Effectiveness of Partial Use of Quadruple Precision Arithmetic with QuPAT to Iterative Methods

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Background & Motivation

- ✓ Iterative methods may not converge because of round-off errors.

- ✓ We apply quadruple precision arithmetic **with QuPAT** to iterative methods.
- ✓ To improve convergence with relatively small cost, we use quadruple precision arithmetic **partially**.

Background & Motivation

- ✓ In floating point arithmetic, we cannot avoid :
  - ✓ Round-off errors
  - ✓ Cancellation
  - ✓ Information loss
- ✓ It is difficult to implement multiple precision arithmetic without any special hardware.

A **convenient** quadruple precision arithmetic environment **QuPAT**[1] on **Scilab** has developed.

[1] T. Saito, E. Ishiwata and H. Hasegawa, Development of quadruple precision arithmetic toolbox qupat on scilab, ICCSA2010, Proceedings Part II, LNCS 6017, pp. 60-70, Springer (2010).

Agenda

- Background & Motivation
- DD and QD arithmetic
- Features of QuPAT
  (Quadruple Precision Arithmetic Toolbox)
- Numerical experiment
  (Partial use of DD arithmetic)
- Conclusion

Multiple precision arithmetic

DD and QD arithmetic (Hida, Li and Bailey [2])

- ✓Using **some double precision numbers**
  - ✓DD : quasi quadruple precision
  - ✓QD : quasi octuple precision
- ✓**Combination** of double precision arithmetic operations

  ⟶ **only** needs **double** precision arithmetic environment

QuPAT uses these arithmetic on Scilab

[2] Y. Hida, X. S. Li and D. H. Bailey, Quad-double arithmetic: algorithms, implementation, and application. Technical Report LBNL-46996, Lawrence Berkeley National Laboratory, Berkeley, CA 94720 (2000).

Number representation

DD number a is represented by 2 double precision numbers as follow:

$$a = a_0 + a_1, \quad \begin{cases} a_0 : \text{higher part of } a \\ a_1 : \text{lower part of } a \end{cases}$$

where a_0 and a_1 satisfy $|a_1| \leq \frac{1}{2}\mathrm{ulp}(a_0)$.

*ulp (units in the last place)

	a_0			a_1		
DD	s	$e_1 \dots e_{11}$	$m_1 \dots m_{52}$	s	$e_1 \dots e_{11}$	$m_1 \dots m_{52}$
IEEE quad.	s	$e_1 \dots e_{15}$	$m_1 \dots m_{112}$			

QD number is represented in the same way as follow:

$$a = a_0 + a_1 + a_2 + a_3$$

Number of operations

		+, −	∗	/	total
DD	addition, subtraction	11	0	0	11
	multiplication	15	9	0	24
	division	17	8	2	27
QD	addition, subtraction	84	0	0	84
	multiplication	163	46	0	209
	division	713	88	5	806

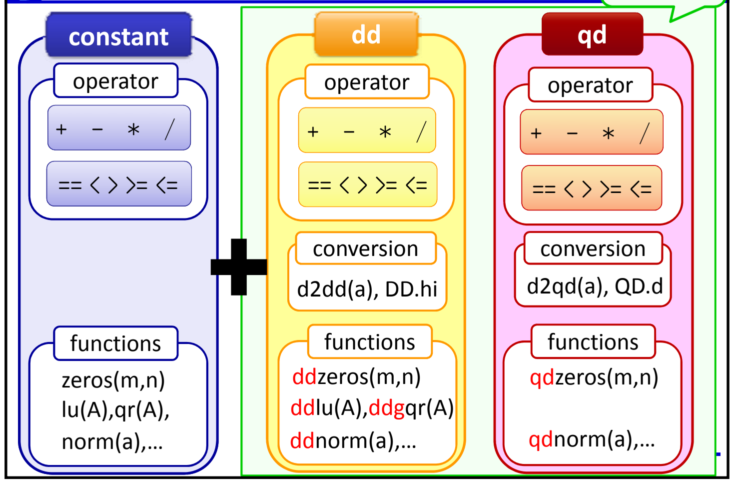
QuPAT(Quadruple Precision Arithmetic Toolbox)

Convenient multiple precision arithmetic toolbox on Scilab

- ✓The same operator (+, −, ∗, /) can be used for double, DD, and QD arithmetic.

  ⇨ We can write a code simply and easily.
- ✓Double, DD, and QD arithmetic can be used at the same time, and also mixed precision arithmetic is available.
- ✓It is independent of any hardware and operating systems.

Relationship between Scilab & QuPAT



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Application of QuPAT

GCR (Generalized Conjugate Residual) method

One of the Krylov subspace method for solving nonsymmetric linear systems $\boldsymbol{Ax} = \boldsymbol{b}$.

