Numerical Optimization Targeting Energy-Efficient Scientific Computing

Roman Iakymchuk
jointly with Yanxiang Chen (UmU) and
Pablo de Oliveira Castro (Paris-Saclay)

Uppsala University and Umeå University, Sweden
roman.iakymchuk@it.uu.se

MS2A: Sustainable Scientific Computing
PASC25, Brugg, Switzerland
June 16, 2025

MS2A: Sustainable Scientific Computing		
14:30	**Roman Iakymchuk**	Numerical Optimization Targeting Energy-Efficient Scientific Computing
15:00	**Michele Weiland**	Sustainable Supercomputing: An Overview of Activities at EPCC
15:30	**Pablo De Oliveira Castro**	Exploring Numerical Accuracy and Mixed-Precision with Verificarlo and Stochastic Rounding
16:00	**El-Mehdi El Arar**	Probabilistic Error Analysis of Limited-Precision Stochastic Rounding

Outline

Outline

Mixed-precision arithmetic

Energy efficiency in computing

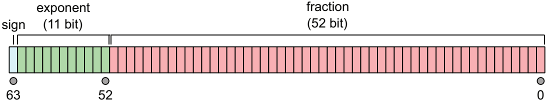
Methodology for energy-efficient algorithms

Summary

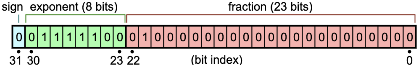
Floating-point formats

IEEE Standard for Floating-Point Arithmetic IEEE 754-2019 is widely supported by hardware and software

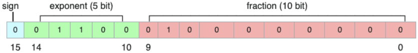
- double - binary64



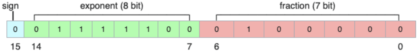
- single - binary32



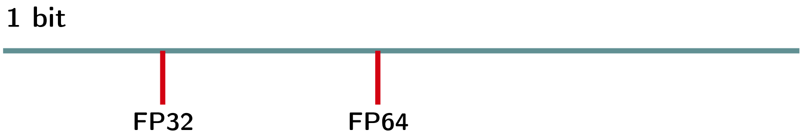
- half - binary16



- bfloat



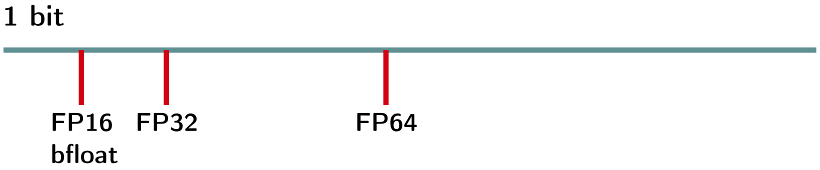
Mixed-precision arithmetic



- double-single plus iterative refinement [a]

[a] Butari et al. 'Mixed-precision iterative refinement techniques for the solution of dense linear systems'. IJPHCA 2007

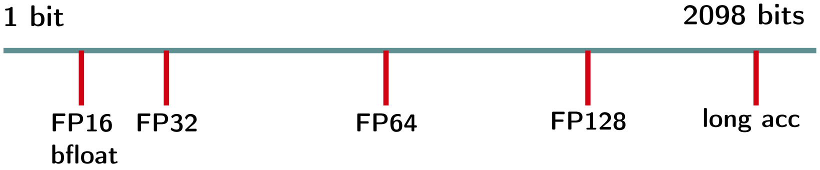
Mixed-precision arithmetic



- double-single plus iterative refinement
- double-single-half/ bfloat
- Over 100 works on mixed precision [a]

[a] N. Higham and Th. Mary. 'Mixed Precision Algorithms in Numerical Linear Algebra'. Acta Numerica. 2022; 31:347-414

Mixed-precision arithmetic



- double-single plus iterative refinement
- double-single-half/ bfloat
- Over 100 works on mixed precision
- Extending precision for exact computations: double plus FPEs or double plus long accumulator

Example: Ariane 5 explosion

- Failed maiden flight of the ESA Ariane 5 rocket
- Causes of the failure
  - Old code from Ariane 4, but Ariane 5 had higher horizontal velocity
  - Overflow in converting numbers (64-bit to 16-bit) for the horizontal velocity
  - This halted the internal navigation system and led to self destruction
- Loss: more than $\$500$ million for satellite

Outline

Energy efficiency: from hardware to NLA

- Supercomputing is constrained by **power consumption**

→ Power-efficient hardware
  - RIKEN's Fugaku w A64FX (FP64:FP32:FP16 = 1:2:4)
  - EPI (ARM, FPGA, RISC-V)
  - **Jülich to host the first EPI-based supercomputer**

- Numerical linear algebra is dominant by **double precision**

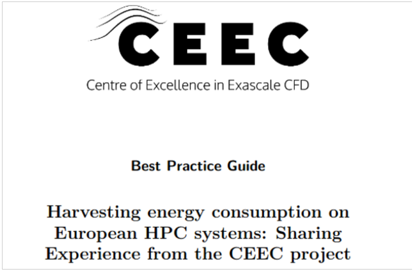
→ **Mixed-precision/ energy-efficient algorithms**

math Mixed and adaptive precision computing

code Communication hiding or avoiding

tools Numerical abnormalities and precision cropping

How to measure energy consumption?


