Enhancing nonlinear optimization through GPU computing

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Outline

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Accelerated Computing in 2024

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Aurora Supercomputer @ Argonne

Mostly powered by GPUs

$=$ 1 million $\times$

iPhone 14 Pro

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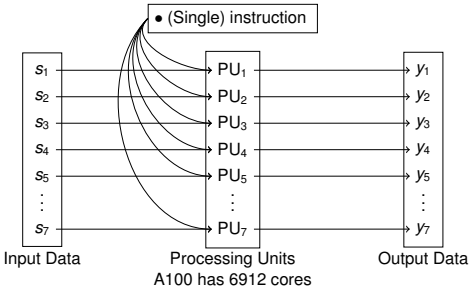
Can we harness these capabilities in the realm of **classical nonlinear optimization** (e.g., energy infrastures, optimal control, operations research)?

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

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



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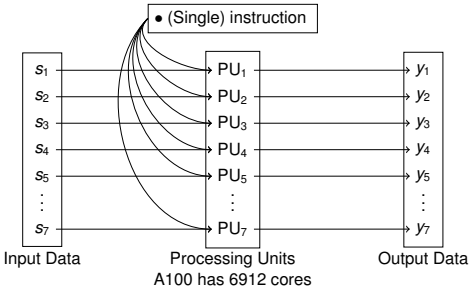

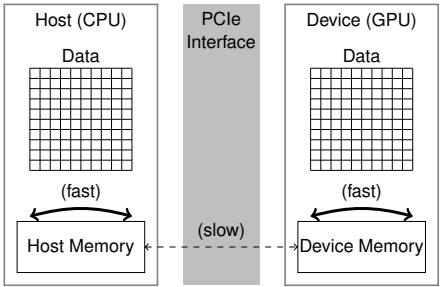

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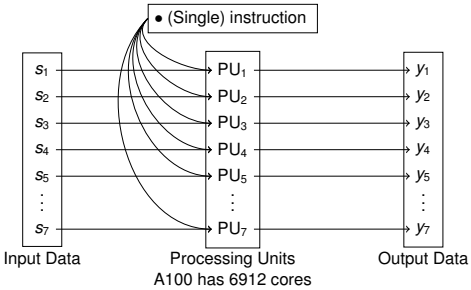

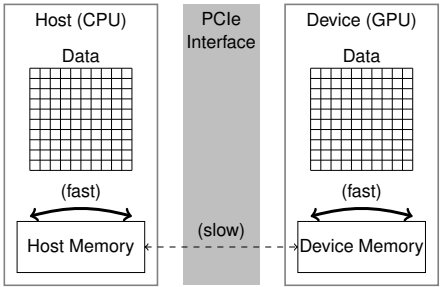

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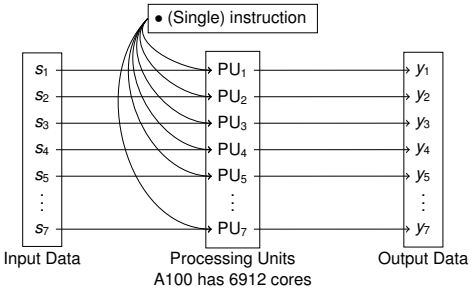

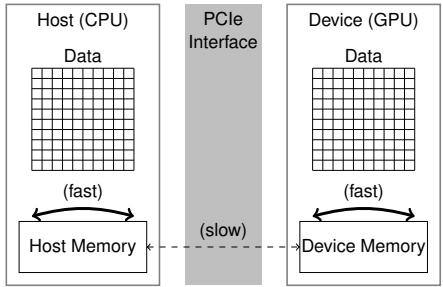

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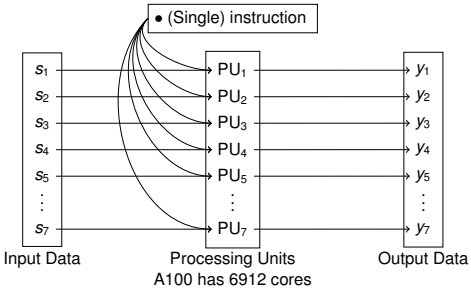

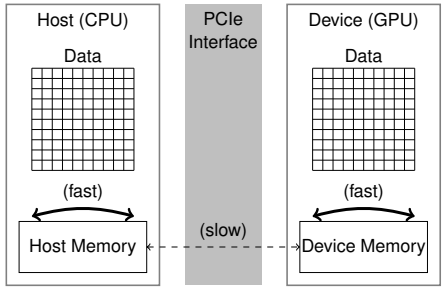

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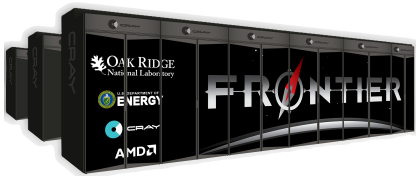
Exascale Computing Project

- **Mission**: Tackle **real-world computational problems** with exascale computing.

