

# Array Programming on GPUs : Challenges and Opportunities

## An Experience Report

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# Org

- GPUs rule
- Energy drives everything
- 50% of energy for math
- Number systems help curb energy / bug tradeoff
  - But what's happening in today's ML-driven world is an explosion of ill-specified systems
  - ML hardware has driven out traditional well-specified FP hardware, resulting in bugs
- The bugs are: FP exceptions; Ill-specified HW; and a lack of formal specs + managing their surfeit
- Exceptions first
  - Pytorch evidence abounds - solutions neither air-tight nor efficient - present table
  - What is a gold-standard for exception handling
  - We know of only one (very good definition) : consistent exception handling
  - But that is not happening
    - SRU example
    - Diagonal boosting in HPC example
    - Closed-source libraries without specs - certainly can't happen under that condition
  - We need to begin concerted efforts
    - Prior GPU-FPX contribution recap
    - Now show how easily we can "go to work with GPU-FPX" and reveal the "rats running around"
    - Show cartoon
    - Then show the 3 examples : SRU, Compressors, GPT
  - New work
    - Support for many number systems, Tensor Core → Community infra
- Ill-specified HW next
  - Eye-opening examples → NFM examples + formal specs under construction → Community infra
- Lack of formal specs last
  - Create many
  - Then
    - Either neutralize to one common denominator, OR
    - See how much one can do to live under a different regime → Work in progress is to make HPC like ML to adapt to new order
- Conclusions
  - Exceptions are an unrecognized threat and you can engage as a PL crowd (start with dyn methods and end with static analysis)
  - Manage specs (develop specs, tests, and have a way for the community to grow this) – say like how the mem model people are doing around litmus tests
  - Grow and manage specs - needs more than numerics-level litmus : need contextual analysis and adjustments

context:

# GPUs Rule

They are key to energy-efficient computing: GPT to watches

# GPUs : The Ama\$\$ing Computing-Engine : H100 (Hopper, source)

## H100: The Foundational Workhorse of Modern AI

The **NVIDIA H100 Tensor Core GPU** remains one of the most versatile and widely deployed GPUs for AI training and inference. Available in both **PCIe** and **SXM** (**via HGX systems**), it offers a solid balance of performance, compatibility, and cost.



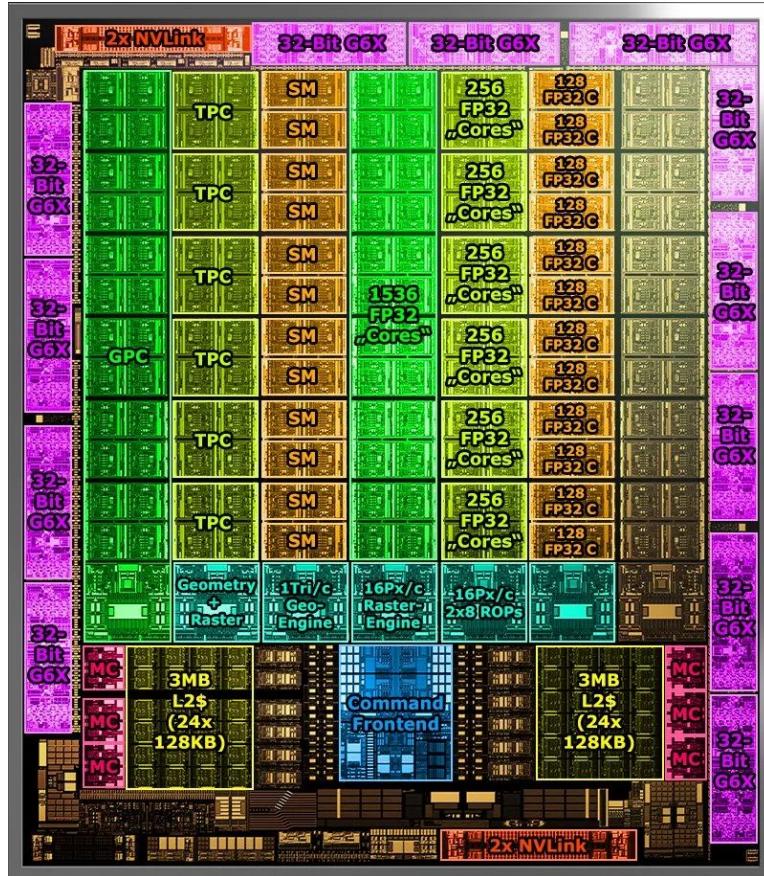
NVIDIA H100 PCIe Form Factor

- **Memory:** 80GB HBM2e
  - **Form Factors:** PCIe and SXM
  - **Peak FP8 Performance:** Up to 4.9 PFLOPs (SXM)
  - **Arc's Availability:**
    - **HGX Systems (SXM):** Starting at **\$215,000 USD** – [View Servers](#)
    - **PCIe Systems:** [Contact Sales](#)
    - **Reserved Cloud (HGX H100):** [Arc's Reserved Cloud](#)
- \$215K ←

## Why Choose H100?

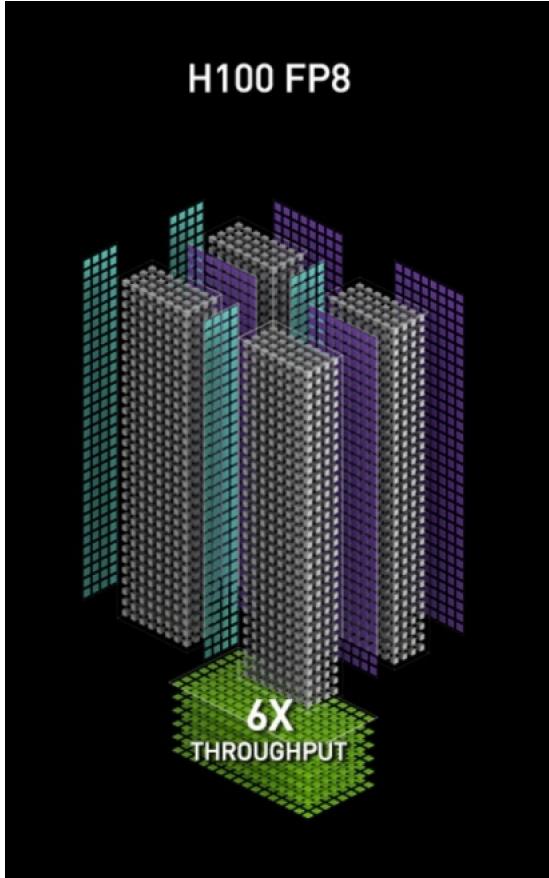
- **PCIe:** Ideal for scalable inference and modular deployments. Broad compatibility and lower entry costs make it great for startups and production-ready GenAI teams.
- **SXM (HGX):** Designed for multi-GPU training. With **NVLINK** and **NVSwitch**, up to 8 GPUs can share memory at high bandwidth, and HGX nodes can be networked for large-scale training.

# GPUs : The Amazing Computing-Engine of This Century (image [source](#))



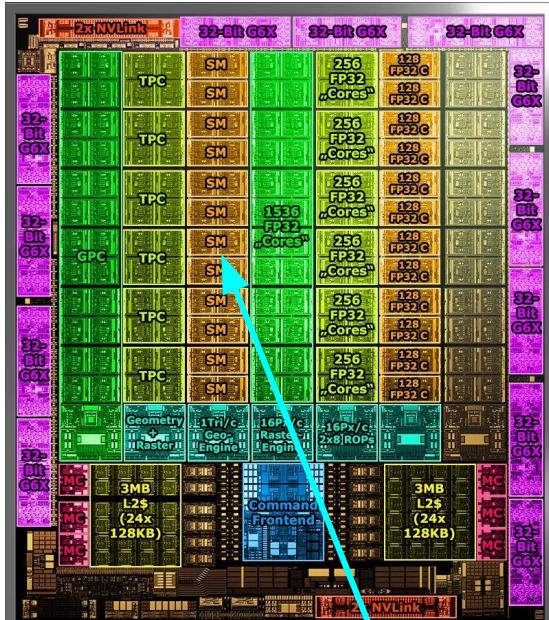
- An affordable GPU: Nvidia GA102
  - Ampere architecture.
    - GeForce RTX 30 series cards,
      - 3090, 3080 Ti, 3080, etc.
  - 128 CUDA cores, 4 Tensor cores,
  - About 350W
  - About \$800 per card bought on eBay

# GPU Tensor Cores : True Workhorses in ML and rising in HPC



- Google TPUs
  - "Only Tensor Cores"
- NVIDIA GPUs
  - Rising support
  - Growing silicon area
- Crucial for Deep ML
- Growing interest in HPC

# GPUs : The Amazing Computing-Engine of This Century ([image source](#))



The SMs contain  
Hardware Warp Schedulers  
The Warps carry  
SIMT-Core instruction "work" and  
Tensor-Core Instruction "work"

CUDA C Code

```
int i = threadIdx.x;  
c[i] = a[i] * b[i];
```



CUDA C Code

```
wmma::mma_sync(c_frag, a_frag, b_frag, d_frag);
```



PTX Code

```
wmma.mma.sync.aligned.m16n16k16.row.row.f32.f16.f32
```



ptxas

PTX Code



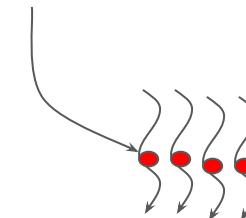
SASS Code

```
/*0008*/ LDG.E.SYS R4, [R1];  
/*0010*/ FMUL R6, R4, R5;  
/*0018*/ STG.E.SYS [R3], R6;
```



Warp

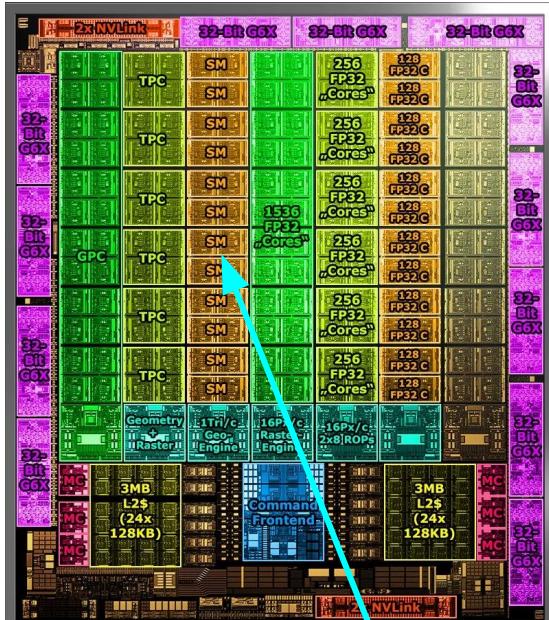
HMMA.1688.F32.F16.F16.F32



Warp

Single  
"small  
matrix  
Multiplicat  
ion" call -  
done in  
Tensore  
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```
int i = threadIdx.x;  
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```



