Solving Large-Scale, Sparse, Constrained Nonlinear Optimization Problems on GPUs

Pivoting-Free Interior Point Methods

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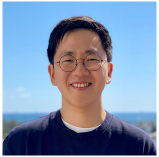
Who are we?

https://madsuite.org/

- Alexis Montoison @ Argonne National Lab
- François Pacaud @ MINES Paris-PSL (an ANL alumnus)
- Sungho Shin @ MIT (an ANL alumnus)
- Mihai Anitescu @ Argonne National Lab
- and friends... Michael Saunders, Dominic Orban, Armin Nurkanović, Anton Pozharskiy, Jean-Baptiste Caillau, ...

GPU-based optimization

- What is GPU? —many-core accelerator with high memory bandwidth
- Traditionally used for graphics, now widely used for ML/AI workloads
- Classical optimization (mathematical program; not ML training problems) has been thought to be unsuitable for GPUs
- Many state-of-the-art solvers (on CPUs) rely on sparse direct factorizations, which has been considered difficult to implement efficiently on GPUs
- This status quo is changing—the focus of this talk

GPU-based optimization: current landscape

- Factoriation-free methods have been the dominant approach
  - PDLP: Primal-dual first-order methods (Applegate et al., 2022; Lu et al., 2025)
  - PCG-based algorithms for convex QPs (Schubiger et al., 2020)
  - ALM + IPM + PCG for nonlinear problems (Cao et al., 2016)
- Factoriztion-free methods only rely on GPU-friendly kernels—`spmv`, `axpy`, `map`, `mapreduce`—makes them easy to implement on GPUs
- Scale to extremely large problems but achieving high precision is difficult
- Can we implement second-order methods with sparse direct solvers on GPUs?

David Applegate et al. (2022). *Practical Large-Scale Linear Programming Using Primal-Dual Hybrid Gradient*. arXiv: 2106.04756 [math]
Haihao Lu et al. (2025). *cuPDLP+: A Further Enhanced GPU-Based First-Order Solver for Linear Programming*. arXiv: 2507.14051 [math]
Michel Schubiger et al. (2020). "GPU Acceleration of ADMM for Large-Scale Quadratic Programming". In: *Journal of Parallel and Distributed Computing*
Yankai Cao et al. (2016). "An Augmented Lagrangian Interior-Point Approach for Large-Scale NLP Problems on Graphics Processing Units". In: *Computers & Chemical Engineering*

Our problem setting

Large-scale, sparse, constrained nonlinear programs

- We consider:

$$\min_{x^\flat \le x \le x^\sharp} f(x) \quad \text{s.t. } g^\flat \le g(x) \le g^\sharp,$$

  … but will particularly focus on:
  - $f : \mathbb{R}^n \to \mathbb{R}$ and $g : \mathbb{R}^n \to \mathbb{R}^m$ twice continuously differentiable
  - n and m are large (millions or more)
  - $\nabla g(x)$ and $\nabla^2_{xx} L(x, \lambda)$ are sparse (tens of nonzeros per row)—$L(\cdot, \cdot)$ is the Lagrangian
- Generally nonconvex—we only seek local solutions
- Most important instances (e.g., energy systems, optimal control) fall into this category
- Most existing solvers (e.g., Ipopt, KNITRO) are optimized for such problems

Our problem setting

Large-scale, sparse, constrained nonlinear programs

- WLOG (via $a = b \iff a \geq b,\ b \geq a$), we consider:

$$\min_{x \in \mathbb{R}^n} f(x) \quad \text{s.t. } g(x) \geq 0,$$

  ... but will particularly focus on:
  - $f : \mathbb{R}^n \to \mathbb{R}$ and $g : \mathbb{R}^n \to \mathbb{R}^m$ twice continuously differentiable
  - n and m are large (millions or more)
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NLP software stack—either on CPUs or GPUs

(1) algebraic modeling system, (2) NLP solver, and (3) sparse, direct linear solver

