Anemoi graphs

anemoi-graphs.readthedocs.io

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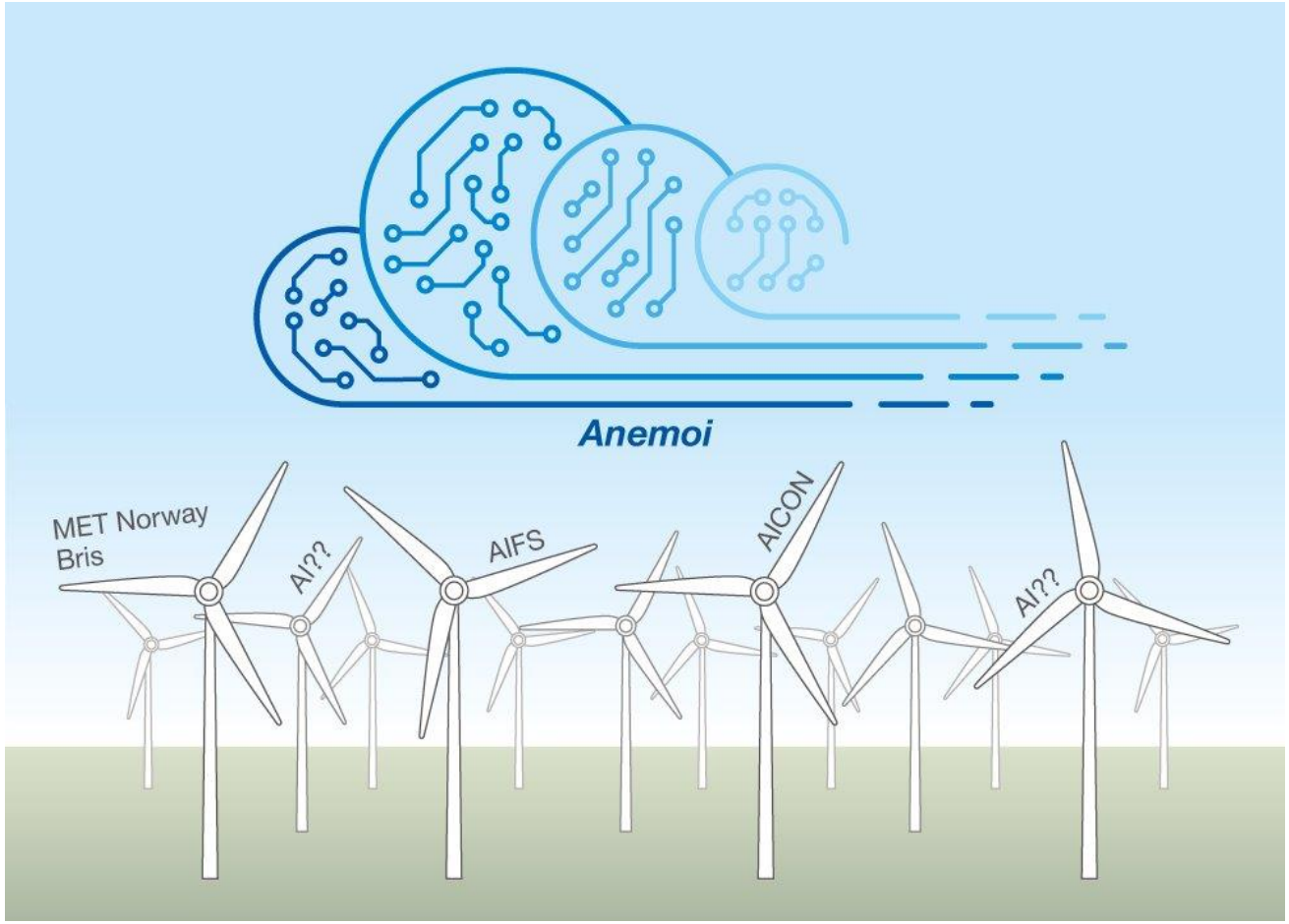
Anemoi framework

- Develop machine learning (ML) weather forecasting models.
  - Dataset preparation tools.
  - Graph creation tools.
  - ML model training support.
  - Inference tools integrated with verification software.
  - Registry for datasets and trained models.
- **Benefits:**
  - Simplifies shared meteorological challenges.
  - Enables training of models using existing recipes and custom data.



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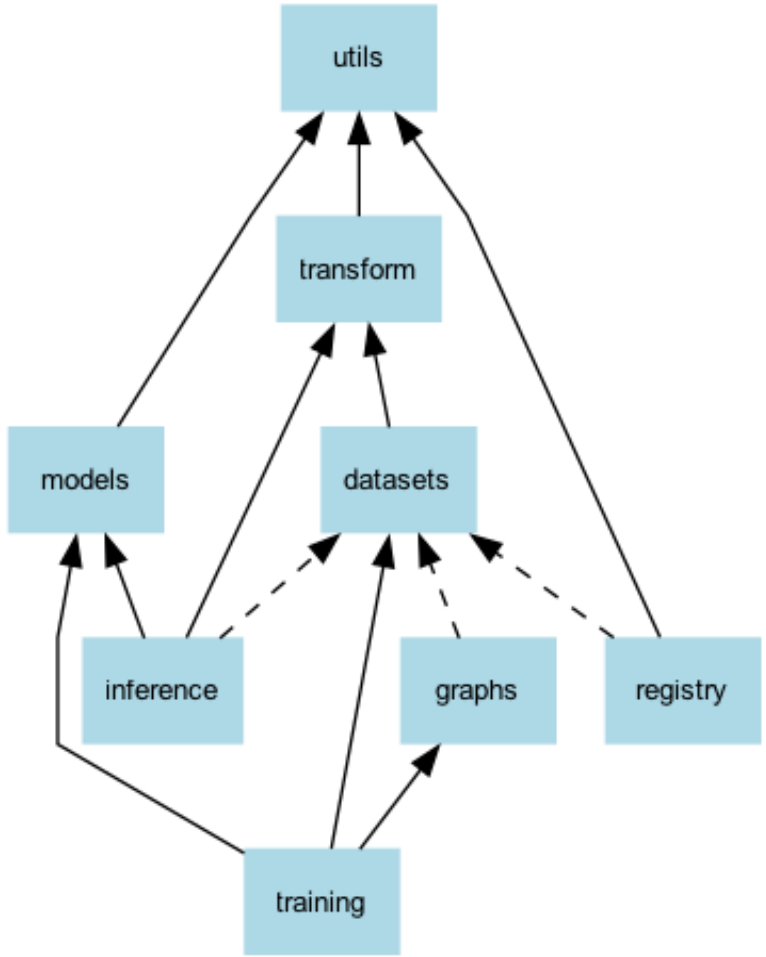
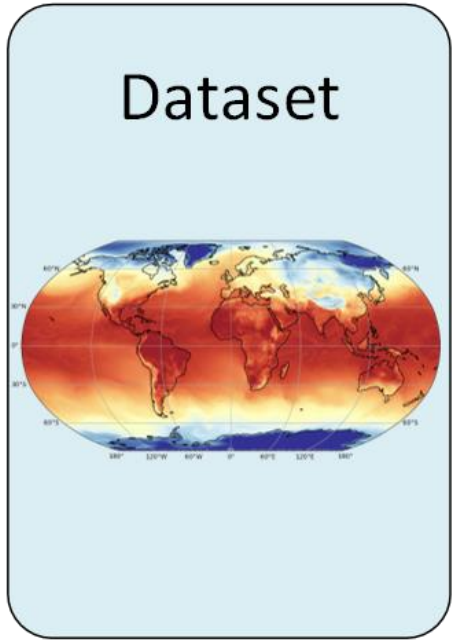
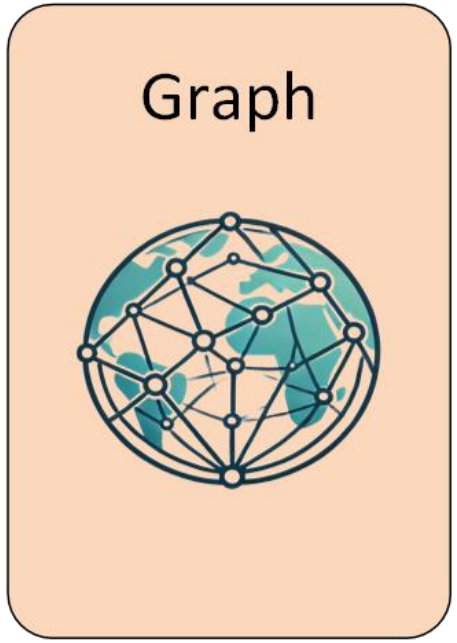


