GEANT4 models for muonic atom processes, and proposed simulation package.

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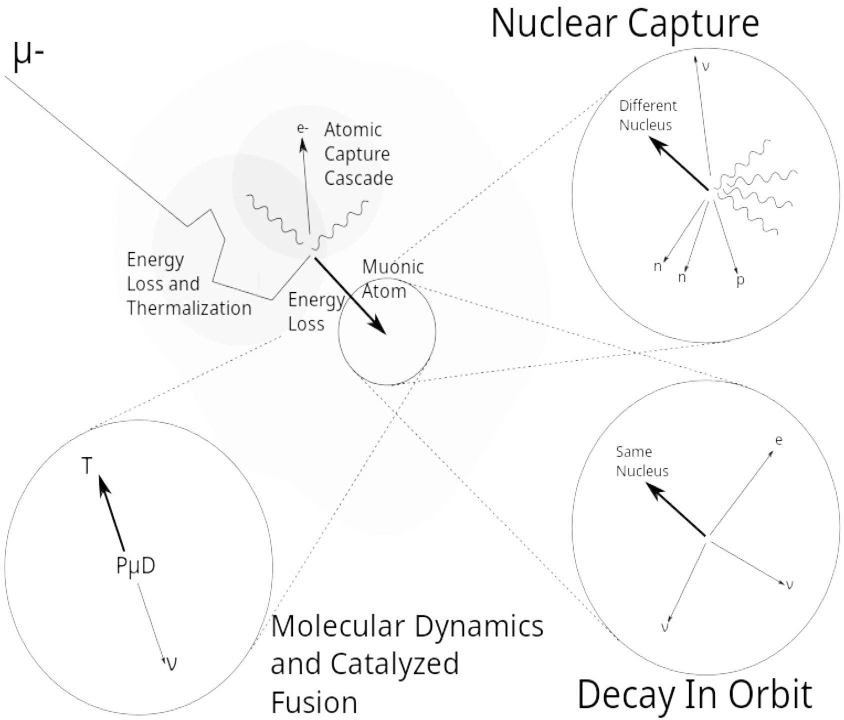
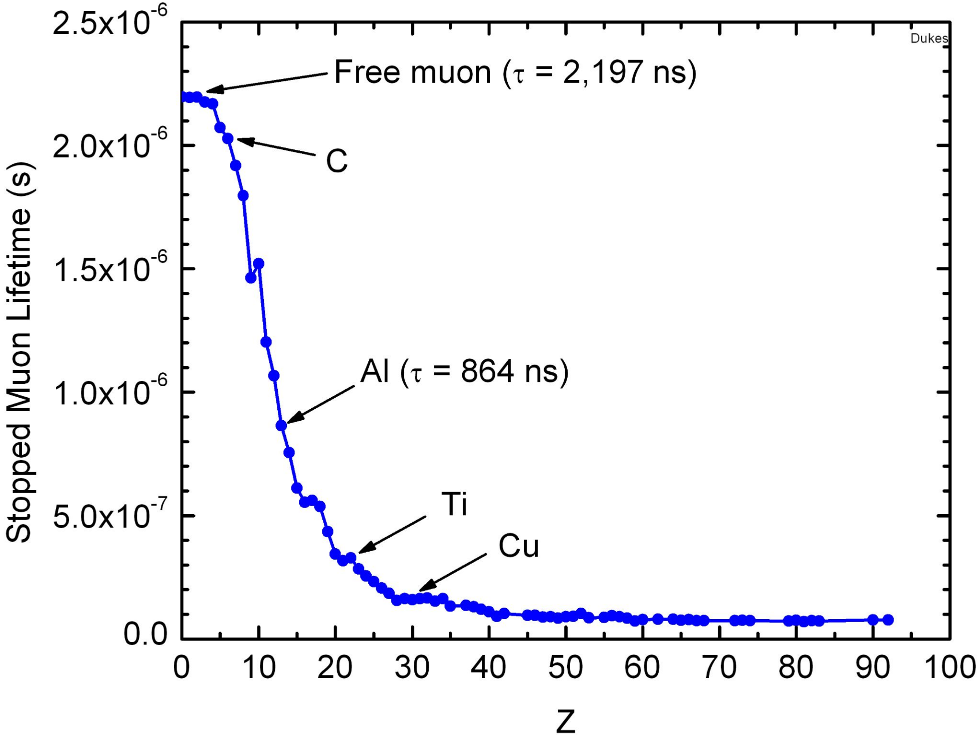
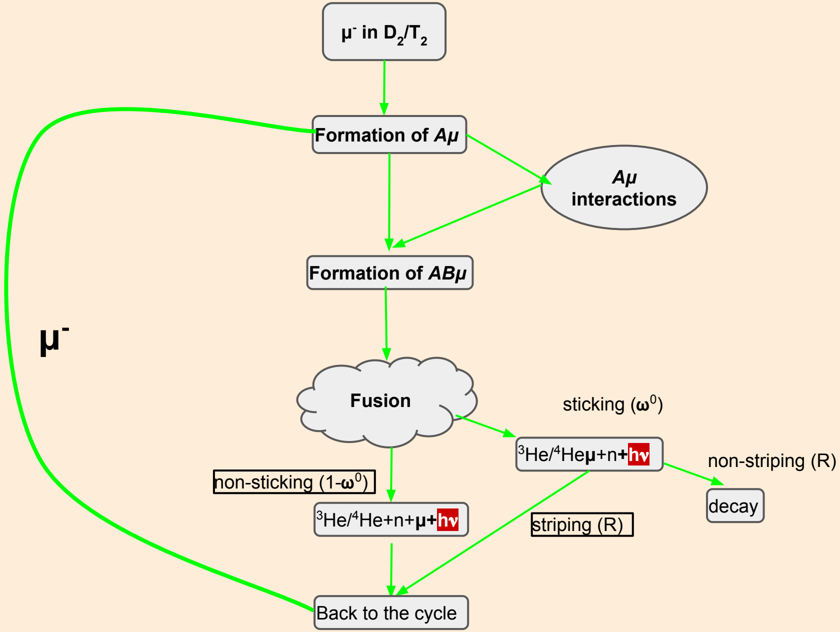
μ^- in matter





- Stopped can undergo DIO, nuclear capture, muonic atom formation
- Accurately modelling MuAtom physics is essential.

