forceLandshoff Function Documentation

Function Overview

The forceLandshoff function calculates the Landshoff interaction forces between fluid particles based on their positions, velocities, and a provided neighborhood list. This function is particularly useful in fluid dynamics simulations where particle interactions determine the system's behavior.

Usage

```
F = forceLandshoff(X, vX [,V, config, verbose])
[F, W, n] = forceLandshoff()
```

Parameters

- X: nX x 3 array of coordinates of atoms.
- vX: nX x 3 array of velocity components.
- V: Optional. nX x 1 cell array containing indices of neighbors within a cutoff distance (output of buildVerletList).
- config: Optional. Structure containing simulation parameters such as gradient kernel, smoothing length, speed of sound, density, mass, and volume.
- verbose: Optional. Boolean flag to control verbosity of the output for debugging purposes.

Outputs

- F: If a single output is provided, nX x 3 vector of Landshoff forces.
- W: If two outputs are provided, nX x 9 array representing virial stress tensor components (reshape W(i), 3,3 to recover the matrix).
- n: nX x 3 array of normal vectors.

Algorithm Details

Initialization and Configuration

#

- · Initializes default values for simulation parameters like smoothing length, density, mass, etc., and adjusts these based on input config if provided.
- · Verifies input consistency and dimensions.
- Prepares for virial stress calculation if required by the number of function outputs.

- Iterates over each particle, calculating forces based on the relative position and velocity vectors between the particle and its neighbors identified in the Verlet list.
- Employs a highly vectorized approach to minimize computational overhead and improve performance.
- Applies a conditional model where the interaction force is calculated only if the relative velocity is directed towards the particle, representing an approaching scenario commonly found in shock tube problems.
- Utilizes an analytical form of the kernel gradient function specified in config for force calculation.

Post-Processing

#

- Calculates the norm of the force vector for each particle and normalizes it to derive the direction.
- If virial stress output is requested, computes the stress tensor based on the interaction forces and the geometric configuration of particle pairs.

Example

```
matlabCopy code% Define coordinates and velocities
2
     X = [0,0,0; 1,0,0; 0,1,0];
3
     vX = [0,0,0; 0,0,1; 0,1,0];
4
5
     % Optional: Define neighbors manually or use buildVerletList function
     V = \{[2;3], [1;3], [1;2]\};
6
7
8
     % Configuration for interaction calculations
9
     config = struct('h', 0.1, 'c0', 10, 'rho', 1000, 'mass', 1, 'vol', 1);
10
11
     % Calculate forces
     [F, W, n] = forceLandshoff(X, vX, V, config, true);
     disp('Forces:');
13
14
     disp(F);
15
     disp('Virial Stress Tensor:');
16
     disp(W);
     disp('Normal Vectors:');
17
18
     disp(n);
```