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Recent Advances in Bounding Transient PDE Models with Parametric Uncertainty

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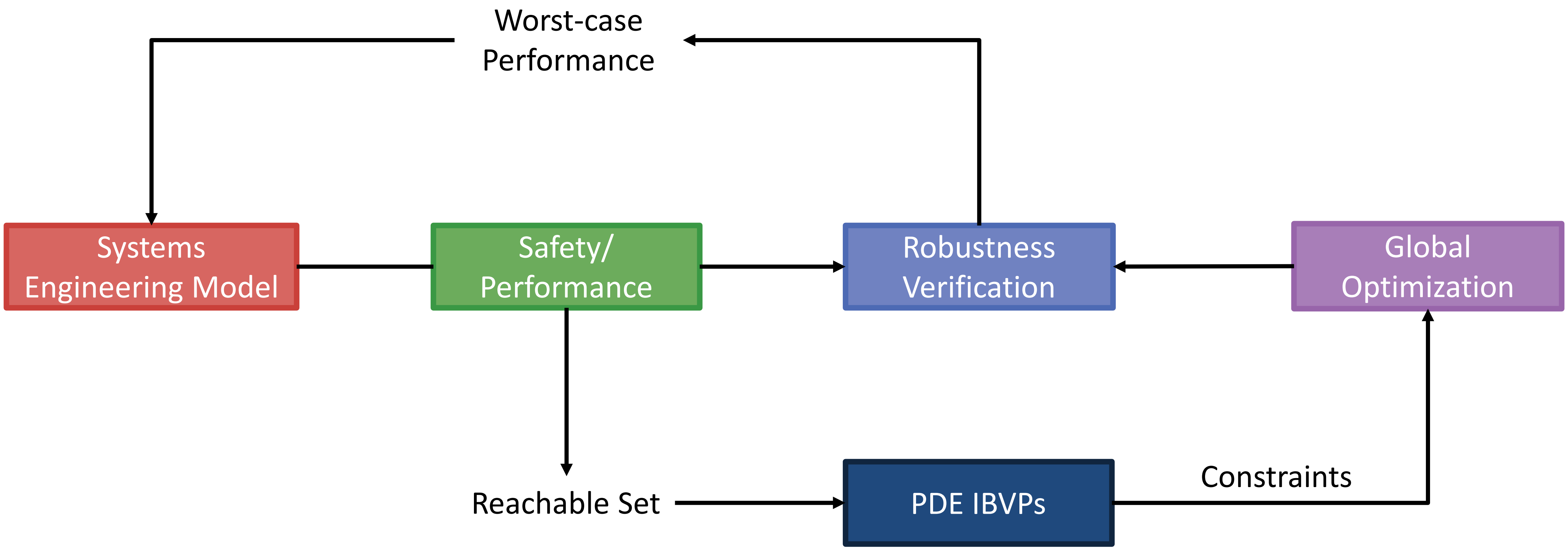
2020 AIChE Annual Meeting

2020 AIChE ANNUAL MEETING

Process Systems and Operations Research Laboratory

Background



[1] C. Wang and M. D. Stuber, *Under Review*, 2020
[2] M. D. Stuber and P. I. Barton, “Robust simulation and design using semi-infinite programs with implicit functions,” *International Journal of Reliability and Safety*, vol. 5, no. 3-4, pp. 378-397, 2011.
[3] M. D. Stuber, A.Wechsung, A. Sundaramoorthy, and P. I. Barton, “Worst-case design of subsea production facilities using semi-infinite programming,” AIChE Journal, vol. 60, no. 7, pp. 2513-2524, 2014.

Parametric Partial Differential Equations

- Provide rigorous bounds for parametric PDE system (IBVP)

$$\partial_t \tilde{\mathbf{x}}(y,t,\mathbf{p}) = \tilde{\mathbf{f}}(y,t,\tilde{\mathbf{x}}(y,t,\mathbf{p}),\partial_y \tilde{\mathbf{x}}(y,t,\mathbf{p}),\partial_{yy}\tilde{\mathbf{x}}(y,t,\mathbf{p}),\mathbf{p}) \quad (1)$$
$$\tilde{\mathbf{x}}(y,t_0,\mathbf{p}) = \tilde{\mathbf{x}}_0(y,\mathbf{p})$$
$$\tilde{\mathbf{f}}_l(\tilde{\mathbf{x}}(y_l,t,\mathbf{p}),\partial_y \tilde{\mathbf{x}}(y_l,t,\mathbf{p}),\mathbf{p}) = \tilde{\mathbf{x}}_l(t,\mathbf{p})$$
$$\tilde{\mathbf{f}}_r(\tilde{\mathbf{x}}(y_r,t,\mathbf{p}),\partial_y \tilde{\mathbf{x}}(y_r,t,\mathbf{p}),\mathbf{p}) = \tilde{\mathbf{x}}_r(t,\mathbf{p}).$$

- Assumptions:
  1. *$\tilde{\mathbf{f}} : Y \times I \times D \times \mathbb{R}^{n_x} \times \mathbb{R}^{n_x} \times P \to \mathbb{R}^{n_x}$, $\tilde{\mathbf{x}}_0 : Y \times P \to D$, $\tilde{\mathbf{f}}_l : D \times \mathbb{R}^{n_x} \times P \to \mathbb{R}^{n_x}$, $\tilde{\mathbf{x}}_l : I \times P \to \mathbb{R}^{n_x}$, $\tilde{\mathbf{f}}_r : D \times \mathbb{R}^{n_x} \times P \to \mathbb{R}^{n_x}$ and $\tilde{\mathbf{x}}_r : I \times P \to \mathbb{R}^{n_x}$ are locally Lipschitz continuous.*
  2. *A solution of (1) is denoted $\tilde{\mathbf{x}} : Y \times I \times P \to D$, and is twice continuously differentiable for all $y \in Y$.*
  3. *For each $y \in Y$, there exists a unique solution over the time domain I for every $\mathbf{p} \in P$.*

