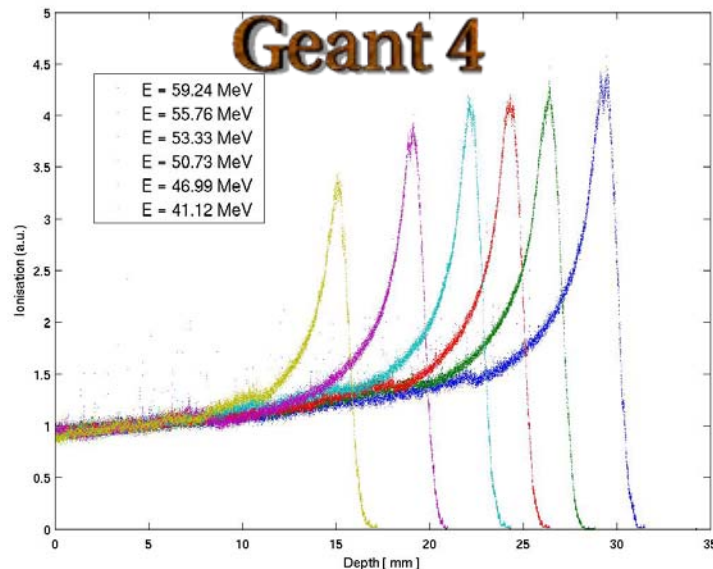


Experimental validation of **Geant 4** models in the pre-equilibrium and nuclear de-excitation phase

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CHEP 2007
Victoria, BC, Canada
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Geant4 physics

- Wide set of physics processes and models
- Versatility of configuration according to use cases
- How to best choose the most appropriate model for my simulation?
- Provide objective criteria to evaluate Geant4 physics models
 - document their **precision** against established experimental data
 - evaluate all available Geant4 physics models **systematically**
 - **publication-quality** results, subject to peer-review process
- Geant4 Physics Book
 - validation of basic Geant4 physics quantities (cross sections, final state distributions etc.)
 - demonstration of Geant4 validation in some typical use cases

K. Amako et al.,

Comparison of Geant4 electromagnetic physics models against the NIST reference data

IEEE Trans. Nucl. Sci., Vol. 52, no. 4, Aug. 2005, pp. 910-918

S. Guatelli et al.,

Validation of Geant4 Atomic Relaxation against NIST Reference Data

IEEE Trans. Nucl. Sci., Vol. 54, no. 3, Jun. 2007, pp. 594-603

● Systematic approach

- cover ALL available models
- start from the bottom (low energy)
- progress towards higher energy on the ground of previous assessments

● Quantitative validation

- rigorous statistical methods to compare simulated and experimental data

● Complementary playgrounds

- Microscopic validation of physics models features (cross sections, spectra etc.)
- Geant4 Advanced Examples: real-life use cases

● Guidance to users based on objective results

- beyond “educated-guess” PhysicsLists

Proton Bragg peak

Space Science



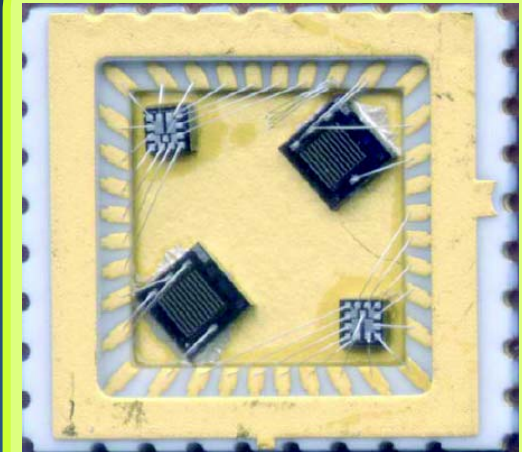
Astronauts' radiation protection

Medical Physics



Oncological radiotherapy

High Energy Physics



LHC Radiation Monitors

- Results directly relevant to various experimental use cases
- This work: performed in the context of a hadrontherapy facility

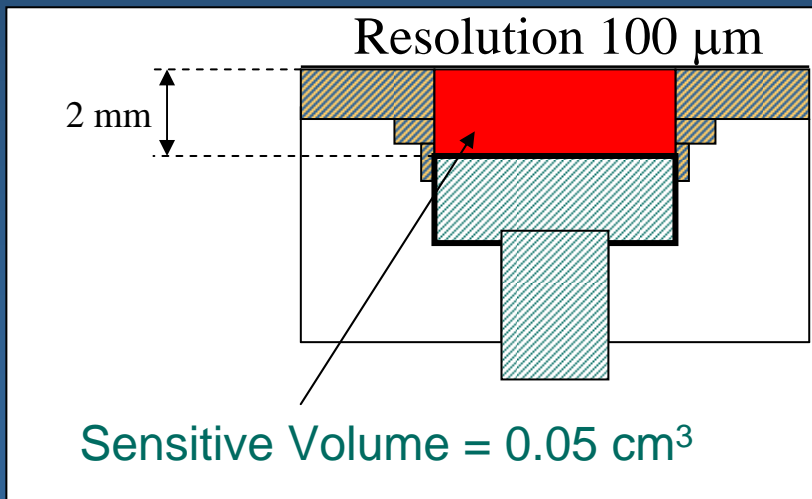
Experimental data



- CATANA hadrontherapy facility in INFN LNS, Catania, Sicily, Italy
 - High precision experimental data satisfying rigorous medical physics protocols
 - **Data taken at INFN LNS** by G.A.P. Cirrone, G. Cuttone, F. Di Rosa, G. Russo
 - Acknowledgment to the hosting laboratory: INFN LNS
 - *No credit to co-authors A.L. and MGP for experimental measurements*

More info in CATANA web site <http://www.lns.infn.it/catana/CATANA>

Markus Ionisation Chamber



Markus Chamber



G. A. P. Cirrone et al., "A 62 MeV proton beam for the treatment of ocular melanoma at Laboratori Nazionali del Sud-INFN (CATANIA)", in *IEEE Trans. Nucl. Sci.*, vol. 51, no. 3, pp. 860-865, 2004.

