WINGS/Pegasus: Semantic Metadata Reasoning for Large Scientific Workflows

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"Semantic Metadata Generation for Large Scientific Workflows"
Jihie Kim, Yolanda Gil, and Varun Ratnakar, ISWC 2006.
http://www.isi.edu/ikcap/scec-it/papers/Wings-metadata-ISWC-2006.pdf

"Wings for Pegasus: A Semantic Approach to Creating Very Large Scientific Workflows"
Yolanda Gil, Varun Ratnakar, Ewa Deelman, Marc Spraragen, and Jihie Kim. (Under review.)

Creation of Workflows in Layers of Increasing Detail

1. Workflow Template (generic)
   - Specifies executables and dataflow
   - No data specified, just their type
2. Workflow Instance (user specific)
   - Specifies data files for a given template
   - Logical file names, not physical file replicas
3. Executable Workflow (actual run)
   - Specifies physical locations of data files, hosts/pools for execution of jobs, and data movement jobs

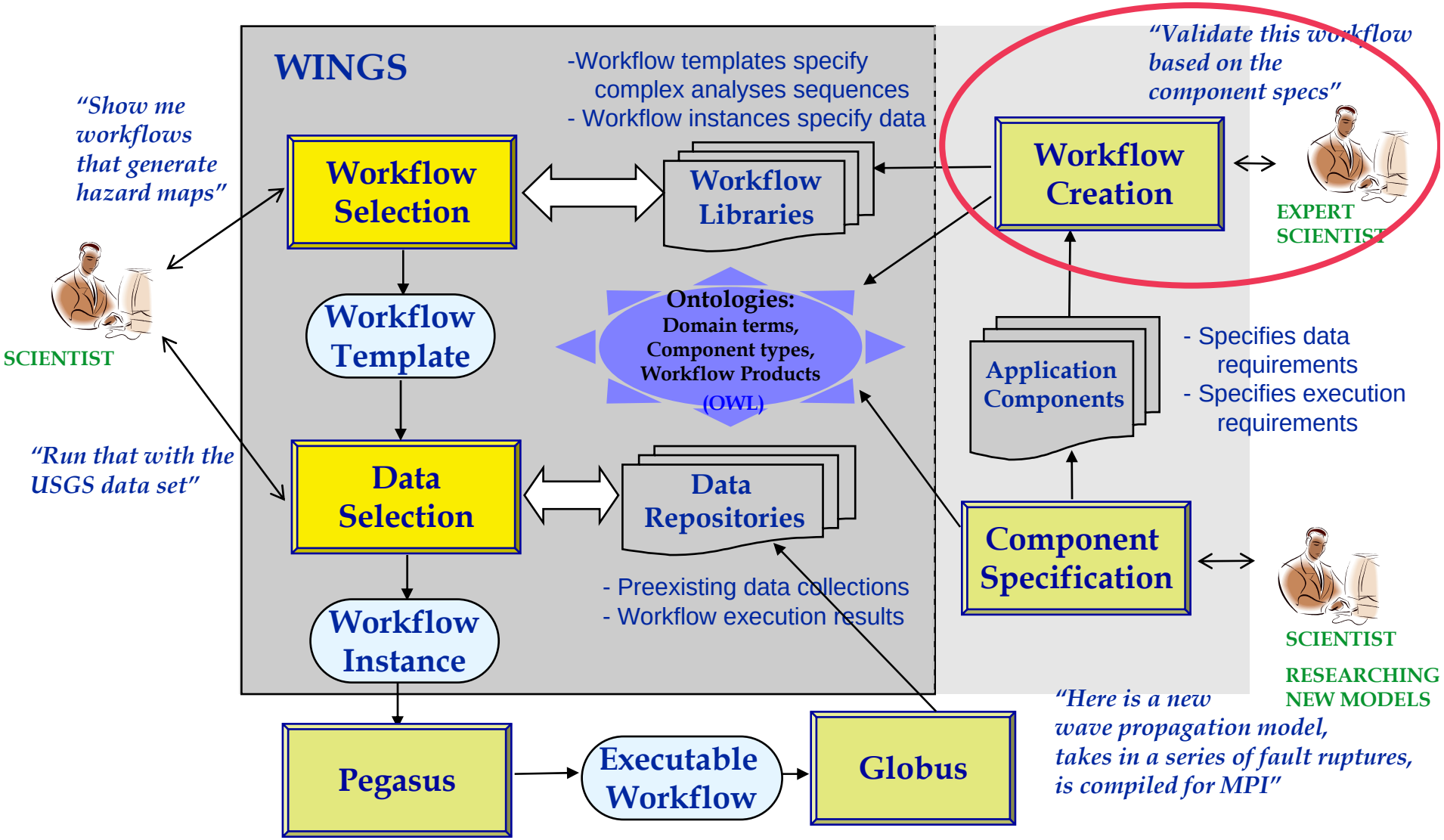
The Process of Creating an Executable Workflow

