Materials in FLUKA

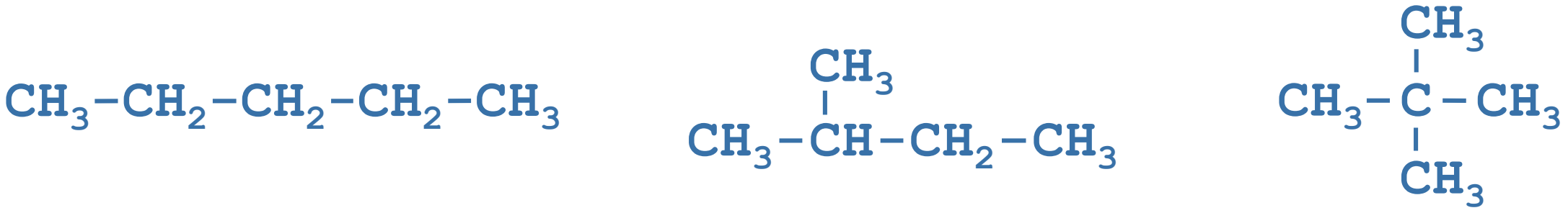
How to define and use (complex) materials in your calculations

Lecture overview

- Introduction
- Pre-defined materials
- Declaring & assigning materials
- Compound materials
- Flair material database
- Special cards

Introduction

- FLUKA assumes that radiation propagates through homogeneous media
  - E.g., within a volume occupied by CO_2, the probability of encountering an O atom is the same at any location within the volume (and double that of encountering a C atom)
  - **Exception:** crystals! (particle propagation depends on the direction with respect to the lattice)
- Therefore, only the stoichiometry and the density matter, as they define the atom density per unit volume for each atomic species (C and O in the above example)
- **Example:** as long as the density is the same, chemical isomers are identical for FLUKA, despite their different molecular structure and other physical properties
  - Pentane, 2-methylbutane, 2,2-dimethylpropane: $\mathbf{C_5H_{12}}$
  - $\rho \approx 6.2$ g/cm^3, but different structure, boiling points etc.



Pre-defined materials

- A number of common materials (23 elements and 12 compounds) are pre-defined and can be assigned to a region without the corresponding material declaration
  - Hydrogen, carbon, oxygen, iron, lead, argon etc. – natural isotopic composition
  - Water, dry air, polyethylene, various biological tissues (bone, muscle etc.)
  - Full lists available in the manual (section 5.2)
- 2 special materials are also included:
  - **`VACUUM:`** obvious definition. Static electrical fields can be defined only in vacuum.
  - **`BLCKHOLE:`** ideal absorber, must be assigned to the “black body” region surrounding your geometry (see Geometry lecture), but can also be used elsewhere in the geometry, e.g., for perfect shielding/collimation, to reduce CPU-time by killing tracking in certain regions etc. – Beware of potential consequences!
- Users may modify the pre-defined materials (except for **`BLCKHOLE`** and **`VACUUM`**)
  - **Note:** Using the name of a predefined material for a user-defined material will override the FLUKA definition.

Declaring materials

- A non-predefined (single element) material is declared with a **`MATERIAL`** card

- Each material must have a different name/identifier (8 character limit!)
  - **Note:** this is the case even when e.g. defining different isotopes of an element as materials, such as **`Boron-10`** and **`Boron-11`** (as opposed to natural boron)

- **Note:** The choice of material name is important for **low-energy neutron group-wise transport**: a **`LOW-MAT`** card may be required to assign correct neutron cross-sections to the material. Conversely, using the FLUKA name will automatically call the corresponding cross-sections (if they exist).

Assigning materials

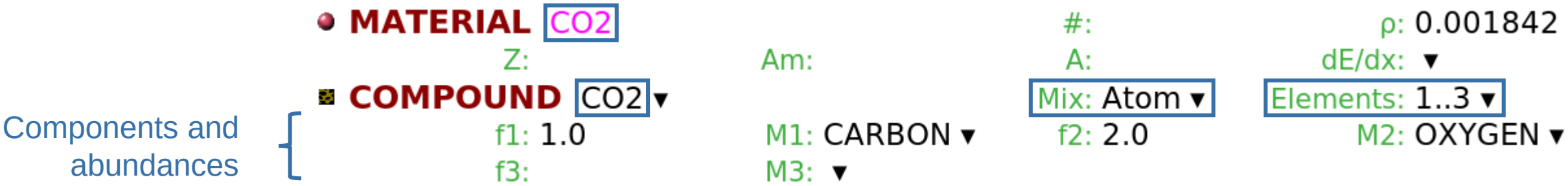
- The **ASSIGNMA** (material assignment) card assigns a material to one or more regions
  - Region: an enclosed finite volume in our geometry
  - Example: here material **COPPER** is assigned to region **TARGET**
  - **Note:** the assignment can be made to more than one region with the **Reg** / **to Reg** / **Step** options

