Parallel reproducibility of the SHYFEM-MPI model

Francesco Carere[1], Giorgio Micaletto[1], Italo Epicoco[1,2], Francesca Mele [1]

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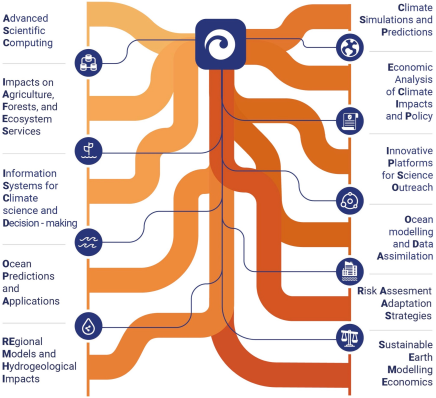
Workshop on Correctness and Reproducibility for Climate and Weather Software

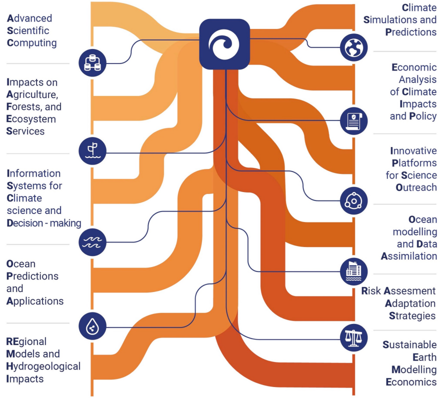
[1]Euro-Mediterranean Center on Climate Change (CMCC), Lecce, Italy
[2]Dep. Engineering for Innovation, University of Salento, Lecce, Italy

CMCC, ASC and SHYFEM-MPI

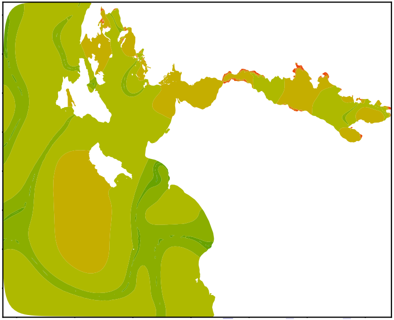


- W&C/society $\xleftrightarrow{\text{interdiscip. sci.}}$ policy
- Science (applied) vs. engineers (SW)

CMCC, ASC and SHYFEM-MPI



- W&C/society $\xleftrightarrow{\text{interdiscip. sci.}}$ policy
- Science (applied) vs. engineers (SW)
- ASC: develop SHYFEM-MPI
- Non-bitwise reproducible (non-BR)



Goal

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Equations $\longrightarrow$ Correct, V&V code $\longrightarrow$ optimised code

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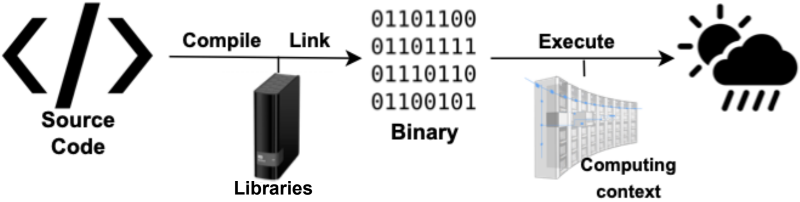
Propose : BR useful for second stage, but **not** needed after optimisation

Losing BR

It is easy to lose BR

Losing BR



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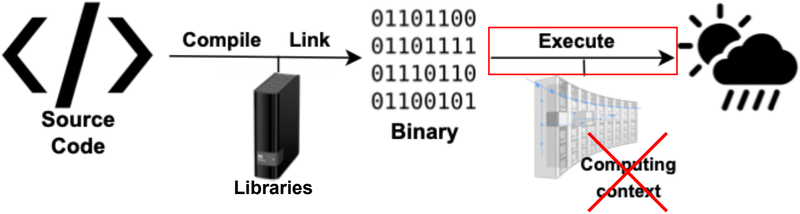

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Our case: parallelized model introduces non-det. during execution/runtime (without changing comp. context)

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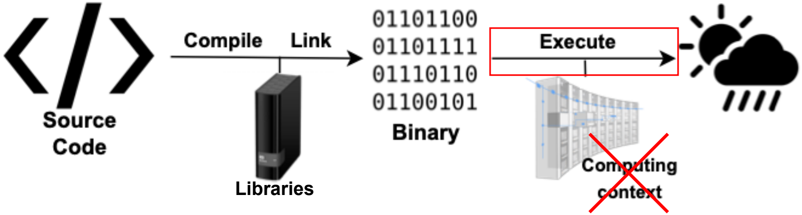

