Targeting Real chemical accuracy at the EXascale

CO DESIGNING A HIGH PERFORMANCE AND PORTABLE LIBRARY (QMCKL): ONE OF THE MAJOR CHALLENGES ADDRESSED BY TREX CoE

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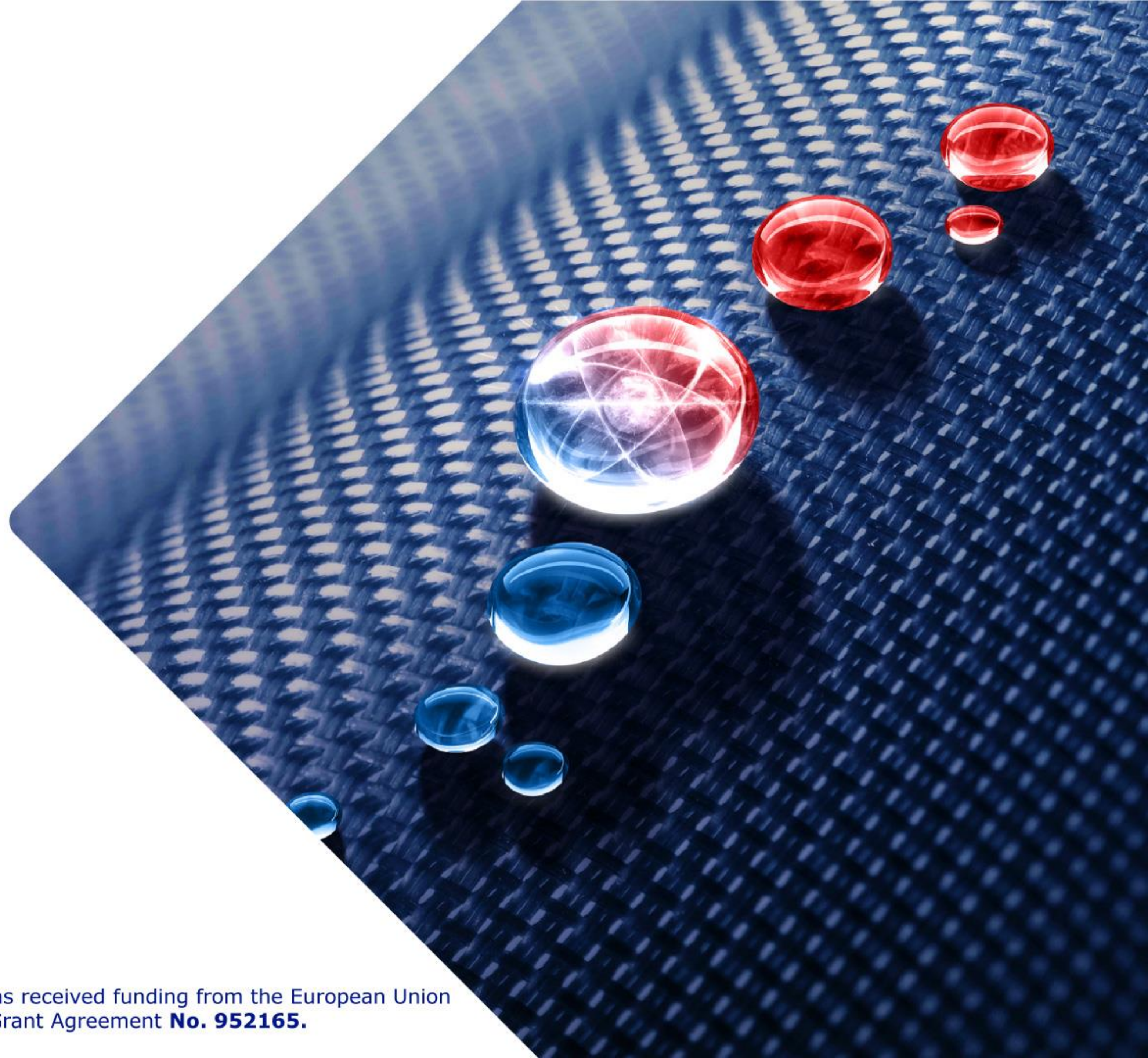