User guided

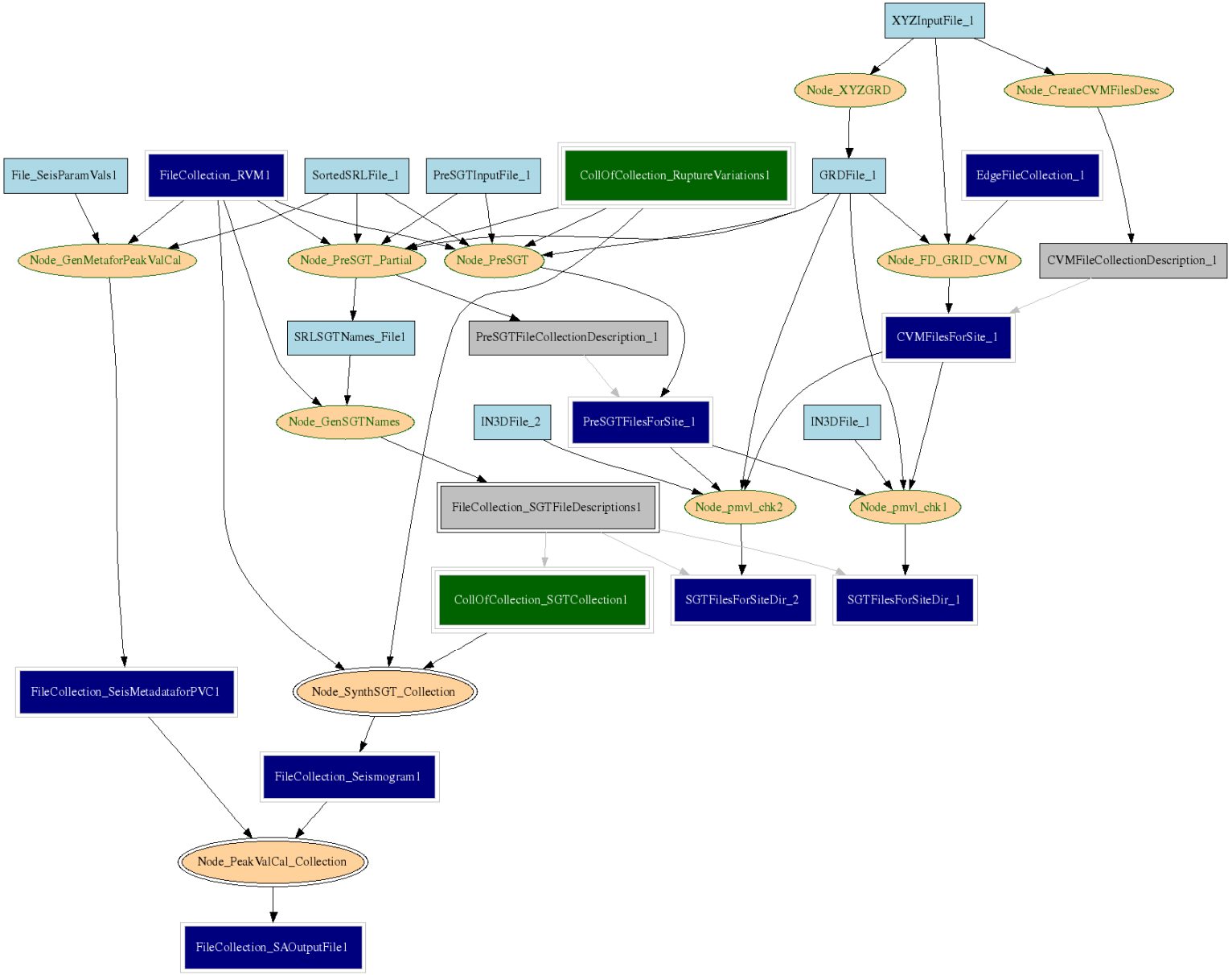
1. Creating a valid workflow template
   - Selecting application components and connecting inputs and outputs to specify data flow
   - Adding other steps for data conversions/transformations
2. Creating instantiated workflow
   - Providing input data to pathway inputs (logical assignments)
3. Creating executable workflow
   - Given requirements of each model, find and assign adequate resources for each model
   - Select physical locations for logical names
   - Include data movement steps, including data deposition steps

