2014 SIAM Conference on Uncertainty Quantification

MS42:

The Reliability of Computational Research Findings:
Reproducible Research, Uncertainty Quantification, and
Verification & Validation

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About me

Lorena A. **Barba group**

Computational Fluid Dynamics
Algorithms *Fluid Mechanics*
HIGH-PERFOMANCE COMPUTING
CFD *Immersed Boundary Methods*
Biomolecular Physics
GPU Computing

New NVIDIA #CUDA Research Center at GW's Barba Group
http://t.co/VOkkGCnShc
@GPUComputing @GWColonialOne @GWGradEngineer
View // Reply // Retweet // Favorite

RESEARCH

New CUDA Research Center at GW

NVIDIA
CUDA RESEARCH CENTER

Not an expert in UQ

Tell stories, express conviction, use examples, avoid jargon—The road to academic success is paved with writing style http://t.co/z9n7lYHDHI
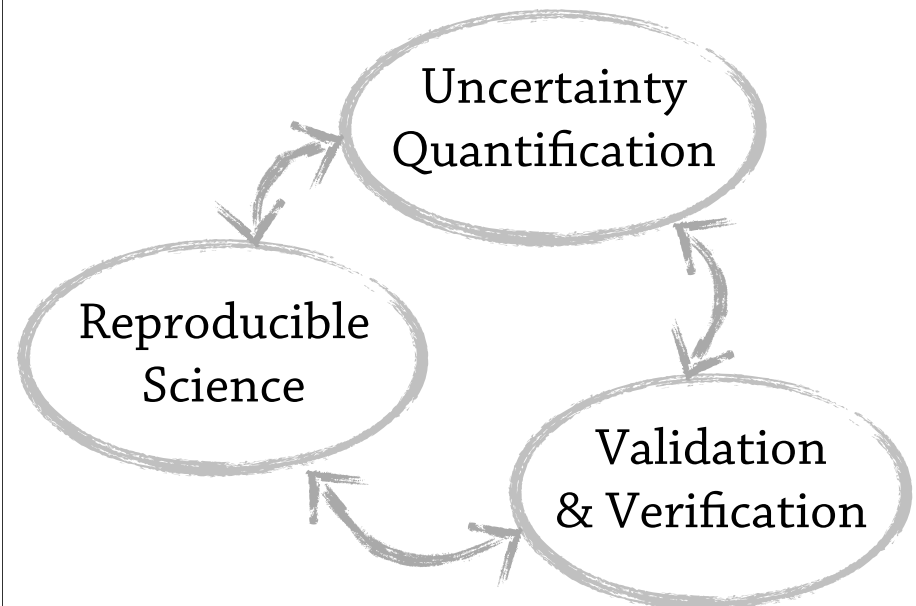View // Reply // Retweet // Favorite

NVIDIA names GW a new CUDA Research Center, in recognition of the research trajectory of Prof. Lorena Barba. The announcement reads as follows. The CUDA Research Center at the George Washington University in Washington,

http://lorenabarba.com

Uncertainty Quantification

Reproducible Science

Validation & Verification

Petascale turbulence simulation using a highly parallel fast multipole method on GPUs

Rio Yokota [a], L.A. Barba [a,*], Tetsu Narumi [b], Kenji Yasuoka [c]

4.6. Reproducibility and open-source policy

The authors of the exaFMM code have a consistent policy of making science codes available openly, in the interest of reproducibility. The entire code that was used to obtain the present results is available from https://bitbucket.org/exafmm/exafmm. The revision number used for the results presented in this paper is 191 for the large-scale tests up to 4096 GPUs. Documentation and links to other publications are found in the project homepage at http://exafmm.org/. Fig. 11, its plotting script and datasets are available online and usage is licensed under CC-BY-3.0 [29].

Petascale turbulence simulation using a highly parallel fast multipole method on GPUs

Rio Yokota [a], L.A. Barba [a,*], Tetsu Narumi [b], Kenji Yasuoka [c]

Can UQ make "irreproducible" large-scale simulations *reliable*?

Why does it matter?

Computer simulations create scientific knowledge.

