Cas d'études de calculs parallèles numériquement reproductibles

Philippe Langlois, Chemseddine Chohra, Rafife Nheili

Retour d'expéRiences sur la Recherche Reproductible
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DALI, Université de Perpignan Via Domitia
LIRMM, UMR 5506 CNRS - Université de Montpellier

DALI, Digits, Architectures
et Logiciels Informatiques

Acknowledgment

Christophe Denis, EDF R&D, Clamart and CMLA, Cachan
Jean-Michel Hervouet, LNE, EDR R&D, Chatou

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Reproducibility failure of one industrial simulation code

- Simulation of free-surface flows in 1D-2D-3D hydrodynamic
- Integrated set of open source Fortran 90 modules, 300 000 loc.
- LNHE (EDF R&D) + international consortium, 20 years, 4000 reg. users

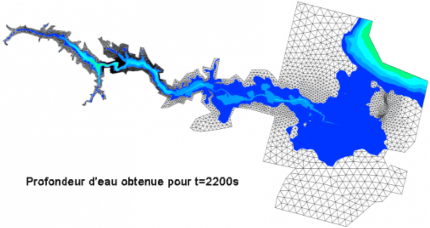
Telemac 2D [5]

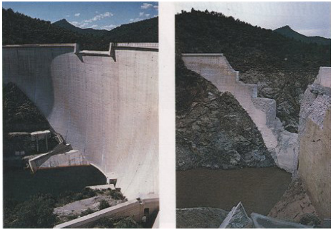
- 2D hydrodynamic: Saint Venant equations
- Finite element method, triangular element mesh, sub-domain decomposition for parallel resolution
- Mesh node unknowns: water depth (H) and velocity (U,V)

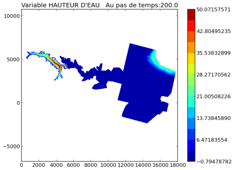
The Malpasset dam break: a reproducible simulation?

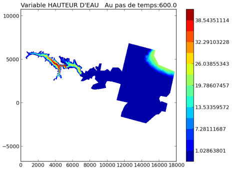
The Malpasset dam break (1959)

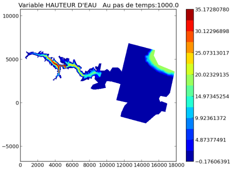
- A five year old dam break: 433 dead people and huge damage
- Simulation mesh: 26000 elements and 53000 nodes
- Simulation: 2200 seconds with a 2 sec. time step











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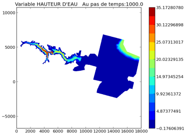

A reproducible simulation?

	velocity U	velocity V	depth H
The sequential run	0.4029747E-02	0.7570773E-02	0.3500122E-01

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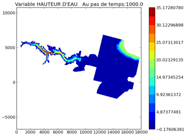

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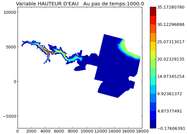

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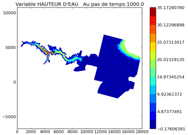

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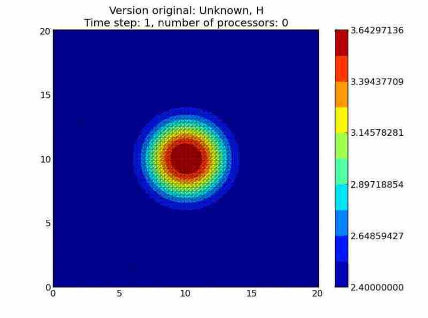
The privileged sequential run? uncertainty: up to $\times$ 2.5

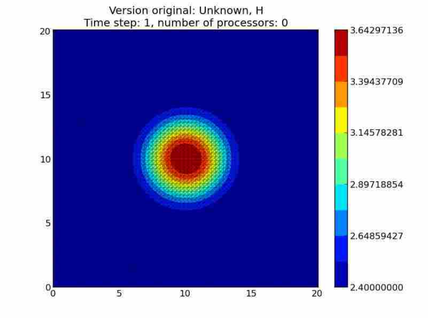
Telemac2D: the simplest gouttedo simulation

Expected numerical reproducibility

time step $= 1, 2, \ldots$



Sequential

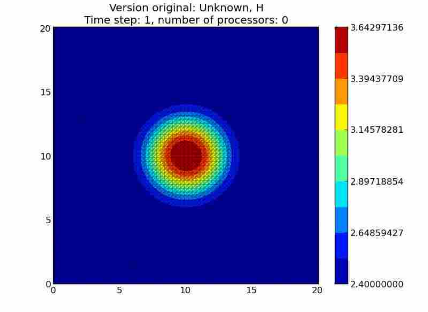


Parallel $p = 2$

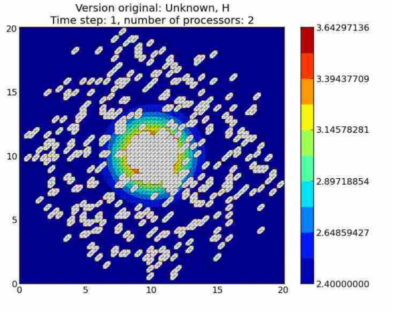
Telemac2D: gouttedo

Numerical reproducibility?

time step $= 1$



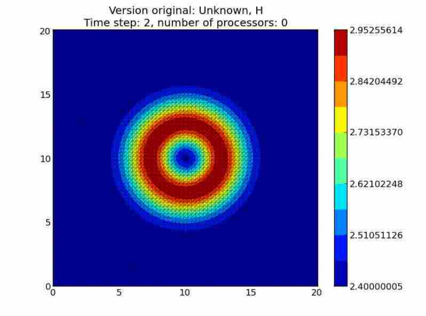
Sequential



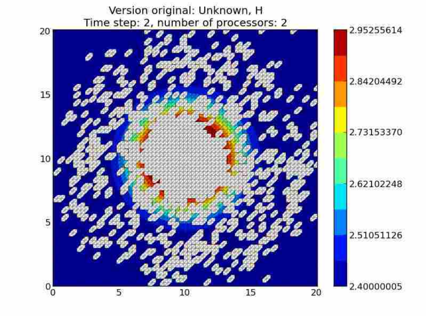
Parallel $p = 2$

Numerical reproducibility?

time step = 2



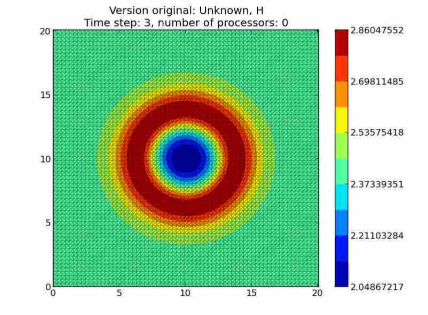
Sequential



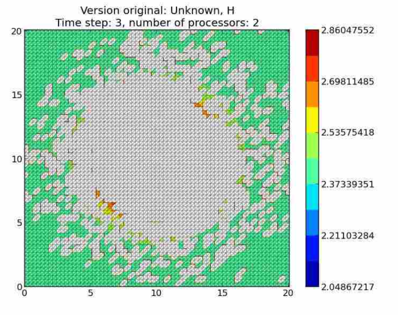
Parallel $p = 2$

Numerical reproducibility?

time step = 3



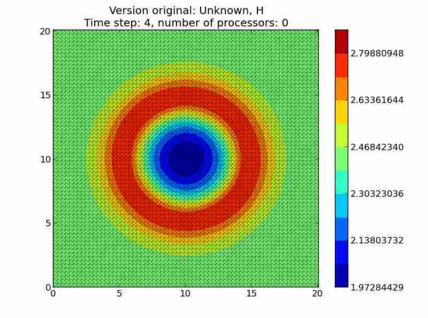
Sequential



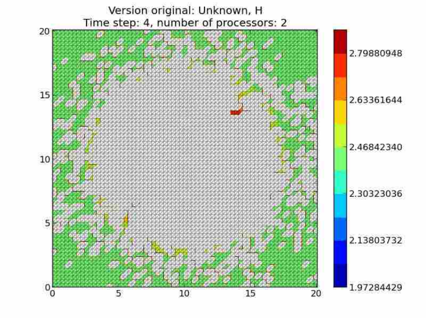
Parallel $p = 2$

Numerical reproducibility?

time step = 4



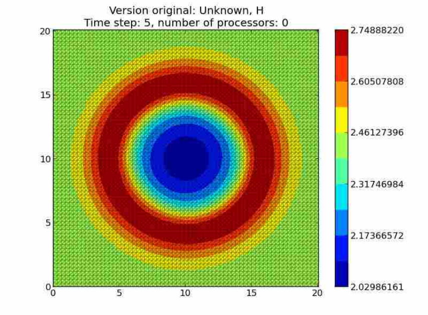
Sequential



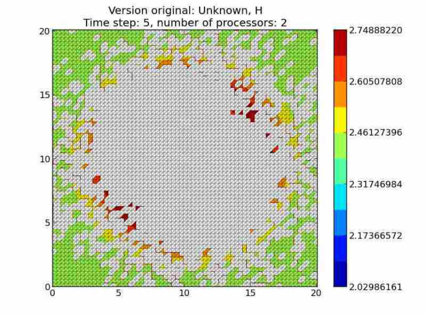
Parallel $p = 2$

Numerical reproducibility?

