Anemoi graphs

anemoi-graphs.readthedocs.io

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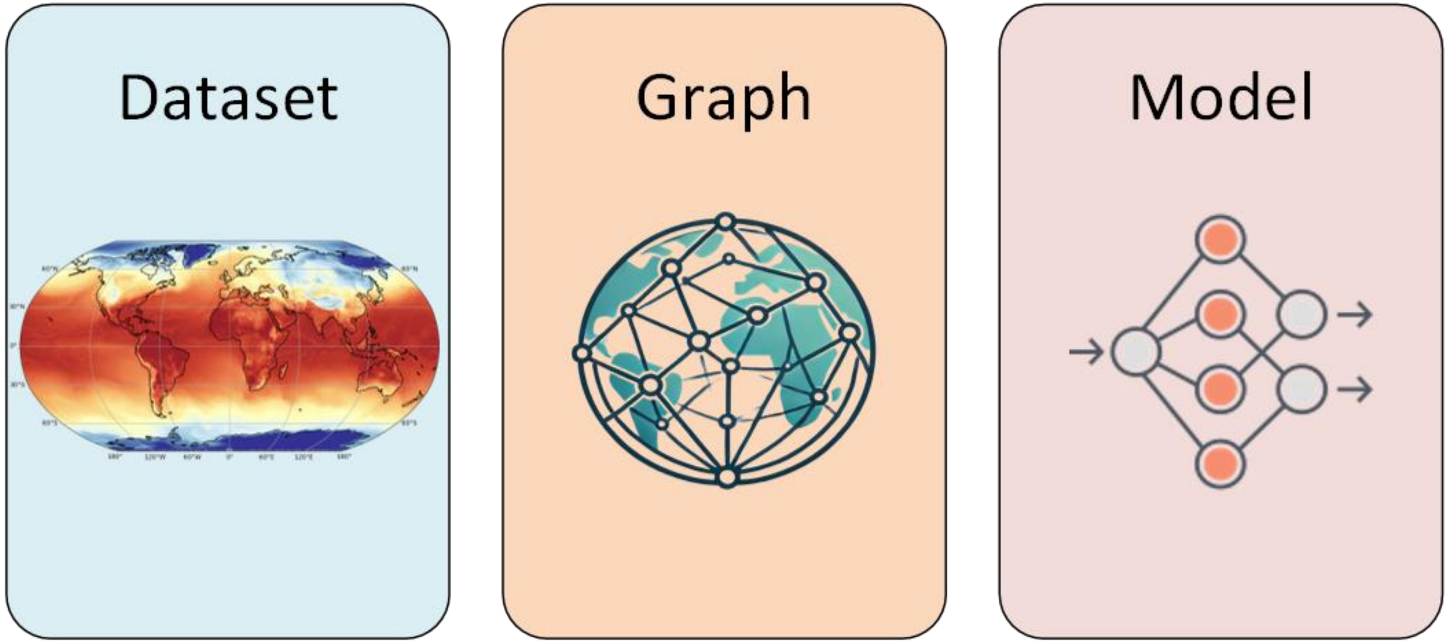
Getting started

To train a data-driven weather forecasting model in **Anemoi**, three main components are needed:



Dataset

Graph

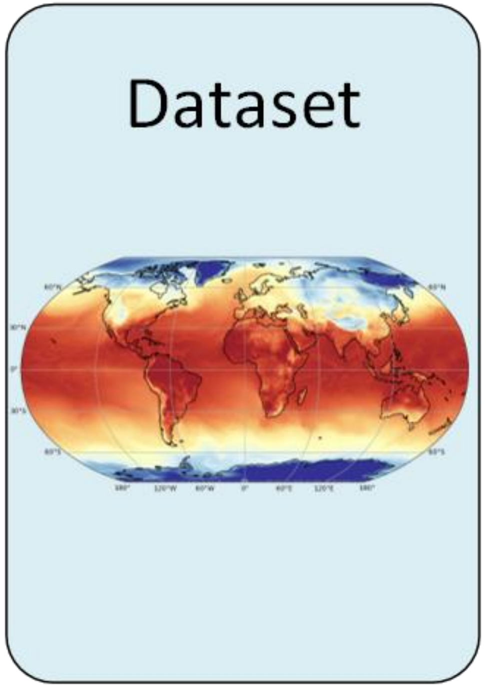
Model

Zarr

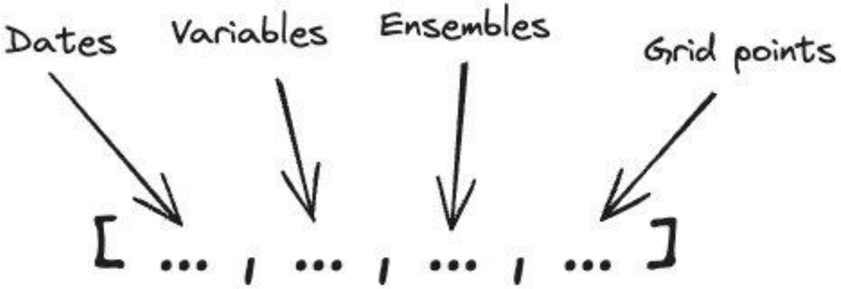
PyG

PyTorch

anemoi-datasets

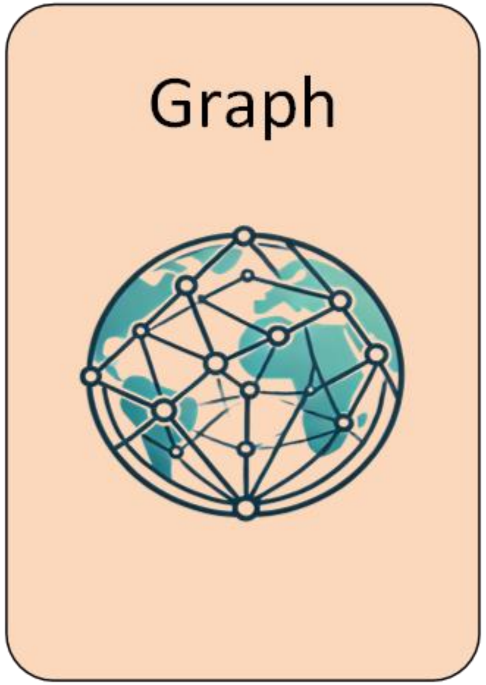


anemoi-datasets.readthedocs.io



- Create "machine-learning ready" datasets for training data-driven weather forecasts.
- Make the loading of data samples as efficient as possible
  - I/O operations are minimised
- Zarr
  - Offers an array-like view on chunks
  - Each file is a single date
- Using datasets
  - Subsetting datasets (time, variables, member, ...)
  - Combining datasets (join, concat, cutout, ensemble, ...)

anemoi-graphs



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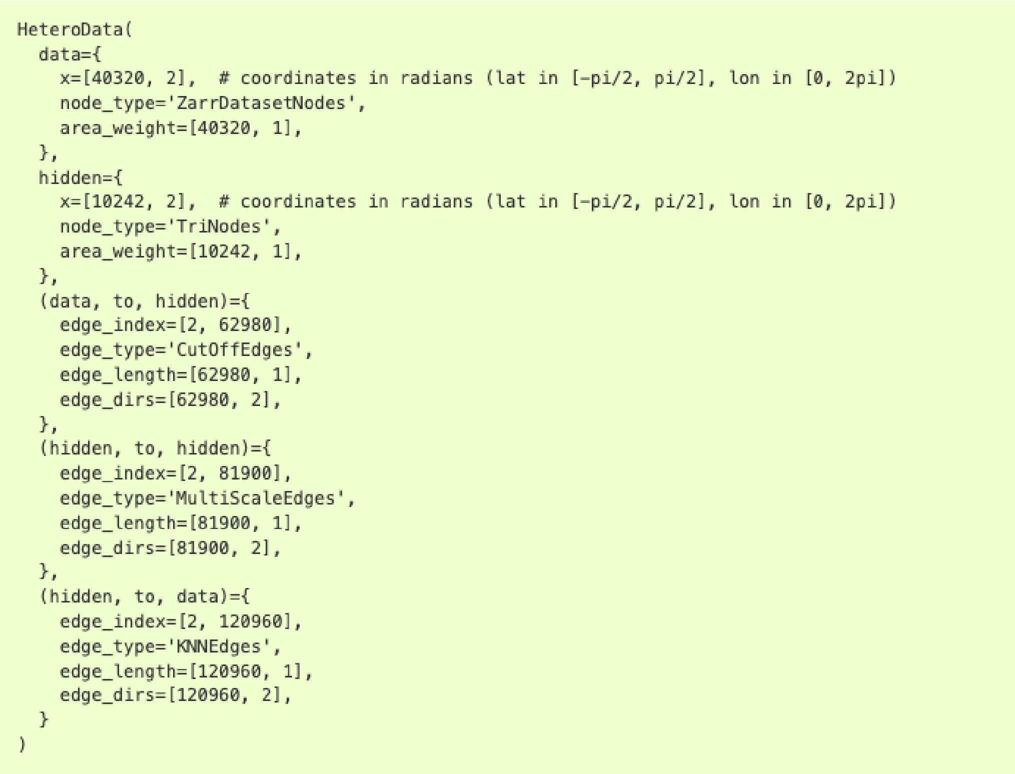
In Anemoi, it is represented by a *torch_geometric.data.**HeteroData*** object, and stored in a .PT file.

