\partial y_{h,i}} \, [\mathcal{I}^x \mathcal{I}_i^\alpha \psi_{HH}]^T \; R_h^x(\mathcal{I}^x \mathcal{I}_i^\alpha u_{HH}; \alpha_i), \quad \alpha_i \in \mathcal{T}_h^\alpha$$

$$\delta J = \sum_i w_i \, \frac{\partial f_h}{\partial y_{h,i}} \, [\psi_{hh} - \mathcal{I}^x \mathcal{I}_i^\alpha \psi_{HH}]^T \; R_h^x(\mathcal{I}^x \mathcal{I}_i^\alpha u_{HH}; \alpha_i), \quad \alpha_i \in \mathcal{T}_h^\alpha$$

- $\psi_{hh} \approx \left(\frac{\partial R_h^x(\mathcal{I}^x \mathcal{I}_i^\alpha u_{HH}; \alpha_i)}{\partial u_h} \right)^{-T} \frac{\partial y_h}{\partial u_h}^T$
- $w_i =$ integration weights for trapezoid rule



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Continuous DWR

Correction and error estimate

$$\Delta J = \sum_q w_q \frac{\partial f_h}{\partial y_{h,q}} \left[\mathcal{I}^x \mathcal{I}_q^\alpha \psi_{HH}\right]^T R_h^x(\mathcal{I}^x \mathcal{I}_i^\alpha u_{HH}; \alpha_q)$$

$$\delta J = \int f'[y] \left(\mathcal{R}^x \left(u_{HH}, \psi - \psi_{HH}; \alpha\right)\right) d\alpha$$

$$\approx \sum_q w_q \frac{\partial f_h}{\partial y_{h,q}} \left[\psi_{hh} - \mathcal{I}^x \mathcal{I}_q^\alpha \psi_{HH}\right]^T R_h^x(\mathcal{I}^x \mathcal{I}_q^\alpha u_{HH}; \alpha_q)$$

- $\psi_{hh} \approx \left(\frac{\partial R_h^x(\mathcal{I}^x \mathcal{I}_q^\alpha u_{HH}; \alpha_q)}{\partial u_h}\right)^{-T} \frac{\partial y_h}{\partial u_h}^T$
- α_q, w_q = LGL integration points and weights

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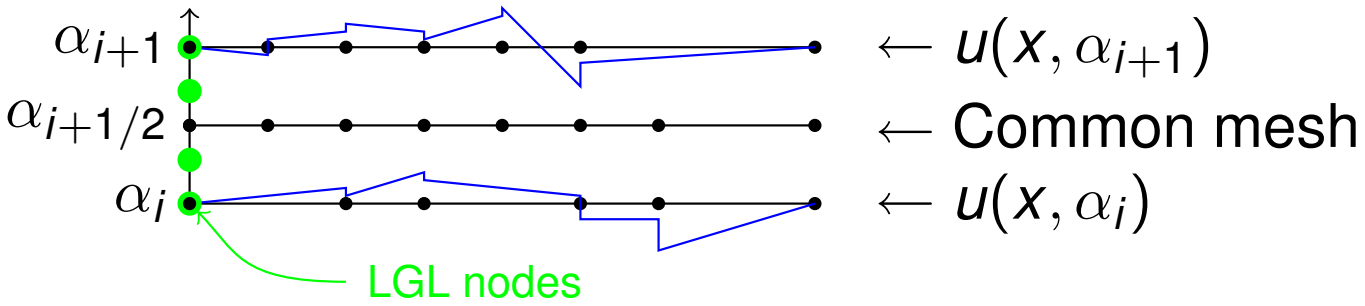
Calculating $R_h^x(\cdot;\alpha_i)$

A common mesh

- Use common mesh within α-slabs
- Tree structure: common mesh = "maximum" mesh
- Intrusiveness: transfer (inject) solutions between meshes



Evaluating residuals

- Discrete (Collocation): if splitting α-slabs, need $R_h^x(\cdot;\alpha_{i+1/2})$
- Continuous (FEM): need to evaluate R_h^x at quad-points α_q

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Adjoint Reconstruction

Correction

- ψ_{HH} ($p_\alpha = 1$: linear interp. in α) injected onto $\mathcal{V}_{hh}$

Error estimate: reconstructing ψ_{hh}

Solve for $\psi(x, \alpha_i)$ exactly	ψ_{hh}
Interpolate ψ_{HH} in x and α	$\tilde{\mathcal{I}}^x \tilde{\mathcal{I}}^\alpha \psi_{HH}$
Solve from appx. fine Jacobian	$\left(\frac{\partial R_h^x(\mathcal{I}^x \mathcal{I}_i^\alpha u_{HH};\alpha_i)}{\partial u_h}\right)^{-T} \frac{\partial y_h}{\partial u_h}^T$
Solve from coarse Jac., interp. in x	$\tilde{\mathcal{I}}^x \left[\left(\frac{\partial R_H^x(\mathcal{I}_i^\alpha u_{HH};\alpha_i)}{\partial u_H}\right)^{-T} \frac{\partial y_H}{\partial u_H}^T\right]$

- New Jacobian assembly or interpolate it in α
- Actually use $\delta\psi = \mathcal{I}^\alpha \left(\Pi^\alpha \psi_{hh} - \mathcal{I}^x \psi_{HH}\right)$ so that $\delta\psi \neq 0$ at α_i, α_{i+1}

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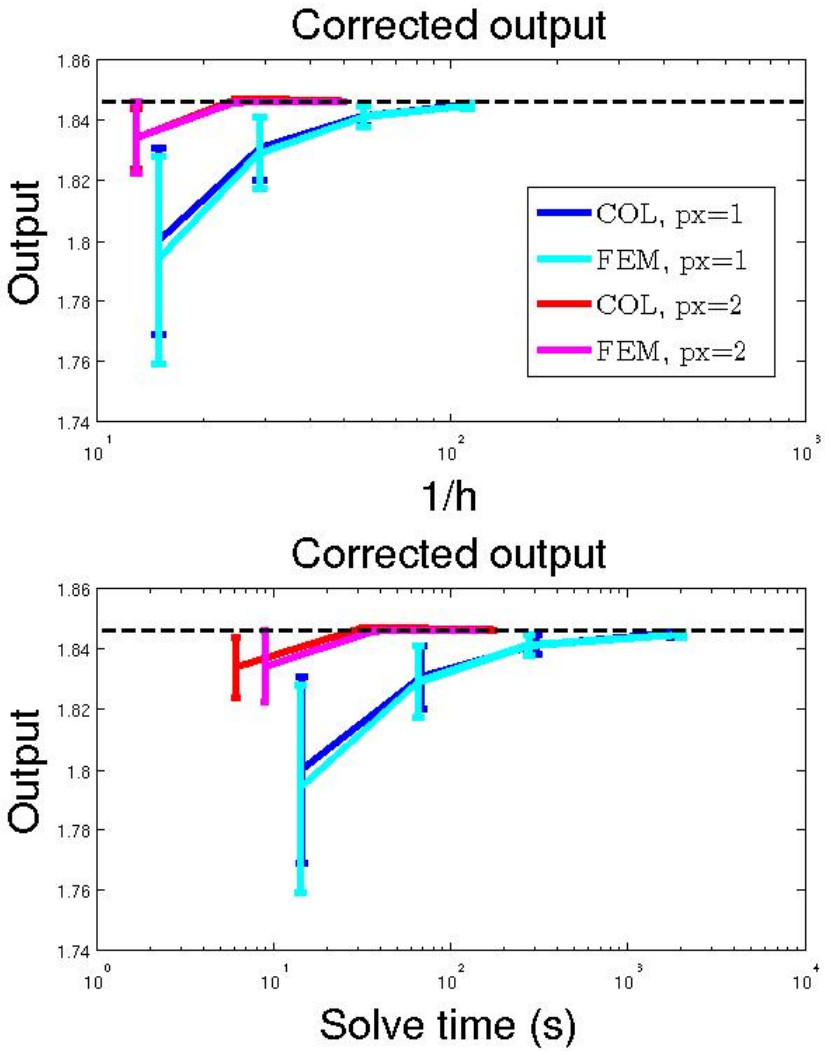
Adjoint Reconstruction



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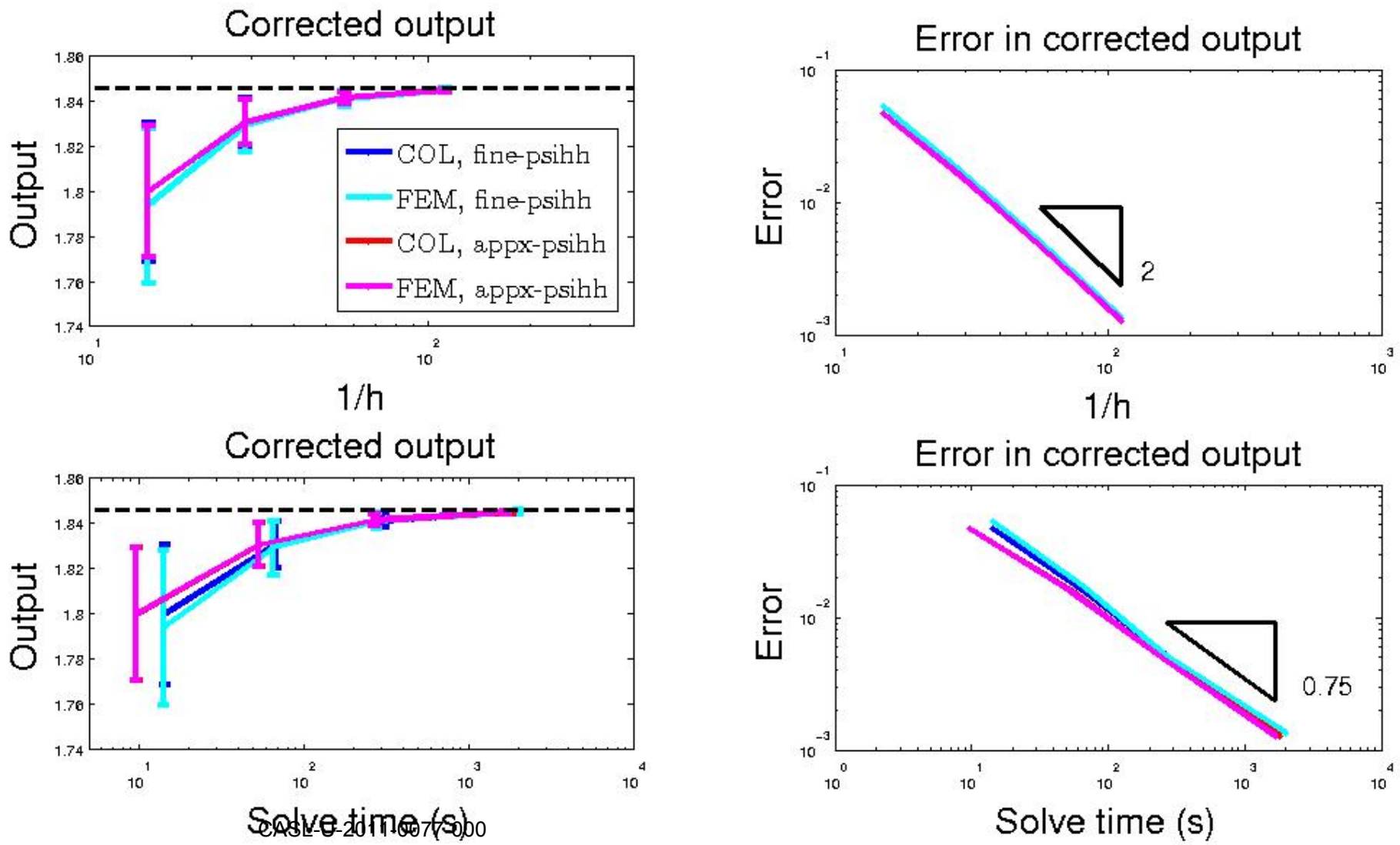
Adjoint Reconstruction

