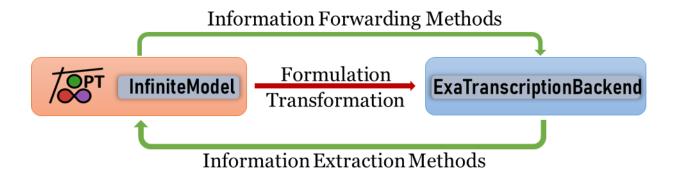


INFINITEEXAMODELS.JL: Accelerating infinite-dimensional Optimization problems on CPU & GPU

7/29/2024

Joshua Pulsipher and Sungho Shin





ACKNOWLEDGEMENTS



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Department of Chemical Engineering





EXASCALE COMPUTING PROJECT



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ENGINEERING

OUTLINE

InfiniteOpt

ExaModels

InfiniteExaModels

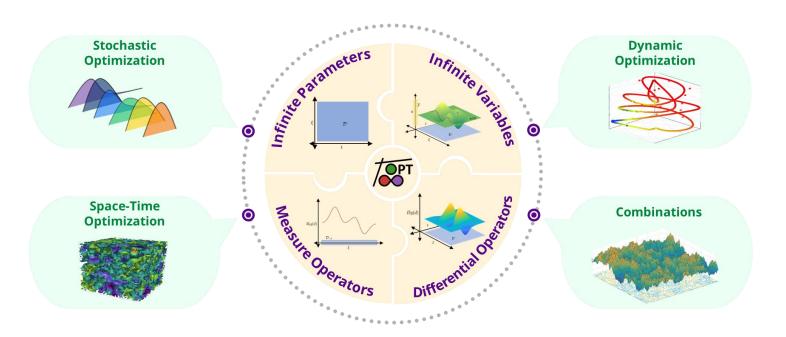


OUTLINE

InfiniteOpt

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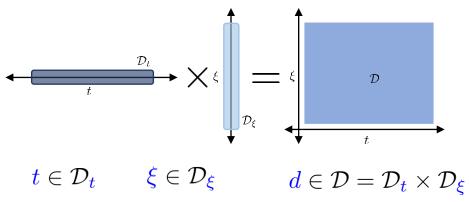




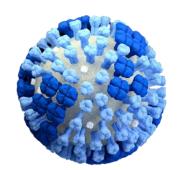
INFINITE-DIMENSIONAL OPTIMIZATION

Infinite Parameters

Index over continuous domains

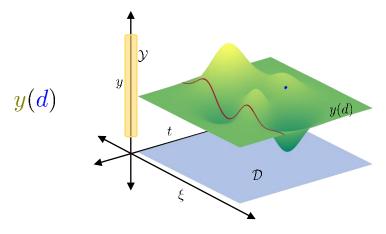


- Example: Disease Control
 - Population dynamics
 - $\mathbf{t} \in [0, t_f]$
 - Uncertain infection rates
 - $\boldsymbol{\xi} \in (-\infty,\infty) \sim \mathcal{N}(\boldsymbol{\mu},\boldsymbol{\Sigma})$



Infinite Variables

• **Decisions** indexed by infinite parameters



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



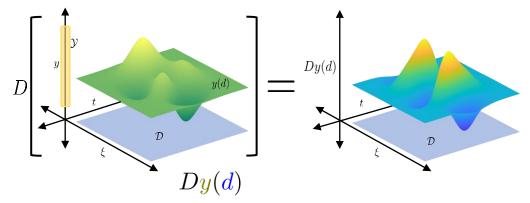
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INFINITE-DIMENSIONAL OPTIMIZATION

Differential Operators

• Capture of **rate of change** in variables



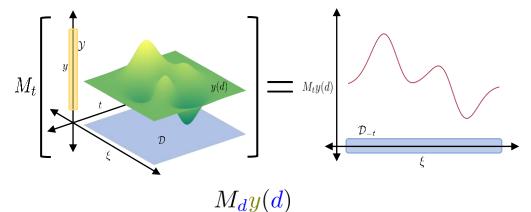
- Example: Disease Control
 - Time derivative
 - SEIR model

