Geant4 Hadronic Physics Working group progress and status.

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Outline

- Status on milestones, and recent developments
- Validation/verification
- News on outside contacts (3rd parties)

The dry numbers…

- Number of packages
  - Released: 27
  - Total: 36
- Number of classes
  - Released: 720
  - Total: 1114
- Lines of source code.
  - Released: ~240,000
  - Total: ~360,000

...

- At present about 30 people are contributing to this effort with some of their time, creativity, or expertise.
- The number of use-case packages considered is currently 14, and we provide a total of 16 physics lists for the various areas of applicability.

The milestones.

- 2002
  1. Distribute ‘educated guess’ physics lists for major use-cases (*)
  2. Include at least one test-beam simulation in pre-release WG level validation (*)
  3. Improved verification suite for the cascade energy range (*)
  4. Release biased MARS re-write for energies below 5 GeV (*)
  5. Include γ-nuclear reactions in quark-gluon string model (*)
  6. Improve the charge-state treatment for recoils/residuals (*)
  7. Bring kinetic model to a releasable state (ongoing)
  8. Release of a cascade code (from HETC milestone 2001, ongoing)
  9. Provide a generic scattering term for cascade type models (*’)
  10. Improve electro-nuclear cross-section to include hard scattering (*)
  11. Publish work - at least 4 papers submitted to refereed journals (2 done)

- (*) = reached

Particle physics relevant requirements collected

- Specifically from LHC:
  - Have starting physics list (done)
  - Improve information flow on V&V (done, to be verified)
  - Provide a cascade code (two focused efforts)
  - Fix known problems in low energy models (released)

A complete sample requirement.

- Name and E-mail: Dennis Wright, SLAC
- Title: Pion and kaon nuclear prodution cross-sections
- Description: 1-5 GeV pions and kaons interacting inelastically. 10% precision would be great.
- Rationale: Representation of how the shower develops.
- Supporting use-cases that require this: Trying to model hadronic interactions in the BaBar intsrumented flux return.
- Responsible cathegory: hadronics
- Fulfillment criterion: Comparison to the data from particles interacting in the beam-pipe and flux return.
- Relevace: very highly relevant for BaBar, relevant also for LHCb
- References: An E-mail from Dennis pointing to the data.

Requirements collected – titles only

- During the last geant4 workshop, the users workshop at SLAC, and in private mails:
  - Ensure that the physics reference manual match the implementation, and the models are mentioned in the applications developers guide, Referencing papers is just fine.
  - Memory usage for G4NDL cross-sections
  - Energy and momentum conservation should be checked in regression independently by the working group for all models, and publish the test-suite.
  - Use ’well known’ international benchmarks to validate; publish results.
  - More understandable hadronic physics lists
  - Get documentation on which model is good/usefull/required for which use-case

Requirements Cont.

- Provide a set of plots, and put them u; i.e. provide a place to put these plots for users.
- Cross-sections for n,p inelastic scattering below 150 MeV in CMS tracker materials at 10% level of precisions.
- Pion and kaon nuclear prodution cross-sections: 1-5 GeV pions and kaons interacting inelastically. 10% precision would be great.
- 10-20% level of description for 10-100GeV incident protons for example on Beryllium or copper.
- Enroll a set of users to validate on complete application; as beta testers so to say.
- Compare inclusive and exclusive cross-sectios to data from the RAL/Durham database

Requirements Cont.

- Description on how to set cuts, and its effects
- Possibility to stop low energy neutral particles (like neutrons)
- Each model should be specified concerning its application area/use-cases
- Provide a list of models per use-case package
- List of models per use-case package
- Include physics list samples, once they exists, into the phsics editor
- Ensure tracability of data to the primary source
- Well defined process for updating the databases on request.
- Parametrizations of hadronic showers in CsI and Iron.
- Parametrizations of neutron background in LHC experiments
- Models for alpha incident inelastic reactions

Requirements Cont.

- Models for alpha incident difractive dissociation reactions
- Where the modelling approach allows to produce the residual, it should be provided.
- Neutron production by alphas at energies below 10 MeV; including reaction cross-sections at 20%precision and kinematics of neutrons and gammas produced.
- Include K0 oszillations
- Provide muon nuclear reactions
- Provide internal conversion
- Provide neutron elastic scattering, in particular recoil energy and momentum distributions for neutrons below 10MeV.
- Dito for n inelastic scattering off Xenon and SiO2, CaCO3, H2O

Requirements Cont.

- Dito for capture
- Provide gamma nuclear reactions for gamma energies of less than 100 MeV, including cross-sections.
- Provide radioactive decay after transmutation.
- Provide k-shell excitation in radioactive decay
- Activation of detector material and environment by shower particles

Note: Almost all of these requirements are by now fulfilled. Many were fulfilled when the issue was entered as a requirement, so only information was to be provided.The rest are to be scheduled for being addressed, according to priorities.

Requirements cont.

- 17 fresh requirements harvested during the geant4 workshop last week.
- Direct interaction with the experts is very productive in this.

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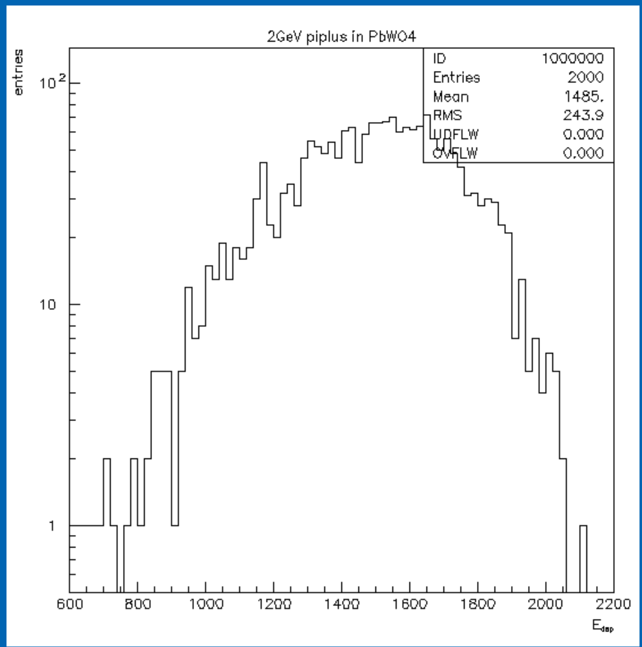
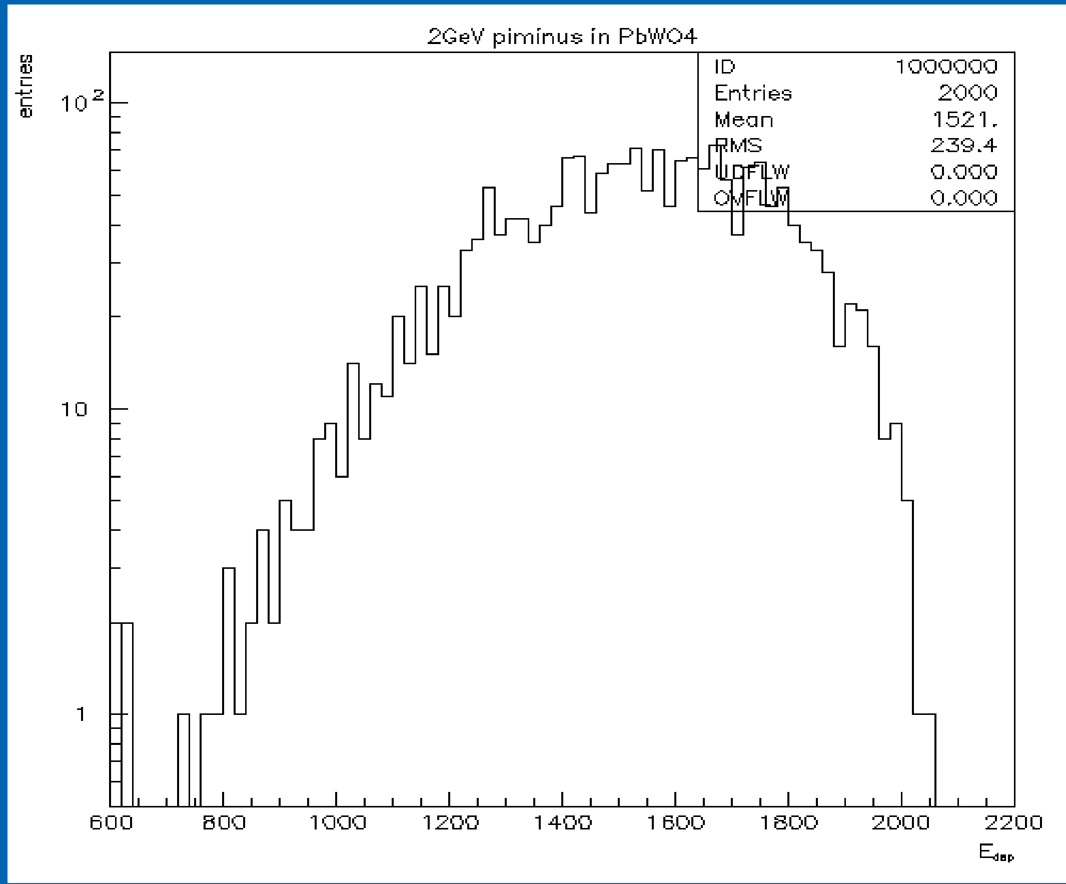
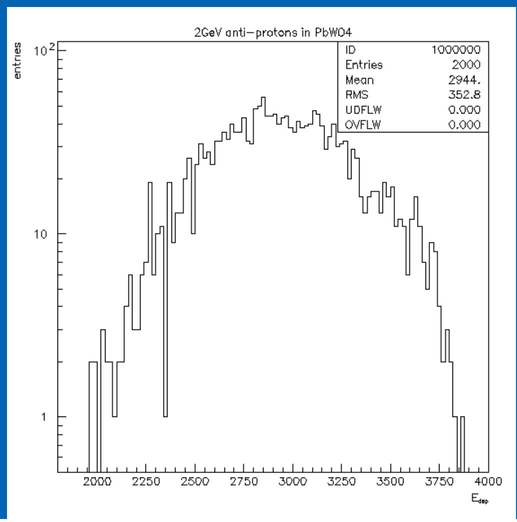
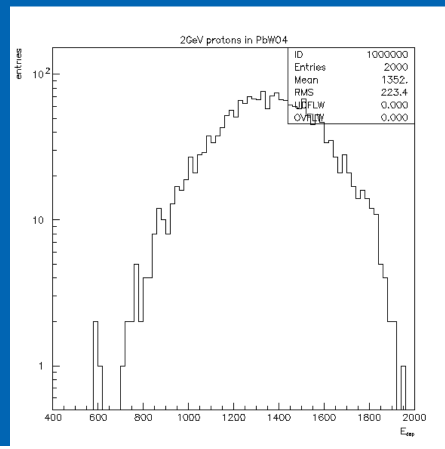
Sample plots energy deposition





