Geant4 Simulation of Very Low Energy Electromagnetic Interactions

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The Geant4 Low Energy EM Physics[1/4]

- Models based on Livermore evaluated data libraries
  - Electrons and Photons processes
  - Validity range 250 eV – 100 GeV
  - Elements from Z=1 to Z=100
  - Validated against reference data
- Models originated from the Penelope Monte Carlo Code
  - Electrons and Photons processes
  - Validity down to ~ 100 eV
  - Validated against reference data
- Models for ions and hadrons
  - Composition of models, including ICRU and Ziegler parametrisations
  - Validity down to ~ 1 keV

The Geant4 Low Energy EM Physics 2/4

- Photons processes based on Livermore data
  - Compton scattering (polarised and unpolarised)
    - Klein-Nishina formula + corrections based on EPDL97 (Evaluated photons data library)
    - Angular distribution based on EPDL97
  - Rayleigh scattering (polarised and unpolarised)
    - As Compton scattering
  - Photoelectric effect
    - Total cross-section and shell selection according to EPDL
    - Deexcitation via the atomic relaxation
  - Gamma conversion
    - Bethe-Heitler cross-sections + Coulomb corrections
    - Angular distribution according Tsai differential cross-section

The Geant4 Low Energy EM Physics 3/4

- Electrons processes based on Livermore data
  - Bremsstrahlung
    - Total cross section based on EEDL (Evaluated electrons data librabry)
    - Angular distribution can be chosen from three models
      - Modified Tsai, 2BS, 2BN
  - Electron ionisation
    - Parametrisation based on 5 parameters for each shell
- Auger effect
  - Based on Livermore libraries
- PIXE
  - Data driven model based on Paul et Sacher evaluated data library
- Atomic relaxation processes based on Livermore data
  - Based on EADL (Evaluated atomic data library)
    - From Z>5

The Geant4 Low Energy EM Physics 4/4

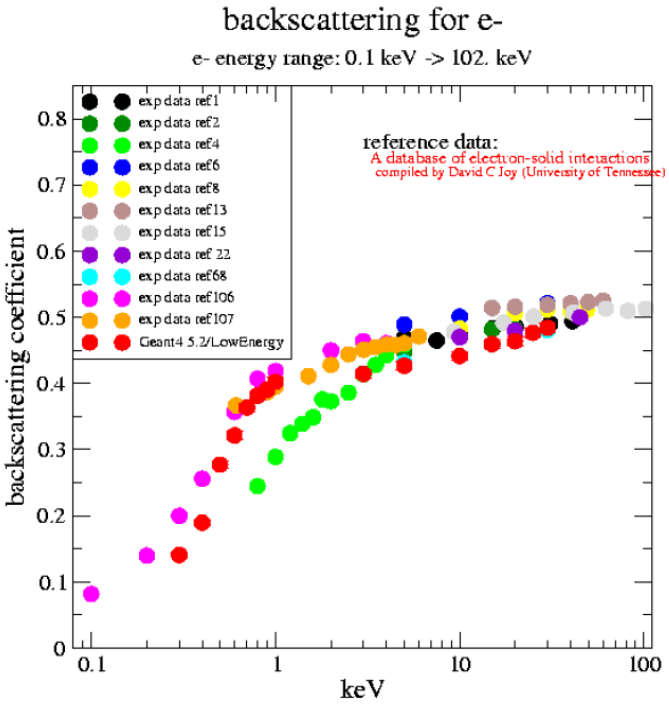
- Penelope Monte Carlo code re-engineered into Geant4
  - Except for multiple scattering
  - Models for protons and electrons
- Validation
  - See Wednesday M. G. Pia talk
  - All Geant4 physics models for electrons, photons, protons and alpha particles has been validated against NIST database
    - Photoelectric, Compton, Rayleigh, pair production cross-sections
    - Photon attenuation coefficients
    - Electron, proton, α stopping power and range
  - Rigorous and quantitative approach

