

const auto & buffer = engine.results()

engine.results() returns a
reference to a std::vector of pointers

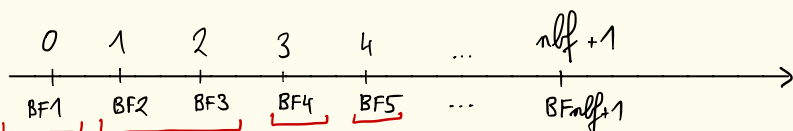
buffer[0] is a pointer to the
first calculated integral of these specific shells
buffer.size() is always 1, so

for (auto sh1=0; sh1!=nsh; ++sh1) {

for (auto sh2=0; sh2!=nsh; ++sh2) {

engine.compute(obs[sh1], obs[sh2]);

example:



sh1 sh2 sh3 sh4 ...
f1 traverses shell 1
f2 traverses shell 2

(BF1 BF2)	(BF1 BF3)	...	
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LIBINT2 STORES
ROW MAJOR FORM

CALCULATED INTEGRALS IN
general index =

calculated_integrals = buffer[0]

$$f1 * nbf - sh2 + f2$$