Socrative

Go to:

`http://m.socrative.com`

‣ Room number : **75443**

True/False?
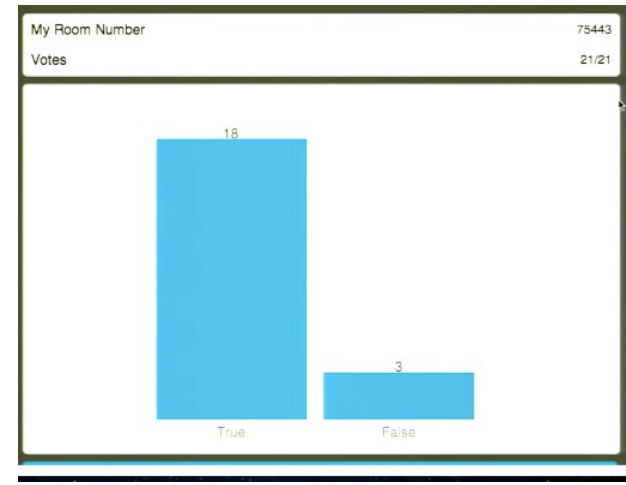
Computer simulations create scientific knowledge.
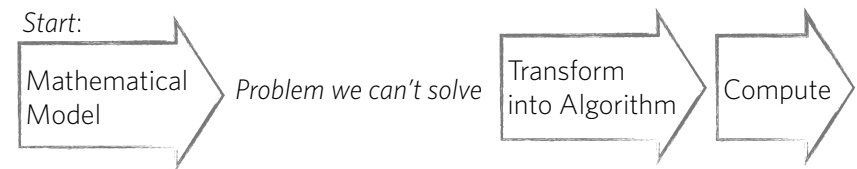
True/False?

Simulation is a method.

When do we have evidence that claims to knowledge from simulation are justified?

E. Winsberg, "Science in the Age of Computer Simulation" (2010)

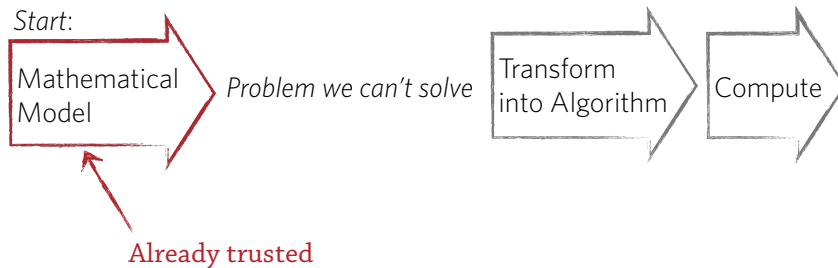
The Method of computer simulation

‣ Same as von Neumann et al. in 1945

Start:

Mathematical Model → *Problem we can't solve* → Transform into Algorithm → Compute

The **Method** of computer simulation

‣ Same as von Neumann et al. in 1945

Start:

Mathematical Model → *Problem we can't solve* → Transform into Algorithm → Compute

↑ Already trusted

The **Method** of computer simulation

‣ Same as von Neumann et al. in 1945

Start:

Mathematical Model → *Problem we can't solve* → Transform into Algorithm → Compute

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The **Method** of computer simulation

‣ Same as von Neumann et al. in 1945

Transform into Algorithm → Compute

↑ Discretize the equations:
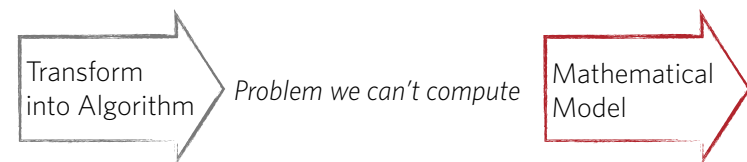...what if accuracy demands a grid that is too fine to compute?