Geant4 test application

Accurate reproduction of the experimental set-up in the simulation

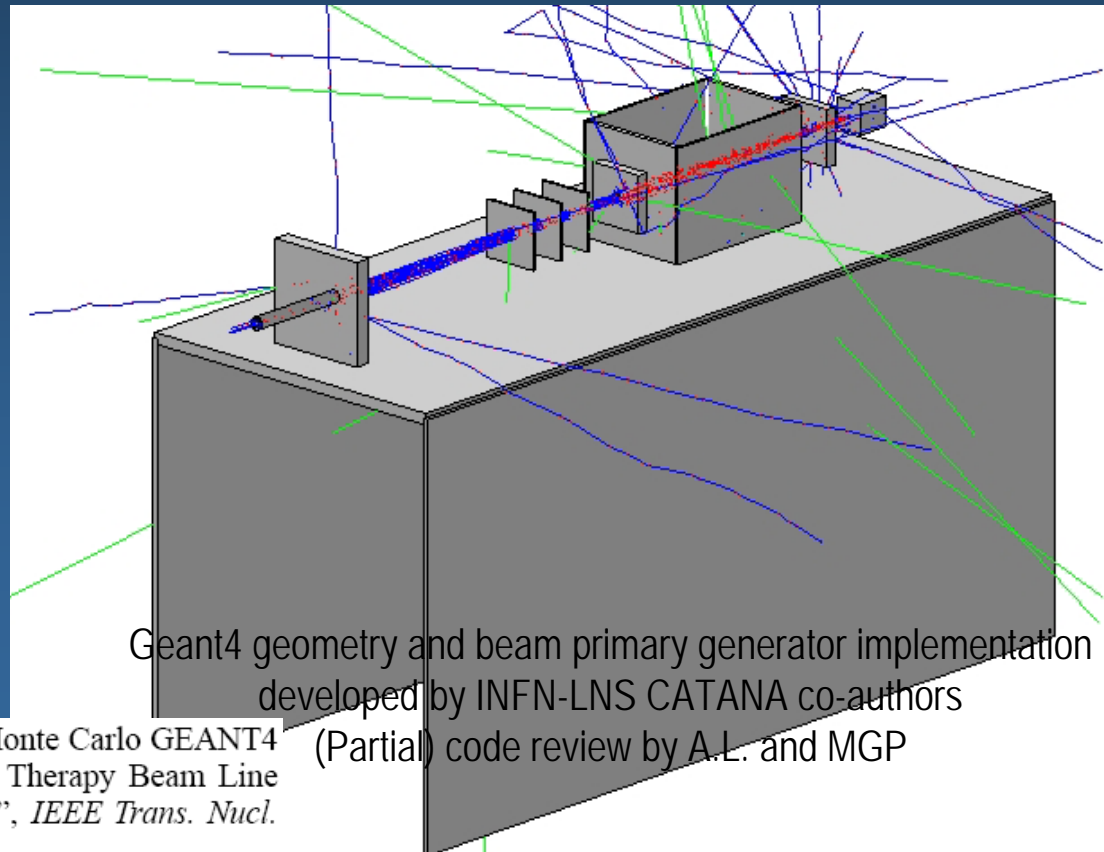
Crucial to achieve a quantitative Geant4 physics validation

Geometry and **beam** characteristics must be known in detail and with high precision



GEANT4 simulation

Geant4 hadrontherapy
Advanced Example



Geant4 geometry and beam primary generator implementation
developed by INFN-LNS CATANA co-authors
(Partial) code review by A.L. and MGP

[14] G. A. P. Cirrone et al., "Implementation of a New Monte Carlo GEANT4 Simulation Tool for the Development of a Proton Therapy Beam Line and Verification of the Related Dose Distributions", *IEEE Trans. Nucl. Sci.*, vol. 52, no. 1, pp. 262-265, Feb. 2005.

Relevant Geant4 models

Electromagnetic

- Standard
- Low Energy – ICRU 49
- Low Energy – Ziegler 1977
- Low Energy – Ziegler 1985
- Low Energy – Ziegler 2000
- *New “very low energy” models*

Assess lower energy range of hadronic interactions
pre-equilibrium + nuclear deexcitation
to build further validation tests on solid ground



Hadronic

- Elastic scattering
 - Parameterized
 - UHadronElastic
 - Bertini
 - CHIPS
- Parameterized (à la GHEISHA)
- Nuclear Deexcitation
 - Default evaporation
 - GEM evaporation
 - Fermi break-up
- Pre-equilibrium
 - Precompound model
 - Bertini model

