GPU-accelerated optimal control

A nonlinear programming point-of-view

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Who are we?

https://madsuite.org/









- Alexis Montoison @ ANL
- Sungho Shin @ MIT
- Mihai Anitescu @ ANL

Outline: today we talk about GPU-accelerated optimal control

We leverage the GPU-accelerated optimization solver MadNLP to solve large-scale optimal control on the GPU

Motivation for today's lecture

New generation of optimization solvers is under way



Figure: Go check Sungho's talk at ScaleOpt!

■ Massive investments in robotics

Nvidia Bets Big on Robots

The chipmaker, which has led a rally in artificial intelligence stocks, laid out a vision for dominating so-called physical A.I. Investors appeared impressed.







By Andrew Ross Sorkin, Ravi Mattu, Bernhard Warner, Sarah Kessler, Michael J. de la Merced and Lauren Hirsch Jan. 7, 2025



Figure: NVIDIA Jetson

Outline

What am I talking about when talking about optimal control?

Primal-dual interior-point method

How to solve the Newton systems on the GPU?

Using MadNLP and ExaModels on the GPU

Applications of optimal control

Finding optimal trajectory in problems with a dynamic structure

- Trajectory planning
- Real-time optimization with model predictive control (MPC)

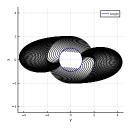


Figure: Trajectory flow for moving a satellite locally close to its orbit

A mature ecosystem already exists!

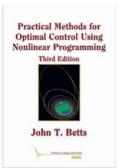
Classical workflow:

- Modeling with casadi
- Solving with Ipopt (or any structure exploiting solver)

Useful references









Disclaimer: We write everything in discrete time

At discrete time k, the *state* of the system is encoded in a vector $x_k \in \mathbb{R}^{n_x}$. After applying a *control* $u_k \in \mathbb{R}^{n_u}$, the system evolves between k and k+1 as

$$x_{k+1} = g_k(x_k, u_k)$$

Most of the time, the dynamics $g_k(\cdot)$ discretizes an ordinary differential equations (e.g. using collocation)

The system is subject to the operational constraints:

$$h_k(x_k,u_k)\leq 0$$

Optimal control problem

Starting from $\underline{x} \in \mathbb{R}^{n_x}$, we minimize the functional $\ell_k(\cdot)$ over an horizon N:

$$\min_{x,u} \sum_{k=0}^{N-1} \ell_k(x_k, u_k) + \ell_N(x_N)$$
s.t. $x_{k+1} = g_k(x_k, u_k)$, $x_0 = \underline{x}$

$$h_k(x_k, u_k) \le 0$$

Let
$$x := (x_0, \dots, x_N)$$
 and $u := (u_0, \dots, u_{N-1})$.

Introducing the nonlinear program

Many degrees-of-freedom approach

For w := (x, u), we abstract the previous dynamic program as:

$$\min_{w} f(w)$$
s.t. $g(w) = 0$, $h(w) \le 0$. (NLP)

Nonlinear programming

- Problem is nonlinear nonconvex:
 we are interested in finding only a local optimum solution
- Solvable using classical nonlinear solvers:
 - IPM (Ipopt, Knitro, MadNLP)
 - SQP (FilterSQP, SNOPT)
 - Augmented-Lagrangian (LANCELOT, Algencan)

Karush-Kuhn-Tucker (KKT) conditions

Using a slack variable $s \ge 0$, NLP is equivalent to

$$\min_{w,s} f(w)$$
s.t. $g(w) = 0$, $h(w) + s = 0$ (NLP)
$$s \ge 0$$

We introduce the Lagrangian:

$$\mathcal{L}(w, y, z) = f(w) + y^{\top}g(w) + z^{\top}h(w).$$

KKT stationary equations

If w is a regular local solution, then there exist dual multipliers (y, z) satisfying

$$\begin{cases} \nabla f(w) + \nabla g(w)^{\top} y + \nabla h(w)^{\top} z = 0 \\ g(w) = 0 \\ h(w) + s = 0 \\ 0 \le s \perp z \ge 0 \end{cases}$$
Complementarity conditions

 \blacksquare Solving the NLP is equivalent to the solution of a system of *nonsmooth* nonlinear equations

