UKAEA NEPTUNE - Preconditioning

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The abstract pattern can be removed or repositioned if required. Be careful to ‘Send to Back’ so that it does not obscure any important information.

Linear solvers

Discretisation of the PDE => a very large linear system ***Ax=b*** must be solved (or series)

$$\boldsymbol{A} = \begin{bmatrix} A_{1,1} & \cdots & A_{1,n} \\ \vdots & \ddots & \vdots \\ A_{n,1} & \cdots & A_{n,n} \end{bmatrix}$$

$A_{i,i}$ represents discretisation of *i*-th PDE

Iterative methods preferable but convergence slow: $\boldsymbol{x}^{(0)}, \boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}, \ldots, \boldsymbol{x}^{(k)} \rightarrow \boldsymbol{x}$

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Linear solvers (2)

Want to (approximately) solve $Ax=b$

Instead find P and/or Q and solve $By=c$, where $B= P^{-1}AQ^{-1}$, $c= P^{-1}b$ and $x=Q^{-1}y$

Choose P/Q that
- improve rate of convergence
- but “cheap” to generate and apply preconditioner

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Our approach

$$A = \begin{bmatrix} A_{1,1} & \cdots & A_{1,n} \\ \vdots & \ddots & \vdots \\ A_{n,1} & \cdots & A_{n,n} \end{bmatrix}$$

Identification of key PDEs and literature search to assess suitability of known preconditioners

- PDE-based (multigrid,…)
- Sparse approximate inverses (Markov Chain Monte Carlo Matrix Inverse,…)

Development of implicit-factorization preconditioners

- Make use of block structure and preconditioners for $A_{i,i}$
- Comparison of implicit-factorization versus SPAI applied to A

Guide NEPTUNE Programme in choice of preconditioner

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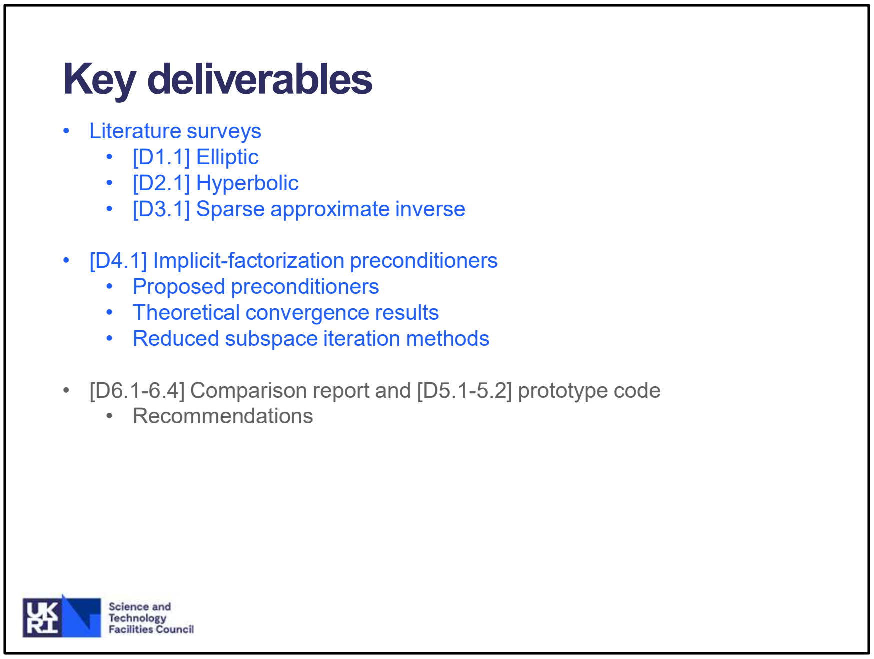

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Prioritisation of Equations

- Elliptic Problems
  - System 2-2: 2D elliptic solver in complex geometry
    - Simplified Grad-Shafranov equation
    - Simplified non-Boussinesq vorticity equation

