Nonlinear Optimization on Graphics Processing Units

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2023 AIChE Meeting, Orlando, Florida



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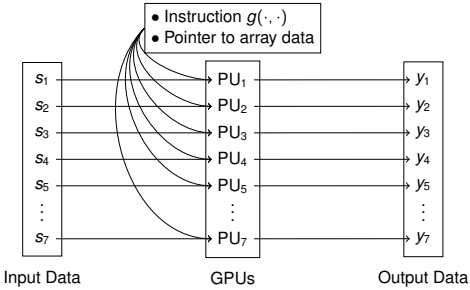
Can we harness these capabilities in the realm of **classical optimization**?
(e.g., energy systems, optimal control, operations research)

How Do GPUs Work? (or, how are they different from CPUs?)

- Single Instruction, Multiple Data (**SIMD**) parallelism,



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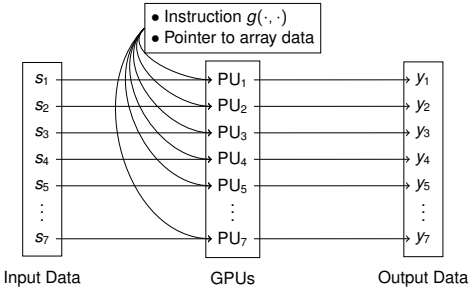

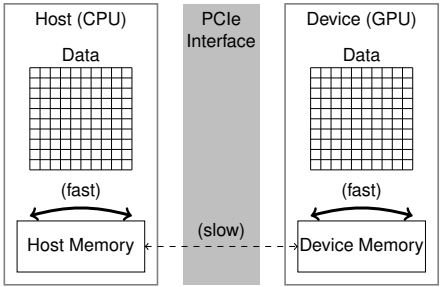

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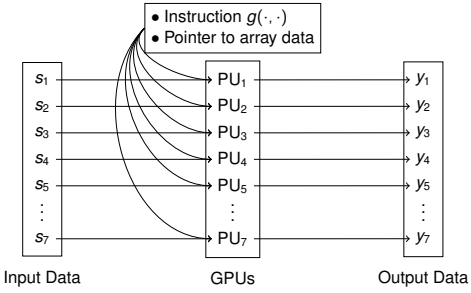

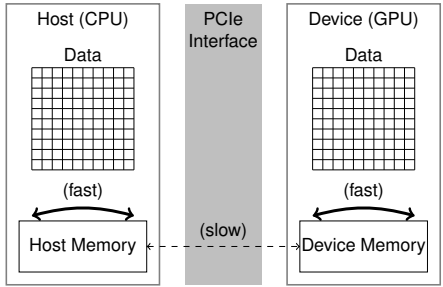

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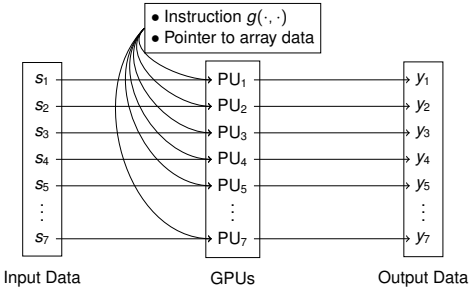

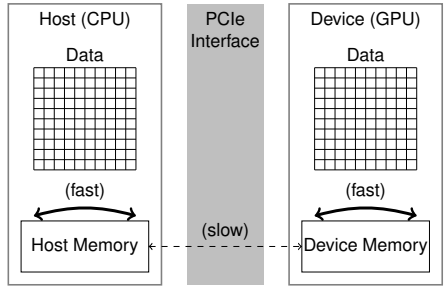

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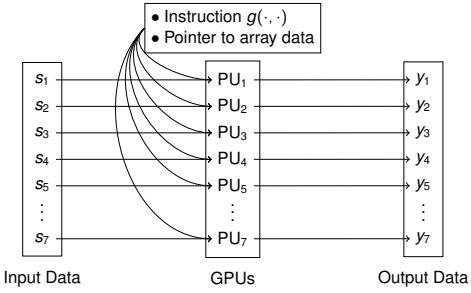

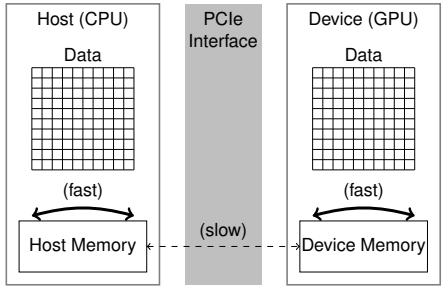

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Adapting CPU algorithms into GPU algorithms is **not merely a matter of software engineering** and often requires a **complete redesign of the algorithm**.

