RIGOROUS OPTIMAL UNCERTAINTY QUANTIFICATION & OPTIMIZATION

DR. ADAM R GERLACH

CONTROL SCIENCES CENTER, AFRL

AFOSR CONTRACTORS MEETING, AUG 2024

The Team

AFOSR Support
- Computational Math
- Dynamics & Controls
- Mathematical Optimization

Control Sciences Center, AFRL

Adam Gerlach

Alex Von Moll

John Schierman

External Collaborators

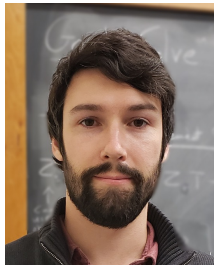
Chris Rackauckas
Department of Mathematics
Massachusetts Institute of Technology
JuliaHub

Avinash Subramanian
JuliaHub

Ben Chung
JuliaHub

Andrew Horning
Department of Mathematics
Rensselaer

AFOSR Summer Faculty Fellowship



"Open" Collaboration

Flemming Holtorf
Massachusetts Institute of Technology

Houman Owhadi
Caltech

Optimal Uncertainty Quantification (OUQ)

Admissible Set of Measures

$$\mathcal{A} = \left\{ \mu \,\middle|\, \begin{array}{c} \boldsymbol{x} \in \Omega \subseteq \mathbb{R}^d \\ \mathbb{E}\left[\varphi_j(\boldsymbol{x}) \,\middle|\, \mu\right] \leq c_j \quad \text{for } j = 1, \dots, N \end{array} \right\}$$

Bound Expectation of Quantity of Interest

"Tightest" possible bounds

∞-D Optimization

$$\underbrace{\operatorname*{infimum}_{\mu \in \mathcal{A}} \ \mathbb{E}[g(\boldsymbol{x}) \mid \mu]}_{\underline{\xi}(\mathcal{A})} \leq \mathbb{E}[g(\boldsymbol{x}) \mid \mu^*] \leq \underbrace{\operatorname*{supremum}_{\mu \in \mathcal{A}} \ \mathbb{E}[g(\boldsymbol{x}) \mid \mu]}_{\overline{\xi}(\mathcal{A})}$$

Owhadi, H., et al., "Optimal Uncertainty Quantification," *SIAM Review*, Vol. 55, No. 2, 2013, pp. 271–345.

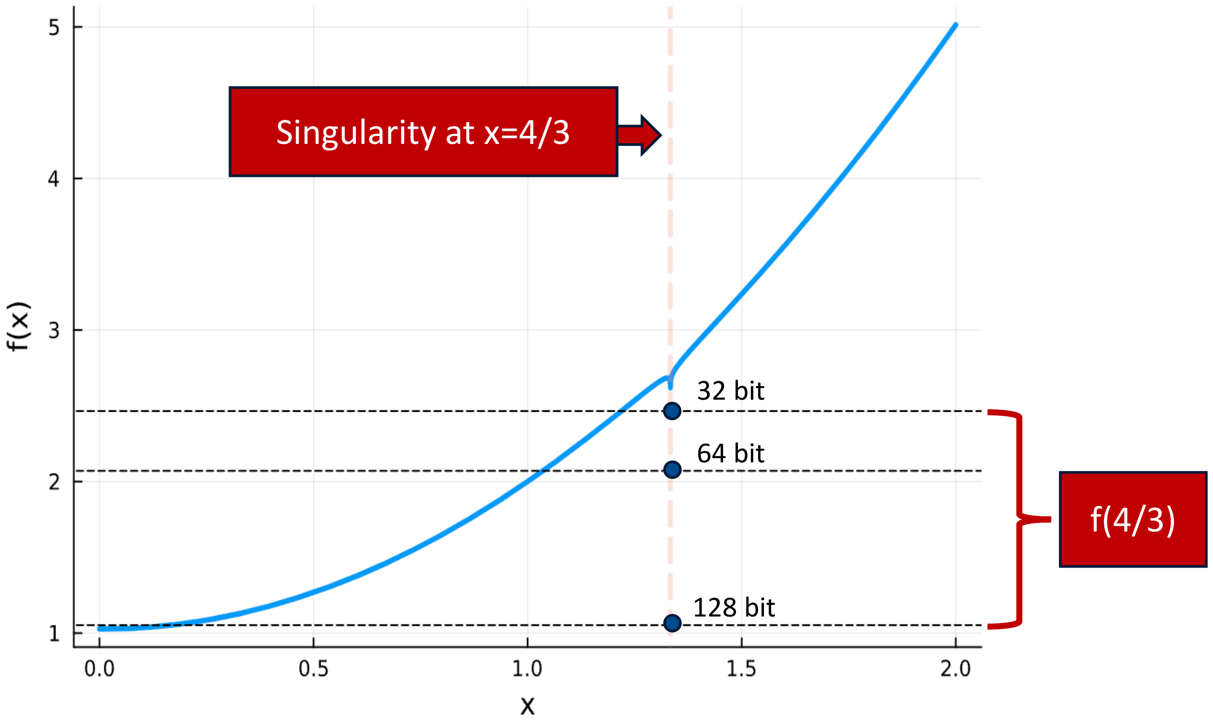
OUQ & Neumaier's classification of algorithms

$$\underset{\mu \in \mathcal{A}}{\text{infimum}} \ \mathbb{E}[g(\boldsymbol{x}) \mid \mu] \leq \mathbb{E}[g(\boldsymbol{x}) \mid \mu^*] \leq \underset{\mu \in \mathcal{A}}{\text{supremum}} \ \mathbb{E}[g(\boldsymbol{x}) \mid \mu]$$

Complete: Reaches global minima within prescribed tol. in finite t *within floating point precision*

Rigorous: Reaches global minima within prescribed tol. in finite t *despite rounding errors*.

$$f(x) = \frac{1}{51}\log(|3(1-x)+1|) + x^2 + 1$$

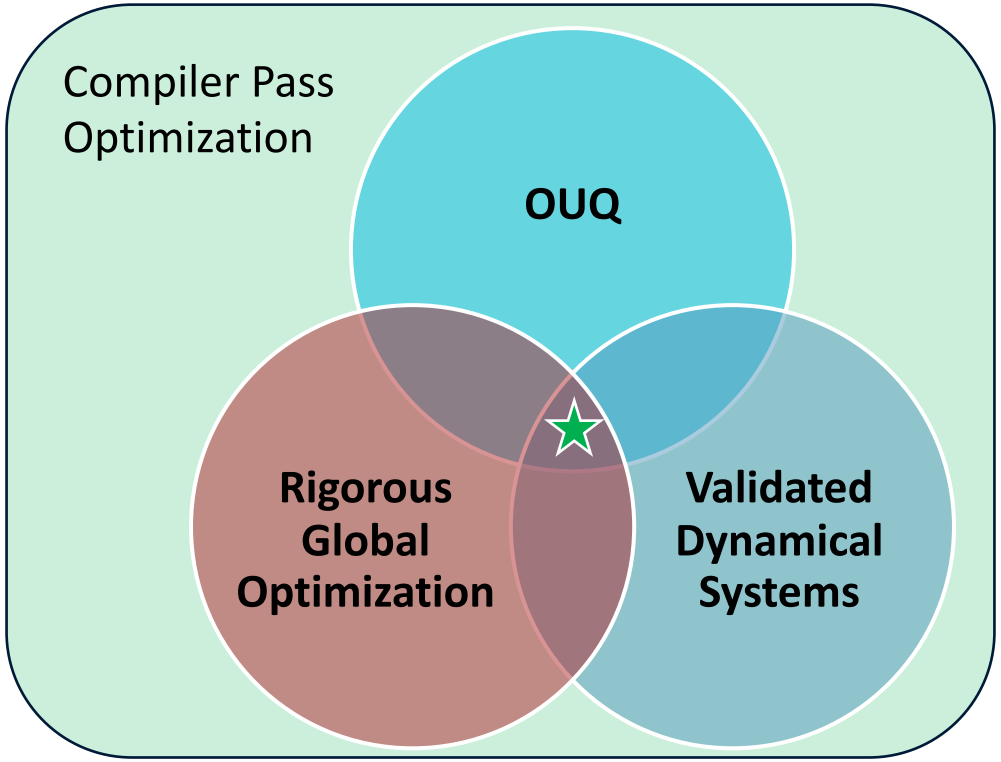


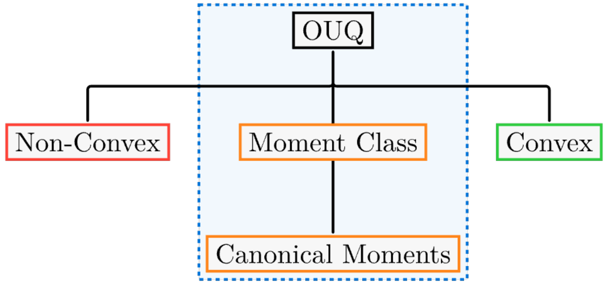
Neumaier, A., "Complete search in continuous global optimization and constraint satisfaction." *Acta numerica* 13 (2004): 271-369.

