A Formal Theory of Granularity

Toward enhancing life science information systems with granularity

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Outline



2 The TOG

- Architecture for a granulated information system
- Types of granularity
- Overview of the TOG
- Granular querying and toward implementation

- Answers
- Summary

Background

- Information overload, (non-)interoperability of software tools [Keet05a]
 - Need for vertical integration for linking databases and ontologies. e.g. the "virtual human", metagenomics, health-GIS, pharmacoinformatics [Keet&Roos&Marshall07]
 - User should be able to select section(s) of interest and retrieve just that
- Too many one-off bioinformatics tools
 - Need for new foundational methodologies to push implementations to the next phase of *in silico* biology and biomedicine

Granularity

- How to (computationally) manage coarser- and finer-grained (less/more detailed) data, information, and knowledge?
- Granular computing at present
 - distinction "structured thinking" & "structured problem solving" pres; a.o. fuzzy logic, (rough) mereology, data mining, rough sets
 - quantitative & a bit (mostly informal) qualitative
- KR: set-theoretic or mereology
- Subject domains: mainly GIS, biology & biomedicine, spatial, temporal
- Theories & languages, a.o.: TGP [ВS03], GMD [FK03] and MultiDimER [MZ06], MADS [PSZ06]

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Problems with granularity

- **Engineering**: are not reusable in the current format beyond the difficult to scale-up software application each one is designed for that are not-interoperable.
- **Informal**: are not usable or reusable for computation and reasoning, are ontologically inconsistent, and underspecified.
- Formal: are more or less compatible partial data-centric theories that neither address what granularity is nor what its components are nor how to use it.

Research question and Aims

- The main **research question**: *Why, how, and where will* usage of granularity improve knowledge representation and knowledge management?
- The **aims**:
 - Develop a formal, domain- and implementation- independent theory of granularity (TOG) that can be used for computational reasoning.
 - This TOG is integrated with data- and knowledge bases and ontologies to enhance data, information and knowledge management, including querying and reasoning across levels of granularity.
 - The TOG will be sufficiently comprehensive to be useful in the subject domain of biology.

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Foundational semantics of granularity



branching points

key requirements

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(a)

Motivation The TOG Conclusions Conclusions Mathematical Architecture for a granulated information system Types of granularity Overview of the TOG Granular querying and toward implementation



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Main characteristics

- Ontologically-motivated, e.g., taxonomy of part-whole relations (Keet06b, Keet&Artale07], characterisation similarity & indistinguishability [Keet07a], DOLCE
- FOL, model theoretic semantics
- 27 definitions, 19 propositions, 19 lemmas, 7 theorems, and 6 corollaries
- Tested with Mace4 model searcher

Architecture for a granulated information system Types of granularity **Overview of the TOG** Granular querying and toward implementation

Graphical rendering of main components



Architecture for a granulated information system Types of granularity **Overview of the TOG** Granular querying and toward implementation

Excerpt (definitions)

DEFINITION 1 (Granular perspective)

 $\forall x \exists !w, y, z, \phi$ such that GP(x) is a concept CN(x), has a definition DF(x, y), relates to its criterion C(z) through the relation RC(x, z), has_granulation type $TG(\phi)$ and is contained in $D^{f}(w)$.

 $\forall x (GP(x) \triangleq \exists w, y, z, \phi (DF(x, y) \land RC(x, z) \land C(z) \land RE(x, w) \land has_granulation(x, \phi)))$

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Excerpt (definitions)

DEFINITION 2 (Granular level)

 $\forall x \exists !v, w, y, z \exists p$ such that GL(x) is a concept CN(x), has a definition DF(x, y), is related to GP(w) with RE(x, w) and uses criterion C(z) with RC(w, z) and has_value(z, v) where the value is in region V(v) for any GL(x) that adheres_to sG, $GL^s(x)$, and z's label for any GL(x) that adheres_to type nG, $GL^n(x)$. Entities residing in $GL^s(x)$ are similar to each other with respect to (the value z of) V(v), entities residing in $GL^n(x)$ are similar to each other with respect to (the label of the universal of) Prop(p) of C(z), and both are φ -indistinguishable with respect to its adjacent coarser-grained level.

$$\forall x (GL(x) \triangleq \exists !v, w, y, z (DF(x, y) \land GP(w) \land RE(x, w) \land C(z) \land RC(w, z) \land R(v) \land has_value(z, v)))$$