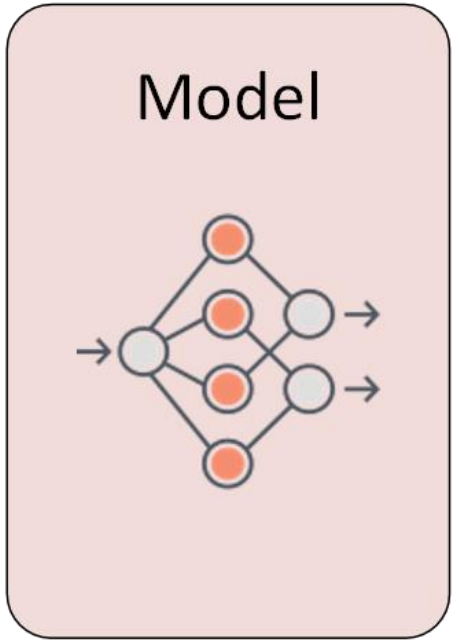
Diagram of dependencies within anemoi packages.

Getting started

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

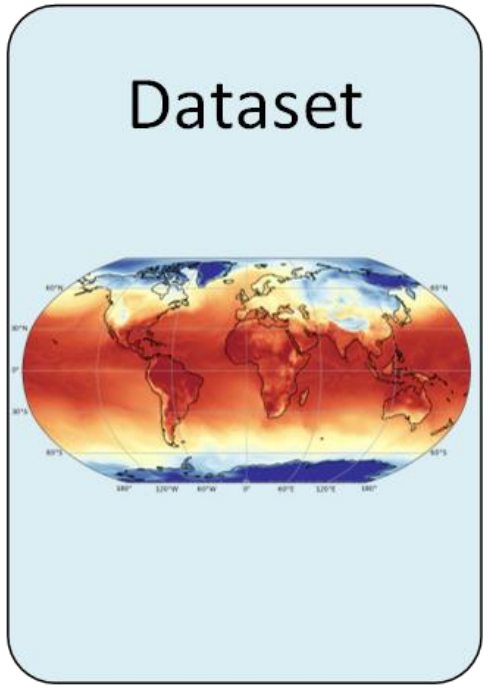






Zarr PyG PyTorch

anemoi-datasets



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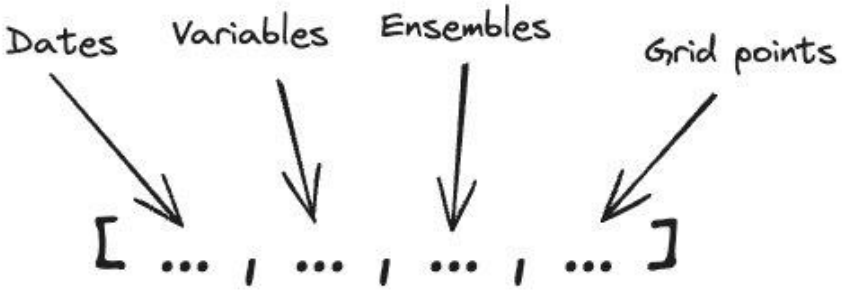
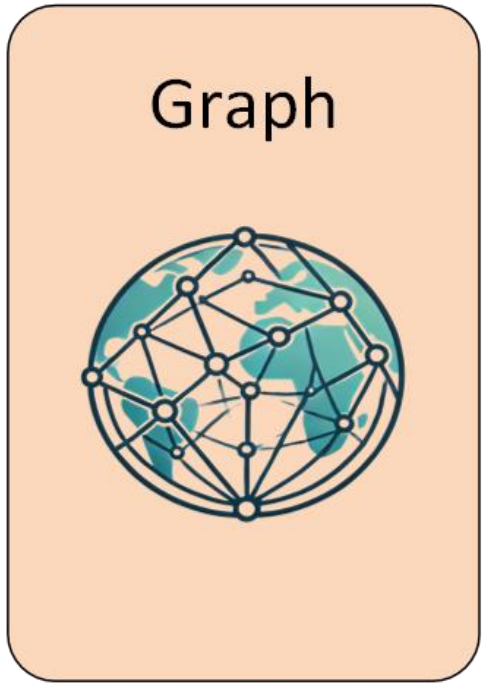


- Create "machine-learning ready" datasets for training data-driven weather forecasts.
- Make the loading of data samples as efficient as possible
  - I/O operations are minimised
- Zarr
  - Offers an array-like view on chunks
  - Each file is a single date
- Using datasets
  - Subsetting datasets (time,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

anemoi-graphs



anemoi-graphs.readthedocs.io

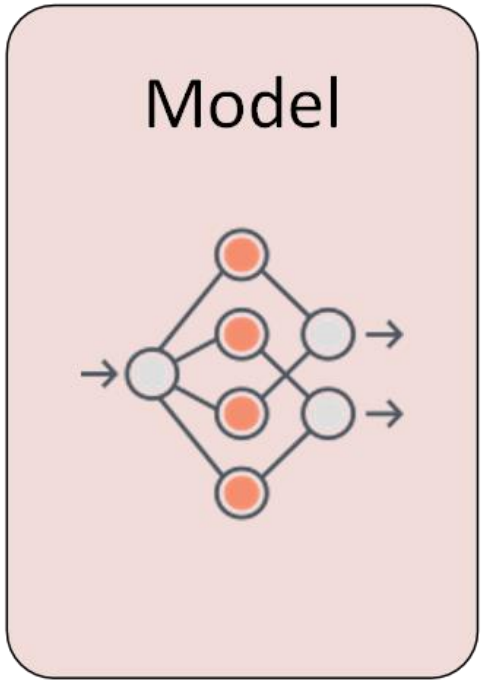
In Anemoi, it is represented by a *torch_geometric.data.**HeteroData*** object, and stored in a .PT file.

