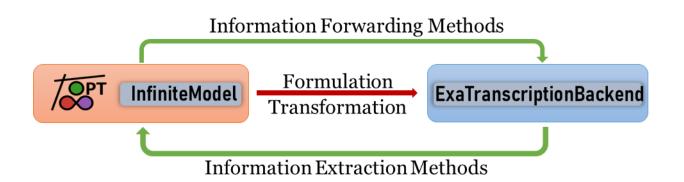




# **INFINITEEXAMODELS.JL: ACCELERATING INFINITE-DIMENSIONAL** OPTIMIZATION PROBLEMS ON CPU & GPU

7/29/2024

Joshua Pulsipher and Sungho Shin





## **ACKNOWLEDGEMENTS**



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François Pacaud Mines Paris Assistant Professor



Mihai Anitescu Argonne Senior Computational Mathematician











# **OUTLINE**

InfiniteOpt

ExaModels

InfiniteExaModels

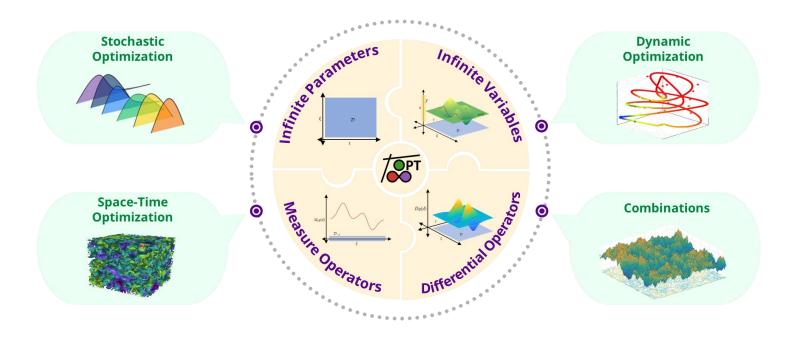


# **OUTLINE**

InfiniteOpt

ExaModels

InfiniteExaModels

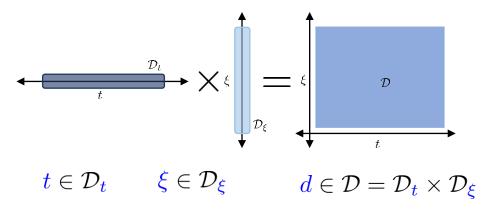




## INFINITE-DIMENSIONAL OPTIMIZATION

#### **Infinite Parameters**

Index over continuous domains

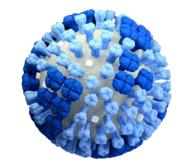


- Example: Disease Control
  - Population dynamics

$$\mathbf{t} \in [0, t_f]$$

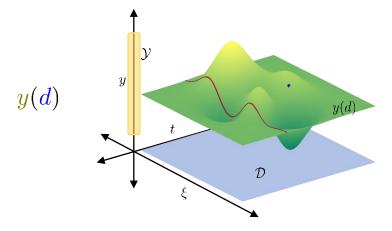
Uncertain infection rates

$$\boldsymbol{\xi} \in (-\infty, \infty) \sim \mathcal{N}(\mu, \Sigma)$$



#### **Infinite Variables**

Decisions indexed by infinite parameters



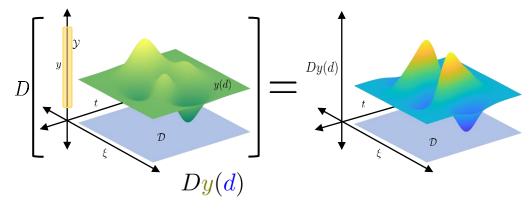
- **Example:** Disease Control
  - Population of infected at a particular time and infection rate  $y_i(t,\xi)$



## INFINITE-DIMENSIONAL OPTIMIZATION

#### **Differential Operators**

Capture of rate of change in variables



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

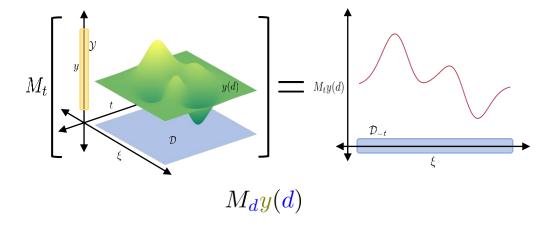
$$\frac{\partial y_i(t,\xi)}{\partial t}$$

