Graph Library: Overview

Document #: P3126r1
Date: 2024-02-05
Project: Programming Language C++
Audience: Library Evolution
          SG19 Machine Learning
          SG14 Game, Embedded, Low Latency
          SG6 Numerics
Revises: D3126r0

Reply-to: Phil Ratzloff (SAS Institute)
          phil.ratzloff@sas.com
          Andrew Lumsdaine
          lumsdaine@gmail.com

Contributors: Kevin Deweese
               Muhammad Osama (AMD, Inc)
               Jesun Firoz
               Michael Wong (Intel)
               Jens Maurer
               Richard Dosselmann (University of Regina)
               Matthew Galati (Amazon)
               Guy Davidson (Creative Assembly)
1 Getting Started

This paper is one of several interrelated papers for a proposed Graph Library for the Standard C++ Library. The Table 1 describes all the related papers.

<table>
<thead>
<tr>
<th>Paper</th>
<th>Status</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>P1709</td>
<td>Inactive</td>
<td>Original proposal, now separated into the following papers.</td>
</tr>
<tr>
<td>P3126</td>
<td>Active</td>
<td>Overview, describes the big picture of what we are proposing.</td>
</tr>
<tr>
<td>P3127</td>
<td>Active</td>
<td>Background and Terminology provides the motivation, theoretical background, and terminology used across the other documents.</td>
</tr>
<tr>
<td>P3128</td>
<td>Active</td>
<td>Algorithms covers the initial algorithms as well as the ones we’d like to see in the future.</td>
</tr>
<tr>
<td>P3129</td>
<td>Active</td>
<td>Views has helpful views for traversing a graph.</td>
</tr>
<tr>
<td>P3130</td>
<td>Active</td>
<td>Graph Container Interface is the core interface used for uniformly accessing graph data structures by views and algorithms. It is also designed to easily adapt to existing graph data structures.</td>
</tr>
<tr>
<td>P3131</td>
<td>Active</td>
<td>Graph Containers describes a proposed high-performance compressed_graph container. It also discusses how to use containers in the standard library to define a graph, and how to adapt existing graph data structures.</td>
</tr>
</tbody>
</table>

Table 1: Graph Library Papers

Reading them in order will give the best overall picture. If you’re limited on time, you can use the following guide to focus on the papers that are most relevant to your needs.

Reading Guide

— If you’re new to the Graph Library, we recommend starting with the Overview paper (P3126) to understand the focus and scope of our proposals.

— If you want to understand the theoretical background that underpins what we’re doing, you should read the Background and Terminology paper (P3127).

— If you want to use the algorithms, you should read the Algorithms paper (P3128) and Graph Containers paper (P3131).

— If you want to write new algorithms, you should read the Views paper (P3129), Graph Container Interface paper (P3130), and Graph Containers paper (P3131). You’ll also want to review existing implementations in the reference library for examples of how to write the algorithms.

— If you want to use your own graph container, you should read the Graph Container Interface paper (P3130) and Graph Containers paper (P3131).

2 Revision History

P3126r0

— Split from P1709r5. Added Getting Started section.

— Rewrite Goals and Priorities section to reflect the structure of the papers and to include a section on our Future Roadmap.

— Added Notes and Considerations section.

— Concepts will be identified as “For exposition only” until we have consensus of whether they belong in the standard or not.

P3126r1

— Added Issues Status section to be open with the issues that have been reported and that we are working on.
3 Overview

Graphs, used in ML and other scientific domains, as well as industrial and general programming, do not presently exist in the C++ standard. In ML, a graph forms the underlying structure of an artificial neural network (ANN). In a game, a graph can be used to represent the map of a game world. In business environments, graphs arise as entity relationship diagrams (ERD) or data flow diagrams (DFD). In the realm of social media, a graph represents a social network.