PTX Code

```
ld.global.f32 , mul.f32 , st.global.f32
```



SASS Code

```
/*0008*/ LDG.E.SYS R4, [R1];  
/*0010*/ FMUL R6, R4, R5; ←  
/*0018*/ STG.E.SYS [R3], R6;
```

CUDA C Code

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wmma.mma.sync.aligned.m16n16k16.row.row.f32.f16.f32
```



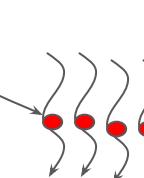
SASS Code

HMMA.1688.F32.F16.F16.F32



Warp

We  
Instrument  
SASS, as  
that's often  
what we  
can access  
+ that's the  
most  
honest !!



Warp

Single  
"small  
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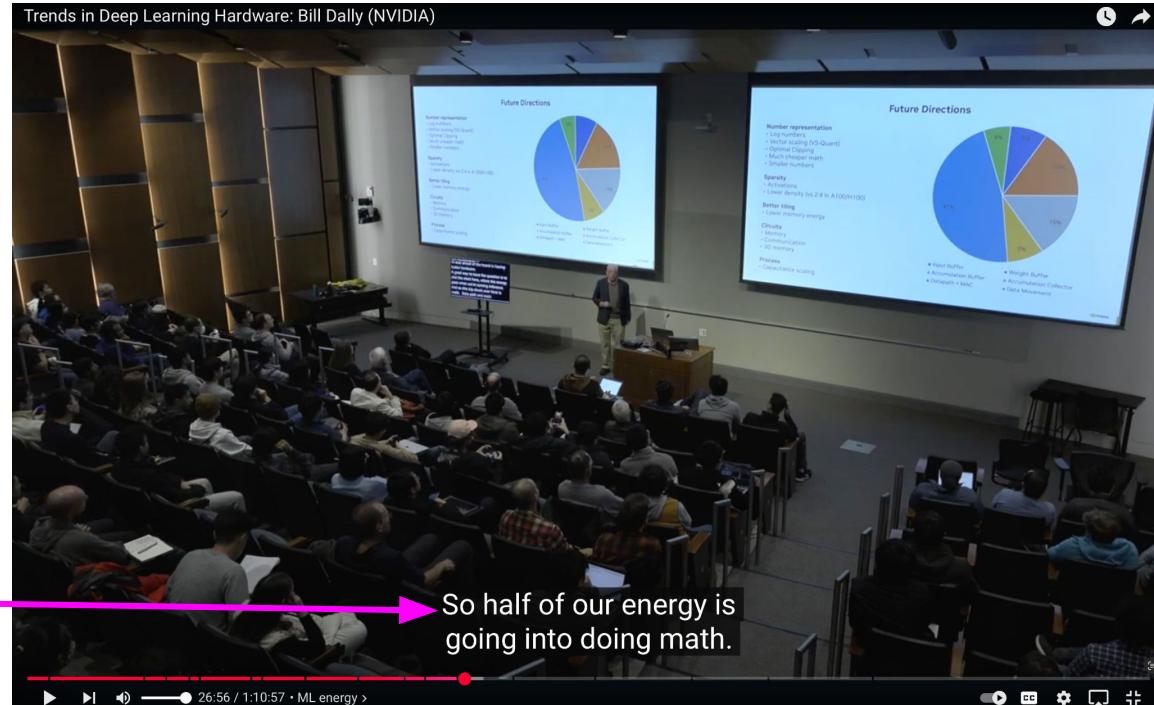
# Energy Drives Decisions

Half the energy goes into doing math (for inference)

# GPU Array Programming Complexities Stem from Measures to Save Energy!

- Why?
  - [Talk-1](#)
    - at UW
  - [Talk-2](#)
    - at HotChips'23
- by Dr. Bill Dally, SVP
  - Chief Scientist @ NVIDIA

Must move fewer bits.  
This causes  
Accuracy and Dynamic Range  
to be reduced , leading to bugs



## Future Directions

### Number representation

- Log numbers
- Vector scaling (VS-Quant)
- Optimal Clipping
- Much cheaper math
- Smaller numbers

### Sparsity

- Activations
- Lower density (vs 2:4 in A100/H100)

### Better tiling

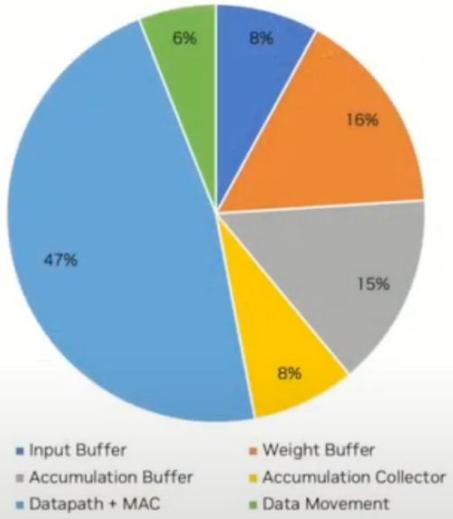
- Lower memory energy

### Circuits

- Memory
- Communication
- 3D memory

### Process

- Capacitance scaling



when we're doing inference.

Play (k)

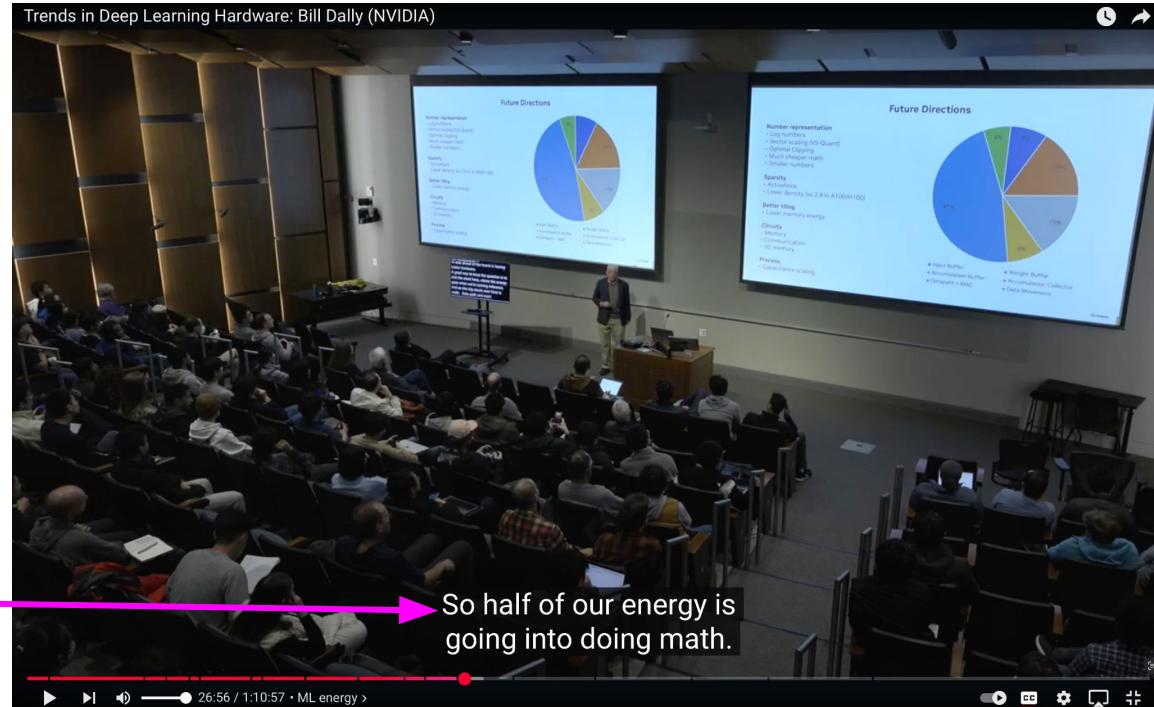
▶ ▶ ⏪ 26:46 / 1:10:57 • ML energy >

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# GPU Array Programming Complexities Stem from Measures to Save Energy!

- Why?
  - [Talk-1](#)
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Must move fewer bits.  
Unfortunately, the types of hardware created by AI companies are ill-specified.

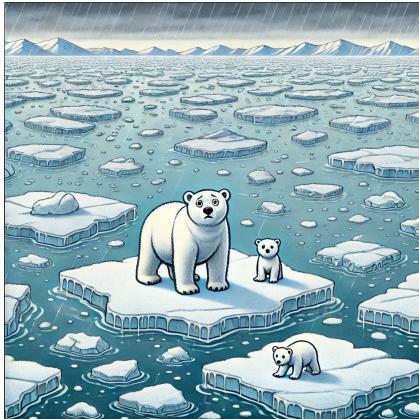


# Number Systems Help Trade Energy and Bugs

The plethora of choices of formats is evidence

# Background: Dynamic Range and Error for various number formats

No.	Fmt	Prec	Exp	Sm. norm.	Lrgst norm.	Unit rnd	u ULP @ e_max	2's comp. bits
1	FP16	11	5	6.10e-5	6.55e4	4.88e-4	2^5	30
2	BF16	8	8	1.18e-38	3.39e38	3.91e-3	2^120	254
3	TF32	11	8	1.18e-38	3.40e38	4.88e-4	2^117	254
4	FP32	24	8	1.18e-38	3.40e38	5.96e-8	2^104	254
5	FP64	53	11	2.23e-308	1.80e308	1.11e-16	2^971	2046
256 values	→ 6	E4M3	4	1.56e-2	2.48e2	6.25e-2	2^4	14 (fwd, for activations.)
	→ 7	E5M2	3	6.10e-5	6.14e4	1.25e-1	2^13	30 (bkwd, for grad.)



The future depends on moving fewer bits while managing the errors caused by this variety of number systems.



We discuss 3 types of bugs / needs



# Floating-Point Numbers : A compromise, with many good properties, that can span a large range with a small number of bits

No.	Fmt	Prec	Exp	Sm. norm.	Lrgst norm.	Unit rnd u	ULP @ e_max	2-comp bits
1	FP16	11	5	6.10e-5	6.55e4	4.88e-4	2^5	30
2	BF16	8	8	1.18e-38	3.39e38	3.91e-3	2^120	254
3	TF32	11	8	1.18e-38	3.40e38	4.88e-4	2^117	254
4	FP32	24	8	1.18e-38	3.40e38	5.96e-8	2^104	254
5	FP64	53	11	2.23e-308	1.80e308	1.11e-16	2^971	2046

- Unit Roundoff ("u") : One unit of rounding (assuming RTN) : rnd to nearest ties to even
- $u = \text{half of the distance from } 1.0 \text{ to the next representable number}$
- Absolute errors are discussed below. Its value is  $\text{NumberRepresented} * u$

- FP32
  - Error measuring earth-to-Moon distance of 384,400 km : 22.9 meters
  - Error measuring height of Human (172 cm) : 0.000103 mm

- BF16
  - Moon: 1500 km
  - Human: 6.7 mm

- FP16
  - Moon: Can't represent - INF
  - Human: 0.84 mm

# Gist of talk

- 
- **What can we do for the PL Community (covering ML and HPC) so that**
  - (contribution 1) : They can detect show-stopper bugs early ?
  - (contribution 2) : Explicate opaque hardware ?
  - (contribution 3) : Develop formal specs ... even synthesize correct code?

# Problem Addressed: GPU variety grows w/o Tools Support

- **Growth in GPU variety, leading to:**
  - Growth in **two primary aspects** of GPU programming that cause bugs:
    - Parallelism varieties (not emphasized in this talk)
    - Number systems (emphasized here)
- **Debugging tools haven't kept up**
  - Inability to reason about the exhibited behaviors
- **Specs don't exist**
  - Must be discovered through testing
- **Having many specs is also undesirable**
  - Which specs can support a given application?

# Three Types of "Bugs"

- (1) **FP exceptions**
- (2) **III-specified HW**
- (3) **Lack of formal specs + Managing their surfeit**

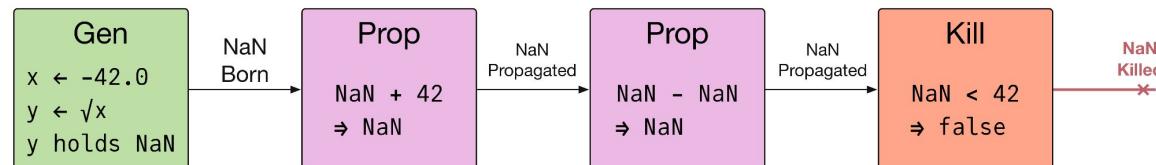
# Why these three types of "bugs"

- Measures to save energy has resulted in
  - Executions that often generate **FP Exceptions** which arrest overall progress
  - (Tensor Core...) Hardware that is **Weird** as well as **Sparingly Specified**
  - (Overall ISA has...) **No Formal Descriptions**
- ML can survive this level of "mystery" ... (or, so it seems – do we have a choice?)
  - Libraries provide API to hardware
- **Unfortunately**
  - **ML's success has driven out standard and well-specified hardware**
- This leads to three challenges that we discuss in this presentation

# FP Exceptions

- FP32: ( $1.9 \times 10^{19}$ )<sup>2</sup> → INF ... (in E4M3,  $16^2 = \text{INF}$ )  
Squaring is widely used (e.g., dot-products)
- INF and NaN are most serious; also they inter-convert INF / INF = NaN
- **#define MAX(x,y) ( (x >= y) ? x : y ) is incorrect**  
hint : consider x == NaN or y == NaN

Exception flow, in general



# Classical (CPU-era) Solution to Exceptions

- Have the hardware generate traps
  - When trap-handling is enabled, handle it in software
- **NVIDIA GPUs do not generate traps!**
- This approach is incongruous with GPU computing
  - Imagine a million threads generating traps!
    - AMD GPUs do "something in-between"

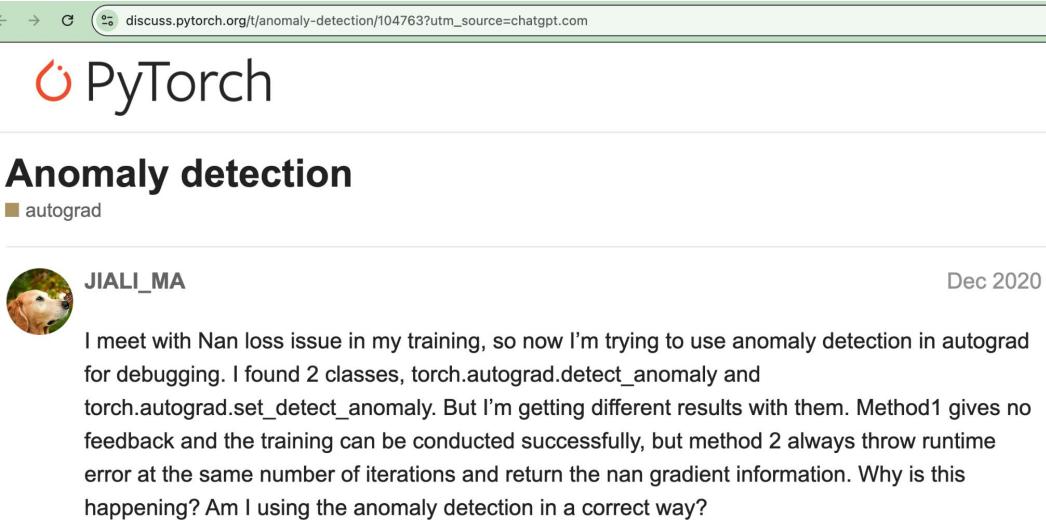
In ML, Frameworks such as PyTorch Silently "Fix" Exceptions, but this can be Slow / Imperfect (believable ChatGPT summary below)

## 2 What PyTorch does automatically

Layer	What happens internally	Key API / behaviour
Forward kernels	Produces INF/NaN normally (IEEE "masked exceptions")—no trap.	<code>torch.isfinite</code> , <code>tensor.isnan()</code> etc. for explicit checks.
autograd anomaly detection	Wrap graph execution; throws when the <i>first</i> backward op creates a non-finite grad and prints the forward traceback.	<code>torch.autograd.detect_anomaly()</code> or <code>set_detect_anomaly(check_nan=True)</code>
Mixed-precision scaler	<code>GradScaler</code> un-scales grads, then runs a fused <code>isfinite</code> reduction <b>on-GPU</b> . If any grad is non-finite the <i>optimizer step is skipped</i> and the loss-scale is halved.	<code>scaler.step(optim) /</code> <code>scaler.update()</code> ; see AMP docs
High-level trainers	Lightning, DeepSpeed, Accelerate all keep a "gradient overflow" flag; a skipped step just logs <b>OVERFLOW</b> and carries on.	DeepSpeed fp16 messages "Overflow detected. Skipping step." <a href="#">GitHub</a>
Linalg ops	PyTorch's <code>torch.linalg</code> wrappers pass inputs to cuSOLVER/CPU LAPACK <b>without extra guards</b> ; docs explicitly warn to pre-check with <code>torch.isfinite</code> .	<a href="#">PyTorch</a>

# Framework-Recommended Solutions Don't Work Always

- Experts have told me how they deal with show-stopper exceptions
  - Try a bag of tricks (similar to those present in PyTorch - listed shortly)
- Thousands of reports that go like this



The screenshot shows a GitHub issue page from the PyTorch repository. The title of the issue is "Anomaly detection". The user "JIALI\_MA" has posted a comment. The comment text is as follows:

I meet with Nan loss issue in my training, so now I'm trying to use anomaly detection in autograd for debugging. I found 2 classes, `torch.autograd.detect_anomaly` and `torch.autograd.set_detect_anomaly`. But I'm getting different results with them. Method1 gives no feedback and the training can be conducted successfully, but method 2 always throw runtime error at the same number of iterations and return the nan gradient information. Why is this happening? Am I using the anomaly detection in a correct way?

In ML, Frameworks such as PyTorch Silently "Fix" Exceptions, but this can be Slow / Imperfect

## 3 Typical user-level counter-measures in PyTorch

Category	Common tricks
Clamp before trouble	<code>logits = torch.clamp(logits, -15, 15)</code> before soft-max
Gradient clipping	<code>torch.nn.utils.clip_grad_norm_(model.parameters(), max_norm)</code>
Loss-scale tuning	Lower <code>init_scale</code> in <code>GradScaler(init_scale=2**14)</code>
Replace non-finites	<code>tensor = torch.nan_to_num(tensor, nan=0.0, posinf=1e4, neginf=-1e4)</code>
Batch filtering	Drop or re-initialise batches whose loss isn't finite
Debug builds	Keep <code>detect_anomaly()</code> on for the first few epochs only

# Current Exception Handling in PyTorch / ML : Sometimes an Overkill

- Key debugging tools in PyTorch: `isnan` and `isfinite`