Exascale Computing Project

- **Mission**: Harness exascale computing capabilities to tackle **real-world challenges**.

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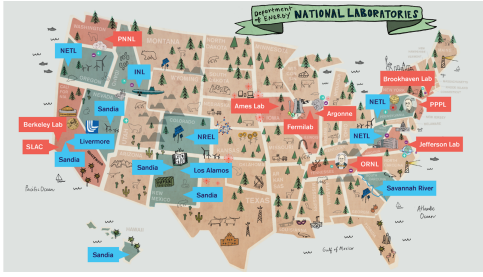

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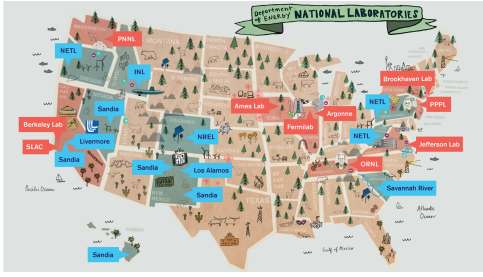

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- **Challenge**: There were no implementations of **sparse automatic differentiation, nonlinear optimization solver, nor sparse indefinite solvers** on GPUs.
- **Goal**: Build a **comprehensive software infrastructure** for nonlinear optimization on GPUs.
  - **Performance**: at least an order of magnitude speedup.
  - **Portability**: compatibility with NVIDIA, AMD, and Intel.
  - **Application**: energy infrastructure problems.

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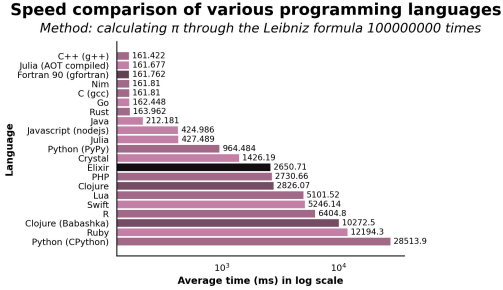

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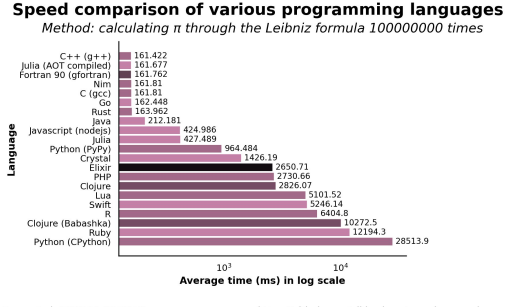
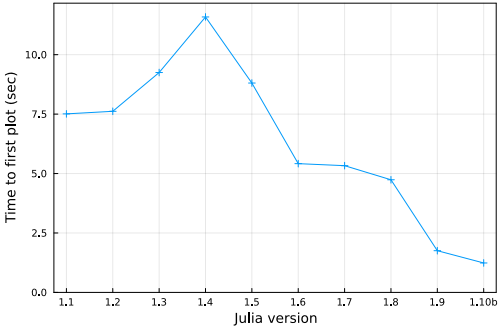
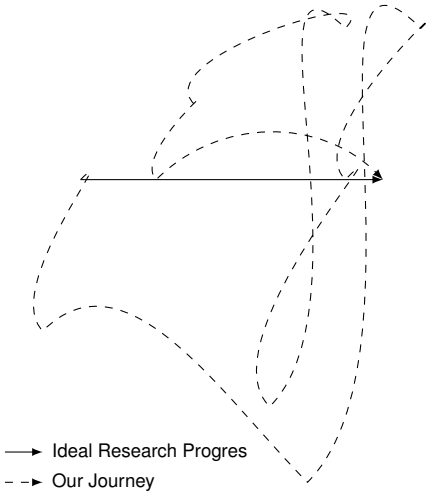
- The initial delay, often referred to as "**time-to-first-call**," has been significantly reduced.