$p_x = 1$



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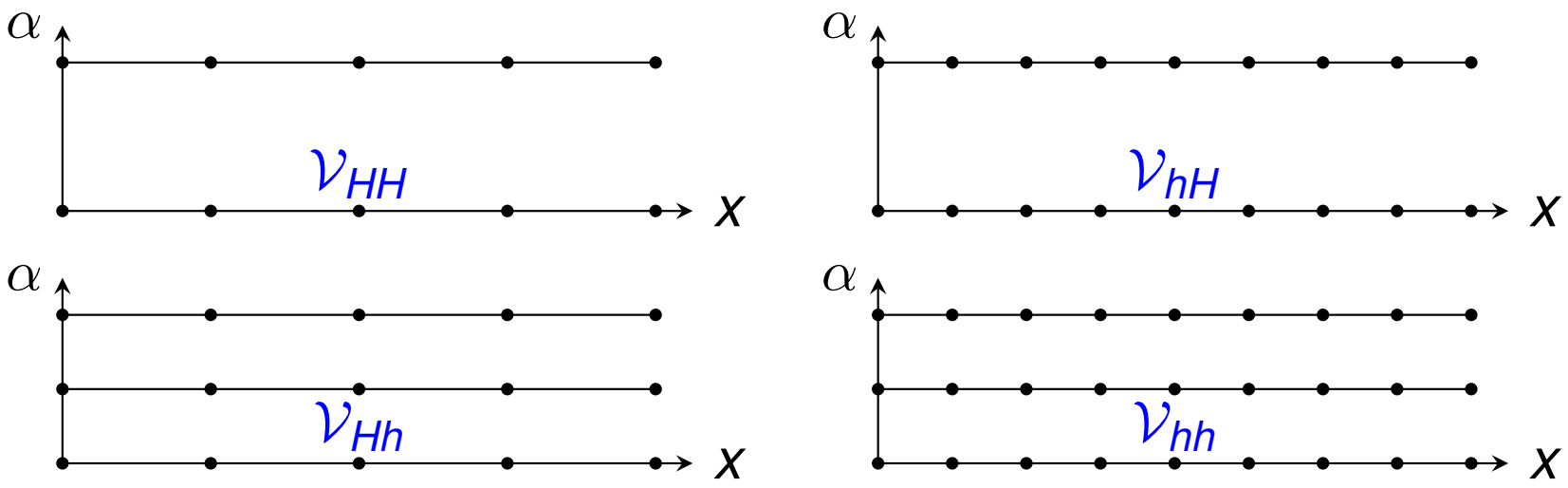
x-α Splitting

- Error estimate for a specific fine space $\rightarrow$ fraction of error
  - x-only: refine x-meshes
  - α-only: new simulations (same x-mesh)
- No error contamination
- Used for efficient anisotropic adaptation



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Adaptive Indicators: Other Methods

- Interpolation error in
  - x: single simulation, fine x-mesh
  - α: interp. of u on coarse x-mesh at $\alpha_{i+1/2}$
- Residuals
  - x: $R_h^x(\mathcal{I}^x u_{HH}; \alpha_i),\ \alpha_i \in \mathcal{T}_H^\alpha$ (old sims on fine mesh)
  - α: $R_H^x(\mathcal{I}_i^\alpha u_{HH}; \alpha_i),\ \alpha_i \in \mathcal{T}_h^\alpha$ (resid. at new α: no eqn. in α)
- Jumps in
  - x: u_{HH} across x-elements
  - α: nearby u_{HH} at $\alpha_{i+1/2}$ (assumes smoothness of jumps; no eqn. or jumps in α)

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Refinement Strategy

Allocating DOFs

- Split x-elements or α-slabs in half
- $C(\{(\alpha_i, \mathcal{T}_j); \alpha_{k+1/2}\})$ = DOFs actually solved for
- Work growth: $C^n \leq f_g C^{n-1}$
- Choosing $\{(i,j); k\}$: knapsack problem
  - Nonlinear cost f'n: $C(\{(1,1),(1,2);\cdot\}) < C(\{(1,1),(2,2);\cdot\})$
  - No polynomial time algorithm for exact solution
  - Appx. sol'n: allocate x and α DOFs (f_α), then add extra x-elements (f_x)

Choosing mesh for $\alpha_{i+1/2}$

- Coarse mesh
- Common mesh, refine if surrounding elements are refined

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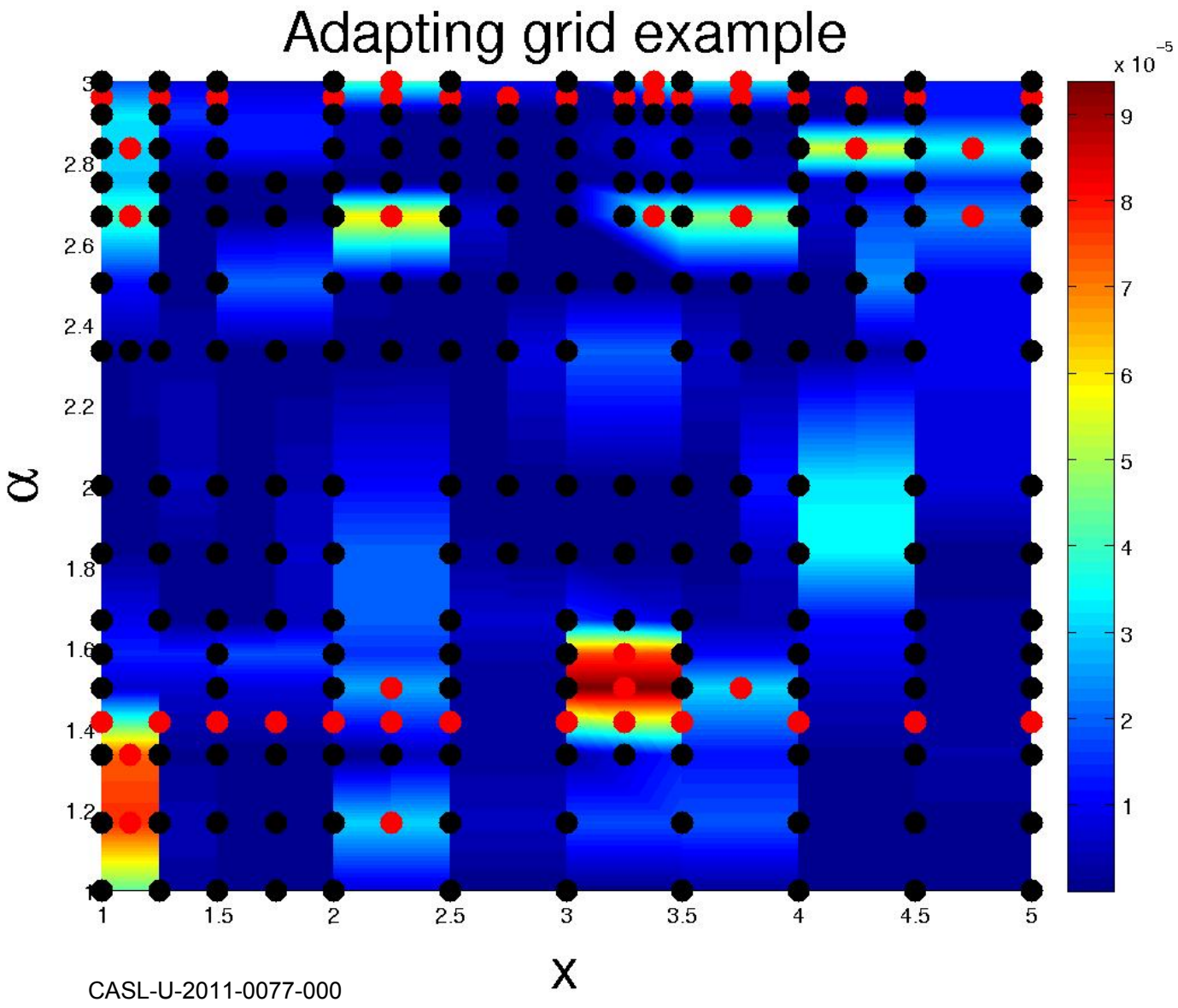
Refinement Strategy



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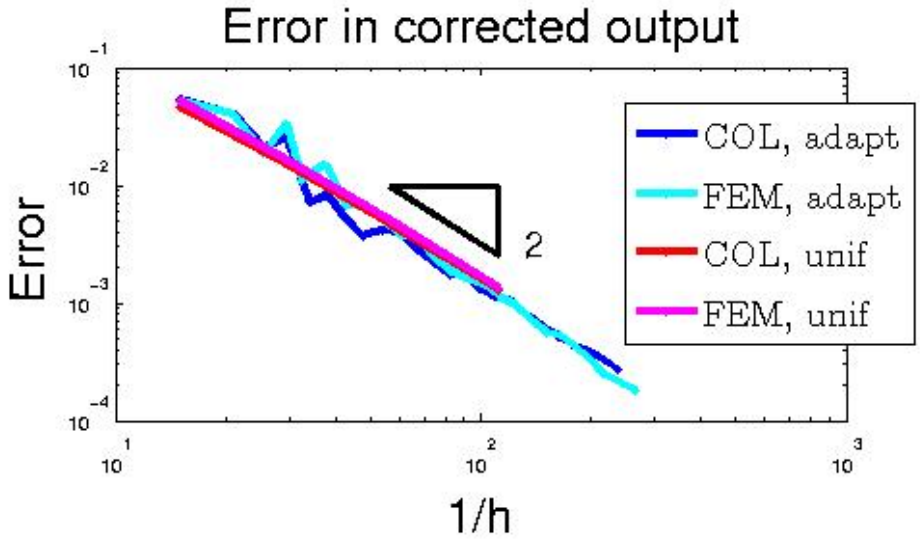
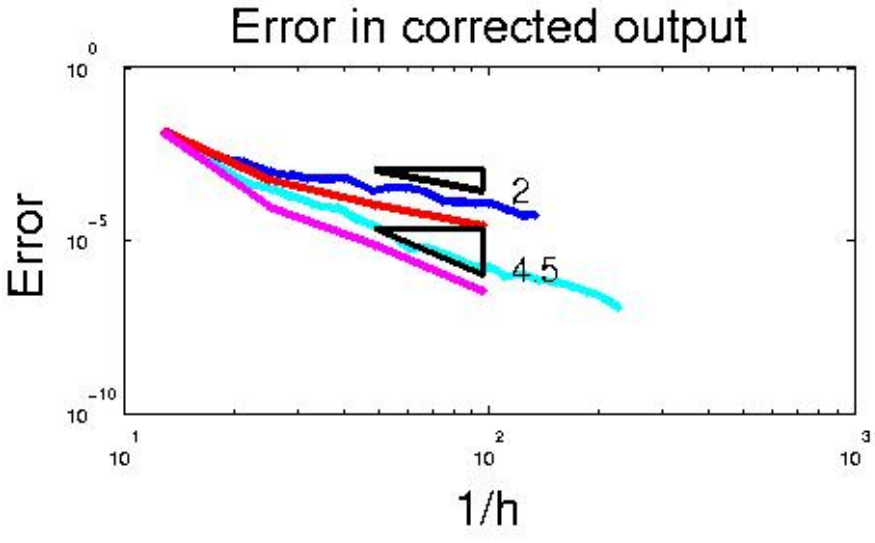
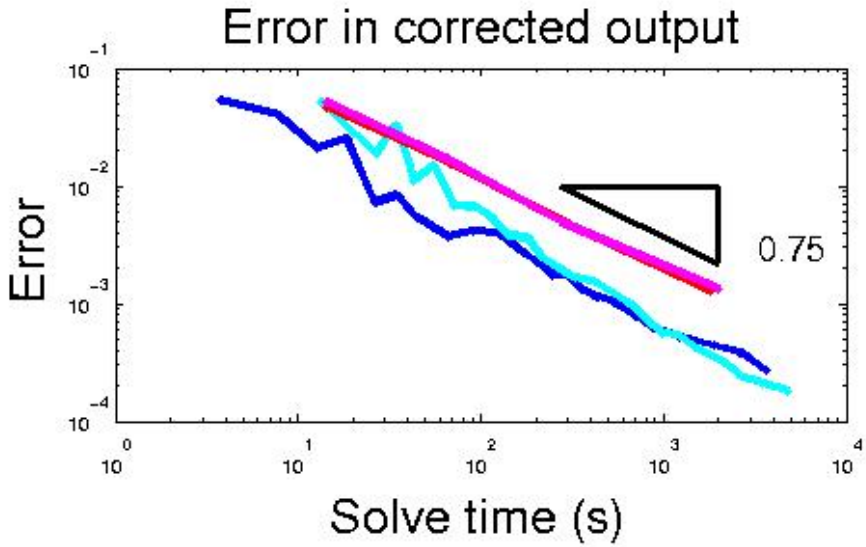
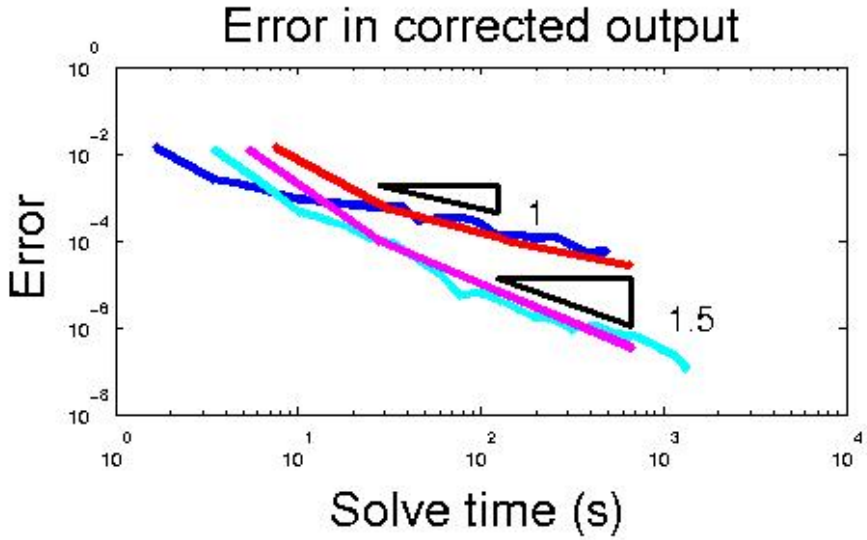






