Accurate simulation of operating system updates in neuroimaging using Monte-Carlo arithmetic

Ali Salari¹, Yohan Chatelain¹, Gregory Kiar², Tristan Glatard¹

¹Department of Computer Science and Software Engineering, Concordia University, Montréal, QC, Canada
²Center for the Developing Brain, Child Mind Institute, New York, NY, USA
m_alari@encs.concordia.ca

Abstract. Operating system (OS) updates introduce numerical perturbations that impact the reproducibility of computational pipelines. In neuroimaging, this has important practical implications on the validity of computational results, particularly when obtained in systems such as high-performance computing clusters where the experimenter does not control software updates. We present a framework to reproduce the variability induced by OS updates in controlled conditions. We hypothesize that OS updates impact computational pipelines mainly through numerical perturbations originating in mathematical libraries, which we simulate using Monte-Carlo arithmetic in a framework called “fuzzy libmath” (FL). We applied this methodology to pre-processing pipelines of the Human Connectome Project, a flagship open-data project in neuroimaging. We found that FL-perturbed pipelines accurately reproduce the variability induced by OS updates and that this similarity is only mildly dependent on simulation parameters. Importantly, we also found between-subject differences were preserved in both cases, though the between-run variability was of comparable magnitude for both FL and OS perturbations. We found the numerical precision in the HCP pre-processed images to be relatively low, with less than 8 significant bits among the 24 available, which motivates further investigation of the numerical stability of components in the tested pipeline. Overall, our results establish that FL accurately simulates results variability due to OS updates, and is a practical framework to quantify numerical uncertainty in neuroimaging.

Keywords: Computational reproducibility · Neuroimaging pipelines · Monte-Carlo arithmetic.

1 Introduction

Numerical round-off and cancellation errors are ubiquitous in floating-point computations. In neuroimaging, they contribute to results uncertainty along with other sources of variability, including population selection, scanning devices, sequence parameters, acquisition noise, and methodological flexibility [3,2]. Numerical errors manifest particularly through variations in elementary mathemat-
Mathematical libraries resulting from operating system (OS) updates. Indeed, due to implementation differences, mathematical functions available in different OS versions provide slightly different results. The impact of such epsilon-like differences on image analysis depends on the conditioning of the problem and the pipeline’s numerical implementation. In neuroimaging, established image processing pipelines have been shown to be substantially impacted: for instance, differences in cortical thicknesses measured by the same Freesurfer version in different execution platforms were shown to reach statistical significance in some brain regions [9], and Dice coefficients as low as 0.6 were observed between FSL or Freesurfer segmentations obtained in different platforms [8,18]. Such observations threaten the validity of neuroimaging results by revealing systematic instabilities.

Despite its possible implications on results validity, the effect of OS updates remains seldom studied due to (1) the lack of closed-form expressions of condition numbers for complex pipelines and non-differentiable non-linear analyses, (2) the technical challenge associated with experimental studies involving multiple OS distributions and versions, (3) the uncontrolled nature of OS updates. As a result, the effect of OS updates on neuroimaging analyses is generally neglected or handled through the use of software containers (Docker or Singularity), static executable builds, or similar approaches. While such techniques improve experiment portability, they only mask numerical instabilities and do not tackle them. Numerical perturbations are bound to reappear due to security updates [14], obsoleting software [17], or parallelization. Therefore, the mechanisms through which numerical instabilities propagate need to be investigated and eventually addressed.

This paper presents “fuzzy libmath” (FL), a framework to simulate OS updates in controlled conditions, allowing software developers to evaluate the robustness of their tools with respect to likely-to-occur numerical perturbations. As we hypothesize that numerical perturbations resulting from OS updates primarily come from implementation differences in elementary mathematical libraries, we leverage Monte-Carlo arithmetic (MCA) [16] to introduce controlled amounts of noise in these libraries. FL enables MCA in mathematical functions used by existing pipelines without the need to modify or recompile them. To demonstrate the approach, we study the effect of common OS updates on the numerical precision of structural MRI pre-processing pipelines of the Human Connectome Project [19], a major neuroimaging initiative.

