

PRC 2022

Final presentation

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11/28/2022

Experimentation with FrontISTR

- Experimental Environment
- CAE Simulation model
- Simulation parameter + visualization results

Experimental Environment

- Intel machine

- CPU: Intel Xeon E5 (36C / 72T)
- Memory: 128 GB DDR4 RAM
- Storage: local Intel NVMe SSD 750 Series 1.2TB



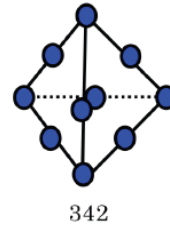
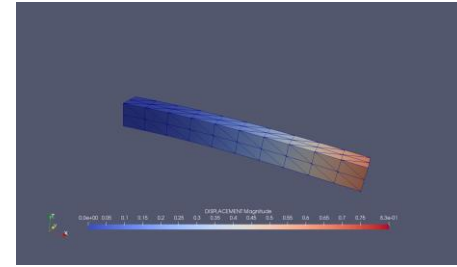
- FrontISTR build

- Version: 5.4 (latest)
- Compilers: **Intel compilers** (mpiifort, mpiicc, mpiicpc) version 20.2.6.20220226
 - options: -O3 -xhost
- Build with cmake 3.16
 - Intel OpenMP 5.1 , Intel MPI 3.1, Scalapack-2.1.0, Intel MKL 2022.1.0 (BLAS, LAPACK)
 - Metis 5.1.0, Trilinos 13.0.1

FrontISTR Simulation: 3D Beam model

● 3D Beam model

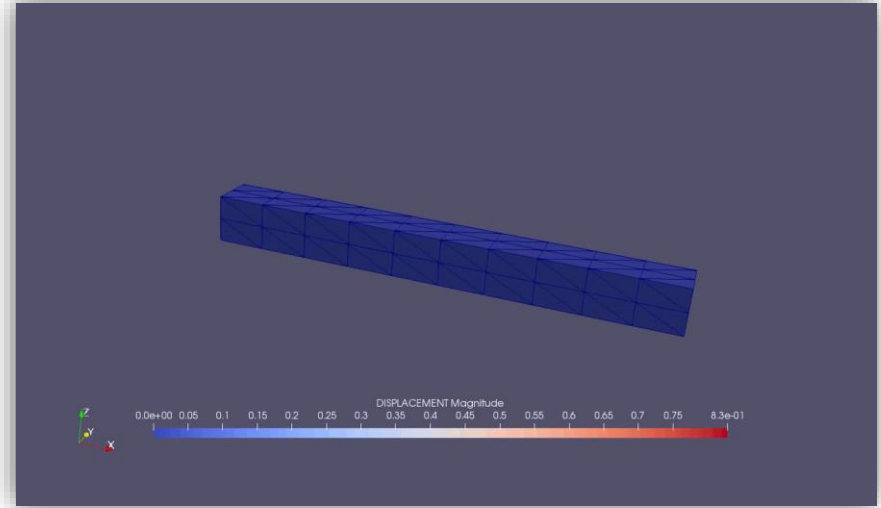
- Application: tutorial, material fatigue
- Mesh: 524 nodes
- Element: 240 elements
- Element type: = 10-nodes tetrahedral quadratic (ID=342)
- Material: Elastic Solid
 - Young modulus=4000
 - Poisson ratio=0.3
 - Density=1.0E-8
- Boundary conditions:
 - left part is fixed
 - concentrated load is applied to other part with given amplitude



FrontISTR Simulation: 3D Beam model

● Simulation parameters

- Analysis type: Dynamic Nonlinear
- Numerical method: Newmark
- Linear Solver: CG-DIAG
- Linear tolerance: 1E-06
- Nonlinear tolerance: 1E-03
- Timesteps: 100,000
- OMP Threads: 72, 36
- Simulation computation time: 796.88 sec