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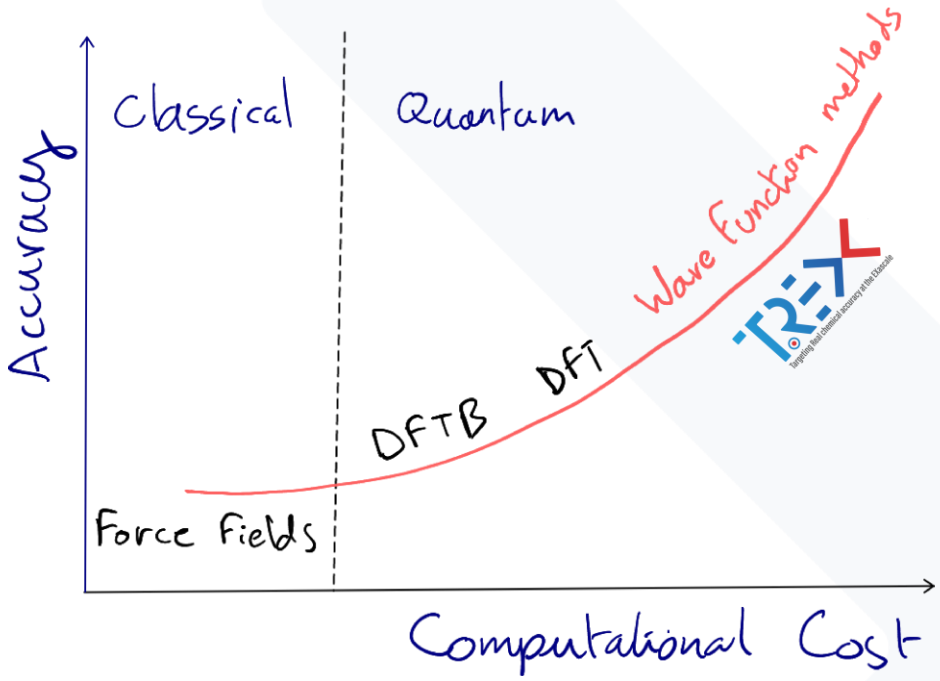
TREX Mission: To develop, promote, and maintain open-source, exascale-ready software solutions in (stochastic) quantum chemistry

Materials modeling at the nanoscale with extreme accuracy

- Scientists in quantum chemistry, physics, and machine learning
- Software and HPC experts
- Tech and communication SMEs
- Representative of user communities



What: Use Quantum Monte Carlo Methods

- Highly accurate
- Massively parallelizable (multiple QMC trajectories)
- No Blocking communications
- CPU intensive (difficult to exploit)

Objective: Make codes ready for exascale

How: Instead of re-writing codes, provide libraries

- A library for exchanging information between codes:

TREXIO ➡ Enables HTC

- A library for high-performance numerical computation:

QMCkl ➡ Enables HPC

Create a platform of interoperable flagship codes extendable and/or operable with codes outside TREX

Objectives

1. **PRODUCTIVITY**: Used and developed by scientists, can be 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.

We need to go beyond these classical objectives:

- Not only performance but also energy consumption should be a major goal
- Numerical accuracy is extremely important

Major axes/guidelines

1. **Focus and Specialization**: focused on well identified objectives (not general)
2. **Ease of interaction with software and hardware environment:** beyond classic portability
3. **Use of Advanced Tuning Tools:** adaptable library via tools instead of static library

Objectives

1. **Application target = QMC**: use of high degree of parallelism present in most QMC applications. Focus on single node/core implementations
2. **Focus on a few reference platforms:** CPU (ISA: X86 + ARM Neoverse), GPU
3. **Specific needs of our target applications:** for example no need of general arbitrary size Matrix Multiplies. Many of our apps are using Rank K Updates: (MxK) x (KxM) with K much smaller than M

GOOD NEWS:

- For our propose (scientific computing) X86 and ARM general architecture share a lot of common characteristics with secondary differences which can be dealt with automatically
- CPU and GPU all strongly require vectors…. But memory constraints are very different