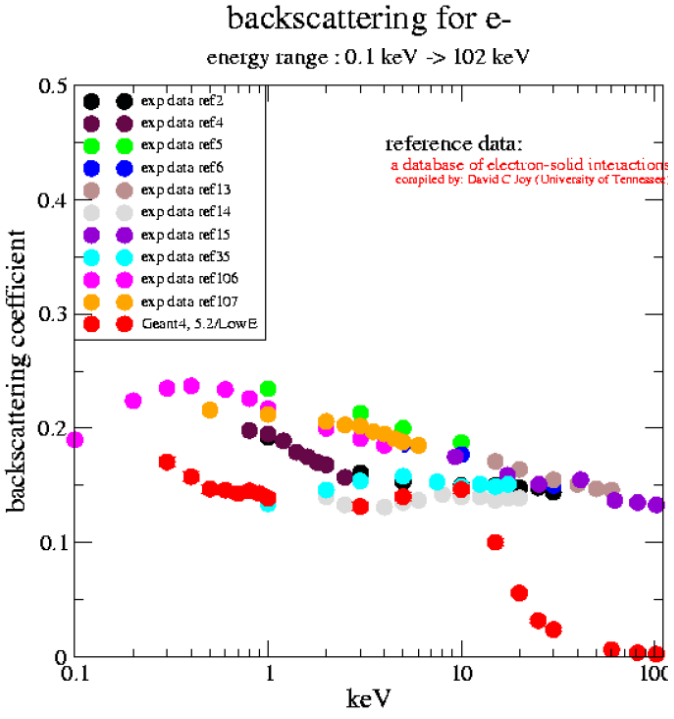
Lower energies extensions 1/2

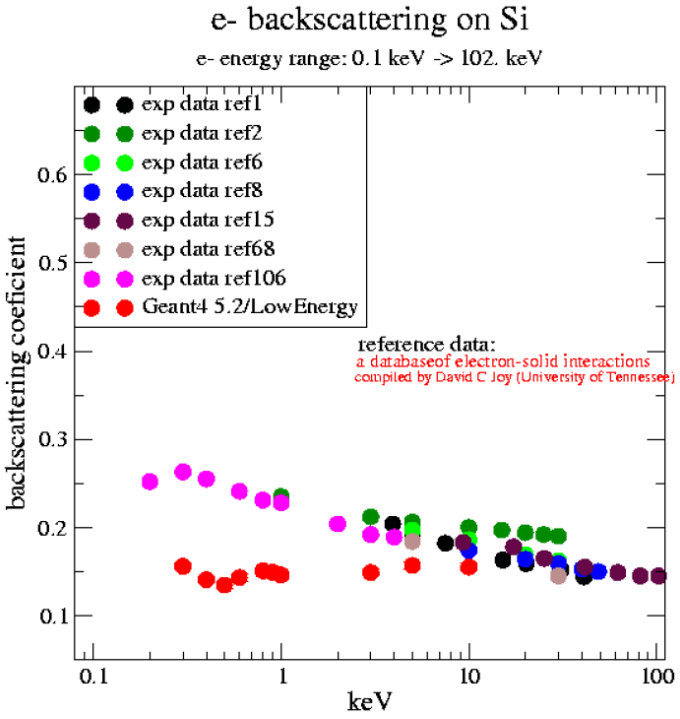
- The extension to lower energies is an important issue both for manned and unmanned space missions
  - The radiation hazard to the crew is critical to the feasibility of interplanetary space missions
    - The REMSIM project has performed a first evaluation of the radiation damage to astronauts
    - The Geant4-DNA activity currently in progress will allow in-depth understanding the effects of radiation on astronauts
  - The radiation effects on electronics are critical to the successful operation of a mission
    - Gaining an understanding of the physical effects of radiation down to the electronvolt scale opens the possibility for microdosimetry and nanodosimetry studies in components of interest for a variety of ESA space missions
- The issue of lower energy extensions has been pointed out in the last year ESA Round Table on radiation effects software

Lower energies extensions[2/2]

- The complexity of the physics processes involved and the need to account for the materials makes the project challenging
- Moreover it is difficult to find reliable data for the physics validation
  - Electron backscattering on Au, Al, Si from a database of experimental data compiled by David C. Joy (University of Tennessee) and compared with Geant4 LowE 5.2 (• Red)







Approaches

- Extension of validity of the Livermore libraries
  - In principle these libraries provides data down to ~ 10 eV
  - The huge task consists in the validation of the models against reliable reference data for all the materials
  - Could be necessary to develop corrections
- Development of step-by-step multiple scattering models
  - Available in literature, materials-dependent
- Development of models to describe the interactions with a specific material
  - Available in literature (water, silicon, air, etc...)
  - Great care must be taken in the design of the code in order to have a maintainable framework

Condensed models limitations[1/2]

- Currently Geant4 implements a condensed (integrated) model for the elastic scattering
  - This is motivated by the fact that a step-by-step simulation is rather CPU expensive
  - Based on the Lewis theory
    - Quite complete and accurate theory, but in the hypothesis of infinite medium
    - This means that steps near or crossing the interface between two media must be considered with particular care

Condensed models limitations 2/2

- Event-by-event even if CPU expensive are more precise and simple to handle
  - Moreover it is easier to find in literature accurate models for single interaction processes
- An alternative hybrid approach is the one of Penelope Monte Carlo
  - Interactions below a fixed angle q are simulated as condensed, while interactions above that angle are simulated in detail
    - Most of the interaction have small deflection angles
    - While problems with condensed models are mainly due to interactions with large deflections

Processes in water

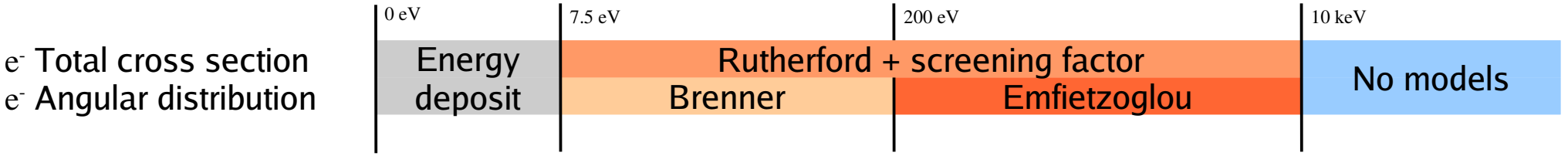
- At the end of May a working group has been formed for the development of low energy processes in the water medium within the Geant4-DNA project
  - Goal of the working group was the development of step-by-step electromagnetic interactions for
    - Electrons between 7 eV and 10 keV
    - Protons and alpha particles between 1 keV and 10 MeV
  - The processes considered are
    - Elastic scattering (relevant only for electrons)
    - Excitation of liquid water molecules
    - Ionization of liquid water molecules