time step $= 5$



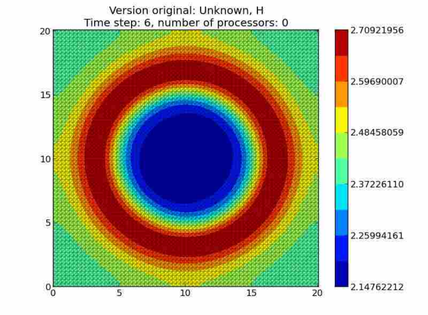
Sequential



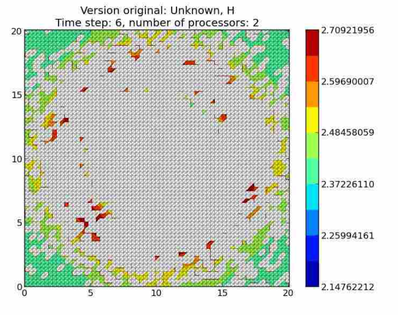
Parallel $p = 2$

Numerical reproducibility?

time step $= 6$



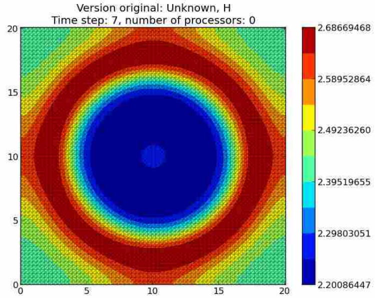
Sequential



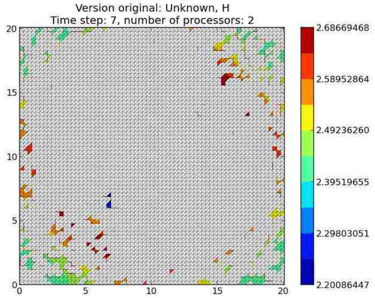
Parallel $p = 2$

Numerical reproducibility?

time step = 7



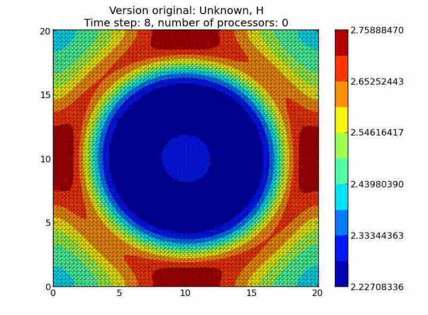
Sequential



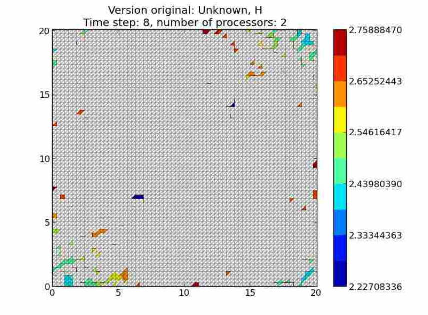
Parallel $p = 2$

Numerical reproducibility?

time step = 8



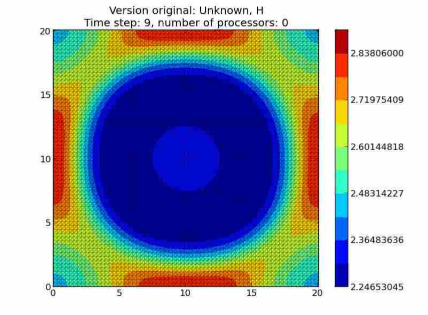
Sequential



Parallel $p = 2$

Numerical reproducibility?

time step = 9



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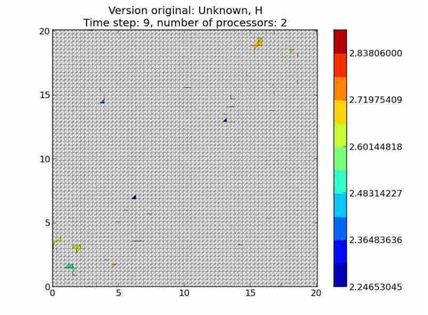
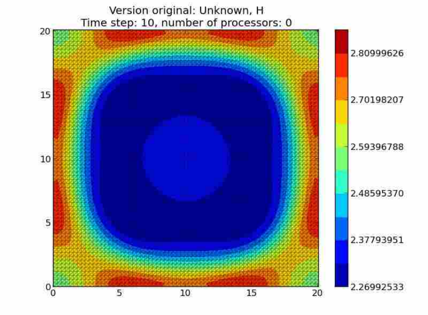


Parallel $p = 2$

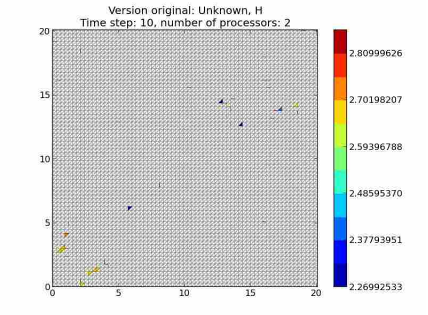
Telemac2D: gouttedo

Numerical reproducibility?

time step = 10



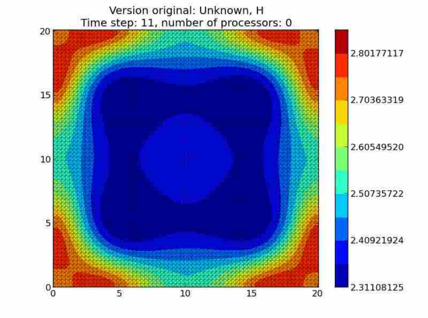
Sequential



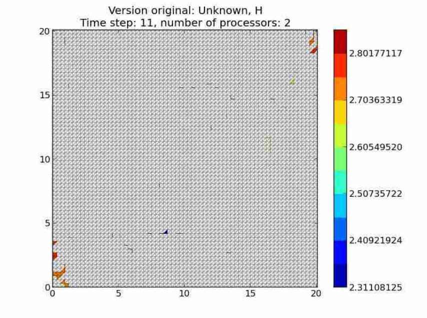
Parallel $p = 2$

Numerical reproducibility?

time step = 11



Sequential

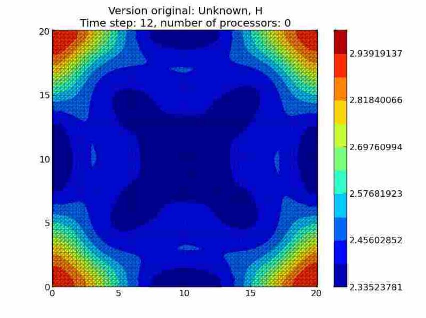


Parallel $p = 2$

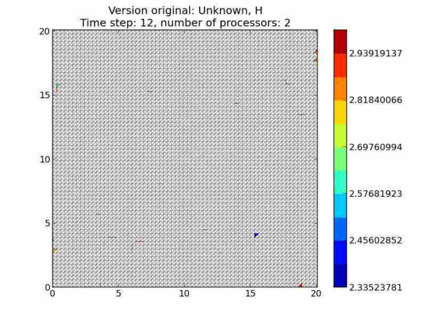
Telemac2D: gouttedo

Numerical reproducibility?

time step $= 12$



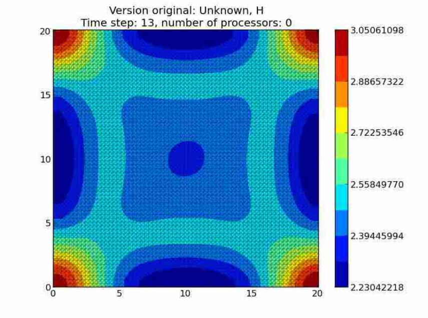
Sequential



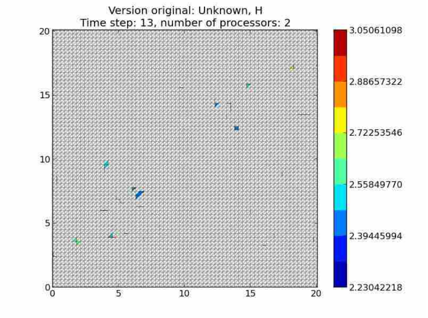
Parallel $p = 2$

Numerical reproducibility?

time step $= 13$



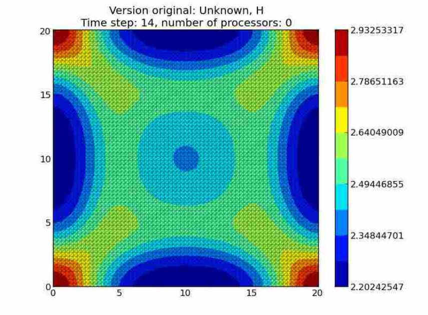
Sequential



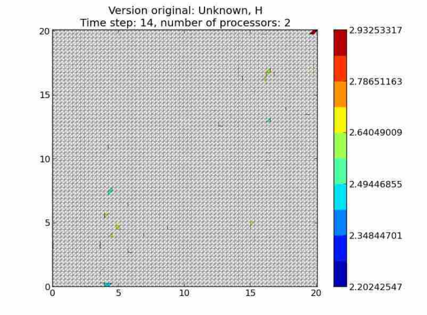
Parallel $p = 2$

Numerical reproducibility?