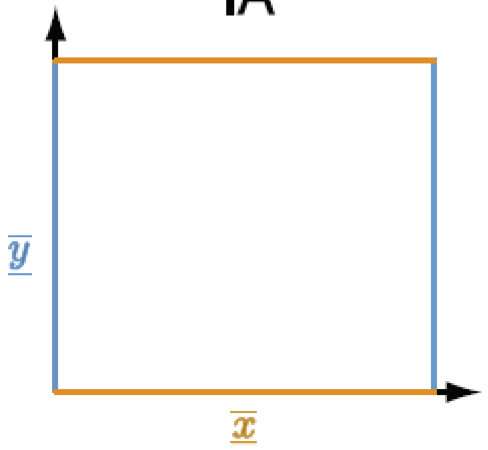
- Reachable set: $\mathrm{R}(y,t) \equiv \{\tilde{\mathbf{x}}(y,t,\mathbf{p}) : \mathbf{p} \in P\}$.

- State bounds: $\tilde{\mathbf{x}}^L, \tilde{\mathbf{x}}^U : Y \times I \to \mathbb{R}^{n_x}$

Interval Arithmetic and Affine Arithmetic

Interval Arithmetic (IA)

$x \in [x^L, x^U] = X$



- $F(X) \supseteq \mathbf{f}(X) = \{\mathbf{f}(\mathbf{x}) | \mathbf{x} \in X\}$
- Dependency problems

$x_0 = (x^L + x^U)/2,$

$x_1 = (x^U - x^L)/2,$

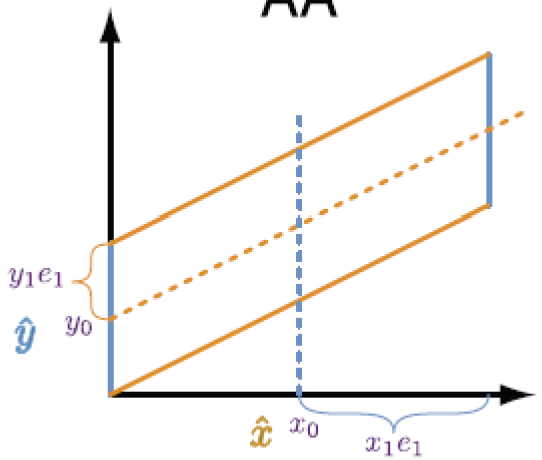
$x_i = 0, \forall i > 1$

Affine Arithmetic (AA)

$\hat{x} = x_0 + \sum_{i=1}^{m} x_i \varepsilon_i$

$\hat{X} = [x_0 - r_x, x_0 + r_x]$

$r_x = \sum_{i=1}^{m} |x_i|$



- Keep track of the dependency;
- Reduce overestimation

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[5] J. Stolfi, L. H. de Figueiredo, "An introduction to affine arithmetic," *Trends in Applied and ComputationalMathematics*, 4 (3) (2003) 297–312.
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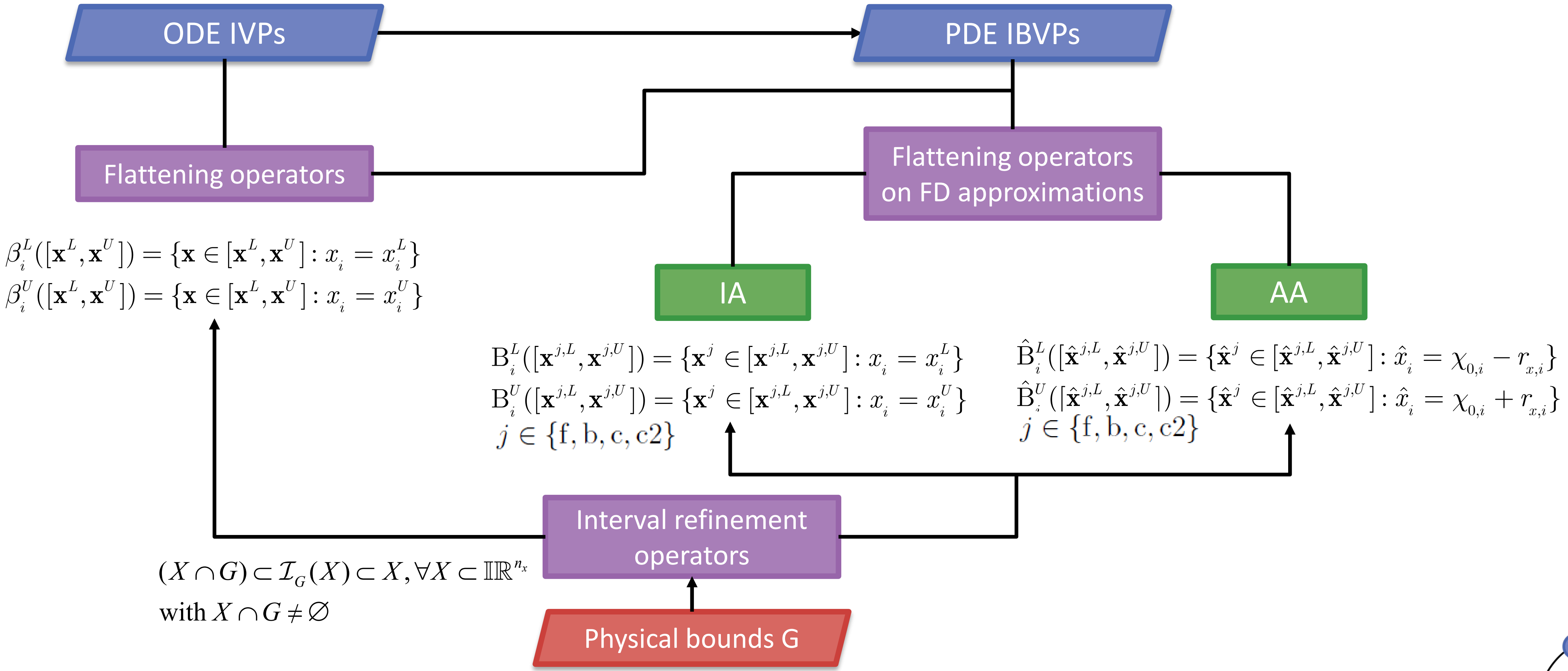
Differential Inequalities