SEIR model

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

#### **Measure Operators**

Summarize variables over continuous domains



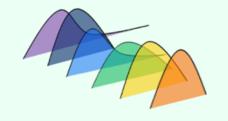
- **Example:** Disease Control
  - Summarize overall infections

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

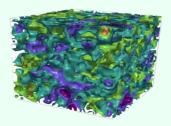


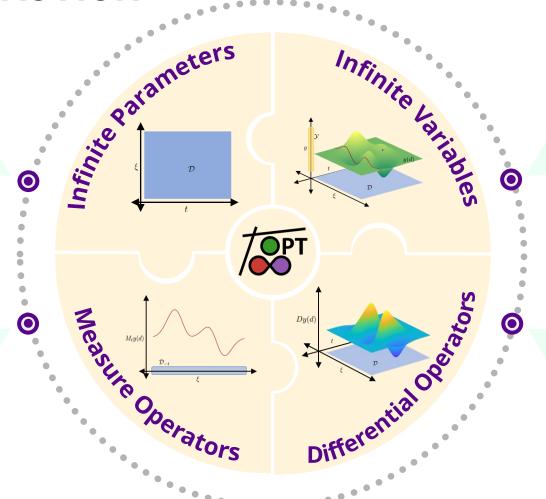
# **UNIFYING ABSTRACTION**

Stochastic Optimization

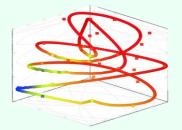


Space-Time Optimization

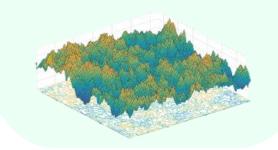




Dynamic Optimization



**Combinations** 



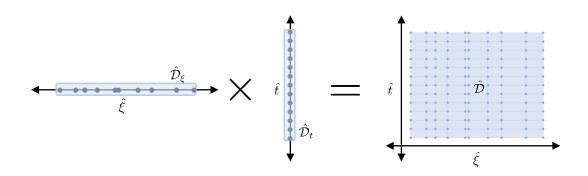


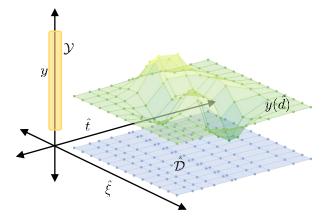
# TRANSFORMING INFINITEOPT PROBLEMS INTO FINITE ONES

#### **Direct Transcription**

**Project** onto set of **finite points**  $\widehat{\mathcal{D}}$ 

$$\hat{\mathcal{D}} := \prod_{\ell \in \mathcal{L}} \{ \hat{d}_{\ell,i} : \hat{d}_{\ell,i} \in \mathcal{D}_{\ell}, i \in \mathcal{I}_{\ell} \}$$

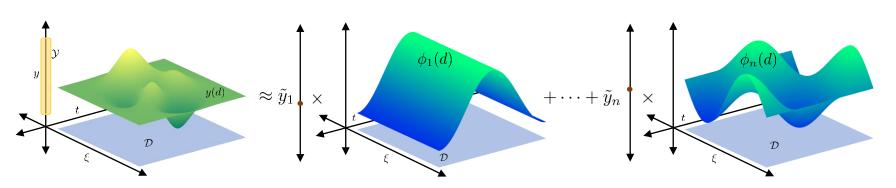




#### **Method of Weighted Residuals**

**Project** onto set of known **basis functions** 

$$y(d) \approx \sum_{i \in \mathcal{I}} \tilde{y}_i \phi_i(d)$$

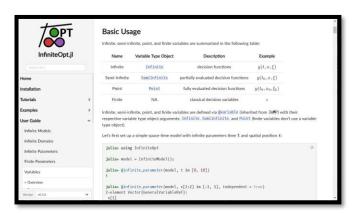






#### Why is it Different?

- 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







#### **Intuitive Modeling API**

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

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

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

@constraint(m, 
$$\partial$$
(yb, t) ==  $2$ yb^2 + ya - z[1])  
@constraint(m,  $\mathbb{E}$ (yc,  $\xi$ )  $\geq \alpha$ )  
@constraint(m, ya(0) + z[2] ==  $\beta$ )

#### **Impact**

1000s of downloads



- Use cases in diverse disciplines
  - e.g., evolutionary biology, rocketry, economics, autonomous vehicles