Objectives

1. **Interaction with context**: routines available in source form so compiler can inline and optimize through calls
2. **Develop optimized but generic code versions:** use tools for generating highly optimized and specific version
3. **Strongly structure arrays within the library:** systematic use of tiled arrays for improving memory hierarchy usage
4. **Systematic use of (1+n) library versions:** a pedagogical/reference version and several optimized versions
5. **OPEN SOURCE + STANDARDS:** easy to modify and integrate. Strong use of standard: OpenMP directives for GPU and vectorization

Objectives

1. **Obtain high performance across a large range of platforms (first CPU)**
2. **Provide input for compilers/library/hardware designers**

Approach

- Start from the generic version perform first level (generic) optimization following tools guidance
- Perform detailed analysis of hardware and software interaction (including low level)
- Use tools (MAQAO) to automate info gathering and performance comparison
- Use tools (MAQAO) for generating specialized versions in partocular auto tuners for last mile optimization

Key issues analyzed

1. **Profile categorizations:** time spent in libraries, binary, loops (innermost/outermost), etc…
2. **Flow complexity:** number of paths, presence of calls, etc…
3. **Array access:** unit/non unit stride access, indirect
4. **Vectorization:** not only amount of vector instruictions but also assess vectorization quality

IMPORTANT:

- All of the above analysis is performed at the ASM level (either statically or dynamically at run time)
- This analysis depends upon compiler and processor used

GOOD NEWS: we can test various compilers and hardware and perform comparative studies. Very usefull for vectorization.

Provide performance estimates when specific optimizations are triggered

1. **Perfect OpenMP/MPI/Pthread:** suppress time spent in these parallelism libraries
2. **Perfect OpenMP/MPI/Pthread + Perfect Load balancing:** suppress time spent in these parallelism libraries + perform perfect load balancing
3. **Perfect compiler**: gets rid of all of the “integer” operations
4. **Perfect arithmetic FP vectorization:** assumes arithmetic FP vectorization
5. **Perfect Full vectorization**: assumes arithmetic FP + Load/Store vectorization
6. **L1 data access:** assumes that all data access are performed from L1

IMPORTANT: all of these performance estimates are computed at the loop level but their performance impact is extrapolated at the whole application.

Target: Unicore Skylake Xeon(R) Platinum 8170 + ICC/IFORT 2021 –O3

▶ Colums Filter

Loop id	Source Location	Source Function	Level	Coverage run_0 (%)	Vectorization Ratio (%)	Vectorization Efficiency (%)	Speedup If No Scalar Integer	Speedup If FP Vectorized	Speedup If Fully Vectorized	Speedup If Perfect Load Balancing run_0	Stride 0	Stride 1	Stride n	Stride Unknown
703	libqmckl.so.0 - qmckl_jastrow_f.F90:2088-2105 [...]	qmckl_compute_factor_een_deriv_e_f	Innermost	12.56	100	50	1.3	1.21	2	1	1	12	0	1
602	libqmckl.so.0 - qmckl_jastrow_f.F90:798-815	qmckl_compute_factor_een_rescaled_e_deriv_e_f	Innermost	7.74	55.56	30.56	1	1	3.55	1	0	6	0	0
640	libqmckl.so.0 - qmckl_jastrow_f.F90:1050-1067	qmckl_compute_factor_een_rescaled_n_deriv_e_f	Innermost	2.15	56.76	31.08	1	1	3.42	1	0	6	0	0
155	libqmckl.so.0 - qmckl_jastrow.c:1649-1653	qmckl_compute_een_rescaled_e_hpc	Innermost	1.98	0	12.5	1	1	8	1	0	2	0	2
603	libqmckl.so.0 - qmckl_jastrow_f.F90:798-815	qmckl_compute_factor_een_rescaled_e_deriv_e_f	Innermost	1.29	0	12.5	1	1	8	1	0	2	0	4
606	libqmckl.so.0 - qmckl_jastrow_f.F90:784-789	qmckl_compute_factor_een_rescaled_e_deriv_e_f	Innermost	1.17	100	44.74	1.02	1.35	2.46	1	0	5	0	0
161	libqmckl.so.0 - qmckl_jastrow.c:1630-1633	qmckl_compute_een_rescaled_e_hpc	Innermost	0.39	0	12.5	1.2	1.5	8	1	0	0	0	0

