

# Fractional PDEs Constrained Optimization: an optimize–then–discretize approach with L–BFGS and Approximate Inverse Preconditioning

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# OVERVIEW

The Control Problem

Fractional Partial Differential Equations

Lagrangian Conditions

Discretization of the FPDEs

The Algorithms: LBFGS and Approximate Inverses

The LBFGS Optimization Routine

Preconditioning

Numerical Results

Conclusions

## THE PROBLEM

$$\begin{cases} \min J(y, u) = \frac{1}{2} \|y - z_d\|_2^2 + \frac{\lambda}{2} \|u\|_2^2, \\ \text{subject to } e(y, u) = 0. \end{cases} \quad (1)$$

$J$  and  $e$  **continuously Fréchet derivable** functionals :

$$J : Y \times U \rightarrow \mathbb{R}, \quad e : Y \times U \rightarrow W,$$

$Y, U$  and  $W$  *reflexive* Banach spaces, if

- ▶  $e_y(\bar{y}, \bar{u}) \in \mathcal{B}(Y, W)$  is a bijection;
- ▶  $y(u)$  is a (*locally*) unique solution to the state equation  $e(y, u) = 0$ .

Then the problem in terms of the *Reduced Cost Functional*  $f(u)$ ,

$$\min_{u \in U} f(u) = \min_{u \in U} J(y(u), u). \quad (2)$$

admits an **optimal solution**, if  $f(u)$  is **continuous**, **convex** and **radially unbounded** (De los Reyes [2015])

## LAGRANGIAN CONDITIONS

To enforce the optimality conditions of the first order for this problem we consider its **Lagrangian formulation**

$$\mathcal{L}(y, u, p) = J(y, u) - \langle p, e(y, u) \rangle_{W', W},$$

where  $\mathcal{L} : Y \times U \times W' \rightarrow \mathbb{R}$ , thus the optimality conditions are stated in terms of  $\mathcal{L}$  as (see De los Reyes [2015]):

$$\begin{cases} e(y(\bar{u}), \bar{u}) = 0, \\ \mathcal{L}_y(y, \bar{u}, p) = 0 \\ \mathcal{L}_u(y, \bar{u}, p) = 0 \end{cases} \quad . \quad (3)$$

### General framework

In the following we will compute the **Lagrangian conditions** for our problems with **Fractional Partial Differential Equations** (FPDEs) state equations and use them to obtain an expression for both  $f(u)$  in (2) and  $\nabla f(u)$ .

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In the following we will compute the **Lagrangian conditions** for our problems with **Fractional Partial Differential Equations** (FPDEs) state equations and use them to obtain an expression for both  $f(u)$  in (2) and  $\nabla f(u)$ .

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Leibniz (1646–1716)

LEIBNIZ: “[. . .] Thus it follows that  $d^{\frac{1}{2}}x$  will be equal to  $x\sqrt{dx} : x$ . This is an apparent paradox from which, one day, useful consequences will be drawn.”

In response to Marquis de l'Hôpital, 1695

We are going to **very briefly** define *some* **Fractional Derivative operators** and their **discretizations**.

## FRACTIONAL DERIVATIVES

- ▶ **Riemann-Liouville:** given  $\alpha > 0$  and  $m \in \mathbb{Z}^+$  such that  $m - 1 < \alpha \leq m$  the left-side Riemann-Liouville fractional derivative reads as

$${}_{\text{RL}}D_{a,x}^{\alpha}y(x) = \frac{1}{\Gamma(m-\alpha)} \left(\frac{d}{dx}\right)^m \int_a^x \frac{y(\xi)d\xi}{(x-\xi)^{\alpha-m+1}},$$

while the right-side Riemann-Liouville fractional derivative

$${}_{\text{RL}}D_{x,b}^{\alpha}y(x) = \frac{1}{\Gamma(m-\alpha)} \left(-\frac{d}{dx}\right)^m \int_x^b \frac{y(\xi)d\xi}{(\xi-x)^{\alpha-m+1}};$$

- ▶ **Symmetric Riesz:** given  $\alpha > 0$  and  $m \in \mathbb{Z}^+$  such that  $m - 1 < \alpha \leq m$  the symmetric Riesz derivative reads as

$$\frac{d^{\alpha}y(x)}{d|x|^{\alpha}} = \frac{1}{2} ({}_{\text{RL}}D_{a,x}^{\alpha} + {}_{\text{RL}}D_{x,b}^{\alpha}) y(x);$$



