Cache-optimierte QR-Zerlegung

Bachelor Kolloquium

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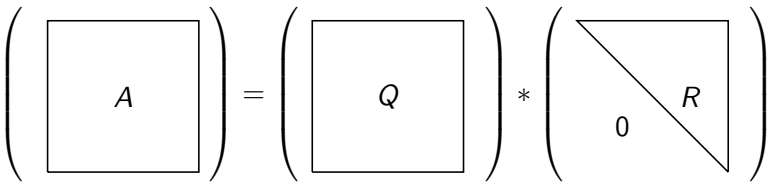
Cache-optimierte QR-Zerlegung

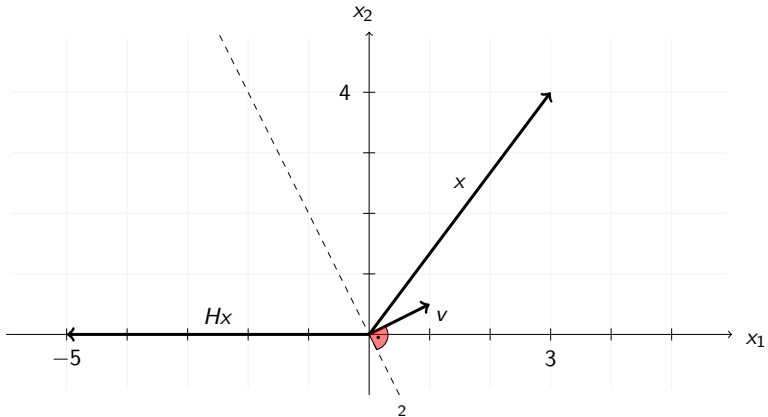
- $A = QR$



- QR-Zerlegung mittels Householder transformation
- Cache-optimierten Algorithmus implementieren
- Anwendungs:
  - LGS $Ax = b$ lösen mit QR
  - Lineares Ausgleichsproblem mittels kleinstes Fehler Quadrat
  - Kern operation im QR-Verfahren (Berechnung von Eigenwerten)

Householder-Transformation

$$H = I - 2\frac{vv^T}{v^T v}$$



Householder-Transformation

- Householder Vektor berechnen
  - Ansatz $Hx = \alpha e_1$
  - Normieren $v_1 = 1$
  - $\tau = \frac{2}{v^T v} \quad \Longrightarrow \quad H = I - 2\frac{vv^T}{v^T v} = I - \tau vv^T$
- Householder-Transformation anwenden

$$HA = (I - \tau vv^T)A = A - \tau(vv^T)A = A - \tau v(v^T A)$$

- Vektor-Rechenoperationen und Vektor-Matrix-Rechenoperationen

QR-Zerlegung mittels Householder

- $A = QR$

$$H_1 A = \begin{pmatrix} * & * & * & * \\ 0 & * & * & * \\ 0 & * & * & * \\ 0 & * & * & * \end{pmatrix}$$

-

$$H_1 = (\hat{H}_1) \quad , \quad H_2 = \left(\begin{array}{c|c} I_1 & 0 \\ \hline 0 & \hat{H}_2 \end{array}\right) \quad , \quad H_i = \left(\begin{array}{c|c} I_{i-1} & 0 \\ \hline 0 & \hat{H}_i \end{array}\right)$$

QR-Zerlegung mittels Householder

- $A = QR$

$$H_2 H_1 A = \begin{pmatrix} * & * & * & * \\ 0 & * & * & * \\ 0 & 0 & * & * \\ 0 & 0 & * & * \end{pmatrix}$$

-

$$H_1 = (\hat{H}_1) \quad , \quad H_2 = \left(\begin{array}{c|c} I_1 & 0 \\ \hline 0 & \hat{H}_2 \end{array}\right) \quad , \quad H_i = \left(\begin{array}{c|c} I_{i-1} & 0 \\ \hline 0 & \hat{H}_i \end{array}\right)$$

QR-Zerlegung mittels Householder

- $A = QR$

$$H_3 H_2 H_1 A = \begin{pmatrix} * & * & * & * \\ 0 & * & * & * \\ 0 & 0 & * & * \\ 0 & 0 & 0 & * \end{pmatrix}$$

-

$$H_1 = (\hat{H}_1) \quad , \quad H_2 = \left(\begin{array}{c|c} I_1 & 0 \\ \hline 0 & \hat{H}_2 \end{array}\right) \quad , \quad H_i = \left(\begin{array}{c|c} I_{i-1} & 0 \\ \hline 0 & \hat{H}_i \end{array}\right)$$

