

**TurboGAP**

# Top 10 kernels before and after

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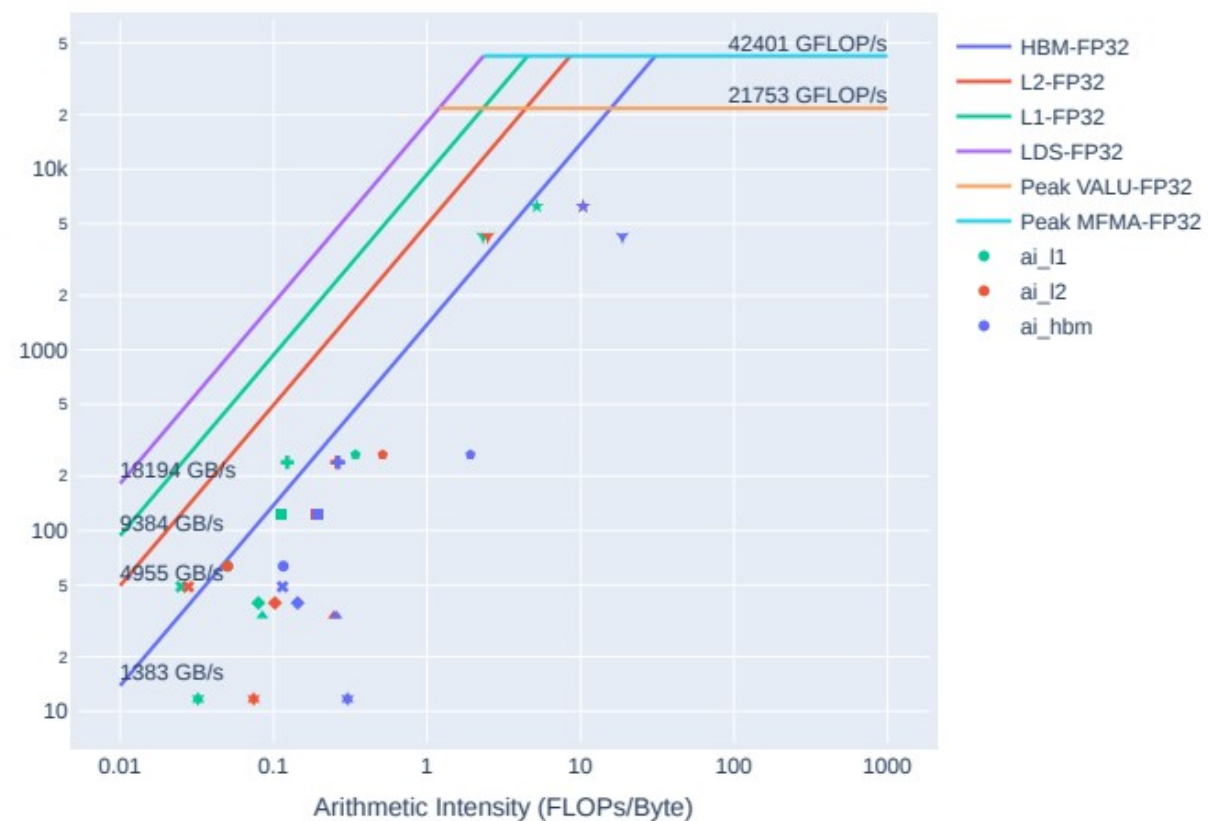
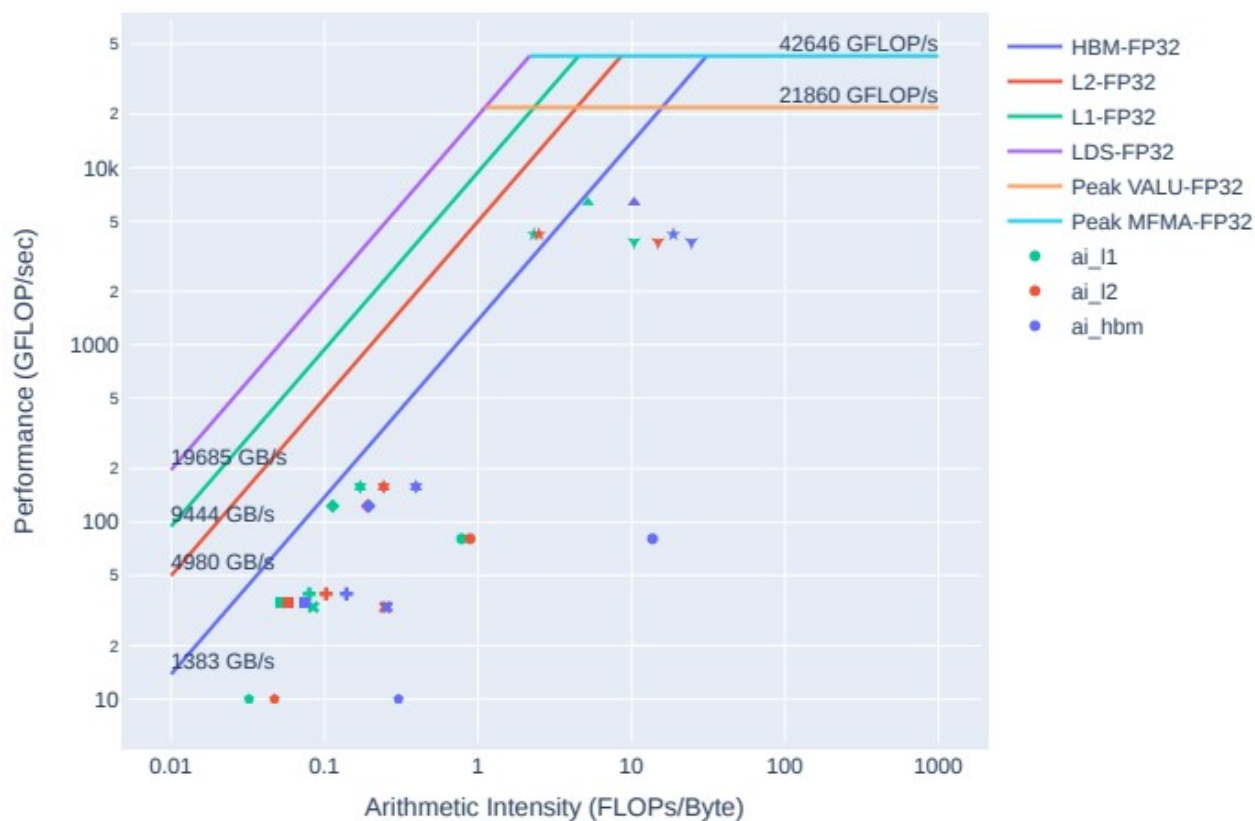
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	KernelName	Count	Sum(ns)	Mean(ns)	Median(ns)	Pct
0	cuda_soap_forces_virial_two(int, double*, int, int*, int*, HIP_vector_type<double, 3u>*, HIP_vector_type<double, 3u>...	441	2685706683.00	6090037.83	6042742.00	38.93
1	cuda_get_soap_der_one(double*, double*, double*, double*, HIP_vector_type<double, 2u>*, HIP_vector_type<double, 2u>*,...	441	2409008202.00	5462603.63	5461140.00	34.92
2	cuda_get_derivatives_new_new(double*, HIP_vector_type<double, 2u>*, double*, HIP_vector_type<double, 2u>*, HIP_vector...	441	582627721.00	1321151.29	1324165.00	8.44
3	cuda_get_exp_coeff_der_one(HIP_vector_type<double, 2u>*, double*, double*, bool*, double*, double*, double, int, int,...	441	362738938.00	822537.27	822723.00	5.26
4	void gemvn_kernel<64, 16, int, double, double, double>(int, int, double, long, double const*, long, int, long...	441	130958571.00	296958.21	297442.00	1.90
5	gpu_pow(double*, double*, double, int) [clone .kd]	882	110287395.00	125042.40	124961.00	1.60
6	cuda_get_soap_p(double*, double*, double*, HIP_vector_type<double, 2u>*, bool*, int, int, int, int) [clone .kd]	441	104922302.00	237919.05	239041.00	1.52
7	Cijk_Alik_Bljk_DB_MT64x16x16_MI16x16x4x1_SN_1LDSB0_APM1_ABV0_ACED0_AF0EM1_AF1EM1	441	74660591.00	169298.39	169281.00	1.08