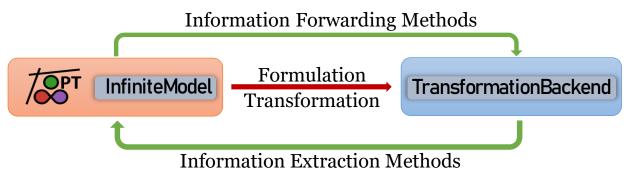




## TRANSFORMING INFINITEOPT MODELS



#### **Transformation Paradigm**

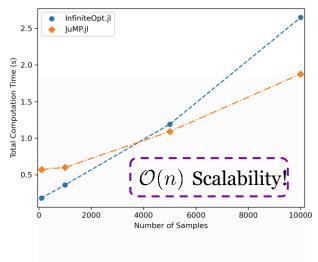


#### **Transformation API**

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

# Automated Transcription (via TranscriptionOpt)

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





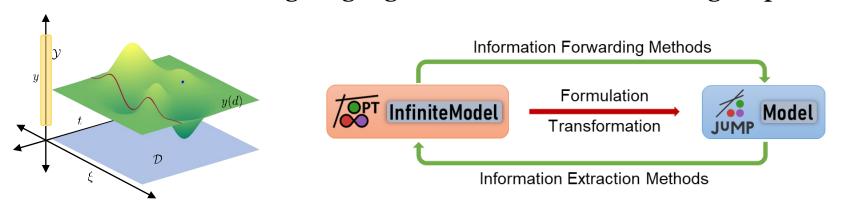


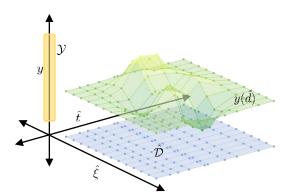


## SOLVING INFINITEOPT PROBLEMS VIA TRANSCRIPTIONOPT

- 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

- $\sin^2(y(t)) \le 42, \ t \in \mathcal{D}_t$   $\sin^2(y_k) \le 42, \ k \in \mathcal{K}$
- Traditional modeling languages like JuMP do not leverage repeated structure