time step = 14



Sequential

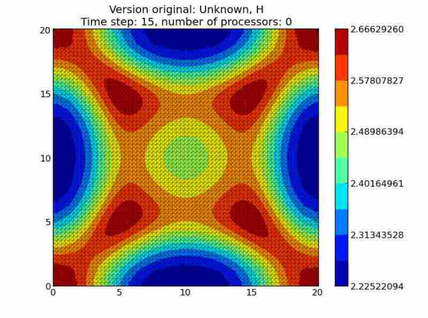


Parallel $p = 2$

Telemac2D: gouttedo

NO numerical reproducibility!

time step = 15



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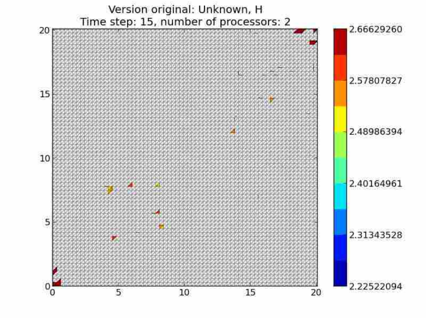

Parallel $p = 2$

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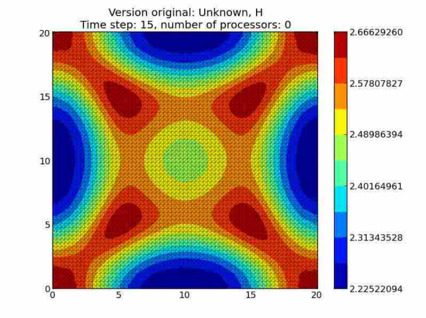

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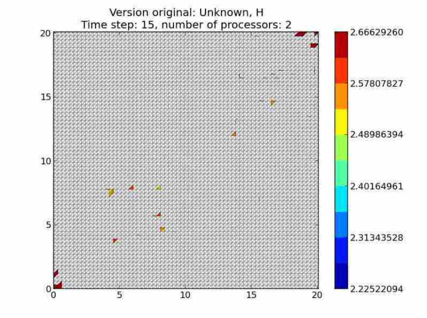

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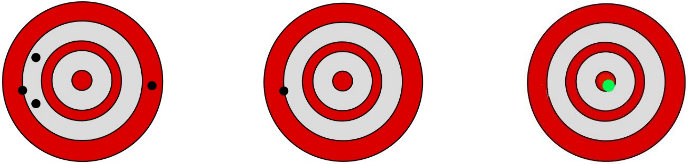
Numerical Reproducibility



1. Motivations
2. Basic ingredients
3. Recovering reproducibility in a finite element resolution
4. Efficient and reproducible BLAS 1
5. Conclusion and work in progress

Motivations

Exascale HPC and numerical simulation

- Moore's rule $\rightarrow 10^{\mathbf{18}}$ flop/sec in 2020
- Massive and heterogeneous parallelism : 1 million of computing units
- Numerical simulation of complex and sensitive physical phenomena

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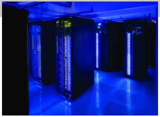

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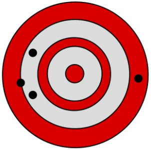
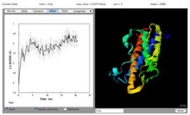
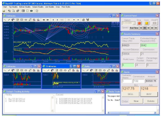
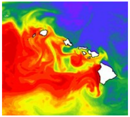
Numerical reproductibility failure of finite precision computations



- Non associative floating-point addition
- Computed value depends on the operation order
- Reproducibility failures reported in numerical simulations for energy [12], dynamical weather science [4], dynamical molecular [11], dynamical fluid [8]







Reproducibility failure (1)

When? why?

- Operation order uncertainty for consecutive executions of a given binary file
- Appears both in parallel and "sequential+SIMD" environments

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- Appears both in parallel and "sequential+SIMD" environments

Parallel reduction: SIMD, openMP, MPI, GPU

- Let p be the number of computing units
- When p varies, the partial computed values before the reduction also vary
- For a given $p > 2$, the computed reduced value depends on the dynamic scheduling of the reduction: omp, mpi, gpu

Reproducibility failure (2)

Reproducibility $\neq$ Portability

- Portability : one source $\rightarrow$ different binaries
- Parameters: compilers and their options, librairies, OS, comput. units
- Reproducibility may fail for a given set of portability parameters

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Reproducibility $\neq$ Accuracy

- Reproducibility: bitwise identical results for every p-parallel run, $p \geq 1$
- Full accuracy = unit roundoff accuracy = bitwise exact result
- Improving accuracy up to correct rounding $\Rightarrow$ reproducibility

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Reproducibility

- Pros: numerical debug, validation, legal agreements
- Cons: numerical debug, stochastic arithmetic

Today's issues

Feasibility

- Do existing techniques easily provide reproducibility to large scale (industrial) scientific software?

Efficiency

- Do correctly rounded summation algorithms provide efficient implementations of reproducible parallel BLAS routines?

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  - openTelemac-Mascaret: Tomawak, Telemac2D
  - finite element assembly, domain decomposition, linear system solving

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  - BLAS 1: asum, dot, nrm2
  - overcost vs. Intel MKL

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  - openTelemac-Mascaret: Tomawak, Telemac2D
  - finite element assembly, domain decomposition, linear system solving
- Compensation yields reproducibility here!

Efficiency

- Do correctly rounded summation algorithms provide efficient implementations of reproducible parallel BLAS routines?
  - BLAS 1: asum, dot, nrm2
  - overcost vs. Intel MKL
- Convincing rtn-BLAS 1 but ...

Basic ingredients

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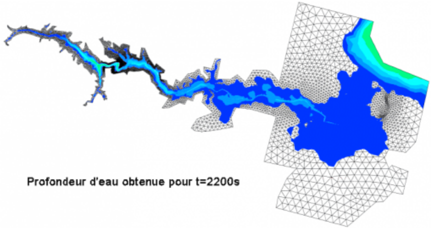
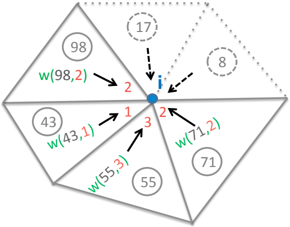
Sequential finite element assembly

Assembly step principle: $V(i) = \sum_{elements} W_e(i)$

- compute the inner node values
- accumulate W_e for every *ielem* that contains *i*





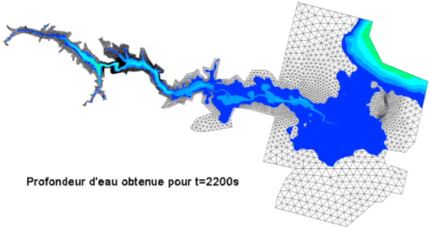
The assembly loop

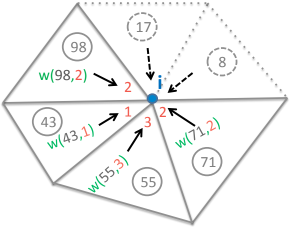
```
for idp = 1, ndp         //idp: triangular local numbering (ndp=3)
  for ielem = 1, nelem
    i = IKLE(ielem, idp)
    V(i) = V(i) + W(ielem, idp)      //i: domain global numbering
```

Sequential finite element assembly

Assembly step principle: $V(i) = \sum_{elements} W_e(i)$

- compute the inner node values
- accumulate W_e for every *ielem* that contains i



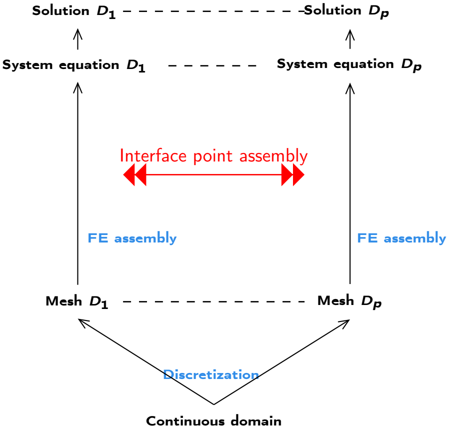


The assembly loop

```
for idp = 1, ndp          //idp: triangular local numbering (ndp=3)
  for ielem = 1, nelem
    i = IKLE(ielem, idp)   <-- LOOP INDEX INDIRECTION
    V(i) = V(i) + W(ielem, idp)      //i: domain global numbering
```

