

A Parallel Approximation Algorithm for Maximizing Submodular b -MATCHING *

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Abstract

We design new serial and parallel approximation algorithms for computing a maximum weight b -matching in an edge-weighted graph with a submodular objective function. This problem is NP-hard; the new algorithms have approximation ratio $1/3$, and are relaxations of the Greedy algorithm that rely only on local information in the graph, making them parallelizable. We have designed and implemented Local Lazy Greedy algorithms for both serial and parallel computers. We have applied the approximate submodular b -matching algorithm to assign tasks to processors in the computation of Fock matrices in quantum chemistry on parallel computers. The assignment seeks to reduce the run time by balancing the computational load on the processors and bounding the number of messages that each processor sends. We show that the new assignment of tasks to processors provides a four fold speedup over the currently used assignment in the NWChemEx software on 8000 processors on the Summit supercomputer at Oak Ridge National Lab.

1 Introduction

We describe new serial and parallel approximation algorithms for computing a maximum weight b -MATCHING in an edge-weighted graph with a submodular objective function. This problem is NP-hard; the new algorithms have approximation ratio $1/3$, and are variants of the Greedy algorithm that rely only on local information in the graph, making them parallelizable. We apply the approximate submodular b -MATCHING algorithm to assign tasks to processors in the computation of Fock matrices in quantum chemistry on parallel computers, in order to balance the computational load on the processors and bound the number of messages that a processor sends.

A b -MATCHING is a subgraph of the given input graph, where the degree of each vertex v is bounded by a given natural number $b(v)$. In linear (or modular)

b -MATCHING the objective function is the sum of the weights of the edges in a b -MATCHING, and we seek to maximize this weight. The well-known maximum edge-weighted matching problem is the 1-matching problem. Although these problems can be solved in polynomial time, in recent years a number of approximation algorithms have been developed since the run time of exact algorithms can be impractical on massive graphs. These algorithms are based on the paradigms of short augmentations (paths that increase the cardinality or weight of the matching) [32]; relaxations of a global ordering (by non-increasing weights) of edges to local orderings [34]; partitioning heavy weight paths in the graph into matchings [12]; proposal making algorithms similar to stable matching [18, 26], etc. Some, though not all, of these algorithms are concurrent and can be implemented on parallel computers; a recent survey is available in [33].

Our algorithm employs the concept of an edge being locally dominant in its neighborhood that was first employed by Preis [34] to design the $1/2$ -approximate matching algorithm for (modular or linear) maximum weighted 1-matching; the approximation ratio is as good as the Greedy algorithm, and Preis showed that the algorithm could be implemented in time linear in the size of the graph. Since then there has been much work in implementing variants of the locally dominant edge algorithm for 1-matching and b -matching on both serial and parallel computational models (e.g., [18, 26]). More details are included in [33].

In this paper we employ the local dominance technique, relaxing global orderings to local orderings, to the b -MATCHING problem with submodular objective. We exploit the fact that the b -MATCHING problem may be viewed as a 2-extendible system, which is a relaxation of a matroid. We show that any algorithm that adds locally optimal edges, with respect to the marginal gain for a submodular objective function, to the matching preserves the approximation ratio of the corresponding global Greedy algorithm. This result offers a blueprint to design many approximation algorithms, of which we develop one: LOCAL LAZY GREEDY algorithm. Testing

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for local optimality in the submodular objective is more expensive than in the linear case due to the variability of the marginal gain. To efficiently maintain marginal gains, we borrow an idea from the lazy evaluation of the Greedy algorithm. Combining local dominance and lazy Greedy techniques, we develop a LOCAL LAZY GREEDY algorithm, which is theoretically and practically faster than the Lazy Greedy algorithm. The runtime of both these algorithms are analyzed under a natural local dependence assumption on the submodular function. Since our algorithm is parallelizable thanks to the local orderings, we show good scaling performance on a shared memory parallel environment. To the best of our knowledge, this is the first parallel implementation of a submodular b -MATCHING algorithm.

Submodular b -MATCHING has applications in many real-life problems. Among these are content spread maximization in social networks [8], peptide identification in tandem mass spectrometry [2, 3], word alignment in natural language processing [25], and diversity maximizing assignment [1, 11]. Here we show another application of submodular b -MATCHING in load balancing the Fock matrix computation in quantum chemistry on a multiprocessor environment. Our approach enables the assignment of tasks to processors leading to scalable Fock matrix computations.

We highlight the following contributions:

- We show that any b -MATCHING that is ϵ -locally dominant w.r.t the marginal gain is $\frac{\epsilon}{2+\epsilon}$ -approximate for submodular objective functions, and devise an algorithm, LOCAL LAZY GREEDY to compute such a matching. Under a natural local dependence assumption on the submodular function, this algorithm runs in $O(\beta m \log \Delta)$ time and is theoretically and practically faster than the popular LAZY GREEDY algorithm. (Here m is the number of edges, Δ is the maximum degree of a vertex, and β is the maximum value of $b(v)$ over all vertices v .)
- We provide a shared memory parallel implementation of the LOCAL LAZY GREEDY algorithm. Using several real-world and synthetic graphs, we show that our parallel implementation scales to more than sixty-five cores.
- We apply submodular b -MATCHING to generate an assignment of tasks to processors for building Fock matrices in the NWChemEx quantum chemistry software. The current assignment method used there does not scale beyond 3000 processors, but our assignment shows a four-fold speedup per

iteration of the Fock matrix computation, and scales to 8000 cores of the Summit supercomputer at ORNL.

2 Background

In this section we describe submodular functions and their properties, formulate the submodular b -MATCHING problem, and discuss approximation algorithms for the problem.