Credits for physics models

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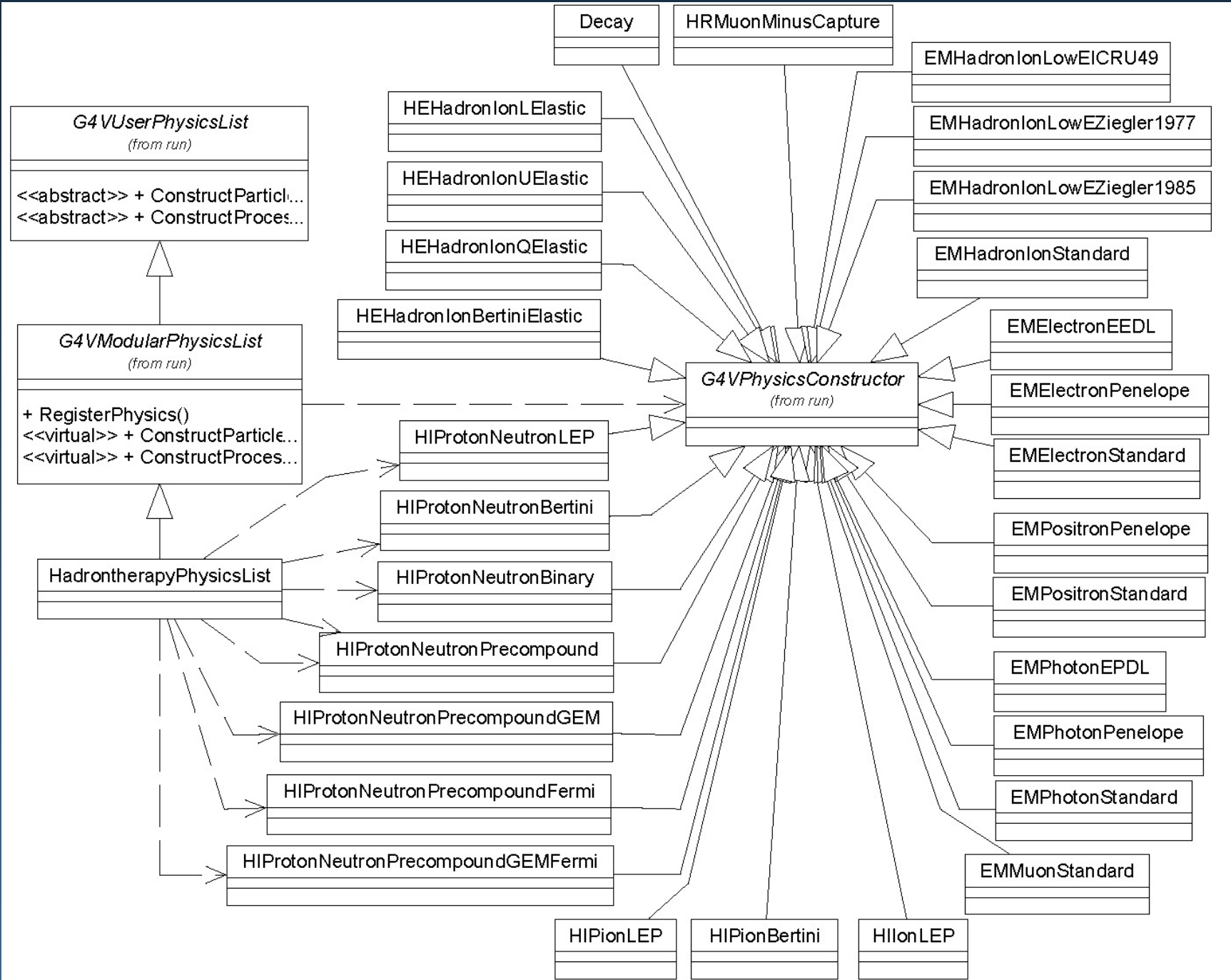
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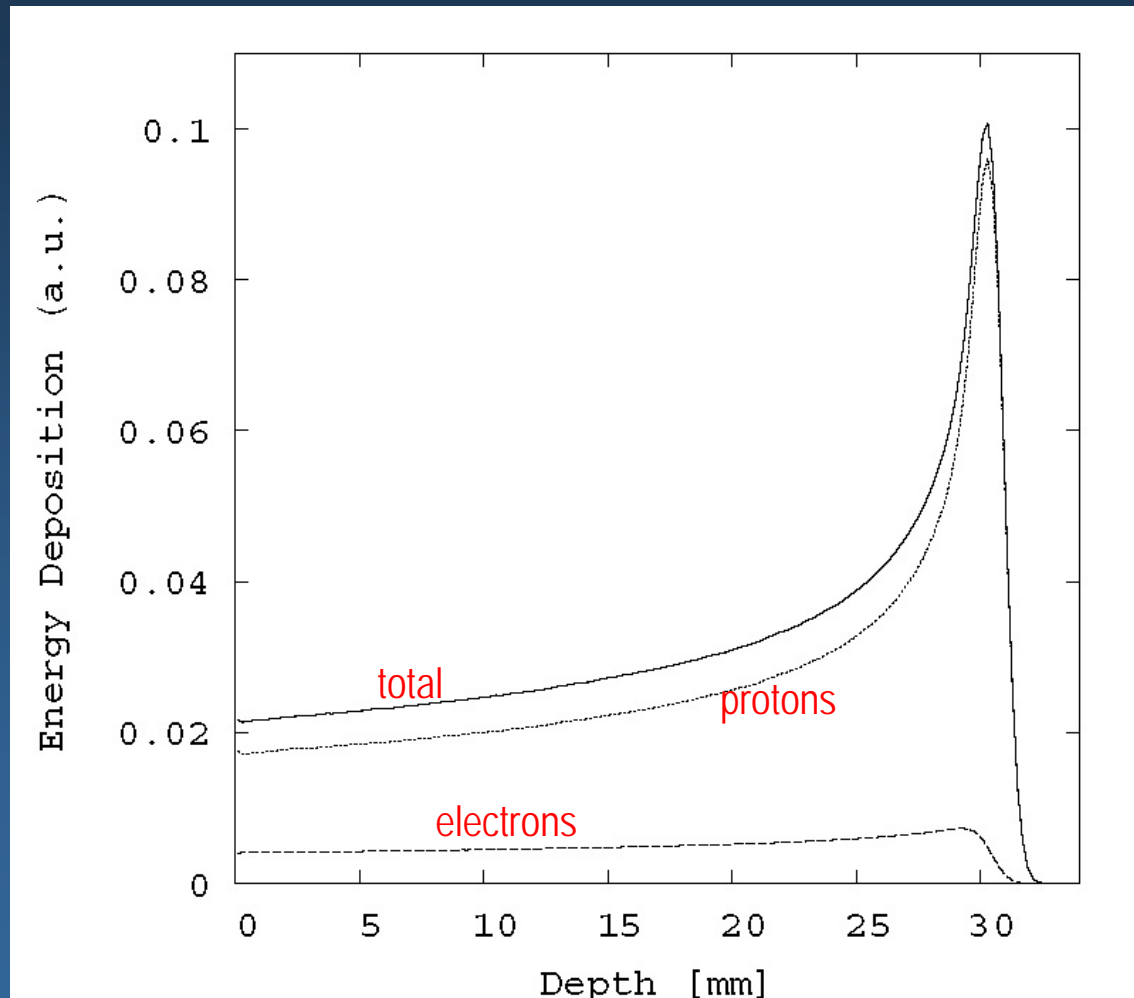
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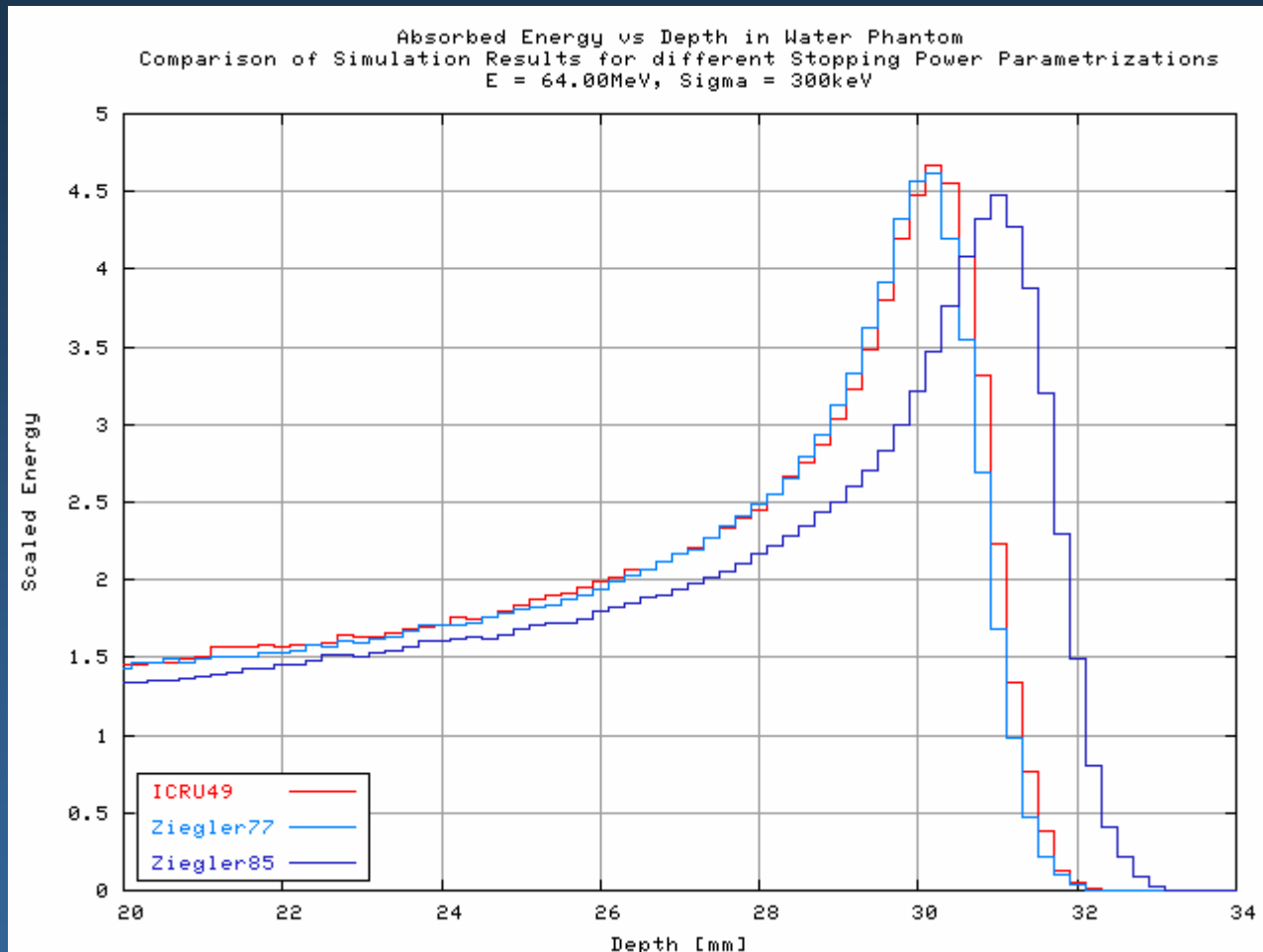
Software configuration