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



## **OUTLINE**

InfiniteOpt

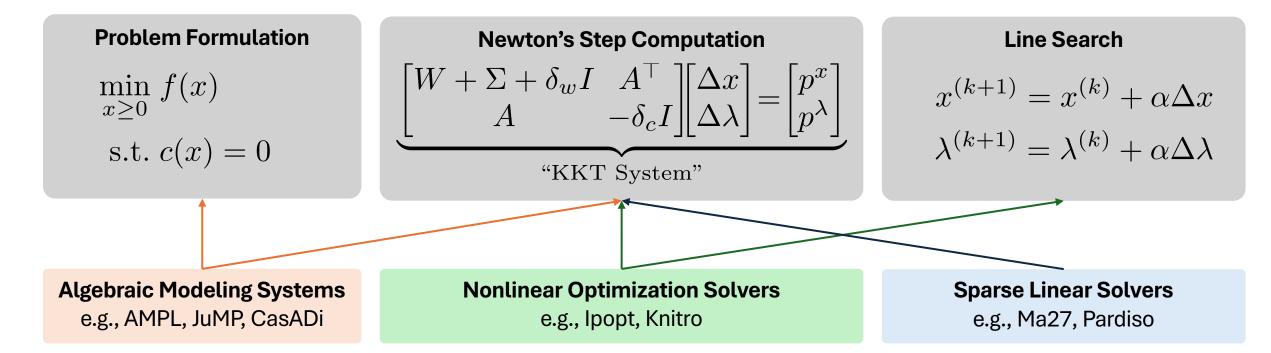
ExaModels



InfiniteExaModels



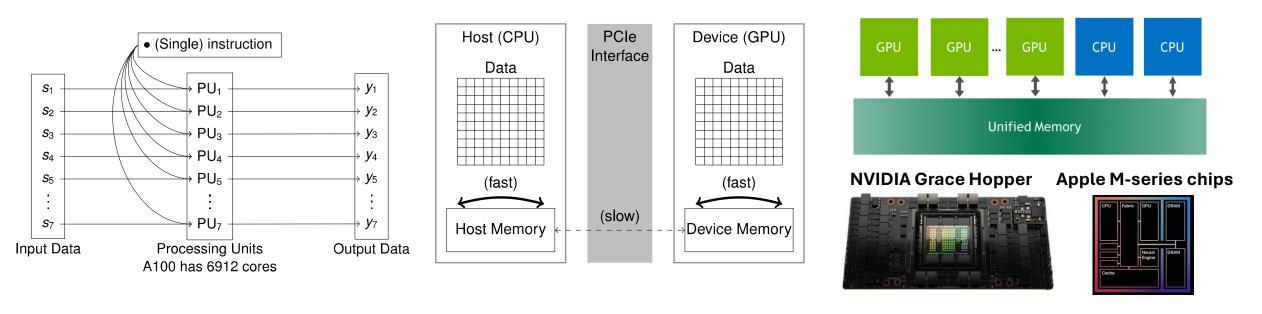
## **Traditional Nonlinear Optimization: Software**



- 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.

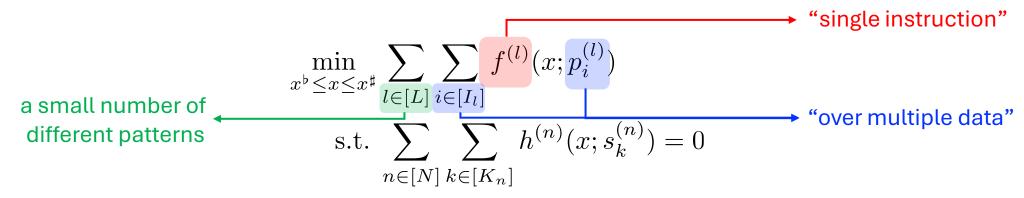


Adapting CPU code to GPU code is not merely a matter of software engineering; it often requires the **redesign of the algorithm** 

#### SIMD Abstraction for NLPs



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

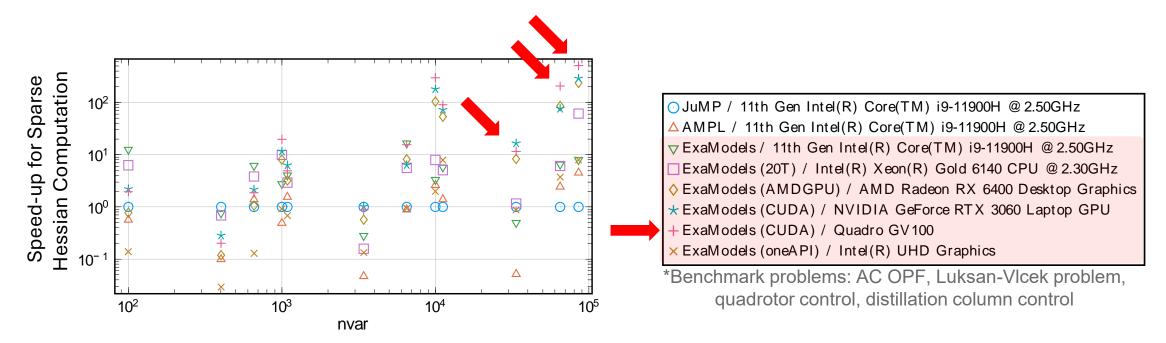


Repeated patterns are inputted as iterators (data can be stored in structured format)

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

## **Sparse AD Benchmark**





- For the largest case, **ExaModels on GPU** is **100× faster** than the state-of-the-art tools on CPUs
- 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**

#### **Problem Formulation**

$$\min_{x \ge 0} f(x)$$

s.t. 
$$c(x) = 0$$

#### **Newton's Step Computation**

$$\begin{bmatrix} W + \Sigma + \delta_w I & A^{\top} \\ A & -\delta_c I \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta \lambda \end{bmatrix} = \begin{bmatrix} p^x \\ p^{\lambda} \end{bmatrix}$$

"KKT System" (ill-conditioned)