2.1 Submodular b -MATCHING

DEFINITION 2.1. (MARGINAL GAIN) *Given a ground set X , the marginal gain of adding an element $e \in X$ to a set $A \subseteq X$ is*

$$\rho_e(A) = f(A \cup \{e\}) - f(A).$$

The marginal gain may be viewed as the discrete derivative of the set A for the element e . Generalizing, the marginal gain of adding a subset Q to another subset A of the ground set X is

$$\rho_Q(A) = f(A \cup Q) - f(A).$$

DEFINITION 2.2. (SUBMODULAR SET FUNCTION)

Given a set X , a real-valued function f defined on the subsets of X is submodular if

$$\rho_e(A) \geq \rho_e(B)$$

for all subsets $A \subseteq B \subseteq X$, and elements $e \in X \setminus B$. The function f is monotone if for all sets $A \subseteq B \subseteq X$, we have $f(A) \leq f(B)$; it is normalized if $f(\emptyset) = 0$.

We will assume throughout this paper that f is normalized. The concept of submodularity also extends to the addition of a set. Formally, for $Q \subseteq X \setminus B$, f is submodular if $\rho_Q(A) \geq \rho_Q(B)$. If f is monotone then $\rho_e(A) \geq 0$, $\forall A \subseteq X$ and $\forall e \in X$.

PROPOSITION 2.1. *Let $S = \{e_1, \dots, e_k\}$, S_i be the subset of S that contains the first i elements of S , and f be a normalized submodular function. Then $f(S) = \sum_{i=1}^k \rho_{e_i}(S_{i-1})$.*

PROPOSITION 2.2. *For sets $A \subseteq B \subseteq X$, and $e \in X$, a monotone submodular function f defined on X satisfies $\rho_e(A) \geq \rho_e(B)$.*

Proof. There are three cases to consider. i) $e \in X \setminus B$: The inequality holds by definition of a submodular function. ii) $e \in A$: Then both sides of the inequality equal zero and the inequality holds again. iii) $e \in B \setminus A$: Then $\rho_e(B) = 0$, and since f is monotone, $\rho_e(A)$ is non-negative. \square

Proposition 2.2 extends to a set, i.e., monotonicity of f implies that for every $A \subseteq B \subseteq X$, and $Q \subseteq X$, $\rho_Q(A) \geq \rho_Q(B)$. Informally Proposition 2.2 states that if f is monotone then the diminishing marginal gain property holds for every subset of X .

We are interested in maximizing a monotone submodular function with b -MATCHING constraints. Let $G(V, E, W)$ be a simple, undirected, and edge-weighted graph, where V, E, W are the set of vertices, edges, and non-negative edge weights, respectively. For each $e \in E$ we define a variable $x(e)$ that takes values from $\{0, 1\}$. Let $M \subseteq E$ denote the set of edges for which $x(e)$ is equal to 1, and let $\delta(v)$ denote the set of edges incident on the vertex $v \in V$. The submodular b -MATCHING problem is

$$(2.1) \quad \begin{aligned} & \max f(M) \\ & \text{subject to} \\ & \sum_{e \in \delta(v)} x(e) \leq b(v) \quad \forall v \in V, \\ & x(e) \in \{0, 1\}. \end{aligned}$$

Here f is a non-negative monotone submodular set function, and $0 \leq b(v) \leq |\delta(v)|$ is the integer degree bound on v . Denote $\beta = \max_{v \in V} b(v)$.

We now consider the b -MATCHING problem on a bipartite graph with two parts in the vertex set, say, U and V , where the objective function is a concave polynomial.

$$(2.2) \quad \begin{aligned} f = \max & \sum_{u \in U} \left(\sum_{e \in \delta(u)} W(e)x(e) \right)^\alpha \\ & + \sum_{v \in V} \left(\sum_{e \in \delta(v)} W(e)x(e) \right)^\alpha \\ \text{subject to} & \\ & \sum_{e \in \delta(u)} x(e) \leq b(u) \quad \forall u \in U, \\ & \sum_{e \in \delta(v)} x(e) \leq b(v) \quad \forall v \in V, \\ & x(e) \in \{0, 1\}. \end{aligned}$$

The objective function Problem 2.2 becomes submodular when $\alpha \in [0, 1]$. This formulation has been used for peptide identification in tandem mass spectrometry [2, 3], and word alignment in natural language processing [25].

2.2 Complexity of Submodular b -MATCHING and Approximation

A *subset system* is a pair (X, \mathcal{I}) ,

where X is a finite set of elements and \mathcal{I} is a collection of subsets of X with the property that if $A \in \mathcal{I}$ and $A' \subseteq A$ then $A' \in \mathcal{I}$. A *matroid* is a subset system (X, \mathcal{I}) which satisfies the property that $\forall A, B \in \mathcal{I}$ and $|A| < |B|$, $\exists e \in B \setminus A$ such that $A \cup \{e\} \in \mathcal{I}$. Here the sets in \mathcal{I} are called *independent sets*. A *subset system* is *k-extendible* [27] if the following holds: let $A \subseteq B$, $A, B \in \mathcal{I}$ and $A \cup \{e\} \in \mathcal{I}$, where $e \notin A$, then there is a set $Y \subseteq B \setminus A$ such that $|Y| \leq k$ and $B \setminus Y \cup \{e\} \in \mathcal{I}$.

Maximizing a monotone submodular function with constraints is NP-hard in general; indeed, it is NP-hard for the simplest constraint of cardinality for many classes of submodular functions [13, 21]. A Greedy algorithm that repeatedly chooses an element with the maximum marginal gain is known to achieve $(1 - 1/e)$ -approximation ratio [31], and this is tight [30]. The Greedy algorithm with matroid constraints is $1/2$ -approximate. More generally, with k -matroid intersection and k -extendible system constraints, the approximation ratio of the Greedy algorithm becomes $1/(k+1)$ [7].

