

# **Reproducible Science and Deep Software Variability**

## Mathieu Acher @acherm

Special thanks to Luc Lesoil, Jean-Marc Jézéguel, Arnaud Blouin, and Benoit Combemale







VaMoS keynote, 24 february 2022

### https://hal.inria.fr/hal-03528889

Abstract : Biology, medicine, physics, astrophysics, chemistry: all these scientific domains need to process large amount of data with more and more complex software systems. For achieving reproducible science, there are several challenges ahead involving multidisciplinary collaboration and socio-technical innovation with software at the center of the problem. Despite the availability of data and code, several studies report that the same data analyzed with different software can lead to different results. I am seeing this problem as a manifestation of deep software variability: many factors (operating system, third-party libraries, versions, workloads, compile-time options and flags, etc.) themselves subject to variability can alter the results, up to the point it can dramatically change the conclusions of some scientific studies. In this keynote, I argue that deep software variability is a threat and also an opportunity for reproducible science. I first outline some works about (deep) software variability, reporting on preliminary evidence of complex interactions between variability layers. I then link the ongoing works on variability modelling and deep software variability in the quest for reproducible science.

**References** at the ~end of the slides!

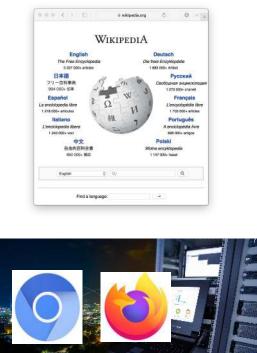


- **Reproducible Science and (Deep) Software (Variability)**
- Deep Software Variability
- Evidence of Deep Software Variability in Science
- Threats and Opportunities

## **SOFTWARE VARIANTS ARE EATING THE WORLD**









## **SOFTWARE IS EATING SCIENCE**



## **Computational science depends on software and its engineering**



design of mathematical model

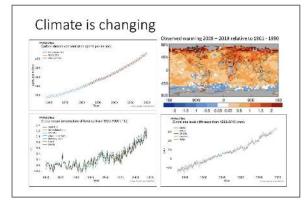
mining and analysis of data

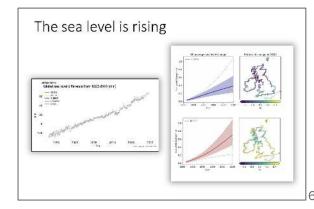
executions of large simulations

problem solving

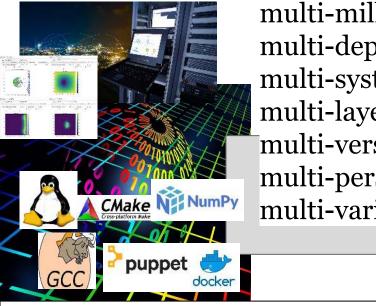
executable paper

from a set of scripts to automate the deployment to... a comprehensive system containing several features that help researchers exploring various hypotheses

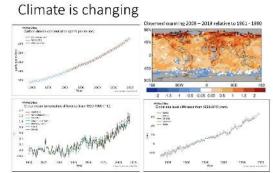


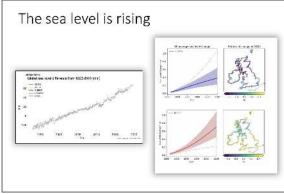


## Computational science depends on software and its engineering



multi-million line of code base multi-dependencies multi-systems multi-layer multi-version multi-person multi-variant





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## **Computational science depends on software and its engineering**



multi-million line of code base multi-dependencies multi-systems multi-layer multi-version multi-person multi-variant



In [6]:	sess.run(	tf.svd(tf_matrix))	)		
Out[6]:	(array([	9.99998987e-01,	1.48747023e-03,	4.88133628e-06,	
		4.69811084e-06,	4.37980998e-06,	3.45290823e-06,	
		1.14686304e-06,	3.10980795e-06,	2.97525912e-06,	
		2.65099743e-06,	1.91537106e-06,	0.00000000e+00,	
-		0.00000000e+00,	0.00000000e+00,	0.00000000e+00,	
		0.00000000e+00,	0.0000000e+00,	0.00000000e+00,	
		0.00000000e+00,	0.00000000e+00],	dtype=float32),	
	array([[	1.00000000e+00,	9.82503479e-05,	-2.52892733e-06,	
1		6.4375694807	-2 6420140806	-3 19651632-06	
		nan,	nan,	nan,	
		0.000000 <mark>0</mark> 0e+00,	nan,	5.08329823e-09,	
		8.60062854e-10,	1.93595340e-09,	0.00000000e+00,	
		-1.24836730e-09,	3.83645737e-09,	-3.90316446e-09,	
		nan,	-7.00323994e-07],	-	
	I	-7.27595761e-11,	7.15255737e-07,	-2.68207733e-02,	
		-6.68754578e-01,	1.68675050e-01,	-2.37232931e-02,	
				<b></b>	

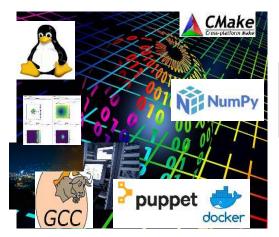
Dealing with software collapse: software stops working eventually Konrad Hinsen 2019

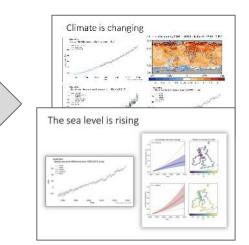
Configuration failures represent one of the most common types of software failures Sayagh et al. TSE 2018

## "Insanity is doing the same thing over and over again and expecting different results"

http://throwgrammarfromthetrain.blogspot.com/2010/10/definition-of-insanity.html



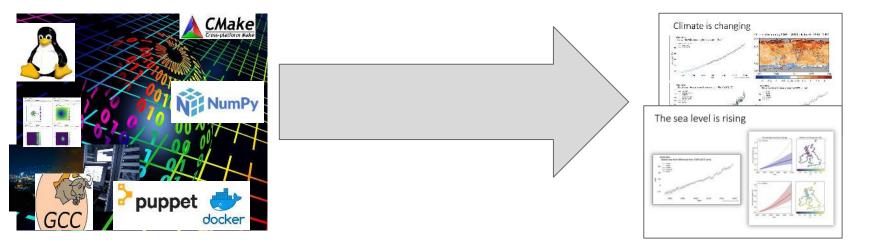






"Authors provide all the necessary data and the computer codes to run the analysis again, re-creating the results." (Claerbout/Donoho/Peng definition)

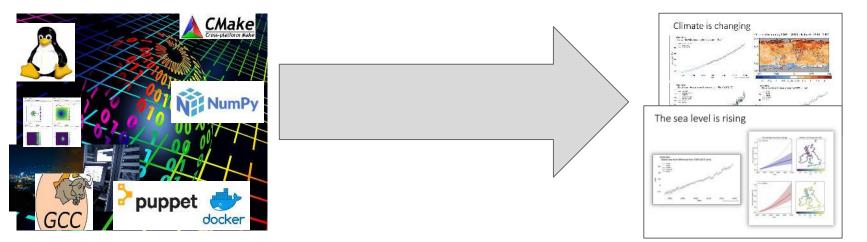
"The actual scholarship is the complete software development environment and the complete set of instructions which generated the figures." (~executable paper)



# **Reproducibility and Replicability**

**Reproducible**: Authors provide all the necessary data and the computer codes to run the analysis again, re-creating the results. **Replication**: A study that arrives at the same scientific findings as another study, collecting new data (possibly with different methods) and completing new analyses. "Terminologies for Reproducible

"Terminologies for Reproducible Research", Lorena A. Barba, 2018

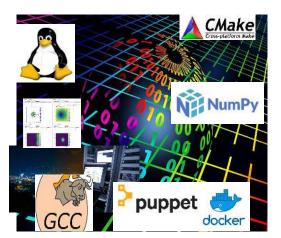


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The Claerbout/Donoho/Peng terminology is broadly disseminated across disciplines (see Table 2). But the recent adoption of an opposing terminology by two large professional groups—ACM and FASEB—make standardization awkward. The ACM publicizes its rationale for adoption as based on the International Vocabulary of Metrology, but a close reading of the sources makes this justification tenuous. The source of the FASEB adoption is unclear, but there's a chance that Casadevall and Fang (2010) had an influence there. They, in turn, based their definitions on the emphatic but essentially flawed work of Drummond (2009).

Table 2: Grouping of terminologies, as in Table 1, but by discipline.

A	B1	B2
political science economics	signal processing scientific computing econometry epidemiology clinical studies internal medicine physiology (neuro) computational biology biomedical research statistics	microbiology, immunology (FASEB) computer science (ACM)

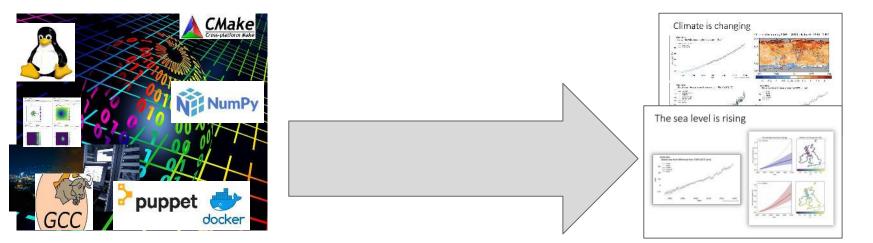
# **Reproducibility and Replicability**

**Methods Reproducibility:** A method is reproducible if reusing the original code leads to the same results.

**Results Reproducibility:** A result is reproducible if a reimplementation of the method generates statistically similar values.

**Inferential Reproducibility:** A finding or a conclusion is reproducible if one can draw it from a different experimental setup.

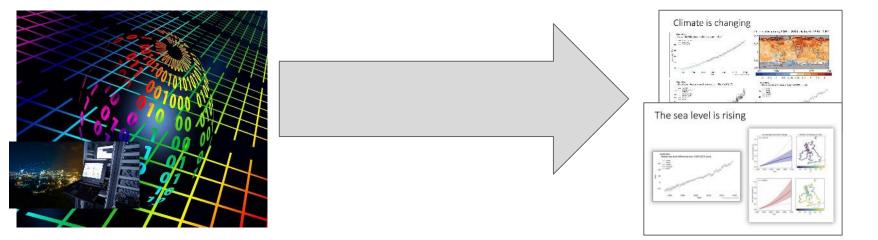
"Unreproducible Research is Reproducible", Bouthillier et al., ICML 2019



"Authors provide all the necessary data and the computer codes to run the analysis again, re-creating the results."