Summary of Exanauts' Journey



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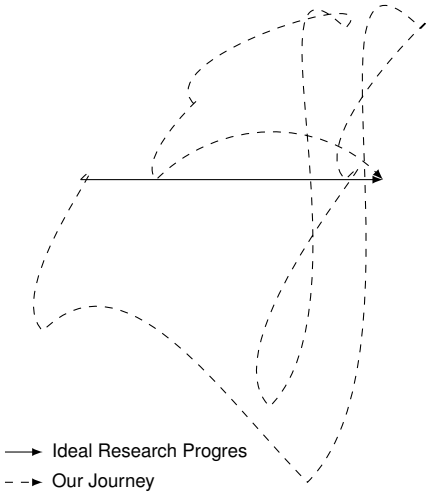

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- **Modeling/automatic differentiation**: batched second-order adjoint sensitivity, SIMD abstraction, ...
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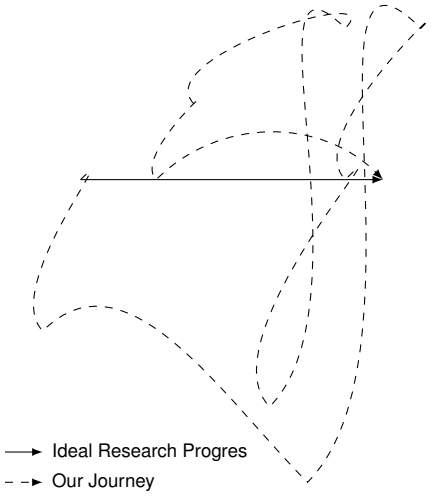

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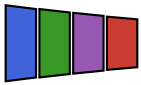
Two Award-Winning Open-Source Projects (2023 COIN-OR Cup)



ExaModels

MadNLP

https://github.com/sshin23/ExaModels.jl

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How {AMPL, IPOPT, Ma27} Have Succeeded on CPUs

Modeling

$$\min_{x \geq 0} f(x)$$
$$\text{s.t. } c(x) = 0$$

Barrier Reformulation

$$\min_{x} f(x) - \mu \log(x)$$
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Newton's Step Comp.

$$\underbrace{\begin{bmatrix} W + \Sigma + \delta_w I & A^\top \\ A & \delta_c I \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta \lambda \end{bmatrix} = \begin{bmatrix} p^x \\ p^\lambda \end{bmatrix}}_{\text{"KKT System"}}$$

Line Search

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

AMPL, JuMP, CasADi, ...

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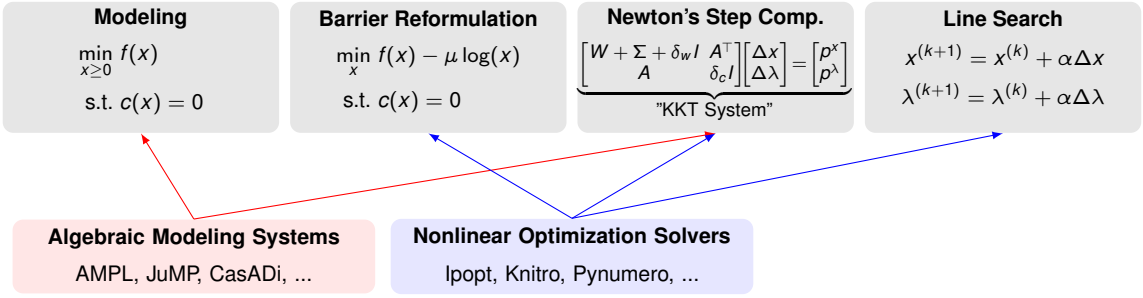

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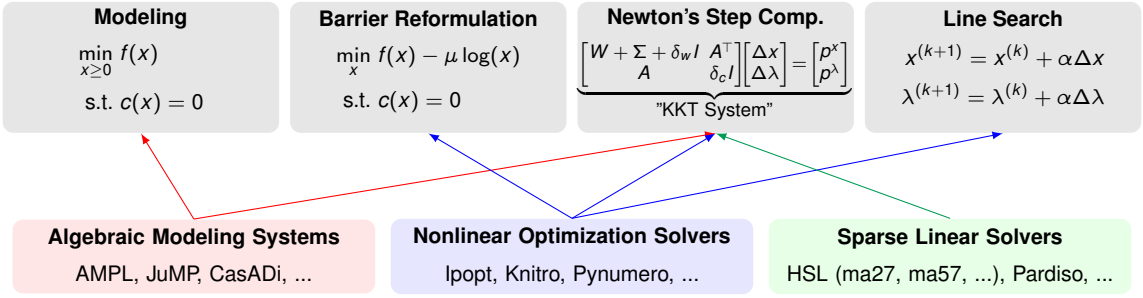

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- Sparse indefinite solvers have enabled **the solution of ill-conditioned linear systems**.