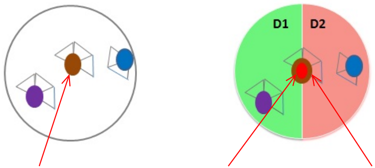
Parallel FE assembly

Parallel FE: subdomain decomposition



Exact arithmetic

sequential | parallel



$V(i) = a$ | $V(i_1) = b$ | $V(i_2) = c$

Interface point assembly

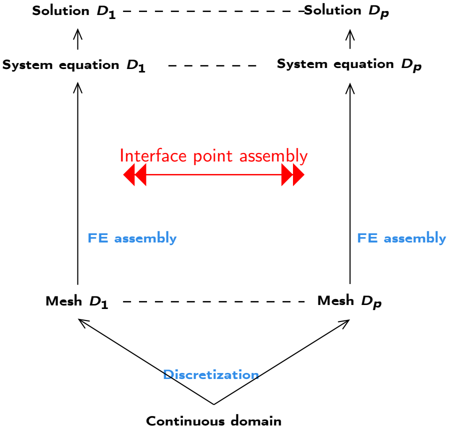
$V(i) = b + c = a$

IP assembly = communications and reductions

$V(i) = \sum_{D_k} V(i)$
subdomains D_k, $k = 1...p$

Parallel FE assembly

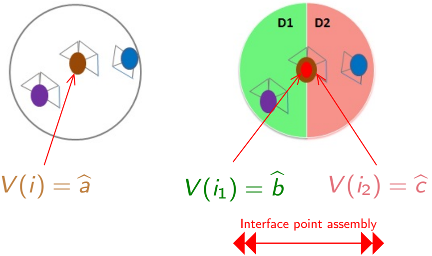
Parallel FE: subdomain decomposition



IP assembly =
communications and reductions

Floating point arithmetic

sequential parallel



$$V(i) = \widehat{b} \oplus \widehat{c} \neq \widehat{a}$$

$$V(i) = \sum_{D_k} V(i)$$

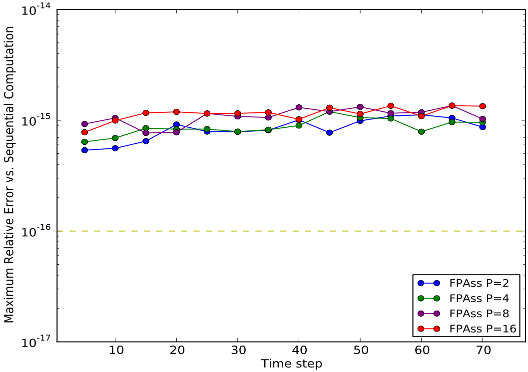
subdomains $D_k, k = 1 \ldots p$

Assembly step: example of reproducibility failure

Sequential vs. p-parallel results differ for $p = 2, 4, 8, 16$

- Assembly with the classical floating-point accumulation
- sequential *FPAss* vs. p-parallel $FPAss_p$

$$\max |FPAss_p - FPAss| / |FPAss|$$



Mean frequency wave, Nice test case, Tomawac

Basic ingredients

1. Motivations
2. Basic ingredients
   - Finite element assembly: sequential and parallel cases
   - Sources of non reproducibility in Telemac2D
   - Compensation
3. Recovering reproducibility in a finite element resolution
   - Reproducible parallel FE assembly
   - Reproducible conjugate gradient
4. Efficient and reproducible BLAS 1
5. Conclusion and work in progress

Sources of non reproducibility in Telemac2D

Culprits: theory

- Building step: interface point assembly
- Resolution with conjugate gradient: matrix-vector and dot products

Culprits: practice = optimizations

- Element-by-element storage of FE matrix and second member
- Wave equation and associated algebraic transformations
- Interface point assembly and system solving are merged

Sources of non reproducibility in Telemac2D

Telemac2D finite element method (FE)

Solution U,V

wave equation

Solution H

conjugate gradient

System equation $Ay = b$

$$\begin{pmatrix} AM1 & 0 & 0 \\ 0 & AM2 & 0 \\ 0 & 0 & AM3 \end{pmatrix} \begin{pmatrix} H \\ U \\ V \end{pmatrix} = \begin{pmatrix} CV1 \\ CV2 \\ CV3 \end{pmatrix}$$

algebraic transformation

$$\begin{pmatrix} A_{hh} & A_{hu} & A_{hv} \\ A_{uh} & A_{uu} & 0 \\ A_{vh} & 0 & A_{vv} \end{pmatrix} \begin{pmatrix} H \\ U \\ V \end{pmatrix} = \begin{pmatrix} B_h \\ B_u \\ B_v \end{pmatrix}$$

FE assembly +

algebraic computation

Mesh (elements, nodes)

Discretization

$CV2 = B_u - A_{uh}H,$

$CV3 = B_v - A_{vh}H.$

Interface node assembly:

$CV2$, $CV3$

H

AM2,AM3

Interface node assembly:

$AM1$ in each iteration

AM1,CV1

$AM2, AM3$: diagonal matrices,

$AM1 = A_{hh} - A_{hu}AM2^{-1}A_{uh} - A_{hv}AM3^{-1}A_{vh},$

$CV1 = B_h - A_{hu}AM2^{-1}B_u - A_{hv}AM3^{-1}B_v,$

Interface node assembly:

$AM2, AM3, CV1$

Sources of non reproducibility in Telemac2D

Telemac2D finite element method (FE)

Solution U,V

wave equation

$CV2 = B_u - A_{uh}H,$

$CV3 = B_v - A_{vh}H.$

Interface node assembly:

$CV2, CV3$

H

AM2,AM3

Solution H

conjugate gradient

Interface node assembly:

$AM1$ in each iteration

AM1,CV1

System equation $Ay = b$

$$\begin{pmatrix} AM1 & 0 & 0 \\ 0 & AM2 & 0 \\ 0 & 0 & AM3 \end{pmatrix} \begin{pmatrix} H \\ U \\ V \end{pmatrix} = \begin{pmatrix} CV1 \\ CV2 \\ CV3 \end{pmatrix}$$

algebraic transformation

$AM2, AM3$: diagonal matrices,

$AM1 = A_{hh} - A_{hu}AM2^{-1}A_{uh} - A_{hv}AM3^{-1}A_{vh},$

$CV1 = B_h - A_{hu}AM2^{-1}B_u - A_{hv}AM3^{-1}B_v,$

Interface node assembly:

$AM2, AM3, CV1$

$$\begin{pmatrix} A_{hh} & A_{hu} & A_{hv} \\ A_{uh} & A_{uu} & 0 \\ A_{vh} & 0 & A_{vv} \end{pmatrix} \begin{pmatrix} H \\ U \\ V \end{pmatrix} = \begin{pmatrix} B_h \\ B_u \\ B_v \end{pmatrix}$$

FE assembly +

algebraic computation

Mesh (elements, nodes)

Discretization

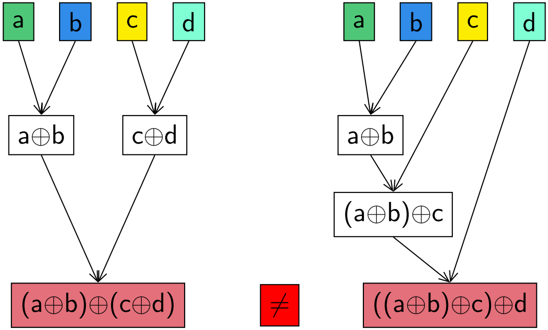
Objective

Correct sources of non-reproducibility
to compute reproducible system and solutions

Basic ingredients

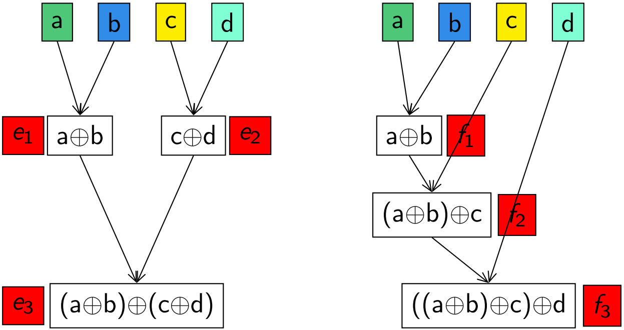
Parallel reduction and compensation techniques

Reproducibility failure of the parallel reduction



Parallel reduction and compensation techniques

Compensation principle

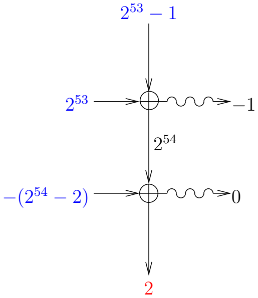


$$((a \oplus b) \oplus (c \oplus d)) \oplus ((e_1 \oplus e_2) \oplus e_3) = (((a \oplus b) \oplus c) \oplus d) \oplus ((f_1 \oplus f_2) \oplus f_3)$$

Compensated summation: one example

IEEE binary64 (double): $x_1 = 2^{53} - 1$, $x_2 = 2^{53}$ and $x_3 = -(2^{54} - 2)$.
Exact sum: $x_1 + x_2 + x_3 = 1$.