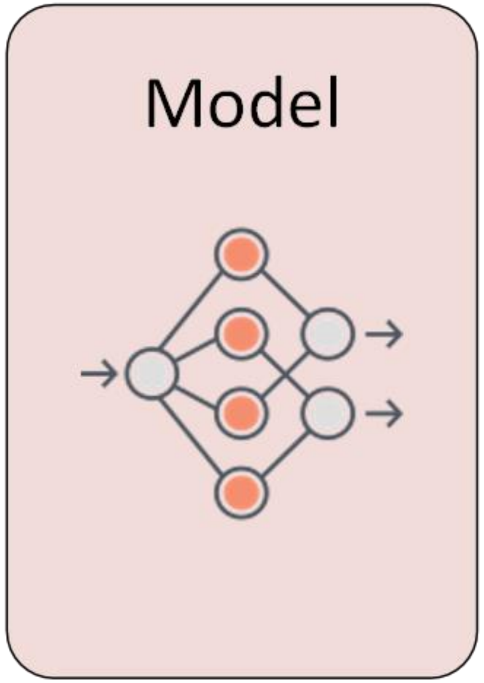
- A graph is a structure composed of:
  - **Nodes**: Represent locations in space.
  - **Edges**: Define how information flows between nodes.



```
HeteroData(
  data={
    x=[40320, 2],  # coordinates in radians (lat in [-pi/2, pi/2], lon in [0, 2pi])
    node_type='ZarrDatasetNodes',
    area_weight=[40320, 1],
  },
  hidden={
    x=[10242, 2],  # coordinates in radians (lat in [-pi/2, pi/2], lon in [0, 2pi])
    node_type='TriNodes',
    area_weight=[10242, 1],
  },
  (data, to, hidden)={
    edge_index=[2, 62980],
    edge_type='CutOffEdges',
    edge_length=[62980, 1],
    edge_dirs=[62980, 2],
  },
  (hidden, to, hidden)={
    edge_index=[2, 81900],
    edge_type='MultiScaleEdges',
    edge_length=[81900, 1],
    edge_dirs=[81900, 2],
  },
  (hidden, to, data)={
    edge_index=[2, 120960],
    edge_type='KNNEdges',
    edge_length=[120960, 1],
    edge_dirs=[120960, 2],
  }
)
```

Console log of a graph created with anemoi-graphs.

anemoi-models



anemoi-models.readthedocs.io

- Graph Neural Networks (GNNs) are a type of neural network designed to operate on **graph-structured** data.
    - GNN (G) = G', where G, G' are graphs
- Node features are update based on *message passing*:
    - Message creation (from node and edge features)
    - Message aggregation
    - Node update
- Permutation-invariance

anemoi-graphs

Tools for creating graphs used in data-driven, deep learning weather forecasting models.

- **High-Level Interface:**
  - YAML recipe file to define graph configuration.
- **Node Definition:**
  - Based on dataset coordinates (e.g., Zarr, NPZ, TXT, ...) or algorithmic methods (e.g., triangular refined icosahedron).
- **Edge Definition:**
  - Methods include cut-off radius or K nearest-neighbors.
- **Attributes:**
  - Supports node and edge attributes (weights, lengths, directions).

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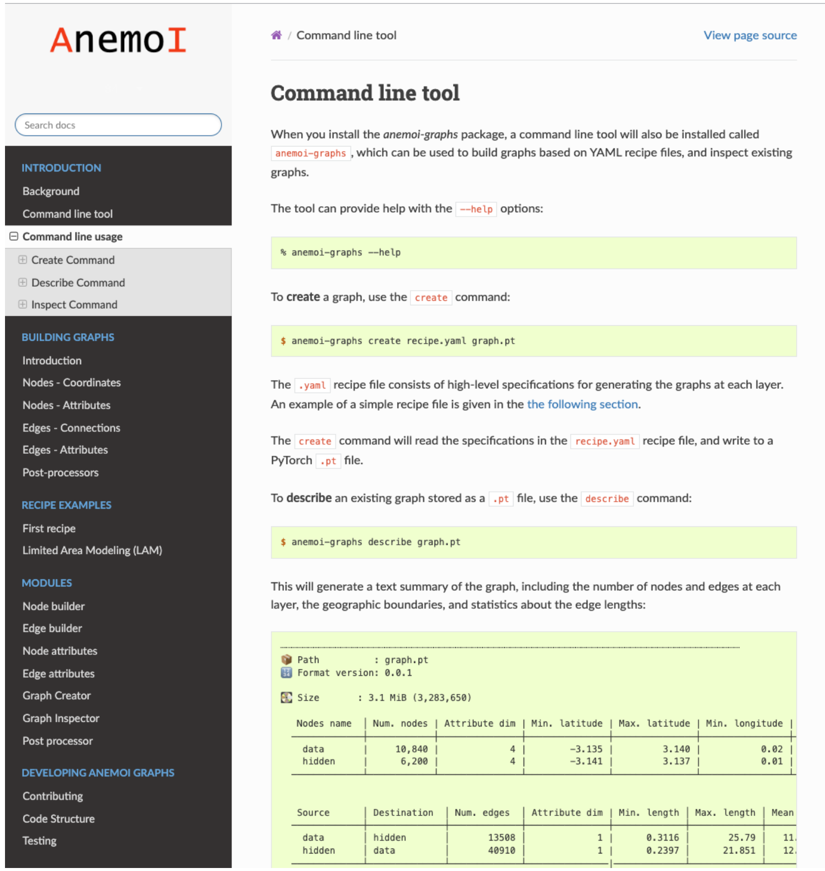


Command line tool

When you install the *anemoi-graphs* package, a command line tool will also be installed called `anemoi-graphs`, which can be used to build graphs based on YAML recipe files, and inspect existing graphs.

The tool can provide help with the `--help` options:

```
% anemoi-graphs --help
```

To **create** a graph, use the `create` command:

```
$ anemoi-graphs create recipe.yaml graph.pt
```

The `.yaml` recipe file consists of high-level specifications for generating the graphs at each layer. An example of a simple recipe file is given in the the following section.

The `create` command will read the specifications in the `recipe.yaml` recipe file, and write to a PyTorch `.pt` file.

To **describe** an existing graph stored as a `.pt` file, use the `describe` command:

```
$ anemoi-graphs describe graph.pt
```

This will generate a text summary of the graph, including the number of nodes and edges at each layer, the geographic boundaries, and statistics about the edge lengths:

```
........................................................................................
📦 Path          : graph.pt
🔢 Format version: 0.0.1

📀 Size        : 3.1 MiB (3,283,650)

  Nodes name   | Num. nodes | Attribute dim | Min. latitude | Max. latitude | Min. longitude |
 --------------+------------+---------------+---------------+---------------+----------------+
   data        |     10,840 |             4 |        -3.135 |         3.140 |           0.02 |
   hidden      |      6,200 |             4 |        -3.141 |         3.137 |           0.01 |
 --------------+------------+---------------+---------------+---------------+----------------+


  Source       | Destination  | Num. edges   | Attribute dim | Min. length | Max. length | Mean
 --------------+--------------+--------------+---------------+-------------+-------------+------
   data        | hidden       |        13508 |             1 |      0.3116 |       25.79 |   11.
   hidden      | data         |        40910 |             1 |      0.2397 |      21.851 |   12.
 --------------+--------------+--------------+---------------+-------------+-------------+------
```

Documentation of anemoi-graphs package.