- 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:**
  - **Y**AML 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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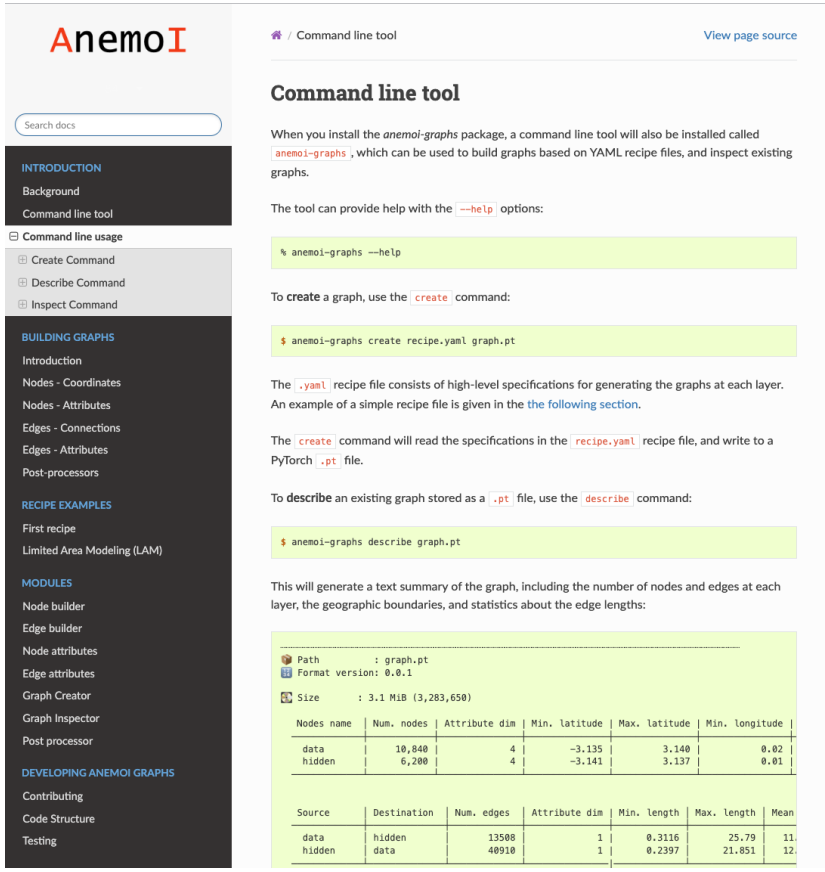


Documentation of anemoi-graphs package.

Command line tool

- Create a new graph:

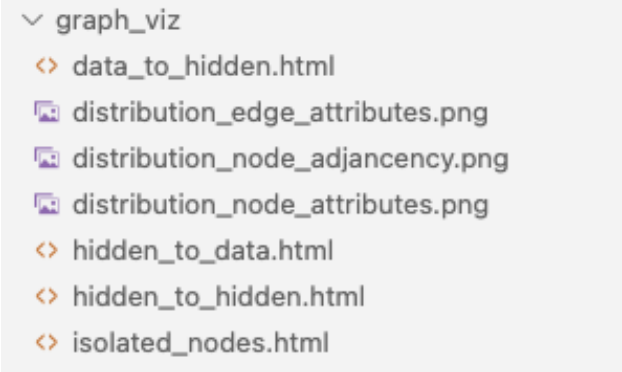
```
>>> anemoi-graphs create recipe.yaml graph.pt
```

- Describe an existing graph:

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

- Inspect visually an existing graph:

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



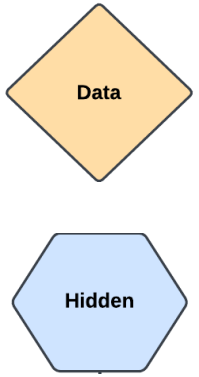
Local files generated to inspect graphs.

```
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.

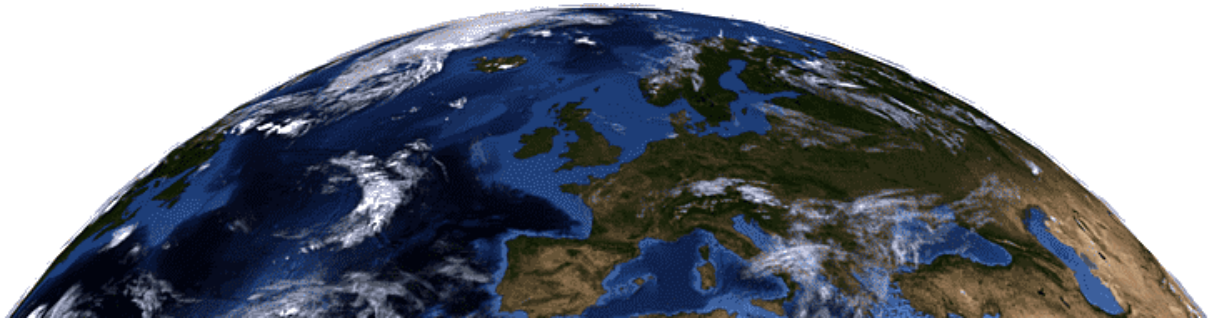
Note: The inspection tools provided are designed for testing different graph configuration but it is not recommendded for high-resolution graphs with a high number of nodes/edges.

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.

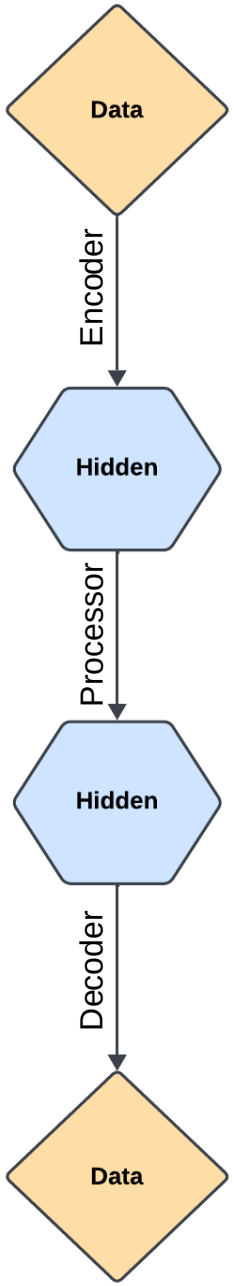


Note: For weather forecasting, the input and output nodes often correspond to the same physical locations. In other use cases (e.g., downscaling), input and output nodes may differ.

Graph recipe

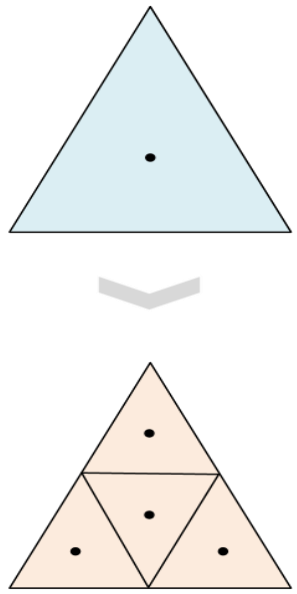
recipe.yaml