3 Related Work

Here we situate our contributions to submodular b -MATCHING in the broader context of earlier work in submodular maximization. A reader who is eager to get to the algorithms and results in this paper could skip this section on a first reading.

The maximum k -cover problem can be reduced to submodular b -MATCHING [16]. Feige [13] showed that there is no polynomial time algorithm for approximating the max k -cover within a factor of $(1 - 1/e + \epsilon)$ for any $\epsilon > 0$. Thus we obtain an immediate bound on the approximation ratio of submodular b -MATCHING.

New approximation techniques have been developed to expedite the greedy algorithm, especially for cardinality and matroid constraints. Surveys on submodular function maximization under different constraints may be found in [6, 20, 36].

Several approximation algorithms have been proposed for maximizing monotone submodular functions with b -MATCHING constraints. If the graph is bipartite, then the b -MATCHING constraint can be represented as the intersection of two partition matroids, and the Greedy algorithm provides a $1/3$ -approximation ratio. But b -MATCHING forms a 2-extendible system and the Greedy algorithm yields a $1/3$ -approximation ratio for non-bipartite graphs. Feldman *et al.* [14] showed that b -MATCHING is also a 2-exchange system, and they provide a $1/(2 + \frac{1}{p} + \epsilon)$ -approximation algorithm based on local search, with time complexity $O(\beta^{p+1}(\Delta - 1)^{pnm}\epsilon^{-1})$. (Here p is a parameter to be chosen.) The continuous

greedy and randomized LP rounding algorithms have been used in [8] to compute a submodular b -MATCHING algorithm that produces a $(\frac{1}{3+2\epsilon})(1 - \frac{1}{e})$ approximate solution in $O(m^5)$ time.

Recently Fuji [16] developed two algorithms for the problem. One of these, Find Walk, is a modified version of the Path Growing approximation algorithm [12] proposed for 1-matching with linear weights. Mestre [27] extended the idea to b -MATCHING. In [16], Fuji extended this further to the submodular objectives. They showed an approximation ratio of $1/4$ with time complexity $O(\beta m)$. The second algorithm uses randomized local search, has an approximation ratio of $1/(2 + \frac{1}{p}) - \epsilon$, and runs in $O(\beta^{p+1}(\Delta - 1)^{p-1}m \log \frac{1}{\epsilon})$ time in expectation. Here a vertex is chosen uniformly at random in each iteration, and the algorithm searches for a certain length alternating path with increasing weights. This algorithm is similar to the $2/3 - \epsilon$ approximation algorithm for linear weighted matching in [32] and the corresponding b -MATCHING variant in [27]. We list several approximation algorithms for submodular b -MATCHING in Table 1.

Now we consider several related problems that do not have the b -MATCHING constraint.

Assigning tasks to machines is a classic scheduling problem. The most studied objective here is minimizing the makespan, i.e., the maximum total time used by any machine. The problem of makespan minimization can be generalized to a General Assignment Problem (GAP), where there is a fixed processing time and a cost associated with each task and machine pair. The goal is to assign the tasks into available machines with the assignment cost bounded by a constant C and makespan at most T . Shmoys and Tardos [35] extended the LP relaxation and rounding approach [24] to GAP. The makespan objective can be a surrogate to the load balancing that we are seeking, but the GAP problem

does not encode the b -matching constraints on the machines. Computationally solving a GAP problem entails computing an LP relaxation that is expensive for large problems.

Another possible approach is to model our load balancing problem as a multiple knapsack problem (MKP). In an MKP, we are given a set of n items and m knapsacks such that each item i has a weight (profit) w_i and a size s_i , and each knapsack j has a capacity c_j . The goal here is to find a subset of items of maximum weight such that they have a feasible packing in the knapsacks. MKP is a special case of GAP [9], and like the GAP, we cannot model the $b(v)$ constraints by MKP.

Our formulation of load balancing has the most similarity with the Submodular Welfare Maximization (SWM) problem [23]. In the SWM problem, the input consists of a set of n items to be assigned to one of m agents. Each agent j has a submodular function v_j , where $v_j(S)$ denotes the utility obtained by this agent if the set of items S is allocated to her. The goal is to partition the n items into m disjoint subsets S_1, \dots, S_m to maximize the total welfare, defined as $\sum_{j=1}^m v_j(S_j)$. The greedy algorithm achieves $1/2$ -approximation ratio [23]. Vondrak's $(1 - 1/e)$ -approximation [37] is the best known algorithm for this problem. This algorithm uses continuous greedy relaxation of the submodular function and randomized rounding. Although we have modeled our objective as the sum of submodular functions, unlike the SWM, we have the same submodular function for each machine; our approach could be viewed as Submodular Welfare Maximization with b -matching constraints. In the original SWM problem, there are no constraints on the partition size, but in our problem we are required to set an upper bound on the individual partition sizes.

4 Greedy and Lazy Greedy Algorithms

A popular algorithm for maximizing submodular b -MATCHING is the GREEDY algorithm [31], where in each iteration, an edge with the maximum marginal gain is added to the matching. In its simplest form the GREEDY algorithm could be expensive to implement, but submodularity can be exploited to make it efficient. The efficient implementation is known as the LAZY GREEDY algorithm [22, 28]. As the maximum gain of each edge decreases monotonically in the course of the algorithm, we can employ a maximum heap to store the gains of the edges. Since the submodular function is normalized, the initial gain of each edge is just the function applied on the edge, and at each iteration we pop an edge e from the heap. If e is an *available edge*, i.e., e can be added to the current matching without violating b -MATCHING constraints,