```
>>> x
tensor([0., 1., nan, inf])
>>> x.isnan()
tensor([False, False, True, False])
>>> x.isfinite()
tensor([ True, True, False, False])
```

- Typical safeguards

- `torch.nn.utils.clip_grad_norm_`
- Add a small number to potentially-zero denominators.
  - These are built into many modules, e.g. [Adam](#) (see the “+  $\epsilon$ ”)

- Current Approach Taken in ML

- Fix NaN / INF exceptions and continue, saving checkpoints
- **If we can't continue, restart from a "good checkpoint"**

- While we can put exception detection everywhere, it will make it VERY slow
  - **3x slowdown** reported when using `torch.autograd.detect_anomaly(check_nan=True)`
- **Need a solid set of concepts to do formal PL work !!**

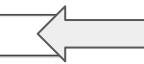
# Current Exception Handling in HPC : Very Situation-Specific

- No real widely used approach
  - Table of results from our paper GPU-FPX below
- Need Binary-Instrumentation Tools (GPU-FPX) to Peek into Codes
  - Necessary (closed-source libraries) + Accurate (compiler opt. effects)

Table 7. Overview of Exception Diagnoses and Repairs using *Analyzer* for Programs with Severe Exceptions

Program	Source available?	Diagnose?	Exceptions Matter?	Fixed?	How Fixed?
GRAMSCHM	yes	yes	yes	yes	Remove 0 from input
LU	yes	yes	yes	yes	Remove 0 from input
myocyte	yes	no	N.A.	N.A.	N.A.
S3D	yes	yes	no	N.A.	N.A.
Interval	yes	yes	no	N.A.	N.A.
Laghos	yes	no	N.A.	N.A.	N.A.
Sw4lite	yes	no	N.A.	N.A.	N.A.
HPCG	no	no	N.A.	N.A.	N.A.
CuMF-Movielens	yes	yes	yes	yes	Enforce variable consistency
cuML-HousePrice	partial	yes	yes	partial	N.A.
CUDA GMRES	partial	yes	yes	partial	Diagonal boosting
SRU-Example	yes	yes	yes	yes	Change input generator

Expert-helped  
Black Magic !!



# FP Exceptions

How to define their "proper handling"?

We've found only one clear definition ... by Demmel

# What is Consistent / Sound Exception Handling? How close are we to it ?

[Submitted on 19 Jul 2022]

## Proposed Consistent Exception Handling for the BLAS and LAPACK

James Demmel, Jack Dongarra, Mark Gates, Greg Henry, Julien Langou, Xiaoye Li, Piotr Luszczek, Wesley Pereira, Jason Riedy, Cindy Rubio-González

Numerical exceptions, which may be caused by overflow, operations like division by 0 or  $\sqrt{-1}$ , or convergence failures, are unavoidable in many cases, in particular when software is used on unforeseen and difficult inputs. As more aspects of society become automated, e.g., self-driving cars, health monitors, and cyber-physical systems more generally, it is becoming increasingly important to design software that is resilient to exceptions, and that responds to them in a consistent way. Consistency is needed to allow users to build higher-level software that is also resilient and consistent (and so on recursively). In this paper we explore the design space of consistent exception handling for the widely used BLAS and LAPACK linear algebra libraries, pointing out a variety of instances of inconsistent exception handling in the current versions, and propose a new design that balances consistency, complexity, ease of use, and performance. Some compromises are needed, because there are preexisting inconsistencies that are outside our control, including in or between existing vendor BLAS implementations, different programming languages, and even compilers for the same programming language. And user requests from our surveys are quite diverse. We also propose our design as a possible model for other numerical software, and welcome comments on our design choices.

cases, in particular when software is used on unforeseen and difficult inputs. As more aspects of society become automated, e.g., self-driving cars, health monitors, and cyber-physical systems more generally, it is becoming increasingly important to design software that is resilient to exceptions,

Sometimes it takes an event like the crash of the Ariane 5 rocket [1], a naval propulsion failure [2], or a crash in a robotic car race [3] to make people aware of the importance of handling exceptions correctly in numerical software [4, 5]! As applications like self-driving cars, health monitors, and cyber-physical systems more generally be-

## EXCvATE: Spoofing Exceptions and Solving Constraints to Test Exception Handling in Numerical Libraries

Jackson Vanover\*, James Demmel\*, Xiaoye Sherry Li†, Cindy Rubio-González\*

\*University of California, Davis

†University of California, Berkeley

‡Lawrence Berkeley National Laboratory

ARITH

2025

Best Paper

When an Overflow, Divide-by-Zero, or Invalid exception occurs, a sound exception-handling policy notifies users by either...

1. The presence of EVs in the output
2. Some library-specific mechanism triggered by checking for their presence at some point during the execution.

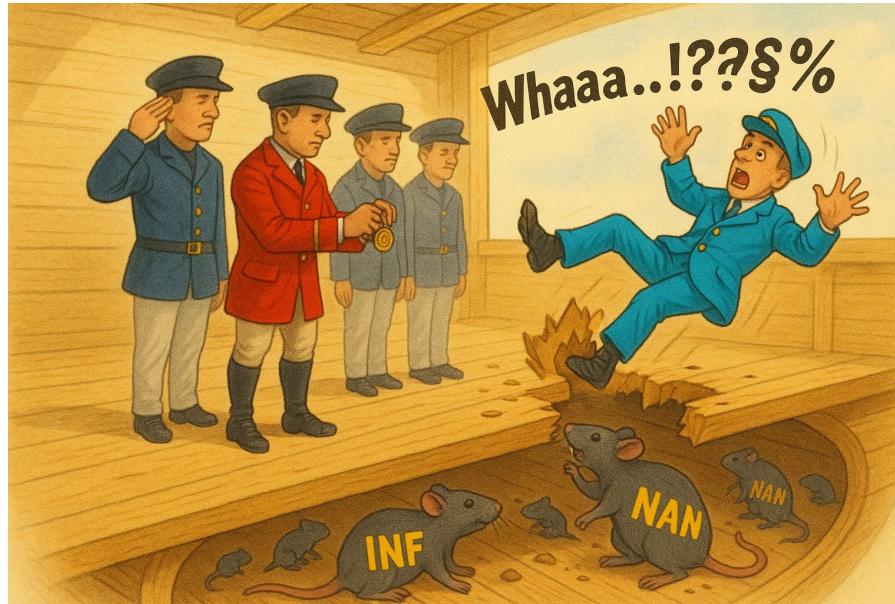
This is the policy adopted by the reference LAPACK/BLAS implementations [1].

> How can we test this?

[1] J. Demmel, et al. "Proposed Consistent Exception Handling for the BLAS and LAPACK".

# We are not even close to consistent exception handling!

- The SRU Example
- The example that needed "diagonal-boosting"
- Two data-compressors illustrated in our paper
- Even the "Baby GPT" of Andrej Karpathy after I ported it to GPU  
(image by ChatGPT with prompts [HERE](#))



**GPU-FPX** (for SIMT-only)

and **nixnan** (for SIMT and Tensor Cores) **are easy to use**  
**and tell you a lot !!** and you can get them !!  
nixnan is being released as part of this workshop!

(... could be slow, but...)



# Ease of use: tracing Karpathy's Baby GPT learning a DFA's n-gram language...

## "Classical" run (w/o our tools)