BTEV: All distributions are in the expected energy range





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Active tasks 2002

- Write 'educated guess' physics lists for major use-cases
- Include at least one test-beam simulation into regular validation
- Include a complete radiation benchmark into WG level validation
- Improved validation suite for the cascade energy range
- Possibly further extension of the high energy validation suite
- Plan to contribute to SATIF-6
- Release fully leading particle biased mars-5 re-write
- Release of cascade part of HETC re-write
- Improve gamma nuclear reactions in QGS model
- Make a validation/verification WWW page

Active tasks 2002, cont.

- Possibly first release of high energy heavy ion reactions in QGS model, with option to further extension to QMD
- Revision of the reaction cross-sections
- Improve the charge state treatment for recoils.
- Bring kinetic model to releasable state
- Bring inucl cascade code to releasable state
- Research the use of CHIPS in string fragmentation for intrinsically 3D fragmentation
- Provide a generic scattering term for cascade type models
- Alternative coherent elastic model (reggee theory based)

Active tasks 2002, cont.

- Improve electro-nuclear cross-sections to take hard scattering into account.
- Investigate JENDL2.2, and LA150 neutron data libraries
- Collect (even more) requirements
- Release work, coordination
- Contribute to maintenance and user support
- Contribute to architecture working group
- Contribute to process improvement/establishment
- Contribute to training
- Publish work (11 papers in the plan…)

Conclusions

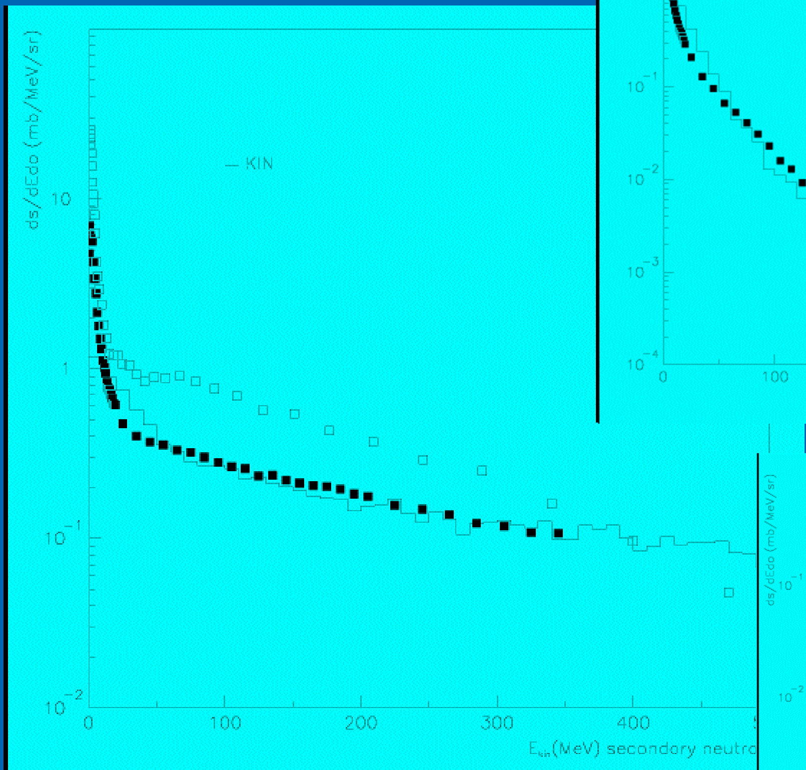
- We have, at TIMENOW, met 8/11 milestones for 2002.
- We get a constant flow of requirements, fee-back, and test-beam results from the detector groups (this is excellent news).
- We have a good team, and we are normally able to attract the expertise needed for modeling.
- We fully depend on visitor and travel money from CERN.
- Front-line support man-power non-trivial to find.

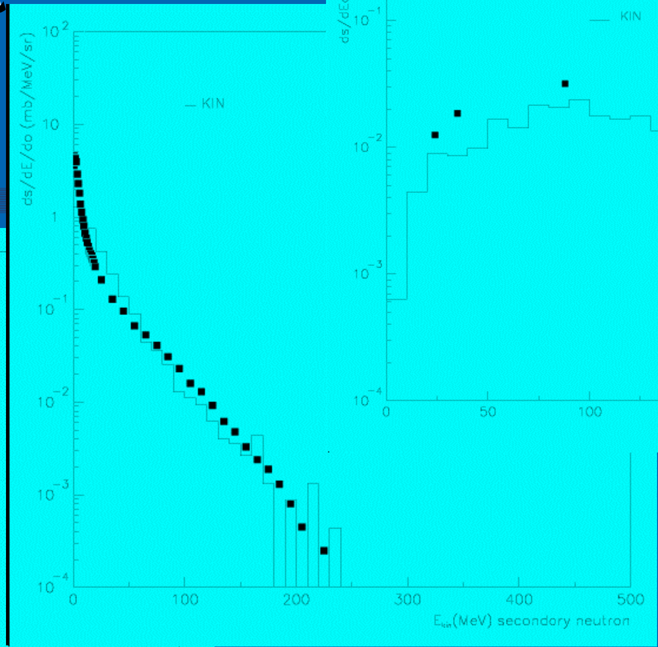
Some hadronic physics highlights of late 2001 and 2002

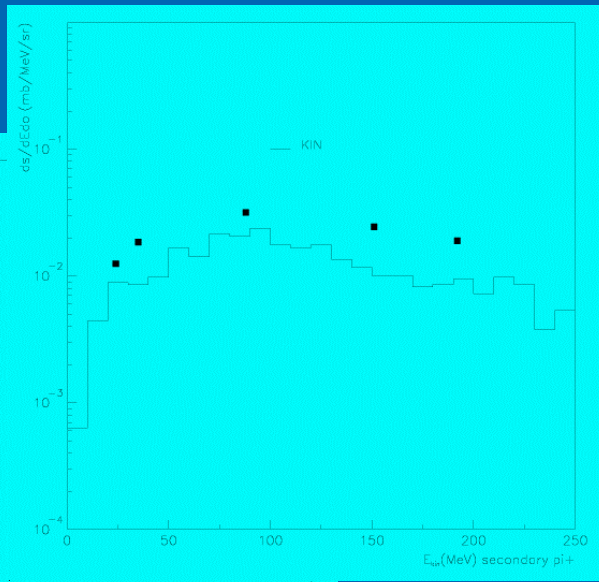
- Neutron spectra from pre-equilibrium decay and a sneak preview on kinetic model performance
- qgs model for pion and kaon (and gamma) induced reactions
- Doppler broadening on the fly
- Internal conversion, and a new photon evaporation data-base
- Chiral invariant phase-space decay
- A propagation test for quantum molecular dynamics

Swapping to show a few transparencies on pre-compound neutron yields.