- Geant4 8.1 p02
 - Most of the results presented
 - Production and data analysis extended over ~ 1 year
- Geant4 9.0 (29 June 2007)
 - Subset of significant results (models updated)
- “User-like” project (with the insight as Geant4 developers)
- 1M events produced for each physics configuration
 - (unless differently stated)
- Statistical Toolkit
 - Version 2.1 (β -version used, to be released Sep. 2007)

Contributions to Bragg peak profile



Electromagnetic models



Different stopping power models produce visibly different Bragg peak profiles

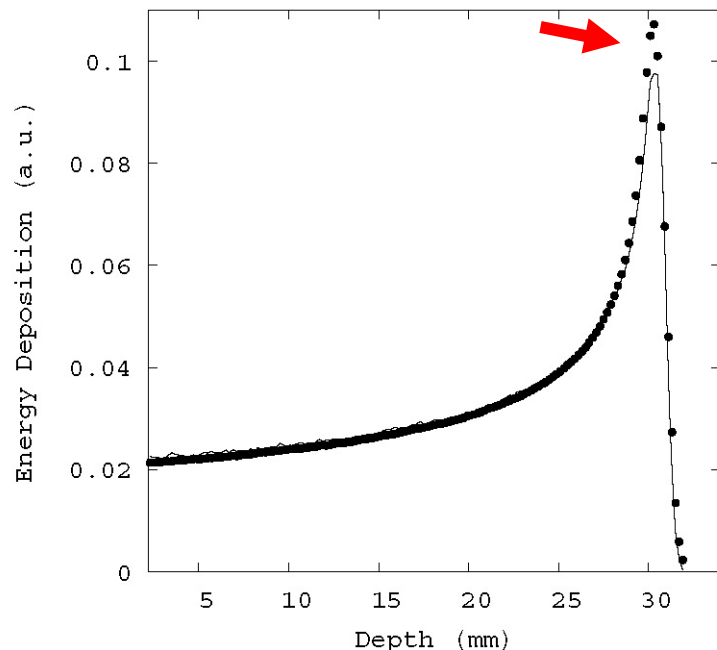
Optimisation of beam parameters

- Energy and energy spread of the CATANA beam are approximately known
 - Feature common to hadrontherapy beams
 - $E \sim 62 \text{ MeV}$, $\sigma(E) \sim 200\text{-}300 \text{ keV}$
 - No problem for therapeutical purpose
- Energy and energy spread must be determined for simulation production
 - Optimised using the experimental data themselves
 - Find beam energy and energy spread best fitting the Bragg peak profile, or best fitting the measured range in water
- No way to use these data for validating the electromagnetic models
 - Only an evaluation of plausibility of electromagnetic models
- Focus on hadronic models, after selecting an electromagnetic set-up
 - Other strategies for electromagnetic validation