MAQAO ANLYSIS OF JASTROW ROUTINE: GLOBAL LEVEL

Target: Unicore Skylake Xeon(R) Platinum 8170 + ICC/IFORT 2021 –O3

Global Metrics

Total Time (s)		54.83
Profiled Time (s)		52.76
Time in analyzed loops (%)		30.9
Time in analyzed innermost loops (%)		29.8
Time in user code (%)		31.3
Compilation Options		OK
Perfect Flow Complexity		1.00
Iterations Count		1.00
Array Access Efficiency (%)		92.8
Perfect OpenMP + MPI + Pthread		1.00
Perfect OpenMP + MPI + Pthread + Perfect Load Distribution		1.00
No Scalar Integer	Potential Speedup	1.04
	Nb Loops to get 80%	2
FP Vectorised	Potential Speedup	1.03
	Nb Loops to get 80%	3
Fully Vectorised	Potential Speedup	1.25
	Nb Loops to get 80%	6
Data In L1 Cache	Potential Speedup	1.10
	Nb Loops to get 80%	1
FP Arithmetic Only	Potential Speedup	1.16
	Nb Loops to get 80%	7

Target: Unicore Skylake Xeon(R) Platinum 8170 + ICC/IFORT 2021 –O3

- [x] Analysis
- [ ] CQA speedup if no scalar integer
- [ ] CQA speedup if FP arith vectorized
- [ ] CQA speedup if fully vectorized
- [x] Number of paths
- [ ] Vectorization Ratio (%)
- [ ] Vectorization Efficiency (%)
- [x] ORIG / DL1
- [ ] Saturation ratio (MAX(DL1,LS)/REF)
- [x] Saturation
- [x] FP/CQA(FP)
- [x] DL1/CQA(DL1)
- [x] FP/LS
- [x] ORIG (cycles per iteration)
- [x] STA (ORIG)
- [x] REF (cycles per iteration)
- [x] STA (REF)
- [x] FP (cycles per iteration)
- [x] STA (FP)
- [x] LS (cycles per iteration)
- [x] STA (LS)
- [x] DL1 (cycles per iteration)
- [x] STA (DL1)
- [x] FES (cycles per iteration)
- [x] STA (FES)
- [x] CQA cycles
- [x] CQA cycles if no scalar integer
- [x] CQA cycles if FP arith vectorized
- [x] CQA cycles if fully vectorized
- [x] Iteration count
- [x] Function
- [x] Source
- [x] Nb FP_ADD / CPI
- [x] Nb FP_MUL / CPI
- [x] CAP(FP)
- [x] BW(FP)
- [x] SAT(FP)
- [x] CAP(L1R)
- [x] BW(L1R)
- [x] SAT(L1R)
- [x] CAP(L1W)
- [x] BW(L1W)
- [x] SAT(L1W)
- [x] CAP(L2)
- [x] BW(L2)
- [x] SAT(L2)
- [x] CAP(L3)
- [x] BW(L3)
- [x] SAT(L3)
- [x] CAP(RAM_R)
- [x] CAP(RAM_W)

Select none

ID	Module	Coverage (% app. time)	Analysis	Number of paths	ORIG / DL1	Saturation	FP/CQA(FP)	DL1/CQA(DL1)	FP/LS	ORIG (cycles per iteration)	STA (ORIG)	REF (cycles per iteration)	STA (REF)	FP (cycles per iteration)	STA (FP)	LS (cycles per iteration)	STA (LS)	DL1 (cycles per iteration)
▼ Loop 703 +	libqmckl.so.0	12.56	RAM bound	1	3.81	SATURATED	1.21	1.36	0.16	95.74	0.75	114.41	0.48	17.54	0.04	112.36	0.46	25.13
○ Bucket 7		66.99	RAM bound	1	3.81	SATURATED	1.21	1.36	0.16	95.74	0.75	114.41	0.48	17.54	0.04	112.36	0.46	25.13
○ Bucket 6		18.57	RAM bound	1	2.75	UNSATURATED	1.19	1.36	0.28	69.18	0.55	72.46	0.48	17.28	0.09	61.54	0.51	25.13
○ Bucket 8		13.42	RAM bound	1	6.12	UNSATURATED	1.20	1.36	0.13	154.00	0.36	143.49	0.79	17.44	0.10	134.72	0.35	25.18