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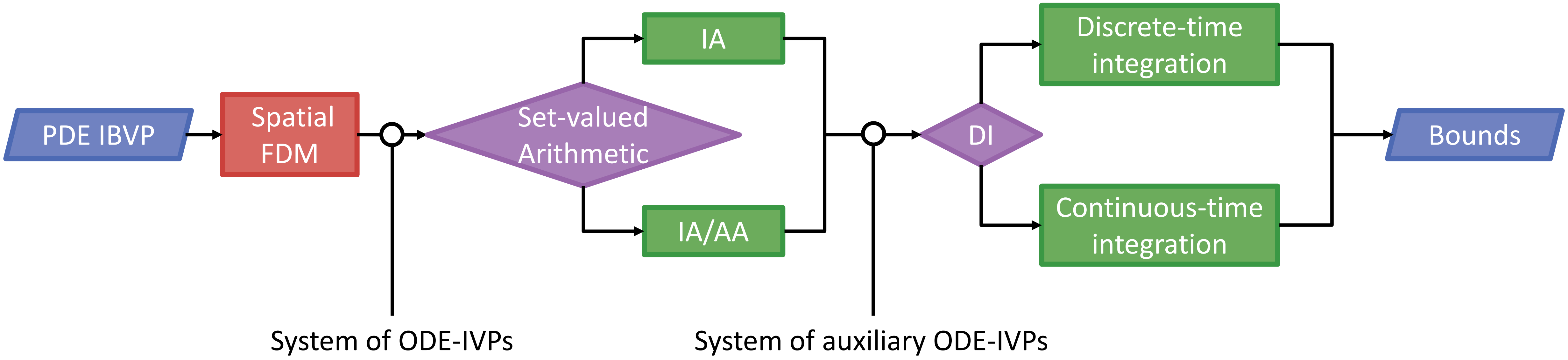
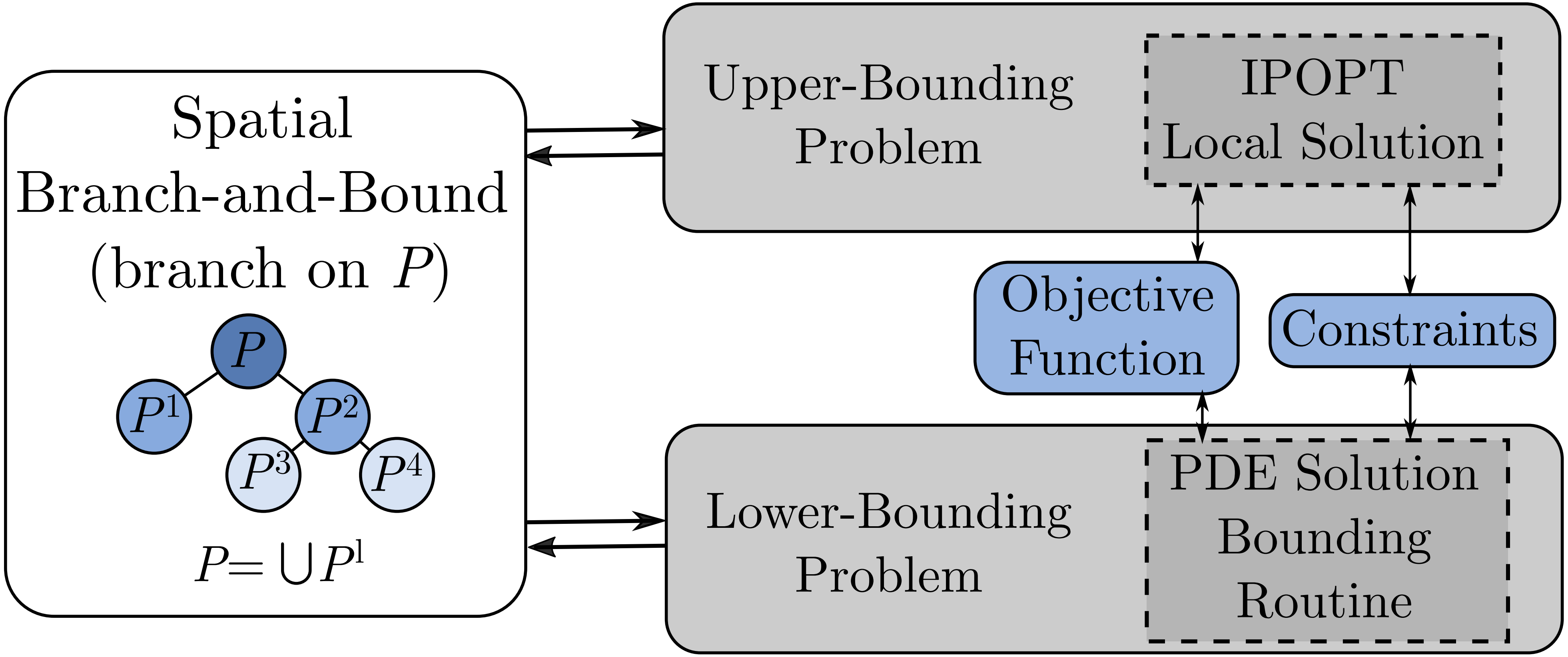
Bounding IBVPs



