DECOMPOSITION OF STENCIL UPDATE FORMULA INTO ATOMIC STAGES

QIQI WANG

Abstract. In parallel solution of partial differential equations, a complex stencil update formula that accesses multiple layers of neighboring grid points sometimes must be decomposed into atomic stages, ones that access only immediately neighboring grid points. This paper shows that this requirement can be formulated as constraints of an optimization problem, which is equivalent to the dual of a minimum-cost network flow problem. An optimized decomposition of a single stencil on one set of grid points can thereby be computed efficiently.

Key words. stencil computation, partial differential equation, parallel computing, computational graph, combinatorial optimization, minimum cost network flow

AMS subject classifications. 65M06, 68W10, 90C35, 90C90

1. Introduction. In large-scale solution of partial differential equations, there is a need to better exploit the computational power of massively parallel systems [15, 30, 23]. Particularly needed are algorithms that hide network and memory latency [9, 32, 19, 31, 12], increase computation-to-communication ratios [28, 11, 5, 7], and minimize synchronization [14, 21, 8]. It is challenging to design and deploy solutions to address these problems, partly due to the variety and complexity of schemes commonly used for solving partial differential equations. A solution may have been demonstrated on a simple scheme with a compact stencil, but to support complex discretization scheme involving arbitrary stencil can sometimes be challenging or cumbersome. Because of this, it would be useful to decompose complex discretization schemes into components that are easier to integrate into stencil computation algorithms.

This paper describes a process that decomposes a general update formula into an optimal series of atomic update formulas, each with a compact stencil that involves only the immediate neighbors in a mesh. This process enables application of algorithms and software that operate only on atomic update formulas to formulas with larger stencils. The algorithm can also serve as a pre-processing step for stencil compilers such as OP2 [25, 26], Patus [10], and Simit [22], as well as loop transforming techniques such as tiling [27].

1.1. Stencil update formula and atomic decomposition. When performing a variety of physical simulations, we discretize space into grid points, and time into time steps. The resulting discretized equation often updates a few values in each grid point every time step, following a predetermined stencil update formula. For example, conduction of heat in one-dimensional, homogeneous structures is often modeled by the 1D heat equation

(1)
$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}.$$

It can be simulated with the update formula

(2)
$$u_i^{n+1} = u_i^n + \Delta t \frac{u_{i-1}^n - 2u_i^n + u_{i+1}^n}{\Delta x^2},$$

where subscript i denotes spatial grid point, and superscript n denotes time step. The set of neighboring grid points involved, $\{i-1,i,i+1\}$, is called the stencil of this update formula. This update formula is derived through manipulation of Taylor

series, formally by approximating the spatial derivative with a linear combination of neighboring values, a technique known as finite difference, in conjunction with a time advancing method called forward Euler.

To automate the manipulation of these update formulas, it is useful to represent them in a computer language. In Python, this update formula can be described as the following function

```
def heat(u0):
    return u0 + Dt/Dx**2 * (im(u0) - 2*u0 + ip(u0))
```

where im and ip represent values at the i-1st grid point and i+1st grid point, respectively. The same stencil update formula (2) is applied at every grid point i, for every time step n.

We can solve a wide variety of problems by applying stencil update formulas at a set of spatial grid points over a series of time steps. More complex update formulas are often used to increase the accuracy, and to solve more complex equations. To increase the accuracy for solving the same 1D heat equation, for example, one may upgrade the time advancing method from forward Euler to the midpoint method. Also known as the second-order Runge-Kutta, it is derived through more complex manipulation of Taylor series. The resulting update formula is

(3)
$$u_i^{n+\frac{1}{2}} = u_i^n + \frac{\Delta t}{2} \frac{u_{i-1}^n - 2u_i^n + u_{i+1}^n}{\Delta x^2},$$
$$u_i^{n+1} = u_i^n + \Delta t \frac{u_{i-1}^{n+\frac{1}{2}} - 2u_i^{n+\frac{1}{2}} + u_{i+1}^{n+\frac{1}{2}}}{\Delta x^2}.$$

Because u_i^{n+1} depends on u_{i-2}^n and u_{i+2}^n , the stencil of this update formula is $\{i-2,i-1,i,i+1,i+2\}$. This update formula can be described as the following function

```
def heatMidpoint(u0):
    u_half = u0 + Dt/Dx**2/2 * (im(u0) - 2*u0 + ip(u0))
    return u0 + Dt/Dx**2 * (im(u_half) - 2*u_half + ip(u_half))
```

Scientists and mathematicians invented numerous updating formulas to simulate various problems. To make them accurate, stable, flexible, and appealing in other aspects, they craft formulas that can involve orders of magnitude more calculations than those in our examples. In this paper, we focus on update formulas that use a fixed number of inputs and produce a fixed number of outputs at every grid points. The outputs depend on the inputs at a stencil, a neighboring set of grid points. The update formula is applied to a set of grid points over a series of time steps.

We can decompose a complex update formula into a sequence of stages. Such decomposition is desirable if the simulation runs on massively parallel computers. Processors in such computers must communicate during a simulation. These communications can be simplified if a complex update formula is decomposed into simpler stages in the following way

- 1. Each stage generates outputs that feed into the inputs of the next stage. The inputs of the first stage and the outputs of the last stage match the inputs and outputs of the entire update formula.
- 2. Each stage is **atomic**, which means that its outputs at each grid point depend on the inputs at no further than the immediately neighboring grid points.

¹Note that running this descriptive function does not necessarily perform the computation. It can merely build a data structure containing information about the steps required to perform the computation.

Some parallel computing method, such as the swept decomposition scheme, is based on the assumption that an update formula is decomposed into atomic stages.

For example, the update formula (2) is an atomic stage. Its input is u_i^n ; its output is u_i^{n+1} . Update formula (3) can be decomposed into two atomic stages in the following way. The input of the first stage is u_i^n , and the outputs include $u_i^{n+\frac{1}{2}}$ and a copy of u_i^n . These outputs must be the inputs of the next stage, whose output is u_i^{n+1} . These stages can be encoded as

```
def heatMidpoint_stage1(u0):
    u_half = u0 + Dt/Dx**2/2 * (im(u0) - 2*u0 + ip(u0))
    return u0, u_half

def heatMidpoint_stage2(inputs):
    u0, u_half = inputs
    return u0 + Dt/Dx**2 * (im(u_half) - 2*u_half + ip(u_half))
```

Decomposition into atomic stages is not unique. In addition to the decomposition above, for example, the same update formula (3) can be decomposed in the following different ways:

```
1. def heatMidpoint_stage1(u0):
    im_plus_ip_u0 = im(u0) + ip(u0)
    return u0, im_plus_ip_u0

def heatMidpoint_stage2(inputs):
    u0, im_plus_ip_u0 = inputs
    u_half = u0 + Dt/Dx**2/2 * (im_plus_ip_u0 - 2*u0)
    return u0 + Dt/Dx**2 * (im(u_half) - 2*u_half + ip(u_half))
```

```
2. def heatMidpoint_stage1(u0):
    u_half = u0 + Dt/Dx**2/2 * (im(u0) - 2*u0 + ip(u0))
    im_plus_ip_u_half = im(u_half) + ip(u_half)
    return u0, u_half, im_plus_ip_u_half

def heatMidpoint_stage2(inputs):
    u0, u_half, im_plus_ip_u_half = inputs
    return u0 + Dt/Dx**2 * (im_plus_ip_u_half - 2*u_half)
```

Note that the first alternative decomposition passes two variables from the first stage to the second stage, the same number as passed by the original decomposition; the second alternative decomposition, however, passes three variables from the first stage to the second stage. Because passing variables between stages may incur communication of data between parallel computing units, we consider it less efficient to pass more variables. In this metric, the second alternative decomposition is inferior to both the original decomposition and the first alternative.