Properties

n : dimension of A

- In theory, the residual norm converges at most n iterations.
- Using floating point arithmetic, the residual norm often stagnates by round-off errors.

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Computational condition

Matrix : olm2000
Dimension : 2000
Condition number : 5.94×10^6
(from The University of Florida Sparse Matrix Collection)

Scilab version 5.1.1 on Windows XP

Maximum iteration : 2000
Initial vector : $\boldsymbol{x_0} = (0, 0, \cdots, 0)^T$
Solution vector : $\boldsymbol{x^*} = (1, 1, \cdots, 1)^T$
Stopping criterion : $\|\boldsymbol{r_k}\|_2 \leq 10^{-12} \|\boldsymbol{r_0}\|_2$

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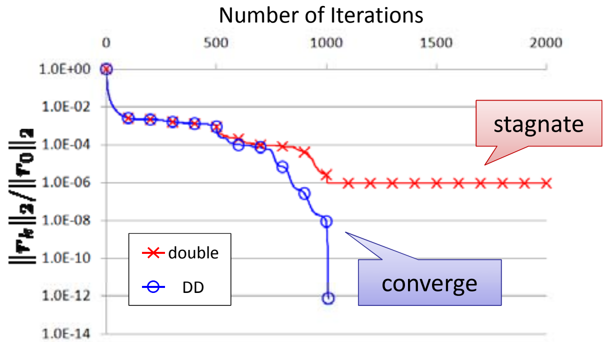
Computational results of double and DD



	Number of Iter.	$\|b-Ax\|_2/\|r_0\|_2$	$\|x-x^*\|_\infty/\|x^*\|_\infty$
double	×	9.11E-07	8.67E-03
DD	1009	7.10E-13	3.56E-09

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Reviewing iterative process of GCR

Let x_0 be an initial guess.
set $r_0 = b - Ax_0,\ p_0 = r_0,\ q_0 = Ap_0,\ k = 0$
while $\|r_k\|_2 < \varepsilon\|r_0\|_2$ and $k < n$ do
$\alpha_k = (r_k, q_k)/(q_k, q_k)$
$x_{k+1} = x_k + \alpha_k p_k$
$r_{k+1} = r_k - \alpha_k q_k$
for $i = 0, \cdots, k$ do
$\beta_{k,i} = -(Ar_{k+1}, q_i)/(q_i, q_i)$
$p_{k+1} = r_{k+1} + \sum_{i=0}^{k} \beta_{k,i} p_i$
$q_{k+1} = Ar_{k+1} + \sum_{i=0}^{k} \beta_{k,i} q_i$
$k = k + 1$

iteration

Updating approximate solution and residual (Strategy 1)

Generating a basis vector (Strategy 2)

DD arithmetic is partially used for α and β [3].

[3] T. Saito, E. Ishiwata and H. Hasegawa, Analysis of the GCR method with mixed precision arithmetic using QuPAT, Journal of Computational Science, in press

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Strategy 1 (using DD arithmetic for α)

Let x_0 be an initial guess.
set $r_0 = b - Ax_0,\ p_0 = r_0,\ q_0 = Ap_0,\ k = 0$
while $\|r_k\|_2 < \varepsilon\|r_0\|_2$ and $k < n$ do
$\alpha_k = (r_k, q_k)/(q_k, q_k)$
$x_{k+1} = x_k + \alpha_k p_k$
$r_{k+1} = r_k - \alpha_k q_k$
for $i = 0, \cdots, k$ do
$\beta_{k,i} = -(Ar_{k+1}, q_i)/(q_i, q_i)$
$p_{k+1} = r_{k+1} + \sum_{i=0}^{k} \beta_{k,i} p_i$
$q_{k+1} = Ar_{k+1} + \sum_{i=0}^{k} \beta_{k,i} q_i$
$k = k + 1$

- α_k (inner product, division)
  x_{k+1}, r_{k+1} (product, sum)
  …DD arithmetic
- α_k, r_{k+1}
  …DD numbers

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Strategy 2 (using DD arithmetic for β)

Let x_0 be an initial guess.
set $r_0 = b - Ax_0,\ p_0 = r_0,\ q_0 = Ap_0,\ k = 0$
while $\|r_k\|_2 < \varepsilon\|r_0\|_2$ and $k < n$ do
$\alpha_k = (r_k, q_k)/(q_k, q_k)$
$x_{k+1} = x_k + \alpha_k p_k$
$r_{k+1} = r_k - \alpha_k q_k$
for $i = 0, \cdots, k$ do
$\beta_{k,i} = -(Ar_{k+1}, q_i)/(q_i, q_i)$
$p_{k+1} = r_{k+1} + \sum_{i=0}^{k} \beta_{k,i} p_i$
$q_{k+1} = Ar_{k+1} + \sum_{i=0}^{k} \beta_{k,i} q_i$
$k = k + 1$