Command line tool

- Create a new graph:

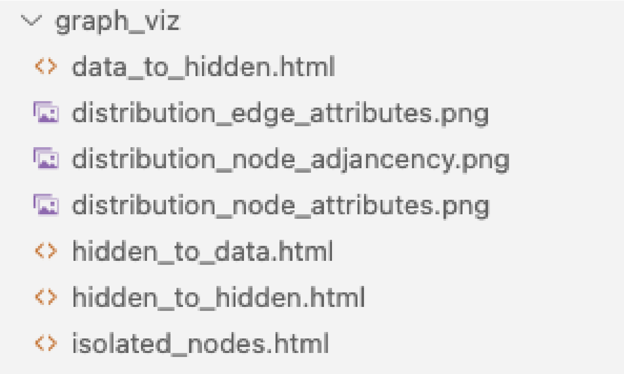
```
>>> anemoi-graphs create recipe.yaml graph.pt
```

- Describe an existing graph:

```
>>> anemoi-graphs describe graph.pt
```

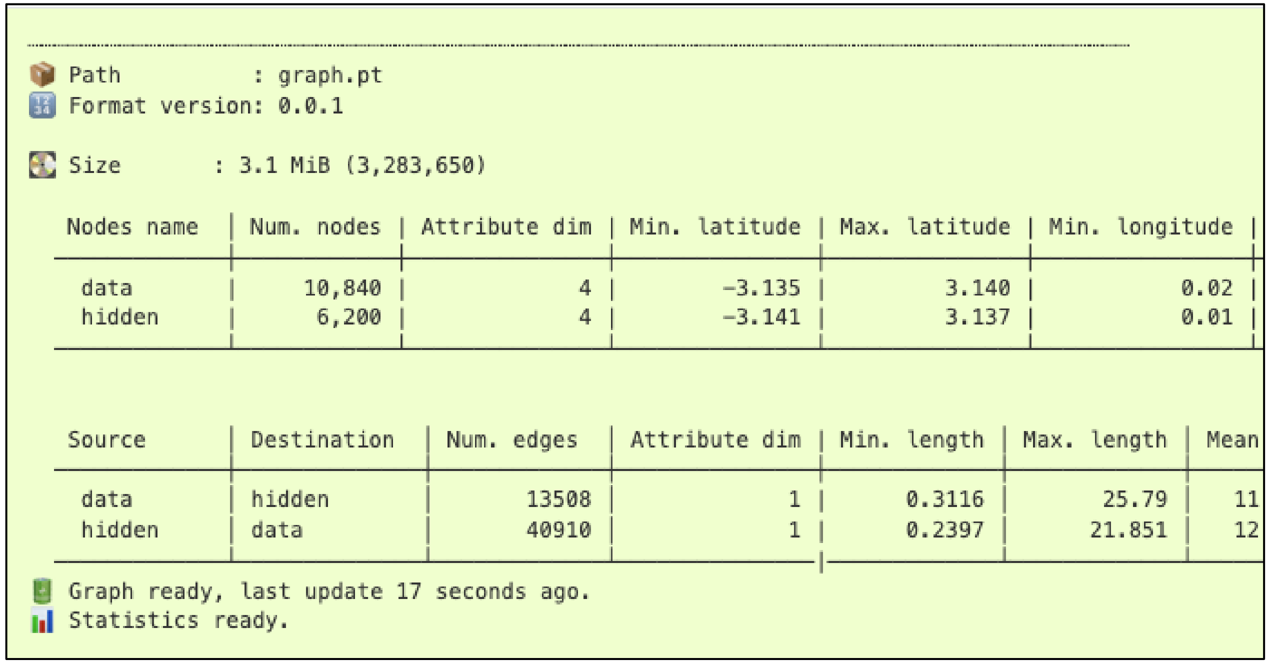
- Inspect visually an existing graph:

```
>>> anemoi-graphs inspect graph.pt graph_viz/
```



- graph_viz
  - data_to_hidden.html
  - distribution_edge_attributes.png
  - distribution_node_adjancency.png
  - distribution_node_attributes.png
  - hidden_to_data.html
  - hidden_to_hidden.html
  - isolated_nodes.html

Local files generated to inspect graphs.

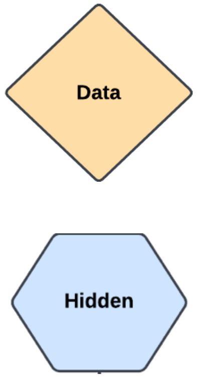


```
📦 Path          : graph.pt
🔢 Format version: 0.0.1

💽 Size        : 3.1 MiB (3,283,650)

  Nodes name   | Num. nodes | Attribute dim | Min. latitude | Max. latitude | Min. longitude |
 ──────────────┼────────────┼───────────────┼───────────────┼───────────────┼────────────────┼
   data        |     10,840 |             4 |        -3.135 |         3.140 |           0.02 |
   hidden      |      6,200 |             4 |        -3.141 |         3.137 |           0.01 |
 ──────────────┴────────────┴───────────────┴───────────────┴───────────────┴────────────────┴


  Source       | Destination   | Num. edges  | Attribute dim | Min. length  | Max. length  | Mean
 ──────────────┼───────────────┼─────────────┼───────────────┼──────────────┼──────────────┼─────
   data        | hidden        |       13508 |             1 |       0.3116 |        25.79 |   11
   hidden      | data          |       40910 |             1 |       0.2397 |       21.851 |   12
 ──────────────┴───────────────┴─────────────┴───────────────┴──────────────┴──────────────┴─────
🔋 Graph ready, last update 17 seconds ago.
📊 Statistics ready.
```

Console log when describing/inspecting a graph with anemoi-graphs.

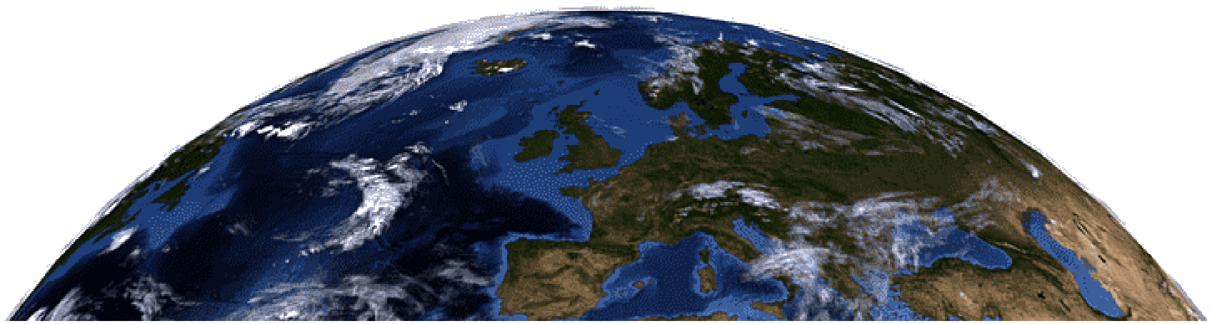
Note: The inspection tools provided are designed for testing different graph configuration but it is not recommendded for high-resolution graphs with a high number of nodes/edges.

Encoder – Processor – Decoder



anemoi-training uses a specific **encoder-processor-decoder** graph structure:

- **Data Nodes**: Represent the locations of input/output data points (e.g., temperature, wind speed).
- **Hidden Nodes**:
  - Operate at a lower spatial resolution than the input/output nodes. (~½)
  - Allow for feature extraction and dimensionality reduction, enabling the model to capture large-scale patterns.

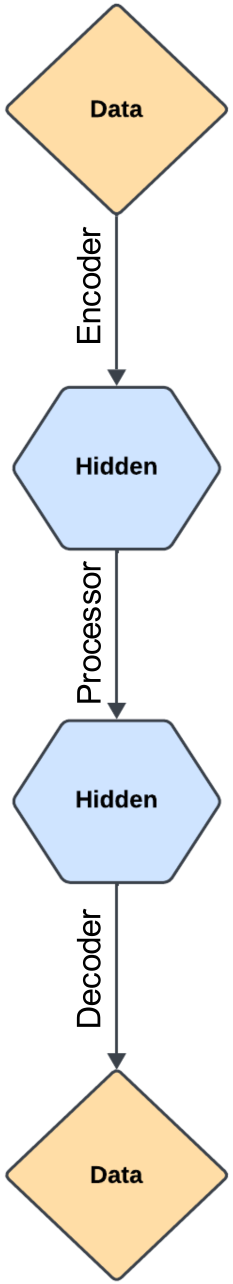


Note: For weather forecasting, the input and output nodes often correspond to the same physical locations. In other use cases (e.g., downscaling), input and output nodes may differ.