Electromagnetic physics only

GEANT4 ELECTROMAGNETIC PROCESSES FOR ELECTRONS, POSITRONS AND PHOTONS

Package	lowenergy		standard
Option	Library-based	Penelope-like	
Electrons			
Ionisation Bremsstrahlung	G4LowEnergyIonisation G4LowEnergyBremsstrahlung	G4PenelopeIonisation G4PenelopeBremsstrahlung	G4eIonisation G4eBremsstrahlung
Positrons			
Ionisation Bremsstrahlung Annihilation		G4PenelopeIonisation G4PenelopeBremsstrahlung G4PenelopeAnnihilation	G4eIonisation G4eBremsstrahlung G4eplusAnnihilation
Photons			
Photoelectric effect Compton scattering Rayleigh scattering Conversion	G4LowEnergyPhotoelectric G4LowEnergyCompton G4LowEnergyRayleigh G4LowEnergyGammaConversion	G4PenelopePhotoelectric G4PenelopeCompton G4PenelopeRayleigh G4PenelopeGammaConversion	G4PhotoElectricEffect G4ComptonScattering G4GammaConversion



GEANT4 ELECTROMAGNETIC PROCESSES FOR HADRONS

Package	lowenergy	standard
Process	G4hLowEnergyIonisation	G4hionisation
Parameterised model	ICRU49 Ziegler77 Ziegler85 Ziegler2000	ICRU49

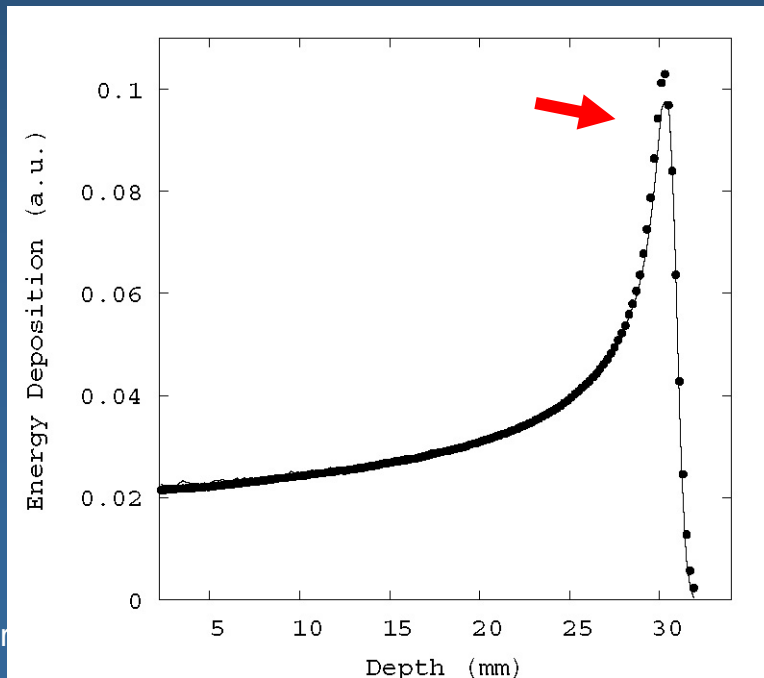
LowE EEDL-EPDL-ICRU49

Elastic Scattering

GEANT4 PROCESSES AND MODELS FOR ELASTIC SCATTERING

Processes	G4HadronElasticProcess		G4UHadronElasticProcess	G4QElastic
Package	processes		models/coherent_elastic	models/chiral_invariant_phase_space
Base class	G4HadronicProcess		G4HadronicProcess	G4VDiscreteProcess
Particle	All hadrons and ions		All hadrons and ions	p,n
Models	G4ElasticCascadeInterface	G4LElastic	G4HadronElastic	
Package	models/cascade/cascade	models/low_energy	models/coherent_elastic	
Base class	G4VIntraNuclearTransportModel	G4HadronicInteraction	G4HadronicInteraction	
Energy	< 10 GeV	Any		
Particle	p, n, π	p, n, π , ions	p, n, π , d, t, α	
Cross sections	G4HadronElasticDataSet		G4QElasticCrossSection	G4QElasticCrossSection

Logical and physical design!



LowE EEDL-EPDL-ICRU49

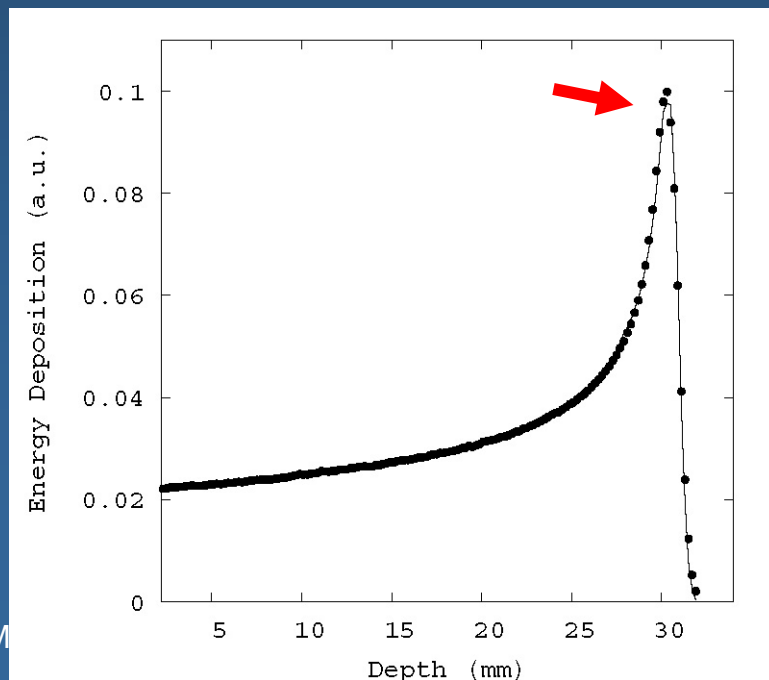
G4UHadronElastic

Hadronic Inelastic Scattering

PROCESS AND MODELS FOR PROTON INELASTIC SCATTERING

Processes	G4ProtonInelasticProcess		
Package	processes		
Base class	G4HadronInelasticProcess		
Cross sections	G4HadronInelasticDataSet G4ProtonInelasticCrossSection		
Models	Parameterised	Precompound	Bertini
Interface	G4LEProtonInelastic	G4PreCompoundModel	G4CascadeInterface
Package	low_energy	pre_equilibrium/exciton_model	cascade/cascade
Energy	< 10 GeV	< 170 MeV	< 10 GeV
Model options		Dovstrovsky evaporation GEM evaporation Fermi break up	