Classic summation

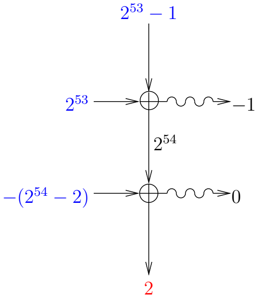


Relative error = 1

Compensated summation: one example

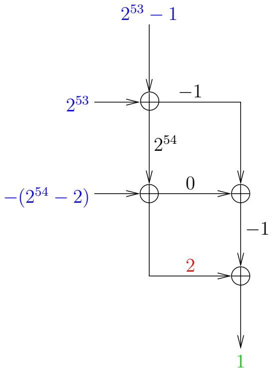
IEEE binary64 (double): $x_1 = 2^{53} - 1$, $x_2 = 2^{53}$ and $x_3 = -(2^{54} - 2)$.
Exact sum: $x_1 + x_2 + x_3 = 1$.

Classic summation



Relative error = 1

Compensation of the rounding errors

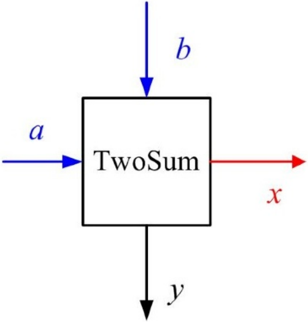


The exact result is computed

Rounding errors are computed with EFT

2Sum (Knuth, 65), Fast2Sum (Dekker, 71) for base ≤ 2 and RTN.

$$a + b = x + y, \text{ with } a, b, x, y \in \mathbb{F} \text{ and } x = a \oplus b.$$



Algorithm (Knuth)

function [x,y] = 2Sum(a,b)

$x = a \oplus b$

$z = x \ominus a$

$y = (a \ominus (x \ominus z)) \oplus (b \ominus z)$

Algorithm ($|a| > |b|$, Dekker)

function [x,y] = Fast2Sum(a,b)

$x = a \oplus b$

$z = x \ominus a$

$y = b \ominus z$

Other existing techniques

Existing techniques to recover numerical reproducibility in summation

- Accurate compensated summation [6]
- Demmel-Nguyen's reproducible sums [3]
- Integer convertion [7]

Recovering reproducibility in a finite element resolution

Recovering reproducibility in Telemac2D

Culprits

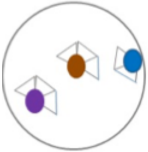
- Building step: interface point assembly
- Resolution: matrix-vector and dot products
- Element-by-element storage of FE matrix and second member
- Wave equation (decoupling) and associated algebraic transformations
- Interface point (IP) assembly and system solving are merged

Reproducible resolution: principles

- Compensate FE assembly of inner nodes
- Propagate rounding errors and compensate while assembling the IP
- Compensate the EBE matrix-vector products
- Compensate the MPI parallel dot products
- vector $V \to [V, E_V] \to V + E_V$

Accurate compensated assembly: the sequential case

for idp= 1, ndp
  for ielem= 1, nelem
    i=IKLE(ielem, idp)
    X(i)=X(i)+W(ielem,idp)



D1

FE assembly

Contribution $W_i(e_1)$ for every node mesh i belonging to element $e_1 \ldots e_n$

Computation and accumulation of rounding errors Δ

$$X(i) = W_i(e_1) + W_i(e_2) + \ldots + W_i(e_n)$$

Δ_1 Δ_2 Δ_n

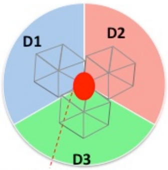
$$E(i) = \Delta_1 + \Delta_2 + \ldots + \Delta_n$$

Compensation of the FE assembly for every mesh node I

$$X(i)=X(i)+E(i)$$

The parallel case is easy to derive

```
for idp=1, ndp
  for ielem=1, nelem
    i=IKLE (ielem, idp)
    X(i)=X(i)+ W(ielem, idp)
```



i : Interface Point

Interface Point assembly

D1 D2 D3

Subdomain FE assembly.

Contribution $W_i(e_k)$ for every node mesh i belonging to elem $e_1,\ldots, e_n$

Computation and accumulation of rounding errors Δ

similar

$X(i) = W_i(e_1) + W_i(e_2) + \ldots + W_i(e_n)$

$\Delta_1 \quad \Delta_2 \quad \Delta_n$

$E(i) = \Delta_1 + \Delta_2 + \ldots + \Delta_n$

similar

Interface point assembly

i : interface point between D1,D2,D3

Accumulation of errors Δ and ε

X(i), E(i)

$X(i) = X(i) + X(i) + X(i)$

$\varepsilon_1 \quad \varepsilon_2$

$E(i) = ((E(i) + E(i) + \varepsilon_1) + E(i) + \varepsilon_2)$

X(i), E(i)

Compensation of the FE assembly for every mesh node i

similar

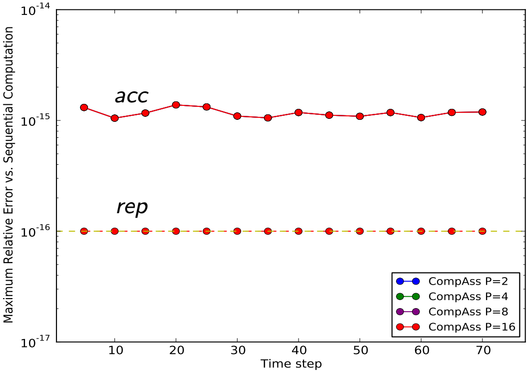
$X(i)=X(i)+E(i)$

similar

Accurate compensated assembly gives reproducibility

Reproducibility in Tomawac

- Reproducibility and accuracy



A^s: sequential, A^p: p-parallel

$\max_{rel}(A_1, A_2) = |A_1 - A_2|/|A_2|$

Accuracy (of FPSum):

$acc = \max_{rel}(CompAss^p, FPAss^s)$

Reproducibility:

$rep = \max_{rel}(CompAss^p, CompAss^s)$

Mean frequency wave, Nice test case, Tomawac

Recovering reproducibility in a finite element resolution

Towards a reproducible conjugate gradient

A=[$AM1$, E_{AM1}]

B=$CV1$

Initialization:

$$r^0 = AX^0 - B;\ \text{a given } d^0$$

$$\rho^0 = \frac{(r^0, d^0)}{(Ad^0, d^0)};\ X^1 = X^0 - \rho^0 d^0$$

Iterations:

$$r^m = r^{m-1} - \rho^{m-1} Ad^{m-1}$$

$$d^m = r^m + \frac{(r^m, r^m)}{(r^{m-1}, r^{m-1})} d^{m-1}$$

$$\rho^m = \frac{(r^m, d^m)}{(d^m, Ad^m)}$$

$$X^{m+1} = X^m - \rho^m d^m$$

$\rightarrow$ X=H

Sources of non-reproducibility :

Matrix-vector product

Dot product

Last steps to compensate

- Conjugate gradient
- Matrix-vector product
- Dot product
  - ponderated dot product
  - MPI reduced dot product

Reproducible conjugate gradient

A=[*AM1*, E_{AM1}]

B=*CV1*

Initialization:

$$r^0 = AX^0 - B; \text{ a given } d^0$$

$$\rho^0 = \frac{(r^0, d^0)}{(Ad^0, d^0)}; \; X^1 = X^0 - \rho^0 d^0$$

Iterations:

$$r^m = r^{m-1} - \rho^{m-1} Ad^{m-1}$$

$$d^m = r^m + \frac{(r^m, r^m)}{(r^{m-1}, r^{m-1})} d^{m-1}$$

$$\rho^m = \frac{(r^m, d^m)}{(d^m, Ad^m)}$$

$$X^{m+1} = X^m - \rho^m d^m$$

$\longrightarrow$ **X=*H***

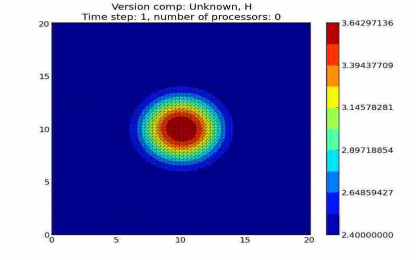
Not necessarily more accurate but reproducible

Same errors in compensated values for both sequential and parallel executions

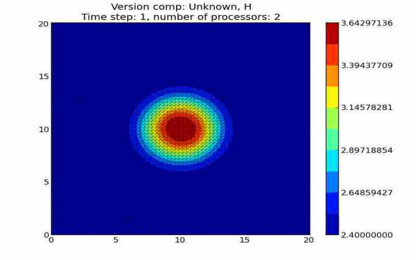
Reproducible Telemac2D!