#### **Line Search**

$$x^{(k+1)} = x^{(k)} + \alpha \Delta x$$

$$\lambda^{(k+1)} = \lambda^{(k)} + \alpha \Delta \lambda$$

**Algebraic Modeling Systems** 

**Nonlinear Optimization Solvers** 

**Sparse Linear Solvers** 



- Parallel AD with SIMD abstraction
- Runs on GPU architectures



- Lifted & Hybrid KKT System
- Runs on NVIDIA GPUs



- Parallel Cholesky factorization
- Runs on NVIDIA GPUs

### **AC Optimal Power Flow**

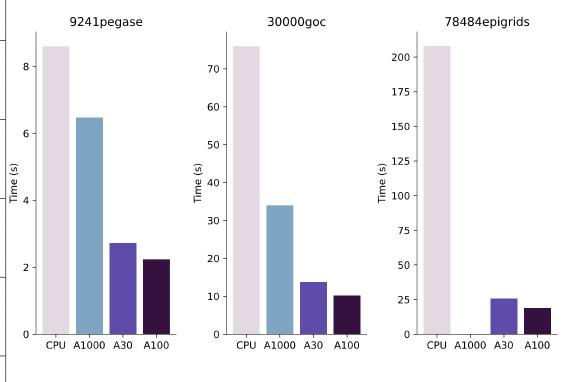








			CPU			Lifted K	KT on G	PU	H	lybrid k	KT on G	iPU
Case	it	init	lin	$\overline{\text{total}}$	it	init	lin	total	it	init	lin	total
89_pegase	32	0.00	0.02	0.03	29	0.03	0.12	0.24	32	0.03	0.07	0.22
179_goc	45	0.00	0.03	0.05	39	0.03	0.19	0.35	45	0.03	0.07	0.25
$500\_goc$	39	0.01	0.10	<b>0.14</b>	39	0.05	0.09	0.26	39	0.05	0.07	0.27
793_goc	35	0.01	0.12	0.18	57	0.06	0.27	0.52	35	0.05	0.10	0.30
$1354$ _pegase	49	0.02	0.35	<b>0.52</b>	96	0.12	0.69	1.22	49	0.12	0.17	0.50
2000_goc	42	0.03	0.66	0.93	46	0.15	0.30	0.66	42	0.16	0.14	0.50
2312_goc	43	0.02	0.59	<b>0.82</b>	45	0.14	0.32	0.68	43	0.14	0.21	0.56
$2742$ _goc	125	0.04	3.76	7.31	157	0.20	1.93	15.49	_	-	-	-
$2869\_pegase$	55	0.04	1.09	$\bf 1.52$	57	0.20	0.30	0.80	55	0.21	0.26	0.73
$3022\_goc$	55	0.03	0.98	1.39	48	0.18	0.23	0.66	55	0.18	0.23	0.68
3970_goc	48	0.05	1.95	2.53	47	0.26	0.37	0.87	48	0.27	0.24	0.80
$4020$ _goc	59	0.06	3.90	4.60	123	0.28	1.75	3.15	59	0.29	0.41	1.08
$4601\_goc$	71	0.09	3.09	4.16	67	0.27	0.51	1.17	71	0.28	0.39	1.12
$4619\_{ m goc}$	49	0.07	3.21	3.91	49	0.34	0.59	$\bf 1.25$	49	0.33	0.31	0.95
$4837\_\mathrm{goc}$	59	0.08	2.49	3.33	59	0.29	0.58	1.31	59	0.29	0.35	0.98
4917_goc	63	0.07	1.97	2.72	55	0.26	0.55	1.18	63	0.26	0.34	0.94
5658_epigrids	51	0.31	2.80	<b>3.86</b>	58	0.35	0.66	1.51	51	0.35	0.35	1.03
$7336_{ m epigrids}$	50	0.13	3.60	$\bf 4.91$	56	0.45	0.95	1.89	50	0.43	0.35	1.13
$8387$ _pegase	74	0.14	5.31	$\bf 7.62$	82	0.59	0.79	2.30	75	0.58	7.66	8.84
$9241_{-}$ pegase	74	0.15	6.11	8.60	101	0.63	0.88	2.76	71	0.63	0.99	$\bf 2.24$
9591_goc	67	0.20	11.14	13.37	98	0.63	2.67	4.58	67	0.62	0.74	1.96
$10000\_\mathrm{goc}$	82	0.15	6.00	8.16	64	0.49	0.81	1.83	82	0.49	0.75	1.82
$10192$ _epigrids	54	0.41	7.79	10.08	57	0.67	1.14	2.40	54	0.67	0.66	1.81
$10480\_goc$	71	0.24	12.04	14.74	67	0.75	0.99	2.72	71	0.74	1.09	2.50
$13659\_pegase$	63	0.45	7.21	10.14	75	0.83	1.05	2.96	62	0.84	0.93	$\bf 2.47$
19402_goc	69	0.63	31.71	36.92	73	1.42	2.28	5.38	69	1.44	1.93	4.31
20758_epigrids	51	0.63	14.27	$\boldsymbol{18.21}$	53	1.34	1.05	3.57	51	1.35	1.55	3.51
30000_goc	183	0.65	63.02	75.95	_	_	_	-	225	1.22	5.59	10.27
78484_epigrids	102	2.57	179.29	207.79	101	5.94	5.62	18.03	104	6.29	9.01	18.90