Elastic scattering

- Step by step model
- Relevant only for electrons

$$e^- + H_20 \rightarrow e^- + H_20$$

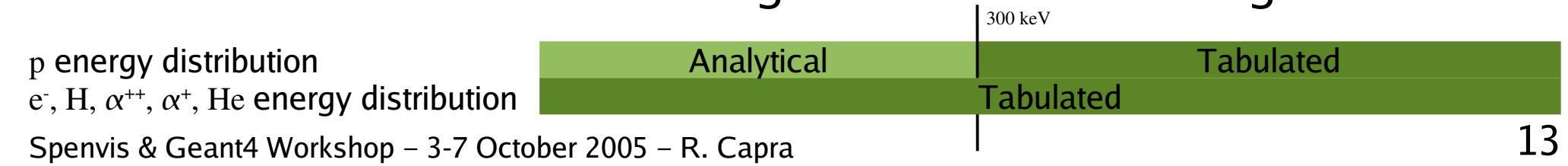
- Analytical total cross section between 7.5 eV and 10 keV
- Two analytical angular distribution models
  - Brenner model between 7.5 and 200 eV
  - Emfietzoglou model between 200 eV and 10 keV
- Electrons below 7.5 eV must be killed and energy must be deposited (UR)
- Water molecule tracking after interaction is neglected



Ionization processes

- Step by step model
- Six incoming particles considered
  - e^-, p, H, α^{++}, α^+, He
- 5 different ionization levels
  - Energy deposit depends on the ionization level
- Total cross sections (for each ionization level) are tabulated
  - Tables are precalculated and stored in files
- Angular distribution of the outgoing electron is analytical
  - Each incoming particle has a different model
- Energy distribution of the outgoing electron is
  - Analytical for protons below 300 keV
  - Based on tables for protons above 300 keV and other particles
    - Tables for outgoing electrons must interpolate on two parameters (Energy of the incoming particle, Energy of the outgoing electron)
- Ionized water molecule tracking after interaction is neglected

$$p + H_20 \rightarrow p + H_20^+ + e^- + \text{Energy Deposit}$$



Electrons exchange

- Step by step model
- Three incoming particles considered
  - p, α^{++}, α^{+}
  - α^{++} can strip one or two electrons to the water molecule
- Total cross sections
  - Analytical for protons
  - Tables for alphas
- Energy of the outgoing particle and the energy deposit depend on the incoming particle and on the number of electrons stripped
- Direction changes are neglected
- Ionized water molecule tracking after interaction is neglected

$$p + H_20 \rightarrow H + H_20^{+} + \text{Energy Deposit}$$

- Three incoming particles considered
  - H, α^{+}, He
  - α can release one or two electrons
- Tabulated total cross section
- Energy of the outgoing particle and the energy deposit depend on the incoming particle and on the number of electrons stripped
- Direction changes are neglected for both particles and electrons
- Water molecule tracking after interaction is neglected

