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High Order Matrix-Free FEM on GPU

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- Traditional Matrix-based FEM typically involves two primary steps:

$$K = \sum_{e=1}^{N_e} P_e^T K_e P_e \qquad \text{(Assembly)}$$

$$K u_1 = u_2 \qquad \text{(Iterative Solver)}$$

- Requires storage for the stiffness matrix (K).
- Element matrices and right-hand side vectors are transferred from local memory to global memory.

- Iterations are carried out in-place.

$$u^2 = \sum_{e=1}^{N_e} P_e^T K^e (P_e u^1) \qquad \text{(Iteration on the fly)}$$

- Stiffness matrix (K) is not stored.
- Only the local solution (u^2) is transferred from local memory to global memory.

Mass Matrix Operator Example:

$$M^e_{mn} = \sum_{q=1}^{N_q} w_q |J^e| \phi_m(\xi_q, \eta_q, \zeta_q) \phi_n(\xi_q, \eta_q, \zeta_q)$$
$$M^e u^1_e = u^2_e$$

- Local element mass matrix (M_e) can be formed and then multiplied by the local solution (u_1).
- The computational complexity for the forming local stiffness matrix is $O((p+1)^{2d})$. (p: degree, d: dimension).

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- Interpolation polynomials are expressed in tensor product of 1-D polynomials.

$$\phi(\xi, \eta, \zeta) = \phi_i(\xi) \otimes \phi_j(\eta) \otimes \phi_k(\zeta)$$

- The evaluation of each shape function at each quadrature point results in a matrix ($I^{1D}_{ia} = \phi_{ia}(\xi_q)$).
- Final form of the mass matrix in tensor notation;

$$M^e = (I^{1D} \otimes I^{1D} \otimes I^{1D})^T J (I^{1D} \otimes I^{1D} \otimes I^{1D})$$

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- The mass matrix operator can be expressed in sum factorization form using index notation:

$$u^e_{ijk} = \sum_{a=0}^{q} \phi_{ia}(\xi_q) \sum_{b=0}^{q} \phi_{jb}(\eta_q) \sum_{c=0}^{q} \phi_{kc}(\zeta_q) \sum_{a,b,c=0}^{q} J_{abc} \sum_{i=0}^{p} \phi_{ia}(\xi_q) \sum_{j=0}^{p} \phi_{jb}(\eta_q) \sum_{k=0}^{p} u^e_{ijk} \phi_{kc}(\zeta_q)$$

- Performing operations in Mat-vec multiplication form reduces computational complexity to $O(d(p+1)^{d+1})$.

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- Our implementations are based on the CEED benchmarks.
- CEED benchmarks can be classified into two main catagories:
  1. Communication-free algorithms (Mass, stiffness matrix operators).
  2. Communication based algorithms (Preconditioned CG).
- As the current algorithms are communication-free, we employ a single GPU.
- Programming models are CUDA and Kokkos.

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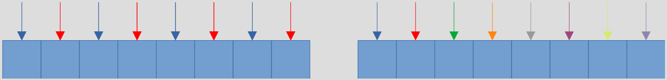
- Optimization techniques for our implementations can be grouped into two main categories.
  1. Thread granularity (block-centric, warp-centric)
  2. Thread-level Data Mapping (strided fashion, simple map)



($\rightarrow$: thread ■ : array entry)

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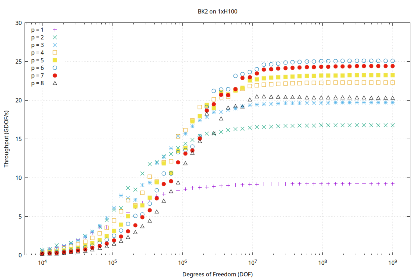
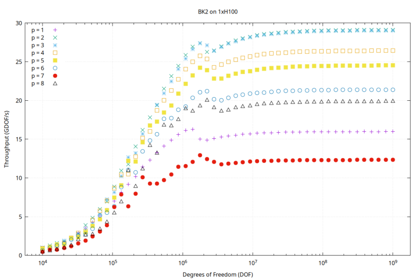
Preliminary Results and Findings

Strided access implementations offer more flexibility in thread block size.



A simple map is approximately 30% faster, but thread block occupancy depends on the polynomial order (i.e p=7, blockDim=729, max thread per SM=2048).



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