2 Simulating OS updates with Monte-Carlo arithmetic

MCA models floating-point roundoff and cancellations errors through random perturbations, allowing for the estimation of error distributions from independent random result samples. MCA simulates computations at a given virtual precision using the following perturbation:

\[
\text{inexact}(x) = x + 2^{e_x - t} \xi
\]  

where \(e_x\) is the exponent in the floating-point representation of \(x\), \(t\) is the virtual precision and \(\xi\) is a random uniform variable of \((-\frac{1}{2}, \frac{1}{2})\).
MCA allows for three perturbation modes: Random Rounding (RR) introduces the perturbation in function outputs, simulating roundoff errors; Precision Bounding (PB) introduces the perturbation in function operands, allowing for the detection of catastrophic cancellations; and, Full MCA combines RR and PB, resulting in the following perturbation:

$$mca\_mode(x \circ y) = inexact_{RR}(inexact_{PB}(x) \circ inexact_{PB}(y))$$  

To simulate OS updates, we introduce random perturbations in the GNU mathematical library, the main mathematical library in GNU/Linux systems. Instrumenting mathematical libraries with MCA raises a number of issues as many functions assume deterministic arithmetic. For instance, applying random perturbations around a discontinuity or within piecewise approximations results in large variations and a total loss of significance that are not relevant in our context. Therefore, we have applied MCA to proxy mathematical functions wrapping those in the original library, such that only the outputs of the original functions were perturbed but not their inputs or the implementations themselves. This technique allows us to control the magnitude of the perturbation as perceived by the application.

We instrumented the GNU mathematical library with MCA using Verificarlo [5], a tool that (1) uses the Clang compiler to generate an LLVM (http://llvm.org) Intermediate Representation (IR) of the source code, (2) replaces floating-point operations in the IR by a call to the Verificarlo API, and (3) compiles the modified IR to an executable using LLVM. The perturbation applied by the Verificarlo API can be configured at runtime, for instance to change the virtual precision applied to single- and double-precision floating-point values.

The resulting MCA-instrumented mathematical library, “fuzzy libmath” (FL), is loaded in the pipeline using LD_PRELOAD, a Linux mechanism to force-load a shared library into an executable. As a result, functions defined in fuzzy libmath transparently overload the original ones without the need to modify or recompile the analysis pipeline. Fuzzy libmath functions call the original functions through dlsym, a function that returns the memory address of a symbol. To trigger MCA instrumentation, a floating-point zero is added to the output of the original function and the result of this sum is perturbed and returned.

Finally, we measure results precision as the number of significant bits among result samples, as defined in [16]:

$$s = -\log_2 \left| \frac{\sigma}{\mu} \right|$$  

where $\sigma$ and $\mu$ are the observed cross-sample standard deviation and average.

3 HCP Pipelines & Dataset

We apply the methodology described above to the minimal structural pre-processing pipeline associated with the Human Connectome Project (HCP) dataset [7], entitled “PreFreeSurfer”. This pipeline consists of many independent components,
including: spatial distortion correction, brain extraction, cross-modal registration, and alignment to standard space. Each high-level component of this pipeline (Fig. 1) consists of several function calls using FSL, the FMRIB Software Library [12]. The pipeline requires T1w and T2w images for each subject. A full description of the pipeline is available at [7].

It should be noted that the PreFreeSurfer pipeline uses both single and double precision functions from the GNU mathematical library. Among the preprocessing steps in the pipeline, it has been shown that linear and non-linear registrations implemented in FSL FLIRT [13,11] and FNIRT [1] are the most sensitive to numerical instabilities [18].

We selected 20 unprocessed subjects from the HCP data release S500 available in the ConnectomDB repository. We selected these subjects from different subject types to cover execution paths sufficiently. For each, the available data consisted of 1 or 2 T1w and T2w images each, with spatial dimensions of $256 \times 320 \times 320$ and voxel resolution of 0.7 mm. Acquisition protocols and parameters are detailed in [19]. Two distinct experimental configurations were tested:

**Operating Systems (OS):** subjects were processed on three different Linux operating systems inside Docker images: CentOS7 (glibc v.2.17), CentOS8 (glibc v.2.28), and Ubuntu20 (glibc v.2.31).

**Fuzzy libmath (FL):** the dataset was processed on an Ubuntu20 system using fuzzy libmath. The virtual precision ($t$) for the perturbations was swept from 53 bits (the full mantissa for double-precision data) down to 1 bit by steps of 2. For $t \geq 24$ bits, only double-precision was altered and single-precision was set to 24 bits, and for $t < 24$ bits, both double- and single-precision simultaneously were changed. Three FL-perturbed samples were generated for each subject and virtual precision, to match the number of OS samples.