$$rac{\partial oldsymbol{y_i}(t,oldsymbol{\xi})}{\partial t}$$

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

Measure Operators

• Summarize variables over continuous domains

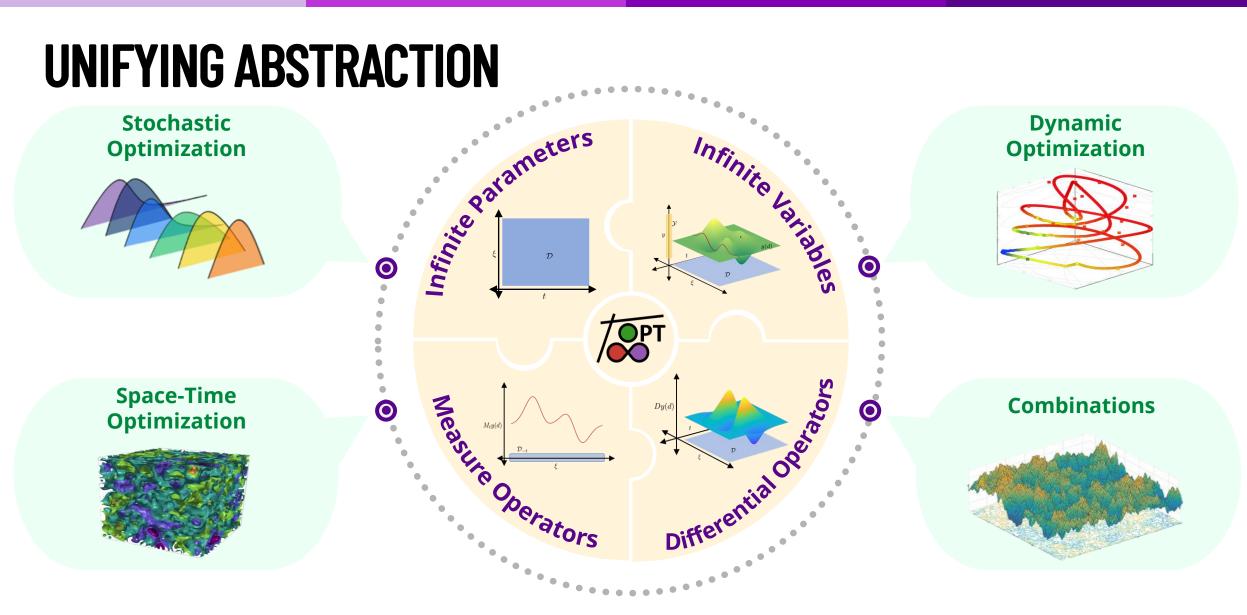


- Example: Disease Control
 - Summarize overall infections

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

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

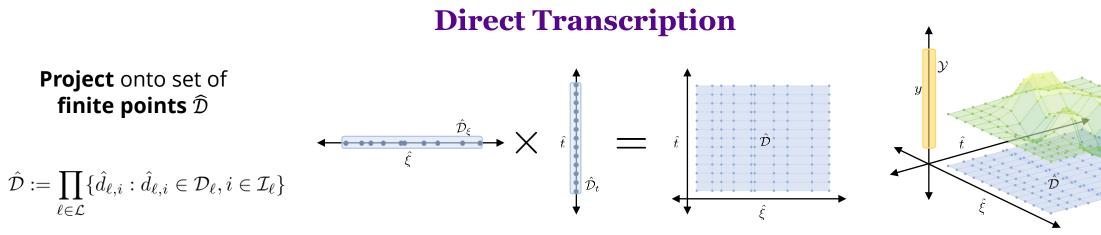




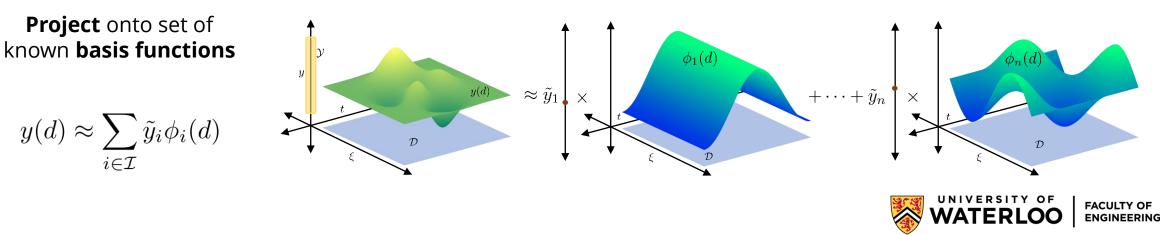


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TRANSFORMING INFINITEOPT PROBLEMS INTO FINITE ONES



Method of Weighted Residuals



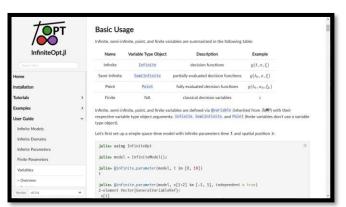
J. L. Pulsipher, W. Zhang, T. J. Hongisto, and V. M. Zavala. "A Unifying Modeling Abstraction for Infinite-Dimensional Optimization." Computers & Chem. Eng. 2022