$p_x = 1, f_x = 0.5$



$p_x = 2, f_x = 0.5$

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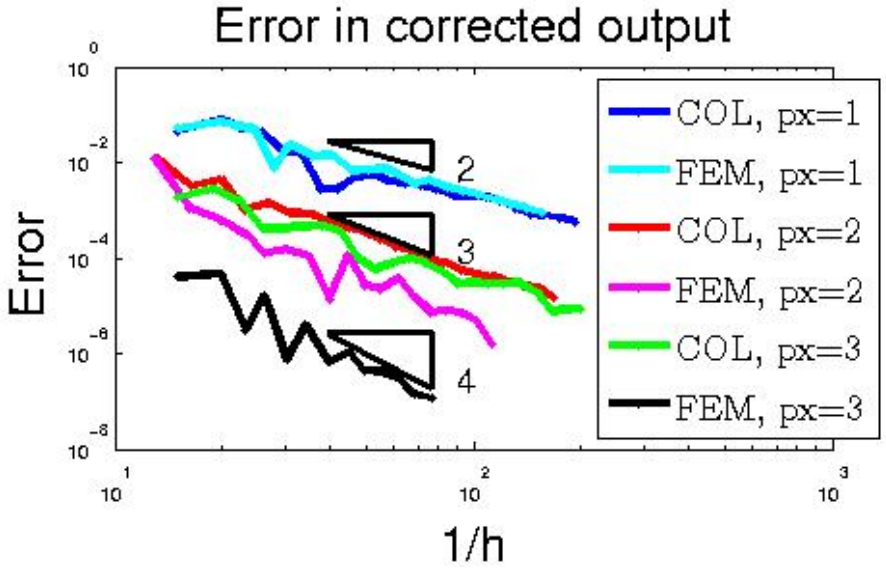
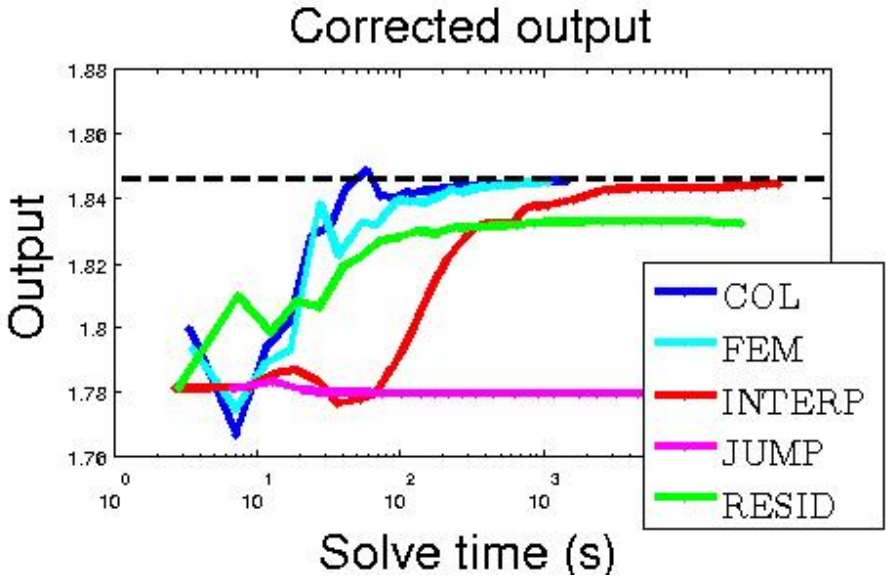
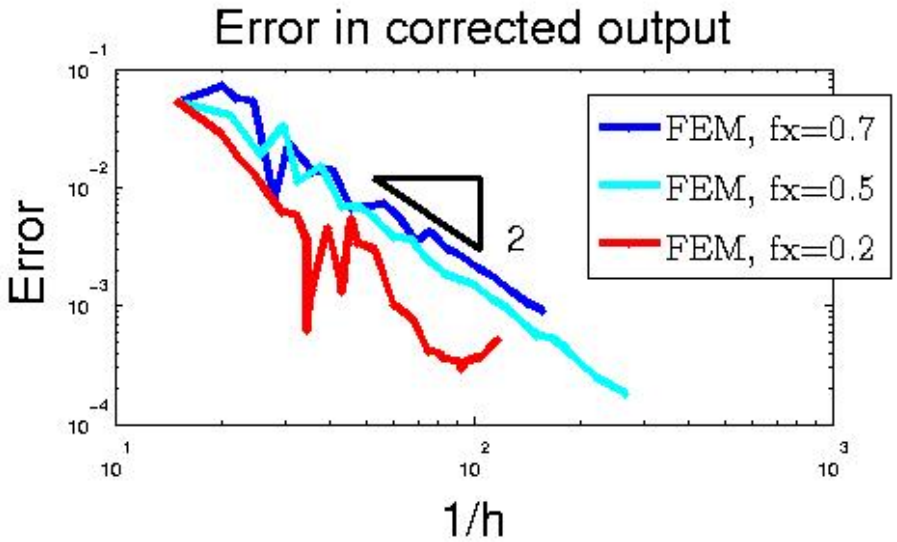


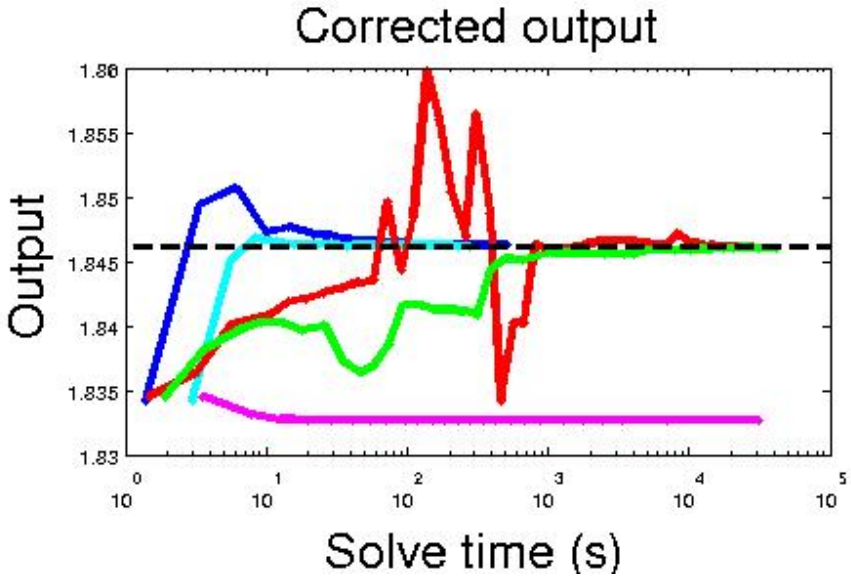
Discrete vs. continuous, $p_x = 1, 2, 3$



Other adaptation metrics, $p_x = 1$



Varying adaptation parameter, $p_x = 1$



Other adaptation metrics, $p_x = 2$

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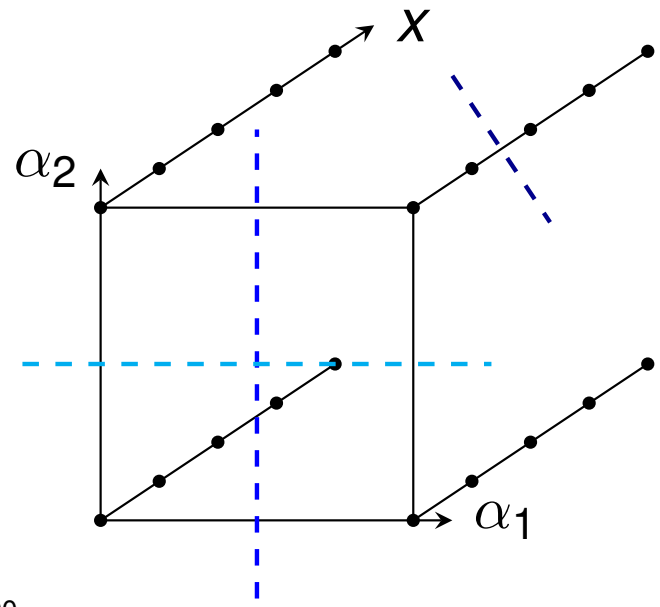
Two Stochastic Dimensions: Discretization and Results

- Tensor product grid for simplicity, adaptive
- Sparse grids give slightly better scaling with dimensionality

$$-\alpha_1 \frac{\partial^2 u}{\partial x^2} + (5 + \alpha_2 x)\frac{\partial u}{\partial x} = 1$$

Solved with $x \in [1, 5]$, $\alpha_1 \in [4, 5]$, $\alpha_2 \in [1, 2]$. BC: $u(1; \cdot) = u(5; \cdot) = 0$.