Muon Catalyzed Fusion



μ^- in D_2/T_2

Formation of *Aμ*

***Aμ* interactions**

Formation of *ABμ*

Fusion

sticking (ω^0)

^{3}He/^{4}He**μ**+n+**hν**

non-striping (R)

decay

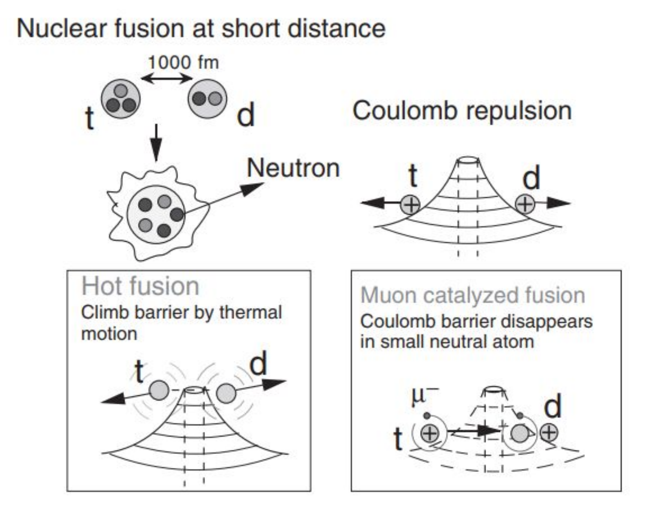
non-sticking (1-ω^0)

^{3}He/^{4}He+n+**μ**+**hν**

striping (R)

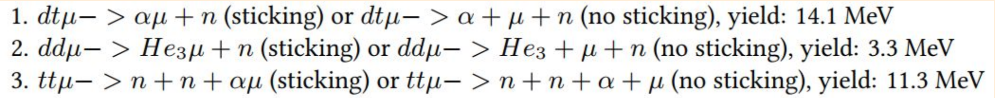
Back to the cycle

μ^-



Concept of μCF in comparison to thermonuclear fusion

Typical fusion reactions:

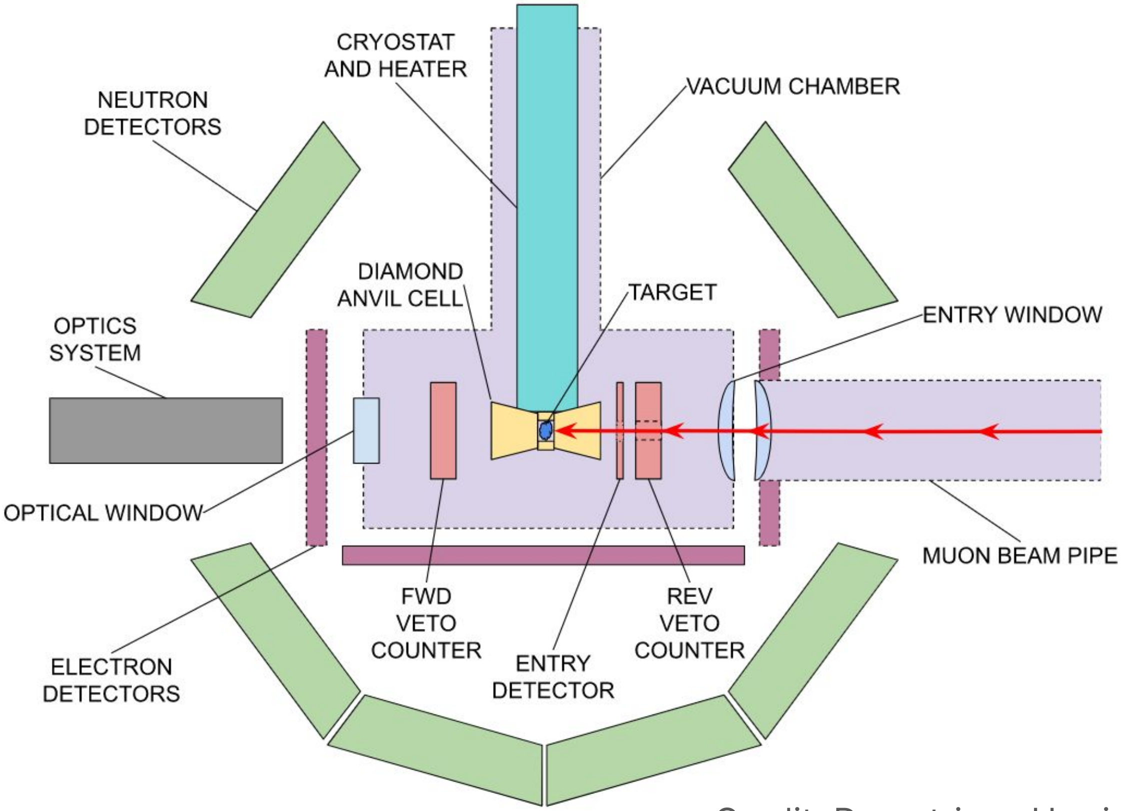


1. $dt\mu- > \alpha\mu + n$ (sticking) or $dt\mu- > \alpha + \mu + n$ (no sticking), yield: 14.1 MeV
2. $dd\mu- > He_3\mu + n$ (sticking) or $dd\mu- > He_3 + \mu + n$ (no sticking), yield: 3.3 MeV
3. $tt\mu- > n + n + \alpha\mu$ (sticking) or $tt\mu- > n + n + \alpha + \mu$ (no sticking), yield: 11.3 MeV

Predominant channels:

1. *ddμ,dtμ,ttμ* (rate >10^8)
2. Other processes like pd*μ*, pt*μ* are not fruitful (rate ~10^5)

Experimental design



- Diamond anvil cell, ~10^5 bar, 7-1500 K
- Veto counters, electron detectors, neutron detectors
- DT mixture target upto 3 LHD
- Muon beam through a window

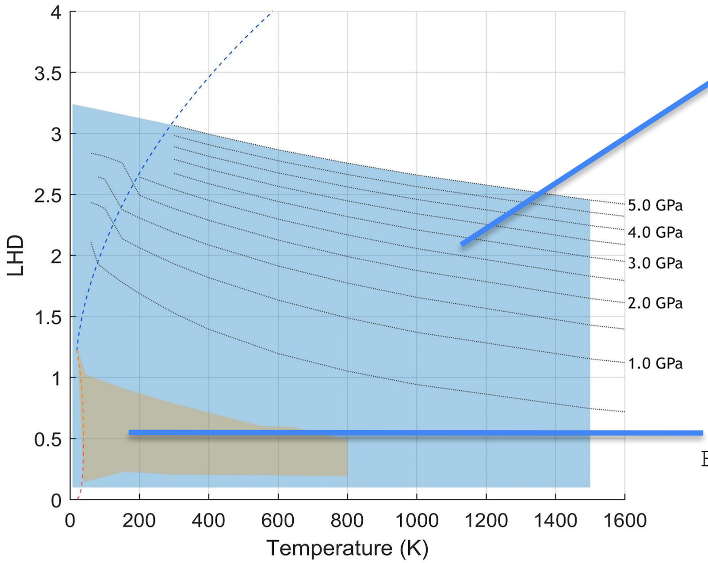
Credit: Demetrious Harrington, NK Labs

Goals

This presentation

- Measure key μCF rate and efficiency parameters at higher temperatures and pressures than have been explored previously

