

Dynamic Load Balancing of Plasma and Flow Simulations

1st Gerrett Diamond

SCOREC

Rensselaer Polytechnic Institute

Institute

Troy, NY

diamog@rpi.edu

2nd Cameron W. Smith

SCOREC

Rensselaer Polytechnic

Institute

Troy, NY

smithc11@rpi.edu

3rd Eisung Yoon

Ulsan National Institute

of Science and Technology

Ulsan, South Korea

esyoon@unist.ac.kr

4rd Mark S. Shephard

SCOREC

Rensselaer Polytechnic

Institute

Troy, NY

shephard@rpi.edu

Abstract—Extracting performance from simulations with complex information dependencies on massively parallel computers requires the computational work to be evenly distributed across the processing resources while maintaining low communication costs. Plasma simulations using a particle-in-cell method and computational fluid dynamics using unstructured mesh-based finite element and volume methods present three distinct distribution requirements. To meet these needs, we present EnGPar’s diffusive partition improvement method. An initial demonstration of EnGPar’s particle distribution improvement is provided along with fluid dynamics mesh partition improvement results on up to 512Ki processes on an IBM BlueGene/Q.

Index Terms—partition improvement, multigraph, hypergraph, dynamic load balancing, particle-in-cell, computational fluid dynamics, plasma physics

I. INTRODUCTION

High performance computing applications have a wide range of partitioning requirements for managing computation and communication costs. For evolving simulations these costs change as the simulation proceeds. In order to maintain good performance throughout the simulation, quick repartitioning methods are required that can deal with incremental changes to the computational load.

In plasma physics simulations using a particle-in-cell (PIC) method and finite element/volume based computational fluid dynamics (CFD), unstructured meshes are utilized as a discretization of the spatial domain of interest. The partitioning of the mesh into sets of elements assigned to a process, a part, results in computational costs associated with the mesh entities and communication costs relative to the number of shared entities between parts. In addition to these basic metrics, applications add further criteria that are critical for performance.

Multilevel graph/hypergraph methods and geometric methods have been successfully applied to balance unstructured

mesh applications. Multilevel graph/hypergraph methods are the most powerful tools to build good static partitions [1]–[4]. These methods construct a graph representing the data of the application. Then, target reducing the imbalance (measured as max divided by average) of the graph vertices while minimizing the edges cut between processes. Multilevel methods are very good at reducing these metrics, but require increasing amounts of memory as they are applied to larger part counts. One way to alleviate these costs is to run multilevel partitioners globally out to thousands of processes, then partition locally on each of those parts to go out further. This approach readily supports partitions with millions of parts, but each local partitioning cannot improve the global partitioning. For meshes, these methods can degrade the final load balance which is a function of not only base mesh entity count, but of a number of mesh level interactions [5], [6].

Geometric methods quickly provide a spatial partition. They are good for getting low imbalances of a single criteria, but often result in poor surface areas of parts and thus large communication costs in the applications [7], [8].

In order to improve the partitions for PIC and CFD applications, we utilize diffusive load balancing procedures to improve the partitions. Diffusive methods iteratively transfer weight from heavily loaded parts to lighter neighboring parts [9], [10]. Diffusive methods have been shown to be able to reduce the large imbalances accounting for a full set of mesh entity considerations [6]. Our tool, EnGPar, uses diffusive methods on a generalized graph structure in order to improve partitions for a diverse set of application needs.

Section II briefly discusses EnGPar. Section III discusses a PIC application and initial results using EnGPar. Section IV describes two different types of CFD codes. Results for CFD mesh partitions are given in Section V. A brief summary of the results closes the paper.

II. ENGPARG

EnGPar [11], [12] is a tool for partition improvement and dynamic load balancing. EnGPar utilizes a multi-hypergraph, called the N-graph, to represent the data of an application in a relational format that allows load balancing of the vertices and edges simultaneously. The N-graph is defined

This research was supported by the National Science Foundation under Grant No. ACI 1533581, (SI2-SSE: Fast Dynamic Load Balancing Tools for Extreme Scale Systems) and the U.S. Department of Energy, Office of Science, under awards DE-AC52-07NA27344 (FASTMath SciDAC Institute) and DE-SC0018275 (Unstructured Mesh Technologies for Fusion Simulation Codes). Any opinions, findings, and conclusions or recommendations expressed in this material are those of the author(s) and do not necessarily reflect the views of the National Science Foundation.

as $G^n = \{V, H^n, P^n\}$ where V is the set of vertices in the graph. The vertices are uniquely assigned to processes and are used to represent the main source of data in an application. $H^n = \{H_1, \dots, H_n\}$ are sets of hyperedges where each hyperedge connects a subset of vertices in V . The pins, $P^n = \{P_1, \dots, P_n\}$, represent the connections from vertices to hyperedges. Each application that utilizes EnGPar represents the data that needs partitioning as an N-graph before running any of the partitioning tools. The general design of the N-graph allows easy representation for different applications that use structures such as meshes, graphs, and other relational structures.