Alg.	Appx. Ratio	Time	Conc.?
Greedy [31]	$1/3$	$O(\beta nm)$	N
Lazy Greedy [28]	$1/3$	$O(\beta m \log m)$ assuming 4.1	N
Local Search [14]	$1/(2 + \frac{1}{p} + \epsilon)$	$O(\beta^{p+1}(\Delta - 1)^{p-1}nm\epsilon^{-1})$	N
Cont. Grdy+ Rand. Round [8]	$(\frac{1}{3+2\epsilon})(1 - \frac{1}{e})$	$O(m^5)$	N
Path Growing [16]	$1/4$	$O(\beta m)$	N
Rand LS [16]	$1/3 - \epsilon$	$O(\beta^2 m \log 1/\epsilon)$ in expectation	N
Local Lazy Greedy	$\frac{\epsilon}{2+\epsilon}$	$O(\beta m \log \Delta)$ assuming 4.1	Y

Table 1: Algorithms for the submodular b -MATCHING problem. The last column lists if the algorithm is concurrent or not.

we update its marginal gain $g(e)$. We compare $g(e)$ with the next best marginal gain of an edge, available as the heap's current top. If $g(e)$ is greater than or equal to the marginal gain of the current top, we add e to the matching; otherwise we push e to the heap. We iterate on the edges until the heap becomes empty. Algorithm 1 describes the LAZY GREEDY approach.

Algorithm 1 LAZY GREEDY Algorithm ($G(V, E, W)$)

```

pq = max heap of the edges keyed by marginal gain
while pq is not empty do
  Edge  $e = \text{pq.pop}()$ 
  Update marginal gain of  $e$ 
  if  $e$  is available then
    if  $\text{marg\_gain of } e \geq \text{marg\_gain of pq.top}()$  then
      Add  $e$  to the matching
      update  $b(\cdot)$  values of endpoints of  $e$ 
    else
      push  $e$  and its updated gain into  $pq$ 
    end if
  end if
end while

```

The maximum cardinality of a b -MATCHING is bounded by βn . In every iteration of the GREEDY algorithm, an edge with maximum marginal gain can be chosen in $O(m)$ time. Hence the time complexity of the GREEDY algorithm is $O(\beta n m)$. The worst-case running time of the LAZY GREEDY algorithm is no better than the GREEDY algorithm [28]. However, by making a reasonable assumption we can show a better time complexity bound for the LAZY GREEDY algorithm.

The adjacent edges of an edge $e = (u, v)$ constitute the set $N(e) = \{e' : e' \in \delta(u) \text{ or } e' \in \delta(v)\}$. Likewise, the adjacent vertices of a vertex u are defined as the set $N(u) = \{v : (u, v) \in \delta(u)\}$.

ASSUMPTION 4.1. *The marginal gain of an edge e depends only on its adjacent edges.*

With this assumption, when an edge is added to the matching only the marginal gains of adjacent edges change. We make this assumption only to analyze the runtime of the algorithms but not to obtain the quality of the approximation. This assumption is applicable to the objective function in Problem 2.2 that has been used in many applications, including the one considered in this paper of load balancing Fock matrix computations.

LEMMA 4.1. *Under Assumption 4.1, the time complexity of Algorithm 1 is $O(\beta m \log m)$.*

Proof. The time complexity of Algorithm 1 depends on the number of push and pop operations in the max

heap. We bound how many times an edge e is pushed into the heap. The edge e is pushed when its updated marginal gain is less than the current top's marginal gain, and thus the number of times the marginal gain of e is updated is an upper bound on the number of push operations on it. From our assumption, the update of the marginal gain of an edge e can happen at most 2β times. Hence an edge is pushed into the priority queue $O(\beta)$ times, and each of these pushes can take $O(\log m)$ time. Thus the runtime for the all pushes is $O(\beta m \log m)$. The number of pop operations are at most the number of pushes. Thus the overall runtime of the LAZY GREEDY algorithm for b -MATCHING is $O(\beta m \log m)$. \square

5 Locally Dominant Algorithm

We introduce the concept of ϵ -local dominance, use it to design an approximation algorithm for submodular b -MATCHING, and prove the correctness of the algorithm.

5.1 ϵ -Local Dominance and Approximation

Ratio The LAZY GREEDY algorithm presented in Algorithm 1 guarantees a $\frac{1}{3}$ approx. ratio [7, 15] by choosing an edge with the highest marginal gain at each iteration, and thus it is an instance of a globally dominant algorithm. We will show that it is unnecessary to select a globally best edge because the same approximation ratio could be achieved by choosing an edge that is best in its neighborhood.

Recall that given a matching M , an edge e is *available w.r.t* M if both of its end-points are unsaturated in M .

DEFINITION 5.1. (LOCALLY DOMINANT MATCHING)

An edge e is locally dominant if it is available w.r.t a matching M , and the marginal gain of e is greater than or equal to all available edges adjacent to it. Similarly, for an $\epsilon \in (0, 1]$, an edge e is ϵ -locally dominant if its marginal gain is at least ϵ times the marginal gain of any of its available adjacent edges. A matching M is ϵ -locally dominant if every edge of M is ϵ -locally dominant when it is added to the matching.

A globally dominant algorithm is also a locally dominant one. Thus our analysis of locally dominant matchings would establish the same approximation ratio for the GREEDY and LAZY GREEDY algorithms.

THEOREM 5.1. *Any algorithm that produces an ϵ -locally dominant b -MATCHING is $\frac{\epsilon}{2+\epsilon}$ -approximate for a submodular objective function.*

Proof. Let M^* denote an optimal matching and M be a matching produced by an ϵ -locally dominant algorithm.

Denote $|M| = k$. We order the elements of M such that when the edge e_i is included in M , it is an ϵ -locally dominant edge. Let M_i denote the locally dominant matching after adding e_i to the set, where $M_0 = \emptyset$ and $M_k = M$.