- Algebraic modeling systems (e.g., JuMP, AMPL, CasADi) generate callback functions—$f(\cdot)$, $g(\cdot)$, $\nabla f(\cdot)$, $\nabla g(\cdot)$, $\nabla^2_{xx} L(\cdot,\cdot)$—for NLP solvers
- NLP solvers (e.g., Ipopt, KNITRO) form KKT systems to find step direction:

$$\underbrace{\begin{bmatrix} \nabla^2_{xx} L(x,s,\lambda) + \delta_p I & & \nabla g(x)^\top \\ & S^{-1}\Lambda & -I \\ \nabla g(x) & -I & -\delta_d I \end{bmatrix}}_{\text{KKT matrix}} \underbrace{\begin{bmatrix} d_x \\ d_s \\ -d_\lambda \end{bmatrix}}_{\text{step direction}} = - \underbrace{\begin{bmatrix} \nabla f(x) - \nabla g(x)^\top \lambda \\ \Lambda e - \mu S^{-1} e \\ g(x) - s \end{bmatrix}}_{\text{residual to KKT conditions}},$$

  where s is the slack variable, $S = \mathrm{diag}(s)$, $\Lambda = \mathrm{diag}(\lambda)$, and $\delta_p, \delta_d \geq 0$ are primal-dual regularization parameters
- Sparse, direct linear solvers (e.g., MA27, PARDISO) factorize and solve KKT systems; iterative method is typically not an option due to ill-conditioning

Full NLP software stack on GPU—is it possible?

(1) algebraic modeling system, (2) NLP solver, and (3) sparse, direct linear solver

- Partially porting on GPU (e.g., AD or linear algebra only) is not sufficient—will be bottlenecked by CPU–GPU communication. We need all three components on GPU
- Porting algebraic modeling system is relatively straightforward. ExaModels.jl provides GPU-compatible modeling capabilities (Shin et al., 2024)—not the focus today
- Porting direct linear solver is more non-trivial; as of now, there is no drop-in replacement of MA27 on GPUs

Our approach

Adapt interior-point method for NLPs so that it can work with GPU direct linear solvers with (relatively) limited capabilities

Sungho Shin et al. (2024). "Accelerating Optimal Power Flow with GPUs: SIMD Abstraction of Nonlinear Programs and Condensed-Space Interior-Point Methods". In: *Electric Power Systems Research*

Sparse direct solvers within interior-point methods

LBL$^\top$ factorization

$$\begin{bmatrix} \nabla^2_{xx} L(x,s,\lambda) + \delta_p I & & \nabla g(x)^\top \\ & S^{-1}\Lambda & -I \\ \nabla g(x) & -I & -\delta_d I \end{bmatrix} = P \times Q \times L \times B \times L^\top \times Q^\top \times P^\top$$

- P: Fill-in-reducing (and parallel-friendly) re-ordering (re-used across IPM iterations)
- Q: Pivoting (computed on-the-fly during factorization)
- $LBL^\top$: Factorization of permuted matrix
- Additionally, pivots may be perturbed, which must be corrected via iterative refinement
- Factorization reveals inertia—number of $+$, 0, and $-$ eigenvalues; primal-dual regularization (δ_p, δ_d) is adjusted to achieve correct inertia (Wächter et al., 2006); this can be merged with pivot perturbation (Nocedal et al., 2006)

Andreas Wächter et al. (2006). "On the Implementation of an Interior-Point Filter Line-Search Algorithm for Large-Scale Nonlinear Programming". In: *Mathematical Programming*

Jorge Nocedal et al. (2006). *Numerical Optimization*. 2nd ed. Springer Series in Operations Research. New York: Springer

Pivoting-free IPM

Montoison, Pacaud, Shin, et al., 2025

- Numerical pivoting is difficult to implement on GPUs (Świrydowicz et al., 2022) because row swapping can potentially destroy parallelism
- Existing GPU solvers (e.g., cuDSS) don't have adequately robust pivoting strategies; currently only have partial pivoting and pivot perturbation (NVIDIA, 2024)
- Factorization may fail without numerical pivoting, unless
  - Symmetric quasi-definite (SQD): factorization exists (Vanderbei, 1995)
  - Symmetric positive definite (SPD): factorization exists and numerically stable

  However, KKT systems for NLPs are generally indefinite
- When pivoting is not required, GPU sparse direct solvers can be very efficient

Can we make IPM pivoting-free?