Why it is Challenging: Sparse Automatic Differentiation

- **Automatic differentiation** is **more efficient** than *finite difference* or *symbolic differentiation*, and is **less prone to error** than *hand-written derivative codes*.

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f(x){ ... }
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df(x){ ... }
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$$y = f(x)$$

$$y' = f'(x)$$

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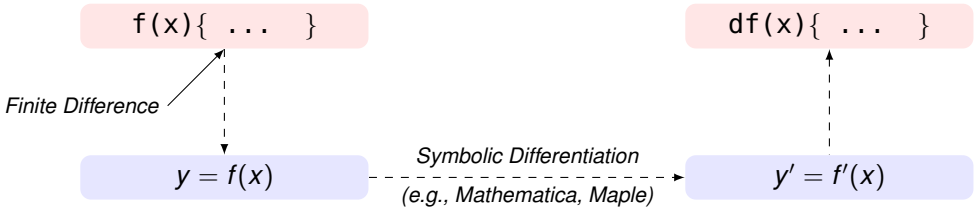

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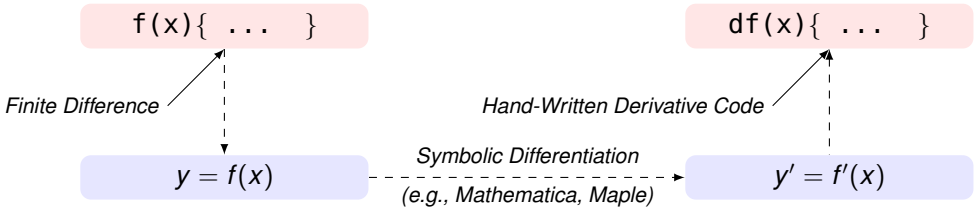

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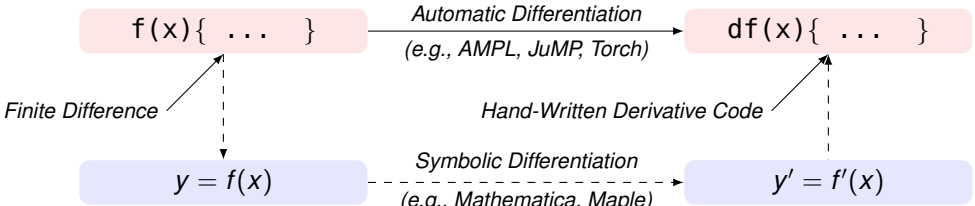

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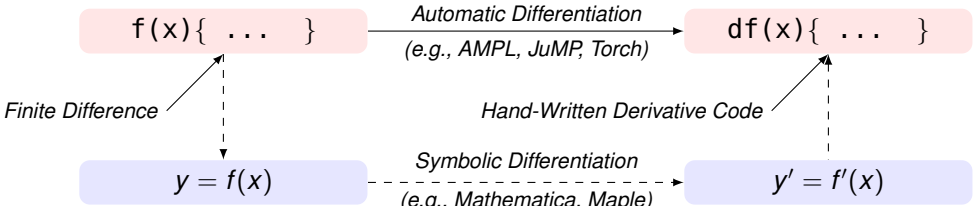

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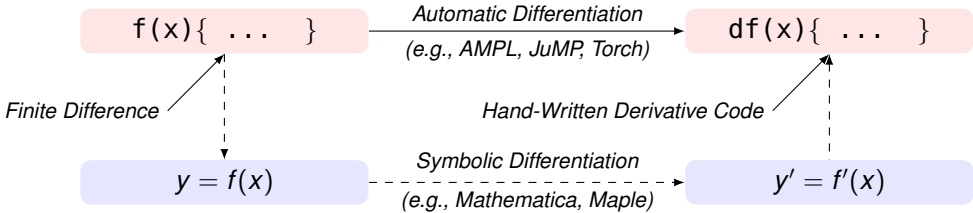

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- **Machine learning frameworks** (e.g., Torch) are not effective for **sparse problems**.

