XHYPRE: A HIGH-PRECISION NUMERICAL SOFTWARE PACKAGE FOR SOLVING LARGE-SCALE SPARSE LINEAR EQUATIONS

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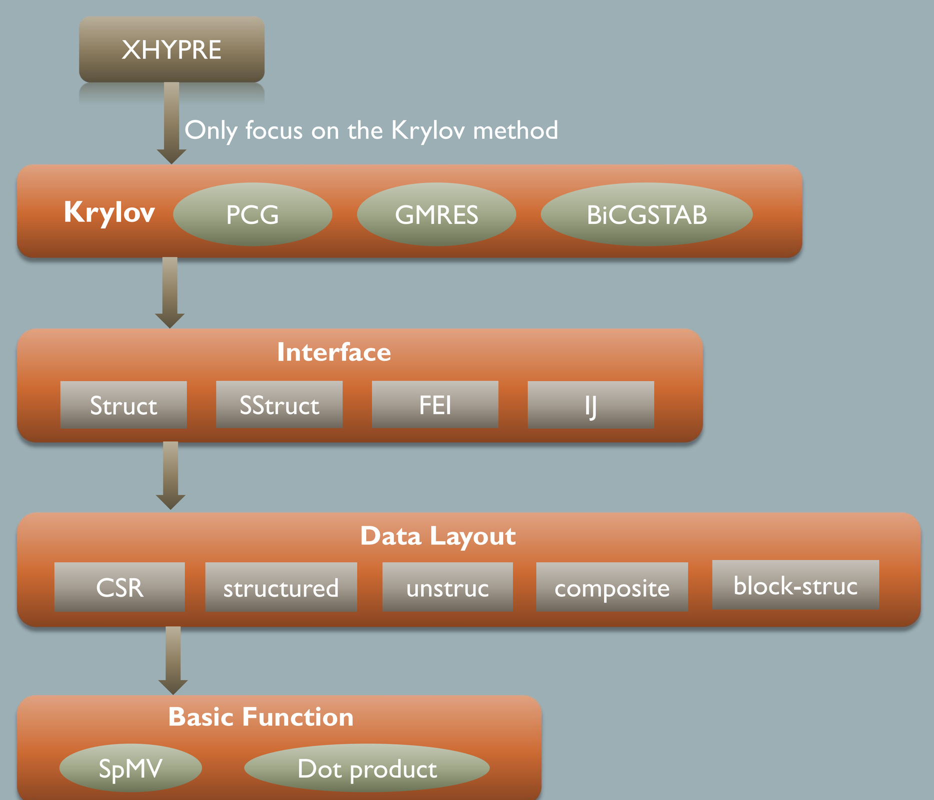
Introduction

When there are floating-point numbers with a limited number of digits representing real numbers, rounding errors will occur. Rounding error is unavoidable in floating-point operations, and it means the numerical difference between the exact value and the approximate value obtained by floating-point computation. We study how to control the cumulative effect of rounding errors because of the inaccurate results of numerical calculations on high-performance computing platforms.



Software design of XHYPRE

In this paper, we adopt the error-free transformation technology to design and implement a high-precision numerical software package XHYPRE with the high-precision algorithms above for large-scale sparse linear equations. It is open-sourced at https://github.com/compilerOpt/-XHYPRE-2.0.0.

Methods

- The high-precision dot product algorithm in XHYPRE uses the Dot2 algorithm[3].
- We improve the TwoProd algorithm in the Dot2 algorithm to the TwoProdFMA algorithm.