QR-Zerlegung mittels Householder

- $A = QR$

$$H_3 H_2 H_1 A = \begin{pmatrix} r_{1,1} & r_{1,2} & r_{1,3} & r_{1,4} \\ v_2^{(1)} & r_{2,2} & r_{2,3} & r_{2,4} \\ v_3^{(1)} & v_3^{(2)} & r_{3,3} & r_{3,4} \\ v_4^{(1)} & v_4^{(2)} & v_4^{(3)} & r_{4,4} \end{pmatrix}$$

-

$$H_1 = (\hat{H}_1) \quad , \quad H_2 = \left(\begin{array}{c|c} I_1 & 0 \\ \hline 0 & \hat{H}_2 \end{array}\right) \quad , \quad H_i = \left(\begin{array}{c|c} I_{i-1} & 0 \\ \hline 0 & \hat{H}_i \end{array}\right)$$

Benchmark

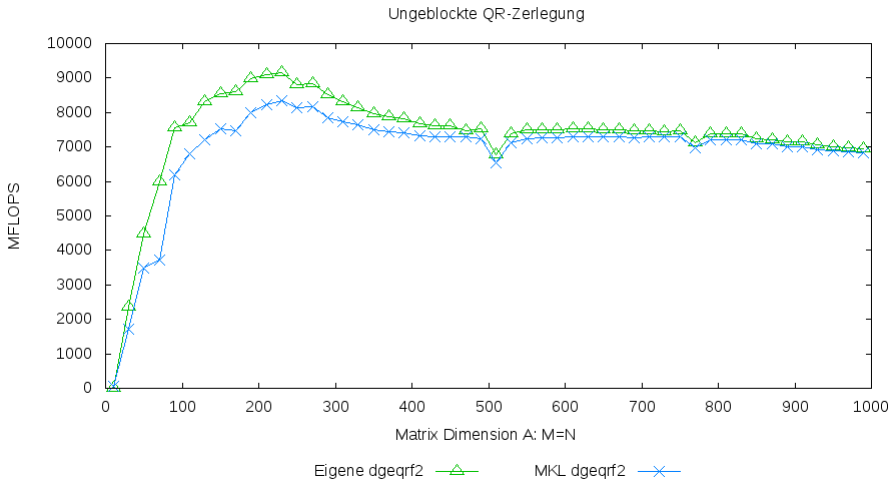
- Peak performance
  25,6 GFLOPS auf dem Testsystem mit i5-3470-CPU
- Aufwand QR mittels Householder $A \in \mathbb{R}^{m \times n}, \quad m \geq n$

$$\#\text{QR} = n \cdot \left(\frac{23}{6} + m + \frac{n}{2} + n \cdot \left(m - \frac{n}{3} \right) + \frac{5}{6} + n \cdot \left(\frac{1}{2} + m - \frac{n}{3} \right) \right) = \mathcal{O}(n^2 m)$$

- Flops

$$\text{FLOPS} = \frac{\text{Aufwand}}{\Delta t}$$

Ungeblockte QR



Mehrere Householder-Transformationen anwenden

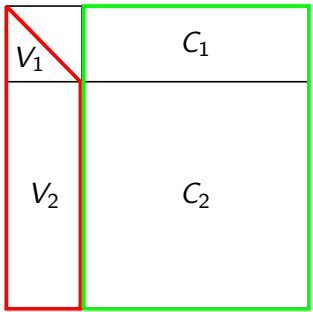
- Ansatz

  $$\hat{H} = H_1 H_2 ... H_k = I - VTV^T \quad \text{mit} \quad H_i = I - \tau_i v_i v_i^T$$

- Vektor-Matrix-Rechenoperationen um T zu berrechen
- Householder-Transformationen anwenden

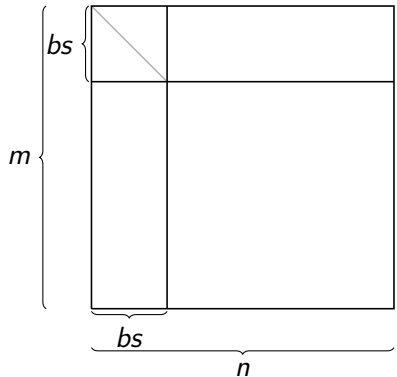
  $$C \leftarrow \hat{H}C = C - VTV^T C$$