## THE TWO FPDES WE CONSIDER AS STATE EQUATIONS

We consider both the **Fractional Advection Dispersion Equation (FADE)**

$$\begin{cases} -a \left( l {}_{\text{RL}}D_{0,x}^{2\alpha} + r {}_{\text{RL}}D_{x,1}^{2\alpha} \right) y(x) + b(x)y'(x) \dots, & x \in \Omega = (0, 1), \\ \dots + c(x)y(x) = u(x) \\ y(0) = y(1) = 0. \end{cases}$$

for  $\alpha \in (1/2, 1)$ ,  $a, l, r > 0$  and  $l + r = 1$ ,  $b(x) \in \mathcal{C}^1(\overline{\Omega})$ ,  $c(x) \in \mathcal{C}(\overline{\Omega})$   
and such that  $c(x) - 1/2b'(x) \geq 0$ ,

## THE TWO FPDES WE CONSIDER AS STATE EQUATIONS

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for  $\alpha \in (1/2, 1)$ ,  $a, l, r > 0$  and  $l + r = 1$ ,  $b(x) \in C^1(\bar{\Omega})$ ,  $c(x) \in C(\bar{\Omega})$  and such that  $c(x) - 1/2b'(x) \geq 0$ , and the **2D Riesz Space Fractional Diffusion equation**

$$\begin{cases} -K_{x_1} \frac{\partial^{2\alpha} y}{\partial |x_1|^{2\alpha}} - K_{x_2} \frac{\partial^{2\beta} y}{\partial |x_2|^{2\beta}} + \mathbf{b} \cdot \nabla y + cy = u, & (x_1, x_2) \in \Omega \\ y \equiv 0, & (x_1, x_2) \in \partial\Omega. \end{cases}$$

where  $\mathbf{b} \in C^1(\Omega, \mathbb{R}^2)$ ,  $c \in C(\Omega)$ ,  $u \in \mathbb{L}^2(\Omega)$ ,  $K_{x_1}, K_{x_2} \geq 0$  and  $K_{x_1} + K_{x_2} > 0$ ,  $\alpha, \beta \in (1/2, 1)$ ,  $\Omega = [a, b] \times [c, d]$ .

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## LAGRANGIAN CONDITIONS FOR THE FADE - I

**Proposition 1: Lagrange Conditions for the FADE**

$U = \mathbb{L}^2(\Omega)$ ,  $Y = H_0^\alpha(\Omega)$  for  $\alpha > 0$  the closure of  $\mathbb{C}_0^\infty(\Omega)$  in the norm,

$$\|u\|_\alpha = (\|u\|_2^2 + \|{}_{\text{RL}}D_{0,x}^\alpha u\|_2^2)^{1/2}, \quad (4)$$

and  $W = Y'$ . The Lagrangian conditions for problem

$$\left\{ \begin{array}{l} \min J(y, u) = \frac{1}{2} \|y - z_d\|_2^2 + \frac{\lambda}{2} \|u\|_2^2, \\ \text{subject to} \quad -a \left( l {}_{\text{RL}}D_{0,x}^{2\alpha} + r {}_{\text{RL}}D_{x,1}^{2\alpha} \right) y(x) + \\ \quad + b(x)y'(x) + c(x)y(x) - u(x) = 0, \\ y(0) = y(1) = 0. \end{array} \right. , \quad (*)$$

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and  $W = Y'$ . The Lagrangian conditions for problem (\*) are expressed in *weak form* as

$$\begin{cases} B(y, v) = F(v), & \forall v \in Y, \\ \tilde{B}(p, w) = \langle y - z_d, w \rangle, & \forall w \in Y, \\ \langle p, h \rangle = -\lambda \langle u, h \rangle, & \forall h \in Y. \end{cases},$$

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$$\|u\|_\alpha = (\|u\|_2^2 + \|\text{RL}D_{0,x}^\alpha u\|_2^2)^{1/2}, \quad (4)$$

and  $W = Y'$ . The Lagrangian conditions for problem (\*) where  $u \in U$ ,  $y \in Y$  and

$$\begin{aligned} B(y, v) &= -al \langle \text{RL}D_{0,x}^\alpha y(x), \text{RL}D_{x,1}^\alpha v(x) \rangle + \\ &\quad - ar \langle \text{RL}D_{x,1}^\alpha y(x), \text{RL}D_{0,x}^\alpha v(x) \rangle \\ &\quad + \langle b(x)y'(x) + c(x)y(x), v(x) \rangle, \\ \tilde{B}(p, w) &= -al \langle \text{RL}D_{0,x}^\alpha w(x), \text{RL}D_{x,1}^\alpha p(x) \rangle + \\ &\quad - ar \langle \text{RL}D_{x,1}^\alpha w(x), \text{RL}D_{0,x}^\alpha p(x) \rangle + \\ &\quad - \langle (b(x)p(x))', w \rangle + \langle c p, w \rangle, \\ F(v) &= \langle u, v \rangle. \end{aligned}$$