EnGPar's partition improvement is driven by local diffusive techniques that migrate weight from heavily weighted parts to lightly weighted parts. This is done by iteratively running a set of steps until the target imbalance is met or no further improvements are found. A diffusive iteration consists of three steps: targeting, selection, and migration. The targeting step consists of gathering information about the current partition and deciding which neighbors should be sent weight and how much weight to send. The selection step constructs a plan of what vertices should be sent to each neighbor in order to satisfy the weights in the targeting step. The final step, migration, is where the vertices are sent to their destinations and the partition is changed.

III. PLASMA SIMULATION

Plasma physics simulated using a PIC method utilize particles in the spatial domain of a mesh. In this work we focus on load balancing the computationally dominant particle push operation that is common to both PIC codes with a fixed field (e.g., GTR [13]) and a self-consistent field (e.g., XGC [14]–[16], M3D-C1 [17], HPIC [18]). Given initial electric and magnetic fields on the mesh, the value of the field for each particle is determined via interpolation from associated mesh vertices. The spatial position of the particles is then updated using a push operation. Particle properties are then interpolated back to the mesh vertices; the reverse of the vertex-to-particle interpolation process. Unless the entire mesh is replicated on all processes, particles that do not have their field dependencies satisfied will need to be sent to a different process that has sufficient field information. As these simulations continue the particles migrate through the mesh causing computational imbalance that degrades performance [19]–[21].

XGC is a gyrokinetic PIC code for plasma turbulence simulation in a tokamak fusion device [14]–[16]. In this work we refer to a development version of XGC named XGCm that supports a mesh-based particle distribution strategy. XGCm decomposes the domain with a 2D mesh of the poloidal plane that is repeated a given number of times in the toroidal direction. Figure 1-a depicts a simplified representation of the tokamak computational domain, the poloidal planes that decompose it in the toroidal direction, and the definition of physics-based geometric features within the planes. Specifically, Figures 1-b and 1-c depict the flux curve and the faces they form. Each flux face is defined as a core and assigned

to a process. To satisfy information dependencies of particles belonging to the core, the sets of elements of neighboring cores are replicated and thus avoid communication during the computationally intensive particle push operation. These replicated elements are referred to as the buffer region. Figures 1-d and 1-e depict a core and buffer flux faces that makes up one part. This decomposition of the poloidal plane is identical for all planes along the toroidal direction and does not change during the simulation.

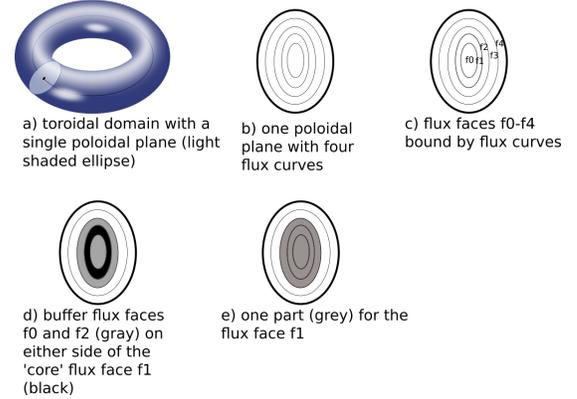


Fig. 1. XGCm mesh distribution in the toroidal and poloidal directions of a tokamak.

The elements in the core flux face of each part, and some layers of the buffer region elements that surround it, are marked as a safe region. Within the safe region there is sufficient mesh field information available to satisfy the dependencies of the push operation. Initially, particles are distributed uniformly over the tokamak volume. The dominant motion of the particles, projected to the poloidal plane, tends to keep them within their initial flux face while a secondary motion drifts them outwards towards the boundary of the plane. If the particle moves outside of the safe region, it is migrated to a process where it resides in the safe region before the next push operation.

To ensure that particles are always migrated to the safe elements of a process, we construct the N-graph carefully such that any partition decision in EnGPar will always maintain this requirement in XGCm. Towards this, we represent each region of overlapping safe zones. Figure 2 depicts a model (a) with four flux faces labeled in (b) as f0–f3. Safe zones for each core are shown in the second row. Each overlapping safe zone set, \bar{S}_i , is in the third row. For an element in one of the \bar{S}_i , the safe zones in the set represent the parts that a particle in the element can migrate to.

The N-graph is then constructed using the set of \bar{S}_i . For each \bar{S}_i a component is constructed consisting of a hyperedge and vertices for each safe zone $S_j \in \bar{S}_i$. The hyperedge connects each of the vertices in the component. The fourth row of Figure 2 shows the N-graph components for the example model. Weights are then applied to each vertex based on the number of particles in the elements for each part. EnGPar is then used in order to determine how to redistribute the weight

associated with particles.

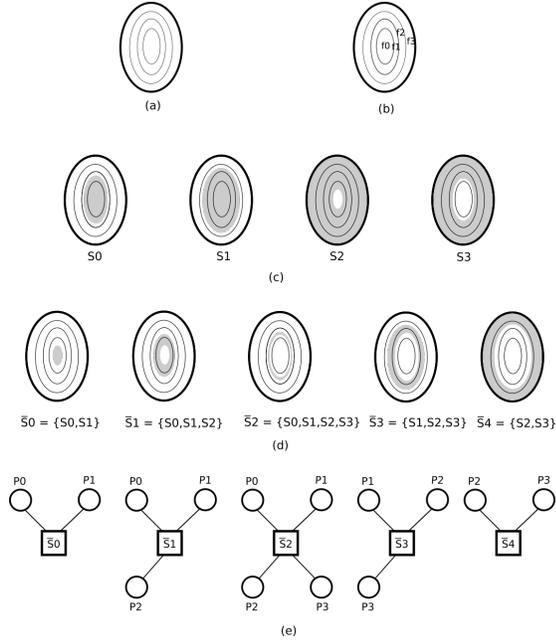


Fig. 2. An example of overlapping safe zones and the N-graph constructed from them. A poloidal plane (a) with four flux faces, f0-f3 (b). Safe zones around each flux face (c). Each overlapping set of safe zones (d) and the N-graph constructed from the overlapping safe zones (e). Vertices are represented with circles and hyperedges with squares.

