




# GridFormat: header-only C++-library for grid file I/O

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## Summary

Numerical simulations play a crucial role in various research domains including mathematics, physics, and engineering. Such simulations typically involve solving a set of model equations that describe the physical system under investigation. To find an approximate solution to these equations on a given domain geometry and with specific boundary conditions, the domain is usually discretized into a grid composed of points and cells, on which discretization schemes such as finite differences, finite volumes, or finite elements are then employed. This process yields a discrete solution defined at specific grid positions, which, depending on the scheme, can be interpolated over the entire domain using its basis functions. Due to the high computational demand of such simulations, developers often implement simulation codes in performant C++ and leverage distributed-memory parallelism through MPI, the *Message Passing Interface* ([Clarke et al., 1994](#); [MPI Forum, 2023](#)), to run them on large high-performance computing systems.

Visualization plays a fundamental role in analyzing numerical results, and one widely-used visualization tool in research is ParaView ([Ahrens et al., 2005](#); [ParaView, 2023](#)), which is based on VTK, the *Visualization Toolkit* ([Schroeder et al., 2006](#); [The Visualization Toolkit, 2023](#)). ParaView can read results from a wide range of file formats, with the [VTK file formats](#) being among the most popular. To visualize simulation results with ParaView, researchers need to write their data into one of the supported file formats. Users of existing simulation frameworks, such as Dune ([Bastian et al., 2008, 2021](#)), Dumux ([Flemisch et al., 2011](#); [Koch et al., 2021](#)), Deal.II ([Arndt et al., 2022](#)), FEniCS ([A. Logg, 2012](#); [FEniCS, 2023](#)) or MFEM ([Anderson et al., 2021](#); [MFEM, 2023](#)), can usually export their results into some standard file formats. However, they are limited to those formats that are supported by the framework. Reusing another framework's I/O functionality is generally challenging, at least without runtime and memory overhead due to data conversions, since the implementation is typically tailored to its specific data structures. As a consequence, the work of implementing I/O into standard file formats is currently repeated in every framework and remains inaccessible for researchers developing new simulation frameworks or other research codes relying on I/O for visualization.

To address this issue, GridFormat aims to provide an easy-to-use and framework-agnostic API for reading from and writing to a variety of grid file formats. By utilizing generic programming with C++ templates and traits, GridFormat is data-structure agnostic and allows developers to achieve full interoperability with their data structures by implementing a small number of trait classes (see discussion below). Users of both simulation frameworks and self-written small codes can write grid-based data into standard file formats with minimal effort and without significant runtime or memory overhead. GridFormat comes with out-of-the-box support for data structures of several widely-used frameworks, namely Dune, Deal.II, FenicsX, MFEM, and CGAL ([CGAL, 2023](#); [The CGAL Project, 2023](#)).

## Statement of Need

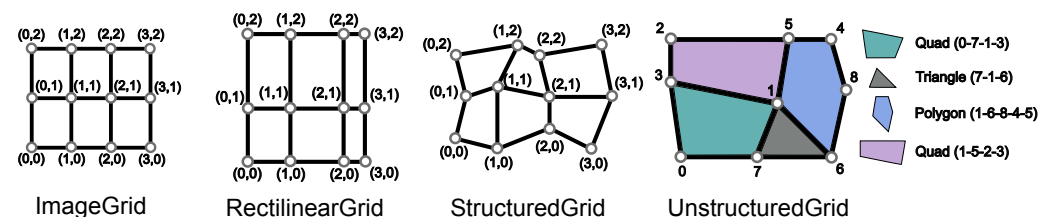
GridFormat addresses the issue of duplicate implementation effort for I/O across different simulation frameworks. By utilizing GridFormat as a backend for visualization file output, framework developers can easily provide their users with access to additional file formats. Moreover, instead of implementing support for new formats within the framework, developers can integrate them into GridFormat, thereby making them available to all other frameworks that use GridFormat. In addition to benefiting framework developers and users, the generic implementation of GridFormat also serves researchers with framework-independent smaller simulation codes.

Three key requirements govern the design of GridFormat: seamless integration, minimal runtime and memory overhead, and support for MPI. Given that C++ is widely used in grid-based simulation codes for performance reasons, we selected C++ as the programming language such that GridFormat can be adopted and used natively. It is lightweight, header-only, free of dependencies (unless opt-in features such as HDF5 output is desired), and supports CMake (CMake, 2023) features that allow for automatic integration of GridFormat in downstream projects.