**Socio-technical issues**: open science, open source software, multi-disciplinary collaboration, incentives/rewards, initiatives, etc.

with many challenges related to data acquisition, knowledge organization/sharing, etc.



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#### **EMSE Open Science Initiative**

Openness in science is key to fostering progress via transparency, reproducibility, and replicability. Especially open data and open source are two fundamental pillars in open science as both build the core for excellence in evidencebased research. The Empirical Software Engineering journal (EMSE) has therefore decided to explicitly foster open science and reproducible research by encouraging and supporting authors to share their (anonymised and curated) empirical data and source code in form of replication packages. The overall goals are:

- Increasing the transparency, reproducibility, and replicability of research endeavours. This supports the immediate credibility of authors' work, and it also provides a common basis for joint community efforts grounded on shared data.
- Building up an overall body of knowledge in the community leading to widely accepted and well-formed software

#### https://github.com/emsejournal/openscience

#### Reproducible Science is good. Replicated Science is better.

ReScience C is a *platinum open-access* peer-reviewed journal that targets computational research and encourages the explicit replication of already published research, promoting new and open-source implementations in order to ensure that the original research is reproducible. You can read about the ideas behind ReScience C in the article *Sustainable computational science: the ReScience initiative* 

#### https://rescience.github.io/

### OpenReview.net

#### https://reproducible-research.inria.fr/





GitHub



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#### **ARTIFACT EVALUATION**

Authors of accepted research papers are invited to submit the artifacts associated paper for evaluation. To do so, they should submit a PDF via Easychair (select the R Artifacts track). The PDF should contain a stable URL (or DOI) to the artifacts. The UF contain the steps or general instructions to execute/analyze the artifact. Each artif

According to ACM's "Result and Artifact Review and Badging" policy, an "artifact" is "a digital object that was either created by the authors to be used as part of the study or generated by the experiment itself [... which can include] software systems, scripts used to run experiments, input datasets, raw data collected in the experiment, or scripts used to analyze results."

CALL FOR CHALLENGE CASES Home / Call for Papers / Call for challenge cases

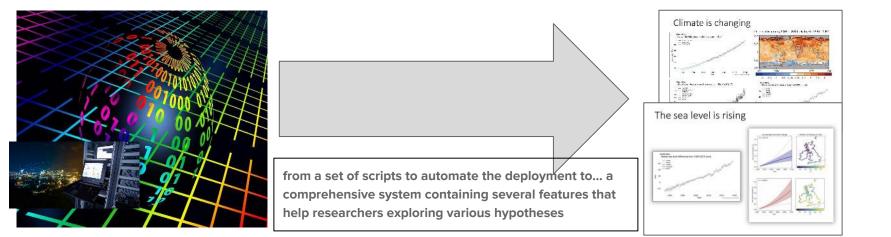
> dea of the challenge track is to provide participants with a set of case studies that tackle relevan ems and challenge the state of the art. The challenge track happens in two phases. In the first p will be a call for cases. Submitted cases will be reviewed by the challenge co-chairs to ensure t red information is clearly described. Accepted cases will be part of the official conference proce-

ICPE 2022 13th ACM/SPEC International Conference on Performance Engineering

In this track, an industrial performance dataset will be provided. The submit participants are invited to come up with research questions about the dataset, and study those. The challenge is open-ended: participants can choose the research questions that they find most interesting. The proposed approaches and/or tools and their findings are discussed in short papers, and presented in the main conference.

"Authors provide all the necessary data and the computer codes to run the analysis again, re-creating the results."

Despite the availability of data and code, several studies report that the same data analyzed with different software can lead to different results.



deep software variability

software application varial input data variability build variability

compiler variability

<mark>container variability</mark>

hypervisor variability

operating system variability

hardware variability

Despite the availability of data and code, several studies report that the same data analyzed with different software can lead to different results

Many *layers* (operating system, third-party libraries, versions, workloads, compile-time options and flags, etc.) themselves subject to variability can alter the results.

Reproducible science and deep software variability: a threat and opportunity for scientific knowledge!



- Reproducible Science and (Deep) Software (Variability)
- **Deep Software Variability**
- Evidence of Deep Software Variability in Science
- Threats and Opportunities









deep software variability

hardware variability

15,000+ options

thousands of compiler flags and compile-time options

dozens of preferences

**100+ command-line parameters** 

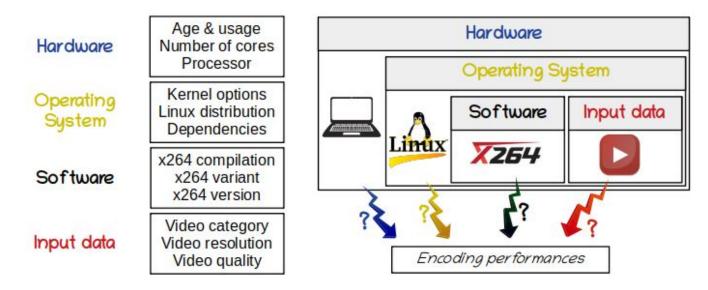
1000+ feature toggles

20

Deep software variability: does it matter? *i.e.* Are *layers/features orthogonal or are there interactions?* 

Variability layers





Luc Lesoil, Mathieu Acher, Arnaud Blouin, Jean-Marc Jézéquel: Deep Software Variability: Towards Handling Cross-Layer Configuration.



## Configuration is hard: numerous options, informal knowledge



--bframes 1 --ref 3 --cabac DiverSE-meeting.mp4 -o meeting13.webm



264

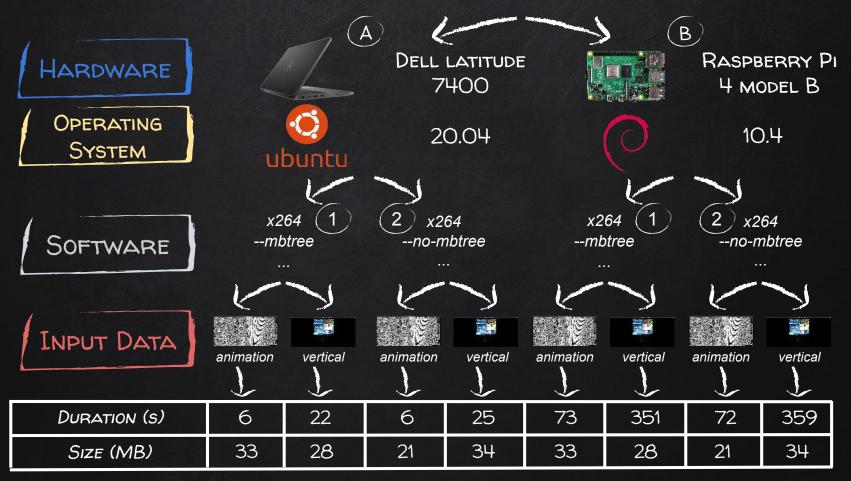
?????

localhost.localdomain ~ x264 --fullhelp | wc -l

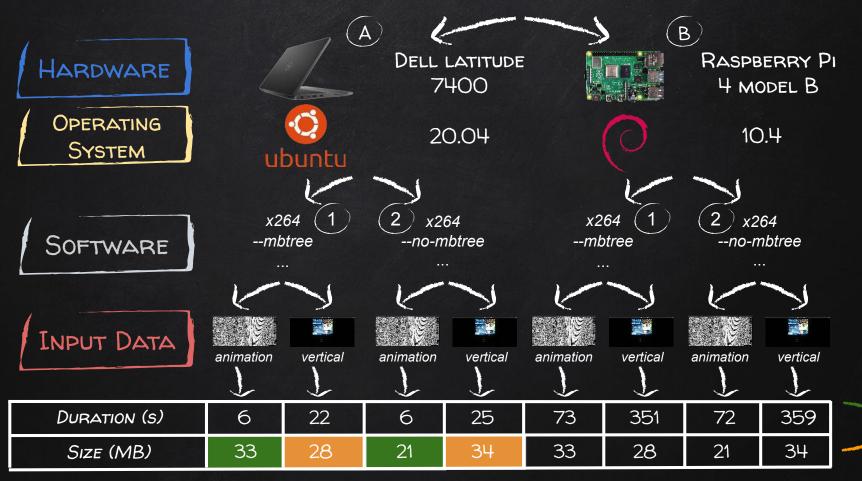
#### 480

Lossless: x264qp 0 -o	<output> <input/></output>	tff bff	'infinite"> Maximum GOP size [250] Enable interlaced mode (top field first Enable interlaced	
245522	cost of speed and visual quality: placebotune psnr -o <output> <input/></output>	pulldown <string></string>	Use soft pulldown - none, 22, : HARDWARE	
Constant bitrate at 1	L000kbps with a 2 second-buffer:	Ratecontrol:		AGE / # CORES / GPU
2012년 2012년 2012년 - 18년 18년 2012년 - 18년 2012년 - 18년 2012년 - 18년 2012년 - 18년 2012년 2012년 2012년 2012년 2012년 2012년	size 2000bitrate 1000 -o <output> <input/></output>	-B,bitrate <integer> crf <float></float></integer>	Set bitrate (kbi <sup>.</sup> Quality-based VBM	
Presets:		vbv-maxrate <integer> vbv-bufsize <integer></integer></integer>	> Max local bitrate ODERATING	
profile <string></string>	Force the limits of an H.264 profile Overrides all settings. – baseline, main, high, high10, high422	-p,pass <integer></integer>	Enable multipass - 1: First p: - 2: Last pa:	VERSION OPTION DISTRIE
preset <string></string>	Use a preset to select encoding settings [m Overridden by user settings. – ultrafast,superfast,veryfast,faster,f – medium,slow,slower,veryslow,placebo	mL	Software	
tune <string></string>	Tune the settings for a particular type of or situation Overridden by user settings. Multiple tunings are separated by comma Only one psy tuning can be used at a ti	as.	INPUT DATA	