Frontier @Oak Ridge



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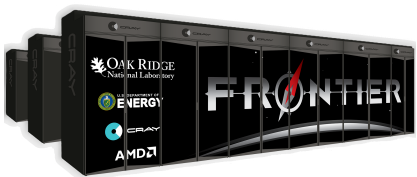

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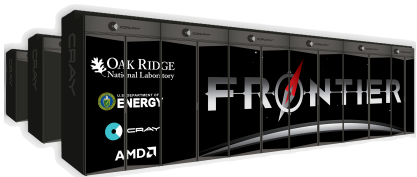

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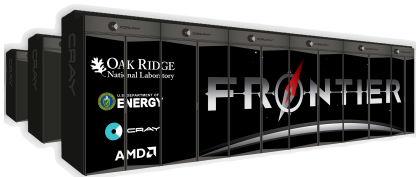

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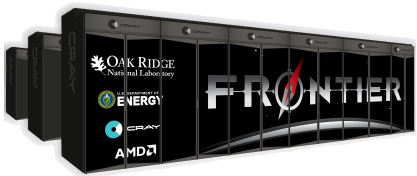

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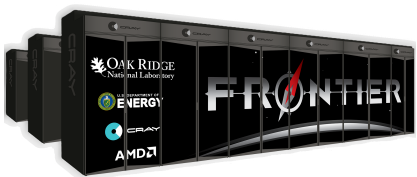

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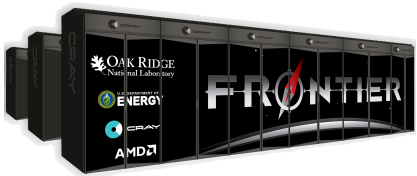

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  - **Performance**: at least an order of magnitude speedup.
  - **Portability**: compatibility with NVIDIA, AMD, and Intel.
  - **Application**: energy infrastructure problems (AC optimal power flow, in particular).

Language of Choice: Julia

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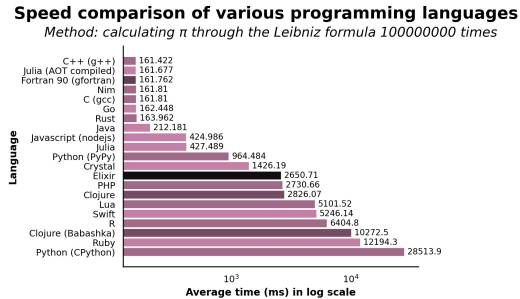

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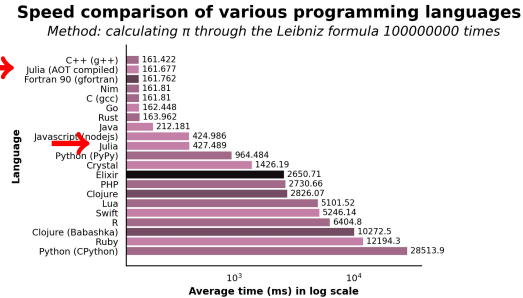

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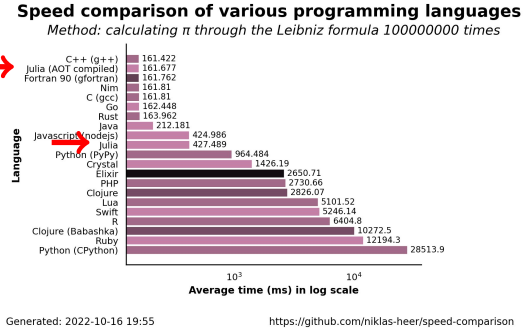