+ neutrons, ions

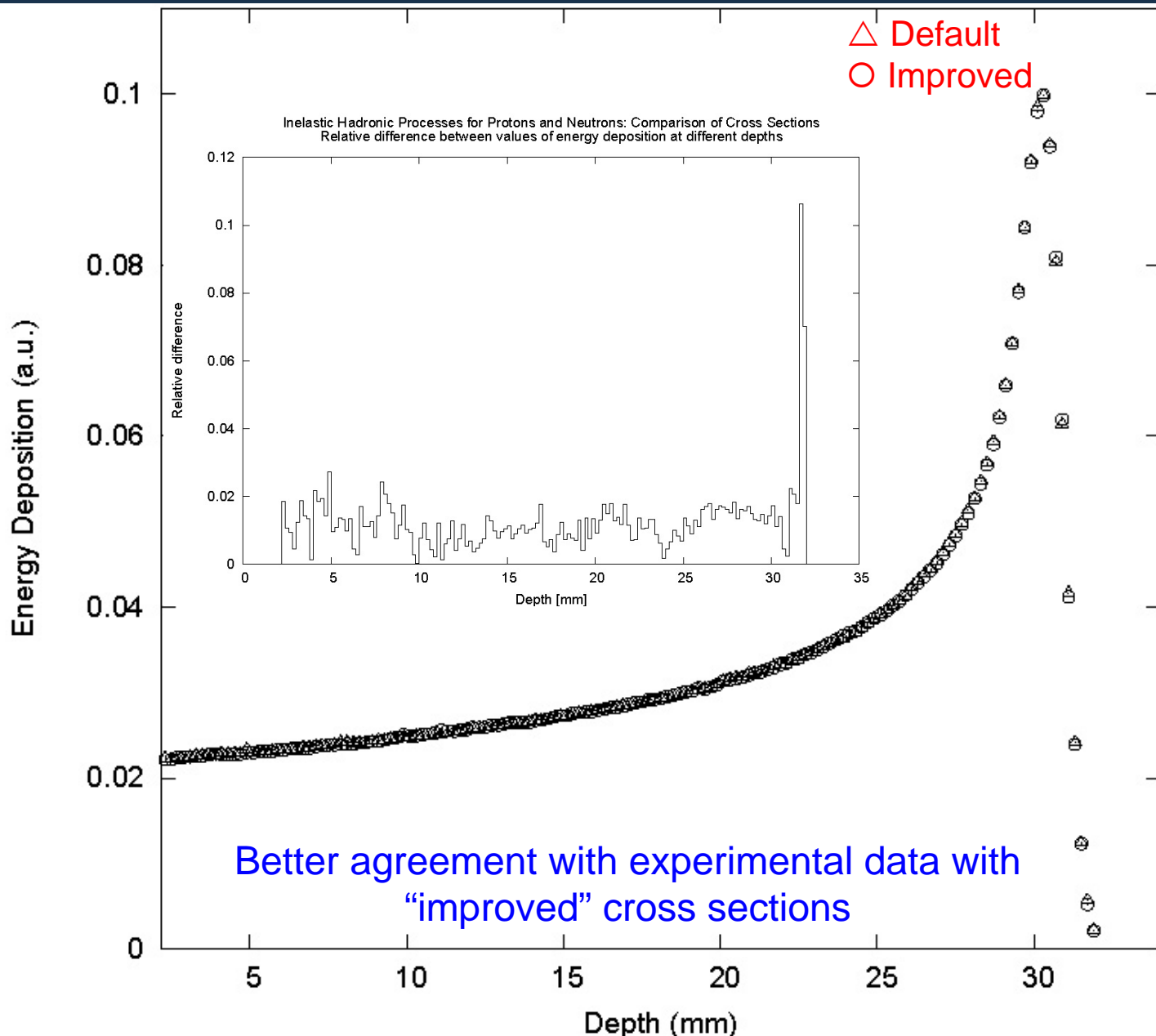


LowE EEDL-EPDL-ICRU49

G4UHadronElastic

Precompound – Dostrovsky Evaporation

Inelastic cross sections



P-value Goodness Of Fit

	Branch	Cramer vonMises	Anderson Darling	Kolmogorov Smirnov	Tiku	Kuiper	Watson
LowE EEDL EPDL ICRU49	left	0.193079	0.066764	0.142372	0.198616	0.342449	0.246875
	right	0.971884	0.986288	0.999999	0.950476	1	0.997859
LowE Penelope ICRU49	left	0.228884	0.0885704	0.186566	0.235461	0.50953	0.322665
	right	0.971884	0.986288	0.999999	0.950476	1	0.997859
EEDL EPDL ICRU49 Elastic-Gheisha	left	0.291799	0.111499	0.186566	0.298635	0.50953	0.311926
	right	0.971884	0.986288	0.999999	0.950476	1	0.979616
EEDL EPDL ICRU49 Elastic-Bertini	left	0.253406	0.0981338	0.186566	0.260319	0.50953	0.304403
	right	0.971884	0.986288	0.999999	0.950476	1	0.997859
EEDL EPDL ICRU49 Elastic-U	left	0.440595	0.178817	0.306021	0.441376	0.692105	0.485139
	right	0.971884	0.986288	0.999999	0.950476	0.999968	0.950093
EE/PDL ICRU49 Elastic-G Precompound Dostrovsky	left	0.998487	0.983378	0.993915	0.746602	0.999989	0.999929
	right	0.971884	0.986288	0.999999	0.950476	0.999968	0.926177
EE/PDL ICRU49 Elastic-G BinaryCascade	left	0.999591	0.995938	0.999408	0.727616	1	0.999996
	right	0.971884	0.986288	0.999999	0.950476	0.999968	0.926177
EE/PDL ICRU49 Elastic-G Precompound GEM	left	0.95757	0.769128	0.928293	0.881608	0.993923	0.975921
	right	0.971884	0.986288	0.999999	0.950476	0.999968	0.926177
EE/PDL ICRU49 Elastic-G Precompound Dostr. FermiBk	left	0.996874	0.987559	0.999408	0.761155	1	0.999985
	right	0.971884	0.986288	0.999999	0.950476	0.999968	0.926177
EE/PDL ICRU49 Elastic-G Precompound GEM FermiBk	left	0.95757	0.769128	0.928293	0.881608	0.993923	0.975921
	right	0.971884	0.986288	0.999999	0.950476	0.999968	0.926177