Algorithm 1 Dot2 Algorithm

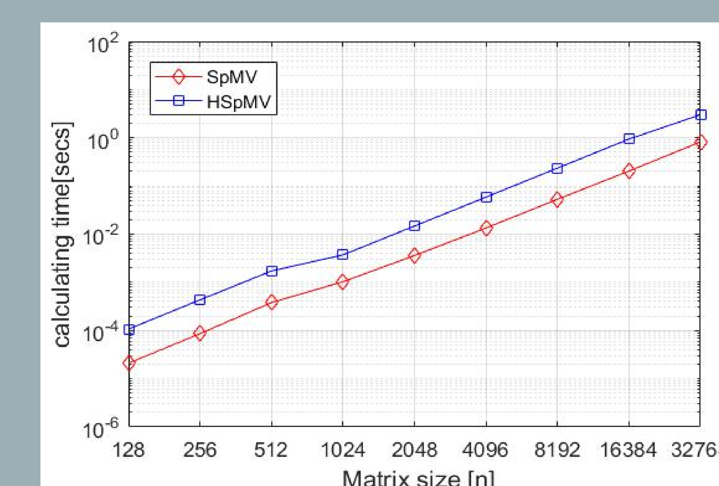
Input:
Two vectors: p, q;
Output:
The result of the dot product: res;
Initialize $th = 0, res = 0$;
for $t = 1$ **to** $tnum$ **do**
  $[h, l]$ = TwoProdFMA(p_t,q_t);
  $[th, tl]$ = TwoSum(th, h);
  $res = res + (l + tl)$;
end for
$res = res + th$;
return res.

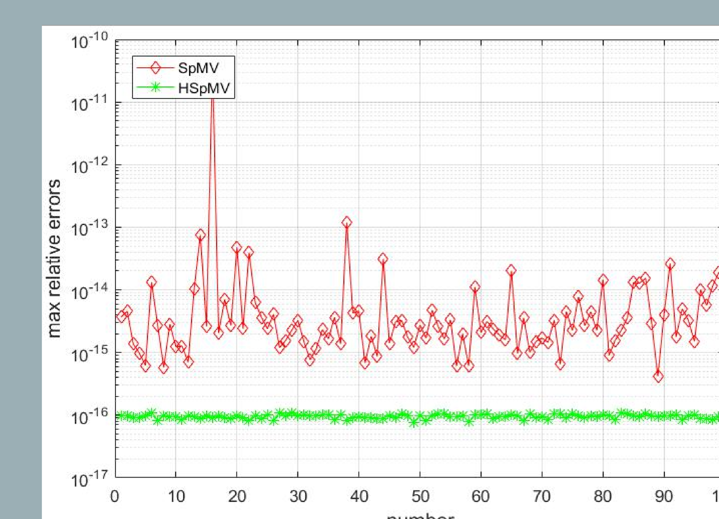
Methods

- The execution process of high-precision sparse matrix-vector multiplication is shown in Algorithm 2.
- Using the high-precision algorithm is the ordinary floating-point result of SpMV that adds the rounding errors.

Algorithm 2 SpMV in XHYPRE (HSpMV)

Input:
$nrows, A\_value, A\_index, A\_pointer, x$;
Output:
Vector: b;
for $i = 0$ **to** $nrows - 1$ **do**
  Initialize $th = 0, res = 0$;
  for $j = A\_pointer[i]$ **to** $j = A\_pointer[i+1] - 1$ **do**
    $[h, l]$ = TwoProdFMA($A\_value[j]$,$x[A\_index[j]]$);
    $[th, tl]$ = TwoSum(th, h);
    res = res + (l + tl);
  end for
  $b_i = res + th$;
end for
return b.





- The following will briefly explain the GMRES algorithm as an example. Algorithm 3 is a high-precision GMRES.
- The implementation process of PCG and BiCGSTAB is similar to the GMRES of high-precision, so we do not introduce them in detail.
- The input and output of the algorithm remain unchanged.

Algorithm 3 High-precision Generalized Minimal Residual method (HGMRES)