The **Method** of computer simulation

Deviates from the mathematical model to make it computable:

‣ Simplifying assumptions— symmetry, ignoring variables

‣ Add elements that are not in the original equations, e.g., eddy viscosity, cloud models
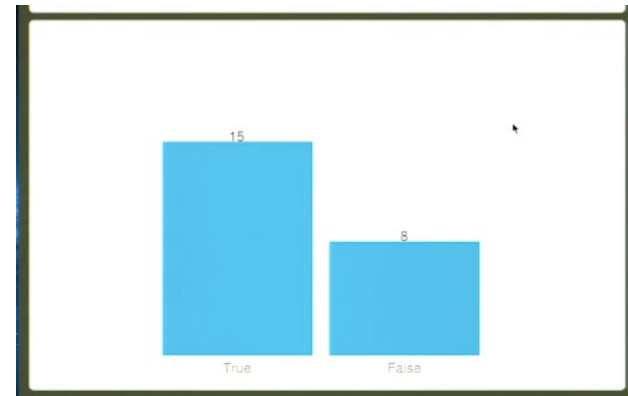
‣ What if the initial algorithm is unstable?

Transform into Algorithm → *Problem we can't compute* → Mathematical Model

True/False?
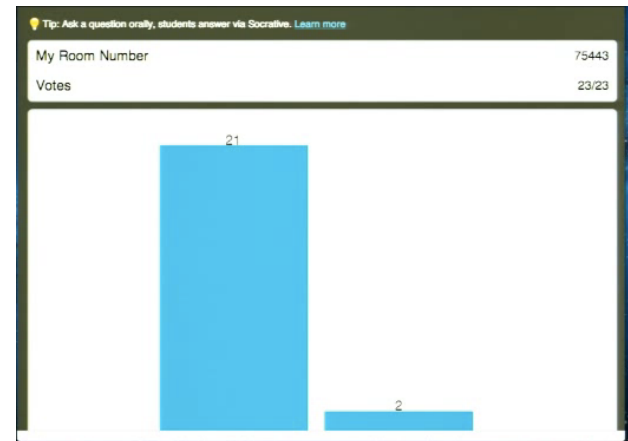
A reproducible simulation does not need to be accurate.

True/False

Is there value to a Reproducible Wrong Answer?

(If yes, V&V and Reproducibility are distinct.)

Validation & Verification

▸ Validation — confirm that the simulation parallels the physics we want to study

▸ Verification — confirm that the simulation results match the solutions to the mathematical model

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Validation & Verification

Fitness of the model

▸ Validation — confirm that the simulation parallels the physics we want to study

▸ Verification — confirm that the simulation results match the solutions to the mathematical model

Fitness of the solver

Validation & Verification

Fitness of the model

▸ Validation — confirm that the simulation parallels the physics we want to study

Fitness of the solver

▸ Verification — confirm that the simulation results match the solutions to the mathematical model

(Can these really be divided neatly?)

How do we show evidence that a simulation gives **reliable** data about the real world?

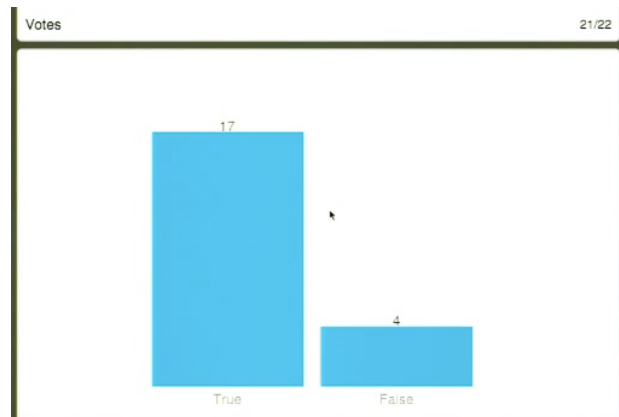How do we come to rationally believe in an *experimental* result?

A. Franklin, "The Neglect of Experiment" (1986)

True/False?

Simulation is an experiment.

Not so neat as V&V

‣ What about comparisons with other simulations?

‣ What is the role of **visualization**?
data interpretation? analysis?

Important for
Reproducibility!

‣ And all the judgements in between …

Not so neat as V&V

‣ What about comparisons with other simulations?

‣ What is the role of **visualization**?
  data interpretation? analysis?

Important for
Reproducibility!