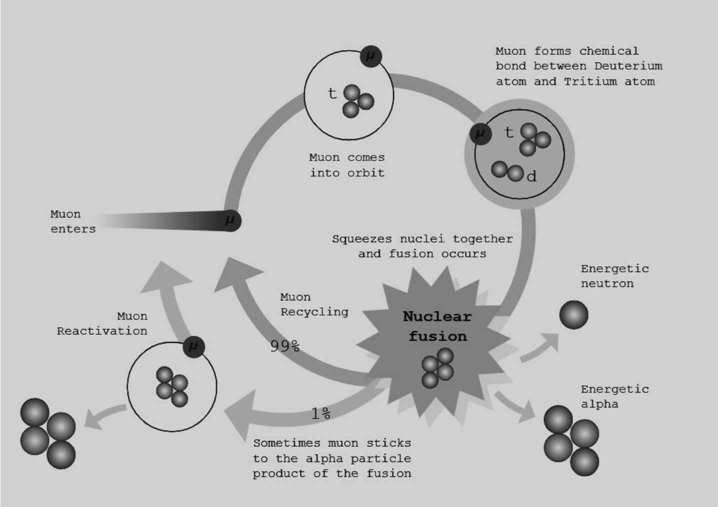
- Create high-fidelity physics process of muon-catalyzed fusion for GEANT4



Design range of our anvil cell target

Range measured historically Bom et al, 2005

Credit: JT hinchen, NK Labs

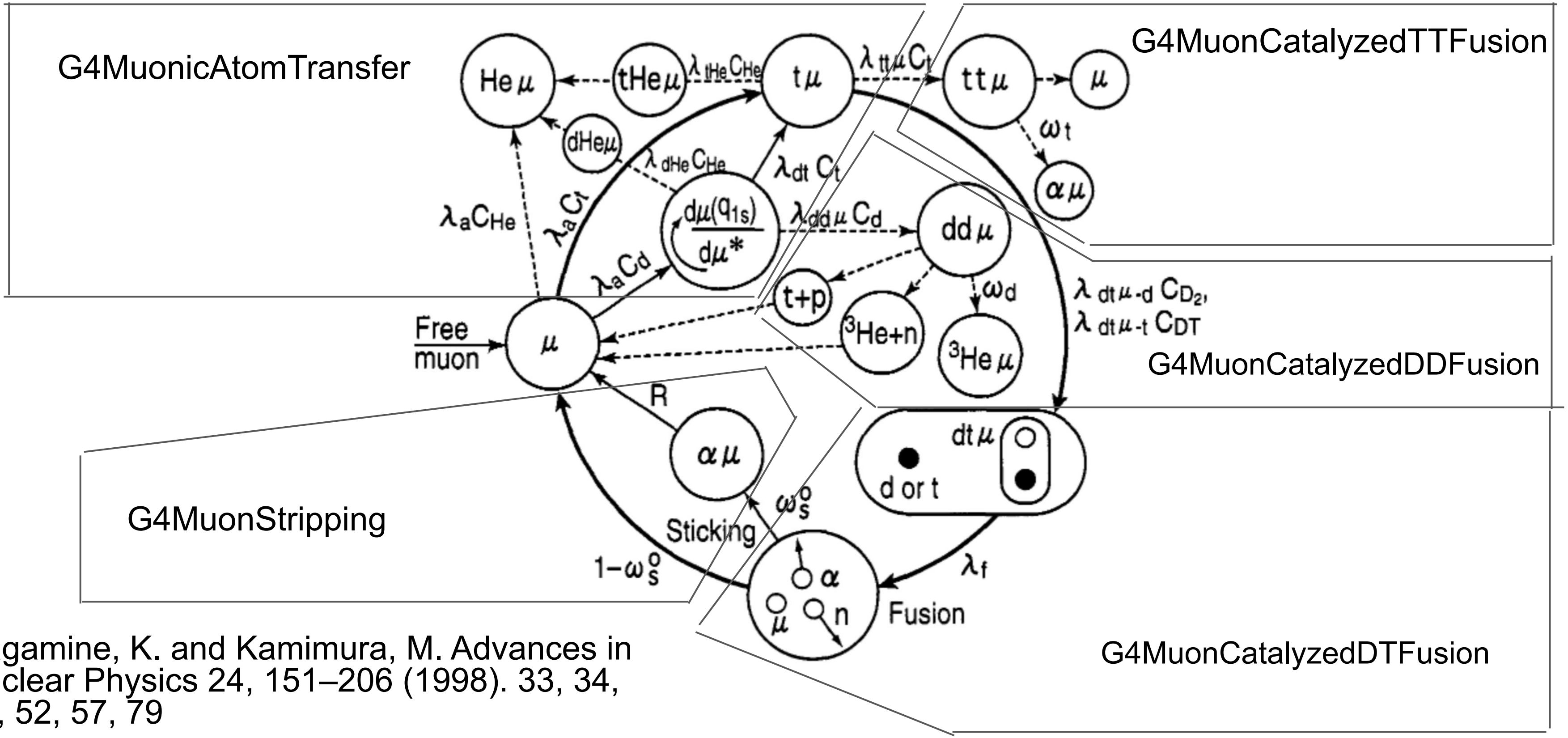


Credit: Sydney Fulkerson, Accelaron

Process models for GEANT4

- Add muon catalyzed fusion and associated muonic atom processes to GEANT4.
- Be a function of: (at least)
  - Temperature
  - Density
  - Mixture fraction of P, D, and T
  - Impurity concentration
- Return reasonably accurate yields, with reasonable matching to experimental data
- Include the time structure, and spatial extent of the reaction.