Many update formulas can be decomposed into a sequence of atomic stages, such that the outputs of each stage is the inputs of the next. The goal of this paper is to automatically find the best decomposition for very complex update formulas, such that the total amount of variables passed between the decomposed stages is as few as possible. After decomposition, a stencil optimization framework such as Modesto [20] can further improve the performance of the stages.

1.2. Motivation by the swept rule. The algorithm developed in this paper is motivated mainly the the swept rule [3, 4]. It is an algorithm designed to break the latency barrier of parallel computing by minimizing synchronization. This algorithm has the potential to significantly increase the strong scaling limit [16] of many simulations, allowing them to better exploit the computational power of massively parallel systems.

The algorithm has been demonstrated on atomic stencil update formulas, i.e., ones with compact stencils, involving only the immediate neighbor in a mesh. Although it

was suggested that a more complex formula can be decomposed into a series of atomic update formulas, it is not obvious how to effectively do so in general. An algorithmic approach to performing such decomposition is desirable.

2. Graph theoretical representation of a stencil update formula and its atomic decomposition. To algorithmically find a decomposition for a given stencil update formula, we view it as a directed acyclic graph (V, E). Vertices in the graph, denoted by integers $0,1,\ldots$, represent intermediate values in the update formula. We interchangeably use Value i and Vertex $i \in V$ in this paper. An edge (i,j) exists if j directly depends on i, i.e., if Value i is directly used in the computation of Value j. Source vertices with no incoming edges are the inputs of the stencil update formula. Sink vertices with no outgoing edges are the outputs. Figure 1 shows an example of such a graph for Update formula (3). Note that each node of the computational graph represents a symbolic value located at all the grid points, as opposed to a value at a particular grid point. We call this directed acyclic graph the computational graph of the update formula. Similar computational graphs have been used in solving other combinatorial problems in the realm of optimizing complex stencil computation [20, 10, 13].

Special edges represent value dependency at neighboring grid points. If Value j at a grid point depends on Value i at a neighboring grid point, then (i,j) is called a 'swept' edge. Operations that create swept edges include im(u) and ip(u). The set of swept edges are denoted by $E_S \subset E$. Swept edges are visualized by triple lines in Figure 1.

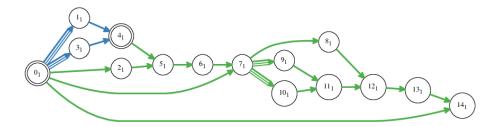
The computational graph helps to visualize not only the update formula but also its decomposition into atomic stages. In the decomposition, the computational graph is divided into a sequence of subgraphs, each representing an atomic stage. An intermediate value can either live within a single atomic stage, or be created in one stage and passed to subsequent stages for further use; therefore, a vertex in the computational graph can belong to either one subgraph or several successive subgraphs. We do not allow a stage to repeat a computation that has been performed in a previous stage; therefore, each vertex is created in one and only one stage, a stage that not only solely owns all the incoming edges of that vertex, but also contains all the vertices from which these edges originate.

This decomposition differs from many classical parallel computing methodologies, which often starts by identifying closely related computational work and assigning them to be executed by a single processor. In contrast, each decomposed stage here corresponds to a subset of computation that needs to be performed on each grid point before the next stage can occur at the same grid point. Neither work or data is assigned to any particular processor during this decomposition. Each decomposed stage is atomic, and thus can be relatively easy to parallelize.

The **source** of each atomic stage is the set of vertices with no incoming edges in the subgraph; these are the inputs of the atomic stage. The **sink** of each atomic stage is the set of vertices with no outgoing edges in the subgraph; they are the outputs. Because the outputs of each state serve as inputs of the next, the sink of one subgraph must be identical to the source of the next subgraph. Also, the source of the first subgraph and the sink of the last subgraph should match the source and sink of the entire computational graph.

Recall that a stage is atomic only if its outputs depend on its inputs at no further than the immediately neighboring grid points. This property can be graphtheoretically enforced, by allowing at most one swept edge in any path within a

```
def heatMidpoint(u0):
    uHalf = u0 + Dt/Dx**2/2 * (im(u0) - 2*u0 + ip(u0))
    return u0 + Dt/Dx**2 * (im(uHalf) - 2*uHalf + ip(uHalf))
```



Vertex	represents intermediate value
0	u0
1	im(u0)
2	2 * u0
3	ip(u0)
4	im(u0) + ip(u0)
5	im(u0) + ip(u0) - 2 * u0
6	dt / dx**2 * (im(u0) + ip(u0) - 2 * u0)
7	uHalf = u0 + dt / dx**2 * (im(u0) + ip(u0) - 2 * u0)
8	2 * uHalf
9	im(uHalf)
10	ip(uHalf)
11	im(uHalf) + ip(uHalf)
12	im(uHalf) + uip(uHalf) - 2 * uHalf
13	dt / dx**2 * (im(uHalf) + ip(uHalf) - 2 * uHalf)
14	u0 + dt / dx**2 * (im(uHalf) + ip(uHalf) - 2 * uHalf)

Fig. 1: Atomic decomposition of the midpoint scheme for the heat equation represented as a computational graph.

subgraph. If every path from a source value to a sink value of the subgraph contains no more than one swept edge, the corresponding output value can only depend on the corresponding input value at the immediately neighboring grid points.

Now we can formulate a graph-theoretical equivalence to the problem of decomposing a stencil update formula into atomic stages. This problem is to decompose a directed acyclic graph (V, E), with swept edges $E_S \subset E$, into a sequence of subgraphs $(V_1, E_1), \ldots, (V_k, E_k)$, such that the three axioms hold:

- 1. Each edge in E belongs to one and only one subgraph. That implies no redundant computation is performed. Also, for each vertex $i \in V$, all incoming edges belong to one subgraph, which corresponds to the stage in which Value i is computed.
- 2. The source of each subgraph, other than the first one, must be contained in the previous subgraph. This disallows communication between non-subsequent stages. Also, the source of the first subgraph (V_1, E_1) must match the source of (V, E); the sink of (V, E) must be contained in V_K .

3. There is no path within any subgraph (V_k, E_k) that contains two edges in E_S . This ensures that each stage is atomic.

Figure 1 shows an example of an atomic decomposition. The source of the stencil update formula is Value 0; the sink is Value 14. Blue and green colors represent edges in the first and second subgraphs. The source of blue subgraph includes only Vertex 0. Vertices 1 and 3 belong exclusively to the blue subgraph; they are created in the blue subgraph and are used to compute values only in the same subgraph. In other words, all their incoming and outgoing edges are blue. Vertices 2 and 5-13 belong exclusively to the green subgraph; all their incoming and outgoing edges are green. Vertices 0 and 5 are shared by both subgraphs. Both are created in the blue subgraph (inputs to the entire update formula are defined to be created in the first subgraph); both are used in blue and green subgraphs. These two vertices are the sink of the blue subgraph, and source of the green subgraph. Neither the blue nor green subgraph contains directed path that goes through more than one swept edges, visualized by the triple-lines.

3. Algebraic representation of an atomic decomposition. Using the graph theoretical representation, we can formulate a set of algebraic constraints, the satisfaction of which leads to an atomic decomposition of an update formula. We can then combine these constraints with an optimization problem to minimize the values passed between the decomposed stages. If satisfaction of the constraints is not only sufficient but also necessary for a valid decomposition, then by solving the constrained optimization problem, we are guaranteed to obtain the best possible decomposition.

The primary challenge of constructing these constraints is the third criterion in the last section, which forbids any path within a subgraph that contains two swept edges. Naively enforcing this criterion requires enumerating all paths, which can be combinatorially many. This section shows that this criterion can be applied more efficiently, along with other criteria, by introducing three integers for each vertex, and prescribing linear equalities and inequalities on these integers.