- 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 @ <u>https://github.com/infiniteopt/InfiniteOpt.jl</u>



Intuitive Modeling API

$$\frac{\partial y_b(t,\xi)}{\partial t} = 2y_b(t,\xi)^2 + y_a(t) - z_1$$
$$\mathbb{E}_{\xi} \left[y_c(t,\xi) \right] \ge \alpha$$
$$y_a(0) + z_2 = \beta$$

Impact

Announcements Welcome to InfiniteOpt.jl Discussions!

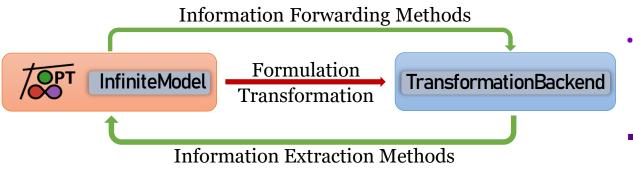
- 1000s of downloads
- Use cases in diverse disciplines
 - e.g., evolutionary biology, rocketry, economics, autonomous vehicles



TRANSFORMING INFINITEOPT MODELS



Transformation Paradigm

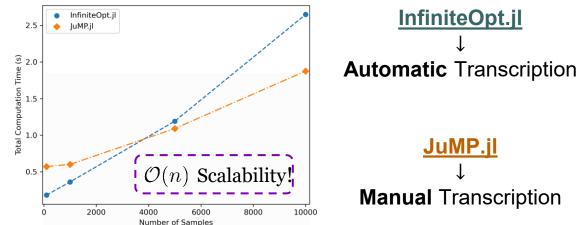


Transformation API

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



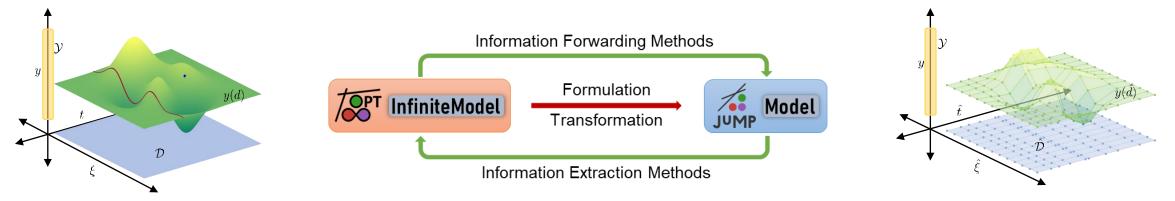
- Many derivative/measure approximations
 - Orthogonal collocation, Gauss quadrature, etc.
- Performant





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**?