Time step 1

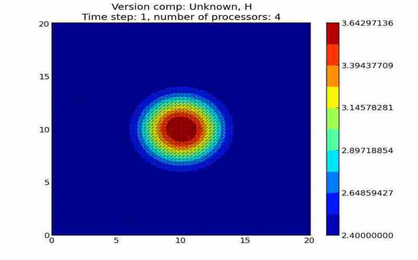
p=1



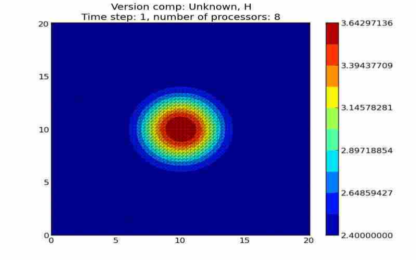
p=2



p=4

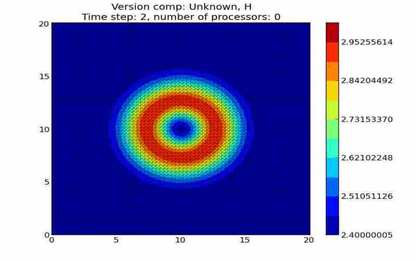


p=8

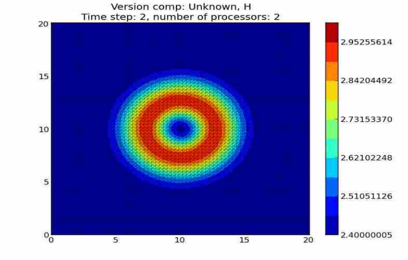


Time step 2

p=1



p=2



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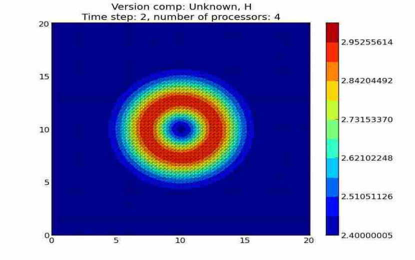

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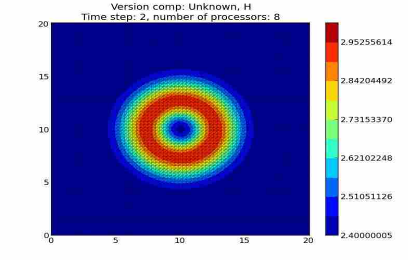
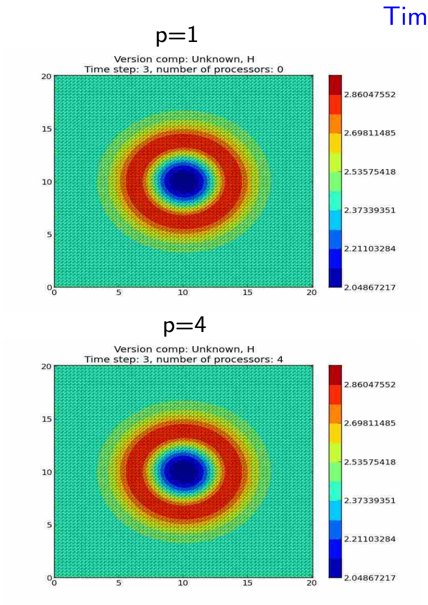
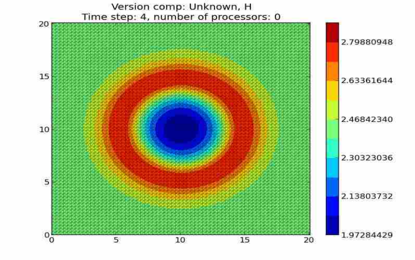


Reproducible Telemac2D!

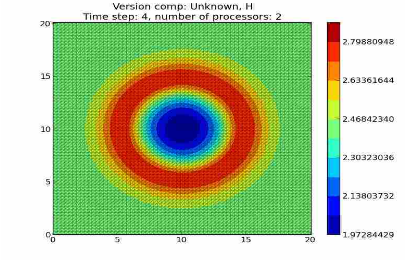


Time step 4

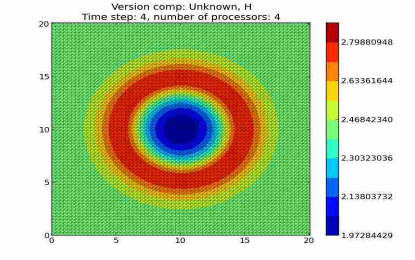
p=1



p=2



p=4



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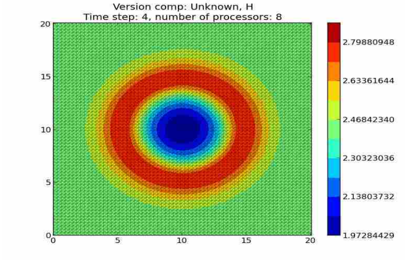
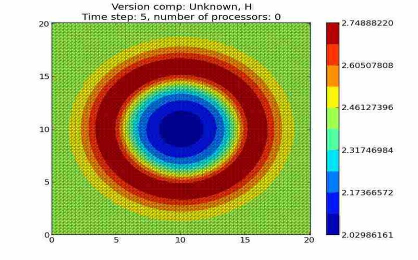
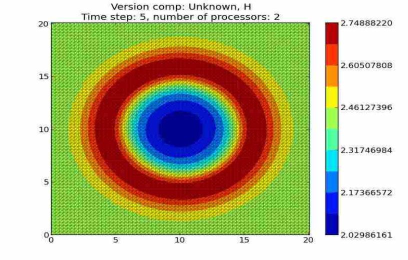


Time step 5

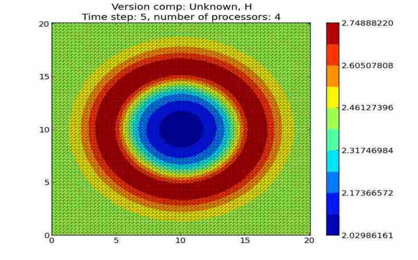
p=1



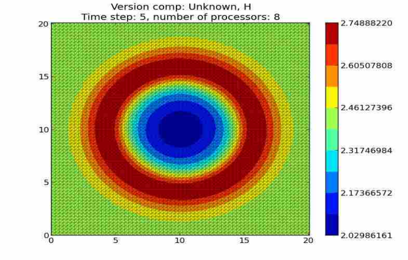
p=2



p=4

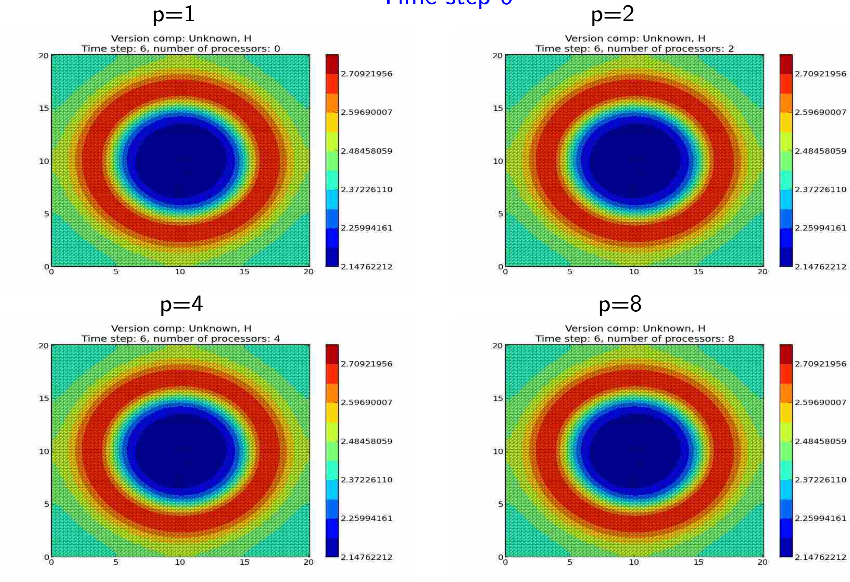


p=8



Reproducible Telemac2D!

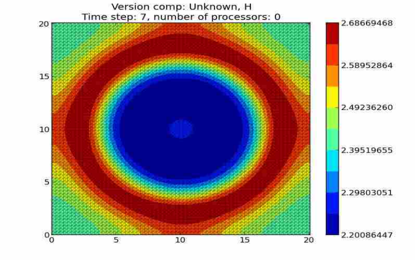
Time step 6



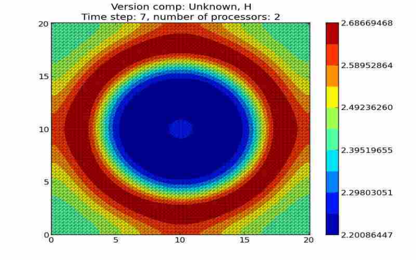
Reproducible Telemac2D!