Our goal is to show that for each edge in the locally dominant algorithm, we may charge at most two distinct elements of M^* . At the i th iteration of the algorithm when we add e_i to M_{i-1} , we will show that there exists a distinct subset $M_i^* \subset M^*$ with $|M_i^*| \leq 2$ such that $\rho_{e_i}(M_{i-1}) \geq \epsilon \rho_{e_j^*}(M_{i-1})$, for all $e_j^* \in M_i^*$. We will achieve this by maintaining a new sequence of sets $\{T_j\}$, where T_{i-1} is the reservoir of potential edges that e_i could be charged to. The initial set of this sequence of sets is T_0 , which holds the edges in the optimal matching M^* . The sequence of T -sets shrink in every iteration by removing the elements charged in the previous iteration, so that it stores only the candidate elements that could be charged in this and future iterations. Formally, $M^* = T_0 \supseteq T_1 \supseteq \dots \supseteq T_k = \emptyset$ such that for $1 \leq i \leq k$, the following two conditions hold.

- i) $M_i \cup T_i$ is also a b -MATCHING and
- ii) $M_i \cap T_i = \emptyset$.

The two conditions are satisfied for M_0 and T_0 because $M_0 \cup T_0 = M^*$ and $M_0 \cap T_0 = \emptyset \cap M^* = \emptyset$.

Now we will describe the charging mechanism at each iteration. We need to construct the reservoir set T_i from T_{i-1} . Recall that e_i is added at the i th step of the ϵ -locally dominant matching to obtain M_i . There are two cases to consider:

- i) If $e_i \in T_{i-1}$, the charging set $M_i^* = \{e_i\}$, $M_i = M_{i-1} \cup \{e_i\}$, and $T_i = T_{i-1} \setminus \{e_i\}$.
- ii) Otherwise, let M_i^* be a smallest subset of T_{i-1} such that $(M_{i-1} \cup \dots \cup \{e_i\} \cup T_{i-1}) \setminus M_i^*$ is a b -MATCHING. Since a b -matching is a 2-extendible system, we know $|M_i^*| \leq 2$. Then $M_i = M_{i-1} \cup \{e_i\}$; and $T_i = T_{i-1} \setminus M_i^*$. Note that the two conditions on M_i and T_i from the previous paragraph are satisfied after these sets are computed from M_{i-1} and T_{i-1} . Since M is a maximal matching, we have $T_k = \emptyset$; otherwise we could have added any of the available edges in T_k to M .

Now when e_i is added to M_{i-1} , all the elements of M_i^* are available. This set M_i^* must be the adjacent edges of e_i . Thus $\forall e_j^* \in M_i^*$, we have $\epsilon \rho_{e_j^*}(M_{i-1}) \leq \rho_{e_i}(M_{i-1})$. We can sum the inequality for each element of $e_j^* \in M_i^*$, leading to $\sum_j \rho_{e_j^*}(M_{i-1}) \leq \frac{2}{\epsilon} \rho_{e_i}(M_{i-1})$.

Rewriting the summation we have,

$$\begin{aligned}
 \rho_{e_i}(M_{i-1}) &\geq \frac{\epsilon}{2} \sum_j \rho_{e_j^*}(M_{i-1}) \\
 &\geq \frac{\epsilon}{2} \sum_j \rho_{e_j^*}(M_{i-1} \cup \{e_1^*, \dots, e_{j-1}^*\}) \\
 &= \frac{\epsilon}{2} \sum_j (f(M_{i-1} \cup \{e_1^*, \dots, e_j^*\}) \\
 &\quad - f(M_{i-1} \cup \{e_1^*, \dots, e_{j-1}^*\})) \\
 &= \frac{\epsilon}{2} (f(M_{i-1} \cup \{e_1^*, \dots, e_{|M_i^*|}^*\}) - f(M_{i-1})) \\
 &= \frac{\epsilon}{2} (f(M_{i-1} \cup M_i^*) - f(M_{i-1})) \\
 &\geq \frac{\epsilon}{2} (f(M \cup M_i^*) - f(M)).
 \end{aligned}$$

In line 2, each of the summands is a superset of M_{i-1} , and the inequality follows from submodularity of f (Proposition 2.2). Line 3 expresses the marginal gains in terms of the function f . The fourth equality is due to telescoping of the sums, the fifth equality replaces the set M_i^* for its elements, and the last inequality follows by monotonicity of f (from Proposition 2.2).

We now sum over all the elements in M as follows.

$$\begin{aligned}
 \sum_i \rho_{e_i}(M_{i-1}) &\geq \frac{\epsilon}{2} \sum_i (f(M \cup M_i^*) - f(M)), \\
 f(M) &\geq \frac{\epsilon}{2} \sum_i (f(M \cup \{M_1^* \cup \dots M_i^*\}) \\
 &\quad - f(M \cup \{M_1^*, \dots, M_{i-1}^*\})) \\
 &= \frac{\epsilon}{2} (f(M \cup M^*) - f(M)) \\
 &\geq \frac{\epsilon}{2} (f(M^*) - f(M)). \\
 f(M) &\geq \frac{\epsilon}{2 + \epsilon} f(M^*).
 \end{aligned}$$

The left side of the second line of the above equations is due to Proposition 2.1, while the right side comes from Proposition 2.2. The next equality telescopes the sum, and the fourth inequality is due to monotonicity of f . Finally the last line is a restatement of the inequality above it. \square

COROLLARY 5.1. *Any algorithm that produces an ϵ -locally dominant semi-matching is $\frac{\epsilon}{1+\epsilon}$ -approximate for a submodular objective function.*

Proof. A semi-matching (there are matching constraints on only one vertex part in a bipartite graph) forms a matroid, which is a 1-extendible system [27]. So by definition of 1-extendible system, $|M_i^*| \leq 1$. We can substitute this value in appropriate places in the proof of Lemma 5.1 and get the desired ratio. \square

5.2 Local Lazy Greedy Algorithm Now we design a locally dominant edge algorithm to compute a b -MATCHING, outlining our approach in Algorithm 3. We say that a vertex v is *available* if there is an available edge incident on it, i.e., adding the edge to the matching does not violate the $b(v)$ constraint.