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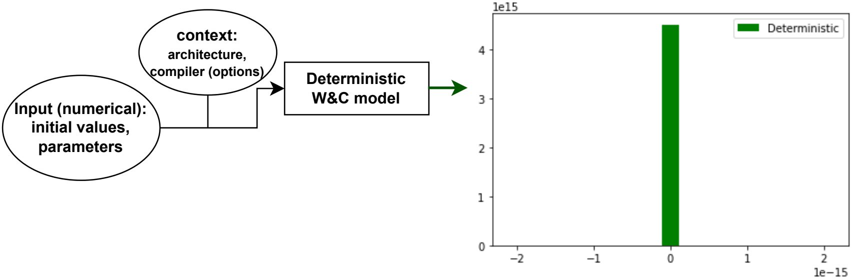
non-BR $\longleftrightarrow$ rounding error

W&C models: probability distributions



Have sequential model

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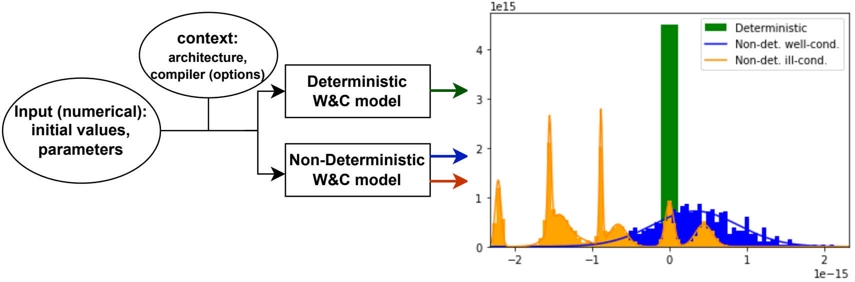

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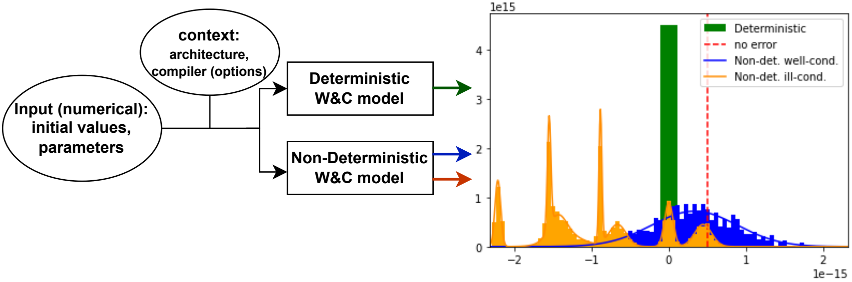

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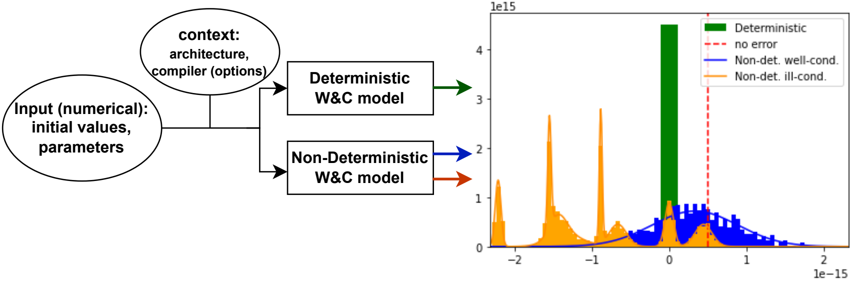

Have sequential model → parallelised (lose BR)

Parallel model: (part of) rounding error emerges

Non-BR: what to do?

Scientists and engineers unhappy with loss of BR. Solutions?

1. Force back BR (e.g. det. comm., little compiler optim., ...)
2. Reachieve BR (e.g. reproBLAS)
3. No BR (influence BR by e.g. precision [Nhe16; Pic18])

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- Section 1: (dis)advantages of BR
- Section 2: introducing parallel reproducibility via permutations
- Section 3: SHYFEM-MPI

1 BR: when to use it

2 Parallel reproducibility: Statistical approach

3 SHYFEM-MPI

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BR: (Dis)advantages

Table: Generally mentioned (dis)advantages of BR

Engineer	**Scientist**

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- Rare behaviour? Decreasing instead of wanting non-BR?