Regularity conditions: first-order

Denote the active set $A(w) = \{i \in [m] \mid h_i(w) = 0\}$ and the active Jacobian

$$J(w) = \begin{bmatrix} \nabla g(w) \\ \nabla h_{\mathcal{A}}(w) \end{bmatrix}$$

First-order constraint qualification

We say that the point w is *qualified* is the local geometry of the feasible can be captured by a *linearized* model near w

(in math language, the tangent cone is equal to the set of linearized feasible directions)

- The Linear Independence Constraint Qualification (LICQ) holds if the active Jacobian J(w) is full row-rank
- The Mangasarian-Fromovitz Constraint Qualification (MFCQ) holds if (y, z) = (0, 0) is the unique solution to the linear system

$$\begin{cases} \nabla g(w)^\top y + \nabla h(w)^\top z = 0 \\ z_i \ge 0 & \forall i \in \mathcal{A}(w) \end{cases}$$

Gauvin's theorem (1979)

MFCQ holds if and only if the set of multipliers (y, z) satisfying KKT is bounded

Regularity conditions: second-order

Let (w, y, z) a primal-dual point satisfying KKT. We define the *critical cone*:

$$\begin{split} \mathcal{C}(w,y,z) &= \{ d \in \mathbb{R}^n \mid \nabla g_i(w)^\top d = 0 \;,\; i \in [m_e] \;, \\ \nabla h_i(w)^\top d &= 0 \;,\; i \in \mathcal{A}(w) \; \text{with} \; z_i > 0 \;, \\ \nabla h_i(w)^\top d &\leq 0 \;,\; i \in \mathcal{A}(w) \; \text{with} \; z_i = 0 \} \;. \end{split}$$

Strict complementarity (SC) holds if $z_i > 0$ for all $i \in A(w)$.

Second-order sufficient condition (SOSC)

We say that (w, y, z) satisfies SOSC if

$$d^\top \nabla^2_{ww} \mathcal{L}(w,y,z) d > 0 \quad \forall d \in \mathcal{C}(w,y,z) \setminus \{0\}$$

Under SOSC, the problem is locally convex near w and the solution is isolated

Proposition

Suppose LICQ and SC hold. Then SOSC holds if and only if

$$Z^\top \nabla^2_{ww} \mathcal{L}(w,y,z) Z \succ 0$$

with Z a basis of the null-space of the active Jacobian J(w).

Are optimal control problems regular?

Well... it depends

State constraints

- Pure state constraints: $h_k(x_k) \leq 0$
- Mixed state constraints: $h_k(x_k, u_k) \leq 0$
- Problems with active state constraints do not satisfy LICQ (not enough degrees of freedom)
- Problems with *singular arcs* do not satisfy SOSC Example: Goddard rocket's problem

Observation

Oftentimes, nonlinear solvers are struggling to solve optimal control instances

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Interior-point method (IPM)

Rewrite the (nonsmooth) KKT system as a smooth nonlinear system

Dual variables
$$F_{\mu}(x,s; \mathbf{y}, \mathbf{z}) := \begin{bmatrix} \nabla f(x) + \nabla g(x)^{\top} \mathbf{y} + \nabla h(x)^{\top} \mathbf{z} \\ g(x) \\ h(x) + s \\ S\nu - \mu e \\ \uparrow \text{ Homotopy, } S = \text{diag}(s) \end{bmatrix} = 0$$

Primal-dual interior-point method

Solve $F_{\mu}(x,s;y,z,
u)=0$ using Newton method while driving $\mu o 0$.

Augmented KKT system

The Newton algorithm translates to the solution of a sequence of linear systems

Denote the primal-dual variable by $v^k := (w^k, s^k, y^k, z^k)$. At iteration k,

1. Compute Newton step d^k as solution of the linear system

$$\nabla F_{\mu}(v^k) d^k = -F_{\mu}(v^k)$$

 $v^{k+1} = v^k + \alpha^k d^k$

2. Update the as

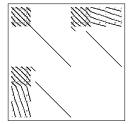


Figure: ∇F_{μ}

Augmented KKT system

After (slight) reformulation, the Newton step writes as

$$\begin{bmatrix} W & 0 & \nabla g^{\top} & \nabla h^{\top} \\ 0 & \Sigma_s & 0 & I \\ \nabla g & 0 & 0 & 0 \\ \nabla h & I & 0 & 0 \end{bmatrix} \begin{bmatrix} d_w \\ d_s \\ d_y \\ d_z \end{bmatrix} = - \begin{bmatrix} r_1 \\ r_2 \\ r_3 \\ r_4 \end{bmatrix}$$

