

Constructing Efficient Monte Carlo Generators

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> VANISH School 03.04.2014



Outline of the lecture

Part I

- Introduction
- General neutrino Monte Carlo scheme
- General optimization tricks

Part II

- Selected interaction channels
- All-in-one example: intranuclear cascade.
- Summary







Introduction



Purpose of MC simulations

- In HEP experiments: simulation of particle interactions.
- Monte Carlo: statistical description and tool to understand your experiment with all its systematic and statistical errors.
- Lots of input and dependencies:

theoretical models, experimental data, engineering knowledge etc.





Purpose of MC simulations

• Shortly: how to put it all together and get from here:



To our Physical Review Letters result:

phase $\delta_{\rm CP}$. In this neutrino oscillation scenario, assuming $|\Delta m_{32}^2| = 2.4 \times 10^{-3} \text{ eV}^2$, $\sin^2 \theta_{23} = 0.5$, $\delta_{\rm CP} = 0$, and $\Delta m_{32}^2 > 0$ ($\Delta m_{32}^2 < 0$), a best-fit value of $\sin^2 2\theta_{13} = 0.140^{+0.038}_{-0.032}$ ($0.170^{+0.045}_{-0.037}$) is obtained.



General neutrino MC scheme



 Our focus: generators for neutrino interactions: beam profile, detector, target nucleus interaction vertex and process (dynamics), final state interactions (FSI) (e.g. GENIE, NEUT, <u>NuWro</u>)





Handling the probabilities

Probability of drawing a neutrino flavor f with energy E interacting at point (x,y,z) with nucleus N through dynamics D producing outgoing particles {X_i}...



What's inside the black box?



NuWro

- Main example during this talk: NuWro, the Wrocław neutrino events generator.
- The project started 2005 at the Wrocław University; an important encouragment from Danuta Kiełczewska from Warsaw
- Main authors: Tomasz Golan, Krzysztof Graczyk, Cezary Juszczak, Jarosław Nowak, Jan Sobczyk, Jakub Żmuda.
- Code written in C++ language.
- First (natural) name: Wrocław Neutrino Generator: WroNG → changed from marketing reasons... (Jan T. Sobczyk, Jaroslaw A. Nowak, Krzysztof M. Graczyk "WroNG - Wroclaw Neutrino Generator of events for single pion production" Nucl.Phys.Proc.Suppl. 139 (2005) 266)



NuWro is not an official MC in any experiment and serves as a laboratory for <u>new developments.</u>

Relatively new components (introduced or developed recently also in GENIE and NEUT):

- 1) Meson exchange currents
- 2) Random phase approximation (on top of RFG)

NuWro

- 3) Spectral function
- 4) Electron simulation coming soon!

http://borg.ift.uni.wroc.pl/nuwro/

Repository, documentation, NuWro on-line



Beam profile

Simple case: ", perfect" beam with only one flavor:



- Uniform bin spacing, *n* bins in neutrino energy, bin width $\Delta E = (E_{max} E_{min})/n$.
- Calculate the cummulative distribution function, invert it, or accept event according to weight~bin height?
- Actually not very effective algorithms!



• Second bin twice as probable as the first one, same widths $\Delta E = (E_{max} - E_{min})/2$.

• Distribution "flip": histogram h[i] with bin heights plus extra element with their sum Σ i=2

a + 2a = sum=3a

- *frand()* random number [0,1], MT19937. $x=frand()*sum; x < a \rightarrow i=0$ else i=1;
- Uniform sampling with second bin twice as probable as first.
- After setting *i* : linear interpolation of energy inside bin (spectrum is continuous!): $E=E_{min}+i^{*}\Delta E + frand()^{*}\Delta E;$



Beam profile

Extension to any number of bins! ;)

All neutrinos with equal weights Only some happen more often



- Beam: some distribution in space+direction of neutrinos
- Detector: geometrical distribution of matter (local density and composition- fraction of isotopes).





- Beam: assume neutrino direction along the z-axis.
- Detector: geometrical distribution of matter (local density and composition- fraction of isotopes).