QMCkl: a QMC driven library

1. **Oriented towards performance/portability/productivity but with customized objectives**
2. **Focused and specialized**
3. **Easy to interact with**
4. **Strongly focused on co design**
5. **Using systematically software tools:** multiple versions depending upon target architectures

STATUS:

- A first X86 version available
- GPU and ARM first versions available within 12 to 18 months

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- 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

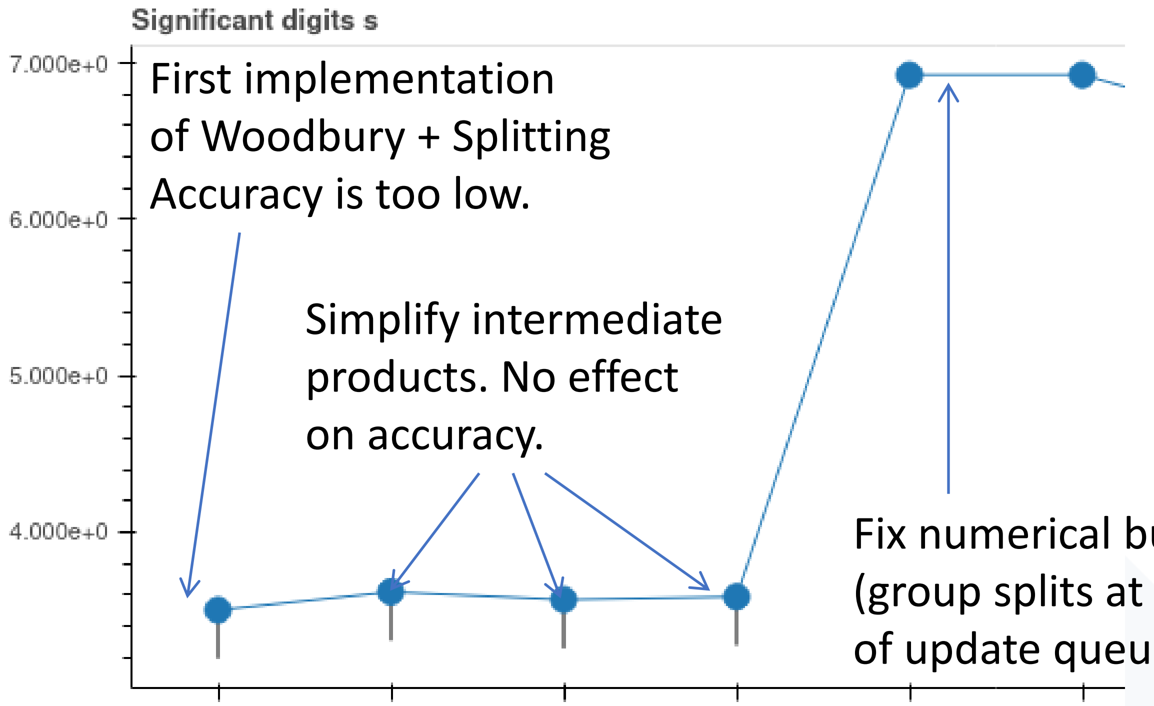
Preserve **numerical accuracy** for new architectures, parallel runtimes, optimizations.
Verificarlo is a tool for assessing the precision of floating point computations.

github.com/verificarlo/verificarlo GPL v3

- **Find numerical bugs in codes** [1]
  - Stochastic arithmetic to simulate round-off and cancellations
  - Localization techniques to pinpoint source of errors
  - Track precision through CI framework
- **Optimize precision** [2]
  - Simulate custom formats for mixed precision (float, bf16)
  - Tune precision in math library calls