To describe the set of constraints, we use integers $1, 2, \ldots, K$ to denote the K decomposed stages. We then introduce the following three integers associated with each vertex in the computational graph:

- 1. The creating stage c_i ,
- 2. The discarding stage d_i ,
- 3. The effective stage e_i ,

In this section, we first introduce c_i, d_i and their governing constraints. Before we proceed to introduce e_i , we prove the Atomic Stage Lemma, which useful for explaining e_i . Finally, we present the Quarkflow Theorem, which lists all the constraints between c_i, d_i , and e_i , and shows that they are equivalent to the three criteria listed in the previous section.

3.1. c_i, d_i , and their governing constraints. The first integer, the creating $stage c_i$, indicates in which stage Value i is created. It is the first subgraph to which vertex i belongs. In other words,

$$c_i := \min\{k : i \in V_k\}.$$

The second integer, the discarding stage d_i , indicates in which stage Value i is last used. It is the last subgraph to which vertex i belongs. In other words,

$$d_i := \max\{k : i \in V_k\}.$$

Because a value must first be created before it is discarded, d_i is always greater or equal to c_i . This leads to our first constraint,

$$(4) c_i - d_i \le 0.$$

Specifically, if $c_i = d_i$, then Vertex *i* belongs exclusively to Stage c_i ; its corresponding vertex has all incoming and outgoing edges in this same stage. If $c_i < d_i$, then Vertex *i* belongs to Stages $c_i, c_i + 1, \ldots, d_i$.

If Vertex i belongs to the source of the update formula, then

$$(5) c_i = 1,$$

i.e., it is created at the first stage. If Vertex i belongs to the sink of the update formula, then

$$(6) d_i = K ;$$

this is to indicate that an output is used after the last stage. These are equality constraints associated with the source and sink of the update formula.

The next set of constraints is based on the following truth. For a valid decomposition satisfying the properties in Section 3, the creating stage satisfies the following property:

Edge Lemma: For a valid decomposition, if $(i, j) \in E_k$, then $c_j := \min\{k' : j \in V_{k'}\} = k$.

Proof. Because $(i,j) \in E_k$, $j \in V_k$. Then by its definition, $c_j \leq k$. It is then sufficient to prove that vertex j cannot be in any $V_{k'}, k' < k$. We prove this by contradiction. Because j has one incoming edge in E_k , all its incoming edges must be exclusively in E_k . If $j \in V_{k'}, k' < k$, then j has no incoming edge in $(V_{k'}, E_{k'})$, and must be a source of the subgraph. If k' = 1, then by Criterion 2 of Section 3, j must be in the source of (V, E), which cannot be true because j has an incoming edge (i, j). If k' > 1, then j being in the source of $(V_{k'}, E_{k'})$ implies, by Criterion 2 again, that j must be in $(V_{k'-1}, E_{k'-1})$, which leads to contradiction by induction.

Edge Corollary: For a valid decomposition, $\forall (i,j) \in E$, then $c_i := \min\{k' : i \in V_{k'}\} \leq c_j$.

Proof. Each (i,j) belongs to one and only one subgraph. Denote $(i,j) \in E_k$. Then $i \in V_k$, and by its definition $c_i \leq k$. By the Edge Lemma, $c_j = k$. Thus $c_i \leq c_j$.

The lemma and corollary indicate that if $(i,j) \in E_k$, then $c_i \leq c_j = k$. In addition, by the definition of a subgraph, both i and j must belong to V_k . Thus the definition of d_i implies that $d_i \geq k$. This leads to our second set of inequality constraints,

$$(7) c_i \le c_i \le d_i$$

3.2. The Atomic Stage Lemma. The next set of constraints is derived from Criterion 3 of Section 3, which enforces that the decomposed stages are atomic. Recall that a stage is atomic if every directed path in its subgraph contains at most one swept edge. Naively enforcing this criterion requires enumerating over all paths in a subgraph, leading to exponentially many constraints. To avoid the combinatorial explosion of constraints, we prove an equivalent definition of an atomic stage that requires fewer constraints to enforce.

Atomic Stage Lemma: A directed acyclic graph (V_k, E_k) with swept edges $E_{S,k} \subset E_k$ is atomic if and only if there exists an $s_{i;k} \in \{0,1\}$ for each $i \in V_k$, such that

1. $\forall (i, j) \in E_k, s_{i;k} \leq s_{j;k},$ 2. $\forall (i, j) \in E_{S:k}, s_{i:k} < s_{j:k}.$

This lemma enables us to efficiently enforce the atomicity of each stage by reducing the necessary constraints from as many as the number of paths, which can scale exponentially to the size of a graph, to the number of edges, which scales linearly. This lemma makes it possible to enforce Criterion 3 in Section 3 at a computational cost that does not scale exponentially with respect to the complexity of the stencil update formula.

Proof of the Atomic Stage Lemma. Let us denote the directed acyclic graph (V, E) with swept edge set E_S as (V, E, E_S) . To prove the theorem, we decompose it into two propositions, such that it is sufficient to prove both propositions.

Proposition 1: If $s_i \in \{0,1\}$ exists for each $i \in V$ and both conditions in the theorem are satisfied, then (V, E, E_S) is atomic.

Proposition 2: If (V, E, E_S) is atomic, then there exists an $s_i \in \{0, 1\}$ for each $i \in V$, such that both conditions in the theorem are satisfied.

Proof. Proof of Proposition 1 by contradiction: If (V, E, E_S) is not atomic, then there exists a path (i_0, \ldots, i_n) that contains two swept edges. Because we can truncate both ends of such a path such that the first and last edges are swept, we can assume $(i_0, i_1) \in E_S$ and $(i_{n-1}, i_n) \in E_S$ without loss of generality. From Condition 2 of the theorem, $(i_0, i_1) \in E_S \Rightarrow s_{i_0} < s_{i_1}$. So $s_{i_0} = 0$ and $s_{i_1} = 1$ because both must either be 0 or 1. Similarly, $(i_{n-1}, i_n) \in E_S \Rightarrow s_{i_{n-1}} < s_{i_n}$. So $s_{i_{n-1}} = 0$ and $s_{i_n} = 1$. From Condition 1 of the theorem, however, $(i_k, i_{k+1}) \in E \Rightarrow s_{i_k} \le s_{i_{k+1}}$, thus the series s_{i_k} must be monotonically non-decreasing, contradicting the previous conclusion that $s_{i_1} = 1$ and $s_{i_{n-1}} = 0$.

To prove of Proposition 2. We first construct a non-negative integer for each vertex with the following recursive formula

(8)
$$s_{j} = \begin{cases} 0, & \text{Vertex j has no incoming edge} \\ \max_{i:(i,j)\in E'} s_{i} + I_{(i,j)\in E_{S}}, & \text{otherwise} \end{cases}$$

where $I_{(i,j)\in E_S} = 1$ if $(i,j) \in E_S$ and 0 otherwise. By construction, these integers satisfy both conditions in the theorem. We then show that if the graph is atomic, then all these integers satisfy the additional condition that $s_i \in \{0,1\}$. This additional condition can be proved with the aid of the following lemma:

Lemma: For every vertex j, there exists a path, consisting of zero or more edges, that ends at j and contains s_j swept edges, where s_j is defined by Equation (8).

Proof. Proof of Lemma by induction: We prove by induction with respect to the length of the longest path that ends at Vertex j. If the length of the longest incoming path is 0, it means Vertex j has no incoming edge; by definition, $s_j = 0$. In this case, an empty path suffices as one that ends at j and contains 0 swept edges. Therefore, the lemma is true if the longest incoming path to j is of length 0.