Graph recipe

recipe.yaml

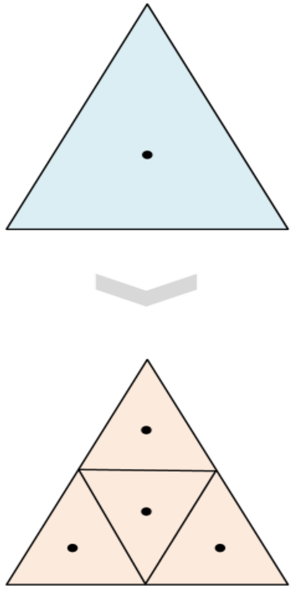
```yaml
nodes:
  data:
    node_builder:
      _target_: anemoi.graphs.nodes.AnemoiDatasetNodes
      dataset: my_anemoi_dataset
  hidden:
    node_builder:
      _target_: anemoi.graphs.nodes.TriNodes
      resolution: 5 # num of refinements

edges:
  # Encoder configuration
  - source_name: data
    target_name: hidden
    edge_builders:
      - _target_: anemoi.graphs.edges.CutOffEdges
        cutoff_factor: 0.6
  # Processor configuration
  - source_name: hidden
    target_name: hidden
     edge_builders:
      - _target_: anemoi.graphs.edges.MultiScaleEdges
        x_hops: 1
  # Decoder configuration
  - source_name: hidden
    target_name: data
    edge_builders:
      - _target_: anemoi.graphs.edges.KNNEdges
         num_nearest_neighbours: 3
```

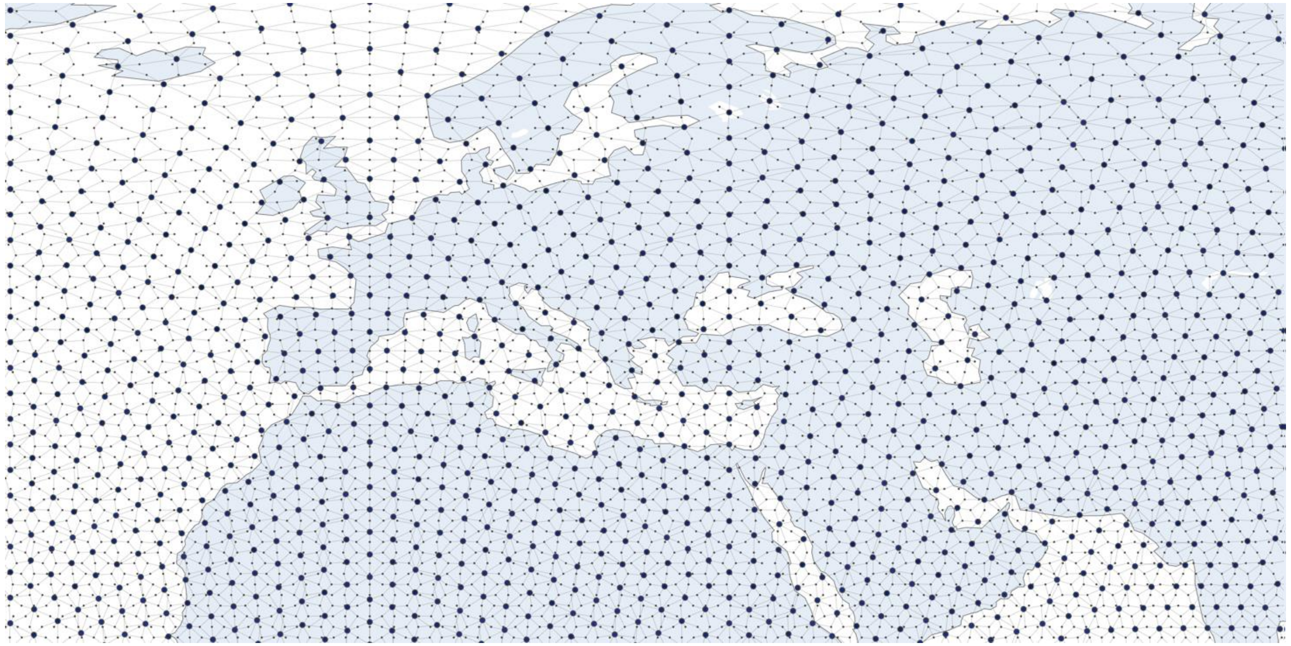


Triangular refined mesh

- It starts with an icosahedron (20 faces) projected to a sphere.
    - Each refinement splits each face into 4 faces.

```
nodes:
  hidden:
    node_builder:
      _target_: anemoi.graphs.nodes.TriNodes
      resolution: 5 # num. of refinements
```





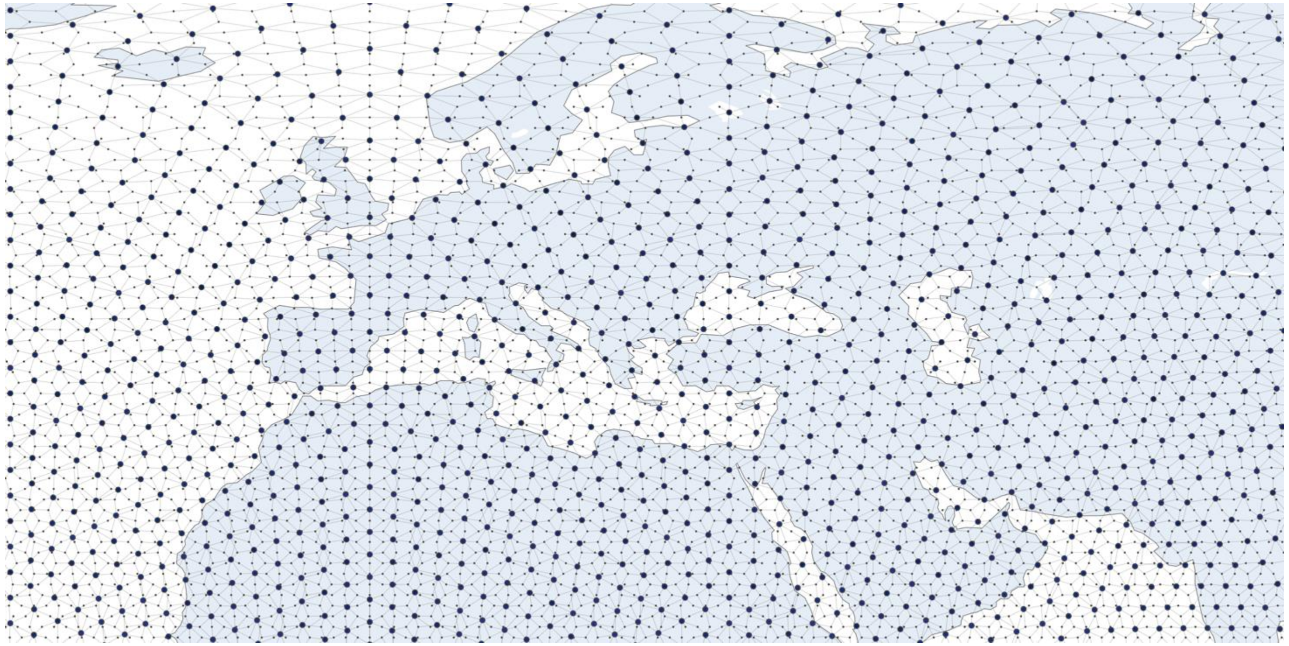
Encoder - CutOffEdges

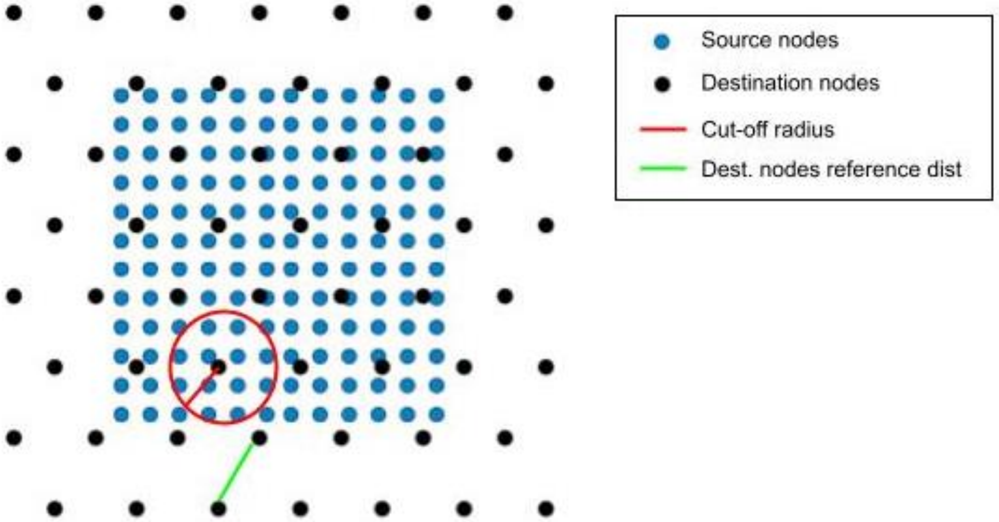
```
edges:
  - source_name: data
    target_name: hidden
    edge_builders:
      - _target_: anemoi.graphs.edges.CutOffEdges
        cutoff_factor: 0.6
```

For each target node, it connects all nodes within a given radius.