Automated

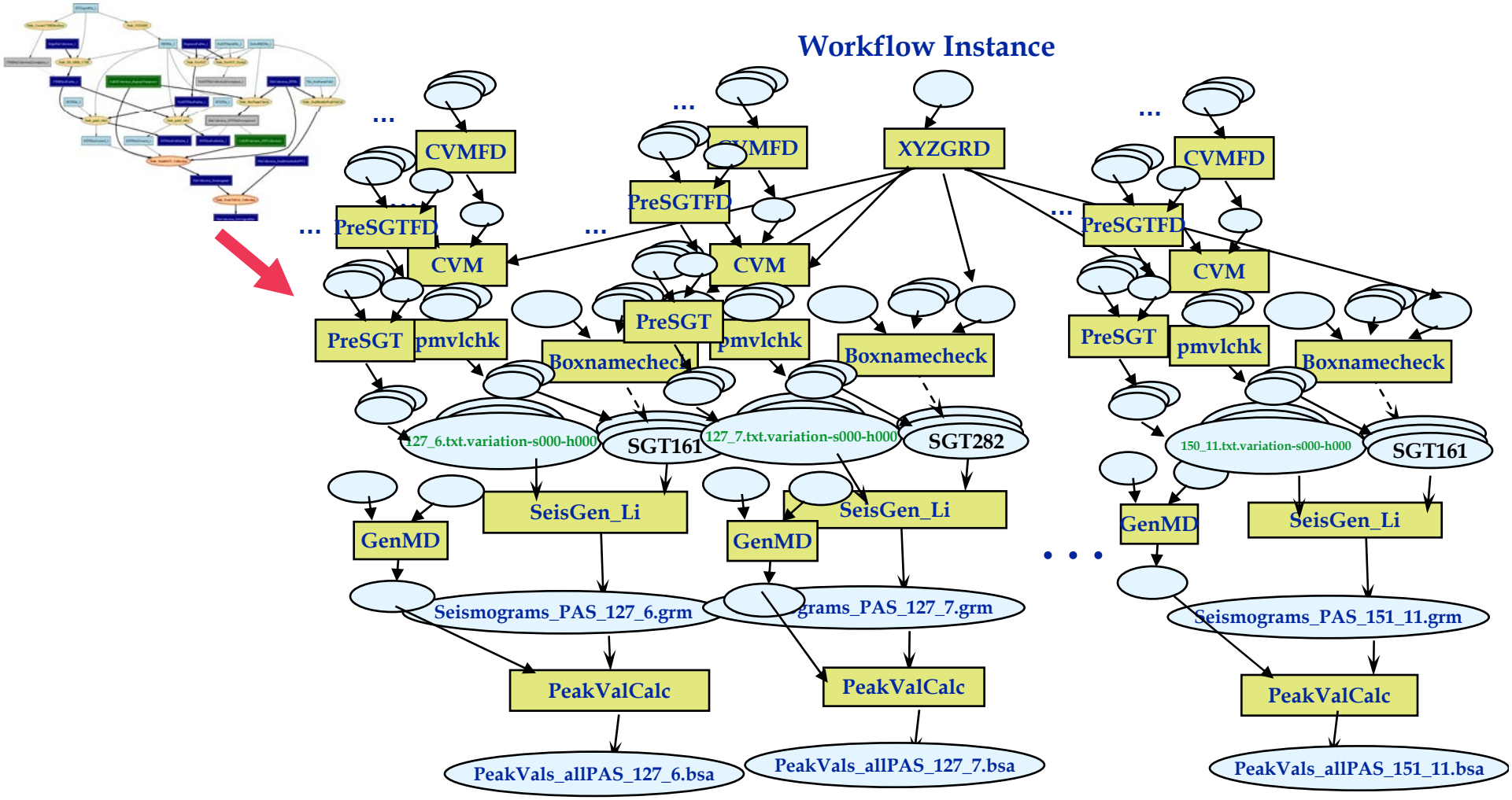
WINGS/Pegasus: Workflow Instance Generation and Selection



An example Workflow Template in Earthquake Science : Seismic Hazard Analysis



Generating Metadata/Provenance *while Creating a Workflow Instance*



~4,000 ruptures,
>100,000 variations for a site,

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Metadata Constraints (in OWL ontology)

- Constraints on Files
  - metadata attributes: data types and default values

  e.g. simulation_out_timesamples of SeisParamValsFile should be an integer and the default value is 1801
- Constraints on collections and collection of collection
  - Type of each element
  - Relations between metadata of a collection and metadata of individual items