In order to balance the particles in the mesh, we target redistributing the weights within each component. We run diffusive techniques on the weights of the vertices rather than the vertices. This means that instead of migrating graph vertices, we migrate the weight of the vertices across hyperedges to neighboring vertices to reduce the imbalance of load in the graph.

After EnGPar's weight diffusion is run, a migration plan is returned that details how much weight to send from each graph vertex on a part to each of its neighboring vertices. In XGCM, particles are migrated in order to match the plan. Since each graph vertex was only connected to processes that could receive the particles from the part, any decision XGCM makes within the \bar{S}_i will satisfy the requirement of particles being in safe zones. Future work will go into different particle selection methods that can be applied to reduce how often dynamic load balancing will be required as particles continue to propagate.

Initial demonstrations of the weighted partitioning approach are run on a 16 process test case. The mesh has around four thousand mesh faces, four flux faces with four processes per flux face, and sixteen thousand particles. The initial distribution of particles has an imbalance of 42%. After running EnGPar, the imbalance of particles is reduced to 18%. The push operation's computational load is statistically proportional to the number of particles on part. This reduction will significantly improve the performance of the computationally dominant push operation.

IV. COMPUTATIONAL FLUID DYNAMICS

Parallel CFD applications using the finite volume and finite element methods distribute their meshes in different ways to efficiently resolve data dependencies. A partition of mesh elements uniquely assigns each mesh element to a process. Lower dimension entities are duplicated as needed to form the closure of the elements. For example, if two triangles share an edge, but are assigned to different processes, the shared edge and its bounding vertices will exist on both processes. A vertex partition of a mesh uniquely assigns vertices to parts while the elements, and their closure, are copied along the boundary to any process that shares them. We first examine both methods of partitioning meshes with EnGPar, and then discuss additional mechanisms to localize semi-structured element stacks defined in boundary layer flow regions.

A. Element-partitioned mesh

For element-partitioned meshes, the N-graph is constructed by first representing the mesh elements as graph vertices. Then, graph hyperedges are constructed for each mesh vertex. Pins are created between each hyperedge and graph vertex where the mesh vertex bounds the mesh element. For higher order finite element simulations, where degrees of freedom are associated with mesh edges and mesh faces, additional graph hyperedge types can be constructed similarly for those mesh dimensions. Figure 3 shows how a 2-D mesh (a) is converted into the N-graph with hyperedges as mesh vertices (b) and with hyperedges for both mesh vertices and mesh edges (c).

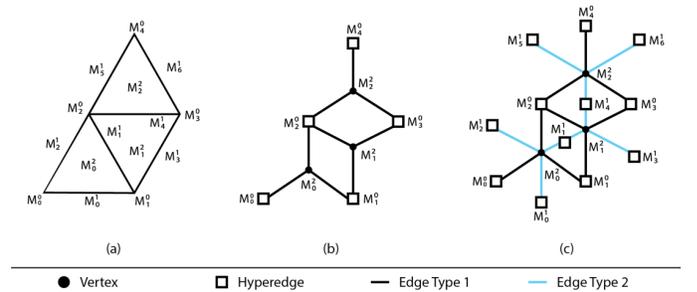


Fig. 3. (a) a 2D unstructured mesh. (b) N-graph construction with elements \rightarrow vertices, vertices \rightarrow hyperedges. (c) Same construction, but with an additional edge type for mesh edges.

In previous work on this case, we used EnGPar to improve partitions of an element-partitioned mesh targeting balancing mesh vertices and mesh elements [11]. For larger process counts, EnGPar fell short balancing mesh vertices. We identified that EnGPar was stagnating due to poor choices of destination part when selecting graph vertices that were on the part boundary of several processes. In order to make better decisions, we choose the destination part based on the largest surface area between the source part and the potential destination part. This results in migrating these vertices to parts that are more connected to the source part instead of parts that may only share a few edges.

B. Vertex-partitioned meshes

To represent the vertex-partitioned mesh in EnGPar, the construction is essentially the opposite of the element-partitioned mesh. Graph vertices are defined by mesh vertices and graph hyperedges are defined by mesh elements. The pins between graph vertices and hyperedges are created for any mesh vertex that bounds a mesh element. Alternatively, the hyperedges could be formed from mesh edges or faces. Defining mesh faces as hyperedges is similar in characteristic to hyperedges formed from elements; they both have low degree.

