# **PARAVIEW Isosurface (1)**

https://s3-us-west-2.amazonaws.com/secure.notion-static.com/cd73088b-bc91-4 078-b62f-e4fa00bbe785/BF3\_esp.cub

https://s3-us-west-2.amazonaws.com/secure.notion-static.com/a13d06d4-6ffe-42 d3-9fdc-4871aa0c746b/BF3\_den\_tot.cub

## 1) Открыть файл



2) Выбрать All Files

| File name:     |               | Navigate |
|----------------|---------------|----------|
| Files of type: | All Files (*) | ~        |

### 3) Открыть с помощью Gaussian Cube Read

| <b>III</b> *   | Open Data With   | ?                | $\sim$      | ^    | × |
|--|--|------------------|-------------|------|---|
| A reader for "/home/lsv<br>Please choose one:  | vt/diffcub/BF3_esp.cub" could  | not be           | four        | nd.  |   |
| AdaptiveCosmoCore<br>ADIOS2VTXReader<br>AVS UCD Reader<br>CityGML Reader<br>CML Molecule Reader<br>CosmoReader<br>CSV Reader<br>DEM Reader<br>Ensemble Data Reade<br>ENZO AMR Particles Re<br>Enzo Reader<br>FLASH AMR Particles R<br>Flash Reader<br>Fluent Case Reader | r<br>eader<br>.eader   |                  |             |      |   |
| Gaussian Cube Reader<br>GDAL Vector Reader<br>GenericIOMultiBlockRe<br>GenericIOReader<br>GITF Reader<br>H5PartReader<br>HDF5 Rage Reader<br>Image Reader<br>Opening the file with an<br>unpredictable behavior  | eader<br>n incompatible reader may rest<br>or a crash. Please choose the<br>OK | ult in<br>correc | t re<br>Cai | ader | • |

## 4) Нажать Apply

| Properties Info | ormation          |          |   |    |
|-----------------|-------------------|----------|---|----|
| Properties      |                   |          |   | đ× |
| Arply           | <b>⊘</b> Reset    | 🗱 Delete | ? |    |
| Search (use Es  | c to clear text)  |          |   | \$ |
| Properties      | (BF3_den_tot.cub) |          |   | B  |
| Display         |                   |          |   | B  |
| - View (Rend    | er View)          |          |   | B  |
| Axes Grid       |                   | Edit     |   |    |
| Center Axes Vi  | sibility          |          |   |    |
| Orientation Axe | 5                 |          |   |    |

- 5) Повторить 1-4 для второго файла
- 6) С зажатым Ctrl выделить 2 грида



7) Ctrl+Space и ввести Append Attrubutes



7.5) Выбрать AppendAttributes1



## 8) Нажать Аррly

| Properties                  | Information             |    |
|-----------------------------|-------------------------|----|
| Properties                  |                         | ð× |
|                             |                         |    |
| 🗬 Appl                      | Reset <b>X</b> Delete ? |    |
| Search (use                 | Esc to clear text)      |    |
| - Propertie                 | es (AppendAttributes1)  |    |
| <ul> <li>Display</li> </ul> |                         |    |
| 🗕 View (Re                  | nder View)              |    |
| Axes Grid                   | Edit                    |    |
| Center Axes                 | Visibility              |    |
| <b>Orientation</b> A        | xes                     |    |
| ✓ Orientation               | Axes Visibility         |    |

9) Выбрать контуры

| <u>F</u> ile <u>I</u> | Edit <u>\</u> | /iew     | <u>S</u> o | urces      | Fi <u>l</u> t€ | ers | E <u>x</u> trac | tors   | <u>T</u> ools | <u>C</u> a | talyst | <u>M</u> ac | ros |
|-----------------------|---------------|----------|------------|------------|----------------|-----|-----------------|--------|---------------|------------|--------|-------------|-----|
|                       | r 🔁           | <u> </u> | <b>,</b>   | 1          | Ŵ              | Ŵ   | 0               | 5      | a             | P          |        | <b>?</b>    |     |
|                       |               | 2        | ₽<br>T     | <b>₽</b> ₽ | ⇔<br>++t       |     | So              | lid Co | lor           |            |        |             |     |
|                       |               |          |            |            | Ø              | ٩   |                 |        |               | 0          | Į      |             | 1   |

