MAX-PLANCK-INSTITUT
FÜR PLASMAPHYSIK

JOREK: Advancements in GPU Porting of MHD Solver

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Outline

- **Motivation**
- **Overview of JOREK code**
- **MHD Solver Algorithm**
- **GPU Porting of Stiffness Matrix Construction**
- **GPU Porting of Iterative Solver**
- **Summary**

JOREK: overview

- **JOREK is an extended nonlinear MHD code used to study large scale plasma instabilities and their control in realistic divertor geometry**
  - **IPP-Garching is hosting one of the main hubs for the code development in the European and international community**
  - **JOREK is written in modern FORTRAN with MPI/OpenMP hybrid parallelization**
- **Several models are implemented in JOREK with different sets of physical quantities, including full-MHD, and various implementations of reduced MHD models**
  - **MHD equations in weak form are spatially discretized on continuous 2D isoparametric Bezier finite element grid in poloidal plane, combined with a toroidal Fourier expansion**
  - **Implicit time integration scheme allows large time stepping for realistic simulations**
- **Several hybrid kinetic-fluid models are also available, e.g. for ITG turbulence, neutrals, impurities, energetic particles, relativistic runaway electrons**

JOREK: MHD solver and global sparse matrix

Generalized form of MHD equation

$$\frac{\partial A(u)}{\partial t} = B(u,t)$$

Linearized implicit time discretization scheme yields

$$\left[(1+\xi)\left(\frac{\partial A}{\partial u}\right)^n - \Delta t\theta\left(\frac{\partial B}{\partial u}\right)^n\right]\delta u^n = \Delta t B^n + \xi\left(\frac{\partial A}{\partial u}\right)^{n-1}\delta u^{n-1}$$

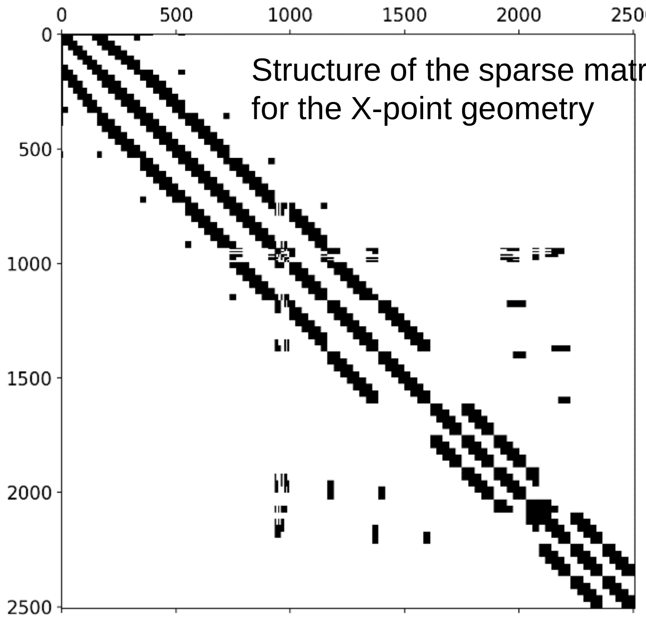
$$\delta u^n = u^{n+1} - u^n$$

Linear system of algebraic equations

$$Ax = b$$

A is a sparse matrix, typically large and ill-conditioned

Example: 30K nodes; 8 physical variables; 4 dof per node; 21 toroidal harmonics: matrix dimension 40 million with 500 billion non-zero elements – requires 8 TB of memory for storage



Structure of the sparse matrix for the X-point geometry

Physics-based preconditioner

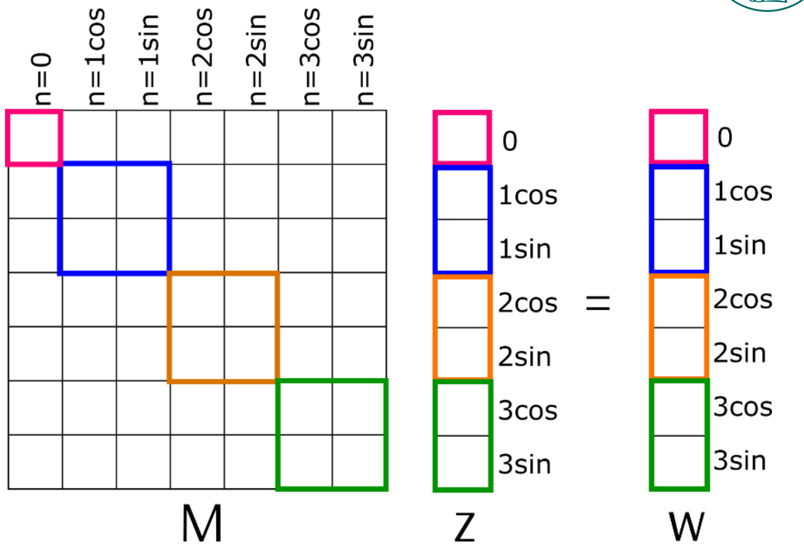
- Direct LU factorization is (usually) prohibitively expensive
- Iterative GMRES method with (left) preconditioning is used