	KernelName	Count	Sum(ns)	Mean(ns)	Median(ns)	Pct
0	naive_transpose_cnk_arrays(HIP_vector_type<double, 2u>*, HIP_vector_type<double, 2u>*, int, int, int) [clone .kd]	1764	602582422.00	341600.01	413281.00	19.98
1	cuda_get_derivatives_new_new(double*, HIP_vector_type<double, 2u>*, double*, HIP_vector_type<double, 2u>*, HIP_vector...	441	582471514.00	1320797.08	1327042.00	19.31
2	cuda_get_exp_coeff_der_one(HIP_vector_type<double, 2u>*, double*, double*, bool*, double*, double*, double, int, int,...	441	358708583.00	813398.15	813281.00	11.89
3	cuda_get_soap_der_one(double*, double*, double*, double*, double*, double*, HIP_vector_type<double, 2u>*, HI...	441	358139467.00	812107.63	814561.00	11.88
4	naive_transpose_soap_rad_azi_pol(double*, double*, int, int) [clone .kd]	2646	154854142.00	58523.86	68080.50	5.13
5	void gemvn_kernel<64, 16, int, double, double, double>(int, int, double, long, double const*, long, int, long...	441	127989122.00	290224.77	291040.00	4.24
6	gpu_pow(double*, double*, double, int) [clone .kd]	882	115731363.00	131214.70	131200.00	3.84
7	cuda_soap_forces_virial_two(int, double*, int, int*, int*, HIP_vector_type<double, 2u>*, HIP_vector_type<double, 2u>...	441	114165445.00	258878.56	258881.00	3.79

# Roofline Profile, before and after



# Optimizations

- Atomic operations
- Memory accesses