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

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



InfiniteOpt

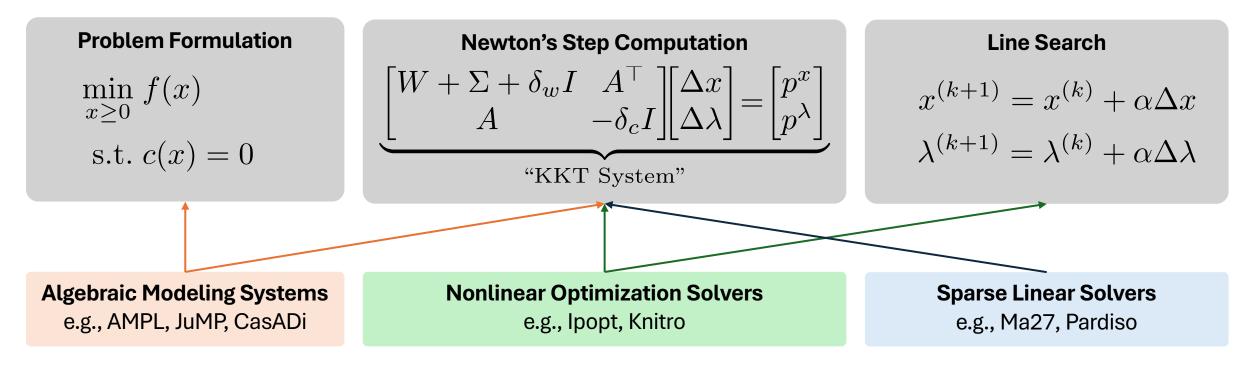
ExaModels



InfiniteExaModels



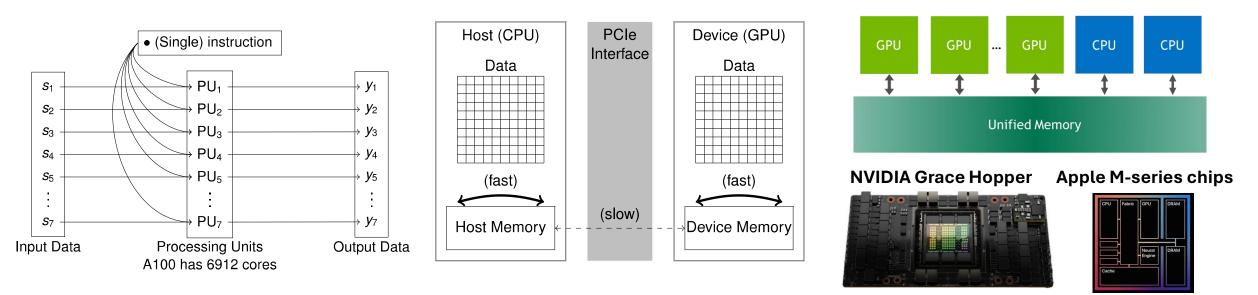
Traditional Nonlinear Optimization: Software



- 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.

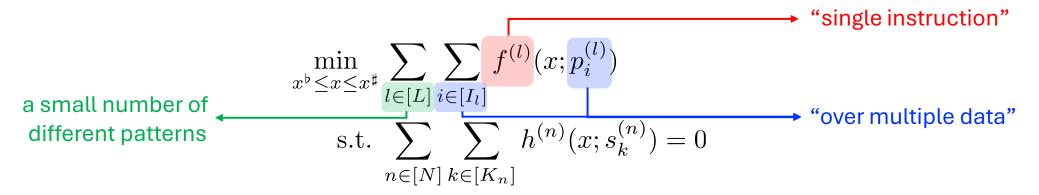


Adapting CPU code to GPU code is not merely a matter of software engineering; it often requires the **redesign of the algorithm**