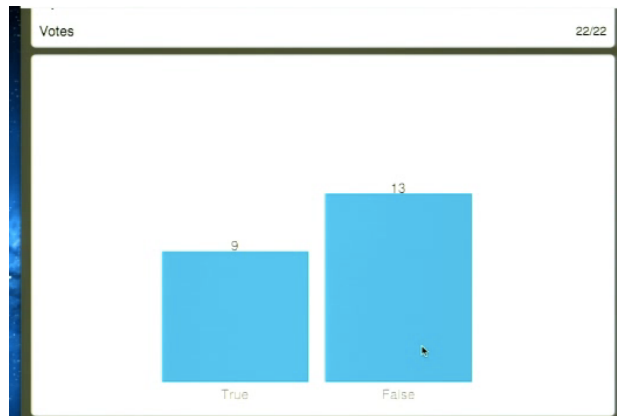‣ And all the judgements in between ...

V&V --> trust the simulation results
R --> trust the science results? trust the scientist?

True/False
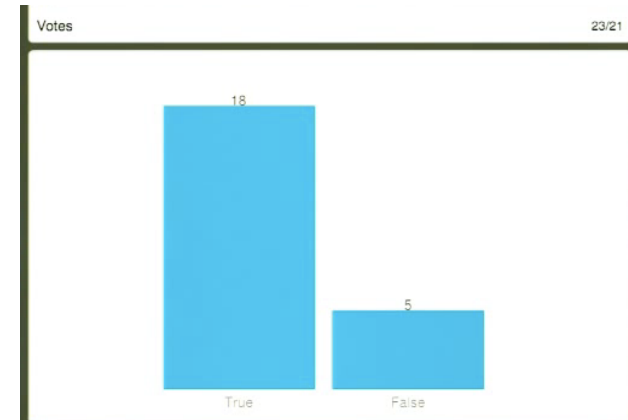Is V&V a pre-requisite to Reproducibility?

Confidence in results ...

‣ mathematical rigor needed, but not enough!

‣ involves physical intuition

‣ often relies in visualizations

‣ requires skilled judgement

‣ value questions

True/False

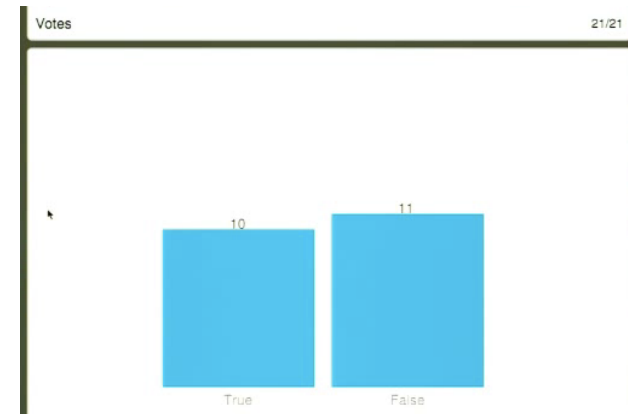UQ aims to give objective confidence levels for the results of simulations.

Votes   23/21

18

5

True   False

True/False

Is V&V a pre-requisite to UQ?

Votes   21/21

10   11

True   False

True/False

UQ presupposes verification and informs validation.