```yaml
nodes:
  data:
    node_builder:
      _target_: anemoi.graphs.nodes.ZarrDatasetNodes
      dataset: my_zarr_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
```

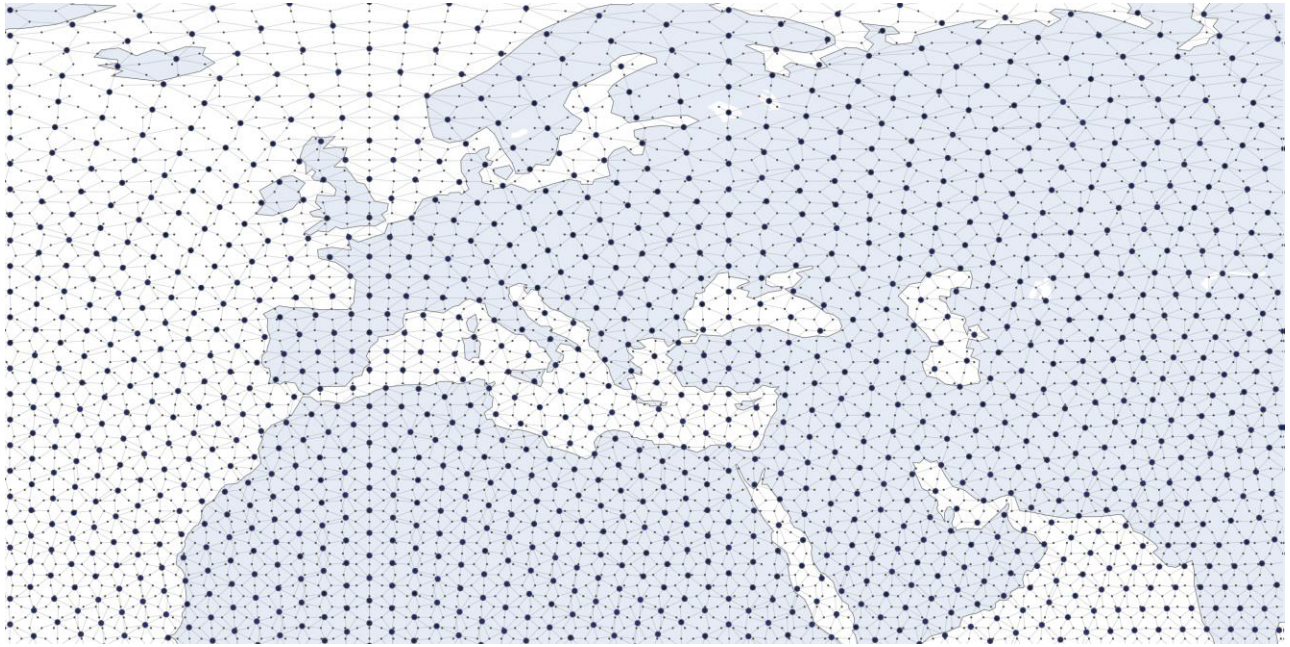


Triangular refined mesh

- 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
```



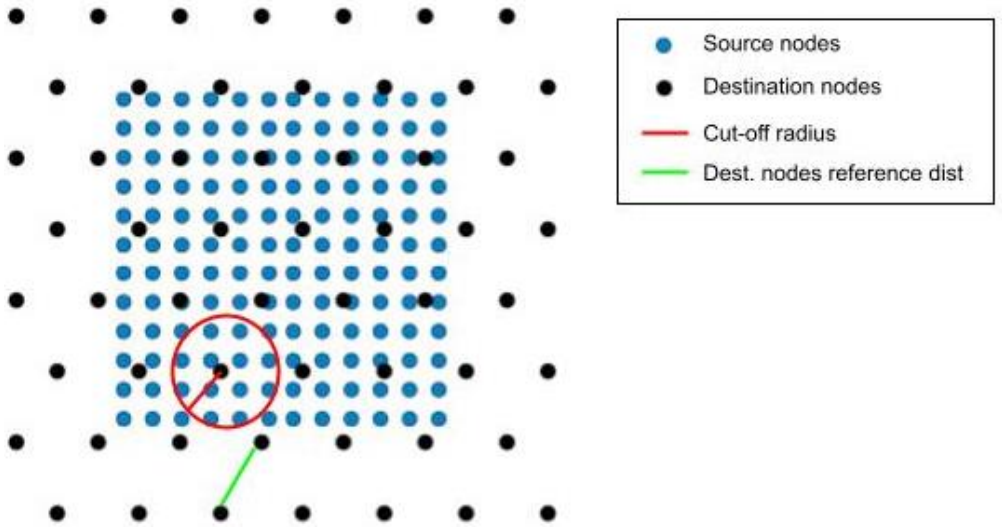
Encoder - CutOffEdges

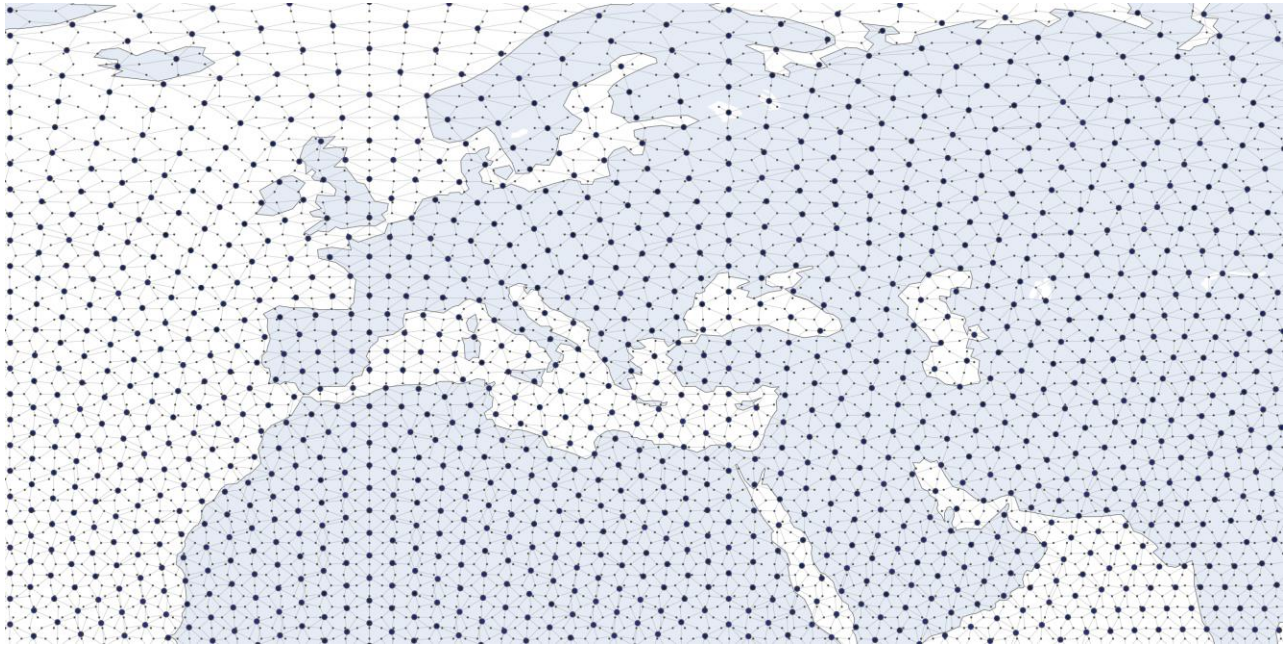
For each target node, it connects all nodes within a given radius.

Why is this important?