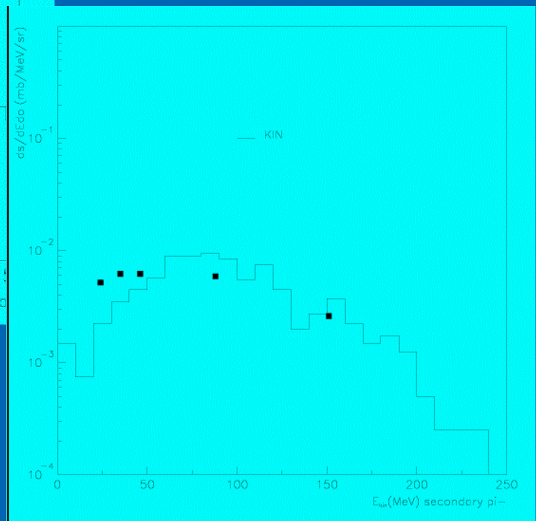
Preview on kinetic model

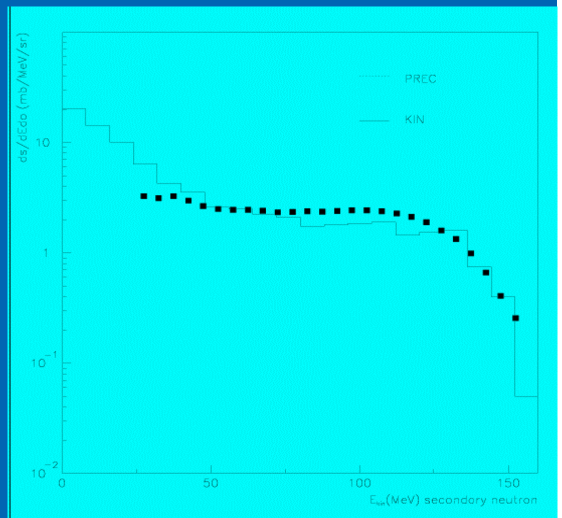






160 MeV p on Pb, forward neutrons





585MeV p on Al, forward And backward n and π

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Low energy neutrons: G4NDL0.2, 3.7

- Are granular selections of data from (alphabetic)
  - Brond 2.1
  - CENDL 2.2
  - EFF-3
  - ENDF/B (VI.0, VI.1, VI.5)
  - ENSDF
  - FENDL/E2.0
  - JEF 2.2
  - JENDL (3.1, 3.2, FF, 3.3 currently under study)
  - MENDL-2(P)
- Large parts of the selection is guided by the FENDL-2 selection
- G4NDL0.2 for non-thermal application

The neutron_hp transport models

- Simulate the cross-sections and interactions of neutrons with kinetic energies below 20 MeV down to thermal energies .
- The upper limit is set only by the evaluated data libraries the code is based on.
- We consider elastic scattering, fission, capture and inelastic scattering as separate models
- Neutron_hp sampling codes for the ENDF/B-VI derived data formats are completely generic (not including general R-matrix for the time being)
  - Note that for fission there is a quite competitive theory driven alternative model, G4ParaFissionModel.

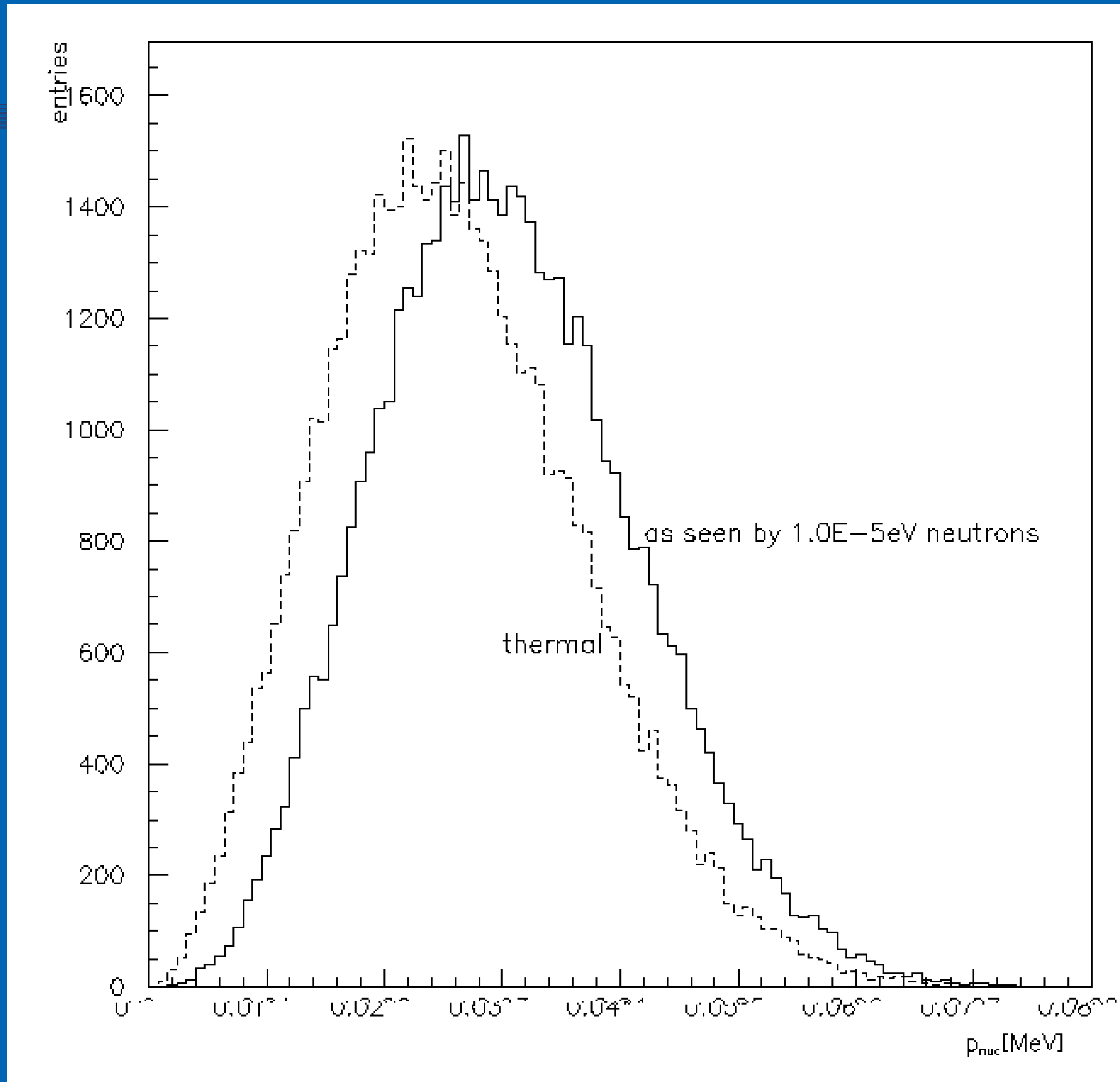
Models for neutron interaction and thermalization.

- neutron_hp models and cross-sections:
  - Uses the unix file-system to ensure granular and transparent access/usage of data sets.
  - More than 10^10 events run.
  - Uses point-wise cross-sections → no artifacts due to multi-group structure.

Doppler broadening

- Does exact doppler broadening on the fly, based on 0K data → no pre-formatting of data to fixed temperatures, and easy simulation of set-ups with mixed temperatures.
- Adds the doppler bias to the nuclear momentum distribution
- Point one is to the best of our knowledge not available from any other transport code (the second is also in MCNP).