Process models for GEANT4



G4MuonicAtomTransfer

G4MuonCatalyzedTTFusion

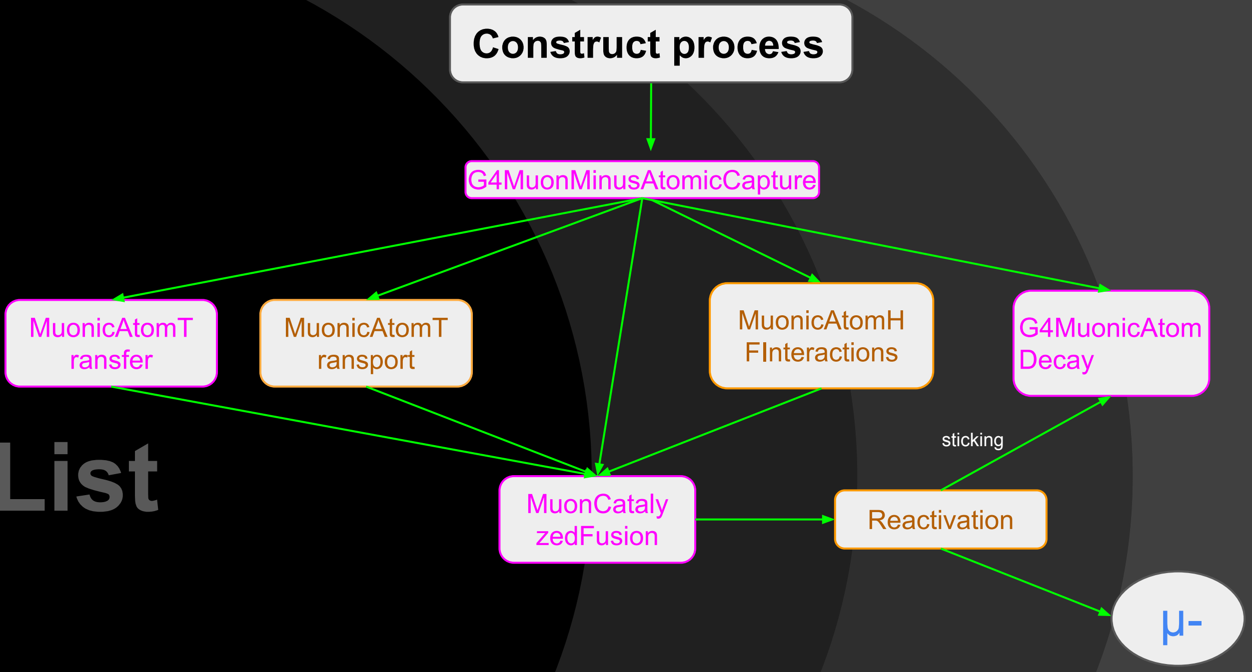
G4MuonCatalyzedDDFusion

G4MuonStripping

G4MuonCatalyzedDTFusion

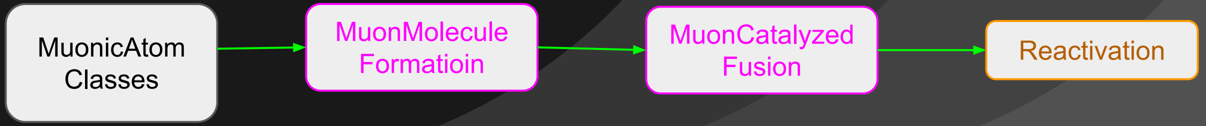
Nagamine, K. and Kamimura, M. Advances in Nuclear Physics 24, 151–206 (1998). 33, 34, 35, 52, 57, 79

Physics List



- ☐ Rest Processes
- ☐ Post-step Processes

More Accurate μCF Channel

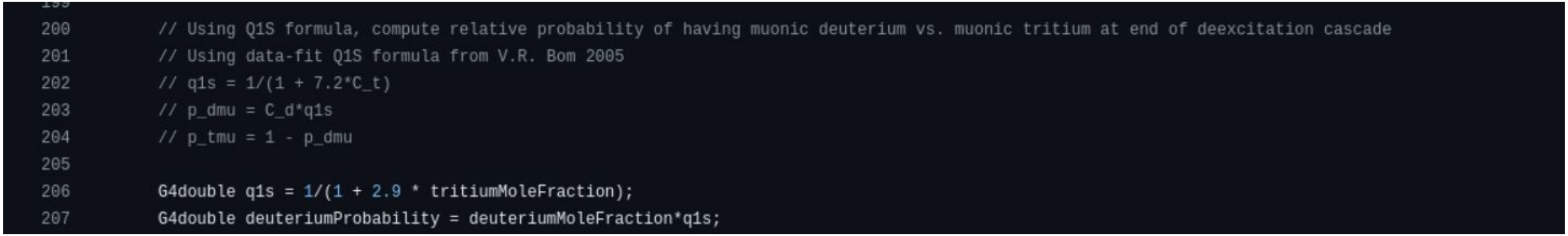


Process models for GEANT4

Processes we have implemented:

- G4MuonMinusAtomicCapture :Modified
- EM processes to act on muonic atoms :Modified
- G4MuonicAtomTransfer :New
- G4MuonicAtomSpinFlip :New
- G4MuonCatalyzedDDFusion :New
- G4MuonCatalyzedDTFusion :New
- G4MuonCatalyzedTTFusion :New
- G4MuonStripping :New

MuonicAtomTransfer



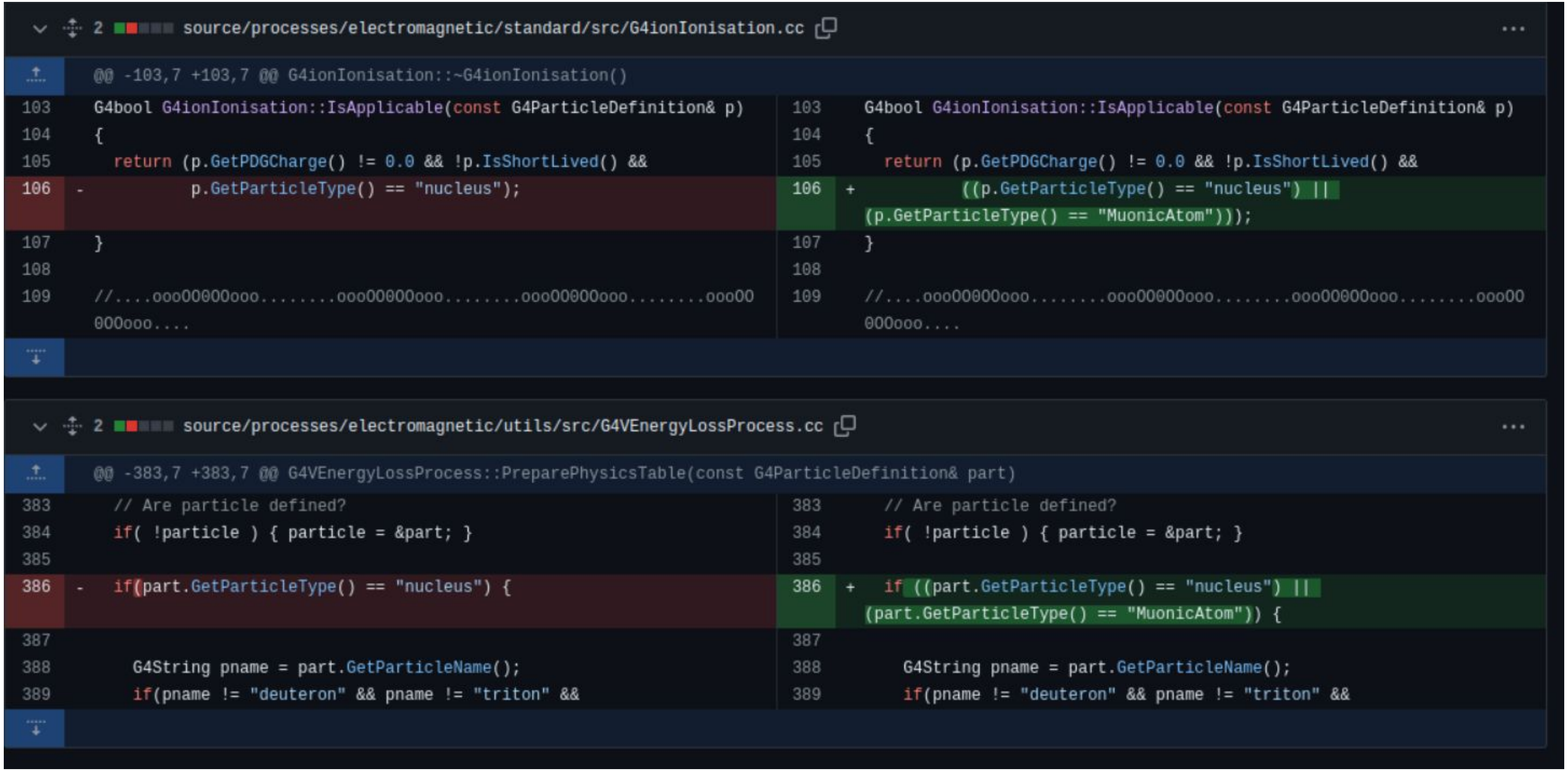
```
        // Using Q1S formula, compute relative probability of having muonic deuterium vs. muonic tritium at end of deexcitation cascade
        // Using data-fit Q1S formula from V.R. Bom 2005
        // q1s = 1/(1 + 7.2*C_t)
        // p_dmu = C_d*q1s
        // p_tmu = 1 - p_dmu

        G4double q1s = 1/(1 + 2.9 * tritiumMoleFraction);
        G4double deuteriumProbability = deuteriumMoleFraction*q1s;
```

