

Workflow

1. Initialization:

- The spatial domain is discretized into a 3D grid with dimensions $n_x \times n_y \times n_z$.
- Each particle is assigned an initial position (x, y, z) corresponding to the release point, and an initial radionuclide label according to the decay chain (Pu → Am → Np).
- Particle numbers are scaled to represent the total activity (Bq) of the release.

2. Velocity and Grid Data Loading:

- Horizontal velocities u and v are read from HYCOM monthly outputs and interpolated linearly to desired times.
- Bathymetry, depth layers, and lat/lon grids are read from external data files.

3. Time Loop:

- The simulation progresses in discrete time steps dt , covering each day of the simulation period.
- At each time step, the model performs: a. Advection: Particle positions are updated according to local currents, considering the Earth's curvature. b. Diffusion: Stochastic horizontal and vertical displacements are applied based on specified diffusion coefficients. c. Decay: Each particle may decay to the next radionuclide in the chain according to probabilistic decay rates derived from physical half-lives. d. Water-Sediment Interaction: Particles can fix to sediments from the water column or resuspend back to water based on local depth and sediment-water interaction coefficients.
- Particles leaving the domain are marked as inactive ("dead").

4. Post-processing:

- Particle counts are aggregated per grid cell to compute concentrations in Bq/m³ (water column) or Bq/m² (sediments).
- Outputs are written for each radionuclide in water and sediment, providing spatial distributions at the end of the simulation.

Additional Model Components:

- **Stochastic Treatment of Decay:** The decay of radionuclides is treated probabilistically at the particle level, enabling the simulation of parent-daughter transformations over time.

- **Sediment Interaction:** The model includes explicit exchange between water column and surface sediments in the bottom 50 m of the water column (in contact with the seabed), incorporating sediment thickness, porosity, and mineral density.
- **Variable Grid Layers:** Depth layers (dz) are non-uniform to reflect realistic bathymetry and stratification.