$$H + H_20 \rightarrow p + H_20 + e^{-} + \text{Energy Deposit}$$

Excitation

- Step by step model

$$p + H_20 \rightarrow p + H_20^*$$

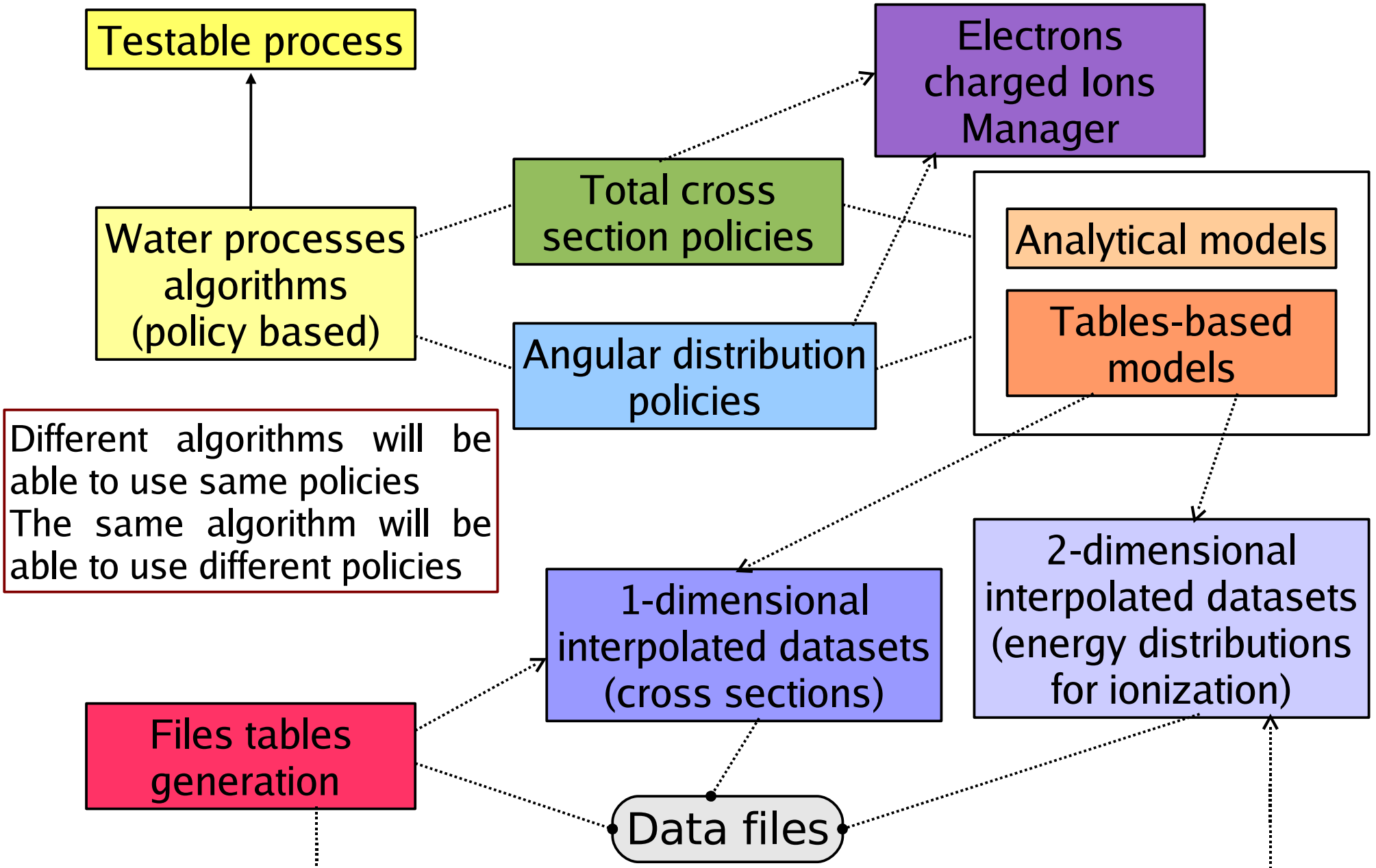
- Six incoming particles considered
  - e^-, p, H, α^{++}, α^{+}, He
- Excited water molecules are not described
  - Excitation energy is deposited
- 5 different excitation levels
  - Energy deposit depends on the excitation level
- Total cross sections (for each excitation level)
  - Analytical for protons
  - Tables for other particles
- Direction changes are neglected

- Excited water molecule tracking after interaction is neglected

Software process

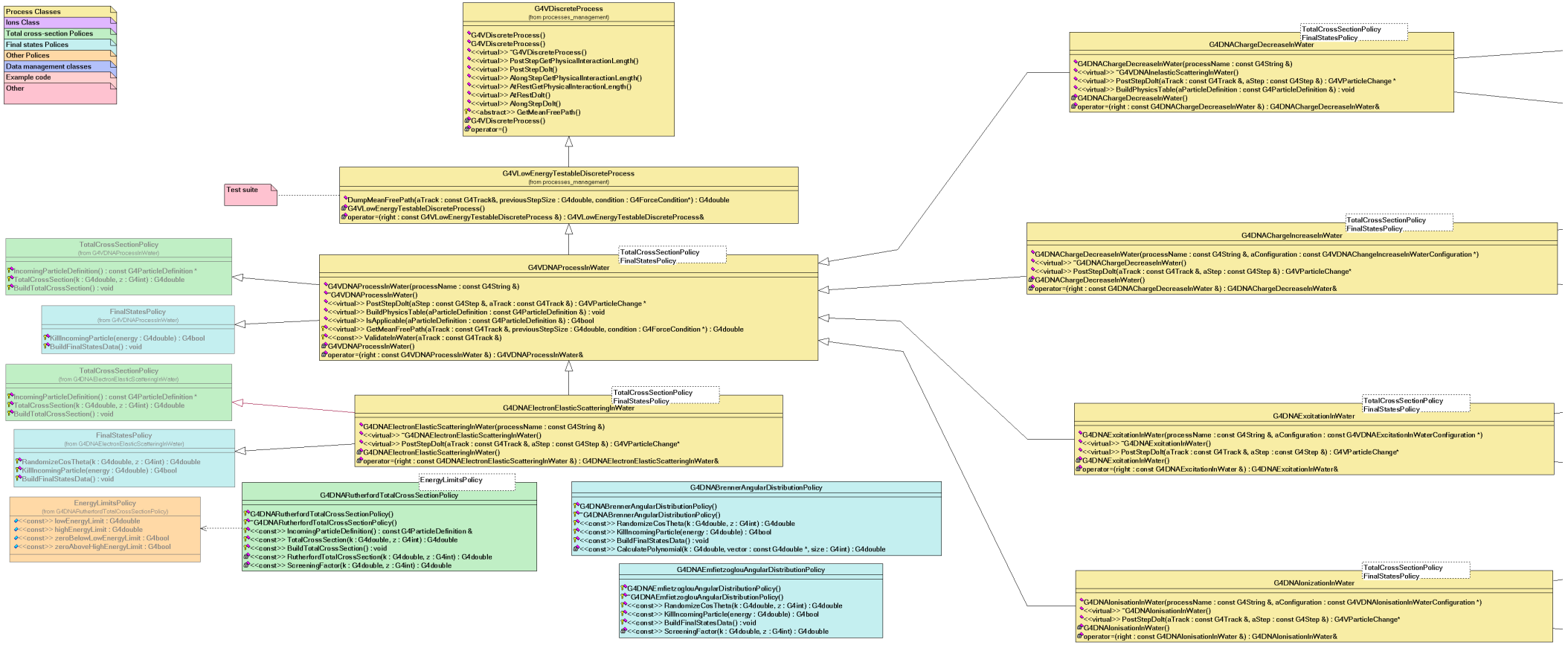
- The development of this set of processes has adopted a rigorous software process
  - Requirements
    - Vision document
    - User requirement document
      - Both available in the Geant4 documentation CVS repository
  - Analysis and design
    - Design model
      - Available in the Geant4 documentation CVS repository
  - Implementation
    - Developed code is available in the Geant4 CVS repository
  - Testing
    - Unit test
    - Validation (some results will be produced for December release)
  - Traceability

