Diseño de Software para Cómputo Científico

Proyecto Final: GriSPy (Grid Search in Python)

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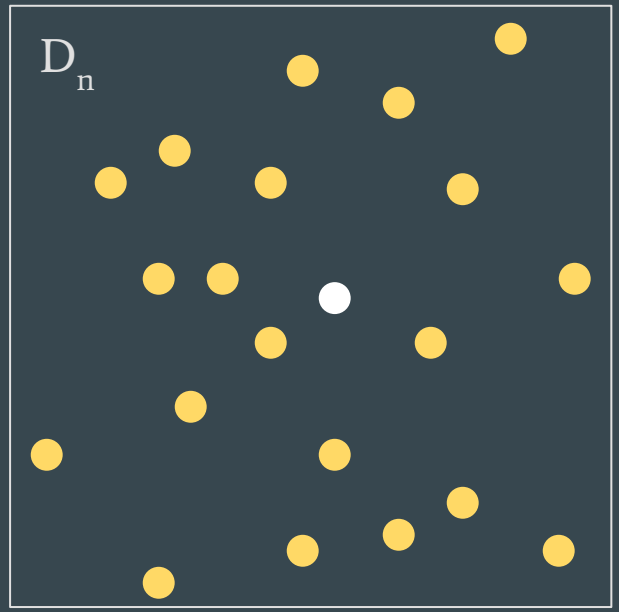
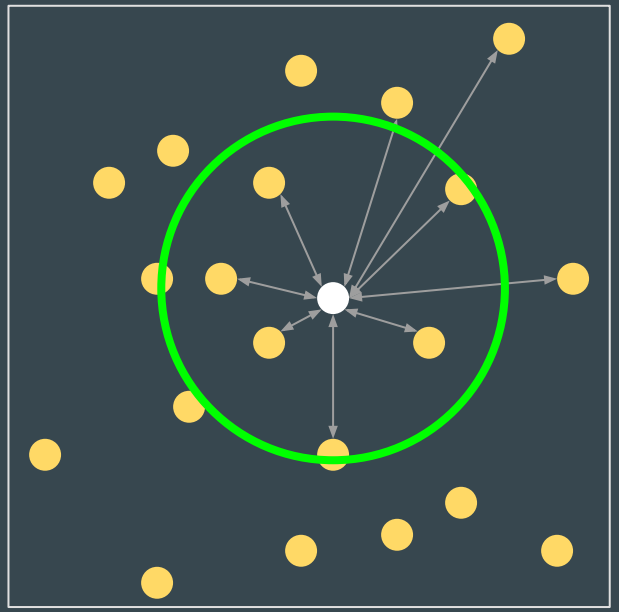
Chalela, M., Sillero, E., Pereyra, L., García, M. A., Cabral, J. B., Lares, M., & Merchán, M. (2019).
GriSPy: A Python package for Fixed-Radius Nearest Neighbors Search. arXiv preprint arXiv:1912.09585.

Problema: Búsqueda de vecinos cercanos

$d(c,x_k) = d_k \in \{d_1, d_2, ..., d_n\}$



k-esimo vecino de c



$P = \{x \in \mathbb{R}^d \mid x \in D_n\}$

$S = \{x_k \in D_n \mid d_k <= r_S\}$

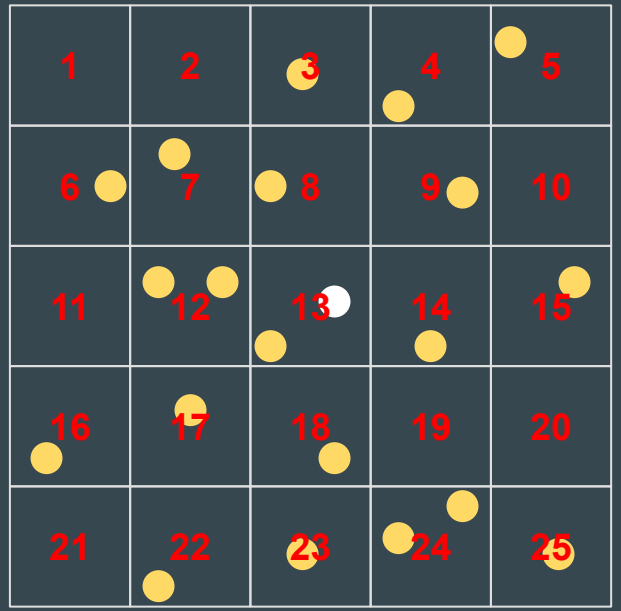
Búsqueda de vecinos más cercano (NNS)

Métodos (según su solución):

- Aproximados (Maneewong-vatana y Mount 1999):
  De interés para conjuntos de alta dimensión y recuperan puntos tal que:
  $$D(q, p) \leq (1+\epsilon)\, D(q, p)^*$$
  donde $D(q, p)^*$ es la distancia real y ϵ el parámetro de incertidumbre.
- Exatos (Particionado - Indexado):
  - Binary tree (k-d tree - Friedman+ 1977 ; Bentley 1975): Dividen el espacio en dos nodos en cada iteración hasta que se alcanza un cierto número de hojas.
  - Cell techniques: Crean una red de hipercubos y cada punto se asigna a su celda. Luego usan el indexado (tabla hash) para consultas futuras.

Objetivo del proyecto:
Desarrollar una paquete (Python) para la búsqueda de vecinos en k-dimensiones

$N \times N = N^d$



$\Delta x_d = [\max(x_d) - \min(x_d)\ ]/N$

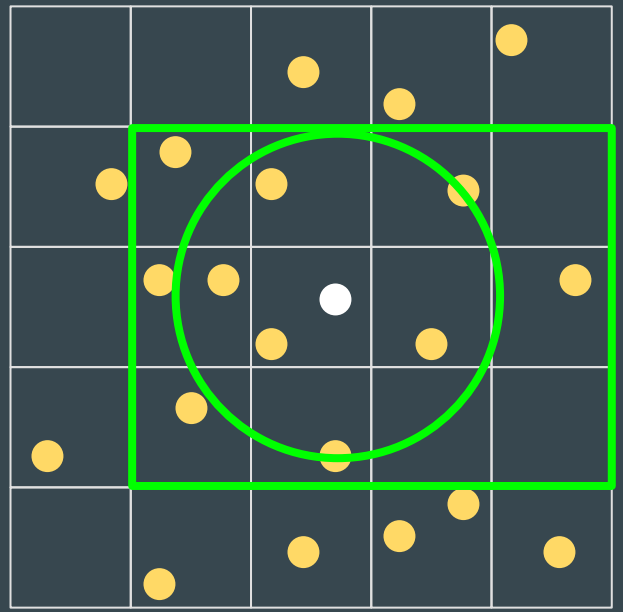
CONSTRUCCIÓN DE LA GRILLA

- Elegir N
- Calcular Δx_d
- Recorrer S indexando x_i

  $g_{i,d} = \text{int}(N\ [(x_{i,d} - \max(x_d)) / \Delta x_d])$

- Aplanar indices $g_{i,d}$
- Agrupar puntos por indice
- Eliminar celdas vacías
- Crear tabla hash

