MPII news

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Overview

- Portability
  - Range and precision of numbers in PEDE

- MINRES solution method
  - New version MINRES-QLP added

Portability

- Precision and range of numbers in PEDE
  - Previously definition platform dependent:
    - `INTEGER, DOUBLE PRECISION, ..`
  - Now explicitly requested:

```
INTEGER, PARAMETER :: mpi = selected_int_kind(9)          !>  4 byte integer
INTEGER, PARAMETER :: mpl = selected_int_kind(18)         !>  8 byte integer
INTEGER, PARAMETER :: mps = selected_real_kind(6, 37)     !>  4 byte float
INTEGER, PARAMETER :: mpd = selected_real_kind(15, 307)   !>  8 byte float
INTEGER, PARAMETER :: mpq = selected_real_kind(33, 4931) !> 16 byte float
```

  - Quad precision (16 byte float)
    - Supported by *gcc* since version 4.5 (`-lquadmath`)
    - First tests: about factor 60-70 slower (than 'mpd')

MINRES

- Iteratively solve $\mathbf{A}\cdot\mathbf{x}=\mathbf{b}$ or minimize $\|\mathbf{A}\cdot\mathbf{x}-\mathbf{b}\|$
  - Transform symmetric matrix ***A*** into ≈ tridiagonal matrix **T** (Lanczos process)
  - At each iteration k solve subproblem by $\mathbf{T}=\mathbf{Q}\cdot\mathbf{R}$ factorization (Q is orthogonal, R upper triangular)
  - Solution $\mathbf{x}_k$ based on Krylov subspace $\mathbf{V}_k=\left\{\mathbf{b},\mathbf{A}\cdot\mathbf{b},..,\mathbf{A}^{k-1}\cdot\mathbf{b}\right\}$
  - Stopping conditions based on estimated (matrix and vector) norms, e.g. $\|\mathbf{r}\|<\|\mathbf{A}\|\cdot\|\mathbf{x}\|\cdot r_{tol}$, $\mathbf{r}=\mathbf{A}\cdot\mathbf{x}-\mathbf{b}$
- Implemented in MP-II
  - Fortran77 version (2003)

MINRES-F90

- Fortran90 version (2007)
  - Additional stopping rule for singular systems

$$\|\mathbf{A}\cdot\mathbf{r}\| < \|\mathbf{A}\|\cdot\|\mathbf{r}\|\cdot r_{tol}, \quad \mathbf{r} = \mathbf{A}\cdot\mathbf{x} - \mathbf{b}$$

(**r≠0** with ***A*·r=0** means nullity(*A*)>0, rank(*A*)<size(*A*))

MINRES-QLP (I)

- ★ Result of (math) PhD thesis at Stanford U.
  - S. Choi, 2006; supervised by MINRES author
  - Improved norm estimates and stopping rules
    - ✦ e.g. $\|\mathbf{r}\| < \left(\|\mathbf{A}\| \cdot \|\mathbf{x}\| + \|\mathbf{b}\|\right) \cdot r_{tol}$
    - ✦ Number of iterations can be different
  - Factorization $\mathbf{T} = \mathbf{Q} \cdot \mathbf{L} \cdot \mathbf{P}$ instead of 'QR'
    (Q,P orthogonal, L lower triangular)
    - ✦ Allows to find for singular systems the minimum length ('pseudo-inverse') solution
    - ✦ Should be numerically superior

MINRES-QLP (II)

- ★ Method implementation
  - MINRES-QLP starts with 'QR' factorization
  - Switches to 'QLP' if matrix condition exceeds limit
- ★ PEDE implementation
  - New solution method:
    - "sparseMINRES-QLP", "fullMINRES-QLP"
  - Additional options (steering parameters)
    - mresmode: 0=QR+QLP, 1=QR, 2=QLP factorization (0)
    - mrestranscond: cond(*A*) to switch from QR to QLP (10^7)

MINRES-QLP (III)

- Some testing
  - With early variant of 2011 alignment (copied to DESY): 200k parameters, 17M tracks
  - Solution compatible with MINRES
  - More homogenous number of (internal) iterations
    - MINRES: 29, 763, 507, 401
    - MINRES-QLP: 517, 524, 523, 443
  - Slightly more CPU time used
    - 28h instead of 26h

Summary & Outlook

- Summary, PEDE in MPII V04-01-00
  - Portability improved
  - Solution by MINRES updated to f90 version
  - Solution by MINRES-QLP added

- Outlook
  - Should try MINRES-QLP with QR or QLP factorization for alignment
    - Especially for weak mode studies