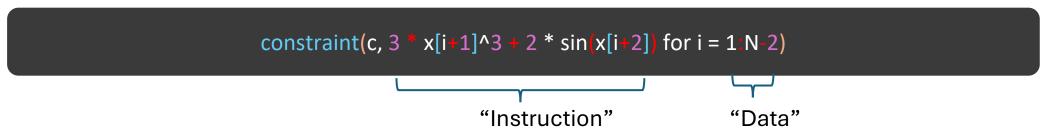
SIMD Abstraction for NLPs



- 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

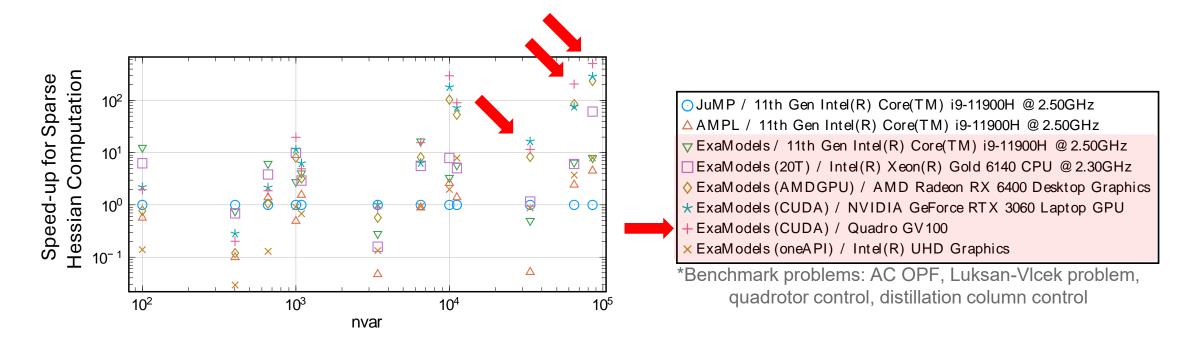
Shin, Pacaud, and Anitescu

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

PSCC 2024

Sparse AD Benchmark

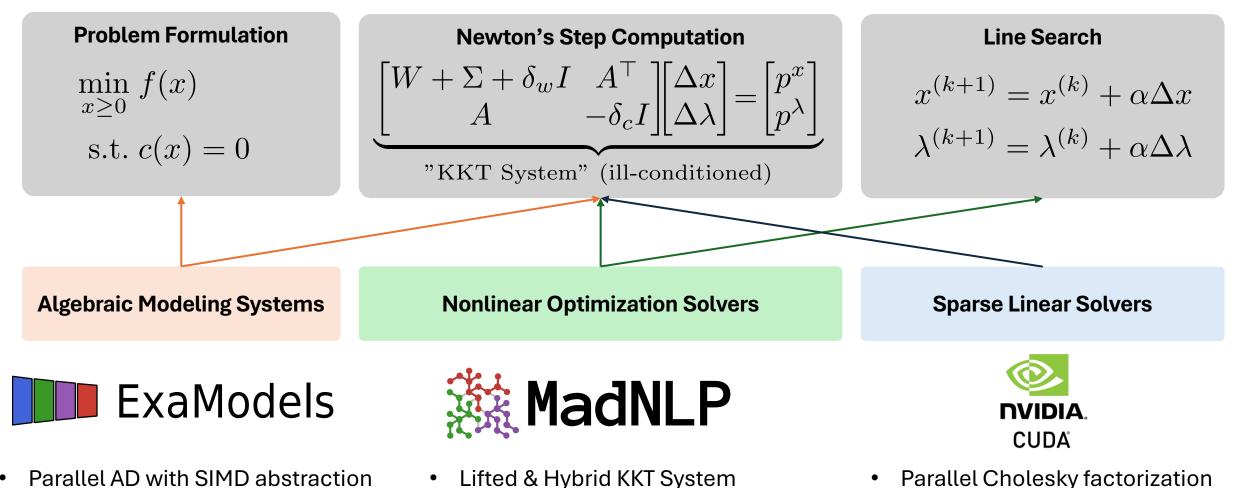




- For the largest case, **ExaModels on GPU** is **100× faster** than the state-of-the-art tools on CPUs
- ExaModels runs on all major GPU architectures and single/multi-threaded CPUs

Sparse AD with SIMD abstraction enables efficient derivative computations on GPUs

Nonlinear Optimization Framework on GPUs



Runs on NVIDIA GPUs

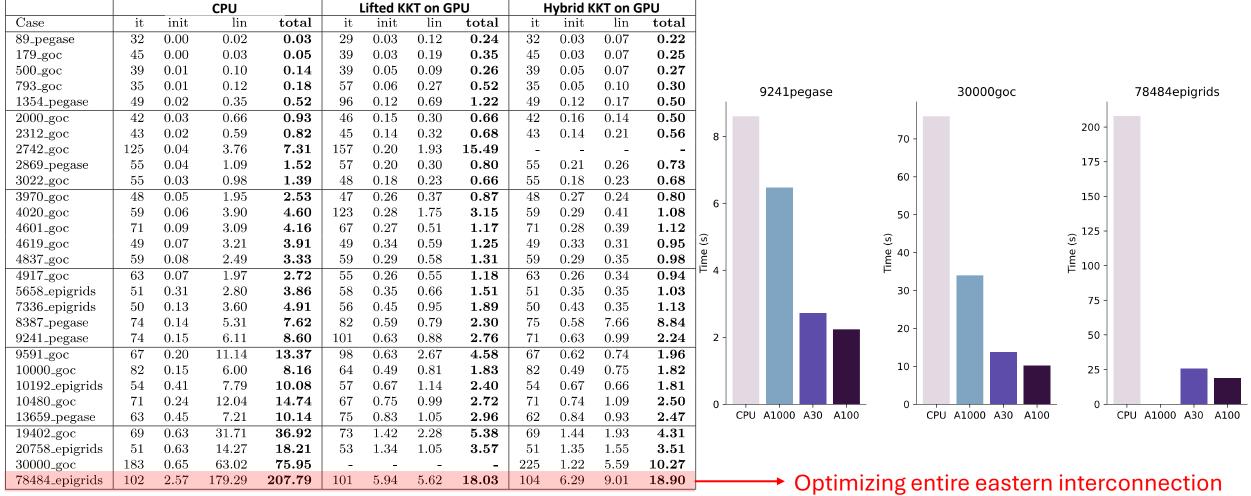
• Runs on GPU architectures

https://github.com/exanauts/ExaModels.jl https://github.com/MadNLP/MadNLP.jl https://docs.nvidia.com/cuda/cudss