A comparable project in Python is meshio (Schlömer, 2022), which supports reading from and writing to a wide range of grid file formats. However, accessing it from within simulators written in C++ would introduce an undesirable performance penalty, as well as memory overhead, since meshio operates on an internal mesh representation that users have to convert their data into. Dune users can employ dune-vtk (Praetorius, 2019), which supports I/O for a number VTK-XML file formats and flavours, however, its implementation is strongly coupled to the dune-grid interface and can therefore not be easily reused in other contexts. To the best of our knowledge, a framework-independent solution that fulfills the above-mentioned requirements does not exist.

## Concept

Following the distinct VTK-XML file formats, GridFormat supports four different *grid concepts*: ImageGrid, RectilinearGrid, StructuredGrid, and UnstructuredGrid. While the latter is fully generic, the first three assume that the grid has a structured topology. A known structured topology makes it obsolete to define cell geometries and grid connectivity, and formats designed for such grids can therefore store the grid in a space-efficient manner. An overview of the different types of grids is shown in the image below, and a more detailed discussion can be found in the [GridFormat documentation](#).



**Figure 1:** Overview over the grid concepts supported in GridFormat. While UnstructuredGrids are fully general, the first three have a structured topology.

GridFormat uses a traits (or meta-function) mechanism to operate on user-given grid types, and to identify which concept a given grid models. As a motivating example, consider the following function template:

```
template<typename Grid>
void do_something_on_a_grid(const Grid& grid) {
```

```
    for (const auto& cell : grid.cells()) {  
        // ...  
    }  
}
```

In the function body, we iterate over all cells of the given grid by calling the `cells` method. This limits the usability of this function to grid types that fulfill such an interface. One could wrap the grid in an adapter that exposes the required interface method. However, this can become cumbersome, especially if there are certain requirements on the cell type in the iterated range. An alternative is to use traits, which allows writing the function generically, accepting any instance of a grid type that the `Cells` trait class template is specialized for (by using (partial) template specialization):

```
namespace Traits { template<typename Grid> struct Cells; }  
  
template<typename Grid>  
void do_something_on_a_grid(const Grid& grid) {  
    for (const auto& cell : Traits::Cells<Grid>::get(grid)) {  
        // ...  
    }  
}
```

Instead of calling a function on grid directly, it is accessed via `Cells`, which can be specialized for any type. If such specialization exists, `do_something_on_a_grid` is invocable with an instance of type `Grid` directly, without the need for wrappers or adapters. Using C++-20 concepts, `GridFormat` can check at compile-time if a user grid specializes all required traits correctly. Error messages emitted by the compiler indicate which trait specializations are missing or incorrect. The traits mechanism makes the `GridFormat` library fully extensible: users can achieve compatibility with their concrete grid type by specializing the required traits within *their* code base, without having to change any code in `GridFormat`. Moreover, `GridFormat` comes with predefined traits for Dune, FenicsX, Deal.II, MFEM and CGAL such that users of these frameworks can directly use `GridFormat` without any implementation effort.

Note that each of the above-mentioned grid concepts requires the user to specialize a certain subset of traits. For instance, to determine the connectivity of an unstructured grid, `GridFormat` needs to know which points are embedded in a given grid cell. The information is not required for writing structured grids into structured grid file formats. An overview of which traits are required for which grid concept can be found in the [GridFormat documentation](#).

The traits are required for writing out grids and associated data, and are not needed when using `GridFormat` to read data from grid files. `GridFormat` provides access to the data as specified by the file format, however, these specifications may not be sufficient in all applications. For instance, to fully instantiate a simulator for parallel computations, information on the grid entities shared by different processes is usually required. Since these requirements are simulator-specific, any further processing has to be done manually by the user and for their data structures. The recommended way to deal with this issue is to add any information required for reinstantiation as data fields to the output. This way, it is readily available when reading the file. For information on how to use these features, we refer to the [API documentation](#) and the [examples](#).