  $\text{Grid} = \{\ (g_c,) : [i, ..., n_c]\ \}$



BÚSQUEDA DE VECINOS

- Esfera

  $S = \{x_k \in D_n \mid d_k <= r_S\}$

- Cascara

  $S = \{x_k \in D_n \mid r_{min} <= d_k <= r_{max}\}$

Radios de búsqueda individuales

- k-esimos vecinos

  $d(c,x_k) = d_k \in \{d_1, d_2, ..., d_n\}$

Calculo de distancias - Metricas

Euclidea

$$D(x_0, x) = \sqrt{\sum_{i=1}^{k} \left(x_{0,i} - x_i\right)^2}$$

Haversine

$$D(x_0, x) = 2\ arcsin\ \sqrt{A + B}$$

$$A = sin^2\left(\frac{\Delta\varphi}{2}\right)$$

$$B = cos^2\varphi_0\ cos^2\varphi\ sin^2\left(\frac{\Delta\lambda}{2}\right)$$

Vincenty

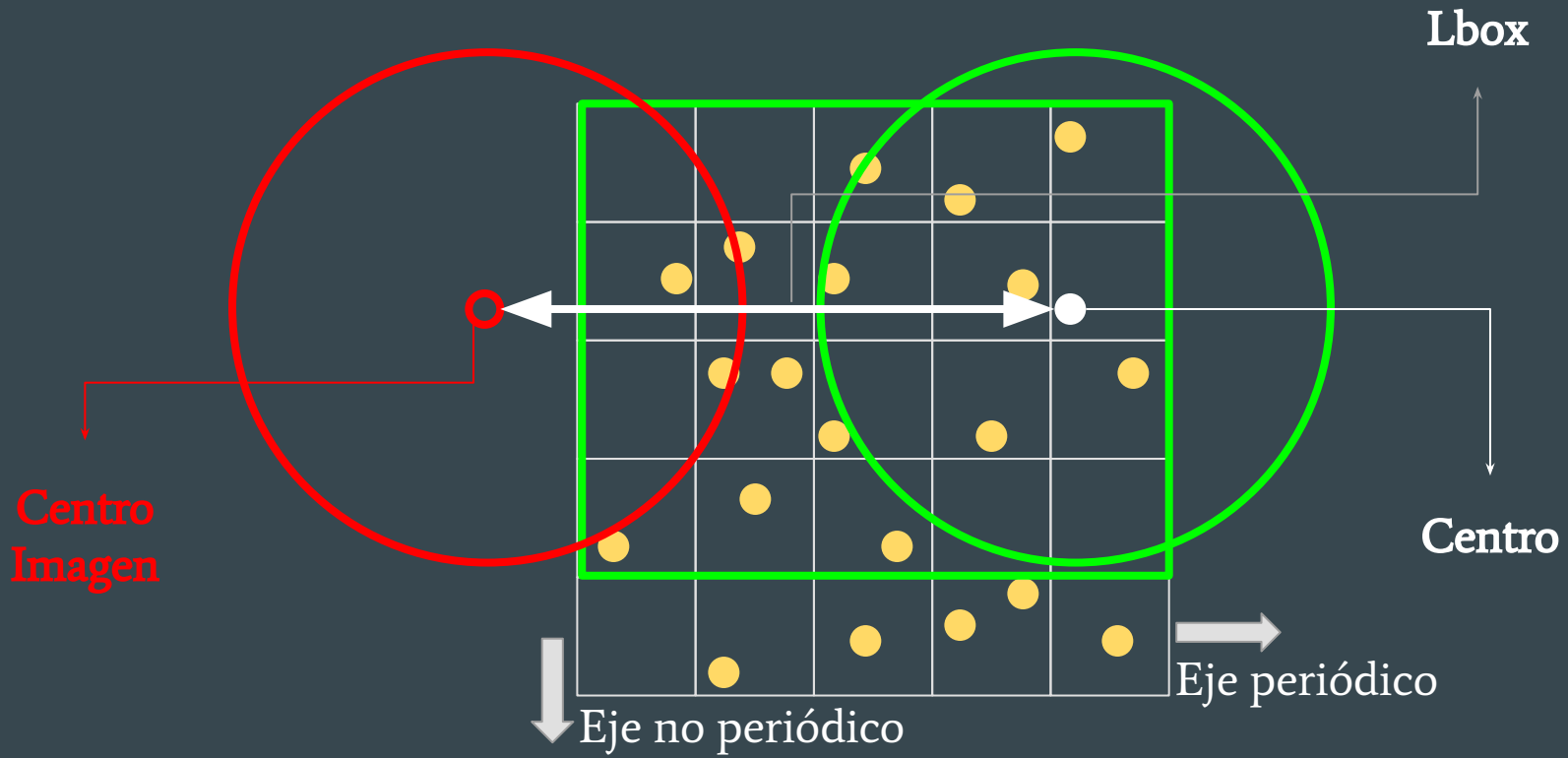
$$D(x_0, x) = arctan\ \frac{\sqrt{E^2 + F^2}}{G}$$

$$E = cos(\varphi)\ sin(\Delta\varphi)$$

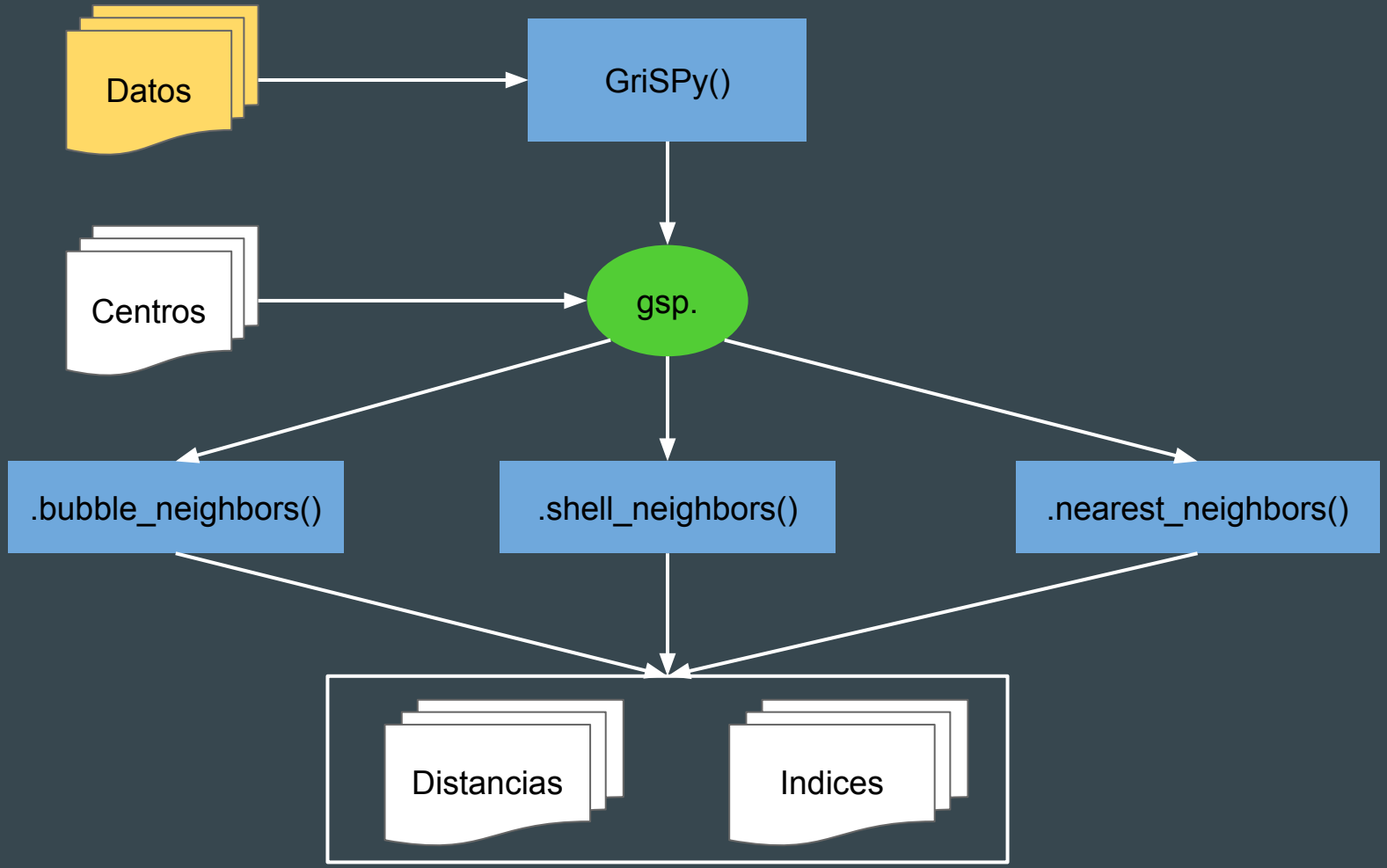
$$F = cos(\varphi_0)\ sin(\varphi) - sin(\varphi_0)\ cos(\varphi)\ (\Delta\lambda)$$

$$G = sin(\varphi_0)\ sin(\varphi) - cos(\varphi_0)\ cos(\varphi)\ (\Delta\lambda)$$

Periodicidad



Desarrollo de GriSPy:
Implementación interna y API


Datos
GriSPy()
Centros
gsp.
.bubble_neighbors()
.shell_neighbors()
.nearest_neighbors()
Distancias
Indices

Dependencias:

```
13  from scipy.spatial.distance import cdist
14  import numpy as np
15  import time
16  import datetime
17  import attr
18  from . import utils
19
```

Construcción de la Grilla:

```
21  @attr.s
22  class GriSPy(object):
23      """Grid Search in Python.
24
25      GriSPy is a regular grid search algorithm for quick nearest-neighbor
26      lookup.
27      """
28
29      # User input params
30      data = attr.ib(
31          default=None, kw_only=False, repr=False, validator=utils.validate_data,
32      )
33      N_cells = attr.ib(default=20, validator=utils.validate_N_cells)
34      periodic = attr.ib(default={})  # The validator runs in set_periodicity()
35      metric = attr.ib(default="euclid", validator=utils.validate_metric)
36      copy_data = attr.ib(
37          default=False, validator=attr.validators.instance_of(bool),
38      )
39
40      def __attrs_post_init__(self):
41          """Init more params and build the grid."""
42          if self.copy_data:
43              self.data = self.data.copy()
44          self.dim = self.data.shape[1]
45          self.set_periodicity(self.periodic)
46          self._build_grid()
47          self._empty = np.array([], dtype=int)  # Useful for empty arrays
```

```python

    def _build_grid(self, epsilon=1.0e-6):
        """Build the grid."""
        t0 = time.time()
        data_ind = np.arange(len(self.data))
        self.k_bins = np.zeros((self.N_cells + 1, self.dim))
        k_digit = np.zeros(self.data.shape, dtype=int)
        for k in range(self.dim):
            k_data = self.data[:, k]
            self.k_bins[:, k] = np.linspace(
                k_data.min() - epsilon,
                k_data.max() + epsilon,
                self.N_cells + 1,
            )
            k_digit[:, k] = self._digitize(k_data, bins=self.k_bins[:, k])

        compact_ind = np.ravel_multi_index(
            k_digit.T, (self.N_cells,) * self.dim, order="F",
        )

        compact_ind_sort = np.argsort(compact_ind)
        compact_ind = compact_ind[compact_ind_sort]
        k_digit = k_digit[compact_ind_sort]

        split_ind = np.searchsorted(
            compact_ind, np.arange(self.N_cells ** self.dim)
        )
        deleted_cells = np.diff(np.append(-1, split_ind)).astype(bool)
        split_ind = split_ind[deleted_cells]
        if split_ind[-1] > data_ind[-1]:
            split_ind = split_ind[:-1]

        list_ind = np.split(data_ind[compact_ind_sort], split_ind[1:])
        k_digit = k_digit[split_ind]

        self.grid = {}
        for i, j in enumerate(k_digit):
            self.grid[tuple(j)] = list(list_ind[i])

        # Record date and build time
        self.time = {"buildtime": time.time() - t0}
        currentDT = datetime.datetime.now()
        self.time["datetime"] = currentDT.strftime("%Y-%b-%d %H:%M:%S")
```