- Beam: assume neutrino direction along the z-axis.
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Nuclear interaction vertex

- Two steps in each event:
- A) Position of vertex inside the nucleus (density-depedent)
- B) Dynamics choice: weights from flux-integrated total cross sections
- Part A) for single-nucleon interaction: relatively easy. Each nucleus: nuclear matter density profile with spherical symmetry $\rho(r)$.
- Normalized probability:

$$P(r) = \frac{4\pi}{A} r^2 \rho(r), \int P(r) dr = 1$$



Nuclear interaction vertex

 To sample vertex position: find maximum probability P_{max} (efficiency/speed tip: do it only once, when your nucleus gets generated for the first time!)

$$P(r) = \frac{4\pi}{A} r^2 \rho(r), \int P(r) dr = 1$$



Each dista	nce \rightarrow P=P(r)/P _{max} .
Choose pr	oton (P=p/(p+n)) or neutron
(P=n/(p+n))). Special case: CCQE:
always ne	utron (neutrinos) or always
proton (anti-neutrinos).	



Test events

- Assume N channels $D_1...D_N$ (CCQE, NC EL, DIS, MEC...)
- No a prori knowledge of $\sigma_1 \dots \sigma_N \rightarrow$ "test events". NuWro: the only generator calculating weights during run \rightarrow flexibility to physical model and parameter (e.g. M_A) changes!
- For each D_i: calculation of flux-integrated total cross section- weight w_i, search for maximum differential cross section w_i^{max}.
- Test events: fast (no FSI, no save to file- unless specified otherwise!).
- Good to have as many test events, as possible, in NuWro 10 000 000 \rightarrow nothing unusual.



Real events





Already covered:

1) General scheme of MC simulation (beam \rightarrow detector \rightarrow event)



Next: general optimization "tricks"



General optimization tricks



Peaked cross sections

For QE and coherent processes: forward-peaked distributions



- Acceptance according to $P = \sigma / w_i^{max}$. Very low efficiency (imagine doing 10 000 coherent events to get 2 accepted)
- Very probable large changes of w^{max}.



Handling physics: growing cross sections

- Another special case; Deep Inelastic Scattering
- Saturation of σ/E for isoscalar targets (source: J. Nowak PhD thesis- early NuWro):



- DIS \rightarrow first rapd, than linear growth of cross section with energy.
- Small flux (above 1 GeV in T2K) and LARGE event weight (DIS cross section).



Handling physics: growing cross sections

Another (typical) re-weight:

 $P(E) \rightarrow P(E) \cdot E$ $\sigma(E) \rightarrow \sigma(E) \div E$

Fix of DIS efficiency and sampling



Discretized probability distributions







Frame of reference





Frame of reference

Boost to neutrino-nucleon centre-of mass frame (CMS)





- Already covered:
- 1) General scheme of MC simulation (beam \rightarrow detector \rightarrow event)
- 2) General optimization tricks (peaked or growing cross sections, sampling from discretized distributions, frame of reference choice)









Selected interaction channels



Physical channels in NuWro





Physical channels in NuWro

Relatively new components (introduced recently also in GENIE and NEUT):

- 1) Meson exchange currents
- 2) Random phase approximation (on top of the RFG)

3) Spectral function

Topic of this section



Meson Exchange Currents

- MEC: growing interest in neutrino community
- First proposals of MEC search in neutrino interactions in T2K!
- MEC "cartoon":



- Need for MC implementation.
- In NuWro three models: Marteu-Martini-like, Transverse Enhancement and <u>Valencia</u> model.
- Each theoretical model above → inclusive muon double-differential cross sections, no information about nucleon kinematics


- Information about actual nucleon dynamics: unavailable \rightarrow effective ansatz.
- Microscopic models predicting inclusive cross sections: (local) Fermi gas ground state → two (or three) random nucleons from local denstiy distribution (NuWro).
- Problem: around 20% nucleons in strongly correlated proton-neutron pairs with back-to-back momenta → developing version with correlated nucleons with momenta randomized from spectral function (J. Sobczyk's talk in Seattle)



- Vertex position inside the nucleus:
- 1) Two nucleons at the same point in space, probability $\sim \rho^2$.
- 2) Two nucleosns at different points in space: both from single-particle distribution $\sim \rho$.
- Second solution: different (local) Fermi momenta, used for Valencia implementation.
- Isospin content: in NuWro free parameter (default 60% mixed p-n initial pairs)



From J. Sobczyk's talk in Seattle

Impact of correlation effects on number of proton pairs in the final state:



Isospin and momentum correlations are analyzed seperately. A possible confusion: In above figures correlations means initial state nucleon momenta are back-to-back.



algorithm by J. Sobczyk Phys. Rev. C86 015504 using hadronic CMS:



The same in each MEC muon inclusive cross section model:





 Example of Valencia MEC model: even with numerical approximations (J. Nieves, I. Ruiz-Simo, M.J. Vicente-Vacas Phys.Rev. C83 (2011) 045501) 5-fold integrals inside double-differential cross section (main model prediction):