[1] C. Wang and M. D. Stuber, *Under Review*, 2020

Deterministic Global Optimization

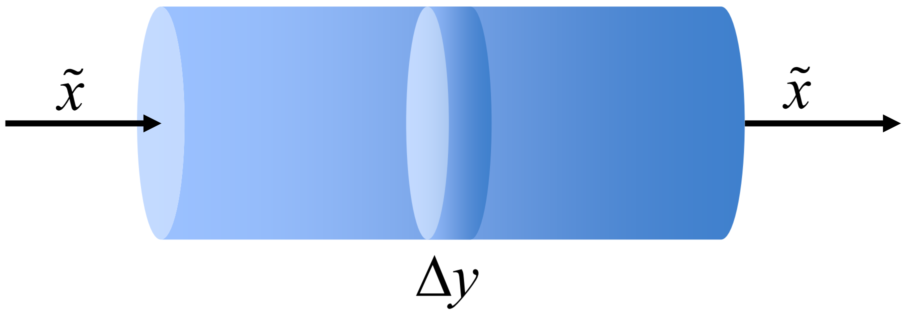
Deterministic Global Optimization Algorithm



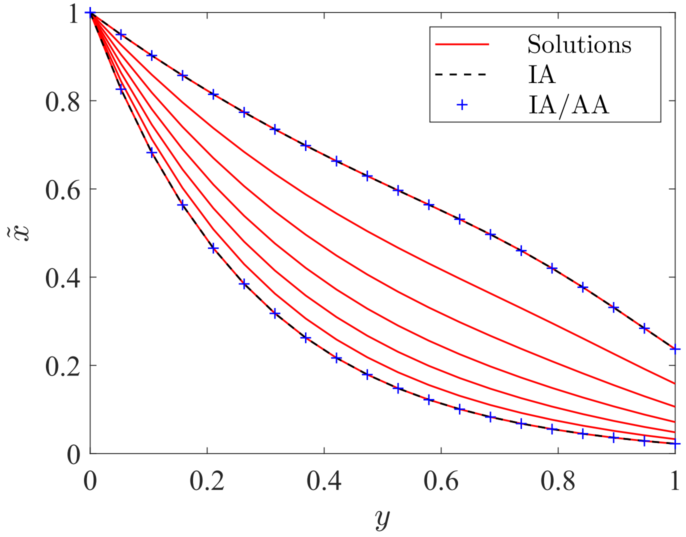
Transient Plug Flow Reactor

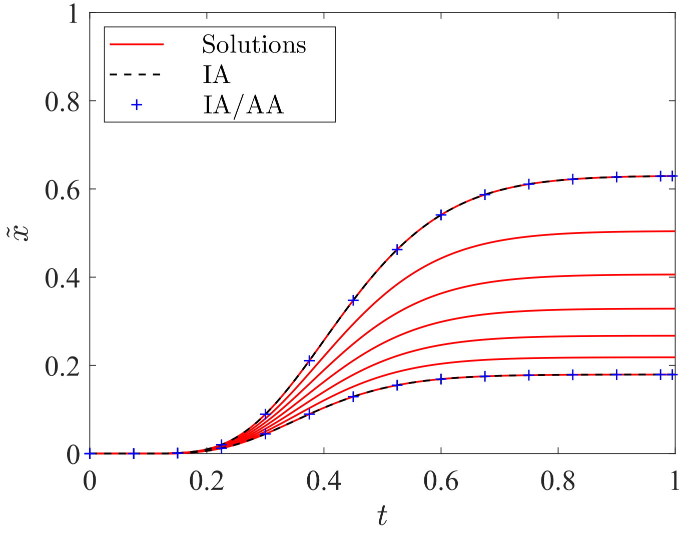
$$\frac{\partial \tilde{x}}{\partial t} = -\frac{\partial \tilde{x}}{\partial y} - Da\tilde{x},\ t \in [0,1],\ y \in [0,1]$$

$$Da = k\tau \qquad k \in [0.1, 0.4]$$



$$\frac{\partial \mathbf{x}}{\partial t} = -\mathbf{x}^{\mathrm{b}} - Da\mathbf{x}$$

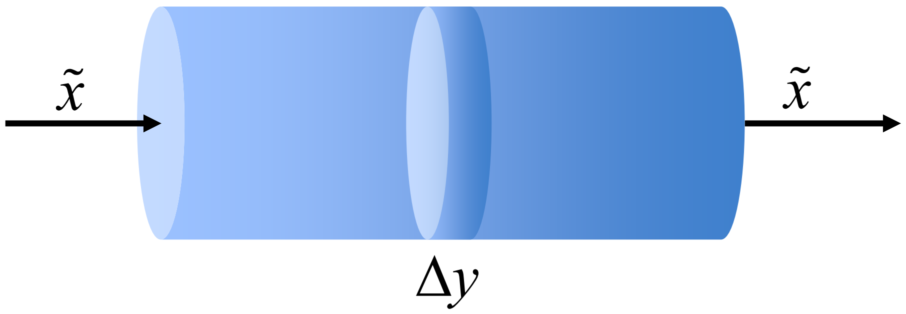




[1] C. Wang and M. D. Stuber, *Under Review*, 2020

Transient Plug Flow Reactor

$$\frac{\partial \tilde{x}}{\partial t} = -\frac{\partial \tilde{x}}{\partial y} - Da\tilde{x}, \ t \in [0,1], \ y \in [0,1]$$



$$\frac{\partial \mathbf{x}}{\partial t} = -\mathbf{x}^{\mathrm{b}} - Da\mathbf{x}$$

$$\min_{p \in P} \ p$$

$$\text{s.t.} \ z_{K,exit} - \lambda \leq 0$$

$$p \in P = [0,1]$$

$$Da = k\tau = (0.1 + 0.3p)\tau$$

$z_{K,exit}$: effluent concentration

Method	Time (s)
Explicit approach	38.7
Implicit approach	382

[1] C. Wang and M. D. Stuber, Under Review, 2020
[8] M. E. Wilhelm and M. D. Stuber. EAGO.jl: easy advanced global optimization in Julia. *Optimization Methods and Software*, pages 1–26, aug 2020
[9] M. E. Wilhelm, A. V. Le, and Matthew D. Stuber. Global optimization of stiff dynamical systems. *AIChE Journal*, 65(12), nov 2019

