NEKRS: OVERVIEW

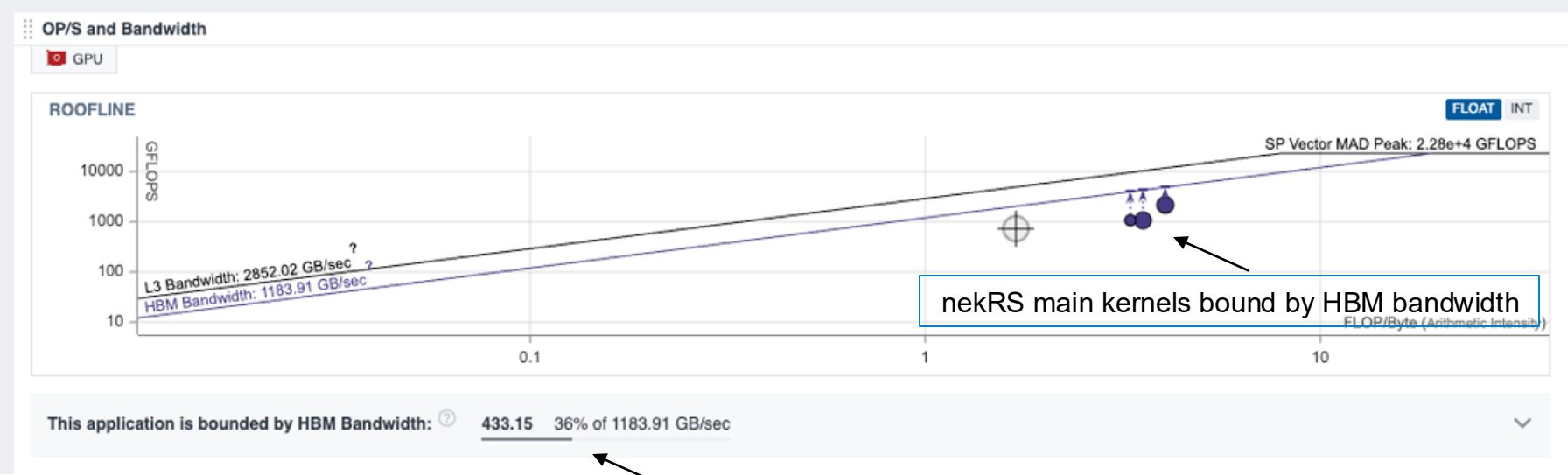
- nekRS solves the governing equations using a spectral element discretization
- nekRS employs high-order spectral elements in which the solution, data, and test functions are represented as locally structured Nth-order tensor product Lagrange polynomials on a set of E globally unstructured curvilinear hexahedral brick elements.
- Within each element, the Gauss–Lobatto–Legendre (GLL) quadrature points are set as the nodes of the Lagrange basis polynomials.
- For polynomial order N, there are $(N+1)^3$ GLL points in an element, leading to $E(N+1)^3$ total GLL points in the mesh.
- nekRS, like many other CFD codes, uses domain decomposition to solve very large meshes on distributed systems with MPI (each sub-domain is assigned to a distinct MPI rank)
- The size of the mesh, E, the polynomial order, N, and the number of MPI ranks, M, determine the computational load on each MPI rank (approx. $E(N+1)^3/M$)

NEKRS: OVERVIEW

- Common polynomial order N for science runs: 7, 9
- Common loading for good nekRS scaling (GLL points per MPI rank):
  - —Aurora: 4-5 million