Búsqueda de vecinos: bubble_neighbors()

```
377     # User methods
378     def bubble_neighbors(self, centres, distance_upper_bound=-1.0,
379         sorted=False, kind="quicksort"):
380         """Find all points within given distances of each centre."""
381
382         # Validate iputs
383         utils.validate_centres(centres, self.data)
384         utils.validate_distance_bound(distance_upper_bound, self.periodic)
385         utils.validate_bool(sorted)
386         utils.validate_sortkind(kind)
387         # Match distance_upper_bound shape with centres shape
388         if np.isscalar(distance_upper_bound):
389             distance_upper_bound *= np.ones(len(centres))
390         else:
391             utils.validate_equalsize(centres, distance_upper_bound)
392
393         # Get neighbors
394         neighbor_cells = self._get_neighbor_cells(
395             centres, distance_upper_bound
396         )
397         neighbors_distances, neighbors_indices = self._get_neighbor_distance(
398             centres, neighbor_cells
399         )
```

```
401         # We need to generate mirror centres for periodic boundaries...
402         if self.periodic_flag:
403             terran_centres, terran_indices = self._mirror_universe(
404                 centres, distance_upper_bound
405             )
406             # terran_centres are the centres in the mirror universe for those
407             # near the boundary.
408             terran_neighbor_cells = self._get_neighbor_cells(
409                 terran_centres, distance_upper_bound[terran_indices]
410             )
411             terran_neighbors_distances, \
412                 terran_neighbors_indices = self._get_neighbor_distance(
413                     terran_centres, terran_neighbor_cells
414                 )
415
416             for i, t in zip(terran_indices, np.arange(len(terran_centres))):
417                 # i runs over normal indices that have a terran counterpart
418                 # t runs over terran indices, 0 to len(terran_centres)
419                 neighbors_distances[i] = np.concatenate(
420                     (neighbors_distances[i], terran_neighbors_distances[t])
421                 )
422                 neighbors_indices[i] = np.concatenate(
423                     (neighbors_indices[i], terran_neighbors_indices[t])
424                 )
425
426         for i in range(len(centres)):
427             mask_distances = neighbors_distances[i] <= distance_upper_bound[i]
428             neighbors_distances[i] = neighbors_distances[i][mask_distances]
429             neighbors_indices[i] = neighbors_indices[i][mask_distances]
430             if sorted:
431                 sorted_ind = np.argsort(neighbors_distances[i], kind=kind)
432                 neighbors_distances[i] = neighbors_distances[i][sorted_ind]
433                 neighbors_indices[i] = neighbors_indices[i][sorted_ind]
434         return neighbors_distances, neighbors_indices
```

1. Celdas vecinas

```python
    # Neighbor-cells methods
    def _get_neighbor_cells(self, centres, distance_upper_bound,
        distance_lower_bound=0, shell_flag=False):

        """Retrieve cells touched by the search radius."""
        cell_point = np.zeros((len(centres), self.dim), dtype=int)
        out_of_field = np.zeros(len(cell_point), dtype=bool)
        for k in range(self.dim):
            cell_point[:, k] = (
                self._digitize(centres[:, k], bins=self.k_bins[:, k])
            )
            out_of_field[
                (centres[:, k] - distance_upper_bound > self.k_bins[-1, k])
            ] = True
            out_of_field[
                (centres[:, k] + distance_upper_bound < self.k_bins[0, k])
            ] = True

        if np.all(out_of_field):
            return [self._empty] * len(centres)  # no neighbor cells

        # Armo la caja con celdas a explorar
        k_cell_min = np.zeros((len(centres), self.dim), dtype=int)
        k_cell_max = np.zeros((len(centres), self.dim), dtype=int)
        for k in range(self.dim):
            k_cell_min[:, k] = (
                self._digitize(
                    centres[:, k] - distance_upper_bound,
                    bins=self.k_bins[:, k],
                )
            )
            k_cell_max[:, k] = (
                self._digitize(
                    centres[:, k] + distance_upper_bound,
                    bins=self.k_bins[:, k],
                )
            )

            k_cell_min[k_cell_min[:, k] < 0, k] = 0
            k_cell_max[k_cell_max[:, k] < 0, k] = 0
            k_cell_min[k_cell_min[:, k] >= self.N_cells, k] = self.N_cells - 1
            k_cell_max[k_cell_max[:, k] >= self.N_cells, k] = self.N_cells - 1
```

```python
        cell_size = self.k_bins[1, :] - self.k_bins[0, :]
        cell_radii = 0.5 * np.sum(cell_size ** 2) ** 0.5

        neighbor_cells = []
        for i in range(len(centres)):
            # Para cada centro i, agrego un arreglo con shape (:,k)
            k_grids = [
                np.arange(k_cell_min[i, k], k_cell_max[i, k] + 1)
                for k in range(self.dim)
            ]
            k_grids = np.meshgrid(*k_grids)
            neighbor_cells += [
                np.array(list(map(np.ndarray.flatten, k_grids))).T
            ]

            # Calculo la distancia de cada centro i a sus celdas vecinas,
            # luego descarto las celdas que no toca el circulo definido por
            # la distancia
            cells_physical = [
                self.k_bins[neighbor_cells[i][:, k], k] + 0.5 * cell_size[k]
                for k in range(self.dim)
            ]
            cells_physical = np.array(cells_physical).T
            mask_cells = (
                self._distance(
                    centres[i], cells_physical
                ) < distance_upper_bound[i] + cell_radii
            )

            if shell_flag:
                mask_cells *= (
                    self._distance(
                        centres[i], cells_physical
                    ) > distance_lower_bound[i] - cell_radii
                )

            if np.any(mask_cells):
                neighbor_cells[i] = neighbor_cells[i][mask_cells]
            else:
                neighbor_cells[i] = self._empty
        return neighbor_cells
```

2. Distancias a los vecinos

```
227
228     def _get_neighbor_distance(self, centres, neighbor_cells):
229         """Retrieve neighbor distances whithin the given cells."""
230         neighbors_indices = []
231         neighbors_distances = []
232         for i in range(len(centres)):
233             if len(neighbor_cells[i]) == 0:  # no hay celdas vecinas
234                 neighbors_indices += [self._empty]
235                 neighbors_distances += [self._empty]
236                 continue
237             # Genera una lista con los vecinos de cada celda
238             # print neighbor_cells[i]
239             ind_tmp = [
240                 self.grid.get(tuple(neighbor_cells[i][j]), [])
241                 for j in range(len(neighbor_cells[i]))
242             ]
243             # Une en una sola lista todos sus vecinos
244             neighbors_indices += [np.concatenate(ind_tmp).astype(int)]
245             neighbors_distances += [
246                 self._distance(centres[i], self.data[neighbors_indices[i], :])
247             ]
248         return neighbors_distances, neighbors_indices
```

```
184     def _distance(self, centre_0, centres):
185         """Compute distance between points."""
186
187         if len(centres) == 0:
188             return self._empty
189
190         if self.metric == "euclid":
191             c0 = centre_0.reshape((-1, self.dim))
192             d = cdist(c0, centres).reshape((-1,))
193             return d
194
195         elif self.metric == "haversine":
196             lon1 = np.deg2rad(centre_0[0])
197             lat1 = np.deg2rad(centre_0[1])
198             lon2 = np.deg2rad(centres[:, 0])
199             lat2 = np.deg2rad(centres[:, 1])
200
201             sdlon = np.sin((lon2 - lon1) / 2.)
202             sdlat = np.sin((lat2 - lat1) / 2.)
203             clat1 = np.cos(lat1)
204             clat2 = np.cos(lat2)
205             num1 = sdlat ** 2
206             num2 = clat1 * clat2 * sdlon ** 2
207             sep = 2 * np.arcsin(np.sqrt(num1 + num2))
208             return np.rad2deg(sep)
209
210         elif self.metric == "vincenty":
211             lon1 = np.deg2rad(centre_0[0])
212             lat1 = np.deg2rad(centre_0[1])
213             lon2 = np.deg2rad(centres[:, 0])
214             lat2 = np.deg2rad(centres[:, 1])
215
216             sdlon = np.sin(lon2 - lon1)
217             cdlon = np.cos(lon2 - lon1)
218             slat1 = np.sin(lat1)
219             slat2 = np.sin(lat2)
220             clat1 = np.cos(lat1)
221             clat2 = np.cos(lat2)
222             num1 = clat2 * sdlon
223             num2 = clat1 * slat2 - slat1 * clat2 * cdlon
224             denominator = slat1 * slat2 + clat1 * clat2 * cdlon
225             sep = np.arctan2(np.sqrt(num1 ** 2 + num2 ** 2), denominator)
226             return np.rad2deg(sep)
```