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If optimised (non-BR) code is correct, verified, validated.
Use for science!

Bitwise reproducibility or an alternative?

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In what sense trust (correctness, V&V) parallelised code?

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We try a statistical definition (not epistemological)

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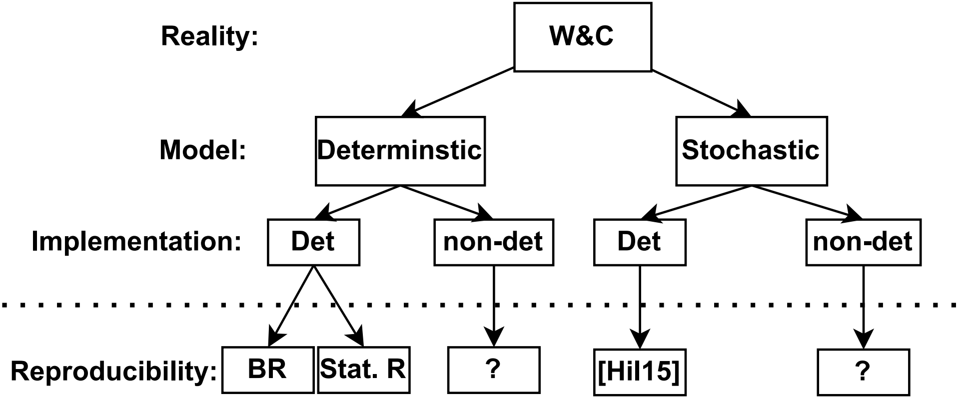
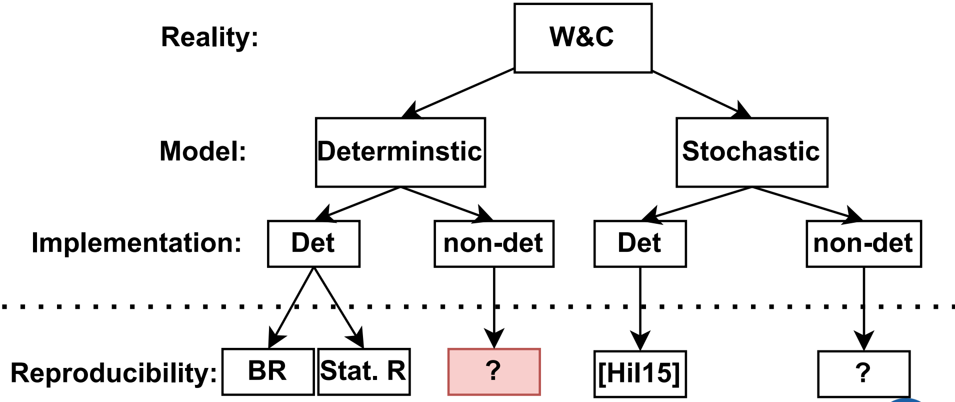
Statistical framework: reproducibility



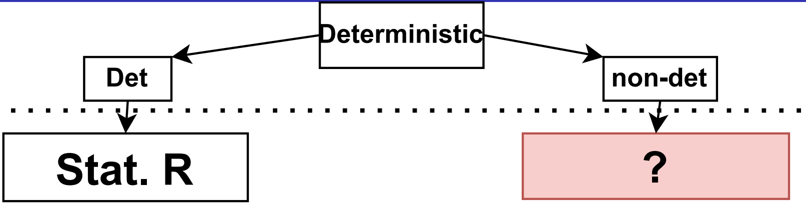
Statistical reproducibility exists [Mah+19] (as for stoch. det. [Hil15])

Statistical framework: reproducibility



Problem: reproducibility for non-det. implementations of det. models

Parallel reproducibility: first try



1. Two version x, y of code, both det.
2. Vary init. vars, to get samples X_i, Y_i
3. Two-sample test using probability metric $d(\{X_i\}_i, \{Y_i\}_i)$
4. Stat. reproducibility: tolerance for test, e.g. [Mah+19]