CEEC
Centre of Excellence in Exascale CFD

Best Practice Guide

Harvesting energy consumption on European HPC systems: Sharing Experience from the CEEC project

Iakymchuk et al. Zenodo, 2024

- **More complex than measuring time-to-solution**
- Measurements require elevated privileges

Objectives

- Facilitate energy measurements on the European HPC systems
- Teach the community how to conduct such measurements
- Provide examples with easy-to-use guide

Practical advices

What can we measure?

- CPU, DRAM, accelerators
- NO: cooling, interconnect

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Energy/ power-meters

- on clusters, use job monitoring systems like **SLURM**, eg energy measurement pluggin `sacct`
- similarly, Energy Aware Runtime (**EAR**) helps to measure energy: `eacct`
- **likwid-powermeter** is another tool that can measure the entire program or its part
- MSR counters – the lowest level possible

Outline

Methodology

Methodology to enable mixed-precision algorithmic solutions in applications with accuracy guarantees.

Original application

↓

Check speed-up (performance models)

↓

Check accuracy (arithmetic tools)

↘

Candidate code-sections

↗

Port to mixed-precision

↑

Expert Validation

↑

Mixed-Precision application

- Conduct classic or probabilistic (aka optimistic) error analysis
  - error bound with constant $\sqrt{n}\mu$ with high probability

EuroHPC JU CoE CEEC

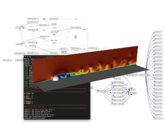
Center of Excellence in Exascale CFD

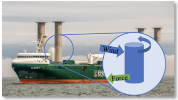
Overview

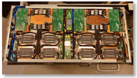
CEEC

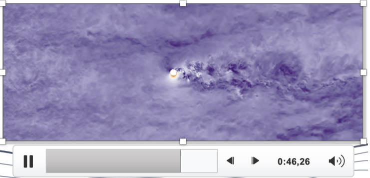
The main goal of CEEC is to address the extreme-scale computing challenge to enable the use of accurate and cost-efficient high fidelity computational fluid dynamics (CFD) simulations at exascale

- Implement **exascale-ready workflows** for addressing grand challenge scientific problems
- Develop **new or improved algorithms** that can efficiently exploit exascale systems.
- Significantly improve **energy efficiency** of simulations
- Demonstrate workflows on **lighthouse cases** relevant for both academia and industry









Courtesy of Niclas Janson, KTH

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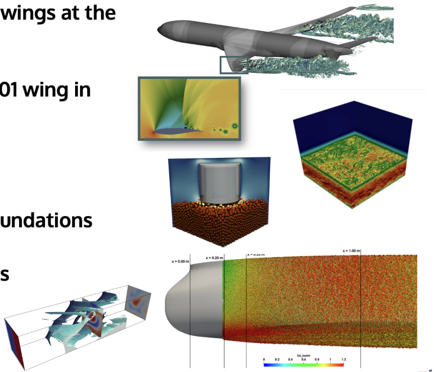
Lighthouse Cases

- **Shock-boundary layer interaction and buffet on wings at the edge of the flight envelope**
  - Codes used: FLEXI
- **High fidelity aeroelastic simulation of the SFB 401 wing in flight conditions**
  - Codes used: Alya
- **Topology optimisation of static mixers**
  - Codes used: Neko
- **Localized erosion of an offshore wind-turbine foundations**
  - Codes used: waLBerla
- **Simulation of Atmospheric Boundary Layer flows**
  - Codes used: NekRS/Nek5000
- **Merchant ship hull**
  - Codes used: Neko



CEEC us out on `https://ceec-coe.eu`

Test case

- **Nek5000/ Neko** are the high order, incompressible Navier-Stokes solvers based on the spectral element method

→ 'matrix-free'

- **Nekbone** is a mini-app of Nek5000 and it solves a Poisson equation using a Conjugate Gradient method with the spectral element multigrid preconditioner