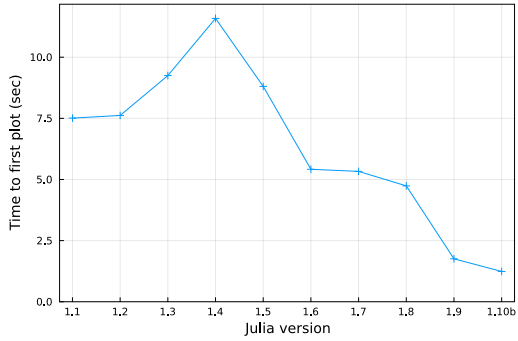

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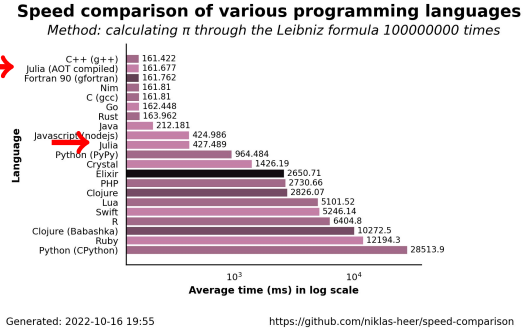

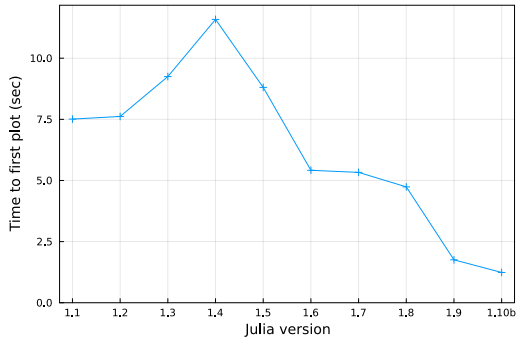

- **Fast development** (like Python, R, Matlab): Julia resolves the "**two-language problem**".

Language of Choice: Julia

- **Multiple dispatch**: High-level abstraction while specializing for specific data types.

```
function solve!(s::Solver{...})
  # NLP algorithm
  ...
  mul!(A, B, C)
  ...

end
```

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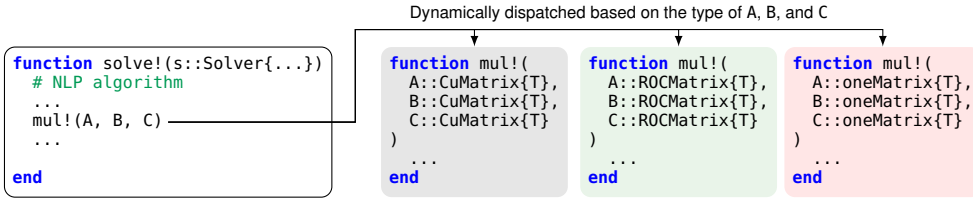

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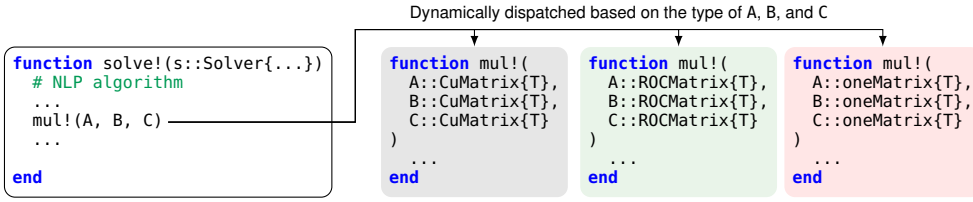

- **Portable kernel programming**: Compatibility across various architectures.

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Dynamically dispatched based on the type of A, B, and C

```
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MySolver.jl

```
function mul!(
  A::CuMatrix{T},
  B::CuMatrix{T},
  C::CuMatrix{T}
)
  ...
end
```

CUDA.jl

```
function mul!(
  A::ROCMatrix{T},
  B::ROCMatrix{T},
  C::ROCMatrix{T}
)
  ...
end
```

AMDGPU.jl