Sungho Shin <u>sshin@anl.gov</u>

Runs on NVIDIA GPUs

AC Optimal Power Flow



CUDA

ExaModels + 🤼 MadNLP +

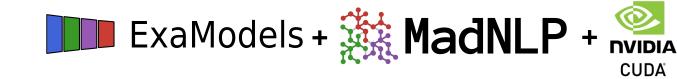
Table 3 OPF benchmark, solved with a tolerance tol=1e-6. (A100 GPU)

• 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

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

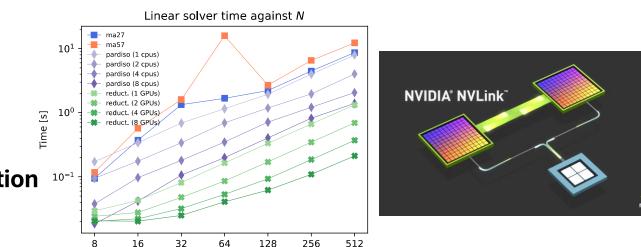
ExaModels, MadNLP, and **CUDSS** provide **efficient and reliable** solution framework for large-scale nonlinear optimization problems

Remaining Challenges

Portable sparse Cholesky factorization

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

- 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



N scenarios

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

EXAMODELSMOI.JL

2

- Provides an MOI optimizer for JuMP models
 - Can use either ExaModels.IpoptOptimizer or ExaModels.MadNLPOptimizer
 - 1 using ExaModels, JuMP, CUDA, MadNLPGPU
 - 3 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

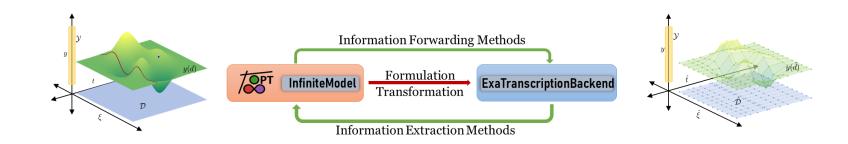
- ExaModels + MadNLP is highly performant for problems with repeated patterns
- Translating InfiniteOpt problems to SIMD is nontrivial
- TranscriptionOpt + ExaModelsMOI has to ignore structure while building the model