All documents, taken as a whole for a Graph Library, proposes the addition of graph algorithms, operators, views, adaptors, the graph container interface, and a graph container implementation to the C++ library to support machine learning (ML), as well as other applications. ML is a large and growing field, both in the research community and industry, that has received a great deal of attention in recent years. This document presents an interface of the proposed algorithms, operators, adaptors, views, graph functions, and containers.

4 Goals and Priorities

Because graphs and their algorithms cover a broad range of capabilities and implementations, we have defined a focused set of goals and priorities that will provide an initial set of useful functionality, as well as a sound foundation for future work.

— Provide a firm theoretical foundation for the library.

— Follow the separation of algorithms, ranges, views, and containers established by the standard library.

— Include a rich enough set of algorithms for the library to be useful.

— The syntax for an algorithm’s implementation should be simple, expressive, and easy to understand.

— The ability to write high-performance algorithms should not be compromised.

— Algorithms can expect vertices to be in a random access range with an integral vertex id initially.

— Include views for common traversals of a graph’s vertices and edges that is concise and consistent without having to use a lower level interface.

— Simple views for vertex list, incidence edges on a vertex, neighbors of a vertex, and edges of a graph.

— Complex views for depth-first search, breadth-first search, and topological sort.

— A Graph Container Interface, used by Views and Algorithms, that provides a consistent interface for different graph data structures. The interface includes concepts, types, traits and functions and provides a similar role to the Ranges library for standard containers.

— Descriptors for a consistent data model for vertex, edge and neighbor by views and edge lists.

— Adjacency list, an outer range of vertices with an inner range of outgoing edges on each vertex.

— Be able to use the algorithms and views with existing graph data structures using customization points.

— Support for optional user-defined value types on an edge, vertex, and/or the graph itself.

— Support bipartite and multipartite graphs.

— Edge list, which is a range of edge descriptors.

— From an edgelist view.

— From a user-defined range that uses std::ranges::transform_view.

— Provide one or more graph containers that can be used with the algorithms.

— A high-performance compressed_graph container, based on the Compressed Sparse Row matrix.
— The ability to create simple graph container from standard containers, e.g. `vector<vector<int>>`.

The design should not hinder the ability to extend the functionality to support expanded functionality identified in the future roadmap that follows.

4.1 Future Roadmap

The following are areas we’d like to see in future proposals, after the initial proposals are accepted. We endeavor to investigate these to assure the existing design will support them.

— Additional graph algorithms. The Graph Algorithms paper identifies tiers of algorithms we’d like to see added in the future, including parallel algorithms.

— Support for sparse vertex ids, implying the use of bi-directional containers such as `map` and `unordered_map` for vertices.

— Bi-directional graphs, where vertices have incoming and outgoing edges.

— Constexpr graphs, where vertices and edges are stored in `std::array` or other constexpr-friendly container.

5 Examples

The following code demonstrates how a simple graph can be created as a range of ranges, using the standard containers.

```cpp
using G = std::vector<std::vector<int>>;
G costar_adjacency_list{
    {1, 5, 6}, {7, 10, 0, 5, 12}, {4, 3, 11}, {2, 11}, {8, 9, 2, 12}, {0, 1}, {7, 0},
    {6, 1, 10}, {4, 9}, {4, 8}, {7, 1}, {2, 3}, {1, 4} }

int main() {
    std::vector<int> bacon_number(size(actors));

    // 1 -> Kevin Bacon
    for (auto& [uid, vid] : basic_sourced_edges_bfs(costar_adjacency_list, 1)) {
        bacon_number[vid] = bacon_number[uid] + 1;
    }

    for (int i = 0; i < size(actors); ++i) {
        std::cout << actors[i] << " has Bacon number " << bacon_number[i] << std::endl;
    }
}
```

target_id(g,uv) defines the required function to get a target_id for an edge in the graph G. Other functions can also be overridden to allow a developer to adapt their own graph data structures to the library.