If the lemma is true for any vertex whose longest incoming path is of length less than n > 0, we prove it for any vertex j whose longest incoming path is of length n. Because n > 0, Vertex j has an incoming edge. By Equation (8), there exists an edge (i,j) such that $s_j = s_i + I_{(i,j) \in E_S}$. Note that Vertex i has no incoming path of length n; if it does, then appending edge (i,j) to that path would result in a path to Vertex j of length n + 1, violating the assumption about the longest incoming path to j. Because the longest incoming path to Vertex i is less than n, by the induction assumption, the lemma holds for Vertex i: there exists a path that ends at Vertex i that contains s_i swept edges. At the end of this path, we append edge (i, j) to

form a path to Vertex j. If $(i,j) \notin E_S$, the path contains the same number of swept edges as the path to i. $(i,j) \notin E_S$ also sets $s_j = s_i$ by Equation (8). Thus this path suffices as one that ends at Vertex j and contains s_j swept edges. The other case is $(i,j) \in E_S$, and the resulting path to j has one more swept edge than the path to i. In this case, $s_j = s_i + 1$ according to Equation (8), and this path still suffices as one that ends at Vertex j and contains s_j swept edges. This shows that the lemma is true for any Vertex j whose longest incoming path is of length n, thereby completing the induction.

Proof. Proof of Proposition 2 by contradiction: If the proposition is not true for an atomic stage, then s_j constructed via Equation (8) must not satisfy $s_j \in \{0,1\}$ for some j. Because s_j are non-negative integers by construction, $s_j \notin \{0,1\}$ means $s_j > 1$. By the lemma, there exists a path that ends at Vertex j that contains more than 1 swept edges. So the graph cannot be an atomic stage, violating the assumption.

3.3. The Quarkflow Theorem. The set of integers $s_{i;k}$ in the lemma, however, is specific to each subgraph k. They can only be defined on top of a valid decomposition. To specify a-priori conditions that can serve as foundation to build a valid decomposition, we construct e_i , the effective stage, for each $i \in V$. The construction of e_i is such that for each $0 \le k < K$,

(9)
$$s_{i;k} := \begin{cases} e_i - c_i , & c_i = k \\ 0, & c_i < k \end{cases}$$

satisfies both conditions in the Atomic Stage Lemma for subgraph k. The introduction of e_i and its associated constraints, together with c_i and d_i and their associated constraints derived previously, leads us to the main theorem of this section. We name it the "Quarkflow" theorem since the triplet of integers (c_i, d_i, e_i) representing each vertex is analogous to quarks forming each subatomic particle.

Quarkflow Theorem: A graph (V, E) is decomposed into K subgraphs, $(V_0, E_0), \ldots, (V_{K-1}, E_{K-1})$. The decomposition satisfies the three criteria stated in Section 3, if and only if there exists a triplet of integers (c_i, d_i, e_i) for vertex $i \in V$, such that the following constraints are satisfied:

- 1. $c_i \leq d_i$ for all $i \in V$
- 2. $c_i = 1$ for all i in the source of V
- 3. $d_i = K$ for all i in the sink of V
- 4. $c_i \leq c_j \leq d_i$ for all $(i, j) \in E$
- 5. $c_i \leq e_i \leq c_i + 1$ for all $i \in V$
- 6. $e_i \leq e_j$ for all $(i, j) \in E$
- 7. $e_i + 1 \le e_j$ for all $(i, j) \in E_S$
- 8. $c_i + 1 \le e_i$ for all $i \in V$ where $\exists (j, i) \in E_S$

and that
$$\forall k = 1, ..., K, V_k = \{i : c_i \le k \le d_i\}, E_k = \{(i, j) \in E : c_j = k\}.$$

This theorem achieves the goal of this section. To find a decomposition, we only need to find the integer triplets, $(c_i, d_i, e_i), \forall i \in V$, together with the number of stages K, satisfying all these constraints. If we can use the same set of integers to describe how good the decomposition is, we can solve an integer program to find the best possible decomposition.

Proof of the Quarkflow Theorem. We split the proof into two subsections. The first shows that for a decomposition that satisfies the three criteria in Section 3, there exists $(c_i, d_i, e_i), \forall i \in V$ satisfying all constraints in the theorem, and the

decomposition matches (V_k, E_k) constructed in the theorem. The second subsection shows that if the triplets satisfy all the constraints in the theorem, then (V_k, E_k) is a valid decomposition satisfying all three criteria in Section 3.

- 3.3.1. Criteria in Section 3 \Longrightarrow Constraints in the Quarkflow Theorem. For a decomposition that satisfies the three criteria in Section 3, we can construct (c_i, d_i, e_i) in the following way:
 - 1. $c_i = \min\{k | i \in V_k\}$
 - 2. $d_i = \max\{k|i \in V_k\}$
 - 3. $e_i = c_i + s_{i;c_i}$, where $\{s_{i;c_i}\}_{i \in V_{c_i}}$ satisfy the two constraints in the Atomic Stage Lemma for subgraph c_i .

Constraints 1, 2, and 3 are satisfied by construction.

For Constraint 4, consider each $(i, j) \in E$ belonging to subgraph E_k . Therefore, $i \in V_k$ and $j \in V_k$. Thus, $c_i \leq k$ and $d_j \geq k$. By the Edge Lemma, $c_j = k$. Constraint 4 therefore holds.

Constraint 5 is satisfied by construction of e_i and by the Atomic Stage Theorem. Constraint 6 and 7 can be proved in two cases. The first case is when $c_i = c_j$. Denote both c_i and c_j as k. From the Atomic Stage Lemma, $s_{i;k} \leq s_{j;k}$, and when $(i,j) \in E_S$, $s_{i;k} + 1 \leq s_{j;k}$. Plug these inequalities, as well as $c_i = c_j = k$, into the definition of e_i and e_j , we get $e_i \leq e_j$ and when $(i,j) \in E_S$, $s_i + 1 \leq s_j$.

The second case is when $c_i < c_j$ (the Edge Corollary ensures that c_i cannot be greater than c_j). Because both c_i and c_j are integers, $c_i + 1 \le c_j$. Also because both $s_{i;c_i}$ and $s_{j;c_j}$ are either 0 or 1, $e_i := c_i + s_{i;c_i} \le c_i \le c_j \le c_j + s_{j;c_j} =: e_j$. In particular, when $(i,j) \in E_S$, the Atomic Stage Lemma ensures that $s_{i;c_j} < s_{j;c_j}$; since both are either 0 or 1, the strict inequality leads to $s_{j;c_j} = 1$. Thus $e_i := c_i + s_{i;c_i} \le c_i + 1 \le c_j = c_j + s_{j;c_j} - 1 =: e_j - 1$, and thus $e_i + 1 \le e_j$.

To prove Constraint 8 for an edge $(i,j) \in E_S$, we use Criterion 1 of Section 3, which specifies that (i,j) is in a unique subgraph, denoted as E_k . By the Edge Lemma, $k = c_j$. Because $(i,j) \in E_S \cap E_k$, the Atomic Stage Lemma guarantees that $s_{i,k} < s_{j;k}$. Because both $s_{i,k}$ and $s_{j,k}$ are 0 or 1, this strict inequality ensures that $s_{j,k} = 1$. Therefore, $e_j := c_j + s_{j,k} \ge c_j + 1$, which is Constraint 8.