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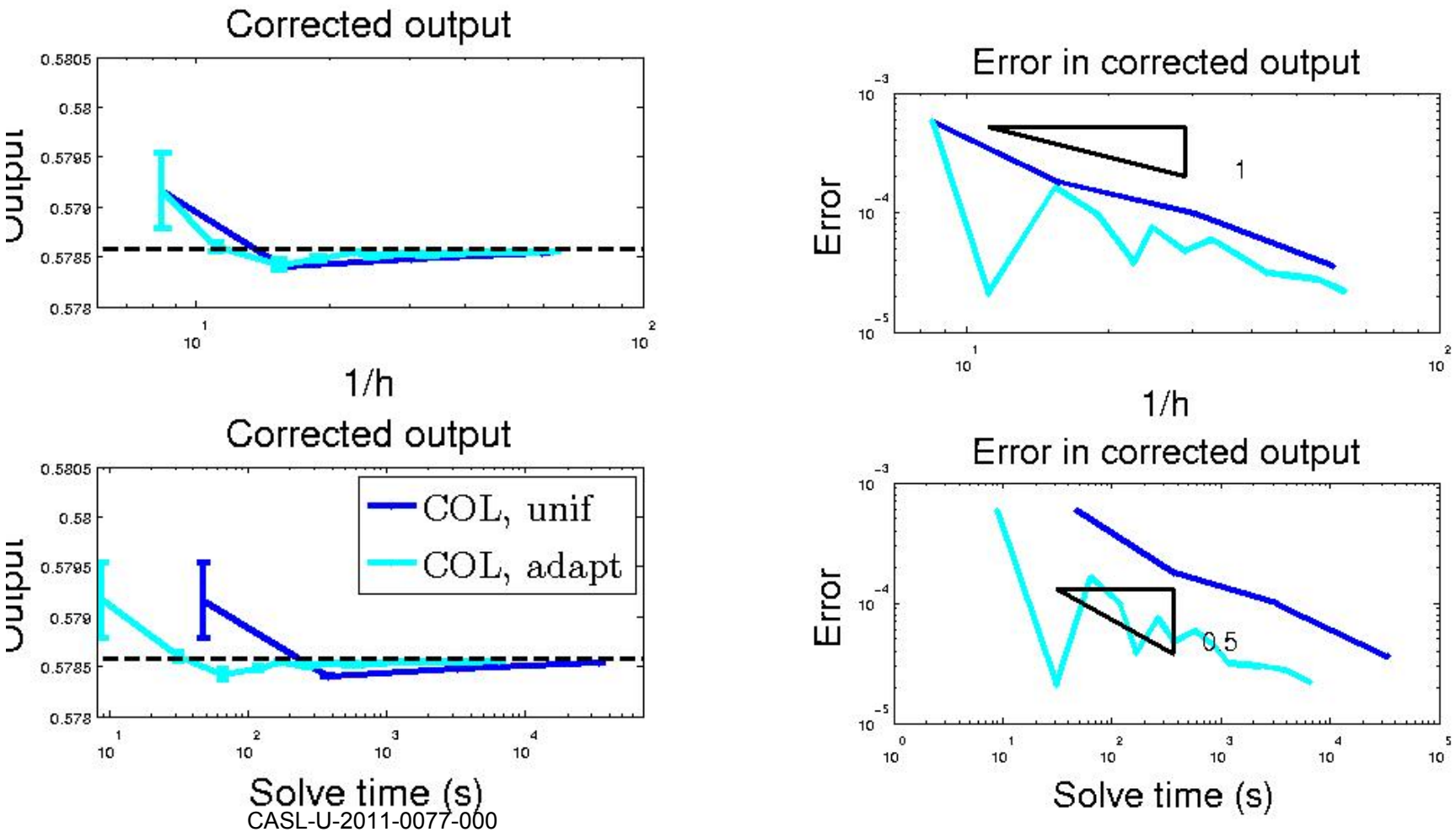
Two Stochastic Dimensions: Discretization and Results

$p_x = 1$, perspective of α_1



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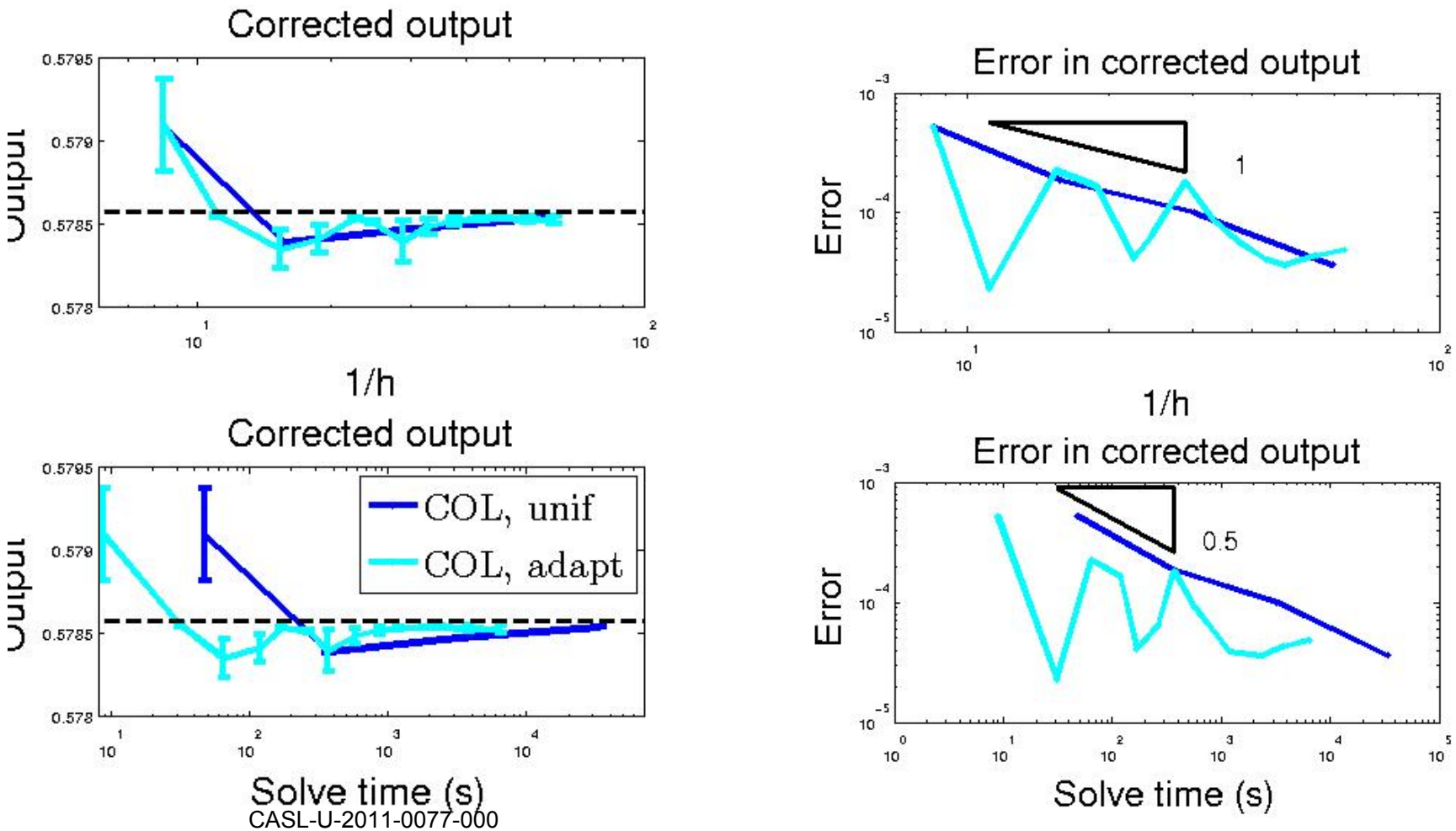
Two Stochastic Dimensions: Discretization and Results

$p_x = 1$, perspective of α_2



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Conclusions

- Developed nonintrusive method for error estimation and adaptation in $\vec{x}$- and $\vec{\alpha}$-spaces; requires ability to
  - Solve for u and ψ
  - Transfer solutions between meshes
  - Evaluate residuals and ψ at intermediate $\vec{\alpha}$
  - Adaptively refine $\vec{x}$-mesh
- Can take advantage of cheap residual evaluations for more accurate error estimates
- Adaptive converges at same rate as uniform, uses same or less computation time, can use fewer DOFs
- Adaptive converges faster than other adaptation metrics, plus error estimates

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Future Work

- Inconsistencies in discretization and non-zero correction, convergence rates
- Adaptation constants (DOF growth factor, extra x-element factor)
- Adaptation mechanics (multiple refinements)
- More deterministic dimensions
- More stocastic dimensions: kriging
  - High-dim. interp, complexity independent of number of dimensions
  - Assumes stochastic nature of parameters (as opposed to response-surface method)

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Thank You!

Funded by the Center for Advanced Simulation of Light-water reactors

[Backup slides]

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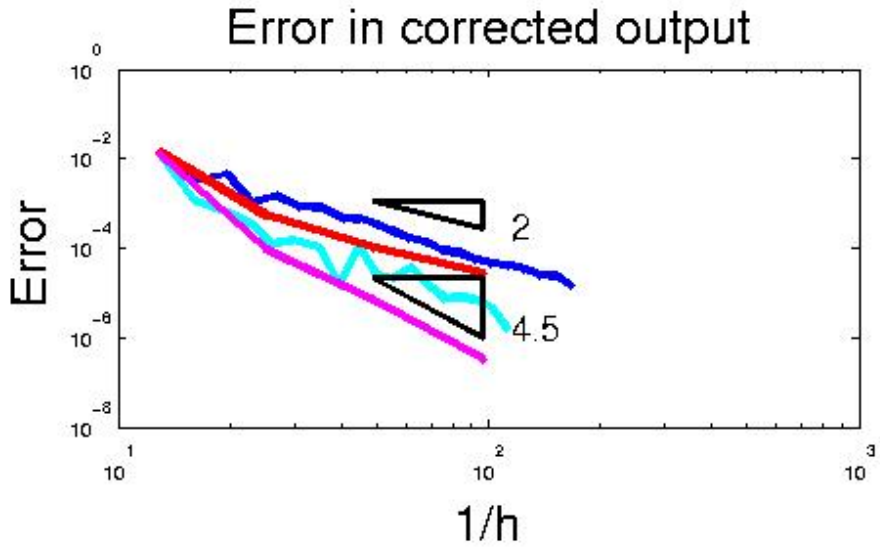
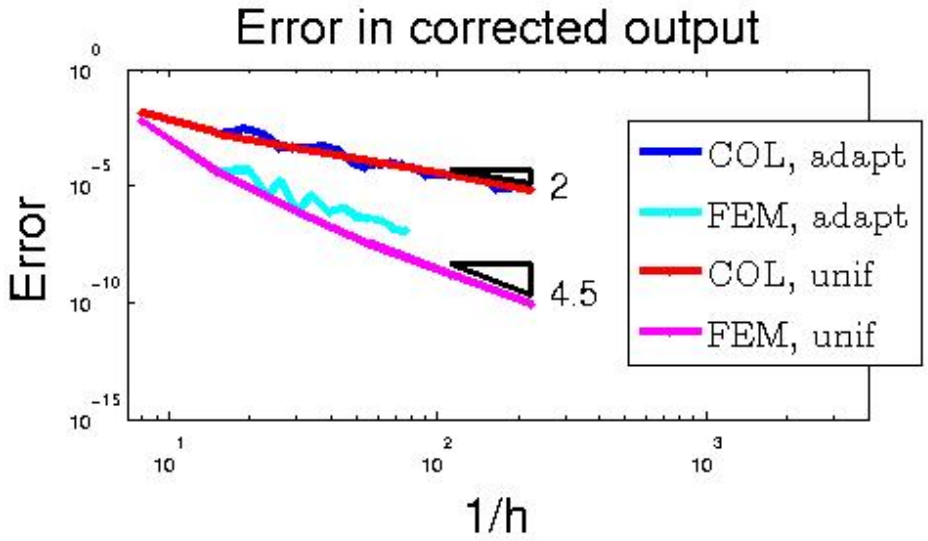
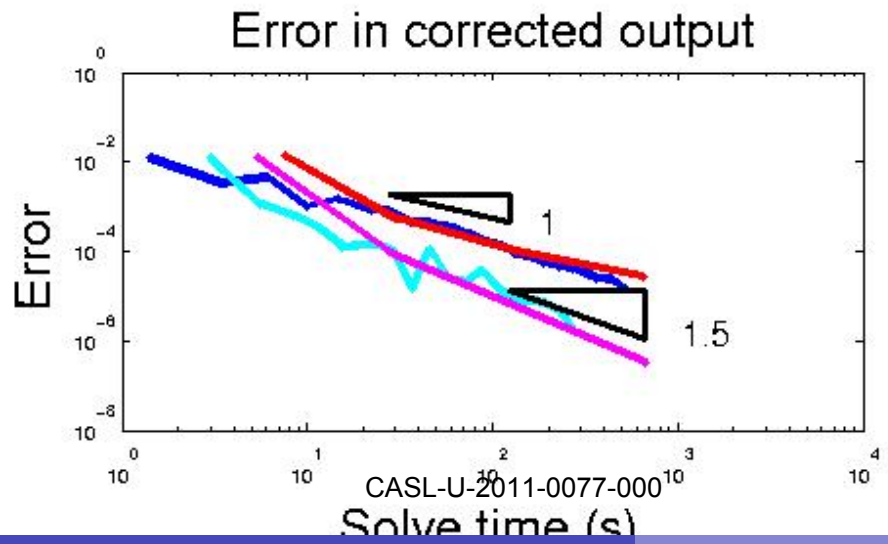
Adaptive vs. uniform refinement, $p_x = 2, 3$

