



## Supplement of

## **GNAQPMS v1.1: accelerating the Global Nested Air Quality Prediction Modeling System (GNAQPMS) on Intel Xeon Phi processors**

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Advanced Hotspots Hotspots vie	ewpoint ( <u>change</u> ) @								INTEL VTUNE AMPLIFIER XE 20
🔄 🛄 Collection Log 🕕 Analysis Target 🔥 Ana	ilysis Type 🛛 Summary 🗟 Bottom-up	🗣 Caller/Callee 🛛 🗳	Top-down 1	Tree 📑	Platform				
Grouping: Source Function / Function / Call Stack									: × Q
, s (	CPU Time (4)								
Source Function / Function / Call Stack	Effective Time by Utilization *	Spin Time				CPI Rate	CPU Frequency Ratio	Module	Function (Full)
	Idle Poor Ok Ideal Over	Communicati	Other	Other					
I MPI COLL SHM GENERIC RELEASE BCAST	378.599s	0s	0s	Os	420,338,800,000	2.524	1.221		I MPI COLL SHM GENERIC REL
Jibm_powf_19	243.909s	0s	0s	0s	1,375,979,600,000	0.495	1.218		_libm_powf_l9
svml_expf4_h9	187.933s	0s	Os	Os	1,149,689,500,000	0.458	1.221		_svml_expf4_h9
mbe_solver	164.855s	05	Os	Os	1,457,884,900,000	0.316	1.219		mbe_solver
libm_log10f_l9	129.002s	0s	0s	Os	361,044,800,000	0.998	1.218		_libm_log10f_l9
libm_expf_19	128.984s	0s	0s	0s	865,887,900,000	0.415	1.214		_libm_expf_19
• main	114.793s	0s	0s	Os	543,388,800,000	0.590	1.218		main
ode_gas	114.042s	<b>O</b> S	Os	Os	534,467,100,000	0.596	1.217		ode_gas
mapgas_com	106.510s	0s	0s	Os	657,475,700,000	0.454	1.222		mapgas_com
troe	100.200s	0s	Os	Os	340,434,500,000	0.825	1.222		troe
peroxyrateconstants	99.208s	0s	0s	0s	721,940,100,000	0.384	1.219		peroxyrateconstants
gasrates_com	82.307s	<b>O</b> S	0s	Os	587,242,900,000	0.393	1.223		gasrates_com
ode_com	67.533s	<b>O</b> S	<b>0</b> 5	Os	361,274,800,000	0.518	1.208		ode_com
advec1d	64.133s	0s	0s	Os	353,965,400,000	0.506	1.217		advec1d
photoparam2	45.788s	Os	Os	Os	313,795,900,000	0.405	1.210		photoparam2
selectgasregime	42.888s	0s	Os	0s	328,173,200,000	0.364	1.215		selectgasregime
libm_sse2_sincosf	42.185s 🛑	Os	Os	Os	255,723,200,000	0.463	1.224		libm_sse2_sincosf
gasrateconstants_com	41.771s 🛑	0s	0s	Os	244,869,500,000	0.473	1.207		gasrateconstants_com
convect	39.821s 🛑	0s	0s	Os	315,323,100,000	0.355	1.225		convect
arr	37.673s 🛑	0s	0s	Os	250,214,700,000	0.418	1.209		arr
LMPLCOLL_SHM_GENERIC_GATHER_REDUCE	28.949s 📕	0s	Os	Os	32,411,600,000	2.500	1.220		L_MPI_COLL_SHM_GENERIC_GA
domassbalance	25.472s 📕	0s	0s	Os	156,158,500,000	0.458	1.224		domassbalance
libm sinf 19	21.192s								libm_sinf_l9

Figure S1. The hotspot functions detected by Vtune in Base-V GNAQPMS. The red bar shows the low CPU utilization of the functions in Base-V GNAQPMS, which could be optimized to improve the code performance.