```
function mul!(
  A::oneMatrix{T},
  B::oneMatrix{T},
  C::oneMatrix{T}
)
  ...
end
```

oneAPI.jl

- **Portable kernel programming**: Compatibility across various architectures.

Portable GPU kernels can be executed on different accelerator backends

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Frontier @Oak Ridge (AMD GPUs)

Aurora @Argonne (Intel GPUs)

Summit @Oak Ridge (NVIDIA GPUs)

Summary

GPU/HPC

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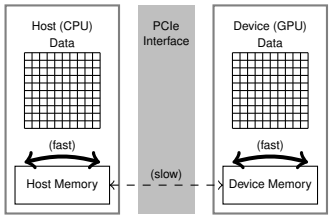
SIMD Architecture



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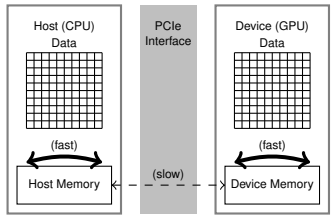

Performance, Fast Development, & Portability

- **Motivation**: **Harness accelerated computing** for **nonlinear programming**.
- Adapting CPU code into GPU code is **not merely an issue of software engineering**.
- **Goal**: Build a **comprehensive software infrastructure** for nonlinear programming on GPUs on **Julia Language**, for its **fast performance**, **fast development speed**, and **portability**.

Outline

CUDA.jl

- CUDA.jl is a Julia library that enables developers to harness the parallel computing capabilities offered by NVIDIA GPUs.
- CUDA.jl provides a native Julia interface for programming GPU kernels with Julia wrappers.
- CUDA.jl functions can be called directly from Julia code, making development and maintenance of code easier.
- CUDA.jl generates efficient and optimized CUDA code, fully leveraging the computing power of NVIDIA GPUs.

CUDSS.jl

NVIDIA cuDSS provides three factorizations (LDU, LDL^T, LL^T) for solving sparse linear systems.

cuDSS follows a well-established three phases approach commonly used in sparse direct solvers:

- reordering and symbolic factorization;
- numerical factorization;
- solve linear system using the computed factors.

This modular approach allows cuDSS to efficiently handle sparse linear systems by reusing the analysis and factorization stages, facilitating the solution of the KKT system in interior point methods.

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Nonlinear Optimization Software: State-of-the-Art on CPU