The doppler bias illustrated for Carbon



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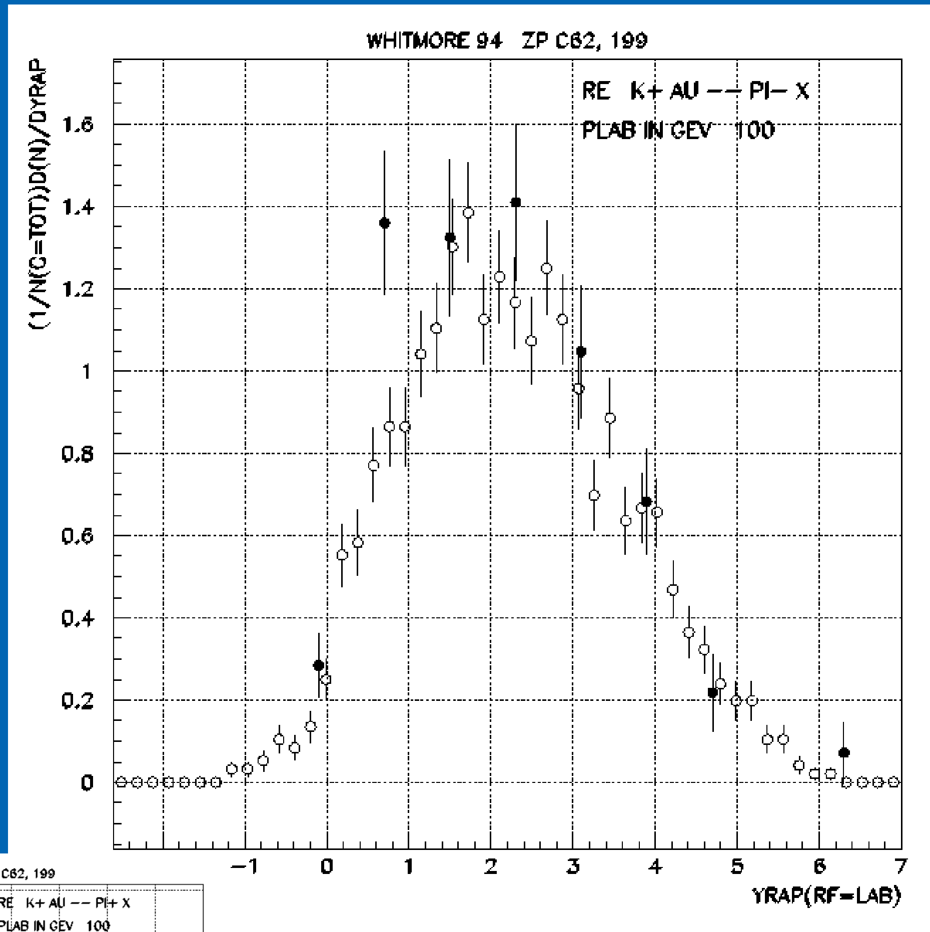
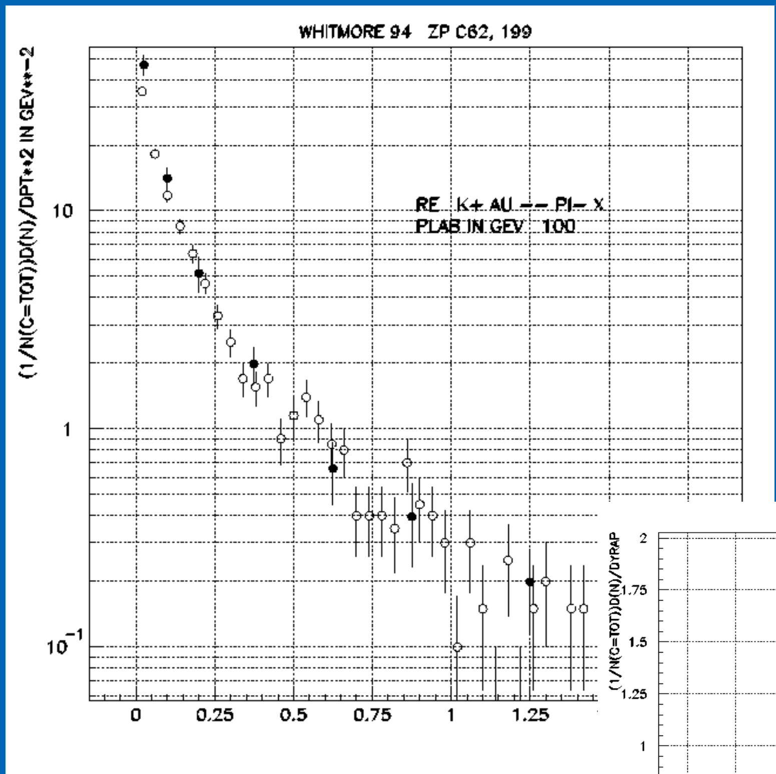
qgs model for π and K induced reactions

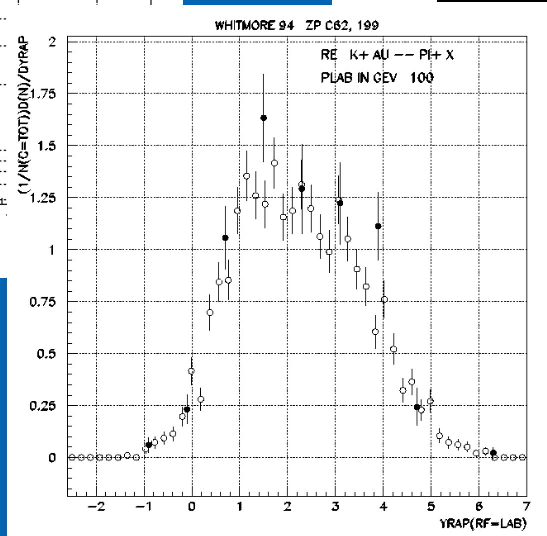
- Pomeron trajectory and vertex parameters tuned to describe elastic, total and diffractive (6% assumed) cross-sections for kaon and pion scattering off nucleons.
- No tuning on final state distributions.
- A few plots to illustrate the quality of prediction

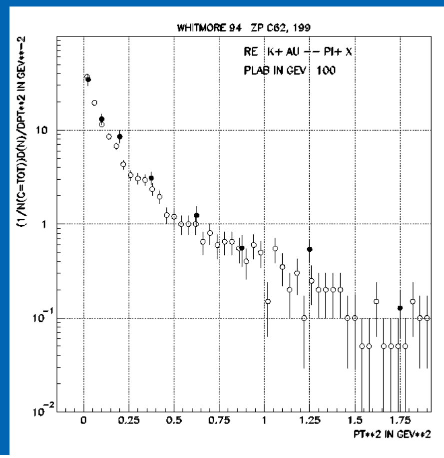
K-, scattering off Au

(for pions see V&V section)









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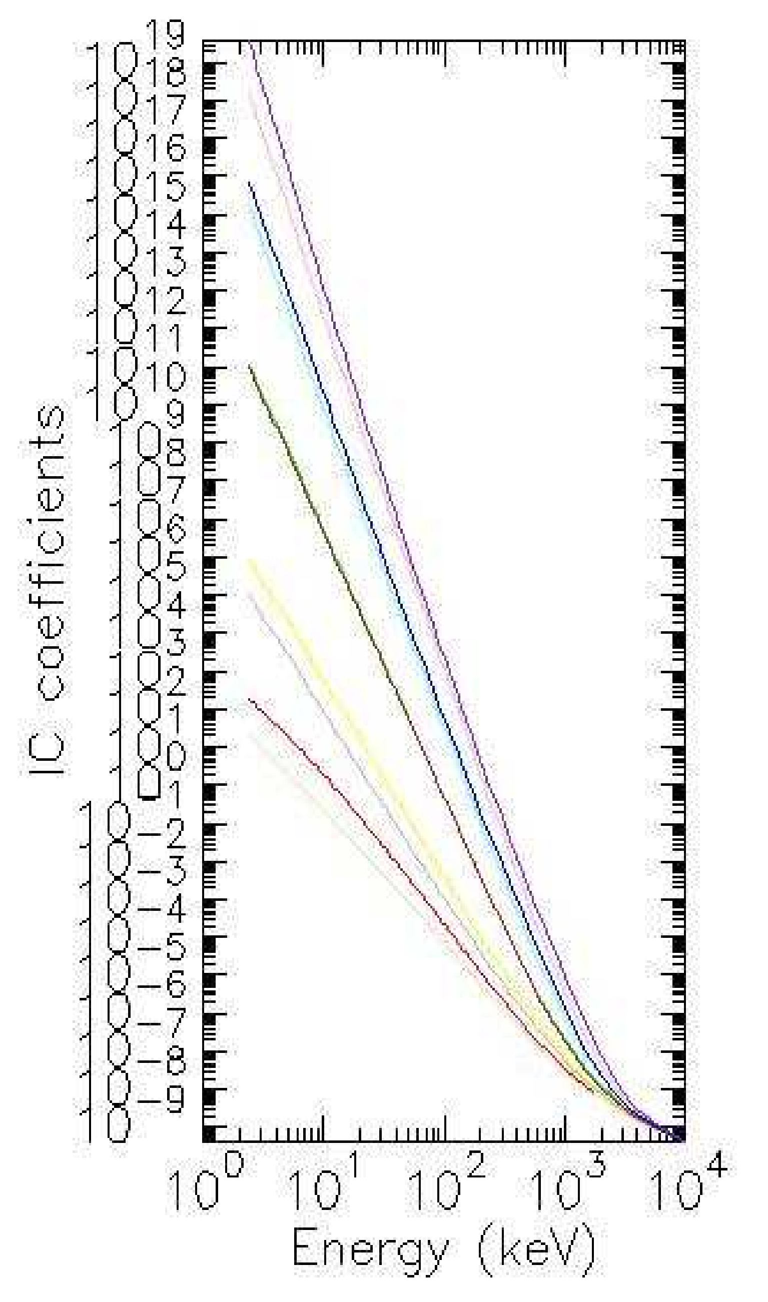
Photon Evaporation data base