- Usual approach: discrete tables for chosen kinematic variables (e.g. E_{ν} , T_{μ} , $\cos(\Theta_{\mu}) \rightarrow$ first attempt in NuWro, then NEUT).
- Limited energy range problem (first:series from J. Nieves only ~3 GeV, then extension up to 30 GeV)
- Optimal binning dependent on flavor, antineutrinos etc. \rightarrow usually non-uniform.
- Linear interpolation for each nucleus 92 (E) x 31 (cos(Θ)) x 31 (T) x 2 (flavors) x 2 (antineutrinos)=353648 points dσ/dT dcos(Θ) [10⁻⁴¹cm²/GeV] ¹²C 0.2 GeV v_u XS tables





Higher energies: cut in momentum transfer to q_{max}=1.2 GeV. Above: effective field theory failure, R. Gran, J. Nieves, F. Sanchez and M.J. Vicente Vacas Phys.Rev. D88 (2013) 113007. Rapid phase-space collapse





- So far separate tables: energy, target, flavor, antiparticle...
- Point of view of nucleus (one boson exchange (OBE), no polarization):



Nucleus "responds" only to what it "knows"!



Unpolarized inclusive double-differential neutrino cross section:





- Idea: keep all complicated cross sections as structure functions:
- 1) No need for separate tables in neutrino energy \rightarrow no upper limit.
- 2) No need for separate tables for flavors.
- 3) No need for separate tables for antineutrinos.
- 4) Same binning always.
- 5) Because 4) \rightarrow simple algorithm for all cases, e.g. linear interpolation with uniform step \rightarrow gain in speed.
- Smaller data set (Carbon+Oxygen muon/electron (anti) neutrino=353 648 points, response function grid Carbon+Oxygen 2*5*120*121/2 = 72 600 points).
- 7) "Natural" cut in momentum transfer.



- Valencia MEC: limited region (q^o<|q| and limited |q|). Other models: response saturation hypothesis, extrapolation for higher values.</p>
- Warning: grid step in q⁰= grid step in T_{μ} . E.g. 10 MeV step in q^{o} for 200 MeV muon neutrino = 8 available points in T_{μ} for interpolation in kinetic energy \rightarrow possible resolution loss near MEC threshold, but at T2K peak ~600 MeV almost 50 points!
- Near threshold: small beam intensity and small MEC cross section, not a real problem?
- For $E-m_i > q_{cut}$ saturation of resolution (whole grid available).



- Thanks to courtesy of J. Nieves and M. J. Vicente Vacas: code for MEC hadronic tensor element production = code for structure functions.
- I0x10 MeV grids for Carbon, Oxygen and Calcium up to momentum cut (NuWro).
- Only physical region stored (q⁰<|q|).</p>
- Our dilemma:





• Sample double-differential cross sections for 1 GeV v_{μ} scattering off ¹²C.

(left- from cross section tables, right – from response functions)





Relative difference in total cross sections:



- At 0.2 GeV difference up to 10%, above 0.5 GeV: differences below 4%, 1-2% at 1 GeV.
- Near 0.2 GeV: small cross section, small T2K flux, at the verge of detector possibilities → no problem, posiible more dense binning
- Response function approach valid!
- For theoretical models predicting inclusive cross sections: store response functions not cross sections.



 Whenever possible, do analytic kinematic limits. e.g. Valencia MEC model solutions both for energy transfer and scattering angle:

$$\cos(\Theta)_{min} = \frac{E_{\nu}^{2} + \vec{l}'^{2} - q_{max}^{2}}{2E_{\nu}|\vec{l}'|} < 1 \Rightarrow E_{\nu}^{2} + (E_{\nu} - q^{0})^{2} - m_{l}^{2} - q_{max}^{2} - 2E_{\nu}\sqrt{(E_{\nu} - q^{0})^{2} - m_{l}^{2}} < 0$$

- For each randomized neutrino energy \rightarrow limits, then:
- 1) Evaluate phase space in energy transfer and in scattering angle.
- 2) Sample inside <u>allowed</u> phase-space.
- 3) Calculate cross section (event weight).
- Less zero weight events, bigger efficiency



 Spectral Function: replacement of usual (local) Fermi distribution for quasielastic event by a probability distribution of removing nucleon with momentum *p* leaving the residual nucleus with excitation energy *E*. Extra integral in cross section:



- Mix of theoretical mean-field calculation (shell model orbitals) and short-range correlations with experimental data on actual orbital occupation numbers and momentum spreadings plus a lot of phenomenological "cooking".
- Works of Omar Benhar's group
- In NuWro: implementation based on A. Ankowski PhD thesis by C. Juszczak



Example Oxygen SF:





- Again, $P(\mathbf{p}, E)$ first-principle computation too complicated for MC.
- Response function: good for cross sections, but here- nucleon kinematics!
- Storage of *P*(*p*,*E*) (two methods in NuWro): ۲
- 1) Two-dimensional grid in momentum and removal energy "grid SF"
- 2) Effective SF with removal energy probabilities as a vector of gaussians

[central value E_{0i} , width w_i , norm N_i] \rightarrow A. Ankowski PhD thesis



Grid SF: ¹²C, ¹⁶O, ⁴⁰Ar, ⁵⁶Fe, gaussian SF ¹⁶O, ⁴⁰Ca, ⁴⁰Ar. ۲

No lepton FSI, which change differential cross section shapes (electron/muon ۲ energy re-distribution -different FSI from hadronic ones)! 44



- Both cases:
- 1) Create spectral function (find a way to do it once for the first interaction with given target!), get $P(p) \rightarrow$ integration (gaussian) or sum (grid) of P(p,E) w.r.t. E. (possible pre-calculation and storage in data files \rightarrow some CPU time saved).
- 2) Get neutrino from the beam.
- 3) Get interaction point from LFG density distribution.
- 4) Sample momentum p according to P(p), uniform sample direction.
- 5) Sample P(E|p).
- 6) Boost to neutrino-nucleon CMS.
- 7) Uniform decay.
- 8) Boost back to laboratory frame
- 9) Check Pauli Blocking

Typical for QE, save for PB

Typical for QE

SF only!



- Pauli Blocking in SF MC: not exactly obvious:
- 1) First method: mean Fermi momentum \rightarrow sharp cutoff
- 2) Second method: interaction point from local density distribution \rightarrow local Femi momentum \rightarrow better, smooth distribution (NuWro)
- 3) Third method: probability $P(p_p)$ translated for occupational number for final

momentum state $n(p_{i})$: check frand() against $n(p_{i}) \rightarrow$ closest to actual SF physics,





Random Phase (Ring) Approximation



 Algebraic solution of Dyson equation (by K. Graczyk – relativistic Ring Approximation)



Random Phase (Ring) Approximation

NuWro RPA implementation



K.M. Graczyk, JTS, Eur. Phys. J C31 (2003) 177

For QE Marteau is basically the same as Martini model.

K. Graczyk

d² RPA $d^2 T_{\mu} d \cos \theta$ doLFG $dT_{\mu}d\cos\theta$





- Already covered:
- 1) General scheme of MC simulation (beam \rightarrow detector \rightarrow event)
- 2) General optimization tricks (peaked or growing cross sections, sampling from discretized distributions, quick sampling from Fermi ball, frame of reference choice)
 3) Handling complicated interaction models (MEC/SF/RPA)



Next: we use all the mentioned tricks for FSI



All-in-one example: Intranuclear cascade



All-in-one example: intranuclear cascade

All particles start inside nucleus. Way out: a lot can happen



FSI: quantum transport equations or intranuclear cascade (NuWro).



All-in-one example: intranuclear cascade

1)Handling probabilities, reference frame change, effective modeling \rightarrow all in one (T. Golan -upcoming PhD thesis!).





All-in-one example: intranuclear cascade – particle step

Probability of interaction with nucleon at distance x:

 $P(\lambda) = \exp(-\lambda/\bar{\lambda})$

Mean free path: dependence on nuclear matter density ρ and cross σ sections (EL, CEX, PB, ABS, n π).

Exponential distribution sampling:

$$\lambda(r) = -\frac{1}{\sigma_p \rho_p(r) + \sigma_n(r) \rho_n(r)} \ln(frand())$$

- Propagation by $\lambda(r) \rightarrow$ sometimes too big w.r.t. typical nuclear matter density changes. Introduction of λ_{max} = e.g. 0.2 fm.
- Cascade step $min[\lambda(r), \lambda_{max}]$. Interaction if $\lambda(r) < \lambda_{max}$.



All-in-one example: intranuclear cascade - particle step

- Example of Formation Zone (FZ) (new particle interaction possible after given distance): first move by the FZ length \rightarrow different model for nucleons and pions.
- Outside of nucleus condition:
- 1) Global FG: $r > r_0 A^{1/3}$; $r_0 = 1.25 + /-0.20 \text{ fm}$.