with
$$W = \nabla_{xx}^2 L(\cdot)$$
, $\Sigma_s = S^{-1} \text{diag}(z)$

This is the system solved by default in Ipopt

Generic case: sparse linear solver for nonlinear programming

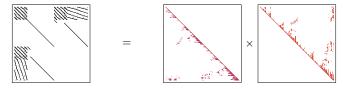


Figure: Matrix factorization using a direct solver

Direct method for sparse indefinite linear systems

- Ill-conditioning of the KKT system
 (= iterative solvers are often not practical)
- Direct solver requires numerical pivoting for stability (= difficult to parallelize)

Computing sparse factorizations

Duff-Reid factorization

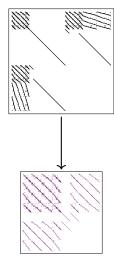
$$A = PQ LBL^{\top} Q^{\top} P^{\top}$$

with

- P: fill-in minimization matrix
- Q: additional pivoting for numerical stability
- L: unit lower-triangular matrix
- B: block diagonal matrix with blocks of dimension 1×1 or 2×2
- The LBL factorization has become competitive only in the 1990s, using a technique known as matching-based preprocessing
- The progress in sparse linear solvers has directly benefited to nonlinear optimization solvers such as Ipopt or Knitro
- \square Numerical pivoting Q impairs the parallelism in the algorithm

Condensed KKT system

We condense the linear system by removing the inequality blocks



Condensed KKT system

The augmented KKT system condenses to

$$\begin{bmatrix} \kappa & \nabla g^{\top} \\ \nabla g & 0 \end{bmatrix} \begin{bmatrix} d_w \\ d_y \end{bmatrix} = - \begin{bmatrix} r_1 + (\nabla h)^{\top} (\Sigma_s r_4 + r_2) \\ r_3 \end{bmatrix}$$

with the condensed matrix $K = W + \nabla h^{\top} \Sigma_s \nabla h$. We recover (d_s, d_z) as

$$\label{eq:ds} \textit{d}_{s} = -\Sigma_{s}^{-1}(\textit{r}_{3} + \textit{d}_{y}) \; , \quad \textit{d}_{z} = \Sigma_{s} \left(\nabla \textit{h} \, \textit{d}_{x} - \textit{r}_{4} \right) - \textit{r}_{2} \; .$$

- Additional fill-in
- Useful when large number of inequality constraints m

Writing the control as a feedback on the state

Proposition

For K positive definite, the solution of the saddle-point linear system

$$\begin{bmatrix} K & G^{\top} \\ G & 0 \end{bmatrix} \begin{bmatrix} w \\ y \end{bmatrix} = \begin{bmatrix} -c \\ b \end{bmatrix}$$

is the primal-dual solution of the convex QP

$$\min_{w} \frac{1}{2} w^{\top} K w + c^{\top} w \quad \text{s.t.} \quad G w = b$$

For problem with a dynamic structure, the condensed KKT system yields the LQR

$$\min_{d_{x},d_{u}} \sum_{k=0}^{N-1} \begin{bmatrix} d_{x,k} \end{bmatrix}^{\top} \begin{bmatrix} K_{xx}^{k} & K_{xu}^{k} \\ K_{ux}^{k} & K_{uu}^{k} \end{bmatrix} \begin{bmatrix} d_{x,k} \\ d_{u,k} \end{bmatrix} + \begin{bmatrix} r_{x,k} \end{bmatrix}^{\top} \begin{bmatrix} d_{x,k} \\ d_{u,k} \end{bmatrix}$$
s.t.
$$d_{x,k+1} = G_{x,k} d_{x,k} + G_{u,k} d_{u,k}$$

- No need to use a sparse linear solver
- Efficient solution with (backward) Riccati recursions
- Require convexification in nonlinear programming

