

# INFINITEEXAMODELS.JL: ACCELERATING INFINITE-DIMENSIONAL OPTIMIZATION PROBLEMS ON CPU & GPU

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**Joshua Pulsipher** and Sungho Shin





# ACKNOWLEDGEMENTS



Sungho Shin MIT *Assistant Professor*



François Pacaud Mines Paris *Assistant Professor*



Mihai Anitescu Argonne *Senior Computational Mathematician*



**Department of Chemical Engineering** 





EXASCALE COMPUTING PROJECT



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# OUTLINE

▪ InfiniteOpt

**ExaModels** 

▪ InfiniteExaModels



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▪ **InfiniteOpt**

**ExaModels** 

▪ InfiniteExaModels





# INFINITE-DIMENSIONAL OPTIMIZATION

### **Infinite Parameters Infinite Variables**

#### ▪ Index over **continuous domains**



- **Example: Disease Control** 
	- Population dynamics
		- $t\in[0,t_f]$
	- Uncertain infection rates
		- $\xi \in (-\infty, \infty) \sim \mathcal{N}(\mu, \Sigma)$



**Decisions** indexed by infinite parameters



- **Example: Disease Control** 
	- Population of infected at a particular time and infection rate  $y_i(t,\xi)$



# INFINITE-DIMENSIONAL OPTIMIZATION

### **Differential Operators Measure Operators**

#### ▪ Capture of **rate of change** in variables



- **Example: Disease Control** 
	- Time derivative
	- SEIR model

$$
\frac{\partial y_i(t,\xi)}{\partial t}
$$

 $\frac{\partial y_i(t,\xi)}{\partial t} = \xi y_e(t) - \gamma y_i(t)$ 

**Summarize variables** over continuous domains



- **Example:** Disease Control
	- Summarize overall infections

 $\mathbb{E}_{\xi}[y_i(t,\xi)]dt$   $\mathbb{E}_{\xi}\left[\int_{t\in\mathcal{D}_t}y_i(t,\xi)dt\right]$ 







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# TRANSFORMING INFINITEOPT PROBLEMS INTO FINITE ONES

# **Direct Transcription**



### **Method of Weighted Residuals**



**J. L. Pulsipher**, W. Zhang, T. J. Hongisto, and V. M. Zavala. "A *Unifying Modeling Abstraction for Infinite-Dimensional Optimization*." Computers & Chem. Eng. 2022

**Zept InfiniteOpt Why is it Different? Intuitive Modeling API**

- Implements **unifying abstraction**
	- Models a wide range of problems
	- Leverages structure to **accelerate solutions**
- Implemented in julia
	- Enables **intuitive** symbolic expressions
	- Highly **performant**

### • **Extensive resources**

• Documentation, tutorials, examples, forum, short courses, videos





Try it @<https://github.com/infiniteopt/InfiniteOpt.jl>



$$
\frac{\partial y_b(t,\xi)}{\partial t} = 2y_b(t,\xi)^2 + y_a(t) - z_1
$$

$$
\mathbb{E}_{\xi} [y_c(t,\xi)] \ge \alpha
$$

$$
y_a(0) + z_2 = \beta
$$

 $\phi$ constraint(m,  $\partial(yb, t) == 2yb^2 + ya - z[1]$ )  $\phi$ constraint(m,  $E(yc, \xi) \ge \alpha$ )  $\phi$ constraint(m, ya(0) + z[2] ==  $\beta$ )

### **Impact**

#### Announcement **Welcome to InfiniteOpt.jl Discussions** (i) pulsipher

- 1000s of downloads
- Use cases in **diverse disciplines**
	- e.g., evolutionary biology, rocketry, economics, autonomous vehicles



# TRANSFORMING INFINITEOPT MODELS



### **Transformation Paradigm**



### **Transformation API**

- Highly extensible to **make advanced solution techniques accessible/automated**
- Detailed templates, tutorials, and docs



- Many **derivative/measure approximations**
	- Orthogonal collocation, Gauss quadrature, etc.
- **Performant**





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# SOLVING INFINITEOPT PROBLEMS VIA TRANSCRIPTIONOPT

- Apply **transformation** to obtain finite JuMP model that can be solved
- InfiniteOpt has a large suite of **discretization** techniques
- Discretized InfiniteOpt problems have **repeated structure**
- Traditional modeling languages like JuMP do not leverage repeated structure



How can we leverage the repeated structure to **accelerate solution performance**?