- Hyperbolic Problems
  - System 2-3: 1D fluid solver with simplified physics but with UQ and realistic boundary conditions
  - Hasegawa-Wakatani: 2D simulation of dynamics across the magnetic field

$$\begin{bmatrix} M + \Delta t(L + \alpha M - D_n K) & 0 & \Delta t(L_n - \alpha M) \\ \alpha \Delta t\, M & M + \Delta t(L - D_\omega K) & \Delta t L_\omega \\ 0 & -M & K \end{bmatrix}$$

$$\begin{bmatrix} M + \Delta t(L_{(K^{-1}M)} + \alpha M - D_n K) & \Delta t(LK^{-1}M - \alpha M K^{-1} M) \\ \alpha \Delta t M & M + \Delta t(L_{\omega(K^{-1}M)} - \alpha M K^{-1} M - D_\omega K) \end{bmatrix}$$

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Plasma density, vorticity, potential
Eliminate potential

Iterative Solution Methods

$$A = \begin{bmatrix} A_{1,1} & \cdots & A_{1,n} \\ \vdots & \ddots & \vdots \\ A_{n,1} & \cdots & A_{n,n} \end{bmatrix}$$

Identified existing methods and preconditioners of interest

- Talk by Anton Lebedev 11/3
- Technical Note 2047353-TN-02 "Linear Systems of Equations and Preconditioners relating to the NEPTUNE Programme"
  - Multigrid for symmetric and non-symmetric problems
    - Algebraic multigrid
  - Sparse approximate inverse preconditioners
    - Markov Chain Monte Carlo for approximate matrix inverse
  - Reduce condition number and/or cluster the eigenvalues

- Deliverables D1.1, D2.1 and D3.1

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Constraint-style preconditioners

$$A = \begin{bmatrix} H & B \\ C & -D \end{bmatrix}$$

$$P = \begin{bmatrix} G & B \\ C & -D \end{bmatrix}$$

- $C \neq B^T \in \mathbb{R}^{m \times n}$ and $D = 0$
  - $2m$ eigenvalues at 1
  - $n - m$ eigenvalues
    $$\hat{Z}^T HZx = \lambda \hat{Z}^T GZx, \qquad CZ = 0, \qquad B^T \hat{Z} = 0$$
  - NEW! Extension of Keller, Gould and Wathen (2001)

- $C \neq B^T \in \mathbb{R}^{m \times n}$ and D non-singular
  - m eigenvalues at 1
  - n eigenvalues
    $$(H + BD^{-1}C)x = \lambda(G + BD^{-1}C)x$$
  - NEW! Extension of Dollar, Gould, Schilders and Wathen (2006)

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Implicit-factorization preconditioners

$$\boldsymbol{A} = \begin{bmatrix} H_{1,1} & H_{1,2} & B_1 \\ H_{2,1} & H_{2,2} & B_2 \\ C_1 & C_2 & -D \end{bmatrix}$$

Family 2

$$\boldsymbol{P} = \begin{bmatrix} 0 & 0 & B_1 \\ 0 & \tilde{G}_{2,2} & B_2 \\ \tilde{G}_{3,1} & 0 & \tilde{G}_{3,3} \end{bmatrix} \begin{bmatrix} 0 & 0 & B_{1,3} \\ 0 & B_{2,2} & 0 \\ B_{3,1} & 0 & 0 \end{bmatrix} \begin{bmatrix} 0 & 0 & G_{1,3} \\ 0 & G_{2,2} & 0 \\ C_1 & C_2 & G_{3,3} \end{bmatrix}$$

$$G_{3,1} = B_{1,3}^{-1}, \qquad G_{1,3} = B_{3,1}^{-1}, \qquad G_{3,3} + \tilde{G}_{3,3} - \tilde{G}_{3,1} B_{1,1} G_{1,3} = -D$$

Total of 14 families for $\boldsymbol{A} = \boldsymbol{A}^T$ derived with constrained optimization as application (Dollar, Gould, Schilders, Wathen, 2006)

Deliverable 4.1: Extended to $\boldsymbol{A} \neq \boldsymbol{A}^T$ for inclusion in Deliverable D6.1 along with the new theoretical results.

For NEPTUNE, particularly want to take advantage of mass matrices

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