For each vertex $v \in V$, we maintain a priority queue that stores the edges incident on v . The key value of the queue is the marginal gain of the adjacent edges. At each iteration of the algorithm we alternate between two operations: *update* and *matching*. In the *update* step, we update a best incident edge of an unmatched vertex v . Similar to LAZY GREEDY, we can make use of the monotonicity of the marginal gains, and the lazy evaluation process is shown in Algorithm 2. After this step, we can consider a best incident edge for each vertex as a candidate to be matched. We also maintain an array (say *pointer*) of size $|V|$ that holds the best vertex found in the *update* step. The next step is the actual *matching*. We scan over all the available vertices $v \in V$ and check whether $\text{pointer}(v)$ also points to v (i.e., $\text{pointer}(\text{pointer}(v)) = v$). If this condition is true, we have identified a locally dominant edge, and we add it to the matching. We continue the two steps until no available edge remains.

Algorithm 2 Lazy Evaluation (Max Heap pq)

```

1: while  $pq$  is not empty do
2:   Edge  $e = pq.\text{pop}()$ 
3:   Update marginal gain of  $e$ 
4:   if  $e$  is available then
5:     if  $\text{marg\_gain of } e \geq \text{marg\_gain of } pq.\text{top}()$  then
6:       break
7:     else
8:       push  $e$  and its updated gain into  $pq$ 
9:     end if
10:  end if
11: end while

```

We omit the short proofs of the following two results.

LEMMA 5.1. *The LOCAL LAZY GREEDY algorithm is locally dominant.*

COROLLARY 5.2. *For the b -MATCHING problem with submodular objective, the LOCAL LAZY GREEDY algorithm is $1/3$ -approximate.*

LEMMA 5.2. *Under Assumption 4.1, the time complexity of Algorithm 3 is $O(\beta m \log \Delta)$.*

Proof. As for the Lazy Greedy algorithm, the number of total push operations is $O(m\beta \log \Delta)$ (the argument of

Algorithm 3 Local Lazy Greedy Algorithm

```

▷ Initialization
1: for  $v \in V$  do
2:    $pq(v) := \text{max-heap of the incident edges keyed by}$ 
    $\text{marginal gain}$ 
3:    $\text{pointer}(v) = pq(v).\text{top}$ 
4: end for

▷ Main Loop
5: while  $\exists$  an edge with both its endpoints available do
▷ Updating
6:   for  $v \in V$  such that  $u$  is available do
7:     Update  $pq(v)$  using Lazy Evaluation ( $pq(v)$ )
8:      $\text{pointer}(v) = pq(v).\text{top}$ 
9:   end for

▷ Matching
10:  for  $u \in V$  such that  $u$  is available do
11:     $v = \text{pointer}(u)$ 
12:    if  $v$  is available and  $\text{pointer}(v) == u$  then
13:       $M = M \cup \{u, v\}$ 
14:    end if
15:  end for
16: end while

```

the logarithm is Δ instead of m because the maximum size of a priority queue is Δ). We maintain two arrays, say *PotentialU* and *PotentialM*, of vertices that hold the candidate vertices for iteration in the *update* and *matching* step, respectively. Initially all the vertices are in *PotentialU* and *PotentialM* is empty. The two arrays are set to empty after their corresponding step. In the *update* phase, we insert the vertices for which the marginal gain changed into *PotentialM*. In the *matching* step, we iterate only over the vertices in *PotentialM* array. When an edge (u, v) is matched in the *matching* step, we insert u, v if they are unsaturated and all their available neighboring vertices into the *PotentialU*. This is the array on which in the next iteration, *update* would iterate. Since a vertex u can be inserted at most $b(u) + \sum_{v \in N(u)} b(v)$ times into the array, the overall size of *PotentialU* array during the execution of the algorithm is $O(m\beta)$. The *PotentialM* is always a subset of *PotentialU*. So it is also bounded by $O(m\beta)$. Combining all these we get, an $O(\beta m \log \Delta)$ time complexity. \square

5.3 Parallel Implementaion of Local Lazy Greedy Both the standard GREEDY and LAZY GREEDY algorithm offer little to no concurrency. The GREEDY algorithm requires global ordering of

Algorithm 4 Parallel Local Lazy Greedy

```

  ▷ Initialization
1: for  $v \in V$  in parallel do
2:    $pq(v) := \text{max-heap of the incident edges keyed by}$ 
    $\text{marginal gain}$ 
3:    $\text{pointer}(v) = pq(v).\text{top}$ 
4: end for

  ▷ Main Loop
5: while  $\exists$  an edge where both endpoints are available do
  ▷ Updating
6:   for  $v \in V$  such that  $v$  is available in parallel do
7:     Update  $pq(v)$  according to Lazy Evaluation
     ( $pq(v)$ )
8:      $\text{pointer}(v) = pq(v).\text{top}$ 
9:   end for

  ▷ Matching
10:  for  $u \in V$  such that  $u$  is available in parallel do
11:     $v = \text{pointer}(u)$ 
12:    if  $v$  is available and  $u < v$  and  $\text{pointer}(v) == u$  then
13:      Mark  $(u, v)$  as a matching edge
14:    end if
15:  end for
16: end while

```

the gains after each iteration, and the LAZY GREEDY has to maintain a global priority queue. On the other hand, the LOCAL LAZY GREEDY algorithm is concurrent. Here local dominance is sufficient to maintain the desired approximation ratio. We present a shared memory parallel algorithm based on the serial LOCAL LAZY GREEDY in Algorithm 4.

