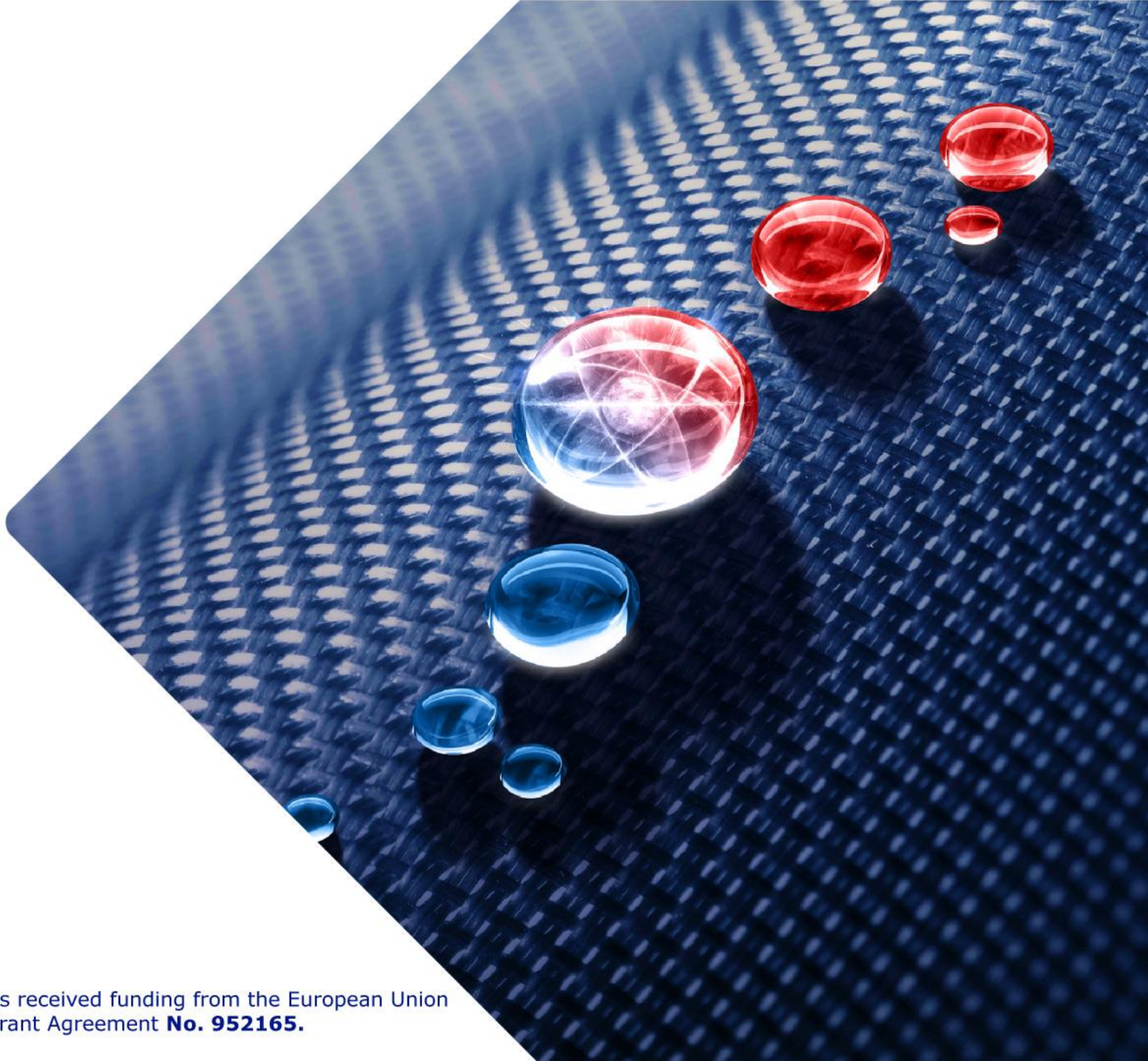




QMCKL RATIONALE

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Objectives

1. **PRODUCTIVITY:** Used and developed by scientists, called from different languages
2. **PORTABILITY:** available on large number of hardware and software platforms
3. **PERFORMANCE:** Must be efficient

“Classical” challenge : be good simultaneously on the 3 objectives. There is a workshop at SC devoted to this triple objective.

Key ingredients of our approach:

- Reasonable limits on our objectives : library specialization
- Use of automatic tools to build and tune the library
- Performance AND numerical accuracy have to be both addressed
- Free Software (Open Science)
- Systematically avoid proprietary technology (cf CUDA) always rely on standards (such as OpenMP)

Limitations/Focal points/Timing

1. **Limited/Specialized functionality:** First single core and later node/multicore (no multimode version)
2. **Limited number of hardware targets:** First X86 (INTEL/AMD) and ARM Neoverse. Later GPU: wait until there is some convergence between NVIDIA, INTEL and AMD
3. **Systematic use of tradeoffs:** for example trade performance in favor of portability
4. **Strong data structures:** a lot of attention will be devoted to structure data and access.

Two major variants

1. **Esay to read and Unoptimised** : essentially used for functionality testing. Code will be simple and compact but already the innermost loops should be vectorizable and stride 1 array access should be systematically favored.
2. **Optimized versions**: multiple versions depending upon target architectures

Develloping optimized versions

GOOD NEWS: our main CPU targets share a lot of common characteristics/organization/technology

BAD NEWS: work around (and not necessarily together) compilers.

Our approach: use of specific vector languages (MIPP) and abstract vector constructs.

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