During initial attempts at improving the partitions, we found that the edge cut was growing at a large rate as we improved edge imbalance. This has been attributed to the differences caused by the vertex-partitioning of the mesh. In an unstructured mesh, vertices have high degree upward adjacencies while elements have low degree downward adjacencies: i.e., four vertices bound a tetrahedron, five for a pyramid, six for a prism, etc. For element-partitioned meshes, the hyperedges represent the mesh vertices. To maintain a low edge cut, mesh vertices that bound many mesh elements should not be cut across partitions. Towards this, EnGPar avoids migrating cavities around these high degree hyperedges by searching for low degree cavities. For vertex-partitioned meshes, this problem is reversed since mesh vertices are represented as graph vertices and hyperedges have low degree. Thus, the problem of edge cut arises from having high degree graph vertices along the partition boundary which leads to a larger edge cut. To avoid increasing the edge cut, when balancing elements in the vertex partition we must consider the degree of the vertices that bound the hyperedges.

To control the edge cut while balancing the graph, we introduce a metric to represent the potential edge cut change for a cavity. The metric is the ratio of hyperedges that will be cut after the cavity is migrated to the hyperedges currently cut around the cavity. We use a tunable parameter in EnGPar that will not migrate a cavity if the metric is above the parameter. Setting this parameter to 1.0 forces EnGPar to migrate cavities that will not increase the edge cut locally. This does not guarantee that the edge cut will decrease as the metric does not take into account other cavities that are migrated in the iteration. Smaller values of this parameter will limit the increase in edge cut, but also limit EnGPar's ability to improve the imbalance and either take more iterations to reach the imbalance tolerance or stagnate at a higher imbalance.

C. Boundary Layer Stacks

Semi-structured boundary layer element stacks growing from geometric model faces can be used to reduce discretization errors and reduce mesh element count (i.e., versus a full unstructured tetrahedral mesh) when there are strong gradients in fields normal to a geometric model surface. Localizing a stack of elements, or vertices along the growth curve, can reduce communications during a PDE solve that uses line relaxation pre-conditioning methods [22] for improved convergence, and during mesh adaptation coarsening procedures [23]–[25].

Algorithm 1 details steps taken to combine the stacks for a vertex-partitioned mesh. The algorithm loops over each vertex classified on a geometric model face to see if it bounds a prism on lines 1-2. From each of these vertices, the algorithm searches for the mesh edge that does not bound any triangles on lines 5-9. An edge that only bounds quad faces is guaranteed to be the edge going up the prism elements. If this edge is found, lines 10-14 find the other vertex that bounds this edge and repeats looking for a new edge from this vertex. This process is continued until no edge is found since once a tetrahedron or pyramid element is hit there will be no edges that are not adjacent to a triangle. Note, the algorithm is simplified to assume each stack exists on a single process. If this were not the case, topological information used to stitch parts together (i.e., which processes have a copy of a given mesh entity and the pointer to the entity on the remote process) would be queried and peer-to-peer communications required to complete the stack traversal.

Algorithm 1 Boundary Layer Stack Collapse

```
1: for all vertices,  $v$ , classified on a geometric model face do
2:   if  $v$  bounds a prism then
3:      $prev\_edge = NULL$ 
4:      $next\_edge = NULL$ 
5:     for all edges,  $e$ , bounded by  $v$  do
6:       if  $e$  bounds no triangles and is not  $prev\_edge$  then
7:          $next\_edge = e$ 
8:       end if
9:     end for
10:    if  $next\_edge$  is not  $NULL$  then
11:       $edge\_prev = e$ 
12:       $v = other\_vertex(v, e)$ 
13:      goto 4:
14:    end if
15:  end if
16: end for
```

To maintain the correct computational and communication load of the stacks, we assign weights to the vertices and hyperedges that represent the stack. Each boundary layer stack vertex accumulates the weight of the mesh vertices in the stack, while the hyperedges accumulate the weight of the elements that share the same graph vertices. If the application does not supply per-vertex and per element weights than a unit weight is assigned.

V. RESULTS

A. Element-partitioned mesh

Tests for the finite element case were run with a one billion element tetrahedral mesh of an airplane's vertical tail structure. EnGPar was run on the Mira BlueGene/Q system at the Argonne Leadership Computing Facility [26] on partitions from 128Ki (128×2^{10}) up to 512Ki parts. These partitions were created by using ParMETIS part k-way [2] globally up to 8Ki parts. Then METIS is run on each part locally to create the 128Ki to 512Ki partitions. The initial mesh element imbalance is 2% and the mesh vertex imbalance ranges from 12% for the 128Ki partition up to 53% at 512Ki parts.

We compare EnGPar to ParMA [6], a diffusive load balancer that works directly on an unstructured mesh. Each tool is run on the partitions with the goal of balancing the mesh vertices down to 5% while keeping the mesh element imbalance below 5%. Figure 4 shows the mesh vertex imbalance from ParMETIS and after EnGPar and ParMA are used. Both tools significantly reduce the mesh vertex imbalance. For the 128Ki and 256Ki cases, both reduce the imbalance to the target 5%. In the 512Ki case, EnGPar reduces the mesh vertex imbalance to 6% while ParMA reduces to the target.

