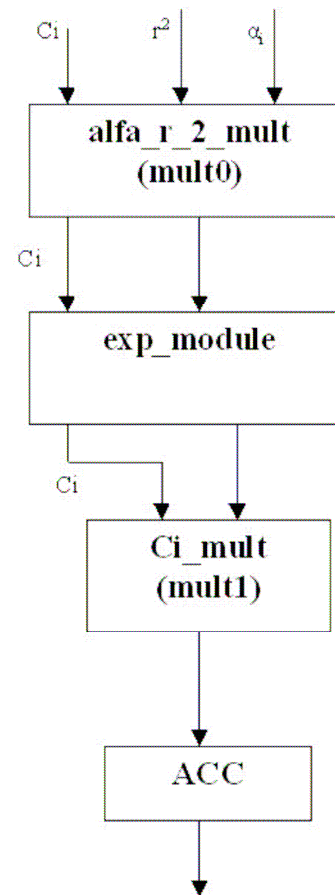


Analysis of the Basic Implementation Aspects of Hardware-accelerated Density Functional Theory Calculations

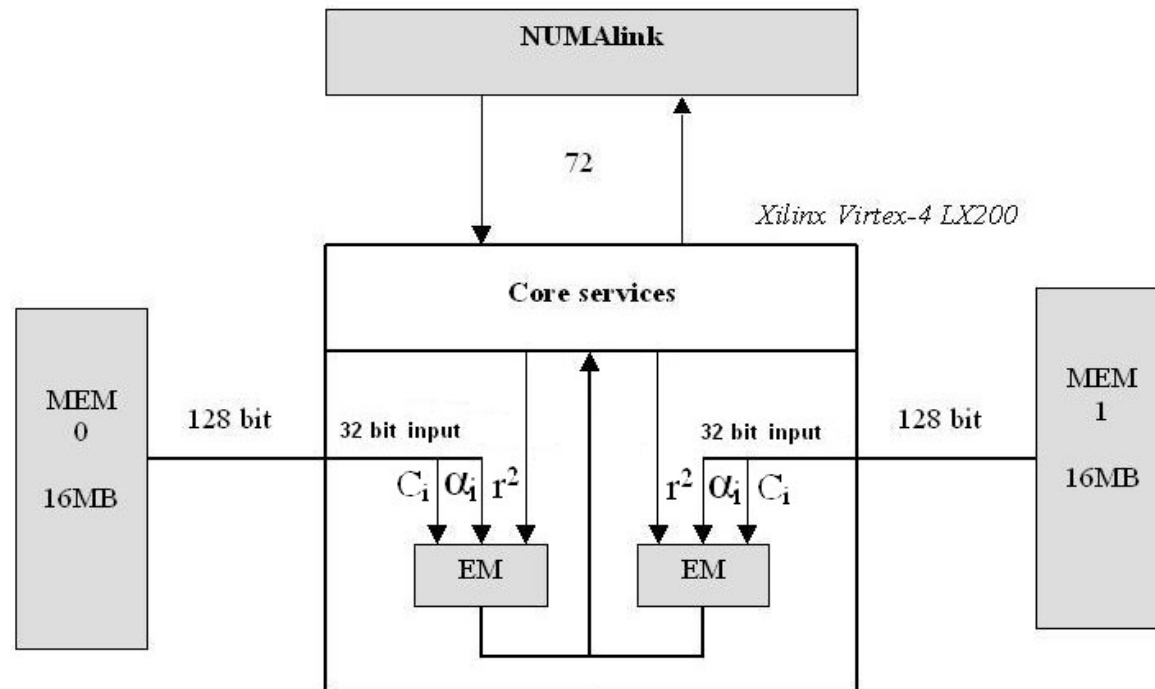
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Application



$$\chi_{klm}(\mathbf{r}) = r_x^k r_y^l r_z^m \sum_i C_i e^{-\alpha_i r^2}$$

Implementation



Implementation results	# 4-input LUT	# flip-flops	# 18-Kb BRAMs
EP module alone	2229 (1%)	1975(1%)	2(0.006%)
EP module with the core services	11560 (7%)	15922(9%)	25(7%)

Acceleration

C code

```
for(t=0;t<size;t++)  
b_c_table[t] = b[t]*c[t];  
  
for(t=0;t<size;t++)  
exp_table[t] = (b_c_table[t]);  
  
for(t=0;t<size;t++)  
result = result + a[t]*exp_table[t];
```

Itanium 2 1.6 Ghz – 20ns

Speed-up

2 EP – 2x

4 EP – 4x

(If Direct_IO mode activated:

4 EP – approx. 8x)