3. Periodicidad

```
335     def _near_boundary(self, centres, distance_upper_bound):
336         mask = np.zeros((len(centres), self.dim), dtype=bool)
337         for k in range(self.dim):
338             if self.periodic[k] is None:
339                 continue
340             mask[:, k] = abs(
341                 centres[:, k] - self.periodic[k][0]
342             ) < distance_upper_bound
343             mask[:, k] += abs(
344                 centres[:, k] - self.periodic[k][1]
345             ) < distance_upper_bound
346         return mask.sum(axis=1, dtype=bool)
347
348     def _mirror(self, centre, distance_upper_bound):
349         mirror_centre = centre - self._periodic_edges
350         mask = self._periodic_direc * distance_upper_bound
351         mask += mirror_centre
352         mask = (mask >= self._pd_low) * (mask <= self._pd_hi)
353         mask = np.prod(mask, 1, dtype=bool)
354         return mirror_centre[mask]
355
356     def _mirror_universe(self, centres, distance_upper_bound):
357         """Generate Terran centres in the Mirror Universe."""
358         terran_centres = np.array([[]] * self.dim).T
359         terran_indices = np.array([], dtype=int)
360         near_boundary = self._near_boundary(centres, distance_upper_bound)
361         if not np.any(near_boundary):
362             return terran_centres, terran_indices
363
364         for i, centre in enumerate(centres):
365             if not near_boundary[i]:
366                 continue
367             mirror_centre = self._mirror(centre, distance_upper_bound[i])
368             if len(mirror_centre) > 0:
369                 terran_centres = np.concatenate(
370                     (terran_centres, mirror_centre), axis=0
371                 )
372                 terran_indices = np.concatenate(
373                     (terran_indices, np.repeat(i, len(mirror_centre)))
374                 )
375         return terran_centres, terran_indices
```

shell_neighbors( )

```python
    def shell_neighbors(self, centres, distance_lower_bound=-1.0,
        distance_upper_bound=-1.0, sorted=False, kind="quicksort"):
        """Find all points within given lower and upper distances of each centre."""

        # Validate inputs
        utils.validate_centres(centres, self.data)
        utils.validate_bool(sorted)
        utils.validate_sortkind(kind)
        utils.validate_shell_distances(
            distance_lower_bound, distance_upper_bound, self.periodic,
        )

        # Match distance bounds shapes with centres shape
        if np.isscalar(distance_lower_bound):
            distance_lower_bound *= np.ones(len(centres))
        else:
            utils.validate_equalsize(centres, distance_lower_bound)
        if np.isscalar(distance_upper_bound):
            distance_upper_bound *= np.ones(len(centres))
        else:
            utils.validate_equalsize(centres, distance_upper_bound)

        # Get neighbors
        neighbor_cells = self._get_neighbor_cells(
            centres,
            distance_upper_bound=distance_upper_bound,
            distance_lower_bound=distance_lower_bound,
            shell_flag=True,
        )
        neighbors_distances, neighbors_indices = self._get_neighbor_distance(
            centres, neighbor_cells)
```

```python
        # We need to generate mirror centres for periodic boundaries...
        if self.periodic_flag:
            terran_centres, terran_indices = self._mirror_universe(
                centres, distance_upper_bound)
            # terran_centres are the centres in the mirror universe for those
            # near the boundary.
            terran_neighbor_cells = self._get_neighbor_cells(
                terran_centres, distance_upper_bound[terran_indices])

            terran_neighbors_distances,\
                terran_neighbors_indices = self._get_neighbor_distance(
                    terran_centres, terran_neighbor_cells)

            for i, t in zip(terran_indices, np.arange(len(terran_centres))):
                # i runs over normal indices that have a terran counterpart
                # t runs over terran indices, 0 to len(terran_centres)
                neighbors_distances[i] = np.concatenate(
                    (neighbors_distances[i], terran_neighbors_distances[t]) )
                neighbors_indices[i] = np.concatenate(
                    (neighbors_indices[i], terran_neighbors_indices[t]) )

        for i in range(len(centres)):
            mask_distances_upper = neighbors_distances[i] <= distance_upper_bound[i]
            mask_distances_lower = neighbors_distances[i][mask_distances_upper]
            mask_distances_lower = mask_distances_lower > distance_lower_bound[i]

            aux = neighbors_distances[i]
            aux = aux[mask_distances_upper]
            aux = aux[mask_distances_lower]
            neighbors_distances[i] = aux

            aux = neighbors_indices[i]
            aux = aux[mask_distances_upper]
            aux = aux[mask_distances_lower]
            neighbors_indices[i] = aux

            if sorted:
                sorted_ind = np.argsort(neighbors_distances[i], kind=kind)
                neighbors_distances[i] = neighbors_distances[i][sorted_ind]
                neighbors_indices[i] = neighbors_indices[i][sorted_ind]

        return neighbors_distances, neighbors_indices
```

nearest_neighbors( )

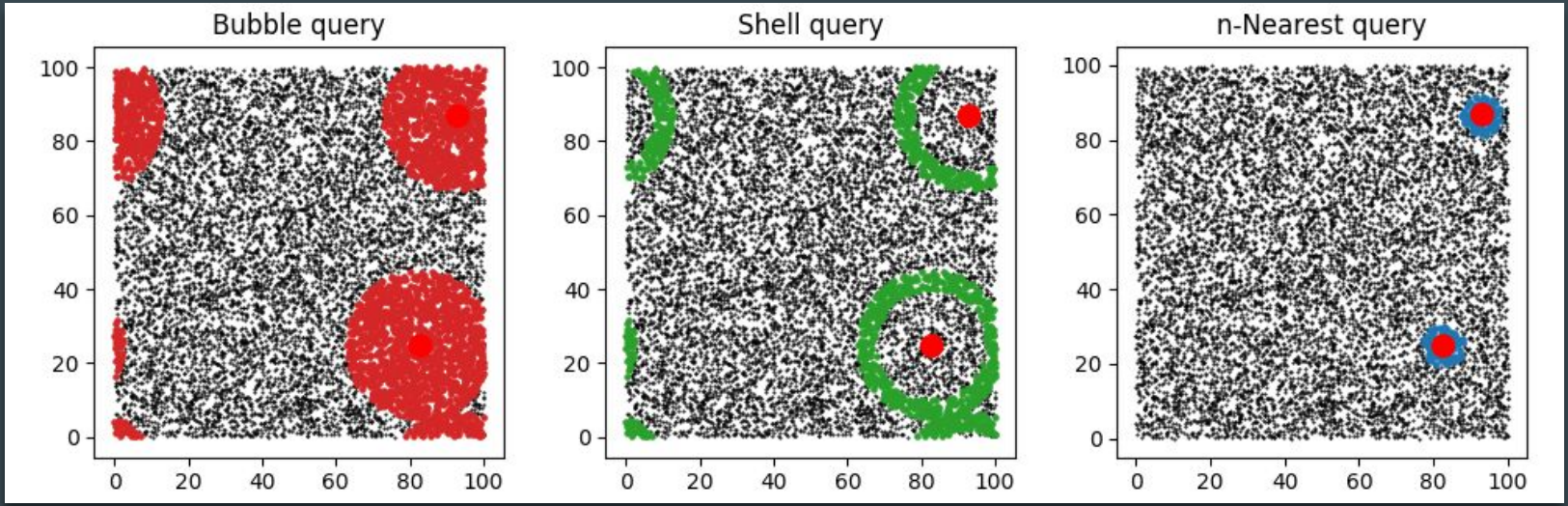
```python
    def nearest_neighbors(self, centres, n=1, kind="quicksort"):
        """Find the n nearest-neighbors for each centre."""

        # Validate input
        utils.validate_centres(centres, self.data)
        utils.validate_n_nearest(n, self.data, self.periodic)
        utils.validate_sortkind(kind)

        # Initial definitions
        N_centres = len(centres)
        centres_lookup_ind = np.arange(0, N_centres)
        n_found = np.zeros(N_centres, dtype=bool)
        lower_distance_tmp = np.zeros(N_centres)
        upper_distance_tmp = np.zeros(N_centres)

        # Abro la celda del centro como primer paso
        centre_cell = self._get_neighbor_cells(
            centres, distance_upper_bound=upper_distance_tmp
        )
        # crear funcion que regrese vecinos sin calcular distancias
        neighbors_distances, neighbors_indices = self._get_neighbor_distance(
            centres, centre_cell
        )

        # Calculo una primera aproximacion con la
        # 'distancia media' = 0.5 * (n/denstiy)**(1/dim)
        # Factor de escala para la distancia inicial
        mean_distance_factor = 1.0
        cell_size = self.k_bins[1, :] - self.k_bins[0, :]
        cell_volume = np.prod(cell_size.astype(float))
        neighbors_number = np.array(list(map(len, neighbors_indices)))
        mask_zero_neighbors = neighbors_number == 0
        neighbors_number[mask_zero_neighbors] = 1
        mean_distance = 0.5 * (n / (neighbors_number / cell_volume)) ** (
            1.0 / self.dim)

        upper_distance_tmp = mean_distance_factor * mean_distance
```

```python
        neighbors_indices = [self._empty] * N_centres
        neighbors_distances = [self._empty] * N_centres
        while not np.all(n_found):
            neighbors_distances_tmp,\
                neighbors_indices_tmp = self.shell_neighbors(
                    centres[~n_found],
                    distance_lower_bound=lower_distance_tmp[~n_found],
                    distance_upper_bound=upper_distance_tmp[~n_found],
                )

            for i_tmp, i in enumerate(centres_lookup_ind[~n_found]):
                if n_found[i]:
                    continue
                if n <= len(neighbors_indices_tmp[i_tmp]) + len(
                    neighbors_indices[i]
                ):
                    n_more = n - len(neighbors_indices[i])
                    n_found[i] = True
                else:
                    n_more = len(neighbors_indices_tmp[i_tmp])
                    lower_distance_tmp[i_tmp] = upper_distance_tmp[
                        i_tmp
                    ].copy()
                    upper_distance_tmp[i_tmp] += cell_size.min()

                sorted_ind = np.argsort(
                    neighbors_distances_tmp[i_tmp], kind=kind
                )[:n_more]
                neighbors_distances[i] = np.hstack(
                    (
                        neighbors_distances[i],
                        neighbors_distances_tmp[i_tmp][sorted_ind],
                    )
                )
                neighbors_indices[i] = np.hstack(
                    (
                        neighbors_indices[i],
                        neighbors_indices_tmp[i_tmp][sorted_ind],
                    )
                )

        return neighbors_distances, neighbors_indices
```