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

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

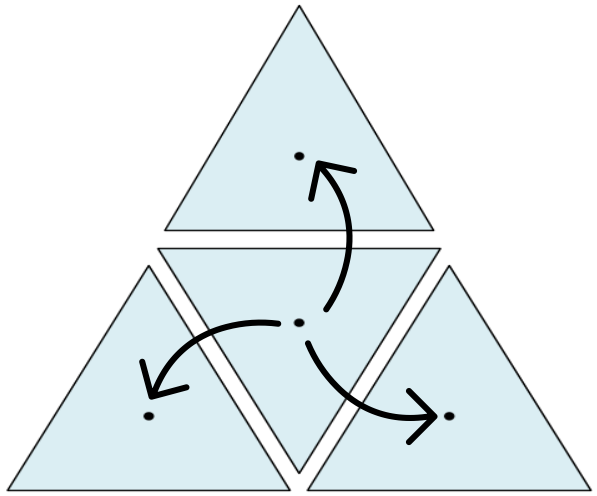


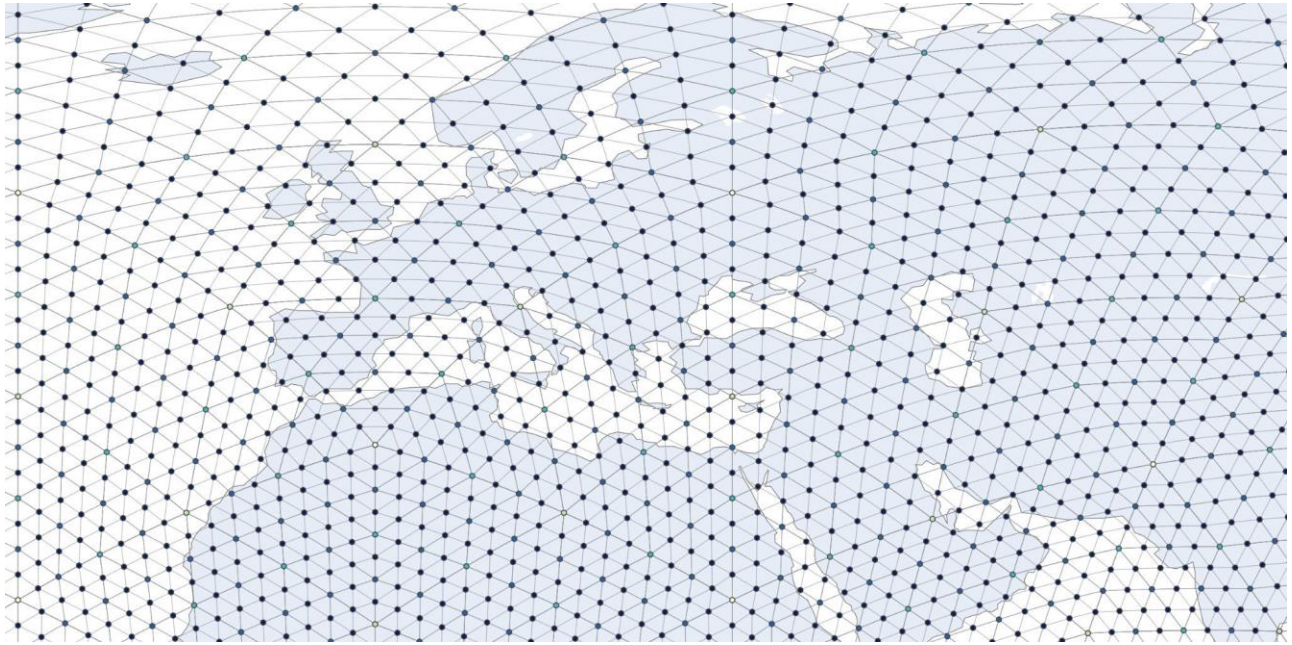


Processor - MultiScaleEdges

- 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
```





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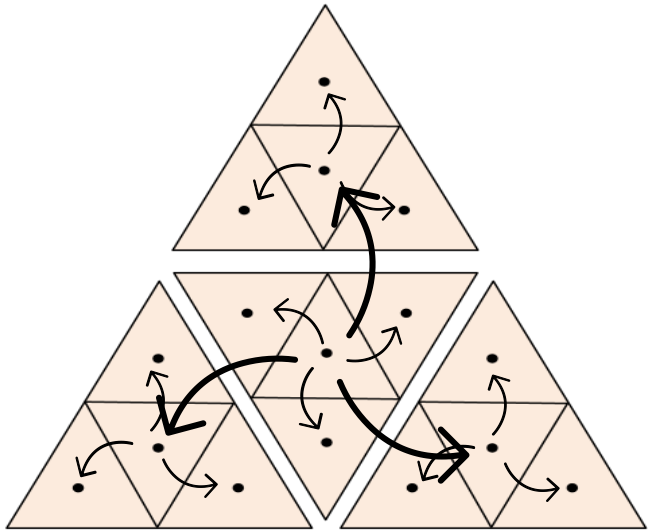
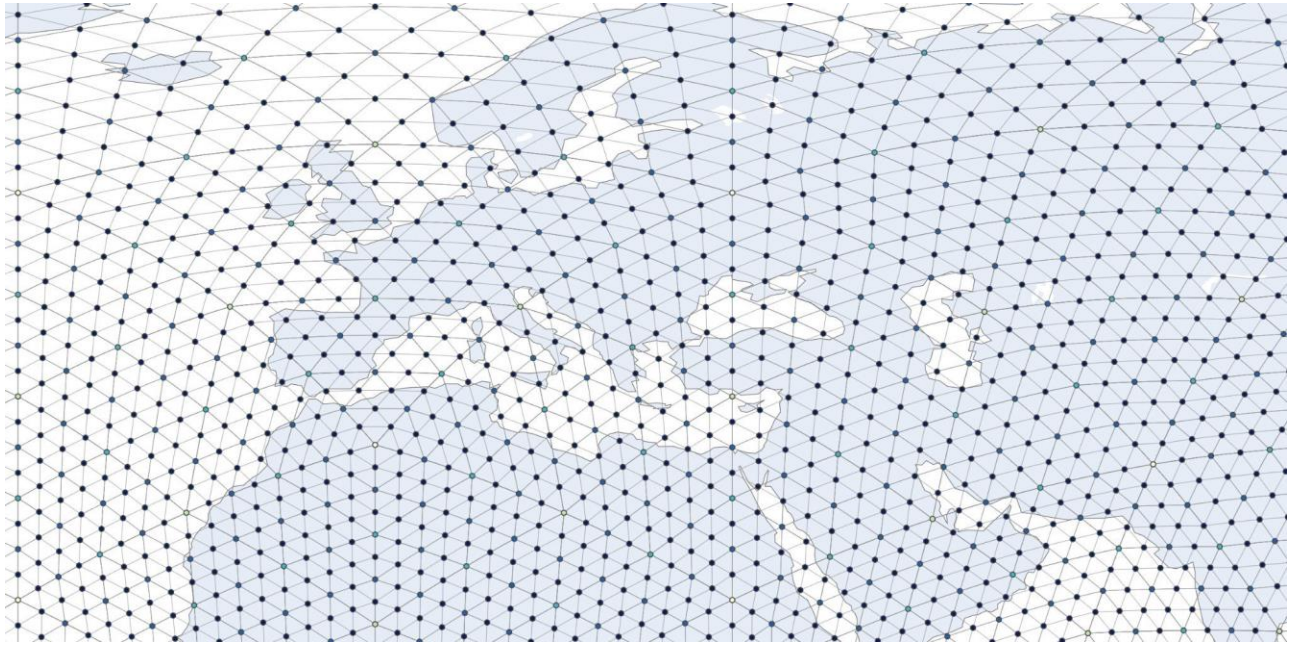
```
edges:
  - source_name: hidden
    target_name: hidden
    edge_builders:
      - _target_: anemoi.graphs.edges.MultiScaleEdges
        x_hops: 1
```

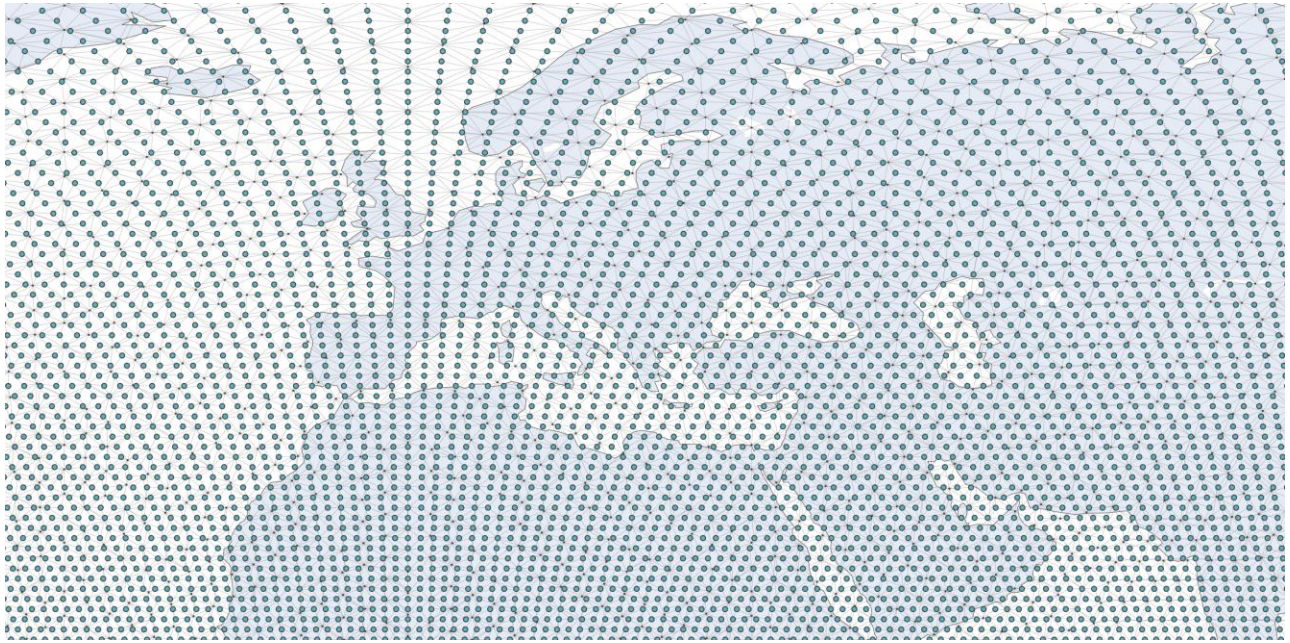




Decoder - KNNEdges

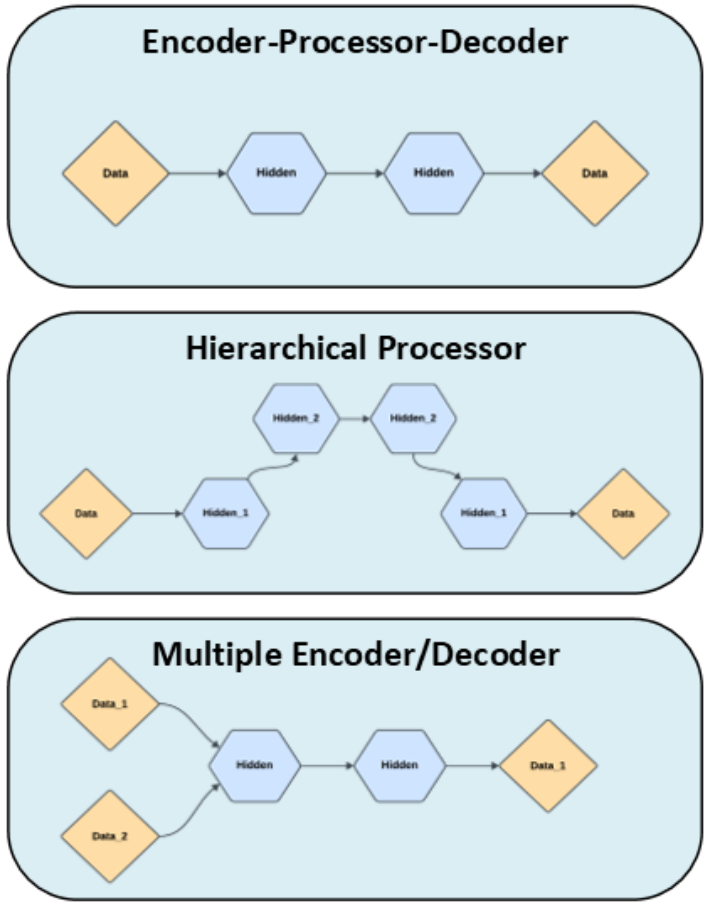