$$q_{1s} = \frac{\lambda_{\mathrm{dex}}}{\lambda_{\mathrm{dex}} + \lambda_{\mathrm{tr}}}.$$

λ_{dex} = de-excitation rate
λ_{tr} = transfer rate

Patch for muonic atoms to experience EM processes



```
2 source/processes/electromagnetic/standard/src/G4ionIonisation.cc

@@ -103,7 +103,7 @@ G4ionIonisation::~G4ionIonisation()
```

```
G4bool G4ionIonisation::IsApplicable(const G4ParticleDefinition& p)
{
  return (p.GetPDGCharge() != 0.0 && !p.IsShortLived() &&
-          p.GetParticleType() == "nucleus");
}

//....ooo00000ooo........ooo00000ooo........ooo00000ooo........ooo00000ooo....
```

```
G4bool G4ionIonisation::IsApplicable(const G4ParticleDefinition& p)
{
  return (p.GetPDGCharge() != 0.0 && !p.IsShortLived() &&
+          ((p.GetParticleType() == "nucleus") || (p.GetParticleType() == "MuonicAtom")));
}

//....ooo00000ooo........ooo00000ooo........ooo00000ooo........ooo00000ooo....
```

```
2 source/processes/electromagnetic/utils/src/G4VEnergyLossProcess.cc

@@ -383,7 +383,7 @@ G4VEnergyLossProcess::PreparePhysicsTable(const G4ParticleDefinition& part)
```

```
  // Are particle defined?
  if( !particle ) { particle = &part; }

-  if(part.GetParticleType() == "nucleus") {

    G4String pname = part.GetParticleName();
    if(pname != "deuteron" && pname != "triton" &&
```

```
  // Are particle defined?
  if( !particle ) { particle = &part; }

+  if ((part.GetParticleType() == "nucleus") || (part.GetParticleType() == "MuonicAtom")) {

    G4String pname = part.GetParticleName();
    if(pname != "deuteron" && pname != "triton" &&
```

Patch for muonic atoms to experience EM processes

```
7 source/processes/electromagnetic/utils/src/G4ionEffectiveCharge.cc
@@ -97,6 +97,13 @@ G4double G4ionEffectiveCharge::EffectiveCharge(const G4ParticleDefinition* p,

   G4double mass   = p->GetPDGMass();
   G4double charge = p->GetPDGCharge();
+
+  // Muon reduces charge of muonic atom by one
+  // TODO is this the right/only place to do this???
+  if (p->GetParticleType() == "MuonicAtom") {
+    charge -= 1.0;
+  }
+
   G4double Zi     = charge*inveplus;

   chargeCorrection = 1.0;
```

G4MuonicAtomTransfer

- Uses temperature-dependent transfer rates between H, D, T, He3, and He4
- Rates to hydrogen isotopes:
  - A. Adamczak, “Differential cross sections for muonic atom scattering from hydrogenic molecules”, PRA 74, 042718 (2006)
  - Newly computed by A. Adamczak for this project from 5 - 1500K
- Rates to helium isotopes:
  - A. V. Kravtsov; A. I. Mikhailov (2000). Temperature dependence of the forma
  - tion rates of hydrogen-helium mesic molecules in collisions of slow hydrogen ato
  - ms with helium. , 90(1), 45–49.
  - Tabulated from 15 - 500K
- Rates for atoms with Z>3 based on scaling of data collected by FAMU collaboration for transfer to oxygen
  - Scaling with temperature, density, and atomic number difference

$$d\mu(1s) + t \longrightarrow t\mu(1s) + d$$

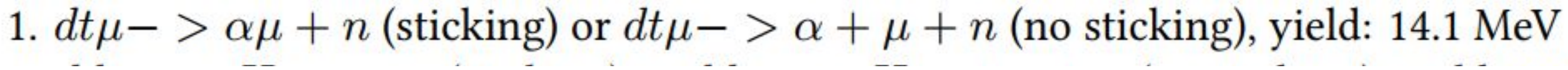
G4MuonicAtomSpinFlip

- Temperature-dependent spin flip modeling is important for accurate time spectra in D-D experiments
- Spin flip rates for H,D,T:
  - A. Adamczak, “Differential cross sections for muonic atom scattering from hydrogenic molecules”, PRA 74, 042718 (2006)
  - Newly computed by A. Adamczak for this project from 5 - 1500K
- Spin flip for Z>1 not modelled

$$d\mu(\uparrow\uparrow) + d \rightarrow d\mu(\uparrow\downarrow) + d$$

G4MuonCatalyzedDTFusion

- Fusion rate depends on temperature and spin of muonic atom
- Rates from
  - Faifman, M.P., Strizh, T.A., Armour, E.A.G. et. al, “Quadrupole corrections to matrix elements of transitions in resonant reactions of muonic molecule formation, Hyperfine Interact 101, 179–189 (1996)”
- Value for initial sticking (0.00857) from
  - M. Kamimura, Y. Kino, T. Yamashite, “Comprehensive study of muon-catalyzed nuclear reaction processes in the dtμ molecule”, 2023 (Arxiv draft)
- Nonlinear density dependence not modeled
- State of matter effects not modeled



1. $dt\mu- > \alpha\mu + n$ (sticking) or $dt\mu- > \alpha + \mu + n$ (no sticking), yield: 14.1 MeV