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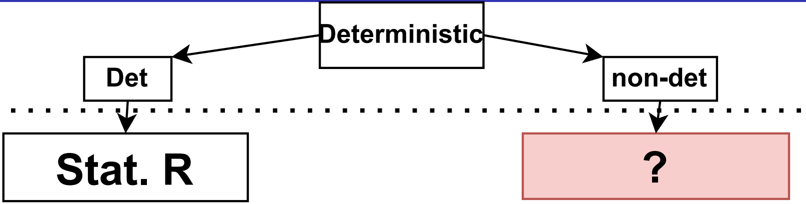

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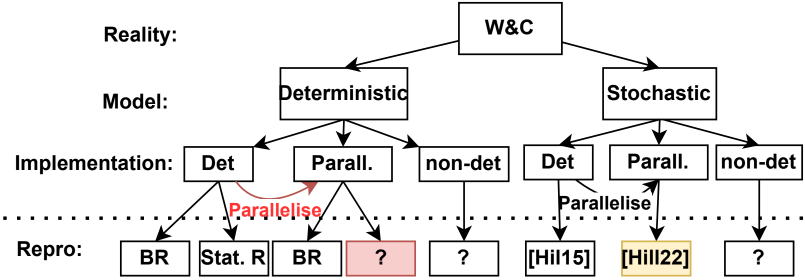
1. One version of code z, non-det
2. Run multiple times to get sample Z_i
3. One-sample test??
4. Reproducibility?

Statistical framework: **parallel** reproducibility



- Goal: **parallel reproducibility** for parallelised model
- [Hil22] defined/treated it in stochastic case

Example: parallel summation

BLAS $\oplus$ not associative: $(x \oplus y) \oplus z \neq x \oplus (y \oplus z)$

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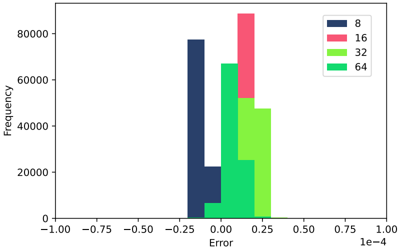

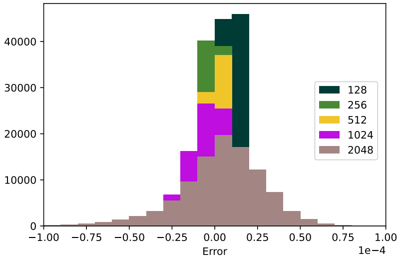

How reproducible is parallel summation?

Parallel summation: rounding error

FLOP $\oplus$ calculates (rel. err. $|\delta_i| \leq \epsilon =$ round. precision)

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$$S := \sum_{i=1}^{n} a_i, \quad s_{i+1} := s_i \oplus a_i = (s_i + a_i)(1 + \delta_i), \qquad s_1 := a_1.$$

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Either estimated error [Rou16]

$$\textbf{estimated:}\ |S - s_n| \leq \frac{(n-1)\epsilon}{1-(n-1)\epsilon} \sum_{i=1}^{n} |a_i| \quad \text{for } n \leq \epsilon{-}1,$$

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or expected [Hen64; Vig93] error:

$$\textbf{expected:}\ S - s_n \sim \mathcal{N}(0, \sqrt{n}\,\sigma) \quad \text{if } \delta_i \sim \mathcal{N}(0,\sigma) \text{ iid } (\sigma = \frac{1}{\sqrt{12}}\epsilon).$$

Parallel reproducibility: try 2

Parallel reproducibility: try 2.

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Sample P_i, parallel code. Probability distribution S of rounding error.

Method 1:

1. Choose probability metric d and $0 < \alpha < 1$
2. Perform one-sample test between P_i and S (e.g. KS)
3. Accept test if passes with tolerance α

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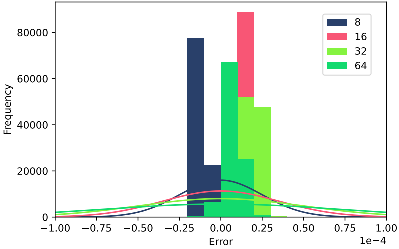
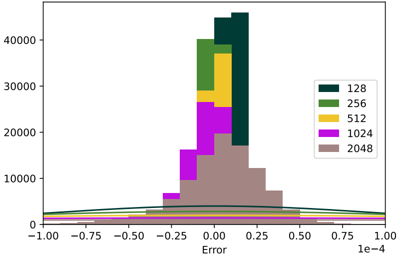
Method 2:

1. Choose tolerance $0 < \alpha < 1$
2. α-confidence interval of mean (of S)
3. Check if P_i lies in α-confidence interval