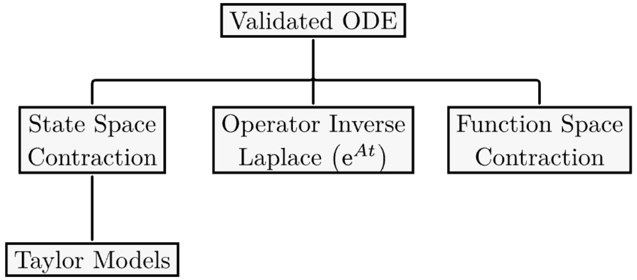
Goals of This Work

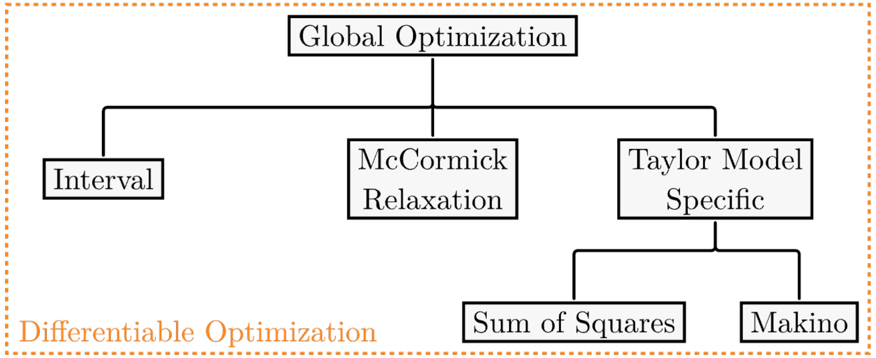
Develop a *computationally rigorous* OUQ framework to support system, control, and mission design and optimization under uncertain and incomplete information

$$\underbrace{\underset{\mu\in\mathcal{A}}{\text{infimum}}\ \mathbb{E}[g(\boldsymbol{x})\,|\,\mu]}_{\underline{\xi}(\mathcal{A})} \leq \mathbb{E}[g(\boldsymbol{x})\,|\,\mu^*] \leq \underbrace{\underset{\mu\in\mathcal{A}}{\text{supremum}}\ \mathbb{E}[g(\boldsymbol{x})\,|\,\mu]}_{\overline{\xi}(\mathcal{A})}$$









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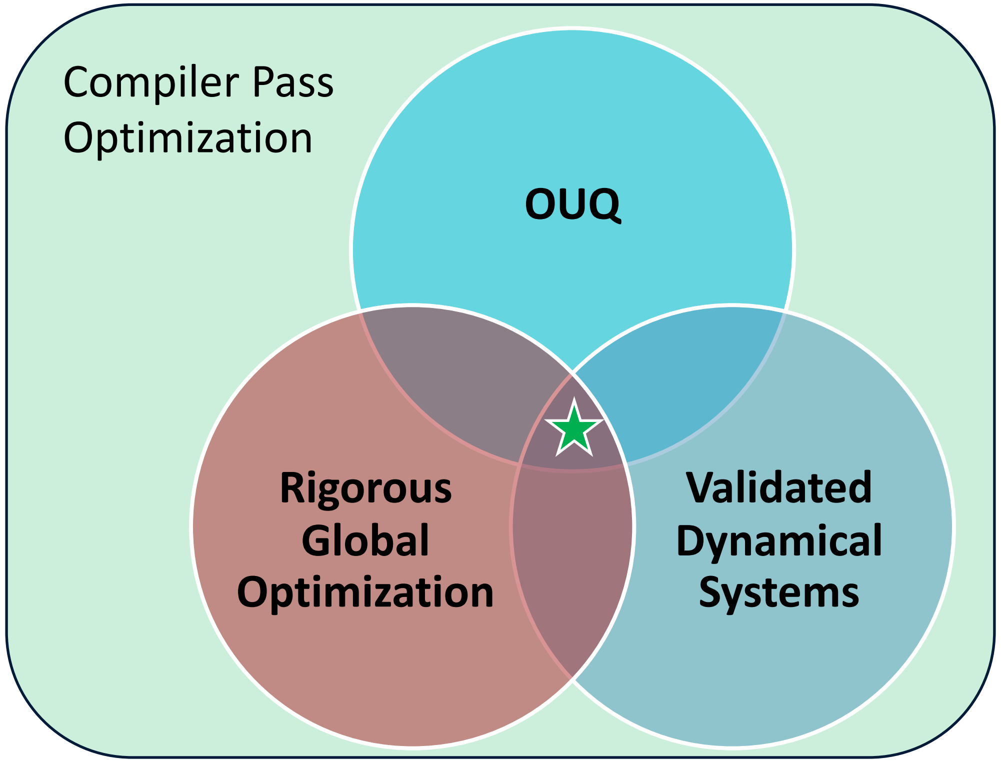
$$\underbrace{\operatorname*{infimum}_{\mu\in\mathcal{A}} \mathbb{E}[g(\boldsymbol{x})\,|\,\mu]}_{\underline{\xi}(\mathcal{A})} \le \mathbb{E}[g(\boldsymbol{x})\,|\,\mu^*] \le \underbrace{\operatorname*{supremum}_{\mu\in\mathcal{A}} \mathbb{E}[g(\boldsymbol{x})\,|\,\mu]}_{\overline{\xi}(\mathcal{A})}$$



Why Compiler Pass Optimizations?

Rigorous Interval Arithmetic is Sub-Distributive

$$a(b+c) \subseteq ab + ac, \quad a,b,c \in \mathbb{IR}$$

$$[\mathrm{LB}^*, \mathrm{UB}^*] = \cap_i\ \rho_i(\mathcal{A}), \rho_i \in \mathfrak{P}$$

Set of equiv. programs

"Quadratic Eq."

$$-b \pm \operatorname{sign}(b)\frac{\sqrt{b^2-4ac}}{2a} \quad \text{vs} \quad \frac{2c}{-b \pm \operatorname{sign}(b)\sqrt{b^2-4ac}}$$

"Tightest" upper bounding code ≠ "Tightest" lower bounding code

Goals of This Work

Develop a *computationally rigorous* OUQ framework to support system, control, and mission design and optimization under uncertain and incomplete information

$$\underbrace{\underset{\mu\in\mathcal{A}}{\text{infimum}}\ \mathbb{E}[g(\boldsymbol{x})\,|\,\mu]}_{\underline{\xi}(\mathcal{A})} \leq \mathbb{E}[g(\boldsymbol{x})\,|\,\mu^*] \leq \underbrace{\underset{\mu\in\mathcal{A}}{\text{supremum}}\ \mathbb{E}[g(\boldsymbol{x})\,|\,\mu]}_{\overline{\xi}(\mathcal{A})}$$

Year 1:

- Enable *computationally rigorous* OUQ for certification & prediction of codes modeling *dynamical systems*
  - Rigorous Polynomial Approximation (RPAs) + Rigorous Global Optimization
  - Develop composable computational tools to support this research.

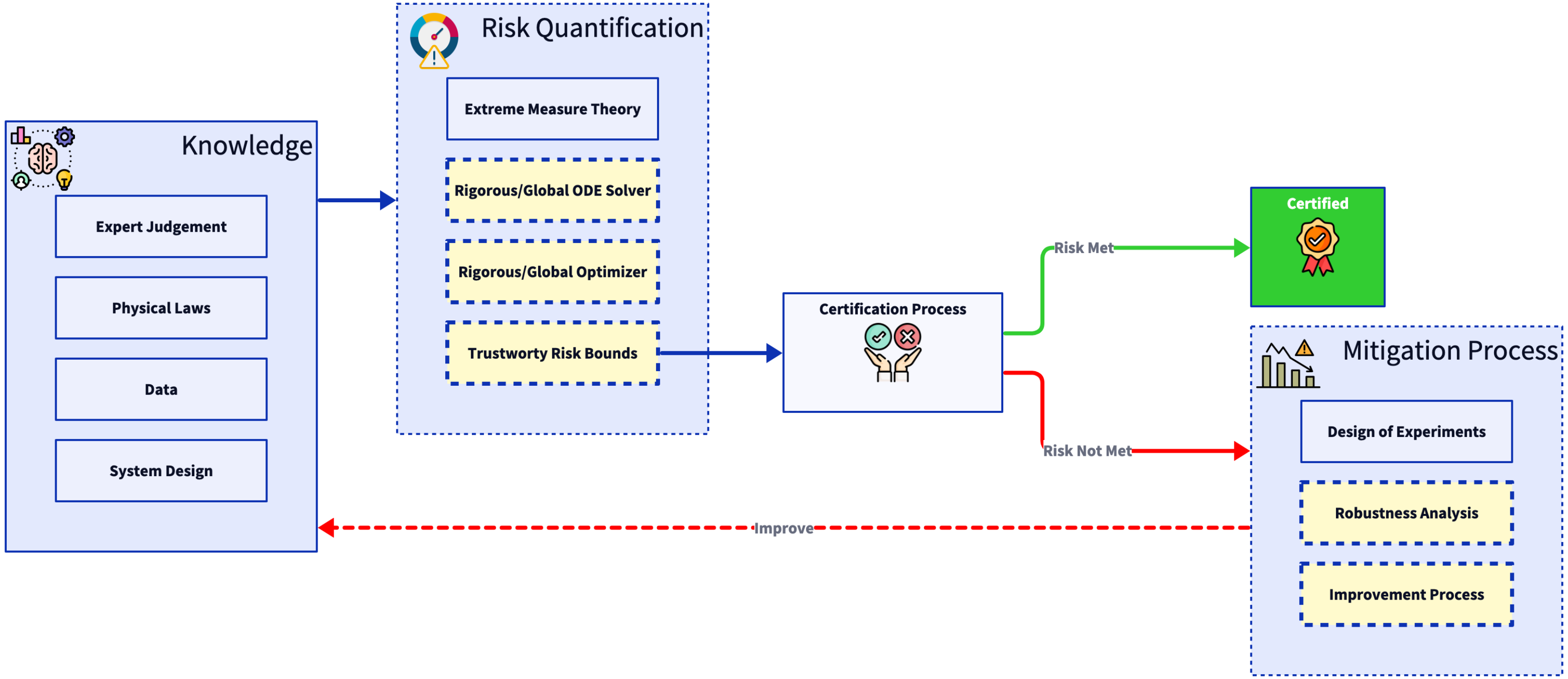
Years 2 & 3:

- Quantify the *uncertainty introduced by finite computation* & how the rigorous computing framework impacts this uncertainty.
- Quantify the *sensitivity/robustness of rigorous bounds* wrt the problem structure and the RPA used.
- Develop *automatic code transformation tools* to optimize expression trees to minimize the effects of over-approximation induced by RPAs.