```
time python KarpathyNGramDFA1.py
...
NOW LOSS DECREASES
...
number of parameters: 12656
0 0.6365983486175537
1 0.601229727268219
2 0.5856719613075256
3 0.5780848264694214
...
46 0.3900260329246521
47 0.3890194892883301
48 0.3880999982357025
49 0.3872622549533844
...
real    0m2.409s
user    0m2.423s
sys 0m1.645s
```

## Instrumented run (with our tools)

```
time LD_PRELOAD=./analyzer.so python KarpathyNGramDFA1.py
```

```
=====
time LD_PRELOAD=./analyzer.so python KarpathyNGramDFA1.py
...
#GPU-FPX: Instrument all kernels.
...
Running #GPU-FPX: kernel [void at::native::(anonymous namespace)::vectorized_layer_norm_kernel] ...
Running #GPU-FPX: kernel [void gemmSN_TN_kernel]
...
Running #GPU-FPX: kernel [void (anonymous namespace)::softmax_warp_forward] ...
#GPU-FPX-ANA SHARED REGISTER: Before executing the instruction @ /unknown_path in [void (anonymous namespace)::softmax_warp_forw:0 Instruction: FSEL R11, R11, R2, !P0 ; We have 3 registers in total. Register 0 is INF. Register 1 is INF. Register 2 is INF.
#GPU-FPX-ANA SHARED REGISTER: After executing the instruction @ /unknown_path in [void (anonymous namespace)::softmax_warp_forw:0 Instruction: FSEL R11, R11, R2, !P0 ; We have 3 registers in total. Register 0 is INF. Register 1 is INF. Register 2 is INF.

number of parameters: 12656
...
Running #GPU-FPX: kernel [void at::native::(anonymous namespace)::indexSelectLargeIndex] ...
Running #GPU-FPX: kernel [ampere_sgemm_32x128_tn] ...
Running #GPU-FPX: kernel [ampere_sgemm_128x32_tn] ...
Running #GPU-FPX: kernel [ampere_sgemm_32x32_sliced1x4_tn] ...
#GPU-FPX-ANA SHARED REGISTER: Before executing the instruction @ /unknown_path in [void (anonymous namespace)::softmax_warp_forw:0 Instruction: FSEL R5, R5, R10, !P0 ; We have 3 registers in total. Register 0 is INF. Register 1 is INF. Register 2 is INF.

...
NOW LOSS DECREASES
...
0 0.6365983486175537
1 0.601229727268219
2 0.5856719613075256
3 0.5780848264694214
...
46 0.3900260329246521
47 0.3890194892883301
48 0.3880999982357025
49 0.3872622549533844
...
#GPU-FPX-ANA SHARED REGISTER: Before executing the instruction @ /unknown_path in [void at::native::reduce_kernel]:0 Instruction EL R6, R6, R13, P0 ; We have 3 registers in total. Register 0 is INF. Register 1 is INF. Register 2 is VAL.
...
#GPU-FPX-ANA SHARED REGISTER: Before executing the instruction @ /unknown_path in [void gemmSN_TN_kernel]:0 Instruction: FSEL R1:12, R17, !P0 ; We have 3 registers in total. Register 0 is VAL. Register 1 is NaN. Register 2 is VAL.
...
real    4m59.125s
user    9m38.729s
sys 0m3.257s
=====
```

# We are not even close to consistent exception handling!

LD\_PRELOAD=./analyzer.so python [KarpathyNGramDFA2.py](#)

#GPU-FPX-ANA SHARED REGISTER: Before executing the instruction @ /unknown\_path in [void (anonymous namespace)::softmax\_warp\_forward]:0 Instruction: FFMA R9, R0, 1.4426950216293334961, -R9 ; We have 3 registers in total. Register 0 is VAL. Register 1 is INF. Register 2 is VAL.

#GPU-FPX-ANA SHARED REGISTER: After executing the instruction @ /unknown\_path in [void (anonymous namespace)::softmax\_warp\_forward]:0 Instruction: FFMA R9, R0, 1.4426950216293334961, -R9 ; We have 3 registers in total. Register 0 is NaN. Register 1 is NaN. Register 2 is NaN.

- We uploaded the traces into ChatGPT
- See how ChatGPT "explains" the situation here, plus also recommends code fixes
  - The fixes did not eliminate the exceptions (promising direction we feel)

# Results obtained when I casually uploaded the GPU-FPX traces to ChatGPT (Seems reasonable. Even if not true, suggests a future direction...)

## What the GPU-FPX trace is telling us

Kernel (FPX label)	Where NaN/Inf shows up	Does it disappear before a store?	Likely root-cause	Severity
softmax_warp_forward	Large-magnitude logits start as <code>±Inf</code> ; <code>FADD</code> turns <code>Inf - Inf</code> into <code>NaN</code> . Many of these NaNs are later fed to exponentials ( <code>MUFU.EX2</code> ) and multiplies	Some NaNs are clamped away by <code>FFMA.SAT</code> , but others survive several instructions and keep popping back up	Logits are not being shifted by the row-max (the classic "log-sum-exp trick") or they already contain Inf from an earlier layer	Needs a fix – risk of NaNs reaching the probability vector or its gradient
GEMM micro-kernels <code>(gemmSN_TN_kernel</code> , <code>ampere_sgemm_*</code> )	You see <code>FSEL ... Register 1 is Nan</code> immediately followed by another <code>FSEL</code> whose destination register is <code>VAL</code> 	Yes – the predicate keeps the good operand, so the NaN never leaves a register	One input tile contained NaN/Inf, but the predicate rejected it	Innocuous so long as the selected value isn't NaN
<code>reduce_kernel</code> (used by <code>torch.max</code> , <code>torch.mean</code> , etc.)	Alternating <code>INF ↔ VAL</code> operands in a chain of <code>FSEL</code> instructions 	Often <code>INF</code> wins the comparison and gets written forward	Up-stream overflow (e.g. <code>exp()</code> on large numbers)	Heed – an <code>Inf</code> in a reduction will survive to host memory unless filtered
Misc. elementwise / layer-norm kernels	Short bursts of NaNs immediately neutralised by <code>FFMA.SAT</code>	Yes	These are saturating clamps or ReLU-like masks	Benign
<code>softmax_warp_backward</code> , <code>embedding_backward</code> , etc.	Only mirror the NaNs created in the forward pass; no new sources	—	Propagation of earlier problems	Depends on fixing the forward pass

# Problem description

- Link: <https://github.com/asappresearch/sru/issues/193>



**hoagy-davis-digges** commented on Nov 2, 2021 · edited

...

I have run the example code in the readme on both 2.6.0 and 3.0.0-dev and both have nan values in both the output and state objects using pytorch 1.9, I've tried this on my computer using a Titan X and also with a fresh install on a cloud T4, this doesn't seem to relate to the other nan issue raised here <https://github.com/asappresearch/sru/issues/185> because this problem appears immediately.



# Problem description

- Link: <https://github.com/asappresearch/sru/issues/193>

taolei87 commented on Nov 5, 2021

Contributor ...

hi @hoagy-davis-digges , did you mean you tried the following example and got NaN?