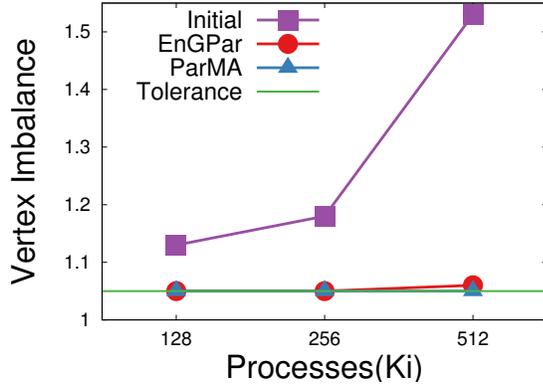


Fig. 4. Vertex imbalance for the initial partitioning and the partitions created by EnGPar and ParMA. Element imbalance is maintained below the 5% tolerance for all cases.

Figure 5 shows the runtime for each partition of ParMA and EnGPar. The timing for EnGPar includes the construction of the N-graph and subsequent repartition of the mesh after running EnGPar to fairly compare with ParMA which doesn't require any conversions of the mesh. In all cases EnGPar runs faster. The speedup ranges from 25% faster at the 256Ki case up to 54% faster for the 512Ki partition.

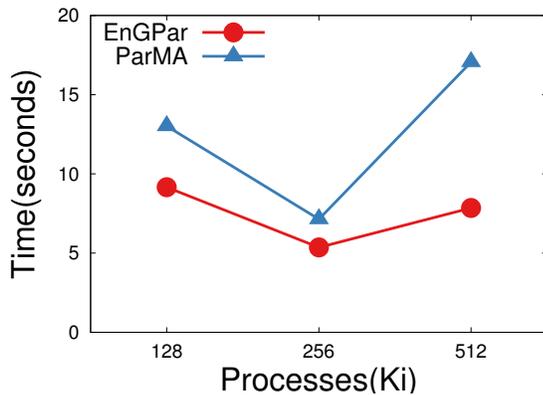


Fig. 5. Time to balance for EnGPar and ParMA

Table I shows the average number of vertices in the mesh for each case. This measurement is related to edge cut in the graph since more average vertices means more surface area of the part and higher edge cut. ParMA slightly reduces the vertex counts in every case. EnGPar increases slightly by around 1%

for each case. As was mentioned for the element-partitioned mesh, the edge cut limit metric was not required to avoid large increases in edge cut.

	128Ki	256Ki	512Ki
Initial	2146.404	1138.881	611.673
ParMA	2141.965	1137.343	610.959
EnGPar	2148.310	1143.970	619.177

TABLE I
AVERAGE NUMBER OF MESH VERTICES PER PART.

B. Vertex-partitioned mesh

Experiments for the vertex-partitioned mesh application were done with a 57 million mixed element mesh (i.e., tetrahedra, prisms, pyramids, and hexahedra) on up to 8192 processes. The mesh is comprised of 32 million tetrahedron, 25 million prisms and 150 thousand pyramids. To show the affect of the edge cut metric, we ran the same test for each process count using values from 0.5 to 1.2 for the metric limit as well as the metric not being used. Each test runs 30 iterations of EnGPar's edge balancer while strictly maintaining the vertex imbalance at 5%. Figure 6 shows the edge cut and edge imbalances for each test; including the initial values of the ParMETIS partitioned mesh. For the 8192 part case, without the metric used, EnGPar reduces the edge imbalance by 24 percentage points while increasing the cut by 34%. Turning on the metric with a value of 1.2 results in limiting the increase of the cut to 17% while reducing the imbalance by 18 percentage points. Results for the metric limit set to 1.0 and 0.8 have similar results following the trend that lower values of the limit result in lower edge cuts and higher edge imbalance. When the limit is set to 0.5, the edge cut increases by 1% while reducing the imbalance by 11 percentage points.

The best edge cut metric parameter is specific to each application. The increase in edge cut means that there will be more elements on each part as well as increased communication between parts. If communication dominates a simulation's scaling then the increase in edge cut, and the associated increase in communications, may negate, or exceed, any savings from improved balance. So, the partition from ParMETIS may be the best choice, or running EnGPar with a low limit for the cut growth metric like in the 0.5 case. However, if the application is very susceptible to imbalance, then a increase in the edge cut would be worth the larger decreases in imbalance as seen in the 0.8 - 1.2 cases.

For the boundary layer collapse, we use the same 57 million element mixed mesh. The N-graph is built in serial from the mesh with the collapsed boundary layers and partitioned out using global ParMETIS for the 1024 to 8192 partitions. Then, EnGPar is run for 30 iterations to reduce the edge imbalance with the same set of configurations for the edge cut metric limit. Figure 7 shows the edge cut and edge imbalance after partitioning with ParMETIS and after EnGPar. Without the metric limit, there is a 41% point reduction in element imbalance with a 38% increase in edge cut. The usage of the metric has a much larger affect than in the uncollapsed

