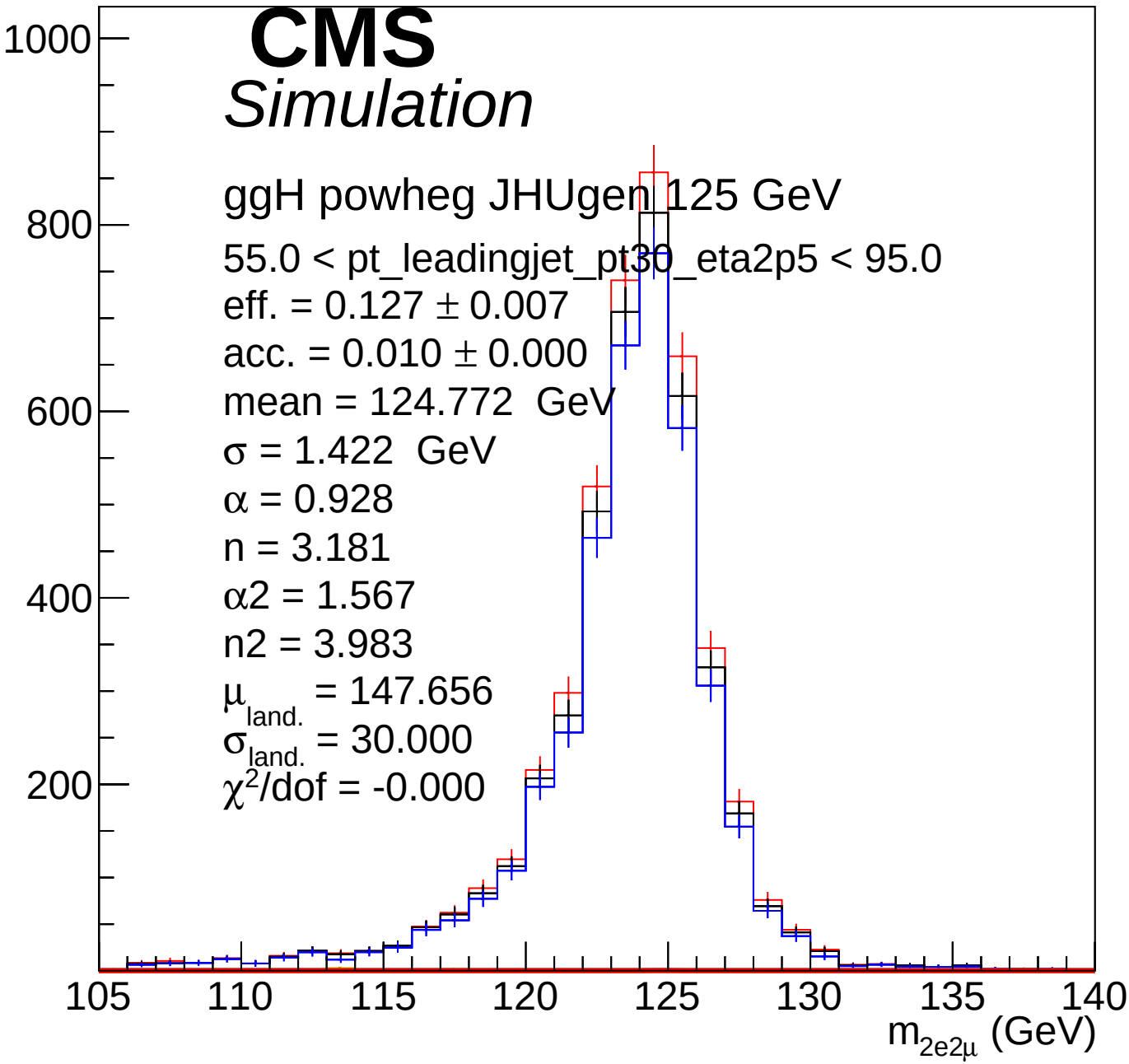mass spectrum