 $\sin^2(y(t)) \leq 42, t \in \mathcal{D}_t$ 

 $\sin^2(y_k) \leq 42, \ k \in \mathcal{K}$ 



**•** InfiniteOpt

▪ **ExaModels**



▪ InfiniteExaModels



### **Traditional Nonlinear Optimization: Software**



- **Algebraic modeling systems** provide **front-end** and **sparse derivative evaluation** capabilities
- **Nonlinear optimization solvers** apply **optimization algorithms**
- **Sparse linear solvers** resolve **KKT systems** using **sparse matrix factorization**
- Many of these tools are developed in the 1980s-2000s (not compatible with GPUs).

## **How Does GPU Work?**

- Single Instruction, Multiple Data **(SIMD) parallelism**
- **Dedicated device memory and slow interface:** all data should reside in device memory only
- **Emerging architectures** employ **unified memory.**



Adapting CPU code to GPU code is not merely a matter of software engineering; it often requires the **redesign of the algorithm**

## **SIMD Abstraction for NLPs**



- **Large-scale optimization problems almost always have repeated patterns**
- **SIMD Abstraction** can capture such repeated patterns:



• Repeated patterns are inputted as **iterators** (data can be stored in structured format)



• **For each pattern**, the AD kernel is **compiled** and **executed over multiple data** in parallel

Shin, Pacaud, and Anitescu

*Accelerating optimal power flow with GPUs: SIMD abstraction of nonlinear programs and condensed-space interior-point methods*.

PSCC 2024

## **Sparse AD Benchmark**





- For the largest case, **ExaModels on GPU** is **100× faster** than the state-of-the-art tools on CPUs
- $\bullet$  ExaModels runs on all major GPU architectures and single/multi-threaded CPUs

### **Sparse AD** with **SIMD abstraction** enables **efficient derivative computations on GPUs**

## **Nonlinear Optimization Framework on GPUs**



• Runs on NVIDIA GPUs

• Runs on GPU architectures

<https://github.com/exanauts/ExaModels.jl> <https://github.com/MadNLP/MadNLP.jl> [https://docs.nvidia.com/cuda/cudss](https://docs.nvidia.com/cuda/cudss/index.html)

Sungho Shin sshin@anl.gov

• Runs on NVIDIA GPUs

## **AC Optimal Power Flow**



**ExaModels + Solution And NLP +** 

**O** 

**CUDA** 

**Table 3** OPF benchmark, solved with a tolerance tol=1e-6. (A100 GPU)

• For large-scale cases (> 20k vars), GPU becomes **significantly faster than CPU** (up to ×10)

#### • **Reliable convergence for** tol=10-6 , but still less reliable than CPUs  $\frac{1}{2}$ .  $\frac{1}{2}$ .

Pacaud, Shin, Montoison, Schanen, and Anitescu. *Approaches to nonlinear programming on GPU architectures*. In preparation.  $\theta$  and  $\theta$  are the section that both L is previous section that  $\theta$  and  $\theta$  and  $\theta$  and  $\theta$  and  $\theta$  and  $\theta$ 

### **Distillation Column**





- "**Symbolic analysis**" is often the bottleneck on GPUs, but this can be computed "**off-line**" thus, **online computation performance** can be **even greater**
- The distillation column control problem can be solved more than 20x faster

**ExaModels**, **MadNLP**, and **CUDSS** provide **efficient and reliable** solution framework for large-scale nonlinear optimization problems

## **Remaining Challenges**

• **Portable sparse Cholesky factorization**



- Currently, we are relying on a **proprietary** Cholesky solver (CUDSS)
- An open-source, **portable Cholesky solver is needed** to run on Exascale **Experience of the COPT of COPPO (Stockholm of Property COPPO)**<br>Molecky colver is needed to run on Expect of Co
- **Multi-GPU optimization tools** 
	- A **single GPU is sometimes limited** in computation & storage capacity
	- Our recent results suggest that there are significant opportunities in **multi-GPU utilization**



Pacaud et. al. *Parallel interior-point solver for block-structured nonlinear programs on SIMD/GPU architectures*, OMS (2024).