One key difference between the parallel and the serial algorithms is on maintaining the *potentialU* and *potentialM* arrays. One option is for each of the processors to maintain individual *potentialU* and *potentialM* arrays and concatenate them after the corresponding steps. These arrays may contain duplicate vertices, but they can be handled as follows. We maintain a bit array of size of n initialized to 0 in each position. This bit array would be reset to 0 at every iteration. We only process vertices that have 0 in its corresponding position in the array. To make sure that only one processor is working on the vertex, we use an atomic **test-and-set** instruction to set the corresponding bit of the array. Thus the total work in the parallel algorithm is the same as of that the serial one i.e., $O(\beta m \log \Delta)$. Since the fragment inside

the while loop is embarrassingly parallel, the parallel runtime depends on the number of iterations. This number depends on the weights and the edges in the graph, but in the worst case, could be $O(\beta n)$. We leave it for future work to bound the number of iterations under different weight distributions (say random) and different graph structures.

6 Experimental Results

The experiments on the serial algorithm were run on an Intel Haswell CPUs with 2.60 GHz clock speed and 512 GB memory. The parallel algorithm was executed on an Intel Knights Landing node with a Xeon Phi processor (68 physical cores per node) with 1.4 GHz clock speed and 96 GB DDR4 memory.

6.1 Dataset We tested our algorithm on both real-world and synthetic graphs shown in Table 2. (All Tables and Figures from this section are at the end of the paper.) We generated two classes of RMAT graphs: (a) G500, representing graphs with skewed degree distributions from the Graph 500 benchmark [29] and (b) SSCA, from the HPCS Scalable Synthetic Compact Applications graph analysis (SSCA#2) benchmark using the following parameter settings: (a) $a = 0.57$, $b = c = 0.19$, and $d = 0.05$ for G500, and (b) $a = 0.6$, and $b = c = d = 0.4/3$ for SSCA. Moreover, we considered eight problems taken from the SuiteSparse Matrix Collection [10] covering application areas such as medical science, structural engineering, and sensor data. We also included a large web-crawl graph(*eu-2015*) [4] and a movie-interaction network(*hollywood-2011*) [5].

6.2 Serial Performance In Table 3 we compare the LOCAL LAZY GREEDY algorithm with the LAZY GREEDY algorithm. Each edge weight is chosen uniformly at random from the set $[1, 5]$. The submodular function employed here is the concave polynomial with $\alpha = 0.5$, and $b = 5$ for each vertex. Since both LAZY GREEDY and LOCAL LAZY GREEDY algorithms have equal approximation ratios, the objective function values computed by them are equal, but the LOCAL LAZY GREEDY algorithm is faster. For the largest problem in the dataset, the LOCAL LAZY GREEDY algorithm is about five times faster than the LAZY GREEDY, and it is about three times faster in geometric mean.

6.3 Parallel Performance Performance of the parallel implementations of the LOCAL LAZY GREEDY algorithm is shown by a scalability plot in Figure 1. Figure 1 reports results from a machine with 68 threads, with all the cores on a single socket. We see that

all problems show good speedups, and all but three problems show good scaling with high numbers of threads.

7 Load Balancing in Quantum Chemistry

We show an application of submodular b -MATCHING in Self-Consistent Field (SCF) computations in computational chemistry [17].

7.1 Background The SCF calculation is iterative, and we focus on the computationally dominant kernel that is executed in every SCF iteration: the two-electron contribution to the Fock matrix build. The algorithm executes forty to fifty iterations to converge to a predefined tolerance.

The two-electron contribution involves a $\Theta(n^4)$ calculation over $\Theta(n^2)$ data elements, where n is the number of basis functions. The computation is organized as a set of n^4 tasks, where only a small percentage ($< 1\%$) of tasks contribute to the Fock matrix build. Before starting the main SCF iterative loop, the work required for the Fock matrix build in each iteration is computed from the number of nonzeros in the matrix, which is proportional to the work across all SCF iterations. This step is inexpensive since it only captures the execution pattern of the Fock matrix build algorithm without performing other computations. The task assignment is recorded prior to the first iteration and then reused across all SCF iterations.

The Fock matrix build itself is also iterative (written as a $\Theta(n^4)$ loop), where each iteration represents a task that computes some elements of the Fock matrix. For a given iteration, a task is only executed upon satisfying some domain constraints based on the values in two other pre-computed matrices, the Schwarz and density matrices.

The default load balancing used in NWChemEx [19] is to assign iteration indices of the outermost two loops in the Fock matrix build across MPI ranks using an atomic counter based work sharing approach. All MPI ranks atomically increment a global shared counter to identify the loop iterations to execute. This approach limits scalability of the Fock build since the work and number of tasks across MPI ranks are not guaranteed to be balanced.

The task assignment problem here naturally corresponds to a b -MATCHING problem. Let $G(U, V, W)$ be a complete bipartite graph, where U, V, W represent the sets of blocks of the Fock matrix, the set of machines, and the load of the (block, machine) pairs, respectively. The b value for each vertex in U is set to 1; for each vertex in V , it is set to $\lceil |U|/|V| \rceil$ in order to balance the number of MPI messages that each processor needs

to send. We will show that a submodular objective with these b -MATCHING constraints implicitly encodes the desired load balance. To motivate this, we use the square root function ($\alpha = 0.5$) as our objective function in Eqn. (2.2).