- For each target node, it connects the N nearest neighbours.

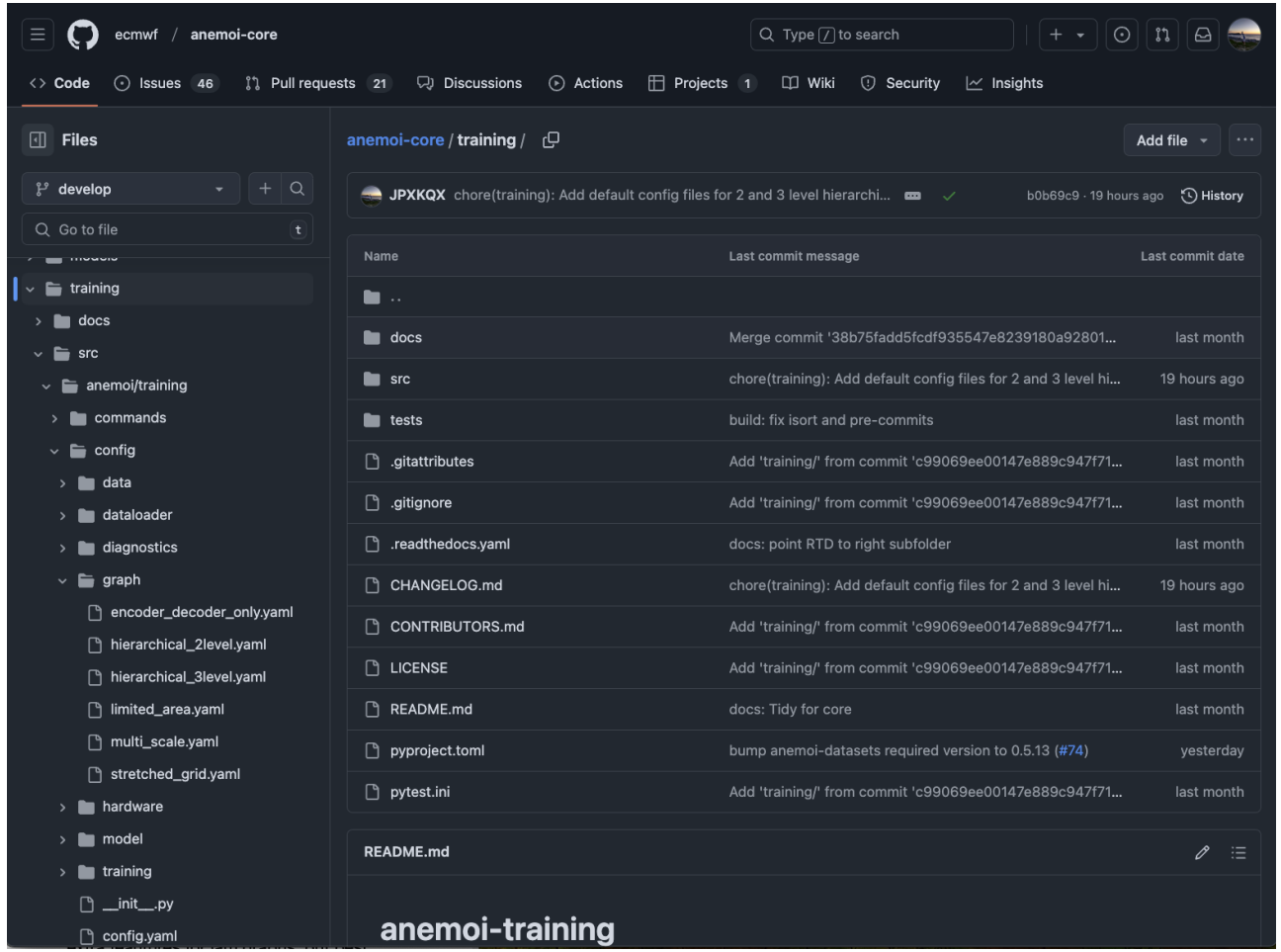
```
edges:
  - source_name: hidden
    target_name: data
    edge_builders:
      - _target_: anemoi.graphs.edges.KNNEdges
        num_nearest_neighbours: 3
```



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

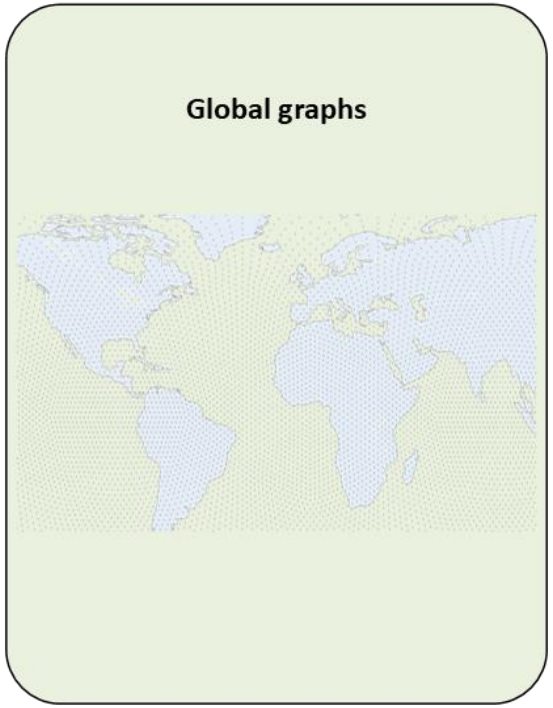
Graph configurations

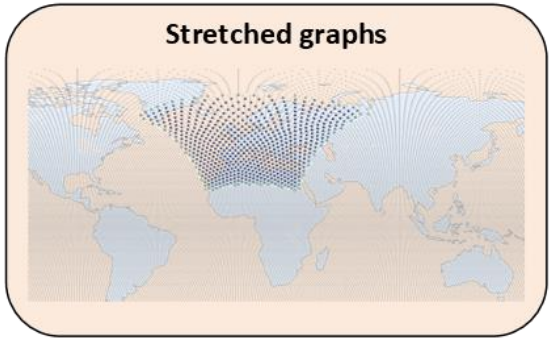


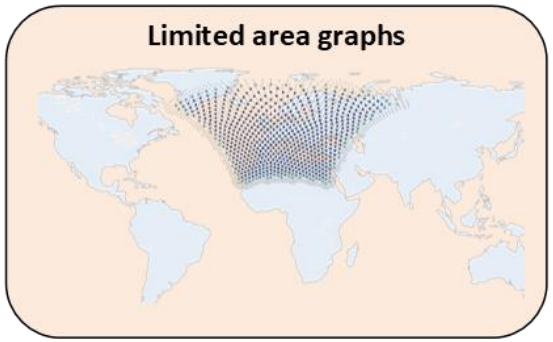


Example [configuration files](#) for different use cases.

Use cases







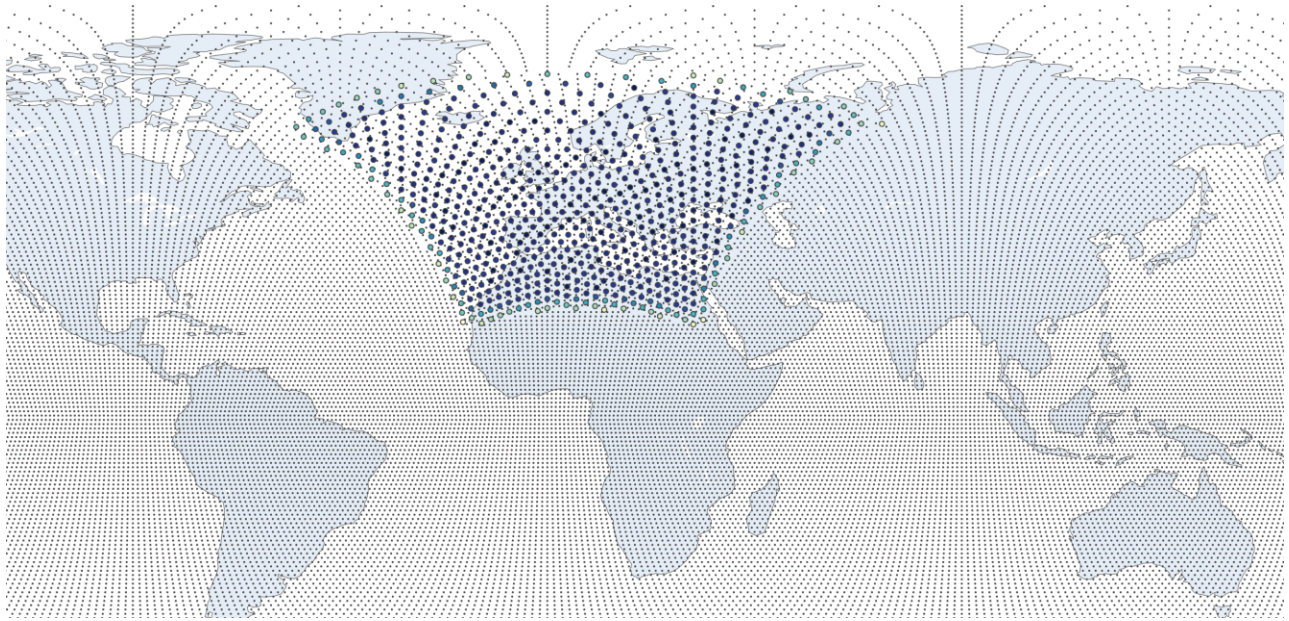
Some user may focus in specific regions of interest. In this case, there are several options:

- **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