Problems domain decomposition

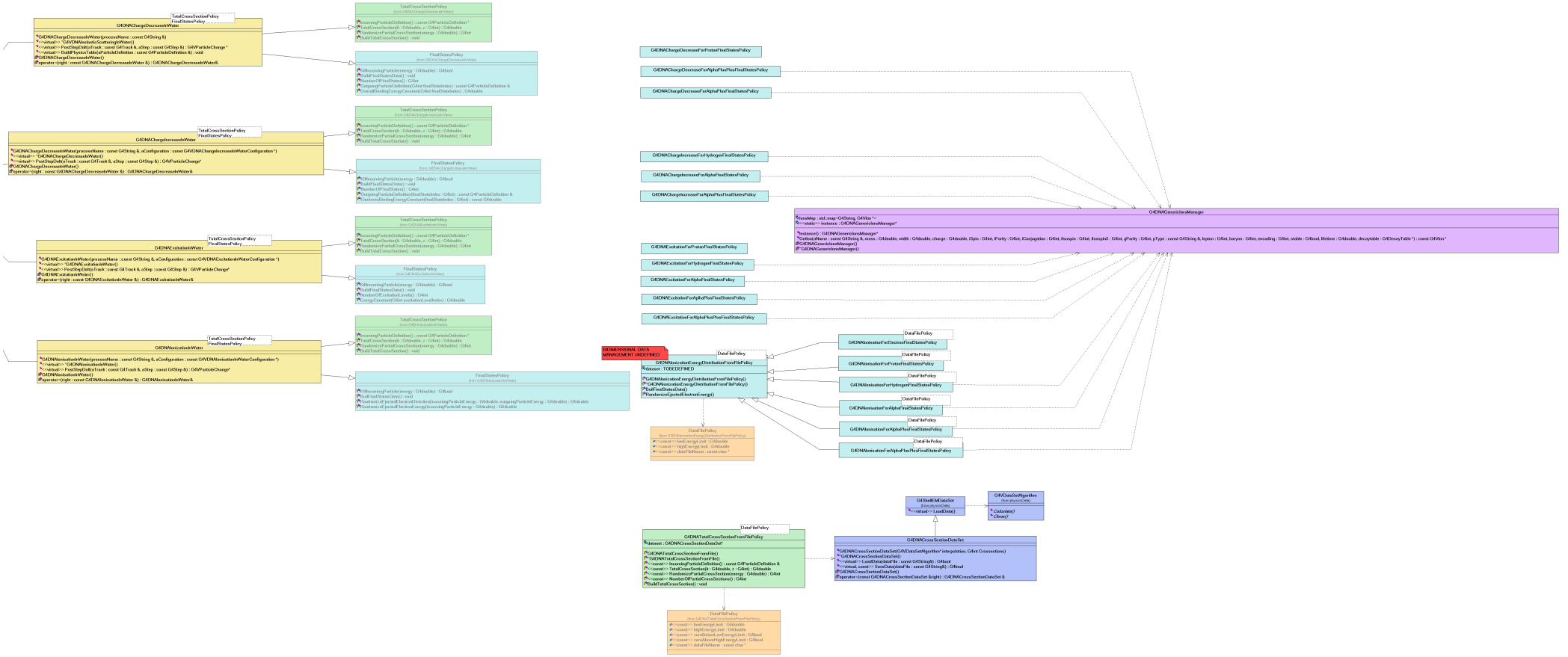


Design overview[1/2]

