Webminar on Reproducible Research: Numerical Reproducibility
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Reproducible Finite Element Simulation: A Case Study

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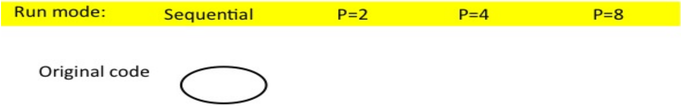
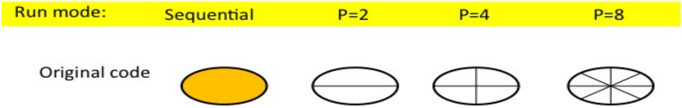

Run mode:
Sequential
P=2
P=4
P=8
Original code

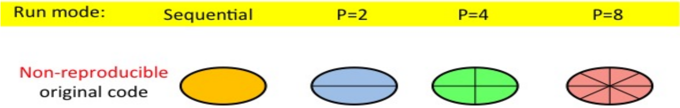
Bitwise identical results for every p-parallel run, $p \geq 1$ II

Run mode:	Sequential	P=2	P=4	P=8
Original code				

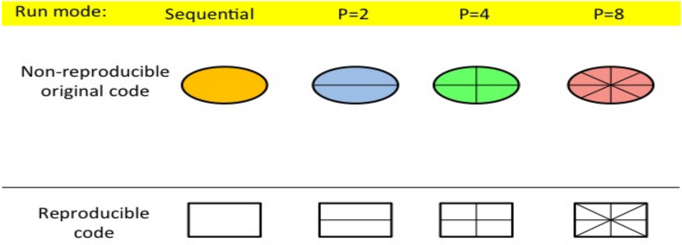
Bitwise identical results for every p-parallel run, $p \geq 1$ III



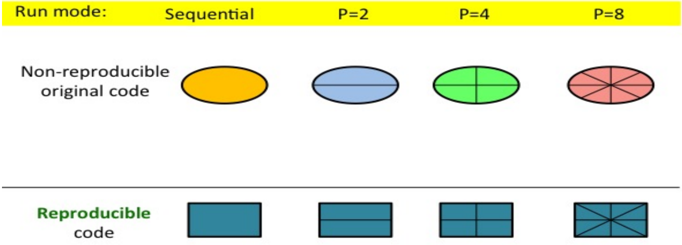
Bitwise identical results for every p-parallel run, $p \geq 1$ IV



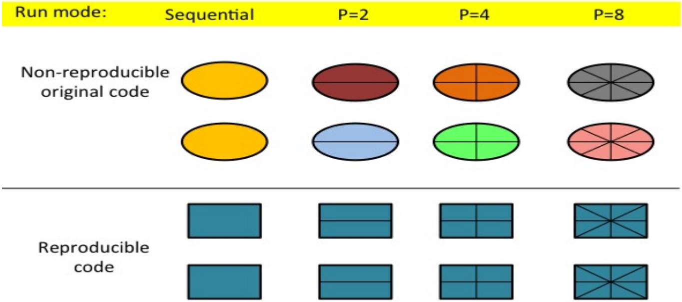
Bitwise identical results for every p-parallel run, $p \geq 1$ V



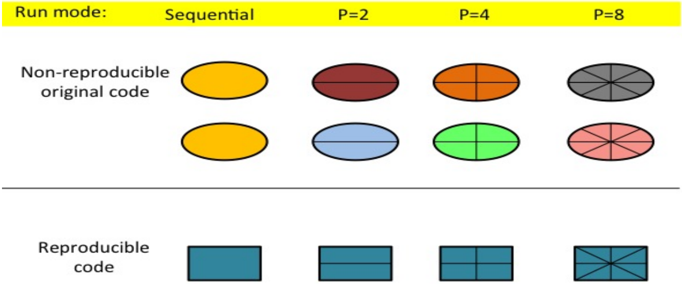
Bitwise identical results for every p-parallel run, $p \geq 1$ VI



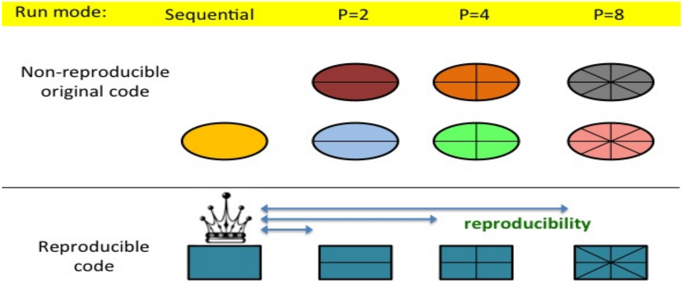
Bitwise identical results for every p-parallel run, $p \geq 1$ VII



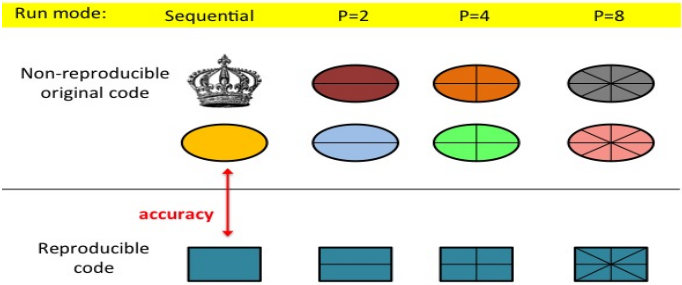
Bitwise identical results for every p-parallel run, $p \geq 1$ VIII



Bitwise identical results for every p-parallel run, $p \geq 1$ IX



Bitwise identical results for every p-parallel run, $p \geq 1$ X



Reproducibility failure of one industrial scale simulation code

- Simulation of free-surface flows in 1D-2D-3D hydrodynamics
- 300 000 loc. of open source Fortran 90
- 20 years, 4000 registered users, EDF R&D + international consortium

Telemac 2D [3]

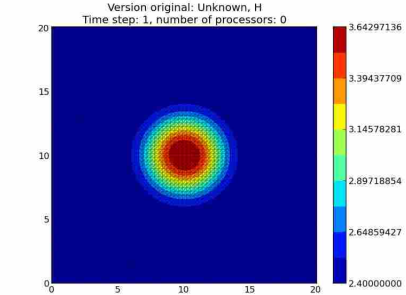
- 2D hydrodynamic: Saint Venant equations
- Finite element method, triangular element mesh, sub-domain decomposition for parallel resolution
- Mesh node unknowns: water depth (H) and velocity (U,V)

Telemac2D: the simplest gouttedo simulation

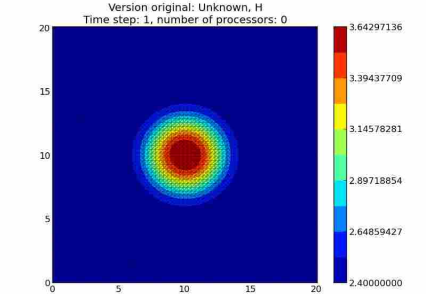
The gouttedo test case

- 2D-simulation of a water drop fall in a square bassin
- Unknown: water depth for a 0.2 sec time step
- Triangular mesh: 8978 elements and 4624 nodes

Expected numerical reproducibility (time step = 1, 2, ...)



Sequential

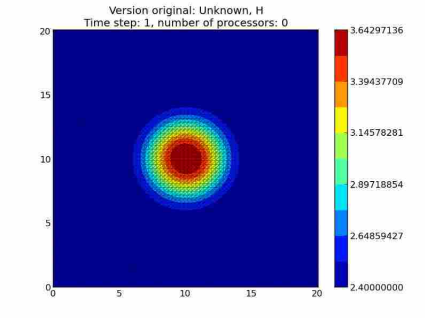


Parallel $p = 2$

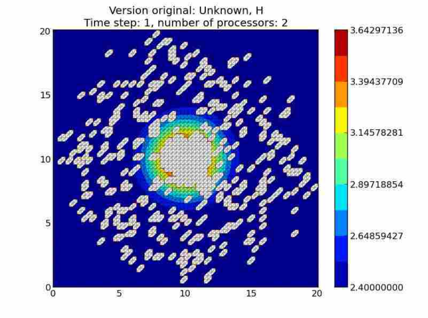
A white plot displays a non-reproducible value

Numerical reproducibility?

time step $= 1$



Sequential



Parallel $p = 2$

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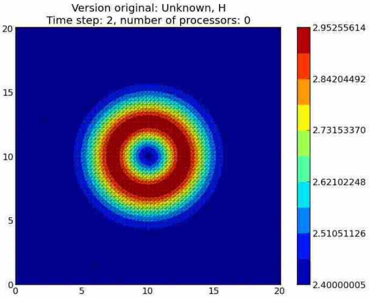
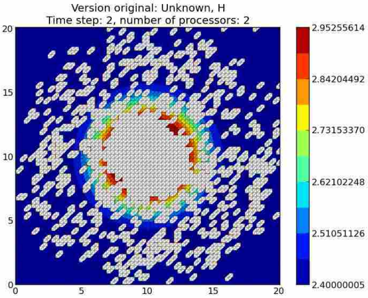
Numerical reproducibility?