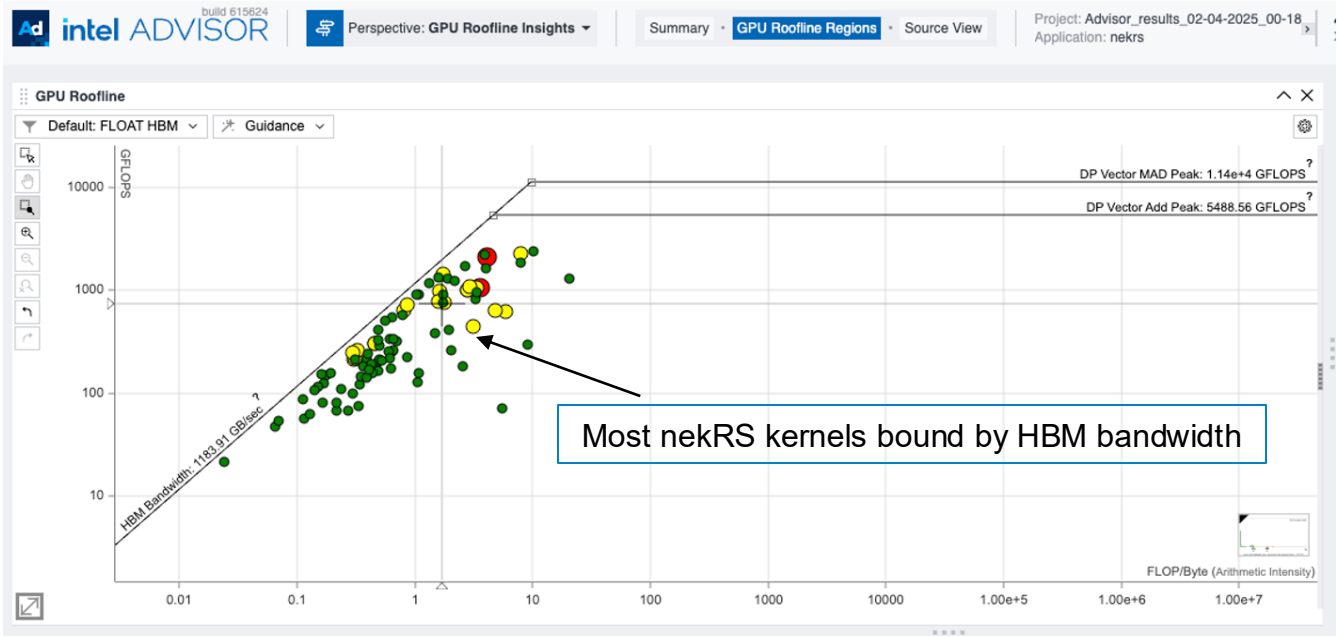
ROOFLINE (4M GLL POINTS PER RANK, N=7)

- nekRS roofline collected with Intel Advisor on single Aurora PVC tile
  - nekRS main kernels are **HMB bandwidth bound**
  - nekRS application as a whole is also **HBM bandwidth bound**



ROOFLINE (4M GLL POINTS PER RANK, N=7)

- nekRS roofline collected with Intel Advisor on single Aurora PVC tile
  - Most nekRS kernels are **HBM bandwidth bound**
  - Dependency on loading (GLL points per GPU) and p-order to be explored further



MPI PROFILES

- nekRS high-speed network usage
  - Collected MPI memory traffic usage with iprof on Aurora
  - **>50% of memory traffic done by Isend/Irecv** (point-to-point communication dominates time step loop)

Explicit memory traffic (BACKEND_MPI) | 1 Hostnames | 1 Processes | 1 Threads |

Name	Byte	Byte(%)	Calls	Average	Min	Max
MPI_Isend	2.19GB	56.25%	45793	47.93kB	0B	100.66MB
MPI_Irecv	1.45GB	37.23%	45996	31.58kB	0B	2.43MB
PMPI_Status_set_elements_x	217.67MB	5.58%	216	1.01MB	4B	1.05MB
MPI_File_write_all	18.14MB	0.46%	9	2.02MB	4B	7.74MB
MPI_Issend_c	18.14MB	0.46%	26	697.66kB	4B	1.05MB
MPI_Recv	187.62kB	0.00%	337	556.72B	8B	27.66kB
MPI_Allreduce	71.62kB	0.00%	3863	18.54B	4B	12.00kB
MPI_Send	15.21kB	0.00%	873	17.42B	0B	56B
MPI_Bcast	9.90kB	0.00%	246	40.23B	1B	1.98kB
MPI_Irecv_c	4.69kB	0.00%	86	54.51B	16B	144B
PMPI_Bcast	4.19kB	0.00%	15	279.40B	4B	4.10kB
PMPI_Allreduce	2.04kB	0.00%	54	37.70B	4B	192B
MPI_Isend_c	416B	0.00%	9	46.22B	16B	144B
MPI_Reduce	216B	0.00%	11	19.64B	16B	24B
MPI_Scan	164B	0.00%	23	7.13B	4B	8B
Total	3.90GB	100.00%	97557			