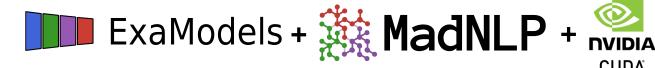
Optimizing entire eastern interconnection

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 to I=10<sup>-6</sup>, but still less reliable than CPUs

Pacaud, Shin, Montoison, Schanen, and Anitescu. Approaches to nonlinear programming on GPU architectures. In preparation.

#### **Distillation Column**



		CPU	-	Lifte	d KKT o	n GPU	Hybrid KKT on GPU				
#time steps	init (s)	it	solve (s)	init (s)	it	solve (s)	init (s)	it	solve (s)		
100	0.1	7	0.1	0.1	11	0.1	0.1	7	0.0		
500	0.1	7	0.5	0.2	12	0.1	0.2	7	0.1		
1,000	0.1	7	1.5	0.4	12	0.2	0.4	7	0.1		
5,000	0.6	7	8.2	2.3	13	0.5	2.3	7	0.4		
10,000	1.3	7	18.7	5.2	13	0.9	5.3	7	0.7		
20,000	4.3	7	38.2	10.7	14	2.1	11.3	7	1.4		
50,000	15.9	7	98.8	30.4	14	5.5	31.2	7	3.8		

- "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

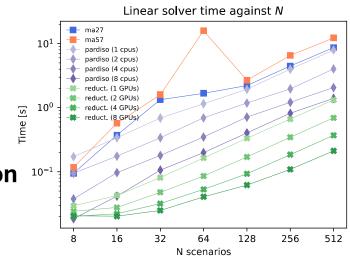
#### Portable sparse Cholesky factorization

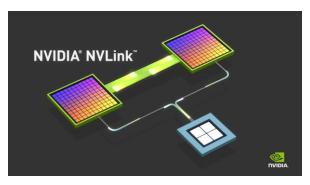
		CPU (single)	CPU (multi)	NVIDIA GPU	AMD GPU	Intel GPU
	AMPL	✓	X	Х	Х	X
Algebraic Modeling Platforms	JuMP	✓	X	×	×	×
	ExaModels	✓	$\checkmark$	$\checkmark$	$\checkmark$	$\checkmark$
NLP Solvers	lpopt	✓	Х	Х	Х	X
INLE Solveis	MadNLP	✓	×	✓	×	X

- Currently, we are relying on a proprietary Cholesky solver (CUDSS)
- An open-source, portable Cholesky solver is needed to run on Exascale