Solution: SIMD Abstraction

- Large-scale optimization problems **almost always have repetitive patterns**.
  e.g., optimal power flow w/ millions of variables can be expressed with a handful of patterns.
  - referencebus voltage angle
  - active and reactive power flow
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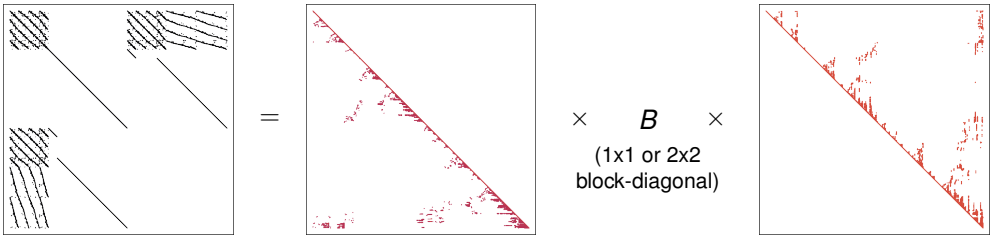
- **For each repeatitive pattern**, the derivative evaluation kernel is constructed & compiled, and it is **executed in parallel over multiple data**.

Why it is Challenging: Sparse Linear Solvers

- Solving KKT systems on CPUs has traditionally relied on **direct LBL$^\top$ factorization**.



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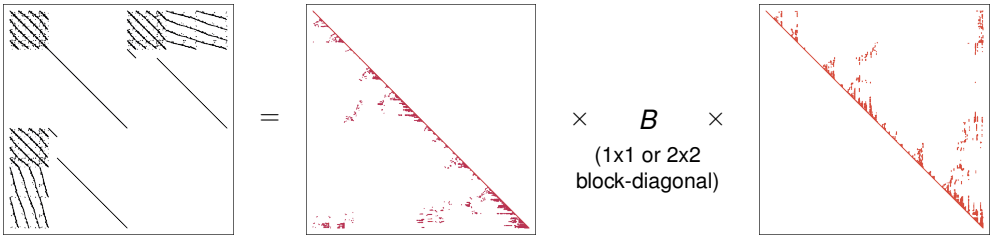
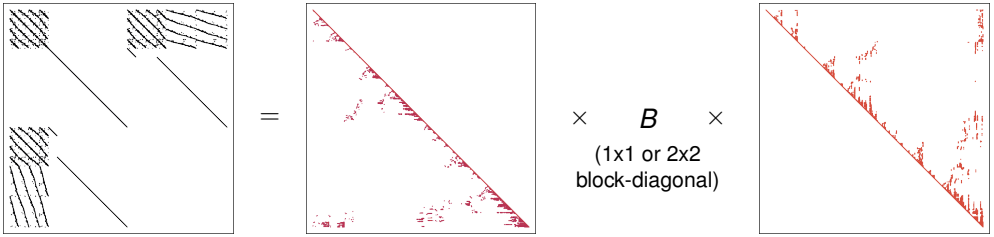


- Achieving numerical stability necessitates **numerical pivoting**, a process that is notoriously **challenging to parallelize**.

Why it is Challenging: Sparse Linear Solvers

- Solving KKT systems on CPUs has traditionally relied on **direct LBL$^\top$ factorization**.



- Achieving numerical stability necessitates **numerical pivoting**, a process that is notoriously **challenging to parallelize**.
- Due to the ill-conditioning of the KKT system, **iterative methods** are generally impractical, although there have been some promising results with **specialized preconditioners**.

Curtis, Huber, Schenk, Waechter. *A note on the implementation of an interior-point algorithm for nonlinear optimization with inexact step computations.* MathProg. (2012)
Cao, Seth, Laird. *An augmented Lagrangian interior-point approach for large-scale NLP problems on graphics processing units.* CACE. (2016)
Gondzio, Matrix-free interior point method, Comput Optim Appl (2012)