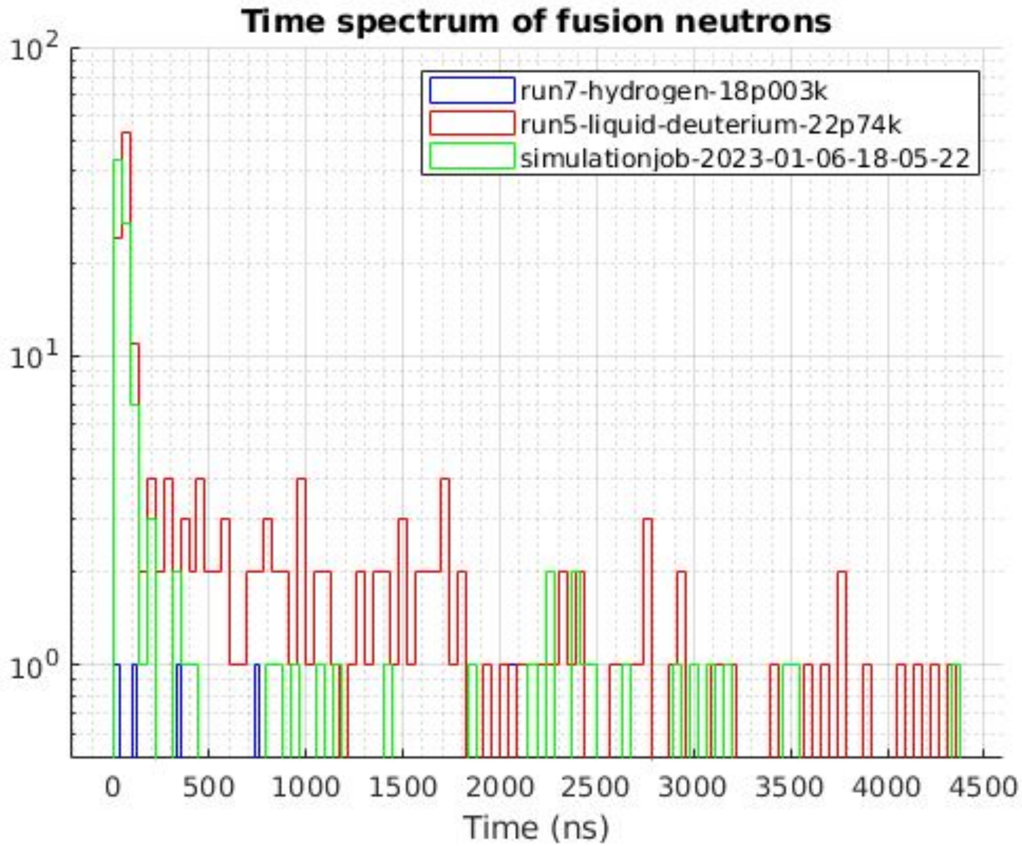
G4MuonStripping

- Stripping of muon from muonic alpha cycling back to fusion cycle is vital.
- Muon stripping in ground-state MuHe3 and MuHe4 due to collisional ionization and transfer processes
- Striping cross-sections are estimated by scaling the data of p-He collisions for muon’s mass following the approach given in

  C.D. Stodden, H.J. Monkhurst, K. Szalewicz, T.G. Winter,
  Physical Review A, Volume 4, Number 3, February 1, 1990, p. 1281

- Excited state of muonic alpha not modelled yet.

Validation of DD fusion



Example for Validation

- Geometry and Parameters:

  Target volume: User-specific HDT mixture in shape of a box.

  Fuel Temp: 300-1500 K

  Fuel Density: 0.3-1.5 LHD

  T_2 concentration: 18-70 %

- Particle Gun:

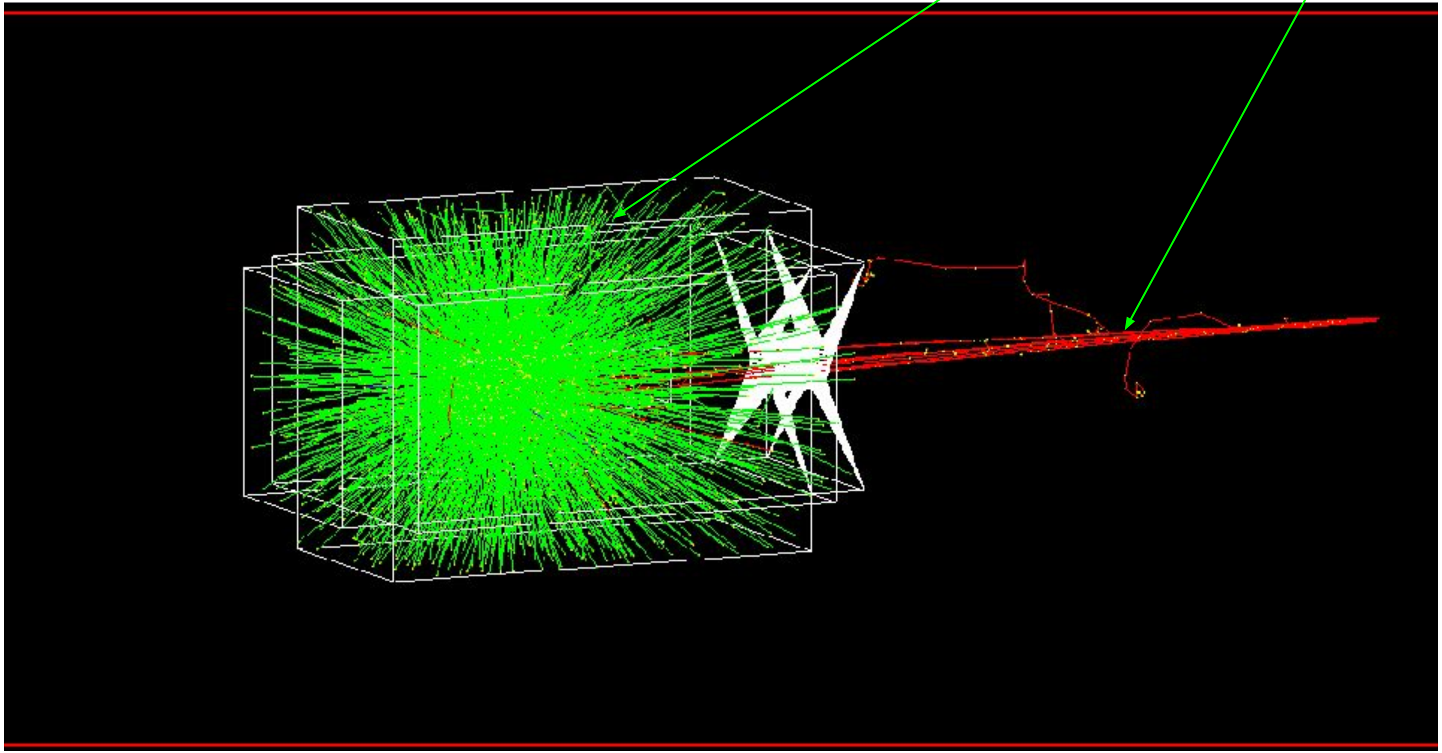
  Muon beam: beam energy, type (collimated/Gaussian, etc.), direction, can be provided in the PrimaryGeneratorAction or Messenger classes via macro.

- MuonicAtomPhysics:

  The example uses QGSP_BIC & user defined G4VPhysicsConstructor for muonic atoms.

- Neutron stops in the detector volumes surrounding the target are identifiers for fusion processes. Muon veto and decay electron detectors to be added.