Finally, we show that $V_k = \{i : c_i \le k \le d_i\}$ and $E_k = \{(i,j) \in E : c_j = k\}$. For $V_k = \{i : c_i \le k \le d_i\}$ to be true, it is sufficient to show that $i \in V_k \Leftrightarrow c_i \le k \le d_i$. If $c_i > k$ or $d_i < k$, then $i \notin V_k$ by the construction of c_i and d_i . It is then sufficient to show that $i \in V_k$ for all k satisfying $c_i \le k \le d_i$. We prove this by contradiction. If the previous statement is not true, then because $i \in V_{c_i}$ and $i \in V_{d_i}$ by the construction of c_i and d_i , there must exist $c_i < k < d_i$ such that $i \in V_{k+1}$ but $i \notin V_k$. By the edge lemma, all incoming edges of i must be in subgraph c_i , so i must be in the source of subgraph k+1. By Criterion 2 of Section 3, $i \in V_k$ which contradicts with $i \notin V_k$. Therefore $i \in V_k \Leftrightarrow c_i \le k \le d_i$ and $V_k = \{i : c_i \le k \le d_i\}$.

For $E_k = \{(i, j) \in E : c_j = k\}$, we know from the edge lemma that $(i, j) \in E_k \Rightarrow c_j = k$. From Criterion 1, each edge can only be in one subgraph. Therefore, $(i, j) \in E_k \Leftarrow c_j = k$. Thus $E_k = \{(i, j) \in E : c_j = k\}$.

3.3.2. Constraints in the Quarkflow Theorem \Longrightarrow Criteria in Section **3.** Now if all 8 constraints are satisfied, we prove that $(V_k := \{i : c_i \le k \le d_i\}, E_k := \{(i,j) \in E : c_j = k\})$ is a graph decomposition satisfying all three criteria specified in Section 3.

First, we need to show that each (V_k, E_k) is a subgraph. If $(i, j) \in E_k$, then by the definition of E_k and Constraint 1 of the Quarkflow Theorem, $k = c_j \leq d_j$. This ensures that $j \in V_k$ by the definition of V_k . On the other hand, Constraint 4 of the

Quarkflow Theorem ensures that $c_i \leq c_j \leq d_i$. Because $c_j = k$, $c_i \leq k \leq d_i$. This ensures that $i \in V_k$ by the definition of V_k . Because $i \in V_k$ and $j \in V_k$ for every $(i,j) \in E_k$, (V_k, E_k) is a valid subgraph.

Now we proceed to prove that the subgraphs satisfy the three criteria of Section 3.

Criterion 1: Each edge (i, j) belongs to Subgraph c_j and no other subgraph by the definition of E_k . Also by this definition, for each vertex $j \in V$, all incoming edges belongs to Subgraph c_j . Criterion 1 therefore holds.

Criterion 2: This criterion has three statements. We first prove the first statement: if vertex j is in the source of Subgraph $(V_k, E_k), k > 1$, then in $j \in V_{k-1}$.

By the definition of V_k , $c_j \leq k \leq d_j$. We now prove that $c_j < k$. This is because if $c_j = k > 1$, then by Constraint 2 of the Quarkflow Theorem, j is not in the source of V, i.e., $\exists (i,j) \in E$. $c_j = k$ also implies, by the definition of E_k , that such $(i,j) \in E_k$. This contradicts with the assumption that j is in the source of (V_k, E_k) .

Now we know that $c_j < k \le d_j$, which implies that $c_j \le k - 1 < d_j$. Therefore, $j \in V_{k-1}$ by the definition of $j \in V_{k-1}$.

We then prove the second statement of the criterion: j is in the source of $(V_1, E_1) \iff$ it is in the source of (V, E).

j being in the source of (V_1, E_1) implies that $j \in V_1$, and by the definition of V_1 , $c_j = 1$. By the definition of E_1 , any $(i, j) \in E$ must be in E_1 . Such incoming edge (i, j) cannot exist if j is in the source of (V_1, E_1) . j, therefore, has no incoming edge and is in the source of (V, E).

On the other hand, by Constraint 2 of the Quarkflow Theorem, j being in the source of (V, E) implies that $c_j = 1$. By Constraint 1 of the Quarkflow Theorem, $c_j = 1 \le d_j$, which means $j \in V_1$ by the definition of V_1 . j has no incoming edge at all, and therefore is in the source of (V_1, E_1) .

We finally prove the third statement of the criterion. if j is in the sink of (V, E), then by Constraint 3 of the Quarkflow Theorem, $d_j = K$. By Constraint 1 of the Quarkflow Theorem, $c_j \leq K = d_j$. Therefore, by the definition of V_k , $j \in V_k$. This completes the proof of Criterion 2 of Section 3.

Criterion 3: To prove Criterion 3, we use Equation (9) to construct a set of $s_{i,k}$ for each subgraph k and $i \in V_k$. We now show that such $s_{i,k}$ satisfies both conditions in the Atomic Stage Lemma. Thus Criterion 3 holds by the Lemma.

To show this, consider any $(i,j) \in E_k$. By the construction of E_k , we have $c_j = k$. By Constraint 4 of the Quarkflow Theorem, $c_i \le c_j = k$. The rest of the proof splits into two cases, $c_i = c_j = k$ and $c_i < c_j = k$.

• If $c_i = c_j = k$, then by Equation (9),

$$s_{i:k} := e_i - c_i = e_i - k, \quad s_{i:k} := e_i - c_i = e_i - k.$$

Constraint 6 and 7 of the Quarkflow Theorem states that

$$e_j - e_i \ge \begin{cases} 1, & (i,j) \in E_S \\ 0, & (i,j) \notin E_S \end{cases}$$

Therefore,

$$s_{j,k} - s_{i,k} = (e_j - k) - (e_i - k) = e_j - e_i \ge \begin{cases} 1, & (i,j) \in E_S \\ 0, & (i,j) \notin E_S \end{cases}$$

which is a sufficient condition for the Atomic Stage Lemma to hold.

• If $c_i < c_j = k$, then by Equation (9),

$$s_{i:k} := e_i - c_i, \quad s_{i:k} := 0.$$

So, $s_{j;k} - s_{i;k} = e_j - c_j$. Using Constraints 5 and 8 of the Quarkflow Theorem, we therefore have

 $s_{j;k} - s_{i;k} \ge \begin{cases} 1, & (i,j) \in E_S \\ 0, & (i,j) \notin E_S \end{cases}$

which is sufficient for the Atomic Stage Lemma. In both cases, we now have proved Criterion 3.

4. Decomposition as the dual of a network flow problem. In Section 2, we formulated three criteria that define a valid decomposition of a stencil update formula into atomic stages. In Section 3, we proved that any such valid decomposition could be represented by a set of integers, K and $(c_i, d_i, e_i), \forall i \in V$ that satisfy a set of linear constraints among them. The reverse is also true: any set of integers satisfying these constraints represents a valid decomposition. In this section, we complete these linear constraints with a linear cost function to form an integer program.

The cost function should model how expensive it is to execute the decomposed formula. This cost, in a massively parallel computation, depends on the interconnect, the domain decomposition, and the solver. In this paper, we use a very simplistic cost function, composed of two factors: the number of stages and the amount of coupling between the stages. These factors correspond to the communication cost of executing the decomposed formula in the swept rule of parallel computing [3]. The number of stages is proportional to how often data needs to be communicated, and thereby models the communication time due to network latency. The amount of coupling between stages can correspond to how much data is communicated, and thereby models how much time is spent due to network bandwidth. Both factors can be represented algebraically using the same integers K and (c_i, d_i, e_i) we use in Section 3.