EE/PDL ICRU49 Elastic-G Inelastic-LE	left	0.983838	0.946415	0.993915	0.815811	0.999989	0.999656
	right	0.971884	0.986288	0.999999	0.950476	0.999968	0.926177
EE/PDL ICRU49 Elastic-G BertiniCascade	left	0.993789	0.950131	0.973296	0.779169	0.999821	0.999445
	right	0.971884	0.986288	0.999999	0.950476	0.999968	0.926177
EE/PDL ICRU49 Elastic-B BertiniCascade	left	0.978608	0.938323	0.993915	0.830678	0.999989	0.999775
	right	0.971884	0.986288	0.999999	0.950476	0.999968	0.979616
EE/PDL ICRU49 Elastic-U Precompound Dostrovsky	left	1	1	1	0.683034	1	1
	right	0.971884	0.986288	0.999999	0.950476	0.999968	0.926177
EE/PDL ICRU49 Elastic-U Precompound GEM	left	0.979687	0.931731	0.993915	0.827739	0.999989	0.999863
	right	0.971884	0.986288	0.999999	0.950476	0.999968	0.950093
EE/PDL ICRU49 Elastic-U Precompound Dostr. FermiBk	left	0.999998	0.999999	1	0.691358	1	0.999998
	right	0.971884	0.986288	0.999999	0.950476	0.999968	0.926177
EE/PDL ICRU49 Elastic-U Precompound GEM FermiBk	left	0.999058	0.993946	0.993915	0.73884	0.999989	0.999978
	right	0.971884	0.986288	0.999999	0.950476	0.999968	0.926177

Statistical analysis - Comments

- Several GoF tests

- Avoid systematics
- Relative consistency among tests
- Strictest: Anderson-Darling

Details of model performance
impossible to appraise
qualitatively

Statistical analysis is essential

- Electromagnetic only: p-value < 0.1

- Elastic: **G4UHadronElastic** consistently the best performing

- Evaporation: **Dostrovsky** better than **GEM**

- Fermi Break-Up: irrelevant

- All-Bertini (Bertini Elastic + Bertini Cascade)

- Worse than G4UHadronElastic + Precompound)

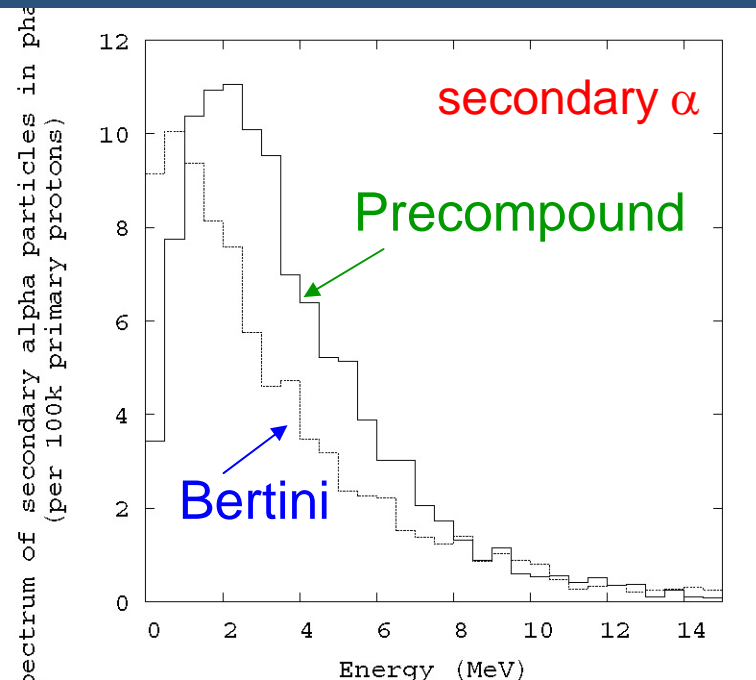
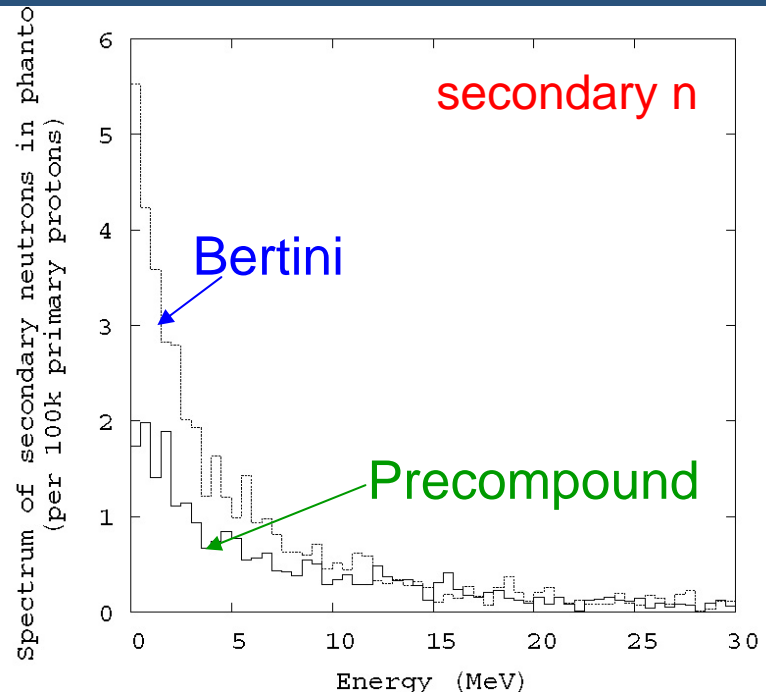
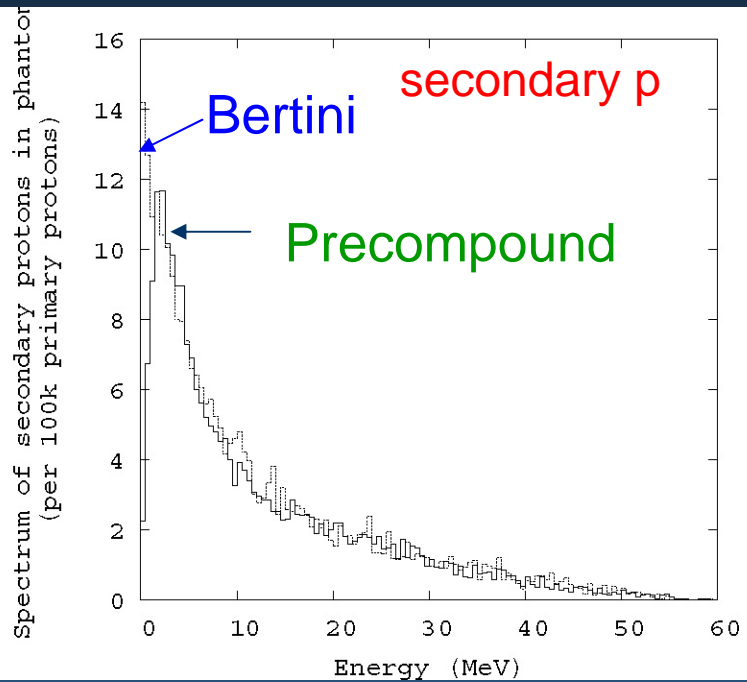
- All-GHEISHA-like (G4LEElastic + G4LE*Inelastic)