- Originally containing adopted level and gamma-ray transition energies, photon intensity, multipolarity, half-life and spin parity for isotopes up to Z=94, A=240
- Expanded to include probability of internal conversion and internal conversion coefficients (ICC) from shells K, L1, L2, L3, M1, M2, M3, M4, M5 and N+
- Based on ENSDF data from LBNL and tabulated theoretical ICC data from Band *et. al.* (used for Z ≤ 80) and Rösel *et . al.* (used 80 ≤ Z ≤ 96)



- ICCs are calculated by cubic spline interpolation using above tables at the required gamma-ray energy
- ICC calculated for Mixed multipolarity M1+E2 if mixing ratio available
- Some changes were introduced in the format of the data base entries to keep the size of the files down (data base is now 4.5 times larger)

Preliminary test results

- ENSDF decay data processed with RADLIST (BNL code) and Geant4 (for 2000 decays)

^{137}Cs

	RADLIST (BNL)		Geant4	
Radiation	Energy (keV)	Intensity (100dks)	Energy (keV)	Intensity (100dks)
CE K	624.216	7.66 (0.23)	624.216	8.70 (0.66)
CE L	655.668	1.39 (0.05)	655.668	1.15 (0.24)
γ	283.500	0.00058		
γ	661.657	85.1 (0.20)	661.657	84.15 (2.05)

^{57}Co

Radiation	RADLIST (BNL) Energy (keV)	RADLIST (BNL) Intensity (100dks)	Geant4 Energy (keV)	Geant4 Intensity (100dks)
CE K	7.301	71.00 (6.0)	7.301	70.55 (1.88)
CE			12.899	10.00 (0.70)
CE L	13.567	7.40 (0.6)	13.562	5.95 (0.54)
CE			13.687	0.35 (0.13)
CE			14.315	0.85 (0.21)
CE			14.405	0.45 (0.19)
CE K	114.949	1.83 (0.14)	114.949	1.95 (0.31)
CE			120.497	5.70 (0.53)
CE L	121.215	0.19 (0.020)		
CE M+	121.968	0.03 (0.005)		
CE K	129.361	1.30 (0.16)	129.362	1.25 (0.25)
CE			134.910	0.25 (0.11)
γ	14.413	9.16 (0.15)	14.413	10.05 (0.71)
γ	122.061	85.60 (0.17)	122.061	86.05 (2.07)
γ	136.474	10.68 (0.08)	136.474	10.05 (0.71)
γ	692.410	0.15 (0.01)	692.030	0.15 (0.09)

A sample development:
Chiral Invariant Phase-space Decay.

- A quark level 3-dimensional event generator for fragmentation of excited hadronic systems into hadrons.
- Based on the QCD idea of asymptotic freedom
- Local chiral invariance restoration lets us consider quark partons massless, and we can integrate the invariant phase-space distribution of quark partons and quark exchange (fusion) mechanism of hadronization
- The only non-kinematical concept used is that of a temperature of the hadronic system (quasmon).

Vacuum CHIPS

- This allows to calculate the decay of free excited hadronic systems:
- In an finite thermalized system of N partons with total mass M, the invariant phase-space integral is proportional to M^{2N-4} , and the statistical density of states is proportional to $e^{-M/T}$. Hence we can write the probability to find N partons with temperature T in a state with mass M as

$$dW \propto M^{2N-4} e^{-M/T} dM$$

- Note that for this distribution, the mean mass square is $\left\langle M^2 \right\rangle = 2N(2N-2)T^2$

Vacuum CHIPS

- We use this formula to calculate the number of partons in an excited thermalized hadronic system, and obtain the parton spectrum

$$\frac{dW}{kdk} \propto \left(1 - \frac{2k}{M}\right)^{N-3}$$

- To obtain the probability for quark fusion into hadrons, we can now compute the probability to find two partons with momenta q and k with the invariant mass μ.

$$P(k, M, \mu) = \int \left(1 - \frac{2q}{M\sqrt{1-2k/M}}\right)^{N-4} \times \delta\left(\mu^2 - \frac{2kq(1-\cos\theta)}{\sqrt{1-2k/M}}\right) qdqd\cos\theta$$

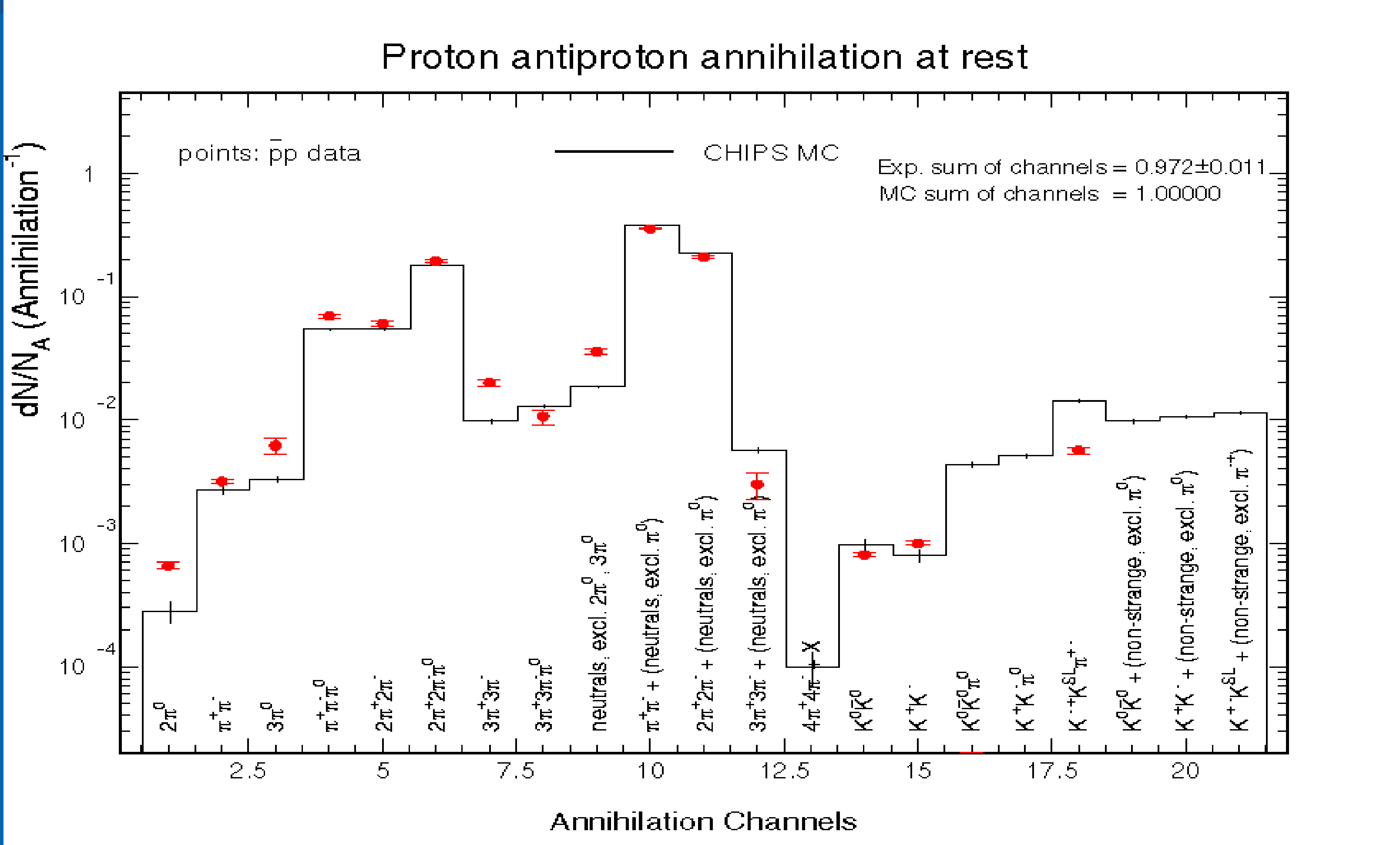
Vacuum CHIPS

- Using the delta function to perform the integration and the mass constraint, we find the total kinematical probability of hadronization of a parton with momentum k into a hadron with mass μ:

$$\frac{M-2k}{4k(N-3)}\left(1-\mu^2/2kM\right)^{N-3}$$

- Accounting for spin and quark content of the final state hadron adds (2s+1) and a combinatorial factor.
- At this level of the language, CHIPS can be applied to p-pbar annihilation