Goals of This Work

Develop a ***computationally rigorous*** OUQ framework to support system, control, and mission design and optimization under uncertain and incomplete information

$$\underbrace{\underset{\mu\in\mathcal{A}}{\text{infimum}}\ \mathbb{E}[g(\boldsymbol{x})\,|\,\mu]}_{\underline{\xi}(\mathcal{A})} \leq \mathbb{E}[g(\boldsymbol{x})\,|\,\mu^*] \leq \underbrace{\underset{\mu\in\mathcal{A}}{\text{supremum}}\ \mathbb{E}[g(\boldsymbol{x})\,|\,\mu]}_{\overline{\xi}(\mathcal{A})}$$



Tractable OUQ Induced by Dynamical Systems

Tractable OUQ

Extreme Measure Theorem [1,2]

The measure that extremizes expectation is discrete and supported on at most N+1 points

$$\mathcal{A} = \left\{ \mu \,\middle|\, \begin{array}{c} \boldsymbol{x} \in \Omega \subseteq \mathbb{R}^d \\ \mathbb{E}\left[\varphi_j(\boldsymbol{x}) \,\middle|\, \mu\right] \leq c_j \quad \text{for } j = 1, \ldots, N \end{array} \right\} \Rightarrow \mathcal{A}_\Delta = \left\{ \mu = \sum_i^{N+1} w_i \delta_{\boldsymbol{x}_i} \,\middle|\, \begin{array}{c} \boldsymbol{x}_i \in \Omega \subseteq \mathbb{R}^d \quad \text{for } i = 1, \ldots, N+1 \\ w_i \in [0,1] \quad \text{for } i = 1, \ldots, N+1 \\ \sum_i^{N+1} w_i = 1 \\ \sum_i^{N+1} w_i \varphi_j(\boldsymbol{x}_i) \leq c_j \quad \text{for } j = 1, \ldots, N \end{array} \right\}$$

$$\underbrace{\underset{\mu \in \mathcal{A}}{\text{infimum}} \; \mathbb{E}[g(\boldsymbol{x}) \,|\, \mu]}_{\underline{\xi}(\mathcal{A})} \leq \mathbb{E}[g(\boldsymbol{x}) \,|\, \mu^*] \leq \underbrace{\underset{\mu \in \mathcal{A}}{\text{supremum}} \; \mathbb{E}[g(\boldsymbol{x}) \,|\, \mu]}_{\overline{\xi}(\mathcal{A})} \Rightarrow \underbrace{\underset{\mu \in \mathcal{A}_\Delta}{\text{infimum}} \sum_{i=1}^{N+1} w_i g(\boldsymbol{x}_i)}_{\underline{\xi}(\mathcal{A}_\Delta)} \leq \mathbb{E}[g(\boldsymbol{x}) \,|\, \mu^*] \leq \underbrace{\underset{\mu \in \mathcal{A}_\Delta}{\text{supremum}} \sum_{i=1}^{N+1} w_i g(\boldsymbol{x}_i)}_{\overline{\xi}(\mathcal{A}_\Delta)}$$

[1] Owhadi, H., et al., "Optimal Uncertainty Quantification," *SIAM Review*, Vol. 55, No. 2, 2013, pp. 271–345.
[2] Winkler, G., "Extreme Points of Moment Sets," *Mathematics of Operations Research*, Vol. 13, No. 4, 1988, pp. 581–587.

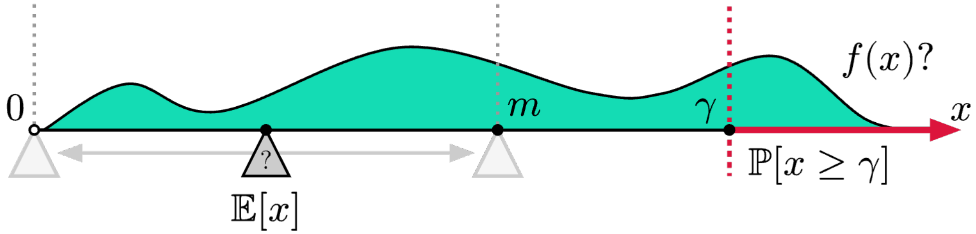
Tractable OUQ

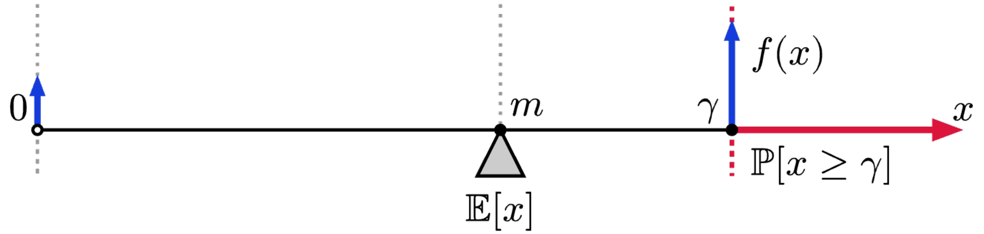
<u>Extreme Measure Theorem [1,2]</u>

The measure that extremizes expectation is <u>discrete</u> and supported on at most <u>N+1 points</u>

$$\underset{\mu \in \mathcal{A}}{\text{supremum}} \; \mathbb{P}[x \geq \gamma \,|\, \mu]$$

$$\mathbb{E}[x] \leq m, \text{for } 0 < m \leq \gamma$$





[1] Owhadi, H., et al., "Optimal Uncertainty Quantification," *SIAM Review*, Vol. 55, No. 2, 2013, pp. 271–345.
[2] Winkler, G., "Extreme Points of Moment Sets," *Mathematics of Operations Research*, Vol. 13, No. 4, 1988, pp. 581–587.

OUQ with Uncertain Response

- Extend Admissible Set to Include Sets of Response Functions

$$\mathcal{A} = \left\{ (\mu, g) \;\middle|\; \begin{matrix} g \in \mathcal{G} \\ \boldsymbol{x} \in \Omega \subseteq \mathbb{R}^d \\ \mathbb{E}\left[\varphi_j(\boldsymbol{x}) \,\middle|\, \mu\right] \leq c_j \quad \text{for } j = 1, \ldots, N \end{matrix} \right\}$$

$$\underset{(\mu,g)\in\mathcal{A}}{\text{infimum}} \;\; \mathbb{E}[g(\boldsymbol{x}) \mid \mu] \leq \mathbb{E}[g^*(\boldsymbol{x}) \mid \mu^*] \leq \underset{(\mu,g)\in\mathcal{A}}{\text{supremum}} \;\; \mathbb{E}[g(\boldsymbol{x}) \mid \mu],$$

OUQ Induced by Dynamical Systems

- Exploit Adjoint relationship with the Push-Forward & Pull-Back Operators

(Frobenious-Perron) (Koopman)

$$\mathbb{E}[g \mid P\mu] = \mathbb{E}[Kg \mid \mu]$$

Push-Forward

Pull-Back

$$Kg = g \circ S$$

$$S(\boldsymbol{x}_k) = \boldsymbol{x}_{k+1}$$

Push-Forward Ambiguity Set [1]	$\underset{\mu \in P\mathcal{A}}{\text{infimum}}\ \mathbb{E}[g \mid \mu] \leq \mathbb{E}[g \mid \mu^*] \leq \underset{\mu \in P\mathcal{A}}{\text{supremum}}\ \mathbb{E}[g \mid \mu]$
Push-Forward Measure	$\underset{\mu \in \mathcal{A}}{\text{infimum}}\ \mathbb{E}[g \mid P\mu] \leq \mathbb{E}[g \mid P\mu^*] \leq \underset{\mu \in \mathcal{A}}{\text{supremum}}\ \mathbb{E}[g \mid P\mu]$
Pull-Back QoI	$\underset{\mu \in \mathcal{A}}{\text{infimum}}\ \mathbb{E}[Kg \mid \mu] \leq \mathbb{E}[Kg \mid \mu^*] \leq \underset{\mu \in \mathcal{A}}{\text{supremum}}\ \mathbb{E}[Kg \mid \mu]$