Alexis Montoison, François Pacaud, Sungho Shin, et al. (2025). *GPU Implementation of Second-Order Linear and Nonlinear Programming Solvers*. arXiv: 2508.16094 [math]
Robert J. Vanderbei (1995). "Symmetric Quasidefinite Matrices". In: *SIAM Journal on Optimization*
Kasia Świrydowicz et al. (2022). "Linear Solvers for Power Grid Optimization Problems: A Review of GPU-accelerated Linear Solvers". In: *Parallel Computing*
NVIDIA (2024). *NVIDIA cuDSS (Preview): A High-Performance CUDA Library for Direct Sparse Solvers — NVIDIA cuDSS Documentation*. https://docs.nvidia.com/cuda/cudss/index.html

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(For now) can we reformulate KKT systems to be SPD or SQD?

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Option 1: Lifted KKT system

Shin et al., 2024

- First, relax equalities by small enough τ (the same as solver tolerances):

$$-\tau \leq h(x) \leq \tau$$

- Condense the KKT system by eliminating slack/dual variables:

$$\begin{bmatrix} \nabla^2_{xx} L(x,s,\lambda) + \delta_p I & & \nabla g(x)^\top \\ & S^{-1}\Lambda & -I \\ \nabla g(x) & -I & -\delta_d I \end{bmatrix} \begin{bmatrix} d_x \\ d_s \\ -d_\lambda \end{bmatrix} = - \begin{bmatrix} \nabla f(x) - \nabla g(x)^\top \lambda \\ \Lambda e - \mu S^{-1} e \\ g(x) - s \end{bmatrix}$$

$$\iff \Big(\underbrace{\nabla^2_{xx} L(x,s,\lambda) + \delta_p I + \nabla g(x)^\top (\delta_d I + \Lambda^{-1} S)^{-1} \nabla g(x)}_{\text{SPD iff the original system has correct inertia}} \Big) d_x = -r_p$$

(and some easy-to-solve equations)

- Enables numerically stable factorization without pivoting or excessive regularization

Sungho Shin et al. (2024). "Accelerating Optimal Power Flow with GPUs: SIMD Abstraction of Nonlinear Programs and Condensed-Space Interior-Point Methods". In: *Electric Power Systems Research*

Option 1: Lifted KKT—numerical results (AC OPF)

Montoison, Pacaud, Shin, et al., 2025

	Tol	Solver	Small $\text{nnz} < 2^{18}$		Medium $2^{18} \leq \text{nnz} < 2^{20}$		Large $2^{20} \leq \text{nnz}$		Total	
			Solved	Time	Solved	Time	Solved	Time	Solved	Time
OPF	10^{-4}	MadNLP (GPU)	**31**	0.4166	**24**	**2.6380**	**11**	**3.7040**	**66**	**1.6979**
		Ipopt (CPU)	**31**	0.3970	**24**	5.0697	11	38.5053	**66**	5.3817
	10^{-8}	MadNLP (GPU)	30	2.5037	**24**	**4.6016**	10	**12.8040**	64	**4.6228**
		Ipopt (CPU)	**31**	0.5100	**24**	5.4292	11	37.7818	**66**	5.5541

- Benchamrk set: AC optimal power flow (Babaeinejadsarookolaee et al., 2021)
- Hardware: NVIDIA GV 100 GPU / Intel Xeon Gold 6130 CPU
- Time: reported as SGM10:= $\prod_{i=1}^{n}(t_i + 10))^{1/n} - 10$, max wall time 900s

Observation

GPU solver is most effective for large-scale problems for moderate accuracy (10^{-4})

Alexis Montoison, François Pacaud, Sungho Shin, et al. (2025). *GPU Implementation of Second-Order Linear and Nonlinear Programming Solvers*. arXiv: 2508.16094 [math]

Sogol Babaeinejadsarookolaee et al. (2021). *The Power Grid Library for Benchmarking AC Optimal Power Flow Algorithms*. arXiv: 1908.02788 [math]