## LAGRANGIAN CONDITIONS FOR THE FADE - II

### Gradient and objective function

The gradient for the objective function  $f(u)$  for the FADE problem reads as

$$\nabla f(u) = \mathcal{L}_u(y(u), u, p(u)) = p + \lambda u,$$

where  $p$  is the solution of the adjoint equation:

$$\begin{cases} -a \left( r_{\text{RL}} D_{0,x}^{2\alpha} + l_{\text{RL}} D_{x,1}^{2\alpha} \right) p(x) - \frac{d}{dx} (b(x)p(x)) + \dots \\ \quad \dots + c(x)p(x) = y(x) - z_d(x), \\ p(0) = p(1) = 0. \end{cases} .$$

## LAGRANGIAN CONDITIONS FOR THE RIESZ FPDE - I

Lagrange Conditions for the Riesz FPDE

$U = \mathbb{L}^2(\Omega)$ ,  $Y = H_0^\alpha(\Omega) \cap H_0^\beta(\Omega)$  and  $W = Y'$ . The Lagrangian conditions (3) for problem

$$\left\{ \begin{array}{l} \min J(y, u) = \frac{1}{2} \|y - z_d\|_2^2 + \frac{\lambda}{2} \|u\|_2^2, \\ \text{subject to } -K_{x_1} \frac{\partial^{2\alpha} y}{\partial |x_1|^{2\alpha}} - K_{x_2} \frac{\partial^{2\beta} y}{\partial |x_1|^{2\beta}} + \mathbf{b} \cdot \nabla y + cy = u \quad (**) \\ y \equiv 0, (x_1, x_2) \in \partial\Omega. \end{array} \right.$$



# LAGRANGIAN CONDITIONS FOR THE RIESZ FPDE - I

## Lagrange Conditions for the Riesz FPDE

$U = \mathbb{L}^2(\Omega)$ ,  $Y = H_0^\alpha(\Omega) \cap H_0^\beta(\Omega)$  and  $W = Y'$ . The Lagrangian conditions (3) for problem (\*\*) are expressed in *weak form* as

$$\left\{ \begin{array}{ll} B(y, v) = F(v), & \forall v \in Y, \\ \tilde{B}(p, w) = \langle y - z_d, w \rangle, & \forall w \in Y, \\ \langle p, h \rangle = -\lambda \langle u, h \rangle, & \forall h \in Y. \end{array} \right. , \quad (***)$$

## LAGRANGIAN CONDITIONS FOR THE RIESZ FPDE - I

### Lagrange Conditions for the Riesz FPDE

$U = \mathbb{L}^2(\Omega)$ ,  $Y = H_0^\alpha(\Omega) \cap H_0^\beta(\Omega)$  and  $W = Y'$ . The Lagrangian conditions (3) for problem where in (\*\*\*)  $u \in U$ ,  $y \in Y$  and, by setting  $C_x = K_{x_1}c_{2\alpha}$  and  $C_{x_2} = K_{x_2}c_{2\beta}$ ,

$$\begin{aligned} B(y, v) = & C_{x_1} \left( \langle \text{RL}D_{a,x_1}^\alpha y, \text{RL}D_{x_1,b}^\alpha v \rangle + \langle \text{RL}D_{x_1,b}^\alpha y, \text{RL}D_{a,x_1}^\alpha v \rangle \right) \\ & + C_{x_2} \left( \langle \text{RL}D_{c,x_2}^\beta y, \text{RL}D_{x_2,d}^\beta v \rangle + \langle \text{RL}D_{x_2,d}^\beta y, \text{RL}D_{c,x_2}^\beta v \rangle \right) \\ & + \langle \mathbf{b} \cdot \nabla y, v \rangle + \langle cy, v \rangle, \end{aligned}$$