Preconditioned system to be solved: $M^{-1}Ax = M^{-1}b$

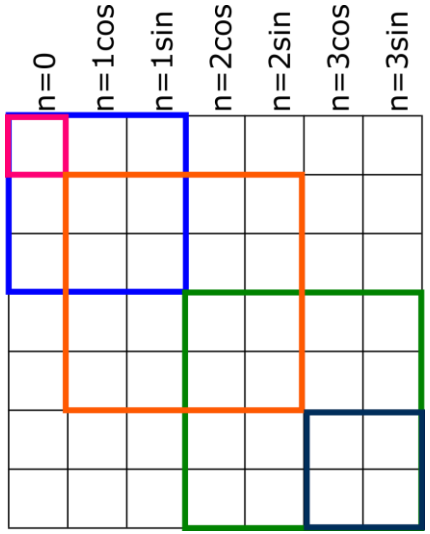
Product $M^{-1}A$ should have low condition number

Solution $z = M^{-1}w$ should be easy to find

Preconditioner matrix doesn't appear explicitly, only in form of a solution



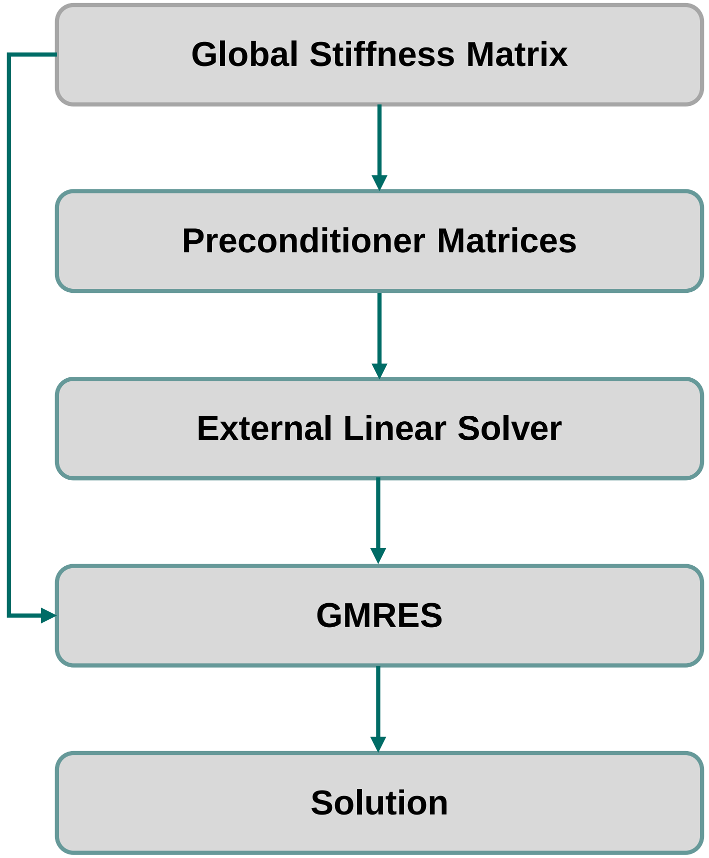
- JOREK preconditioner is bases on decoupling individual toroidal Fourier modes of mode families
    - Full preconditioner matrix is equivalent to the original matrix A with omitted mode coupling
    - Each diagonal block has similar sparsity pattern as A
    - Each diagonal block can be solved independently



Solver algorithm

Solver algorithm:

- Construct global stiffness matrix and RHS – *every time step*
- Construct/distribute preconditioner matrix – ***once per several steps***
- Analyze/build elimination graph – *once per simulation run*
- Perform LU factorization – ***once per several steps***
- Perform GMRES/BICGSTAB iterations – *every step*
  - Find solution for preconditioner matrix – *every iteration*