# EXAMODELSMOI.JL

 $\overline{2}$ 

### ▪ Provides an **MOI optimizer** for JuMP models

- Can use either ExaModels.IpoptOptimizer or ExaModels.MadNLPOptimizer
	- $\mathbf 1$ using ExaModels, JuMP, CUDA, MadNLPGPU
	- 3  $model = Model(() \rightarrow ExaModels.MadNLPOptimize(CUDABackend())$
- Searches for repeated algebraic structure via a **bin search**

■ Doesn't necessary yield the most efficient ExaModel structure



# ACCELERATING NLP PERFORMANCE ON CPUS AND GPUS

- $\blacksquare$  ExaModels + MadNLP is highly performant for problems with repeated patterns
- Translating InfiniteOpt problems to SIMD is nontrivial
- TranscriptionOpt + ExaModelsMOI has to ignore structure while building the model





# **OUTLINE**

▪ InfiniteOpt



**ExaModels** 

▪ **InfiniteExaModels**



# INFINITEEXAMODELS.JL

- **•** Bridges the gap between  $\overline{Q}^F$  InfiniteOpt &  $\overline{Q}$  ExaModels
- **Automates transcription** via established transformation interface
- Leverages repeated structure to **drastically reduce model creation time**
	- More efficient than manual transcription directly given to ExaModels





# IMPLEMENTATION DETAILS

- Supports the use of **JSO NLP solvers** (e.g., Ipopt, MadNLP, KNITRO)
- **Defined via an** ExaTranscriptionBackend
	- using InfiniteOpt, InfiniteExaModels, NLPModelsIpopt  $\mathbf{1}$
	- model = InfiniteModel(ExaTranscriptionBackend(IpoptSolver))  $\mathcal{L}$
- Rapidly transcribes infinite model into **efficient ExaModels**
- **Model build** time is nearly **independent of the discretization** size



# BENCHMARK PROBLEMS

- Compare performance with JuMP, AMPL, ExaModels, and InfiniteExaModels
- Run on CPU with Ipopt and GPU with MadNLP

#### **2-Stage Stochastic Program**

- Stochastic optimal power flow
- 1,000 to 16,000 random scenarios

#### **Optimal Control**

- Model predictive control of quadcopter
- Track trajectory setpoint and vary grid size



#### **Stochastic Optimal Control**

- Control isolation policy to combat disease
- Uncertain transmission rate





# NUMERICAL RESULTS (CPU W/ IPOPT)

- AD is **5 – 20 times faster**
- Model build time is **1 – 2 orders-of-magnitude faster**



using InfiniteOpt, InfiniteExaModels, NLPModelsIpopt  $\mathbf{1}$ 

 $\overline{2}$  $model = InfiniteModel(ExaTransactionBackend(IpoptSolver))$ 



# NUMERICAL RESULTS (GPU W/ MADNLP)

- All AD and solve times are up to **~20 faster on GPU**
- InfiniteExaModels.jl builds models **orders-of-magnitude faster** than ExaModels



- using InfiniteOpt, InfiniteExaModels, MadNLPGPU, CUDA  $\mathbf{1}$
- transform\_backend = ExaTranscriptionBackend(MadNLPSolver, backend = CUDABackend())  $2<sup>1</sup>$
- $model = InfiniteModel(transform *backend*)$  $\overline{3}$



# TRY IT OUT!





**InfiniteExaModels**







### **InfiniteExaModels**

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Our greatest impact happens together.