time step $= 2$



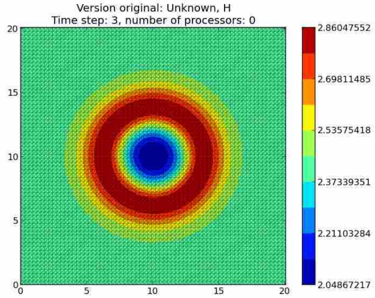
Sequential



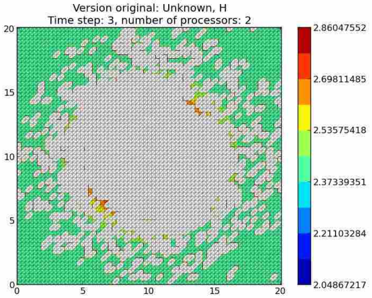
Parallel $p = 2$

Numerical reproducibility?

time step $= 3$



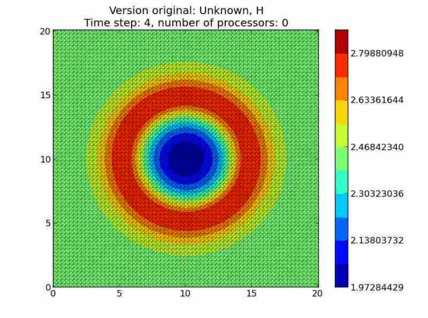
Sequential



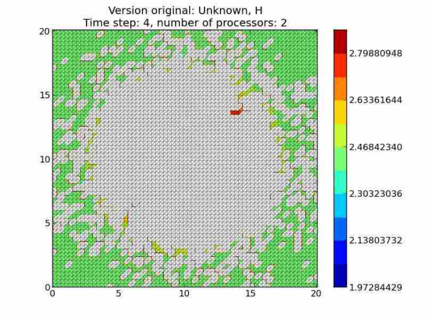
Parallel $p = 2$

Numerical reproducibility?

time step = 4



Sequential

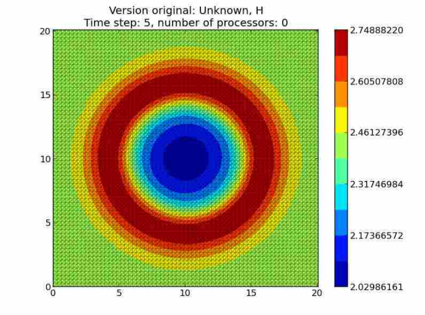


Parallel $p = 2$

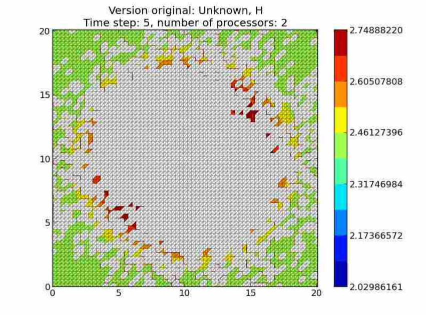
A white plot displays a non-reproducible value

Numerical reproducibility?

time step = 5



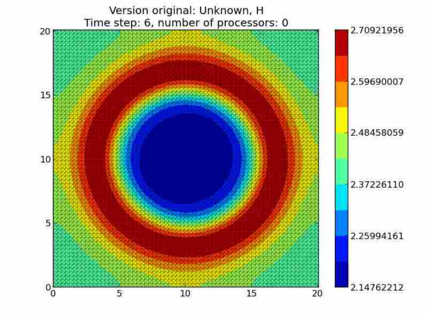
Sequential



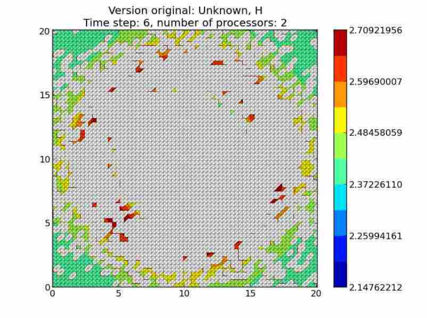
Parallel $p = 2$

Numerical reproducibility?

time step = 6



Sequential

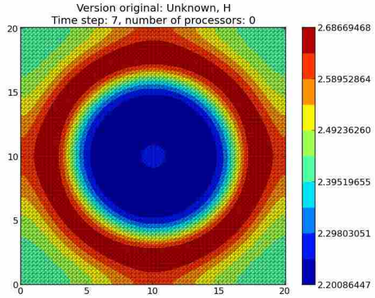


Parallel $p = 2$

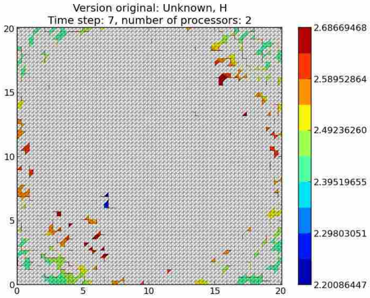
A white plot displays a non-reproducible value

Numerical reproducibility?

time step $= 7$



Sequential

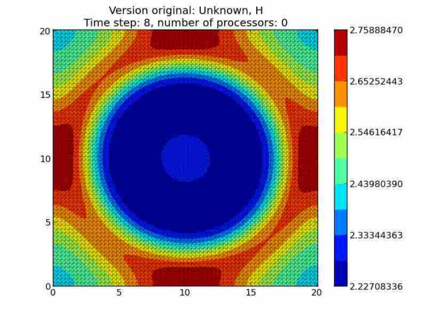


Parallel $p = 2$

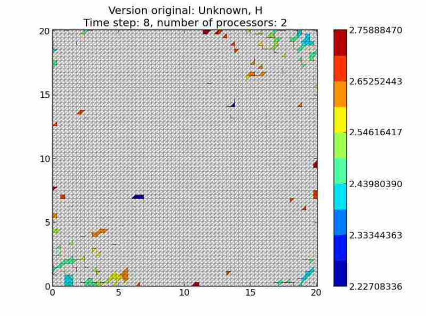
A white plot displays a non-reproducible value

Numerical reproducibility?

time step = 8



Sequential

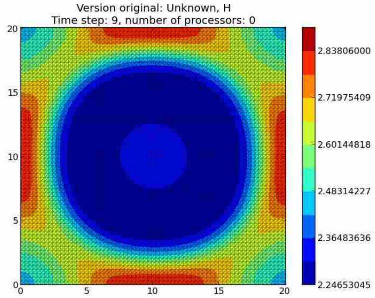


Parallel $p = 2$

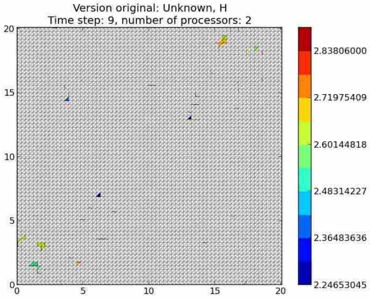
A white plot displays a non-reproducible value

Numerical reproducibility?

time step = 9



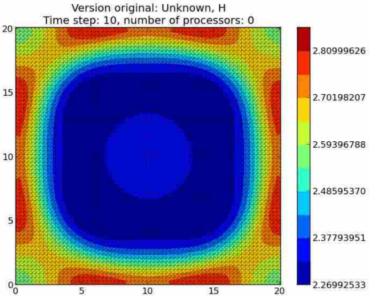
Sequential



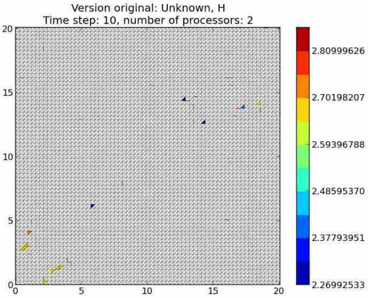
Parallel $p = 2$

Numerical reproducibility?

time step $= 10$



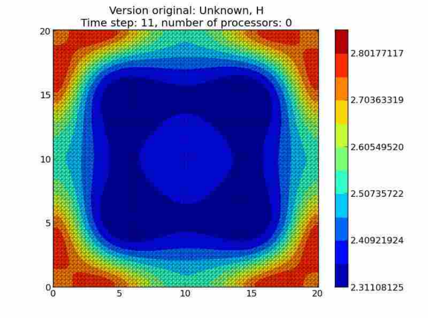
Sequential



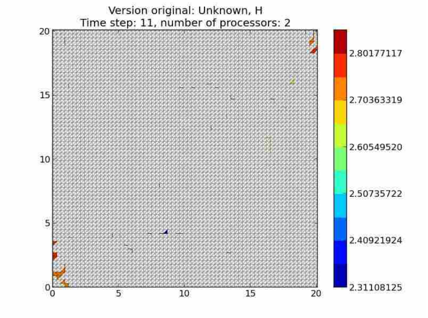
Parallel $p = 2$

Numerical reproducibility?