Excerpt (constraints)

- Part-whole relations for RE, RL, and GR.
- Why some entity (/type) resides in a level, with similarity, indistinguishability, and equivalence [Keet07a], resulting in:

THEOREM 1 (3.2)

A granular perspective GP must contain at least two granular levels GL: $\forall x (GP(x) \rightarrow \exists^{\geq 2} y (RE^{-}(x, y) \land GL(y)))$

THEOREM 2 (3.1)

The combination of some C(y) with a $TG(\phi)$ determines uniqueness of each GP(x).

more theorems

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Functions

- Querying the TOG components [Keet08a]
 - 19 functions for: level assignment; selection and retrieval of the domain, perspective, and level; retrieval of contents of a level and intersection of contents from different levels; and selection of one or more entities (/types) and subsequent retrieval of the one or more levels it (/they) reside in.
 ⇒ One can define functions to retrieve each component of the TOG.

Motivation The TOG Conclusions Conclusions Motive trees of granularity Overview of the TOG Granular querying and toward implementation

Functions

- Querying the TOG components [Keet08a]
- Abstraction & expansion functions [Keet05b, Keet07b]
 - 3 Main modes of abstraction
 - $\bullet~27$ entity (/type)-focussed abstraction and expansion functions
 - Using, a.o., the granulation relations for abstractions
 - Use of *types of granularity* to achieve correct behaviour of expansions
- Reasoning over role hierarchies with the *RBox compatibility service* [Keet&Artale07]

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Basic experiments and examples

- TOG verified with Mace4 model searcher data; computed proofs with Prover9
- Investigation from FOL to DL, complexity of language required to represent the TOG (at least ExpTime) analysis

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Basic experiments and examples

- Infectious diseases [Keet&Kumar05, Keet06e]
- Other (manual) examples, with, a.o., Second messenger system, OBO Foundry [Keet08a] View
- Querying the GO database and FMA through OQAFMA [Keet06d]

more scenarios

Answers Summary

- Foundational semantics of granularity is disambiguated and structured in a taxonomy of types of granularity [Keet06a];
- The static components of granularity—such as levels, indistinguishability, how finer- and coarser-grained levels and entities relate, and granulation criteria—were subjected to an ontological analysis and formalised in a consistent and satisfiable logical theory (TOG) with model-theoretic semantics;
- An extensible set of domain- and implementationindependent **functions** were defined for both the TOG elements to enable granular querying and reasoning over the theory and for moving between entities residing in different levels through abstractions and expansions. [Keet07b]

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Answers Summary

Future work

- Relation between mereology and granularity (w.r.t. mereogeometry [BM07] and aggregates), rough/fuzzy extensions for level specification, integrating rules for conditional level
- DL languages (DLRx and/or OWL 1.1), granularity-enhanced conceptual data modelling, vertical integration of ontologies or conceptual data models
- Types of granularity as extension to DOLCE
- Address Ontology Comprehension Problem with granularity and abstraction and visualisation of metabolic pathways.
- Ontology linking and cross-granular querying: experiment with the OBO Foundry [Keet08a, Keet&Roos&Marshall07, 3]

Answers Summary

Main Research Question

Why, how, and where will usage of granularity improve knowledge representation and knowledge management?

Answers Summary

Granularity is a novel way of structured knowledge representation that is orthogonal to extant modelling methods. It enables a *structured and consistent way for carving up the subject domain* through granularity type selection and criterion-selection for a particular granular perspective and at different levels of detail so that a user can avoid unnecessary detail or too coarse generalisations, yet have the full domain at one's disposal for reasoning across levels of granularity, and also be deployed for users with different foci. The formal, hence unambiguous, Theory Of Granularity, TOG, can be added to ontologies, knowledge bases, database, and conceptual data models with a formal foundation. That is, the hitherto data-centric solutions for dealing with granularity are lifted to the ontological and logical layers and the informal subject domain and philosophical contributions are precisiated in a formal theory, thereby providing easily reusable modelling constructs for granularity components such as level, perspective, type of granularity, and granulation criterion. These static components are augmented with *clear*, *extensible functions for granular querying* and reasoning that are reusable across implementation scenarios.