Why is this important?

- ○ You want to maximise the information flowing to the hidden nodes.
- ○ You want to minimise the number of edges (efficiency)

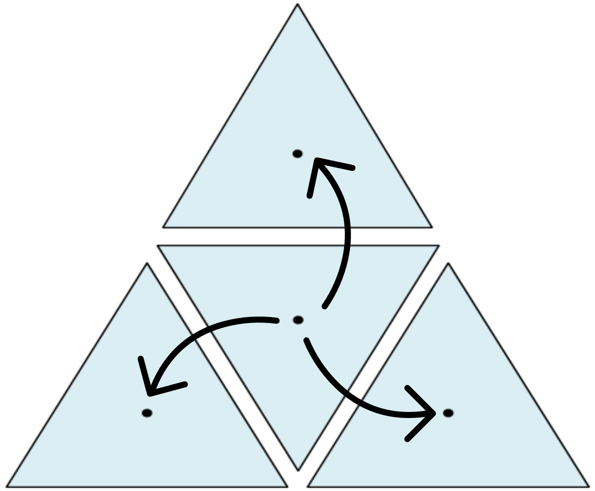


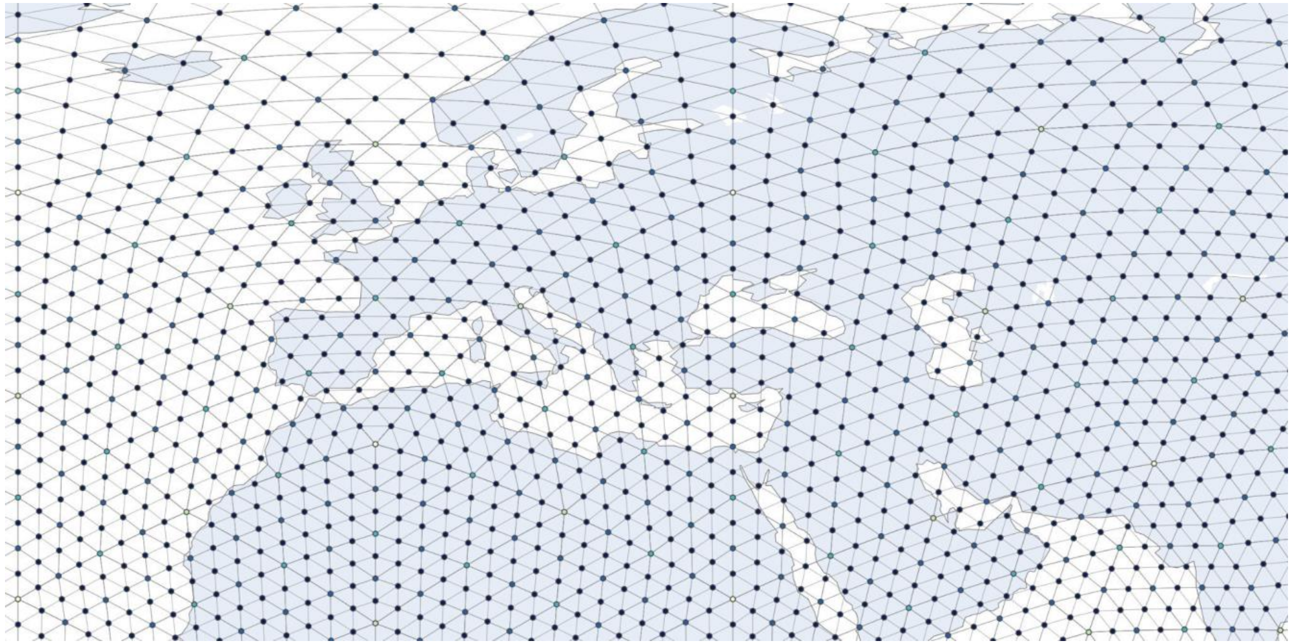


Processor - MultiScaleEdges

- The processor connections define how far the information flows.
    - Connections are created for each level of refinement.

```
edges:
  - source_name: hidden
    target_name: hidden
    edge_builders:
      - _target_: anemoi.graphs.edges.MultiScaleEdges
        x_hops: 1
```

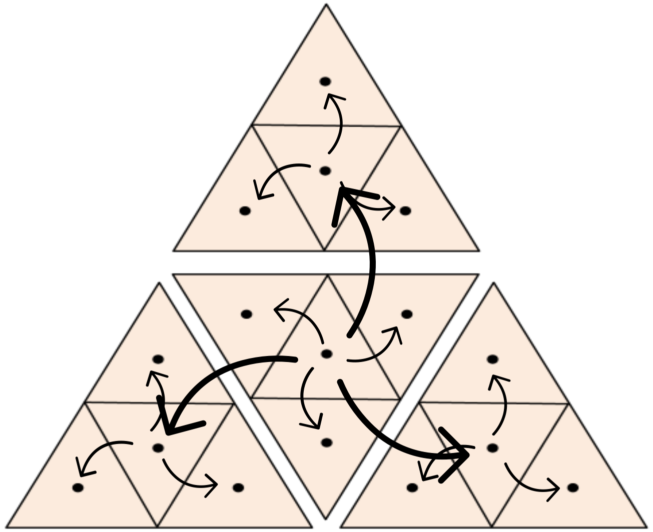


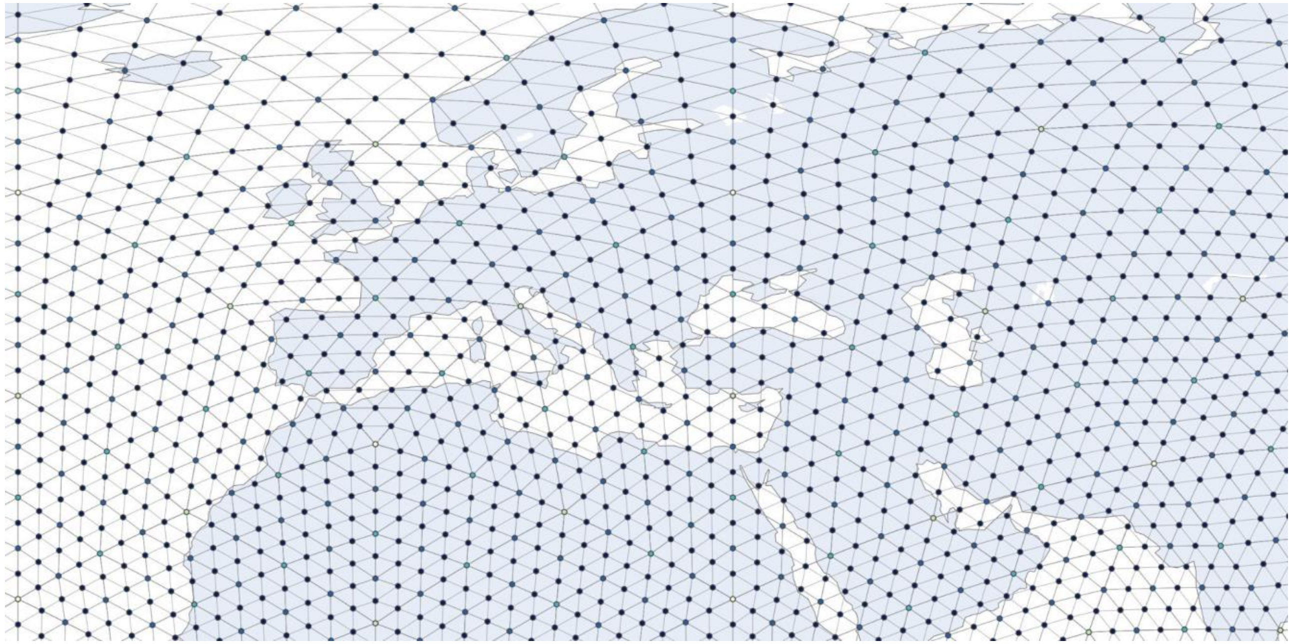


Processor - MultiScaleEdges

- The processor connections define how far the information flows.
  - Connections are created for each level of refinement.

```
edges:
  - source_name: hidden
    target_name: hidden
    edge_builders:
      - _target_: anemoi.graphs.edges.MultiScaleEdges
        x_hops: 1
```