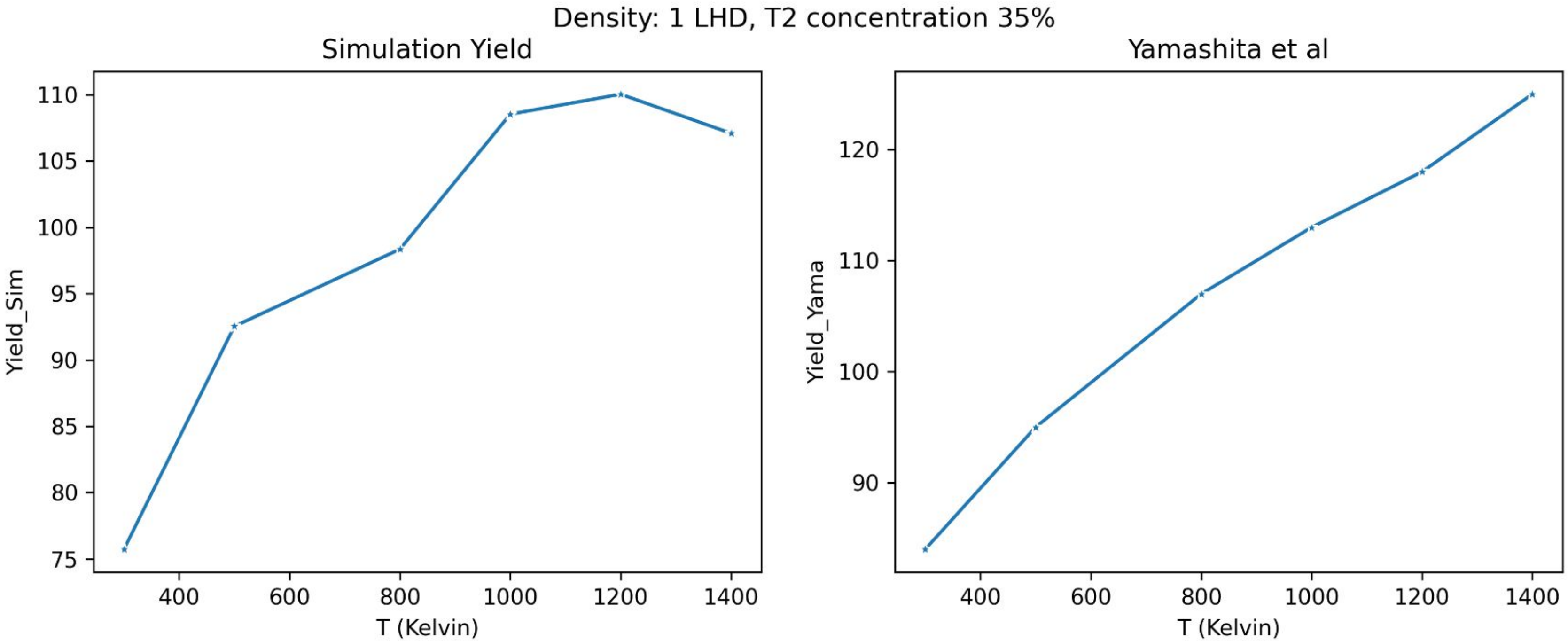
Example for Validation



Surrounding
Neutron Detectors

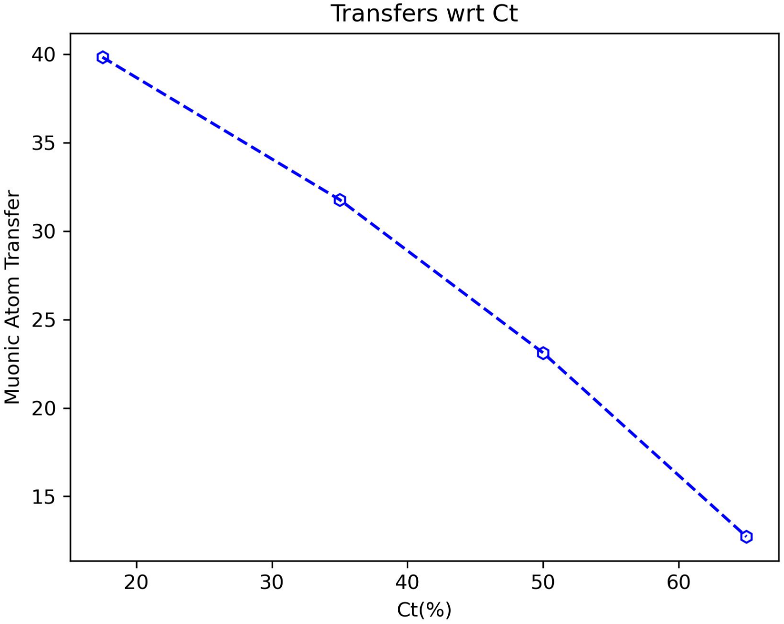
Muon Beam

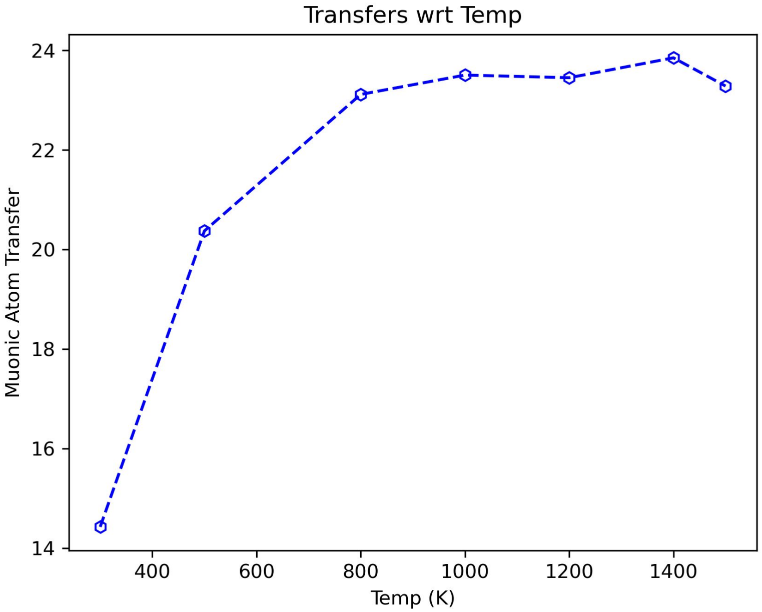
Validation: Temp vs Fusion Yield



- Observed fusion yield for a nominal density and 35% T_2 concentration, The model has been simulated b/w 300-1400 K
- Yamashita et al, Scientific Reports volume 12, Article number: 6393 (2022)