Answers Summary

Where

The structured and consistent representation of granularity enabled by the TOG contributes to good modelling methodology and practice, hence, to the overall quality of the data source. The genericity of the TOG can guarantee interoperability between granulated data sources, such as GISs and bio-ontologies, because its FOL representation is implementation- and scenario-independent. Further, it offers an additional method for linking data sources that contain contents at different levels of granularity, and, subsequently, reasoning across those levels of granularity.

Answers Summary

Summary

- General problems (vertical integration, visualisation, foundational methodolgies) and specific for granularity (data-centric, informal or partial formal theories, non-reusable engineering solutions)
- Overview of architecture for a granulated information system
- Main characteristics of the TOG
 - From a data-centric treatment of granularity to the ontological and logical layers
 - Elements of granularity have become ontologically-motivated modelling constructs proper
 - Representation of granularity is now domain- and implementation independent
 - Reusability across implementations is ensured, which in turn facilitates interoperability among information systems
- Toward implementation, with exploration into DLs and bio-experiments

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Answers Summary

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Answers Summary

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Answers Summary

The TOG and OBO Foundry's approach to granulation



Figure: A: [Seta107] B: preliminary manual granulation with the TOG [Keet08a].

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Answers Summary

Example

- The Foundational Model of Anatomy [RM03, 2] with some 70k types and 1.9mln relations (subsumption, parthood, containment hierarchies etc.).
- Built manually with Protégé, reengineered for query optimization in OQAFMA [MBR03]
- Sample queries:
 - What are the cellular components of blood?
 - so Blood resides in another level as the cells it has as parts.
 - Which hormones are located in the kidney, and where in the kidney?
 - The different people tries, structural for bidney with its parts and functional for horizons.

Answers Summary

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Answers Summary

Example

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Answers Summary

Example (cont'd)

- Blood has a list of 13 direct parts. Which ones are cells, which are not? Is it a complete list of cell-parts?
- $\bullet \Rightarrow$ Combine the taxonomy & partonomy in one query.



Answers Summary

Summary of the general requirements for any theory of granularity

- Use with contents at the instance level and in a format for defining a domain granularity framework at the type level;
- The logic-based representation has to permit both set theoretical and mereological granularity;
- Accommodate both the quantitative and qualitative aspects of granularity (or: arbitrary scale and non-scale-dependent granularity);
- There have to be at least two levels within a perspective, else there is no granularity;

Answers Summary

Summary of the general requirements for any theory of granularity

- A higher level simplifies, makes indistinguishable, the finergrained details that are indistinguishable at that higher level;
- The entities (/types) in a granular level have at least one aspect in common, which is a criterion by which to granulate the data, information, or knowledge;

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Foundational semantics of granularity

Table: Distinguishing characteristics at the branching points in the taxonomy of types of granularity.

| Branching point | Distinguishing feature | | | | | |
|-----------------|--|--|--|--|--|--|
| sG – nG | scale – non-scale (or, roughly: quantitative – qualitative) | | | | | |
| sgG - saG | grain size – aggregation (or: scale <i>on</i> entity – scale <i>of</i> entity) | | | | | |
| sgrG – sgpG | resolution – size of the entity | | | | | |
| saoG – samG | overlay aggregated – entities aggregated according to scale | | | | | |
| naG – nrG – nfG | semantic aggregation – one type of relation between entities in different levels – different type of relation between entities in levels and relations among entities in level | | | | | |
| nacG – nasG | parent-child not taxonomic and relative independence of contents of higher/lower level – parent-child with taxonomic inheritance | | | | | |

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Answers Summary

Part-whole relations

- Ground Mereology [Keet06c]
 - with *part_of*, which is reflexive, antisymmetric, and transitive
 - ppart_of, irreflexive, asymmetric, transitive
 - other relations one can define with it, such as *overlap* and *overcross*
- Other non-mereological part-whole relations that can be used to granulate
- Part-whole relations formalised and structured in a taxonomy [Keet06b, Keet&Artale07]

Answers Summary

Part-whole relations



 $\forall x, y (involved_{in}(x, y) \triangleq part_of(x, y) \land PD(x) \land PD(y))$

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Answers Summary

Excerpt (constraints)

THEOREM 3 (3.5)

RL is of the same type, s_ppart_of, not only within some particular instance of *GP*, but it is of the same type between granular levels in all granular perspectives.