Save & Load

```
652     def save_grid(self, file="grispy.gsp", overwrite=False):
653         """Save all grid attributes in a binary file for future use."""
654 
655         # Validate input
656         utils.validate_filename(file)
657         utils.validate_bool(overwrite)
658         utils.validate_canwrite(file, overwrite)
659 
660         import pickle
661         with open(file, "wb") as fp:
662             pickle.dump(self, fp, protocol=pickle.HIGHEST_PROTOCOL)
663 
664         print("GriSPy grid attributes saved to: {}".format(file))
665         return None
666 
667     @classmethod
668     def load_grid(cls, file):
669         """Load a GriSPy instance previously saved with the save_grid() method."""
670 
671         # Validate input
672         utils.validate_filename(file)
673 
674         import os.path
675         if not os.path.isfile(file):
676             raise FileNotFoundError("There is no file named {}".format(file))
677 
678         import pickle
679         with open(file, "rb") as fp:
680             gsp = pickle.load(fp)
681             if not isinstance(gsp, cls):
682                 raise TypeError("Unpickled object is not a GriSPy instance.")
683 
684         print(
685             "Succsefully loaded GriSPy grid created on {}".format(
686                 gsp.time["datetime"])
687         )
688         return gsp
```

Ejemplo



Calidad:
Testing e integración continua

Testing

Se divide en cuatro áreas:

- Core (13)
- Distancias (12)
- Consistencia de datos (25)
- I/O (7)

Testing

Core:

- GriSPy (8)
  - Orden correcto del vector de distancias en `nearest_neighbors`.
  - Puntos dentro de la burbuja en `bubble_neighbors`.
  - Puntos dentro del rango en `shell_neighbors`.
  - Precisión para todos los métodos de búsqueda de vecinos.
- Periodicidad (2)
  - Control para `bubble_neighbors y shell_neighbors`.
- Hiperesfera (3)
  - Pruebas de cálculo para todos los métodos de búsqueda de vecinos.

Testing

Distancias:

Se ejecuta un test de cada condición para cada una de las métricas (`euclid`, `vincenty` y `haversine`).

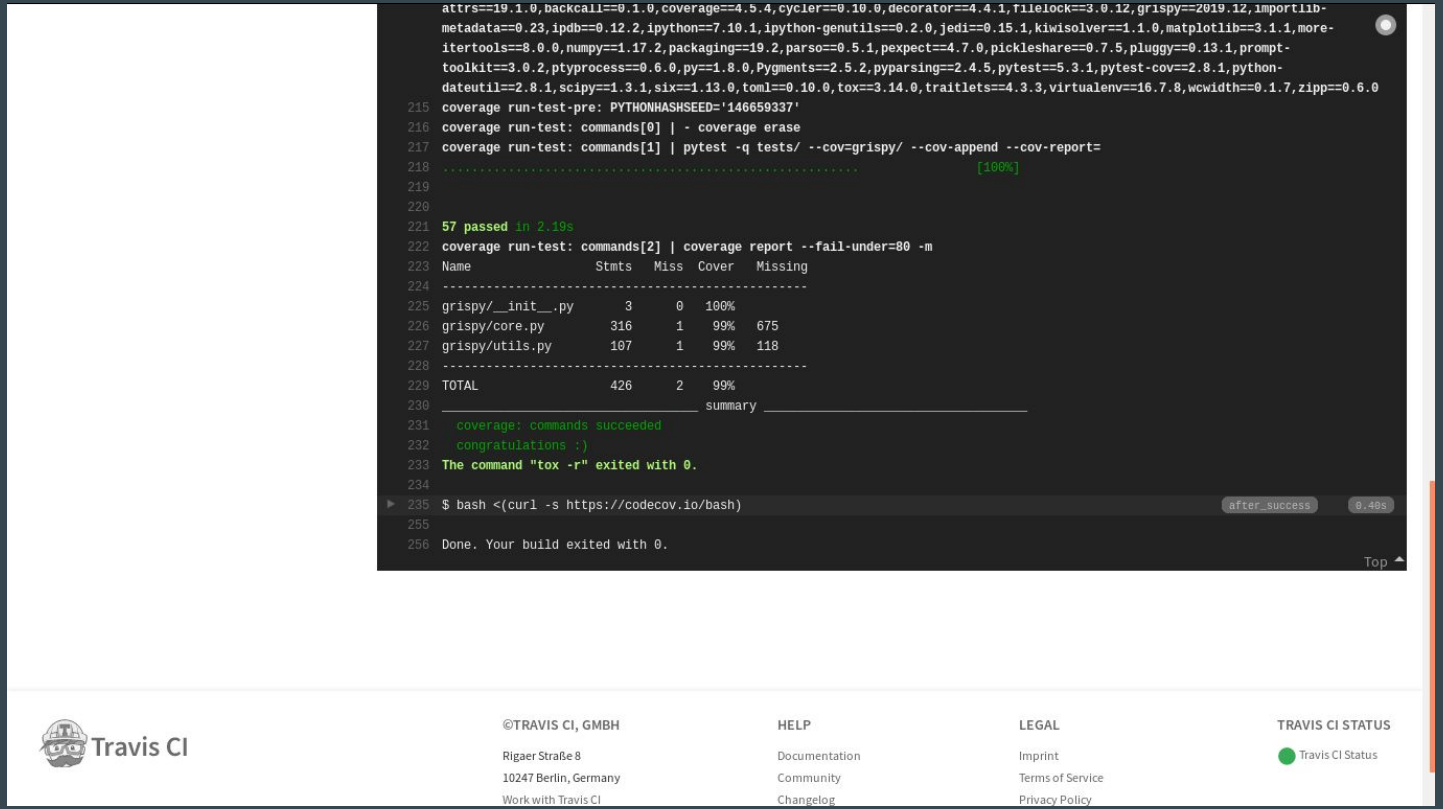
- Condición I (3)
  - dist(a, b) != NaN
- Condición II (3)
  - $0 \leq$ dist(a, b)
- Condición III (3)
  - dist(a, b) = dist(b, a)
- Condición IV (3)
  - dist(a, c) $\leq$ dist(a, b) + dist(b, c)

Testing

Consistencia de datos:

- Datos retornados (9)
  - Tipo y tamaño de los datos retornados para todos los métodos de búsqueda de vecinos (un centro y múltiples centros).
  - Periodicidad. Tipo y tamaño de datos retornados por `mirror_universe`, `_mirror` y `_near_boundary`.
- Inicialización (10)
  - Tipo, valor y estructura de `data`.
  - Tipo y valor de `periodic`, `metric`, `copy_data`, y `N_cells`.
- Inputs de queries (6)
  - En `bubble_neighbors`, tipo y forma forma de centros y radios, valor y tipo de `kind` y `sorted`.
  - En `shell_neighbors`, tipo y forma forma de centros y radios.
  - En `nearest_neighbors`, tipo y valor de `n`.