[1] Aolaritei, L., Lanzetti, N., Chen, H., and Dörfler, F., “Distributional Uncertainty Propagation via Optimal Transport.” https://doi.org/10.48550/arXiv.2205.00343

OUQ Induced by Dynamical Systems

- Exploit Adjoint relationship with the Push-Forward & Pull-Back Operators

$$\dot{\boldsymbol{x}} = F(\boldsymbol{x}), \quad \boldsymbol{x}(0) = \boldsymbol{x}_0$$

$$S_t(\boldsymbol{x}_0) = \boldsymbol{x}(t) = \boldsymbol{x}_0 + \int_0^t F(\boldsymbol{x}(\tau))\,\mathrm{d}\tau, \quad \text{for } t \geq 0.$$

What if S_t is only know implicitly?

$$\{K_t\}_{t\geq 0}$$

$$K_t g = g \circ S_t$$

Pull-Back QoI

$$\underset{\mu\in\mathcal{A}}{\text{infimum}} \ \mathbb{E}[K_t g \,|\, \mu] \leq \mathbb{E}[K_t g \,|\, \mu^*] \leq \underset{\mu\in\mathcal{A}}{\text{supremum}} \ \mathbb{E}[K_t g \,|\, \mu]$$

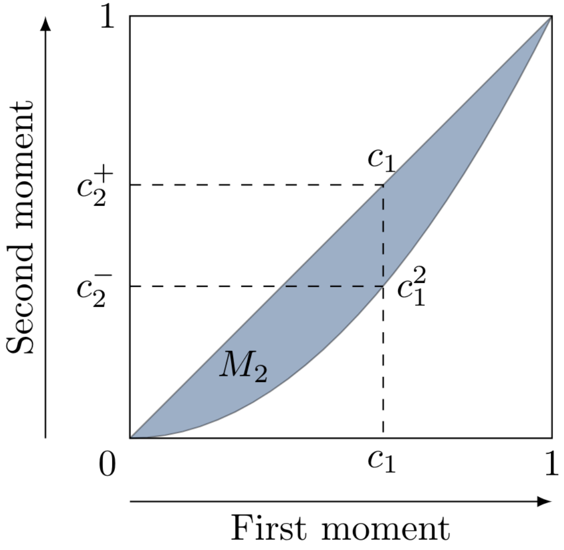
How do we account for effects of finite computation?
(Spatial, Temporal, Floating Point Discretization)

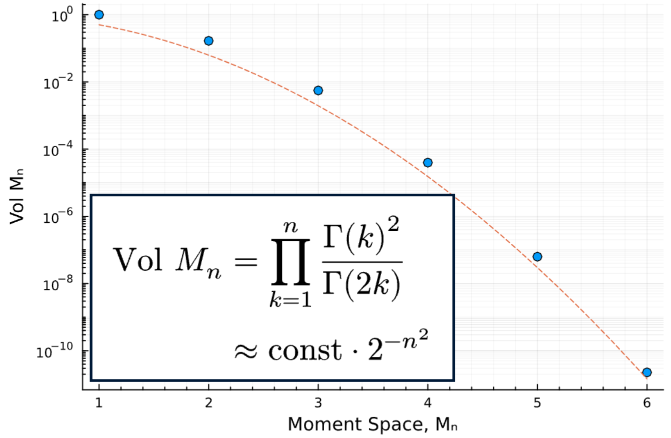
OUQ via Moment Class

$$\mathcal{A} = \left\{ \mu \;\middle|\; \begin{array}{c} \boldsymbol{x} \in \Omega \subseteq \mathbb{R}^d \\ \underline{c}_1^{\{j\}} \leq \mathbb{E}\left[x_1^j \,\middle|\, \mu^*\right] \leq \overline{c}_1^{\{j\}} \quad \text{for } j = 1, \ldots, m_1 \\ \vdots \\ \underline{c}_d^{\{j\}} \leq \mathbb{E}\left[x_d^j \,\middle|\, \mu^*\right] \leq \overline{c}_d^{\{j\}} \quad \text{for } j = 1, \ldots, m_d \end{array} \right\}$$

"normalize" via Canonical Moments

$$\hat{\mathcal{A}} = \left\{ \mu_{\boldsymbol{q}} \;\middle|\; \begin{array}{c} \boldsymbol{x} \in \Omega \subseteq \mathbb{R}^d \\ \boldsymbol{q}_1 \in [0,1]^{m_1+1} \\ \vdots \\ \boldsymbol{q}_d \in [0,1]^{m_d+1} \end{array} \right\}$$





$$\underset{\mu_{\boldsymbol{q}} \in \hat{\mathcal{A}}}{\text{infimum}} \; \mathbb{E}\left[g \circ h \,\middle|\, \mu_{\boldsymbol{q}}\right] \leq \mathbb{E}[g \,|\, \mu^*] \leq \underset{\mu_{\boldsymbol{q}} \in \hat{\mathcal{A}}}{\text{supremum}} \; \mathbb{E}\left[g \circ h \,\middle|\, \mu_{\boldsymbol{q}}\right]$$

$$h\left(\boldsymbol{q}_1, \ldots, \boldsymbol{q}_d; \Omega, \underline{\overline{c}}_1, \ldots, \underline{\overline{c}}_d\right) : [0,1]^{m_1+1} \times \ldots \times [0,1]^{m_d+1} \to \Omega$$

[1] Dette, H., and Studden, W. J., "The Theory of Canonical Moments with Applications in Statistics, Probability, and Analysis," Wiley-Interscience, New York, 1997.
[2] Stenger, J., "Optimal Uncertainty Quantification of a Risk Measurement from a Computer Code," phdthesis. Paul Sabatier. Université Toulouse III - Paul Sabatier (UPS), Toulouse, FRA., 2020.

OUQ: Dynamical System + Response Sets + Canonical Moments

$$\underset{(\mu_{\boldsymbol{q}}, K_t g) \in \mathcal{A}}{\text{infimum}} \; \mathbb{E}\left[K_t[g \circ h] \,\middle|\, \mu_{\boldsymbol{q}}\right] \leq \mathbb{E}[K_t^* g \mid \mu^*] \leq \underset{(\mu_{\boldsymbol{q}}, K_t g) \in \mathcal{A}}{\text{supremum}} \; \mathbb{E}[K_t[g \circ h] \mid \mu]$$

Transform from Canonical to State/Parameter Space

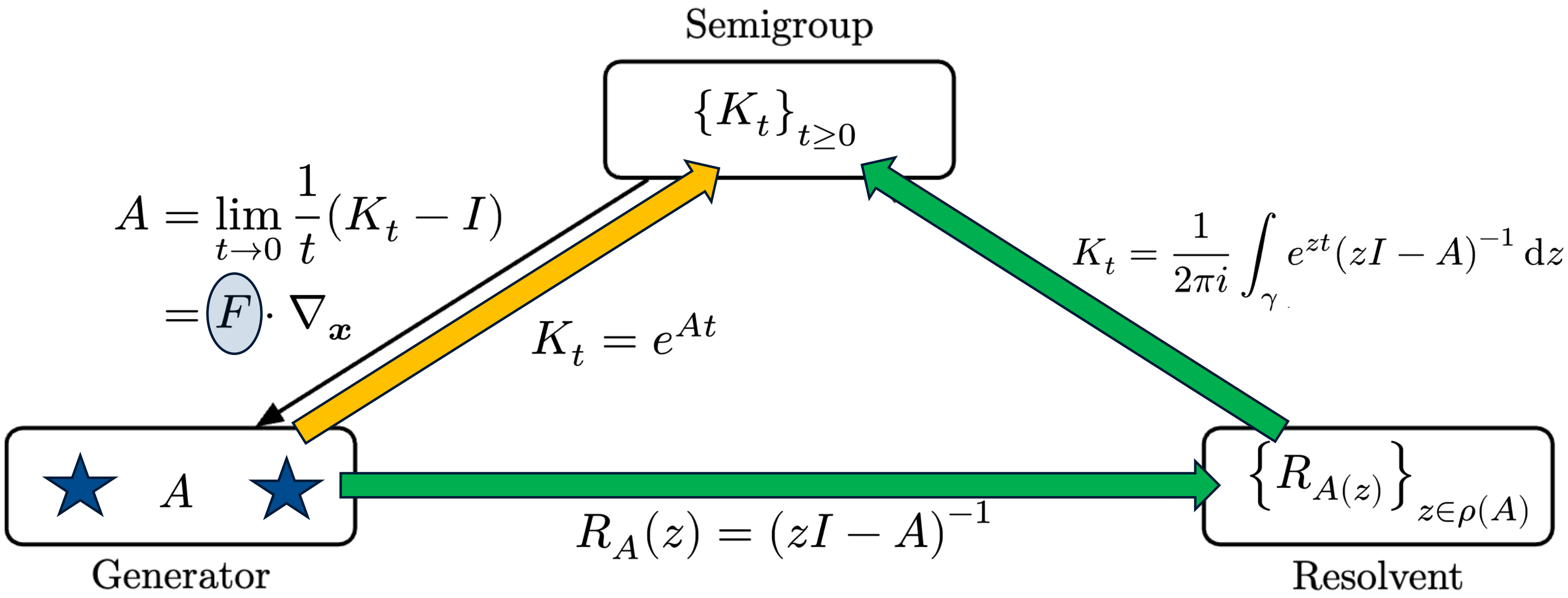
$$\mathcal{A} = \left\{ \left(\mu_{\boldsymbol{q}}, K_t g\right) \,\middle|\, \begin{array}{c} K_t g \in \mathcal{G} \\ \boldsymbol{x} \in \Omega \subseteq \mathbb{R}^d \\ \boldsymbol{q}_1 \in [0,1]^{m_1+1} \\ \vdots \\ \boldsymbol{q}_d \in [0,1]^{m_d+1} \end{array} \right\}$$