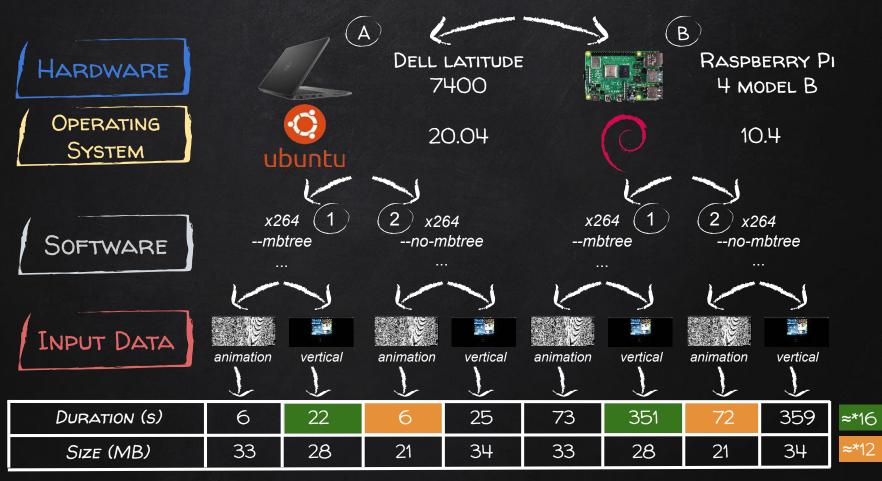
## REAL WORLD EXAMPLE (X264)



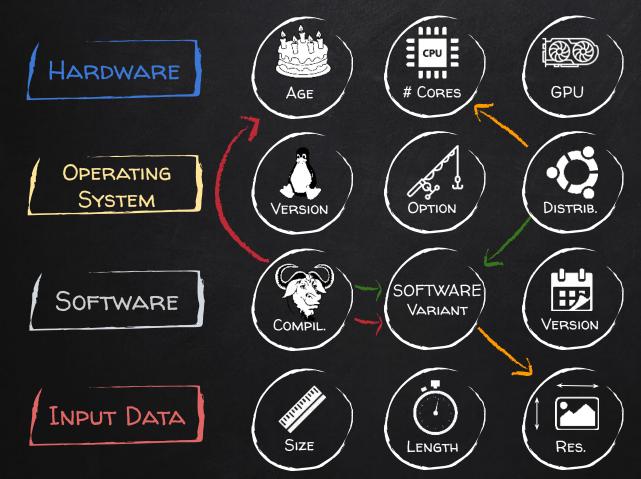
## REAL WORLD EXAMPLE (X264)



## REAL WORLD EXAMPLE (X264)



### DEEP VARIABILITY



The "best"/default software variant might be a bad one.

Influential software options and their interactions vary.

Performance prediction models and <mark>variability</mark> knowledge may not generalize



Bug

PERF. /

**L. Lesoil**, M. Acher, A. Blouin and J.-M. Jézéquel, "Deep Software Variability: Towards Handling Cross-Layer Configuration" in VaMoS 2021

### Transferring Performance Prediction Models Across Different Hardware Platforms Valov et al. ICPE 2017

Table 3: Sum ber of feature					
systems were sured configu		red;	NMC	– Number	r of mea-
	System	Ne	NM	NMC	

x264 7 11 165	System	$N_f$	NM	NMC
영향했던 그 것이 엄마 나면서?	XZ	7	7	154
SQLite 5 10 32	x264	7	11	165
	SQLite	5	10	32

Table 2: Summary of hardware platforms on which configurable software systems were measured; MID – Machine ID in DataMill cluster; NC – Number of CPUs; IS – Instruction set; CCR – CPU clock rate (MHz): RAM – RAM memory size (MB)

	Syster	ms	Machines							
XZ	x264	SQLite	MID	NC	IS	CCR	RAM			
1			73	2	i686	1733	1771			
1	~	1	75	2	i686	3200	977			
1			77	2	i686	2992	2024			
1			78	1	i686	1495	755			
1			79	4	x86_64	3291	7961			
1			80	8	x86_64	3401	7907			
~	$\checkmark$		81	16	x86_64	2411	32193			
	~		87	1	i686	1595	249			
	~		88	1	i686	1700	978			
		1	90	2	i686	3200	977			
	~		91	1	i686	2400	1009			
	~	1	97	2	i686	2992	873			
	~	~	98	2	i686	2992	873			
		1	99	2	i686	2793	880			
	$\checkmark$		103	2	i686	3200	881			
	\$		104	1	i686	1800	502			
	1	~	105	2	i686	3200	881			
	~		106	2	i686	3192	494			
		$\checkmark$	125	4	x86_64	3301	7960			
	~		128	2	i686	2993	2024			
		~	130	2	i686	3198	880			
		$\checkmark$	146	2	i686	2998	872			
		1	157	36	x86_64	2301	15954			

"Linear model provides a good approximation of transformation between performance distributions of a system deployed in different hardware environments"

what about variability of input data? compile-time options?



### Transfer Learning for Software Performance Analysis: An Exploratory Analysis Jamshidi et al. ASE 2017

SPEAR (SAT Solver)	X264 (video end	ode	r)	SQLite	
Analysis time	<b>Encoding time</b>	Query t			
14 options	16 options			14 optio	
16,384 configurations	4,000 configurat	figurations			
SAT problems	Video quality/si	DB Que 2 hardw 2 versio			
3 hardware	2 hardware				
2 versions	3 versions				
	$ec_1: [h_2 \rightarrow h_1, w_3, v_3]$	SM S	0.97 0.96		
	$ec_2: [h_2 \to h_1, w_1, v_3]$ $ec_3: [h_1, w_1 \to w_2, v_3]$	M	0.65		
	$ec_4: [h_1, w_1  ightarrow w_3, v_3]$	Μ	0.67		
	$ec_5: [h_1, w_3, v_2 \rightarrow v_3]$	L	0.05		
	$ec_6: [h_1, w_3, v_1  ightarrow v_3]$	L	0.06		
	$ec_7: [h_1, w_1 \rightarrow w_3, v_2 \rightarrow v_3]$	L	0.08		
	$egin{aligned} oldsymbol{e} oldsymbol{e}_8 &: [h_2  o h_1, w_1  o w_3, v_2  o v_3] \end{aligned}$	VL	0.09		

**Insight**. For non-severe hardware changes, we can linearly transfer performance models across environments.

**Insight**. The strength of the influence of configuration options is typically preserved across environments.

**Insight**. A large percentage of configurations are typically invalid in both source and target environments.

#### SQLite (DB engine) Query time

14 options 1,000 configurations DB Queries 2 hardware 2 versions

#### SaC (Compiler) Execution time

50 options 71,267 configurations 10 Demo programs



## Transfer Learning for Software Performance Analysis: An Exploratory Analysis Jamshidi et al. ASE 2017

SPEAR (SAT Solver) Analysis time 14 options 16,384 configurations SAT problems 3 hardware 2 versions	X264 (video enc Encoding time 16 options 4,000 configurat Video quality/siz 2 hardware 3 versions	tions	SQLite (DB engine) Query time 14 options 1,000 configurations DB Queries 2 hardware 2 versions	SaC (Compiler) Execution time 50 options 71,267 configurations 10 Demo programs
	$\begin{array}{l} \boldsymbol{ec_1}: [h_2 \rightarrow h_1, w_3, v_3] \\ \boldsymbol{ec_2}: [h_2 \rightarrow h_1, w_1, v_3] \\ \boldsymbol{ec_3}: [h_1, w_1 \rightarrow w_2, v_3] \\ \boldsymbol{ec_4}: [h_1, w_1 \rightarrow w_3, v_3] \\ \boldsymbol{ec_5}: [h_1, w_3, v_2 \rightarrow v_3] \\ \boldsymbol{ec_6}: [h_1, w_3, v_1 \rightarrow v_3] \\ \boldsymbol{ec_7}: [h_1, w_1 \rightarrow w_3, v_2 \rightarrow v_3] \\ \boldsymbol{ec_8}: [h_2 \rightarrow h_1, w_1 \rightarrow w_3, v_2 \rightarrow v_3] \end{array}$	SM         0.97           S         0.96           M         0.65           M         0.67           L         0.05           L         0.06           L         0.08           VL         0.09	HA	

- **mixing deep variability:** hard to assess the specific influence of each layer
- **very few hardware, version, and input data...** but lots of runtime configurations (variants)

Let's go deep with input data!



## Let's go deep with input data!



Intuition: video encoder behavior (and thus runtime configurations) hugely depends on the input video (different compression ratio, encoding size/type etc.)

- Is the best software configuration still the best?
- Are influential options always influential?

Does the configuration knowledge generalize?

two performance models  $f_1$  and  $f_2$  $f_1 = \beta imes f_2 + lpha$ 



YouTube User General Content dataset: **1397 videos** Measurements of **201 soft. configurations** (with <u>same</u> hardware, compiler, version, etc.): encoding time, bitrate, etc.