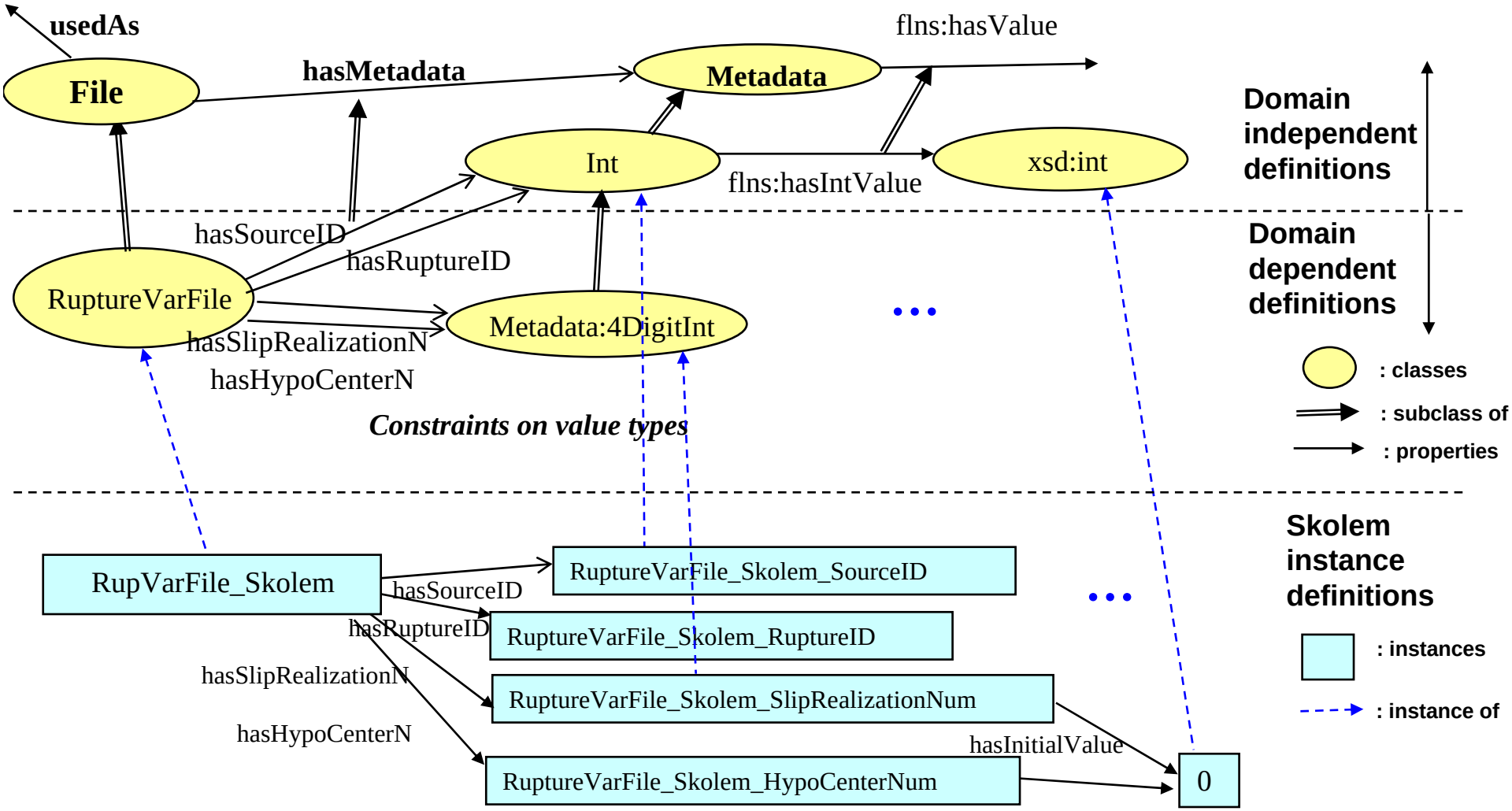
  e.g. Each rupture variation has the same source/rupture ids as the rupture variation collection
- Component level constraints on metadata attributes of input/output files or collections
  - Deriving metadata of output files from metadata of input files

  e.g. The output of PeakValCalc (SA output file) should have the same site name as the seismogram file
- Template level constraints on metadata attributes of files or collections
  - Input/output files of different components can have the same metadata

  e.g. The RVM collection input for SeismogramGen should have the same site name as the CollOfCollection rupture variations input
  - Checking number of items in collections