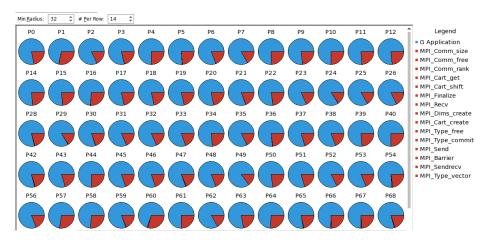


Figure S2. Load balance situation of GANQPMS on single CPU nodes. The pie figures shows the contributions from MPI and application codes for the GNAQPMS on the MPI processes. The almost equal blues parts indicate that the load balance is not the bottleneck of Base-V GNAQPMS.

Advanced Hotspots Hotspots view	point (change) @							INTEL VTUNE AMPLIFIER XE 201
								INTEL VIUNE AMPLIFIER AE 20
🔺 📟 Collection Log 🔮 Analysis Target 🛛 🗛 Analys	is Type 🛛 🛍 Summary 🚳 Bottom-up 📢	Caller/Calle	e 🛛 🗳 Top-down T	ree 🛛 🖻 Platform				
Grouping: Source Function / Function / Call Stack								÷ 🛠 Q
Source Function / Function / Call Stack	CPU Time a							
	Effective Time by Utilization *	Spin Time	Overhead Time	Instructions Retired	CPI Rate	CPU Frequency Ratio	Module	
svml_expf8_l9	317.008s	Os	0s	1,046,095,200,000	0.818	1.177		svml_expf8_l9
gasrates_com	158.629s	0s	0s	312,029,500,000	1.371	1.175		gasrates_com
▶ ode_gas	135.309s	0s	0s	314,757,300,000	1.155	1.171		ode_gas
▶ adv_hori	112.086s	0s	0s	194,191,300,000	1.551	1.171		adv_hori
I_MPI_COLL_SHM_GENERIC_RELEASE_BCAST	102.508s	0s	0s	108,640,500,000	2.628	1.214		I_MPI_COLL_SHM_GENERIC_RELEASE
peroxyrateconstants	97.101s	0s	0s	297,369,300,000	0.883	1.179		peroxyrateconstants
ode_com	88.283s	0s	0s	343,072,600,000	0.688	1.166		ode_com
gasrateconstants_com	86.685s	0s	0s	323,971,100,000	0.724	1.178		gasrateconstants_com
convect	60.367s	0s	0s	79,453,500,000	2.046	1.174		convect
> mbe_solver	43.196s	0s	0s	164,949,100,000	0.705	1.173		mbe_solver
MAIN_\$omp\$parallel_for@3793	38.604s 📕	0s	0s	153,564,100,000	0.698	1.211		MAIN\$omp\$parallel_for@3793
intel_avx_rep_memset	29.173s	0s	0s	53,456,600,000	1.501	1.199		intel_avx_rep_memset
selectgasregime	26.321s	0s	0s	126,509,200,000	0.547	1.146		selectgasregime
main_hotspots_mp_hotspot5_\$omp\$parallel_for@39	25.748s	0s	0s	5,032,400,000	13.770	1.173		main_hotspots_mp_hotspot5_\$omp\$
cfcalc	23.374s	0s	0s	69,234,600,000	0.922	1.190		cfcalc
libm_powf_19	23.052s	0s	0s	92,365,700,000	0.675	1.179		libm_powf_l9
mapgas_com	20.603s	0s	0s	49,785,800,000	1.103	1.162		mapgas_com
ode_het	20.583s	0s	0s	66,612,600,000	0.839	1.183		ode_het
mapgasspecies	19.638s	0s	0s	85,730,200,000	0.618	1.176		mapgasspecies
photoparam2	19.527s	0s	0s	72,406,300,000	0.731	1.182		photoparam2
libm_cosf_19	19.302s	0s	0s	60,128,900,000	0.871	1.183		libm_cosf_l9
gasrates_het	18.697s 🛢	0s	Os	34,431,000,000	1.457	1.170		gasrates_het
▶ ode_urb	18.176s							

Figure S3. Hotspot functions detected by Vtune in Opt-V GNAQPMS. The green bars

indicate the high CPU utilization directly.