Parallel summation

Method 2:





Parallel summation

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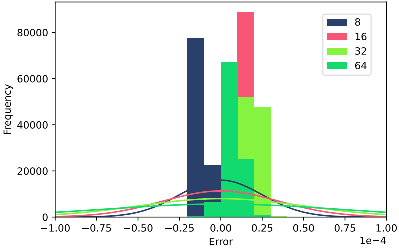

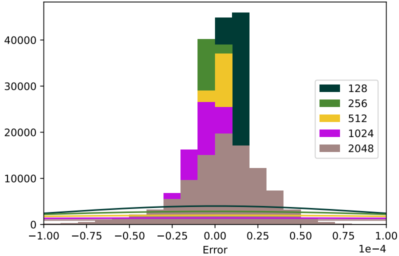

Method 1:

Kolmogorov-Smirnov test: negative outcome. Not drawn from the same distribution

Rounding-error and non-associativity

Problem with this approach:

Distribution of rounding error often hard to find.

[3] See [PN20] for similar tests

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Sample rounding-error. But how?

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Non-associativity → reorder index set **of BR code**[3].

[3] See [PN20] for similar tests

Parallel reproducibility: definition

Samples parallel/sequential P_i and S_i.

Two methods

Two-sample test:

1. Given probability metric d, tolerance $0 < \alpha < 1$
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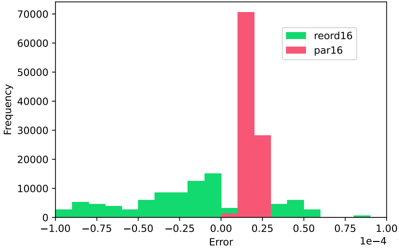
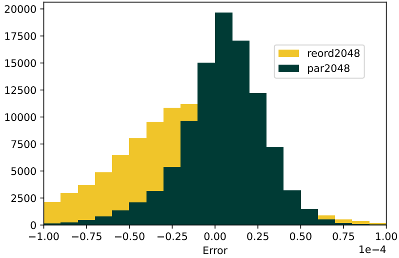
Confidence interval

1. Given tolerance $0 < \alpha < 1$
2. Assume $S_i \sim \mathcal{N}(\mu, \sigma)$ (assume CLT)
3. Check if P_i in confidence interval for given tolerance?

Parallel reproducibility for sums





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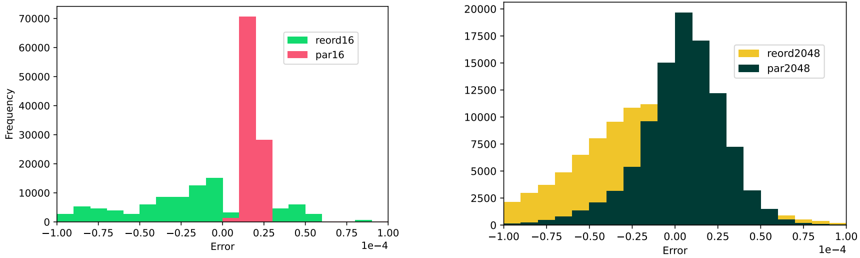

Again negative KS test: negligible value of hypothesis statistic (not equal)

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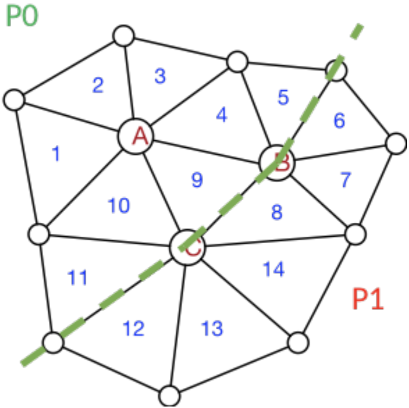
SHYFEM-MPI: reproducibility



- Domain partitioned
- Communication over boundaries
  Non-associativity → BR

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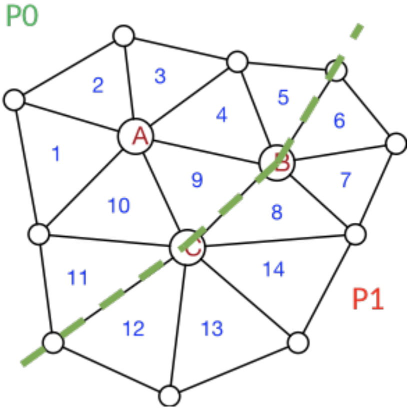