- Worse than G4UHadronElastic + Precompound)
- Slightly better than all-Bertini

Preequilibrium Evaporation

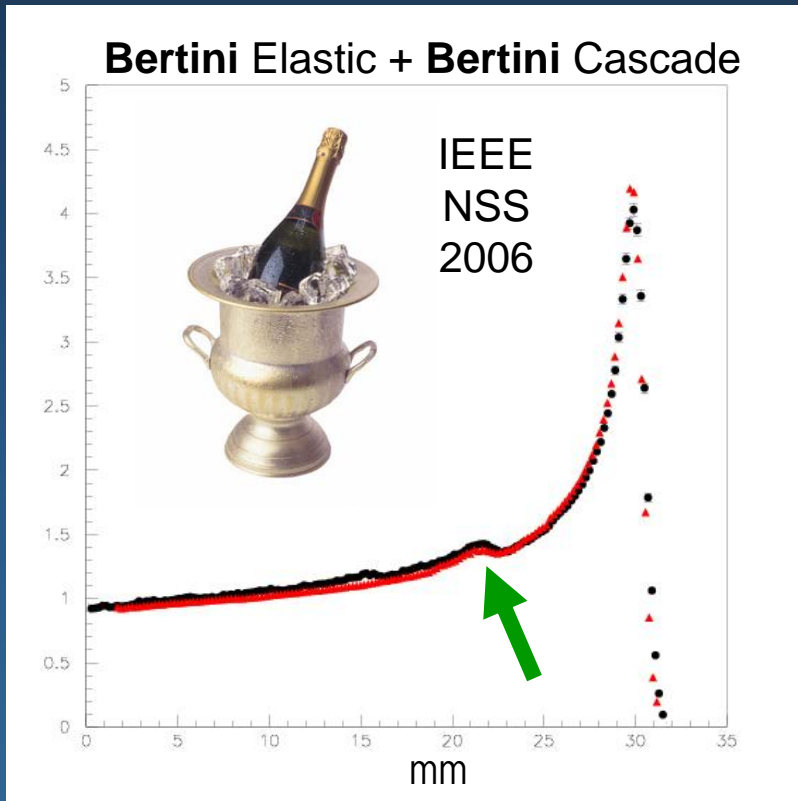
Hadronic inelastic models do behave differently

e.g. different secondary spectra produced



Evolution from preliminary results

- Different experimental data set
 - CHEP 2007: higher quality data
- Larger simulated statistics
 - CHEP 2007: factor 2-20 more events
- Higher quality software
 - Hadrontherapy design and code review
 - Statistical Toolkit code review
- Software process
 - RUP enforced
 - Team respectful of software process
 - NSS 2006: G4CascadeElasticInterface produced neutrons!!! Not verified by NSS 2006 hadrontherapy developer



Evolution in Geant4 9.0 (*preliminary*)

- Major known change relevant to Bragg peak profile
 - “Improved” version of G4UHadronElastic
- Effects observed
 - Significantly reduced filtering effect in beam line
 - ~15% primary protons reach the phantom
 - Previously: ~5%
 - Worse overall agreement between simulated Bragg peak and experimental data
- Surprise!
 - No difference between “default” and “improved” hadronic inelastic cross sections
 - Change management?
- Electromagnetic, hadronic inelastic (Precompound-Dostrovsky)
 - No difference observed

Conclusion

- ...after 4 years' work
 - First results presented at NSS 2003 by G.A.P. Cirrone
- Quantitative evaluation of Geant4 models in the pre-equilibrium and evaporation phases + elastic scattering for $E < \sim 100$ MeV
- PhysicsList based on objective ground
- More work needed for the electromagnetic models
 - Current hadrontherapy data not adequate to quantitative evaluation of models
 - Complementary data are needed
 - HEP/medical worlds
- Part of the Geant4 Physics Book project
- To be submitted for publication in IEEE Trans. Nucl. Sci.

CHEP 2007



Anton Lechner

Austrian Doctoral Student
CERN IT/PSS

A BIG thank you!

Their support for
simulation production
and data analysis
has been crucial to
the project



Jürgen Knobloch



Patricia Mendez Lorenzo



Kuba Moscicki



Andreas Pfeiffer

Maria Grazia Pia

CERN IT/PSS

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