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A. Logg, G. N. W. et al, K.-A. Mardal. (2012). *Automated solution of differential equations by the finite element method*. Springer. <https://doi.org/10.1007/978-3-642-23099-8>

Ahrens, J., Geveci, B., & Law, C. (2005). ParaView: An end-user tool for large-data visualization. *The Visualization Handbook*. <https://doi.org/10.1016/B978-012387582-2/50038-1>

Anderson, R., Andrej, J., Barker, A., Bramwell, J., Camier, J.-S., Cervený, J., Dobrev, V., Dudouit, Y., Fisher, A., Kolev, Tz., Pazner, W., Stowell, M., Tomov, V., Akkerman, I., Dahm, J., Medina, D., & Zampini, S. (2021). MFEM: A modular finite element methods library. *Computers & Mathematics with Applications*, 81, 42–74. <https://doi.org/10.1016/j.camwa.2020.06.009>

Arndt, D., Bangerth, W., Feder, M., Fehling, M., Gassmüller, R., Heister, T., Heltai, L., Kronbichler, M., Maier, M., Munch, P., Pelteret, J.-P., Sticko, S., Turcksin, B., & Wells, D. (2022). The deal.II library, version 9.4. *Journal of Numerical Mathematics*, 30(3), 231–246. <https://doi.org/10.1515/jnma-2022-0054>

Bastian, P., Blatt, M., Dedner, A., Dreier, N.-A., Engwer, C., Fritze, R., Gräser, C., Grüninger, C., Kempf, D., Klöforn, R., Ohlberger, M., & Sander, O. (2021). The Dune framework: Basic concepts and recent developments. *Computers & Mathematics with Applications*, 81, 75–112. <https://doi.org/10.1016/j.camwa.2020.06.007>

Bastian, P., Blatt, M., Dedner, A., Engwer, C., Klöforn, R., Kornhuber, R., Ohlberger, M., & Sander, O. (2008). A generic grid interface for parallel and adaptive scientific computing. Part II: Implementation and tests in DUNE. *Computing*, 82(2), 121–138. <https://doi.org/10.1007/s00607-008-0004-9>

CGAL. (2023). Website: <https://www.cgal.org/>, code repository: <https://github.com/CGAL/cgal>.

Clarke, L., Glendinning, I., & Hempel, R. (1994). The MPI message passing interface standard. In K. M. Decker & R. M. Rehmann (Eds.), *Programming environments for massively parallel distributed systems* (pp. 213–218). Birkhäuser Basel. ISBN: 978-3-0348-8534-8

CMake. (2023). Website: <https://cmake.org/>.

FEniCS. (2023). Website: <https://fenicsproject.org/>, code repository: <https://github.com/FEniCS>.

Flemisch, B., Darcis, M., Erbertseder, K., Faigle, B., Lauser, A., Mosthaf, K., Müthing, S., Nuske, P., Tatomir, A., Wolff, M., & Helmig, R. (2011). DuMux: DUNE for multi-{phase, component, scale, physics, ...} flow and transport in porous media. *Advances in Water Resources*, 34(9), 1102–1112. <https://doi.org/10.1016/j.advwatres.2011.03.007>

Koch, T., Gläser, D., Weishaupt, K., & others. (2021). DuMu<sup>x</sup> 3 - an open-source simulator for solving flow and transport problems in porous media with a focus on model coupling. *Computers & Mathematics with Applications*, 81, 423–443. <https://doi.org/10.1016/j.camwa.2020.02.012>

MFEM. (2023). Website: <https://mfem.org/>, code repository: <https://github.com/mfem/mfem>.

MPI Forum. (2023). Website: <https://www.mpi-forum.org/docs/>.

ParaView. (2023). Website: <https://www.paraview.org/>.

Praetorius, S. (2019). *Dune-vtk*. Published on the Dune GitLab server at <https://gitlab.dune-project.org/extensions/dune-vtk>.

Schlömer, N. (2022). *MeshIO: Input/output for many mesh formats*. Published on GitHub <https://github.com/nschloe/meshio> and also accessible via [Software Heritage Permalink](#).

Schroeder, W., Martin, K., & Lorensen, B. (2006). *The visualization toolkit (4th ed.)*. Kitware. ISBN: 978-1-930934-19-1

The CGAL Project. (2023). *CGAL user and reference manual* (5.5.2 ed.). CGAL Editorial Board. <https://doc.cgal.org/5.5.2/Manual/packages.html>

*The visualization toolkit*. (2023). Website: <https://vtk.org/>.