- Domain partitioned
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  Non-associativity → BR
- Sample by reordering grid

SHYFEM-MPI: reproducibility

Difference parallel runs (non-BR) 2 causes [Mic+22]:

1. MPI communications: different order of operations in **reductions** and **non-blocking recv-send**
2. Assembly of matrix by PETSc library

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Differences between sequential and parallel executions:

1. Different order of floating point operations (regardless of communications)
2. Internal optimization of PETSc
3. Compiler optimization (out of order execution, FMA, vectorization)

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Parallel reproducibility: multivariate case

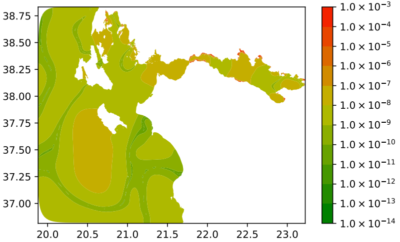
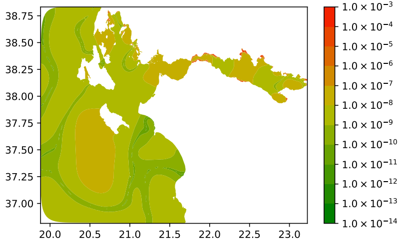


Figure: L_1 norm between parallel run and ensemble average of SST

Look at case study

- Grid: Zakynthos island
- #Processes fixed

Parallel reproducibility: multivariate case



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- Ensemble runs (sequential: reordering)
- Long run (weather: 1 year)

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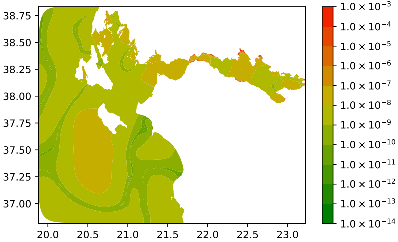

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Have statistical distribution over space and time.

Parallel reproducibility: Multivariate case

Two possibilities:

Multivariate version:

two-sample test and **confidence radius**

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Pointwise version &reduce:

two-sample test and **confidence interval** as above. Then reduce to one-dimension

Parallel reproducibility: Confidence interval

For every point have 2σ confidence interval of the mean

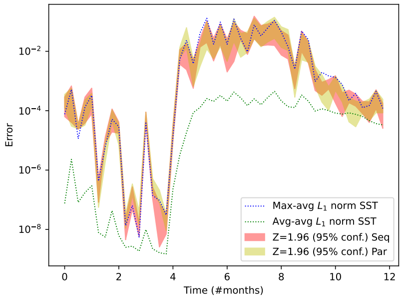

Figure: L_1 norm between ensemble and ensemble-mean. (Maximum and average over grid)

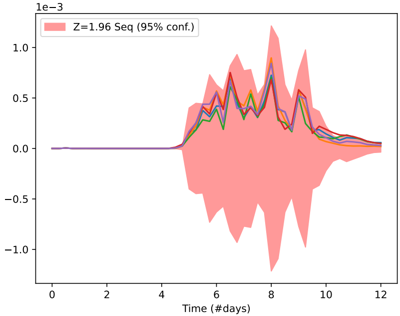

Figure: 90th percentile largest (over grid) 2σ confidence interval (over ensemble), and L_1 error of ensemble runs

Parallel reproducibility

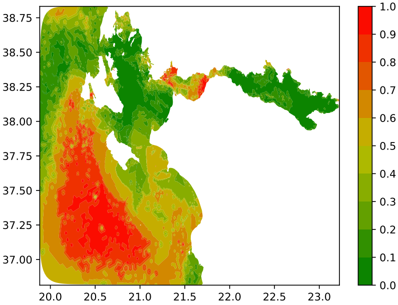

Figure: Kolmogorov-Smirnov test at final time

Define reproducibility using grid?

Parallel reproducibility: thoughts

Define/measure/influence reproducibility in larger sense than BR?

- Two-sample test ($S = P$) not right
- Confidence interval good: parallel code P "more reproducible" than seq. code S. In some sense

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- If $X \leq Y$ V&V follows from the sequential code.

Good for well-conditioned systems (sum, SHYFEM-MPI without turbulence)

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Thoughts:

- **Parallel reproducibility**: Useful if BR code in development $\rightarrow$ non-BR in optimisation (not necessarily parallelisation)

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