We consider the execution of the Greedy algorithm for Submodular b -MATCHING on a small example consisting of four tasks with work loads of 300, 200, 100 and 50 on two machines $M1$ and $M2$. The b -MATCHING constraint requires each processor to be assigned two tasks. At the first iteration, we assign the first block (load 300) to machine $M1$. Note that assigning the second block to machine $M1$ would have the same marginal gain as assigning it to $M2$ if the objective function were linear. But since the square root objective function is submodular, the marginal gain of assigning the second block to the second machine is higher than assigning it to the first machine. So we will assign the second block (load 200) to machine $M2$. Then the third block of work 100 would be assigned to $M2$ rather than $M1$, due to the higher marginal gain, and finally the last block with load 50 would be assigned to $M1$ due to the b -MATCHING constraint. We see that modeling the objective by a submodular function implicitly provides the desired load balance, and the experimental results will confirm this.

7.2 Performance Results As a representative bio-molecular system we chose the Ubiquitin protein to test performance, varying the basis functions used in the computation to represent molecular orbitals, and to demonstrate the capability of our implementation to handle large problem sizes. The assignment algorithm is general enough to be applied to any scenario where such computational patterns exist, and does not depend on the molecule or the basis functions used.

We visualize the load on the processors in Fig. 2. The standard deviation for the current assignment is 10^5 , and the coefficient of variation (Std./Avg.) is 7.5×10^{-2} ; while these quantities for the submodular assignment are 436 and 3×10^{-4} , respectively. It is clear that the latter assignment achieves much better load balance than the former. The run time is plotted against the number of processors in Figure 3. It can be seen that the current assignment does not scale beyond 3000 processors, where as the submodular assignment scales to 8000 processors of Summit. The better load balance also leads to a four-fold speedup over the default assignment. Since the Fock matrix computation takes about fifty iterations, we reduce the total run time from 30 minutes to 8 minutes on Summit.

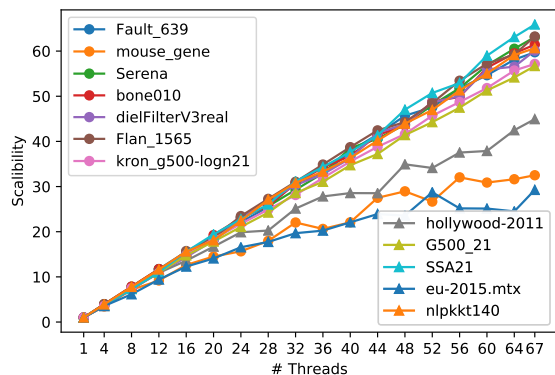


Figure 1: Scalability of the LOCAL LAZY GREEDY algorithm for submodular b -matching with 67 threads.

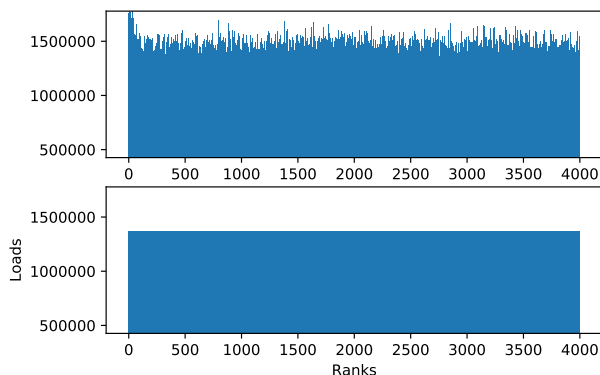


Figure 2: Visualizing the load distribution for the Fock matrix computation for the Ubiquitin protein. Results from: Top, current assignment on NWChemEx. Bottom, submodular assignment.

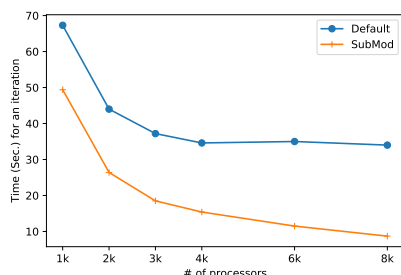


Figure 3: Runtime per iteration for the current (default) and submodular assignments with the 6-31g basis functions for the Ubiquitin protein in NWChemEx on Summit.

Problems	Vertices	Edges	Mean Degree
Fault_639	638,802	13,987,881	44
mouse_gene	45,101	14,461,095	641
Serena	1,391,349	31,570,176	45
bone010	986,703	35,339,811	72
dielFilterV3real	1,102,824	44,101,598	80
Flan_1565	1,564,794	57,920,625	74
kron_g500-logn21	2,097,152	91,040,932	87
hollywood-2011	2,180,759	114,492,816	105
G500_21	2,097,150	118,594,475	113
SSA21	2,097,152	123,097,397	117
eu-2015	11,264,052	257,659,403	46
nlpkkt240	27,993,600	373,239,376	27

Table 2: The properties of the test graphs listed by increasing number of edges.

Problems	Weight	Time (sec.)		Rel. Perf
		LG	LLG	
Fault_639	3.07E+06	61.05	16.83	3.63
mouse_gene	1.90E+05	50.68	22.41	2.26
Serena	6.69E+06	155.81	40.27	3.87
bone010	4.80E+06	177.37	44.15	4.02
dielFilterV3real	5.35E+06	221.92	62.22	3.57
Flan_1565	7.63E+06	310.31	72.00	4.31
kron_g500-logn21	3.69E+06	304.85	105.58	2.89
hollywood-2011	8.59E+06	622.73	163.26	3.81
G500_21	3.93E+06	344.13	137.06	2.51
SSA21	9.46E+06	588.16	285.79	2.06
eu-2015	2.40E+07	1098.40	396.16	2.77
nlpkkt240	1.31E+08	2456.34	465.30	5.28
Geo. Mean				3.29

Table 3: The objective function values and comparison of the serial run times for the LAZY GREEDY and LOCAL LAZY GREEDY algorithms.

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