Time step 7

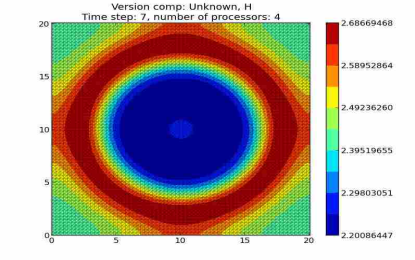
p=1



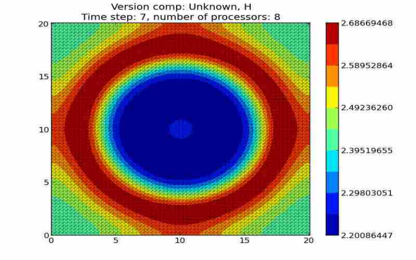
p=2



p=4



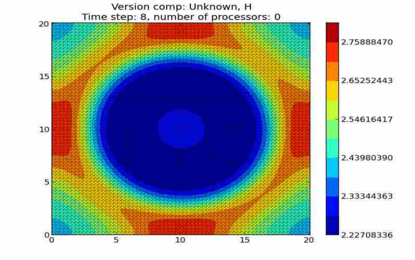
p=8



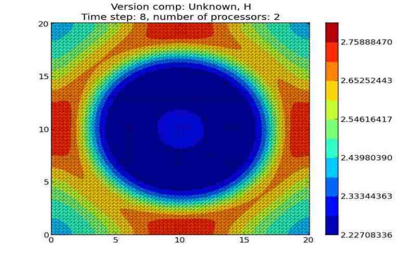
Reproducible Telemac2D!

Time step 8

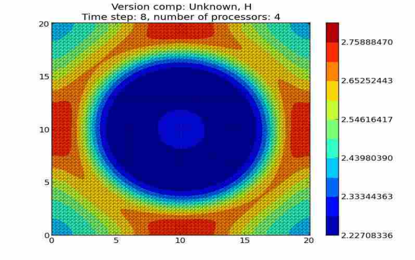
p=1



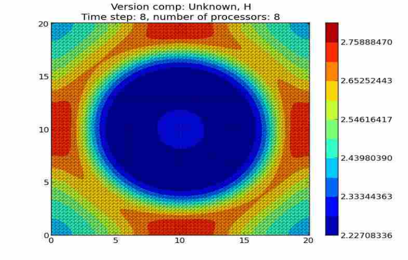
p=2



p=4



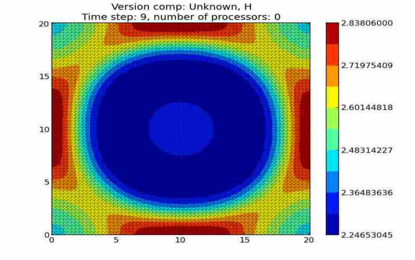
p=8



Reproducible Telemac2D!

Time step 9

p=1



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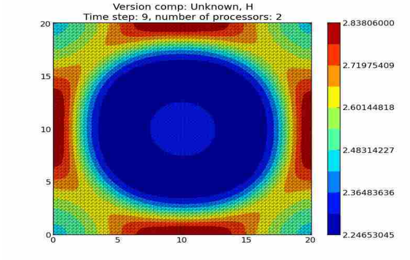

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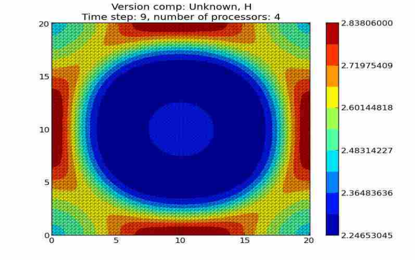

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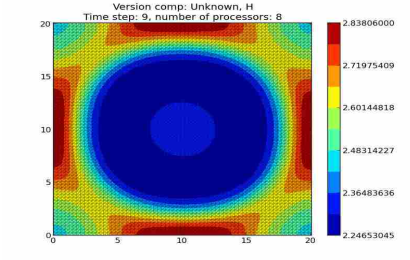
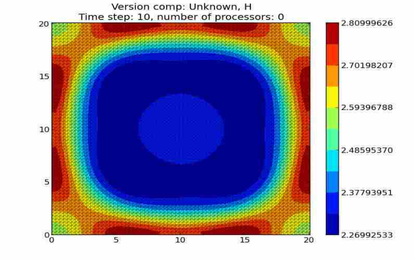


Reproducible Telemac2D!

Time step 10

p=1



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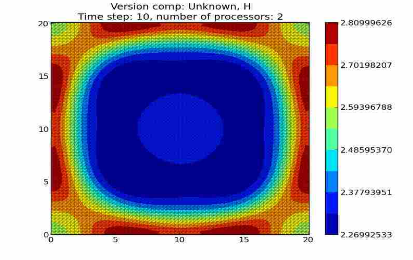

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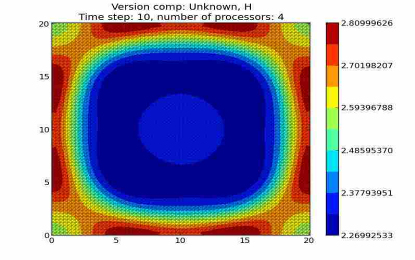

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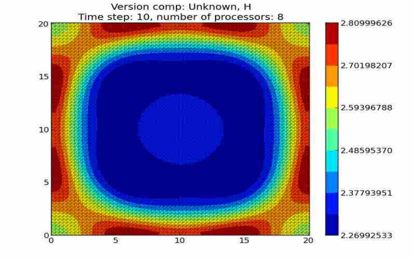
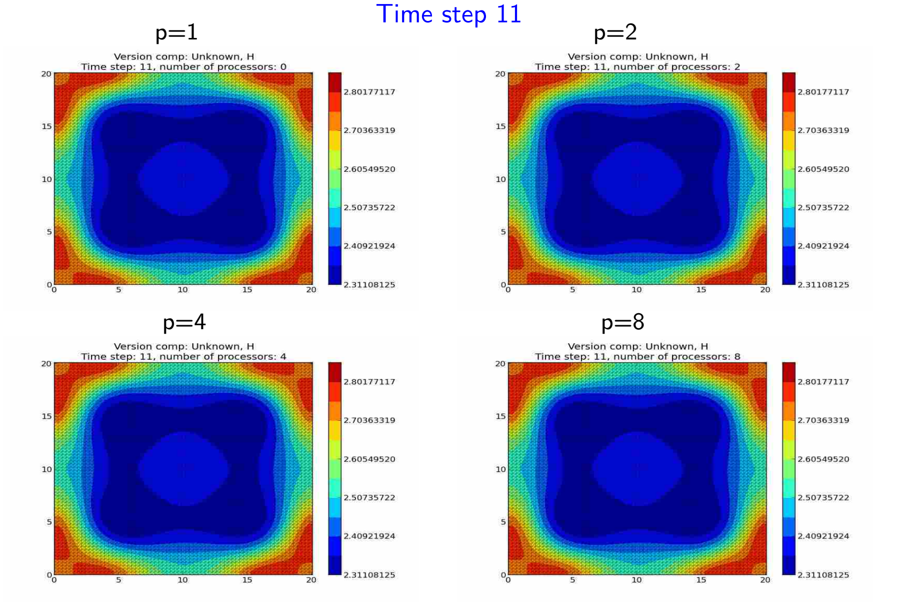
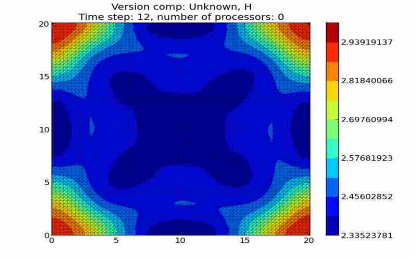


Reproducible Telemac2D!



Time step 12

p=1



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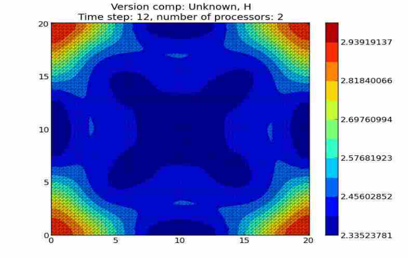

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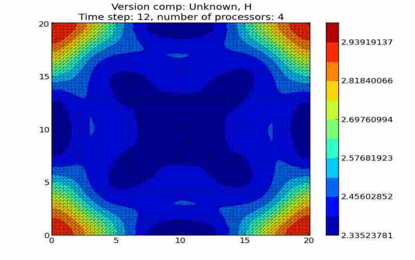

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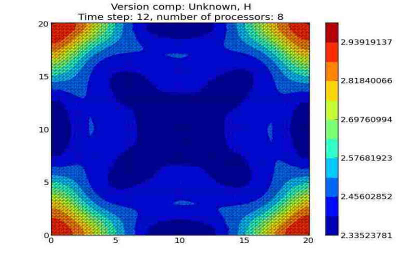
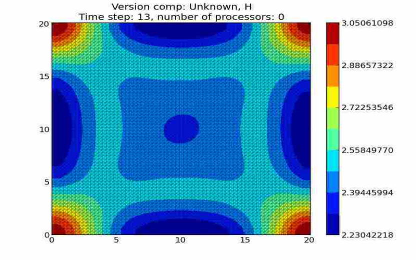


Reproducible Telemac2D!