# Do x264 software performances stay consistent across inputs?

- Encoding time: very strong correlations
   o low input sensitivity
- FPS: very strong correlations

 $\,\circ\,$  low input sensitivity

- CPU usage : moderate correlation, a few negative correlations
   o medium input sensitivity
- Bitrate: medium-low correlation, many negative correlations
  - High input sensitivity
- Encoding size: medium-low correlation, many negative correlations
   High input sensitivity

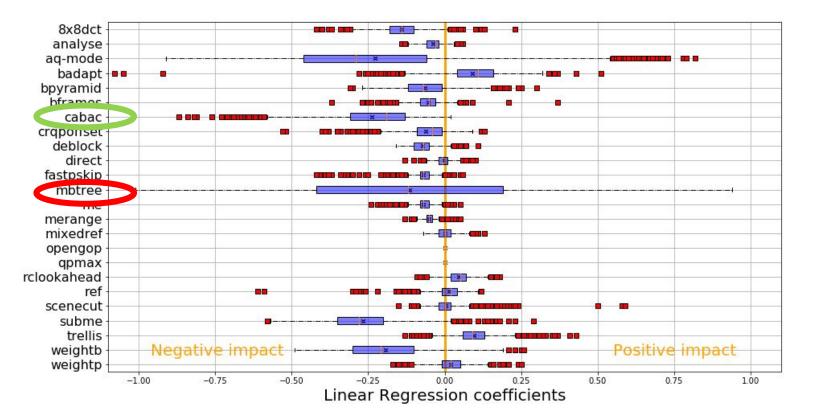
two performance models  $f_1$  and  $f_2$   $f_1 = \beta \times f_2 + \alpha$ 

1397 videos x 201 software configurations



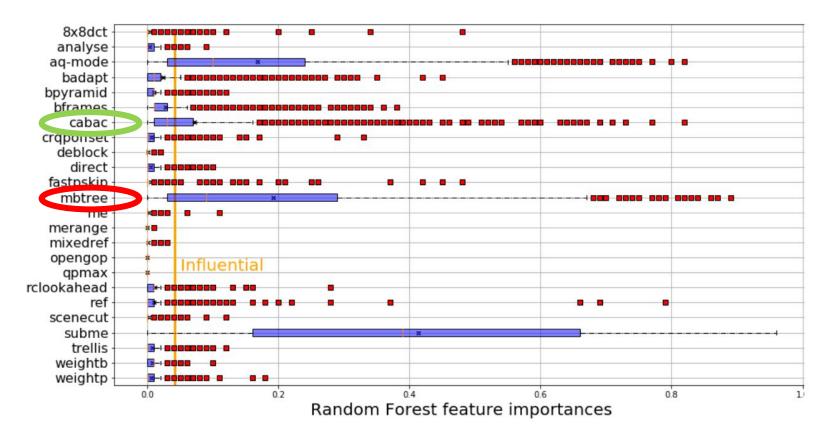
# Are there some configuration options more sensitive to input videos? (bitrate)





# Are there some configuration options more sensitive to input videos? (bitrate)





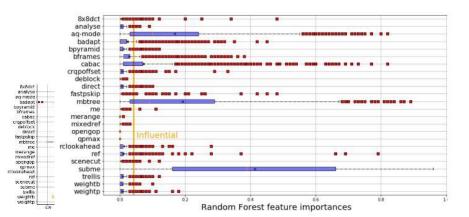
# Practical impacts for users, developers, scientists, and self-adaptive systems

Threats to variability knowledge for performance property bitrate



- optimal configuration is specific to an input; a good configuration can be a bad one
- some options' values have an opposite effect depending on the input
- effectiveness of sampling strategies (random, 2-wise, etc.) is input specific (somehow confirming Pereira et al. ICPE 2020)
- predicting, tuning, or understanding configurable systems

without being aware of inputs can be inaccurate and... pointless





# Practical impacts for users, developers, scientists, and self-adaptive systems

**Threats** to variability knowledge: predicting, tuning, or understanding configurable systems without being aware of inputs can be inaccurate and... pointless

**Opportunities:** for some performance properties (P) and subject systems, some stability is observed and performance remains consistent!

Sys	System Domain		Commit Configs #		C	C Inputs I		#I		
gcc Compilation		mpilation		ccb4e07 80		Ĵ	.c programs		30	
Imagel	ImageMagick Image proces		e processin	g	5ee49d6	100		iı	nages	1000
linge	lingeling SA		AT solver		7d5db72	100		SAT	formulae	351
nod	leJS	JS r	untime env	÷.	78343bb	50		.js	scripts	1939
pop	poppler PDI		F rendering		42dde68	16	. j	.pc	<i>lf</i> files	1480
SQ	SQLite		DBMS		53fa025	50		dat	abases	150
x2	x264 V		eo encoding	;	e9a5903 201		0	videos		1397
x	xz Data System gcc		compressio	m	n e7da44d 30			system files		48
			#M	Performance(s) P size, ctime, exec			D	Docker Datase		1
			2400				I	link	Link	1
	ImageMa	agick	100 000	size, time			I	ink	Link	1
	lingeli	ng	35 100	#confl.,#reduc.		I	Link	Link	1	
	poppler 2		96 950	#operations/s size, time 15 query times q1-q15		I	ink	Link	1	
			23 680			Link		Link Link	1	
			7500			mes q1-q15 Link	1			
	x264		280797	C]	pu, fps, kbs,	size, time	I	link	Link	1
	xz		1440	1	size, ti	me	I	ink	Link	1

L. Lesoil, M. Acher, A. Blouin and J.-M. Jézéquel "The Interaction between Inputs and Configurations fed to Software Systems: an Empirical Study" https://arxiv.org/abs/2112.07279



## x264 video encoder (compilation/build)

x264 --bframes 1 --ref 3 --cabac DiverSE-meeting.mp4 -o meeting13.webm

mathieuacher

#### localhost.localdomain

../x264-SLIMFAST/x264 x264-gcov □

--disable-thread
 --disable-win32thread
 --disable-interlaced
 --bit-depth=BIT\_DEPTH
 --chroma-format=FORMAT

disable multithreaded encoding disable win32threads (windows only) disable interlaced encoding support set output bit depth (8, 10, all) [all] output chroma format (400, 420, 422, 444, all) [all]

disable platform-specific assembly optimizations

Advanced options:

- --disable-asm --enable-lto --enable-debug
- --enable-gprof
- --enable-strip
- --enable-pic

f add -pg p add -s build position-independent code

add -g

Cross-compilation:

- --host=HOST --cross-prefix=PREFIX
- --sysroot=SYSROOT

External library support:

- --disable-avs --disable-swscale --disable-lavf --disable-ffms
- --disable-gpac

fms disable ff pac disable gp smash disable ls

build programs to run on HOST use PREFIX for compilation tools root of cross-build tree

enable link-time optimization

disable avisynth support disable swscale support disable libavformat support disable ffmpegsource support disable gpac support disable lsmash support



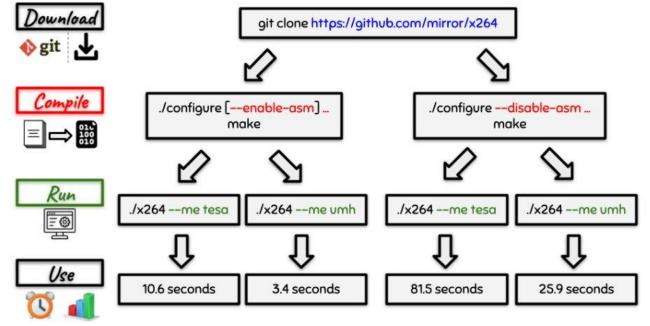


./configure --help

# Is there an interplay between compile-time and runtime options?



L. Lesoil, M. Acher, X. Tërnava, A. Blouin and J.-M. Jézéquel "The Interplay of Compiletime and Run-time Options for Performance Prediction" in SPLC '21



This paper investigates how compile-time options can affect software performances and how compile-time options interact with run-time options.

Figure 1: Cross-layer variability of x264



## Key results (for x264)

L. Lesoil, M. Acher, X. Tërnava, A. Blouin and J.-M. Jézéquel "The Interplay of Compiletime and Run-time Options for Performance Prediction" in SPLC '21

*Worth tuning software at compile-time*: gain about 10 % of execution time with the tuning of compile-time options (compared to the default compile-time configuration). The improvements can be larger for some inputs and some runtime configurations.

**Stability of variability knowledge:** For all the execution time distributions of x264 and all the input videos, the worst correlation is greater than 0.97. If the compile-time options change the scale of the distribution, they do not change the rankings of run-time configurations (i.e., they do not truly interact with the run-time options).

<u>Reuse of configuration knowledge</u>:  $f_1 = \beta \times f_2 + \alpha$ 

- Linear transformation among distributions
- Users can also trust the documentation of run-time options,

consistent whatever the compile-time configuration is.



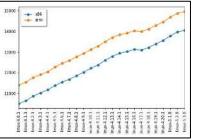


H. Martin, M. Acher, J. A. Pereira, L. Lesoil, J. Jézéquel and D. E. Khelladi, "Transfer learning across variants and versions: The case of linux kernel size" Transactions on Software Engineering (TSE), 2021

- Linux as a subject software system (not as an OS interacting with other layers)
- Targeted non-functional, quantitative property: <u>binary size</u>
  - interest for maintainers/users of the Linux kernel (embedded systems, cloud, etc.)
  - challenging to predict (cross-cutting options, interplay with compilers/build systems, etc/.)
- Dataset: version 4.13.3 (september 2017), x86\_64 arch, measurements of 95K+ random configurations
  - paranoiac about deep variability since 2017, Docker to control the build environment and scale
  - diversity of binary sizes: from 7Mb to 1.9Gb
  - 6% MAPE errors: quite good, though costly...

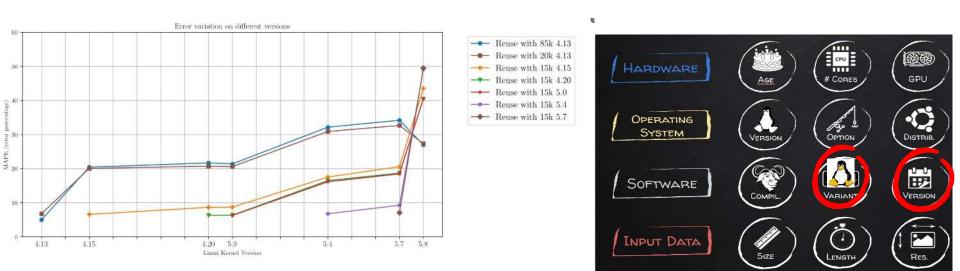






Version	Release Date	LOC	Files	Examples	Seconds/config	Options	Features	Deleted features	New features	$\Delta$ Commits	Files changes
4.13	2017/09/03	16,616,534	60,530	92,562	not available	12,776	9,468	-	2 <b>-</b> 2	-	-
4.15	2018/01/28	17,073,368	62,249	39,391	not available	12,998	9,425	342	299	31,052	934,628
4.20	2018/12/23	17,526,171	62,423	23,489	225	13,533	10,189	468	1,189	104,691	1,972,020
5.0	2019/03/03	17,679,372	63,076	19,952	247	13,673	10,293	494	1,319	118,778	2,170,935
5.4	2019/10/24	19,358,903	67,915	25,847	285	14,159	10,813	663	2,008	181,308	3,827,025
5.7	2020/05/31	19,358,903	67,915	20,159	258	14,586	11,338	715	2,585	225,804	4,393,117
5.8	2020/08/02	19,729,197	69,303	21,923	289	14,817	11,530	730	2,792	242,381	4,681,313

4.13 version (sep 2017): 6%. What about **evolution?** Can we reuse the 4.13 Linux prediction model? No, accuracy quickly decreases: **4.15 (5 months after): 20%; 5.7 (3 years after): 35%** 



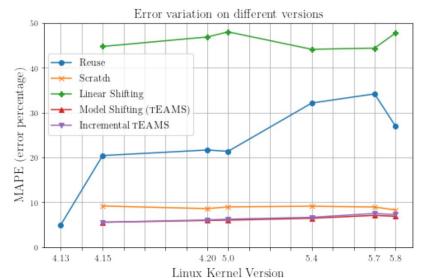
H. Martin, M. Acher, J. A. Pereira, L. Lesoil, J. Jézéquel and D. E. Khelladi, "Transfer learning across variants and versions: The case of linux kernel size" Transactions on Software Engineering (TSE), 2021

## Transfer learning to the rescue

- Mission Impossible: Saving variability knowledge and prediction model 4.13 (15K hours of computation)
- Heterogeneous transfer learning: the feature space is different



• TEAMS: transfer evolution-aware model shifting







DEEP VARIABILITY

Sometimes, variability is consistent/stable and knowledge transfer is immediate.