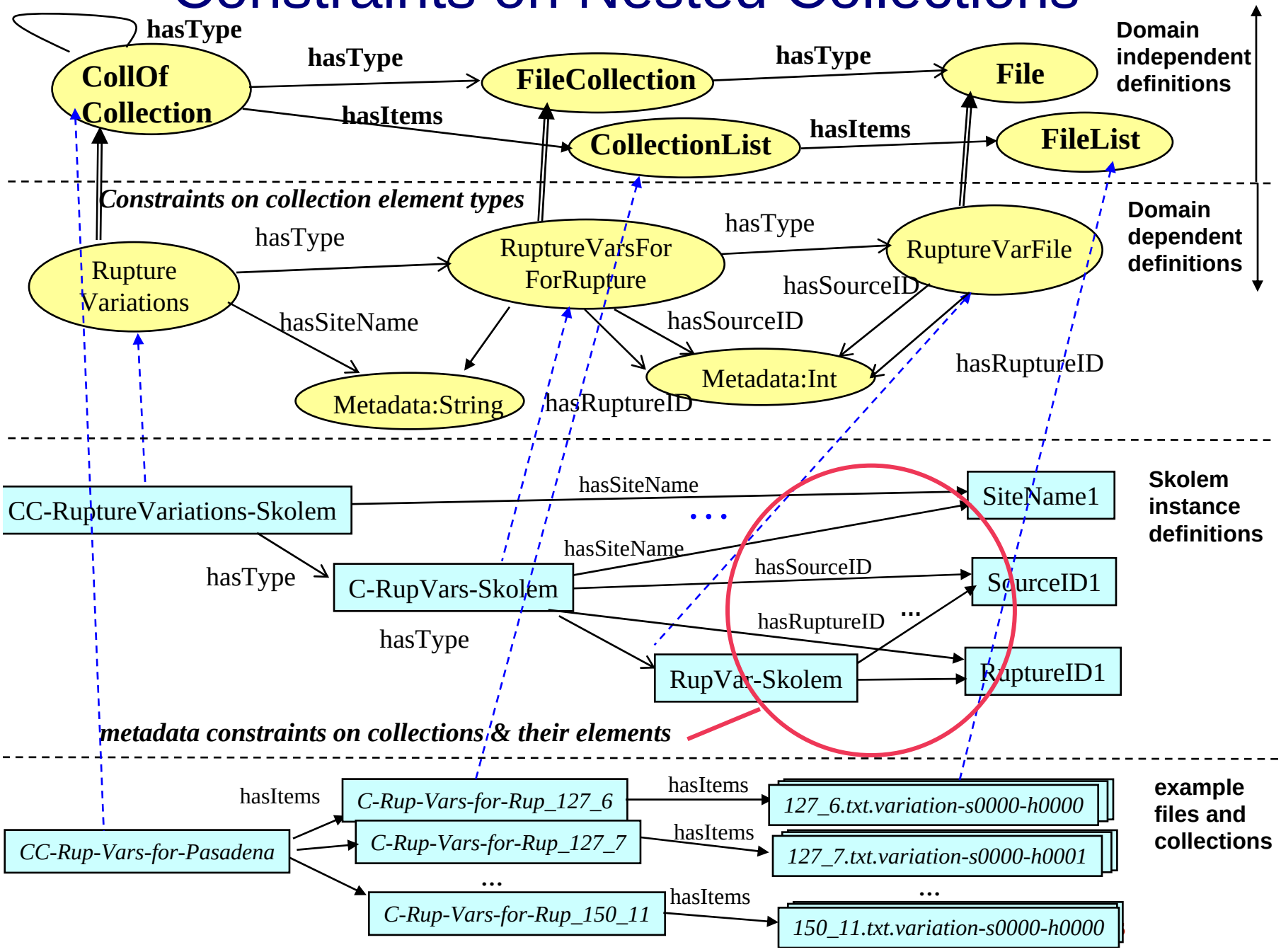
  e.g. number of RVM files and the number of rupture var collections should be equal