time step = 11



Sequential

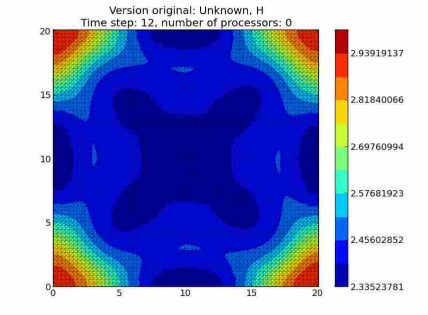


Parallel $p = 2$

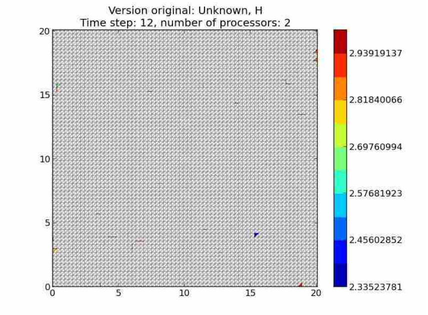
A white plot displays a non-reproducible value

Numerical reproducibility?

time step = 12



Sequential

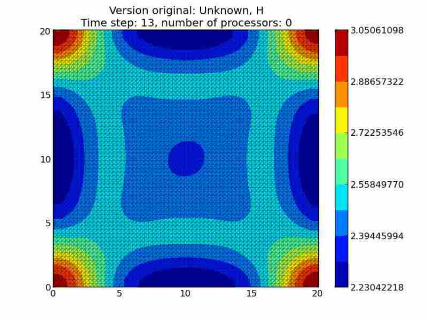


Parallel $p = 2$

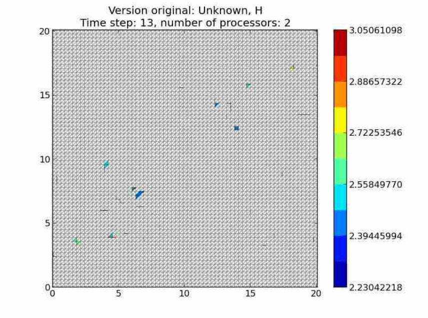
A white plot displays a non-reproducible value

Numerical reproducibility?

time step $= 13$



Sequential

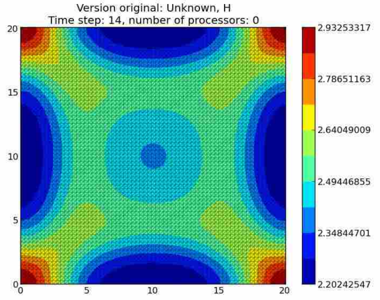


Parallel $p = 2$

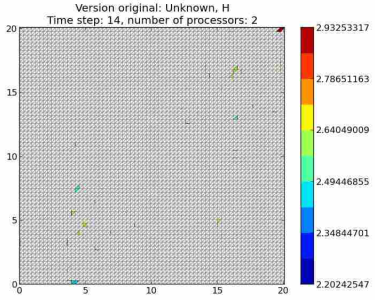
A white plot displays a non-reproducible value

Numerical reproducibility?

time step = 14



Sequential

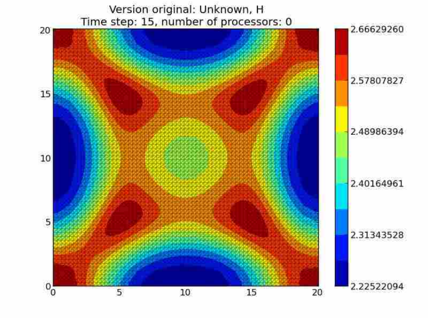


Parallel $p = 2$

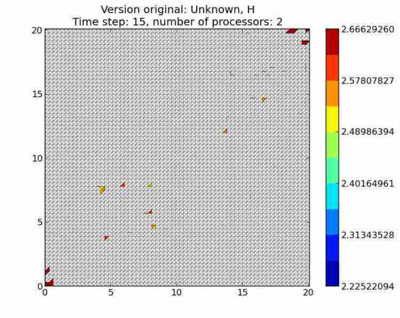
A white plot displays a non-reproducible value

NO numerical reproducibility!

time step $= 15$

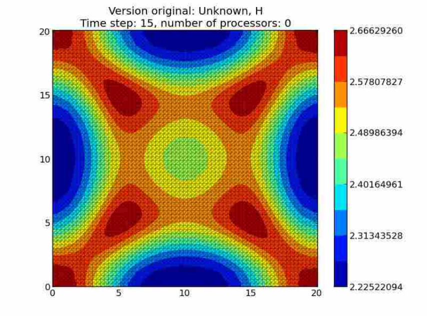


Sequential

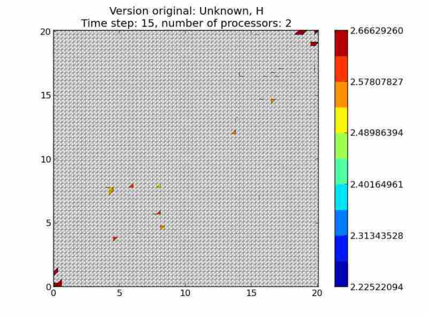


Parallel $p = 2$

NO numerical reproducibility!



Sequential



Parallel $p = 2$

Motivations

Reproducibility failures reported in numerical simulation in many domains

- energy [10],
- dynamic weather science [2],
- dynamic molecular [9],
- dynamic fluid [8]

Motivations

- How to debug?
- How to test?
- How to validate?
- How to receive legal agreements?

Today's issues

Case study

- Industrial scale software: openTelemac-Mascaret
- Finite element simulation, domain decomposition, linear system solving
- 2 modules: Tomawac, Telemac2D

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Feasibility

- How to recover reproducibility?
- Sources of non-reproducibility?
- Do existing techniques apply? how easily?
- Compensation yields reproducibility here!

Today's issues

Case study

- Industrial scale software: openTelemac-Mascaret
- Finite element simulation, domain decomposition, linear system solving
- 2 modules: Tomawac, Telemac2D

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- How to recover reproducibility?
- Sources of non-reproducibility?
- Do existing techniques apply? how easily?
- Compensation yields reproducibility here!

Efficiency

- How much to pay for reproducibility?
- $\times 1.2 \leftrightarrow \times 2.3$ extra-cost which decreases as the problem size increases
- OK to debug, to validate and even to simulate!

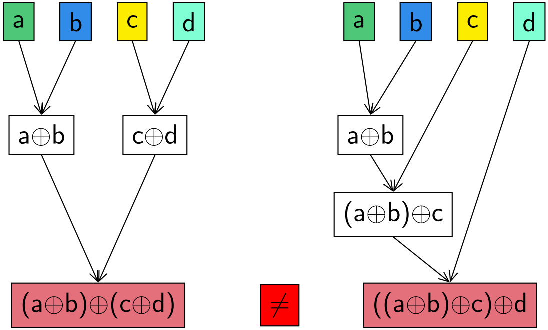
Basic ingredients

Parallel reduction and compensation techniques

Weakness of floating point arithmetic

- Rouding errors, non associative floating-point addition
- The computed value depends on the operation order

Parallel reduction: undefined order generates reproducibility failure



Parallel reduction and compensation techniques

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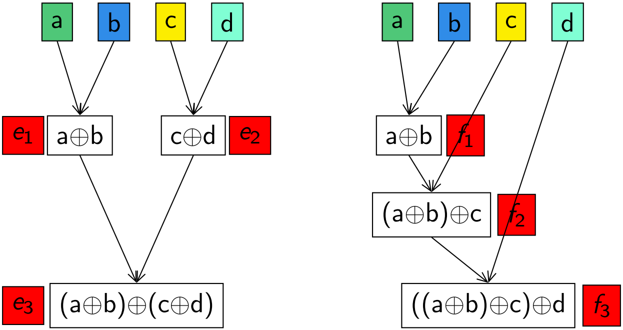
Compensation principle



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

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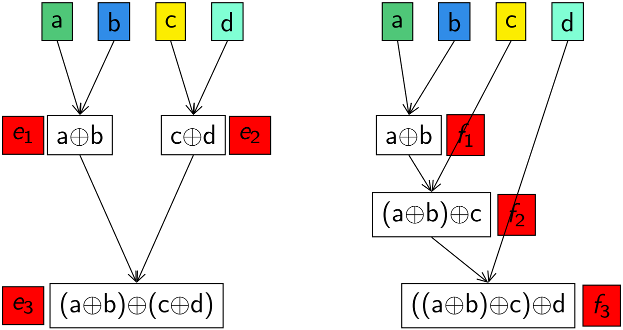