THEOREM 4 (3.6)

The multiplicity (cardinality) of RL and RL⁻ is 1:1, i.e. $\forall x \exists ! y(RL(x, y))$ and $\forall x \exists ! y(RL^{-}(x, y))$.

Answers Summary

Excerpt (constraints)

LEMMA 1 (3.19)

Two levels in different perspectives can overcross: $\forall x, y(overcross(x, y) \land GL(x) \land GL(y) \land \neg(x = y) \rightarrow \exists v, w(R_E(x, v) \land R_E(y, w) \land \neg(v = w))).$

THEOREM 5 (3.7)

If two levels in different perspectives overcross, then their perspectives overcross: $\forall x_1, x_2, y_1, y_2(overcross(x_1, x_2) \land GL(x_1) \land GL(x_2) \land GP(y_1) \land$ $GP(y_2) \land R_E(x_1, y_1) \land R_E(x_2, y_2) \rightarrow overcross(y_1, y_2)).$

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Answers Summary

Tested with Mace4 model searcher

- *Known* to be satisfiable if indistinguishability is made a primitive relation, acyclicity hard-coded, no quantification over universals
- With that input, *known* that there are models up to at least domain size 8
- So, is the TOG within the decidable fragment of FOL, and what is the complexity of the language needed to represent it?

Answers Summary

Mace4 model searcher statistics



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"Interesting" constructors used in the TOG

- *RL* is acyclic. Complexity of DL languages: the only DL language that has a constructor for it, \mathcal{DLR}_{μ} [CGL99], is ExpTime like its base language \mathcal{DLR} and sister languages \mathcal{DLR}_{ifd} and \mathcal{DLR}_{reg} [CGL98, CDGLR03].
- *GP* is uniquely identified by the combination of its *C* and *TG*, which means it is, in ER terminology, a weak entity type: **id** constructor of \mathcal{DLR}_{ifd} [CGL01].
- Others: qualified number restrictions (*RE⁻*, *CP*, and *conv*), a ternary relation (*conv*), and transitivity of relations (*RL*, *RE*, and mereological parthood).

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Answers Summary

A comparison

| \Box Language \Rightarrow | OWL | | | DL-Lite | | | DLR | | |
|-----------------------------------|------|----|------|---------------|---------------|-----------------|-----|-------|-----|
| Feature ↓ | Lite | DL | v1.1 | \mathcal{F} | \mathcal{R} | $ \mathcal{A} $ | ifd | μ | reg |
| Role hierarchy | + | + | + | - | + | + | + | + | + |
| N-ary roles (where $n \ge 2$) | - | - | - | ± | ± | ± | + | + | + |
| Role concatenation | - | - | + | - | - | - | - | - | + |
| Role acyclicity | - | - | - | - | - | - | - | + | - |
| Symmetry | + | + | + | - | + | + | - | - | - |
| Role values | - | - | - | - | - | + | - | - | - |
| Qualified number restrictions | - | - | + | - | - | - | + | + | + |
| One-of, enumerated classes | - | + | + | - | - | - | - | - | - |
| Functional dependency | + | + | + | + | - | + | + | - | + |
| Covering constraint over concepts | - | + | + | - | - | - | + | + | + |
| Complement of concepts | - | + | + | + | + | + | + | + | + |
| Complement of roles | - | - | + | + | + | + | + | + | + |
| Concept identification | - | - | - | - | - | - | + | - | - |
| Range typing | - | + | + | - | + | + | + | + | + |
| Reflexivity * | - | - | + | - | - | - | - | + | + |
| Antisymmetry * | - | - | - | - | - | - | - | - | - |
| Transitivity * [‡] | + | + | + | - | - | - | - | + | + |
| Asymmetry ‡ | + | + | + | - | + | + | - | ± | - |
| Irreflexivity [‡] | - | - | + | - | - | - | - | + | - |

Table: Differences between DL-based ontology and conceptual modelling languages (after [Keet&Rodríguez07]).

Answers Summary

What to do with it?

- For its own sake, 'paper exercise' for developing perspectives and levels, stay in FOL and then alike a global view with LAV
- Orthogonally positioned to conceptual data model or integrated in a conceptual data model
- As meta-layer for conceptual data modelling languages or ontology languages
- Advanced querying & reasoning
- ...

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