6 What this proposal is not

The Graph Library proposal limits itself to adjacency graphs and edgelists only. An adjacency graph is an outer range of vertices with an inner range of outgoing edges on each vertex. An edgelist is a view of edges, which is either all the edges in the adjacency graph or a projection of a user-defined range.
Parallel versions of the algorithms are not included for several reasons. The executors proposal in P2300r5 [1] is expected to introduce new and better ways to do parallel algorithms beyond that used in the parallel STL algorithms and we would like to wait for finalization of that proposal before committing to parallel implementations. Secondly, many graph algorithms don’t benefit from parallel implementations so there is less need to offer an implementation. Lastly, it will help limit the size of this proposal which is already looking to be large without it. It is expected that future proposals will be submitted for parallel graph algorithms.

Hypergraphs are not supported.

7 Impact on the Standard
This proposal is a pure library extension.

8 Interaction with Other Papers
Other than the papers identified as part of the Graph Library, there is no interaction with other proposals to the standard.

9 Implementation Experience
The github github.com/stdgraph repository contains an implementation for this proposal.

10 Usage Experience
There is no current use of the library. There are plans to begin using it in 2024 in a commercial setting.

11 Deployment Experience
There is no current deployment experience of the library. There are plans for this to follow the usage experience.

12 Performance Considerations
The algorithms are being ported from NWGraph to the github.com/stdgraph implementation used for this proposal. Performance analysis from those algorithms can be found in the peer-reviewed papers for NWGraph [2, 3].

13 Prior Art

boost::graph has been an important C++ graph implementation since 2001. It was developed with the goal of providing a modern (at the time) generic library that addressed all the needs of a graph library user. It is still a viable library used today, attesting to the value it brings.

However, boost::graph was written using C++98 in an “expert-friendly” style, adding many abstractions and using sophisticated template metaprogramming, making it difficult to use by a casual developer.

NWGraph ([4] and [2]) was published in 2022 by Lumsdaine et al, bringing additional experience gained since creating boost::graph, to create a modern graph library using C++20 for its implementation that was more accessible to the average developer.

While NWGraph made important strides to introduce the idea of the graph as a range-of-ranges and implemented many important algorithms, there are some areas it didn’t address that come a practical use in the field. For instance, it didn’t have a well-defined API for graph data structures that could be applied to existing graphs, and there wasn’t a uniform approach to properties.
This proposal takes the best of NWGraph, with previous work done for P1709 to define a Graph Container Interface, to provide a library that embraces performance, ease-of-use, and the ability to use the algorithms and views on externally defined graph containers.

GraphBLAS Graph algorithms are traditionally developed, and then implemented, using explicit loops over a graph data structure—“pointer chasing” to put it perhaps somewhat pejoratively. An alternative formulation of graph algorithms leverages the close inherent relationship between graphs and sparse matrices to formulate graph algorithms as sequences of higher-level operations: sparse matrix multiplication (and other similar operations) over a semiring [5].

The GraphBLAS is an ad-hoc standardization effort to develop a set of kernel operations for supporting classical graph algorithms. As an API specification, the GraphBLAS is not a a graph library per se, but rather is intended to be used to implement graph algorithms (much as the linear algebra BLAS are used to implement linear algebra libraries such as LAPACK).

A C language binding that specifically implements the API is available as part of SuiteSparse. However, the resulting library relies on its own (opaque) data structures for representing graphs and would not be inter-operable with modern C++ approaches to library and application design. There have been early attempts at native C++ realizations of GraphBLAS, e.g., the GraphBLAS Template Library (GBTL).

(NB: Andrew is a co-author of boost::graph; Scott and Andrew were participants in GraphBLAS standardization and co-authors of GBTL; Andrew, Scott, and Phil are co-authors of NWGraph.)

14 Alternatives

Although the prior efforts have served, and do serve, important roles, they do not meet the needs or expectations of modern C++ development. We are currently unaware of any existing graph library that meets the same requirements and uses concepts and ranges from C++20.

15 Feature Test Macro

The __cpp_lib_graph feature test macro is recommended to represent all features in this proposal including algorithms, views, concepts, traits, types, functions, and graph container(s).