Nonlinear dynamic analysis

- Governing Equation
- Algorithm
- Numerical Method

Governing Equation

- Dynamic equation of motion:

$$M\ddot{u}_n + r(u_n, \dot{u}_n) = f(t_n)$$
$$u(t_0) = u_0, \quad \dot{u}(t_0) = \dot{u}_0$$

with:

M : mass matrix

r : restoring force

f : external force vector

$u_n, \dot{u}_n, \ddot{u}_n$: displacement, velocity, acceleration at timestep t_n

$M\ddot{u}_n$: inertial force

$r(u_n, \dot{u}_n)$: damping + internal forces

Dynamic Nonlinear Implicit Algorithm

- Dynamic Nonlinear Implicit Algorithm:
 - Initialization
 - For each timestep {
 - For each nonlinear iteration {
 - Stiffness Matrix Generation
 - Linear Solver
 - Update Newton
 - Write Results

Newmark method

- Newmark method is used to compute next timestep acceleration (\rightarrow velocity and position)

1. $\ddot{u}_{k+1} \leftarrow 0$

2. $u_{k+1} = u_k + \dot{u}_k \Delta t + \ddot{u}_k \left(\frac{1}{2} - \beta\right)\Delta t^2 + \ddot{u}_{k+1}\beta\Delta t^2$

3. $\dot{u}_{k+1} = \dot{u}_k + \ddot{u}_k (1 - \gamma)\Delta t + \ddot{u}_{k+1}\gamma\Delta t$

4. $\boldsymbol{\varepsilon} \leftarrow f(t_{k+1}) - r(u_{k+1}, \dot{u}_{k+1}) - M\ddot{u}_{k+1}$ # $\boldsymbol{\varepsilon}$ is the nonlinear residual value

5. **while** $\|\boldsymbol{\varepsilon}\| \geq$ nonlinear tolerance **do**

i. $\Delta\ddot{u}_{k+1} \leftarrow (M + C\gamma\Delta t + K\beta\Delta t^2)^{-1} \boldsymbol{\varepsilon}$ # $\mathbf{x} \leftarrow \mathbf{A}^{-1}\mathbf{b} \implies$ solving $\mathbf{Ax}=\mathbf{b}$ requires a linear solver

ii. $\ddot{u}_{k+1} \leftarrow \ddot{u}_{k+1} + \Delta\ddot{u}_{k+1}$

iii. $\dot{u}_{k+1} \leftarrow \dot{u}_{k+1} + \Delta\ddot{u}_{k+1} \gamma\Delta t$

iv. $u_{k+1} \leftarrow u_{k+1} + \Delta\ddot{u}_{k+1} \beta\Delta t^2$

v. $\boldsymbol{\varepsilon} \leftarrow f(t_{k+1}) - r(u_{k+1}, \dot{u}_{k+1}) - M\ddot{u}_{k+1}$

6. **end while**

The numerical precision of simulation results $(u_n, \dot{u}_n, \ddot{u}_n)$ depends directly on the linear solver solution $(\Delta\ddot{u}_n)$.

FrontISTR and Numerical Precision

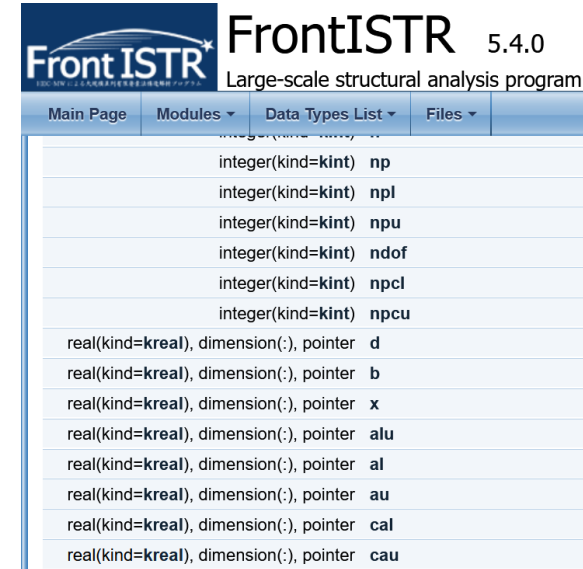
- Research scope
- Numerical Precision in FrontISTR
- Double precision FP number
- QPBLAS

Research Scope

- Focus on **improving numerical precision of Linear Solver**.
➔ will improve the numerical precision of CAE simulation.
- Target specific linear solver: the **Conjugate Gradient method with Diagonal Scaling preconditioner** (widely used in numerical simulation).