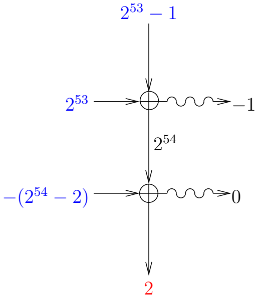
$$((a\oplus b)\oplus(c\oplus d)) \oplus ((e_1 \oplus e_2) \oplus e_3) = (((a\oplus b)\oplus c)\oplus d) \oplus((f_1 \oplus f_2) \oplus f_3)$$

Should be repeted for too ill-conditionned sums

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

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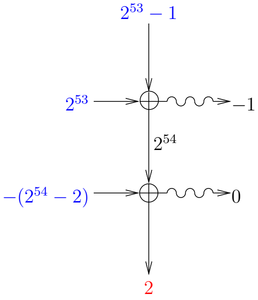
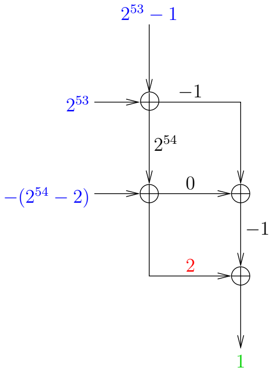


Relative error = 1

Compensation of the rounding errors

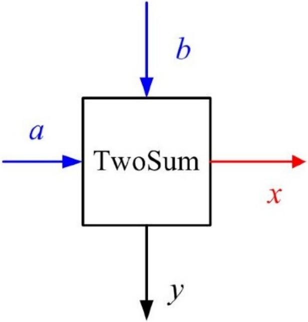


The exact result is computed

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)

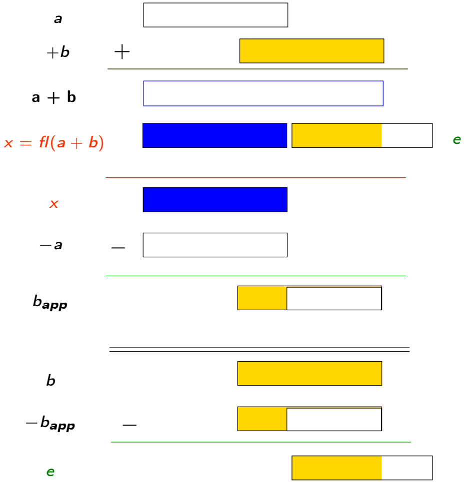
$x = a \oplus b$

$z = x \ominus a$

$y = b \ominus z$

The underlined idea of EFT

Fast2Sum computes the rouding error e in $a \oplus b$ ($|a| > |b|$)



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

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

$x = a \oplus b$

$z = x \ominus a$

$y = b \ominus z$

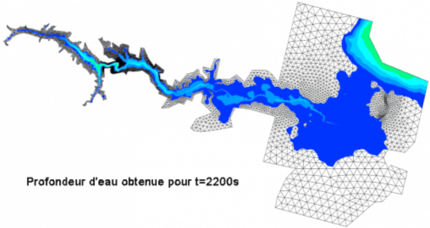
Other EFT for the product, FMA, ...

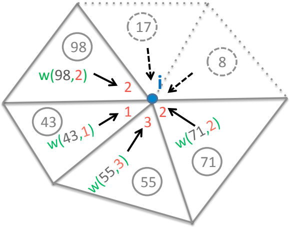
Reproducibility failure in a FE simulation

Finite element assembly: the sequential case

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

- compute the inner node values $V(i)$
- accumulating local W_e for every *ielem* that contains *i*





The assembly loop:

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

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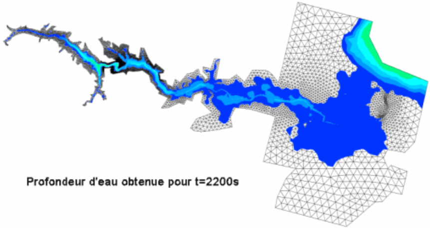
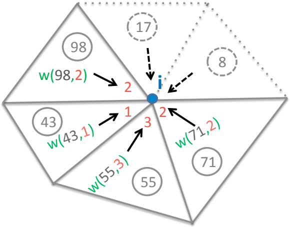
- accumulating local W_e for every *ielem* that contains i



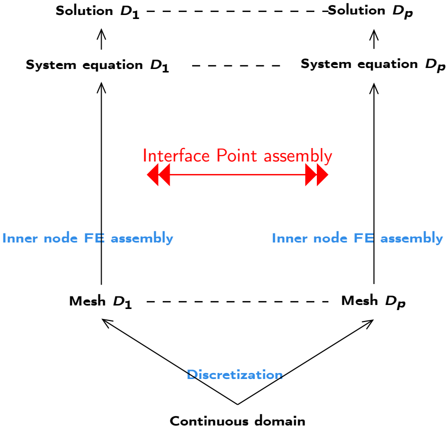


The assembly loop: managing local vs. global numbers

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

Finite element assembly: the parallel case

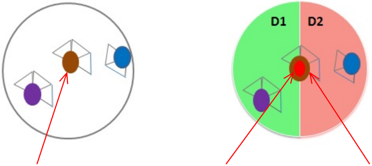
Parallel FE: subdomain decomposition



$\boxed{\text{IP assembly = communications and reductions}}$

Exact arithmetic

sequential | parallel



$V(i) = a$ $\quad V_{D1}(i) = b \quad V_{D2}(i) = c$

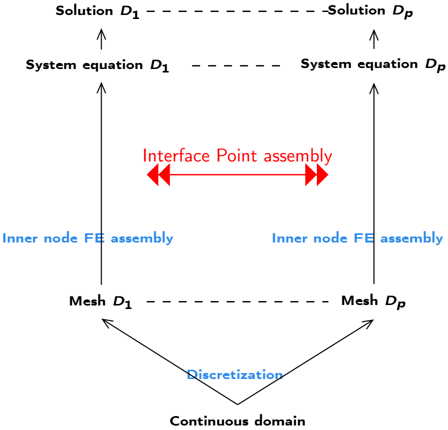
Interface point assembly

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

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

Finite element assembly: the parallel case

Parallel FE: subdomain decomposition

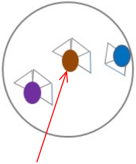


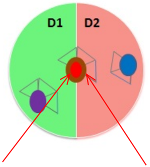
IP assembly =
communications and reductions

Floating point arithmetic

sequential

parallel





$V(i) = \widehat{a}$

$V_{D1}(i) = \widehat{b}$ $\quad V_{D2}(i) = \widehat{c}$

Interface point assembly

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

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

subdomains $D_k, k = 1...p$

The parallel finite element assembly is non-reproducible

Tomawac: the Telemac's module for wave propagation in coastal areas

- Transport equation: 1st order PDE $\rightarrow$ ODEs along its characteristic curves
- Integration reduces to accumulation (and interpolation) over the finite element mesh
- Unknowns: significant wave height, mean wave frequency and direction
- The Nice test case:
  effect of high-speed ferry waves

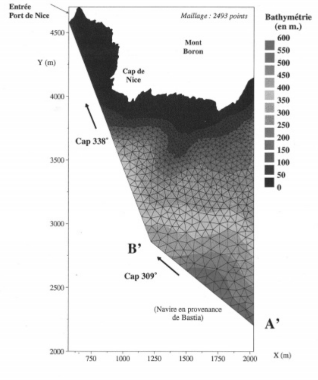


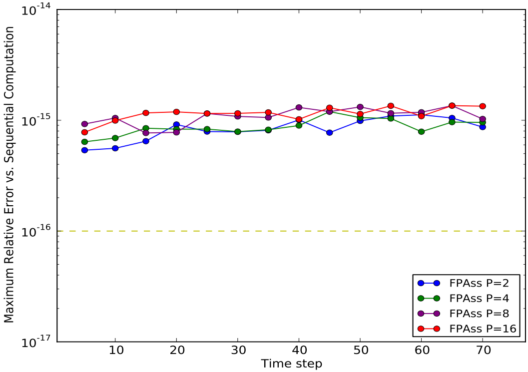
Figure 1 - Bathymétrie et maillage du domaine étudié

Reproducibility failure of the FE assembly step

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. Failure of numerical reproducibility: what, when, why
   - Motivation
   - Today's case study
   - Compensation in floating-point arithmetic
2. Reproducibility failure in a finite element simulation
   - Sequential and parallel FE assembly
   - Non reproducible Tomawac
   - Sources of non reproducibility in Telemac2D
3. Recovering reproducibility
   - Reproducible parallel FE assembly
   - Reproducible algebraic operations
   - Reproducible conjugate gradient
   - Reproducible Telemac2D
4. Efficiency
5. Conclusion and work in progress