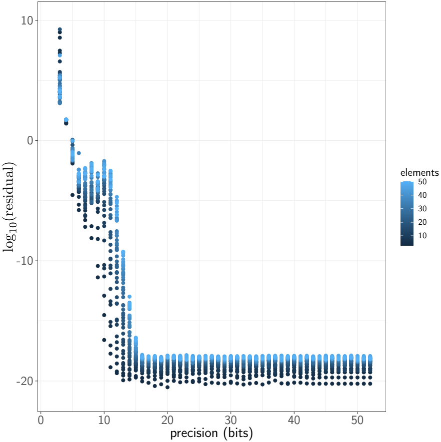
Nekbone w Vprec

$$\boxed{Ax = b}$$

while $(\tau > \tau_{\max})$

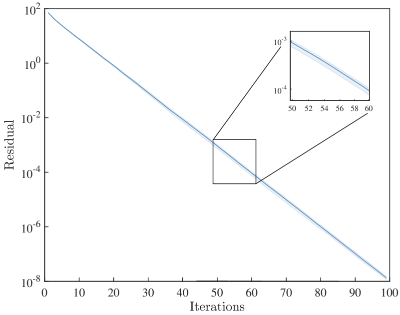
Step	Operation
$S1:$	$w := Ad$
$S2:$	$\rho := \beta / < d, w >$
$S3:$	$x := x + \rho d$
$S4:$	$r := r - \rho w$
$S5:$	$z := M^{-1} r$
$S6:$	$\beta := < z, r >$
$S7:$	$d := (\beta / \beta_{old}) d + z$
$S8:$	$\tau := < r, r >$

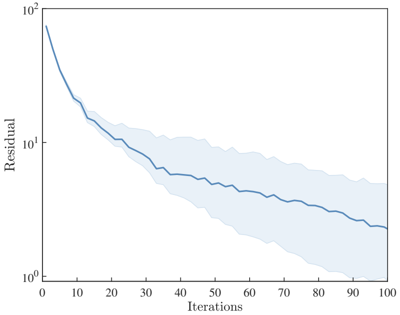
end while



Nekbone w MCA for FP32

Entire program, no preconditioner

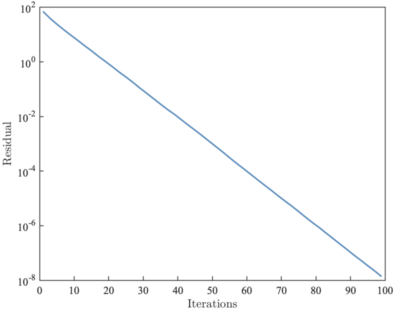


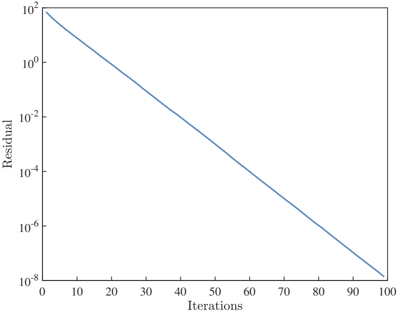


- Random Rounding (rr) mode (left)
- MCA (mca) mode (right)
- Issue in initialization $10^9 \times \cos(x) \rightarrow$ focus on the solver only

Nekbone w MCA for FP32

Only the CG loop, no preconditioner





- Random Rounding (rr) mode (left)
- MCA (mca) mode (right)

Performance of mixed-precision Nekbone

Parallel tests: gain in execution time w/o preconditioner

On LUMI-C, AMD EPYC 7763 CPU with 64 cores @2.45 GHz

(a) Whole program

MPI ranks	1	4	8	16	32	64	128
Mixed	0.741	0.905	0.995	1.642	1.694	2.096	2.641
Double	0.775	1.026	1.857	2.920	3.151	3.562	4.452
Gain	1.05x	1.13x	1.87x	1.78x	1.86x	1.70x	**1.69x**

(b) Solve time

MPI ranks	1	4	8	16	32	64	128
Mixed	0.165	0.178	0.190	0.256	0.430	0.445	0.476
Double	0.182	0.239	0.596	1.115	1.161	1.207	1.245
Gain	1.10x	1.34x	3.14x	4.36x	2.70x	2.71x	2.62x

- time is in seconds
- run each test five times, report median

energy-to-solution of mixed-precision Nekbone

LUMI-C

MPI ranks	32	stddev	64	stddev	128	stddev
Mixed	451.6	4.1%	653.6	2.4%	1089.4	1.0%
Double	990.6	3.9%	1424.8	4.5%	2061.2	3.2%
Gain	2.20x		2.18x		**1.89x**	

- run each test five times, compute mean & standard deviation (stddev)
- energy numbers are in joules measured by `sacct` (Slurm)
- On LUMI-C, 2x AMD EPYC 7763 CPU with 64 cores @2.45 GHz