Coverage: 99%


attrs==19.1.0,backcall==0.1.0,coverage==4.5.4,cycler==0.10.0,decorator==4.4.1,filelock==3.0.12,grispy==2019.12,importlib-metadata==0.23,ipdb==0.12.2,ipython==7.10.1,ipython-genutils==0.2.0,jedi==0.15.1,kiwisolver==1.1.0,matplotlib==3.1.1,more-itertools==8.0.0,numpy==1.17.2,packaging==19.2,parso==0.5.1,pexpect==4.7.0,pickleshare==0.7.5,pluggy==0.13.1,prompt-toolkit==3.0.2,ptyprocess==0.6.0,py==1.8.0,Pygments==2.5.2,pyparsing==2.4.5,pytest==5.3.1,pytest-cov==2.8.1,python-dateutil==2.8.1,scipy==1.3.1,six==1.13.0,toml==0.10.0,tox==3.14.0,traitlets==4.3.3,virtualenv==16.7.8,wcwidth==0.1.7,zipp==0.6.0
215 coverage run-test-pre: PYTHONHASHSEED='146659337'
216 coverage run-test: commands[0] | - coverage erase
217 coverage run-test: commands[1] | pytest -q tests/ --cov=grispy/ --cov-append --cov-report=
218 ..... [100%]
219
220
221 57 passed in 2.19s
222 coverage run-test: commands[2] | coverage report --fail-under=80 -m
223 Name Stmts Miss Cover Missing
224 --
225 grispy/__init__.py 3 0 100%
226 grispy/core.py 316 1 99% 675
227 grispy/utils.py 107 1 99% 118
228 --
229 TOTAL 426 2 99%
230 _____ summary _____
231 coverage: commands succeeded
232 congratulations :)
233 The command "tox -r" exited with 0.
234
235 $ bash <(curl -s https://codecov.io/bash) after_success 0.40s
255
256 Done. Your build exited with 0.
Top
Travis CI
©TRAVIS CI, GMBH
Rigaer Straße 8
10247 Berlin, Germany
Work with Travis CI
HELP
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Community
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LEGAL
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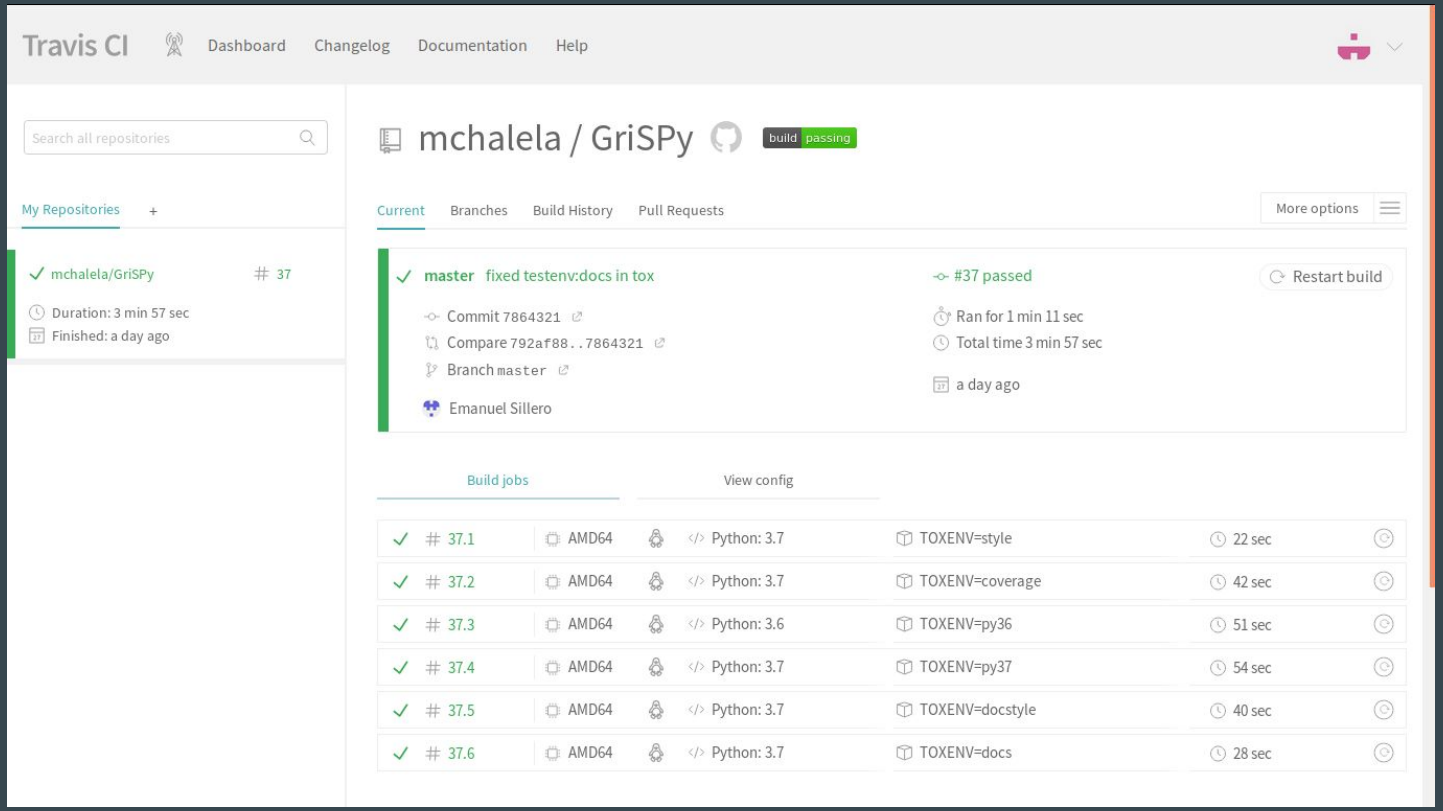
TRAVIS CI STATUS
Travis CI Status

Integración continua con Travis CI



Optimización:
Profiling, paralelización...

Benchmarking (Medición de tiempos)

Métodos

El código puede separarse en dos partes

- Build
- Query

Objetivo

Encontrar los mejores parámetros que minimicen los tiempos Build y Query.

Además entender las limitaciones de nuestro código (Peores Casos)

Parámetros libres del problema

- N - Celdas
- N - Puntos
- N - Centros
- K - dimensiones
- Radio de búsqueda
- Métrica
- Condiciones Periódicas
- El grado de clustering de los datos

Parámetros libres del problema

- N - Celdas
- N - Puntos
- N - Centros
- K - dimensiones
- Radio de búsqueda — **fracción del Box**
- Métrica — **Euclidiana**
- Condiciones Periódicas — **No periódicas**
- El grado de clustering de los datos — **Uniforme**

Variando K-dim [2 - 3 - 4]

Lbox = [0.0, 1.0]

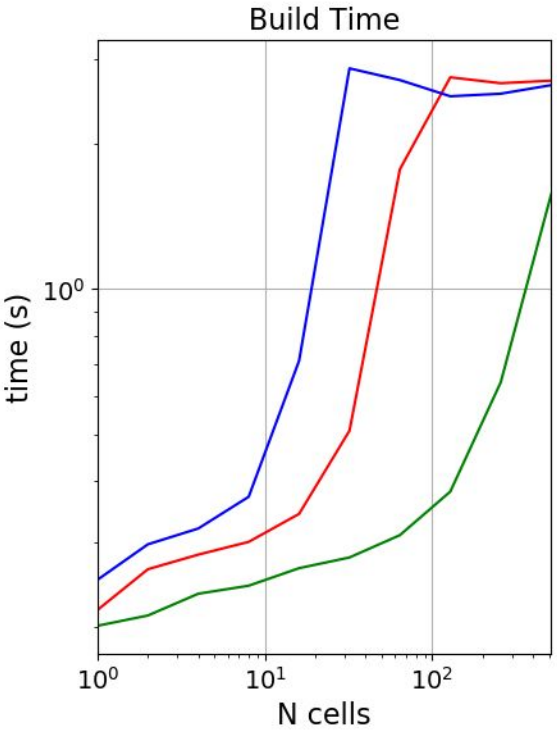
Núm. de centros - Ncent = 10^3

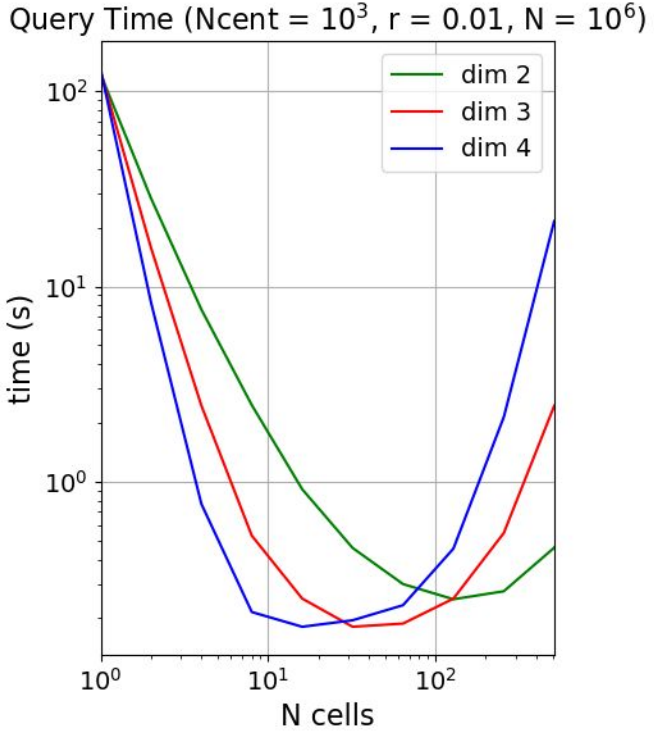
Núm. de puntos - N = 10^6

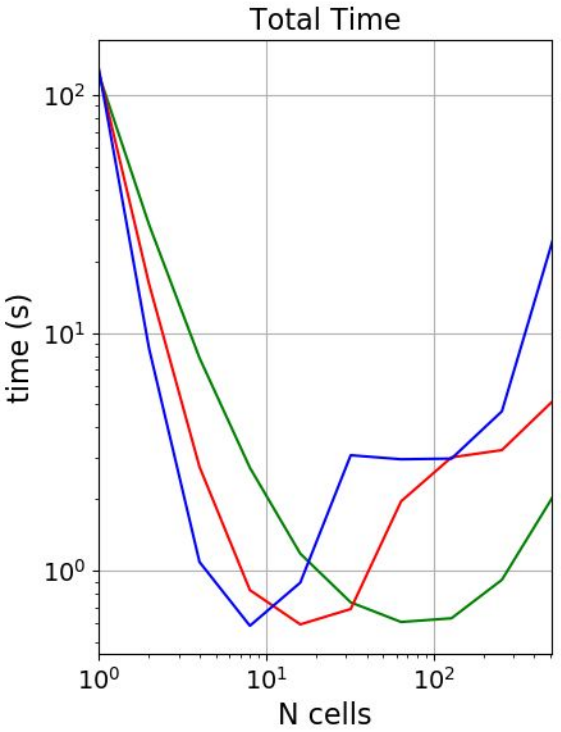
Núm. de celdas -

[1, 2, 4, 8, 16, 32, 64, 128, 264, 512]

UNIFORME


Build Time
time (s)
10^0
10^0
10^1
10^2
N cells


Query Time (Ncent = 10^3, r = 0.01, N = 10^6)
dim 2
dim 3
dim 4
time (s)
10^2
10^1
10^0
10^0
10^1
10^2
N cells


Total Time
time (s)
10^2
10^1
10^0
10^0
10^1
10^2
N cells

Variando N
$[10^3, 10^4, 10^5, 10^6]$

Lbox = [0.0, 1.0]