46 8.9492673e+86 8.27e-84 2.51e+82 -3.8 1.52e+81 - 3.48e-81 2.27e-81f 1	iter objective inf_pr inf_du lg(mu) d lg(rg) alpha_du alpha_pr ls
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48 8.9486888e+86 7.66e-84 1.54e+82 -3.8 9.81e+88 - 3.81e-81 2.86e-81h 1	51 8.9481836e+86 1.55e-01 1.33e+88 -3.8 4.37e+88 -3.9 1.00e+88 7.27e-81h 1
49 8.9484865e+86 9.46e-84 1.82e+82 -3.8 6.78e+88 - 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 1
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59 8.9488584e+86 4.68e-85 2.35e-82 -5.7 1.46e-81 - 1.88e+88 9.96e-81h 1	62 8.9480501e+86 8.70e-03 3.87e-82 -5.7 1.48e-01 -9.1 1.00e+80 9.94e-01h 1
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In iteration 62, 1 Slack too small, adjusting variable bound 63 8.9488498e+86 2.85e-86 1.35e-81 -8.6 3.85e-82 - 9.88e-81 9.81e-81h 1	6/ 8.9488466e+86 8.68e-87 2.86e-82 -8.6 2.38e-83 -6.6 8.35e-81 1.88e+88h 1
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66 8.94884698+86 2.588-89 6.118-89 -8.6 3.228-84 - 1.888+88 1.888+88 1	78 8.9488466e+86 8.89e-87 2.248-89 -8.6 6.45e-84 -6.6 1.88e+88 1.88e+88 1 71 8.9488466e+86 8.89e-18 2.86e-18 -8.6 4.23e-85 -5.3 1.88e+88 1.88e+88h 1
Number of Iterations: 66	
	Number of Iterations: 71
(scaled) (unscaled)	
Objective: 6.8689868522388895e+84 8.9488489176823249e+86	(scaled) (unscaled)
Dual infeasibility: 6.1111782827239337e-89 7.9689641939457634e-87	Objective 6.8689050407876275e+84 8.9480465578552410e+06
Constraint violation: 2.5823698668746874e-89 2.5823698668746874e-89	Dual infeasibility: 2.8585968359393939e-18 2.6817182673681384e-88
Variable bound violation: 1.9973768772274525e-87 1.9973768772274525e-87	Constraint violation: 8.8916429112676269e-18 8.8916429112676269e-18
Complementarity: 4.5931745136391954e-89 5.9834775924759131e-87	Complementarity: 1.9536168379976883e-11 2.5449539861788477e-89
Dverall NLP error: 6.1111782827239337e-89 7.9689641939457634e-87	Overall NLP error: 2.5449539861708477e-89 2.5449539861708477e-89
	Number of objective function evaluations = 76
Number of objective function evaluations = 79	Number of objective radicities = 70
Number of objective radient evaluations = 67	Number of constraint evaluations = 76
Number of equality constraint evaluations = 79	Number of constraint Jacobian evaluations = 72
Number of inequality constraint evaluations = 79	Number of Lagrangian Hessian evaluations = 72
Number of equality constraint Jacobian evaluations = 67	Total wall-clock secs in solver (w/o fun, eval./lin, alg.) = 2.565
Number of inequality constraint Jacobian evaluations = 67	Total wall-clock secs in Solver (w/o fun. eval./lin. alg.) = 2.565
Number of Lagrangian Hessian evaluations = 66	Total wall-clock secs in NLP function evaluations = 8.127
Total seconds in IPOPT = 18.372	Total wall-clock secs in MLP renetion evaluations = 0.127
EXIT: Optimal Solution Found.	EXIT: Optimal Solution Found (tol = 1.0e-08).
"Execution stats: first-order stationary"	"Execution stats: Optimal Solution Found (tol = 1.0e-08)."
julia>	julia>



OUTLINE

InfiniteOpt



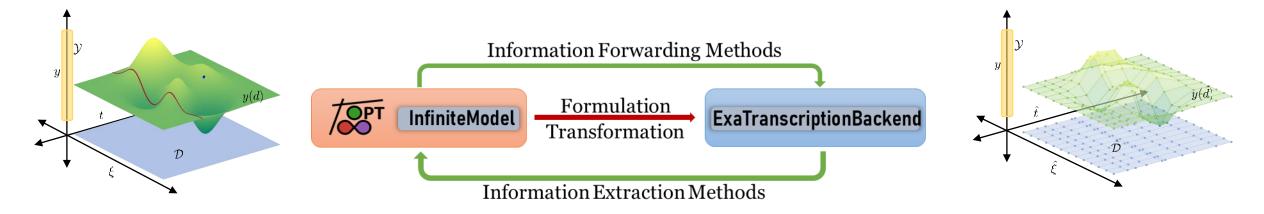
ExaModels

InfiniteExaModels



INFINITEEXAMODELS.JL

- Bridges the gap between This 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

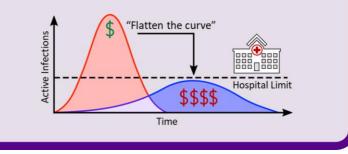
Optimal Control

- 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

	Stochastic 2-Stage		Optimal Control				Stochastic Control					
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
	99.3					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

1 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	otima	l Contr	ol	Stochastic Control			
Approach	Build	AD	Solve	Tot.	Build	AD	Solve	Tot.	Build	AD	Solve	Tot.
ExaModelsMOI.jl	83	0.09	3.15	86.1	133	0.1	6.55	140	8.21	0.51	20.4	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)												

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

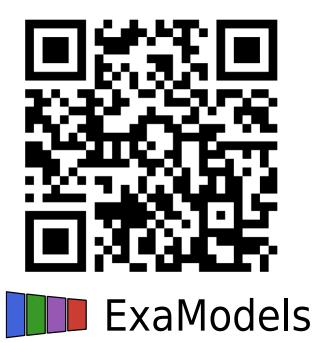


TRY IT OUT!





InfiniteExaModels







InfiniteExaModels

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