Anti proton annihilation



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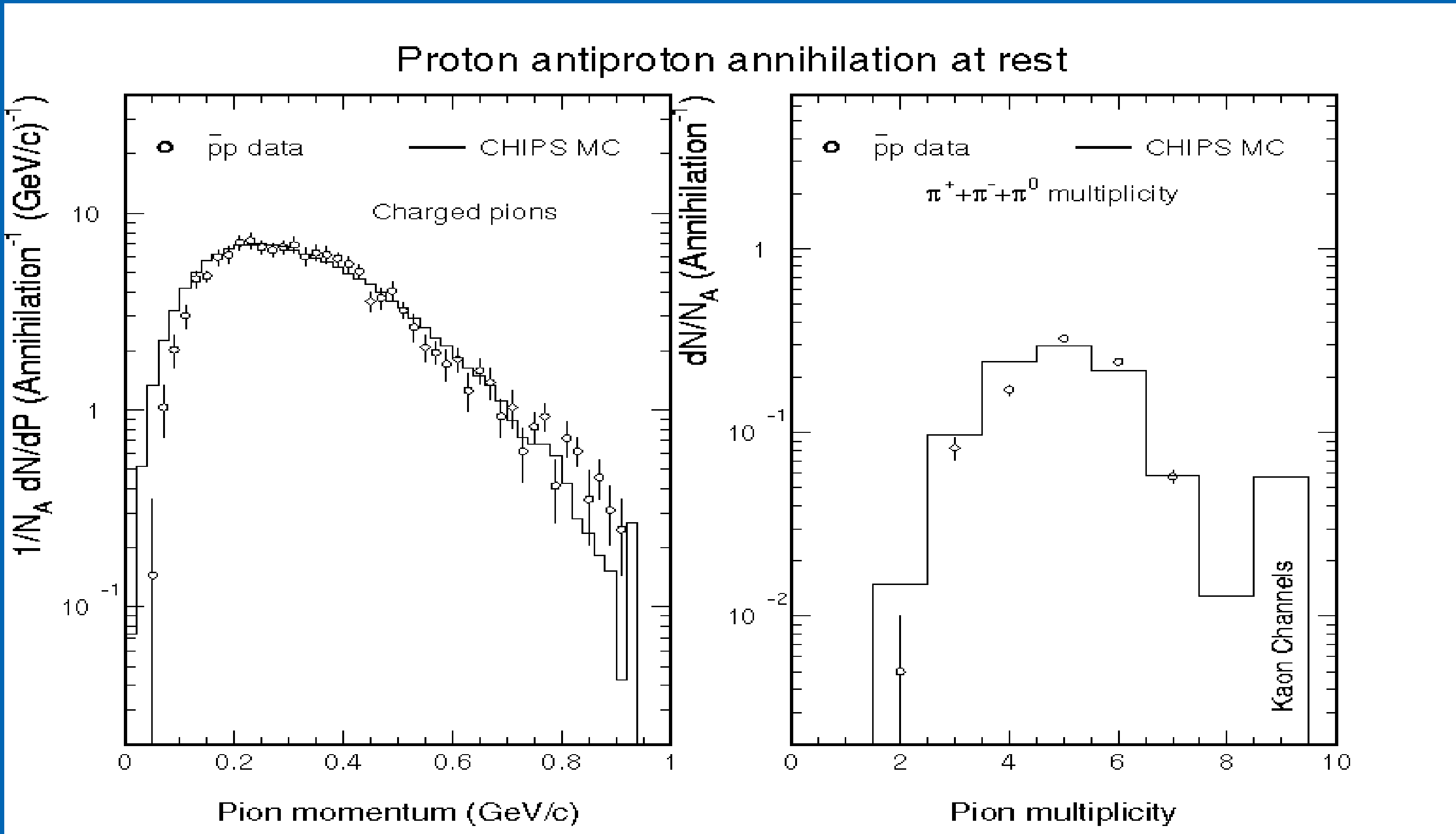
Anti proton annihilation



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Nuclear CHIPS

- In order to apply CHIPS for an excited hadronic system within nuclei, we have to add parton exchange with nuclear clusters to the model
- The kinematical picture is, that a color neutral quasmon emits a parton, which is absorbed by a nucleon or a nuclear cluster. This results in a colored residual quasmon, and a colored compound.
- The colored compound then decays into an outgoing nuclear fragment and a ‘recoil’ quark that is incorporated by the colored quasmon.

Nuclear CHIPS

- Applying mechanisms analogue to vacuum CHIPS, we can write the probability of emission of a nuclear fragment with mass μ as a result of the transition of a parton with momentum k from the quasmon to a fragment with mass μ′ as:

$$P(k,\mu',\mu)=\int\left(1-\frac{2(k-\Delta)}{\mu'+k(1-\cos\theta_{kq})}\right)^{n-3}\frac{\mu'(k-\Delta)}{2\left[\mu'+k(1-\cos\theta_{kq})\right]^{2}}\,d\cos\theta_{kq}$$

- Here, n is the number of quark-partons in the nuclear cluster, and Δ is the covariant binding energy of the cluster, and the integral is over the angle between parton and recoil parton.

Nuclear CHIPS

- To calculate the fragment yields it is necessary to calculate the probability to find a cluster of ν nucleons within a nucleus. We do this using the following assumptions:
  - A fraction $\varepsilon 1$ of all nucleons is not clusterising
  - A fraction $\varepsilon 2$ of the nucleons in the periphery of the nucleus is clustering into two nucleon clusters
  - There is a single clusterization probability ω
- and find, with a being the number of nucleons involved in clusterization

$$P_\nu = \frac{C_\nu^a \omega^{\nu-1}}{(1+\omega)^{a-1}}$$

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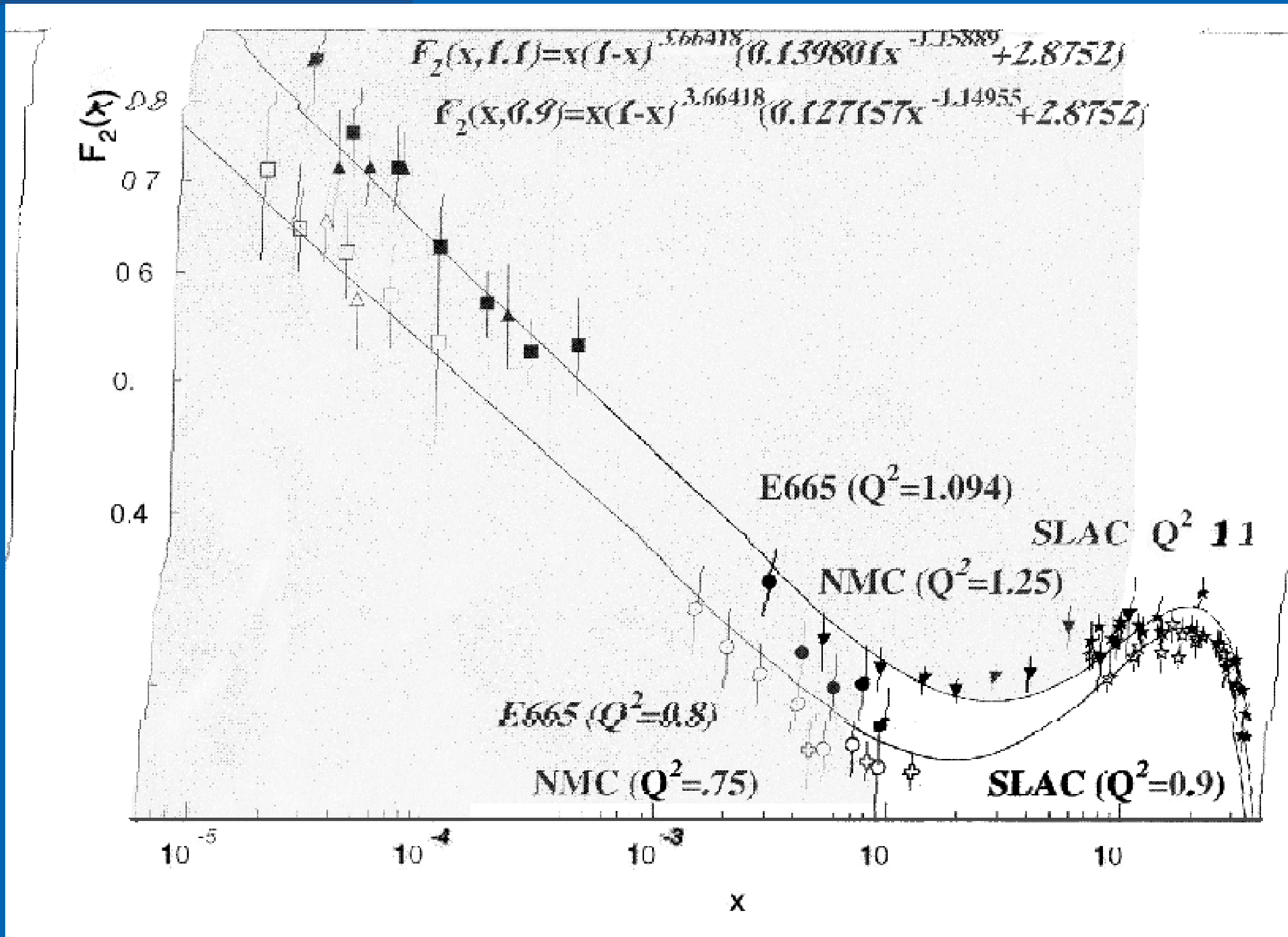
Nuclear CHIPS