Sources of non reproducibility in Telemac2D

Culprits: theory

1. Building step: interface point assembly
2. Solving step (with conjugate gradient): parallel matrix-vector and dot products

Sources of non reproducibility in Telemac2D

Culprits: theory

1. Building step: interface point assembly
2. Solving step (with conjugate gradient): parallel matrix-vector and dot products

Culprits: practice = optimizations

- Element-by-element storage of the FE matrix
  - Everything is vector, no matrix!
  - No BLAS parallel matrix-vector product
- Wave equation, "mass-lumping" and associated algebraic transformations
  - System decoupling and many diagonal matrices
  - Everything is vector, no matrix!
- Interface point assembly and linear system solving are merged

Sources of non reproducibility in Telemac2D

The Telemac2D FE steps

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

---

wave equation →

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

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

Interface node assembly:

$CV2, CV3$

conjugate gradient →

Interface node assembly:

$AM1$ in each iteration

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:

$AM2, AM3, CV1$

H

AM2,AM3

AM1,CV1

Sources of non reproducibility in Telemac2D

The Telemac2D FE steps

Solution U,V

wave equation

$$CV2 = B_u - A_{uh}H,$$
$$CV3 = B_v - A_{vh}H.$$

Interface node assembly:

$CV2$, $CV3$

Solution H

conjugate gradient

Interface node assembly:

$AM1$ in each iteration

H

AM2,AM3

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

Recovering reproducibility in Telemac2D

Sources

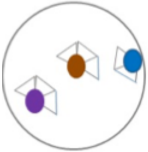
- FE assembly: matrix and second member
- Wave equation: algebraic transformations and diagonal resolutions
- Resolution: matrix-vector and dot products

Reproducible resolution: principles

- vector $V \rightarrow [V, E_V] \rightarrow V + E_V$
- Inner nodes: compensate FE assembly
- Interface nodes: propagate rounding errors
  and compensate within interface node assembly (also denoted IP)
- Compensate the EBE matrix-vector products that include IP assembly
- Compensate the MPI parallel dot products that include MPI reduction

Accurate compensated FE 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

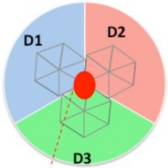
$$E(i) = \Delta_1 + \Delta_2 + \ldots + \Delta_n$$

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

$$X(i) = \underbrace{W_i(e_1)}_{\Delta_1} + \underbrace{W_i(e_2)}_{\Delta_2} + \ldots + \underbrace{W_i(e_n)}_{\Delta_n}$$

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

similar

Interface point assembly

i : interface point between D1,D2,D3

Accumulation of errors Δ and $\mathcal{E}$

$X(i), E(i)$ ⟺ $X(i) = X(i) \underbrace{+}_{\mathcal{E}_1} X(i) \underbrace{+}_{\mathcal{E}_2} X(i)$ ⟺ $X(i), E(i)$

$$E(i) = ((E(i) + E(i) + \mathcal{E}_1) + E(i) + \mathcal{E}_2)$$

Compensation of the FE assembly for every mesh node i

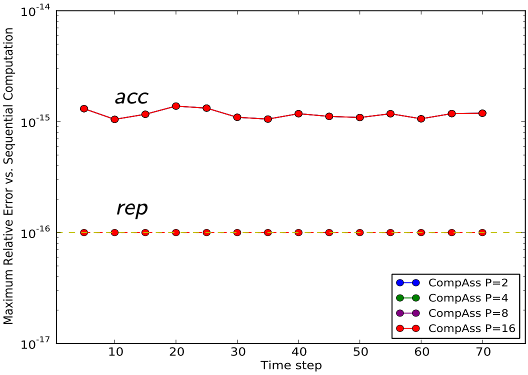
similar

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

similar

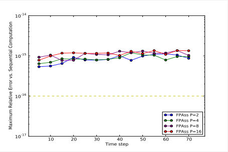
Accurate compensated assembly gives reproducibility

Reproducibility in Tomawac: the Nice test case



Mean frequency wave, Nice test case, Tomawac

rep in the original FE assembly



A^s: sequential, A^p: p-parallel
$\max_{rel}(A_1, A_2) = |A_1 - A_2|/|A_2|$

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

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

Reproducible algebraic operations

Algebraic operation: the vector case

Reproducible vector algebraic operations

- openTelemac's included library: BIEF
- Entry-wise vector ops: copy, opp/inv., add/sub, Hadamard prod., ...
- Applies also for diagonal matrix
- Every op. is applied to FE assembled vectors with/without IP assembly
- Principle: propagate rounding errors and compensate while assembling IP

Example:
Hadamard product

Original version

1. $V = X \circ Y$
2. IP assembly if necessary for interface node i

Reproducible version

1. compute errors:
   $[V, E_V] = [X, E_X] \circ [Y, E_Y]$
   with $(V, e_V) = 2\text{Prod}(X, Y)$
   and $E_V = X \circ E_Y + Y \circ E_X + e_V$
2. compensate at inner nodes k:
   $V(k) + E_V(k)$:
3. propagate and compensate at the IP assembly if necessary for IP i: $V(i) + E_V(i)$

What is reproducible now?

Most of the linear system:

- FE assembly
- algebraic vector operations
- interface point assembly

except:

- the matrix of the H system
- its dependencies: the second members of the U and V systems

Partially reproducible Telemac2D

wave equation :

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

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

Interface node assembly:

$CV2, CV3$

Solution U,V

H

AM2,AM3

conjugate gradient :

Interface node assembly:

$AM1d$ in each iteration

Solution H

AM1,CV1

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:

$AM2, AM3, CV1$

Towards a reproducible conjugate gradient

The last step

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:

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

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

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

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

X=H

Non-reproducibility: sources and solutions [5]

Towards a reproducible conjugate gradient

The last step

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

$B = CV1$

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:

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

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

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

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

$X = H$

Non-reproducibility: sources and solutions [5]

- EBE matrix-vector product
  - is followed by one IP assembly at every iteration
  - reproducible with compensated IP assembly

Towards a reproducible conjugate gradient

The last step

A=[$AM1$, E_{AM1}] → ; B=$CV1$ →

Initialization:

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

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

Iterations:

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

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

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

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

→ X=H

Non-reproducibility: sources and solutions [5]

- EBE matrix-vector product
  - is followed by one IP assembly at every iteration
  - reproducible with compensated IP assembly
- MPI `all_reduced` dot product
  - a parallel version of the compensated `dot2` [6]