Ozone System: Coupled IBVPs

$$O + O_2 \xrightarrow{k_1} O_3$$

$$O + O_3 \xrightarrow{k_2} 2O_2$$

$$O_2 \xrightarrow{k_3(t)} 2O$$

$$O_3 \xrightarrow{k_4(t)} O + O_2$$

$$\frac{\partial c_O}{\partial t} + u_1 \frac{\partial c_O}{\partial y} = D_1 \frac{\partial^2 c_O}{\partial y^2} + r_{c_O},$$

$$\frac{\partial c_{O_2}}{\partial t} + u_2 \frac{\partial c_{O_2}}{\partial y} = D_2 \frac{\partial^2 c_{O_2}}{\partial y^2} + r_{c_{O_2}},$$

$$\frac{\partial c_{O_3}}{\partial t} + u_3 \frac{\partial c_{O_3}}{\partial y} = D_3 \frac{\partial^2 c_{O_3}}{\partial y^2} + r_{c_{O_3}},$$

$$r_{c_O} = -k_1 c_O c_{O_2} - k_2 c_O c_{O_3} + 2k_3(t) c_{O_2} + k_4(t) c_{O_3},$$

$$r_{c_{O_2}} = -k_1 c_O c_{O_2} + k_2 c_O c_{O_3} - k_3(t) c_{O_2} + k_4(t) c_{O_3},$$

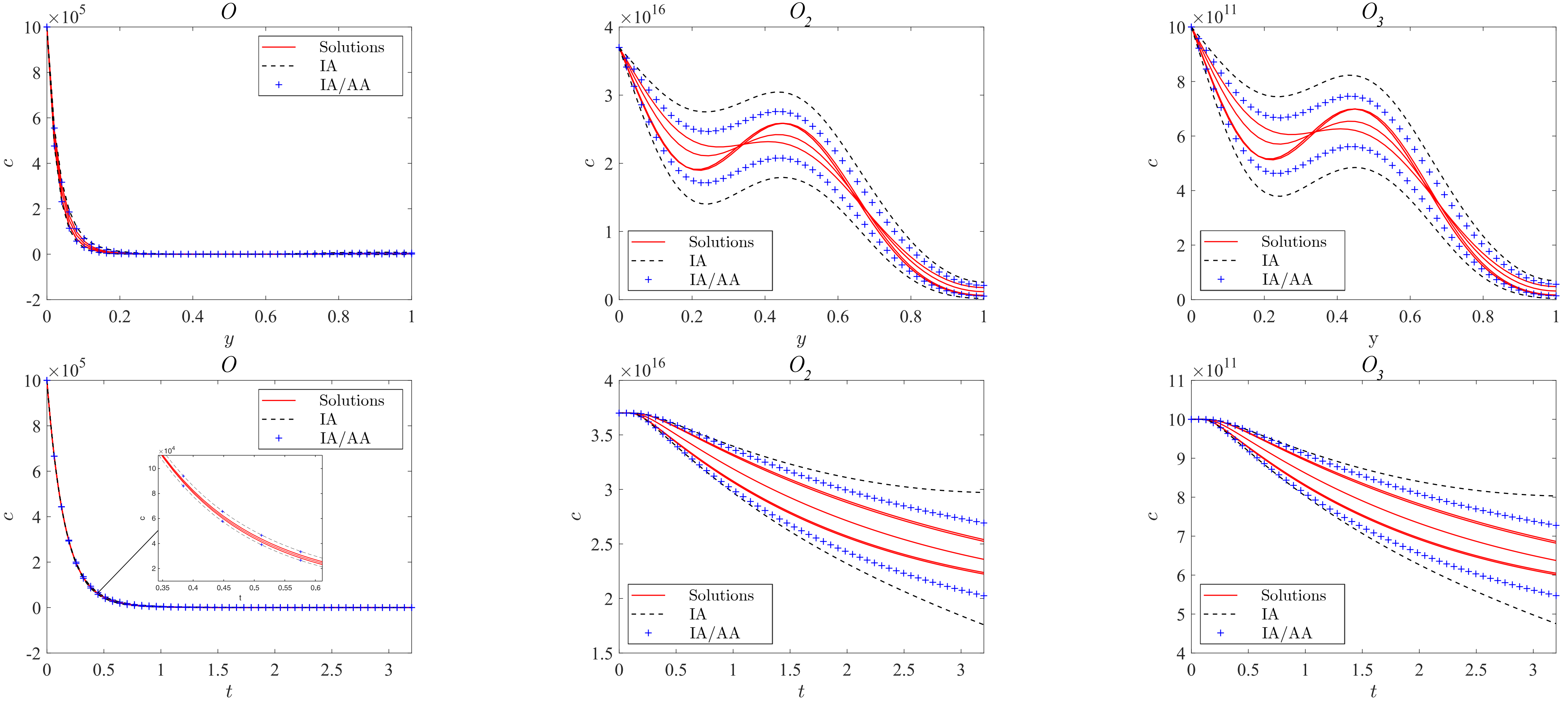
$$r_{c_{O_3}} = k_1 c_O c_{O_2} - k_2 c_O c_{O_3} - k_4(t) c_{O_3}.$$

$u = u_1 = u_2 = u_3$ $\quad u \in$ [4e-3,6e-3]

$D = D_1 = D_2 = D_3$ $\quad D \in$ [4e-3,6e-3]

[10] J. Makungu, H. Haario, W. C. Mahera, “A generalized 1-dimensional particle transport method for convection diffusion reaction model,” *Afrika Matematika*, 23 (1) (2012) 21–39.