The first factor, the number of atomic stages, is simply K. The second factor, the amount of coupling, can be modeled as the amount of values shared between stages. If a value belongs to only one stage, i.e., $c_i = d_i$, it does not contribute to the amount of coupling. If a value belongs to multiple stages, it couples these stages c_i, \ldots, d_i . It then adds an amount $w_i(d_i - c_i)$ to the total coupling. $w_i, i \in V$ here are the weights of the vertices in the graph. If all vertices represent values of the same size, we can set $w_i \equiv 1$. If vertices can represent values of different size, i.e., vectors, matrices, and tensors, then w_i can be adjusted to the number of bytes required to store the ith intermediate value at each grid point. The two factors can be blended using a positive weight factor W_K , the only tuning parameter of the cost function. Curiously, the choice of W_K does not appear to affect the outcome of the optimization in the test cases we have so far examined. The blended cost function combines with the constraints in the Quarkflow Theorem of Section 4 to form the following integer programming problem,

(10)
$$\min_{K,c_i,d_i,e_i,i\in V} W_K K + \sum_i w_i (d_i - c_i)$$
$$s.t. K, c_i, d_i, e_i \in \mathcal{Z}, \text{ and}$$

all 8 conditions in the Quarkflow Theorem are satisfied.

Here \mathcal{Z} represent integers.

This integer program problem can be solved by solving the equivalent linear program, ignoring the requirement that the solutions must be integers, by a simplex method. This is a characteristic shared by all integer programming problems in which the constraint matrix is totally unimodular [29] and the constraint constants are integers. This problem (10) has a unimodular constraint matrix because all its constraints involve the difference between pairs of variables [18]. Therefore, each row of the constraint matrix has exactly two entries; one equals to 1, the other equals to -1. The transpose of this matrices has the same property as the constraint matrix of a flow network. Because the constraint matrix of flow networks are totally unimodular [2], our constraint matrix is totally unimodular.

Not only is the constraint matrix transpose to that of a flow network, the linear program is the symmetric dual of a minimum-cost flow problem on a flow network. In this flow network, each variable in Problem (10), including c_i, d_i, e_i and K, is a vertex. An additional vertex, denoted as 0, is introduced for the single-variable constraints $c_i = 1, \forall i \in V_S$. The dual of Problem (10) as a linear program is

Choose
$$\forall i \in V_S, \quad x_{c_i,0} \in R,$$

$$\forall i \in V_T, \quad x_{d_i,K} \in R,$$

$$\forall i \in V, \quad x_{c_i,d_i} \geq 0,$$

$$x_{c_i,e_i} \geq 0,$$

$$x_{e_i,c_i} \geq 0,$$

$$\forall (i,j) \in E, \quad x_{c_i,c_j} \geq 0,$$

$$x_{c_j,d_i} \geq 0,$$

$$x_{e_i,e_j} \geq 0$$

in order to

(11)
$$\min \sum_{i \in V_S} x_{c_i,0} + \sum_{i \in V} (x_{e_i,c_i} - I_{\exists (j,i) \in E_S} x_{c_i,e_i}) - \sum_{(i,j) \in E_S} x_{e_i,e_j}$$

$$s.t. \sum_{i \in V_T} x_{d_i,K} = W_K, \quad \text{and } \forall i \in V,$$

$$I_{i \in V_S} x_{c_i,0} + x_{c_i,d_i} + x_{c_i,e_i} - x_{e_i,c_i}$$

$$+ \sum_{j:(j,i) \in E} (x_{c_i,d_j} - x_{c_j,c_i}) + \sum_{j:(i,j) \in E} x_{c_i,c_j} = w_i$$

$$I_{i \in V_T} x_{d_i,K} - x_{c_i,d_i} - \sum_{j:(i,j) \in E} x_{c_j,d_i} = -w_i$$

$$- x_{c_i,e_i} + x_{e_i,c_i} + \sum_{j:(i,j) \in E} x_{e_i,e_j} - \sum_{j:(j,i) \in E} x_{e_j,e_i} = 0$$

The constraints are flow balance equations on all vertices in the flow network, except for vertex 0, whose balance equation is a redundant linear combination of the constraints listed above:

$$\sum_{i \in V_S} x_{c_i,0} = -W_K$$

Adding this redundant constraint to the above problem, it becomes clear that this is a minimum cost flow network problem [1], one that can leverage specialized, fast solvers, such as the out-of-kilter algorithm [17, 2] and relaxation algorithms [6].

5. Implementation, Tests and Results. To demonstrate the algorithm developed in this paper, the minimum cost flow network problem (11) is solved using the out-of-kilter algorithm [17], implemented in the open source package GLPK [24]. The out-of-kilter algorithm returns the solution of both the linear program (11) and its dual (10). The dual solution includes c_i for each vertex $i \in V$, indicating the stage in which the corresponding value should be created. The solution also includes d_i for each vertex. Comparing it to c_i tells us whether Value i is used only in its creating stage, or should be passed to subsequent stages for further use.

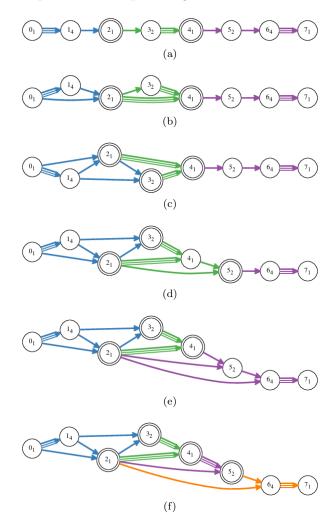


Fig. 2: Atomic decomposition of manufactured test cases. These graphs are not generated from real stencil update formulae but are constructed for testing and illustration purposes. The number and subscript shown in each vertex represent the index i and weight w_i of the vertex. Triple-lined edges represent "swept" edges. Different colors represent different stages. Double circles represent vertices shared by more than one stages.

"pascal" ¹ . The algorithm is first tested in a series of manufactured test cases, as shown in Figure 2.

In (a), our algorithm is asked to decompose a graph of eight vertices; each vertex only depends on the previous one. Three out of the seven dependencies are swept. Under the constraints of atomic decomposition, the optimal decomposition should split the graph into three subgraphs, each containing one swept edge. It should also minimize the total weight of the vertices shared by two subgraphs. The outcome of our algorithm produces this behavior; both shared vertices are of weight 1.

In (b), two additional edges are added, but without affecting the decomposition. The creating stage and discarding stage of each variable can stay the same, thereby creating no more shared vertices. Our algorithm still chooses a similar decomposition as before.

In (c), an edge is added from Vertex 1 to Vertex 3. If Vertex 3 had the same creating stage, green, as in (b), Vertex 1 must be shared between the blue and green stages. This sharing would increase the cost function by 4, the weight of Vertex 1. To reduce the cost, the algorithm moves Vertex 3 into the blue stage, sharing it between the blue and green stages. Because Vertex 3 has a weight of 2, sharing it would increase the cost function only by 2.

In (d), another edge is added from Vertex 2 to Vertex 5. Keeping the creating stage of Vertex 5 would require now sharing Vertex 2 between all three stages, increasing the cost function of (10) by 1. Instead, our algorithm changed the creating stage of Vertex 5, sharing it between the green and purple stages. The resulting increase of the cost function is also 1. Multiple integer optimums exist in this case. Note that any linear combination of these integer optimums also solves the linear program. The out-of-kilter algorithm always chooses one of the integer optimums.

In (e), an edge is added from Vertex 2 to Vertex 6. Now Vertex 2 must be shared among all three stages anyway, our algorithm found it unnecessary to share Vertex 5, and reverts to sharing the cheaper Vertex 4 between the green and purple stages.

In (f), the edge from 4 to 5 is changed to a swept edge. It forces an additional stage to be created, by splitting from the purple stage in (e), sharing Vertices 2 and 5 with the remaining purple stage. Sharing Vertices 2 and 3, the combined weight of which is 3, is cheaper than the alternative splitting of sharing Vertex 6, which alone has a weight of 4.