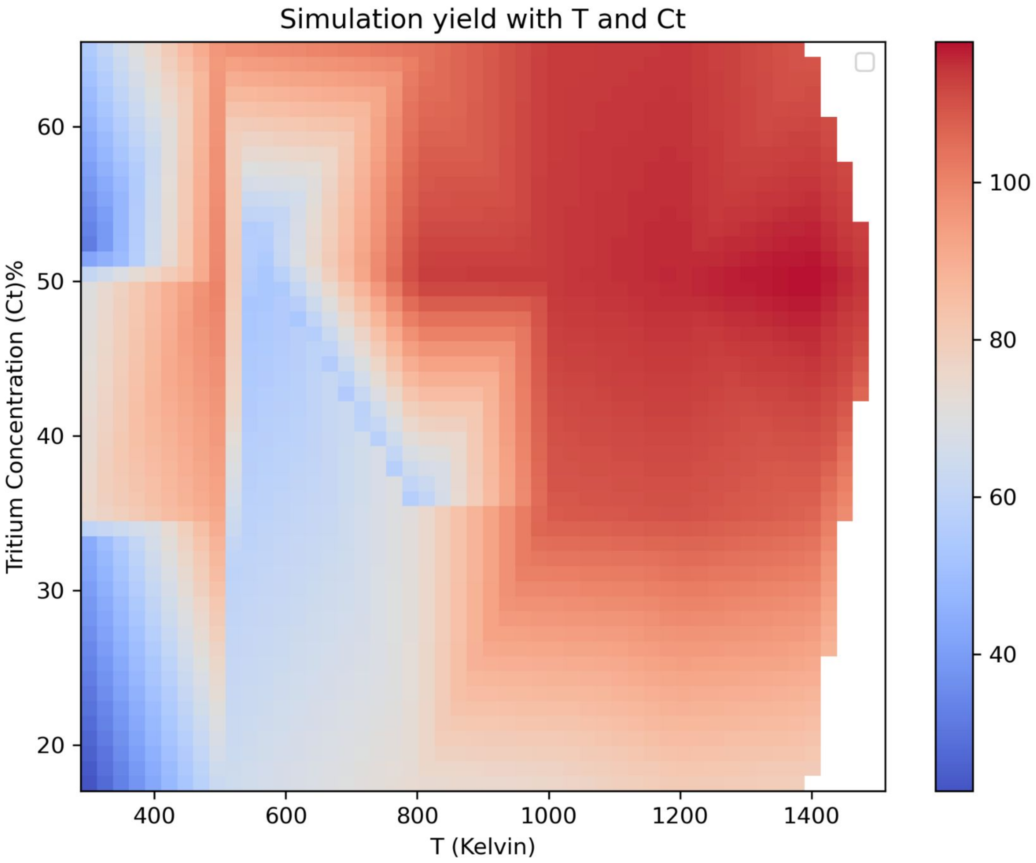
Validation: Muonic Atom Transfer rate


Transfers wrt Ct


Transfers wrt Temp

- Transfer of muonic atom to another isotope observed with respect to different temperature and T2 concentration.

Validation: Fusion Yield vs Temp, T2 Concentration.



Summary

- Several processes modelled for muonic atom and muon catalyzed fusion based on theoretical and experimental studies from literature.
- Working with G4 hadronic group for integration.
- Validation being carried out for simulation vs archival data, fusion yield, sticking fraction, etc.
- Variation with temperature, density, and concentrations
- The dMu/DT collaboration is studying fusion parameters at a relatively higher temperature, 7-1500 K and pressure, ~10^5 bar

Thank You!

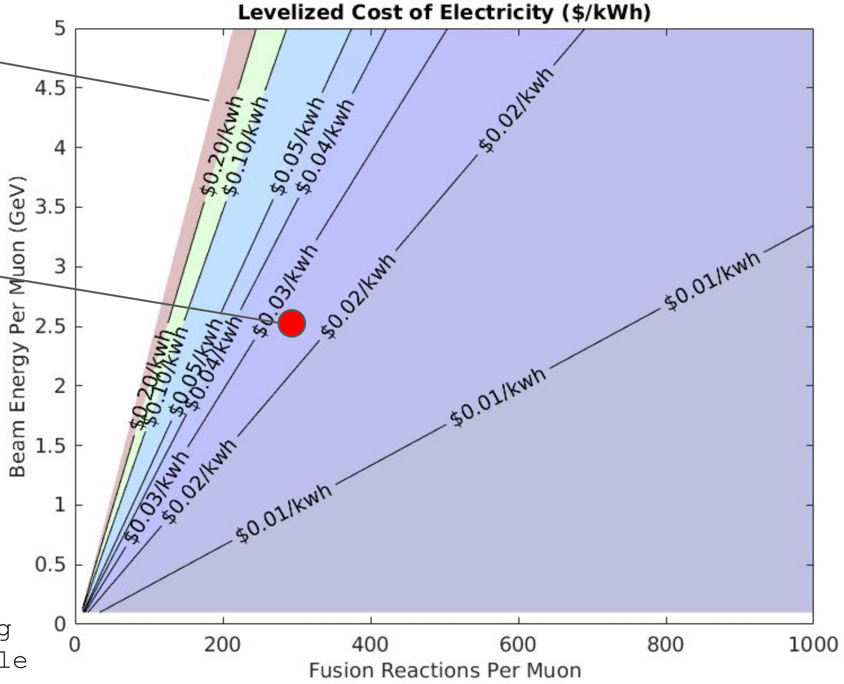
Competition Among Several Processes

Processes	Rate of Reactions at 300K, 1 LHD
Muon decay rate (λ_0)	0.45x 10^6 s^{-1}
Atomic Capture (λ_a)	4 x 10^{12} s^{-1}
Isotopic Exchange (λ_{dt})	2.8 x 10^8 s^{-1}
HF Interactions	~ 10^7 s^{-1}
Molecule Formation ($\lambda_{dt\mu}$)	10^8-10^9 s^{-1}
Fusion Rates($\lambda^f_{dt\mu}$)	10^{12} s^{-1}
Muon Cycling Rates (λ_c)	~ 10^8 s^{-1}

- With the cross-sections and reaction rates given, Geant4 calculates the interaction-lengths step by step and carries out the simulation.
- The temp. and density of the gas volume affects the parameters significantly, however currently 300K data is taken for simulation.
- It is planned to implement the cross-section tables normal atoms with similar atomic properties for $A\mu$, like the case of $\alpha\mu \mapsto {}^{4}\mathrm{H}$.

Ref: Annu. Rev. Nucl. Part. Sci. 1989.39: 311-56

Cost of electricity versus physics parameters



Engineering breakeven

Target operating point for a reactor

(Using a superconducting accelerator, Brayton cycle balance of plant, and revenue from heat sales.)

Cost of baseload power by source, $/kWh (1)

Coal	$0.089
Biomass	$0.077
Nuclear fission	$0.071
Gas:	$0.043

Target operating point:

Fusion (?):	$0.025

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(1) Levelized Costs of New Generation Resources in the Annual Energy Outlook 2023, US Energy Information Administration, Document #AEO2023

- Diamond Anvil Cell: DT sample, 2.5 mm diameter, 0.5 mm thick when compressed, 1 mg at 3 LHD
- Veto counters: plastic scintillators, Neutron detectors: EJ309 liquid scintillators, e det: thin flat plastic scintillators, SiPMs
- Liquid Hydrogen Density = 4.25e+22 atoms/c
- Optical system for pressure monitoring