```
import torch
from sru import SRU, SRUCell

# input has length 20, batch size 32 and dimension 128
x = torch.FloatTensor(20, 32, 128).cuda()

input_size, hidden_size = 128, 128

rnn = SRU(input_size, hidden_size,
           num_layers = 2,           # number of stacking RNN layers
           dropout = 0.0,            # dropout applied between RNN layers
           bidirectional = False,    # bidirectional RNN
           layer_norm = False,       # apply layer normalization on the output of each layer
           highway_bias = -2,        # initial bias of highway gate (<= 0)
           )
rnn.cuda()

output_states, c_states = rnn(x)      # forward pass
```



# Use Detector

```
Running #GPU-FPX: kernel [void at::native::vectorized_elementwise_kernel] ...
Running #GPU-FPX: kernel [ampere_sgemm_32x128_nn] ...
#GPU-FPX LOC-EXCEP INFO: in kernel [ampere_sgemm_32x128_nn], NaN found @ /unknown_path in [ampere_sgemm_32x128_nn]:0 [FP32]
#GPU-FPX LOC-EXCEP INFO: Warning: in kernel [ampere_sgemm_32x128_nn], very small quantity (SUB) found
@ /unknown_path in [ampere_sgemm_32x128_nn]:0 [FP32]
Running #GPU-FPX: kernel [void (anonymous namespace)::sru_cuda_forward_kernel_simple] ...
#GPU-FPX LOC-EXCEP INFO: in kernel [void (anonymous namespace)::sru_cuda_forward_kernel_simple], NaN
found @ /unknown_path in [void (anonymous namespace)::sru_cuda_forward_kernel_simple]:0 [FP32]
#GPU-FPX LOC-EXCEP INFO: in kernel [void (anonymous namespace)::sru_cuda_forward_kernel_simple], INF
found @ /unknown_path in [void (anonymous namespace)::sru_cuda_forward_kernel_simple]:0 [FP32]
#GPU-FPX LOC-EXCEP INFO: in kernel [void (anonymous namespace)::sru_cuda_forward_kernel_simple], DIV0
found @ /unknown_path in [void (anonymous namespace)::sru_cuda_forward_kernel_simple]:0 [FP32]
#GPU-FPX LOC-EXCEP INFO: Warning: in kernel [void (anonymous namespace)::sru_cuda_forward_kernel_simple],
very small quantity (SUB) found @ /unknown_path in [void (anonymous namespace)::sru_cuda_forward_kernel_simple]:0 [FP32]
Running #GPU-FPX: kernel [void at::native::(anonymous namespace)::CatArrayBatchedCopy] ...
#GPU-FPX LOC-EXCEP INFO: in kernel [void at::native::vectorized_elementwise_kernel], NaN found @ /unk
nown_path in [void at::native::vectorized_elementwise_kernel]:0 [FP32]
#GPU-FPX LOC-EXCEP INFO: Warning: in kernel [void at::native::vectorized_elementwise_kernel], very sm
all quantity (SUB) found @ /unknown_path in [void at::native::vectorized_elementwise_kernel]:0 [FP32]
Running #GPU-FPX: kernel [void at_cuda_detail::cub::DeviceReduceSingleTileKernel] ...
Running #GPU-FPX: kernel [void at_cuda_detail::cub::DeviceCompactInitKernel] ...
Running #GPU-FPX: kernel [void at_cuda_detail::cub::DeviceSelectSweepKernel] ...
Running #GPU-FPX: kernel [void at::native::index_elementwise_kernel] ...
Running #GPU-FPX: kernel [void at::native::unrolled_elementwise_kernel] ...
Running #GPU-FPX: kernel [void at::native::reduce_kernel] ...
```

Closed-source library

# Use Detector

```
Running #GPU-FPX: kernel [void at::native::vectorized_elementwise_kernel] ...
Running #GPU-FPX: kernel [ampere_sgemm_32x128_nn] ...
#GPU-FPX LOC-EXCEP INFO: in kernel [ampere_sgemm_32x128_nn], NaN found @ /unknown_path in [ampere_sgemm_32x128_nn]:0 [FP32]
#GPU-FPX LOC-EXCEP INFO: Warning: in kernel [ampere_sgemm_32x128_nn], very small quantity (SUB) found
@ /unknown_path in [ampere_sgemm_32x128_nn]:0 [FP32]
Running #GPU-FPX: kernel [void (anonymous namespace)::sru_cuda_forward_kernel_simple] ...
#GPU-FPX LOC-EXCEP INFO: in kernel [void (anonymous namespace)::sru_cuda_forward_kernel_simple], NaN
found @ /unknown_path in [void (anonymous namespace)::sru_cuda_forward_kernel_simple]:0 [FP32]
#GPU-FPX LOC-EXCEP INFO: in kernel [void (anonymous namespace)::sru_cuda_forward_kernel_simple], INF
found @ /unknown_path in [void (anonymous namespace)::sru_cuda_forward_kernel_simple]:0 [FP32]
#GPU-FPX LOC-EXCEP INFO: in kernel [void (anonymous namespace)::sru_cuda_forward_kernel_simple], DIV0
found @ /unknown_path in [void (anonymous namespace)::sru_cuda_forward_kernel_simple]:0 [FP32]
#GPU-FPX LOC-EXCEP INFO: Warning: in kernel [void (anonymous namespace)::sru_cuda_forward_kernel_simple],
very small quantity (SUB) found @ /unknown_path in [void (anonymous namespace)::sru_cuda_forward_kernel_simple]:0 [FP32]
Running #GPU-FPX: kernel [void at::native::(anonymous namespace)::CatArrayBatchedCopy] ...
#GPU-FPX LOC-EXCEP INFO: in kernel [void at::native::vectorized_elementwise_kernel], NaN found @ /unk
nown_path in [void at::native::vectorized_elementwise_kernel]:0 [FP32]
#GPU-FPX LOC-EXCEP INFO: Warning: in kernel [void at::native::vectorized_elementwise_kernel], very sm
all quantity (SUB) found @ /unknown_path in [void at::native::vectorized_elementwise_kernel]:0 [FP32]
Running #GPU-FPX: kernel [void at_cuda_detail::cub::DeviceReduceSingleTileKernel] ...
Running #GPU-FPX: kernel [void at_cuda_detail::cub::DeviceCompactInitKernel] ...
Running #GPU-FPX: kernel [void at_cuda_detail::cub::DeviceSelectSweepKernel] ...
Running #GPU-FPX: kernel [void at::native::index_elementwise_kernel] ...
Running #GPU-FPX: kernel [void at::native::unrolled_elementwise_kernel] ...
Running #GPU-FPX: kernel [void at::native::reduce_kernel] ...
```

# Use Detector

Closed-source library

```
Running #GPU-FPX: kernel [void at::native::vectorized_elementwise_kernel] ...
Running #GPU-FPX: kernel [ampere_sgemm_32x128_nn] ...
#GPU-FPX LOC-EXCEP INFO: in kernel [ampere_sgemm_32x128_nn], NaN found @ /unknown_path in [ampere_sgemm_32x128_nn]:0 [FP32]
#GPU-FPX LOC-EXCEP INFO: Warning: in kernel [ampere_sgemm_32x128_nn], very small quantity (SUB) found
@ /unknown_path in [ampere_sgemm_32x128_nn]:0 [FP32]
Running #GPU-FPX: kernel [void (anonymous namespace)::sru_cuda_forward_kernel_simple] ...
#GPU-FPX LOC-EXCEP INFO: in kernel [void (anonymous namespace)::sru_cuda_forward_kernel_simple], NaN
found @ /unknown_path in [void (anonymous namespace)::sru_cuda_forward_kernel_simple]:0 [FP32]
#GPU-FPX LOC-EXCEP INFO: in kernel [void (anonymous namespace)::sru_cuda_forward_kernel_simple], INF
found @ /unknown_path in [void (anonymous namespace)::sru_cuda_forward_kernel_simple]:0 [FP32]
#GPU-FPX LOC-EXCEP INFO: in kernel [void (anonymous namespace)::sru_cuda_forward_kernel_simple], DIV0
found @ /unknown_path in [void (anonymous namespace)::sru_cuda_forward_kernel_simple]:0 [FP32]
#GPU-FPX LOC-EXCEP INFO: Warning: in kernel [void (anonymous namespace)::sru_cuda_forward_kernel_simple],
very small quantity (SUB) found @ /unknown_path in [void (anonymous namespace)::sru_cuda_forward_kernel_simple]:0 [FP32]
Running #GPU-FPX: kernel [void at::native::(anonymous namespace)::CatArrayBatchedCopy] ...
#GPU-FPX LOC-EXCEP INFO: in kernel [void at::native::vectorized_elementwise_kernel], NaN found @ /unk
nown_path in [void at::native::vectorized_elementwise_kernel]:0 [FP32]
#GPU-FPX LOC-EXCEP INFO: Warning: in kernel [void at::native::vectorized_elementwise_kernel], very sm
all quantity (SUB) found @ /unknown_path in [void at::native::vectorized_elementwise_kernel]:0 [FP32]
Running #GPU-FPX: kernel [void at_cuda_detail::cub::DeviceReduceSingleTileKernel] ...
Running #GPU-FPX: kernel [void at_cuda_detail::cub::DeviceCompactInitKernel] ...
Running #GPU-FPX: kernel [void at_cuda_detail::cub::DeviceSelectSweepKernel] ...
Running #GPU-FPX: kernel [void at::native::index_elementwise_kernel] ...
Running #GPU-FPX: kernel [void at::native::unrolled_elementwise_kernel] ...
Running #GPU-FPX: kernel [void at::native::reduce_kernel] ...
```

Not clear how to fix it

# Use Analyzer

# Speedup by enabling necessary kernels

```
Running #GPU-FPX: kernel [void deactivate::vectorized_elementwise_kernel] ...
Running #GPU-FPX: kernel [ampere_sgemm_32x128_nn] ...
#GPU-FPX LOC-EXCEP INFO: in kernel [ampere_sgemm_32x128_nn], NaN found @ /unknown_path in [ampere_sgmm_32x128_nn]:0 [FP32]
#GPU-FPX LOC-EXCEP INFO: Warning: in kernel [ampere_sgemm_32x128_nn], very small quantity (SUB) found
@ /unknown_path in [ampere_sgemm_32x128_nn]:0 [FP32]
```

First and most exceptions happened in this kernel, so  
we can limit our instrumentation in this kernel