16 Freestanding

We believe this library can be used in a freestanding C++ implementation.

17 Namespaces

Graph containers and their views and algorithms are not interchangeable with existing containers and algorithms. Additionally, there are some domain-specific terms that may clash with existing or future names, such as degree and partition_id. For these reasons, we recommend their own namespaces. The following assumption is used in this proposal.

std::graph and std::graph::views

Alternative locations include the following:

std::ranges and std::ranges::views

std::ranges/graph and std::ranges::graph::views

The advantage of these two options are that there would be no requirement to use the ranges:: prefix for things in the std::ranges namespace, a common occurrence.
18 Notes and Considerations

There are some interesting observations that can be made about graphs and how they compare and contrast to the standard library that may not be obvious.

— The adjacency list, the primary data structure for this proposal, is a compound data structure of a range of ranges. This introduces a new form of container beyond a simple range.

— There is more than one possible value type, one each for edge, vertex, and graph. Each is optional. This is in contrast to existing practice where the value type is the distinguishing difference between different containers, such as for set and map.

— Algorithms will often use views, though they can use the GCI functions when needed.

— Algorithms and Views often need to allocate memory internally to achieve their purpose. This is a departure from common practice in the standard.

There are other observations we’ve also discovered along the way that may not be obvious.

— Storing vertices in a map (bi-directional range) requires a different style of programming algorithms, compared to being kept in a vector (random access range). When using a vector, edges(g,uid) would normally be used without much thought. Using that with a map would incur a $O(\log(V))$ cost. Instead, it will use vertex id once to get the vertex reference and then use edges(g,uv). This is expected to result in overloading of existing algorithms based on the range type of a container, distinguished with concepts.

The addition of concepts to the standard library is a serious consideration because, once added, they cannot be removed. We believe that graphs as a range-of-ranges merits the addition new concepts but we recognize that it may be a controversial decision. Toward that end, we will continue to include them to help clarify the examples given and are assumed to be 'For exposition only' as suggested implementation until clear decisions to include them, or not, is made.

19 Issues Status

This sections lists the known and open issues for the Graph Library proposal across all papers. They are organized by the paper they are associated with.

19.1 Open Design Issues

— P3130 Graph Container Interface

  1. Complete the definition of the edgelist concepts, types and CPO functions. This is distinct from the existing edgelist view.

— Pxxxx: Graph Operators (paper not yet submitted)

  1. Complete the paper for additional utility functions including degree, sort, relabel, transpose and join.

— Build on mdspan and try to standardize (or at least understand) what might reasonably be called an unstructured span

  — The statement assumes vertices are in a random-access range and prevents the use of bi-directional ranges like std::map, which could be used for sparse vertex ids. The existing design should be able to adept easily to mdspan.

  — I don’t think I expressed myself very well here. I completely take your point about not assuming that vertices are in a random-access range. But what I’m trying to get at is as follows.

Suppose someone standardizes unstructured span, as a natural extension of mdspan. What could we learn from its api that may be relevant for graphs? In both cases, we will presumably have a method which allows iteration over the ith partition (or edges of a given node, for graphs). Consistency of the stl may mean we want these to have the same look/feel.
19.2 Open Reported Issues

— P3127 Background and Terminology

1. P1709 has lots of details which I think to be irrelevant. (P1709 is the original proposal that was split into multiple papers)

   — Clarification: I don’t find the discussion about adjacency matrices helpful, but rather a distraction. It’s not that it shouldn’t be there in some form, but at the moment it has a prominence which I don’t think is commensurate with its importance to the paper, perhaps exacerbated by the fact that the paper lacks many salient details (see next point).

2. It is very hard to follow

   — Clarification: As it stands, the paper lacks a discussion of the authors’ standpoint on graph terminology, defining features (e.g. self loops, multi-edges) and the sort of trade-offs you get by allowing/not allowing them. Put another way, I think the paper would be easier to follow if there’s a technical narrative that reveals the way the authors are thinking about this huge area.