Our algorithm is then tested on a stencil update formula for solving the 3D heat equation using a two-stage Runge-Kutta scheme. The formula is described in Python as following.

```
uh = u + 0.5 * dt / dx**2 * (im(u) + ip(u) - 2 * u + jm(u) + jp(u) - 2 * u + km(u) + kp(u) - 2 * u)

return u + dt / dx**2 * (im(uh) + ip(uh) - 2 * uh + jm(uh) + jp(uh) - 2 * uh + km(uh) + kp(uh) - 2 * uh)
```

The code above is fed into the software "pascal"¹, which automatically builds the computational graph using operator overloading, then calls "quarkflow" to decompose the graph, then translates each subgraph into C code for execution on parallel architectures. Figure 3 illustrates the decomposed computational graph in this example. The computational graph contains 39 vertices connected by 56 directed edges, among which 6 are swept. The decomposition algorithm completed in about 0.38

 $^{^1 \}rm https://github.com/qiqi/pascal,$ branch master, commit df01f76a8bf1bc64237d2e346616dd67e6dd8116

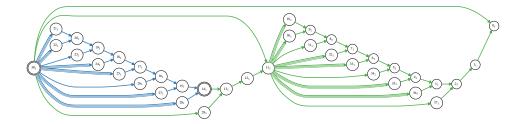


Fig. 3: Atomic decomposition of a 3D heat equation, integrated using the midpoint rule (two-stage Runge-Kutta). The number and subscript shown in each vertex represent the index i and weight w_i of the vertex. Triple-lined edges represent "swept" edges. Different colors represent different stages. Double circles represent vertices shared by more than one stages.

milliseconds on an Intel(R) Core(TM) i7-6650U processor clocked at 2.20GHz. The update formula is decomposed into two stages, containing 22 and 34 edges, respectively. They include 16 and 25 vertices, sharing Vertices 14 and 38.

Finally, our algorithm is applied to an update formula for the Euler equation of gas dynamics. The spatial discretization, described in Appendix A, is the conservative, skew-symmetric finite difference scheme, with a conservative, symmetric, negative-definite 4th order numerical dissipation. The temporal discretization is the 4th order Runge-Kutta scheme. Each spatial discretization requires information from the neighbor of neighboring grid points. Each time step requires 4 level of spatial discretization, thereby requiring access to 8 levels of neighboring grid points. The formula was encoded in Python below and is automatically decomposed. Figure 4 shows the decomposition into 8 stages of this update formula. The computational graph has 1424 vertices and 2106 edges, among which 432 are swept. The decomposition algorithm completed in about 0.25 seconds on an Intel(R) Core(TM) i7-6650U processor clocked at 2.20GHz. The update formula is decomposed into eight stages, containing an average of 186.625 nodes. An average of 6.785 nodes in each stage is shared with subsequent stages.

6. Conclusion. This paper shows that we can decompose a complex stencil update formula by solving the dual of a minimum cost flow network problem. This is a highly nontrivial result because brute force solution of the original problem is an integer program of combinatorial complexity. Instead, the reformulation presented in this paper leads to a linear program of appealing structure, amenable to some very efficient algorithms. As a result, even complex stencils can be decomposed efficiently.

Efficient and automatic decomposition of complex stencil update formulas, such as the one for the Euler equation presented in Section 6, simplifies application of the swept decomposition rule [3]. To use the swept decomposition rule to a numerical scheme, one only need to encode the stencil update formula of the scheme in Python. The update formula is then quickly and automatically decomposed into a series of atomic stages, each can be translated into low level computer code. The resulting code can then be inserted into a software framework for executing the scheme in the swept decomposition rule.

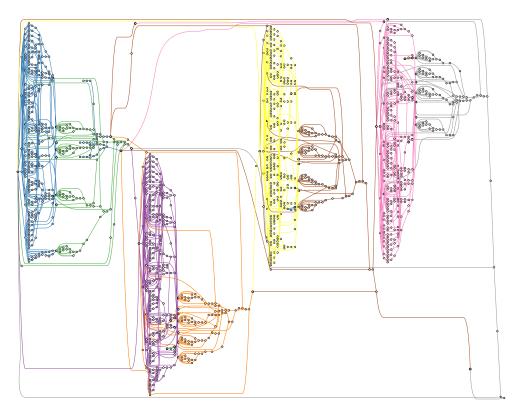


Fig. 4: Automatic decomposition of a complex time step into eight atomic stages. The update formula is for the Euler equation of gas dynamics in three spatial dimensions, using a second-order finite-difference spatial discretization scheme, and a fourth-order Runge-Kutta time integrator.

Acknowledgment. The author acknowledges support from the NASA TTT program Award NNX15AU66A under Dr. Mujeeb Malik and technical monitor Dr. Eric Nielsen, and from the DOE Office of Science ASCR program Award DE-SC-0011089 under Dr. Sandy Landsberg and Dr. Steve Lee. This paper significantly benefited from discussions with Dr. David Gleich, Dr. Christopher Maes, and Dr. Michael Saunders, as well as comments from the anonymous reviewers.

Appendix A. Discretization of the 3D Euler equation.

```
def diffx(w): return (ip(w) - im(w)) / (2 * dx)
def diffy(w): return (jp(w) - jm(w)) / (2 * dy)
def diffz(w): return (kp(w) - km(w)) / (2 * dz)

def div_dot_v_phi(v, phi):
    return diffx(v[0] * phi) + diffy(v[1] * phi) + diffz(v[2] * phi)

def v_dot_grad_phi(v, phi):
    return v[0] * diffx(phi) + v[1] * diffy(phi) + v[2] * diffz(phi)

def dissipation(r, u):
    laplace = lambda u: (ip(u) + im(u) + jp(u) + jm(u) + jp(u) + jm(u)) / 6 - u
    return laplace(DISS_COEFF * r * r * laplace(u))

def assemble_rhs(mass, momentum_x, momentum_y, momentum_z, energy):
    rhs_w = zeros(w.shape)
```

```
rhs_w[0] = -mass
    rhs_w[1] = -momentum_x
     rhs_w[2] = -momentum_y
     rhs_w[3] = -momentum_z
    rhs_w[4] = -energy
     return rhs_w
def rhs(w):
     r, rux, ruy, ruz, p = w
    ux, uy, uz = rux / r, ruy / r, ruz / r
     ru, u = (rux, ruy, ruz), (ux, uy, uz)
     mass = div_dot_v_phi(ru, r)
     mom_x = (div_dot_v_phi(ru, rux) + r * v_dot_grad_phi(ru, ux)) / 2 + diffx(p)
    mom_y = (div_dot_v_phi(ru, ruy) + r * v_dot_grad_phi(ru, uy)) / 2 + diffy(p)
mom_z = (div_dot_v_phi(ru, ruz) + r * v_dot_grad_phi(ru, uz)) / 2 + diffz(p)
     energy = gamma * div_dot_v_phi(u, p) - (gamma-1) * v_dot_grad_phi(u, p)
     dissipation_x = dissipation(r, ux) * c0 / dx
     dissipation_y = dissipation(r, uy) * c0 / dy
    dissipation_z = dissipation(r, uz) * c0 / dz
    rhs_r = c0 * fan * (r - r_fan)

rhs_ux = c0 * fan * (ux - ux_fan) + c0 * obstacle * ux
    rhs_uy = c0 * fan * (uy - uy_fan) + c0 * obstacle * uy
rhs_uz = c0 * fan * (uz - uz_fan) + c0 * obstacle * uz
    rhs_p = c0 * fan * (p - p_fan)
     return assemble_rhs((mass - rhs_r) / (2 * r) + fan * (r - r_fan),
                              (mom_x + dissipation_x - rhs_ux) / r,
(mom_y + dissipation_y - rhs_uy) / r,
(mom_z + dissipation_z - rhs_uz) / r, (energy - rhs_p))
def step(w):
    dw0 = dt * rhs(w)
    dw1 = dt * rhs(w + 0.5 * dw0)
    dw2 = dt * rhs(w + 0.5 * dw1)
    dw3 = dt * rhs(w + dw2)
    return w + (dw0 + dw3) / 6 + (dw1 + dw2) / 3
```