Solution #1: Condensed-Space Interior Point Method

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$$\begin{bmatrix} W^{(\ell)} + \delta_w^{(\ell)} I & & A^{(\ell)\top} & -I & I & & & \\ & \delta_w^{(\ell)} I & -I & & & -I & I & \\ A^{(\ell)} & -I & -\delta_c^{(\ell)} I & & & & & \\ Z_x^{(\ell)\flat} & & & X^{(\ell)} - X^\flat & & & & \\ -Z_x^{(\ell)\sharp} & & & & X^\sharp - X^{(\ell)} & & & \\ & Z_s^{(\ell)\flat} & & & & S^{(\ell)} - S^\flat & & \\ & -Z_s^{(\ell)\sharp} & & & & & S^\sharp - S^{(\ell)} & \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta s \\ \Delta y \\ \Delta z_x^\flat \\ \Delta z_x^\sharp \\ \Delta z_s^\flat \\ \Delta z_s^\sharp \end{bmatrix} = \begin{bmatrix} p_x^{(\ell)} \\ p_s^{(\ell)} \\ p_y^{(\ell)} \\ p_{z_x^\flat}^{(\ell)} \\ p_{z_x^\sharp}^{(\ell)} \\ p_{z_s^\flat}^{(\ell)} \\ p_{z_s^\sharp}^{(\ell)} \end{bmatrix}$$

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- These systems can be solved **without numerical pivoting** (routines available in CUDA).

Solution #2: Reduction & Dense Reformulation

- Oftentimes, the decision variables can be **splitted into state** and **control variables**.

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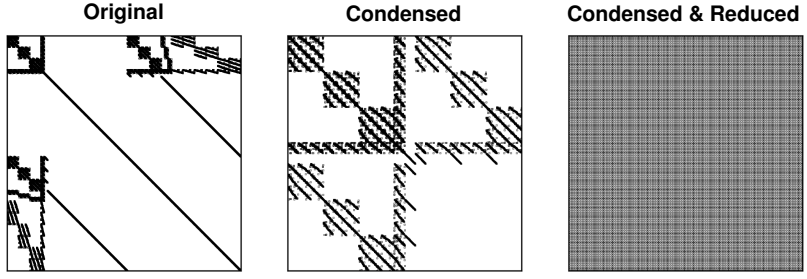

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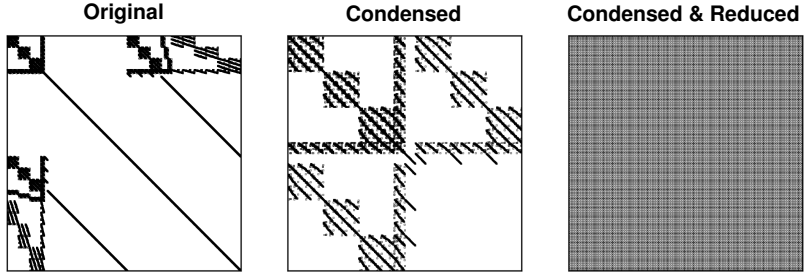

- **The elimination is a bottleneck**, but can be accelerated by exploiting structures (e.g., Riccati recursion for optimal control).

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Highlight: AC Optimal Power Flow (single GPU)

- Standard form polar form AC optimal power flow (AC OPF) problems.
- The condensed-space interior point method is employed.
- Solved up to 10^{-4} precision (note that by default, Ipopt solves up to 10^{-8} precision).

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Case	# vars	# cons	**MadNLP+ExaModels+cuSOLVER (GPU*)**			**Ipopt+AMPL+Ma27 (CPU**)**		
			# iter	AD†	total†	# iter	AD†	total†
10480_goc	96.8k	150.9k	70	0.13	14.26	64	16.93	38.04
13659_pegase	117.4k	170.6k	63	0.12	7.15	64	19.70	35.66
19402_goc	179.6k	281.7k	79	0.17	23.28	70	36.50	95.34
24464_goc	203.4k	313.6k	63	0.11	70.63	58	33.50	70.15
30000_goc	208.6k	307.8k	162	0.33	22.05	180	101.98	249.81

AD = Automatic Differentiation

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- Automatic differentiation is $\times 300$ faster, and the rest of computation is $\times 8$ faster.

Highlight: Security-Constrained AC OPF (multi GPU)

- Standard security-constrained AC optimal power flow (SC AC OPF) problems.
- The **reduction & dense formulation** and the **classical Schur-complement method for block-structured problems** are employed.