Set of response functions induced by the dynamical system

Admissible Set in terms of Canonical Moments

Rigorous Pull-Backs

Pullbacks via Semigroup Theory

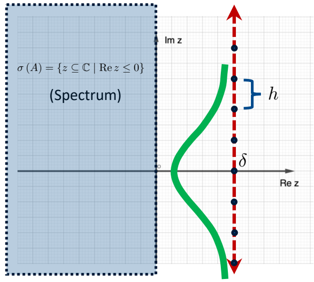


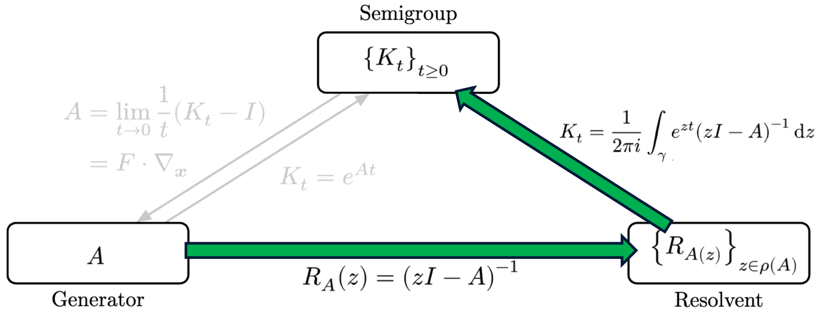
[22] K. Makino and M. Berz, "Taylor Models and Other Validated Functional Inclusion Methods," *International Journal of Pure and Applied Mathematics*, vol. 4, no. 4, Jan. 2003.

Pullbacks via Semigroup Theory #1

- 2023 Review (Series Acceleration)

$$\hat{K}_t g \approx \frac{h}{2\pi}(2\delta - A)^2 \sum_{k=-N}^{N} e^{-(\sigma hk)^2} \frac{e^{t(\delta+ihk)}}{(\delta - ihk)^2} R_A(\delta + ihk)g, \text{for } g \in D(A)$$





- New: Family of High Order Methods http://arxiv.org/abs/2408.07691

$$r(A)e^{At}g = \frac{1}{2\pi i}\int_{\delta - i\infty}^{\delta + i\infty} r(z)e^{zt}R_A(z)g\,\mathrm{d}z$$

How to select $r(\cdot)$?

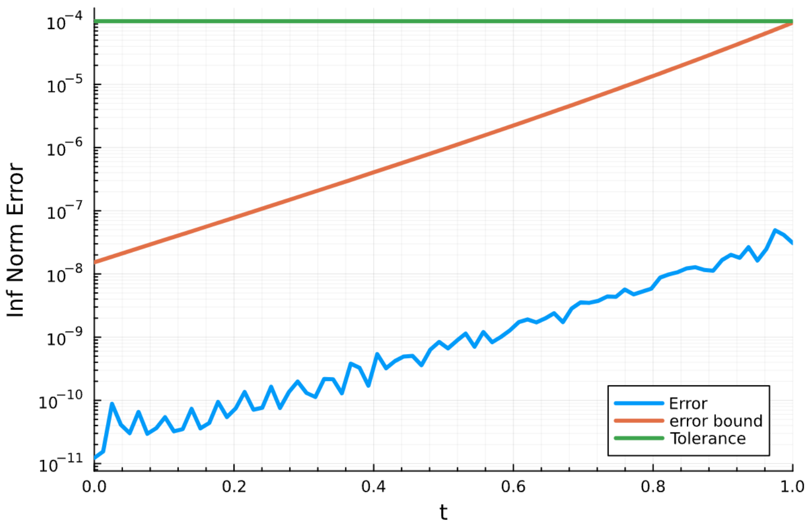
Complexity of $r(A)^{-1}$	Regularity of g	Analyticity/Decay of $r(z)$

$$r(z) = (2\delta - z)^{-m}$$

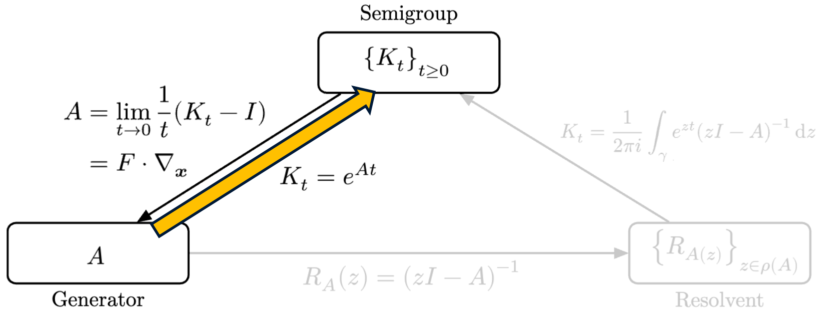
$$\hat{K}_t g \approx \frac{h}{2\pi}\sum_{k=-N}^{N} \frac{e^{t(\delta+ihk)}}{(\delta - ihk)^m}[R_A(\delta + ihk)[(2\delta - A)^m g]], \text{for } g \in D(A^m)$$

$$\|\varepsilon(t)\| = \left(\underbrace{e^{\frac{3}{2}\delta t} f_D(\delta, m, h)}_{\text{Discretization}} + \underbrace{e^{\delta t} f_T(\delta, m, h, N)}_{\text{Truncation}}\right)\|(2\delta - A)^m g\|$$

$$K_t g \in \left\{\hat{K}_t g + \alpha \mid \alpha \in [-\|\varepsilon(t)\|, \|\varepsilon(t)\|]\right\}$$



Pullbacks via Semigroup Theory #2



$$K_t g = e^{At} g = \sum_{k=0}^{\infty} \frac{A^k g}{k!} t^k \qquad \hat{K}_t g = \sum_{k=0}^{n} \frac{A^k g}{k!} t^k$$

$$K_t g \in \underbrace{\left\{ \hat{K}_t g + \alpha \,\middle|\, \alpha \in \underline{I} \in \mathbb{IR}, t \in [0, t_f] \right\}}_{\mathcal{K}}$$

Picard Operator $$[Q_F h_t](\boldsymbol{x}) = \boldsymbol{x} + \int_0^t F(h_\tau(\boldsymbol{x}))\,\mathrm{d}\tau \text{ for } h_t(\boldsymbol{x}) = \boldsymbol{x}_i(t)$$

State Observable

$$\mathcal{J} = \left\{ Q_F h_t \,\middle|\, h_t \in \mathcal{K}, t \in [0, t_f] \right\}$$

Contraction $$\mathcal{J} \subseteq \mathcal{K} \longrightarrow K_t g \in \mathcal{K} \text{ for } g(\boldsymbol{x}) = \boldsymbol{x}_i \longrightarrow S_{t\in[0,t_f]} \in \mathcal{K}$$

Rigorous Flow Map Surrogate

$$K_t g \in \{ g \circ S_t \mid S_t \in \mathcal{K} \} \text{ for } t \in [0, t_f]$$

Definition 8.1 (Taylor Model [22]): Let $f : \Omega \subset \mathbb{R}^n \to \mathbb{R}$ be an $m+1$ times continuously partially differentiable function on an open set containing the domain Ω. Let $\boldsymbol{x}_0$ be a point in Ω, p_m be the m^{th} order Taylor polynomial of f around $\boldsymbol{x}_0 \in \Omega$, and $\underline{I} \in \mathbb{IR}$ be an *interval remainder* such that

$$f(\boldsymbol{x}) \in p_m(\boldsymbol{x} - \boldsymbol{x}_0) + \underline{I}, \quad \forall \boldsymbol{x} \in \Omega \tag{60}$$

The pair $\mathcal{T} := (p_m, \underline{I})$ is then called the m^{th} order Taylor model of f about $\boldsymbol{x}_0$ on Ω.

[22] K. Makino and M. Berz, "Taylor Models and Other Validated Functional Inclusion Methods," *International Journal of Pure and Applied Mathematics*, vol. 4, no. 4, Jan. 2003.