Ozone System: Coupled IBVPs



[1] C. Wang and M. D. Stuber, *Under Review*, 2020

Ozone System: Coupled IBVPs

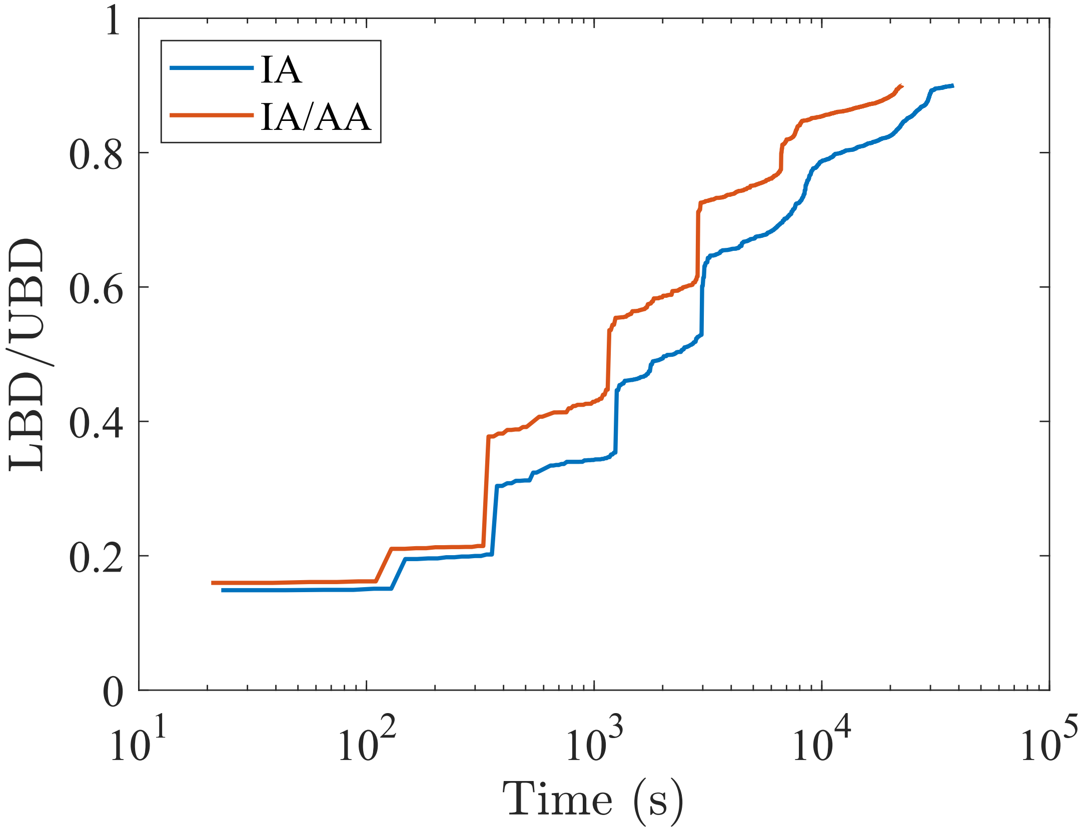
$$\min_{\mathbf{p}\in P} \sum_{j=1}^{10}\sum_{k=1}^{K}(x_{3,5j,k}(\mathbf{p}) - c^{\text{data}}_{O_3,i,k})^2$$

$$\text{s.t.}\quad \mathbf{z}_0(\mathbf{p}) = \mathbf{x}(0,\mathbf{p})$$

$$\mathbf{z}_{k+1}(\mathbf{p}) = \mathbf{z}_k(\mathbf{p}) + h\mathbf{f}(t_k, \mathbf{z}_k(\mathbf{p}), \mathbf{z}_k^{c}(\mathbf{p}), \mathbf{z}_k^{c2}(\mathbf{p}), \mathbf{p})$$

$$\mathbf{p} = (u, D) \in P = [\text{4e-3,6e-3}] \times [\text{4e-3,6e-3}]$$

Method	Time (h)
IA	11
IA/AA	6.5



[1] C. Wang and M. D. Stuber, *Under Review*, 2020

Transport Model in Tumor

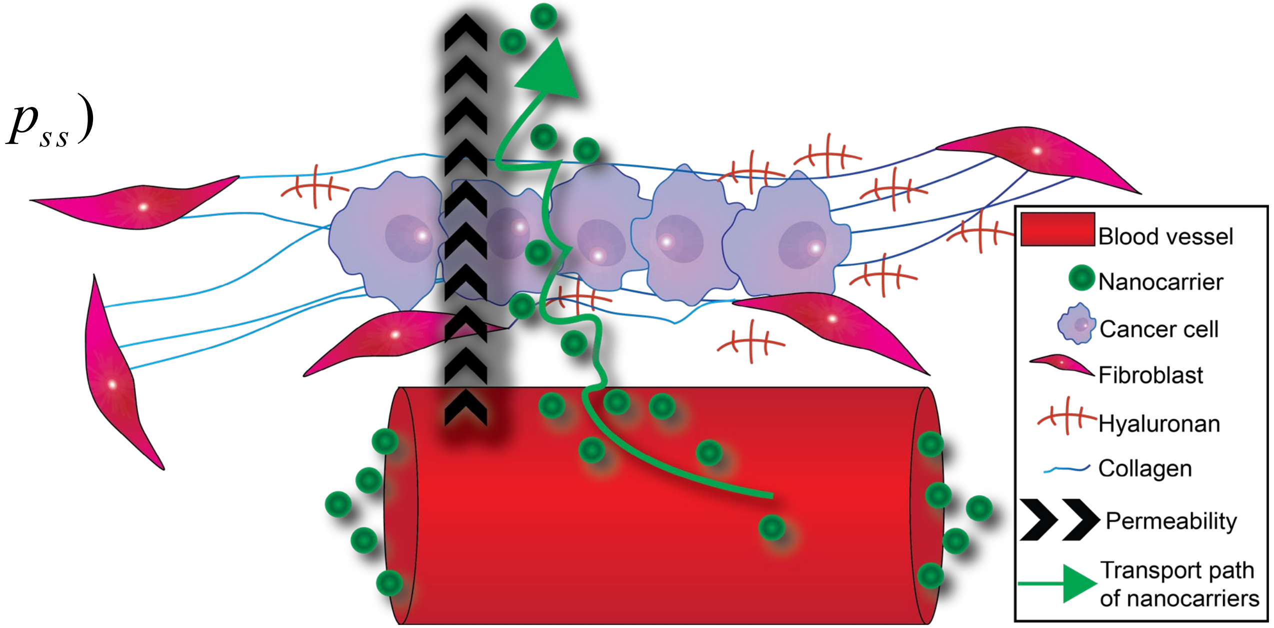
- Fluid Transport Model
  - Darcy's law $u = -K\frac{dp}{dr}$
  - Continuity equation