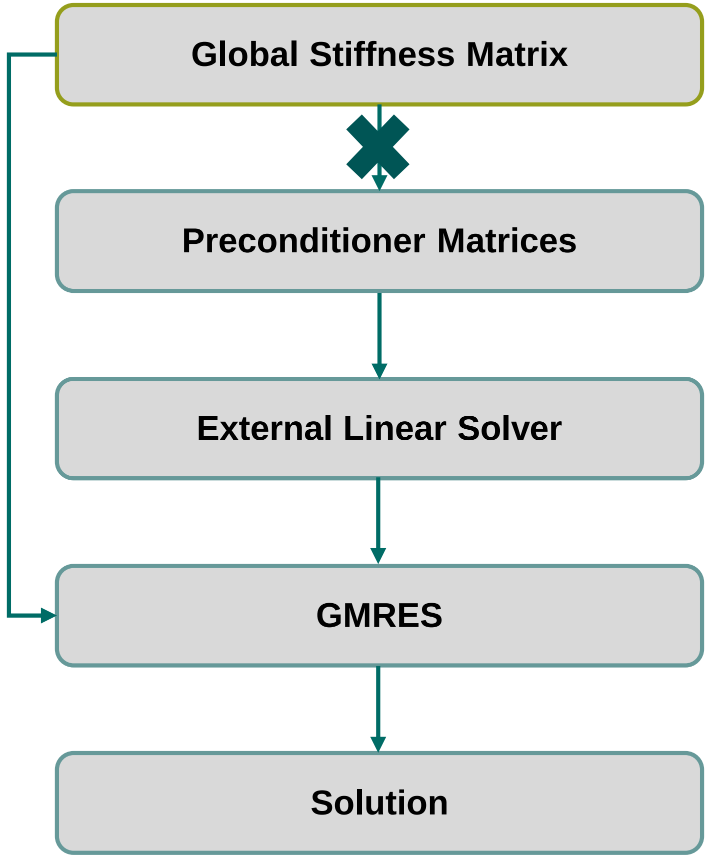
GPU Acceleration Strategy

Acceleration of Preconditioner Solver

- Vendor specific

Acceleration of Matrix Construction/Iterative Solver

- Global Matrix constructed/residing on GPU
- Matrix-vector product in iterative cycle calculated on GPU
- Direct construction used for Preconditioner matrices



GPU Accelerated Matrix Construction

CPU Approach

- Finite Elements distributed among MPI tasks and OpenMP threads
- Element matrices are computed using SIMD vectorization

GPU Approach using OpenMP Offloading

- Element distributed among MPI tasks and OpenMP *teams*
- Element matrices are computed in batches of many elements
- Loop over elements and internal loops are distributed over *teams* and *SM threads*
  - Loop restructuring was necessary to obtain good performance on accelerators

Optimized FFT Libraries

- The Fast Fourier Transform is performed using *CuFFT/RocFFT*
- The transforms for multiple elements are batched for maximum efficiency.

GPU Accelerated Matrix Construction

Element coloring

- Element coloring is used to…
  - …remove synchronization bottleneck
  - …reduce memory cost by element batching.

Performance

- Efficiency is very setup dependent.
- A reasonable setup can lead to a decent speed up of ~2 on HCP Raven node (2x Intel Xeon IceLake-SP 8360Y, 72 cores per node, 4x Nvidia A100)

GPU Accelerated Matrix-Vector Product

Original CPU approach based on matrix block structure:

- **Blocks distributed among OpenMP threads**
- **MKL BLAS used for individual block multiplication**

Better performance achieved using compressed sparse row (CSR) format

- **Row pointers distributed among OpenMP threads**
- **Explicit summation over column indices with SIMD distribution**
- **COO-to-CSR mapping is pre-calculated**

GPU implementation using CSR format

- **Row pointers distributed among OpenMP teams**
- **Explicit summation over column indices with SM thread distribution**

Matrix block-structure (bs=3)

11,12,13 21,22,23 31,32,33	14,15,16 24,25,26 34,35,36

11,12,13,21,22,23,31,32,33,14,15,16,…

Summary

- **GPU offloading of JOREK MHD Solver components has been implemented using OpenMP library**
  - **GPU acceleration of stiffness matrix construction with coloring method**
  - **GPU acceleration of matrix-vector product in the iterative solver**
- **The unification of these components is currently underway**