#### 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





## **EXAMODELSMOI.JL**

- Provides an MOI optimizer for JuMP models
  - Can use either ExaModels. IpoptOptimizer or ExaModels. MadNLPOptimizer

```
using ExaModels, JuMP, CUDA, MadNLPGPU

model = Model(() -> ExaModels.MadNLPOptimizer(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

- 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

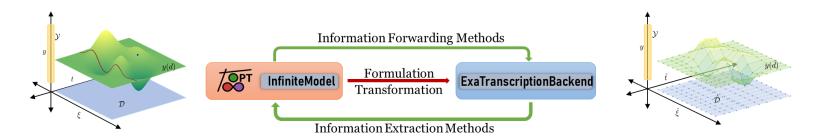
```
5.52e-81 2.96e-81f
                                                                                      58 8.9482184e+86 3.24e-81 3.22e+88 -3.8 1.93e+88
                                                        3.81e-81 2.86e-81h
                                                                                      51 8.9481836e+86 1.55e-81 1.33e+88 -3.8 4.37e+88 -3.9 1.88e+88 7.27e-81h
                                                        7.38e-81 3.69e-81h 1
                                                                                      52 8.9481716e+86 1.95e-81 8.32e-84 -3.8 9.45e+88 -4.4 1.88e+88 1.88e+88h
    8.9484865e+86 9.46e-84 1.82e+82 -3.8 6.78e+88
      objective inf_pr inf_du lg(mu) ||d|| lg(rg) alpha_du alpha_pr ls
                                                                                      53 8.9481718e+86 2.32e-81 2.13e-85 -3.8 1.27e+81 -4.9 1.88e+88 1.88e+88h
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     8.9483344e+86 1.15e-83 5.46e+81 -3.8 4.62e+88
                                                        7.24e-81 4.63e-81h 1
     8.9482821e+86 8.39e-84 1.12e+81 -3.8 2.67e+88
                                                        8.29e-81 7.97e-81h
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     8.9481722e+86 2.24e-85 2.73e-84 -3.8 6.22e-81
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                                                                                      57 8.9481213e+86 4.88e-83 1.95e-81 -5.7 2.14e+88 -6.8 5.36e-81 4.89e-81h
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                                                                                     58 8.9481835e+86 4.93e-83 1.84e+88 -5.7 1.43e+88 -7.2 6.18e-81 2.47e-81h
     8.9481213e+86 6.65e-85 5.97e+88 -5.7 2.15e+88
                                                        5,49e-81 4,18e-81f 1
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                                                        6.87e-81 2.47e-81h
                                                        5.97e-81 6.94e-81h 1
                                                                                    iter objective inf_pr inf_du lg(mu) ||d|| lg(rg) alpha_du alpha_pr
                                                        2.98e-81 4.34e-81h
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                                                      - 1.88e+88 1.88e+88h
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   teration 62, 1 Slack too small, adjusting variable bound
                                                                                      67 8.9488466e+86 4.87e-86 1.25e-81 -8.6 7.66e-83 -11.5 7.47e-81 1.88e+88h
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                                                                                     68 8.9488466e+86 8.68e-87 2.86e-82 -8.6 2.38e-83 -6.6 8.35e-81 1.88e+88h
    8.9488498e+86 2.85e-86 1.35e-81 -8.6 3.85e-82
    8.9488489e+86 2.53e-87 1.87e-87 -8.6 9.47e-83
                                                        1.88e+88 1.88e+88h 1
                                                                                     69 8.9488466e+86 2.36e-86 9.53e-89 -8.6 1.62e-83 -7.1 1.88e+88 1.88e+88h
  5 8.9488489e+86 3.52e-88 3.12e-88 -8.6 1.98e-83
                                                                                    iter objective inf.pr inf.du lg(mu) |||d|| lg(rg) alpha_du alpha.pr ls
78 8.9488466e+85 3.69e-87 2.24e-89 -8.6 6.45e-84 -6.6 1.88e+88 1.88e+88h
71 8.9488466e+85 8.89e-18 2.86e-18 -8.6 4.23e-85 -5.3 1.88e+88 1.88e+88h
                                                       - 1.88e+88 1.88e+88h
    8.9488489e+86 2.58e-89 6.11e-89 -8.6 3.22e-84
                                                                                    Number of Iterations ... . 71