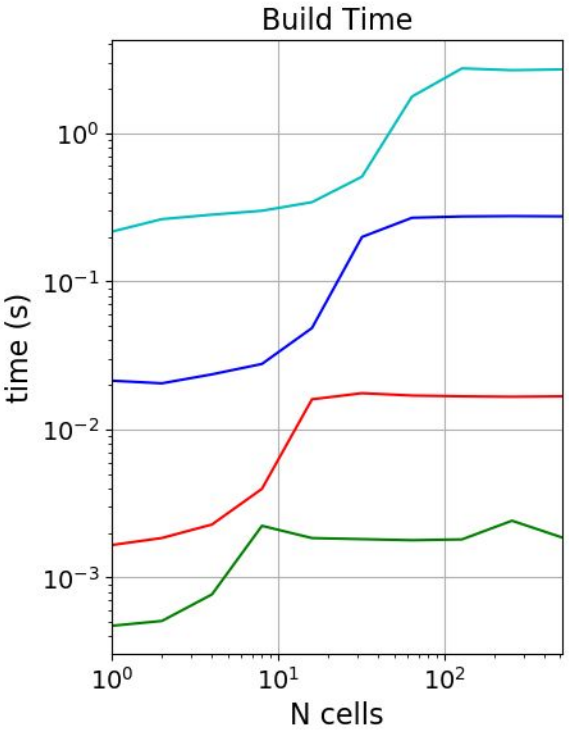
Núm. de centros - Ncent = 10^3

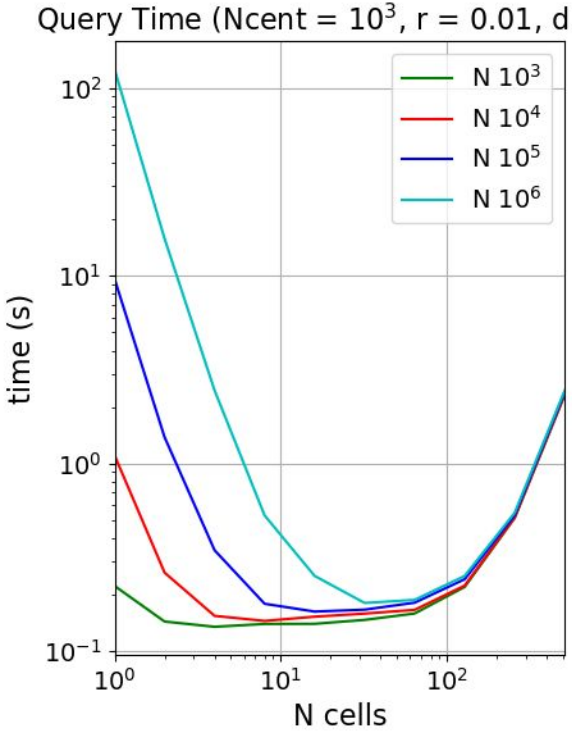
Núm. de dimensiones - K = 3

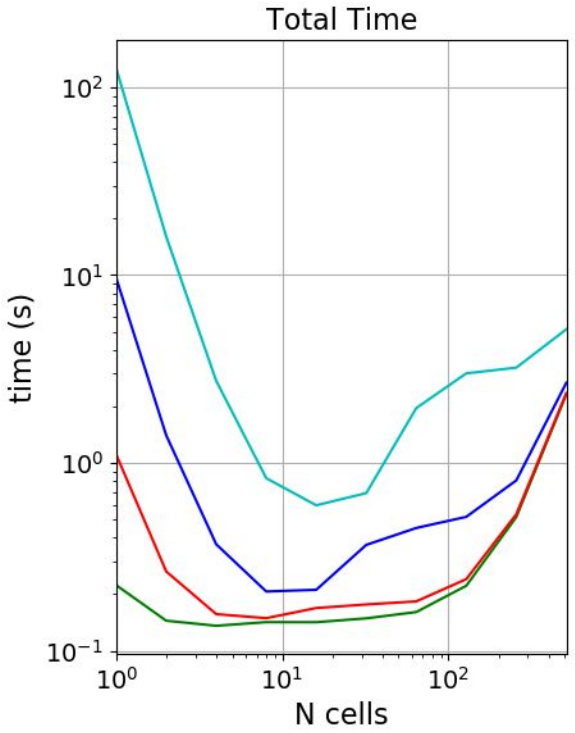
Núm. de celdas -

[1, 2, 4, 8, 16, 32, 64, 128, 264, 512]

UNIFORME


Build Time
time (s)
N cells


Query Time (Ncent = 10^3, r = 0.01, dim 3)
N 10^3
N 10^4
N 10^5
N 10^6
time (s)
N cells


Total Time
time (s)
N cells

Variando Ncentros $[10^3, 10^4, 10^5, 10^6]$

Lbox = [0.0, 1.0]

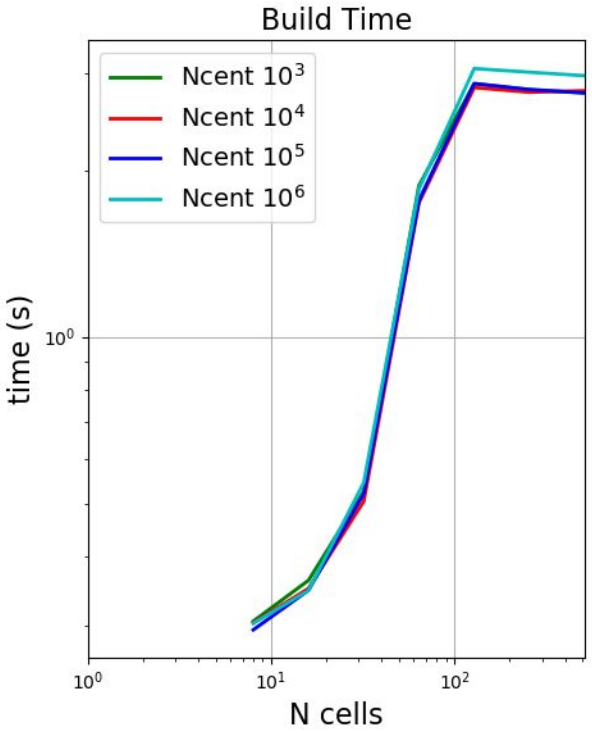
Núm. de centros - N = 10^6

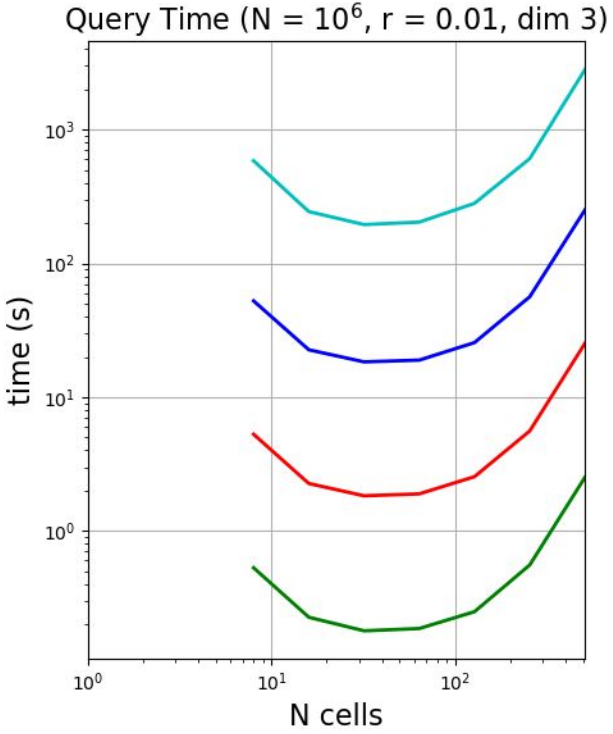
Núm. de dimensiones - K = 3

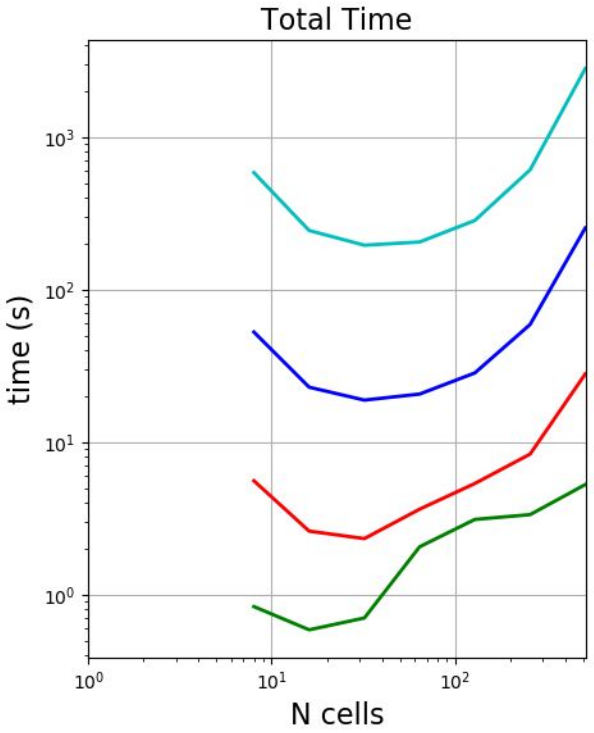
Núm. de celdas -

[8, 16, 32, 64, 128, 264, 512]

UNIFORME


Build Time
Ncent 10^3
Ncent 10^4
Ncent 10^5
Ncent 10^6
time (s)
10^0
10^0
10^1
10^2
N cells