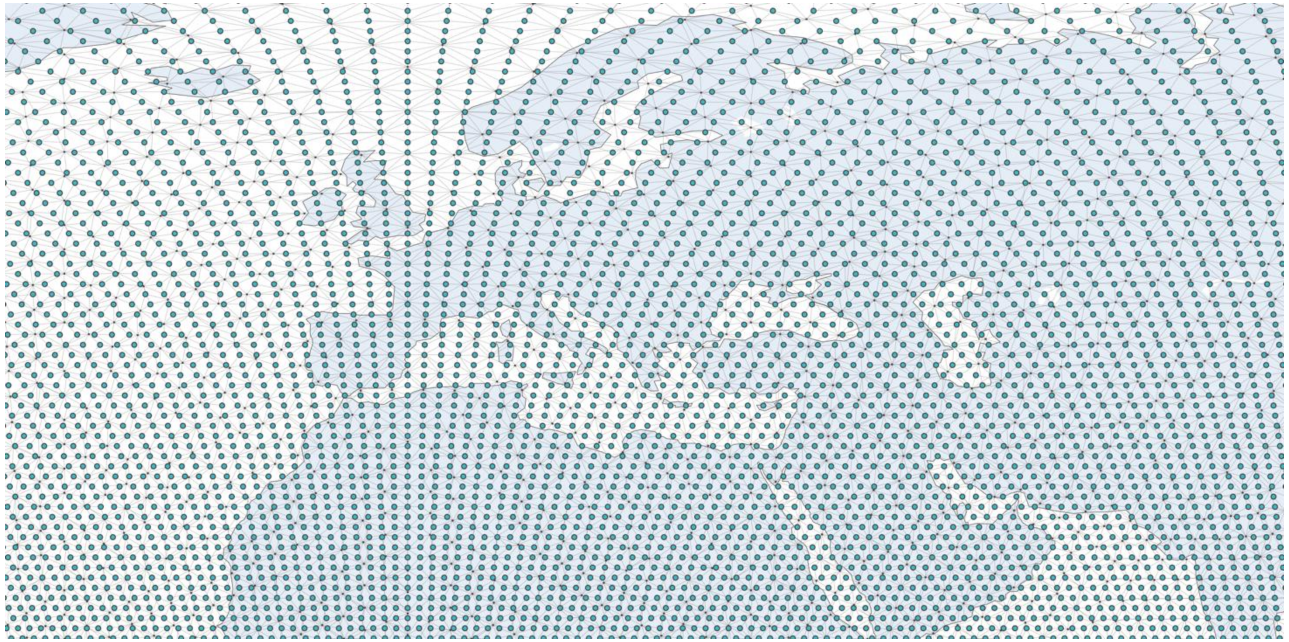




Decoder - KNNEdges

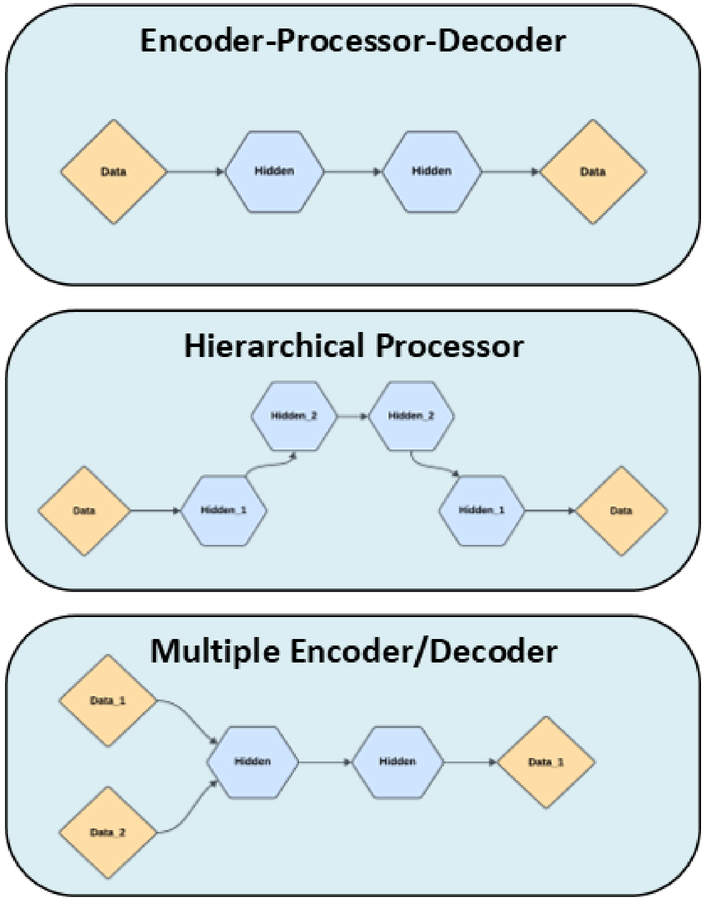
- For each target node, it connects the N nearest neighbours.

```
edges:
  - source_name: hidden
    target_name: data
    edge_builders:
      - _target_: anemoi.graphs.edges.KNNEdges
        num_nearest_neighbours: 3
```



NOTE: The decoder is the part of the graph with more edges.

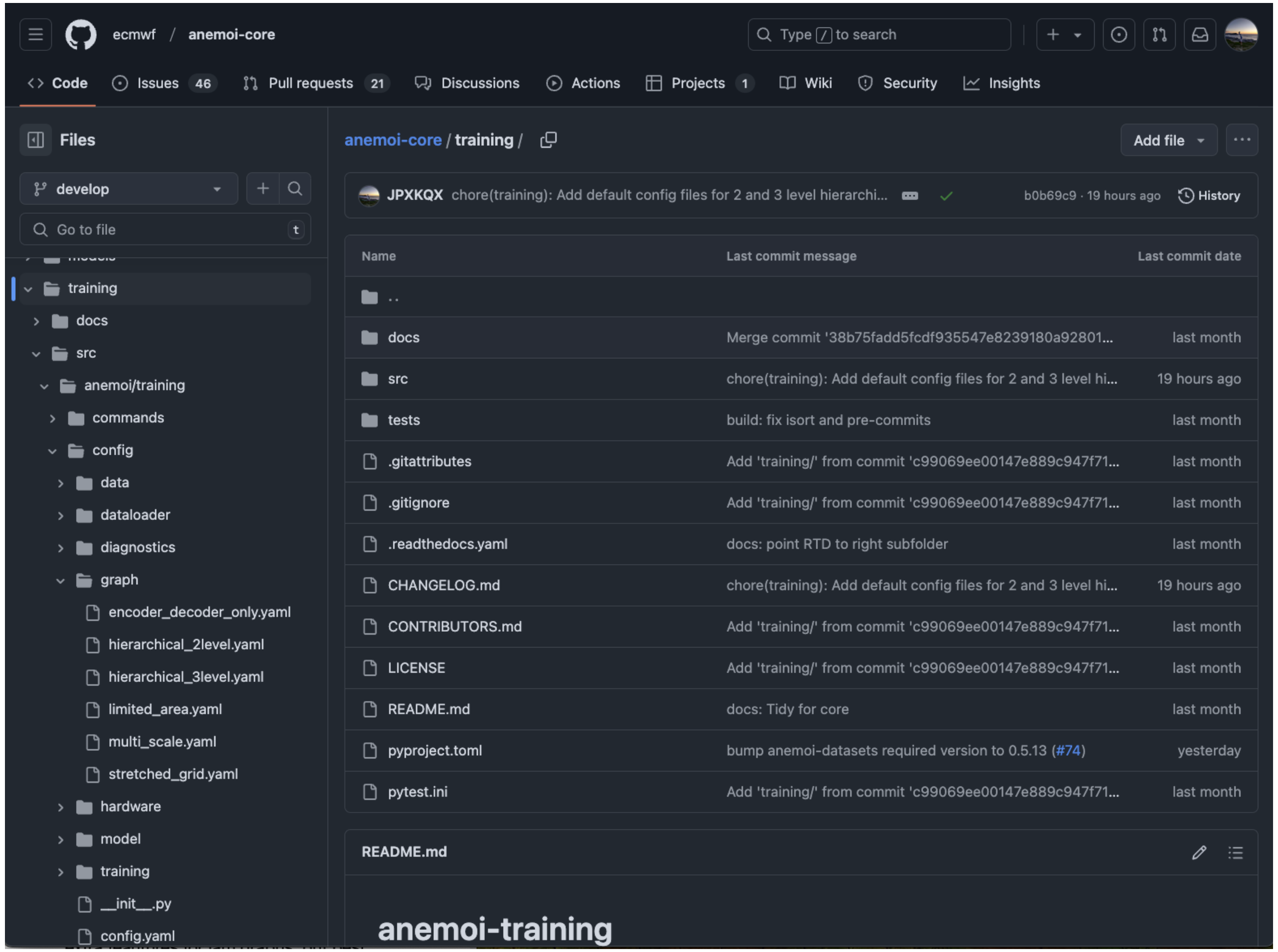
Graph configurations



Encoder-Processor-Decoder

Hierarchical Processor

Multiple Encoder/Decoder



- models
- training
  - docs
  - src
    - anemoi/training
      - commands
      - config
        - data
        - dataloader
        - diagnostics
        - graph
          - encoder_decoder_only.yaml
          - hierarchical_2level.yaml
          - hierarchical_3level.yaml
          - limited_area.yaml
          - multi_scale.yaml
          - stretched_grid.yaml
        - hardware
        - model
        - training
        - __init__.py
        - config.yaml

anemoi-core / training /

JPXKQX chore(training): Add default config files for 2 and 3 level hierarchi... b0b69c9 · 19 hours ago