Problem Formulation

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

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  - the objective and constraints are **smooth**
  - **large number of variables and constraints**
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- Interior-point methods
  - Inequalities $x \geq 0$ replaced by smooth log-barrier functions $f(x) - \mu \sum_i \log(x[i])$.
  - **Newton's Step** is computed by solving a "**KKT system**" (large, sparse, symmetric indefinite, ill-conditioned system).

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  - Line search (along with several additional heuristics) ensures **global convergence**.

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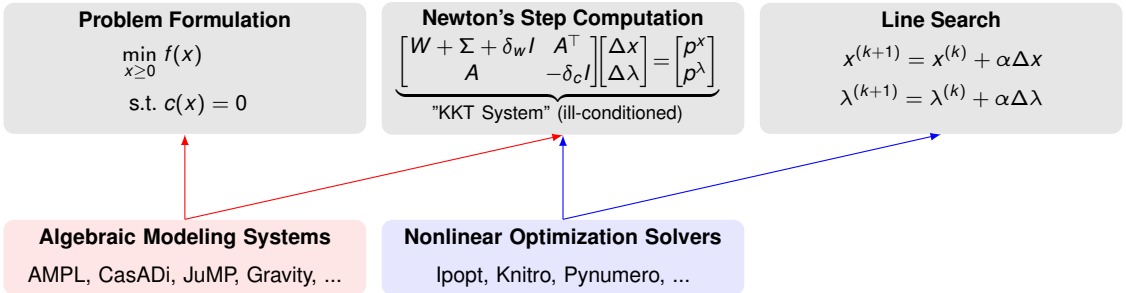
Algebraic Modeling Systems

AMPL, CasADi, JuMP, Gravity, ...

- Algebraic modeling systems provides **front-end** to specify models and (often) provides **derivative computation capabilities**.

Nonlinear Optimization Software: State-of-the-Art on CPU



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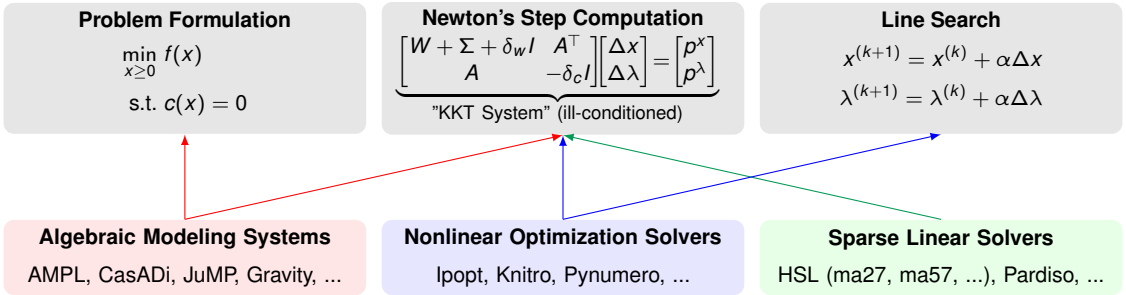

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- Sparse linear solvers solves KKT systems using **sparse matrix factorization**.

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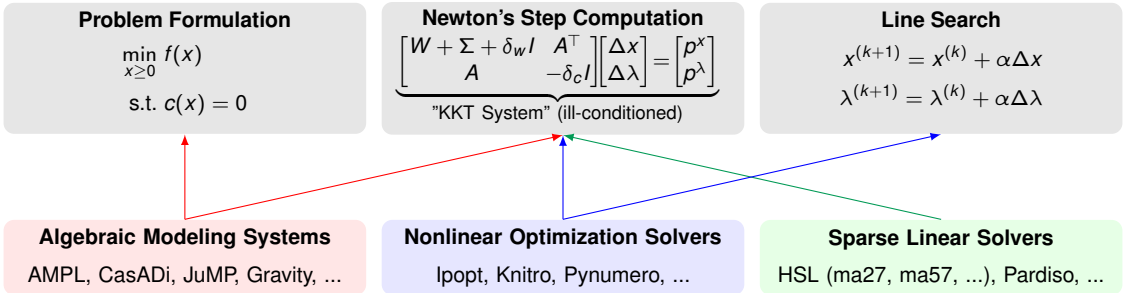

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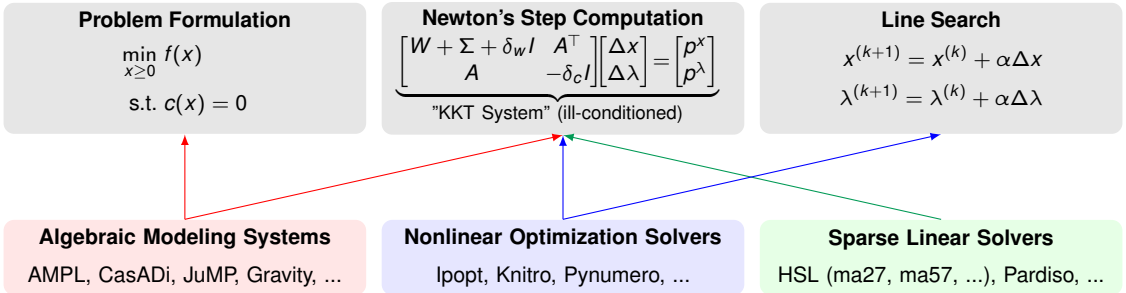

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- Many software tools have been developed in 80s-90s (**heavily optimized for CPUs**).

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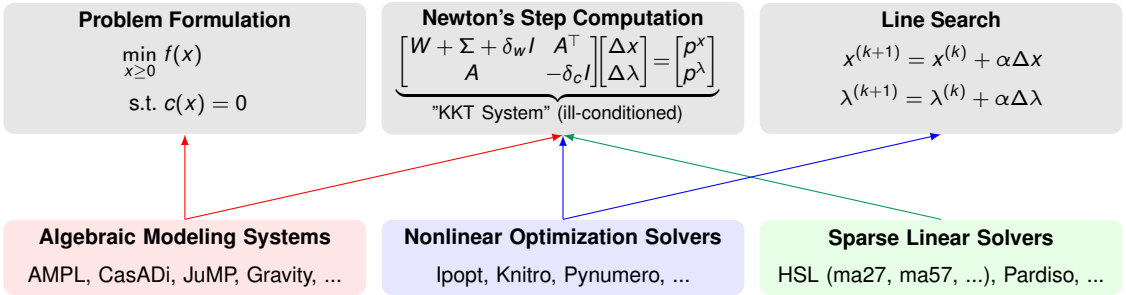

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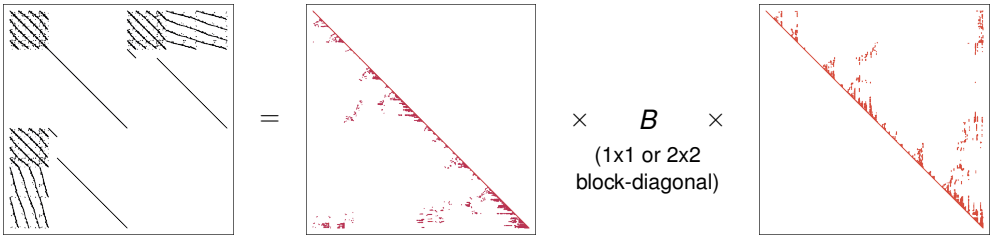
- Many software tools have been developed in 80s-90s (**heavily optimized for CPUs**).
- Now we need **GPU-equivalent** of these tools.

Outline

Why it is Challenging: Sparse Linear Solvers

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



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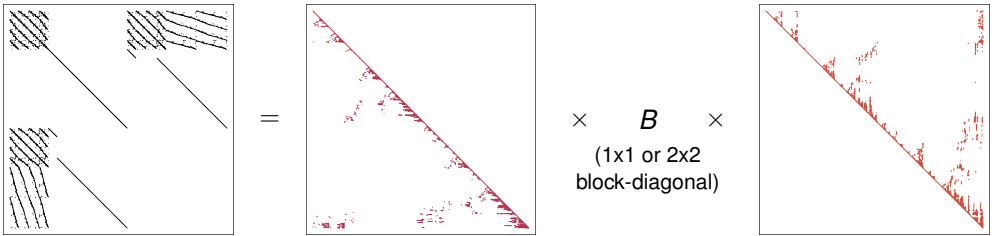