Numerical precision in FrontISTR

- In FrontISTR, linear solver are defined in the HECMW library.
- Linear solver data (matrix and vector) are defined in the `hecmwST_matrix` structure.
- The Fortran data type used for matrix/vector is `real(kind=kreal)` with `kreal=8` → 8-bytes floating point number = 64-bits FP number = **double precision**



FrontISTR 5.4.0
Large-scale structural analysis program

Main Page	Modules	Data Types List	Files
		integer(kind=kint)	np
		integer(kind=kint)	npl
		integer(kind=kint)	npu
		integer(kind=kint)	ndof
		integer(kind=kint)	npcl
		integer(kind=kint)	npcu
		real(kind=kreal), dimension(:), pointer	d
		real(kind=kreal), dimension(:), pointer	b
		real(kind=kreal), dimension(:), pointer	x
		real(kind=kreal), dimension(:), pointer	alu
		real(kind=kreal), dimension(:), pointer	al
		real(kind=kreal), dimension(:), pointer	au
		real(kind=kreal), dimension(:), pointer	cal
		real(kind=kreal), dimension(:), pointer	cau

◆ kreal

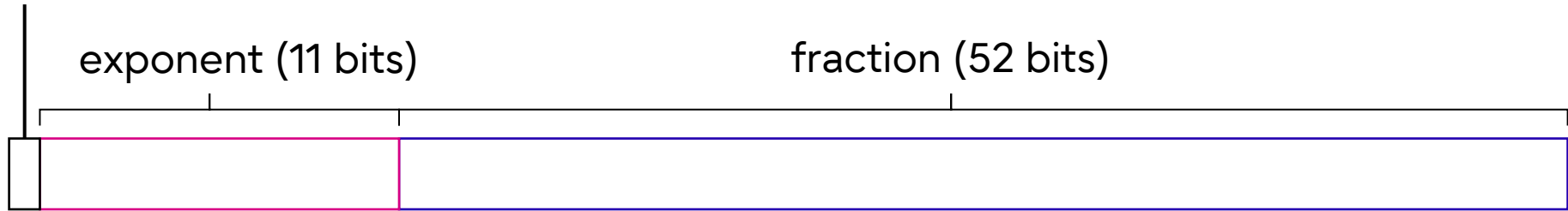
integer(kind=4), parameter hecmw_util::kreal = 8

Definition at line 16 of file `hecmw_util_f.F90`.

Problem of Double precision FP number

- double-precision floating point numbers

sign (1 bit)



- Representation: $(-1)^s \times (1 + \text{fraction}) \times 2^E$
- Exponent field size impacts the range.
- Fraction field size impacts the precision.
- When fraction part of computation results contains more than 52 bits, rounding occurs. → **rounding error.**

QPBLAS for rounding error reduction

- **Quadruple Precision BLAS Routines** (QPBLAS) has been developed by JAEA.
- QPBLAS provides high-precision linear algebra routines.
- QPBLAS simulates 128 bits computation using **double-double algorithm** (two 64-bits numbers represent one 128-bits number).
- QPBLAS leverages fast double-precision computation with almost the same precision of hardware-based 128 bits computation.