But there are also interactions among variability layers and variability knowledge may not generalize

PERF. >

PERF. /

Poppler

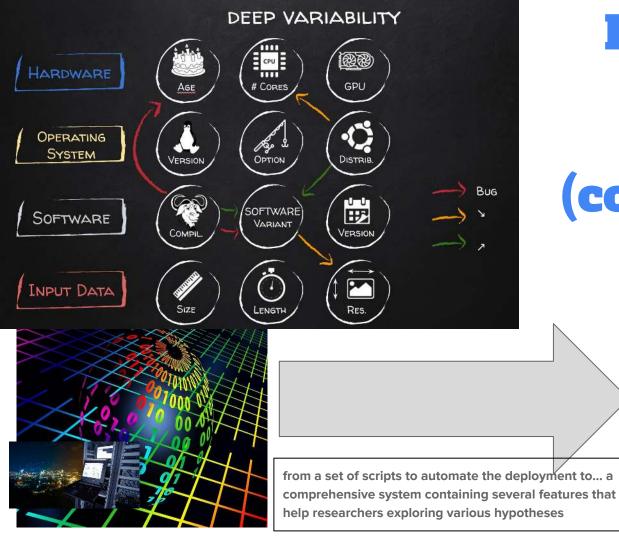
264

nøde

🖹 X2



- Reproducible Science and (Deep) Software (Variability)
- Deep Software Variability
- **Evidence of Deep Software Variability in Computational** Science
- Threats and Opportunities



It's all about software... Where is (computational) science?

# "Neuroimaging pipelines are known to generate different results depending on the computing platform where they are compiled and

> PLoS One. 2012;7(6):e38234. doi: 10.1371/journal.pone.0038234. Epub 2012 Jun 1.

Left

0.000

The effects of FreeSurfer version, workstation type, and Macintosh operating system version on anatomical volume and cortical thickness measurements

Ed H B M Gronenschild <sup>1</sup>, Petra Habets, Heidi I L Jacobs, Ron Mengelers, Nico Rozendaal, Jim van Os, Machteld Marcelis

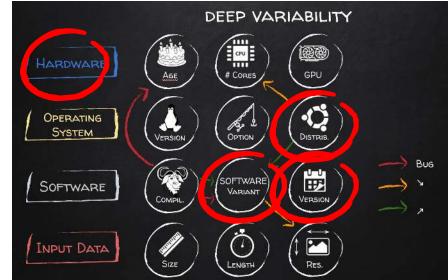
Right

15.000

GM

**see also** Krefting, D., Scheel, M., Freing, A., Specovius, S., Paul, F., and Brandt, A. (2011). "Reliability of quantitative neuroimage analysis using freesurfer in distributed environments," in *MICCAI Workshop on High-Performance and Distributed Computing for Medical Imaging*. (Toronto, ON)

Significant differences were revealed between FreeSurfer version v5.0.0 and the two earlier versions. [...] About a factor two smaller differences were detected between Macintosh and Hewlett-Packard workstations and between OSX 10.5 and OSX 10.6. The observed differences are similar in magnitude as effect sizes -reported in <u>accuracy</u> evaluations and neurodegenerative studies.



"Neuroimaging pipelines are known to generate different results depending on the computing platform where they are compiled and executed."

Reproducibility of neuroimaging

analyses across operating systems,

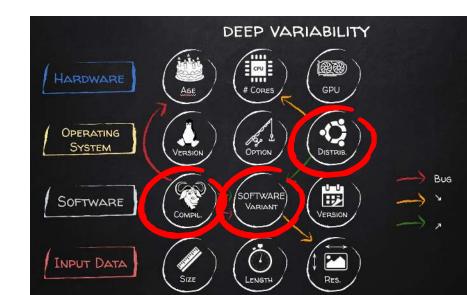
Glatard et al., Front. Neuroinform., 24

<mark>April 2015</mark>



	Cluster A	Cluster B
2 2012 - 5		2 10 20201-000
Applications	Freesurfer 5.3.0, build 1	Freesurfer 5.3.0, build 1 and 2
	FSL 5.0.6, build 1	FSL 5.0.6, build 1 and 2
	CIVET 1.1.12-UCSF, build 1	CIVET 1.1.12-UCSF, build 1
Interpreters	Python 2.4.3, bash 3.2.25,	Python 2.7.5, bash 4.2.47,
	Perl 5.8.8, tcsh 6.14.00	Perl 5.18.2, tcsh 6.18.01
glibc version	2.5	2.18
OS	CentOS 5.10	Fedora 20
Hardware	x86_64 CPUs (Intel Xeon)	x86_64 CPUs (Intel Xeon)

The implementation of mathematical functions manipulating single-precision **floating-point numbers in libmath** has evolved during the last years, leading to numerical differences in computational results. While these differences have little or no impact on simple analysis pipelines such as brain extraction and cortical tissue classification, their **accumulation creates important differences in longer pipelines** such as the subcortical tissue classification, RSfMRI analysis, and cortical thickness extraction.



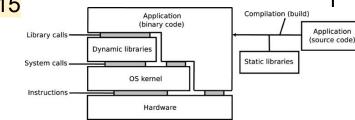
"Neuroimaging pipelines are known to generate different results depending on the computing platform where they are compiled and executed."

Reproducibility of neuroimaging

analyses across operating systems,

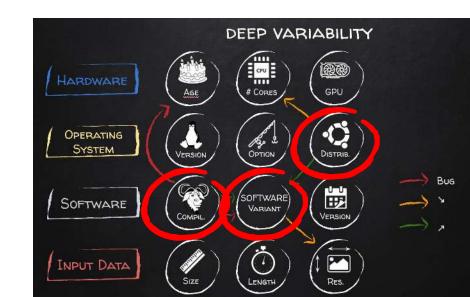
Glatard et al., Front. Neuroinform., 24

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	Cluster A	Cluster B
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Interpreters	Python 2.4.3, bash 3.2.25,	Python 2.7.5, bash 4.2.47,
	Perl 5.8.8, tcsh 6.14.00	Perl 5.18.2, tcsh 6.18.01
glibc version	2.5	2.18
OS	CentOS 5.10	Fedora 20
Hardware	x86_64 CPUs (Intel Xeon)	x86_64 CPUs (Intel Xeon)

Statically building programs improves reproducibility across OSes, but small differences may still remain when dynamic libraries are loaded by static executables[...]. When static builds are not an option, software heterogeneity might be addressed using virtual machines. However, such solutions are only workarounds: differences may still arise between **static executables built on different OSes**, or between **dynamic executables executed in different VMs**.



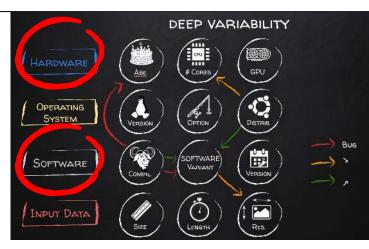
Explanatory variable	Meaning	
entcoef	Entrainment coefficient	
ct	Accretion constant	
rhcrit	Critical relative humidity	
vf1	Ice fall speed through clouds	
eacf	Empirically adjusted cloud fraction	
cw	Threshold for precipitation	
dtice	Temperature range of ice albedo variation	
ice	Nonspherical ice	
midware	Client middleware	
ice_size	Ice particle size	
alpham	Albedo at melting point of ice	
processor_name	CPU classification	
clock_classic	Processor clock speed recorded under classic middleware	
ram_size	Hardware RAM	
clock_boinc_i	Integer processor clock speed recorded under BOINC middleware	
clock_boinc_f	Floating point processor clock speed recorded under BOINC middleware	
os_name	Operating system	
dtheta	Perturbations to initial conditions on a given level	

Association of parameter, software, and hardware variation with large-scale behavior across 57,000 climate models

Christopher G. Knight, Sylvia H. E. Knight, Neil Massey, Tolu Aina, Carl Christensen, Dave J. F... + See all authors and affiliations

PNAS July 24, 2007 104 (30) 12259-12264; https://doi.org/10.1073/pnas.0608144104

We demonstrate that effects of parameter, hardware, and software variation are detectable, complex, and interacting. However, we find most of the effects of parameter variation are caused by a small subset of parameters. Notably, the entrainment coefficient in clouds is associated with 30% of the variation seen in climate sensitivity, although both low and high values can give high climate sensitivity. We demonstrate that the effect of hardware and software is small relative to the effect of parameter variation and, over the wide range of systems tested, may be treated as equivalent to that caused by changes in initial conditions.