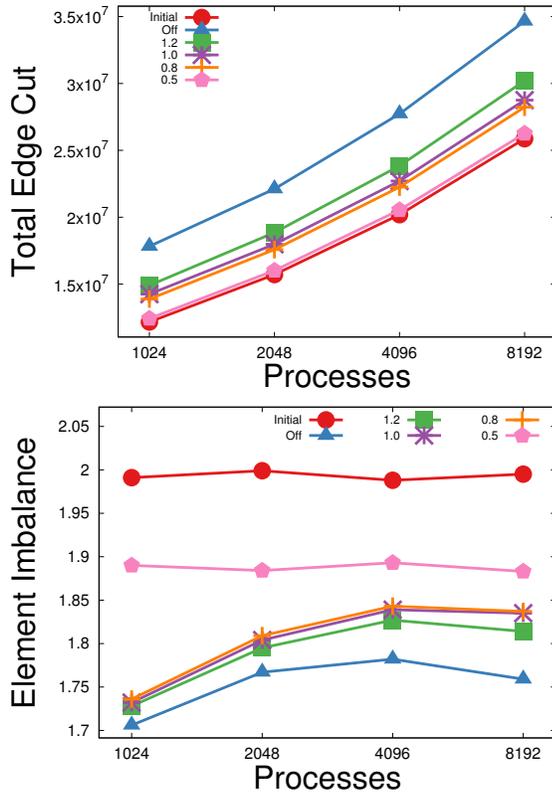


Fig. 6. Edge cut and imbalance for various values of the metric used to reduce the growth of edge cut. Initial values from ParMETIS and not using the metric are also provided. Vertex imbalance is 5% for all cases.

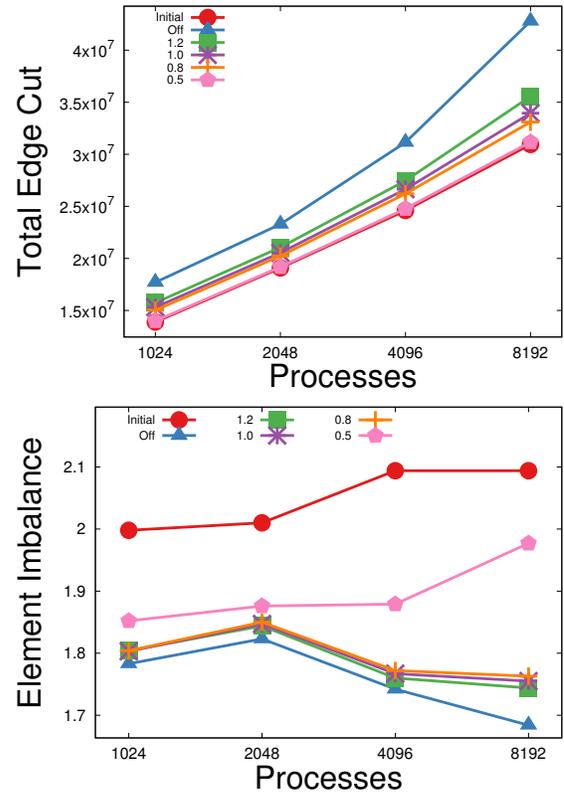


Fig. 7. Edge cut and imbalance for the graph with collapsed boundary layer stacks. Initial values from ParMETIS are provided. Vertex imbalance is 5% for all cases.

boundary layer case. For a value of 1.2 there is a 35% point drop in imbalance with a 15% increase in edge cut. Similar trends are seen for the 1.0 and 0.8 limit. The 0.5 metric reduces the imbalance by 11 percentage points with a less than 1% increase in the edge cut.

VI. CLOSING REMARKS

EnGPar was used to improve the partitions of three different application data. A graph was constructed that compactly represents particles in a fusion application. This graph was designed such that the partition requirements of particles were always satisfied regardless of decisions made by EnGPar. An initial test reduces the particle imbalance by 24 percentage points. In the future, larger simulations will be run to further test EnGPar’s graph construction and balancing procedures.

Previous results using EnGPar to improve the partitions for an element-based CFD application were revisited. Improvements were made that further reduced the imbalance while not sacrificing significant imbalance of the primary vertices, edge cut, or runtime.

Vertex-partitioned meshes for CFD were considered. The diffusive methods used previously for element-partitioned meshes were not able to control the edge cut while improving the partitions. A new metric was introduced that with tuning is able to give a range for trading between edge cut and imbalance. Additionally, combining boundary layer stacks was

explored. The metric for the edge cut was more effective in decreasing imbalance and limiting the increase in edge cut.

VII. ACKNOWLEDGEMENTS

Consultation on CFD methods was provided by members of the NISC SI2-S2I2 Conceptualization of CFDSI: Model, Data, and Analysis Integration for End-to-End Support of Fluid Dynamics Discovery and Innovation; Award Number 1743185 and 1743178.

Computational resources and system support were provided by the Rensselaer Polytechnic Institute Computational Center for Innovations. An award of computer time was provided by the Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program and a separate award of computer time by the Theta Early Science program. This research used resources of the Argonne Leadership Computing Facility, which is a DOE Office of Science User Facility supported under Contract DE-AC02-06CH11357.

REFERENCES

- [1] U. Çatalyürek, M. Deveci, K. Kaya, and B. Uçar, “UMPa: A multiobjective, multi-level partitioner for communication minimization,” *Contemporary Math.*, vol. 588, no. 1, pp. 53–64, Feb. 2013.
- [2] G. Karypis and V. Kumar, “Parallel multilevel series k-way partitioning scheme for irregular graphs,” *Siam Rev.*, vol. 41, no. 2, pp. 278–300, Jun. 1999.