QPBLAS x FrontISTR

- Build FrontISTR with QPBLAS library
- CG with DD arithmetic and QPBLAS
- Data Structure modification
- Integration of DD arithmetic inside FrontISTR source code

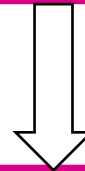
Compilation of FrontISTR with DD library

- We want to incorporate QPBLAS routine in FrontISTR for high-precision CAE simulation.
- Build phase: we add this line to the fistr1/CMakeLists.txt
 - `target_link_libraries(fistr hecmw -lblas -lddblas)`

Implementation of DD arithmetic in FrontISTR

- Implementation of DD arithmetic in `hecmw_dd` module
 - dd version of: add, sub, mul and div
- Integration of DD arithmetic for CG solver: we modified:
 - `hecmw_solve_CG`
 - `solver_misc::hecmw_InnerProduct_R`
 - `solver_misc:: hecmw_xpay_R`
 - `solver_misc:: hecmw_axpy_R`
 - `solver_las::hecmw_matvec`
 - `hecmw_matvec_33, hecmw_matvec_33_inner`
 - `solver_las::hecmw_matresid`
 - `hecmw_matresid_33`
 - `hecmw_solver_scaling_33`
 - `hecmw_precond_apply` (Diagonal Scaling preconditioner in DD has been implemented)
 - `hecmw_precond_apply_33, hecmw_precond_DIAG_33`

`original_fistr_routine(X,Y,alpha)`



`dd_routine(XH,YH,alphaH,XL,YL,alphaL)`
`real(kind=kreal), optional :: XL(:), YL(:), alphaL`


Use of QPBLAS routines in FrontISTR

- Original hecmw code has been replaced by QPBLAS routines:

- **hecmw_solver_misc.f90:**

- hecmw_innerproduct_R → **DDDOT**
- hecmw_axpy_R → **DDAXPY**
- hecmw_copy_R → **DDCOPY**

```
do i = 1, hecMESH%nn_internal * ndof
  Y(i) = X(i)
end do
```



```
if (present(XL)) then
  call DDCOPY(hecMESH%nn_internal*ndof, XH, XL, 1, YH, YL, 1)
```

Data structure modification

- CG solver of HECMW library relies on QPBLAS routine to perform high precision computation with DD algorithm.
 - CG solves $Ax=b$ with DD variables: `solve_lineq(hecMAT)`
 - CG outputs `xh` and `xl`, the solution vector (= incremental displacement) into `hecMAT%xh` and `hecMAT%xl` new attributes.

hecMAT: new attributes

```
type hecmwST_matrix
routine fstr_mat_init
routine hecMAT_init
```

hecMAT: new attributes: memory allocation

```
884 890   hecMAT%AL = 0.0d0
885 891   hecMAT%AU = 0.0d0
886 892   hecMAT%B  = 0.0d0
887 893 +   hecMAT%BH = 0.0d0
887 894 +   hecMAT%BL = 0.0d0
887 895   hecMAT%X  = 0.0d0
887 896 +   hecMAT%XH = 0.0d0
887 897 +   hecMAT%XL = 0.0d0
888 898   hecMAT%ALU = 0.0d0
889 899   end subroutine hecMAT_init
868 872   allocate (hecMAT%X(ndof*hecMAT%NP) ,stat=ierror )
873 +   allocate (hecMAT%XH(ndof*hecMAT%NP) ,stat=ierror )
874 +   allocate (hecMAT%XL(ndof*hecMAT%NP) ,stat=ierror )
```

FrontISTR code: from x to disp results (1)

- `type(hecmwST_matrix), pointer :: hecMATmpc`
- For each timestep:
 - For each nonlinear iteration:
 - solution vector is stored into `hecMATmpc%XH` and `hecMATmpc%XL`
 - call `solve_LINEQ(hecMESHmpc,hecMATmpc)`
 - `hecMATmpc%X[H/L]` is copied into `hecMAT%X[H/L]`
 - call `hecmw_mpc_tback_sol(hecMESH, hecMAT, hecMATmpc)`
 - !the solution x (= incremental displacement) is added to the displacement value as an "update".
 - do `j=1,hecMESH%n_node*ndof`
 - `fstrSOLID%dunode(j) = fstrSOLID%dunode(j)+hecMAT%X(j)`
 - enddo