Input:
Matrix A, vector b;
Output:
Approximate solution of linear system $Ax = b$;
1: Compute $r_0 = b - \text{HSpMV}(A, x_0)$, $\beta = \sqrt{\text{Dot2}(r_0, r_0)}$, and $v_1 = r_0/\beta$;
2: **for** $t = 1$ **to** $tnum$ **do**
3:   Compute $w_t = \text{HSpMV}(A, v_t)$;
4:   **for** $m = 1$ **to** t **do**
5:     $h_{mt} = \text{Dot2}(w_t, v_t)$;
6:     $w_t = \text{Dot2}(w_t, h_{mt}v_t)$;
7:   **end for**
8:   $h_{t+1,t} = \sqrt{\text{Dot2}(w_t, w_t)}$. If $h_{t+1,t} = 0$ set $tnum = t$ and go to 11
9:   $v_{t+1} = w_t/h_{t+1,t}$;
10: **end for**
11: Define the $(tnum + 1) \times tnum$, Hessenberg matrix $\overline{H}_{tnum} = \{h_{mt}\}_{1 \le m \le m+1, 1 \le t \le tnum}$.
12: Compute y_{tnum} the minimizer of $\|\beta e_1 - \overline{H}_{tnum} y\|_2$ and $x_{tnum} = x_0 + V_{tnum} y_{tnum}$
13: **return** x.

The dot product and SpMV become a high-precision solution, which reduces the accumulation of rounding errors and makes the calculation more accurate.

Experiment

Extensive experiments were conducted on the AMD platform, and the results illustrate that XHYPRE is effective.

Experiment

- Solverchallenge21_01 is derived from the three-dimensional photon equation of radiation fluid mechanics and is a structural grid.
- Solverchallenge21_03 is derived from the linear elastic equation of the contact mechanics of the centrifuge device and is a first-order nodal finite element.

Table 1: Specific information of the matrix

name	order	non-zero element	Application area	Convergence
solverchallenge21_01	2,097,152	14,581,760	Laser fusion	<1e-10
solverchallenge21_03	83,073	2,826,927	Engineering mechanics	<1e-8

The two matrices solved in HYPRE do not converge but converge in XHYPRE.

Table 1: Test results of HYPRE and XHYPRE (number of iterations)

Name	HYPRE	XHYPRE	Remark
solverchallenge21_01	not convergent	4431	without precondition
solverchallenge21_03	not convergent	704	with ILU(0)

It can prove the convergence of XHYPRE, and XHYPRE can alleviate the problem of non-convergence in the calculation of HYPRE.

We use an example to perform a detailed experiment to illustrate the performance of XHYPRE, which can be solved by both HYPRE and XHYPRE.

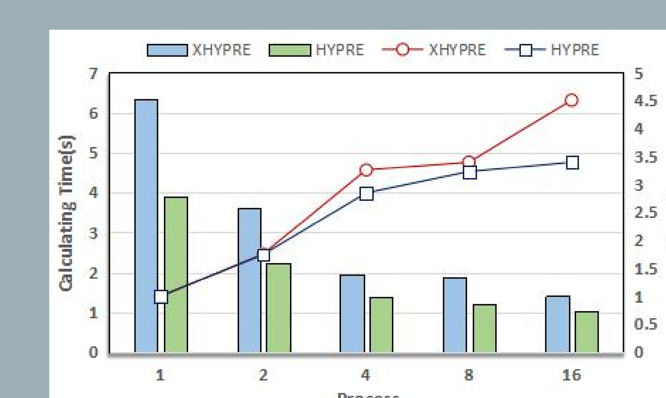


Figure : (a)The calculation time and speedup(N=122500).(b)The calculation time and speedup(N=2^26)

Therefore, while the accuracy is improved to make the result more accurate, the calculation time of XHYPRE does not increase too much.

Conclusion

- We propose a high-precision sparse matrix-vector multiplication algorithm based on error-free transformation techniques.
- We design high-precision GMRES, PCG, and BiCGSTAB algorithms to reduce rounding errors in calculations.
- We propose a high-precision numerical algorithm library XHYPRE for large-scale sparse linear equations, which is used to solve the rounding error problem of large-scale numerical simulation calculations. It is open-sourced at https://github.com/compilerOpt/-XHYPRE-2.0.0.

References

[1] W. Kahan. Pracniques: further remarks on reducing truncation errors. Communications of the ACM, 8 (1): 40, 1965.

[2] D. E. Knuth. The art of computer programming. Pearson Education, 1997.

[3] T. Ogita, S. Rump, S. Oishi. Accurate sum and dot product.SIAM Journal on Scientific Computing, 26(6): 1955-1988, 2005.