- At this level of the language, CHIPS can be applied to capture of pions and photo-nuclear reactions.

Intra-nuclear CHIPS

- Extensions to include the behavior of multiple quasmons within one nucleus have been added.

Hard scattering in electro-nuclear



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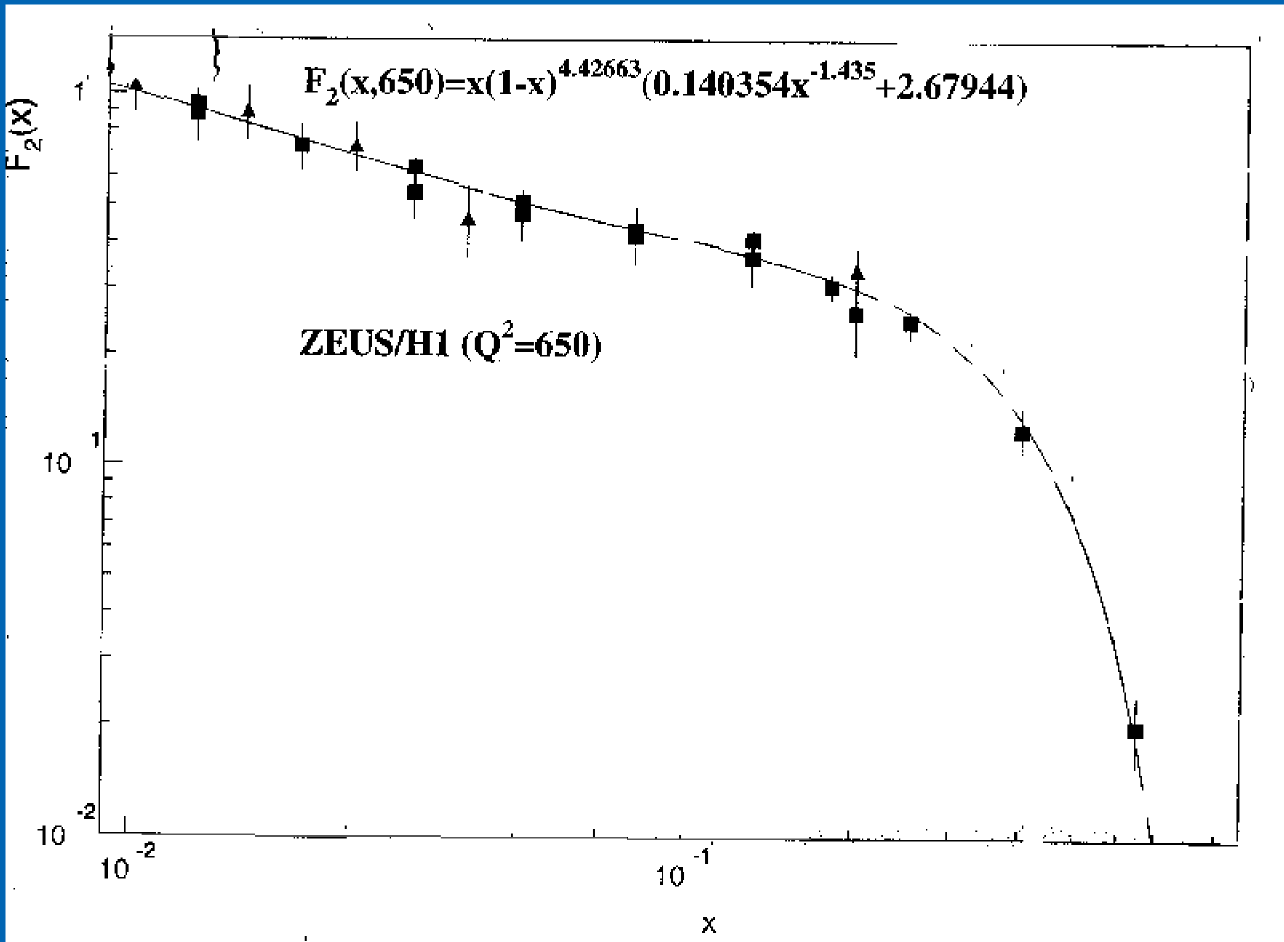
Hard scattering in electro-nuclear



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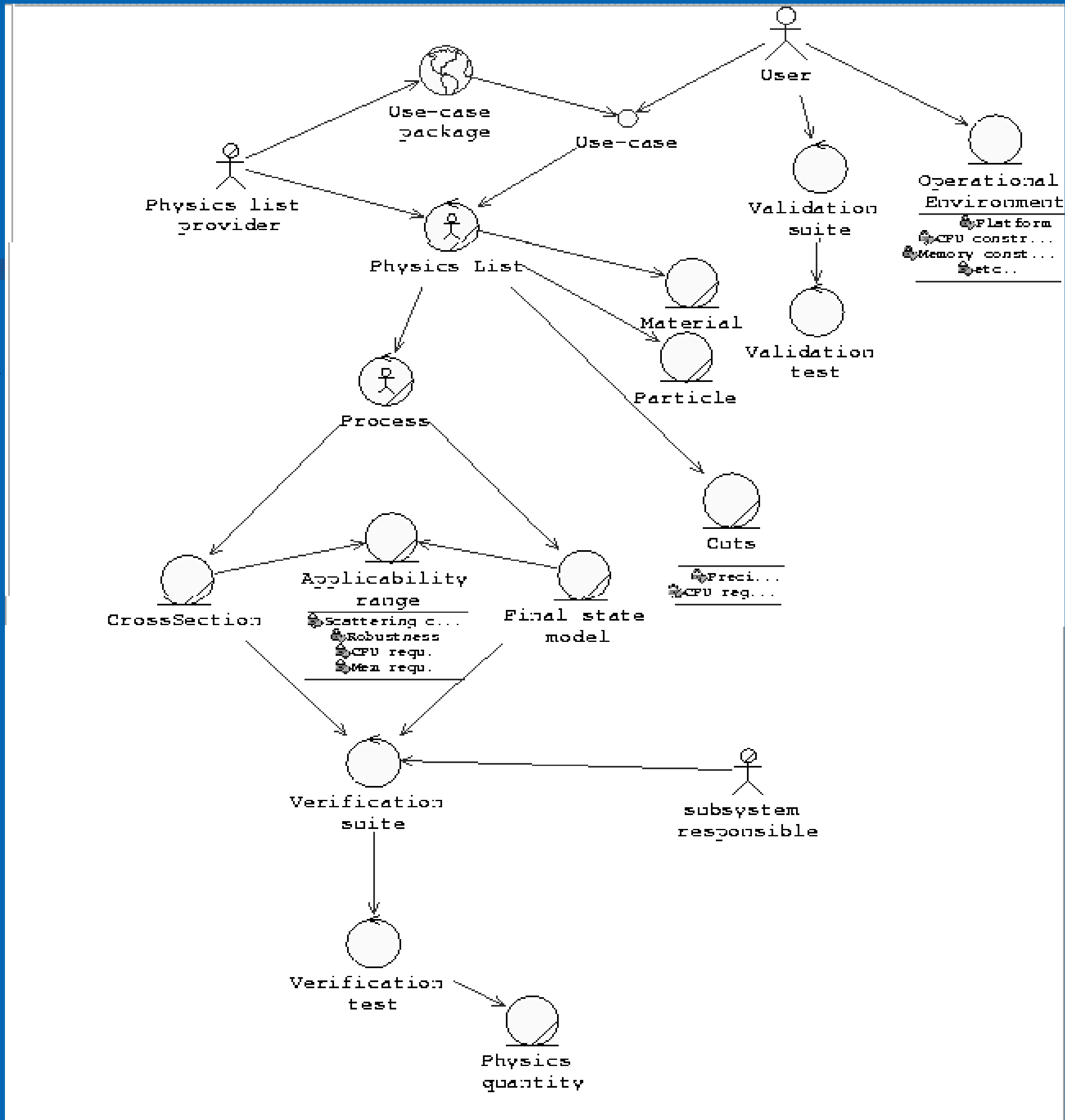
A propagation test for QMD development

- Some characteristics of QDM:
  - A kinematical cascade with detailed modeling of the nucleus.
  - Nuclear Hamiltonian calculated from 2 and 3 body potentials of all hadrons present in the system.
  - Solving the equation of motion by integrating this time-dependent Hamiltonian.
  - Scattering term in terms of localized interactions and decays.
  - Etc..