OUQ Induced by Dynamical System Revisited

$$\underset{(\mu_{\boldsymbol{q}},K_t g)\in\mathcal{A}}{\text{infimum}}\ \mathbb{E}\big[K_t[g\circ h]\,\big|\,\mu_{\boldsymbol{q}}\big] \le \mathbb{E}[K_t^* g\,|\,\mu^*] \le \underset{(\mu_{\boldsymbol{q}},K_t g)\in\mathcal{A}}{\text{supremum}}\ \mathbb{E}[K_t[g\circ h]\,|\,\mu]$$

$$\mathcal{A} = \left\{ (\mu_{\boldsymbol{q}}, K_t g) \;\middle|\; \begin{array}{c} K_t g \in \mathcal{G} \\ \boldsymbol{x} \in \Omega \subseteq \mathbb{R}^d \\ \boldsymbol{q}_1 \in [0,1]^{m_1+1} \\ \vdots \\ \boldsymbol{q}_d \in [0,1]^{m_d+1} \end{array} \right\}$$

$$\mathcal{G} = \hat{K}_t g + \underline{I}(t)$$

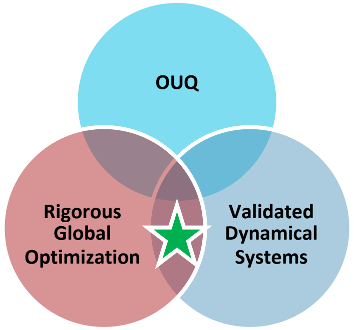
Dense in time & space

$$\underset{\mu_{\boldsymbol{q}}\in\mathcal{A}}{\text{infimum}}\ \mathbb{E}\Big[\hat{K}_t[g\circ h] + \underline{I}(t)\,\Big|\,\mu_{\boldsymbol{q}}\Big] \le \mathbb{E}[K_t^* g\,|\,\mu^*] \le \underset{\mu_{\boldsymbol{q}}\in\mathcal{A}}{\text{supremum}}\ \mathbb{E}\Big[\hat{K}_t[g\circ h] + \overline{I}(t)\,\Big|\,\mu_{\boldsymbol{q}}\Big]$$

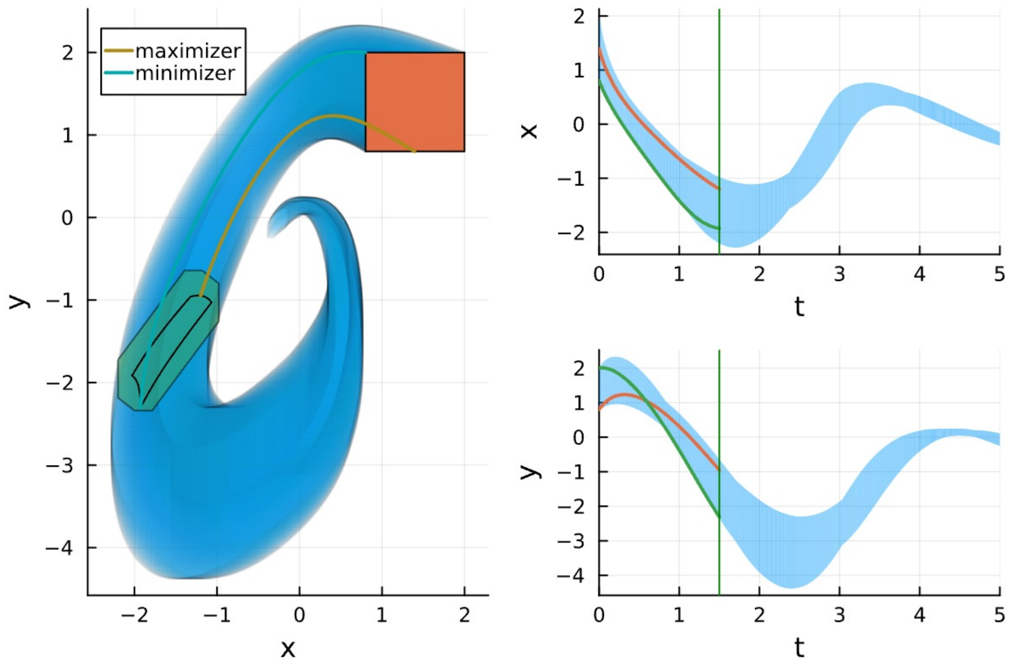
Preliminary Results

Validated ODE + Rigorous Optimization

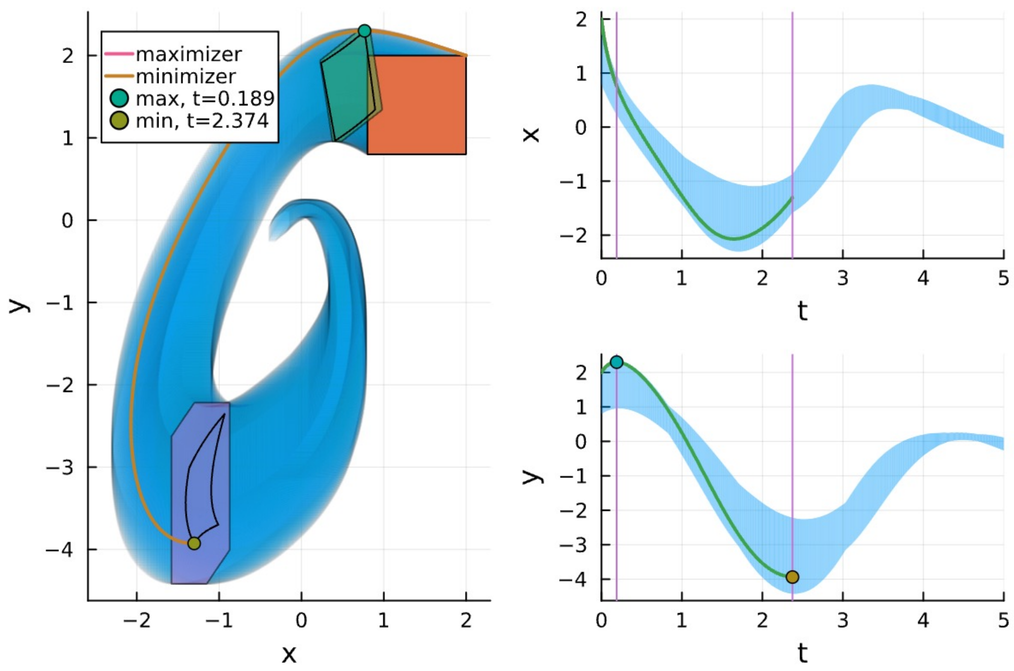
$$\dot{\boldsymbol{x}} = \begin{bmatrix} -x_2 - \frac{3}{2}x_1^2 - \frac{1}{2}x_1^3 + \frac{1}{2} \\ 2x_1 - x_2 \end{bmatrix}, \boldsymbol{x}(0) \in [0.8, 2] \times [0.8, 2] \qquad g(\boldsymbol{x}) = x_2$$



Optimize @ t = 1.5 s



Optimize $\forall t$

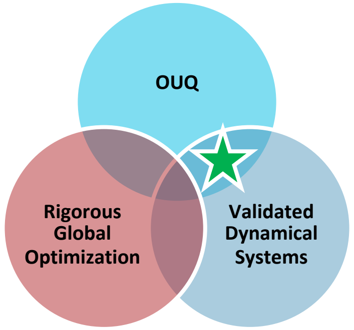


Validated ODE + OUQ

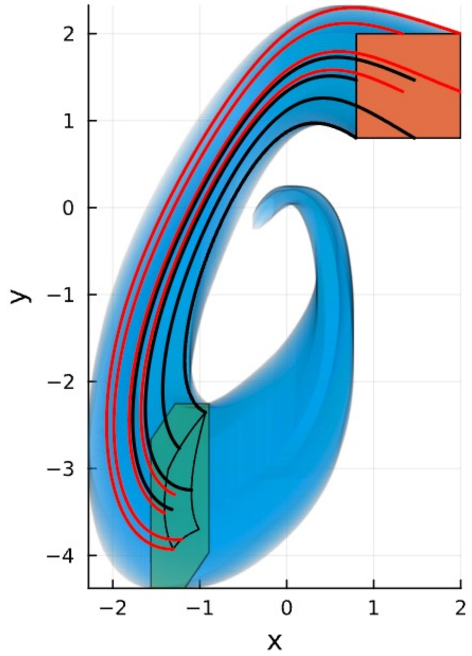
$$\dot{\boldsymbol{x}} = \begin{bmatrix} -x_2 - \frac{3}{2}x_1^2 - \frac{1}{2}x_1^3 + \frac{1}{2} \\ 2x_1 - x_2 \end{bmatrix}, \boldsymbol{x}(0) \in [0.8, 2] \times [0.8, 2]$$