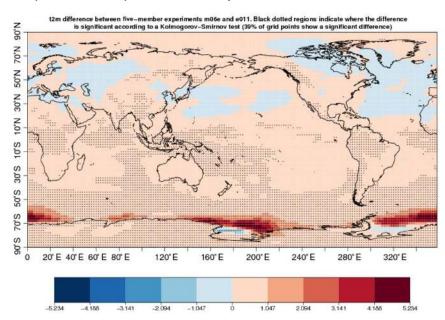
57,067 climate model runs. These runs sample parameter space for 10 parameters with between two and four levels of each, covering 12,487 parameter combinations (24% of possible combinations) and a range of initial conditions

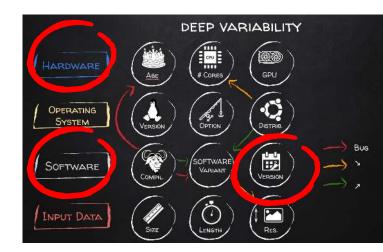
### Replicability of the EC-Earth3 Earth system model under a change in computing environment

François Massonnet<sup>1,2</sup>, Martin Ménégoz<sup>2,3</sup>, Mario Acosta<sup>2</sup>, Xavier Yepes-Arbós<sup>2</sup>, Eleftheria Exarchou<sup>2</sup>, and Francisco J. Doblas-Reyes<sup>2,4</sup>



Can a coupled ESM simulation be restarted from a different machine without causing climate-changing modifications in the results? Using two versions of EC-Earth: one "non-replicable" case (see below) and one replicable case.





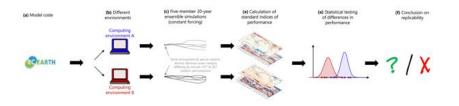
### Replicability of the EC-Earth3 Earth system model under a change in computing environment

François Massonnet<sup>12,2</sup>, Martin Ménégoz<sup>2,2,3</sup>, Mario Acosta<sup>2,2</sup>, Xavier Yepes-Arbós<sup>2,2</sup>, Eleftheria Exarchou<sup>2,4</sup>, and Francisco J. Doblas-Reyes<sup>2,4</sup>

# Can a coupled ESM simulation be restarted from a different machine without causing climate-changing modifications in the results?

A study involving eight institutions and seven different supercomputers in Europe is currently ongoing with EC-Earth. This ongoing study aims to do the following:

- evaluate different computational environments that are used in collaboration to produce CMIP6 experiments (can we safely create large ensembles composed of subsets that emanate from different partners of the consortium?);
- detect if the same CMIP6 configuration is replicable among platforms of the EC-Earth consortium (that is, can we safely exchange restarts with EC-Earth partners in order to initialize simulations and to avoid long spin-ups?); and
- systematically evaluate the impact of **different compilation flag options** (that is, what is the highest acceptable level of optimization that will not break the replicability of EC-Earth for a given environment?).





Joelle Pineau "Building Reproducible, Reusable, and Robust Machine Learning Software" ICSE'19 keynote "[...] results can be brittle to even minor perturbations in the domain or experimental procedure"

### **Deep Reinforcement Learning that Matters**

Peter Henderson<sup>1\*</sup>, Riashat Islam<sup>1,2\*</sup>, Philip Bachman<sup>2</sup> Joelle Pineau<sup>1</sup>, Doina Precup<sup>1</sup>, David Meger<sup>1</sup> What is the magnitude of the effect hyperparameter settings can have on baseline performance?

How does the choice of **network architecture** for the policy and value function approximation affect performance?

How can the **reward scale** affect results?

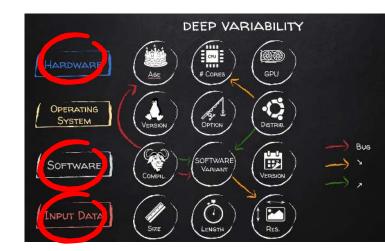
Can random seeds drastically alter performance?

How do the **environment properties** affect variability in reported RL algorithm performance?

Are commonly used baseline **implementations** comparable?



In this paper I investigate the effect of random seed selection on the accuracy when using popular deep learning architectures for computer vision. I scan a large amount of seeds (up to 10<sup>4</sup>) on CIFAR 10 and I also scan fewer seeds on Imagenet using pre-trained models to investigate large scale datasets. The conclusions are that even if the variance is not very large, it is surprisingly easy to find an outlier that performs much better or much worse than the average.



### Reproducible and replicable CFD: it's harder than you think

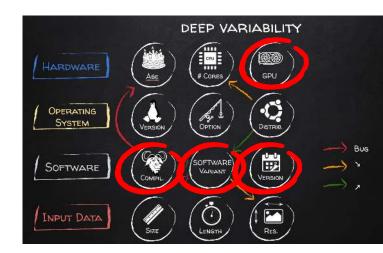
Olivier Mesnard, Lorena A. Barba Mechanical and Aerospace Engineering, George Washington University, Washington DC 20052

"Completing a full replication study of our previously published findings on bluff-body aerodynamics was harder than we thought. <u>Despite the fact that we have good</u> <u>reproducible-research practices</u>, sharing our code and data openly."

Story 1: Meshing and boundary conditions can ruin everything

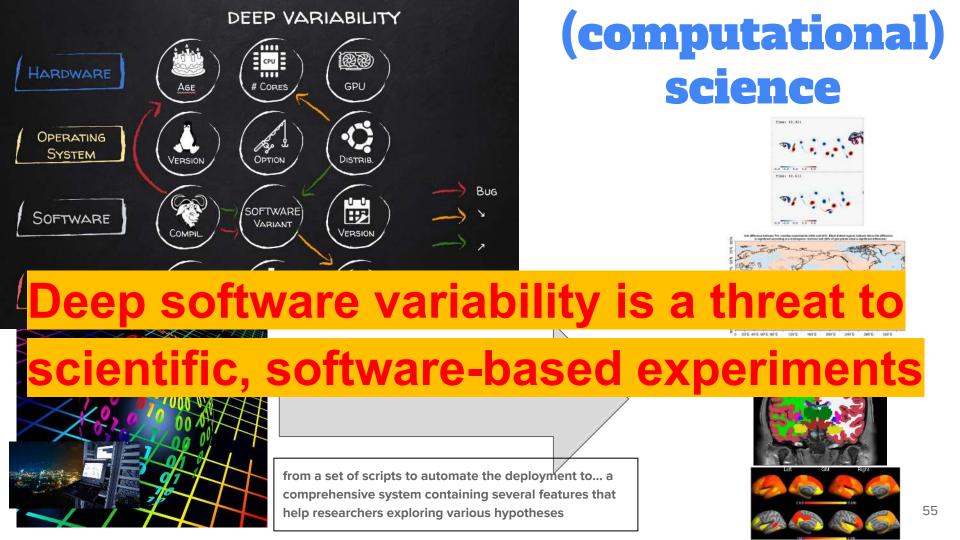
Story 3: All linear algebra libraries are not created equal

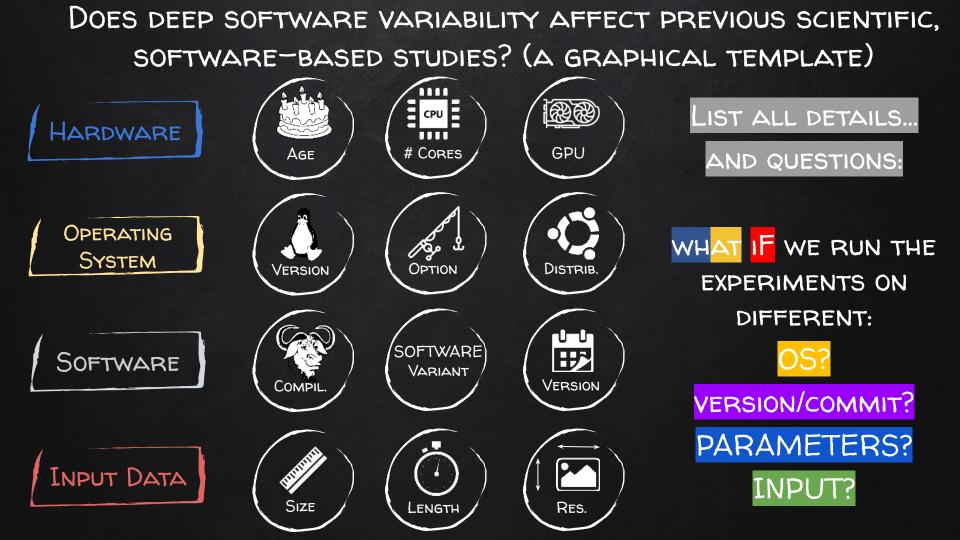
Story 4: Different versions of your code, external libraries or even compilers may challenge reproducibility





- Reproducible Science and (Deep) Software (Variability)
- Deep Software Variability
- Evidence of Deep Software Variability in Computational Science
- **Threats and Opportunities**





# What can we do? (#1 studies)

**Empirical studies** about deep software variability

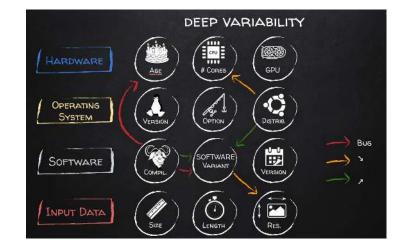
- more subject systems
- more variability layers, including interactions
- more quantitative (e.g., performance) properties

with challenges for gathering measurements data:

- how to scale experiments? Variant space is huge!
- how to fix/isolate some layers? (eg hardware)
- how to measure in a reliable way?