   I like the style of the motivation in P1709R5; if this could be greatly extended to include the mathematical background that Andrew is working on, this would be really helpful. And beyond the mathematical background, as discussion of the computational tradeoffs for both graph implementations and the associated algorithms, given certain choice, would be great to have.

   — This paper includes much of the content from P1709R5 for motivation. Andrew will be extending the paper to include a more rigorous mathematical description.

3. We need to add a mathematical perspective to the paper.

   — P3127 includes some of this. We plan on extending it to include a more rigorous mathematical description.

4. There needs to be a proper discussion about whether the paper’s definition of graph is what some authors call a multigraph and whether it does/doesn’t include loops.

   — The current version of P3128 Algorithms has a summary table for each algorithm that includes Complexity, Directed?, Multi-edge?, Cycles?, Self-loops?, and Throws?. We still need to make a pass through the algorithms to assure the values are correct.

   — The summary tables for the algorithms are necessary but not sufficient:

     — There needs to be a discussion of these aspects for graph implementations themselves. Various graph operations may be more efficient if the graph structure is more constrained. However, not allowing e.g. multiple edges between pairs of nodes prohibits representing many useful systems. There are trade-offs and these need to be discussed.

     — A justification of the choices made for the algorithms may be helpful.

5. The electrical circuit example has issues in P3127, section 6.1.

   — We acknowledge this and will remove it, or replace it with a better example.

   — I think it’s very valuable to include electrical circuits in addition to a simpler example. As we’ve discussed, electrical circuits are surprisingly subtle to represent using graphs, but I think users of a graph library should rightly expect that it can be elegantly done. I think signs of a good design for std::graph is that people can do this. So I think electrical circuits should stay in, in all their glory, but complemented by something less subtle.

— P3128 Graph Algorithms

1. A concern is that the DFS and BFS functionality isn’t flexible enough, especially when compared to boost::graph’s visitors.
We agree having a more general and flexible BFS and DFS would be valuable. We are investigating the merits of implementations based on coroutines and boost::graph-like visitors.

If we propose the use of coroutines we should explain our choice when compared to boost::graph’s visitors, which are the closest to a defacto standard available. The purpose of the standard library is to adopt standard practice, and it would help smooth the process to justify our decision.

— **Comparison to boost::graph** (paper not yet submitted)

1. My comment about the structure of the paper changing was a reference to previous comparisons with boost::graph. I’m sure these were in an earlier version, or am I misremembering?

   — We never had any comparisons to boost::graph.

   — We are planning on adding a new paper to compare it to graph-v2 in regards to syntax and performance.

### 19.3 Resolved Issues

— **P3126 Overview**

1. GraphBLAS is not included as part of the prior art.

   — Added in P3126r1.

— **P3130 Graph Container Interface**

1. I’m not convinced by the load API.

   — We agree because the use of both load functions and constructors creates ambiguity and complexity when both are defined. Even though constructors weren’t in the paper it wasn’t clear whether they should be included or not. We have removed the load functions and added constructors for `compressed_graph` to simplify the interface.

### Acknowledgements

*Phil Ratzloff’s* time was made possible by SAS Institute.

Portions of *Andrew Lumsdaine’s* time was supported by NSF Award OAC-1716828 and by the Segmented Global Address Space (SGAS) LDRD under the Data Model Convergence (DMC) initiative at the U.S. Department of Energy’s Pacific Northwest National Laboratory (PNNL). PNNL is operated by Battelle Memorial Institute under Contract DE-AC06-76RL01830.

*Michael Wong’s* work is made possible by Codeplay Software Ltd., ISOCPP Foundation, Khronos and the Standards Council of Canada.

*Muhammad Osama’s* time was made possible by Advanced Micro Devices, Inc.

The authors thank the members of SG19 and SG14 study groups for their invaluable input.
References