$$\begin{aligned} \tilde{B}(p, w) = & C_{x_1} \left( \langle \text{RL}D_{a,x_1}^\alpha p, \text{RL}D_{x_1,b}^\alpha w \rangle + \langle \text{RL}D_{x_1,b}^\alpha p, \text{RL}D_{a,x_1}^\alpha w \rangle \right) \\ & + C_{x_2} \left( \langle \text{RL}D_{c,x_2}^\beta p, \text{RL}D_{x_2,d}^\beta w \rangle + \langle \text{RL}D_{x_2,d}^\beta p, \text{RL}D_{c,x_2}^\beta w \rangle \right) \\ & - \langle \nabla \cdot (\mathbf{b}p), w \rangle + \langle cp, w \rangle, \end{aligned}$$

$$F(v) = \langle u, v \rangle .$$

## LAGRANGIAN CONDITIONS FOR THE RIESZ FPDE - II

### Gradient and objective function

The gradient for the objective function  $f(u)$  for the Riesz problem reads as

$$\nabla f(u) = \mathcal{L}_u(y(u), u, p(u)) = p + \lambda u,$$

where  $p$  is the solution of the adjoint equation for  $\mathbf{x} \in \Omega$ :

$$\begin{cases} -K_{x_1} \frac{\partial^{2\alpha} p}{\partial |x_1|^{2\alpha}} - K_{x_2} \frac{\partial^{2\beta} p}{\partial |x_2|^{2\beta}} - \nabla \cdot (p\mathbf{b}) + cp = y - z_d, & (x_1, x_2) \in \Omega \\ p \equiv 0, & (x_1, x_2) \in \partial\Omega. \end{cases}$$

## DISCRETIZATIONS

We used, for the solution of both the *state* and *adjoint* equation the *finite difference discretizations* over a grid  $\{x_k\}_k = \{a + kh\}_k$  on the domain  $\Omega = [a, b]$  with stepsize  $h = (b-a)/n$  with the **right  $p$ -shifted Grünwald–Letnikov formula** as

$${}_{\text{RL}}D_{a,x}^{\alpha}y(x)|_{x=x_k} \approx \frac{1}{h^{\alpha}} \sum_{j=0}^{k+p} \omega_j^{(\alpha)} [y(x_{k-j+p}) - y(a)] + \frac{y(a)x_k^{-\alpha}}{\Gamma(1-\alpha)} + O(h^2),$$

where the coefficients  $\omega_j^{(\alpha)}$  are defined as  $\omega_j^{(\alpha)} = (-1)^j \binom{\alpha}{j}$ , and similarly for the **left-sided operator** as

$${}_{\text{RL}}D_{x,b}^{\alpha}y(x)|_{x=x_k} \approx \frac{1}{h^{\alpha}} \sum_{j=0}^{n-k+p} \omega_j^{(\alpha)} [y(x_{k+j-p}) - y(b)] + \frac{y(b)x_k^{-\alpha}}{\Gamma(1-\alpha)} + O(h^2).$$

Discretization of *Riesz Space Fractional derivative* is done in an analogous way.

## DISCRETIZATIONS: MATRIX REPRESENTATION - I

In the **1D** case, i.e., the FADE we have that:

$$A\mathbf{y} = \mathbf{u}, \text{ with}$$

$$A = a(lT_{(\alpha)} + rT_{(\alpha)}^T) + O_n,$$

with,

$$T_{(\alpha)} = -\frac{1}{h^\alpha} \begin{bmatrix} \omega_1 & \omega_0 & 0 & \dots & 0 \\ \omega_2 & \omega_1 & \omega_0 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ \vdots & & \ddots & \omega_1 & \omega_0 \\ \omega_{n-1} & \dots & \dots & \omega_2 & \omega_1 \end{bmatrix}$$

## DISCRETIZATIONS: MATRIX REPRESENTATION - I

In the **1D case**, i.e., the FADE we have that:

$$A\mathbf{y} = \mathbf{u}, \text{ with}$$

$$A = a(lT_{(\alpha)} + rT_{(\alpha)}^T) + O_n,$$

with,

$$O_n = \begin{bmatrix} c_1 & \frac{b_1}{2h} & & & \\ -\frac{b_2}{2h} & \ddots & \ddots & & \\ & \ddots & & c_3 & \frac{b_{n-2}}{2h} \\ & & & -\frac{b_{n-1}}{2h} & c_{n-1} \end{bmatrix}$$

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$$A\mathbf{y} = \mathbf{u}, \text{ with}$$

$$A = a(lT_{(\alpha)} + rT_{(\alpha)}^T) + O_n,$$

with,

$$\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_{n-1} \end{bmatrix}, \quad \mathbf{u} = \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_{n-1} \end{bmatrix}.$$