Constraints on Files

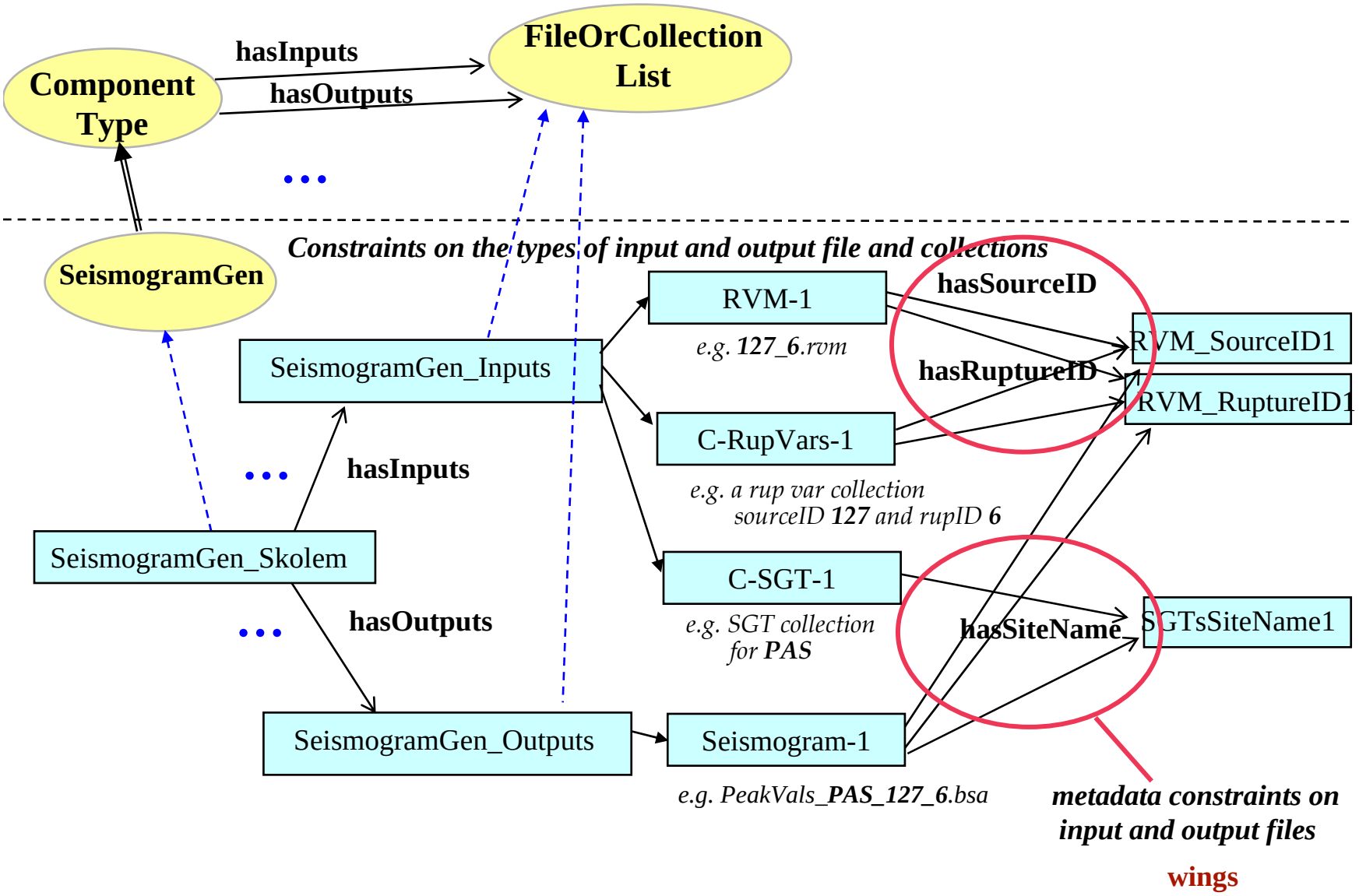


<RuptureVariationFile rdf:ID="RuptureVarFile_Skolem"> <rdf:type rdf:resource="&flns;FileSkolem"/>
<hasRuptureID rdf:resource="#RuptureVarFile_Skolem_RuptureID"/>
<hasSlipRealizationNumber rdf:resource="#RuptureVarFile_Skolem_SlipRealizationNum"/>
…</RuptureVariationFile>
<flns:Int rdf:ID="RuptureVariationFile_Skolem_RuptureID"/>
<FourDigitInt rdf:ID="RuptureVarFile_Skolem_SlipRealizationNum"> <flns:hasInitialValue rdf:datatype="&xsd;int">0</flns:hasInitialValue>
…</FourDigitInt>