$$\mathbb{E}\left[x_j \,\middle|\, \mu^*\right] = 1.4$$

$$\operatorname{std}\left(x_j \mid \mu^*\right) = 0.2$$

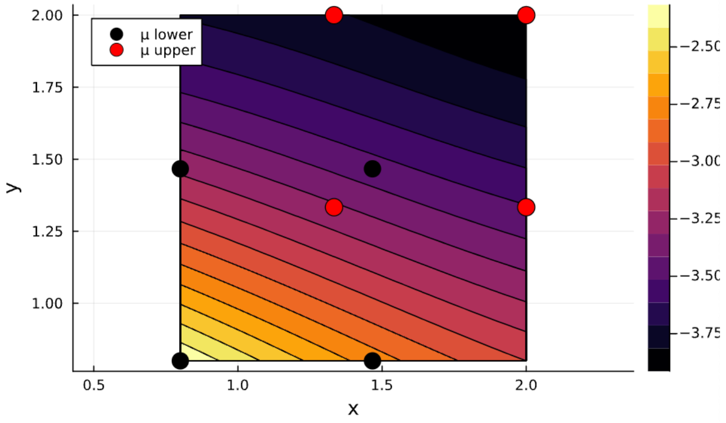


Optimize @ t = 2.374 s

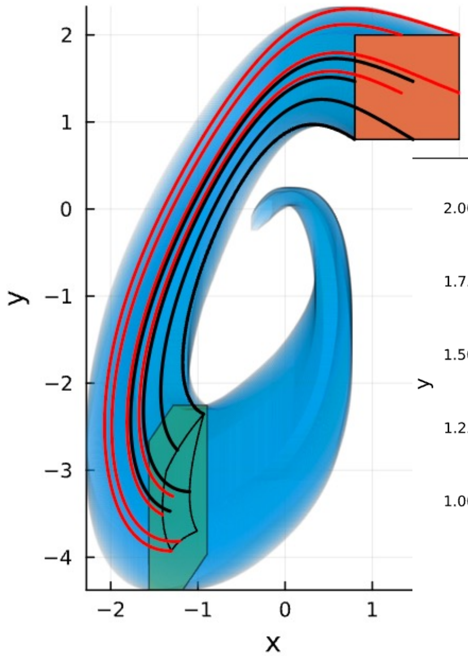


$$g(\boldsymbol{x}) = x_2$$

$$\mathbb{E}[K_t^* g \,|\, \mu^*] \in [-3.375, -3.370]$$

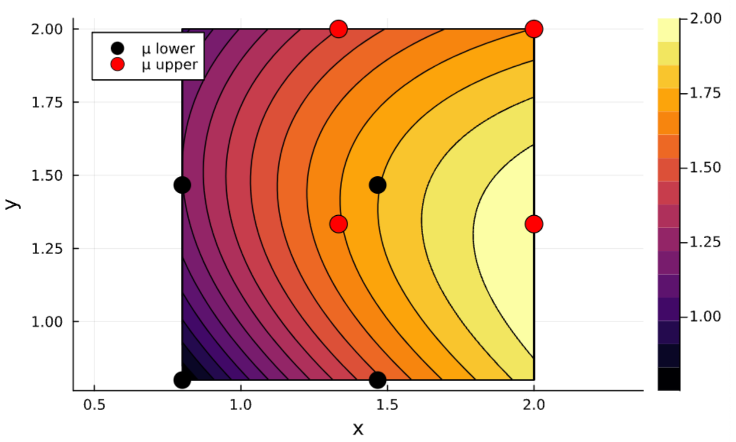


Optimize @ t = 2.374 s

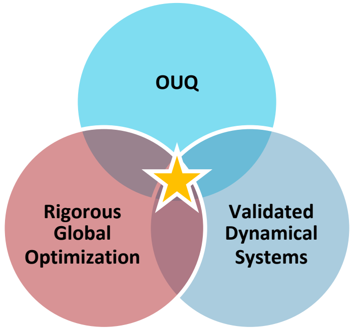


$$g(\boldsymbol{x}) = x_1^2$$

$$\mathbb{E}[K_t^* g \,|\, \mu^*] \in [1.617, 1.755]$$



Validated ODE + **Complete** Optimization + OUQ



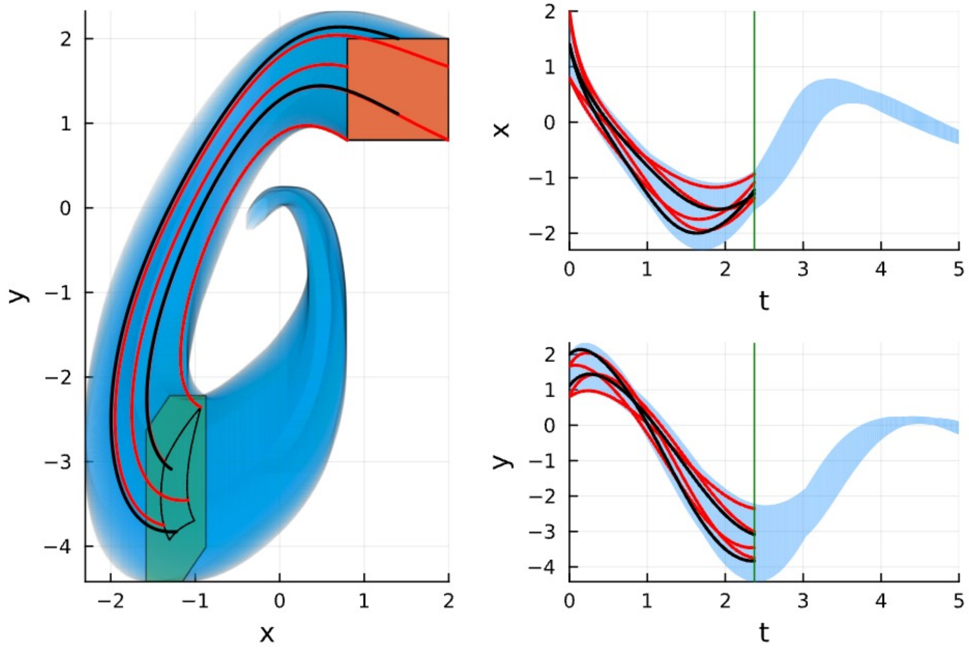
$$\dot{\boldsymbol{x}} = \begin{bmatrix} -x_2 - \frac{3}{2}x_1^2 - \frac{1}{2}x_1^3 + \frac{1}{2} \\ 2x_1 - x_2 \end{bmatrix}, \boldsymbol{x}(0) \in [0.8, 2] \times [0.8, 2]$$

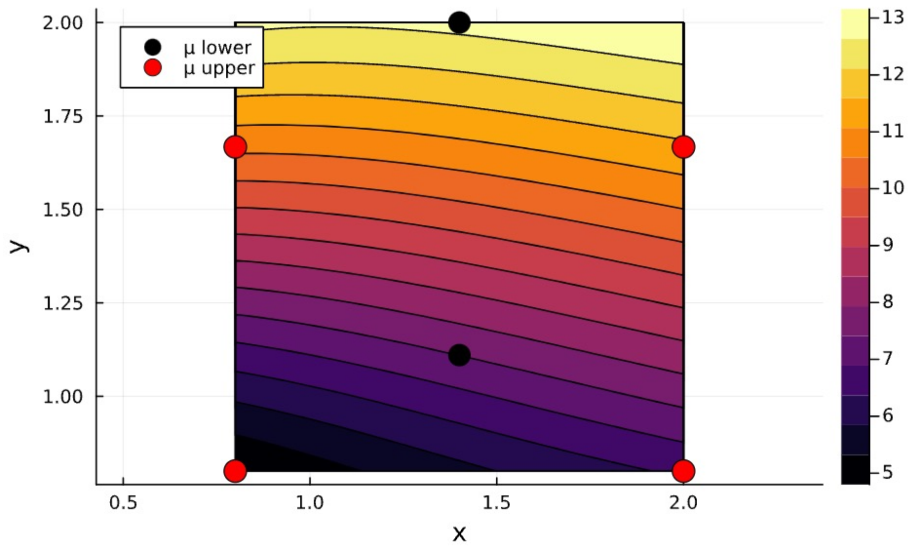
$$\mathbb{E}\left[x_j \,\middle|\, \mu^*\right] = 1.4$$

