Computational Gastronomy : API Creation and Management

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Abstract

*The project addresses the challenge of retrieving specific data from **FlavorDB2**, a vast database of over **25,000** flavor molecules and **900+** food categories. Researchers in computational gastronomy and food science often face difficulties performing dynamic and multidimensional searches due to the lack of efficient tools. This project aimed to develop robust search APIs that enhance accessibility and usability by enabling precise queries based on molecular identifiers, regulatory statuses, food categories, and synthesis methods. The work bridges the gap between raw data and actionable insights, making FlavorDB2 a more powerful resource for researchers.*

Methodology

Data Migration: *Transformed raw CSV datasets into a structured MongoDB database with optimized schemas.*

API Development: *Designed RESTful APIs using the Spring Boot framework to support complex query functionalities.*

Performance Optimization: *Applied indexing, aggregation frameworks, and pagination to ensure scalability and efficiency.*

Testing and Validation: *Used tools like Postman for functional testing and JMeter for performance evaluation under varying loads.*

Class Relations

Design

The project architecture follows a layered **MVC (Model-View-Controller)** pattern to ensure modularity, scalability, and maintainability

Architectural WorkFlow

- **Controller:** *Handles user requests and input validation.*
- **Service:** *Implements business logic and interacts with the repository.*
- **Repository:** *Manages database queries with MongoDB's native query language.*
- **Database:** *Stores data in logically structured collections with indexed fields for efficient retrieval.*

