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

Pivoting-Free Interior-Point Methods

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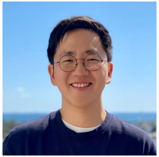
Who are we?

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

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- Many state-of-the-art solvers on CPUs rely on sparse direct factorizations, which are viewed as difficult to implement efficiently on GPUs
- This status quo is changing—the focus of this talk

GPU-based optimization: current landscape

- Factorization-free methods have been the dominant approach:
  - PDLP: first-order method for LPs (Applegate et al., 2022; Lu et al., 2025)
  - PCG within ADMM for convex QPs (Schubiger et al., 2020)
  - ALM + IPM + PCG for nonlinear problems (Cao et al., 2016)

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Can we implement solvers based on second-order methods and direct linear algebra on GPUs?

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Our problem setting

Large-scale, sparse, constrained nonlinear programs

- We consider:

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

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- Most important instances (e.g., energy systems, optimal control) fall into this category

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

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- 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 slack; $S = \mathrm{diag}(s)$; $\Lambda = \mathrm{diag}(\lambda)$; and $\delta_p, \delta_d \geq 0$ are regularization parameters

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  where s is slack; $S = \mathrm{diag}(s)$; $\Lambda = \mathrm{diag}(\lambda)$; and $\delta_p, \delta_d \geq 0$ are 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

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

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Our approach

Adapt interior-point method (IPM) for NLPs so that it can utilize GPU direct linear solvers

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Linear algebra within IPM (on CPUs)

Sparse LBL$^\top$ factorization (Duff et al., 1983)

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Numerical pivoting on GPU is challenging

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- Linear solver relies on pivot perturbation $\Rightarrow$ poor factorization accuracy $\Rightarrow$ iterative refinement failure $\Rightarrow$ forced primal-dual regularization $\Rightarrow$ slow convergence or failure

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Pivoting-free IPM

Montoison, Pacaud, Shin, et al., 2025

- KKT systemes can be factorized without numerical pivoting if
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(For now) can we reformulate KKT systems to be SPD or SQD?

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Option 1: Lifted KKT method

Shin et al., 2024

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

$$h(x) = 0 \quad \Longrightarrow \quad h(x) + s = 0 \quad \text{and} \quad -\tau \leq s \leq \tau$$

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

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

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

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

- Enables numerically stable factorization without pivoting or excessive regularization

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

Option 1: Lifted KKT method—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
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

- Benchmark set: AC optimal power flow (Babaeinejadsarookolaee et al., 2021)
- Hardware: NVIDIA GV100 GPU / Intel Xeon Gold 6130 CPU
- Time: reported as SGM10:$= \prod_{i=1}^{n}(t_i + 10))^{1/n} - 10$ with max wall time 900s

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Observation

GPU solver is most effective for large instances solved up to moderate accuracy (10^{-4})

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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
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

- Benchmark set: COPS Benchmark (Dolan et al., 2001)
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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):

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

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

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

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

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Options 3, 4, 5, ...

- There can be lots of other ways to implement pivoting-free solvers

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Montoison, Pacaud, Saunders, et al. (2025). *MadNCL: A GPU Implementation of Algorithm NCL for Large-Scale, Degenerate Nonlinear Programs*. arXiv: 2510.05885 [math]

Options 3, 4, 5, ...

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- 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)

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- MadIPM: Solver for convex quadratic programs; uses regularization to avoid pivoting (Montoison, Pacaud, Shin, et al., 2025)
- Directly solving augmented systems without pivoting? —currently under investigation

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Concluding remarks

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- Existing GPU solvers have focused on factorization-free (e.g. first-order) methods, but

$$\text{GPU optimization solvers} \supsetneq \text{Factorization-free solvers}$$

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$$\begin{aligned}\text{GPU optimization solvers} &\supsetneq \text{Factorization-free solvers}\\ &\supset \text{Factorization-baesd, but pivoting-free solvers}\end{aligned}$$

- We presented Lifted KKT and Hybrid KKT, but there can be many others

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