```
simple] ...
rd_kernel_simple], NaN
simple]:0 [FP32]
rd_kernel_simple], INF
round @ /unknown_path in [void (anonymous namespace)::sru_cuaa_forwara_kernel_simple]:0 [FP32]
#GPU-FPX LOC-EXCEP INFO: in kernel [void (anonymous namespace)::sru_cuda_forward_kernel_simple], DIV0
found @ /unknown_path in [void (anonymous namespace)::sru_cuda_forward_kernel_simple]:0 [FP32]
#GPU-FPX LOC-EXCEP INFO: Warning: in kernel [void (anonymous namespace)::sru_cuda_forward_kernel_simple], very small quantity (SUB) found @ /unknown_path in [void (anonymous namespace)::sru_cuda_forward_kernel_simple]:0 [FP32]
Running #GPU-FPX: kernel [void at::native::(anonymous namespace)::CatArrayBatchedCopy] ...
#GPU-FPX LOC-EXCEP INFO: in kernel [void at::native::vectorized_elementwise_kernel], NaN found @ /unk
nown_path in [void at::native::vectorized_elementwise_kernel]:0 [FP32]
#GPU-FPX LOC-EXCEP INFO: Warning: in kernel [void at::native::vectorized_elementwise_kernel], very sm
all quantity (SUB) found @ /unknown_path in [void at::native::vectorized_elementwise_kernel]:0 [FP32]
Running #GPU-FPX: kernel [void at_cuda_detail::cub::DeviceReduceSingleTileKernel] ...
Running #GPU-FPX: kernel [void at_cuda_detail::cub::DeviceCompactInitKernel] ...
Running #GPU-FPX: kernel [void at_cuda_detail::cub::DeviceSelectSweepKernel] ...
Running #GPU-FPX: kernel [void at::native::index_elementwise_kernel] ...
Running #GPU-FPX: kernel [void at::native::unrolled_elementwise_kernel] ...
Running #GPU-FPX: kernel [void at::native::reduce_kernel] ...
```

# Analysis

```
Running #gpu-fpx. Kernel [ampere_sgemm_32x128_nn] ...
#GPU-FPX-ANA SHARED REGISTER Before executing the instruction @ /unknown_path in [ampere_sgemm_32x1
28_nn]:0 Instruction: FFMA R1, R32.reuse, R40.reuse, R1 ; We have 4 registers in total. Register 0 is
VAL. Register 1 is VAL. Register 2 is NaN. Register 3 is VAL.

#GPU-FPX-ANA SHARED REGISTER Before executing the instruction @ /unknown_path in [ampere_sgemm_32x1
28_nn]:0 Instruction: FFMA R0, R32, R41.reuse, R0 ; We have 4 registers in total. Register 0 is VAL.
Register 1 is VAL. Register 2 is NaN. Register 3 is VAL.

#GPU-FPX-ANA SHARED REGISTER: After executing the instruction @ /unknown_path in [ampere_sgemm_32x12
8_nn]:0 Instruction: FFMA R1, R32.reuse, R40.reuse, R1 ; We have 4 registers in total. Register 0 is
NaN. Register 1 is VAL. Register 2 is NaN. Register 3 is NaN.

#GPU-FPX-ANA SHARED REGISTER: After executing the instruction @ /unknown_path in [ampere_sgemm_32x12
8_nn]:0 Instruction: FFMA R0, R32, R41.reuse, R0 ; We have 4 registers in total. Register 0 is NaN. R
egister 1 is VAL. Register 2 is NaN. Register 3 is NaN.
```

# Analysis

```
Running #nvprof kernel [ampere_sgemm_32x128_nn] ...
#GPU-FPX-ANA SHARED REGISTER Before executing the instruction @ /unknown_path in [ampere_sgemm_32x128_nn]:0 Instruction: FFMA R1, R32.reuse, R40.reuse, R1 VAL. Register 1 is VAL. Register 2 is NaN. Register 3 is NaN.
#GPU-FPX-ANA SHARED REGISTER Before executing the instruction @ /unknown_path in [ampere_sgemm_32x128_nn]:0 Instruction: FFMA R0, R32, R41.reuse, R0 ; We have 4 registers in total. Register 0 is VAL. Register 1 is VAL. Register 2 is NaN. Register 3 is VAL.
#GPU-FPX-ANA SHARED REGISTER: After executing the instruction @ /unknown_path in [ampere_sgemm_32x128_nn]:0 Instruction: FFMA R1, R32.reuse, R40.reuse, R1 ; We have 4 registers in total. Register 0 is NaN. Register 1 is VAL. Register 2 is NaN. Register 3 is NaN.
#GPU-FPX-ANA SHARED REGISTER: After executing the instruction @ /unknown_path in [ampere_sgemm_32x128_nn]:0 Instruction: FFMA R0, R32, R41.reuse, R0 ; We have 4 registers in total. Register 0 is NaN. Register 1 is VAL. Register 2 is NaN. Register 3 is NaN.
```

**Nan seems already exists within the initial data!**

# Analysis

This creates a tensor with uninitialized data on GPU memory.

```
import torch
from sru import SRU, SRUCell

# input has length 20, batch size 32 and dimension 128
x = torch.FloatTensor(20, 32, 128).cuda()

input_size, hidden_size = 128, 128

rnn = SRU(input_size, hidden_size,
           num_layers = 2,          # number of stacking RNN layers
           dropout = 0.0,           # dropout applied between RNN layers
           bidirectional = False,   # bidirectional RNN
           layer_norm = False,      # apply layer normalization on the output of each layer
           highway_bias = -2,       # initial bias of highway gate (<= 0)
           )
rnn.cuda()

output_states, c_states = rnn(x)      # forward pass
```



# Fix

This creates a tensor with uninitialized data on GPU memory.

```
import torch
from sru import SRU, SRUCell

# input has length 20, batch size 32 and dimension 128
x = torch.FloatTensor(20, 32, 128).cuda() → torch.randn(20,32,128).cuda()

input_size, hidden_size = 128, 128

rnn = SRU(input_size, hidden_size,
           num_layers = 2,          # number of stacking RNN layers
           dropout = 0.0,           # dropout applied between RNN layers
           bidirectional = False,   # bidirectional RNN
           layer_norm = False,      # apply layer normalization on the output of each layer
           highway_bias = -2,       # initial bias of highway gate (<= 0)
)
rnn.cuda()

output_states, c_states = rnn(x)      # forward pass
```



# How GPU-FPX can provide added help in AI/ML and also HPC

- GPU-FPX inspects a lower level than `isnan` and `isfinite` but is slower.
  - You can see exceptions in temporary registers that `isnan` and `isfinite` won't see.
- Fused kernels such as FlashAttention can hide NaN and infinity
  - this can slow down training
  - or only cause an obvious error only MANY steps later.
- Even if you see exceptions in PyTorch...
  - GPU-FPX can pinpoint their first appearance
  - Useful for ambitious custom kernels.
- While we can put exception-suppression everywhere, it will make it VERY slow
  - **3x slowdown** reported when using `torch.autograd.detect_anomaly(check_nan=True)`

# How a custom-made AI assistant might help explain exceptions

- Learn facts about code-base (Pytorch, Numerical Solver, ...) each time a user obtains a trace (and also fixes it)
  - Conversations with experts (two I shall name privately) suggests that this is how humans deal with the infamous NaN or INF
- Can obtain traces at different levels
  - Machine instructions (as with GPU-FPX)
  - LLVM (as with [FPChecker](#))

# Summary : Binary Instrumentation-based Exception Checker

- GPU-FPX Tool has been extended to create a new tool called **nixnan**
  - Released as part of this paper's artifact (see reference [2] but also the QR Code / URL below)
  - Proven success in finding exceptions in HPC Codes
  - GPU-FPX has been **bug-fixed** and **extended to record exceptions from Tensor Cores**
- **Tensor-Cores are Hugely Important for future HPC and AI/ML**
  - **nixnan** now covers many number formats,
  - and also ships amalgamated exception-reports across threads
    - A valuable community infrastructure
    - Please use it
    - All our experiments **plus paper PDF** are [HERE](#) ➔



# III-Specified Hardware

Discovering specs through tests; Grounding them via FM

# Blocked FMA

“Each Tensor Core operates on a 4x4 matrix”

$$\mathbf{D} = \left( \begin{array}{cccc} \mathbf{A}_{0,0} & \mathbf{A}_{0,1} & \mathbf{A}_{0,2} & \mathbf{A}_{0,3} \\ \mathbf{A}_{1,0} & \mathbf{A}_{1,1} & \mathbf{A}_{1,2} & \mathbf{A}_{1,3} \\ \mathbf{A}_{2,0} & \mathbf{A}_{2,1} & \mathbf{A}_{2,2} & \mathbf{A}_{2,3} \\ \mathbf{A}_{3,0} & \mathbf{A}_{3,1} & \mathbf{A}_{3,2} & \mathbf{A}_{3,3} \end{array} \right) \left( \begin{array}{cccc} \mathbf{B}_{0,0} & \mathbf{B}_{0,1} & \mathbf{B}_{0,2} & \mathbf{B}_{0,3} \\ \mathbf{B}_{1,0} & \mathbf{B}_{1,1} & \mathbf{B}_{1,2} & \mathbf{B}_{1,3} \\ \mathbf{B}_{2,0} & \mathbf{B}_{2,1} & \mathbf{B}_{2,2} & \mathbf{B}_{2,3} \\ \mathbf{B}_{3,0} & \mathbf{B}_{3,1} & \mathbf{B}_{3,2} & \mathbf{B}_{3,3} \end{array} \right) + \left( \begin{array}{cccc} \mathbf{C}_{0,0} & \mathbf{C}_{0,1} & \mathbf{C}_{0,2} & \mathbf{C}_{0,3} \\ \mathbf{C}_{1,0} & \mathbf{C}_{1,1} & \mathbf{C}_{1,2} & \mathbf{C}_{1,3} \\ \mathbf{C}_{2,0} & \mathbf{C}_{2,1} & \mathbf{C}_{2,2} & \mathbf{C}_{2,3} \\ \mathbf{C}_{3,0} & \mathbf{C}_{3,1} & \mathbf{C}_{3,2} & \mathbf{C}_{3,3} \end{array} \right)$$

FP16 or FP32                          FP16                          FP16 or FP32

- V100 whitepaper

The matrix multiplications

$$\mathbf{D} = \mathbf{A}^* \mathbf{B} + \mathbf{C}$$

Involve block-FMA steps  
(error in blocks of 4 are one  
rounding for \*/+ ...  
as in a standard FMA

"Multi-Term Adders"

**Each matrix accelerator unit operate on a small size matrix multiplication!**

# Porting danger illustrated

- $D = C - A \cdot B$
- Fill A,B,C "cleverly"
  - See paper
- Code run on five TCs
  - Ideal answer : 191.984375
  - Other ans:
    - 0.0 on A100, V100, MI250, CPU
    - 255.875 on MI100
    - 191.875 on H100
- Extreme porting danger!

generally, computations of the form  $D = C - A \cdot B$  fall under the Level-3 category of the Basic Linear Algebra Subprograms (BLAS) standard.

To investigate the numerical behavior of this pattern, we design a test case involving matrices A, B, and C, each of size  $2^{13} \times 2^{13}$  (i.e.,  $8192 \times 8192$ ). The matrices are populated with carefully chosen values to exercise edge cases in potential multi-term implementations, as detailed in [24].

Specifically, we initialize  $C_{i,j} = 2^{20}$  for all  $i, j$ ;  $A_{i,0} = 2^{10}$ ;  $A_{i,j} = 2^{-2}$  for odd  $j$ ; and  $A_{i,j} = 2^{-3}$  for even  $j$  (excluding  $j = 0$ ). For matrix B, we set  $B_{0,j} = 2^{10}$  and all other  $B_{i,j}$  entries to  $2^{-3}$ . All values are represented in FP16 precision. Under real-number semantics, this construction yields  $D_{i,j} \approx 191.99218$  for all  $i, j$

$$\begin{aligned} D_{i,j} &= -(A_{i,0} \cdot B_{0,j} + \sum_{j \% 2 = 1} A_{i,j} \cdot B_{i,j} + \sum_{\substack{j \% 2 = 0 \\ j \neq 0}} A_{i,j} \cdot B_{i,j}) + C_{i,j} \\ &= -(2^{10} \cdot 2^{10} - \sum_{2^{12}} 2^{-2} \cdot 2^{-3} - \sum_{2^{12}-1} 2^{-3} \cdot 2^{-3}) + 2^{20} \\ &= 2^7 + 2^6 - 2^{-6} = 191.984375 \end{aligned}$$

Unfortunately (as specified under “Story-2” earlier), thanks to the differences in multi-term addition implementation, the answer can be “all zeros” on NVIDIA A100, V100, AMD MI250, and a CPU; a matrix filled with 255.875 on the AMD MI100; and one filled with 191.875 on the NVIDIA H100.

# Can discover specs via tests : Block-FMA width illustrated

(details not important – see our HPDC'23 paper...)

---

**Algorithm 1:** Test Minimum Unit for FMA property preservation. The idea is to assign a moving position the  $2^{-1}ulp$  value and when that position goes beyond the width of the block FMA, we get a 1 output. That index is the FMA block width.

---

**Data:** Matrices  $a$ ,  $b$ ,  $c$ , and  $d$ .  $a$ 's row's length  $K$ .