- Design mainly due to the Genoa group



Design overview 2/2



Status and release plans

- For the December release probably all the processes will be implemented and tested
  - It is expected to start the validation process before the December release
- Currently implemented processes
  - Implementation work mainly due to Clermont-Ferrand and Bordeaux
    - All processes implemented have passed the unit tests

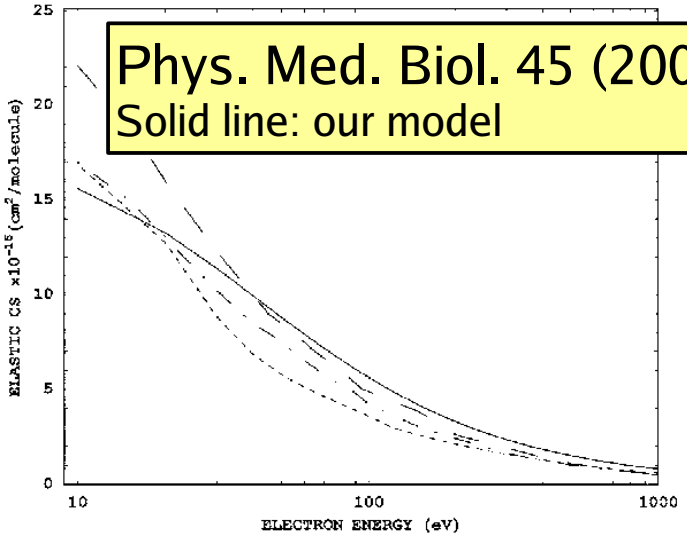
Implemented model
Alternative implemented model
To be done
Does not apply
Neglected

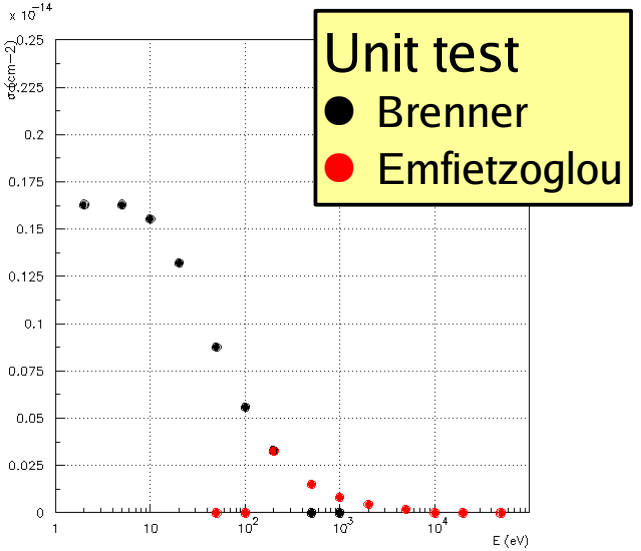
	Electrons	Protons (H+)	Hydrogen (H)	Alpha (He++)	He+	He
Elastic	Brenner (7.5 - 200 eV) Emfietzoglou (> 200 ev)	Neglected	Neglected	Neglected	Neglected	Neglected
Excitation	Emfietzoglou Born (7 ev – 10 keV)	Miller and Green Born (100 eV – 10 MeV)	Neglected	Miller and Green (1 keV – 15 MeV)	Miller and Green (1 keV – 15 MeV)	Miller and Green (1 keV – 15 MeV)
Charge decrease	Does not apply	Dingfelder (100 eV – 2 MeV)	Does not apply	To be done	To be done	Does not apply
Charge increase	Does not apply	Does not apply	Miller and Green Dingfelder (0.1 Kev – 100 MeV)	Does not apply	To be done	To be done
Ionization	To be done	Rudd (0.1 - 500 keV) To be done (> 500 keV)	Rudd (0.1 – 100 MeV)	To be done	To be done	To be done