```yaml
nodes:
  data:
    node_builder:
      _target_: anemoi.graphs.nodes.ZarrDatasetNodes
      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.

```yaml
  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.

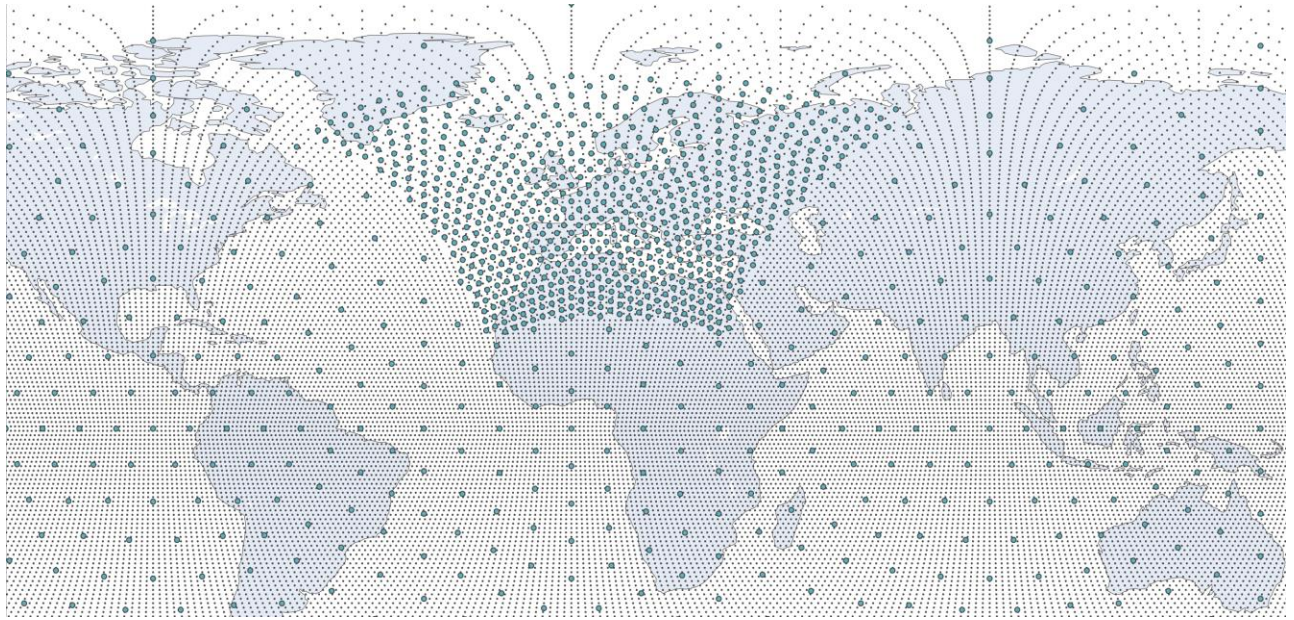
```yaml
  hidden:
    node_builder:
      _target_: anemoi.graphs.nodes.StretchedTriNodes
      lam_resolution: 5
      global_resolution: 3
      reference_node_name: data
      node_attr_name: cutout_mask
```

Graph recipe file containing the nodes configuration for stretched graphs.

Regional modeling