- Matrix-Produkte um Householder-Transformationen anzuwenden



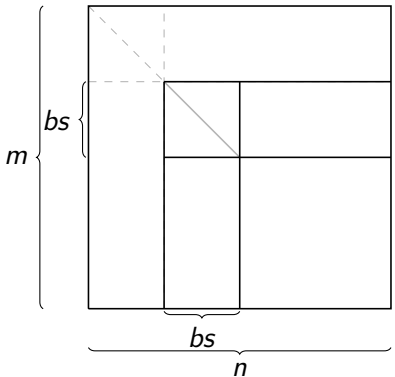
Geblockte QR-Zerlegung

- Matrix A



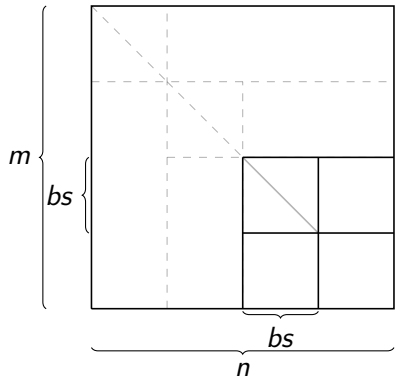
Geblockte QR-Zerlegung

- Matrix A



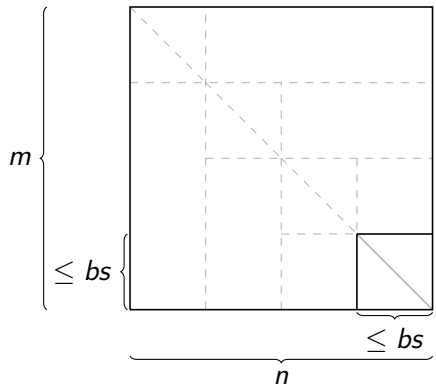
Geblockte QR-Zerlegung

- Matrix A

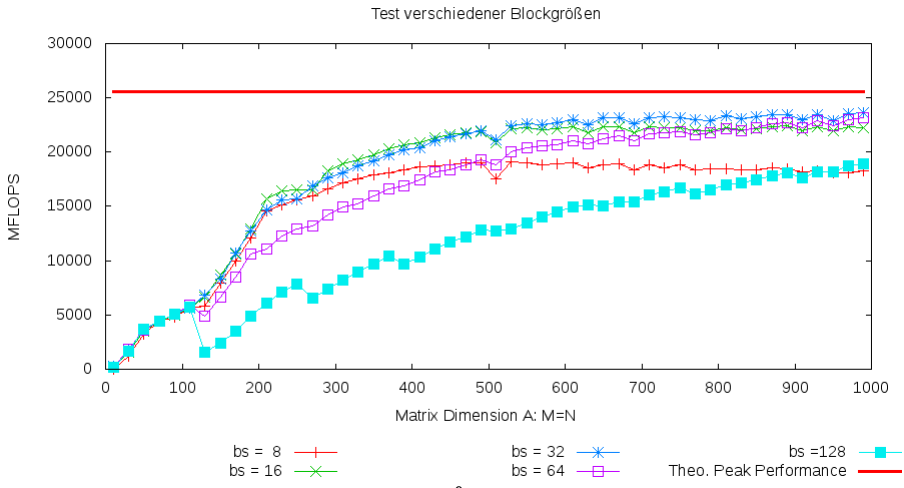


Geblockte QR-Zerlegung

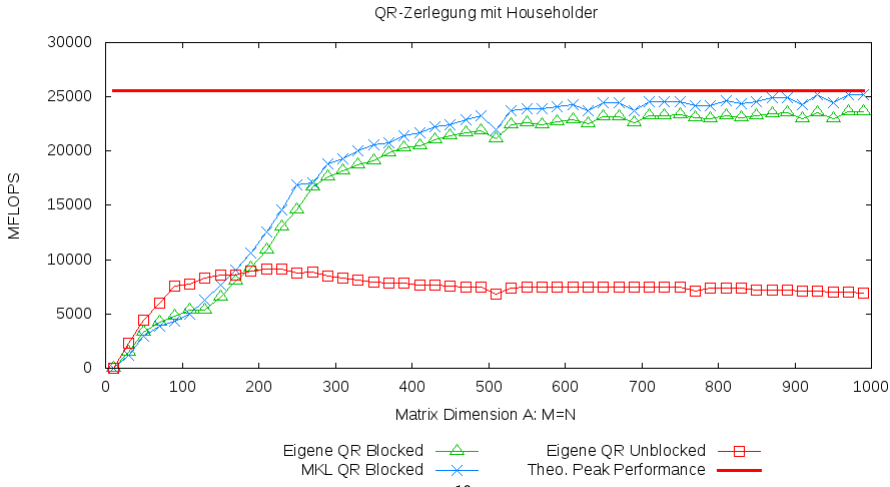
- Matrix A



Verschiedene Blockgrößen



Geblockte QR - Blocksizes



Fazit

- Ungeblockter Algorithmus erreicht nicht die *peak performance*.
- Eigener ungeblockte Algorithmus ist etwa 5% schneller als MKL.
- Geblockte Algorithmus erreicht fast die *peak performance*.
- Der geblockte Algorithmus *dgeqrf* der MKL ist etwas schneller. Der selbst implementierten Algorithmus erreicht bis zu 94% die Performance der MKL.
- Der geblockte Algorithmus ist um den Faktor 3 schneller als der ungeblockte Algorithmus.