FrontISTR code: from x to disp results (2)

- For each timestep:
 - For each nonlinear iteration:
 - !updates the stress, strain and internal forces (not related to displacement value so not modified)
 - fstr_UpdateNewton(fstrSOLID, hecMAT)
 - !computation of new displacement, velocity and acceleration
 - do j = 1, ndof*nnod
 - fstrDYNAMIC%ACC(j,1:2) = -a1*fstrDYNAMIC%ACC(j,1) - a2*fstrDYNAMIC%VEL(j,1) + a3*fstrSOLID%dunode(j)
 - fstrDYNAMIC%VEL(j,1:2) = -b1*fstrDYNAMIC%ACC(j,1) - b2*fstrDYNAMIC%VEL(j,1) + b3*fstrSOLID%dunode(j)
 - fstrSOLID%unode(j) = fstrSOLID%unode(j) + fstrSOLID%dunode(j)
 - fstrDYNAMIC%DISP(j,2) = fstrSOLID%unode(j)
 - enddo
 - !! Output the values
 - call fstr_dynamic_Output(hecMESH, fstrSOLID, fstrDYNAMIC, fstrPARAM)

↑
Final simulation results

Code snippet

```
!DD arithmetic
fstrSOLID%dunodeH = fstrSOLID%dunode
fstrSOLID%dunodeL = 0.0d0

do j=1,hecMESH%n_node*ndof
  !fstrSOLID%dunode(j) = fstrSOLID%dunode(j)+hecMAT%X(j) !original code
  call dd_add(fstrSOLID%dunodeH(j), fstrSOLID%dunodeL(j), hecMAT%XH(j), hecMAT%XL(j), ch, c1)
  fstrSOLID%dunodeH(j) = ch
  fstrSOLID%dunodeL(j) = c1
enddo

!DD Integration
fstrSOLID%dunode = fstrSOLID%dunodeH
```

Code snippet

```
! DD arithmetic
!fstrSOLID%unode(j) = fstrSOLID%unode(j)+fstrSOLID%dunode(j) !original code
call dd_add(fstrSOLID%unodeH(j), fstrSOLID%unodeL(j), fstrSOLID%dunodeH(j), fstrSOLID%dunodeL(j), ch, cl)
fstrSOLID%unodeH(j) = ch
fstrSOLID%unodeL(j) = cl

!fstrDYNAMIC%DISP(j,2) = fstrSOLID%unode(j) !original code
fstrDYNAMIC%DISPH(j,2) = fstrSOLID%unodeH(j)
fstrDYNAMIC%DISPL(j,2) = fstrSOLID%unodeL(j)
```

Evaluation

- Simulation results
- Numerical precision: number of digits
- Calculation time
- Conclusion
- PRC output

Comparison: simulation results

- We compare the original FrontISTR results with the one obtained with QPBLASxFrontISTR after 1000 timesteps analysis:

fistrDYNAMIC%DISP
computed from original hecMAT%X

fistrDYNAMIC%DISP
computed from hecMAT%XH

Timestep: 1k

DISPLACEMENT Magnitude
0.0e+00 0.0005 0.001 0.0015 0.002 0.0025 0.003 0.0035 0.004 0.0045 0.005 0.0055 0.006 0.0065 7.3e-03

Timestep: 1k

DISPLACEMENT Magnitude
0.0e+00 0.0005 0.001 0.0015 0.002 0.0025 0.003 0.0035 0.004 0.0045 0.005 0.0055 0.006 0.0065 7.3e-03

- Results are identical, showing that XH part is same as original X
- However, we also have XL part which increases the precision of XH

Comparison: numerical precision (digits number)

- We look at the numerical precision of:

Original FrontISTR
hecMAT%X

Last value of hecMAT%X:

1.047940573281168E-010

Double precision number:
16 digits

QPBLASxFrontISTR
hecMAT%XH
hecMAT%XL

Last value of hecMAT%XH:

1.047940573281168E-010

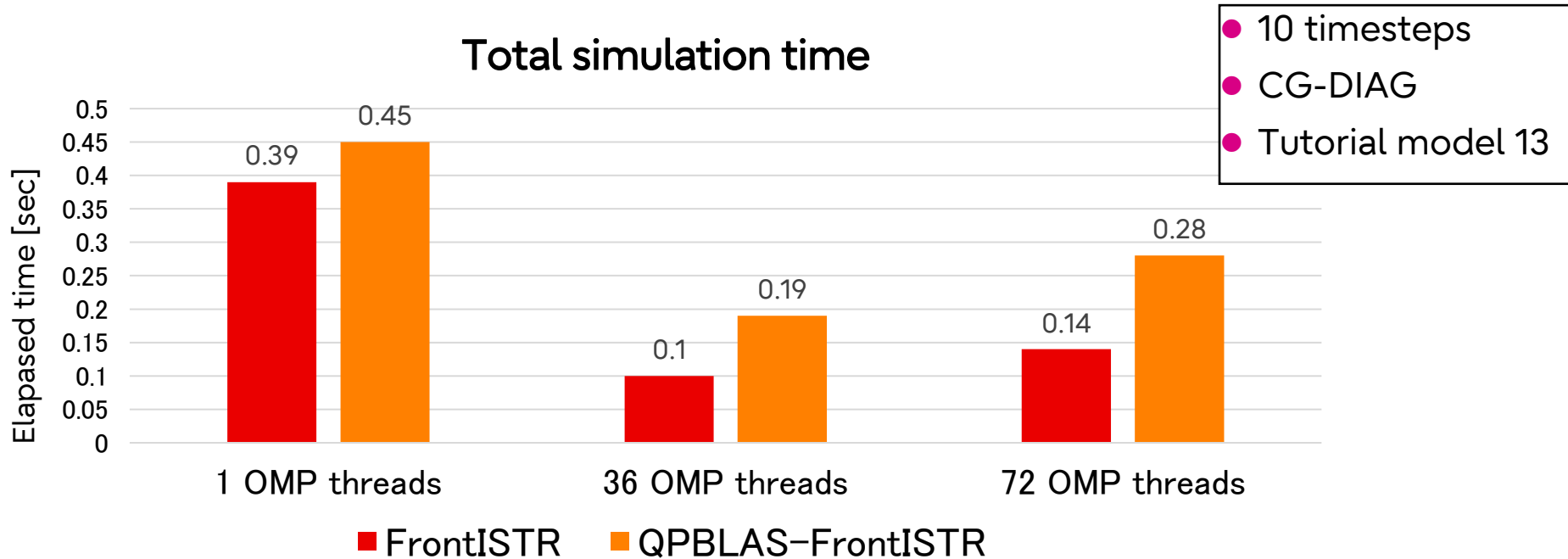
and corresponding hecMAT%XL value:

-2.351042639634128E-027

XH+XL= 1.0479405732811679764895736036587E-10

Quadruple precision number
32 digits → rounding error is reduced

Computation time comparison



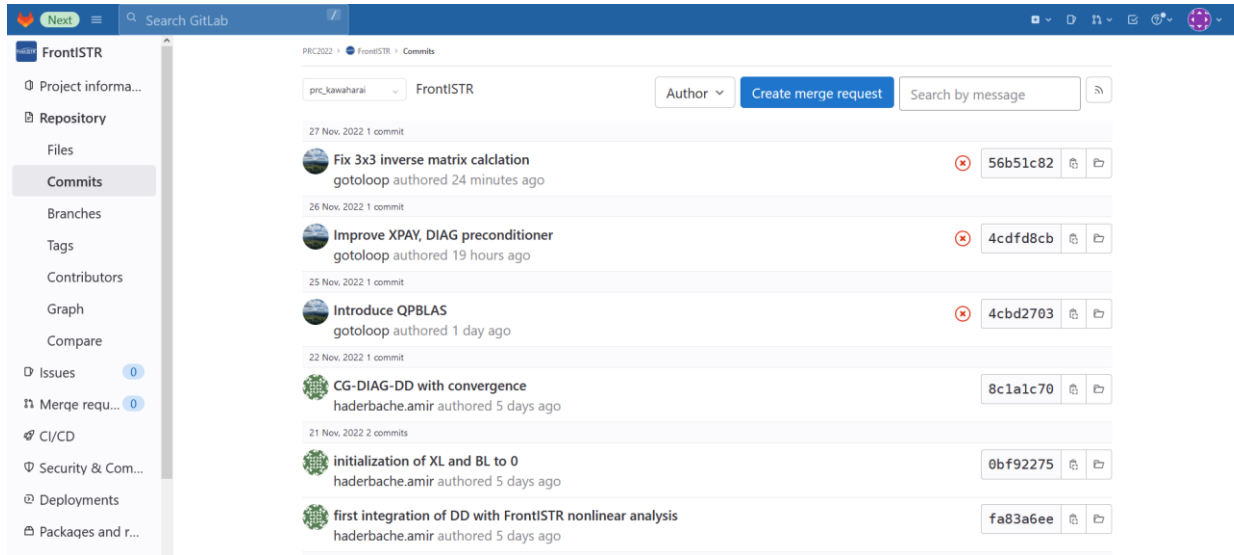
It looks like QPBLAS has some overhead compared with original FrontISTR. We want to investigate such results in future work. Todo: check solver iteration numbers, check how it evolves with increased problem size.

Conclusion

- We implemented and integrated QPBLAS calculation into FrontISTR FEM simulation in the scope of CG-DIAG solver.
- We confirmed that displacement results have higher numerical precision (32 digits versus original 16) with DD algorithm.
- Next work:
 - Find a simulation model which cannot converge with original FrontISTR CG-DIAG and shows that enhanced numerical precision allows convergence for difficult problem. Try high condition number, poisson ratio=0.4999
 - Optimize QPBLASxFrontISTR computational time.
 - Implement I/O to output results files for DD values.

PRC Project: output

- QPBLAS X FrontISTR source code can be found at:
 - https://gitlab.com/prc2022/FrontISTR/-/tree/prc_kawaharai
 - https://gitlab.com/prc2022/FrontISTR/-/tree/prc_amir



The screenshot shows the GitLab interface for the FrontISTR repository. The left sidebar contains navigation options: Project information, Repository, Files, Commits (selected), Branches, Tags, Contributors, Graph, Compare, Issues (0), Merge requests (0), CI/CD, Security & Compliance, Deployments, and Packages and releases. The main content area displays a list of commits for the 'prc_kawaharai' branch. The commits are as follows:

Commit Date	Commit Message	Author	Commit ID
27 Nov, 2022 1 commit	Fix 3x3 inverse matrix calculation	gotoloop	56b51c82
26 Nov, 2022 1 commit	Improve XPAY, DIAG preconditioner	gotoloop	4cfd8cb
25 Nov, 2022 1 commit	Introduce QPBLAS	gotoloop	4cbd2703
22 Nov, 2022 1 commit	CG-DIAG-DD with convergence	haderbache.amir	8c1a1c70
21 Nov, 2022 2 commits	initialization of XL and BL to 0	haderbache.amir	0bf92275
21 Nov, 2022 2 commits	first integration of DD with FrontISTR nonlinear analysis	haderbache.amir	fa83a6ee