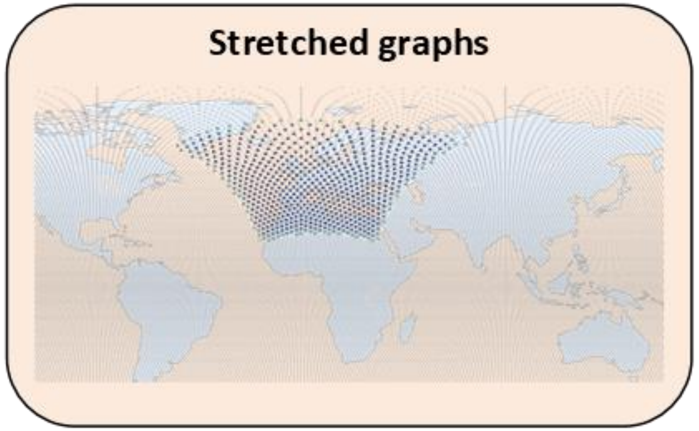
Name	Last commit message	Last commit date
..		
docs	Merge commit '38b75fadd5fcdf935547e8239180a92801...	last month
src	chore(training): Add default config files for 2 and 3 level hi...	19 hours ago
tests	build: fix isort and pre-commits	last month
.gitattributes	Add 'training/' from commit 'c99069ee00147e889c947f71...	last month
.gitignore	Add 'training/' from commit 'c99069ee00147e889c947f71...	last month
.readthedocs.yaml	docs: point RTD to right subfolder	last month
CHANGELOG.md	chore(training): Add default config files for 2 and 3 level hi...	19 hours ago
CONTRIBUTORS.md	Add 'training/' from commit 'c99069ee00147e889c947f71...	last month
LICENSE	Add 'training/' from commit 'c99069ee00147e889c947f71...	last month
README.md	docs: Tidy for core	last month
pyproject.toml	bump anemoi-datasets required version to 0.5.13 (#74)	yesterday
pytest.ini	Add 'training/' from commit 'c99069ee00147e889c947f71...	last month

README.md

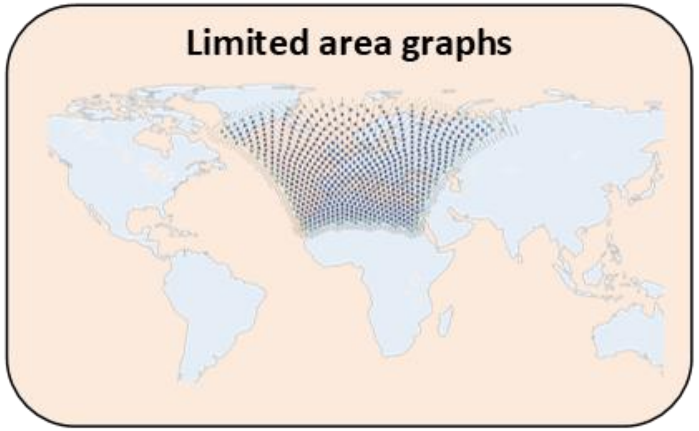
anemoi-training

Example configuration files for different use cases.

Use cases



Stretched graphs



Limited area graphs

Some user may focus in specific regions of interest. In this case, there are several options:

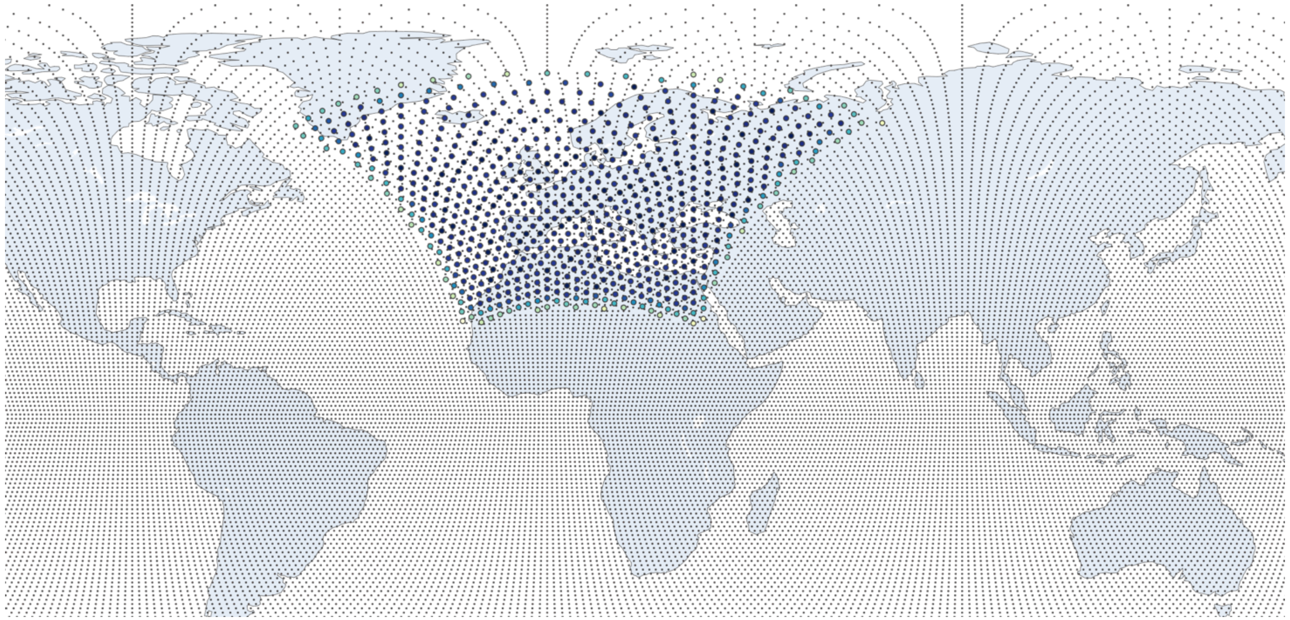
- **Stretched graphs**
  - Increases resolution over a region of interest while maintaining a coarser grid elsewhere.

- **Limited area graphs**
  - Nodes are restricted to a specific region.
  - A coarser dataset can be used as *boundary forcing.*

Regional modeling

```
nodes:
  data:
    node_builder:
      _target_: anemoi.graphs.nodes.AnemoiDatasetNodes
      dataset:
        cutout:
        - my_local_zarr_dataset
        - my_global_zarr_dataset
        adjust: all
    attributes:
      area_weight:
        _target_: anemoi.graphs.nodes.attributes.SphericalAreaWeights
        norm: unit-max
      cutout_mask:
        _target_: anemoi.graphs.nodes.attributes.CutOutMask
```

Graph recipe file containing the data nodes configuration.



Data and hidden nodes for a limited area graph.

```
  hidden:
    node_builder:
      _target_: anemoi.graphs.nodes.LimitedAreaTriNodes
      resolution: 5
      reference_node_name: data
      node_attr_name: cutout_mask
```

Graph recipe file containing the nodes configuration for LAM.