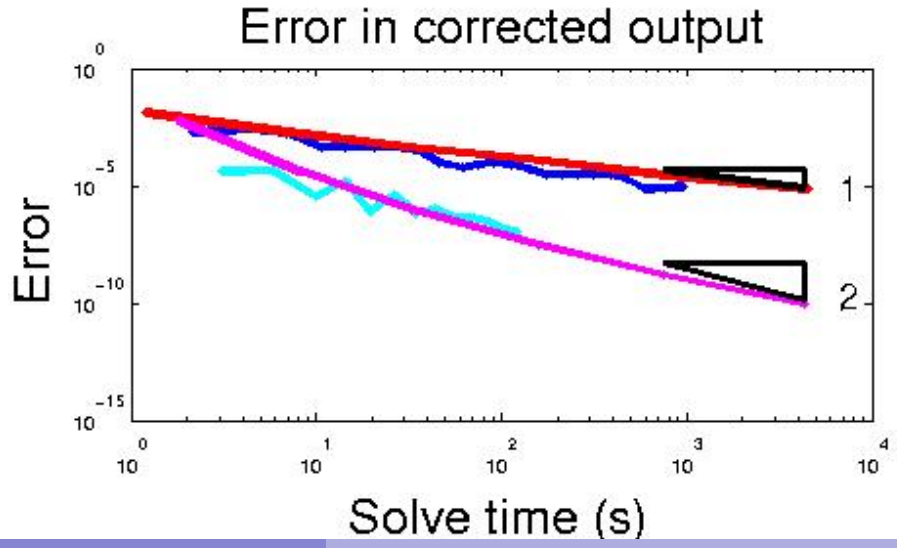
$p_x = 2, f_x = 0.7$



$p_x = 3, f_x = 0.7$







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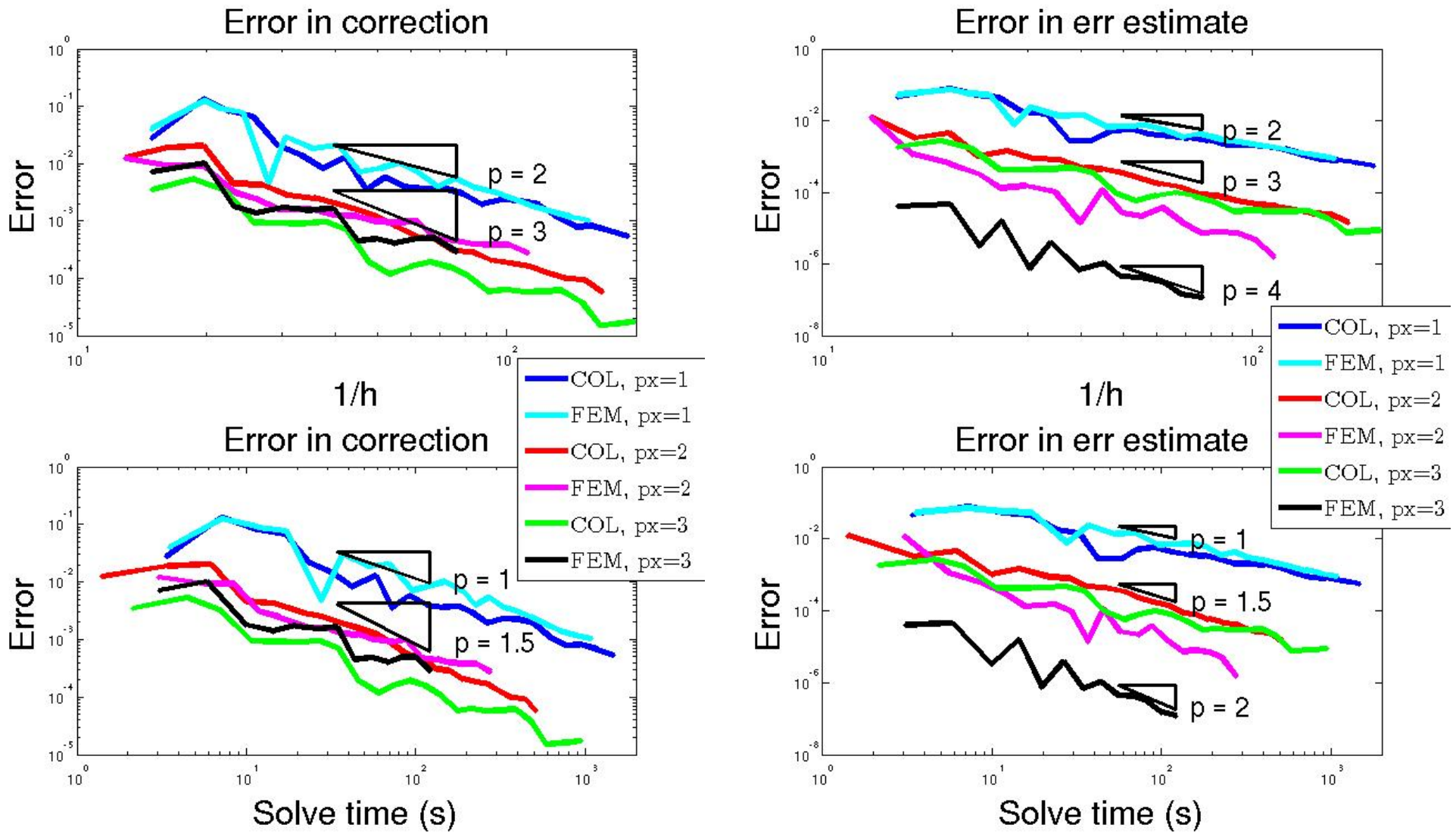
Convergence of correction and error estimate



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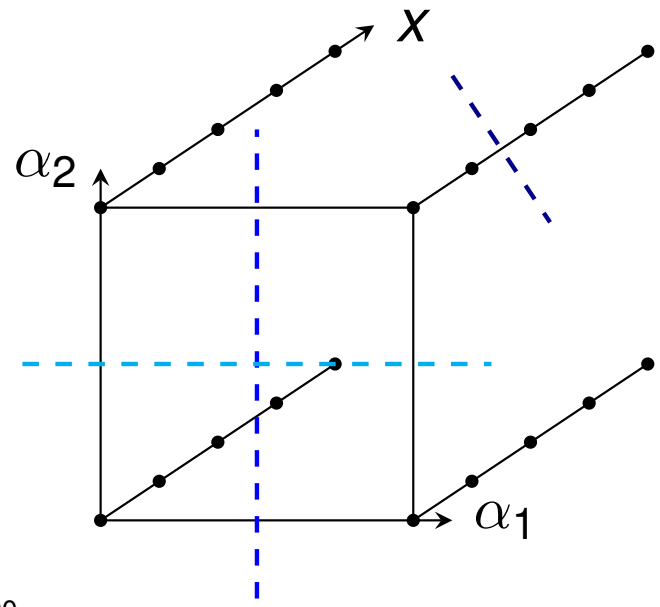

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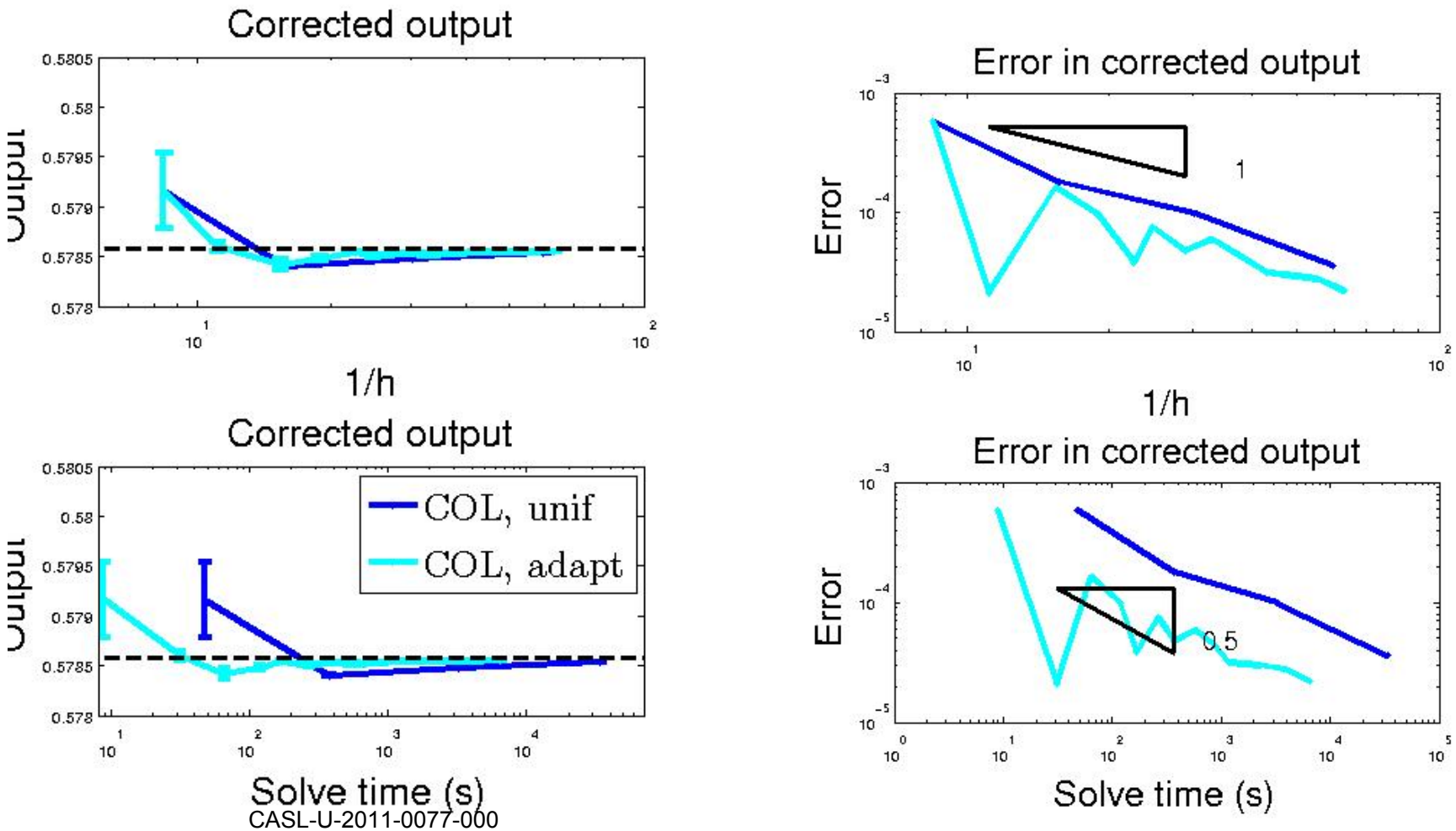
Two Stochastic Dimensions: Discretization and Results