REFERENCES

- R. K. Ahuja, T. L. Magnanti, and J. B. Orlin, Network flows, tech. report, DTIC Document, 1988.
- [2] R. K. Ahuja, T. L. Magnanti, and J. B. Orlin, Network flows: theory, algorithms, and applications, Prentice hall, 1993.
- [3] M. ALHUBAIL AND Q. WANG, The swept rule for breaking the latency barrier in time advancing pdes, Journal of Computational Physics, 307 (2016), pp. 110–121.
- [4] M. M. ALHUBAIL, Q. WANG, AND J. WILLIAMS, The swept rule for breaking the latency barrier in time advancing two-dimensional PDEs, submitted to the Journal of Computational Physics, arXiv preprint arXiv:1602.07558, (2016).
- [5] B. BARNEY ET AL., Introduction to parallel computing, Lawrence Livermore National Laboratory, 6 (2010), p. 10.
- [6] D. P. BERTSEKAS AND P. TSENG, Relaxation methods for minimum cost ordinary and generalized network flow problems, Operations Research, 36 (1988), pp. 93–114.
- [7] E. L. BOYD, G. A. ABANDAH, H.-H. LEE, AND E. S. DAVIDSON, Modeling computation and communication performance of parallel scientific applications: A case study of the ibm sp2, Ann Arbor, 1001 (1995), pp. 48109–2122.
- [8] E. CARSON, N. KNIGHT, AND J. DEMMEL, Avoiding communication in nonsymmetric lanczosbased krylov subspace methods, SIAM Journal on Scientific Computing, 35 (2013), pp. S42– S61
- [9] T.-F. CHEN AND J.-L. BAER, Reducing memory latency via non-blocking and prefetching caches, in ASPLOS V Proceedings of the fifth international conference on Architectural support for programming languages and operating systems, ACM, 1992, pp. 51–61.
- [10] M. CHRISTEN, O. SCHENK, AND H. BURKHART, Patus: A code generation and autotuning framework for parallel iterative stencil computations on modern microarchitectures, in Parallel & Distributed Processing Symposium (IPDPS), 2011 IEEE International, IEEE,

- 2011, pp. 676-687.
- [11] M. CROVELLA, R. BIANCHINI, T. LEBLANC, E. MARKATOS, AND R. WISNIEWSKI, Using communication-to-computation ratio in parallel program design and performance prediction, in Parallel and Distributed Processing, 1992. Proceedings of the Fourth IEEE Symposium on, IEEE, 1992, pp. 238–245.
- [12] K. Datta, S. Kamil, S. Williams, L. Oliker, J. Shalf, and K. Yelick, Optimization and performance modeling of stencil computations on modern microprocessors, SIAM review, 51 (2009), pp. 129–159.
- [13] K. Datta, M. Murphy, V. Volkov, S. Williams, J. Carter, L. Oliker, D. Patterson, J. Shalf, and K. Yelick, Stencil computation optimization and auto-tuning on stateof-the-art multicore architectures, in Proceedings of the 2008 ACM/IEEE conference on Supercomputing, IEEE Press, 2008, p. 4.
- [14] J. DEMMEL, M. HOEMMEN, M. MOHIYUDDIN, AND K. YELICK, Avoiding communication in sparse matrix computations, in Parallel and Distributed Processing, 2008. IPDPS 2008. IEEE International Symposium on, IEEE, 2008, pp. 1–12.
- [15] J. Dongarra, J. Hittinger, J. Bell, L. Chacon, R. Falgout, M. Heroux, P. Hovland, E. Ng, C. Webster, and S. Wild, Applied mathematics research for exascale computing, tech. report, Lawrence Livermore National Laboratory (LLNL), Livermore, CA, 2014.
- [16] P. F. FISCHER, K. HEISEY, AND M. MIN, Scaling limits for PDE-based simulation, in 22nd AIAA Computational Fluid Dynamics Conference, 2015, p. 3049.
- [17] D. R. Fulkerson, An out-of-kilter method for minimal-cost flow problems, Journal of the Society for Industrial and Applied Mathematics, 9 (1961), pp. 18–27.
- [18] R. S. GARFINKEL AND G. L. NEMHAUSER, Integer programming, vol. 4, Wiley New York, 1972.
- [19] P. GHYSELS, T. J. ASHBY, K. MEERBERGEN, AND W. VANROOSE, Hiding global communication latency in the GMRES algorithm on massively parallel machines, SIAM Journal on Scientific Computing, 35 (2013), pp. C48–C71.
- [20] T. GYSI, T. GROSSER, AND T. HOEFLER, Modesto: Data-centric analytic optimization of complex stencil programs on heterogeneous architectures, in Proceedings of the 29th ACM on International Conference on Supercomputing, ACM, 2015, pp. 177–186.
- [21] M. HOEMMEN, Communication-avoiding Krylov subspace methods, PhD thesis, University of California, Berkeley, 2010.
- [22] F. KJOLSTAD, S. KAMIL, J. RAGAN-KELLEY, D. I. LEVIN, S. SUEDA, D. CHEN, E. VOUGA, D. M. KAUFMAN, G. KANWAR, W. MATUSIK, ET AL., Simit: A language for physical simulation, ACM Transactions on Graphics (TOG), 35 (2016), p. 20.
- [23] J. LARSSON AND Q. WANG, The prospect of using large eddy and detached eddy simulations in engineering design, and the research required to get there, Philosophical Transactions of the Royal Society of London A: Mathematical, Physical and Engineering Sciences, 372 (2014), p. 20130329.
- [24] A. Makhorin, GLPK (GNU linear programming kit), 2008.
- [25] G. MUDALIGE, M. GILES, I. REGULY, C. BERTOLLI, AND P. J. KELLY, Op2: An active library framework for solving unstructured mesh-based applications on multi-core and many-core architectures, in Innovative Parallel Computing (InPar), 2012, IEEE, 2012, pp. 1–12.
- [26] I. Z. REGULY, G. R. MUDALIGE, C. BERTOLLI, M. B. GILES, A. BETTS, P. H. KELLY, AND D. RADFORD, Acceleration of a full-scale industrial cfd application with op2, IEEE Transactions on Parallel and Distributed Systems, 27 (2016), pp. 1265–1278.
- [27] L. RENGANARAYANAN, D. KIM, S. RAJOPADHYE, AND M. M. STROUT, Parameterized tiled loops for free, in ACM SIGPLAN Notices, vol. 42, ACM, 2007, pp. 405–414.
- [28] S. ROSTRUP AND H. DE STERCK, Parallel hyperbolic PDE simulation on clusters: Cell versus GPU, Computer Physics Communications, 181 (2010), pp. 2164–2179.
- [29] A. Schrijver, Theory of linear and integer programming, John Wiley & Sons, 1998.
- [30] J. SLOTNICK, A. KHODADOUST, J. ALONSO, D. DARMOFAL, W. GROPP, E. LURIE, AND D. MAVRIPLIS, CFD vision 2030 study: a path to revolutionary computational aerosciences, tech. report, NASA, 2014.
- [31] V. STRUMPEN AND T. L. CASAVANT, Exploiting communication latency hiding for parallel network computing: Model and analysis, in Parallel and Distributed Systems, 1994. International Conference on, IEEE, 1994, pp. 622–627.
- [32] D. WONNACOTT, Using time skewing to eliminate idle time due to memory bandwidth and network limitations, in Parallel and Distributed Processing Symposium, 2000. IPDPS 2000. Proceedings. 14th International, IEEE, 2000, pp. 171–180.