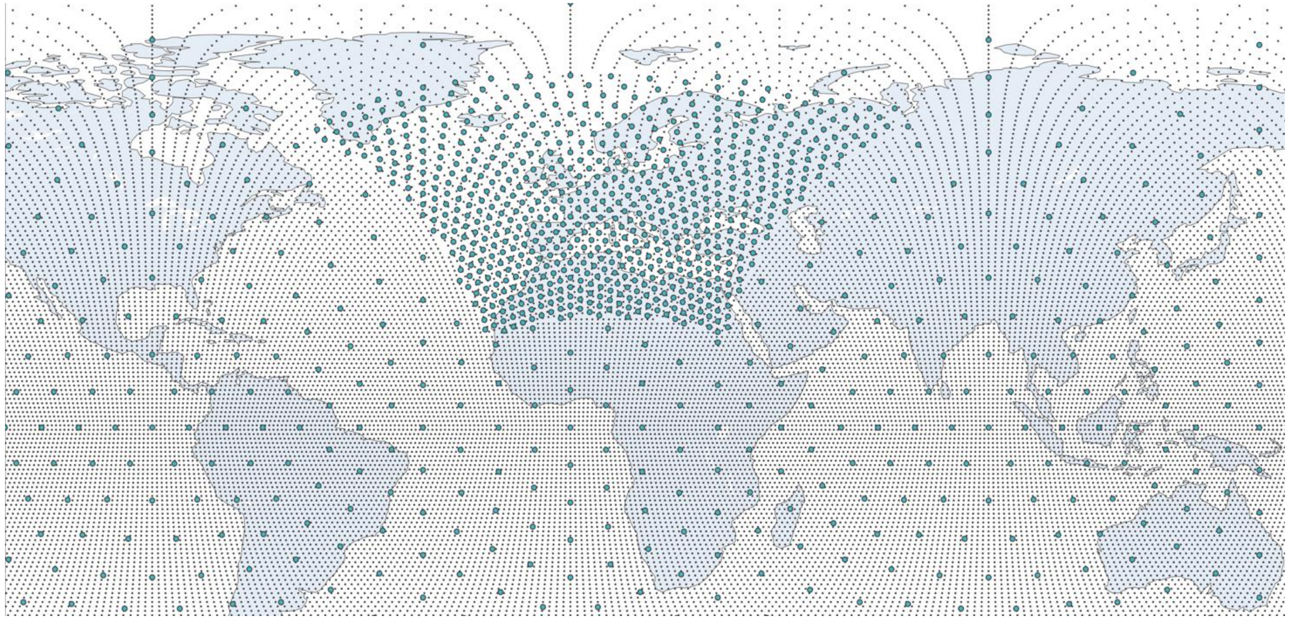
```
  hidden:
    node_builder:
      _target_: anemoi.graphs.nodes.StretchedTriNodes
      lam_resolution: 5
      global_resolution: 3
      reference_node_name: data
      node_attr_name: cutout_mask
```

Graph recipe file containing the nodes configuration for stretched graphs.

Regional modeling

```
nodes:
  data:
    node_builder:
      _target_: anemoi.graphs.nodes.AnemoiDatasetNodes
      dataset:
        cutout:
        - my_local_zarr_dataset
        - my_global_zarr_dataset
        adjust: all
    attributes:
      area_weight:
        _target_: anemoi.graphs.nodes.attributes.SphericalAreaWeights
        norm: unit-max
      cutout_mask:
        _target_: anemoi.graphs.nodes.attributes.CutOutMask
```

Graph recipe file containing the data nodes configuration.



Data and hidden nodes for a streched graph.

```
  hidden:
    node_builder:
      _target_: anemoi.graphs.nodes.LimitedAreaTriNodes
      resolution: 5
      reference_node_name: data
      node_attr_name: cutout_mask
```

Graph recipe file containing the nodes configuration for LAM.

```
  hidden:
    node_builder:
      _target_: anemoi.graphs.nodes.StretchedTriNodes
      lam_resolution: 5
      global_resolution: 3
      reference_node_name: data
      node_attr_name: cutout_mask
```

Graph recipe file containing the nodes configuration for stretched graphs.

Limited Area Modeling

```
edges:
  # Encoder configuration
  - source_name: data
    target_name: hidden
    edge_builders:
     - _target_: anemoi.graphs.edges.CutOffEdges
       cutoff_factor: 0.6
   attributes:
      edge_length:
        _target_: anemoi.graphs.edges.attributes.EdgeLength
  # Processor configuration
  - source_name: hidden
    target_name: hidden
    edge_builders:
     - _target_: anemoi.graphs.edges.MultiScaleEdges
       x_hops: 1
   attributes:
      edge_length:
        _target_: anemoi.graphs.edges.attributes.EdgeLength
  # Decoder configuration
  - source_name: hidden
    target_name: data
    edge_builders:
     - _target_: anemoi.graphs.edges.KNNEdges
       target_mask_attr_name: cutout_mask
       num_nearest_neighbours: 3
    attributes:
      edge_length:
        _target_: anemoi.graphs.edges.attributes.EdgeLength
```

Cont.: Graph recipe file containing the edge configuration for LAM.

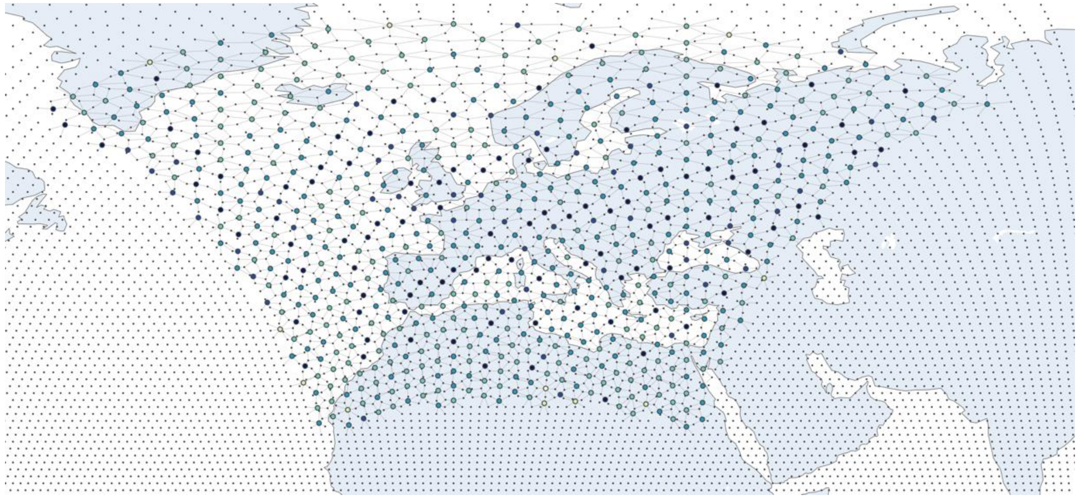


Diagram of encoder connections.

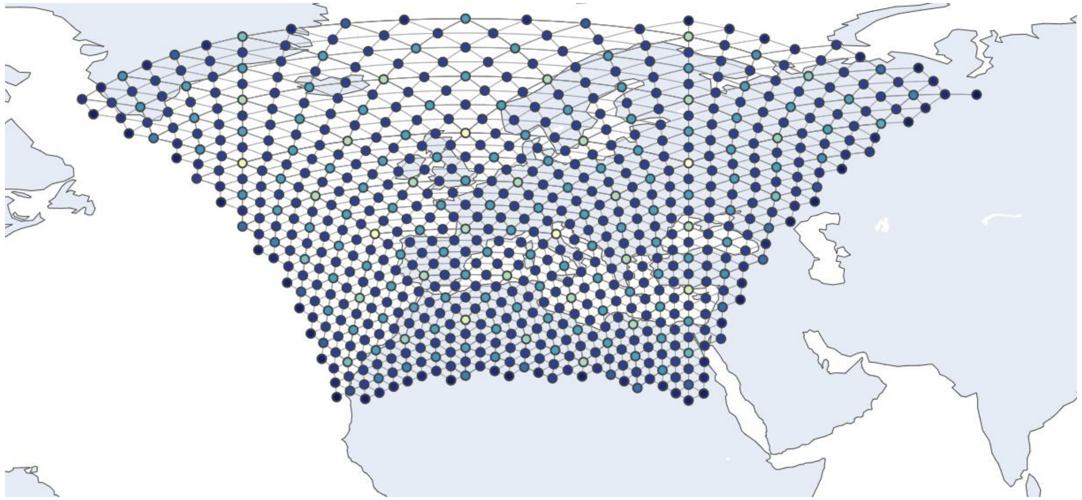


Diagram of processor connections.

Wrap up

- *anemoi-graphs* is used by *anemoi-training* to create the graphs on the fly.
- *anemoi-training* contains recipes for all use cases
- *anemoi-graphs* has a command line tool to create and inspect graphs
- *anemoi-graphs* is designed to be extended with new node, edge and attribute builders.
- *anemoi-graphs* supports different use cases:
  - Global graphs
  - Limited area graphs
  - Stretched graphs
- More complex setups (multi-encoder/decoder, dynamic graphs, …) are not supported outside *anemoi-graphs*.
- Graph configuration plays a key role in the flow of information and the efficiency of the model.

Questions?

anemoi-graphs.readthedocs.io