## DISCRETIZATIONS: MATRIX REPRESENTATION - II

For the 2D *Riesz Space Fractional Diffusion equation*, we get, through the use of Kronecker sums, given an  $(i, j)$ -finite difference grid with  $N_{x_1}, N_{x_2}$  nodes and amplitude  $h, k$  respectively

$$A = K_{x_1}(R_{x_1}^{(\alpha)} \otimes I_{x_2}) + K_{x_2}(I_{x_1} \otimes R_{x_2}^{(\beta)}) \\ + B_{x_1}(T_{x_1} \otimes I_{x_2}) + B_{x_2}(I_{x_1} \otimes T_{x_2}) + C,$$

where

- ▶  $I_{x_i}$ , for  $i = 1, 2$  for the relative grid size,
- ▶  $R_{x_1}^{(\alpha)}$  and  $R_{x_2}^{(\beta)}$  are the **dense Toeplitz matrix** for the 1D fractional order derivatives in the two directions,
- ▶  $T_{x_i}$  are the finite difference matrix for the **convective terms** obtained with centered differences,
- ▶ the  $\{B_{x_i}\}_{i=1,2}$  and  $C$  are respectively the evaluation of the functions  $\mathbf{b} = (b^{(1)}, b^{(2)})$  and  $c$  on the relative nodes of the grid.



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## OPTIMIZATION ROUTINE: L-BFGS

**Input:**  $\mathbf{x}_0$  starting point,  $M \in \mathbb{N}$ ;  
 Compute  $f_0 = f(\mathbf{x}_0)$  and  $\mathbf{g}_0 = \nabla f(\mathbf{x}_0)$  ;  
 Set  $\mathbf{d}_0 = -\mathbf{g}_0$ ,  $\gamma_0 = 1$ ,  $i = 0$  ;  
**while**  $\|\mathbf{g}_i\| > 0$  **do**  
   Choose an initial Hessian approx.:  
    $H_i^0 = \gamma_i I$ ;  
   Compute the step direction  $\mathbf{d}_i = -\mathbf{r}$   
   using *TwoLoopRecursion*;  
   Compute the step length  $\alpha_i$  and set  
    $\mathbf{x}_{i+1} = \mathbf{x}_i + \alpha_i \mathbf{d}_i$ ;  
   Set  $\mathbf{g}_i = \nabla f(\mathbf{x}_{i+1})$ ;  
   **if**  $i > M$  **then**  
   |   Discard vectors  $\{\mathbf{s}_{i-M}, \mathbf{y}_{i-M}\}$   
   |   from storage ;  
   **end**  
   Set and store  $\mathbf{s}_i = \mathbf{x}_{i+1} - \mathbf{x}_i$  and  
    $\mathbf{y}_i = \mathbf{g}_{i+1} - \mathbf{g}_i$ ;  
   Set  $i = i + 1$ ;  
**end**  
**Output:** Output  $\mathbf{x}_i \approx \mathbf{x}_*$  ;

The L-BFGS method, originally introduced in Liu and Nocedal [1989], continuously updates the quasi-Newton matrix, approximation of the Hessian of problem (2), using a **fixed limited amount of storage**.

# OPTIMIZATION ROUTINE: L-BFGS

**Input:**  $\mathbf{x}_0$  starting point,  $M \in \mathbb{N}$ ;

Compute  $f_0 = f(\mathbf{x}_0)$  and  $\mathbf{g}_0 = \nabla f(\mathbf{x}_0)$  ;

Set  $\mathbf{d}_0 = -\mathbf{g}_0$ ,  $\gamma_0 = 1$ ,  $i = 0$  ;

**while**  $\|\mathbf{g}_i\| > 0$  **do**

    Choose an initial Hessian approx.:

$$H_i^0 = \gamma_i I;$$

    Compute the step direction  $\mathbf{d}_i = -\mathbf{r}$

        using *TwoLoopRecursion*;

    Compute the step length  $\alpha_i$  and set

$$\mathbf{x}_{i+1} = \mathbf{x}_i + \alpha_i \mathbf{d}_i;$$

    Set  $\mathbf{g}_i = \nabla f(\mathbf{x}_{i+1})$ ;

**if**  $i > M$  **then**

        Discard vectors  $\{\mathbf{s}_{i-M}, \mathbf{y}_{i-M}\}$   
        from storage ;