$$\nabla \cdot \mathbf{u} = \phi_v(r)$$

$$\phi_v(r) = L_p \frac{S}{V}(p_v - p)$$

$$\nabla^2 p = \frac{\alpha^2}{R^2}(p - p_{ss})$$

$K \in [2.75\text{E-}7, 2.85\text{E-}7]$ $\quad L_p \in [1.65\text{E-}6, 1.75\text{E-}6]$



- Solute Transport Model

$$\frac{\partial C}{\partial t} + \underbrace{\frac{1}{r^2}\frac{\partial (r^2 u C)}{\partial r}}_{\text{Convection}} = \underbrace{D\frac{1}{r^2}\frac{\partial}{\partial r}(r^2 \frac{\partial C}{\partial r})}_{\text{Diffusion}} + \phi_s$$

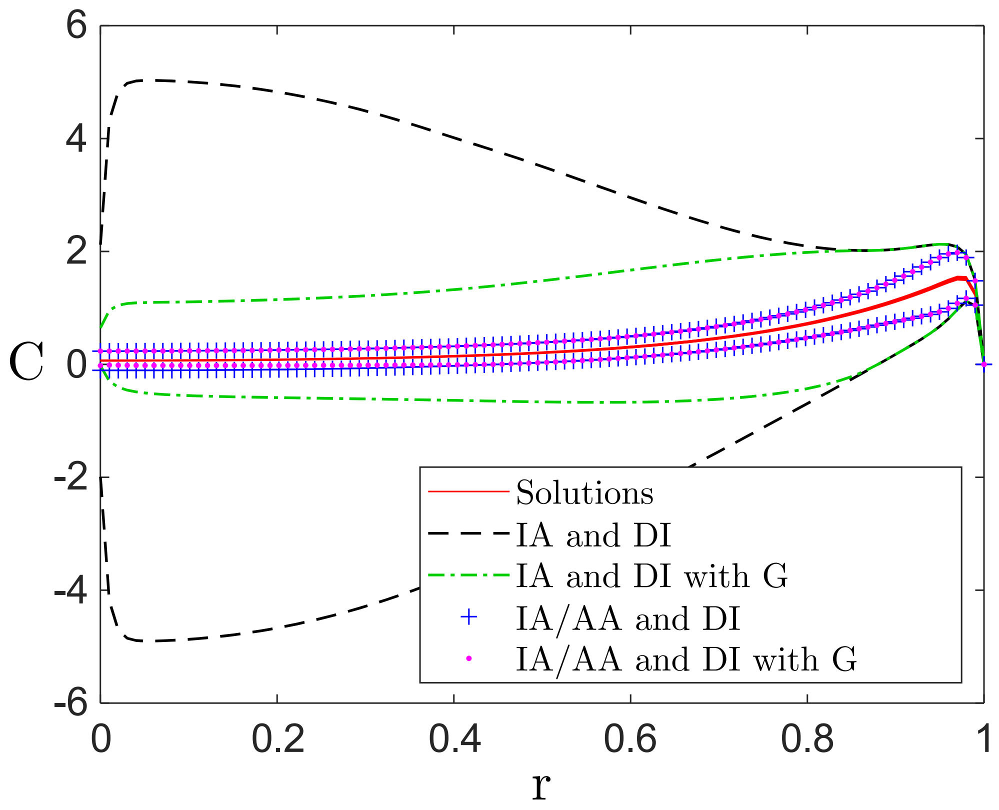
- Pore Theory

$$L_p = \frac{\gamma r_o^2}{8\mu L} \qquad P = \frac{\gamma H D_o}{L} \qquad \sigma = 1 - W$$

