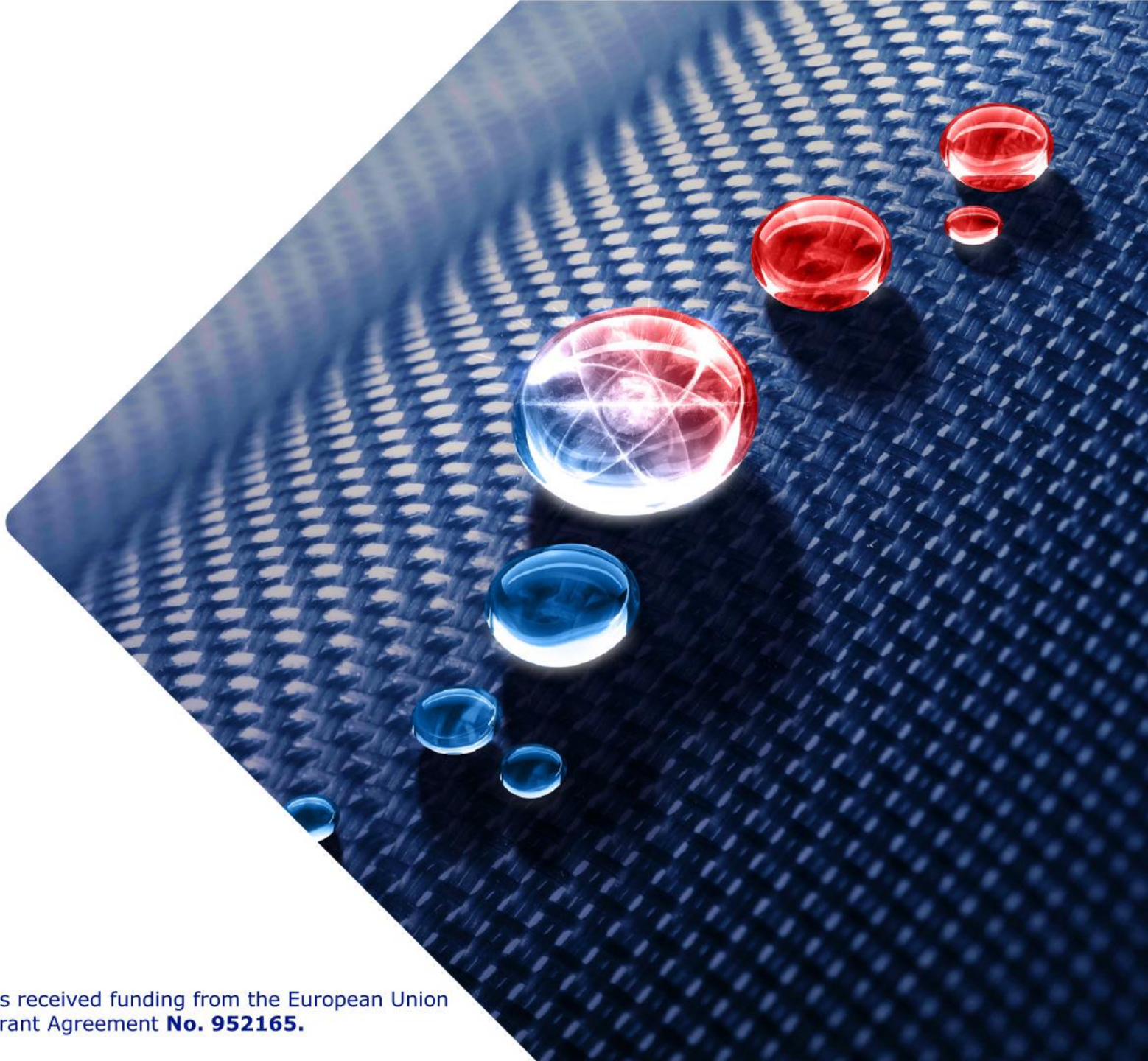




RECENT HPC EVOLUTIONS, LESSONS FROM TREX CODES

W. Jalby (UVSQ)



CPU: INTEL, AMD, ARM

Smooth evolution : more FU, more ports, more memory channels, larger caches, etc..... Better Out of Order and memory hierarchy

Some innovations:

- Support for FP16
- Heterogeneous cores: Performance Cores, Efficiency cores (Alder Lake)
- AMX: matrix operations (FP16 and Integer)

GPU: NVIDIA, INTEL, AMD

Only early access to AMD and INTEL GPU

- Shared memory between GPUs
- Still waiting for shared memory between CPU and GPU: AMD has some partial solutions working.

LLVM

1. **Major industry players are now relying on LLVM:** INTEL, AMD, ARM, NVIDIA
2. **Be cautious:** LLVM does not mean that all of the modules are open source!! Proprietary solutions are embedded into LLVM: backend and also Front End Fortran
3. **GOOD NEWS:** easy to integrate new technology. For example, VERIFICARLO (Numerical Accuracy tool) is fully integrated in LLVM

GPU/SIMD programming

A lot of alternatives to proprietary CUDA: more or less open (DPC++, HIP, etc...), standard (OpenMP)

SIMD directives available in OpenMP

1. **Poorly structured arrays** : having well structured array is essential for vectorization
2. **Loops with low iteration**: unfortunately, compiler offer very little support for such cases
3. **Opportunities for developing new tools: generate specialized code variants SISSA**
4. **Deal with large I/O**

- TREX web site: <https://trex-coe.eu>
- TREXIO: <https://github.com/trex-coe/trexio>
- QMCKI: <https://github.com/trex-coe/qmckl>
- QMCKI documentation: <https://trex-coe.github.io/qmckl>
- MAQAO: <http://www.maqao.org>
- Verificarlo: <https://github.com/verificarlo/verificarlo>