**end**

    Set and store  $\mathbf{s}_i = \mathbf{x}_{i+1} - \mathbf{x}_i$  and

$$\mathbf{y}_i = \mathbf{g}_{i+1} - \mathbf{g}_i;$$

    Set  $i = i + 1$ ;

**end**

**Output:** Output  $\mathbf{x}_i \approx \mathbf{x}_*$  ;

$$H_i = (I - \rho \mathbf{s} \mathbf{y}^T) H (I - \rho \mathbf{y} \mathbf{s}^T) + \rho \mathbf{s} \mathbf{s}^T$$

**Input:**  $\mathbf{g}_i = \nabla f(\mathbf{x}_i)$ ;

Set  $\mathbf{q} = \mathbf{g}_i$ ;

**for**  $k = i - 1, \dots, i - M$  **do**

$$a_k = \frac{\mathbf{s}_k^T \mathbf{q}}{\mathbf{y}_k^T \mathbf{s}_k} ;$$

$$\mathbf{q} = \mathbf{q} - a_k \mathbf{y}_k;$$

**end**

$\mathbf{r} = H_i^0 \mathbf{q}$ ;

**for**  $k = i - M, i - M + 1, \dots, i - 1$  **do**

$$b = \frac{\mathbf{y}_k^T \mathbf{r}}{\mathbf{y}_k^T \mathbf{s}_k} ;$$

$$\mathbf{r} = \mathbf{r} + (a_k - b) \mathbf{s}_k;$$

**end**

**Output:** Output  $\mathbf{r} = H_i \mathbf{g}_i$  ;

## OPTIMIZATION ROUTINE: L-BFGS

**Input:**  $\mathbf{x}_0$  starting point,  $M \in \mathbb{N}$ ;  
 Compute  $f_0 = f(\mathbf{x}_0)$  and  $\mathbf{g}_0 = \nabla f(\mathbf{x}_0)$  ;  
 Set  $\mathbf{d}_0 = -\mathbf{g}_0$ ,  $\gamma_0 = 1$ ,  $i = 0$  ;  
**while**  $\|\mathbf{g}_i\| > 0$  **do**  
   Choose an initial Hessian approx.:  
    $H_i^0 = \gamma_i I$ ;  
   Compute the step direction  $\mathbf{d}_i = -\mathbf{r}$   
   using *TwoLoopRecursion*;  
   **Compute the step length**  $\alpha_i$  and set  
    $\mathbf{x}_{i+1} = \mathbf{x}_i + \alpha_i \mathbf{d}_i$ ;  
   Set  $\mathbf{g}_i = \nabla f(\mathbf{x}_{i+1})$ ;  
   **if**  $i > M$  **then**  
     Discard vectors  $\{\mathbf{s}_{i-M}, \mathbf{y}_{i-M}\}$   
     from storage ;  
   **end**  
   Set and store  $\mathbf{s}_i = \mathbf{x}_{i+1} - \mathbf{x}_i$  and  
    $\mathbf{y}_i = \mathbf{g}_{i+1} - \mathbf{g}_i$ ;  
   Set  $i = i + 1$ ;  
**end**  
**Output:** Output  $\mathbf{x}_i \approx \mathbf{x}_*$  ;

The computational cost of the L-BFGS algorithm:

1.  $O(Mn)$  flops of the optimization procedure,
2. The cost required for the evaluation of the **function** and the **gradient**  $\Rightarrow$  **this costs at least two solutions of FPDEs!**

## BUILDING THE PRECONDITIONER

We consider sparse approximations for nonsymmetric matrices, the **AINV preconditioner** of the form:

$$A^{-1} \approx WD^{-1}Z^T.$$

with

- ▶  $W$  lower triangular,
- ▶  $Z$  upper triangular,
- ▶  $D$  diagonal.

Computed within a **GPU architecture**, see Bertaccini and Filippone [2016].

We stress that for *nonsymmetric* or *non Hermitian* matrices we speak about *biorthogonalization* and *conjugation* for symmetric or Hermitian ones.

## SHORT-MEMORY PRINCIPLE

Lets look into some properties of the matrices  $T_{(\alpha)}$  and  $T_{(\alpha)}^T$ :

1. They are *Toeplitz* matrices,
2. The entries are such that:

$$|\omega_j^{(\alpha)}| = O(j^{-\alpha-1}), \quad \text{for } j \rightarrow +\infty.$$

- ▶ Property (1) have been used to develop **preconditioners for iterative Toeplitz solvers**, e.g., [Donatelli et al., 2016].
- ▶ Property (2) have been used to **discard entries** from  $T_{(\alpha)}$  and  $T_{(\alpha)}^T$  and then use **direct solvers**, e.g., [Popolizio, 2013].
- ▶ In Bertaccini and Durastante [2017] **Property (2)** have been exploited for obtaining sparse approximate inverses of the discretization matrix  $A$ .