Towards a reproducible conjugate gradient

The last step

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:
```

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

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

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

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

X=H

Non-reproducibility: sources and solutions [5]

- EBE matrix-vector product
  - is followed by one IP assembly at every iteration
  - reproducible with compensated IP assembly
- MPI `all_reduced` dot product
  - a parallel version of the compensated `dot2` [6]
- with ponderation for interface node shared by p subdomains
  - $(1/p, 1/p, \ldots, 1/p) \to (0, \ldots, 0, 1, 0 \ldots, 0)$

A reproducible conjugate gradient

$$\mathbf{A} = [AM1,\ E_{AM1}] \quad \mathbf{B} = CV1$$

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:

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

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

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

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

$$\longrightarrow \mathbf{X} = H$$

Not necessarily more accurate but reproducible

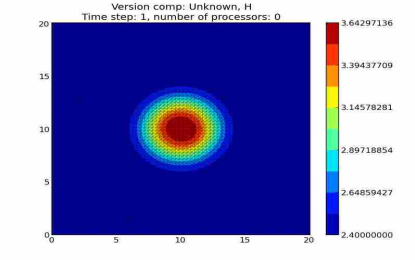
Same errors in the compensated values for both sequential and parallel executions

Recovering reproducibility in a finite element resolution

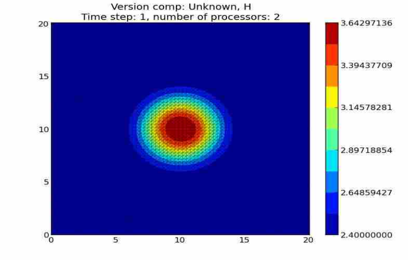
Reproducible gouttedo!

Time step 1

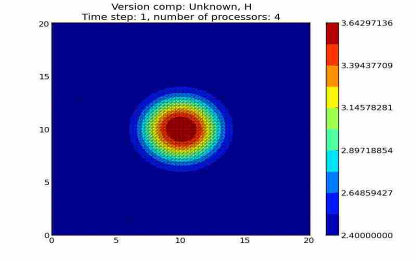
p=1



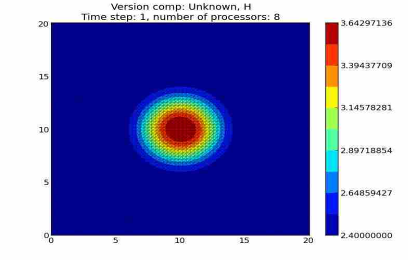
p=2



p=4



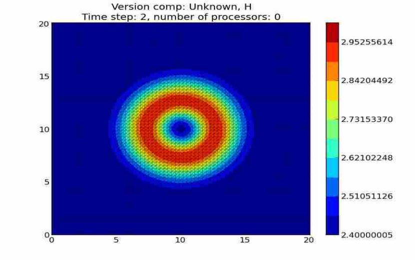
p=8



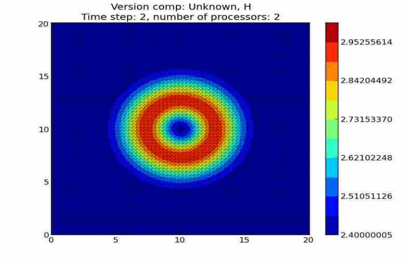
Reproducible gouttedo!

Time step 2

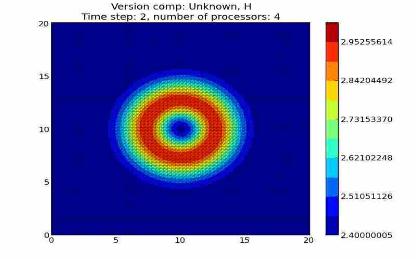
p=1



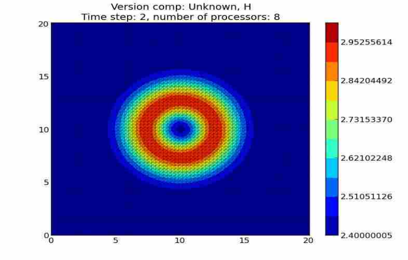
p=2



p=4



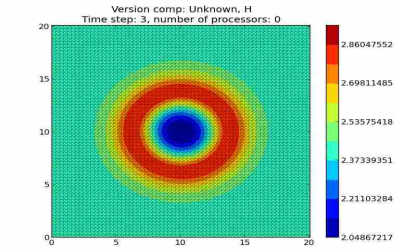
p=8



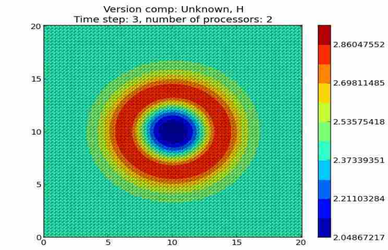
Reproducible gouttedo!

Time step 3

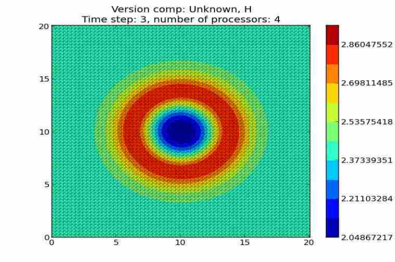
p=1



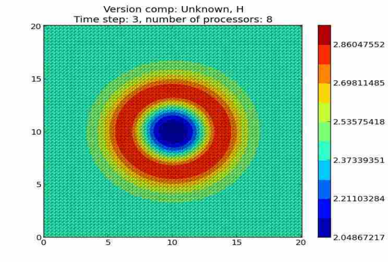
p=2



p=4

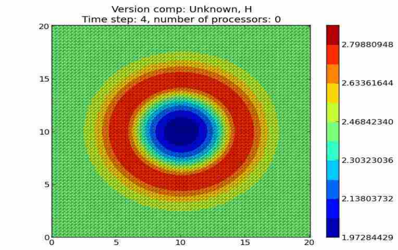


p=8

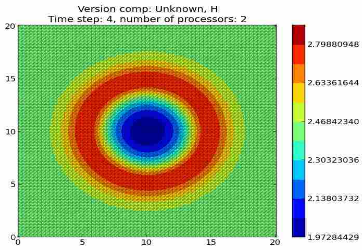


Time step 4

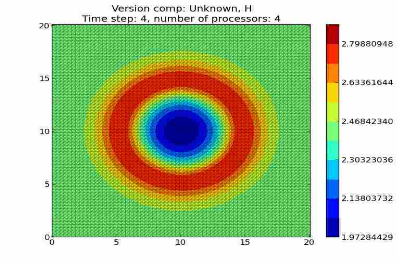
p=1



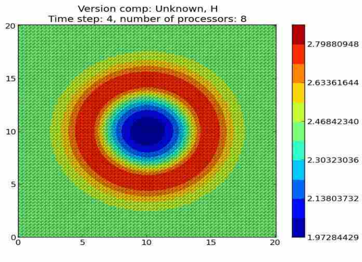
p=2



p=4



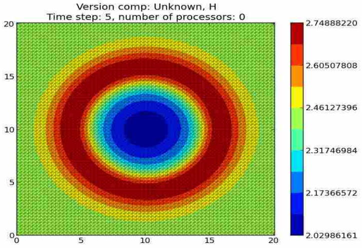
p=8



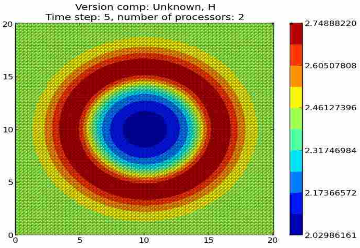
Reproducible gouttedo!

Time step 5

p=1



p=2



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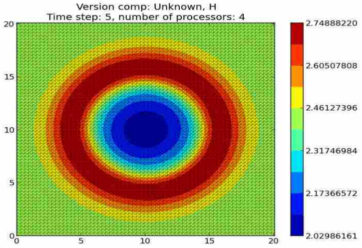

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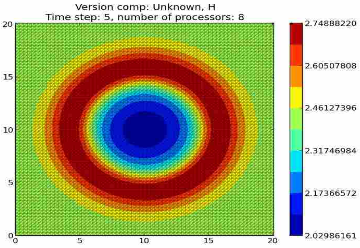

Time step 6

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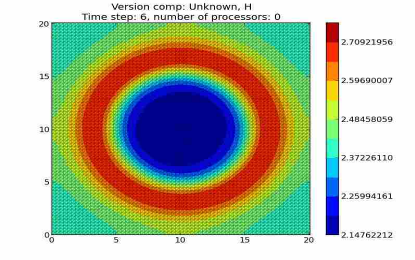

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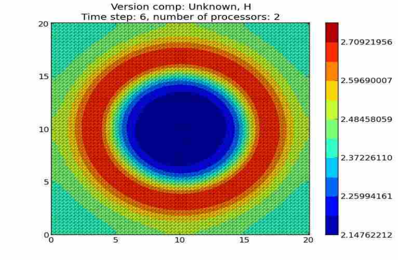

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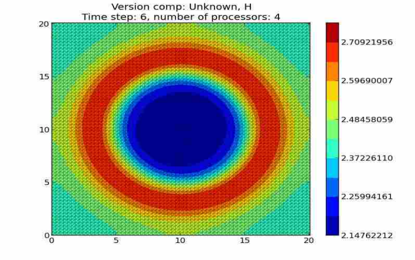