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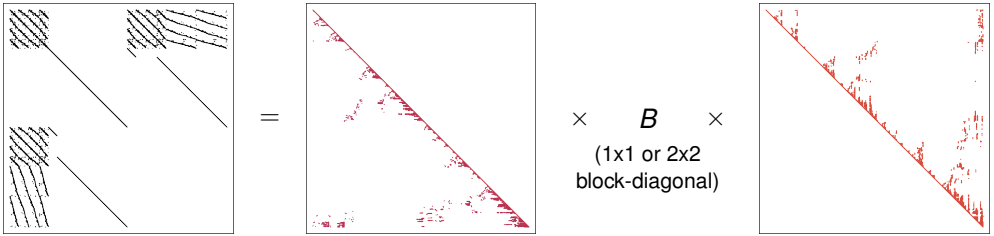

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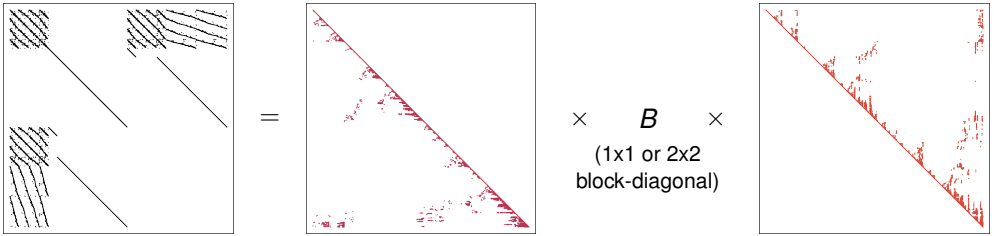

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- Then, how about **iterative solvers** (e.g., GMRES)? Due to ill-conditioning of the KKT system, iterative methods are generally not effective, unless **specialized preconditioners** are used.

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- The relaxation and condensation may cause **ill-conditioning** in the KKT system.

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Highlight: AC Optimal Power Flow (single GPU)

MadNLP

- Standard polar form AC optimal power flow (AC OPF) problems.

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- For large-scale cases, GPU becomes **significantly faster than CPU** (up to $\times$20 speedup).

Case	nvars	ncons	MadNLP+ExaModels+cuDSS (GPU)				Ipopt+ExaModels+Ma27 (CPU)			
			iter	deriv.†	lin.†	total†	iter	deriv.†	lin.†	total†
89_pegase	1.0k	1.6k	28	0.02	0.03	0.15	31	0.01	0.06	0.06
179_goc	1.5k	2.2k	35	0.03	0.07	0.24	46	0.01	0.10	0.11
500_goc	4.3k	6.1k	40	0.05	0.11	0.40	40	0.02	0.21	0.23
793_goc	5.4k	8.0k	39	0.03	0.06	0.28	37	0.03	0.25	0.28
1354_pegase	11.2k	16.6k	55	0.06	0.23	0.62	49	0.07	0.69	0.76
2312_goc	17.1k	25.7k	47	0.04	0.24	0.70	46	0.10	1.12	1.22
2000_goc	19.0k	29.4k	42	0.04	0.12	0.53	43	0.13	1.26	1.38
3022_goc	23.2k	35.0k	53	0.05	0.33	0.90	58	0.18	1.93	2.11
2742_goc	24.5k	38.2k	231	0.28	0.59	2.92	106	0.49	5.63	6.13
2869_pegase	25.1k	37.8k	61	0.06	0.14	0.73	59	0.21	2.22	2.43
3970_goc	35.3k	54.4k	124i	0.13	1.93	3.73	66	0.36	4.87	5.24
4020_goc	36.7k	57.0k	60	0.06	0.42	1.35	60	0.35	6.82	7.17
4917_goc	37.9k	56.9k	59	0.06	0.41	1.15	65	0.34	3.98	4.32
4601_goc	38.8k	59.6k	82	0.08	0.69	1.81	73	0.44	5.84	6.28
4837_goc	41.4k	64.0k	56	0.06	0.30	1.14	59	0.39	4.78	5.17
4619_goc	42.5k	66.3k	53	0.07	0.19	1.20	50	0.34	5.93	6.27
5658_epigrids	48.6k	74.8k	49	0.05	0.31	1.17	51	0.41	5.46	5.87
7336_epigrids	62.1k	95.3k	55	0.06	0.38	1.46	50	0.49	7.08	7.57
10000_goc	76.8k	112.4k	65	0.08	0.48	3.64	84	0.96	12.51	13.47