## SHORT-MEMORY PRINCIPLE

To build the preconditioner we need only another *ingredient*:

- ▶ transport the **decay** of the element of the **discretization matrix** to a **decay** of the element of the **inverse**.

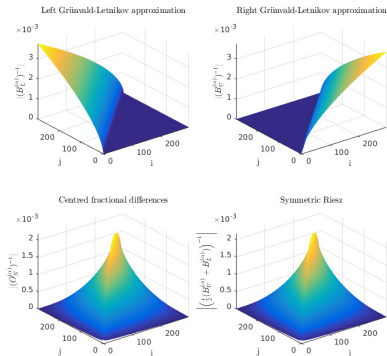
This **decaying property** of these entries is a **structural property** of the fractional differential operators:

$$E(x) = |\text{RL}D_{a,x}^\alpha y(x) - \text{RL}D_{x-L,x}^\alpha y(x)|$$

$$\leq \frac{\sup_{x \in [a,b]} y(x)}{L^\alpha |\Gamma(1-\alpha)|},$$

where  $a \leq L < x$ , is a *memory length*: the

**Short-Memory Principle**.



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## A 2D EXAMPLE

As a last example, we consider the following choice of coefficients for the problem,

$$\left\{ \begin{array}{l} \min J(y, u) = \frac{1}{2} \|y - z_d\|_2^2 + \frac{\lambda}{2} \|u\|_2^2, \\ \text{subject to } -K_{x_1} \frac{\partial^{2\alpha} y}{\partial |x_1|^{2\alpha}} - K_{x_2} \frac{\partial^{2\beta} y}{\partial |x_2|^{2\beta}} + \mathbf{b} \cdot \nabla y + cy = u \\ y \equiv 0, (x_1, x_2) \in \partial\Omega. \end{array} \right.$$

with coefficients

$$\begin{aligned} K_{x_1} &= 2, K_{x_2} = 1.5, c(x, y) = 1 + 0.5 \cos(x_1 x_2), \\ \mathbf{b} &= (\beta + 0.5 \sin(4\pi x_1) \cos(5\pi x_2), \dots \\ &\quad \dots \alpha + 0.7 \sin(7\pi x_2) \cos(4\pi x_1)), \end{aligned}$$

On  $\Omega = [0, 1]^2$  for the desired state

$$z_d(x_1, x_2) = \sin(5\pi x_1) \sin(5\pi x_2).$$

## A 2D EXAMPLE

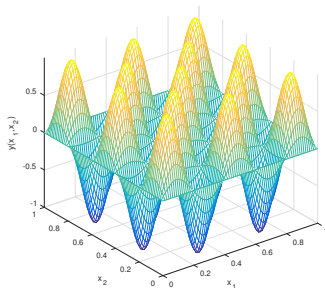
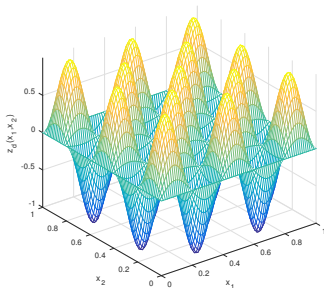
Preconditioner		BiCGstab, $2\alpha = 1.3, 2\beta = 1.2, \lambda = 1e - 6$					Direct
	I	$\#Av$	$\#A'v$	Func. Eval.	$\ \nabla f\ _2$	T(s)	T(s)
N	20	46476	73524	976	2.71e-04	4.9912	6.23
	40	80834	130061	899	1.15e-03	25.4829	146.40
	60	92609	158198	745	3.19e-03	116.5496	1669.18
	80	108270	197247	710	5.49e-03	488.6336	6029.44
AINV(1e-1)		$\#Av$	$\#A'v$	Func. Eval.	$\ \nabla f\ _2$	T(s)	T(s)
N	20	20832	41173	1155	2.99e-04	3.2712	6.2328
	40	36156	73400	976	1.21e-03	16.1750	146.40
	60	51793	109713	958	3.35e-03	89.8328	1669.18
	80	66275	140296	933	5.70e-03	385.6470	6029.44
AINV(1e-2)		$\#Av$	$\#A'v$	Func. Eval.	$\ \nabla f\ _2$	T(s)	T(s)
N	20	10216	12361	947	3.22e-04	<b>1.7162</b>	6.23
	40	24771	38206	1497	1.40e-03	<b>14.2141</b>	146.40
	60	20346	34563	836	2.99e-03	<b>46.0631</b>	1669.18
	80	33924	59922	1079	4.37e-03	<b>207.9970</b>	6029.44