```
1 Initialize all values in  $a$ ,  $b$ ,  $c$  to 0
2  $c_{11} \leftarrow 1$ .
3  $a_{11} \times b_{11} \leftarrow 2^{-1} \times \text{ulp}$ 
4 for  $i \leftarrow 1$  to  $K$  do
5   if  $i > 1$  then
6      $a_{1(i-1)} \times b_{(i-1)1} \leftarrow 0$ 
7      $(a_{1i} \times b_{i1}) \leftarrow (2^{-1} \times \text{ulp})$ 
8     Call wmma( $a$ ,  $b$ ,  $c$ ,  $d$ )
9     if  $d_{11} = 1$ . then
10      break
11 if  $\text{index} < K$  then
12    $\text{min\_preserve\_uint} \leftarrow \text{index}$ 
13 else
14    $\text{min\_preserve\_uint}$  is larger than  $K$ 
```

---

Here are the kinds of features we've discovered via tests

Inputs	GPU	Subnormal inputs handled?	Subnormal outputs handled?	Extra bit present? How many?	Rounding mode exhibited	FMA unit width	Order within one FMA unit is controllable?	Rounding mode for: 1. outputting FP16/BF16 (only for FP16/BF16 inputs) 2. product (only for FP32/FP64 inputs)
FP16	V100	✓	✓	0	truncate	N.A.	N.A.	RTN-TE
	A100	✓	✓	1	truncate	8	✗	RTN-TE
	H100	✓	✓	≥ 2	truncate	≥ 16	✗	RTN-TE
	MI100	✓	✓	3	RTN-TE	4	✗	RTN-TE
	MI250X	✗	✗	3	RTN-TE	1	N.A.	RTN-TE
BF16	A100	✓	✓	1	truncate	8	✗	N.A.**
	H100	✓	✓	≥ 2	truncate	≥ 16	✗	RTN-TE
	MI100	✓	✓	3	RTN-TE	2	✗	RTN-TE
	MI250X	✗	✗	3	RTN-TE	1	N.A.	RTN-TE
TF32(NVIDIA) FP32(AMD)	A100	✓	✓	1	truncate	4	✗	N.A.
	H100	✓	✓	≥ 2	truncate	4	✗	N.A.
	MI100	✓	✓	3	RTN-TE	1	N.A.	RTN-TE
	MI250X	✓	✓	3	RTN-TE	1	N.A.	RTN-TE
FP64	A100	✓	✓	3	RTN-TE	1	✗	RTN-TE
	H100	✓	✓	3	RTN-TE	1	✗	RTN-TE
	MI250X	✓	✓	3	RTN-TE	1	N.A.	RTN-TE

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## Subnormal supported

Inputs	GPU	Subnormal inputs handled?	Subnormal outputs handled?	Extra bit present? How many?	Rounding mode exhibited	FMA unit width	Order within one FMA unit is controllable?	Rounding mode for: 1. outputting FP16/BF16 (only for FP16/BF16 inputs) 2. product (only for FP32/FP64 inputs)
FP16	V100	✓	✓	0	truncate	N.A.	N.A.	RTN-TE
	A100	✓	✓	1	truncate	8	✗	RTN-TE
	H100	✓	✓	≥ 2	truncate	≥ 16	✗	RTN-TE
	MI100	✓	✓	3	RTN-TE	4	✗	RTN-TE
	MI250X	✗	✗	3	RTN-TE	1	N.A.	RTN-TE
BF16	A100	✓	✓	1	truncate	8	✗	N.A.**
	H100	✓	✓	≥ 2	truncate	≥ 16	✗	RTN-TE
	MI100	✓	✓	3	RTN-TE	2	✗	RTN-TE
	MI250X	✗	✗	3	RTN-TE	1	N.A.	RTN-TE
TF32(NVIDIA) FP32(AMD)	A100	✓	✓	1	truncate	4	✗	N.A.
	H100	✓	✓	≥ 2	truncate	4	✗	N.A.
	MI100	✓	✓	3	RTN-TE	1	N.A.	RTN-TE
	MI250X	✓	✓	3	RTN-TE	1	N.A.	RTN-TE
FP64	A100	✓	✓	3	RTN-TE	1	✗	RTN-TE
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## Extra bits and rounding mode

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FP16	V100	✓	✓	0	truncate	N.A.	N.A.	RTN-TE
	A100	✓	✓	1	truncate	8	✗	RTN-TE
	H100	✓	✓	> 2	truncate	≥ 16	✗	RTN-TE
	MI100	✓	✓	3	RTN-TE	4	✗	RTN-TE
	MI250X	✗	✗	3	RTN-TE	1	N.A.	RTN-TE
BF16	A100	✓	✓	1	truncate	8	✗	N.A.**
	H100	✓	✓	> 2	truncate	≥ 16	✗	RTN-TE
	MI100	✓	✓	3	RTN-TE	2	✗	RTN-TE
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TF32(NVIDIA) FP32(AMD)	A100	✓	✓	1	truncate	4	✗	N.A.
	H100	✓	✓	> 2	truncate	4	✗	N.A.
	MI100	✓	✓	3	RTN-TE	1	N.A.	RTN-TE
	MI250X	✓	✓	3	RTN-TE	1	N.A.	RTN-TE
FP64	A100	✓	✓	3	RTN-TE	1	✗	RTN-TE
	H100	✓	✓	3	RTN-TE	1	✗	RTN-TE
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	H100	✓	✓	≥ 2	truncate	≥ 16	✗	RTN-TE
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	MI250X	✓	✓	3	RTN-TE	1	N.A.	RTN-TE
FP64	A100	✓	✓	3	RTN-TE	1	✗	RTN-TE
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	A100	✓	✓	1	truncate	8	✗	RTN-TE
	H100	✓	✓	≥ 2	truncate	≥ 16	✗	RTN-TE
	MI100	✓	✓	3	RTN-TE	4	✗	RTN-TE
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BF16	A100	✓	✓	1	truncate	8	✗	N.A.**
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	MI100	✓	✓	3	RTN-TE	1	N.A.	RTN-TE
	MI250X	✓	✓	3	RTN-TE	1	N.A.	RTN-TE
FP64	A100	✓	✓	3	RTN-TE	1	✗	RTN-TE
	H100	✓	✓	3	RTN-TE	1	✗	RTN-TE
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	A100	✓	✓	1	truncate	8	✗	RTN-TE
	H100	✓	✓	≥ 2	truncate	≥ 16	✗	RTN-TE
	MI100	✓	✓	3	RTN-TE	4	✗	RTN-TE
	MI250X	✗	✗	3	RTN-TE	1	N.A.	RTN-TE
BF16	A100	✓	✓	1	truncate	8	✗	N.A.**
	H100	✓	✓	≥ 2	truncate	≥ 16	✗	RTN-TE
	MI100	✓	✓	3	RTN-TE	2	✗	RTN-TE
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	MI250X	✓	✓	3	RTN-TE	1	N.A.	RTN-TE
FP64	A100	✓	✓	3	RTN-TE	1	✗	RTN-TE
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	H100	✓	✓	≥ 2	truncate	≥ 16	✗	RTN-TE
	MI100	✓	✓	3	RTN-TE	4	✗	RTN-TE
	MI250X	✗	✗	3	RTN-TE	1	N.A.	RTN-TE
BF16	A100	✓	✓	1	truncate	8	✗	N.A.**
	H100	✓	✓	≥ 2	truncate	≥ 16	✗	RTN-TE
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	MI100	✓	✓	3	RTN-TE	1	N.A.	RTN-TE
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FP64	A100	✓	✓	3	RTN-TE	1	✗	RTN-TE
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	H100	✓	✓	≥ 2	truncate	≥ 16	✗	RTN-TE
	MI100	✓	✓	3	RTN-TE	4	✗	RTN-TE
	MI250X	✗	✗	3	RTN-TE	1	N.A.	RTN-TE
BF16	A100	✓	✓	1	truncate	8	✗	N.A.**
	H100	✓	✓	≥ 2	truncate	≥ 16	✗	RTN-TE
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FP64	A100	✓	✓	3	RTN-TE	1	✗	RTN-TE
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	H100	✓	✓	≥ 2	truncate	≥ 16	✗	RTN-TE
	MI100	✓	✓	3	RTN-TE	4	✗	RTN-TE
	MI250X	✗	✗	3	RTN-TE	1	✓	RTN-TE
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	MI250X	✓	✓	3	RTN-TE	1	✓	RTN-TE
FP64	A100	✓	✓	3	RTN-TE	1	✗	RTN-TE
	H100	✓	✓	3	RTN-TE	1	✗	RTN-TE
	MI250X	✓	✓	3	RTN-TE	1	✓	RTN-TE

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# Rounding errors are a concern... but Exceptions are more of a concern

- FP32
  - Error measuring **Earth-to-Moon Distance** of 384,400 km : **22.9 meters**
  - Error measuring **Height of Human** (172 cm) : **0.000103 mm**
- BF16
  - Moon: **1500 km**
  - Human: **6.7 mm**
- FP16
  - Moon: Can't represent - **INF**
  - Human: **0.84 mm**

# Rounding errors often "OK"; Exceptions are Show-Stoppers!

- How much rounding error is too much?
  - No definite answer
    - ML → matters
      - but backprop is "one-stop redemption of all evil"
    - HPC → matters more
      - still if the residual converges, things will often work
- However, exceptions are almost always show-stoppers!
  - Value-ranges being exceeded → INF
    - ( e.g.  $1.9 \times 10^{19}$  ) when squared → INF in FP32
      - dot-products and mat-mat sum such squares
  - INF / INF → NaN
    - NaN : a showstopper in most cases!
- `#define MAX(x,y) ( x >= y ? x : y )` ← buggy MAX macro in FP...

# What are some challenges of Array Programming on GPUs?

- How Pytorch guards against NaNs
  - [https://discuss.pytorch.org/t/outputting-nan-as-predictions-in-my-neural-network-training-loop/183151/2?utm\\_source=chatgpt.com](https://discuss.pytorch.org/t/outputting-nan-as-predictions-in-my-neural-network-training-loop/183151/2?utm_source=chatgpt.com)
- How "Lightning" helps implement NaN callbacks and help debug NaNs
  - <https://chaimrand.medium.com/debugging-the-dreaded-nan-ac3f9feac5b2>
- CuSparse notes on NaN-handling
  - [https://docs.nvidia.com/cuda/archive/12.8.1/pdf/CUDA\\_Toolkit\\_Release\\_Notes.pdf?utm\\_source=chatgpt.com](https://docs.nvidia.com/cuda/archive/12.8.1/pdf/CUDA_Toolkit_Release_Notes.pdf?utm_source=chatgpt.com)
- ChatGPT link of a lot of NaN solutions
  - <https://chatgpt.com/share/683db7c8-6520-8013-b4d2-baab767bbc65>
- NaN in training
  - [https://discuss.pytorch.org/t/anomaly-detection/104763/7?utm\\_source=chatgpt.com](https://discuss.pytorch.org/t/anomaly-detection/104763/7?utm_source=chatgpt.com)

# Lack of formal specs + Managing their surfeit

Create specs; then manage surfeit by  
Either finding ways to bridge to standard APIs, or by  
Adapting applications to work using the new math

# Specifying GPUs and their Versions

- A Huge Variety of Behaviors
  - Unclear how the community can keep up
    - Test-based Spec Discovery is always handy
    - Maybe we can automate tests → Spec creation
- One attractive use of Specs
  - Automated code synthesis
    - Users might do this anyhow (example given in paper)
    - So it behooves some of us to provide verification safety-nets
- How to manage the surfeit of specifications?
  - Simulate all variants on top of one fixed scheme
    - e.g. IEEE FP32
  - OR, Find a way to run existing code on the given platform
    - ... and find a way to detect and recover from failures
      - Many HPC and ML codes may run robustly on "strange" HW anyhow

# Synthesized efficient code: find the max element in a matrix seems correct here – but in general, is fallible in subtle ways