The support process – static view



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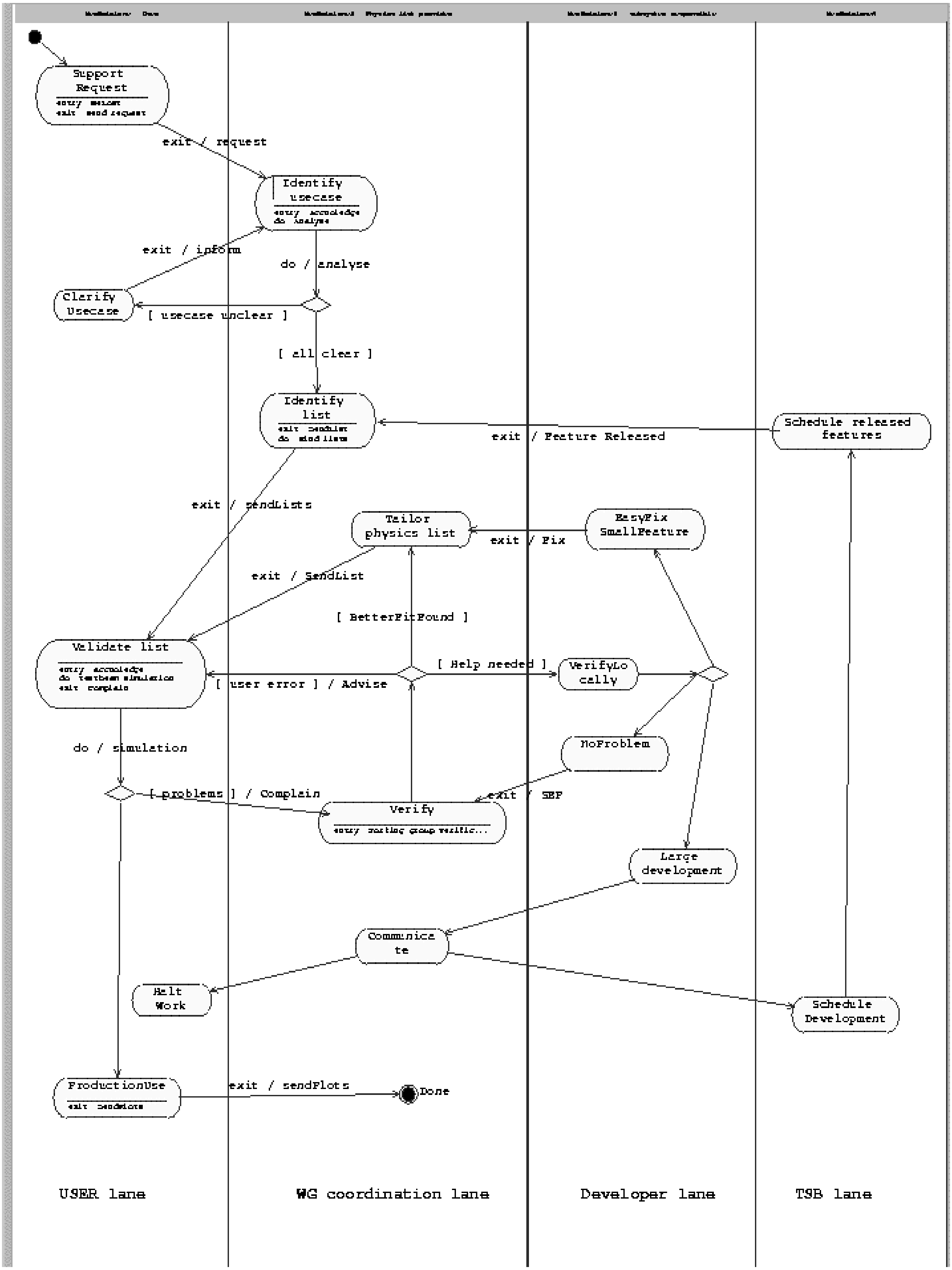
Support Request
exit / request
Identify usecase
exit / inform
do / analyse
Clarify Usecase
[usecase unclear]
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Identify list
Schedule released features
exit / Feature Released
exit / sendLists
Tailor physics list
EasyFix SmallFeature
exit / Fix
exit / SendList
[BetterFitFound]
Validate list
[Help needed]
VerifyLocally
[user error] / Advise
NoProblem
do / simulation
[problems] / Complain
exit / SBP
Verify
Large development
Communicate
Halt Work
Schedule Development
ProductionUse
exit / sendPlots
Done
USER lane
WG coordination lane
Developer lane
TSB lane

Test-beams

- Hadronic test-beam comparisons come from collaboration of experiments' detector groups with 'core' geant4 personnel.
  - ATLAS Tile test-beam
  - CMS Tile test-beam
  - ATLAS HEC test-beam
  - ATLAS FCAL test-beam
  - BTEV crystal test-beam
  - CMS combined test-beam
  - CsI test-beam benchmark
  - GLAST (starting) test-beam

  - Plots being solicited as courtesy of the experimental groups.

Other areas of known usage (likely incomplete)

- Tracker performance
  - ATLAS, CMS, BaBar
- Medical
  - Uppsala, TERA
- Neutron dosimetry, measurement, beam-lines
  - SNO, Los Alamos, CERN/PS, DoD/Can, etc..
- Radiation schielding, activation, thermalization
  - DYNAMIX, MECO, ALICE?, CMS, ESA, etc..
- Oil search and similar
  - Mitsubishi, General electrics, EXXON, ALCATEL…

The hopefully no longer dry numbers…

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- We are normally able to attract the expertise we need
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- Front-line support man-power non-trivial to find

Conclusions

- The main focus of all these developments is of course on LHC and BaBar shower physics, and dosimetry.
- ALL efforts that want to contribute to physics in the geant4 context are welcome.
- Physics modeling, physics V&V, and physics research is both the scope and concern of the geant4 hadronic working group
  - Note that we strive to make sure that individual activities are integrated to avoid duplication of work, but also trivial mistakes

Collaboration with 3rd parties
Some of the reasoning:

- Geant3 had used two strategies. There were shower packages released with geant3, and there were interfaces released with geant3; the latter were interfacing to external packages. The first was a working model, for the latter, geant3 always was claimed to be obsolete.
- GISMO: the no physics situation, but only interfacing to external packages. They never really got support for the use of these codes with GISMO.
- MCNPX: Gets it right. They encourage and help 3rd parties to release MCNP interfaces with their 3rd party code. It solves the support question.

Collaboration with 3rd parties

- Basis: We provide a set of well defined, published, and highly stable interfaces that allows interested 3rd parties to release adapters to use their code, or to use geant4 physics implementations within their infrastructure.
- EGS: geant4 chips code for γ-nuclear reactions also in EGS
- HETC: Being re-written to become natively available in G4
- INUCL: Being integrated to become natively available in G4
- UrQMD: In the process of being re-engineered to become natively available in geant4
- MCNP: Discussion on using the geant4 interfaces in MCNP
- G-FLUKA: Interfaced by 'air shower' users for their own use.
- Liege Cascade code: Discussion in progress. We hope that they will release a G4 interface soon, and are of course happy to help.

Conclusions

- It is very important that individual contributors are enfranchised to join the collaboration, in particular in the area of physics modeling.
- They must feel assured that they are well protected from any attempt to deprive them off (or copy/steal/subltiliser) the work that built their careers, I.e. their code.
- They otherwise would be asked to contribute at their own peril.
- We should explicitly state a policy ensuring this in the MoU revision.