Unit test example

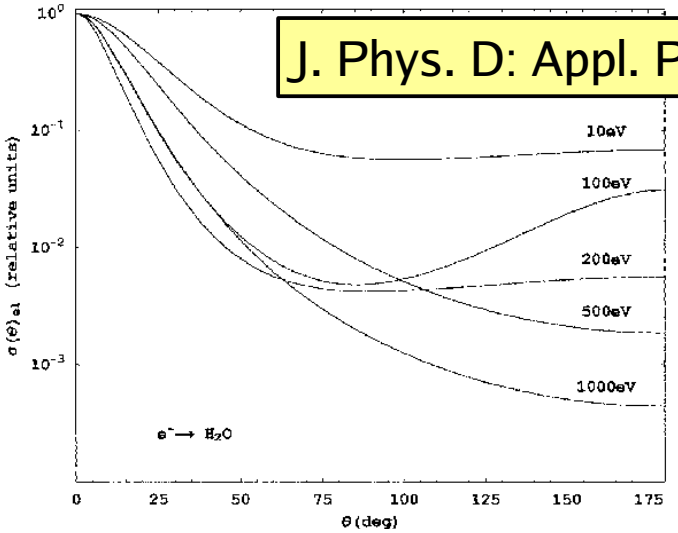
$$e^- + H_2O \rightarrow e^- + H_2O$$

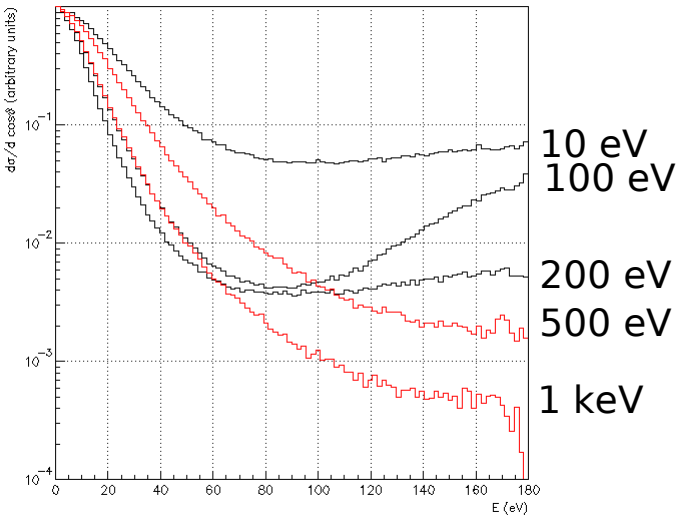
- Total cross section





- Angular distribution





Review of the work in progress[1/5]

- In order to minimize the code duplication each process is obtained using three classes
  - Total cross section (Half of the processes use tabulated total cross sections)
  - Final states distributions (Each model has a different final state distribution)
  - Process kinematics (5 kinematics categories)
- This choice is essential in order not to duplicate portions of code in several processes (like the kinematics of the process or the access to a file)
  - Each distribution, total cross-section has its reference
  - However this means a lot of files/classes
    - 14 processes developed up to now
    - 33 classes
    - 65 files
  - This puts some difficulties in the management of all these files

Review of the work in progress 2/5

- Total cross sections

	Electrons	Protons (H+)	Hydrogen (H)	Alpha (He++)	He+	He
Elastic	Brenner (7.5 - 200 eV) Emfietzoglou (> 200 ev)	Neglected	Neglected	Neglected	Neglected	Neglected
Excitation	Emfietzoglou Born (7 ev – 10 keV)	Miller and Green Born (100 eV – 10 MeV)	Neglected	Miller and Green (1 keV – 15 MeV)	Miller and Green (1 keV – 15 MeV)	Miller and Green (1 keV – 15 MeV)
Charge decrease	Does not apply	Dingfelder (100 eV – 2 MeV)	Does not apply	To be done	To be done	Does not apply
Charge increase	Does not apply	Does not apply	Miller and Green Dingfelder (0.1 Kev – 100 MeV)	Does not apply	To be done	To be done
Ionization	To be done	Rudd (0.1 - 500 keV) To be done (> 500 keV)	Rudd (0.1 – 100 MeV)	To be done	To be done	To be done

- Final states

	Electrons	Protons (H+)	Hydrogen (H)	Alpha (He++)	He+	He
Elastic	Brenner (7.5 - 200 eV) Emfietzoglou (> 200 ev)	Neglected	Neglected	Neglected	Neglected	Neglected
Excitation	Emfietzoglou Born (7 ev – 10 keV)	Miller and Green Born (100 eV – 10 MeV)	Neglected	Miller and Green (1 keV – 15 MeV)	Miller and Green (1 keV – 15 MeV)	Miller and Green (1 keV – 15 MeV)
Charge decrease	Does not apply	Dingfelder (100 eV – 2 MeV)	Does not apply	To be done	To be done	Does not apply
Charge increase	Does not apply	Does not apply	Miller and Green Dingfelder (0.1 Kev – 100 MeV)	Does not apply	To be done	To be done
Ionization	To be done	Rudd (0.1 - 500 keV) To be done (> 500 keV)	Rudd (0.1 – 100 MeV)	To be done	To be done	To be done

Review of the work in progress 3/5

- Kinematics

	Electrons	Protons (H+)	Hydrogen (H)	Alpha (He++)	He+	He
Elastic	Brenner (7.5 - 200 eV) Emfietzoglou (> 200 ev)	Neglected	Neglected	Neglected	Neglected	Neglected
Excitation	Emfietzoglou Born (7 ev – 10 keV)	Miller and Green Born (100 eV – 10 MeV)	Neglected	Miller and Green (1 keV – 15 MeV)	Miller and Green (1 keV – 15 MeV)	Miller and Green (1 keV – 15 MeV)
Charge decrease	Does not apply	Dingfelder (100 eV – 2 MeV)	Does not apply	To be done	To be done	Does not apply
Charge increase	Does not apply	Does not apply	Miller and Green Dingfelder (0.1 Kev – 100 MeV)	Does not apply	To be done	To be done
Ionization	To be done	Rudd (0.1 - 500 keV) To be done (> 500 keV)	Rudd (0.1 – 100 MeV)	To be done	To be done	To be done