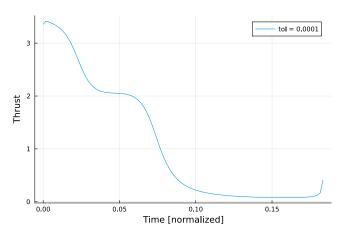


Figure: Optimal solution of the Goddard rocket problem with $\mathit{nh} = 100$

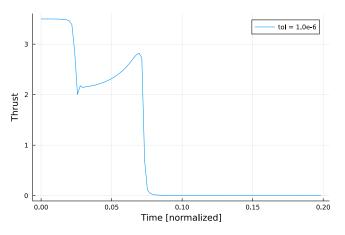


Figure: Optimal solution of the Goddard rocket problem with $\mathit{nh} = 100$

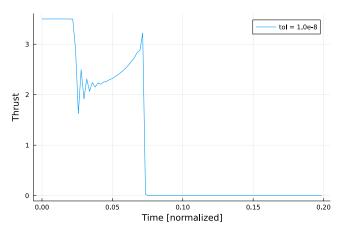


Figure: Optimal solution of the Goddard rocket problem with $\mathit{nh} = 100$

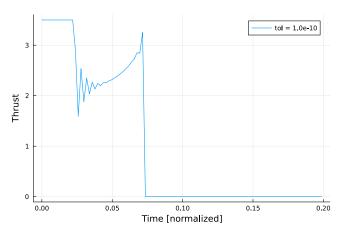


Figure: Optimal solution of the Goddard rocket problem with $\mathit{nh} = 100$

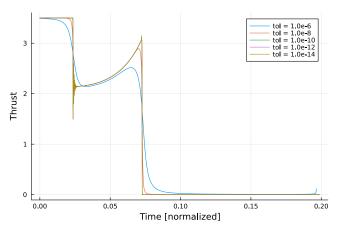


Figure: Optimal solution of the Goddard rocket problem with nh = 1000

Outline

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How to solve the Newton systems on the GPU?

Using MadNLP and ExaModels on the GPU

Why is it challenging?

Current status

- Implementing a sparse linear solver on the GPU is highly non-trivial
- Before the release of NVIDIA cuDSS, there was no efficient sparse linear solver available on the GPU
- Solving the KKT systems in IPM with an iterative solver remains an open research question

Two solution methods for GPU-accelerated optimization method:

- 1. Rewrite the KKT system as a dense matrix;
- 2. Use a pivoting-free factorization (at the price of sacrificing slightly the accuracy).

Few degrees of freedom

Proposition

Suppose the Jacobian ∇g is full rank. Let Z be a matrix whose columns encode a basis of the Jacobian null-space ((∇g)Z=0). Then the condensed KKT system is equivalent to

$$Z^{\top}KZd_{u}=\overline{r}_{red}$$

Oftentimes, the matrix $Z^{\top}KZ$ is dense.

Example of null space for optimal control:

$$\nabla g = \begin{bmatrix} G_x & G_u \end{bmatrix} \implies Z = \begin{bmatrix} -G_x^{-1} G_u \\ I \end{bmatrix}$$

Works best if number of control is small (e.g. PDE constrained optimization)!

How to avoid numerical pivoting?

Reformulate the KKT system either as

a positive definite (PD) system

$$A \succ 0$$

a symmetric quasidefinite (SQD) system

$$\begin{bmatrix} A & B^{\top} \\ B & -C \end{bmatrix} \quad \text{with} \quad A \succ 0 \; , \; C \succ 0$$

In both cases, the sparse system can be factorized using only *static pivoting*, e.g. using a signed Cholesky factorization

$$A = PLDL^{\top}P^{\top}$$

with P static pivoting, L lower triangular, D diagonal matrix.

How to avoid numerical pivoting in nonlinear programming?

Objective

How to avoid numerical pivoting in the algorithm?

We look again at the condensed KKT system (sparse symmetric indefinite):

$$\begin{bmatrix} \kappa & \nabla g^{\top} \\ \nabla g & 0 \end{bmatrix} \begin{bmatrix} d_w \\ d_y \end{bmatrix} = - \begin{bmatrix} r_1 \\ r_2 \end{bmatrix}$$

with the condensed matrix $K = W + \nabla h^{\top} \Sigma_s \nabla h$.