Query Time (N = 10^6, r = 0.01, dim 3)
time (s)
10^3
10^2
10^1
10^0
10^0
10^1
10^2
N cells


Total Time
time (s)
10^3
10^2
10^1
10^0
10^0
10^1
10^2
N cells

Pruebas con Clustering (datos reales)

Variando N $[10^3, 10^4, 10^5, 10^6]$

Lbox = [0.0, 1.0]

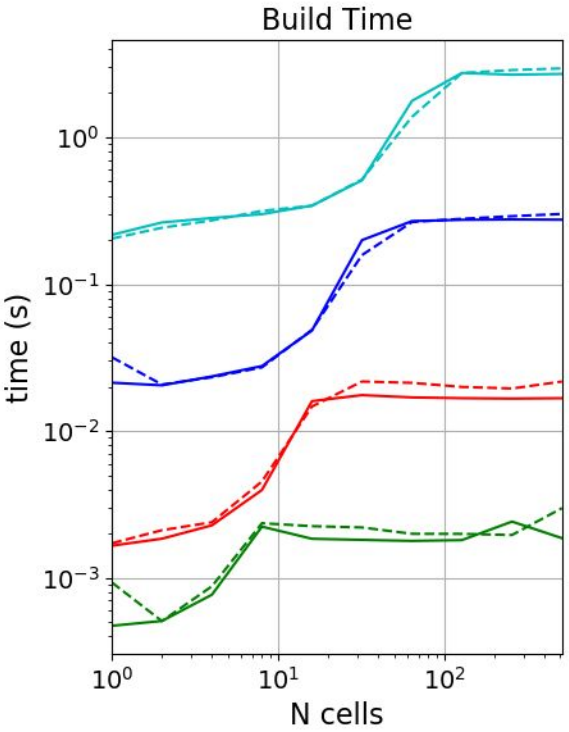
Núm. de centros - Ncent = 10^3

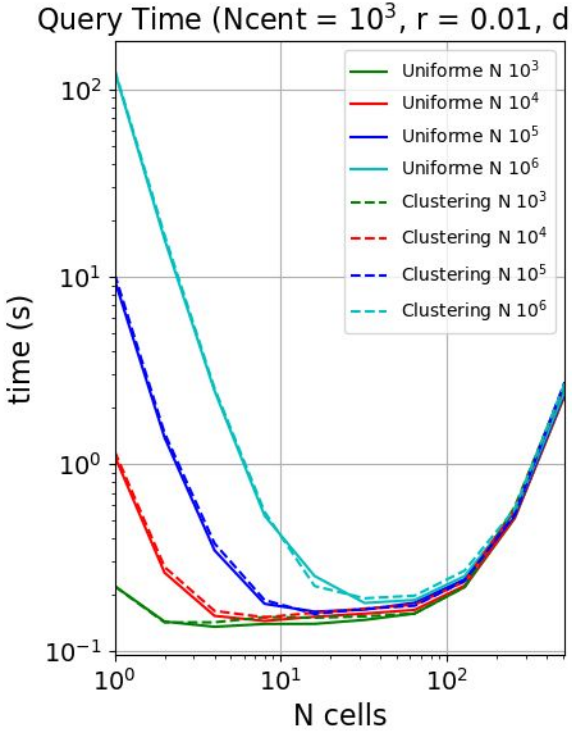
Núm. de dimensiones - K = 3

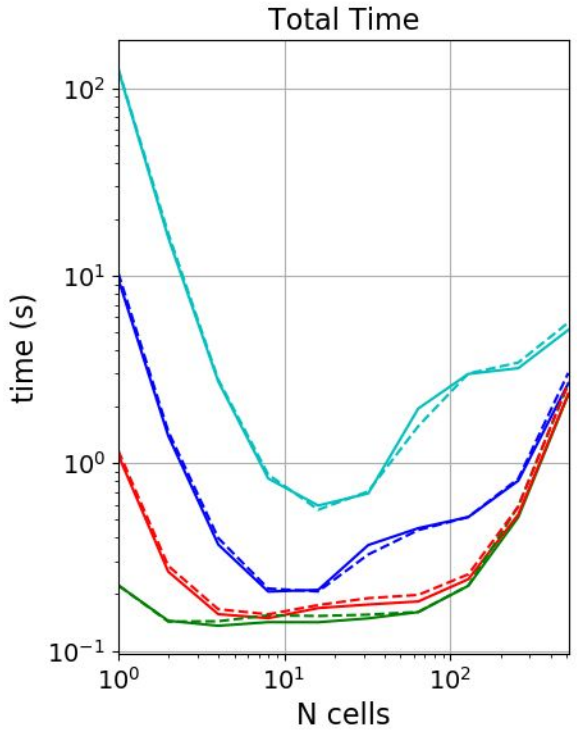
Núm. de celdas -

[1, 2, 4, 8, 16, 32, 64, 128, 264, 512]

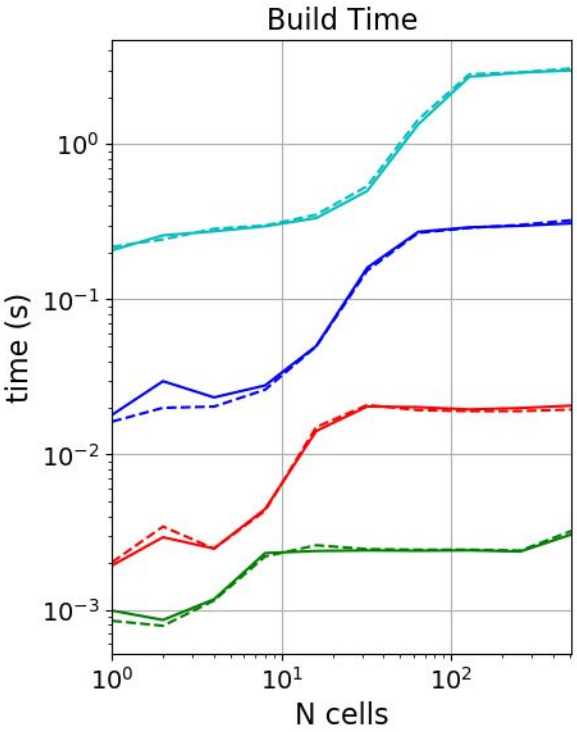
CLUSTERING
Centros Random simulación vs Centros Random uniforme

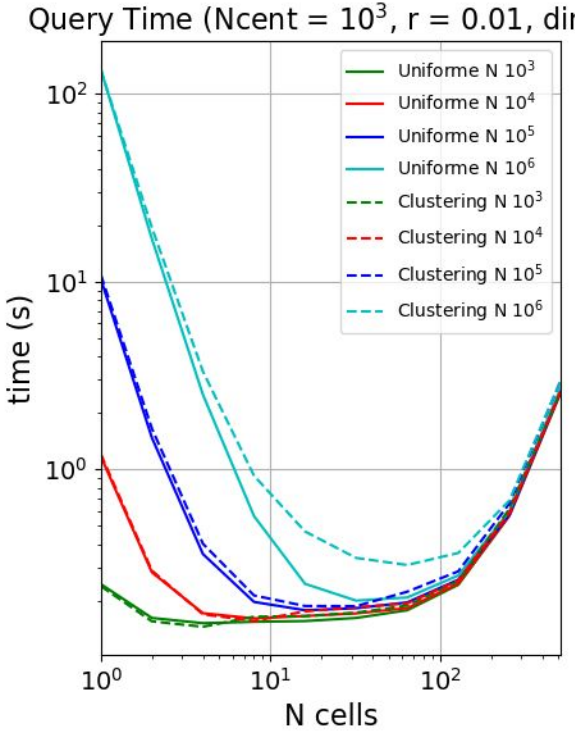


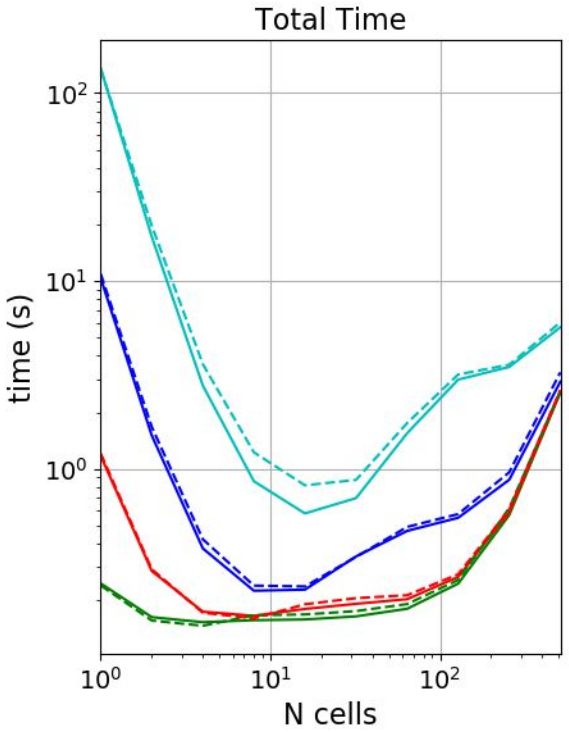




CLUSTERING
Centros FoF vs Centros Random en la simulación







Resumen

Dimensiones	• Se comporta de manera adecuada con el número de dimensiones
Número de centros	• En el rango de prueba el tiempo de Query escala bien con el número de centros
Número de celdas	• Número óptimo depende de la dimensión • Aumentar Ncells no mejora la performance • Depende de la dimensión y el grado de Clustering de los datos

Publicar!

Publicar!

GriSPy: A Python package for Fixed-Radius Nearest Neighbors Search

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