After conducting both experiments, we selected the virtual precision that most closely simulated the variability observed across OSes via the root-mean-square error (RMSE) between the number of significant bits per voxel in all subjects and conditions. This precision is referred to as the global nearest virtual precision and was used to compare results obtained in both the FL and OS versions.
4 Results

The fuzzy libmath source code, Docker image specifications, and analysis code to reproduce the results are available at https://github.com/big-data-lab-team/MCA-libmath-paper. All experiments were conducted on the Béluga HPC computing cluster made available by Compute Canada through Calcul Québec. Béluga is a general-purpose cluster with 872 available nodes. All nodes contain 2× Intel Gold 6148 Skylake @ 2.4 GHz (40 cores/node) CPU, and node memory can range between 92 to 752 GB. The average processing time of the pipeline without FL instrumentation was 69 minutes (average of 3 executions). The FL perturbation increased it to 93 minutes.

We ensured that the pipeline does not use pseudo-random numbers by processing each subject twice on the same operating system. To validate that FL was correctly instrumented with Verificarlo, we used Veritracer [4], a tool for tracing the numerical quality of variables over time. For one subject, the traces showed that the number of significant bits in the function outputs varied over time, confirming the instrumentation with MCA. Throughout the pipeline execution, Veritracer reported approximately 4 billion calls to FL, with the following ratio of calls: 47.12% log, 40.96% exp, 6.92% expf, 3.39% logf, 1.55% sincosf, and 0.06% of cumulated calls to atan2f, pow, sqrt, exp2f, powf, log10f, log10, cos, and asin. We also checked that long double types were not used.

4.1 Fuzzy libmath accurately simulates the effect of OS updates

Fuzzy libmath accurately reproduced the effect of OS updates, both globally (Fig. 2a) and locally (Fig. 2b). The distributions of significant bits in the atlas registered T1w images were nearly identical (p > 0.05, KS test) on the average and individual subject distributions for 15/20 subjects, after correcting for multiple comparisons. Locally, the spatial distribution of significant digits also appeared to be preserved. Losses in significance were observed mainly at the

![Distribution of significant bits](image1.png)

(a) Distribution of significant bits

![Significance map (subject average)](image2.png)

(b) Significance map (subject average)

Fig. 2: Comparison of OS and FL effects on the precision of PreFreeSurfer results for n=20 subjects. FL samples were obtained at the global nearest virtual precision of t=37 bits.
brain-skull interface and between brain lobes, indicating spatial dependency of numerical properties.

The average number of significant bits in either the FL or OS conditions were 7.76 out of 24 available, which corresponds to 2.32 significant (base 10) digits. This relatively low precision motivates future investigations of the stability of pipeline components, in particular for image registration.

4.2 Fuzzy libmath preserves between-subjects image similarity

Numerically-perturbed samples remained primarily clustered by individual subjects (Fig. 3), indicating that neither FL nor OS perturbations were impactful enough to blur the differences between subjects. Notably, the similarity between subjects was also preserved by the numerical perturbation, leading to the same subject ordering in the dendrograms. However, the average RMSE within samples of a given subject was approximately $13 \times$ lower than the average RMSE between different subjects. The fact that between-subject variabilities were nearly on the same order of magnitude as OS and FL variability demonstrates the potential severity of these instabilities.

![Fig. 3: RMSE-based hierarchical clustering of OS (left) and FL (right) samples. Colors identify different subjects, showing that similarities between subjects are preserved by the numerical perturbations. Horizontal gray lines represent average RMSEs between (top line) and within (bottom line) subject clusters.](image)

4.3 Results are stable across virtual precision

The FL results presented previously were obtained at the global nearest virtual precision of $t=37$ bits, determined as the precision which minimized the RMSE between FL and OS average maps of significant bits. We varied the virtual precision in steps of 2 between $t=1$ and $t=53$ bits (Fig. 4). On average, no noticeable RMSE change was observed between the FL and OS variability for
Fig. 4: Comparison of RMSE values computed between OS and FL results for different virtual precisions.

precisions ranging from $t=21$ to $t=53$ bits, which shows that FL can robustly approximate OS updates.