$p_x = 1$, iap=1



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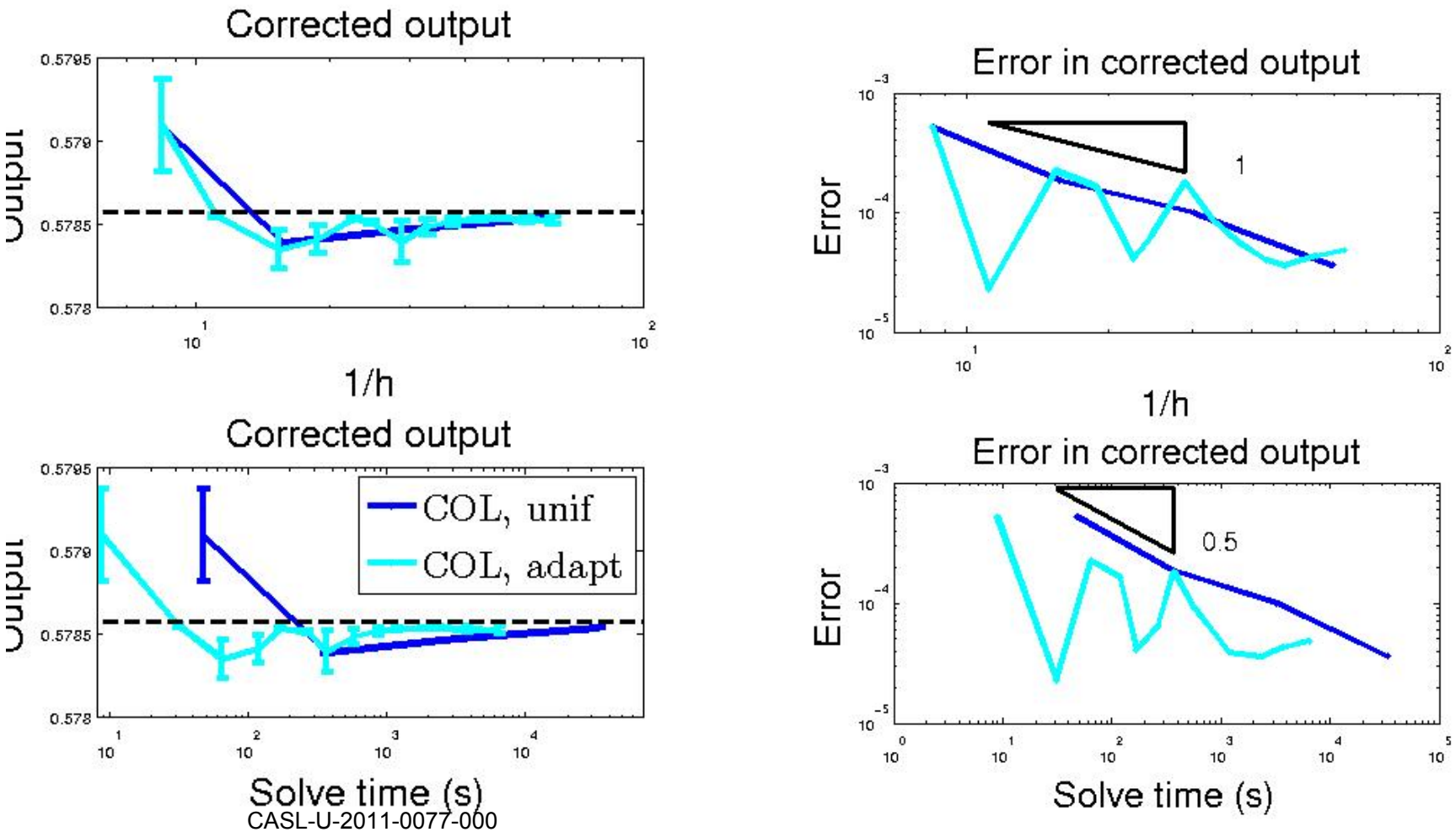
Two Stochastic Dimensions: Discretization and Results

$p_x = 1$, iap=2



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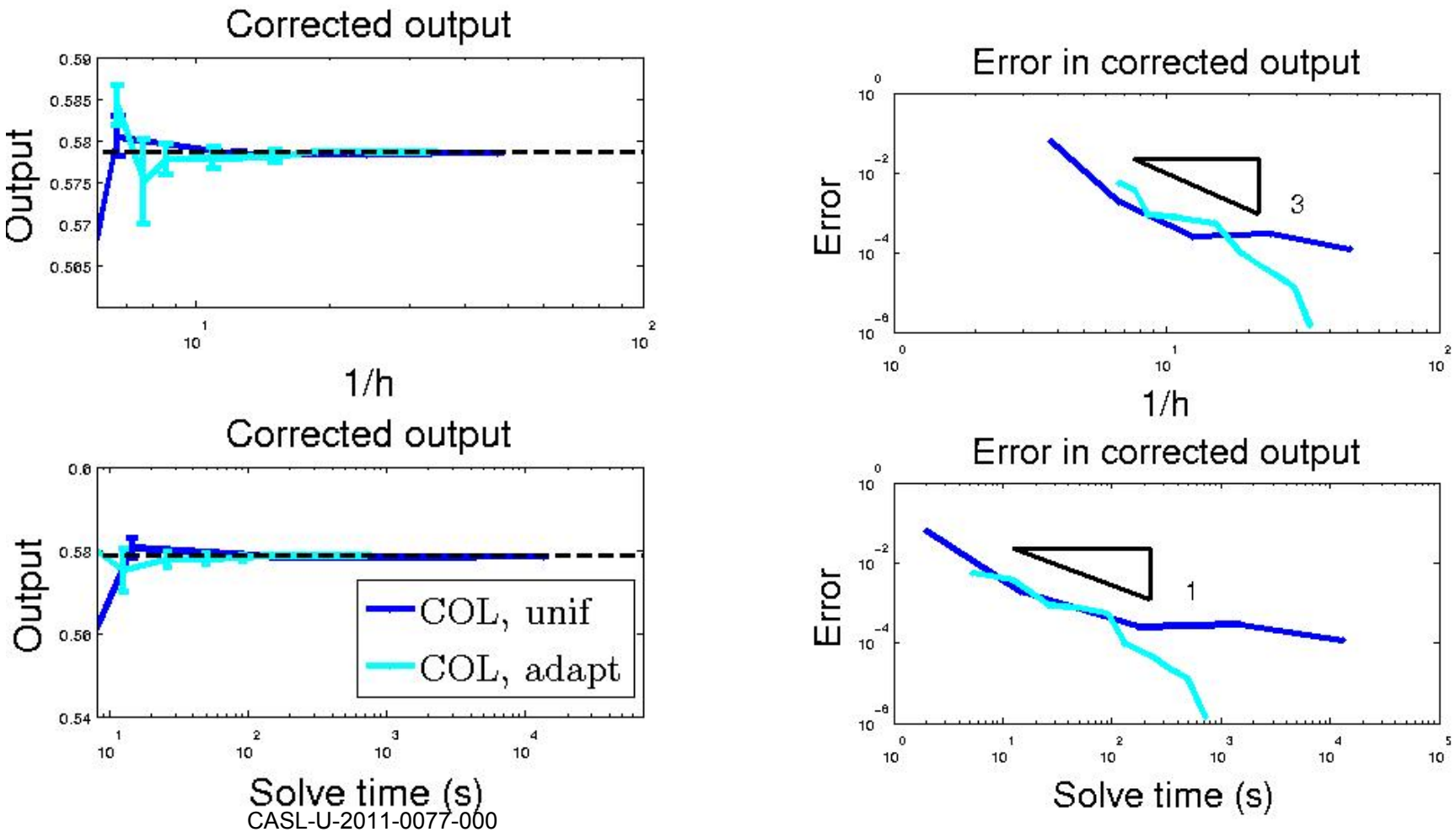
Two Stochastic Dimensions: Discretization and Results

$p_x = 2$, iap=1



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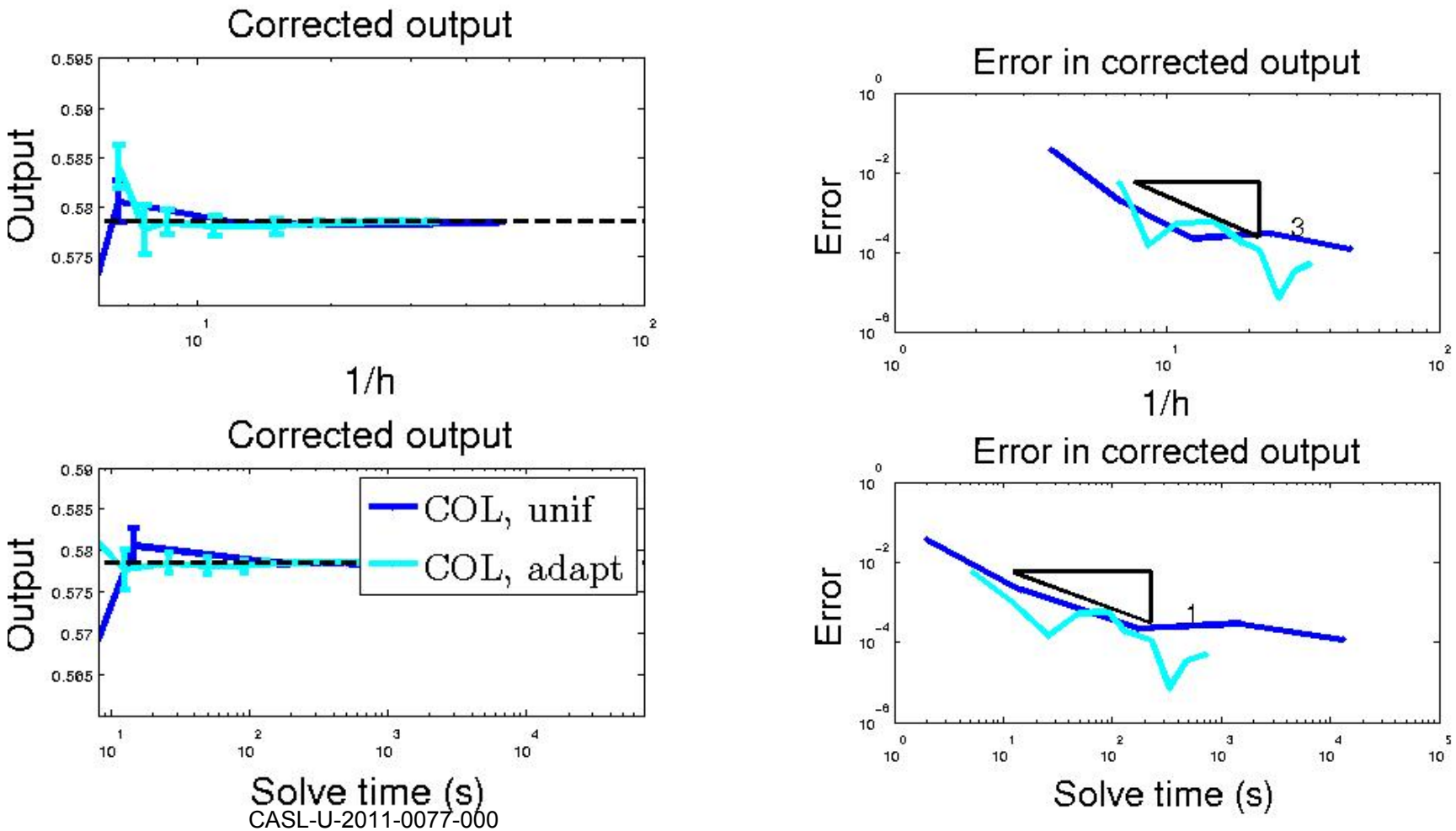
Two Stochastic Dimensions: Discretization and Results