Expected outcomes:

- significance of deep software variability in the wild
- identification of **stable** layers: sources of variability that should not affect the conclusion and that can be eliminated/forgotten
- identification/quantification of **sensitive** layers and interactions that matter
- variability knowledge



# What can we do? (#2 cost)

## Reducing the cost of exploring the variability spaces

Many directions here (references at the end of the slides):

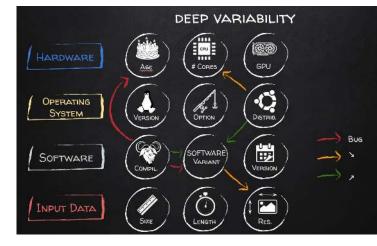
- learning
  - many algorithms/techniques with tradeoffs interpretability/accuracy
  - transfer learning (instead of learning from scratch)
- sampling strategies
  - uniform random sampling? t-wise? distance-based? ...
  - sample of hardware? input data?
- incremental build of configurations
- white-box approaches

DEEP VARIABILITY HARDWARE OPERATING SYSTEM OFTION SOFTWARE COMPIL INPUT DATA DEEP VARIABILITY OFTION OFTION SOFTWARE COMPIL SOFTWARE COMPIL SOFTWARE COMPIL SIZE COMPIL SIZE COMPIL COMPIL SIZE COMPIL COMPIL

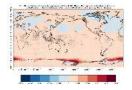
# What can we do? (#3 modelling)

## **Modelling variability**

- Abstractions are definitely needed to...
  - reason about logical constraints and interactions
  - integrate domain knowledge
  - synthesize domain knowledge
  - automate and guide the exploration of variants
  - scope and prioritize experiments
- Challenges:
  - Multiple systems, layers, concerns
  - Different kinds of variability: technical vs domain, accidental vs essential, implicit vs explicit... when to stop modelling?
  - $\circ$  reverse engineering

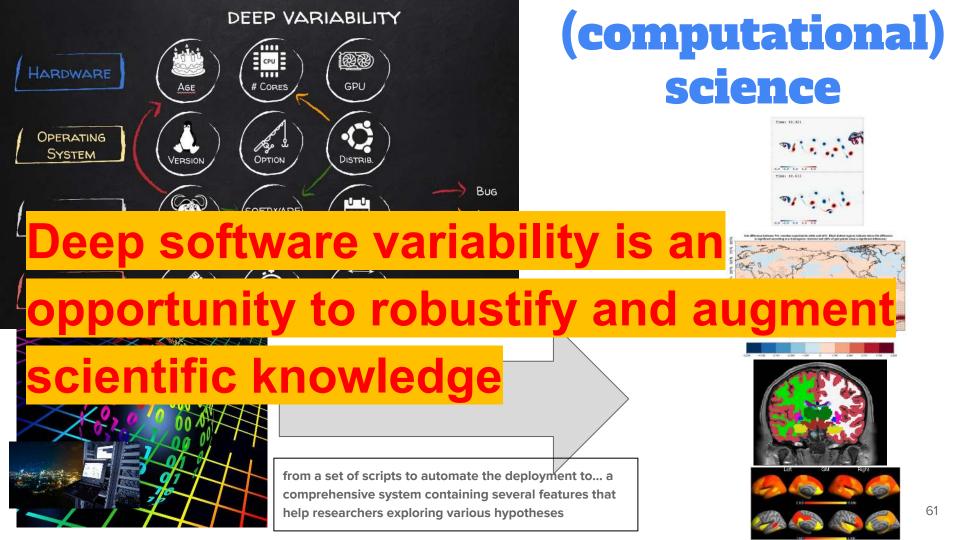


# What can we do? (#4 robustness)



- Robustness (trustworthiness) of scientific results to sources of variability
- I have shown many examples of sources of variations and non-robust results...
- Robustness should be rigorously defined (hint: it's not the definition as given in computer science)
- How to verify the effect of sources of variations on the robustness of given conclusions?
  - actionable metrics?
- methodology? (eg when to stop?)
- variability can actually be leveraged to augment confidence





#### Variability in the analysis of a single neuroimaging dataset by many teams

Rotem Botvinik-Nezer, Felix Holzmeister, ... Tom Schonberg 🗠 🛛 + Show authors

Nature 582, 84–88 (2020) Cite this article 42k Accesses | 203 Citations | 2056 Altmetric | Metrics

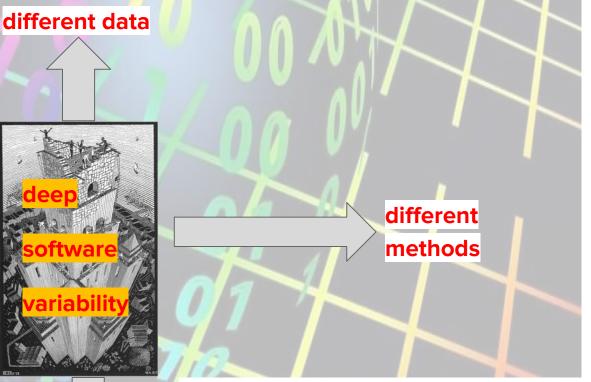
> different assumptions

**Increasing Transparency Through a Multiverse** Analysis

Sara Steegen<sup>1</sup>, Francis Tuerlinckx<sup>1</sup>, Andrew Gelman<sup>2</sup>, Wolf Vanpaemel<sup>3</sup>

Affiliations + expand PMID: 27694465 DOI: 10.1177/1745691616658637





Many Analysts, One Data Set: Making Transparent How Variations in Analytic Choices Affect Results

R. Silberzahn, E. L. Uhlmann, D. P. Martin, more.,

First Published August 23, 2018 Research Article 🖪 Clinication updates https://doi.org/10.1177/2515245917747646

Show all authors v

### different analyses

62

"When you are a researcher, you want to be the first. Research is about discovery, inventing things that others have not done. It is by definition a form of competition. You have to accept that." CNRS CEO





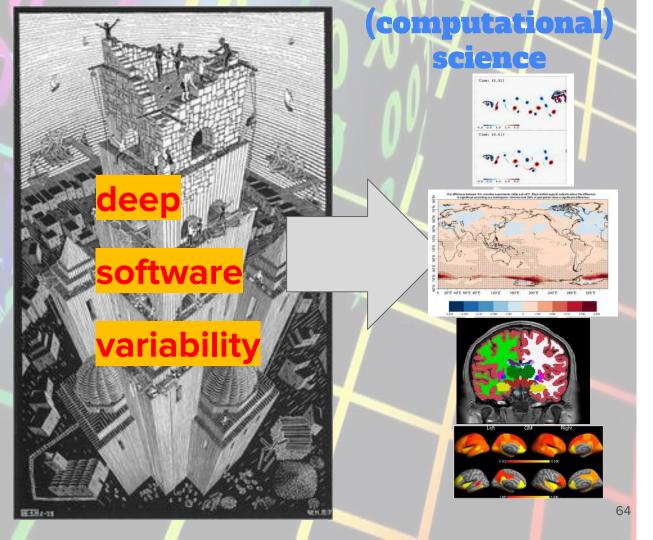
At a time of global pandemics, global warming and unprecedented public distrust of politics and democracy, research is anything but an individualistic competition.

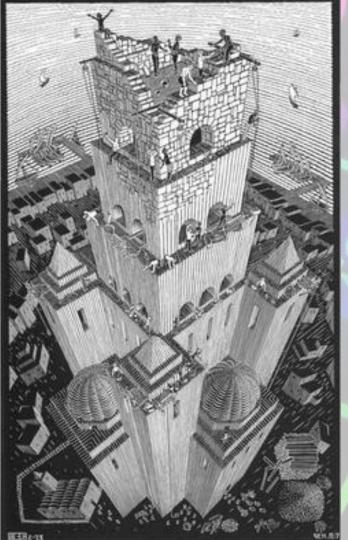
Above all, let us value the need for reproducibility in research. Let us prefer the "discovery" that will be verified or even falsified and encourage collaboration.

Deeply exploring the variability space cannot be done alone. Collaborative, distributed effort needed. Are we in ivory towers?

I mean: We're studying software... for the sake of improving software engineering (and it's nice!).

But should we stay?





### Deep software variability is...

### a threat for reproducible research

"Authors provide all the necessary data and the computer codes to run the analysis again, re-creating the results."

### an opportunity for replication

"A study that arrives at the same scientific findings as another study, collecting new data (possibly with different methods) and completing new analyses."

"A study that refutes some scientific findings of another study, through the collection of new data (possibly with different methods) and completion of new analyses."

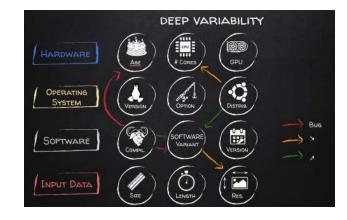
### robustifying and augmenting

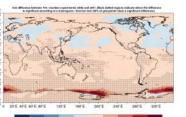
scientific knowledge



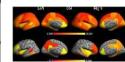
# **Reproducible Science and Deep Software Variability**











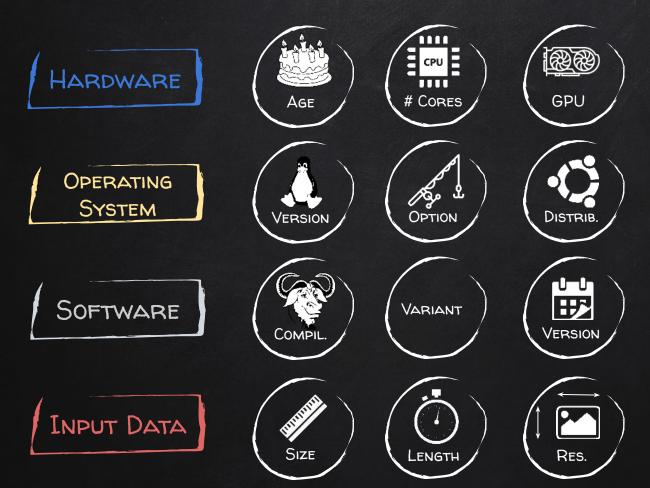








### (BEYOND X264) EMPIRICAL AND FUNDAMENTAL QUESTION



HOW DOES DEEP SOFTWARE VARIABILITY MANIFEST IN THE WILD?

SOFTWARE SCIENTISTS SHOULD OBSERVE THE JUNGLE/ GALAXY!