Time step 13

p=1



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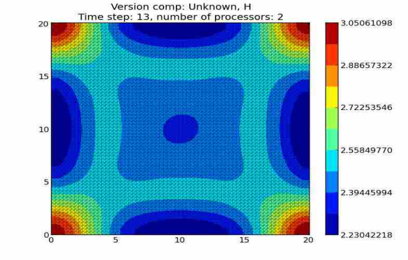

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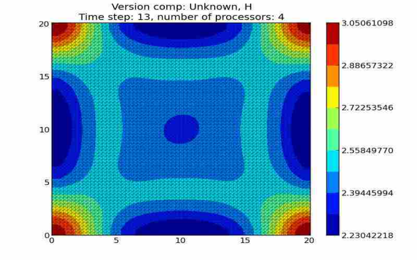

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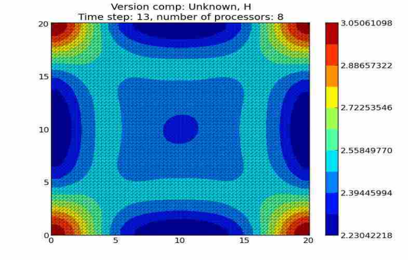
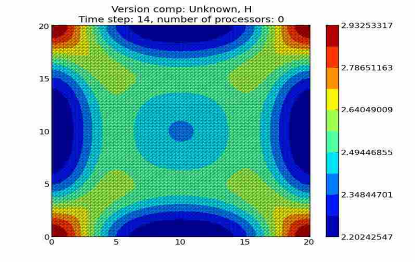


Reproducible Telemac2D!

Time step 14

p=1



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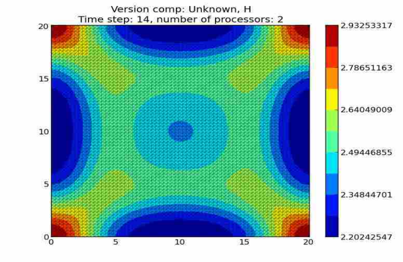

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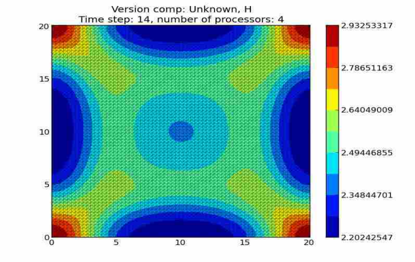

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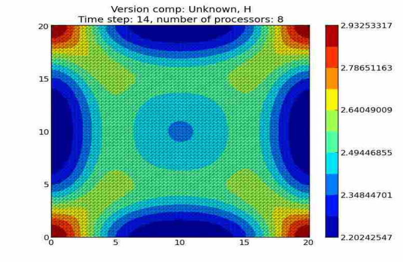
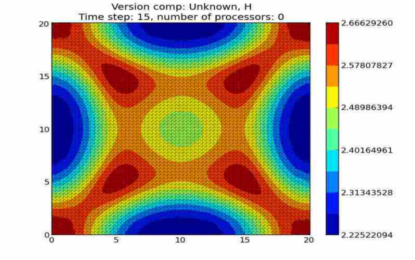


Reproducible Telemac2D!

Time step 15

p=1



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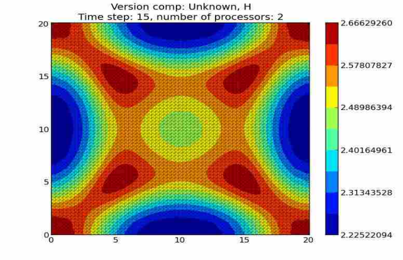
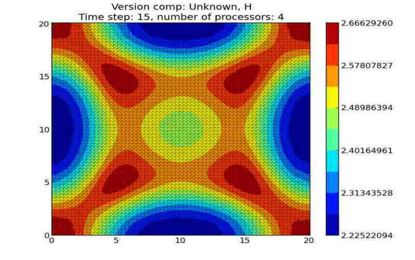
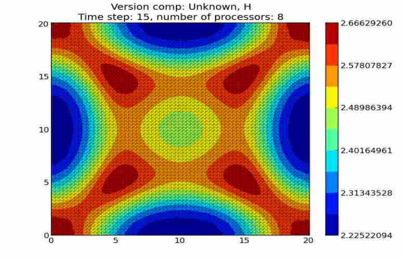


p=4



p=8



Efficient and reproducible BLAS 1

Numerical reproducibility for the BLAS

BLAS + correctly rounded sums

- Dot product of length $n \to$ sum of length $2n$
- A correctly rounded result is reproducible
- A large panel of algorithms for faithful or correctly rounded sums

Motivation

- How to benefit from these CR sums for reproducible BLAS?
- Is the over-cost acceptable in practice for reproducible BLAS?

Current results

- BLAS 1 : asum, dot, norm2
- openMP for shared memory
- Hybrid openMP-MPI for shared+distributed memory

Overview I

Our methodology

1. Optimization and choice of the best sequential CR sums
2. Deriving parallel CR sums
3. Application to reproducible BLAS-1 routines

The starting point: sequential summation algorithms

- Accurate: Sum-K [6]
- Faithful: AccSum [10], FastAccSum [9]
- Correctly rounded (in RtN): iFastSum, HybridSum [14], OnlineExact sum [15]

Overview II

Reproducible parallel BLAS-1: algorithmic choice

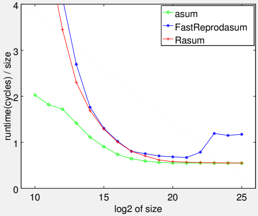
- Rasum: parallel Sum K as in [13] with $K = 2$ for $n \leq 10^7$.
- Rdot: FastAccSum (small n) or modified OnLineExact (large n)
- Rnrm2: Rdot+IEEE sqrt $\rightarrow$ reproducible only

All details in [1]

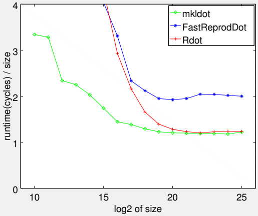
Efficiency of Reproducible Level 1 BLAS,
C. Chohra, Ph. L., D. Parello.
SCAN 2014 Post-Conference Proceedings
Lecture Notes of Computer Science (2015).
`http://hal-lirmm.ccsd.cnrs.fr/lirmm-01101723`

Parallel BLAS-1: Runtime overcost for reproducibility

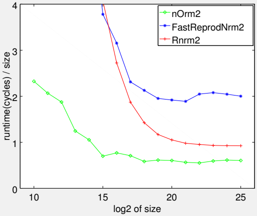
Runtime/size of parallel level 1 BLAS, up to 16 threads, cond=10^{32}



asum



dot



nrm2

Hardware and software env.

- socket: Xeon E5-2660 (L3 cache = 20 M).
- 2 cores, 8 cores on each socket.
- OpenMP 4.0 (Intra socket parallelism).
- Compare vs. Intel MKL 11

Parallel BLAS-1: Scalability

Hardware and software env.

- OCCIGEN: 26^{th} supercomputer in top500 list.
- 4212 cores, 12 cores on each socket.
- OpenMP 4.0 (Intra socket parallelism).
- OpenMPI (Inter socket communications).

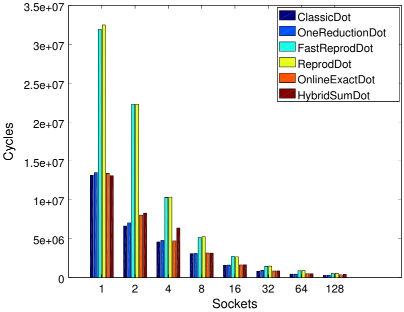
Parallel BLAS-1: Scalability

Configurations

- #sockets = 1 .. 128.
- #threads = 12 per socket.

Dataset

- Entry vectors size = 10^7.
- Condition number = 10^{32}.



Results

- Good scaling for large datasets.
- Two communications cost limits ReprodDot and FastReprodDot.
- We need only one communication for OneReduction, HybridSum and OnlineExact.

Time to conclude

To conclude

Feasibility ?

Do existing techniques easily provide reproducibility
to large scale industrial scientific software?

Efficiency ?

Do correctly rounded summation algorithms provide
efficient implementations of reproducible parallel BLAS routines?

Conclusion I

Numerical reproducibility

- How to remain confident facing the complexity of today's computational systems? and tomorrow?
- Sources: floating-point peculiarities and parallel reduction, data alignment, operator choices, compiler optimizations

Feasability

- Existing techniques are efficient enough and more or less easy to apply
- More precision, less errors or even exact computation

Reproducibility at the large scale: the openTelemac case

- Complex, large and real simulations are tractable
- Difficult to automatize but easier to pass the methodology on to software developpers
- Next step for Telemac 2D: more complex physical and numerical issues

Conclusion II

Efficiency

- Convincing reproducible BLAS level 1
- Hybrid openMP+MPI and scalability "in the large"
- Current step: Intel MIC (Xeon Phi)
- Next steps: BLAS-2, optimistic but BLAS-3, no future!

Numerical reproducibilty: cons/pros

- *Non reproducibility reveals bugs or numerical problems!*
- *just return 1 ... it is reproducible indeed!*
- Reproducibility is one factor towards numerical quality . . . as theorems, experiments, tools that yields error bounds, stability conditions, accuracy
- Reproducibility for the validation steps, not for the actual/operating mode
- Sequential $\rightarrow$ parallel implementation: reproducibility = no more bug . . . both implementations can be wrong!

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