- [3] D. LaSalle and G. Karypis, "Multi-threaded graph partitioning," in *Parallel & Distributed Process. (IPDPS), IEEE 27th Int. Symp.*, May 2013, pp. 225–236.
- [4] K. Schloegel, G. Karypis, and V. Kumar, "Parallel static and dynamic multi-constraint graph partitioning," *Concurrency and Computation: Practice and Experience*, vol. 14, no. 3, pp. 219–240, Mar. 2002.
- [5] M. Zhou, O. Sahni, T. Xie, M. S. Shephard, and K. E. Jansen, "Unstructured mesh partition improvement for implicit finite element at extreme scale," *The J. Supercomputing*, vol. 59, no. 3, pp. 1218–1228, Dec. 2012.
- [6] C. W. Smith, M. Rasquin, D. Ibanez, K. E. Jansen, and M. S. Shephard, "Improving unstructured mesh partitions for multiple criteria using mesh adjacencies," *SIAM J. Scientific Comput.*, pp. C47–C75, Feb. 2018.
- [7] M. Deveci, S. Rajamanickam, K. Devine, and U. Çatalyürek, "Multi-jagged: A scalable parallel spatial partitioning algorithm," *Parallel and Distributed Syst., IEEE Trans.*, vol. 27, no. 3, pp. 803–817, Mar. 2015.
- [8] M. J. Berger and S. H. Bokhari, "A partitioning strategy for nonuniform problems on multiprocessors," *Comput., IEEE Trans.*, vol. 100, no. 5, pp. 570–580, May 1987.
- [9] G. Cybenko, "Dynamic load balancing for distributed memory multiprocessors," *J. Parallel and Distributed Comput.*, vol. 7, no. 2, pp. 279–301, Oct. 1989.
- [10] R. Subramanian and I. D. Scherson, "An analysis of diffusive load-balancing," in *Proc. sixth Annu. ACM Symp. Parallel algorithms and architectures*, Jun. 1994, pp. 220–225.
- [11] G. Diamond, C. W. Smith, and M. S. Shephard, "Dynamic load balancing of massively parallel unstructured meshes," in *Proceedings of the 8th Workshop on Latest Advances in Scalable Algorithms for Large-Scale Systems*, ser. *Scala '17*. New York, NY, USA: ACM, Nov. 2017, pp. 9:1–9:7.
- [12] SCOREC. (2016) EnGPar GitHub repository. [Online]. Available: <https://github.com/SCOREC/EnGPar>
- [13] T. Younkin, D. Green, R. Doerner, D. Nishijima, J. Drobny, J. Canik, , and B. Wirth, "Gitr simulation of helium exposed tungsten erosion and redistribution in pscs-a," in *59th Annual Meeting of the APS Division of Plasma Physics*, Oct. 2017.
- [14] C. Chang, S. Ku, and H. Weitzner, "Numerical study of neoclassical plasma pedestal in a tokamak geometry," *Physics of Plasmas*, vol. 11, no. 5, pp. 2649–2667, 2004.
- [15] S. Ku, R. Hager, C. Chang, J. Kwon, and S. Parker, "A new hybrid-lagrangian numerical scheme for gyrokinetic simulation of tokamak edge plasma," *J. Computational Physics*, vol. 315, pp. 467–475, 2016.
- [16] S. Ku, C. Chang, and P. Diamond, "Full-f gyrokinetic particle simulation of centrally heated global itg turbulence from magnetic axis to edge pedestal top in a realistic tokamak geometry," *Nucl. Fusion*, 2009.
- [17] S. C. Jardin, N. M. Ferraro, J. Breslau, and J. Chen, "Multiple timescale calculations of sawteeth and other global macroscopic dynamics of tokamak plasmas," *Computational Sci. & Discovery*, vol. 5, no. 1, p. 014002, 2012.
- [18] R. Khaziev and D. Curreli, "hPIC: A scalable electrostatic Particle-in-Cell for Plasma-Material Interactions," *Computer Physics Communications*, vol. 229, pp. 87–98, 2018.
- [19] E. A. Carmona and L. J. Chandler, "On parallel pic versatility and the structure of parallel pic approaches," *Concurrency: Practice and Experience*, vol. 9, no. 12, pp. 1377–1405, 1997.
- [20] S. J. Plimpton, D. B. Seidel, M. F. Pasik, R. S. Coats, and G. R. Montry, "A load-balancing algorithm for a parallel electromagnetic particle-in-cell code," *Computer Physics Communications*, vol. 152, no. 3, pp. 227 – 241, 2003.
- [21] P. H. Worley, E. D'Azevedo, R. Hager, S.-H. Ku, E. Yoon, and C. Chang, "Balancing particle and mesh computation in a particle-in-cell code," in *Proc. Cray Users Group Meeting*, May 2016, pp. 1–10.
- [22] P. Wesseling and C. Oosterlee, "Geometric multigrid with applications to computational fluid dynamics," *Journal of Computational and Applied Mathematics*, vol. 128, no. 1, pp. 311 – 334, 2001, numerical Analysis 2000. Vol. VII: Partial Differential Equations.
- [23] K. C. Chitale, O. Sahni, M. S. Shephard, S. Tendulkar, and K. E. Jansen, "Anisotropic adaptation for transonic flows with turbulent boundary layers," *AIAA J.*, vol. 53, no. 2, pp. 367–378, Feb. 2014.
- [24] O. Sahni, K. E. Jansen, M. S. Shephard, C. A. Taylor, and M. W. Beall, "Adaptive boundary layer meshing for viscous flow simulations," *Eng. with Comput.*, vol. 24, no. 3, pp. 267–285, Sep. 2008.
- [25] A. Loseille and R. Löhner, "On 3d anisotropic local remeshing for surface, volume and boundary layers," in *Proc. 18th Int. Meshing Roundtable*, Oct. 2009, pp. 611–630.
- [26] R. Haring, M. Ohmacht, T. Fox, M. Gschwind, D. Satterfield, K. Sugavanam, P. Coteus, P. Heideberger, M. Blumrich, R. Wisniewski, a. gara, G. Chiu, P. Boyle, N. Chist, and C. Kim, "The IBM Blue Gene/Q compute chip," *IEEE Micro*, vol. 32, no. 2, pp. 48–60, Mar. 2012.