Thank you very
much for your time

Additional Materials

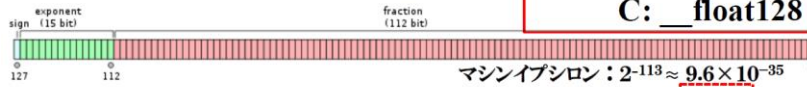
- DD Algorithm
- Interval Arithmetic

Linear system $\mathbf{Ax}=\mathbf{b}$

- A system of linear equation $\mathbf{Ax} = \mathbf{b}$ is solved, where:
 - $\mathbf{A} = \mathbf{M} + \mathbf{C}\gamma\Delta t + \mathbf{K}\beta\Delta t^2 \rightarrow$ the “stiffness matrix”
 - $\mathbf{x} = \Delta\ddot{\mathbf{u}}_{k+1} \rightarrow$ the increment of acceleration
 - $\mathbf{b} = \boldsymbol{\varepsilon} = \mathbf{f}(\mathbf{t}_{k+1}) - \mathbf{r}(\mathbf{u}_{k+1}, \dot{\mathbf{u}}_{k+1}) - \mathbf{M}\ddot{\mathbf{u}}_{k+1} \rightarrow$ the nonlinear residual
- The “stiffness matrix” \mathbf{A} is the sum of 3 sub-matrices:
 - The Mass matrix \mathbf{M}
 - The Damping matrix \mathbf{C}
 - The “linear” stiffness matrix \mathbf{K}
 - γ and β are constant parameter of Newmark method

DD Algorithm

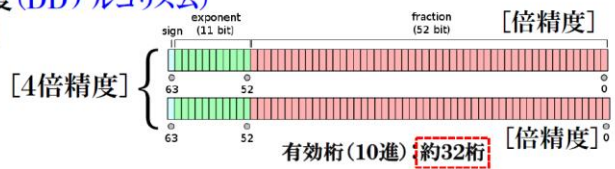
- 4倍精度[128bit, IEEE745形式]



マシンイプシロン: $2^{-113} \approx 9.6 \times 10^{-35}$
有効桁(10進) 約34桁

↕ → ソフトウェア的実装(低速)

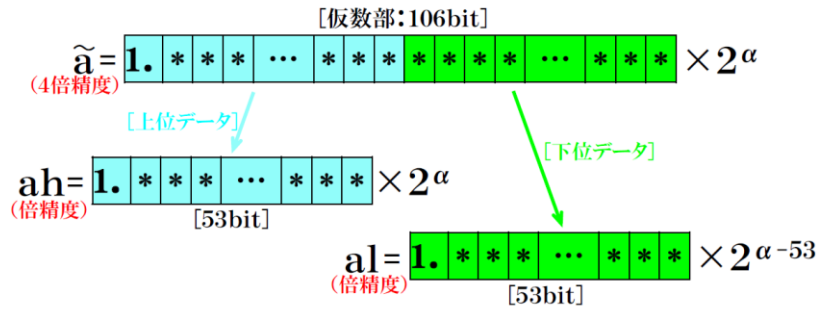
- [擬似]4倍精度(DDアルゴリズム)
[64bit + 64bit]



19/100

DDアルゴリズム

※ 倍精度を2つ組み合わせて4倍精度を構成



$$\tilde{a} = ah + al \rightarrow (ah, al)$$

[上位] [下位]

34/100

FrontISTR code: from x to disp results (summary)

- call `solve_LINEQ(hecMESHmpc,hecMATmpc)`
- call `hecmw_mpc_tback_sol(hecMAT, hecMATmpc)`
- do `j=1,hecMESH%n_node*ndof`
 - `fstrSOLID%dunode(j) = fstrSOLID%dunode(j)+hecMAT%X(j)`
 - `fstrSOLID%unode(j) = fstrSOLID%unode(j) + fstrSOLID%dunode(j)`
 - `fstrDYNAMIC%DISP(j,2) = fstrSOLID%unode(j)`
- The final displacement results is into `fstrDYNAMIC%DISP` and is written into output `res/vtk` files