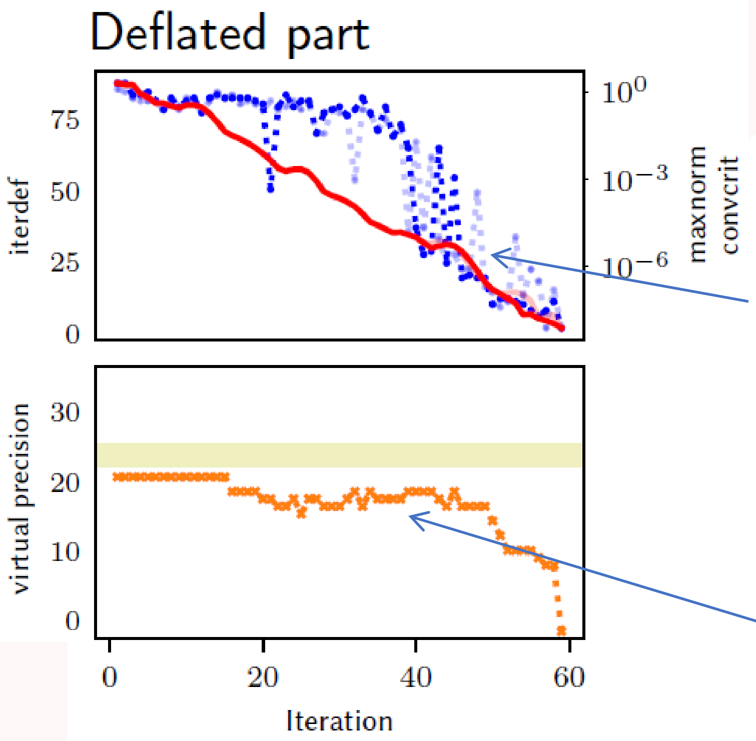
[1] Numerical uncertainty in analytical pipelines leads to impact ul variability in brain networks. Kiar et al. 2021 PLOS ONE.
[2] Study of the effects and benefits of Custom-Precision Mathematical libraries in HPC codes. Brun et al. 2021 IEEE TETC.

Track kernel accuracy during the development process of QMCkl.



Git commits (QMCkl – SMWB kernels)

Harness mixed-precision: 30% speed-up in deflated conjugate gradient (560 cores / YALES2). [3]



Convergence is preserved and…

…the deflated solver runs on **single precision**.

[3] Automatic exploration of reduced floating-point representations in iterative methods. Chatelain et al. Europar'19.

Objectives

1. **Use of automatic generation tools**: from a high level generic ASM generate X86 and ARM versions. This will allow to directly embed low level code (“ASM volatile”).
2. **Use of autotuning tools:** very useful for last mile optimization, explore automatically different code variants and parameters.
3. **Use of advanced performance analysis tools:** monitor not only vectorization ration (% of vector instructions) but also vectorization efficiency (vector width used).
4. **Use of numerical accuracy monitoring tools:** in particular identify code fragments sensitive to accuracy.

A few hundreds of source code lines but restructured for heavy use of dense matrix multiplication operations

The initial equation implemented in CHAMP is:

$$J_{\text{een}}(\mathbf{r},\mathbf{R}) = \sum_{\alpha=1}^{N_{\text{nucl}}} \sum_{i=1}^{N_{\text{elec}}} \sum_{j=1}^{i-1} \sum_{p=2}^{N_{\text{nord}}} \sum_{k=0}^{p-1} \sum_{l=0}^{p-k-2\delta_{k,0}} c_{lkp\alpha} \left(r_{ij}\right)^k \left[\left(R_{i\alpha}\right)^l + \left(R_{j\alpha}\right)^l\right] \left(R_{i\alpha}\, R_{j\alpha}\right)^{(p-k-l)/2}$$

It was rewritten as

$$J_{\text{een}}(\mathbf{r},\mathbf{R}) = \sum_{p=2}^{N_{\text{nord}}} \sum_{k=0}^{p-1} \sum_{l=0}^{p-k-2\delta_{k,0}} \sum_{\alpha=1}^{N_{\text{nucl}}} c_{lkp\alpha} \sum_{i=1}^{N_{\text{elec}}} \bar{\mathrm{R}}_{i,\alpha,(p-k-l)/2}\, \bar{\mathrm{P}}_{i,\alpha,k,(p-k+l)/2}$$

with

$$\bar{\mathrm{P}}_{i,\alpha,k,l} = \sum_{j=1}^{N_{\text{elec}}} \bar{\mathrm{r}}_{i,j,k}\, \bar{\mathrm{R}}_{j,\alpha,l}.$$