                                                   8.9488489176823249e+86
 nstraint violation...: 2.5823698668746874e-89
                                                                                    Dual infeasibility.....: 2.0585960359393939e-10
                                                                                                                                          2.6817182673681384e-88
 mplementarity.....: 4.5931745136391954e-89
                                                                                     Complementarity.....: 1.9536168379976883e-11 2.5449539861788477e-89
                                                                                    Number of objective function evaluations
umber of objective function evaluations
                                                                                    Number of objective gradient evaluations
lumber of objective gradient evaluations
                                                                                    Number of constraint evaluations
 mber of equality constraint evaluations
                                                                                   Number of constraint Jacobian evaluations
mber of inequality constraint evaluations
                                                                                    Total wall-clock secs in solver (w/o fun. eval./lin. alg.)
 mber of equality constraint Jacobian evaluations
 mber of inequality constraint Jacobian evaluations = 67
                                                                                    Total wall-clock secs in linear solver
                                                                                    Total wall-clock secs in NLP function evaluations
 mber of Lagrangian Hessian evaluations
XIT: Optimal Solution Found.
                                                                                    EXIT: Optimal Solution Found (tol = 1.0e-08).
 xecution stats: first-order stationary
                                                                                    "Execution stats: Optimal Solution Found (tol = 1.8e-88)."
```



# **OUTLINE**

InfiniteOpt

ExaModels

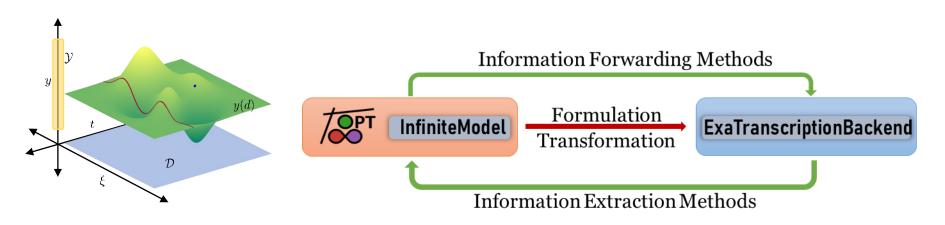


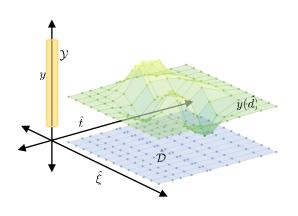
InfiniteExaModels



## INFINITEEXAMODELS.JL

- Bridges the gap between 🎏 InfiniteOpt & 🔲 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

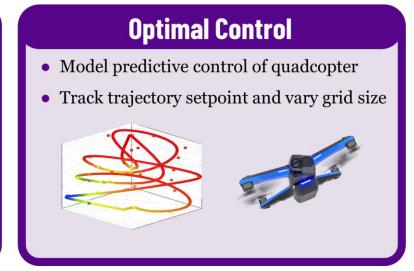
- Supports the use of **JSO NLP solvers** (e.g., Ipopt, MadNLP, KNITRO)
- Defined via an ExaTranscriptionBackend
  - 1 using InfiniteOpt, InfiniteExaModels, NLPModelsIpopt
  - 2 model = InfiniteModel(ExaTranscriptionBackend(IpoptSolver))
- Rapidly transcribes infinite model into efficient ExaModels
-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

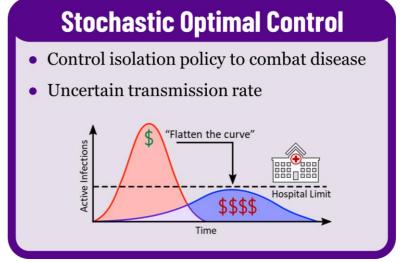


## BENCHMARK PROBLEMS

- 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





# NUMERICAL RESULTS (CPU W/ IPOPT)

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

	Stoc	hasti	c 2-Sta	age	Op	tima	l Contr	ol	Sto	chast	ic Con	trol
Approach	Build	AD	Solve	Tot.	Build	AD	Solve	Tot.	Build	AD	Solve	Tot.
JuMP.jl	87.1	21.4	63.7	151	143	6.3	28.6	172	10.9	60.7	386	397
AMPL	99.3	11.5	90.3	190	153	5	26.4	179	10.6	23.4	364	375
ExaModelsMOI.jl	86.6	3.05	56.3	143	139	1.1	23.1	162	8.63	3.45	368	376
InfiniteExaModels.jl	1.94	2.03	43	45	9.34	1	22.6	31.9	0.12	3.01	369	369

- using InfiniteOpt, InfiniteExaModels, NLPModelsIpopt
- 2 model = InfiniteModel(ExaTranscriptionBackend(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

	Stochastic 2-Stage				Op	tima	l Contr	ol	Stochastic Control			
Approach	Build	AD	Solve	Tot.	Build	AD	Solve	Tot.	Build	AD	Solve	Tot.
ExaModelsMOI.jl							6.55					28.6
InfiniteExaModels.jl	1.8	0.14	3.03	4.82	8.63	0.1	6.44	15.1	0.06	0.74	21	21_
	(151 on CPU) (172 on CPU) (397 on CPU)									CPU) -		

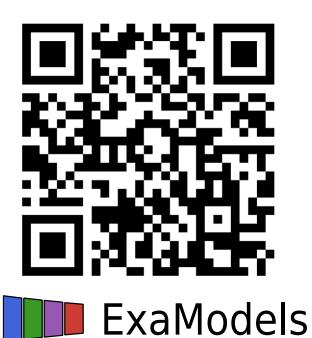
- 1 using InfiniteOpt, InfiniteExaModels, MadNLPGPU, CUDA
- 2 transform\_backend = ExaTranscriptionBackend(MadNLPSolver, backend = CUDABackend())
- 3 model = InfiniteModel(transform\_backend)



## TRY IT OUT!















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