8387_pegase	78.7k	118.7k	110a	0.13	0.47	2.72	79	0.98	12.01	12.99
9591_goc	83.6k	130.6k	67	0.09	0.95	2.85	70	0.96	21.24	22.20
9241_pegase	85.6k	130.8k	500f	1.57	4.17	13.26	73	0.93	12.96	13.89
10192_epigrids	89.8k	139.5k	58	0.10	0.79	2.55	59	0.99	16.38	17.37
10480_goc	96.8k	150.9k	68	0.09	0.61	2.71	70	1.02	22.63	23.65
13659_pegase	117.4k	170.6k	77	0.11	0.79	3.01	66	1.14	16.06	17.20
20758_epigrids	179.2k	274.9k	200a	0.44	5.24	12.59	51	1.63	29.84	31.47
19402_goc	179.6k	281.7k	72	0.14	0.75	4.42	72	2.26	60.80	63.06
24464_goc	203.4k	313.6k	65	0.14	0.90	4.41	63	2.11	41.28	43.39
30000_goc	208.6k	307.8k	179	0.43	3.65	9.57	153	6.17	93.02	99.20
78484_epigrids	674.6k	1.0m	105	0.61	4.37	20.38	104	21.50	345.93	367.43

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- Work-arounds?
  - Using CPUs as we approach the solution.
  - Quadruple precision—challenging due to low-level kernel supports.
  - Hopefully, some breakthrough in sparse linear algebra (e.g., scalable parallel pivoting).

Future Outlook: Towards Portability

Table: GPU Compatibility of Nonlinear Optimization Frameworks

		CPU (single)	CPU (multi)	NVIDIA GPU	AMD GPU	Intel GPU	Apple Metal
Algebraic Modeling Platforms	**AMPL**	✓	✗	✗	✗	✗	✗
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	ExaModels	✓	✓	✓	✓	✓	✗
NLP Solvers	**Ipopt**	✓	✗	✗	✗	✗	✗
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- Work-arounds?
  - Preconditioned iterative solver with reduction.
  - Domain-specific linear solvers (e.g., Riccati solver for optimal control).

Krylov.jl: A Julia Basket of Hand-Picked Krylov Methods `https://github.com/JuliaSmoothOptimizers/Krylov.jl`
Cole et. al., Exploiting GPU/SIMD Architectures for Solving Linear-Quadratic MPC Problems, ACC (2023).

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- Chellenges remain: **Ill-conditioning of condensed KKT system** and **portability**.
- We envision **expanding the application scope of nonlinear programming**.
  - **Extremely large-scale** problems (coupled infrastructures, multi-stage, multiscale).
  - Problems involving **expensive surrogate models** (neural nets, simulations).