10) Нажать Арріу

11) Выбрать данные для Contour и Coloring, нажать Apply и потом Rescale to data range(на картинке)

| Properties    | Information            |           |               |          |                       |
|---------------|------------------------|-----------|---------------|----------|-----------------------|
| Properties    |                        |           |               |          | ð×                    |
| 🔗 Apply       | 🖉 🥝 Res                | set       | 🗱 Delete      |          | ?                     |
| Search (u     | se Esc to clear t      | text)     |               |          | -                     |
| - Proper      | ties (Contour:         | 1)        |               |          | C E -                 |
| Contour By    | Electron de            | nsity fro | m Total SCF D | ensity   | •                     |
| ✔ Compute     | Normals                |           |               |          |                       |
| Compute       | Gradients              |           |               |          |                       |
| ✔ Generate    | Triangles              |           |               |          |                       |
| Isosurfaces   |                        |           |               |          |                       |
| Value Rang    | <b>e:</b> [1.72287e-10 | 0, 2.174  | 93]           |          |                       |
| <b>1</b> 0.01 |                        |           |               | +        | ]                     |
| 0.0           | 01                     |           |               |          | )<br>)<br><b>X. C</b> |
| 💻 Display     | / (GeometryRe          | eprese    | ntation)      |          |                       |
| Representati  | on Surface             |           |               |          | •                     |
| Coloring      |                        |           |               |          |                       |
| Electros      | tatic potential f      | rom Tot   | al SCF Den 🔻  |          | -                     |
|               | 🎴 Edit                 |           |               |          |                       |
| Styling       |                        |           | Rescale to    | data rar | ige                   |
| Opacity       |                        |           | 1             |          |                       |
| Lighting      |                        |           |               |          |                       |
| Specular      | 0                      |           | 0             |          |                       |
|               |                        |           |               |          |                       |

12) Итог:



Доп картинки



## КАК СОХРАНИТЬ ПОЛУЧЕННЫЕ ДАННЫЕ

## ВАРИАНТ 1

1) Оставить видимым и выбрать что нужно



### 2) Нажать Save Data

|              | *            |              |                 |         |                     |               |                  |                |              |                  |   |     |
|--------------|--------------|--------------|-----------------|---------|---------------------|---------------|------------------|----------------|--------------|------------------|---|-----|
| <u>F</u> ile | <u>E</u> dit | <u>V</u> iew | <u>S</u> ources | Filters | E <u>x</u> tractors | <u>T</u> ools | <u>C</u> atalyst | <u>M</u> acros | <u>H</u> elp |                  |   |     |
|              |              |              | <b>,</b>        | r i     | 0 🔊                 | a             | e 🗐              | 🥐 🛛            |              | $\triangleright$ |   | Ľ\$ |
|              |              | <b>2</b>     |                 |         | Electro             | static p      | otential fro     | om Total S     | CF Dens      | ity 👻            |   | ~   |
|              |              |              |                 | 1       | ) 🗊 ⊿               | 0             |                  | F              | ©@<br>+***** | -                | * | {   |

#### 3) Выбрать тип и название

| File name:     | DATA                        | Navigate | ОК     |
|----------------|-----------------------------|----------|--------|
| Files of type: | ParaView Data Files(*.pvd ) | *        | Cancel |

## 4) Выбрать массивы для сохранения и Ascii если нужен текстовый а не бинарный формат

| III ×   | Configure Writer (XMLPVDWriter) $? \lor \land \times$              |  |  |  |  |  |  |  |  |
|---|--|--|--|--|--|--|--|--|--|
| ✓ Choose Arrays To Write  |  |  |  |  |  |  |  |  |  |
| <ul> <li>Array Selection</li> <li>Electron de</li> <li>Electrostati</li> <li>Normals</li> </ul> | nsity from Total SCF Density<br>c potential from Total SCF Density |  |  |  |  |  |  |  |  |
| Ghost Level   | 0  |  |  |  |  |  |  |  |  |
| Data Mode   | Ascii  |  |  |  |  |  |  |  |  |
| Encode Appende  | d Data   |  |  |  |  |  |  |  |  |
| Compressor Type   | None (fastest write)   |  |  |  |  |  |  |  |  |
| Compression Level   | 6  |  |  |  |  |  |  |  |  |
| Write Time Step   | 5  |  |  |  |  |  |  |  |  |
|   |  |  |  |  |  |  |  |  |  |
|   | <u>⊘</u> cancel <u>√</u> <u>O</u> K                                |  |  |  |  |  |  |  |  |

## 5) Нажать ОК

Появится файл и папка с данными

## ВАРИАНТ 2

L

Добавить фильтр (Ctrl + Space) <u>Convert to Point Cloud</u> и можно будет сохранить как csv

| File name:     | Navigate   | ОК     |
|----------------|--|--------|
| Files of type: | Comma or Tab Delimited Files(*.csv *.tsv *.tsv ) | Cancel |

Но минус в том, что потом сложно прочитать