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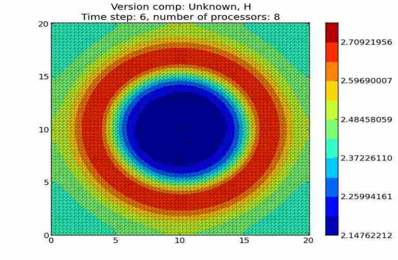
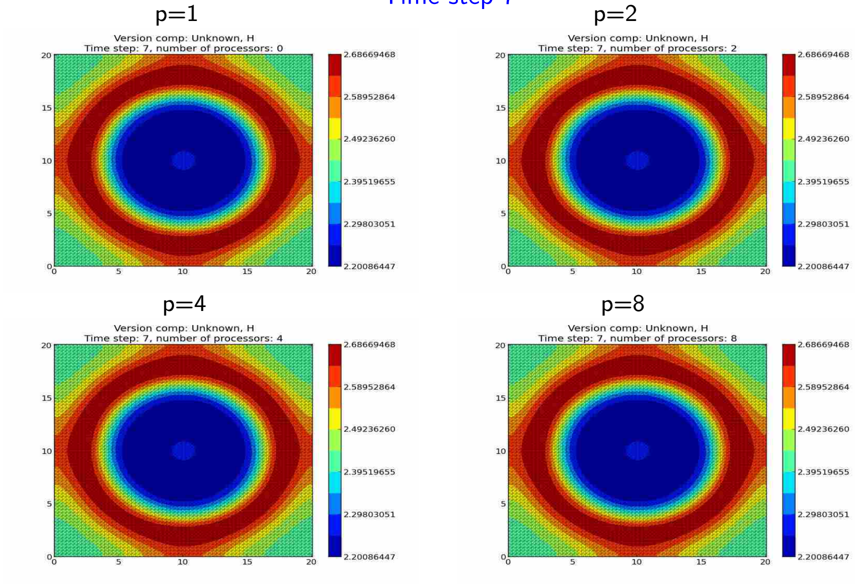


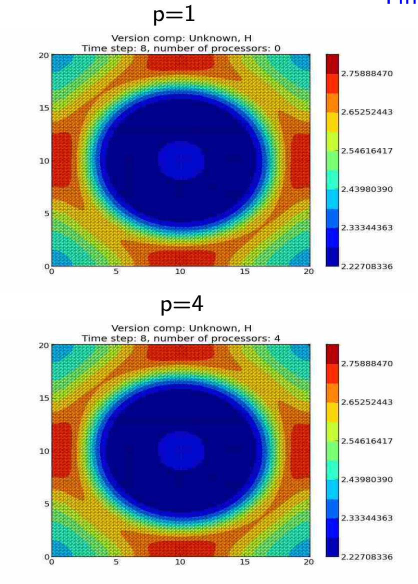
Reproducible gouttedo!

Time step 7



Reproducible gouttedo!

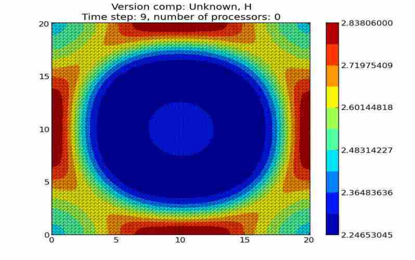
Time step 8



Reproducible gouttedo!

Time step 9

p=1



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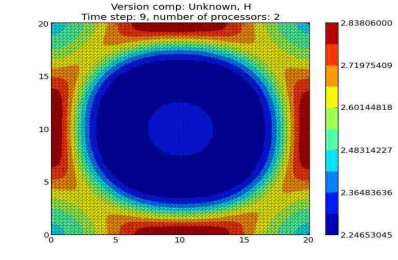

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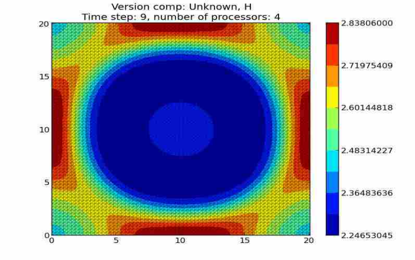

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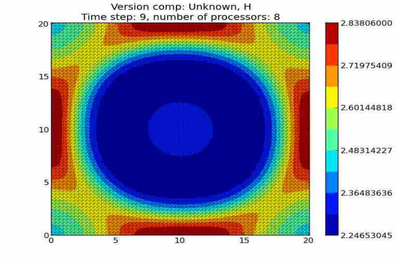
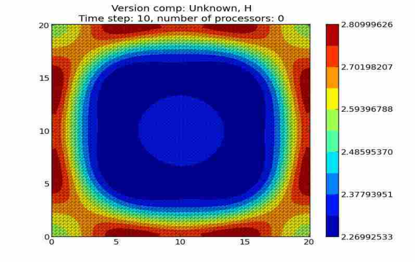


Reproducible gouttedo!

Time step 10

p=1



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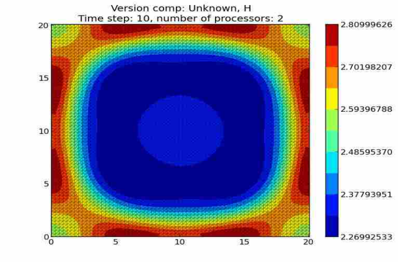

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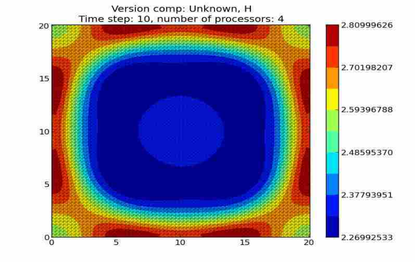

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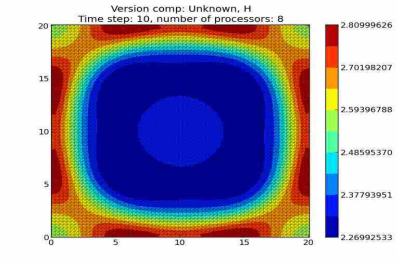
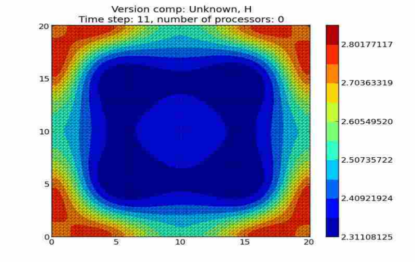


Reproducible gouttedo!

Time step 11

p=1



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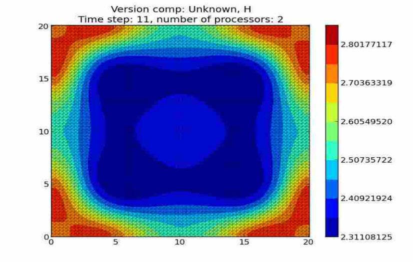

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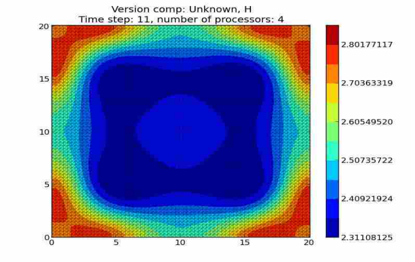

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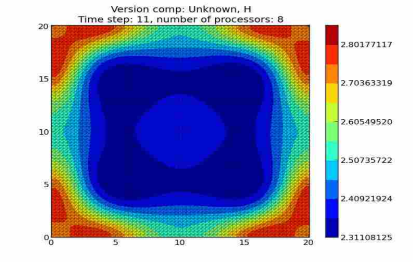
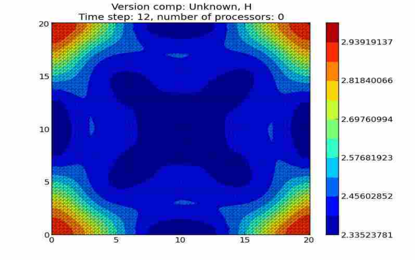


Reproducible gouttedo!

Time step 12

p=1



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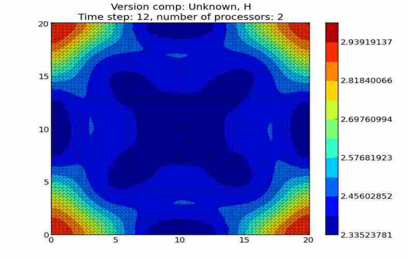

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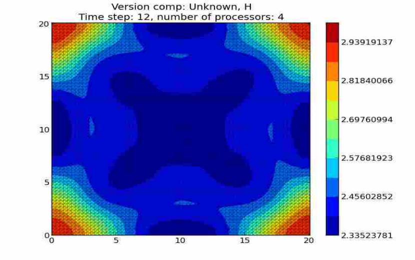

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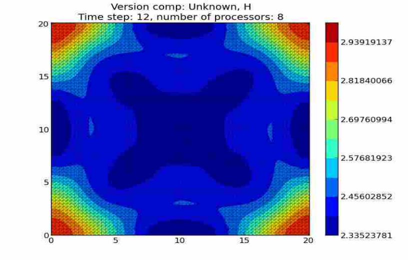

Reproducible gouttedo!

Time step 13

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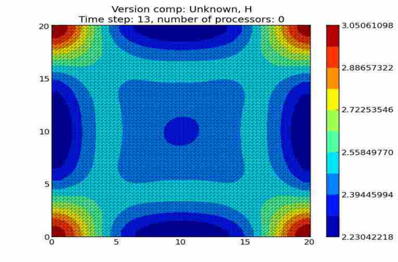

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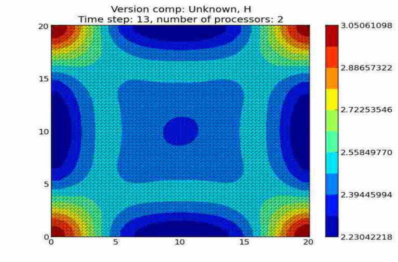

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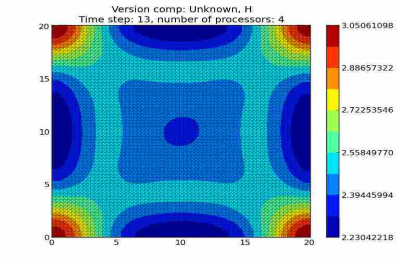

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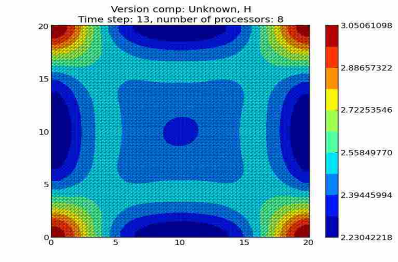
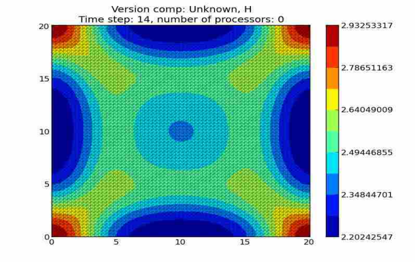


Reproducible gouttedo!

Time step 14

p=1



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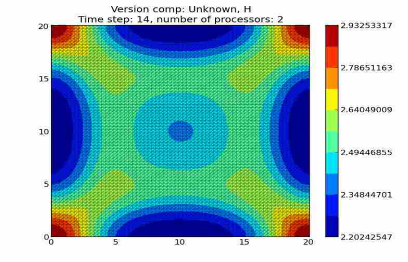

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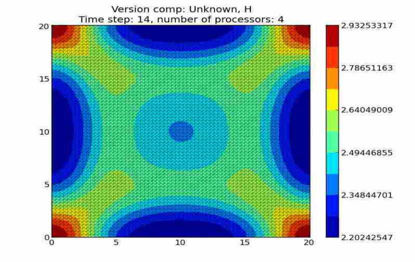

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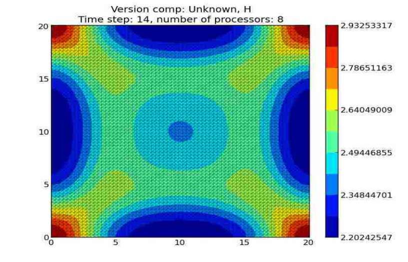

Reproducible gouttedo!

Time step 15

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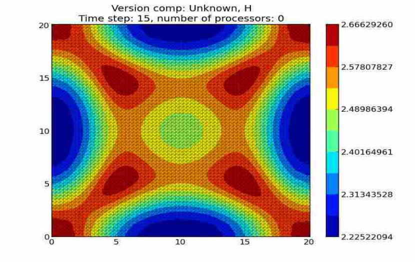

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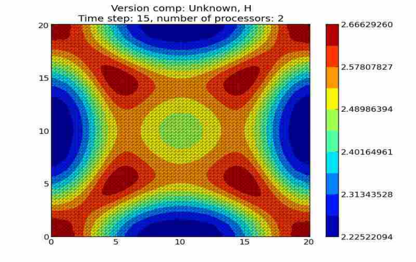

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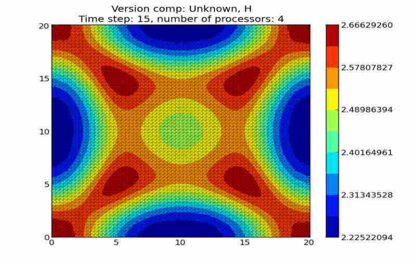