- $\beta_{k,i}$ (inner product, division)
  p_{k+1}, q_{k+1} (product, sum)
  …DD arithmetic
- $\beta_{k,i}, q_{k+1}$
  …DD numbers

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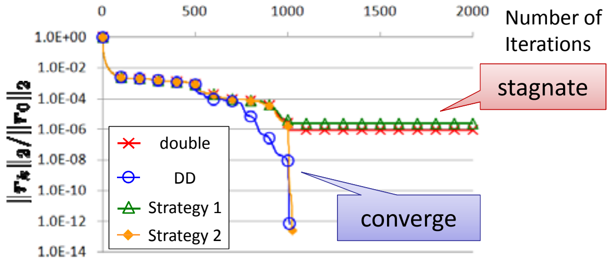
Computational results of 2 strategies



	Number of Iter.	$\|b - Ax\|_2/\|r_0\|_2$	$\|x - x^*\|_\infty/\|x^*\|_\infty$
double	×	9.11E-07	8.67E-03
DD	1009	7.10E-13	3.56E-09
Strategy 1	×	2.38E-06	2.28E-02
Strategy 2	1025	2.87E-11	5.92E-09

Strategy 2 shows almost the same convergence as DD !

Relation between α_k and convergence

Let x_0 be an initial guess.

set $r_0 = b - Ax_0,\ p_0 = r_0,\ q_0 = Ap_0,\ k = 0$

while $\|r_k\|_2 < \varepsilon\|r_0\|_2$ and $k < n$ do

$\alpha_k = (r_k, q_k) / (q_k, q_k)$ ← $\alpha_k \approx 0$ ⇒ $r_{k+1} \approx r_k$

$x_{k+1} = x_k + \alpha_k p_k$

$r_{k+1} = r_k - \alpha_k q_k$

for $i = 0, \cdots, k$ do

$\beta_{k,i} = -(Ar_{k+1}, q_i) / (q_i, q_i)$

$p_{k+1} = r_{k+1} + \sum_{i=0}^{k} \beta_{k,i} p_i$

$q_{k+1} = Ar_{k+1} + \sum_{i=0}^{k} \beta_{k,i} q_i$

$k = k + 1$

iteration

α_k is reflected by the accuracy of q_k

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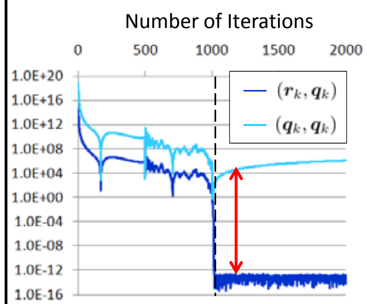
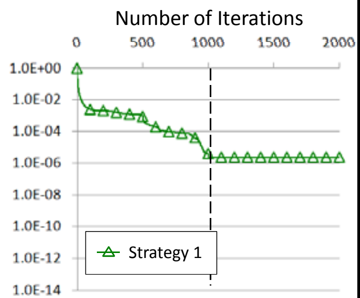
The reason of stagnation is α_k

$|\alpha_k|$ in Strategy 1



Convergence history



$\alpha_k \approx 0$ → Stagnate

$$\alpha_k = \frac{(r_k, q_k)}{(q_k, q_k)}$$

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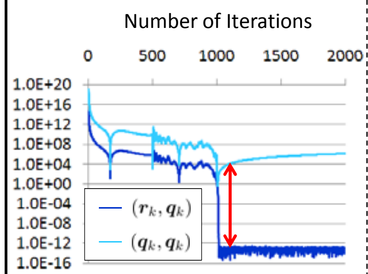
Compare two strategies

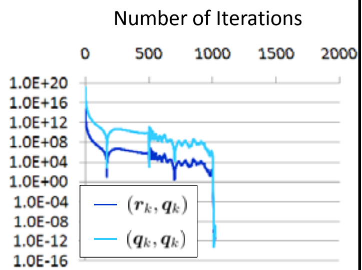
$$\alpha_k = \frac{(r_k, q_k)}{(q_k, q_k)}$$

Strategy 1



$\alpha_k \approx 0$ → Stagnate

Strategy 2



Maintain convergence

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Conclusion

- Partial use of DD arithmetic to GCR is effective!
  - Using DD for only $\beta_{k,i}$ and q_k achieves **almost the same convergence** as full DD
- QuPAT enable us to write multiple precision code **simply** on Scilab!
  - Can be used **the same operators** $(+, -, *, /)$
  - **Independent** of any hardware and operating systems

QuPAT is available at
http://www.mi.kagu.tus.ac.jp/qupat.html

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