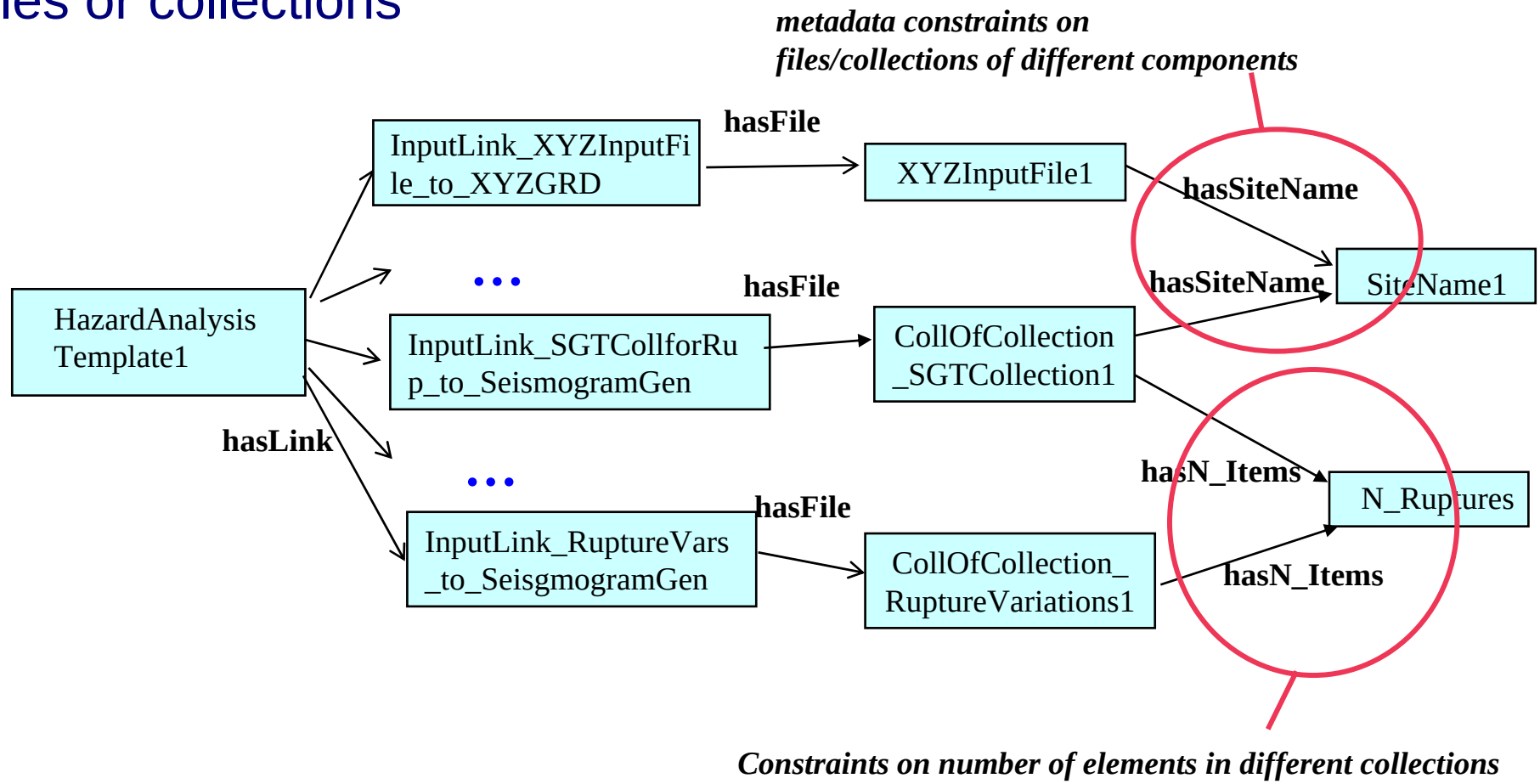
Constraints on Nested Collections



Component level constraints on metadata attributes of input/output files or collections



Template level (global) constraints on metadata attributes of files or collections



<scecflns:XYZInputFile rdf:ID="XYZInputFile_1"> <scecflns:hasSiteName rdf:resource="#**SiteName_1**"/> </scecflns:XYZInputFile>

<scecflns:SGTCollection rdf:ID="CollOfCollection_SGTCollection1"> <scecflns:hasSiteName rdf:resource="#**SiteName_1**"/>
<flns:hasN_items rdf:resource="#**N_Ruptures**"/> <flns:hasCollectionType
rdf:resource="&sceccIns;SynthSGTInput_SGTCollectionforRupture"/> <flns:hasDescriptionFile
rdf:resource="#FileCollection_SGTFileDescriptions1"/> </scecflns:SGTCollection>

<scecflns:RuptureVariations rdf:ID="CollOfCollection_RuptureVariations1"> <scecflns:hasSiteName
rdf:datatype="&xsd;string"></scecflns:hasSiteName> <flns:hasN_items rdf:resource="#**N_Ruptures**"/> <flns:hasCollectionType
rdf:resource="#RuptureVariationsforRupture_1"/> </scecflns:RuptureVariations>

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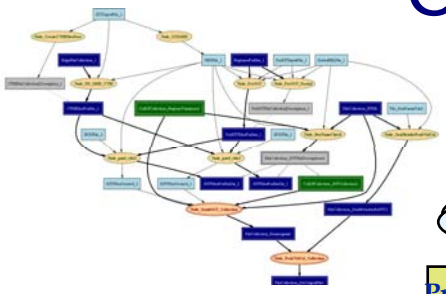
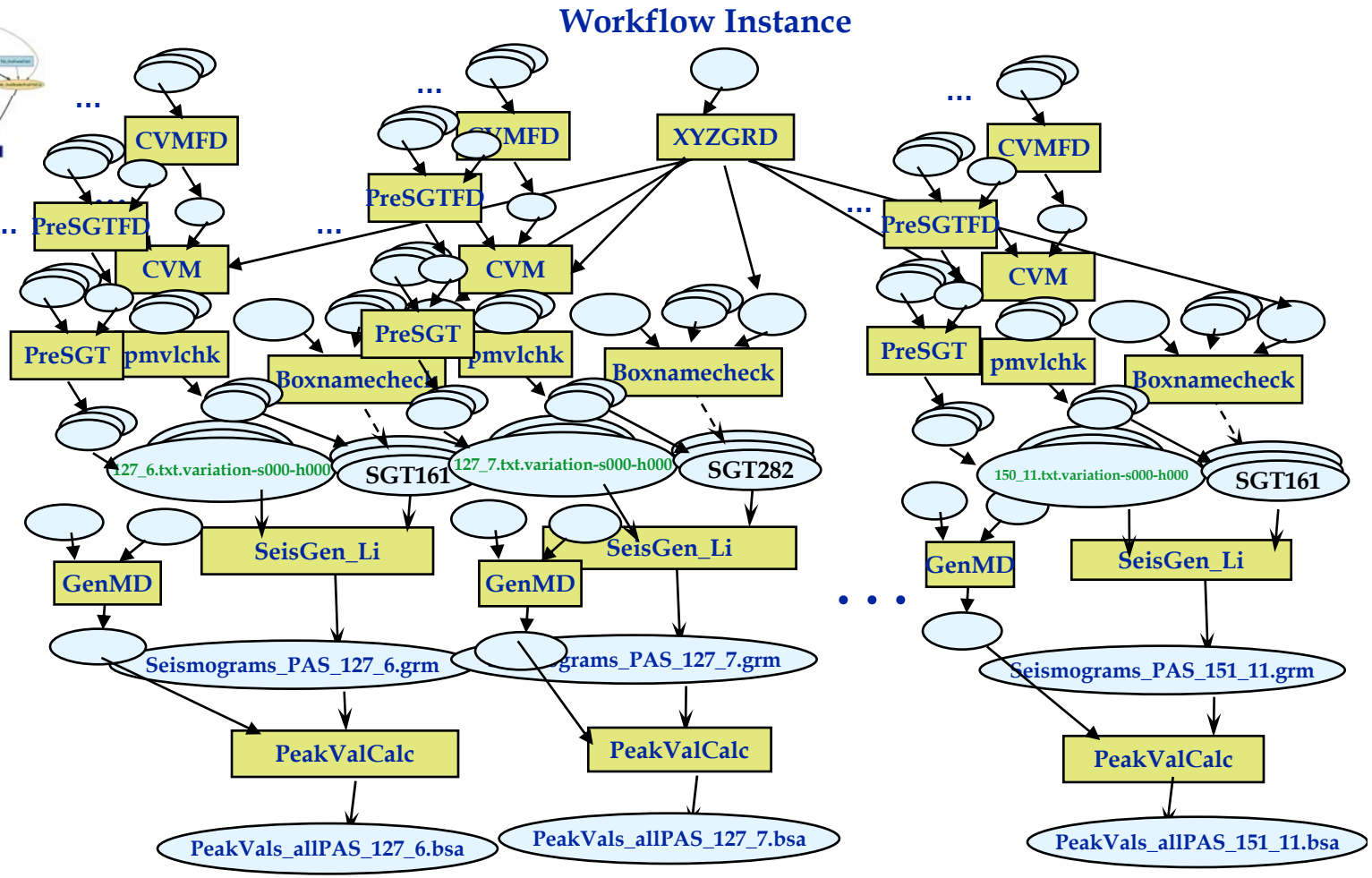
Metadadata/Provenance Generation & Validation