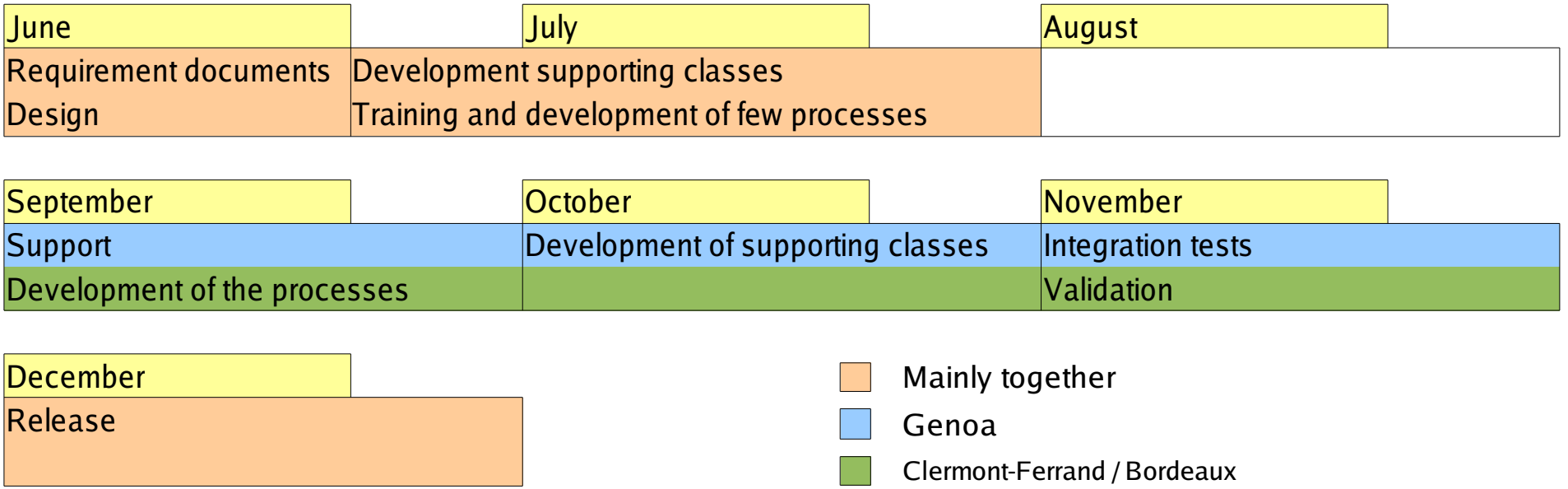
- Supporting classes
  - 3 classes
  - 6 files

Review of the work in progress[4/5]

- The same unit test is used to check all the processes separately
  - This allows developing a unique detailed, reliable and flexible unit test
  - Allows comparing different processes that operate on the same particles and in the same energy range
- The choice of Policy based classes
  - In principle a Strategy pattern could give the same results
    - But with worse performances
    - Templates classes have some more flexibility
  - We expect some extra work in the integration test phase
    - As template classes are a rather new C++ feature is, we expect some extra work to let the code build on all supported platform
    - Integration test will start soon in order to have the code ready for December release

Review of the work in progress 5/5

- Overview of the development phases
  - After an initial phase of
    - Design of the code
    - Training
    - Development of the supporting classes
- The development is going rather fast and independently



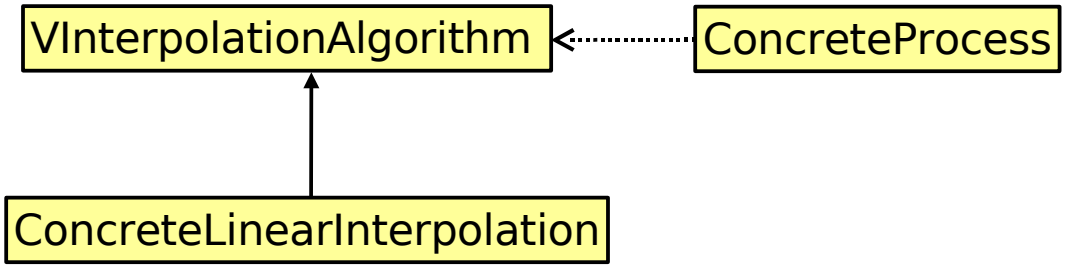
Conclusions

- It has been presented the current status of the Low Energy Package
  - Models currently implemented cover a range of energies down to 100-200 eV
  - Extensions to lower energies are feasible
    - Validating the Livermore processes down to 10 eV
    - Developing step-by-step material dependent models
- Processes based on the second approach has been recently developed for water material
  - The encouraging results
  - All the planned processes should be released in December
- The same approach could be used for other materials (silicon, air, etc.)
  - The design phase and the file management need extra care
    - A lot of models with limited validity (energy range/materials)
    - Risk of code duplication and problems in the management of the files

Extra slides

Policy based classes

- The design makes deep use of policy based classes
  - There classes are parametrized classes that implement an algorithm delegating some operations to their class parameters, called policies
  - Policy based classes have something in common with Strategy pattern



- But with some difference
  - Do not require that policies inherit from specific base classes
    - This means a weaker dependency of the policy and the policy based class from the policy interface. In complex situations this makes a design more flexible and open to extensions
  - They are compile bound
    - In other words there is no need of virtual methods, resulting in faster execution code