- Three strategies to avoid numerical pivoting:
 - 1. LiftedKKT
 - 2. HyKKT
 - 3. NCL (Augmented Lagrangian)

Strategy 1: LiftedKKT

Idea: equality relaxation

For a $\tau > 0$ small enough, solve the relaxed problem

$$\min_{w \in \mathbb{R}^n} f(w) \quad \text{s.t.} \quad \begin{cases} -\tau \le g(w) \le \tau \\ h(w) \le 0 \end{cases}$$

Reformulating the problem with slack variables:

$$\min_{w \in \mathbb{R}^n, s \in \mathbb{R}^m} f(w)$$
 subject to $h^{ au}(w) + s = 0 \; , \; s \geq 0$

with
$$h^{\tau}(w) = (g(w) - \tau, -g(w) - \tau, h(w))$$

Condensed KKT system

The augmented KKT system is equivalent to

$$K_{\tau}$$
 $d_w = -r_1 + (\nabla h^{\tau})^{\top} (\Sigma_s r_4 + r_2)$

with the condensed matrix $K_{\tau} = W + (\nabla h^{\tau})^{\top} \Sigma_{s} (\nabla h^{\tau})$.

 \rightarrow the condensed KKT system can be solved without numerical pivoting!

S. Shin, F. Pacaud, and M. Anitescu. Accelerating optimal power flow with GPUs: SIMD abstraction of nonlinear programs and condensed-space interior-point me

Strategy 2: HyKKT (aka Golub & Greif method)

Idea: augmented Lagrangian reformulation

For $\gamma >$ 0, the condensed KKT system is equivalent to

$$\begin{bmatrix} \kappa_{\gamma} & \nabla g^{\top} \\ \nabla g & 0 \end{bmatrix} \begin{bmatrix} d_{w} \\ d_{y} \end{bmatrix} = - \begin{bmatrix} r_{1} + \gamma \nabla g^{\top} r_{2} \\ r_{2} \end{bmatrix}$$

with
$$K_{\gamma} = K + \gamma \nabla g^{\top} \nabla g$$

$$(\nabla g) \ \mathcal{K}_{\gamma}^{-1} \ (\nabla g)^{\top} d_y = w_2 - \ \mathcal{K}_{\gamma}^{-1} \ (w_1 + \gamma \nabla g^{\top} w_2)$$

- abla Keep K_{γ}^{-1} implicit by solving the normal equations *iteratively* with a conjugate gradient (CG) algorithm!
- ∇ For large γ , CG converges in few iterations

Strategy 3: NCL

Augmented Lagrangian methods have always been popular in optimal control

At iteration k, the algorithm solves:

$$\begin{aligned} & \min_{w,r} f(w) - (y_k^e)^\top r + \frac{\rho_k}{2} \|r\|^2 \\ \text{subject to} & g(w) + r_g = 0 \ , \\ & h(w) + r_h \leq 0 \ , \end{aligned} \tag{NCL}_k)$$

with $r = (r_g, r_h)$ regularization variables

- Subproblem (NCL_k) is always feasible, solvable by IPM!
- ullet Only the objective changes between k and k+1
- Regularization r stabilizes internal IPM iterations

$\mathsf{NCL}\ \mathsf{algorithm} \equiv \mathsf{Auglag}\ \mathsf{algorithm}$

- Solve (NCL_k) down to a tolerance ω_k
- Update parameters as
 - If $||r_{k+1}|| \le \eta_k$, set $y_{k+1}^e = y_k^e \rho_k r_{k+1}$
 - Else $\rho_{k+1} = 10 \times \rho_k$.

Algorithm NCL is more robust, but converges in more iterations than IPM.

Strategy 3: Stabilized KKT system

Rockafellar: Augmented Lagrangian adds a natural dual regularization to the KKT system!

For the two diagonal matrices $C_g:=\frac{1}{\rho_k}I$ and $C_h:=\frac{1}{\rho_k}I+Z^{-1}S$, let

$$\begin{bmatrix} W & \nabla g^{\top} & \nabla h^{\top} \\ \nabla g & -C_g & 0 \\ \nabla h & 0 & -C_h \end{bmatrix} \begin{bmatrix} d_w \\ d_y \\ d_z \end{bmatrix} = - \begin{bmatrix} r_1 \\ r_2 \\ r_3 \end{bmatrix}$$
 (K_{2r})

Observation

NCL can compute its descent direction by solving K_{2r} .