```yaml
nodes:
  data:
    node_builder:
      _target_: anemoi.graphs.nodes.ZarrDatasetNodes
      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.

```yaml
  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.

```yaml
  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.

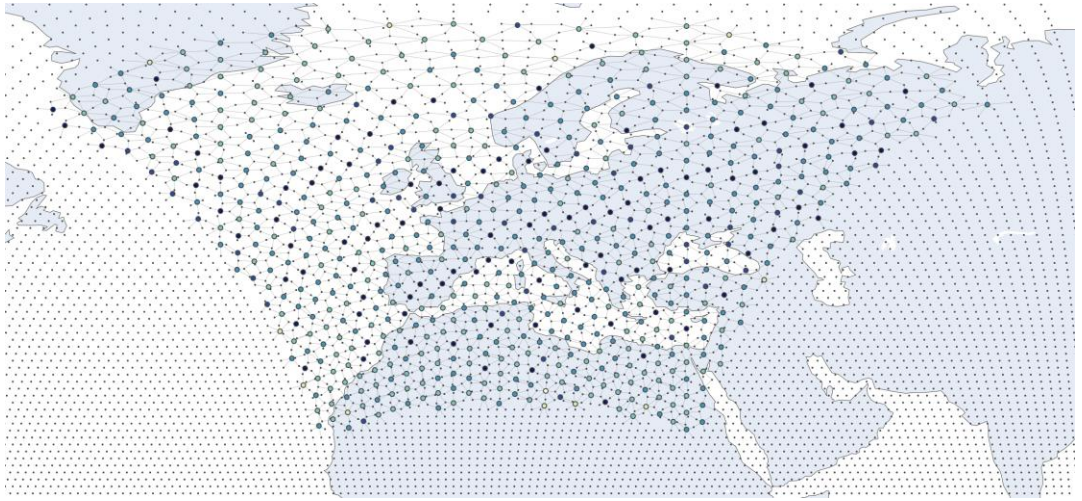


Diagram of encoder connections.

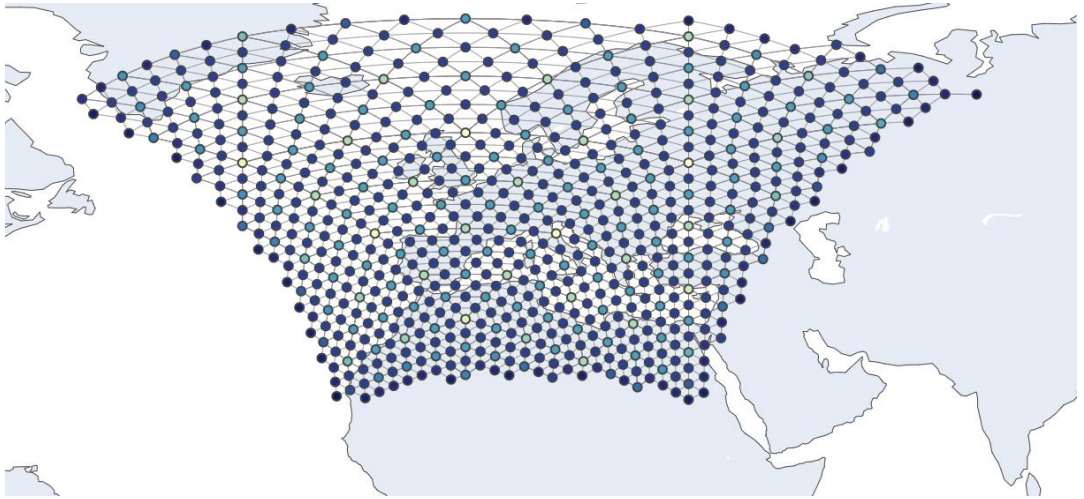


Diagram of processor connections.

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