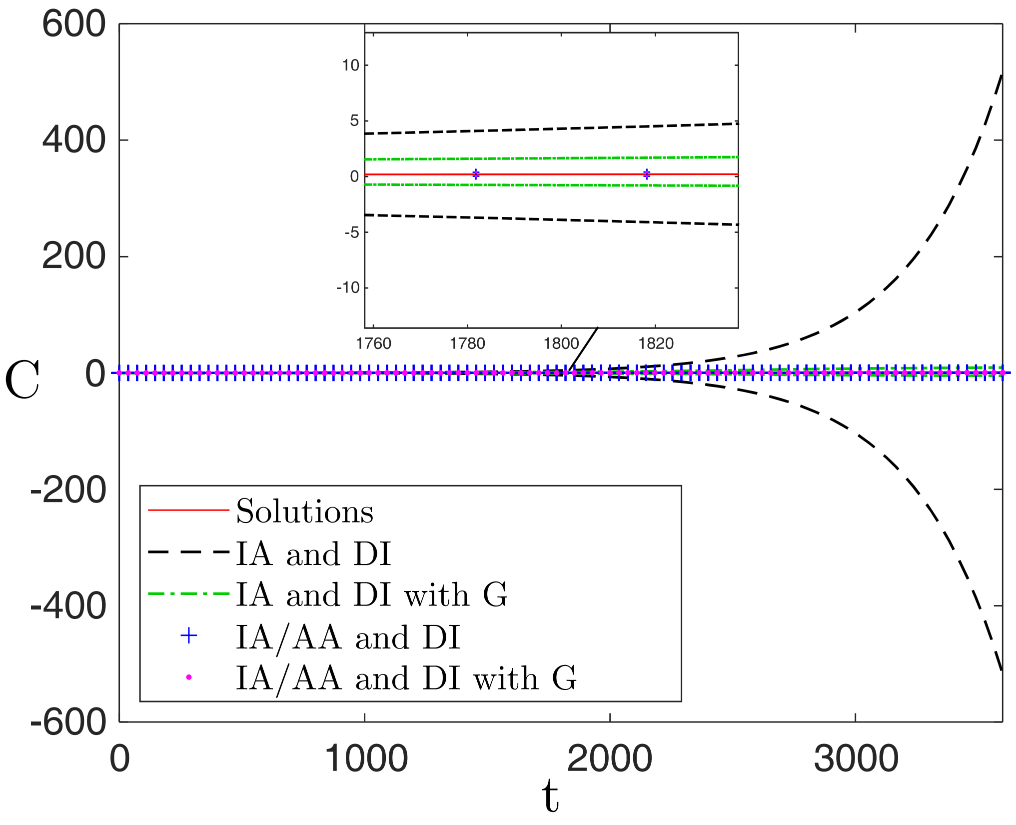
[11] J. D. Martin, M. Panagi, C. Wang, T. T. Khan, M. R. Martin, C. Voutouri, K. Toh, P. Papageorgis, F. Mpekris, C. Polydorou, et al., "Dexamethasone increases cisplatin-loaded nanocarrier delivery and efficacy in metastatic breast cancer by normalizing the tumor microenvironment," *ACS nano*.

Transport Model in Tumor

Concentration at 30 min post injection



Concentration at medium radius



Transport Model in Tumor

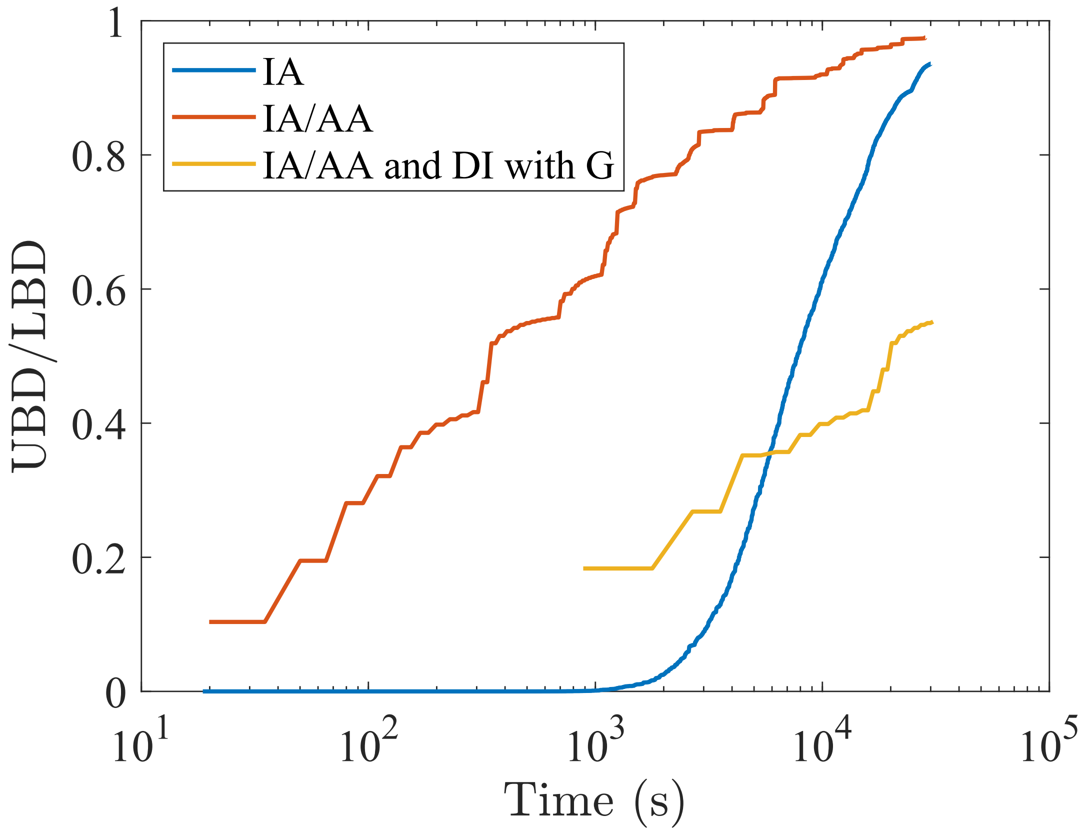
- Purpose: optimal therapy design under uncertainty

$$\max_{\boldsymbol{\pi}\in\Pi} C_{avg}(t_f, \boldsymbol{\pi})$$

$$\text{s.t.} \quad \sum_{i=1}^{n} C_{avg}(t_i, \boldsymbol{\pi}) \leq \lambda$$

$$\pi = (L_p, K) \in \Pi$$

$$\Pi = [1.65\text{E-}5, 1.75\text{E-}6] \times [2.75\text{E-}7, 2.85\text{E-}7]$$



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Any questions?

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