A HIGHLY SCALABLE KERNEL BASED CLUSTERING ALGORITHM FOR MOLECULAR DYNAMICS

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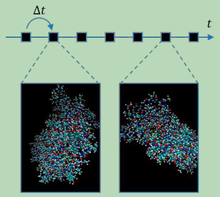
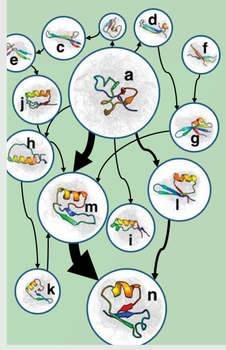
CLUSTERING MD TRAJECTORIES

A BIG DATASET IN HIGHLY DIMENSIONAL SPACE



- **MD trajectory:** discretized **time evolution of the atomic positions** for an entire molecular system.
- Up to $\mathbf{10^{10}}$ **frames** (10μs simulation, 2fs timestep)
- Each frame: $\sim\mathbf{10^5}$ **atom coordinates** in 3D space



GETTING VALUE OUT OF DATA

- Biomolecular processes of interest evolve through a series of metastable states. *How do we define those states in a rigorous unbiased way? Can we build reliable kinetic models?*
- Clustering is the core tool in probabilistic coarse grained model such as **Markov State Models** [1].
- Clustering by itself can be used to extract human-interpretable mesostates to describe a process [2].

A NOVEL ALGORITHM SUITED FOR MD: MINIBATCH DISTRIBUTED KERNEL K-MEANS

DESIGN GUIDELINES

- **Avoid featurization procedures:** they are expensive and inaccurate, our algorithm is based on **Kernel K-means** which **does not require an explicit feature space**. Indeed the whole algorithm requires just a distance metric being expressed in terms of a kernel matrix with the following form,

$$K_{i,j} = e^{-\gamma\, d^2(x_i,x_j)}\,;\; d^2 = \text{aligned RMSD}^2(x_i,x_j) = \frac{1}{N_{atoms}}\sum_{k=1}^{N_{atoms}}\left\|x_{i,k}-x_{j,k}\right\|^2$$

- **Target HPC facilities:** being inspired by the work of Zhang, Rudnicky [3] we devised a **fully distributed algorithm** based on the following quantities,

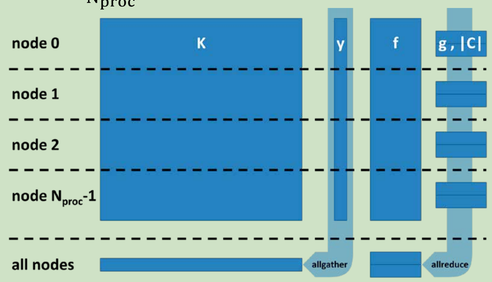
$$f(x_i, C) = -\frac{2}{|C|}\sum_{x_j\in C} K(x_i,x_j);\; g(C) = \frac{1}{|C|^2}\sum_{x_i\in C}\sum_{x_j\in C} K(x_i,x_j)$$

- **Think big:** to scale on large datasets we **divide the data into mini-batches** which are presented to the algorithm one after the other [4].

e.g. 10^6 frames › 16 nodes, 32 GB /node › 4 minibatches (dobule precision), 3 minibatches (single precision)

DISTRIBUTION STRATEGY

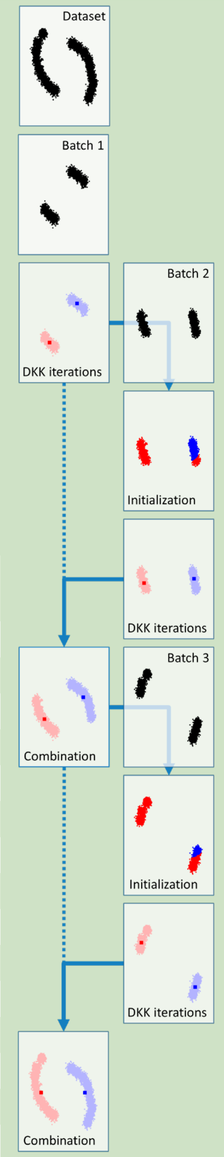
- K, f matrices as well as labels y are fully distributed.
- Each node holds a partial copy of g and |C| .
- Each node deals with $\frac{N^2}{N_{proc}}$ kernel elements.
- $2N_c + \frac{N}{N_{proc}}$ all-to-all communications per step.