Votes 21/22

16

5

True False

True/False

Verification should be done before validation.
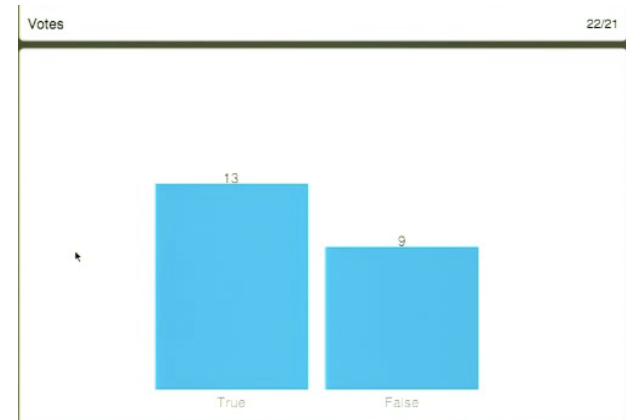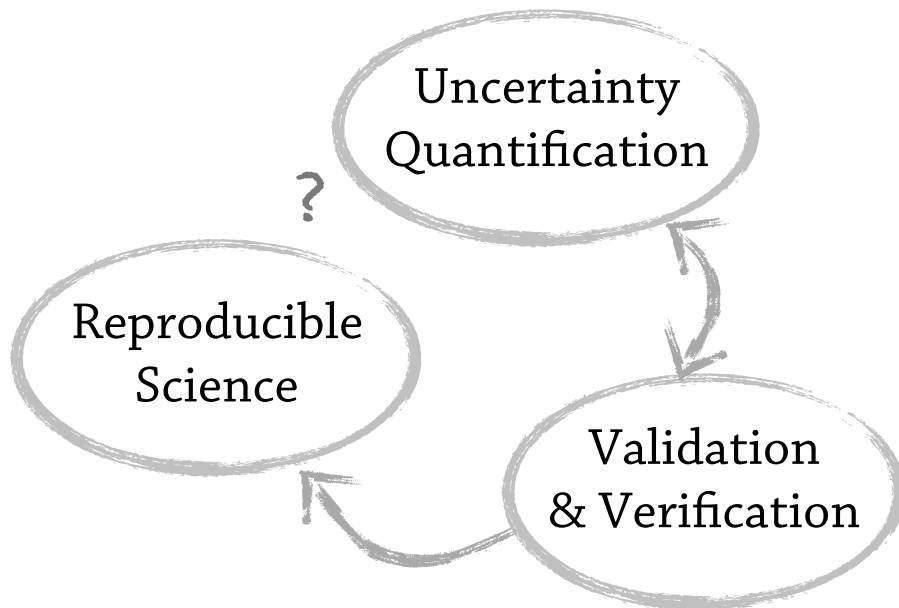
Votes 22/21

19

3

True False

True/False

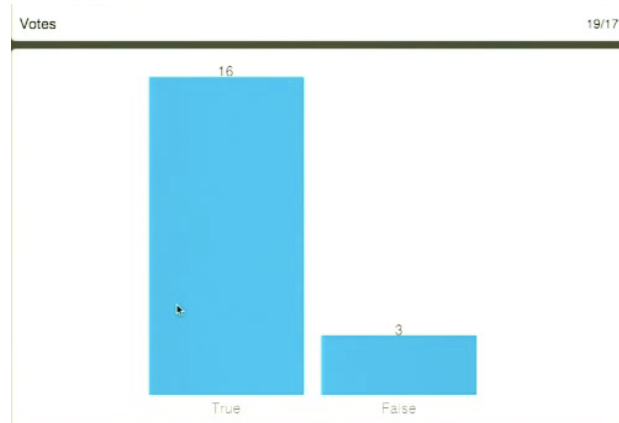In verification, the actual value of the error is generally unknown.

True/False

Can reproducible science be uncertain?

Repeatability & Reproducibility

‣ Repeatability — ability to re-run the same experiment with the same method on the same syste, and obtain the same/similar results

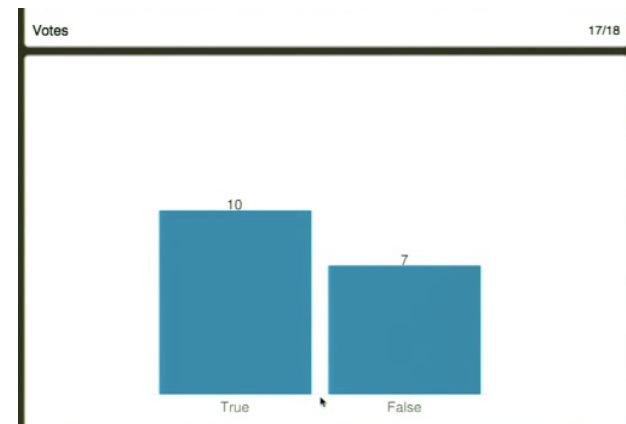‣ Reproducibility — ability to independently confirm a scientific hypothesis via reproduction of published work

Vitek & Kalibera, "R3—Repeatability, Reproducibility, Rigor" (2011)

True/False

UQ is a requirement of reproducibility.

My conclusion

My **Reproducibility PI Manifesto** [*] is incomplete. Making code/data open and publicly available is not all, we need to publish our uncertainties, our judgements.

Lorena A. Barba

[*] http://lorenabarba.com/gallery/reproducibility-pi-manifesto/

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