Option 1: Lifted KKT—numerical results (COPS)

Montoison, Pacaud, Shin, et al., 2025

	Tol	Solver	Small $\text{nnz} < 2^{18}$ Solved	Time	Medium $2^{18} \leq \text{nnz} < 2^{20}$ Solved	Time	Large $2^{20} \leq \text{nnz}$ Solved	Time	Total Solved	Time
COPS	10^{-4}	MadNLP (GPU)	**13**	**0.8665**	**15**	**4.8665**	**16**	**3.8194**	**44**	**3.2314**
		Ipopt (CPU)	**13**	5.2315	**15**	15.9701	15	45.8411	43	19.2243
	10^{-8}	MadNLP (GPU)	**13**	**0.8575**	**16**	**1.5572**	**16**	**8.3549**	**45**	**3.3797**
		Ipopt (CPU)	**13**	5.9413	**15**	17.6758	15	40.8639	43	19.2999

- Benchamrk set: COPS Benchmark (Dolan et al., 2001)
- Hardware: NVIDIA GV 100 GPU / Intel Xeon Gold 6130 CPU
- Time: reported as SGM10:$= \prod_{i=1}^{n}(t_i + 10))^{1/n} - 10$, max wall time 900s

Observation

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Option 2: Hybrid KKT system

Golub et al., 2003; Pacaud et al., 2024; Regev et al., 2023

- We keep the equality constraints $h(x) = 0$ and eliminate the inequalities (slack/dual):

$$\begin{bmatrix} K_{\text{cond}} + \delta_p I & \nabla h(x)^\top \\ \nabla h(x) & -\delta_d I \end{bmatrix} \begin{bmatrix} d_x \\ -d_\lambda \end{bmatrix} = - \begin{bmatrix} r_x \\ r_\lambda \end{bmatrix}$$

$$\xrightarrow[\text{(w/o changing solution)}]{\text{Regularization}} \begin{bmatrix} K_{\text{cond}} + \delta_p I + \rho \nabla h(x)^\top \nabla h(x) & \nabla h(x)^\top \\ \nabla h(x) & -\delta_d I \end{bmatrix} \begin{bmatrix} d_x \\ -d_\lambda \end{bmatrix} = - \begin{bmatrix} r'_x \\ r_\lambda \end{bmatrix}$$

Then, the Schur complement can be solved with an iterative method (e.g., CG)

$$\Bigg(\underbrace{\nabla h(x)^\top \Big(\overbrace{K_{\text{cond}} + \delta_p I + \rho \nabla h(x)^\top \nabla h(x)}^{\text{SPD for sufficiently large } \rho \text{ iff correct inertia}} \Big)^{-1} \nabla h(x)}_{\text{converges to } I \text{ as } \rho \to \infty} + \delta_d I \Bigg) d_\lambda = r'_\lambda$$

Gene H. Golub et al. (2003). "On Solving Block-Structured Indefinite Linear Systems". In: *SIAM Journal on Scientific Computing*

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Options 3, 4, 5, ...

- There can be lots of other ways to implement pivoting-free solvers
- MadIPM: Solver for convex quadratic programs; uses regularization to avoid pivoting (Montoison, Pacaud, Shin, et al., 2025)
- MadNCL: ALM-based algorithm—ALM is more GPU-friendly due to the quadratic penalty term. Uses nonlinearly-constrained Lagrangian (NCL) formulation and applies condensation techniques (Montoison, Pacaud, Saunders, et al., 2025)
- Directly solving augmented systems without pivoting? —currently under investigation

Concluding remarks

- It is an exciting time to develop optimization solvers!
- Existing GPU solvers have focused on factorization-free (e.g. first-order) methods, but

$$\text{GPU optimization solver} \supsetneq \text{Factorization-free solver.}$$

- With GPU direct solvers, second-order methods on GPUs has now become possible
- To harness these GPU direct solvers, we need pivoting-free algorithms
- We presented Lifted KKT and Hybrid KKT, but there can be many others

Check out our project page!

https://madsuite.org/

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