Fig.1 : Workflow
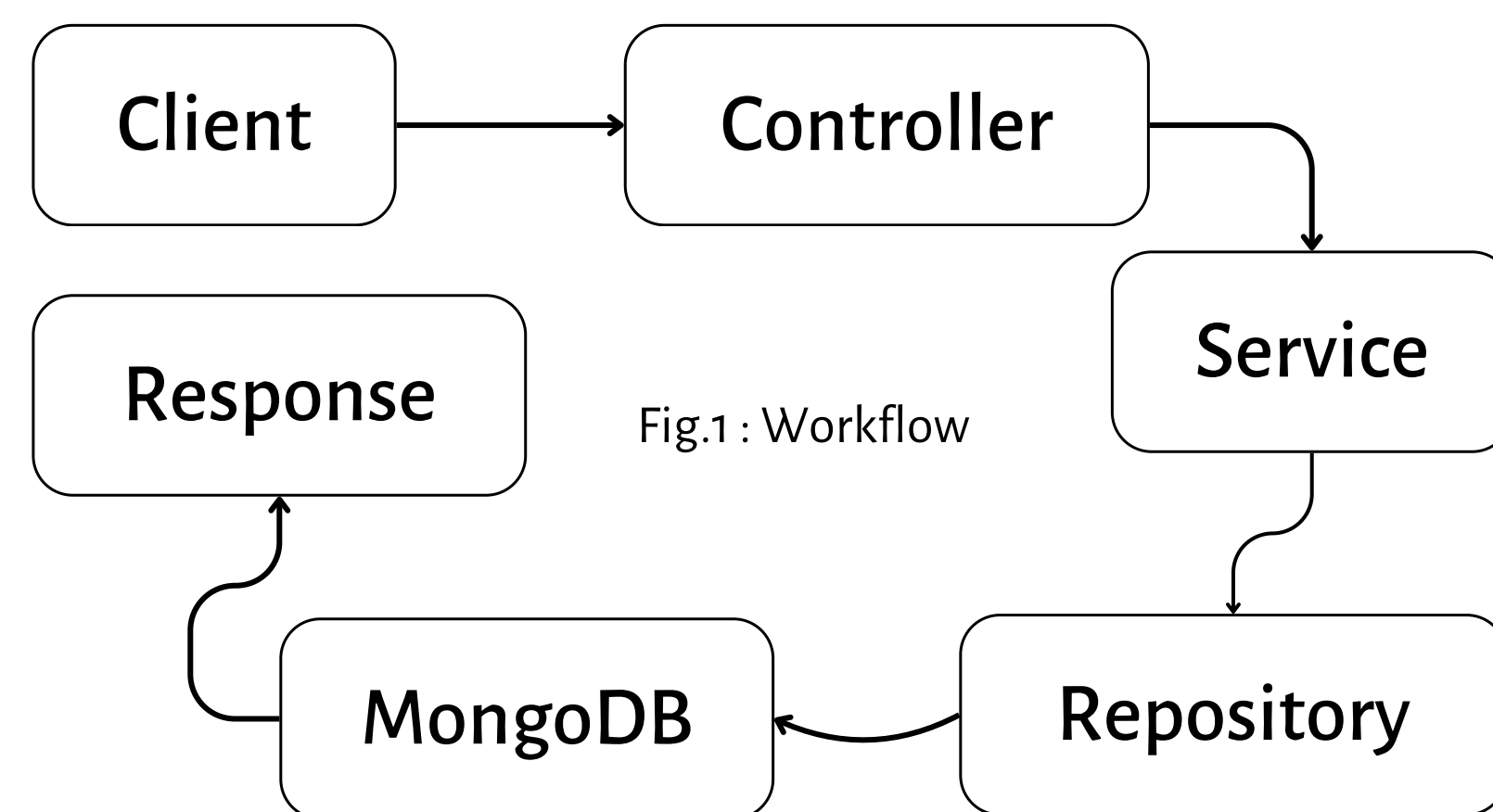
Technology Stack

- **Backend:** *Java, Spring Boot.*
- **Database:** *MongoDB.*
- **Tools:** *Postman for testing and MongoDB Compass for schema visualization.*

Results

- **Sample Endpoint**

  http://localhost:8080/api/more_properties/by-aromaticRings?aromatic_rings=10

```
[
    {
        "id": "66e95076444d020dbaca8ee8",
        "pubchemId": 14969,
        "numberOfAtoms": 101,
        "molecularFormula": "C66H75Cl2N9O24",
        .....
        "numberOfAromaticBonds": 30,
        "numberOfAromaticRings": 10,
        "hbaCount": 14,
        "hbdCount": 18,
        "numberOfHAcceptor": 26,
        "numberOfHAcceptorLipinski": 33,
        "numberOfHDonor": 19,
        "numberOfHDonorLipinski": 21,
        "numberOfHBonds": 0,
        "numRings": 10,
        "numRotatableBonds": 13,
    }
]
```

- **Sample Endpoint (Advanced Query)**

  http://localhost:8080/api/properties/taste-threshold?values=spicy@creamy

```
[
    {
        "id": "66ebe2a43c6a59d5ee5ccf28",
        "name": "4-HYDROXY-3-METHOXYBENZOIC ACID",
        ...
        ...
        "tasteThreshold": "Taste characteristics at 100 ppm; weak sweet resinous vanilla, creamy with a smooth sweetness and body, slightly chocolate-like with a spicy vanitrop nuance ",
        "synthesis": "Prepared by bioconversion of ferulic acid by means of a vanillate-negative mutant of Pseudomonas fluorescens strain BS13. Also prepared by whole-cell bioconversion of vanillin to vanillic acid by Streptomyces viridosporus",
        "food_category": "[['Alcoholic beverages', '5.00', '25.00'], ['Frozen dairy', '5.00', '25.00'], ['Confectionary frostings', '5.00', '25.00'], ['Milk products', '3.00', '15.00']]" ,
        {
            ....
        }
    }
]
```

System Features

- **Comprehensive Search:**
  1. Query by molecular identifiers (e.g., CAS number, IUPAC name).
  2. Filter by food categories (e.g., fruits, spices) and synthesis methods.
  3. Search based on regulatory statuses from FDA and IOFI.

- **Advanced Query Capabilities:**
  1. Logical operators (AND, OR).
  2. Range-based filtering for precise results.
  3. Multidimensional queries combining multiple criteria.

- **Enhanced User Experience:**
  1. Quick, accurate responses in lightweight JSON format.
  2. Scalable design for handling large datasets.

Future Work

- *Expand functionality by Developing API's for the RecipeDB dataset, which encompasses recipes, processes, and ingredient details.*
- *Rigorous testing of all APIs to identify and resolve edge cases, ensuring a robust and error-free system.*

References

1. Garg, N., Sethupathy, A., Tuwani, R., Rakhi, N. K., Dokania, S., Iyer, A., Gupta, A., et al. (2018). FlavorDB: A Database of Flavor Molecules. Nucleic Acids Research, 46(D1), D1210–D1216. . [https://doi.org/10.1093/nar/gkx957]
2. Grover, N., Goel, M., Batra, D., Garg, N., Tuwani, R., Sethupathy, A., & Bagler, G. (2022). FlavorDB2: An Updated Database of Flavor Molecules. Computational Gastronomy Repository. . [https://cosylab.iiitd.edu.in/flavordb2/]
3. MongoDB Documentation [https://www.mongodb.com/docs/]
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