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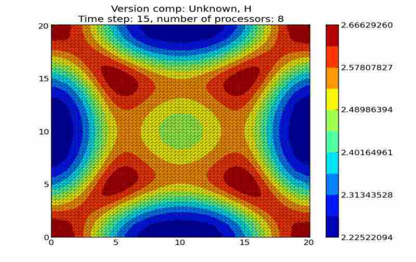
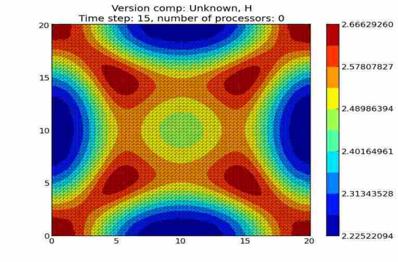


Reproducible gouttedo!

Time step 15

p=1



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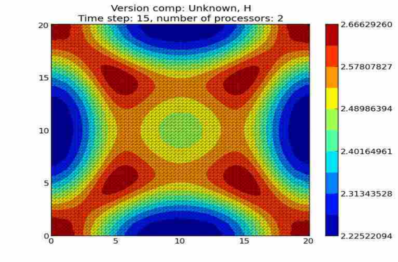

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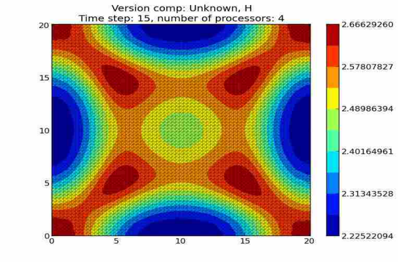

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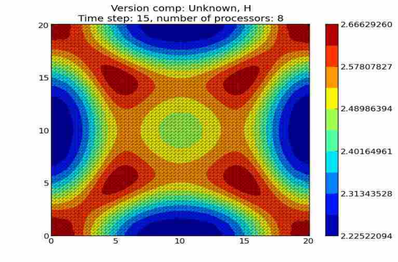


Runtime extra-cost for reproducible simulations

Measures, test cases and mesh sizes

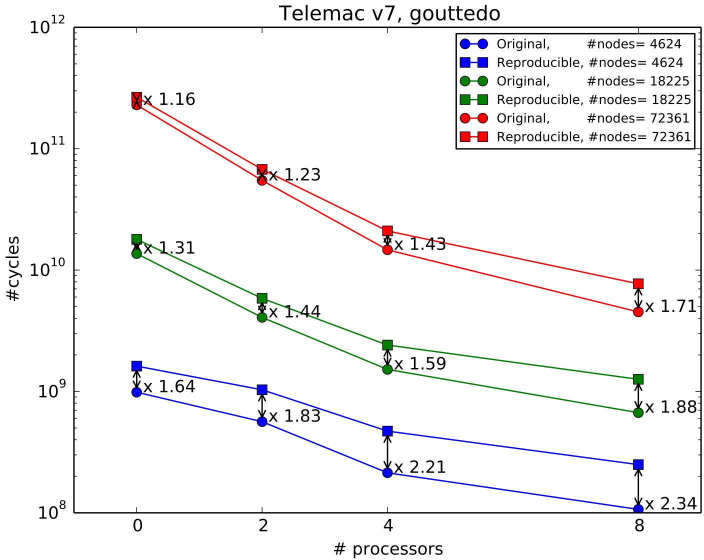
- hardware cycle counter: `rdtsc`
- `gouttedo`
- meshe sizes: 4624, 18225, 72361 nodes ($\approx 1, \times 4, \times 16$)

Hardware and software env.

- openTelemac v7.2
- socket: Intel Xeon E5-2660 2.20GHz (L3 cache = 20 M)
- 2 sockets of 8 cores each
- GNU Fortran 4.6.3, -O3
- OpenRTE (openMPI) 1.5.4
- Linux 3.5.0-54-generic

The core runtime extra-cost for reproducible gouttedo

gouttedo core: no input/output steps, just building+solving



Time to conclude

Conclusion

Recovering numerical reproducibility

- Industrial scale software: openTelemac-Mascaret
- Finite element simulation, domain decomposition, linear system solving
- 2 reproducible modules: Tomawac, Telemac2D
- Integration in the next openTelemac version: in progress

Conclusion

Recovering numerical reproducibility

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Feasibility

- How to recover reproducibility? Sources of non-reproducibility? Do existing techniques apply? how easily?
- Hand-made analysis of the computing workflow
- Compensation yields reproducibility here!
- Fits well to the openTelemac's vector library
- Other existing techniques also apply and more or less easily [4]

Conclusion

Efficiency

- How much to pay for reproducibility?
- $\times 1.2 \leftrightarrow \times 2.3$: OK to debug, to validate and even to simulate!

Conclusion

Efficiency

- How much to pay for reproducibility?
- $\times 1.2 \leftrightarrow \times 2.3$: OK to debug, to validate and even to simulate!

Reproducibility at a larger scale: the whole openTelemac software suite

- Does it still working for complex, large and real-life simulations?
- The two FE test cases are significant enough to validate the methodology
- Localization of the failure sources is difficult to automatize
- but it's easier to pass the methodology on to software developpers

Acknowledgment

Christophe Denis, EDF R&D, Clamart and CMLA, Cachan
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Chemseddine Chohra, DALI/LIRMM, UPVD, Perpignan

DALI, Digits, Architectures et Logiciels Informatiques

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Other existing techniques

Existing techniques to recover numerical reproducibility in summation

- Accurate compensated summation [6]
- Demmel-Nguyen's reproducible sums [1]
- Integer convertion [7]