- For a penalty ρ_k high-enough, there exists a LDL factorization for K_{2r}
- Otherwise, use a pivot regularization strategy inside LDL to return the factorization of a perturbed matrix
- Recover the original descent direction using iterative refinement

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GPU-accelerated optimization

New solvers are blossoming everywhere

Most solvers are specialized on convex problems:

First-order

cuPDLP and all affiliated variants
 OSQP
 cuHALLaR / cuLORADS
 (LP, QP)
 (QP)
 (Iow-rank SDP)

Second-order

- QPTH (dense QP)
- CuClarabel (conic)

MadSuite: an optimization software suite for GPUs	madsuite.org
• ExaModels	(NLP modeler)
MadNLP	(NLP)
MadNCL	(degenerate NLP)
MadIPM	(LP)

State-of-the-art solvers for optimal control

Support for GPU-accelerated optimization is coming

Observations

State-of-the-art solvers are all exploiting the problem's dynamic structure

Differential dynamic programming

(Altro, ProxDDP)

Condensation strategy

(HPIPM)

Riccati recursion

(FATROP)

Further, the ecosystem leverages mature tools:

- BLAS library for embedded system: BLASFEO
- Efficient modeler: Casadi

Question

So, what do we gain by solving optimal control instances on the GPU?

GPU-accelerated sparse automatic differentiation with ExaModels.jl

Large-scale optimization problems almost always have repetitive patterns

$$\begin{aligned} & \min_{x^{\flat} \leq x \leq x^{\sharp}} \sum_{l \in [L]} \sum_{i \in [l_l]} f^{(l)}(x; p_i^{(l)}) & \text{(SIMD abstraction)} \\ & \text{subject to } \left[g^{(m)}(x; q_j) \right]_{j \in [J_m]} + \sum_{n \in [N_m]} \sum_{k \in [K_n]} h^{(n)}(x; \boldsymbol{s}_k^{(n)}) = 0, \quad \forall m \in [M] \end{aligned}$$

Repeated patterns are made available by specifying the models as iterable objects

constraint(c,
$$3 * x[i+1]^3 + 2 * sin(x[i+2])$$
 for $i = 1:N-2$)

For each repeatitive pattern, the derivative evaluation kernel is constructed & compiled, and executed in parallel over multiple data

■ Perfect settings for optimal control (repeated pattern: cost and dynamics)

How fast can we get with ExaModels?

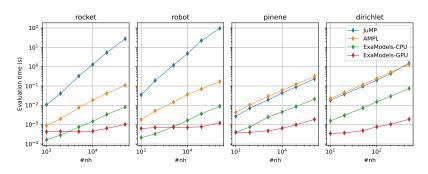


Figure: Time to evaluate the derivatives (Jacobian + Hessian) on various COPS instances with a dynamic structure

Now, combining ExaModels with NVIDIA cuDSS

N.B.: here, we are not exploiting the problem's dynamic structure

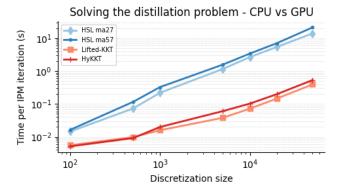


Figure: Solving the infamous distillation column instance

How expensive should be your GPU?

Observation

☑ No need to buy a professional GPU to get fast performance with ExaModels+cuDSS

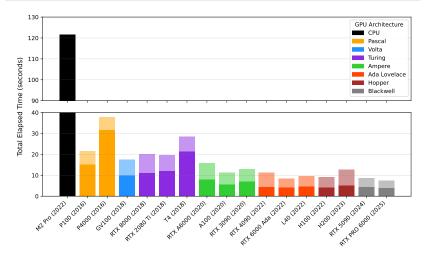


Figure: Time to optimality, here for a large-scale optimal power flow instance.

The KKT system is a block tridiagonal system:

$$\begin{bmatrix} A_{1,1} & A_{2,1}^{\top} & & & & \\ A_{2,1}^{\top} & \ddots & \ddots & & & \\ & \ddots & \ddots & A_{N,N-1}^{\top} & A_{N,N} \end{bmatrix} \begin{bmatrix} d_{w1} & & & \\ \vdots & & & \\ \vdots & & \vdots & \\ d_{wN} & & \end{bmatrix} = \begin{bmatrix} r_1 \\ \vdots \\ \vdots \\ r_N \end{bmatrix}$$

Two different path way:

- Parallel Cycling Reduction (PCR)
- Partitionned Dynamic Programming

Integration is under way in MadNLP!

Conclusion

GPU-accelerated optimal control is currently happening!

ExaModels

Fast evaluations of derivatives in nonlinear models

frapac.github.io/tutorials/powertech/

MadNLP

Fast solution of nonlinear programs on the GPU