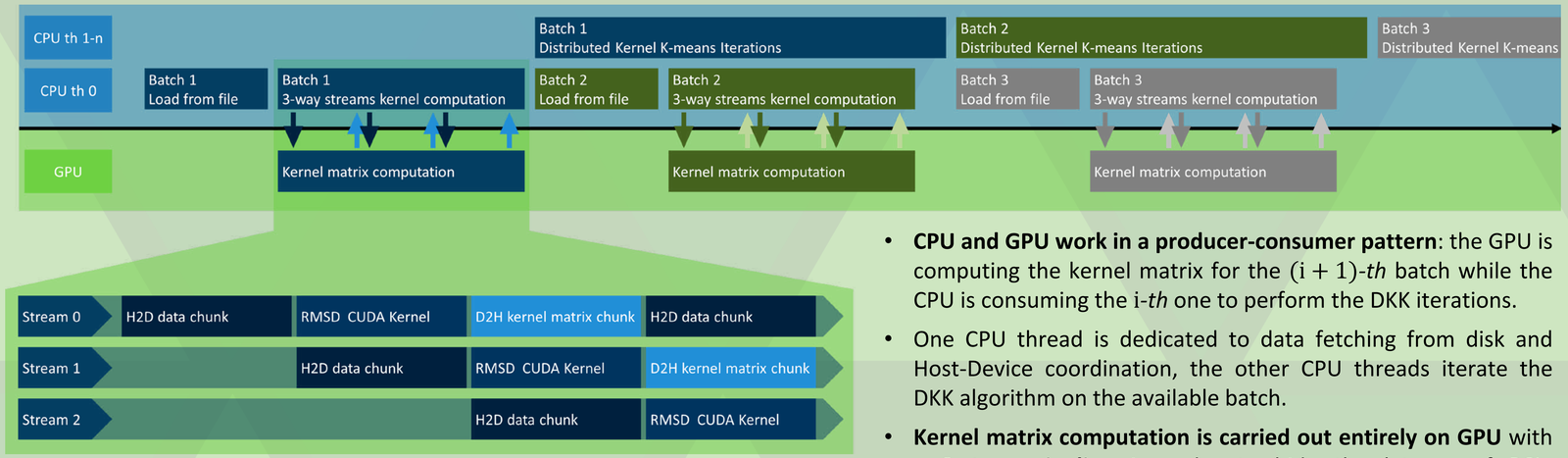
ALGORITHM PSEUDOCODE

D: dataset, B: batch, N: batch size, K: kernel matrix, m: medoids, y: labels

for i=1 to |D|/N **do**
  B ← N frames uniformly sampled from D
  K ← compute distributed kernel matrix
  if (i==1) **then** m_i ← kernelized k-means++ init
  y ← label according to nearest neighbor medoid
  while not converged **do**
    compute local f, g, |C| based on K, y
    allreduce g, |C|
    for every sample: $y_j \leftarrow \text{argmin}_c\,(\, f(x_j,C) + g(C)\,)$
    allgather updated y on each node
  end do
  m_{i+1} ← find mini-batch medoids
  $m_{i+1} \leftarrow a \cdot m_i + (1\text{-}a) \cdot m_{i+1}$; $a=|C|_i/(|C|_i+|C|_{i+1})$
end for



GPU ACCELERATION



- **CPU and GPU work in a producer-consumer pattern**: the GPU is computing the kernel matrix for the $(i+1)$-*th* batch while the CPU is consuming the i-*th* one to perform the DKK iterations.
- One CPU thread is dedicated to data fetching from disk and Host-Device coordination, the other CPU threads iterate the DKK algorithm on the available batch.
- **Kernel matrix computation is carried out entirely on GPU** with a **3-stage pipeline** in order to hide the latency of PCIe communications.

RMSD CUDA KERNEL

- Among the possible algorithms to compute **best-aligned RMSD** we picked the **quaternion based method proposed by Theobald** [5].
- It is **fast and stable** (can be implemented successfully in **mixed single/double precision** fashion).
- To the best of our knowledge the only publicly available GPU implementation of such algorithm is the one introduced by Gil and Guallar [6] in the python package pyRMSD. Such an implementation shows good speedups but still there is **room for improvements**.
- It's our plan to work on the data layout in memory to improve GPU performances (in particular **AoS to SoA transition will be explored to allow coalesced memory access**).

CONCLUSIONS AND OUTLOOKS

- We present a distributed kernel k-means based **algorithm to perform large scale clustering on MD trajectories**. The algorithm is **fully implemented in C++, distributed over MPI**, modular and extensible.
- Single node performances are not sufficient for real-world scenarios without GPU acceleration. **The offload strategy presented here is ideally paired with a self-tuning procedure in order to maximally squeeze the hardware of modern HPC GPU-endowed facilities.**
- The exploitation of approximate techniques where **sparsity on the kernel matrix is induced** by randomly selecting a subset of samples as representation basis [7], **aiming at unprecedented scales** (10^9 - 10^10 frames), which are compatible with the huge amount of simulative data produced in the foreseeable future.

REFERENCES

[1] Voelz, Vincent A., et al. *Journal of the American Chemical Society* 132.5: 1526-1528 (2010).
[2] Decherchi, Sergio, et al. *Nature communications* 6 (2015).
[3] Zhang, Rong, et al. *Pattern Recognition, 16th International Conference on*. Vol. 4. IEEE (2002).
[4] Sculley, David. *Proceedings of the 19th international conference on WWW*. ACM,(2010).
[5] Theobald, Douglas L. *Acta Crystallographica Section A* 61.4: 478-480 (2005): .
[6] Gil, Víctor A., and Víctor Guallar. *Bioinformatics*: btt402 (2013).
[7] Chitta, Radha, et al. *Proceedings of the 17th ACM SIGKDD*. ACM (2011).

ACKNOWLEDGEMENTS

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