- It can also activate the magnetic or electric field (the latter only in vacuum) in the same region(s)
  - To be used in conjunction with a magnetic/electric field definition (see relevant lecture)
  - **Note:** Only one of the two types of field may be defined in a given (vacuum) region

- **Note:** a declared material does not have to be assigned to any region (but it will not be initialised), or it may be assigned only under certain conditions (see lecture on preprocessor commands)

Compound materials

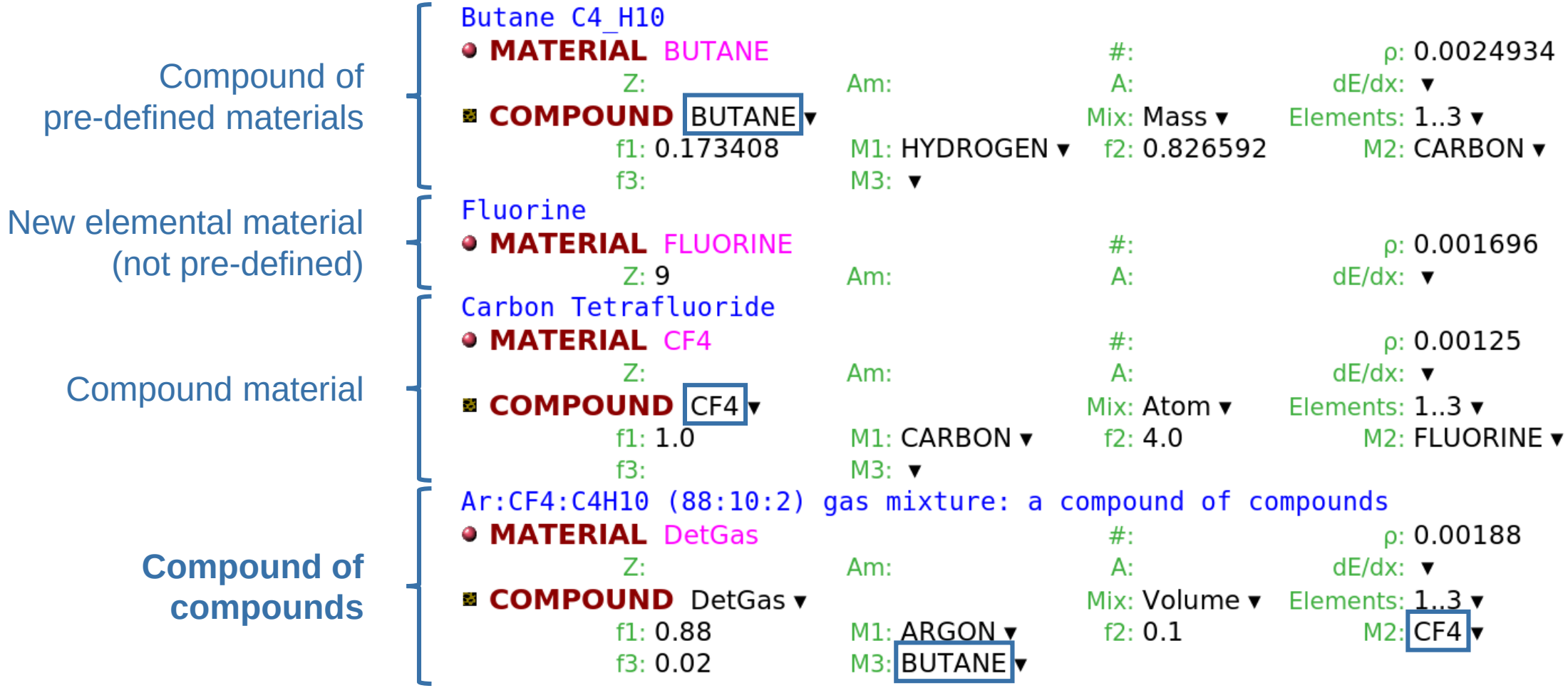
- Composite materials can be defined via the **COMPOUND** card
- Each **COMPOUND** card must be associated to a **MATERIAL** declaration through a matching name/identifier



- The number of components can be increased via the Elements option
- The abundances can be expressed in terms of:
  - Atom content (as in the above example)
  - Mass fractions
  - Volume fractions
- **Note 1:** Mass and volume fractions do not need to add up exactly to 1 (or 100), they are automatically scaled
- **Note 2:** The density of the components is not relevant in a compound and may even be unknown