Bind&ValidateWorkflow (WorkflowTemplate wt, InputLinks ILinks)

1. Assign ILinks to LinksToProcess.
2. While LinksToProcess is not empty
   2.2. Remove one from LinksToProcess and assign it to L1.
   2.2. Let F1 be the link skolem for binding files or collections to L1.
   2.3. *If metadata for F1 should be generated from an execution of a component*
      2.3.1. *if the execution results are not available, continue.*
         ;; i.e. exclude this link in the sub-workflow
   2.4. If any metadata of F1 depends on a link L2 that is not bound yet,
      2.4.1. mark L1 as a dependent of L2 and continue.
   2.5. If L1 is an input link,
      2.5.1. get metadata of the file from the user or a file server
      2.5.1. check consistencies with links that L1 depends on ;; **consistency check**
      2.5.2. check consistencies with existing bindings based on template-level constraints
         ;; **consistency check**
      2.5.3. If any metadata are inconsistent, report inconsistency and return.
      2.5.4. Bind file/collection name and metadata to F1.
      2.5.5. If the file type for F1 is a collection, recursively get the metadata of its elements
   2.6. Else (i.e. L1 is InOutLink or OuputLink)
      2.6.1. Generate file names and metadata base on the definition of the depending links.
         ;; **metadata propagation**
   2.7. For each link L2 that is dependent on l1,
      2.7.1. if all the links that L2 is depending on are bound, put L2 in LinksToProcess.
   2.8. If L1 is an output link, continue.
   2.9. Else (L1 is InputLink or InOutLink)
      2.9.1. If all the inputs to the destination node (i.e. the component that L1 provides an input to) have been bound,
         2.9.1.1. Add all the OutputLinks and InOutLinks from the destination node to the LinksToProcess.

Generating Metadata/Provenance while Creating a Large Workflow Instance





	Creation time	Number of files	Number of OWL individuals
Sub workflow	7 mins 59 sec	15,888	322,473
Full workflow	22 mins 52 sec	117,379	**2,001,972**

~4,000 ruptures,
>100,000 variations for a site,

wings

Technical Contributions: Semantic Metadata Approach to Creating Large Scientific Workflows

- Semantic representations of workflow templates to express **repetitive computational structures and collections**
- Expanding template to instances that **orchestrate large amounts of computations** reflecting the workflow template structure
- Generating appropriate **metadata descriptions for all the new data** created during execution and full elaboration of workflow specs
- **Ensuring validity** of workflow instance (Bind&Validate algorithm)
  - Keeping track of constraints on dataset used, including global constraints among multiple components as well as local constraints within individual components.
- Mapping equivalent datasets, detecting pre-existing intermediate data, and **prevent unnecessary execution** of workflow parts when datasets already exist.

http://www.isi.edu/ikcap/scec-it/