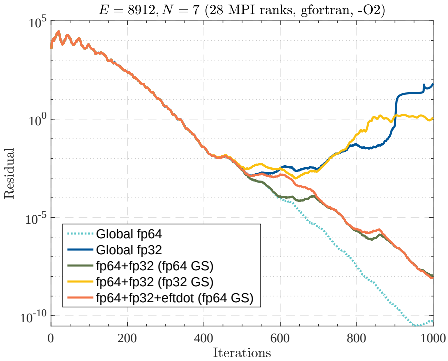
energy-to-solution of mixed-precision Nekbone

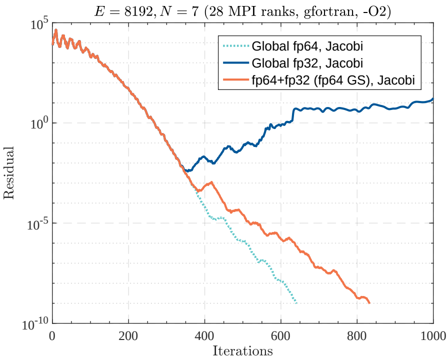
MareNostrum5

MPI ranks	20	40	80
Mixed	637	865	1221
Double	1042	2473	4685
Gain	1.64x	2.86x	**3.84x**

- Energy measurements with EAR
- On MN5, 2x Intel Sapphire Rapids 8460Y+ @2.3Ghz

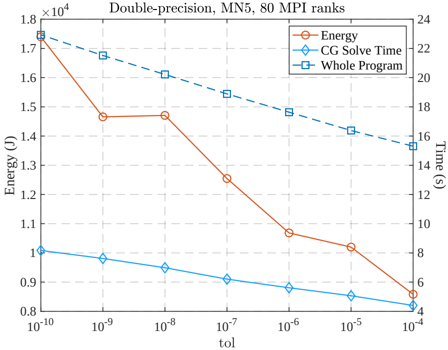
Neko: CG with preconditioner

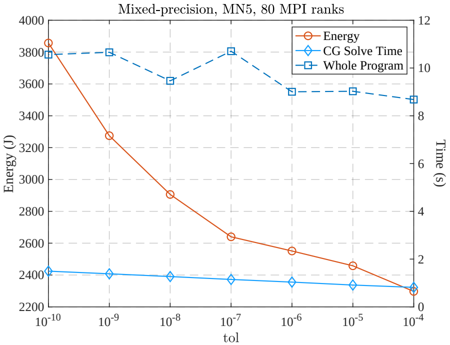




- Results from the real-world Neko code
- Comparable convergence for mixed-precision

Accuracy vs Energy vs Time





- Nekbone with the multigrid preconditioned CG
- 3.7x-4.5x gain in energy and 1.8x-2.2x in time

Outline

Summary

- Computer arithmetic operates with finite precisions
- Use computer arithmetic tools to
  - detect cancellations
  - get the right FP format
  - verify sensitivity of reduced precision
- Start measuring energy consumption
- Enabled mixed-precision in Nekbone and Neko:
  - use tools: Verificarlo, gprof, Intel Advisor
  - target the most time-consuming part
  - reduced time-to-solution by up to 2.2x and **energy-to-solution by up to 3.8x** on 80 MPI ranks at MareNostrum5

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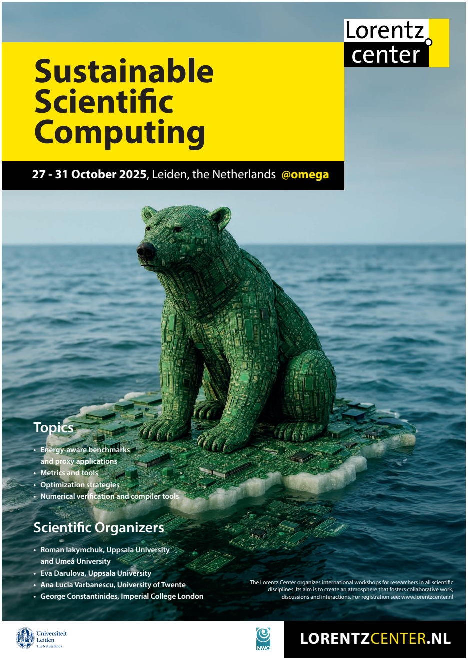
Thank you for your attention !

This research is partially supported by EuroHPC JU CoE CEEC (No. 101093393), TDB and eSSENCE at Uppsala University.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Topics
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Metrics and tools
Optimization strategies
Numerical verification and compiler tools
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Eva Darulova, Uppsala University
Ana Lucia Varbanescu, University of Twente
George Constantinides, Imperial College London
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References

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