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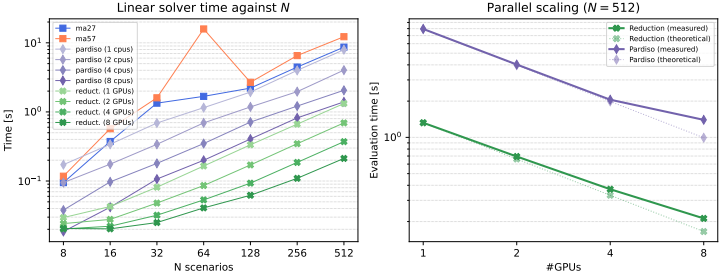
- Leveraging **multiple GPUs** allows us to **overcome the limitations** of a single GPU.

	1354pegase				**2869pegase**				**9241pegase**			
	# iter	AD	LA	total	# iter	AD	LA	total	# iter	AD	LA	total
CPU*	44	2.6	4.2	7.0	77	11.9	27.4	40.3	136	205.6	771.8	984.1
1 GPU**	44	0.3	1.8	2.1	93	1.1	11.7	12.8	98	5.5	112.3	117.8
2 GPUs**	44	0.3	1.1	1.4	93	0.8	7.4	8.2	98	3.4	56.8	60.2
4 GPUs**	44	0.3	1.0	1.3	93	0.8	5.7	6.5	98	2.3	35.8	38.1
8 GPUs**	44	0.2	1.0	1.2	93	0.6	5.1	5.7	98	1.4	26.4	27.7
# vars	20k				42k				139k			
# cons	53k				119k				404k			

AD = Automatic Differentiation, LA = Linear Algebra (KKT System Solver)
*AMD CPU Epyc "Milan" **NVIDIA A100 (4 GPUs per node)

Highlight: Security-Constrained AC OPF (multi GPU)

- Our approach is $\times 6$ faster than commercial multi-CPU solver.



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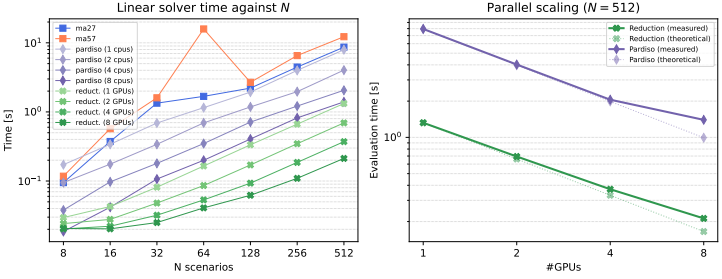
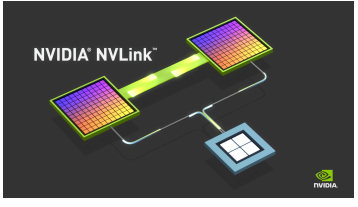


- Single-node, multi-GPU parallelism is more efficient than multi-node, multi-GPU.



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- Modern GPU hardware offers significant potential for accelerating large-scale optimization.
- Implementing algorithms on GPUs can be challenging and often **requires reevaluating key aspects of existing algorithms**.
- We have achieved promising results: up to **10x faster solutions with moderate accuracy**, though challenges remain for high-accuracy solutions.
- GPU-based optimization opens up opportunities to address previously intractable problems:
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Acknowledgement

U.S. Department of Energy, Office of Science, Advanced Scientific Computing Research (DE-AC02-06CH11347)

U.S. Department of Energy, Office of Science and National Nuclear Security Administration, Exascale Computing Porject (17-SC-20-SC)

[1] M. Anitescu, K. Kim, Y. Kim, A. Maldonado, F. Pacaud, V. Rao, M. Schanen, S. Shin, and A. Subramanian. Targeting Exascale with Julia on GPUs for multiperiod optimization with scenario constraints. *SIAG/OPT Views and News*, 2021.

[2] F. Pacaud, M. Schanen, S. Shin, D. A. Maldonado, and M. Anitescu. Parallel interior-point solver for block-structured nonlinear programs on SIMD/GPU architectures, 2023, arXiv:2301.04869. Under Review.

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[4] S. Shin, F. Pacaud, and M. Anitescu. Accelerating optimal power flow with GPUs: SIMD abstraction of nonlinear programs and condensed-space interior-point methods, arXiv:2307.16830. Under Review.

Nonlinear Optimization on Graphics Processing Units

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2023 AIChE Meeting, Orlando, Florida