2) Local FG: local densty smaller, than some small fraction of ρ_{max} (e.g. $10^{-6}\rho_{max}$)





All-in-one example: intranuclear cascade - particle step

Importance of Formation Zone effect





- Case of Formation Zone (FZ) (new particle interaction possible after given distance): first move by the FZ length → different model for nucleons and pions.
- Cascade step $min[\lambda(r), \lambda_{max}]$. Interaction if $\lambda(r) < \lambda_{max}$.
- Outside of nucleus condition:
- 1) Global FG: $r > r_0 A^{1/3}$; $r_0 = 1.25 + -0.20$ fm.

2) Local FG: local densty smaller, than some small fraction of ρ_{max} (e.g. $10^{-6}\rho_{max}$)

Tip for nucleon propagation: remember about nucleus potential energy V(r) and density reduction after removal from nucleus (proportional local density reduction). Otherwise constant density (unlimited nucleon supply) + Fermi motion (extra energy for interactions) = 20+ protons knocked out by 300 MeV neutrino of Carbon nucleus !



All-in-one example: intranuclear cascade – interaction models

- Cross sections for nucleons:
 - Metropolis et al. model from Phys.Rev. 105 (1957) 302-310
 - plus some corrections and extra points from modern experimental data.
 - Storage in data tables in function of nucleon kinetic energy between 350 and 3900 MeV. Below 350 MeV \rightarrow analytic function of velocity from fit to higher energy data, above: constant values.
- Cross sections for pions: either Metropolis et al. (Phys.Rev. 110 (1958) 204-219) experimental data model or microscopic calculation (default):
 - E. Oset, L.L. Salcedo, D. Strottman, Phys.Lett. B165 (1985) 13-18 \rightarrow L.L. Salcedo,
 - E. Oset, M.J. Vicente-Vacas, C. Garcia-Recio Nucl. Phys. A484 (1988) 557



All-in-one example: intranuclear cascade – interaction models

• Probabilities in microscopic model ($N\pi^{\lambda} \rightarrow N\pi^{\lambda'}$):



- Delta self- energy calculated and parametrized by E. Oset and L.L. Salcedo, Nucl. Phys. A468 (1987) 631.
- Metropolis-like tables in pion kinetic energy AND nuclear matter density (constant steps for quick search and interpolation).



All-in-one example: intranuclear cascade

- After random interaction choice: random momentum sampling from local Fermi ball, kinematics done in hadronic CMS (symmetries!).
- Path randomization \rightarrow covered, cross section \rightarrow covered, kinematics \rightarrow covered, interaction choice \rightarrow covered
- Challenge: hadrons go but also new hadrons (one and two-pion production) come.
- Solution: put your hadrons to a queue:



• "Attended" and new hadrons \rightarrow to the back. Outgoing: remove



All-in-one example: intranuclear cascade

Take all hadrons created in primary vertex, move each by formation zone distance





Summary

- We opened the "black box" of MC:
- 1) General scheme of neutrino interaction generator algorithm
- 2) Handling complicated physical models including MEC and FSI with step-by step algorithms
- Many ways to improve your MC:
- 1) Choice of probability sampling order (beam-detector-interaction).
- 2) Choice of sampling routines \rightarrow fast cummulative distributions from histograms.
- 3) Weights: possible to compute while running code (test events) \rightarrow new processes/parameter changes done easy.
- 4) Troublesome (peaked/ growing with neutrino energy) cross sections: sampling stabilization through re-weighting.
- 5) As much as possible analytical solutions (e.g. kinematic limits) : better efficiency/speed.
- 6)Appropriate CMS = higher symmetry \rightarrow easy phase-space and kinematics.
- 7)Complicated (time-consuming) cross section computations: choice of minimal information set (e.g. response functions for MEC or probability grid for SF), pre-computation and storage.



Thank you for your attention!

Special thanks to T. Golan, K. Graczyk, C. Juszczak J. Sobczyk for discussion and guidance and thanks to T. Golan for giving me access to his thesis. Last, but not least -to the Organizers for wonderful time in Valencia!






All-in-one example: intranuclear cascade

• "Generate Interaction" for pions (*x*=frand(), x_i -process probabilities, "ii" \rightarrow same isospins in target nucleon pair)





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All-in-one example: intranuclear cascade

• "Generate Interaction" for nucleons (x=frand(), x_i -process probabilities)