## DEEP SOFTWARE VARIABILITY

## 4 CHALLENGES AND OPPORTUNITIES

Luc Lesoil, Mathieu Acher, Arnaud Blouin, Jean-Marc Jézéquel: Deep Software Variability: Towards Handling Cross-Layer Configuration. VaMoS 2021: 10:1-10:8

## IDENTIFY THE INFLUENTIAL LAYERS

1



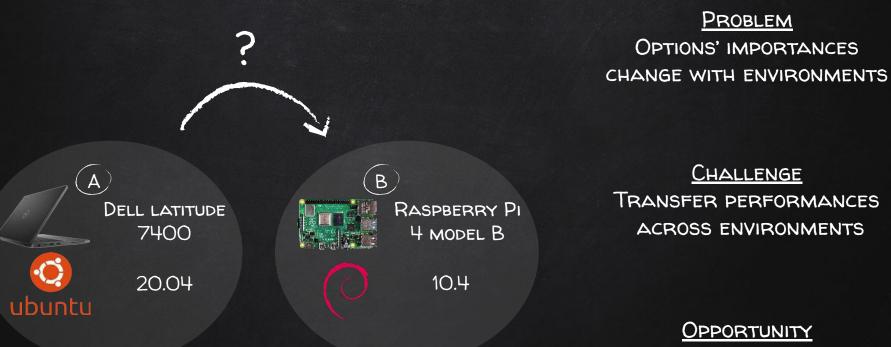
## TEST & BENCHMARK ENVIRONMENTS



DIMENSIONALITY REDUCTION

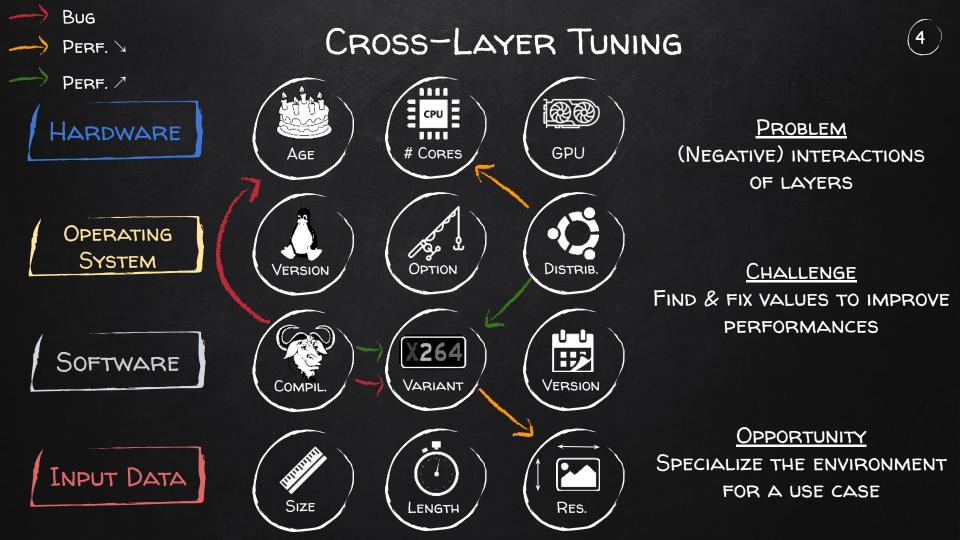
(2)

## TRANSFER PERFORMANCES ACROSS ENVIRONMENTS



REDUCE COST OF MEASURE

(3)



## CHALLENGES FOR DEEP SOFTWARE VARIABILITY

IDENTIFY THE INFLUENTIAL LAYERS

TEST & BENCHMARK ENVIRONMENTS

TRANSFER PERFORMANCES ACROSS ENVIRONMENTS

CROSS-LAYER TUNING

## Wrap-up

Deep software variability is a thing...

miracle and smooth fit of variability layers?

or subtle interactions among layers?

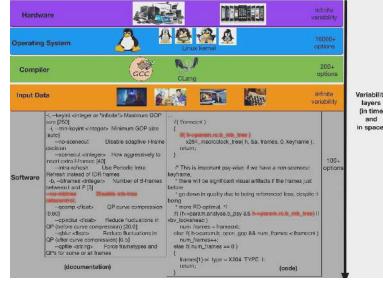
software scientists should **systematically study** the phenomenon

Many challenges and opportunities

cross-layer tuning at affordable cost

configuration knowledge that generalizes to any context and usage

Dimensionality reduction and transfer learning



## Impacts of deep software variability

Users/developers/scientists: missed opportunities due to (accidental) variability/complexity

Deep software variability can be seen as a **threat** to knowledge/validity

### Claim: Deep software variability is a threat to scientific, software-based experiments

Example #1: in the results of neuroimaging studies

- applications of different analysis pipelines (Krefting et al. 2011)
- alterations in software version (Glatard et al. 2015)
- changes in operating system (Gronenschild2012 et al.)

version OS

have both shown to cause variation (up to the point it can change the conclusions).

Example #2: on a modest scale, our ICPE 2020 (Pereira et al.) showed that a variation in inputs could change the conclusion about the effectiveness of a sampling strategy for the same software system.

<u>Example #3:</u> I'm reading Zakaria Ournani et al. "Taming Energy Consumption Variations In Systems Benchmarking" ICPE 2020 as an excellent inquiry to control deep variability factors

Example #4: Similar observations have been made in the machine learning community (Henderson et al. 2018)

## Impacts of deep software variability

Users/developers/scientists: missed opportunities due to (accidental) complexity

Deep software variability can be seen as a threat to knowledge/validity

Claim: Deep software variability is a threat to scientific, software-based experiments

I propose an exercise that might be slightly disturbing:

# Does deep software variability affect (your|a known) previous scientific, software-based studies?

(remark: it's mainly how we've investigated deep software variability so far... either as a threat to our own experiments or as a threat identified in papers)

Applications of different analysis pipelines, alterations in software version, and even changes in operating system have both shown to cause variation in the results of a neuroimaging study. Example:

Reproducibility of neuroimaging analyses across operating systems

👰 Tristan Glatard ?, 🛛 Lindsay B. Lewis , 🐒 Rafael Ferreira da Silva , 🦷 Roza Adalat', Natacha Beck', Claudo Lepage', Pierre Rioux , Marc-Etienne Rousseau', 📓 Tarek Sherif , Ewa Deelman , 🛐 Najmeh Khalili-Mahani' and 🎆 Alan C. Evans''

Neuroimaging pipelines are known to generate different results depending on the computing platform where they are compiled and executed. We quantify these differences for brain tissue classification, fMRI analysis, and cortical thickness (CT) extraction, using three of the main neuroimaging packages (FSL, Freesurfer and CIVET) and different versions of GNU/Linux. We also identify some causes of these differences using library and system call interception. We find that these packages use mathematical functions based on single-precision floating-point arithmetic whose implementations in operating systems continue to evolve. While these differences have little or no impact on simple analysis pipelines such as brain extraction and cortical tissue classification, their accumulation creates important differences in longer pipelines such as subcortical tissue classification, fMRI analysis, and cortical thickness extraction. With FSL, most Dice coefficients between subcortical

### DEEP SOFTWARE VARIABILITY

### Deep Bisioftware svar Rabiacity and Sawthreat to "[...] results an be brittle to even minor perturbations in the domain of experimental procedure" Example:

# scientific, southward and seed (3407) is all you need: On the influence of experiments

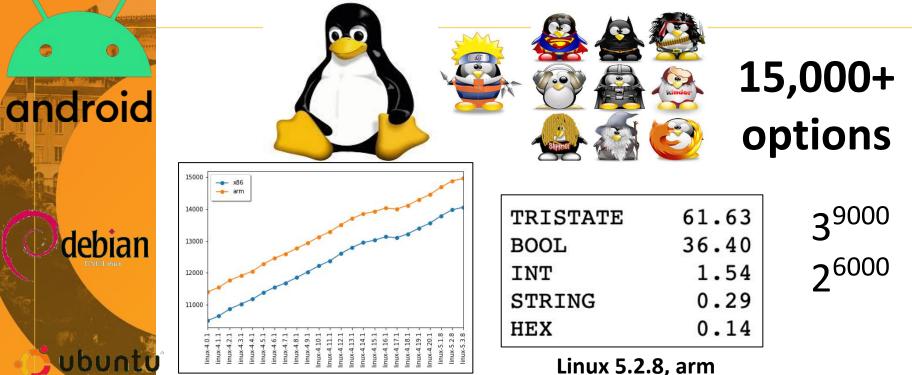
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#### DEEP SOFTWARE VARIABILITY

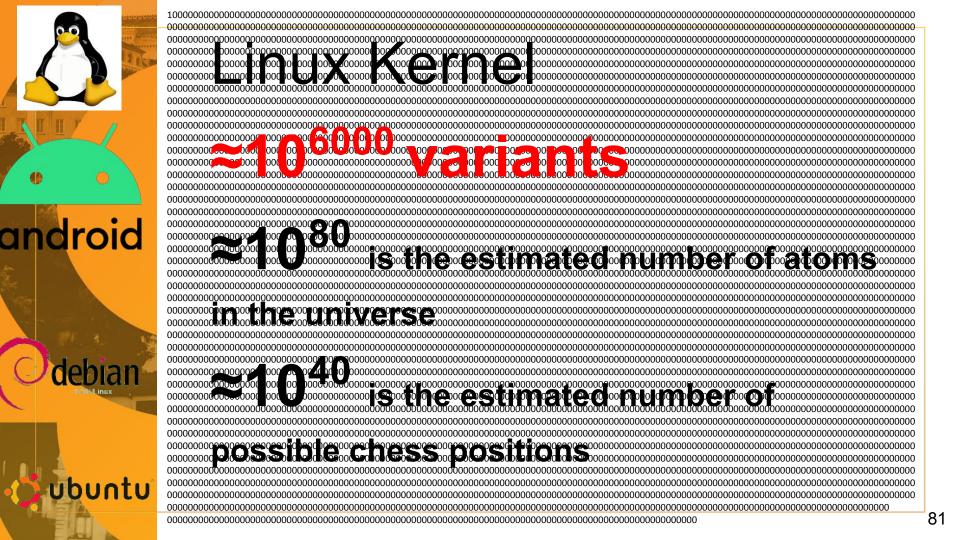
#### Abstract

In this paper I investigate the effect of random seed selection on the accuracy when using popular deep learning architectures for computer vision. I scan a large amount of seeds (up to 10<sup>4</sup>) on CIFAR 10 and I also scan fewer seeds on Imagenet using pre-trained models to investigate large scale datasets. The conclusions are that even if the variance is not very large, it is surprisingly easy to find an outlier that performs much better or much worse than the average. DEEP QUESTIONS?



≈10<sup>6000</sup> variants

(without constraints)



Reproducible Science and Deep Software Variability

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