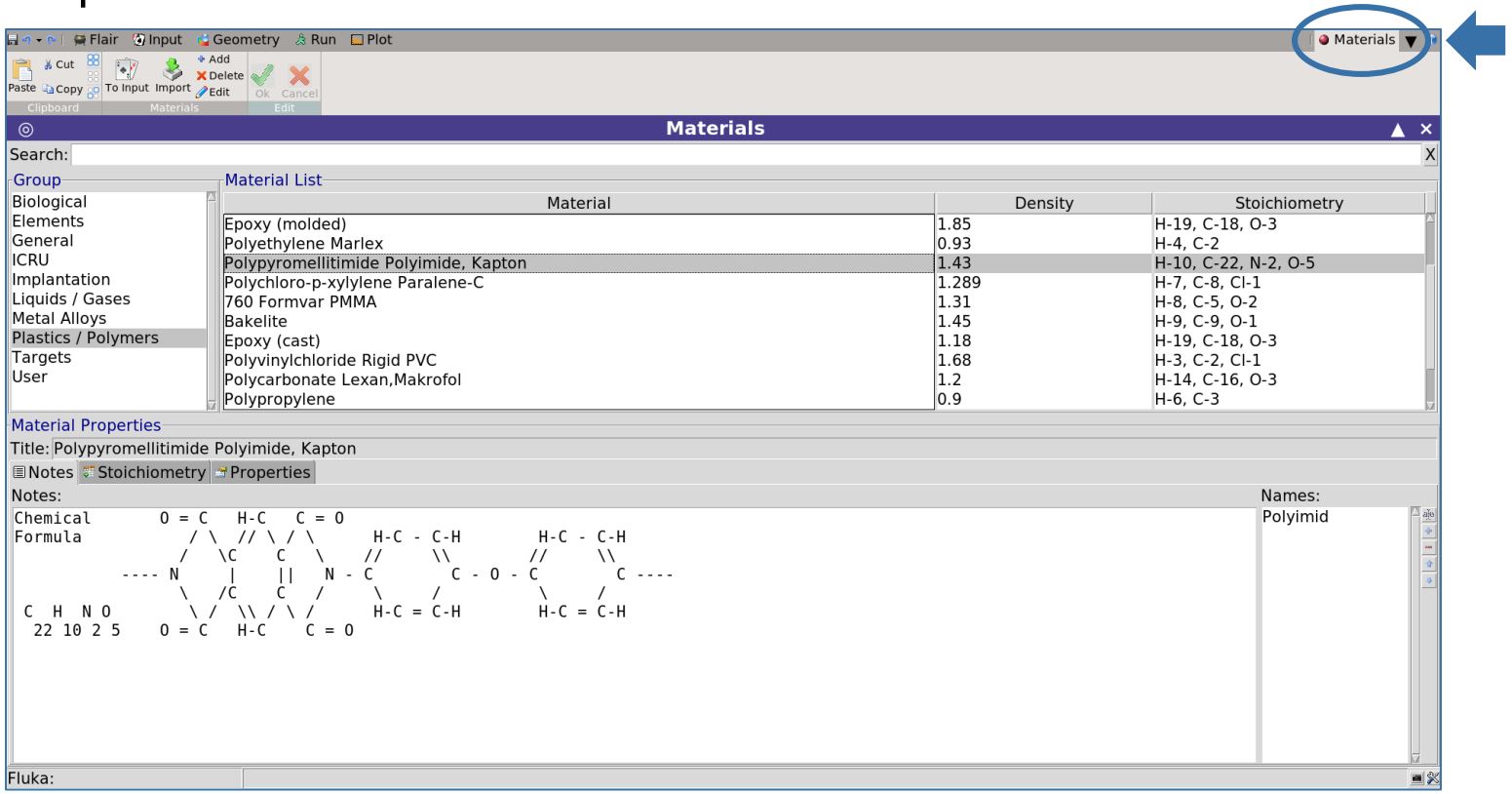
Compound of compounds: an example

- Compound materials can be used as components of other compound materials:



The material database

- Flair comes with an extensive library of ~500 predefined materials (elemental and compounds) that can be imported into the input



- **Caution:** verify material properties before importing
  - E.g. multiple (similar) versions of the material with different properties may exist
- The database can be edited and populated with user-defined materials/compounds

Special material cards (less frequently required)

- The **`MAT-PROP`** card
  - Modification of density and average ionisation potential, setting threshold for DPAs (Displacements Per Atom), request call to **`usrmed.f`** routine when particles are transported in specific material

- The **`CORRFACT`** card
  - Modification of material density for energy loss calculation purposes and nuclear processes on a region-by-region basis
  - Relevant for voxel geometries obtained from CT scans

- The **`STERNHE`** card
  - Allows to modify the recommended Sternheimer density effect parameters used for the stopping power calculations (Sternheimer *et al.*, DOI: 10.1016/0092-640X(84)90002-0) for a material

Summary

- An introduction to materials in FLUKA, including declaration and definition of (compound) materials, the FLUKA pre-defined materials and the Flair material database

- Essential cards to remember:
  - **`MATERIAL:`** material declaration
  - **`ASSIGNMA:`** material assignment to region(s)
  - **`COMPOUND:`** definition of compound material

- Special cards (used more rarely)
  - **`MAT-PROP, CORRFACT, STERNHEI`**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