$p_x = 2$, iap=2



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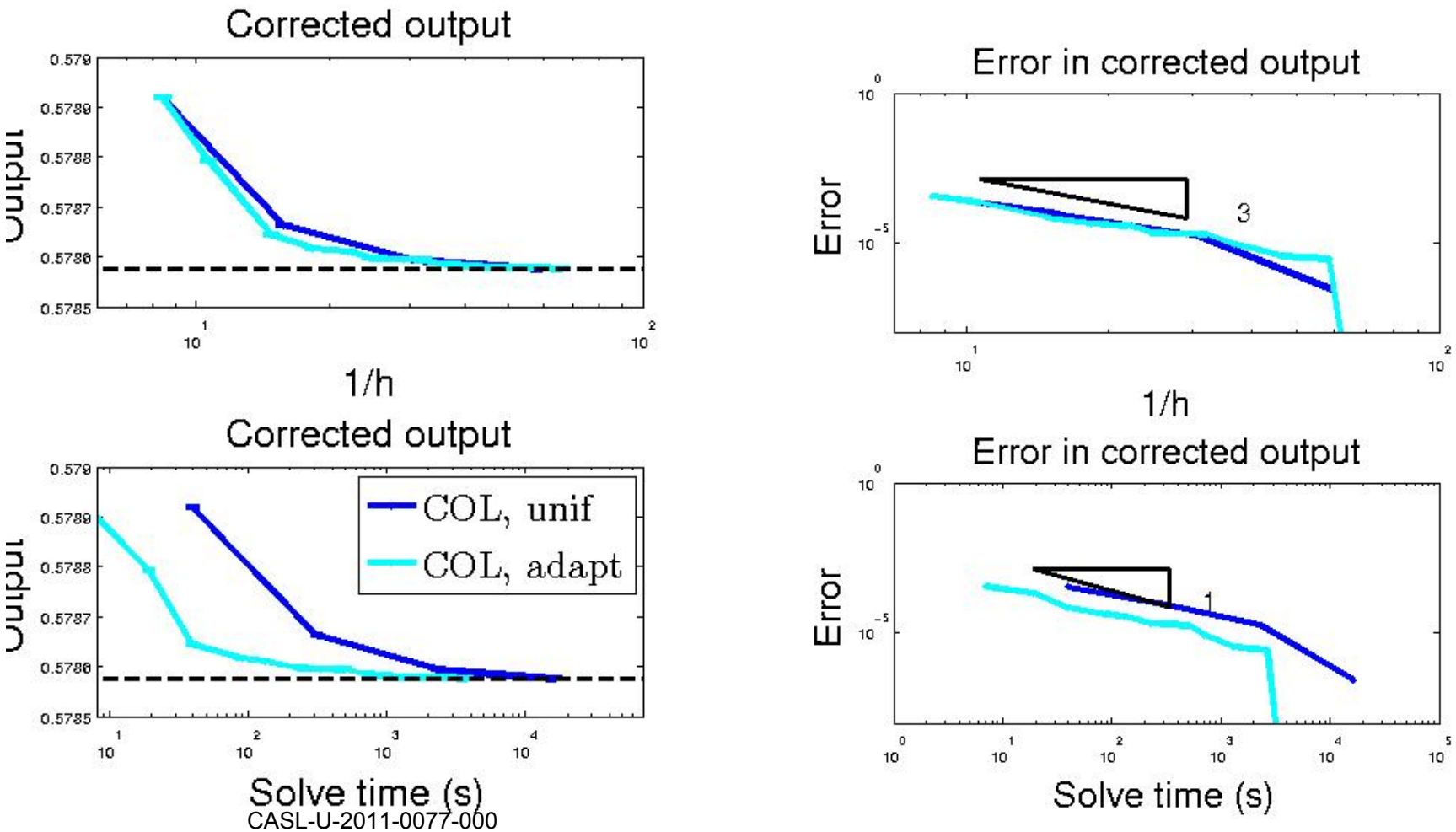
Two Stochastic Dimensions: Discretization and Results

$p_x = 3$, iap=1



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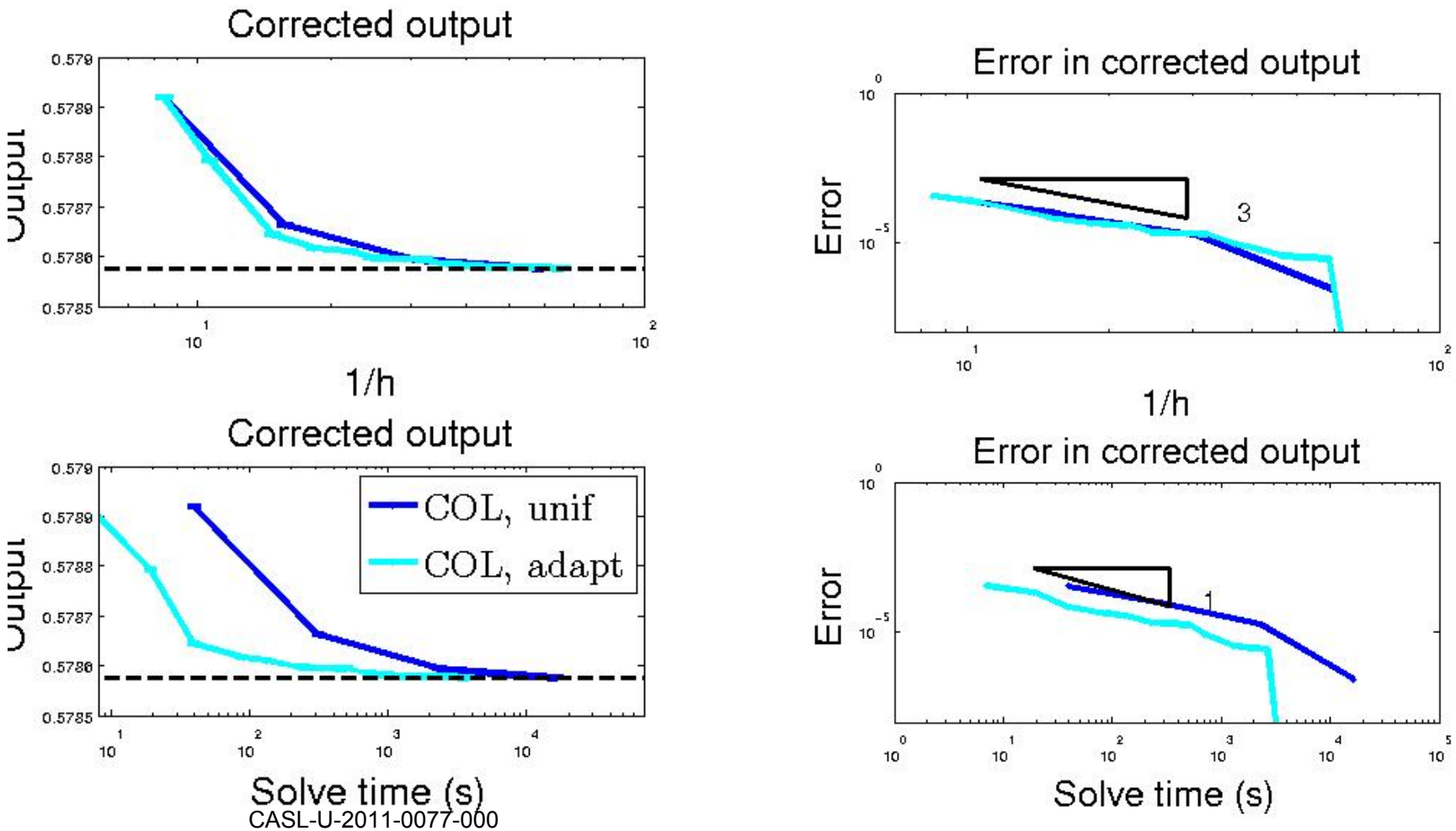
Two Stochastic Dimensions: Discretization and Results

$p_x = 3$, iap=2



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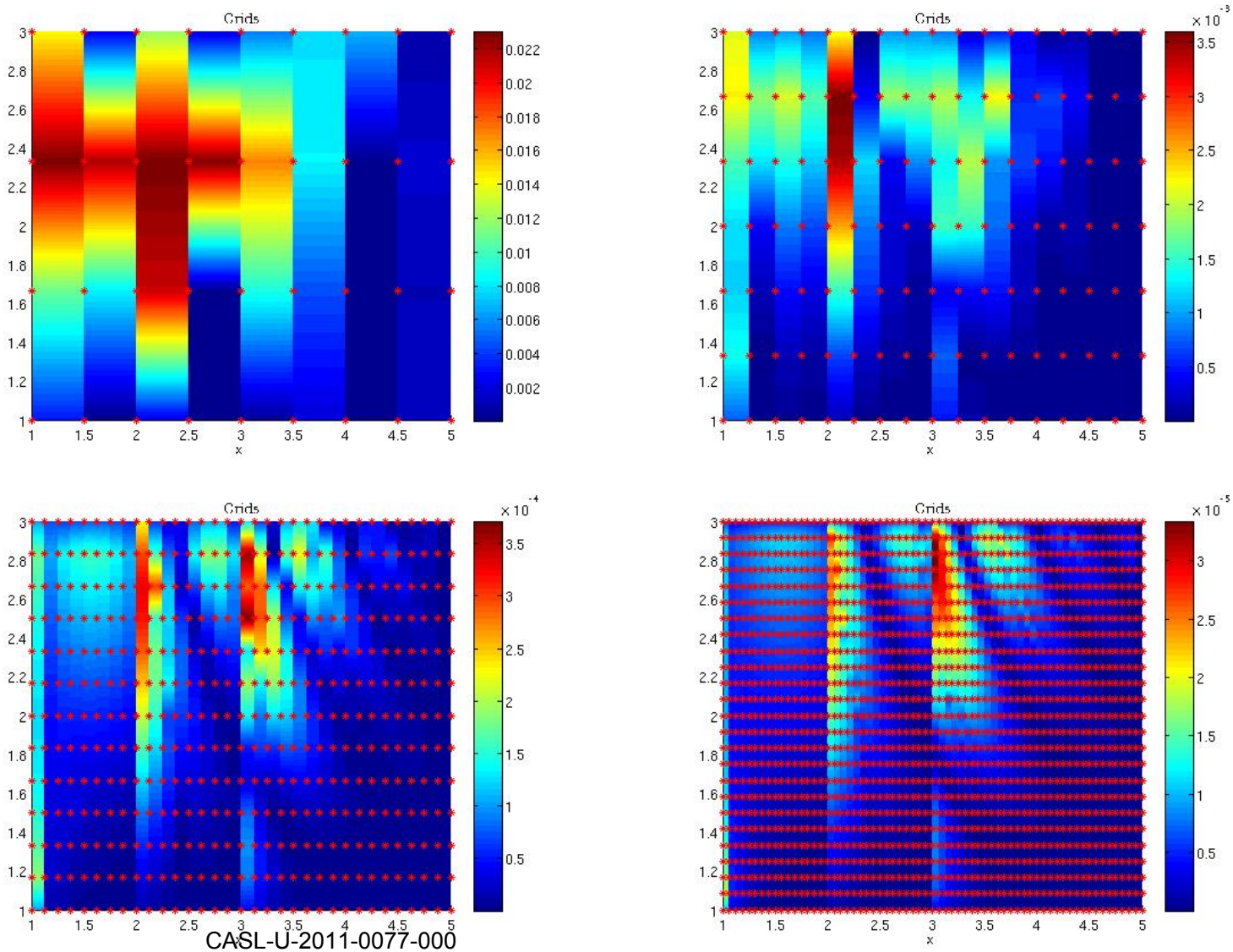
Non-zero correction