The observed plateau suggests the existence of an “intrinsic precision” for the pipeline, above which no improvement in results precision is expected. For the tested pipeline, this intrinsic precision was observed at $t=21$ bits, which indicates that the pipeline could be implemented exclusively with single-precision floating-point representations (24 bits of mantissa) without loss of results precision. This would substantially decrease the pipeline memory footprint and computational time, as approximately 88% of operations used in this pipeline made use of double-precision data. In addition, the presence of such a plateau suggests that numerical perturbations introduced by OS updates might be in the range of machine error ($t=53$ bits), although it is also possible that the extent of the plateau results from the numerical conditioning of the tested pipeline. It is possible in contrast that the absence of such a plateau would suggest an unstable pipeline that would benefit either from correction or larger datatypes. The ability to capture stability across a range of precisions importantly demonstrates a key advantage of using FL to simulate OS variability.

The relationship between RMSE of individual subjects was generally consistent with the average line, with the notable exception of subject 18. The observed discrepancies between this subject and potential others might be leveraged for quality control checks and, as a result, inform tool development.

The pipeline failed to complete for at least one subject below the virtual precision of $t=13$ bits, also referred to as the tolerance of the pipeline. Specifically, 51% of pipeline executions crashed among all subjects for precisions ranging from 1–11 bits, and there was no relationship between tolerance-level and precision. The error raised was in the Readout Distortion Correction portion of the pipeline, and appears to stem from the FSL FAST tissue segmentation. The
specific source of the error within this component is presently unknown, but is an open question for further exploration.

5 Conclusion & Discussion

We demonstrated fuzzy libmath as an accurate method to simulate variability in neuroimaging results due to OS updates. Alongside this evaluation, fuzzy libmath can be used by pipeline developers or consumers to evaluate the numerical uncertainty of tools and results. Such evaluations may also help decrease pipeline memory usage and computational time through the controlled use of reduced numerical precision. Fuzzy libmath does not require any modification of the pipeline as it operates on the level of shared libraries. The accuracy of the simulations were shown to be robust across a wide range of virtual precisions, which reinforces the applicability of the method.

The proposed technique is directly applicable to MATLAB code executed with GNU Octave, to Python programs executed on Linux, and to C programs that depend on GNU libmath. Numerical noise can be introduced in other libraries, such as OpenBLAS or NumPy, using our https://github.com/verificarlo/fuzzy environment.

A commonly used approach to address instabilities resulting from OS version updates in practice is to sweep the issue under the rug of software containers or static linking. While such solutions are undoubtedly helpful to improve code portability or strict re-executability, a more honest position is to consider computational results as realizations of random variables depending on numerical error. The presented technique enables estimating result distributions, a first step toward making analyses reproducible across heterogeneous execution environments. While this work did not investigate the precise cause of numerical instabilities by tracing the system function calls, this is a topic for future work.

The tested OS versions span a timeframe of 7 years (2012–2020) and focused on GNU/Linux, a widely-used platform in neuroimaging [10]. Given that our experiments focused on numerical perturbations applied to mathematical functions, which are implemented similarly across OSes, our findings are likely to generalize to OS/X or MS Windows, although future work would be needed to confirm that. The tested pipeline is the official solution of the HCP project to pre-process data, and is considered the state-of-the-art. This pipeline assembles software components from the FSL toolbox consistent with common practice in neuroimaging, such as in fMRIPrep [6] or the FSL feat workflow [12], to which fuzzy libmath can be directly applied. Efforts are on-going to use fuzzy libmath in fMRIPrep software tests, to guarantee that bug fixes do not perturb results beyond numerical uncertainty.

The fact that the induced numerical variability preserves image similarity between subjects is reassuring and, in fact, exciting. OS updates provide a convenient, practical target to define a virtual precision leading to a detectable but still reasonable numerical perturbation. However, it is also of importance that OS- and FL-induced variability were on a similar order of magnitude as
subject-level effects. This suggests that the preservation of relative between-subject differences may not hold in all pipelines, and such a comparison could be used to evaluate the robustness of a pipeline to OS instabilities. The fact that the results observed across OS versions and FL perturbations arise from equally-valid numerical operations also suggests that the observed variability may contain meaningful signal. In particular, signal measured from these perturbations might be leveraged to enhance biomarkers, as suggested in [15] where augmenting a diffusion MRI dataset with numerically-perturbed samples was shown to improve age classification.

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