Optimize @ t = 2.374 s

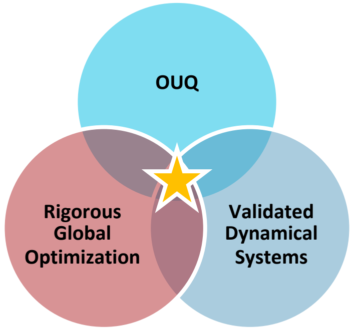
$$g(\boldsymbol{x}) = x_1^3 + x_2^2$$

$$\mathbb{E}[K_t^* g \,|\, \mu^*] \in [-3.388, -3.248]$$





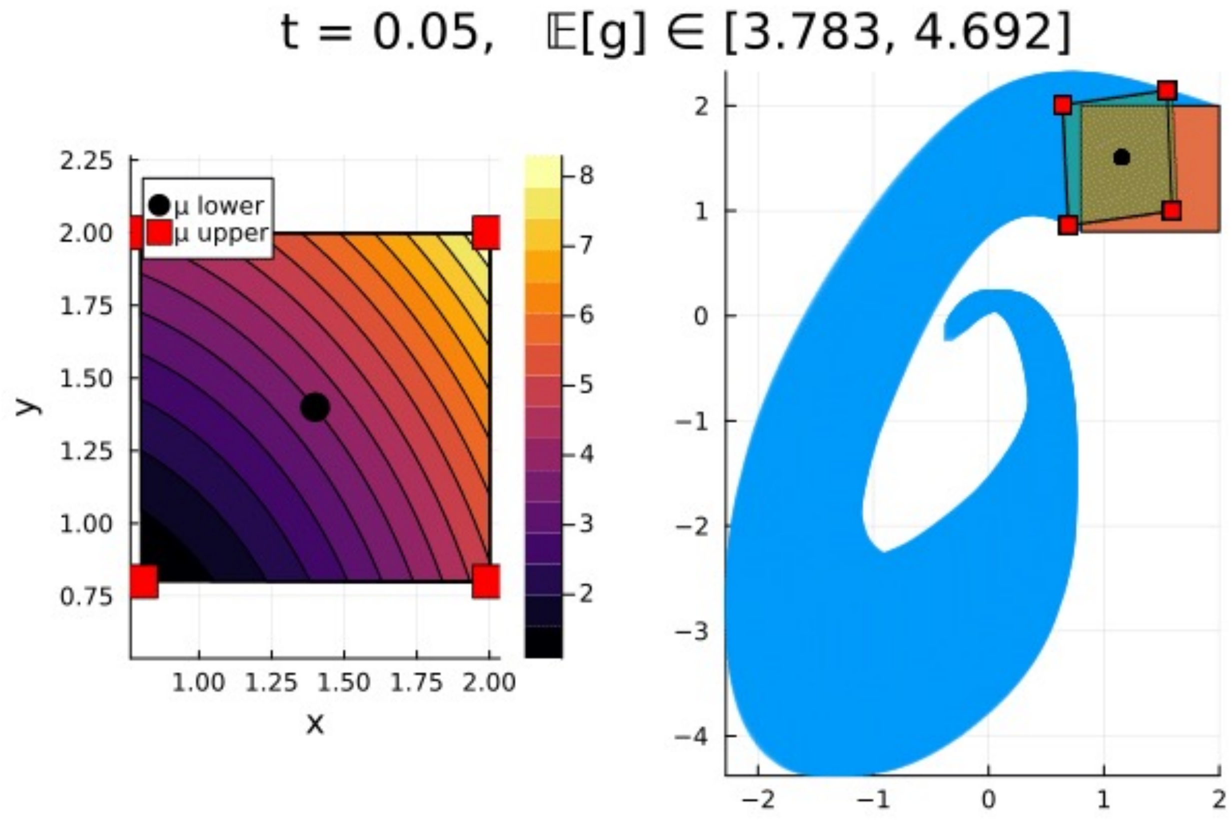
Validated ODE + **Complete** Optimization + OUQ

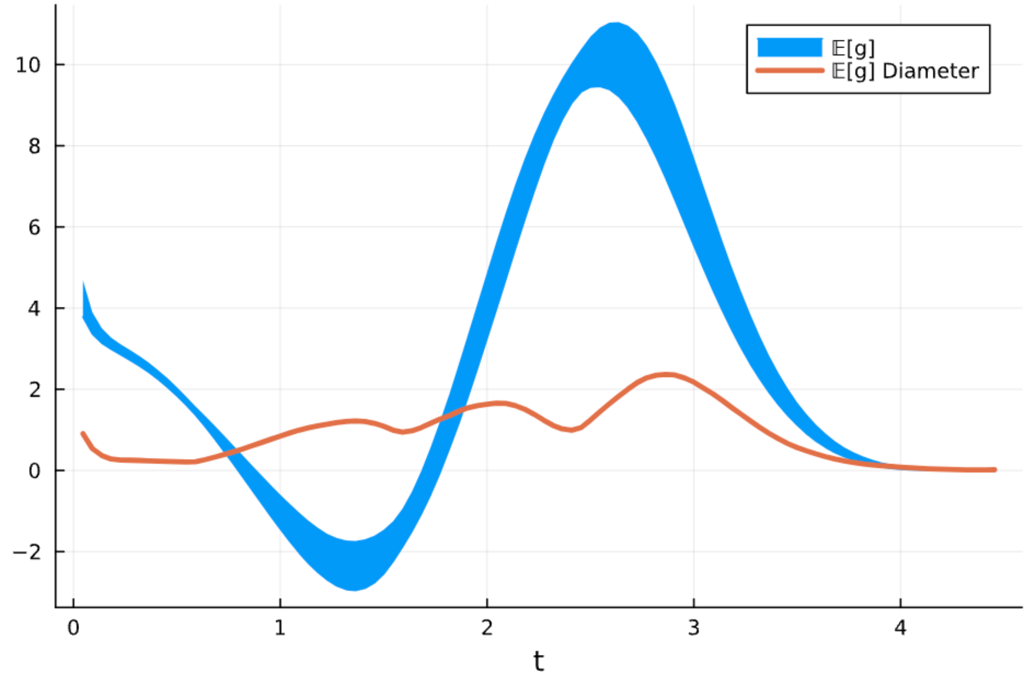


$$\dot{\boldsymbol{x}} = \begin{bmatrix} -x_2 - \frac{3}{2}x_1^2 - \frac{1}{2}x_1^3 + \frac{1}{2} \\ 2x_1 - x_2 \end{bmatrix}, \boldsymbol{x}(0) \in [0.8, 2] \times [0.8, 2]$$

$$\mathbb{E}\left[x_j \mid \mu^*\right] = 1.4$$

$$g(\boldsymbol{x}) = x_1^3 + x_2^2$$

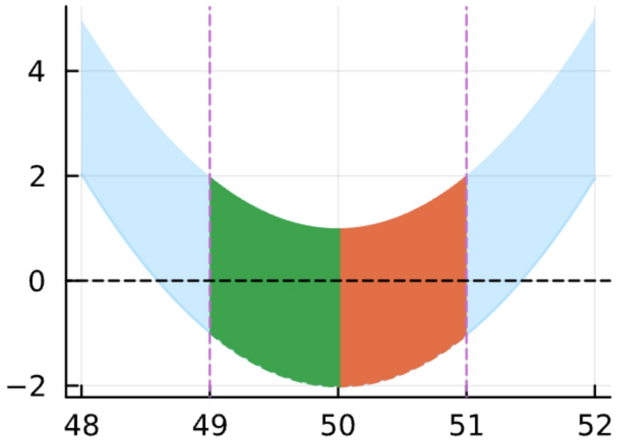




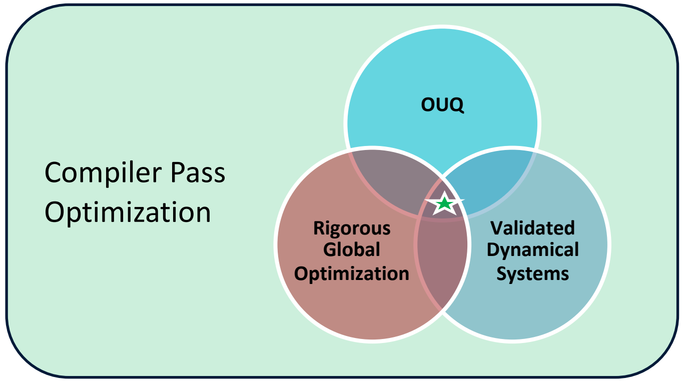
Planned Next Steps

- End-to-End <u>Rigorous</u> OUQ + ODE + Global Opt.
  - Rigorous Canonical Moments $h\left(\boldsymbol{q}_1, \ldots, \boldsymbol{q}_d; \Omega, \underline{\overline{c}}_1, \ldots, \underline{\overline{c}}_d\right) : [0,1]^{m_1+1} \times \ldots \times [0,1]^{m_d+1} \rightarrow \Omega$
  - **Challenge:** Interval Coefficient Polynomial Root Finding
    - Possibility of Repeated Roots
- Global Optimization
  - Extensible SW framework for scalable global dynamic optimization
  - GPU accelerated branch and bound solver
  - Leverage Semidefinite/Second-Order Cone Program (Taylor Model specific)
- Extend Picard Iteration → contraction to the Operator level.
- Develop automatic code transformation tools

$$[\mathrm{LB}^*, \mathrm{UB}^*] = \cap_i\, \rho_i(\mathcal{A}),\, \rho_i \in \boxed{\mathfrak{P} \quad \text{Set of equiv. programs}}$$



$$\begin{bmatrix} 1 & 1 \\ \boxed{[49, 50.05]} & \boxed{[49.95, 51]} \end{bmatrix} \boldsymbol{x} = b$$



Publications to Date

- Horning, A., Gerlach, A., “A family of high-order contour integral methods for strongly continuous semigroups”, In preparation for *Foundations of Computational Mathematics.* http://arxiv.org/abs/2408.07691
- Bakker, C., Rupe, A., Von Moll, A., Gerlach, A., “Operator-Theoretic Methods for Differential Games”, In preparation for *J of Computational Physics.*
- Von Moll, A., Gerlach, A., et al., “Constrained Turret Defense with Fixed Final Time” Modeling, Estimation, and Control, American Automatic Control Council 2024 (accepted)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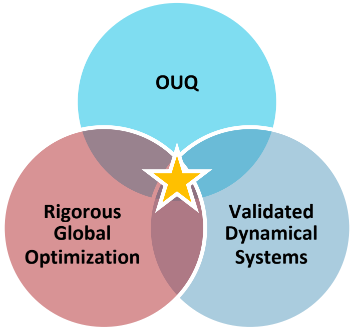
QUESTIONS?

Validated ODE + **Complete** Optimization + OUQ



$$\dot{\boldsymbol{x}} = \begin{bmatrix} -x_2 - \frac{3}{2}x_1^2 - \frac{1}{2}x_1^3 + \frac{1}{2} \\ 2x_1 - x_2 \end{bmatrix}, \boldsymbol{x}(0) \in [0.8, 2] \times [0.8, 2]$$

$$\mathbb{E}\left[x_j \mid \mu^*\right] = 1.4$$

t = 0.05, $\mathbb{E}$[g] ∈ [3.72, 4.57]

$$g(\boldsymbol{x}) = x_1^3 + x_2^2$$