APPENDIX A

ARTIFACT DESCRIPTION APPENDIX: DYNAMIC LOAD BALANCING OF PLASMA AND FLOW SIMULATIONS

A. Abstract

Information is provided to create the vertex partitions of the Aeroelastic Prediction Workshop mesh that are described in Section V of the ScalA18 workshop paper titled “Dynamic Load Balancing of Plasma and Flow Simulations”. The meshes and graphs used for the vertical tail problem contain sensitive design information that cannot be published at this time.

B. Description

1) Check-list:

- **Algorithm:** diffusive partition improvement
- **Program:** EnGPar
- **Compilation:** GNU GCC 4.7.2
- **Transformations:** unstructured conformal mesh to hypergraph
- **Data set:** <https://doi.org/10.5281/zenodo.1409558>
- **Hardware:** IBM Blue Gene/Q
- **Output:** <https://github.com/SCOREC/EnGPar-Docs/tree/1a0a1cbe503f6dfa084f05e23765c1ae97ec5120/scala18>
- **Publicly available?:** Yes

2) *How software can be obtained:* EnGPar is available on Github at <https://github.com/SCOREC/EnGPar>. For reproducibility, we list the specific versions (via Git SHA1 hash) used for the experiments.

- element-partitioned mesh (Section IV-A): f6feb49ccee3d475ca3b66d318773fcb022e9e8
- vertex-partitioned mesh (Section IV-B): 246a25c51ad813408a0b1b95b1c3304ebbef374f
- plasma simulation (Section III): 5357ec528c878965006dfb8cfe0251e83a418b1a

3) *Hardware dependencies:* The experiments were performed on the IBM Blue Gene/Q at Argonne National Laboratories and Rensselaer Polytechnic Institute’s Center for Computational Innovations.

4) *Software dependencies:* EnGPar depends on the following libraries:

- ParMETIS 4.0.3 - initial partitioning
- PCU - peer-to-peer communications and non-blocking sparse neighborhood exchanges
- PUMI - load PUMI unstructured meshes and query them for (hyper)graph construction

A compatible version of PUMI and PCU is <https://github.com/SCOREC/core/tree/b623e021a03fa29c54858222127cc669dc708a4>.

5) *Datasets:* The Zenodo dataset containing the input graphs of the Aeroelastic Prediction Workshop mesh is available at <https://doi.org/10.5281/zenodo.1409558>.

C. Installation

For the CCI BGQ we load modules:

```
module load cmake \  
gcc/4.7.2 \  
zoltan/gcc/4.7.2 \  
parmetis/gcc/4.7.2
```

To build EnGPar:

```
mkdir build  
cd build  
cmake .. \  
-DCMAKE_C_COMPILER="mpicc" \  
-DCMAKE_CXX_COMPILER="mpicxx" \  
-DCMAKE_C_FLAGS="-O2" \  
-DCMAKE_CXX_FLAGS="-O2 -std=c++11" \  
-DENABLE_PARMETIS=ON \  
-DENABLE_PUMI=OFF \  
-DScoreC_PREFIX=/path/to/core/install \  
-DBIG_ENDIAN=ON  
make
```

D. Experiment workflow

The script below was used to run EnGPar’s diffusive load balancing on the vertex-partitioned mesh.

```
#!/bin/sh  
#SBATCH --job-name=BALANCE  
#SBATCH -t 01:00:00  
#SBATCH --partition medium  
#SBATCH --nodes 512  
  
engpar=/path/to/EnGPar/build/test  
graph=/path/to/graphs/$1  
  
srun --ntasks $2 -o balance/$1_$2_$3.out \  
Sengpar/balance $graph/$2/ 1 1.05 1.05 $3
```

An example of running the script with 1024 processes and without the edge cut metric limit is:

```
sbatch balance.sh aepw 1024
```

An example of running the script on the collapsed boundary layer graphs with 8192 processes and the edge cut metric limit set to 1.0 is:

```
sbatch balance.sh aepw_collapsed 8192 1.0
```

E. Evaluation and expected result

Expected results are located in the <https://github.com/SCOREC/EnGPar-Docs/tree/1a0a1cbe503f6dfa084f05e23765c1ae97ec5120/scala18> repo.

Plots of vertex and edge imbalances and edge cut are produced by running the bash script `parseAndPlot.sh` in the `plots/aepw_edgeCut_collapse_results` directory. GNUPlot is required for plotting.