FEM, $p_x = 1$



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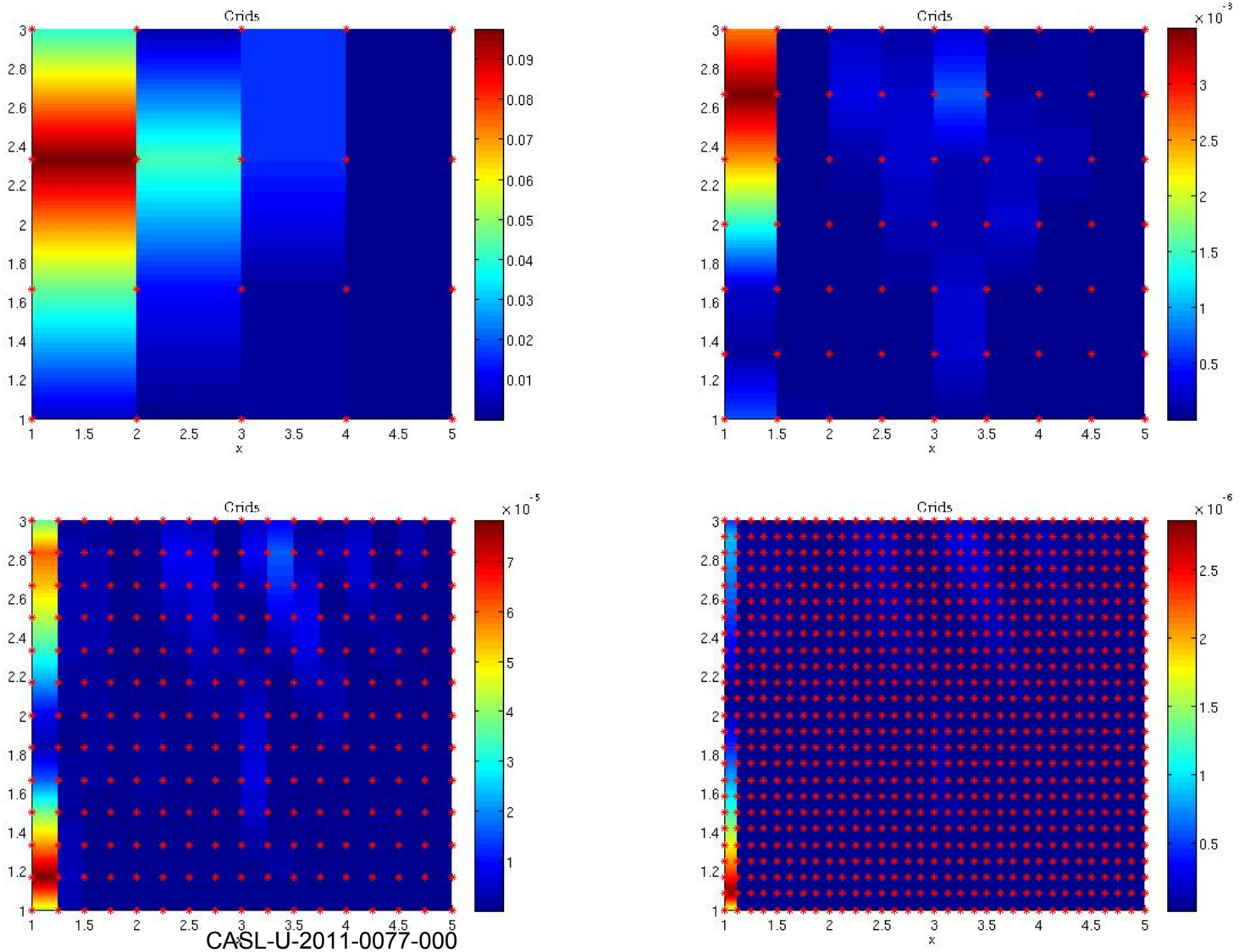
Non-zero correction

FEM, $p_x = 2$



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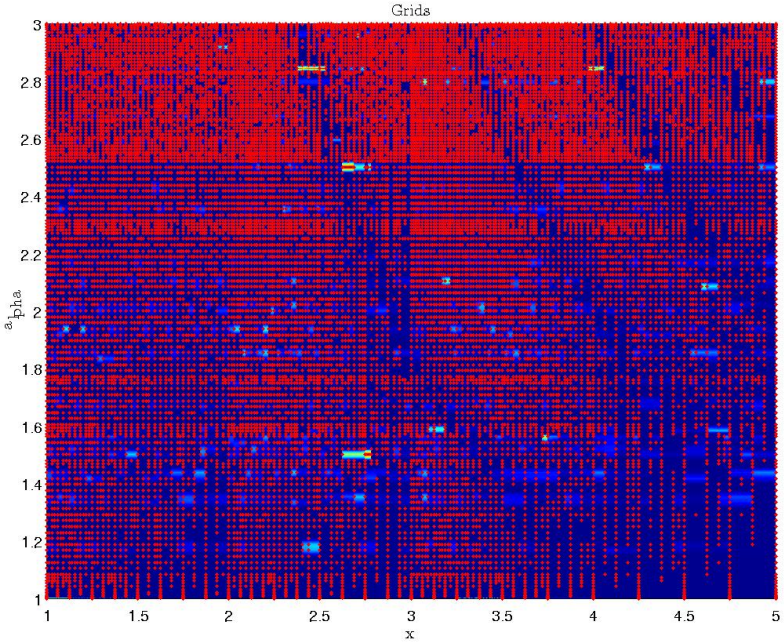
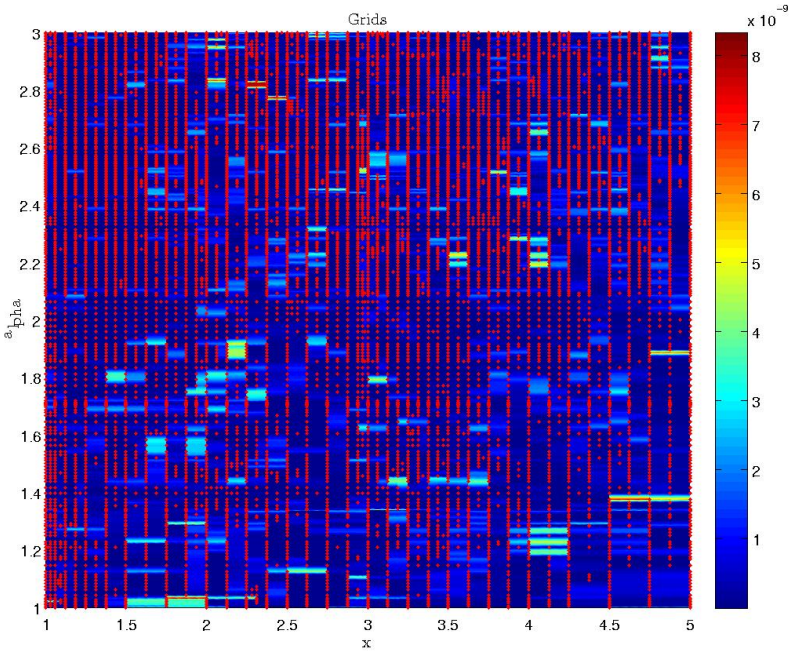
Adapted Grids

Col, $p_x = 1$



Col, $p_x = 2$



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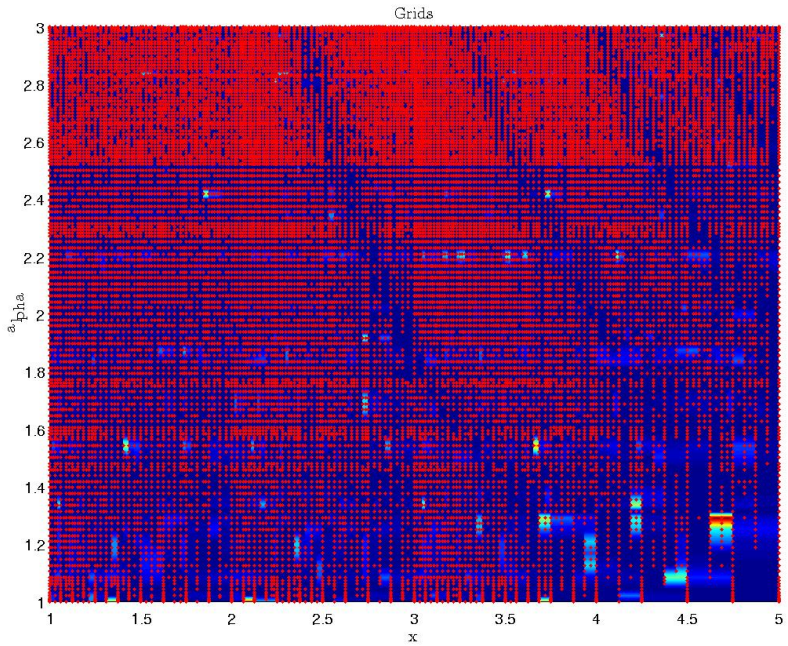
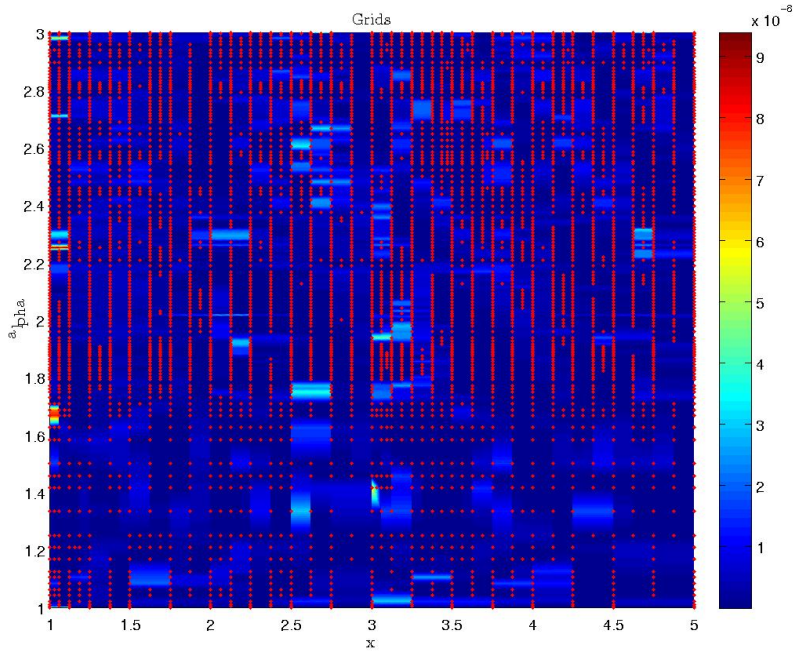
Adapted Grids

FEM, $p_x = 1$



FEM, $p_x = 2$



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