```
// local thread ID within a warp
int warpThreadId = threadIdx.x & (WARP_SIZE - 1);
float localMax  = -65504.0f; // half-prec. min is roughly -65504

// Step 1: Each thread checks some subset of D
for (int idx = warpThreadId; idx < M * N; idx += WARP_SIZE) {
    float val   = __half2float(D[idx]);
    localMax   = fmaxf(localMax, val);
}

// Step 2: Warp-wide reduce using shuffle intrinsics
unsigned int mask = __activemask(); // active lanes
#pragma unroll
for (int offset = WARP_SIZE / 2; offset > 0; offset >>= 1) {
    float temp = __shfl_down_sync(mask, localMax, offset);
    localMax   = fmaxf(localMax, temp);
}

// Step 3: The lane 0 in the warp stores the final max to MaxVal
if (warpThreadId == 0) {
    *MaxVal = __float2half(localMax);
}
```

This best paper award winner at NFM 2025 + released SMT artifacts is a significant step in this direction...

# An SMT Formalization of Mixed-Precision Matrix Multiplication Modeling Three Generations of Tensor Cores

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Gopalakrishnan<sup>2[0000–0002–4161–9278]</sup>

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<sup>2</sup> University of Utah, Salt Lake City, UT 84112, USA `{xin_yi.li@utah.edu, ganesh@cs.utah.edu}`

# The types of questions one can answer once we have formal specifications for GPU Hardware:

Do numerical algorithms such as this port reliably across GPUs?

- Will we get the same convergent results, provided the dynamic range and unit-roundoff are within acceptable limits
  - many choices at each stage of such algorithms

**repeat**

Solve:  $Ax = b$  @ prec.  $u_1 < u_2$

Compute Residual:  $r = b - Ax$  @ prec.  $u_2$

Solve:  $Ae = r$  @ prec.  $u_3 < u_2$

Update solution:  $x = x + e$  @ prec.  $u_2$

**until** Convergence

Figure 3: Steps in Iterative Refinement

# Concluding Remarks

- Need for energy reduction causes GPU number-system variety
- Exceptions are a given... due to reduced precision
  - Credible PL methods critically depend on robust and versatile solutions to handle exceptions
- Test-based specification discovery is quite handy
  - Even when formal specs are available
    - Easily shared amongst groups
      - May help create specs, one day
      - Test-fusion enabled by formal specs...
        - One concrete test that covers many features
  - Must manage surfeit of specs
    - Either emulate common number system
      - or migrate to it with an abundance of caution

## Concluding Remarks (added..)

- Tooling in the GPU space needs a lot of attention
- Tooling such as Binary Instrumentation
  - Is provided by manufacturers
    - Long-term availability is unknown
  - Tool bug-fixes must be incorporated by tool-users
    - Community that helps convey "undocumented knowledge" (blogs, word-of-mouth, BoF,...) yet to grow
- Other tool bugs are also show-stoppers
  - e.g. how we found and helped fix an nvcc bug
- Conclusion : without sufficient number of tools and experience reports, Array Programming on GPUs will not be reliable and trustworthy.

# Tensor core register layout

Each thread holds part of the matrices in its registers

T1							
R0	R1	R2	R3	R4	R5	R6	R7
A0	A1	A2	A3	B0	B1	C0	C1

T2							
R0	R1	R2	R3	R4	R5	R6	R7
A4	A5	A6	A7	B2	B3	C2	C3

T3							
R0	R1	R2	R3	R4	R5	R6	R7
A8	A9	A10	A11	B4	B5	C4	C5

T4							
R0	R1	R2	R3	R4	R5	R6	R7
A12	A13	A14	A15	B6	B7	C6	C7

$$\begin{array}{|c|c|c|c|} \hline A0 & A1 & A2 & A3 \\ \hline A4 & A5 & A6 & A7 \\ \hline A8 & A9 & A10 & A11 \\ \hline A12 & A13 & A14 & A15 \\ \hline \end{array} + = \begin{array}{|c|c|} \hline B0 & B1 \\ \hline B2 & B3 \\ \hline B4 & B5 \\ \hline B6 & B7 \\ \hline \end{array} \times \begin{array}{|c|c|c|c|} \hline C0 & C2 & C4 & C6 \\ \hline C1 & C3 & C5 & C7 \\ \hline \end{array}$$

A                    B                    C

# Tensor core register layout

Each thread holds part of the matrices in its registers

Thread T1 holds:

- The first four elements of A

T1							
R0	R1	R2	R3	R4	R5	R6	R7
A0	A1	A2	A3	B0	B1	C0	C1
A4	A5	A6	A7	B2	B3	C2	C3

T2							
R0	R1	R2	R3	R4	R5	R6	R7
A4	A5	A6	A7	B2	B3	C2	C3
A12	A13	A14	A15	B6	B7	C6	C7

T3							
R0	R1	R2	R3	R4	R5	R6	R7
A8	A9	A10	A11	B4	B5	C4	C5
A12	A13	A14	A15	B6	B7	C6	C7

$$\begin{array}{c|c|c|c} \text{A0} & \text{A1} & \text{A2} & \text{A3} \\ \hline \text{A4} & \text{A5} & \text{A6} & \text{A7} \\ \hline \text{A8} & \text{A9} & \text{A10} & \text{A11} \\ \hline \text{A12} & \text{A13} & \text{A14} & \text{A15} \end{array} + = \begin{array}{c|c} \text{B0} & \text{B1} \\ \hline \text{B2} & \text{B3} \\ \hline \text{B4} & \text{B5} \\ \hline \text{B6} & \text{B7} \end{array} \times \begin{array}{c|c|c|c} \text{C0} & \text{C2} & \text{C4} & \text{C6} \\ \hline \text{C1} & \text{C3} & \text{C5} & \text{C7} \end{array}$$

C

# Tensor core register layout

Each thread holds part of the matrices in its registers

Thread T1 holds:

- The first four elements of A
- The first two elements of B

T1							
R0	R1	R2	R3	R4	R5	R6	R7
A0	A1	A2	A3	B0	B1	C0	C1
A4	A5	A6	A7	B2	B3	C2	C3

T2							
R0	R1	R2	R3	R4	R5	R6	R7
A4	A5	A6	A7	B2	B3	C2	C3
A12	A13	A14	A15	B6	B7	C6	C7

$$\begin{array}{c|c|c|c|c} \text{A0} & \text{A1} & \text{A2} & \text{A3} & \\ \hline \text{A4} & \text{A5} & \text{A6} & \text{A7} & \\ \hline \text{A8} & \text{A9} & \text{A10} & \text{A11} & \\ \hline \text{A12} & \text{A13} & \text{A14} & \text{A15} & \end{array} + \begin{array}{c|c} \text{B0} & \text{B1} \\ \hline \text{B2} & \text{B3} \\ \hline \text{B4} & \text{B5} \\ \hline \text{B6} & \text{B7} \end{array} \times \begin{array}{c|c|c|c} \text{C0} & \text{C2} & \text{C4} & \text{C6} \\ \hline \text{C1} & \text{C3} & \text{C5} & \text{C7} \end{array}$$

A                    B                    C

# Tensor core register layout

Each thread holds part of the matrices in its registers

Thread T1 holds:

- The first four elements of A
- The first two elements of B
- The first two elements of C