## A 2D EXAMPLE

Preconditioner		BiCGstab, $2\alpha = 1.1, 2\beta = 1.8, \lambda = 1e - 9$					Direct
	I	#Av	#A'v	Func. Eval.	$\ \nabla f\ _2$	T(s)	T(s)
N	20	34008	40346	380	3.02e-04	3.1414	2.67
	40	49603	58500	245	1.22e-03	13.0047	32.82
	60	81056	94216	237	3.02e-03	81.4658	335.74
	80	121244	140609	233	5.21e-03	421.9529	1432.13
AINV(1e-1)		#Av	#A'v	Func. Eval.	$\ \nabla f\ _2$	T(s)	T(s)
N	20	13098	12349	388	3.11e-04	1.3566	2.67
	40	15854	14694	218	1.20e-03	4.8374	32.82
	60	23496	24406	237	3.15e-03	30.9931	335.74
	80	29293	29717	215	5.18e-03	112.3551	1432.13
AINV(1e-2)		#Av	#A'v	Func. Eval.	$\ \nabla f\ _2$	T(s)	T(s)
N	20	5715	6036	382	3.03e-04	<b>0.8399</b>	2.67
	40	7682	7841	228	1.15e-03	<b>3.3400</b>	32.82
	60	13626	13914	238	3.18e-03	<b>25.2802</b>	335.74
	80	18825	20112	219	5.21e-03	<b>90.6548</b>	1432.13

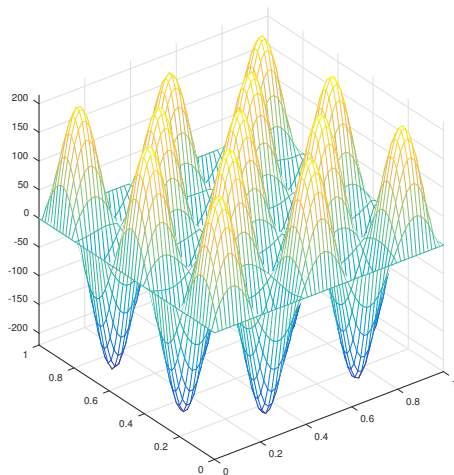
# A 2D EXAMPLE

The **desired state** and the **computed solution**.



# A 2D EXAMPLE

Obtained with the **control**



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## CONCLUSIONS AND FUTURE WORK

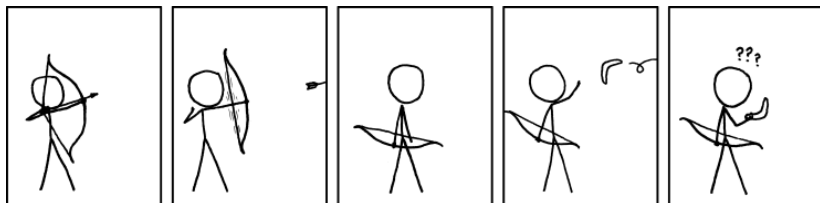
We have,

- ▶ Fully described two FPDEs–constrained optimization problem with tracking type cost functional,
- ▶ Devised a suitable coupling of the L-BFGS algorithm and an approximate inverse preconditioner for speeding up the computations,

We plan to,

- ▶ Add box–constraints on both *state* and *control* variable,
- ▶ Extend the model to account for fractional operators in the definition of  $J(y, u)$ ,
- ▶ Extend the technique for considering also time–fractional problems,
- ▶ Adapt LQN optimization algorithms for these cases; see Cipolla et al. [2015].

# QUESTIONS?



(From XKCD: <http://xkcd.com>)

**Thanks for your attention!**



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## INFINITE VS FINITE

We interpret **discretized optimal control problems** as **optimization problems** and then solve them by a quasi-Newton method.

Discretized problems **do not** solve the original infinite-dimensional control problem but rather approximate it up to a certain accuracy!

This is justified by the **mesh independence property**; see De los Reyes [2015], Kelley and Sachs [1987]